



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 02:23 PM EDT

PDB ID : 7KWP  
Title : Dihydrodipicolinate synthase (DHDPS) from *C.jejuni* with pyruvate bound in the active site and L-lysine bound at the allosteric site in C2221 space group  
Authors : Saran, S.; Sanders, D.A.R.  
Deposited on : 2020-12-01  
Resolution : 2.26 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](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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.35.1  
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) : 2.35.1

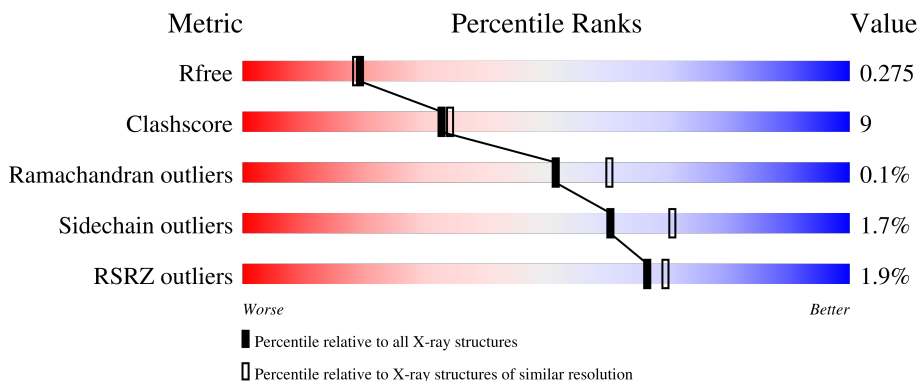
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.26 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	310	 2% 78% 17% 5%
1	B	310	 % 82% 13% 5%
1	C	310	 2% 74% 20% 5%
1	D	310	 % 81% 14% 5%
1	E	310	 2% 76% 18% 5%

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Mol	Chain	Length	Quality of chain
1	F	310	<p>2% 78% 17% 5%</p>

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
2	LYS	F	301	-	-	X	-
4	EDO	B	302	-	-	X	-
4	EDO	D	303	-	-	X	-
5	PEG	C	303	-	-	X	-

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 14194 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-hydroxy-tetrahydrodipicolinate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	296	2274	1446	378	437	13	0	0	0
1	B	296	2274	1446	378	437	13	0	0	0
1	C	296	2278	1449	379	437	13	0	0	0
1	D	296	2274	1447	377	437	13	0	0	0
1	E	296	2266	1440	376	437	13	0	0	0
1	F	296	2278	1449	379	437	13	0	0	0

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	expression tag	UNP Q9PPB4
A	-10	ARG	-	expression tag	UNP Q9PPB4
A	-9	GLY	-	expression tag	UNP Q9PPB4
A	-8	SER	-	expression tag	UNP Q9PPB4
A	-7	HIS	-	expression tag	UNP Q9PPB4
A	-6	HIS	-	expression tag	UNP Q9PPB4
A	-5	HIS	-	expression tag	UNP Q9PPB4
A	-4	HIS	-	expression tag	UNP Q9PPB4
A	-3	HIS	-	expression tag	UNP Q9PPB4
A	-2	HIS	-	expression tag	UNP Q9PPB4
A	-1	GLY	-	expression tag	UNP Q9PPB4
A	0	SER	-	expression tag	UNP Q9PPB4
B	-11	MET	-	expression tag	UNP Q9PPB4
B	-10	ARG	-	expression tag	UNP Q9PPB4
B	-9	GLY	-	expression tag	UNP Q9PPB4
B	-8	SER	-	expression tag	UNP Q9PPB4
B	-7	HIS	-	expression tag	UNP Q9PPB4

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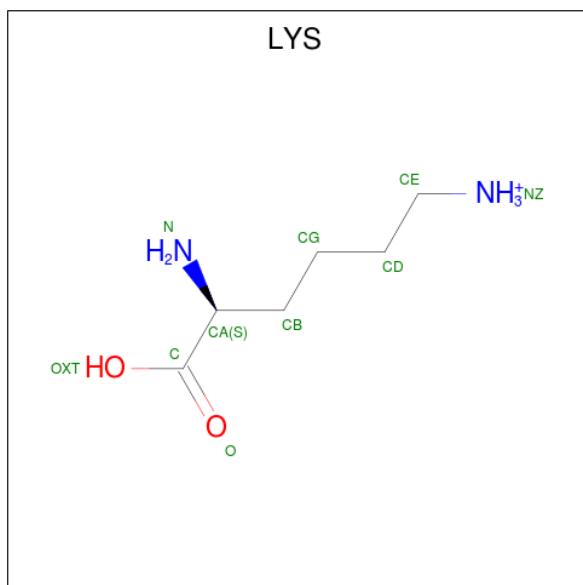
Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	HIS	-	expression tag	UNP Q9PPB4
B	-5	HIS	-	expression tag	UNP Q9PPB4
B	-4	HIS	-	expression tag	UNP Q9PPB4
B	-3	HIS	-	expression tag	UNP Q9PPB4
B	-2	HIS	-	expression tag	UNP Q9PPB4
B	-1	GLY	-	expression tag	UNP Q9PPB4
B	0	SER	-	expression tag	UNP Q9PPB4
C	-11	MET	-	expression tag	UNP Q9PPB4
C	-10	ARG	-	expression tag	UNP Q9PPB4
C	-9	GLY	-	expression tag	UNP Q9PPB4
C	-8	SER	-	expression tag	UNP Q9PPB4
C	-7	HIS	-	expression tag	UNP Q9PPB4
C	-6	HIS	-	expression tag	UNP Q9PPB4
C	-5	HIS	-	expression tag	UNP Q9PPB4
C	-4	HIS	-	expression tag	UNP Q9PPB4
C	-3	HIS	-	expression tag	UNP Q9PPB4
C	-2	HIS	-	expression tag	UNP Q9PPB4
C	-1	GLY	-	expression tag	UNP Q9PPB4
C	0	SER	-	expression tag	UNP Q9PPB4
D	-11	MET	-	expression tag	UNP Q9PPB4
D	-10	ARG	-	expression tag	UNP Q9PPB4
D	-9	GLY	-	expression tag	UNP Q9PPB4
D	-8	SER	-	expression tag	UNP Q9PPB4
D	-7	HIS	-	expression tag	UNP Q9PPB4
D	-6	HIS	-	expression tag	UNP Q9PPB4
D	-5	HIS	-	expression tag	UNP Q9PPB4
D	-4	HIS	-	expression tag	UNP Q9PPB4
D	-3	HIS	-	expression tag	UNP Q9PPB4
D	-2	HIS	-	expression tag	UNP Q9PPB4
D	-1	GLY	-	expression tag	UNP Q9PPB4
D	0	SER	-	expression tag	UNP Q9PPB4
E	-11	MET	-	expression tag	UNP Q9PPB4
E	-10	ARG	-	expression tag	UNP Q9PPB4
E	-9	GLY	-	expression tag	UNP Q9PPB4
E	-8	SER	-	expression tag	UNP Q9PPB4
E	-7	HIS	-	expression tag	UNP Q9PPB4
E	-6	HIS	-	expression tag	UNP Q9PPB4
E	-5	HIS	-	expression tag	UNP Q9PPB4
E	-4	HIS	-	expression tag	UNP Q9PPB4
E	-3	HIS	-	expression tag	UNP Q9PPB4
E	-2	HIS	-	expression tag	UNP Q9PPB4
E	-1	GLY	-	expression tag	UNP Q9PPB4

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Chain	Residue	Modelled	Actual	Comment	Reference
E	0	SER	-	expression tag	UNP Q9PPB4
F	-11	MET	-	expression tag	UNP Q9PPB4
F	-10	ARG	-	expression tag	UNP Q9PPB4
F	-9	GLY	-	expression tag	UNP Q9PPB4
F	-8	SER	-	expression tag	UNP Q9PPB4
F	-7	HIS	-	expression tag	UNP Q9PPB4
F	-6	HIS	-	expression tag	UNP Q9PPB4
F	-5	HIS	-	expression tag	UNP Q9PPB4
F	-4	HIS	-	expression tag	UNP Q9PPB4
F	-3	HIS	-	expression tag	UNP Q9PPB4
F	-2	HIS	-	expression tag	UNP Q9PPB4
F	-1	GLY	-	expression tag	UNP Q9PPB4
F	0	SER	-	expression tag	UNP Q9PPB4

- Molecule 2 is LYSINE (three-letter code: LYS) (formula:  $C_6H_{15}N_2O_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	10	6	2	2	0	0
2	B	1	10	6	2	2	0	0
2	C	1	10	6	2	2	0	0
2	D	1	10	6	2	2	0	0

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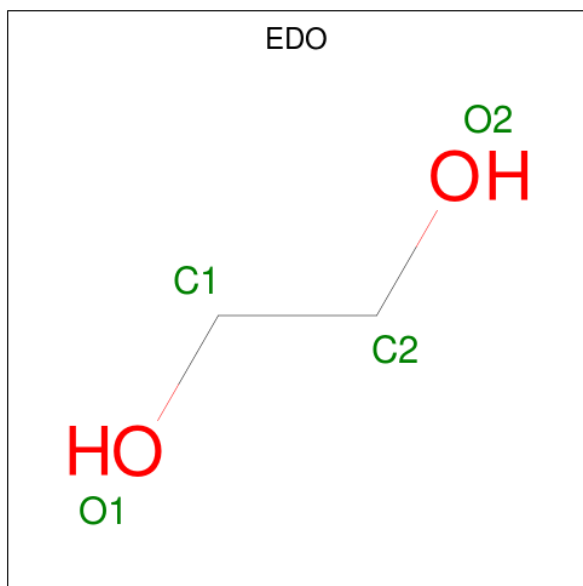
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	E	1	Total	C	N	O	0	0
			10	6	2	2		
2	F	1	Total	C	N	O	0	0
			10	6	2	2		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg	0	0
			2	2		
3	B	3	Total	Mg	0	0
			3	3		
3	C	1	Total	Mg	0	0
			1	1		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



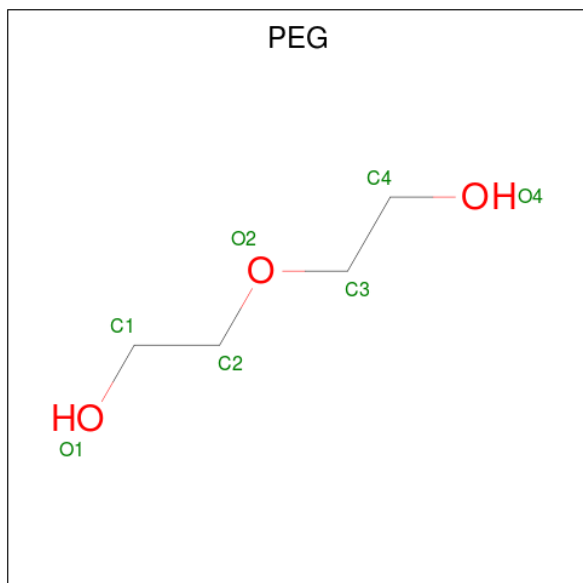
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		

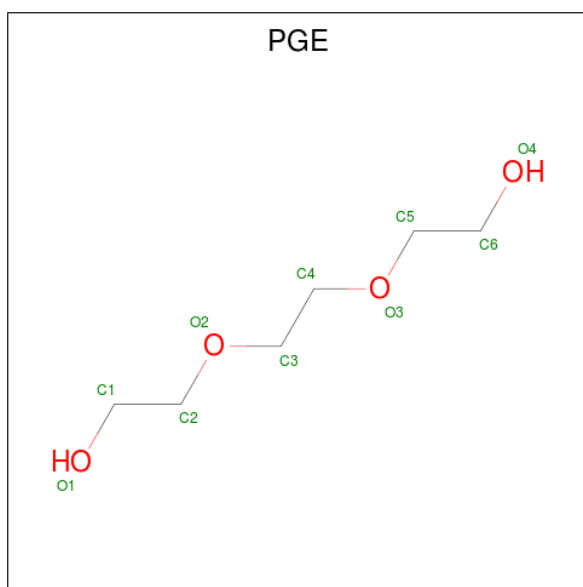
- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	C O	0	0
			10	6 4		

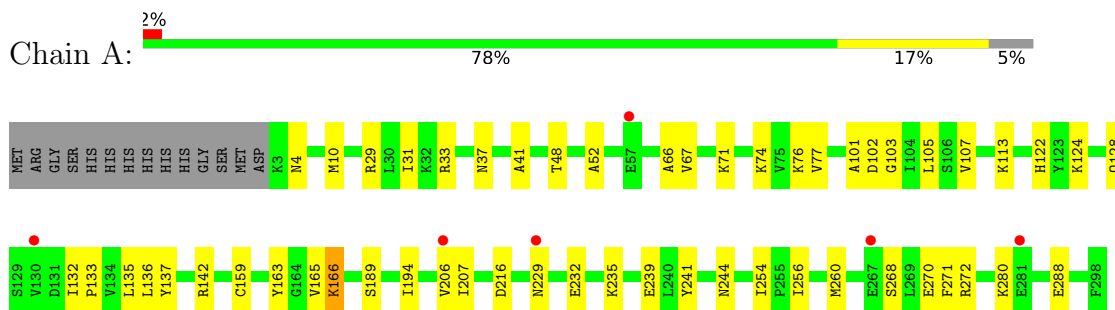
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	83	Total	O	0	0
			83	83		
7	B	87	Total	O	0	0
			87	87		
7	C	72	Total	O	0	0
			72	72		
7	D	62	Total	O	0	0
			62	62		
7	E	70	Total	O	0	0
			70	70		
7	F	73	Total	O	0	0
			73	73		

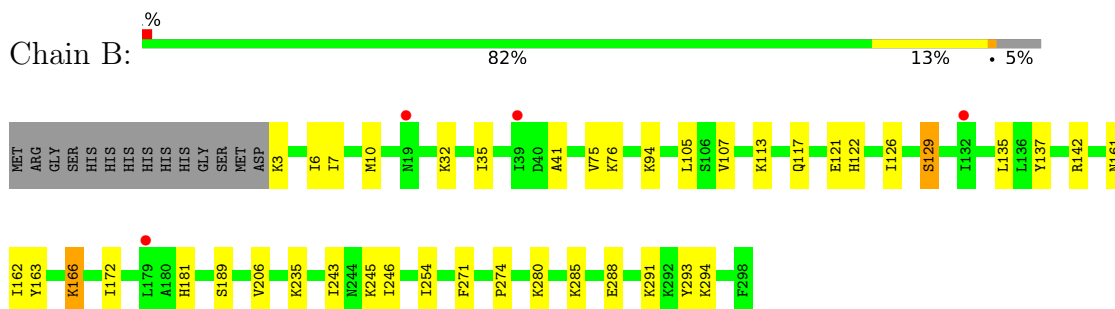
### 3 Residue-property plots [i](#)

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.

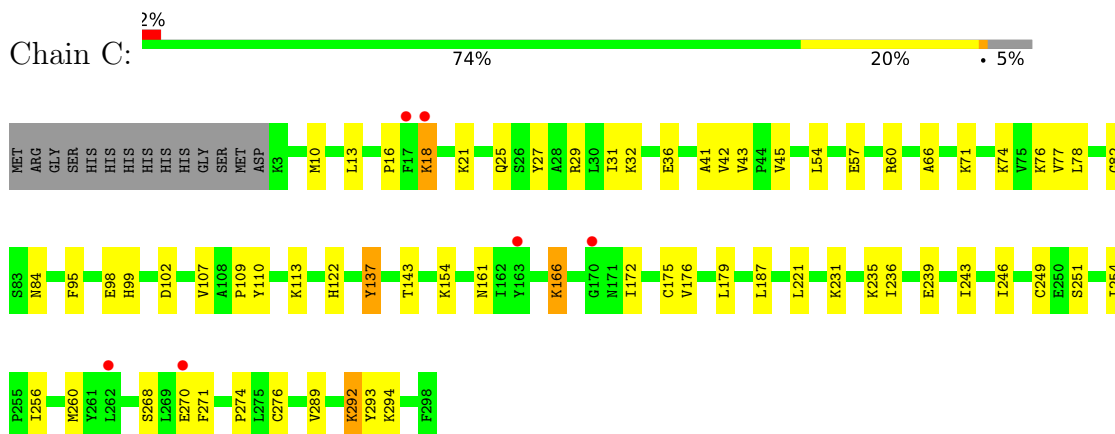
- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase



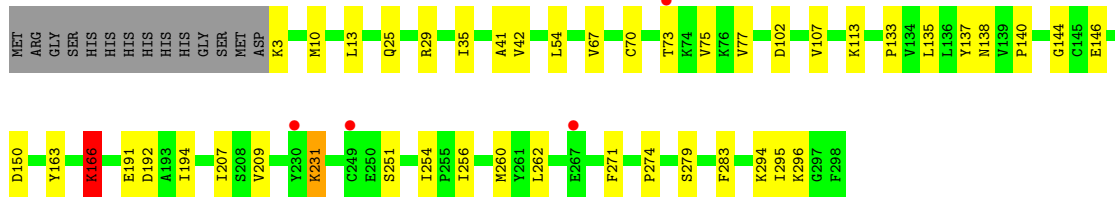
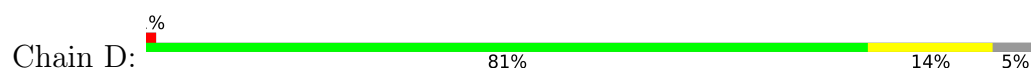
- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase



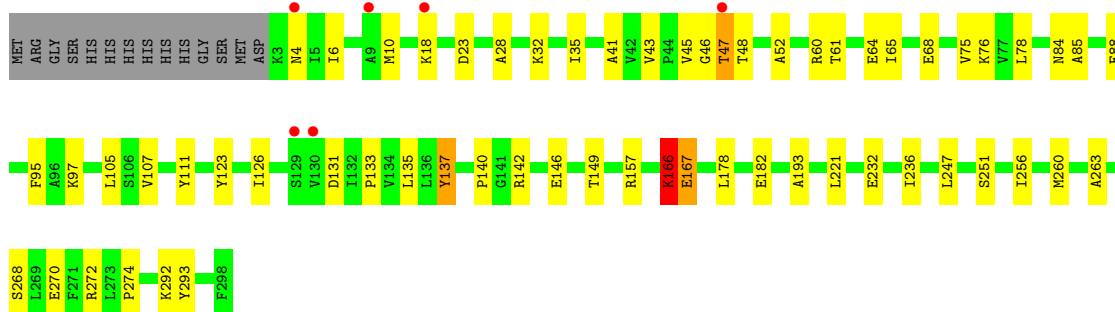
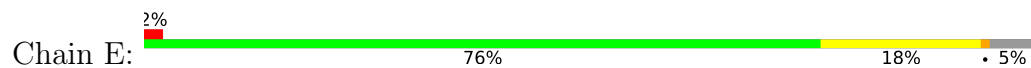
- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase



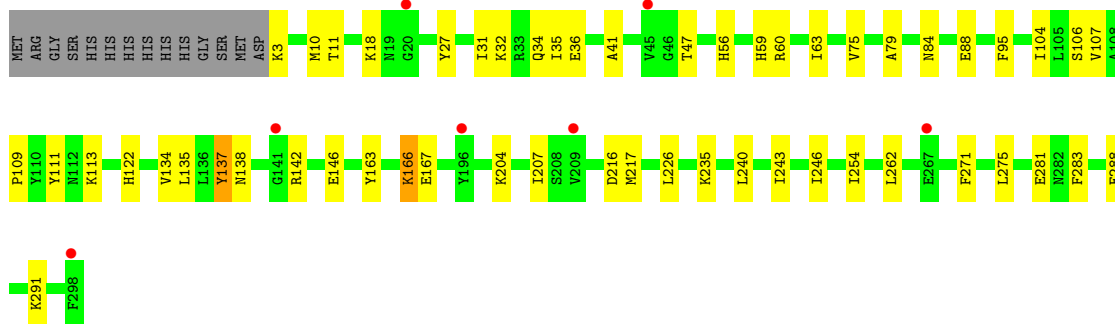
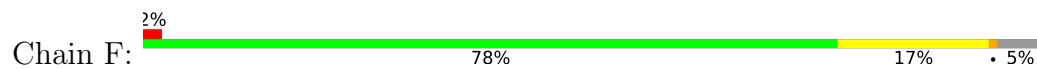
- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase



- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase



- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.40Å 231.13Å 199.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.84 – 2.26 45.84 – 2.26	Depositor EDS
% Data completeness (in resolution range)	99.8 (45.84-2.26) 92.2 (45.84-2.26)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.53 (at 2.27Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.244 , 0.277 0.246 , 0.275	Depositor DCC
$R_{free}$ test set	4623 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.5	Xtrriage
Anisotropy	0.339	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 44.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	14194	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% 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 i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, KPI, MG, PEG, PGE

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	0.52	0/2296	0.61	0/3105
1	B	0.34	0/2296	0.53	0/3105
1	C	0.42	0/2300	0.54	0/3109
1	D	0.39	0/2296	0.55	0/3105
1	E	0.50	1/2288 (0.0%)	0.65	3/3097 (0.1%)
1	F	0.42	2/2300 (0.1%)	0.54	0/3109
All	All	0.44	3/13776 (0.0%)	0.57	3/18630 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
1	E	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	167	GLU	CD-OE2	-6.40	1.18	1.25
1	F	167	GLU	CD-OE1	-5.49	1.19	1.25
1	E	46	GLY	C-N	5.19	1.46	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	47	THR	O-C-N	11.79	141.57	122.70
1	E	47	THR	CA-C-N	-9.01	97.37	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	46	GLY	N-CA-C	-5.00	100.60	113.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	166	KPI	Mainchain
1	E	166	KPI	Mainchain

## 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	2274	0	2305	42	0
1	B	2274	0	2305	33	0
1	C	2278	0	2316	56	0
1	D	2274	0	2302	46	0
1	E	2266	0	2283	44	0
1	F	2278	0	2317	35	0
2	A	10	0	12	1	0
2	B	10	0	12	0	0
2	C	10	0	12	1	0
2	D	10	0	12	1	0
2	E	10	0	12	2	0
2	F	10	0	12	7	0
3	A	2	0	0	0	0
3	B	3	0	0	0	0
3	C	1	0	0	0	0
4	B	8	0	12	9	0
4	D	8	0	12	10	0
4	E	4	0	6	1	0
5	C	7	0	10	7	0
6	D	10	0	14	2	0
7	A	83	0	0	4	0
7	B	87	0	0	0	0
7	C	72	0	0	3	0
7	D	62	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	E	70	0	0	1	0
7	F	73	0	0	3	0
All	All	14194	0	13954	240	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 9.

All (240) 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:192:ASP:N	4:D:303:EDO:H21	1.58	1.16
1:D:192:ASP:H	4:D:303:EDO:H21	1.05	1.13
1:E:47:THR:HG22	1:F:111:TYR:OH	1.49	1.13
1:B:7:ILE:N	4:B:302:EDO:H11	1.62	1.11
1:C:154:LYS:HZ2	5:C:303:PEG:H32	1.03	1.05
1:F:56:HIS:NE2	2:F:301:LYS:HD3	1.76	1.00
1:B:7:ILE:H	4:B:302:EDO:H11	0.84	0.99
1:B:7:ILE:H	4:B:302:EDO:C1	1.77	0.98
1:A:270:GLU:O	1:A:271:PHE:HB2	1.57	0.98
1:C:154:LYS:HZ2	5:C:303:PEG:C3	1.80	0.94
1:D:192:ASP:H	4:D:303:EDO:C2	1.80	0.94
1:F:56:HIS:CE1	2:F:301:LYS:HD3	2.02	0.93
1:C:154:LYS:NZ	5:C:303:PEG:H32	1.87	0.90
1:A:105:LEU:HD11	1:A:137:TYR:HB2	1.54	0.90
1:D:140:PRO:HG3	1:D:146:GLU:OE1	1.72	0.89
1:C:10:MET:HG2	1:C:41:ALA:HB3	1.52	0.88
1:B:6:ILE:HA	4:B:302:EDO:H12	1.55	0.87
1:B:6:ILE:HA	4:B:302:EDO:C1	2.10	0.81
2:E:301:LYS:HA	2:F:301:LYS:HA	1.62	0.81
1:E:47:THR:HG21	1:E:137:TYR:OH	1.82	0.80
1:A:103:GLY:HA2	1:A:132:ILE:HD12	1.64	0.79
1:C:246:ILE:HD12	1:C:249:CYS:HB3	1.64	0.78
1:D:294:LYS:HZ1	1:D:296:LYS:HG2	1.46	0.78
2:F:301:LYS:HG2	7:F:414:HOH:O	1.84	0.77
1:D:35:ILE:HG12	1:D:75:VAL:HG21	1.68	0.76
1:A:124:LYS:HG2	1:A:128:GLN:OE1	1.86	0.75
1:E:47:THR:HG22	1:F:111:TYR:HH	1.51	0.75
1:F:88:GLU:OE2	2:F:301:LYS:HG2	1.88	0.74
1:F:63:ILE:HD12	1:F:79:ALA:HB1	1.70	0.73
1:C:16:PRO:HD2	1:C:27:TYR:HD1	1.52	0.73
1:D:73:THR:HG23	1:D:75:VAL:H	1.52	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:97:LYS:HE2	1:E:131:ASP:OD1	1.89	0.71
1:D:107:VAL:HA	1:D:137:TYR:HB3	1.72	0.70
1:C:10:MET:CG	1:C:41:ALA:HB3	2.21	0.70
1:D:191:GLU:CA	4:D:303:EDO:H21	2.21	0.70
1:D:191:GLU:HA	4:D:303:EDO:H21	1.74	0.69
1:E:137:TYR:HA	1:E:166:KPI:O	1.93	0.69
1:A:107:VAL:HA	1:A:137:TYR:HB3	1.74	0.68
1:F:3:LYS:N	7:F:402:HOH:O	2.27	0.68
1:D:231:LYS:H	1:D:231:LYS:HD2	1.59	0.68
1:D:113:LYS:HE3	1:D:144:GLY:O	1.94	0.67
1:A:229:ASN:ND2	1:A:232:GLU:OE2	2.27	0.67
1:A:136:LEU:HB2	1:A:165:VAL:HG23	1.77	0.67
1:A:189:SER:HB3	1:A:206:VAL:HG12	1.77	0.66
1:E:47:THR:CG2	1:E:137:TYR:OH	2.43	0.66
1:C:32:LYS:O	1:C:36:GLU:HG2	1.95	0.66
1:E:107:VAL:HA	1:E:137:TYR:HB3	1.78	0.66
1:A:10:MET:HG2	1:A:41:ALA:HB3	1.78	0.65
1:B:245:LYS:HE3	4:B:303:EDO:H22	1.76	0.65
1:D:150:ASP:HB3	6:D:304:PGE:H5	1.77	0.65
1:D:191:GLU:C	4:D:303:EDO:H21	2.17	0.65
1:C:294:LYS:NZ	7:C:401:HOH:O	2.30	0.65
1:C:235:LYS:O	1:C:239:GLU:HG3	1.98	0.64
1:C:74:LYS:HG2	1:E:263:ALA:O	1.98	0.64
1:D:191:GLU:HA	4:D:303:EDO:C2	2.27	0.63
1:D:3:LYS:HA	7:D:427:HOH:O	1.98	0.63
1:A:67:VAL:HG22	1:A:77:VAL:HG11	1.81	0.62
1:A:124:LYS:HG3	1:A:159:CYS:SG	2.38	0.62
1:C:246:ILE:CD1	1:C:249:CYS:HB3	2.30	0.62
1:A:235:LYS:O	1:A:239:GLU:HG3	1.99	0.61
1:A:74:LYS:O	1:A:74:LYS:HG2	1.99	0.61
1:F:10:MET:HG2	1:F:41:ALA:HB3	1.82	0.61
1:A:268:SER:OG	1:A:270:GLU:HG3	2.01	0.61
1:E:6:ILE:HG12	1:E:76:LYS:HD3	1.82	0.61
1:E:123:TYR:HA	1:E:126:ILE:HD12	1.83	0.60
1:A:244:ASN:ND2	7:A:402:HOH:O	2.24	0.60
1:E:18:LYS:HE2	1:E:23:ASP:OD2	2.02	0.60
1:A:254:ILE:HA	1:A:271:PHE:CZ	2.38	0.59
1:C:154:LYS:HE3	5:C:303:PEG:H11	1.85	0.59
1:C:154:LYS:CE	5:C:303:PEG:H11	2.32	0.59
1:F:11:THR:HG21	1:F:34:GLN:OE1	2.03	0.59
1:A:270:GLU:O	1:A:271:PHE:CB	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:70:CYS:O	1:D:73:THR:HG22	2.03	0.59
1:A:33:ARG:O	1:A:37:ASN:ND2	2.36	0.59
1:E:47:THR:OG1	1:E:166:KPI:O2	2.16	0.58
1:B:137:TYR:CD1	1:B:166:KPI:HD	2.38	0.58
1:E:111:TYR:O	1:F:142:ARG:HD2	2.04	0.58
1:F:243:ILE:HA	1:F:246:ILE:HG22	1.84	0.58
1:B:274:PRO:HB3	1:C:122:HIS:HB2	1.86	0.58
1:F:288:GLU:HA	1:F:291:LYS:HG3	1.85	0.57
1:F:138:ASN:HD21	1:F:146:GLU:HG3	1.68	0.57
1:C:243:ILE:HA	1:C:246:ILE:HG22	1.86	0.57
1:D:294:LYS:NZ	1:D:296:LYS:HG2	2.20	0.57
1:C:16:PRO:HD2	1:C:27:TYR:CD1	2.39	0.56
1:E:10:MET:HG2	1:E:41:ALA:HB3	1.86	0.56
1:E:47:THR:HG1	1:E:166:KPI:OX2	2.15	0.56
1:E:142:ARG:HH21	1:E:251:SER:HB3	1.71	0.56
1:D:10:MET:HG2	1:D:41:ALA:HB3	1.87	0.56
1:A:52:ALA:O	2:A:301:LYS:N	2.39	0.56
1:A:105:LEU:CD1	1:A:137:TYR:HB2	2.33	0.55
1:E:221:LEU:HB2	1:E:236:ILE:HG21	1.89	0.54
1:A:103:GLY:CA	1:A:132:ILE:HD12	2.37	0.54
1:C:289:VAL:HG13	1:C:292:LYS:HE2	1.90	0.54
1:F:35:ILE:HG12	1:F:75:VAL:HG21	1.88	0.54
1:B:94:LYS:HG3	1:B:129:SER:OG	2.08	0.54
1:A:113:LYS:HE3	1:D:251:SER:OG	2.08	0.54
1:D:35:ILE:HD13	1:D:73:THR:HG21	1.89	0.53
1:A:29:ARG:NH1	7:A:406:HOH:O	2.41	0.53
1:A:10:MET:CG	1:A:41:ALA:HB3	2.39	0.53
1:A:194:ILE:HG21	1:B:172:ILE:HG23	1.90	0.53
1:D:166:KPI:HE	1:D:207:ILE:HB	1.90	0.53
1:F:275:LEU:HA	7:F:435:HOH:O	2.08	0.53
1:C:107:VAL:HA	1:C:137:TYR:HB3	1.91	0.52
1:B:32:LYS:HA	1:B:35:ILE:HD12	1.91	0.52
1:B:105:LEU:HD11	1:B:137:TYR:HB2	1.91	0.52
1:E:35:ILE:HG12	1:E:75:VAL:HG21	1.91	0.52
1:A:142:ARG:HD3	1:D:113:LYS:HD2	1.91	0.52
1:C:254:ILE:HA	1:C:271:PHE:CE1	2.45	0.52
1:C:154:LYS:NZ	5:C:303:PEG:C1	2.73	0.52
1:F:217:MET:HB3	1:F:240:LEU:HD11	1.92	0.52
1:E:105:LEU:HD13	1:E:135:LEU:HD23	1.93	0.51
1:D:254:ILE:HA	1:D:271:PHE:CE2	2.46	0.51
1:F:59:HIS:O	1:F:63:ILE:HG12	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:HIS:HB2	1:D:274:PRO:HB3	1.91	0.51
1:C:77:VAL:N	1:C:102:ASP:OD2	2.34	0.51
1:E:32:LYS:HA	1:E:35:ILE:HD12	1.92	0.51
1:C:54:LEU:O	2:C:301:LYS:HE3	2.11	0.50
1:B:6:ILE:HG12	1:B:76:LYS:HD3	1.93	0.50
1:A:67:VAL:O	1:A:71:LYS:HG2	2.11	0.50
1:D:146:GLU:OE2	7:D:401:HOH:O	2.20	0.50
1:B:76:LYS:HD2	4:B:302:EDO:O2	2.12	0.50
1:D:192:ASP:N	4:D:303:EDO:C2	2.48	0.50
1:D:150:ASP:CB	6:D:304:PGE:H5	2.42	0.50
1:E:52:ALA:O	2:E:301:LYS:N	2.44	0.50
1:B:246:ILE:HD11	1:B:285:LYS:HE3	1.94	0.49
1:D:140:PRO:CG	1:D:146:GLU:OE1	2.53	0.49
1:D:294:LYS:HG2	1:D:295:ILE:N	2.26	0.49
1:A:166:KPI:HE	1:A:207:ILE:HB	1.94	0.49
1:A:229:ASN:HD21	1:A:232:GLU:CD	2.14	0.49
1:E:4:ASN:HB2	1:E:133:PRO:HG3	1.93	0.49
1:C:268:SER:HB2	1:C:270:GLU:HG3	1.93	0.49
1:C:256:ILE:O	1:C:260:MET:HG2	2.12	0.49
1:D:138:ASN:HD21	1:D:146:GLU:CD	2.16	0.49
1:C:268:SER:CB	1:C:270:GLU:HG3	2.44	0.48
1:D:209:VAL:H	4:D:303:EDO:H11	1.78	0.48
1:E:47:THR:OG1	1:E:48:THR:N	2.45	0.48
1:F:107:VAL:HA	1:F:137:TYR:HB3	1.96	0.48
1:D:102:ASP:O	1:D:133:PRO:HD2	2.14	0.48
1:C:82:GLY:HA3	1:C:107:VAL:HG12	1.96	0.47
1:C:172:ILE:HG23	1:D:194:ILE:HG21	1.95	0.47
1:C:292:LYS:HG3	1:C:293:TYR:CD1	2.49	0.47
1:E:232:GLU:O	1:E:236:ILE:HG12	2.14	0.47
1:E:274:PRO:HB3	1:F:122:HIS:HB2	1.97	0.47
1:B:6:ILE:HA	4:B:302:EDO:H11	1.92	0.47
1:E:251:SER:OG	1:F:113:LYS:HE2	2.15	0.47
1:F:27:TYR:O	1:F:31:ILE:HG13	2.13	0.47
1:B:288:GLU:OE2	1:B:291:LYS:HE2	2.14	0.47
1:C:176:VAL:HA	7:C:425:HOH:O	2.13	0.47
1:E:64:GLU:O	1:E:68:GLU:HG2	2.14	0.47
1:E:293:TYR:CE1	4:E:302:EDO:H12	2.50	0.47
1:B:243:ILE:HB	1:B:293:TYR:CE2	2.50	0.47
1:E:149:THR:HG23	1:E:178:LEU:HD23	1.95	0.47
1:E:45:VAL:HG12	1:E:45:VAL:O	2.14	0.47
1:C:60:ARG:HB3	1:C:95:PHE:CZ	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:LEU:HD13	1:A:163:TYR:CZ	2.49	0.47
1:C:25:GLN:HG2	1:C:29:ARG:HH22	1.80	0.47
1:F:60:ARG:HB3	1:F:95:PHE:CZ	2.51	0.46
1:B:126:ILE:O	1:B:129:SER:HB3	2.16	0.46
1:E:256:ILE:O	1:E:260:MET:HG2	2.15	0.46
1:E:268:SER:OG	1:E:270:GLU:HB2	2.14	0.46
1:B:3:LYS:NZ	1:B:162:ILE:O	2.49	0.46
1:B:107:VAL:HA	1:B:137:TYR:HB3	1.98	0.46
1:D:279:SER:HB3	7:D:410:HOH:O	2.14	0.45
1:A:77:VAL:CG1	1:A:101:ALA:HA	2.47	0.45
1:C:175:CYS:HB3	1:C:187:LEU:HD21	1.99	0.45
1:F:135:LEU:HD13	1:F:163:TYR:CZ	2.51	0.45
1:A:76:LYS:NZ	7:A:412:HOH:O	2.49	0.45
1:F:166:KPI:HE	1:F:207:ILE:HB	1.99	0.45
1:C:10:MET:HA	1:C:41:ALA:O	2.17	0.45
1:C:179:LEU:HD21	1:C:187:LEU:HB2	1.98	0.45
1:E:61:THR:O	1:E:65:ILE:HG13	2.16	0.45
1:F:137:TYR:CD1	1:F:166:KPI:HD	2.52	0.45
1:E:193:ALA:HA	7:E:413:HOH:O	2.17	0.44
1:D:262:LEU:HD21	1:D:283:PHE:CZ	2.52	0.44
1:E:84:ASN:OD1	2:F:301:LYS:O	2.36	0.44
1:E:111:TYR:HH	1:F:47:THR:HG1	1.65	0.44
1:B:254:ILE:HA	1:B:271:PHE:CE2	2.53	0.44
1:C:98:GLU:OE1	1:C:99:HIS:NE2	2.47	0.44
1:C:161:ASN:OD1	1:C:161:ASN:N	2.41	0.44
1:F:56:HIS:CD2	2:F:301:LYS:HD3	2.50	0.44
1:C:43:VAL:HA	1:C:78:LEU:O	2.17	0.44
1:D:54:LEU:O	2:D:301:LYS:HE3	2.18	0.44
1:B:10:MET:HG2	1:B:41:ALA:HB3	2.00	0.43
1:B:189:SER:HB3	1:B:206:VAL:HG12	2.00	0.43
1:D:135:LEU:HD13	1:D:163:TYR:CZ	2.53	0.43
1:F:32:LYS:O	1:F:36:GLU:HG3	2.18	0.43
1:B:142:ARG:HG2	1:C:113:LYS:HD2	2.00	0.43
1:B:122:HIS:HB2	1:C:274:PRO:HB3	1.99	0.43
1:A:241:TYR:CD2	1:B:181:HIS:HE1	2.36	0.43
1:D:294:LYS:HG2	1:D:294:LYS:HZ3	1.75	0.43
1:F:262:LEU:HD21	1:F:283:PHE:CE1	2.53	0.43
1:E:85:ALA:HB3	1:E:88:GLU:HB2	2.01	0.43
1:F:216:ASP:OD1	1:F:216:ASP:N	2.52	0.43
1:B:35:ILE:HG12	1:B:75:VAL:HG21	2.00	0.43
1:C:137:TYR:CD1	1:C:166:KPI:HD	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:ASN:HA	1:C:109:PRO:HB3	2.01	0.43
1:C:154:LYS:NZ	5:C:303:PEG:H11	2.34	0.43
1:C:246:ILE:HD12	1:C:246:ILE:HA	1.81	0.43
1:E:142:ARG:NH2	1:E:251:SER:HB3	2.32	0.43
1:D:25:GLN:CD	1:D:25:GLN:H	2.23	0.43
1:F:104:ILE:HG13	1:F:134:VAL:HG13	2.01	0.42
1:A:102:ASP:O	1:A:133:PRO:HD2	2.18	0.42
1:E:28:ALA:O	1:E:32:LYS:HG3	2.19	0.42
1:A:31:ILE:HD13	1:A:66:ALA:HA	2.01	0.42
1:F:10:MET:HA	1:F:41:ALA:O	2.20	0.42
1:A:48:THR:OG1	1:A:166:KPI:O1	2.21	0.42
1:A:216:ASP:OD1	1:A:216:ASP:N	2.52	0.42
1:B:117:GLN:NE2	1:B:121:GLU:OE2	2.37	0.42
1:D:67:VAL:HA	1:D:77:VAL:HG21	2.02	0.42
1:F:204:LYS:HA	1:F:226:LEU:HD21	2.02	0.42
1:D:13:LEU:HD11	1:D:42:VAL:HB	2.01	0.42
1:D:256:ILE:O	1:D:260:MET:HG2	2.19	0.41
1:C:221:LEU:HD12	1:C:236:ILE:HG22	2.01	0.41
1:C:243:ILE:HB	1:C:293:TYR:CE1	2.56	0.41
1:A:4:ASN:ND2	7:A:411:HOH:O	2.48	0.41
1:E:60:ARG:HB3	1:E:95:PHE:CZ	2.56	0.41
1:C:45:VAL:HG12	1:C:45:VAL:O	2.20	0.41
1:C:110:TYR:HA	1:C:143:THR:HB	2.02	0.41
1:C:292:LYS:HG3	1:C:293:TYR:CE1	2.56	0.41
1:D:10:MET:HA	1:D:41:ALA:O	2.21	0.41
1:C:13:LEU:HD11	1:C:42:VAL:HB	2.03	0.41
1:E:43:VAL:HA	1:E:78:LEU:O	2.21	0.41
1:A:10:MET:HA	1:A:41:ALA:O	2.20	0.41
1:B:6:ILE:CA	4:B:302:EDO:H11	2.50	0.41
1:C:54:LEU:HD23	1:C:54:LEU:HA	1.89	0.41
1:D:191:GLU:HA	4:D:303:EDO:H22	1.99	0.41
1:B:135:LEU:HD13	1:B:163:TYR:CZ	2.56	0.41
1:A:256:ILE:O	1:A:260:MET:HG2	2.20	0.40
1:C:18:LYS:N	1:C:21:LYS:O	2.40	0.40
1:E:140:PRO:HG3	1:E:146:GLU:OE1	2.21	0.40
1:E:247:LEU:HD23	1:E:247:LEU:HA	1.92	0.40
1:A:142:ARG:CD	1:D:113:LYS:HD2	2.51	0.40
1:B:161:ASN:OD1	1:B:161:ASN:N	2.45	0.40
1:C:276:CYS:SG	7:C:435:HOH:O	2.45	0.40
1:E:157:ARG:NE	1:E:182:GLU:OE1	2.33	0.40
1:F:254:ILE:HA	1:F:271:PHE:CE2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:ARG:HG2	1:C:95:PHE:CD1	2.56	0.40
1:B:113:LYS:HE3	1:C:251:SER:OG	2.21	0.40
1:C:31:ILE:HD13	1:C:66:ALA:HA	2.03	0.40
1:F:84:ASN:HA	1:F:109:PRO:HB3	2.03	0.40

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	293/310 (94%)	286 (98%)	7 (2%)	0	100	100
1	B	293/310 (94%)	288 (98%)	5 (2%)	0	100	100
1	C	293/310 (94%)	288 (98%)	5 (2%)	0	100	100
1	D	293/310 (94%)	288 (98%)	5 (2%)	0	100	100
1	E	293/310 (94%)	286 (98%)	6 (2%)	1 (0%)	41	46
1	F	293/310 (94%)	288 (98%)	5 (2%)	0	100	100
All	All	1758/1860 (94%)	1724 (98%)	33 (2%)	1 (0%)	51	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	167	GLU

### 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	246/260 (95%)	243 (99%)	3 (1%)	71	80
1	B	246/260 (95%)	242 (98%)	4 (2%)	62	73
1	C	247/260 (95%)	240 (97%)	7 (3%)	43	52
1	D	245/260 (94%)	243 (99%)	2 (1%)	81	88
1	E	244/260 (94%)	240 (98%)	4 (2%)	62	73
1	F	247/260 (95%)	242 (98%)	5 (2%)	55	64
All	All	1475/1560 (95%)	1450 (98%)	25 (2%)	60	71

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	272	ARG
1	A	280	LYS
1	A	288	GLU
1	B	129	SER
1	B	235	LYS
1	B	280	LYS
1	B	294	LYS
1	C	18	LYS
1	C	57	GLU
1	C	71	LYS
1	C	76	LYS
1	C	137	TYR
1	C	231	LYS
1	C	292	LYS
1	D	29	ARG
1	D	231	LYS
1	E	137	TYR
1	E	167	GLU
1	E	272	ARG
1	E	292	LYS
1	F	18	LYS
1	F	106	SER
1	F	137	TYR
1	F	235	LYS
1	F	281	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	128	GLN
1	C	242	ASN
1	E	4	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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
1	KPI	F	166	1	11,13,14	1.74	3 (27%)	10,15,17	1.69	2 (20%)
1	KPI	D	166	1	11,13,14	1.25	1 (9%)	10,15,17	2.54	6 (60%)
1	KPI	B	166	1	11,13,14	1.76	2 (18%)	10,15,17	1.32	1 (10%)
1	KPI	C	166	1	11,13,14	1.92	3 (27%)	10,15,17	2.06	4 (40%)
1	KPI	E	166	1	11,13,14	1.99	2 (18%)	10,15,17	2.04	5 (50%)
1	KPI	A	166	1	11,13,14	1.19	2 (18%)	10,15,17	2.45	5 (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
1	KPI	F	166	1	-	0/13/14/16	-
1	KPI	D	166	1	-	0/13/14/16	-
1	KPI	B	166	1	-	0/13/14/16	-
1	KPI	C	166	1	-	1/13/14/16	-
1	KPI	E	166	1	-	0/13/14/16	-
1	KPI	A	166	1	-	0/13/14/16	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	166	KPI	CX2-CX1	-5.11	1.43	1.49
1	C	166	KPI	CX2-CX1	-4.87	1.44	1.49
1	F	166	KPI	CX2-CX1	-4.31	1.44	1.49
1	B	166	KPI	CX2-CX1	-4.16	1.44	1.49
1	B	166	KPI	O1-CX2	-3.20	1.21	1.30
1	E	166	KPI	O1-CX2	-3.18	1.21	1.30
1	D	166	KPI	O1-CX2	-2.89	1.22	1.30
1	F	166	KPI	O1-CX2	-2.70	1.22	1.30
1	A	166	KPI	O1-CX2	-2.58	1.23	1.30
1	C	166	KPI	O1-CX2	-2.50	1.23	1.30
1	C	166	KPI	CA-N	-2.29	1.41	1.48
1	F	166	KPI	CA-N	-2.24	1.41	1.48
1	A	166	KPI	CA-N	-2.20	1.41	1.48

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	166	KPI	CD-CE-NZ	-4.35	102.74	110.66
1	A	166	KPI	CE-NZ-CX1	3.89	132.29	121.70
1	A	166	KPI	CX2-CX1-NZ	3.81	124.25	114.98
1	D	166	KPI	O1-CX2-CX1	3.62	124.22	116.35
1	F	166	KPI	CE-NZ-CX1	3.53	131.31	121.70
1	F	166	KPI	C1-CX1-CX2	3.43	121.49	118.17
1	C	166	KPI	O2-CX2-CX1	-3.34	117.11	121.38
1	C	166	KPI	C1-CX1-CX2	3.34	121.41	118.17
1	C	166	KPI	CD-CE-NZ	-3.10	105.02	110.66
1	B	166	KPI	CE-NZ-CX1	3.09	130.13	121.70
1	A	166	KPI	O1-CX2-O2	-2.91	116.95	123.61
1	D	166	KPI	O1-CX2-O2	-2.89	116.99	123.61
1	E	166	KPI	O2-CX2-CX1	-2.89	117.69	121.38
1	D	166	KPI	CX2-CX1-NZ	2.76	121.71	114.98
1	E	166	KPI	CE-NZ-CX1	2.74	129.15	121.70
1	D	166	KPI	CE-NZ-CX1	2.64	128.89	121.70
1	E	166	KPI	O1-CX2-CX1	2.63	122.07	116.35
1	A	166	KPI	CD-CE-NZ	2.63	115.44	110.66
1	C	166	KPI	CE-NZ-CX1	2.41	128.27	121.70
1	E	166	KPI	CX2-CX1-NZ	2.37	120.76	114.98
1	A	166	KPI	C1-CX1-CX2	-2.34	115.89	118.17
1	E	166	KPI	CD-CE-NZ	-2.21	106.63	110.66
1	D	166	KPI	O2-CX2-CX1	-2.03	118.79	121.38

There are no chirality outliers.



All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	166	KPI	O-C-CA-CB

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	F	166	KPI	2	0
1	D	166	KPI	1	0
1	B	166	KPI	1	0
1	C	166	KPI	1	0
1	E	166	KPI	3	0
1	A	166	KPI	2	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 6 are monoatomic - leaving 13 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
6	PGE	D	304	-	9,9,9	0.38	0	8,8,8	1.67	3 (37%)
2	LYS	F	301	-	8,9,9	0.88	1 (12%)	9,10,10	1.20	1 (11%)
4	EDO	E	302	-	3,3,3	0.38	0	2,2,2	0.27	0
2	LYS	C	301	-	8,9,9	0.89	1 (12%)	9,10,10	1.13	2 (22%)
2	LYS	B	301	-	8,9,9	0.85	1 (12%)	9,10,10	1.13	2 (22%)
2	LYS	D	301	-	8,9,9	0.84	1 (12%)	9,10,10	1.18	2 (22%)
4	EDO	D	303	-	3,3,3	0.39	0	2,2,2	0.54	0
2	LYS	A	301	-	8,9,9	1.00	1 (12%)	9,10,10	1.52	2 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	PEG	C	303	-	6,6,6	0.31	0	5,5,5	0.68	0
2	LYS	E	301	-	8,9,9	0.84	1 (12%)	9,10,10	1.21	2 (22%)
4	EDO	D	302	-	3,3,3	0.36	0	2,2,2	0.48	0
4	EDO	B	302	-	3,3,3	0.28	0	2,2,2	0.72	0
4	EDO	B	303	-	3,3,3	0.41	0	2,2,2	0.19	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PGE	D	304	-	-	5/7/7/7	-
2	LYS	F	301	-	-	1/9/9/9	-
4	EDO	E	302	-	-	1/1/1/1	-
2	LYS	C	301	-	-	1/9/9/9	-
2	LYS	B	301	-	-	2/9/9/9	-
2	LYS	D	301	-	-	1/9/9/9	-
4	EDO	D	303	-	-	1/1/1/1	-
2	LYS	A	301	-	-	0/9/9/9	-
5	PEG	C	303	-	-	2/4/4/4	-
2	LYS	E	301	-	-	0/9/9/9	-
4	EDO	D	302	-	-	1/1/1/1	-
4	EDO	B	302	-	-	1/1/1/1	-
4	EDO	B	303	-	-	1/1/1/1	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	LYS	OXT-C	-2.76	1.21	1.30
2	F	301	LYS	OXT-C	-2.38	1.22	1.30
2	C	301	LYS	OXT-C	-2.21	1.23	1.30
2	E	301	LYS	OXT-C	-2.20	1.23	1.30
2	B	301	LYS	OXT-C	-2.15	1.23	1.30
2	D	301	LYS	OXT-C	-2.12	1.23	1.30

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	LYS	OXT-C-O	-3.37	116.44	124.09
6	D	304	PGE	O4-C6-C5	-3.02	94.31	111.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	LYS	OXT-C-CA	2.78	122.84	113.38
2	E	301	LYS	OXT-C-O	-2.74	117.87	124.09
2	F	301	LYS	OXT-C-O	-2.71	117.94	124.09
2	D	301	LYS	OXT-C-O	-2.59	118.20	124.09
2	C	301	LYS	OXT-C-O	-2.49	118.44	124.09
2	B	301	LYS	OXT-C-O	-2.41	118.61	124.09
6	D	304	PGE	O1-C1-C2	-2.34	98.26	111.81
2	B	301	LYS	OXT-C-CA	2.18	120.80	113.38
2	E	301	LYS	OXT-C-CA	2.16	120.73	113.38
2	D	301	LYS	OXT-C-CA	2.14	120.69	113.38
6	D	304	PGE	O3-C5-C6	-2.12	100.77	110.07
2	C	301	LYS	OXT-C-CA	2.04	120.34	113.38

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	304	PGE	O2-C3-C4-O3
5	C	303	PEG	O1-C1-C2-O2
6	D	304	PGE	O3-C5-C6-O4
2	B	301	LYS	CG-CD-CE-NZ
4	B	303	EDO	O1-C1-C2-O2
4	D	302	EDO	O1-C1-C2-O2
4	D	303	EDO	O1-C1-C2-O2
2	D	301	LYS	CG-CD-CE-NZ
6	D	304	PGE	O1-C1-C2-O2
4	B	302	EDO	O1-C1-C2-O2
4	E	302	EDO	O1-C1-C2-O2
2	B	301	LYS	CE-CD-CG-CB
2	C	301	LYS	CG-CD-CE-NZ
2	F	301	LYS	CG-CD-CE-NZ
6	D	304	PGE	C6-C5-O3-C4
5	C	303	PEG	O2-C3-C4-O4
6	D	304	PGE	C1-C2-O2-C3

There are no ring outliers.

11 monomers are involved in 40 short contacts:

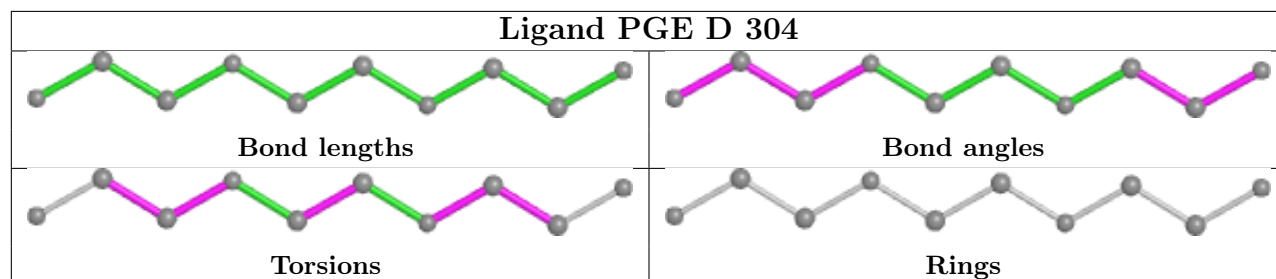
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	304	PGE	2	0
2	F	301	LYS	7	0

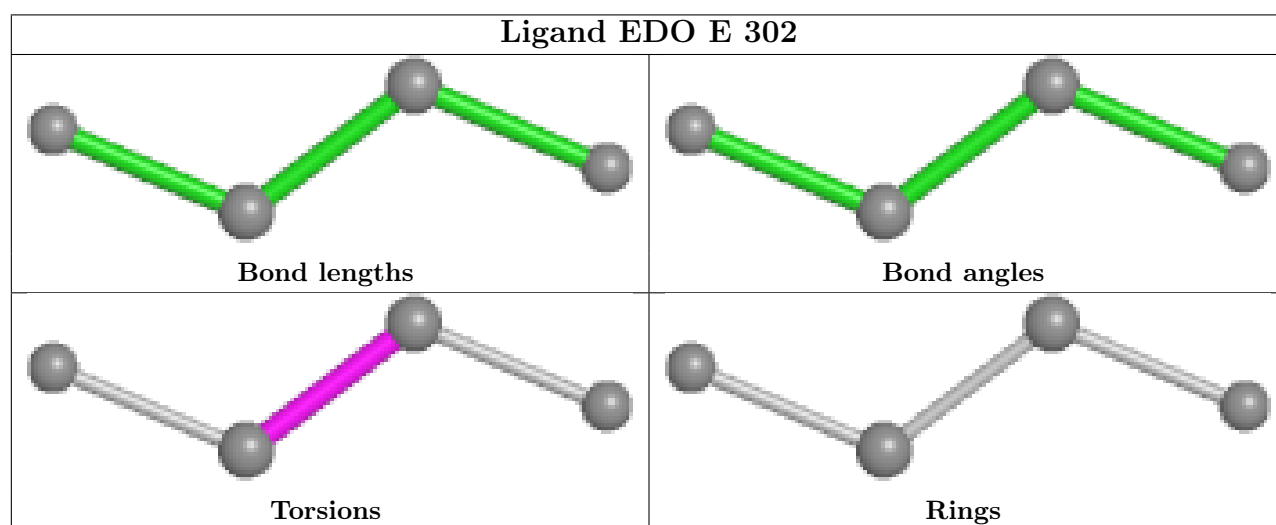
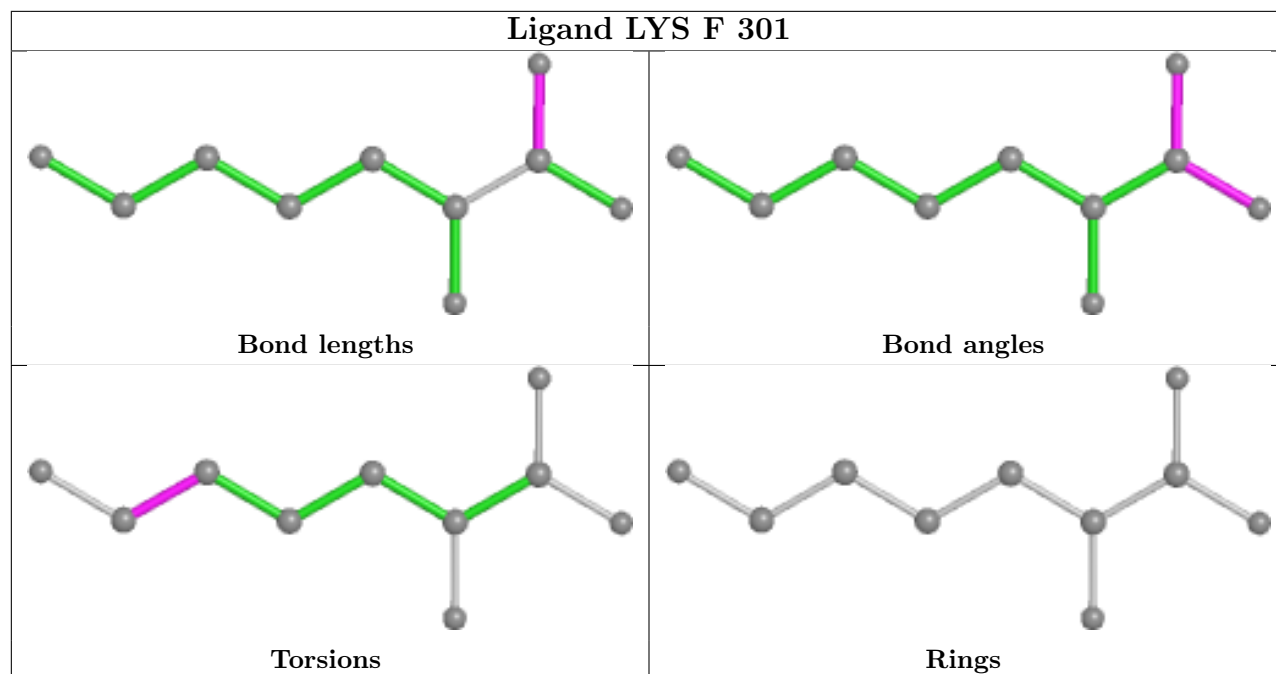
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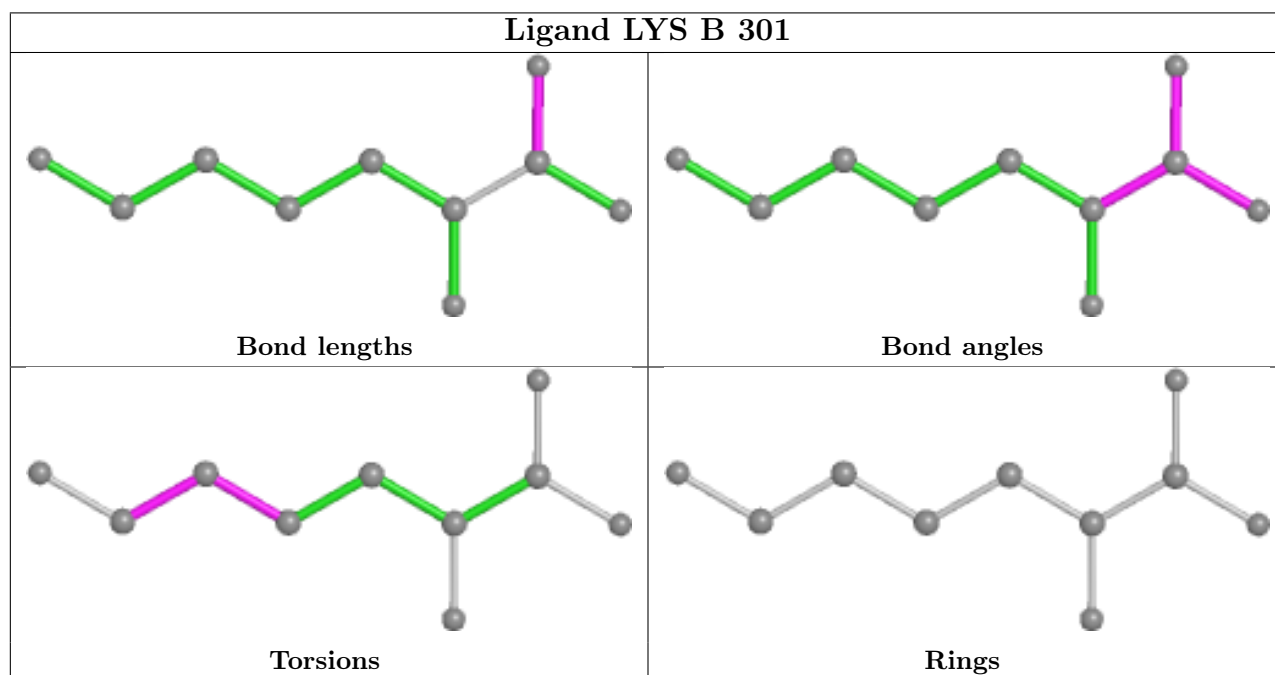
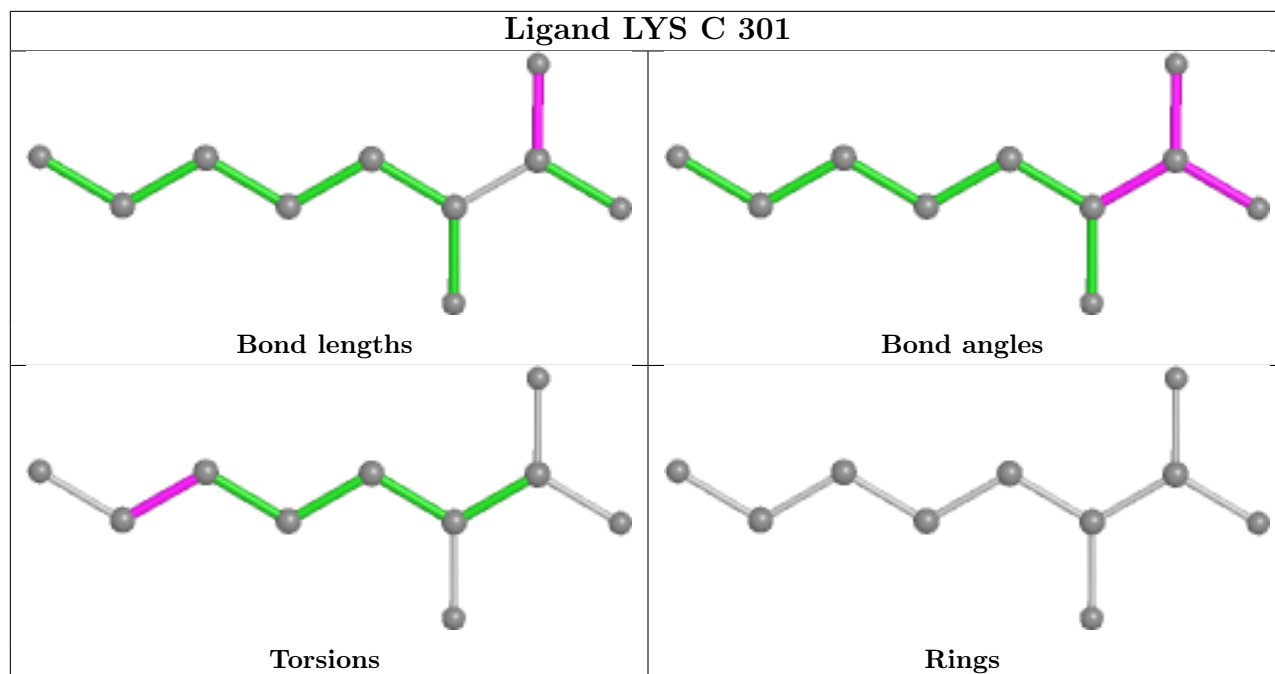
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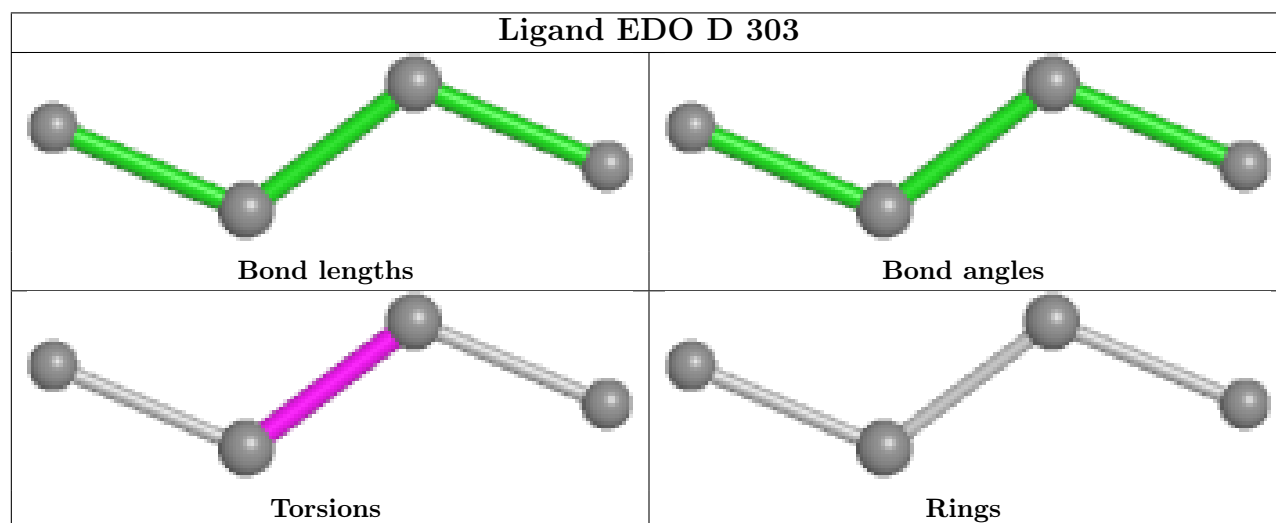
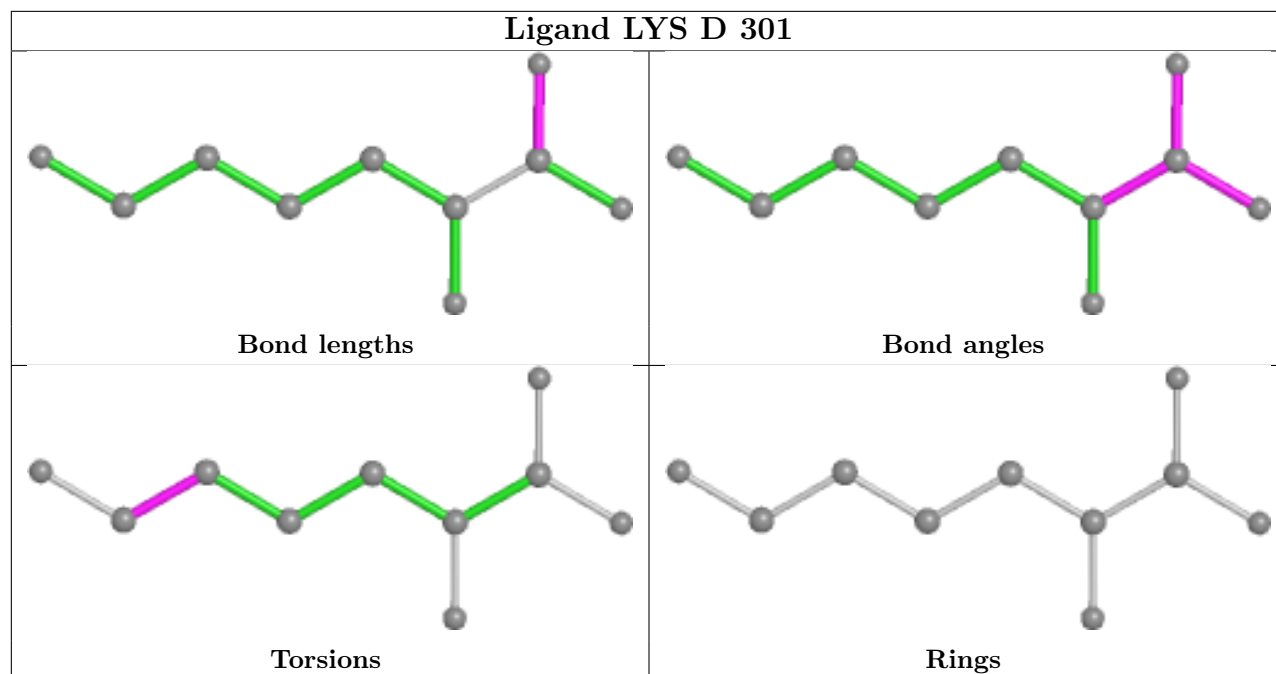
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	302	EDO	1	0
2	C	301	LYS	1	0
2	D	301	LYS	1	0
4	D	303	EDO	10	0
2	A	301	LYS	1	0
5	C	303	PEG	7	0
2	E	301	LYS	2	0
4	B	302	EDO	8	0
4	B	303	EDO	1	0

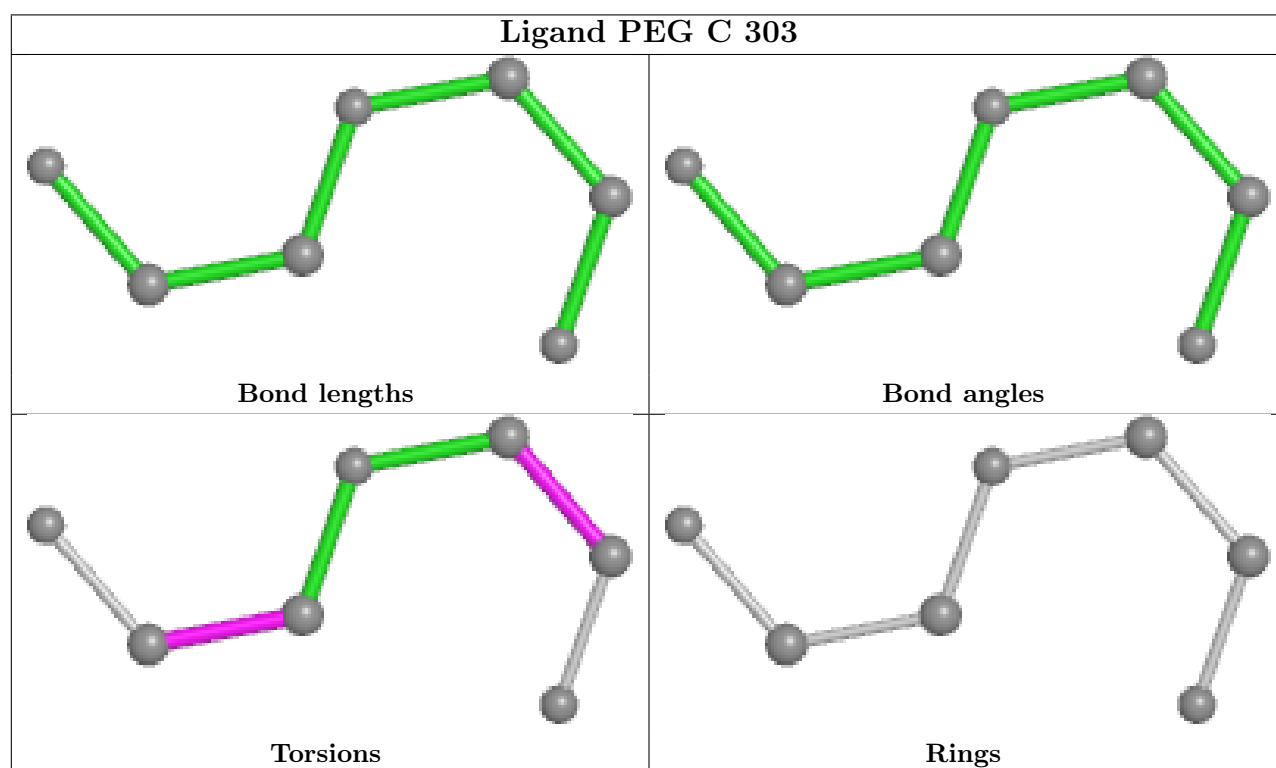
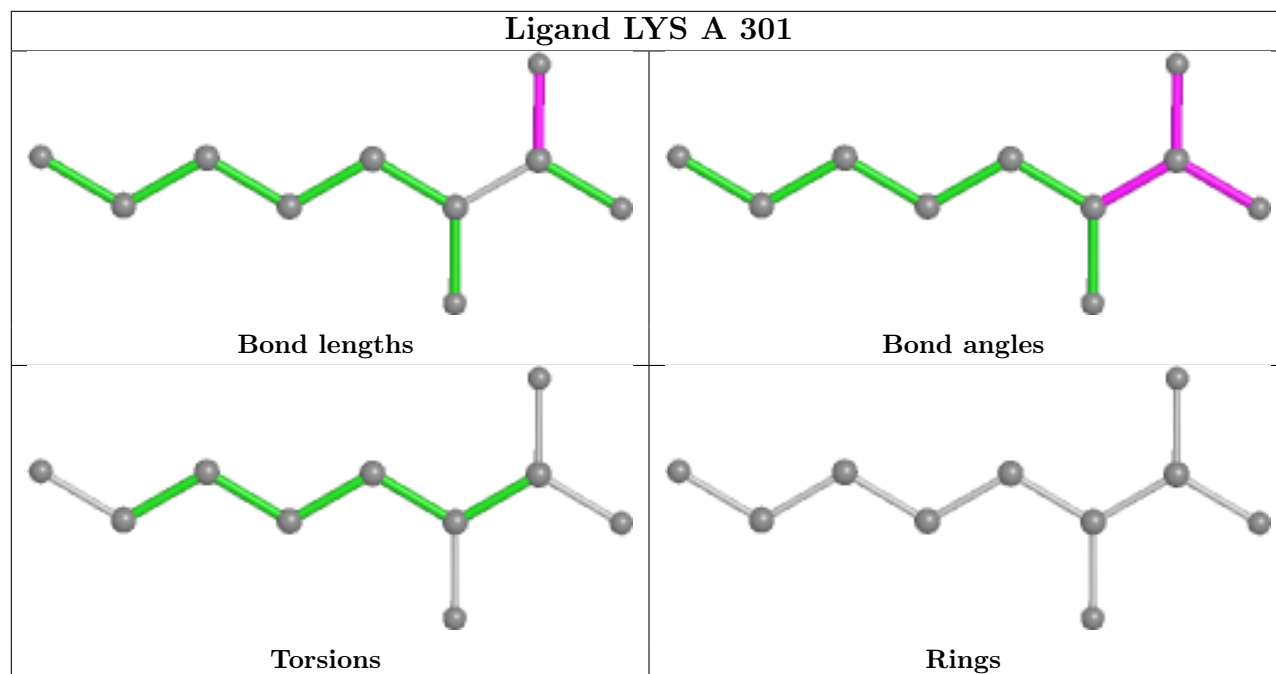
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



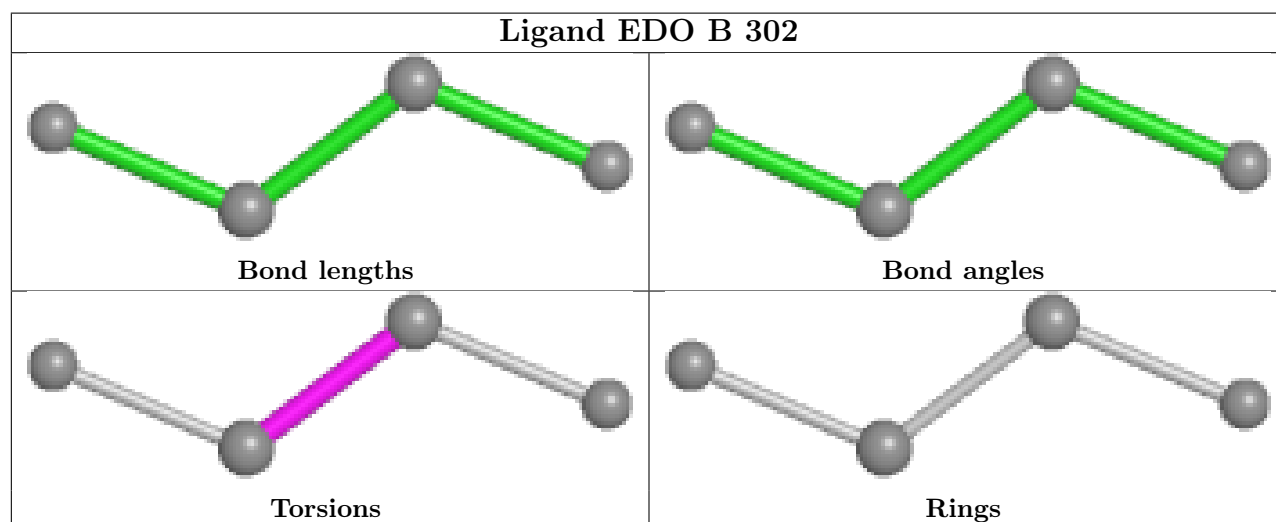
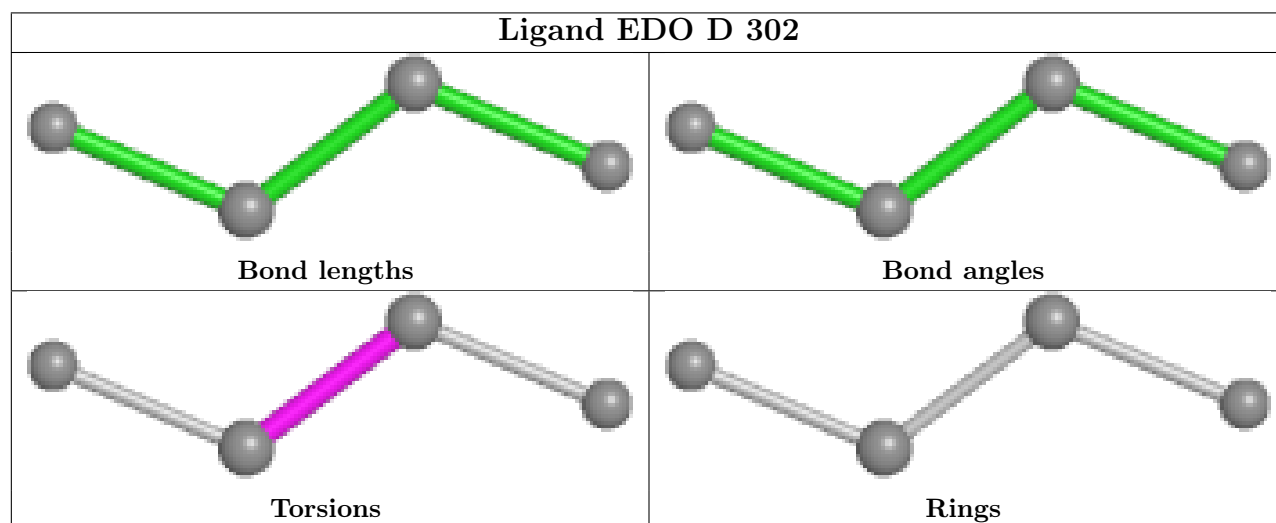
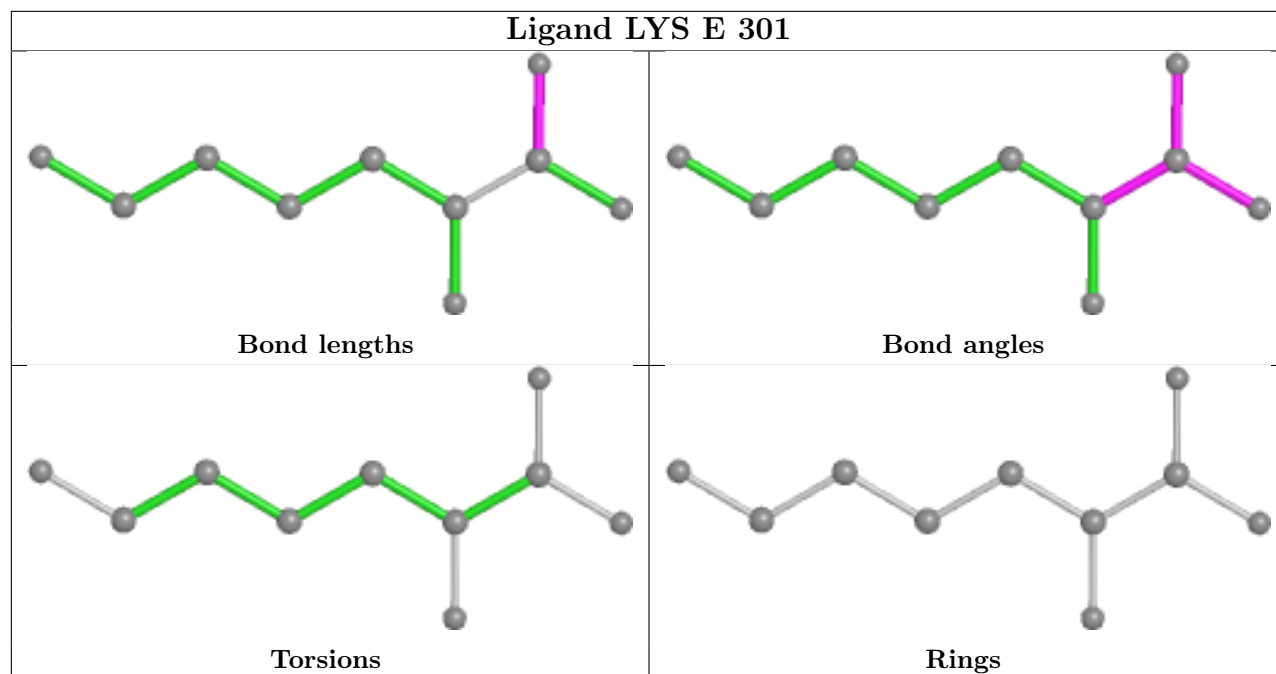


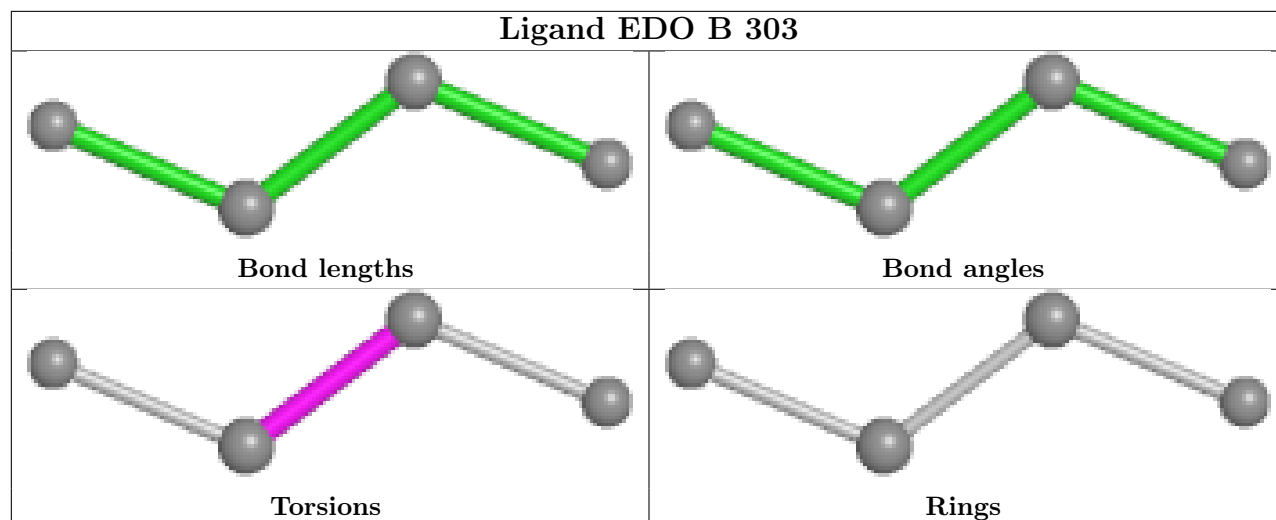












## 5.7 Other polymers [i](#)

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<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	295/310 (95%)	0.43	6 (2%) 65 68	26, 35, 51, 65	0
1	B	295/310 (95%)	0.33	4 (1%) 75 77	26, 34, 49, 61	0
1	C	295/310 (95%)	0.51	6 (2%) 65 68	26, 36, 49, 63	0
1	D	295/310 (95%)	0.44	4 (1%) 75 77	27, 37, 53, 74	0
1	E	295/310 (95%)	0.47	6 (2%) 65 68	26, 38, 53, 63	0
1	F	295/310 (95%)	0.50	7 (2%) 59 62	28, 39, 55, 74	0
All	All	1770/1860 (95%)	0.45	33 (1%) 66 69	26, 36, 52, 74	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	47	THR	4.1
1	A	206	VAL	3.4
1	D	267	GLU	3.2
1	A	229	ASN	3.2
1	C	18	LYS	3.1
1	F	141	GLY	2.8
1	F	267	GLU	2.7
1	C	270	GLU	2.7
1	F	20	GLY	2.6
1	E	4	ASN	2.6
1	F	209	VAL	2.5
1	C	17	PHE	2.5
1	B	132	ILE	2.5
1	B	19	ASN	2.4
1	C	170	GLY	2.4
1	A	267	GLU	2.4
1	E	129	SER	2.3
1	A	281	GLU	2.3
1	E	9	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	57	GLU	2.2
1	C	262	LEU	2.2
1	D	249	CYS	2.2
1	B	39	ILE	2.2
1	B	179	LEU	2.2
1	D	230	TYR	2.1
1	F	196	TYR	2.1
1	C	163	TYR	2.1
1	D	73	THR	2.1
1	A	130	VAL	2.1
1	E	18	LYS	2.1
1	F	45	VAL	2.1
1	F	298	PHE	2.0
1	E	130	VAL	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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<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
1	KPI	C	166	14/15	0.88	0.16	23,27,31,34	0
1	KPI	F	166	14/15	0.89	0.18	33,37,46,48	0
1	KPI	E	166	14/15	0.90	0.18	38,44,61,63	0
1	KPI	A	166	14/15	0.90	0.14	25,30,41,46	0
1	KPI	B	166	14/15	0.92	0.14	24,29,35,36	0
1	KPI	D	166	14/15	0.93	0.15	29,34,44,47	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

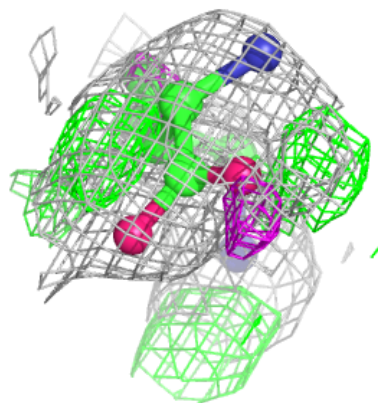
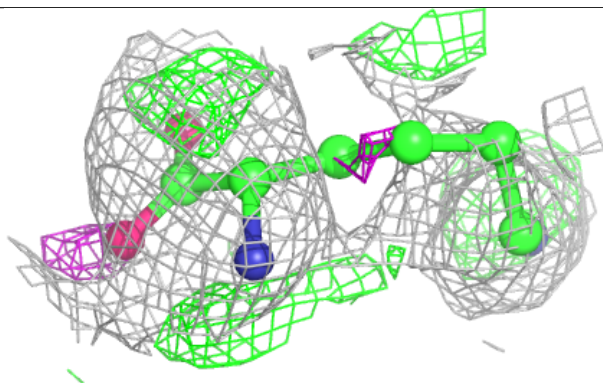
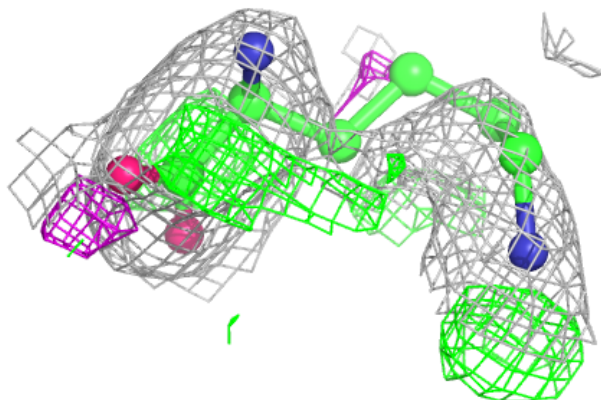
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	LYS	F	301	10/10	0.68	0.35	31,42,46,47	0
5	PEG	C	303	7/7	0.71	0.28	20,20,20,20	0
4	EDO	E	302	4/4	0.72	0.24	20,20,20,20	0
3	MG	B	305	1/1	0.73	0.10	30,30,30,30	0
4	EDO	B	303	4/4	0.75	0.28	20,20,20,20	0
3	MG	B	306	1/1	0.77	0.13	30,30,30,30	0
4	EDO	D	302	4/4	0.78	0.36	20,20,20,20	0
3	MG	A	302	1/1	0.78	0.08	30,30,30,30	0
2	LYS	A	301	10/10	0.78	0.23	20,20,20,20	0
4	EDO	B	302	4/4	0.81	0.34	20,20,20,20	0
6	PGE	D	304	10/10	0.82	0.32	20,20,20,20	0
2	LYS	C	301	10/10	0.89	0.19	24,26,27,28	0
2	LYS	D	301	10/10	0.89	0.17	27,29,37,39	0
3	MG	A	303	1/1	0.91	0.12	30,30,30,30	0
2	LYS	E	301	10/10	0.91	0.18	31,33,39,39	0
4	EDO	D	303	4/4	0.91	0.20	20,20,20,20	0
3	MG	B	304	1/1	0.92	0.11	30,30,30,30	0
2	LYS	B	301	10/10	0.94	0.12	25,28,33,35	0
3	MG	C	302	1/1	0.98	0.15	30,30,30,30	0

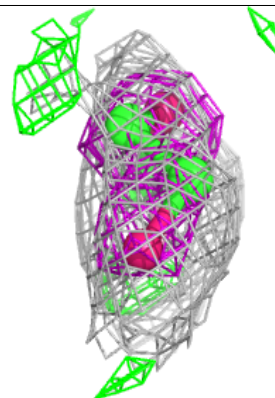
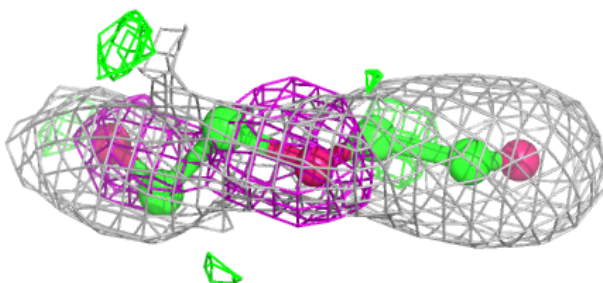
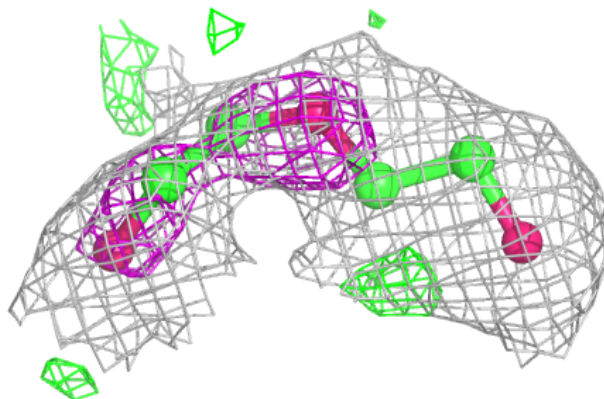
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

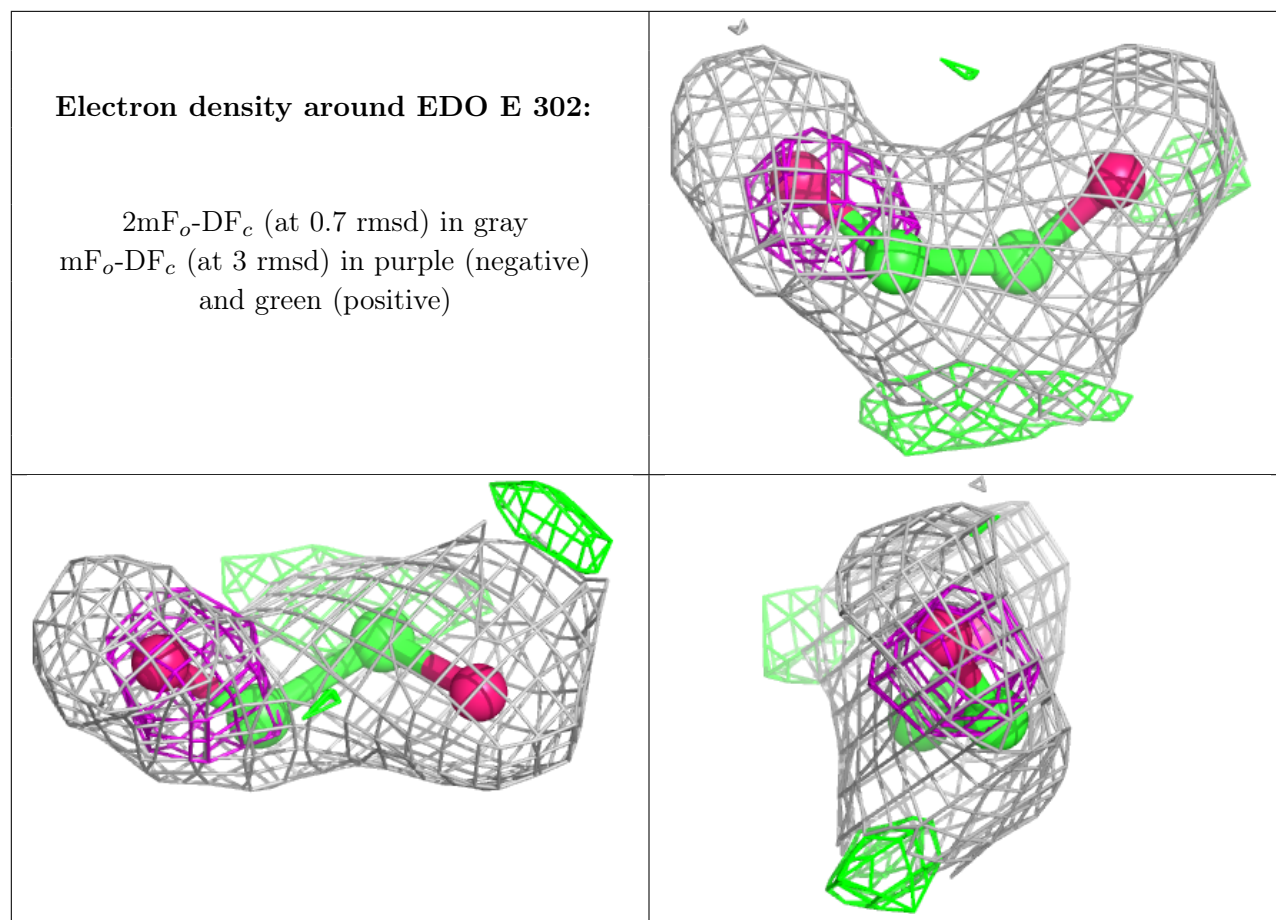
**Electron density around LYS F 301:**

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

**Electron density around PEG C 303:**

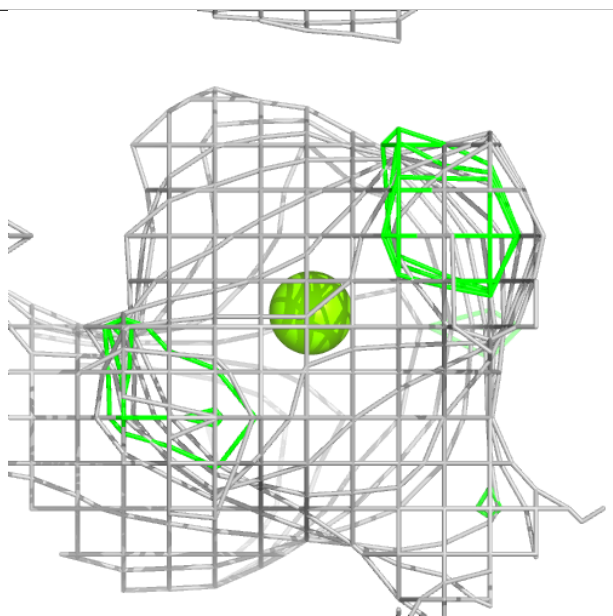
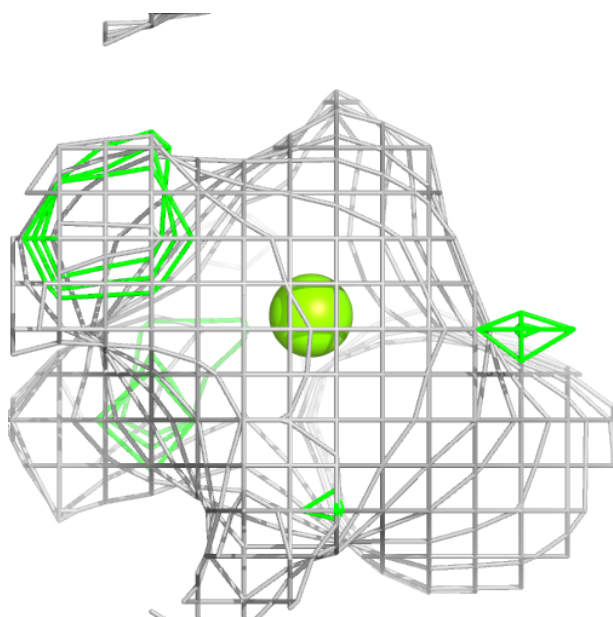
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around MG B 305:**

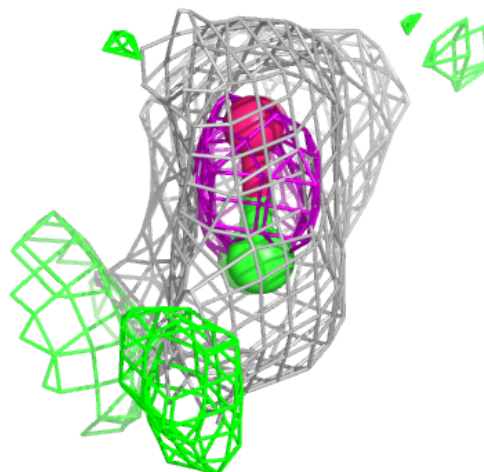
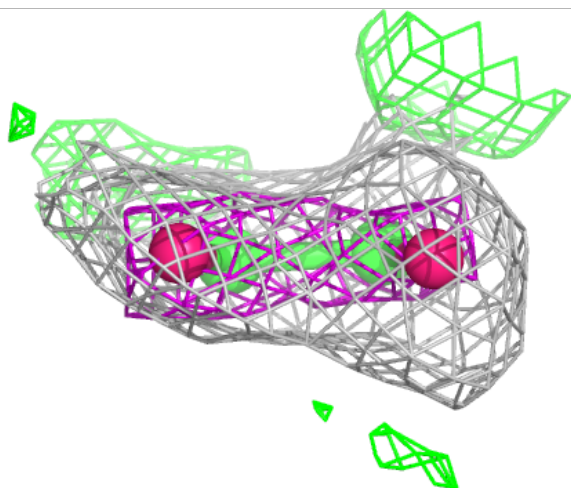
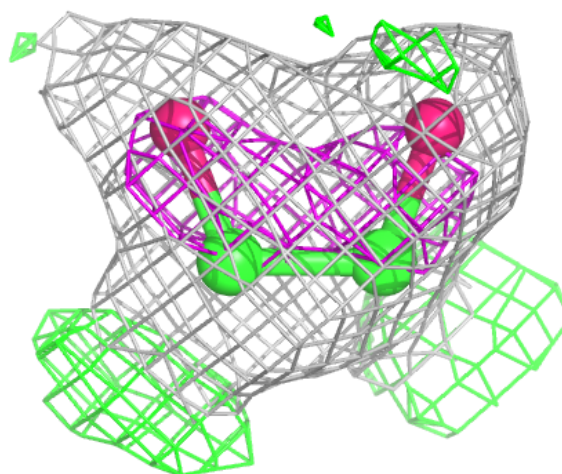
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





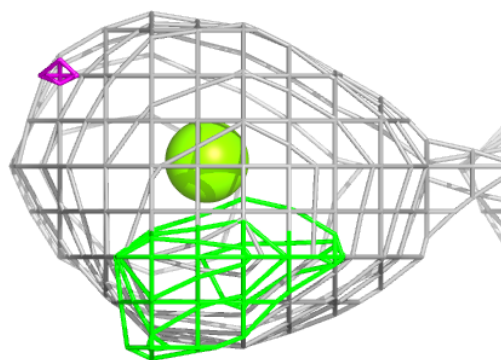
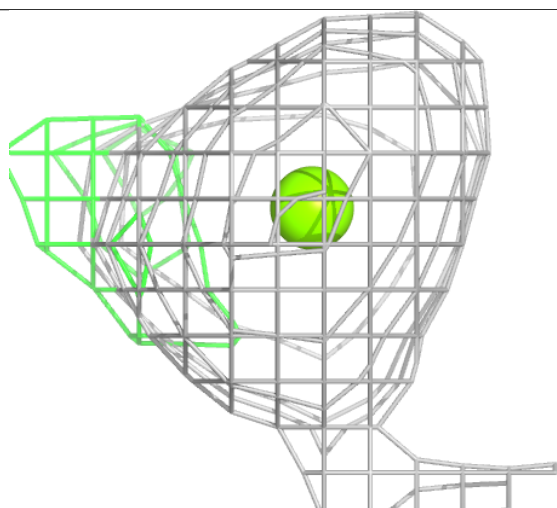
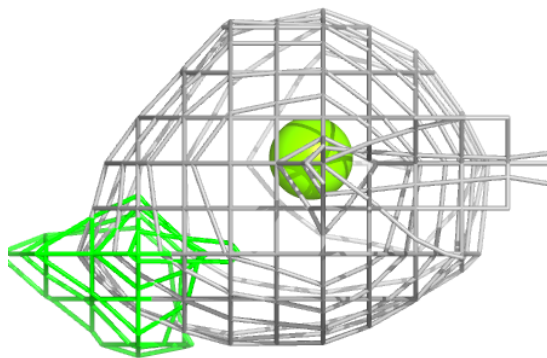
**Electron density around EDO B 303:**

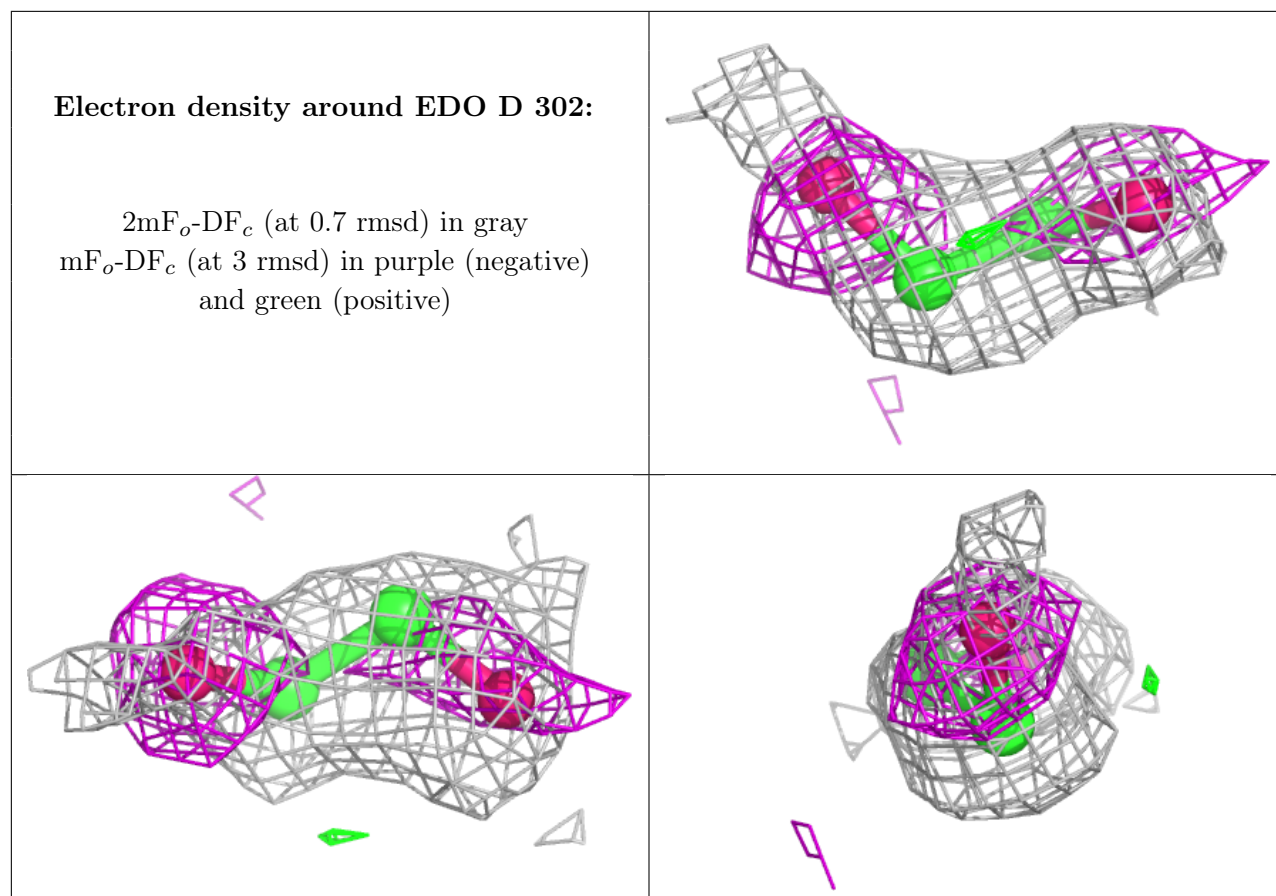
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around MG B 306:**

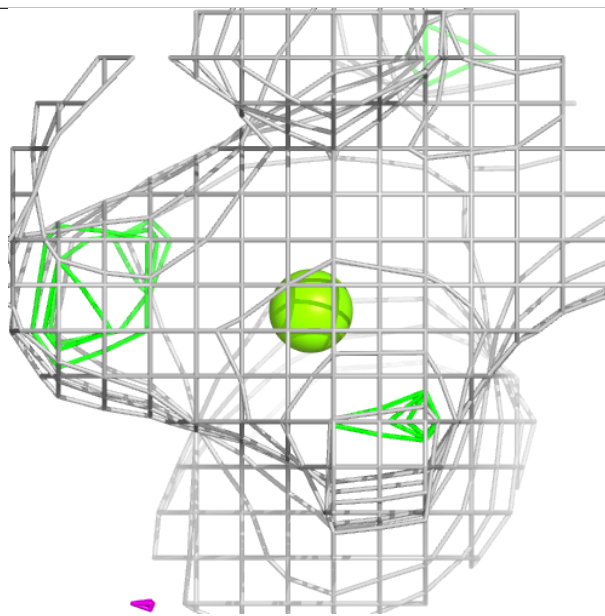
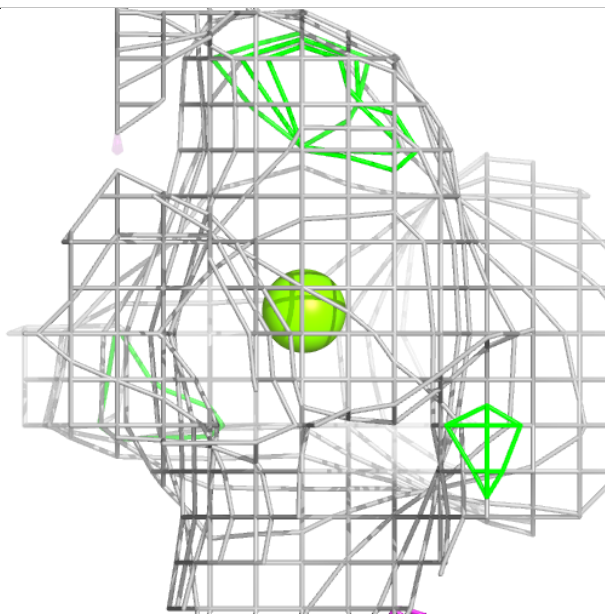
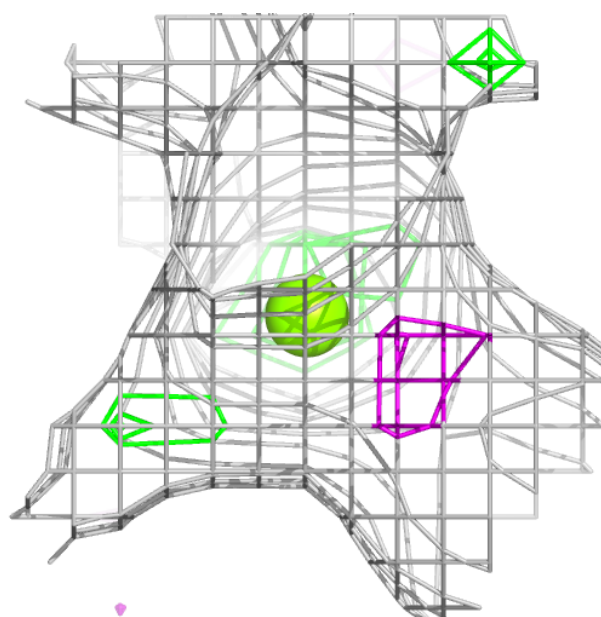
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





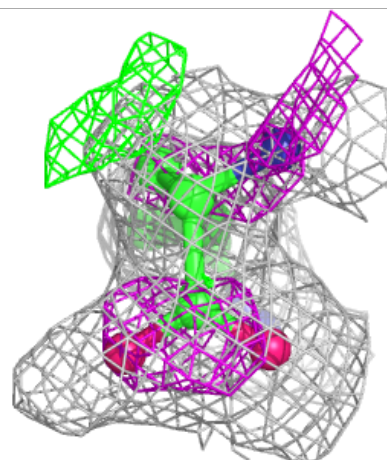
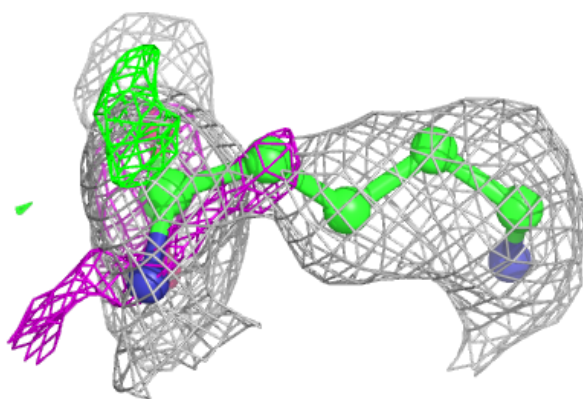
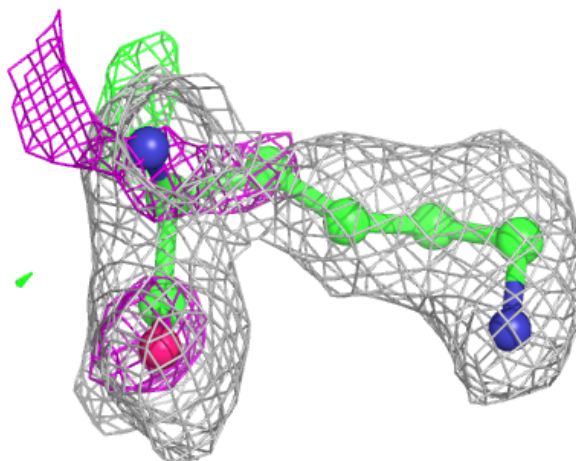
**Electron density around MG A 302:**

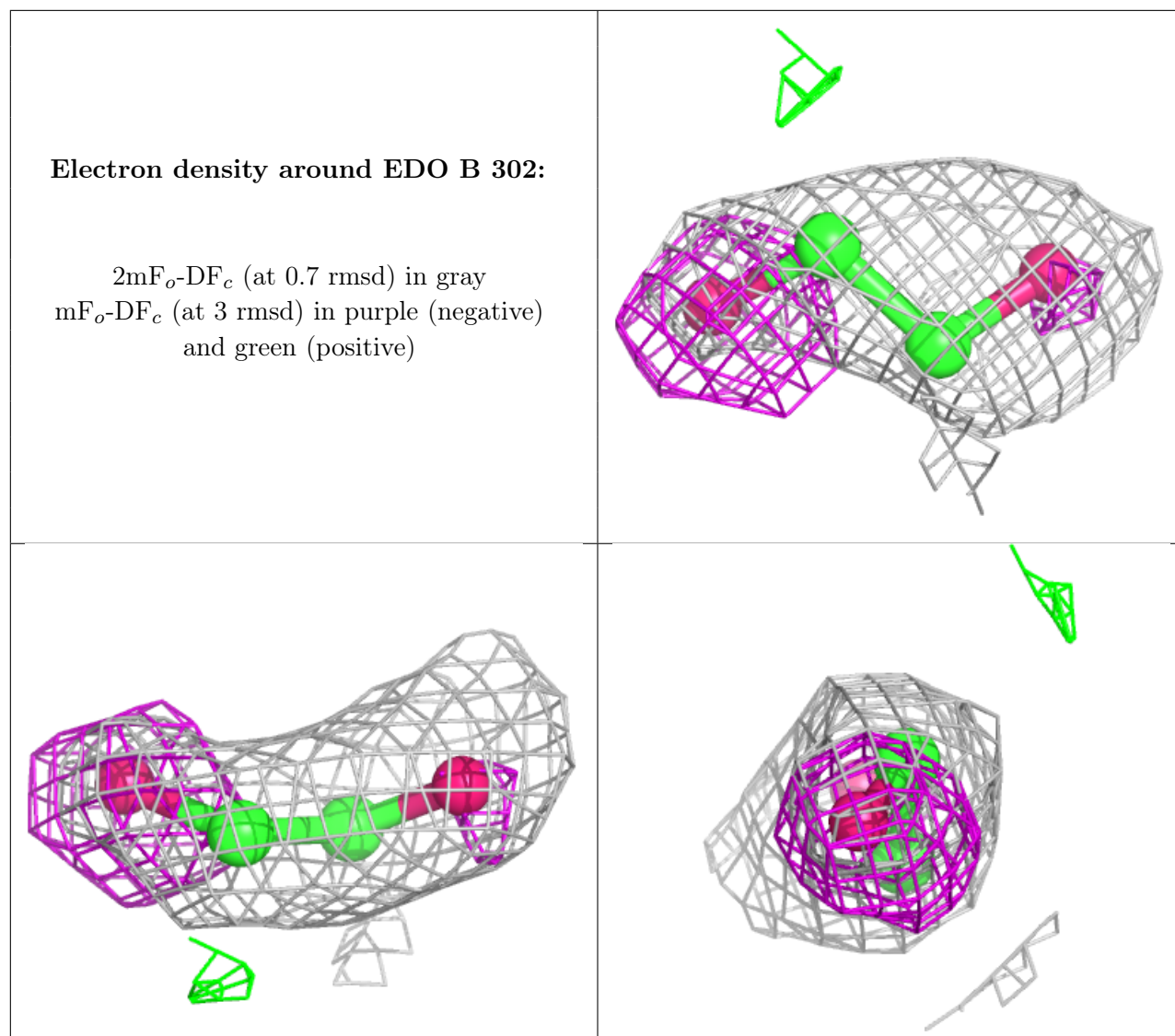
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around LYS A 301:**

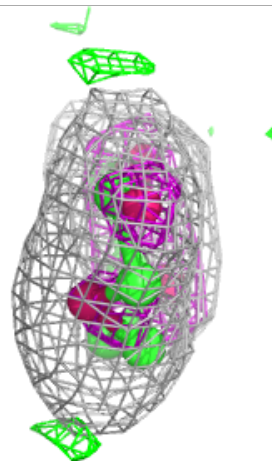
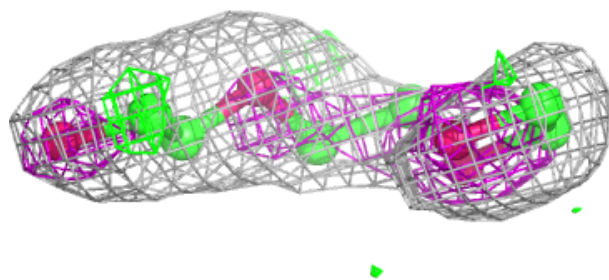
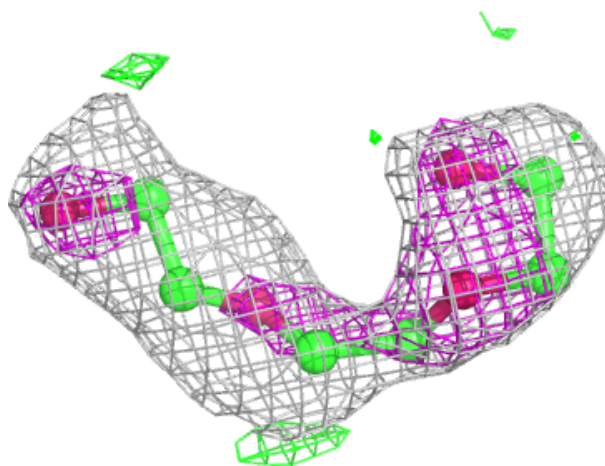
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





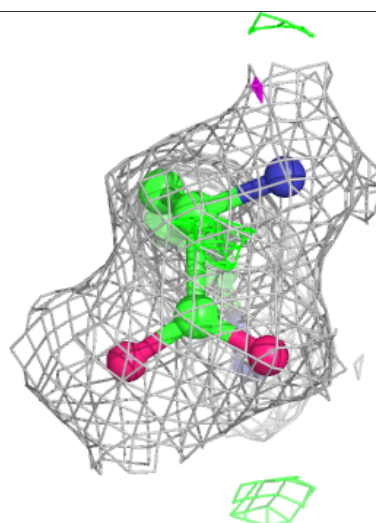
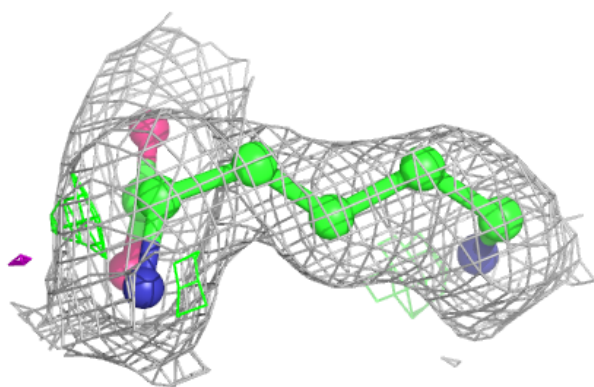
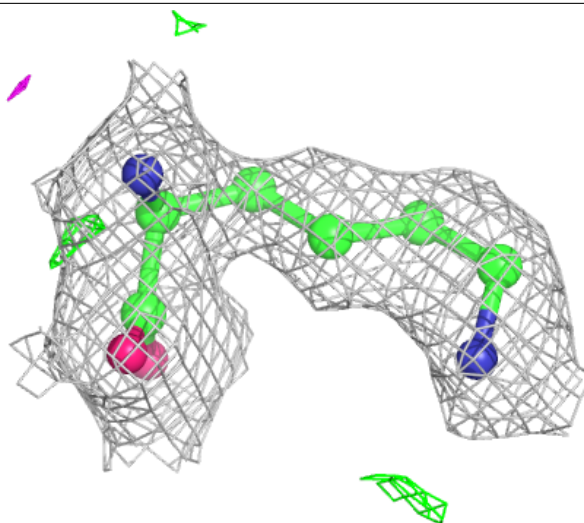
**Electron density around PGE D 304:**

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



**Electron density around LYS C 301:**

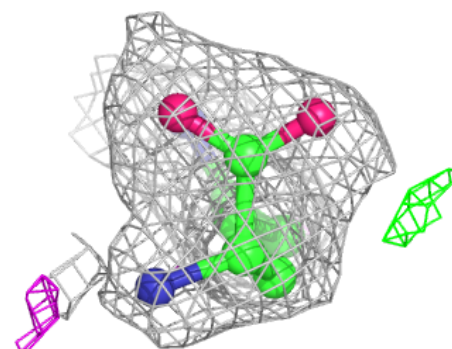
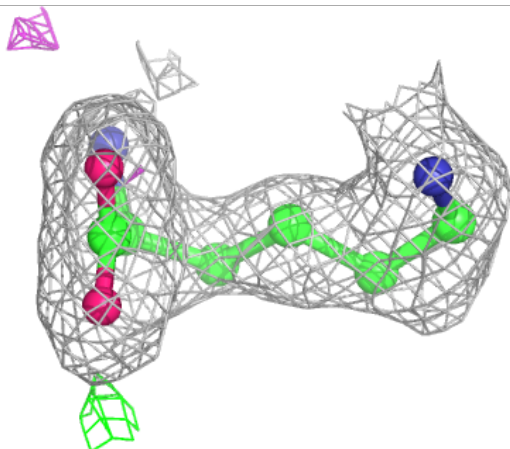
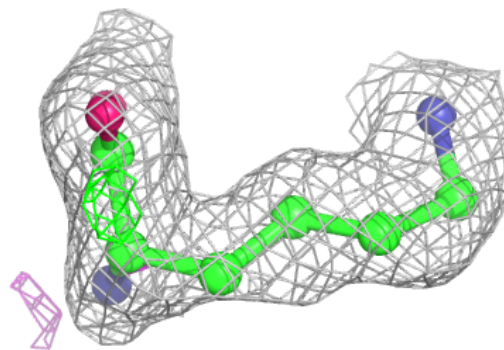
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





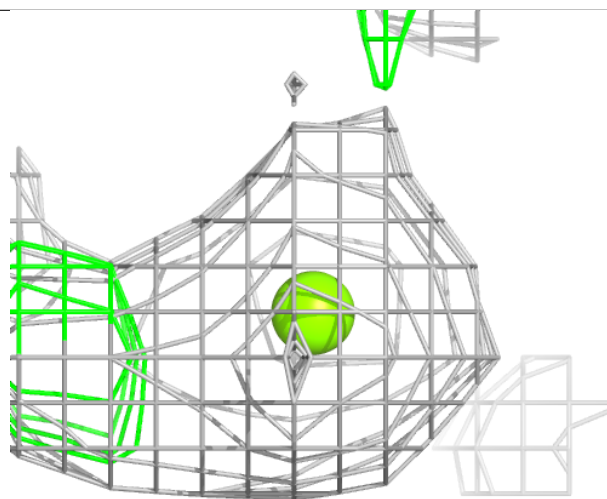
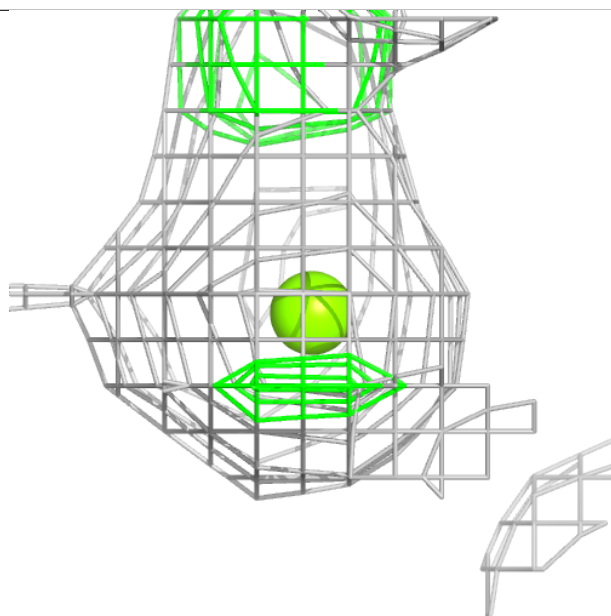
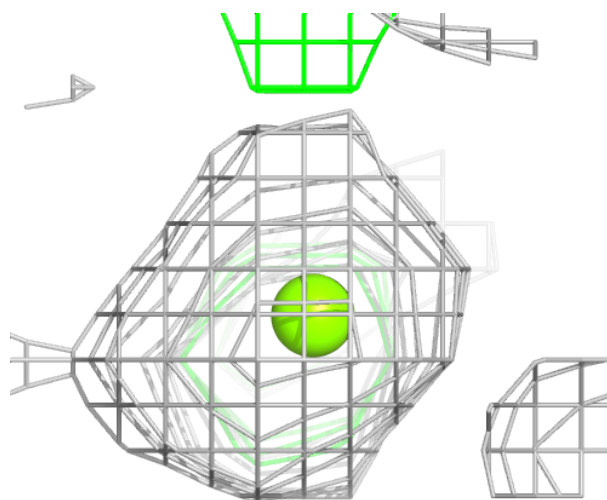
**Electron density around LYS D 301:**

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



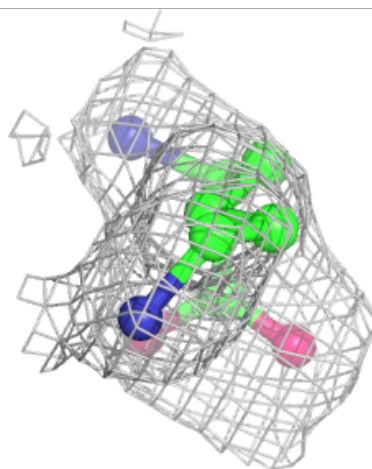
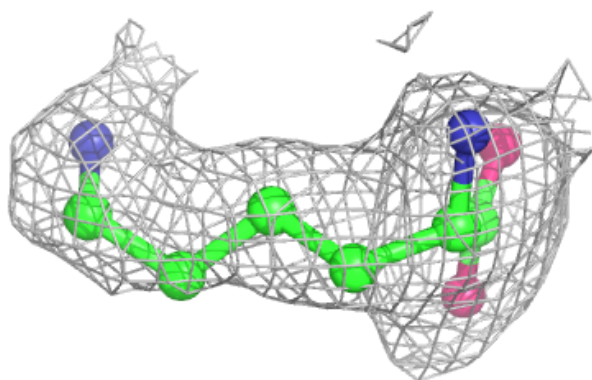
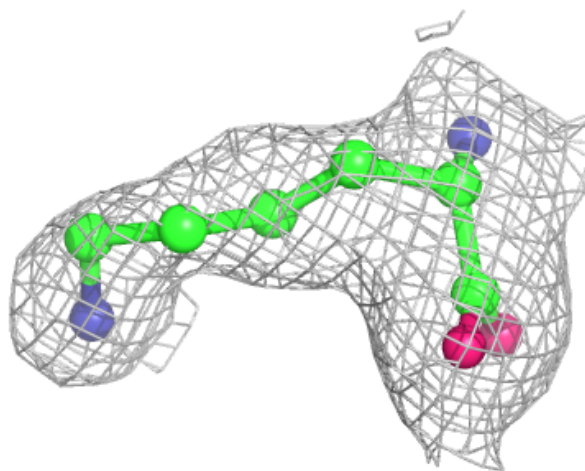
**Electron density around MG A 303:**

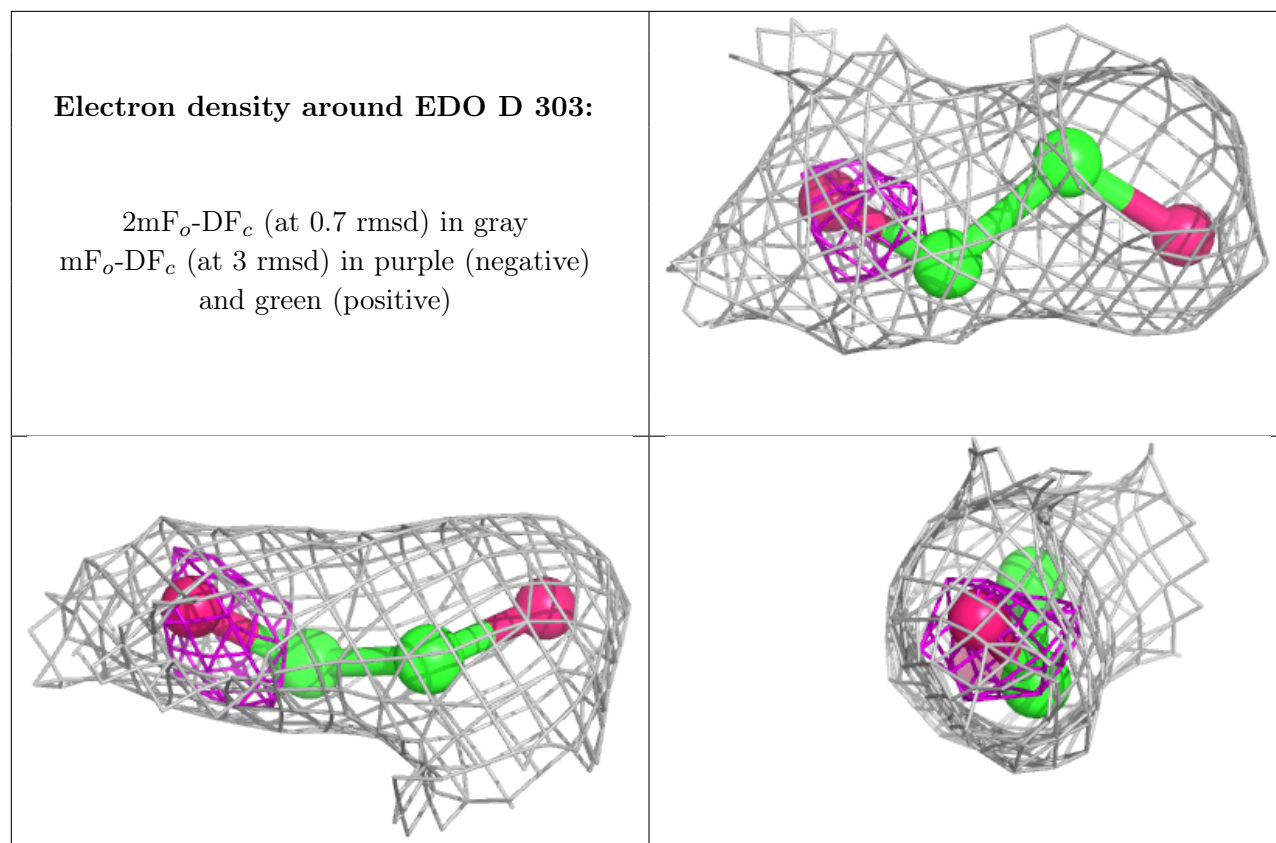
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around LYS E 301:**

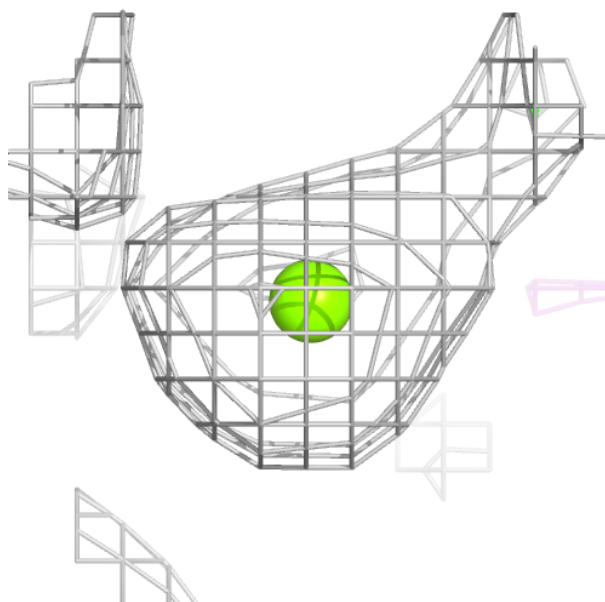
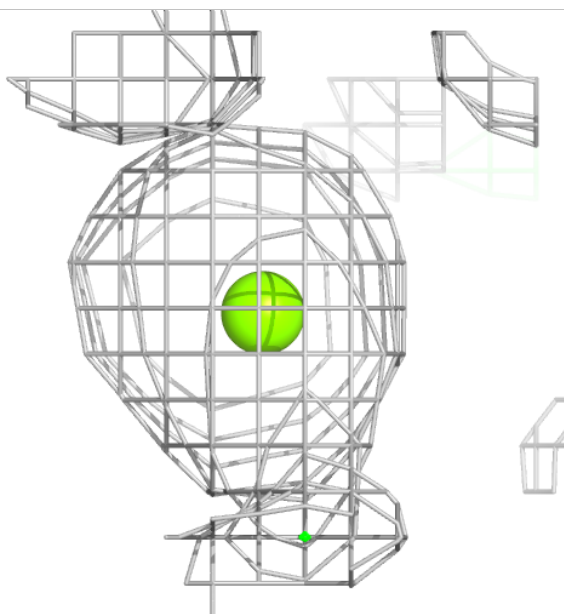
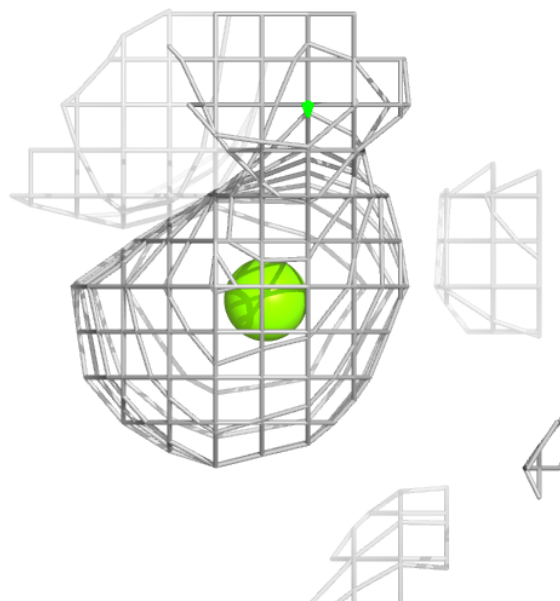
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





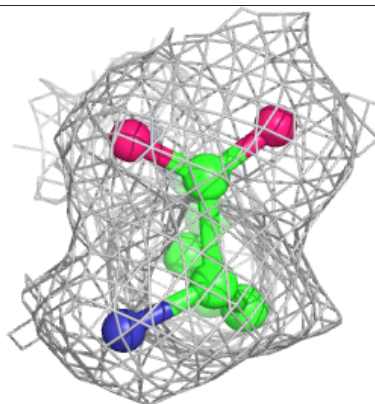
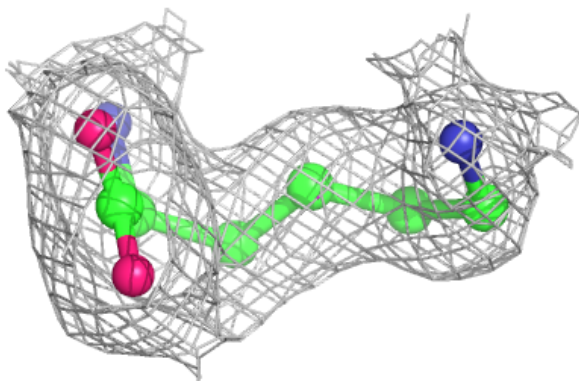
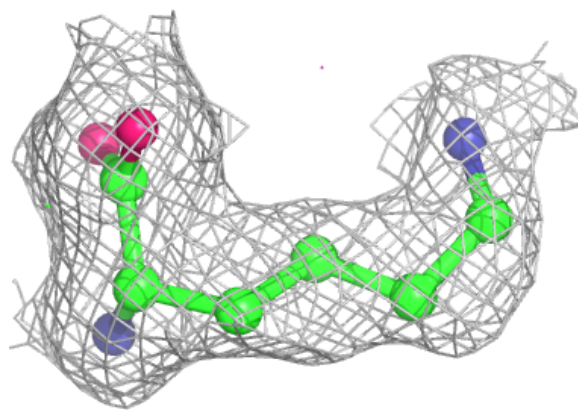
**Electron density around MG B 304:**

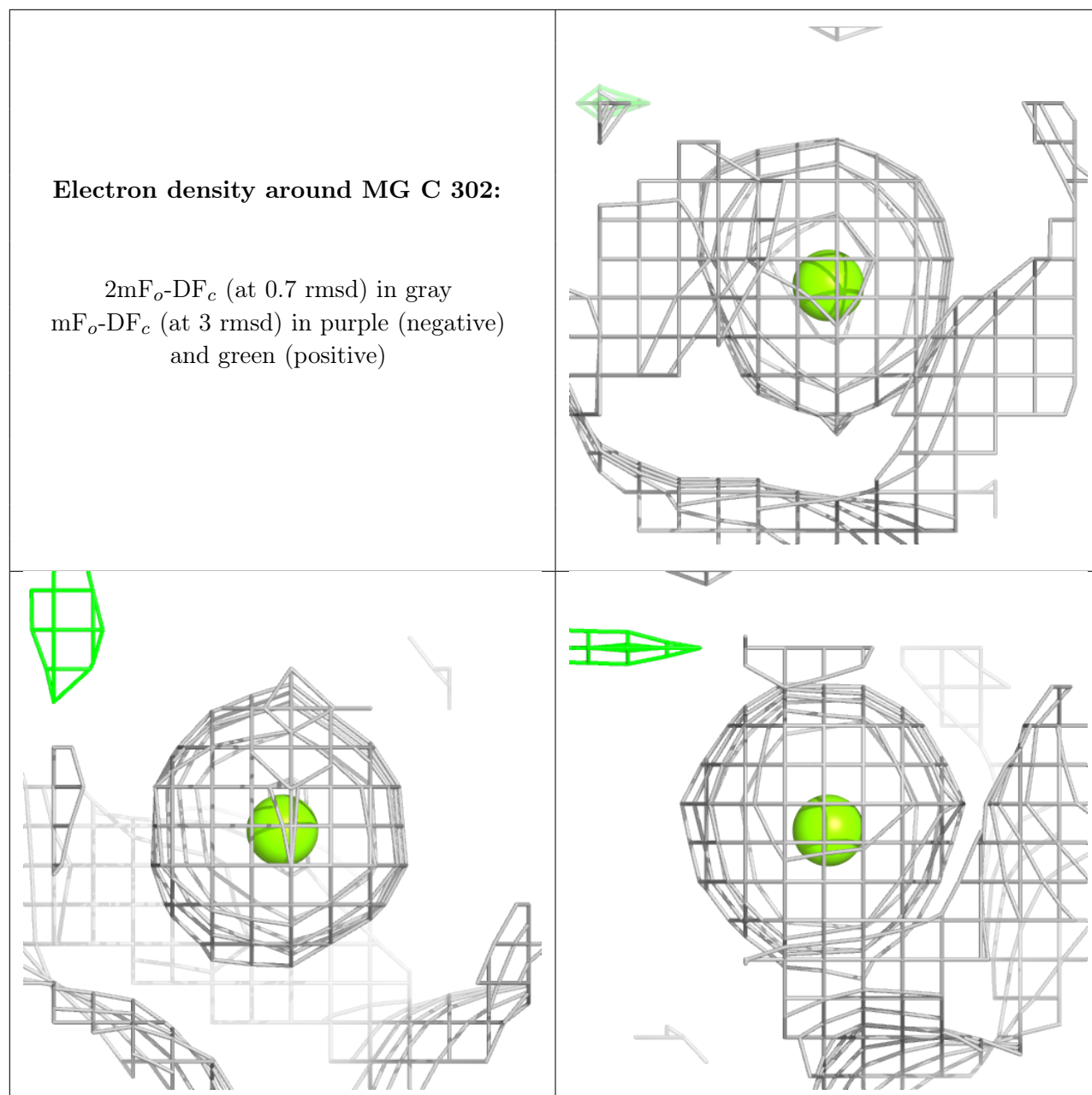
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around LYS B 301:**

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





## 6.5 Other polymers ⓘ

There are no such residues in this entry.