



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 11:31 AM UTC

PDB ID : 7CWZ / pdb_00007cwz
Title : Crystal structure of a tyrosine decarboxylase from *Enterococcus faecalis* K392A mutant in complex with the cofactor PLP and L-dopa
Authors : Yu, X.; Gong, M.; Huang, J.; Liu, W.; Chen, C.; Guo, R.
Deposited on : 2020-09-01
Resolution : 2.97 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (

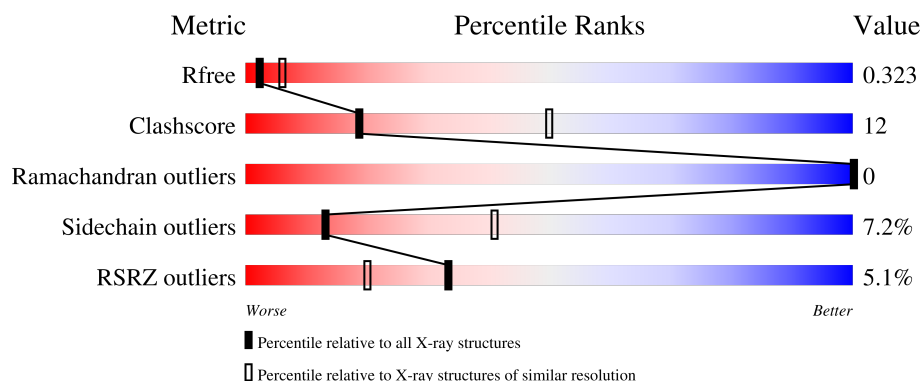
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.97 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers		

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14274 atoms, of which 51 are hydrogens and 0 are deuteriums.

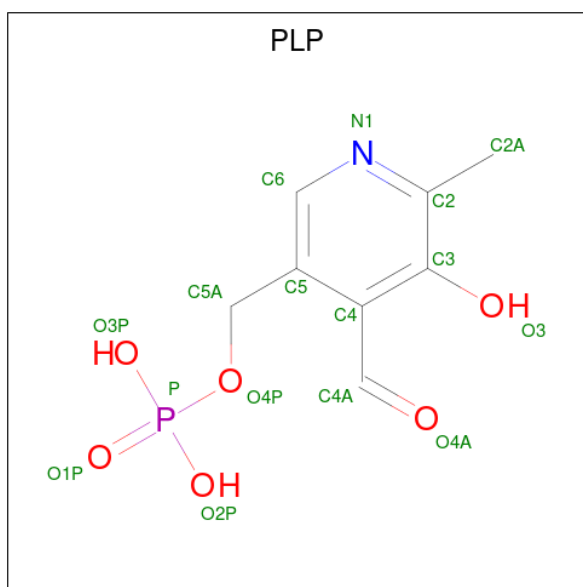
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Decarboxylase.

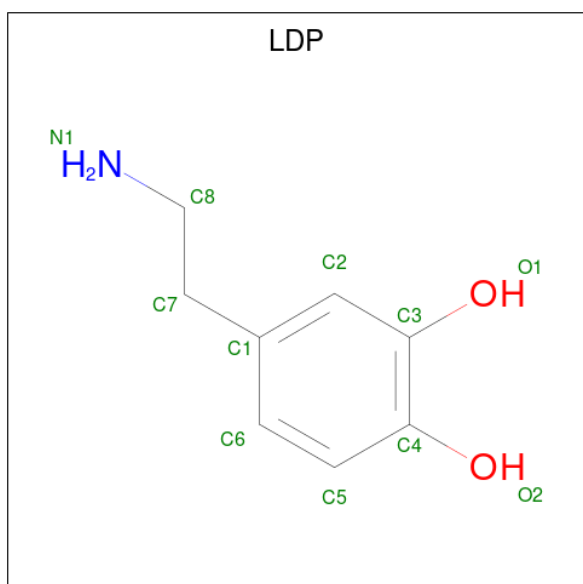
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	601	Total	C	N	O	S	0	0	0
			4711	3008	780	902	21			
1	B	601	Total	C	N	O	S	0	0	0
			4748	3032	786	909	21			
1	C	592	Total	C	N	O	S	0	0	0
			4628	2957	766	886	19			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled
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- Molecule 4 is L-DOPAMINE (CCD ID: LDP) (formula: $C_8H_{11}NO_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	0	0
			20	8	9	1	2		
4	B	1	Total	C	H	N	O	0	0
			20	8	9	1	2		
4	C	1	Total	C	H	N	O	0	0
			20	8	9	1	2		

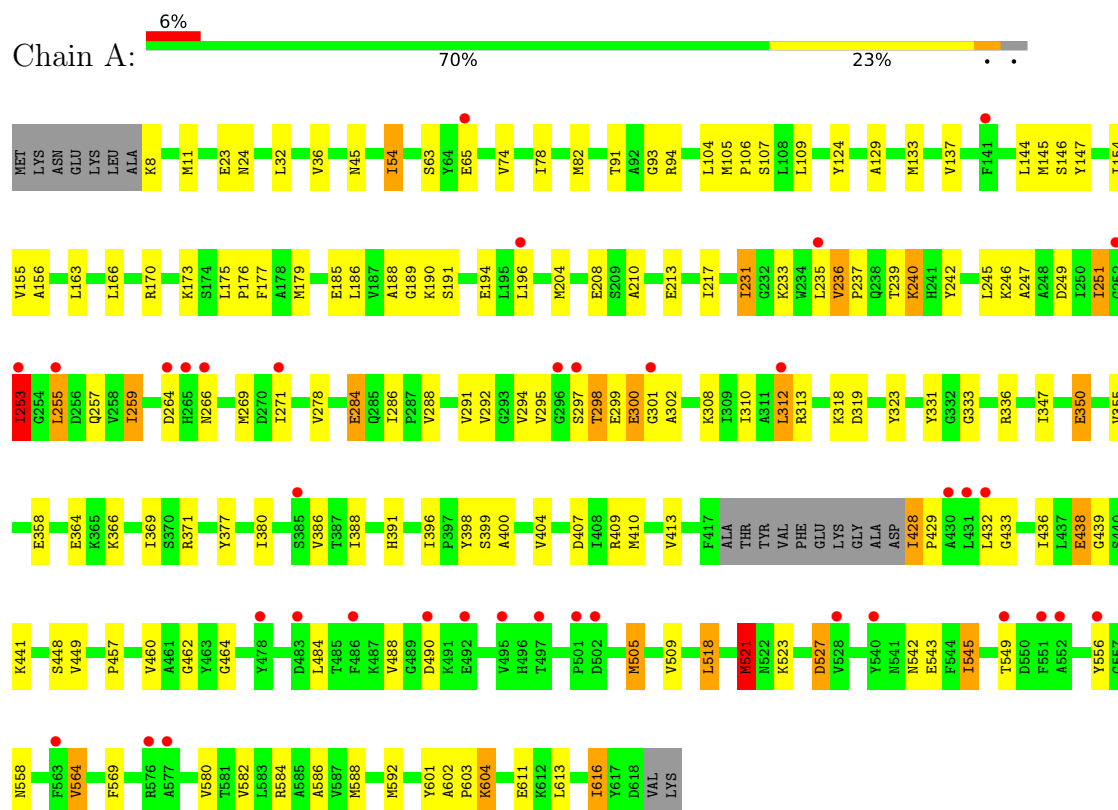
- Molecule 5 is water.

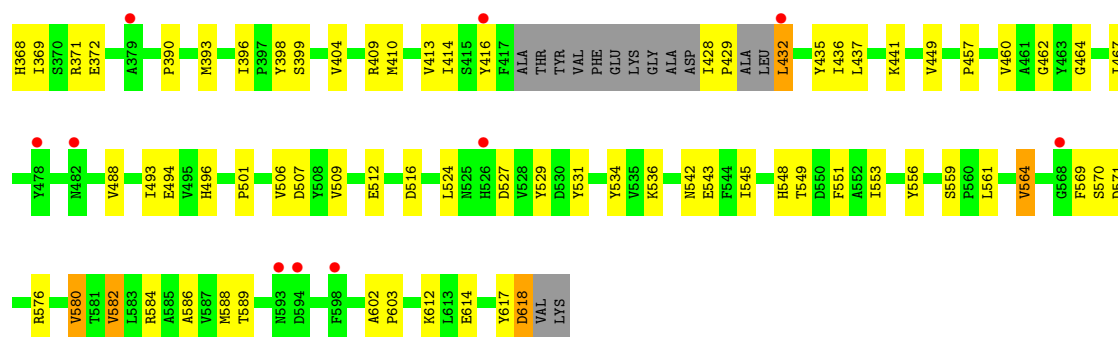
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	17	Total	O	0	0
			17	17		
5	B	18	Total	O	0	0
			18	18		
5	C	21	Total	O	0	0
			21	21		

3 Residue-property plots

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: Decarboxylase





4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	133.31Å 133.31Å 390.63Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.85 – 2.97 24.85 – 2.97	Depositor EDS
% Data completeness (in resolution range)	98.1 (24.85-2.97) 97.9 (24.85-2.97)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.70 (at 2.99Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.243 , 0.293 0.254 , 0.323	Depositor DCC
R_{free} test set	647 reflections (1.49%)	wwPDB-VP
Wilson B-factor (Å ²)	58.3	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 21.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.39$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of		

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PLP, MG, LDP

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	0.65	1/4829 (0.0%)	1.04	16/6564 (0.2%)
1	B	0.68	0/4864	1.10	14/6602 (0.2%)
1	C	0.58	0/4742	0.96	12/6447 (0.2%)
All	All	0.64	1/14435 (0.0%)	1.03	42/19613 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	266	ASN	C-N	-5.92	1.25	1.33

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4711	0	4466	118	0
1	B	4748	0	4547	97	0
1	C	4628	0	4377	130	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	15	8	7	0	0
3	B	15	8	7	1	0
3	C	15	8	7	1	0
4	A	11	9	9	0	0
4	B	11	9	10	0	0
4	C	11	9	10	0	0
5	A	17	0	0	0	0
5	B	18	0	0	0	0
5	C	21	0	0	0	0
All	All	14223	51	13440	329	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 12.

The worst 5 of 329 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	597/620 (96%)	560 (94%)	37 (6%)	0	100	100
1	B	595/620 (96%)	552 (93%)	43 (7%)	0	100	100
1	C	582/620 (94%)	546 (94%)	36 (6%)	0	100	100
All	All	1774/1860 (95%)	1658 (94%)	116 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	489/524 (93%)	453 (93%)	36 (7%)	13	40
1	B	499/524 (95%)	454 (91%)	45 (9%)	9	32
1	C	479/524 (91%)	455 (95%)	24 (5%)	22	

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	PLP	C	701	4</						

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	LDP	C	702	3	-	0/3/3/3	0/1/1/1
3	PLP	B	702	4	-	3/6/6/8	0/1/1/1
4	LDP	A	703	3	-	2/3/3/3	0/1/1/1

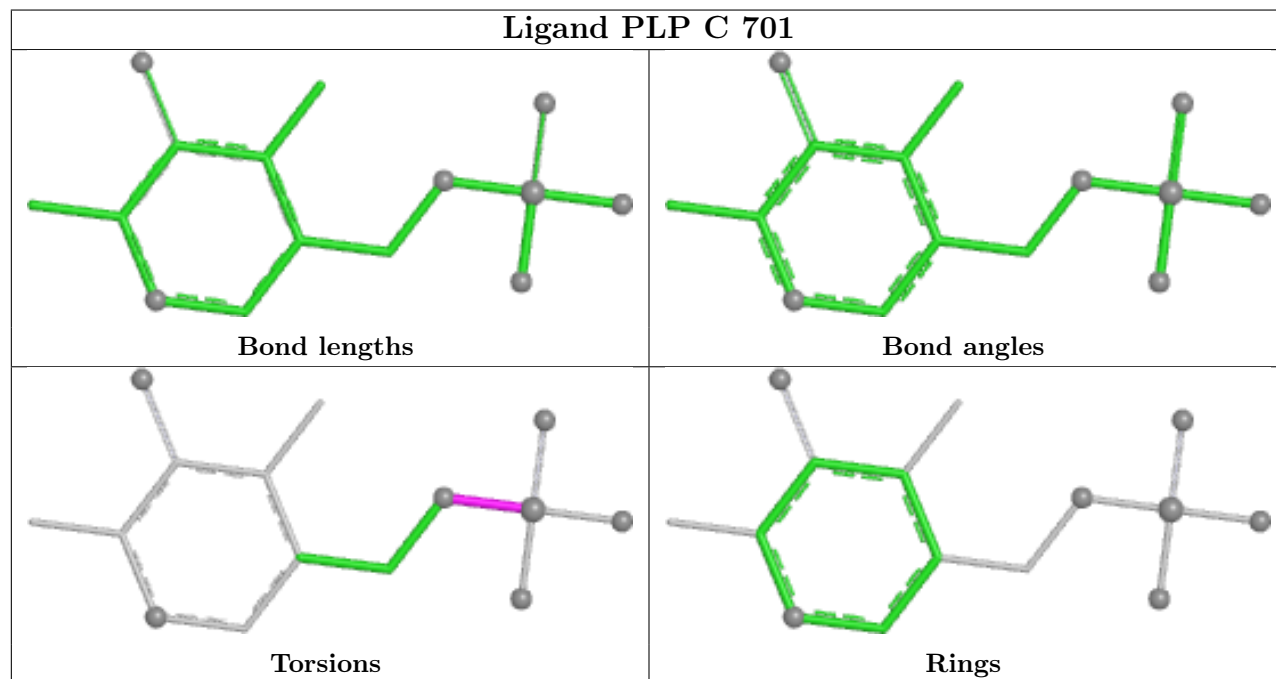
All (5) bond length outliers are listed below:

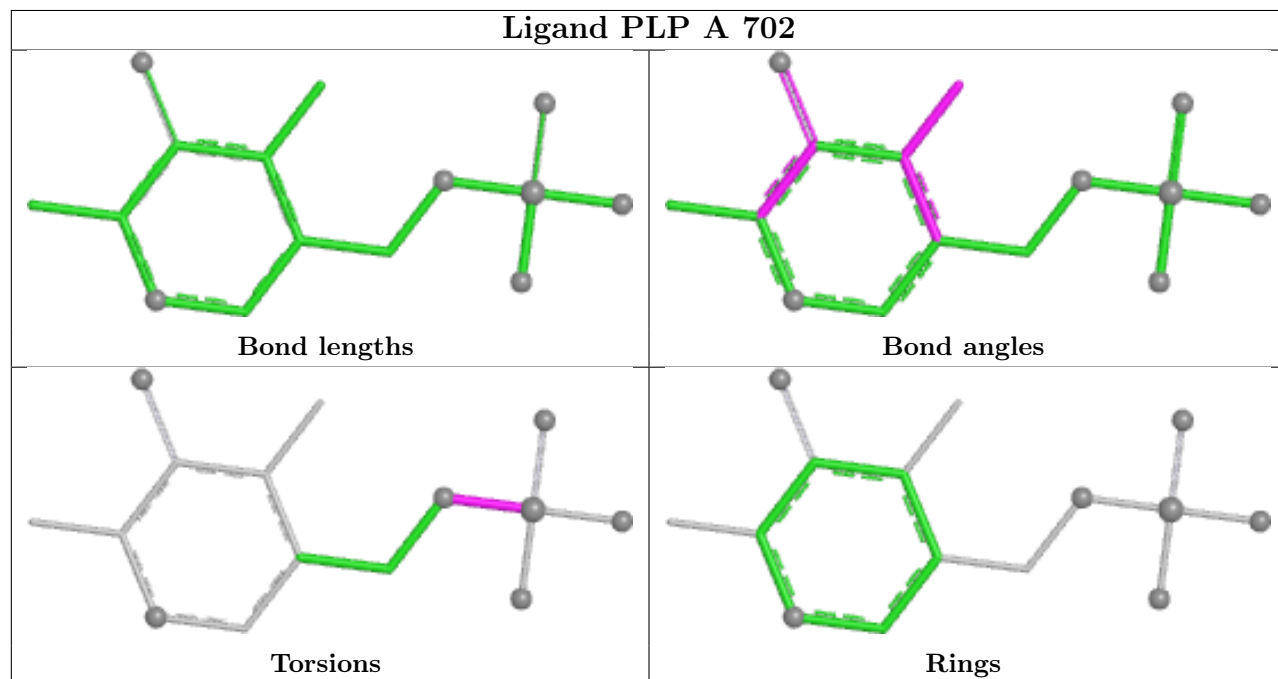
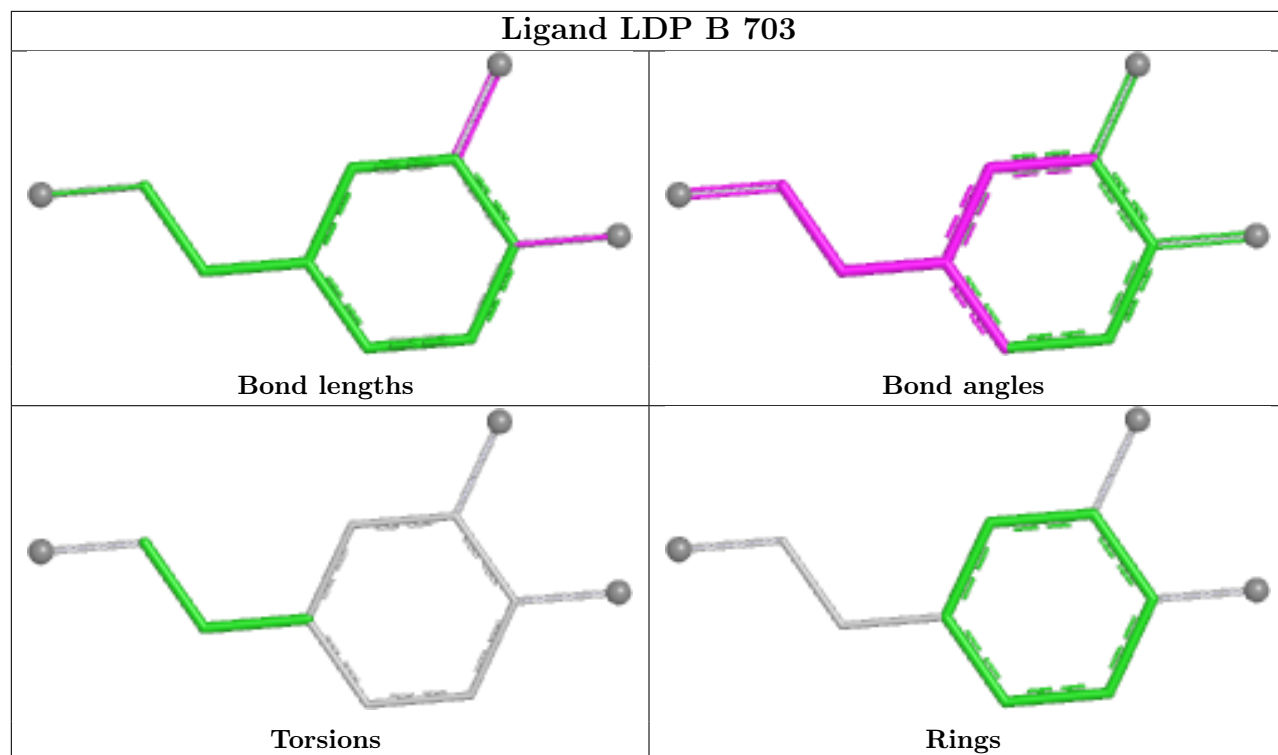
Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	703	LDP	O1-C3	2.28	1.40	1.36
4	C	702	LDP	O2-C4	2.16	1.40	1.36
4	B	703	LDP	O2-C4	2.13	1.40	1.36
4	C	702	LDP	O1-C3	2.12	1.40	1.36
4	B	703	LDP	O1-C3	2.06	1.40	1.36

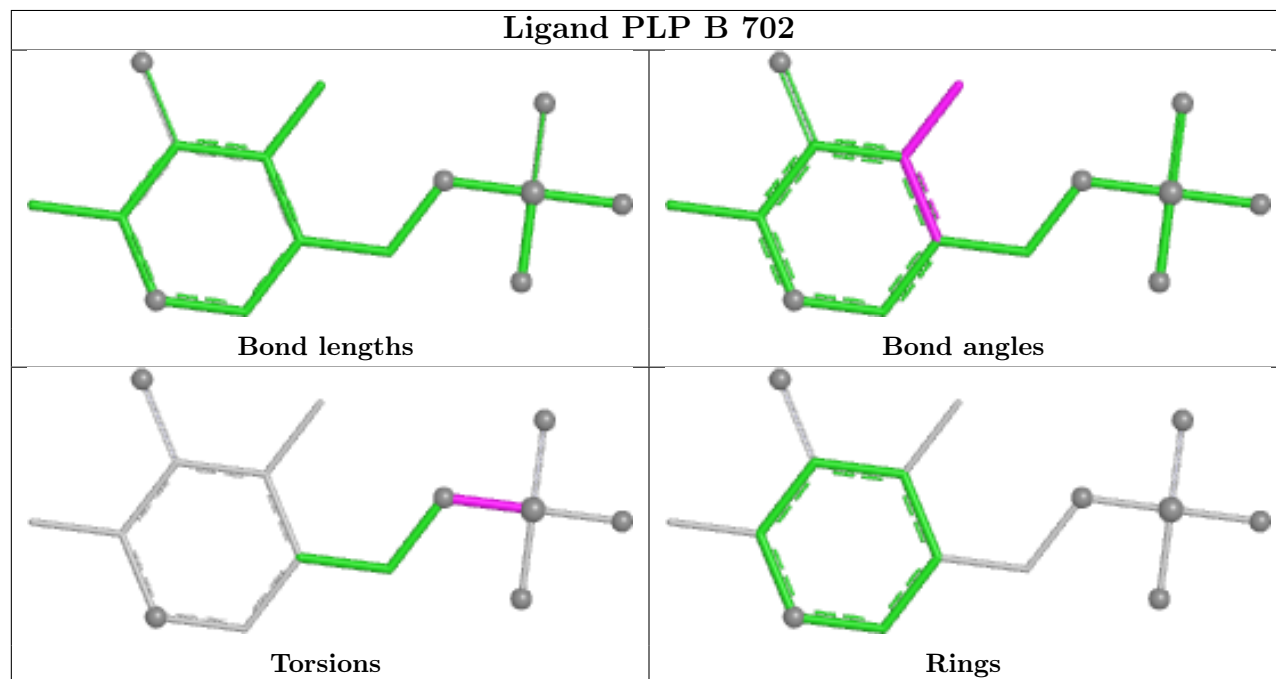
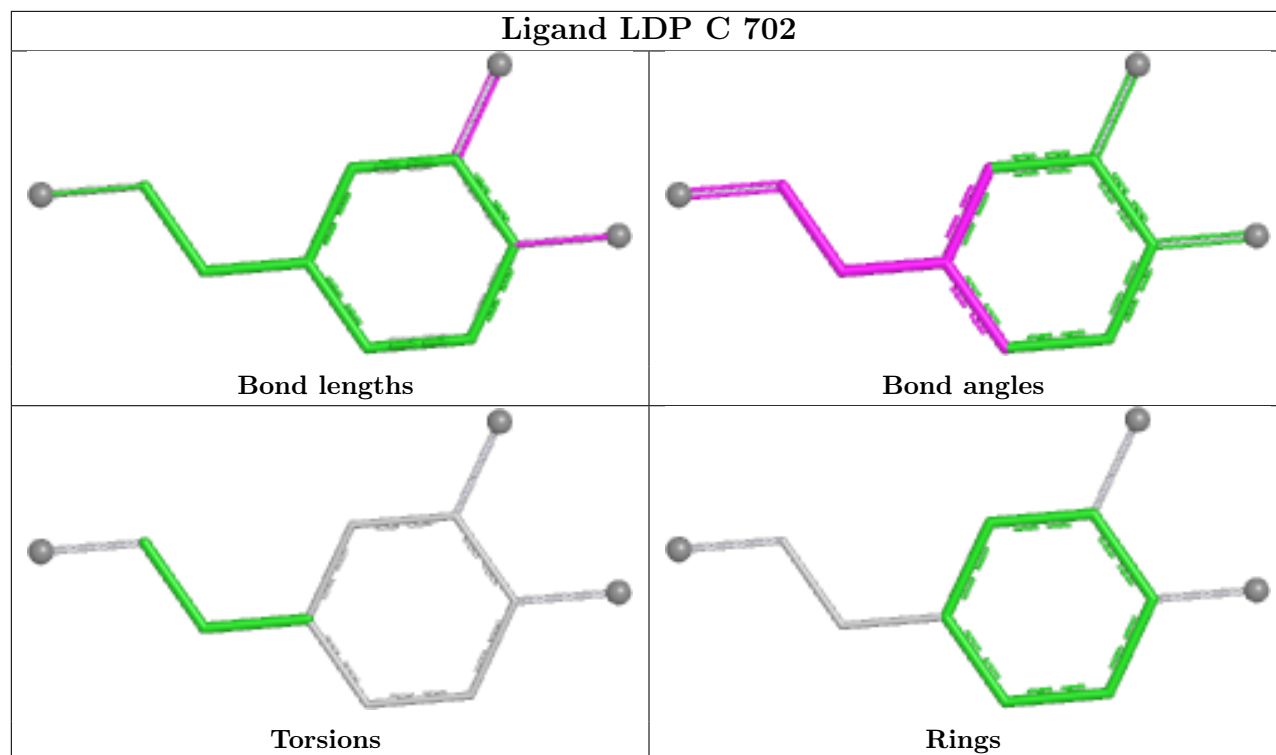
The worst 5 of 11 bond angle outliers are listed below:

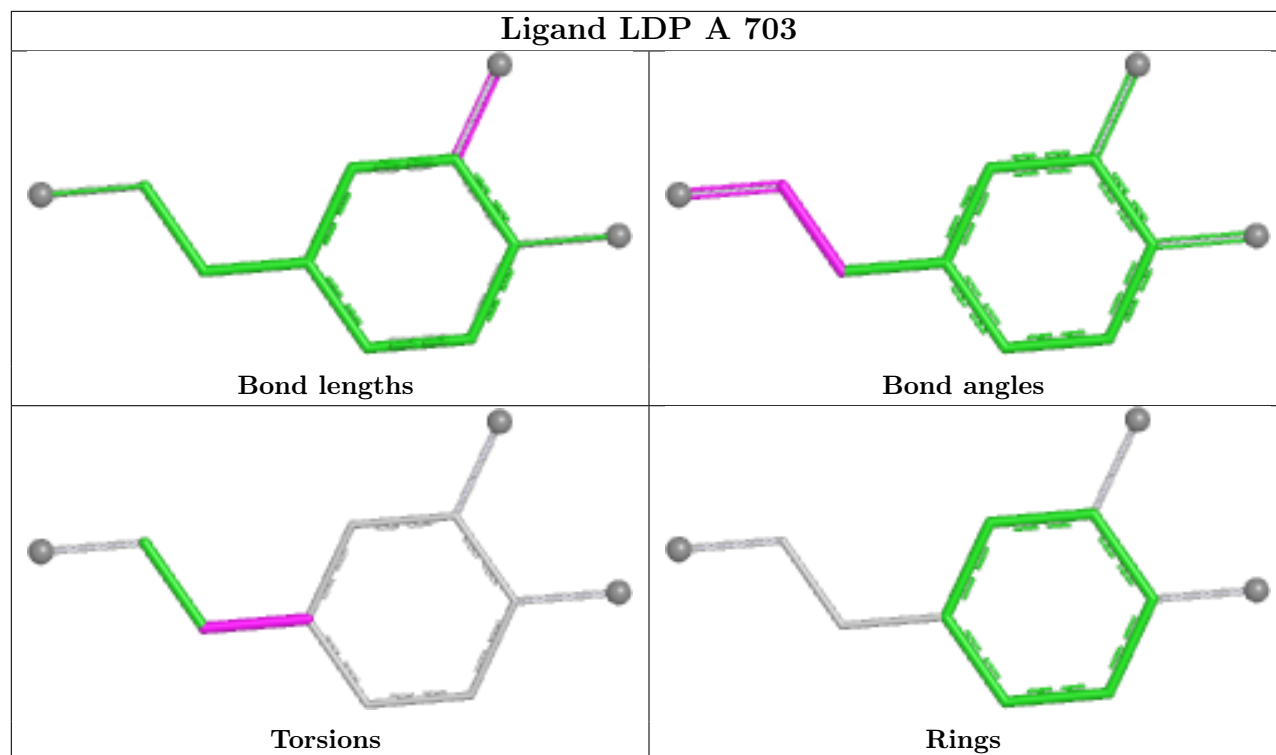
Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	703	LDP				

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 [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	601/620 (96%)	0.70	37 (6%) 26 16	28, 49, 74, 89	0
1	B	601/620 (96%)	0.59	28 (4%) 36 22	27, 53, 77, 95	0
1	C	592/620 (95%)	0.56	26 (4%) 39 24	26, 51, 83, 100	0
All	All	1794/1860 (96%)	0.62	91 (5%) 33 20	26, 51, 79, 100	0

The worst 5 of 91 RSRZ outliers are listed below:

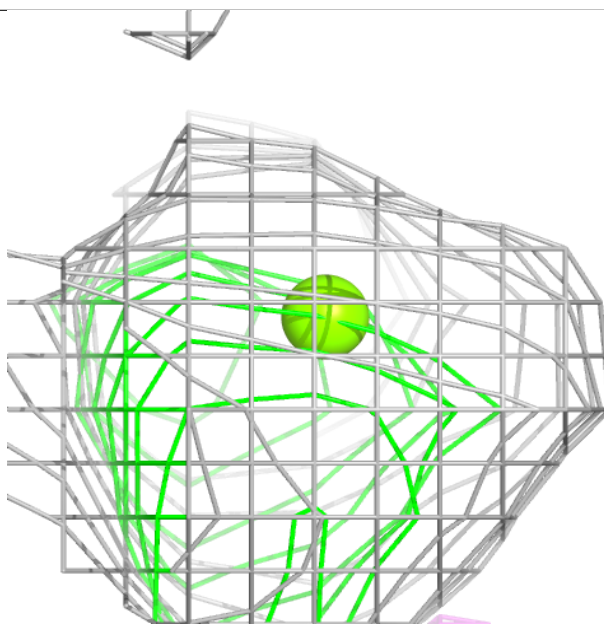
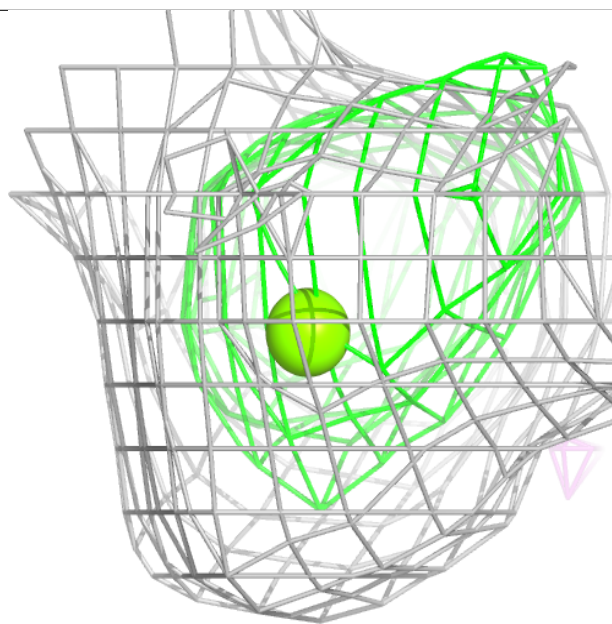
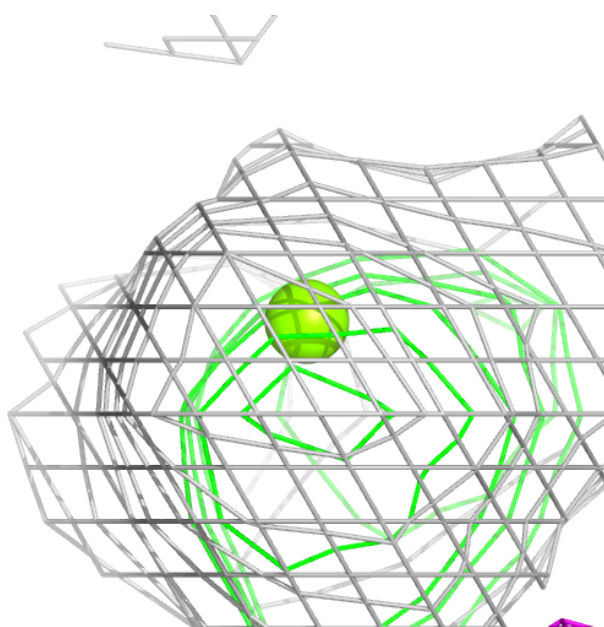
Mol	Chain	Res	Type	RSRZ
1	C	520	ALA	7.1
1	C	580	VAL	4.8
1	C</			

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	B	701	1/1	0.50	0.30	58,58,58,58	0
2	MG	A	701	1/1	0.70	0.28	87,87,87,87	0
4	LDP	A	703	11/11	0.72	0.22	52,60,72,72	0
4	LDP	B	703	11/11	0.83	0.22	44,52,62,62	0
3	PLP	B	702	15/16	0.86	0.12	46,54,65,67	0
3	PLP	A	702	15/16	0.87	0.13	45,53,63,65	0
4	LDP	C	702	11/11	0.88	0.18	45,54,67,67	0
3	PLP	C	701	15/16	0.93	0.09	44,53,64,67	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.

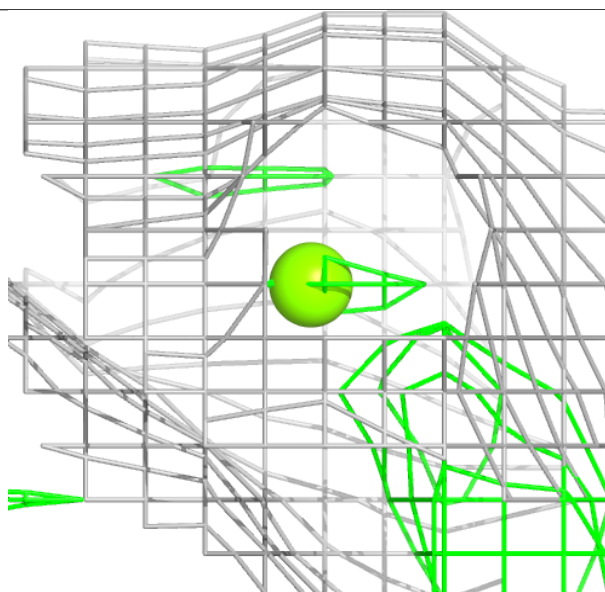
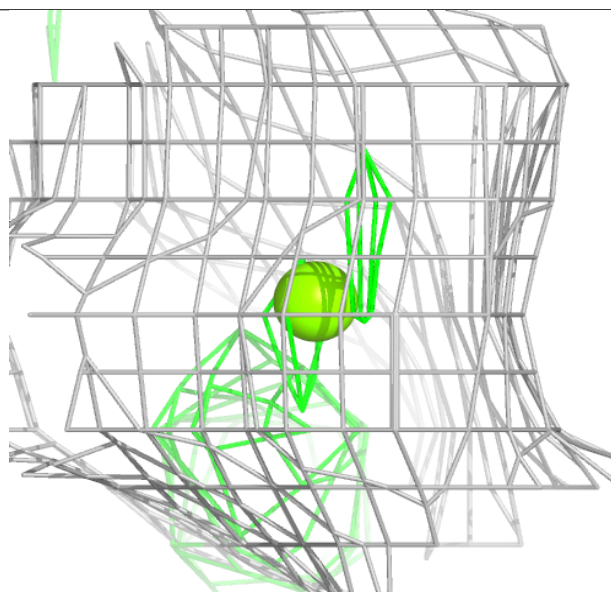
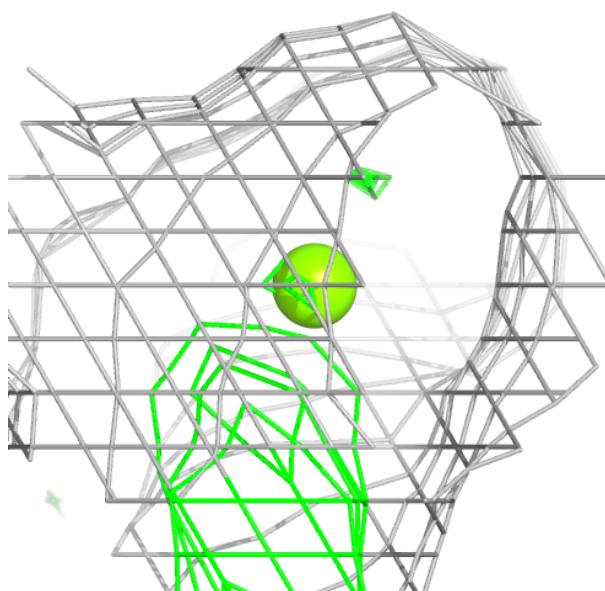
Electron density around MG B 701:

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



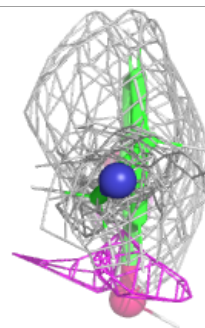
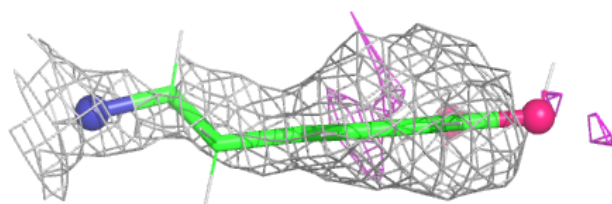
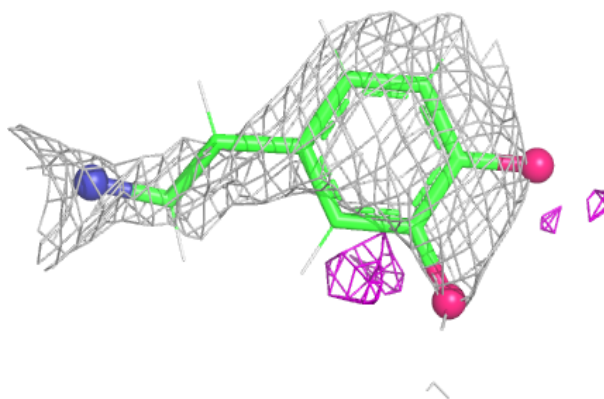
Electron density around MG A 701:

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

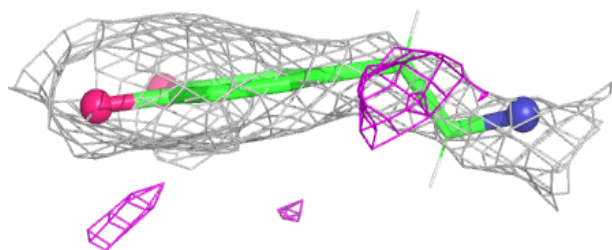
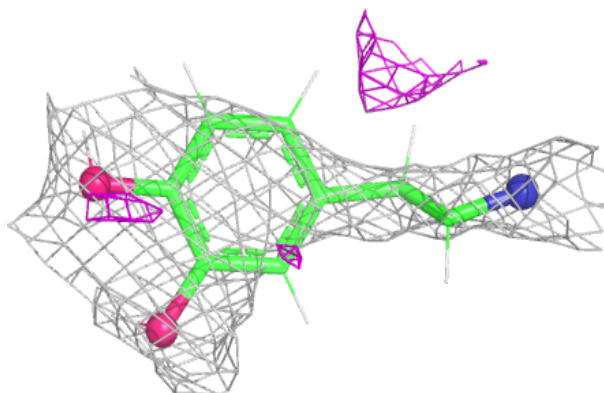


Electron density around LDP A 703:

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

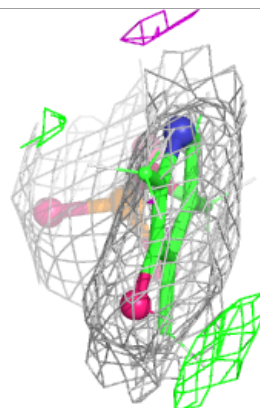
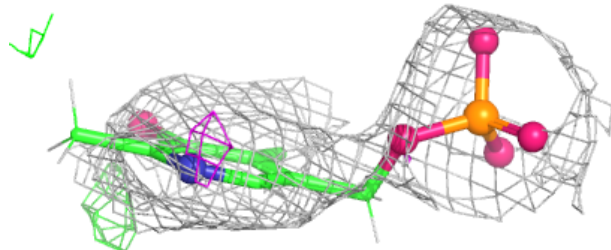
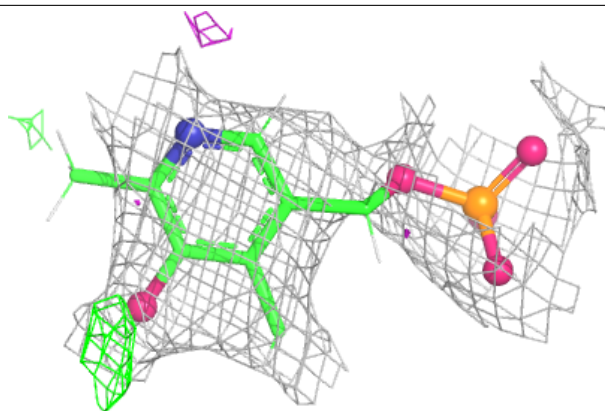
**Electron density around LDP B 703:**

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

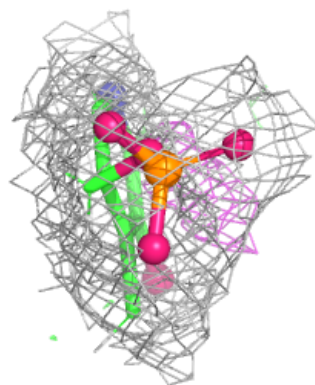
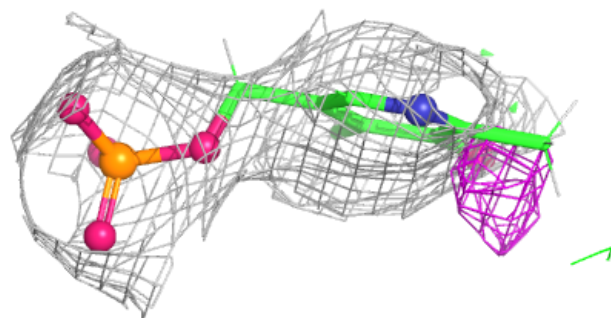
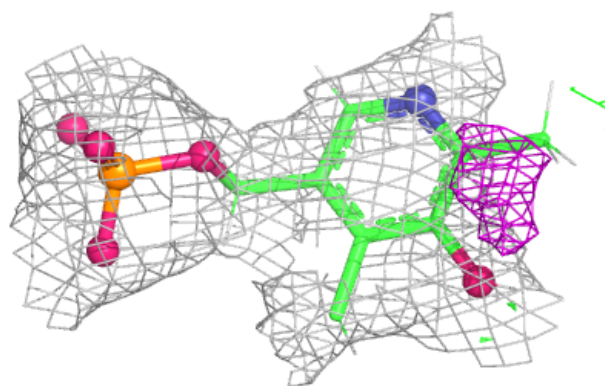


Electron density around PLP B 702:

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

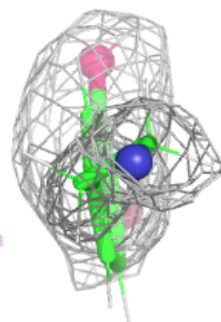
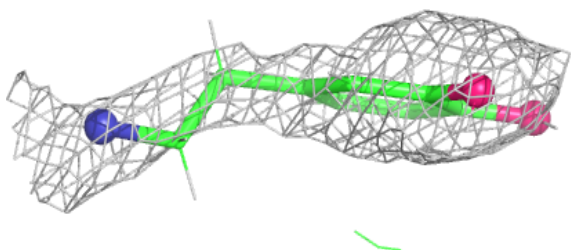
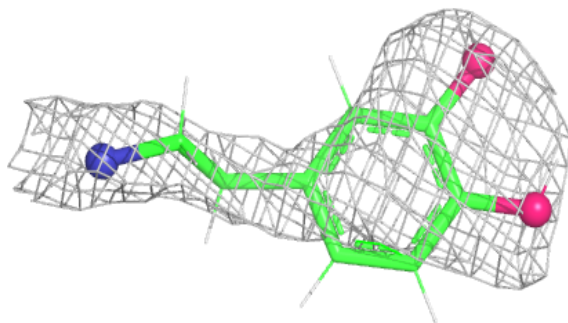
**Electron density around PLP A 702:**

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

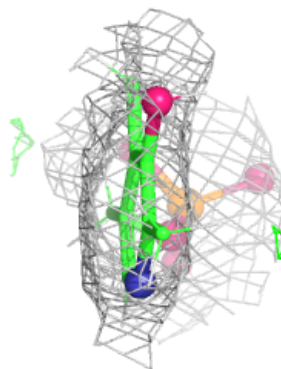
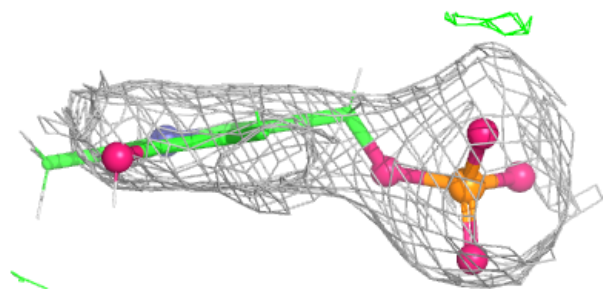
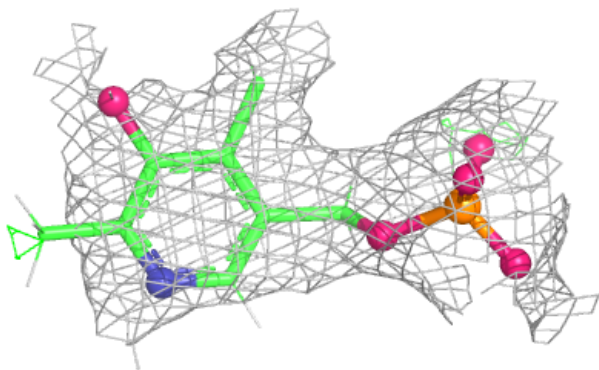


Electron density around LDP C 702:

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

**Electron density around PLP C 701:**

$2mF_o-DF_c$ (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.