



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2021 – 02:11 PM JST

PDB ID : 7CX0
Title : Crystal structure of a tyrosine decarboxylase from *Enterococcus faecalis* in complex with the cofactor PLP and inhibitor carbidopa
Authors : Yu, X.; Gong, M.; Huang, J.; Liu, W.; Chen, C.; Guo, R.
Deposited on : 2020-09-01
Resolution : 2.66 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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 : 2.23.1
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) : 2.23.1

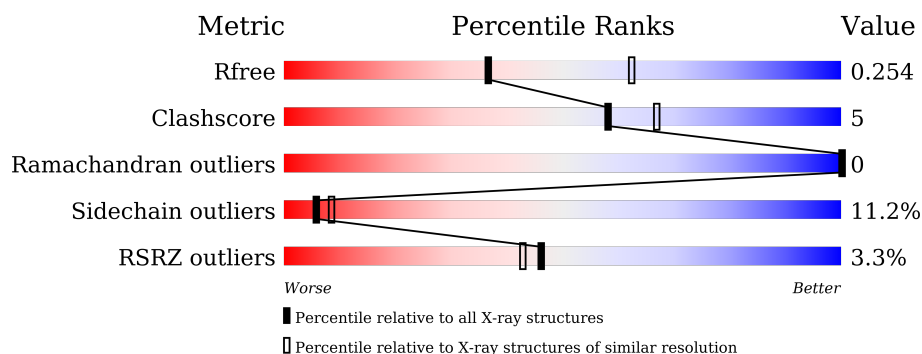
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.66 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	620	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>14%</div> <div>• •</div> </div> </div>
1	B	620	<div> <div>4%</div> <div> <div></div> <div>81%</div> <div>14%</div> <div>• •</div> </div> </div>
1	C	620	<div> <div>4%</div> <div> <div></div> <div>79%</div> <div>12%</div> <div>• 5%</div> </div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 14273 atoms, of which 57 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.

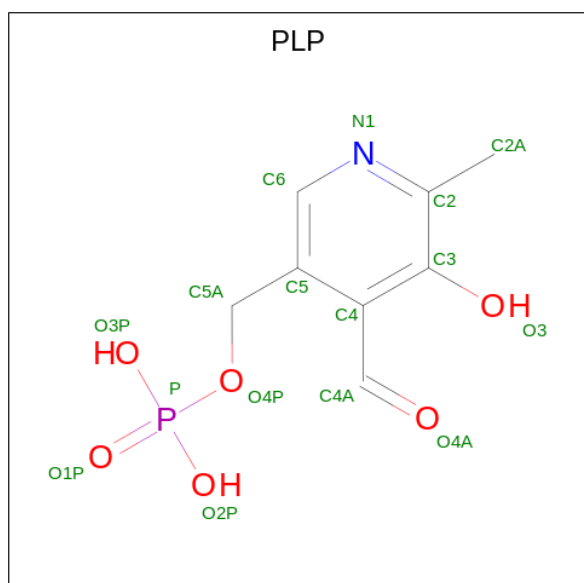
- Molecule 1 is a protein called Decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	602	Total	C	N	O	S	0	0	0
			4757	3035	788	913	21			
1	B	603	Total	C	N	O	S	0	0	0
			4747	3023	789	914	21			
1	C	588	Total	C	N	O	S	0	0	0
			4586	2921	761	884	20			

There are 3 discrepancies between the modelled and reference sequences:

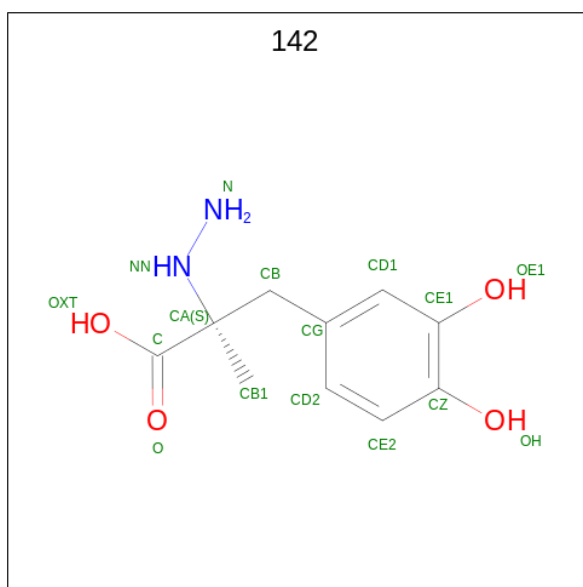
Chain	Residue	Modelled	Actual	Comment	Reference
A	62	LYS	GLU	conflict	UNP Q8KXD2
B	62	LYS	GLU	conflict	UNP Q8KXD2
C	62	LYS	GLU	conflict	UNP Q8KXD2

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	
			23	8	8	1	5	1	
2	B	1	Total	C	H	N	O	P	
			23	8	8	1	5	1	
2	C	1	Total	C	H	N	O	P	
			23	8	8	1	5	1	

- Molecule 3 is CARBIDOPA (three-letter code: 142) (formula: $C_{10}H_{14}N_2O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O		
			27	10	11	2	4	0	0
3	B	1	Total	C	H	N	O		
			27	10	11	2	4	0	0
3	C	1	Total	C	H	N	O		
			27	10	11	2	4	0	0

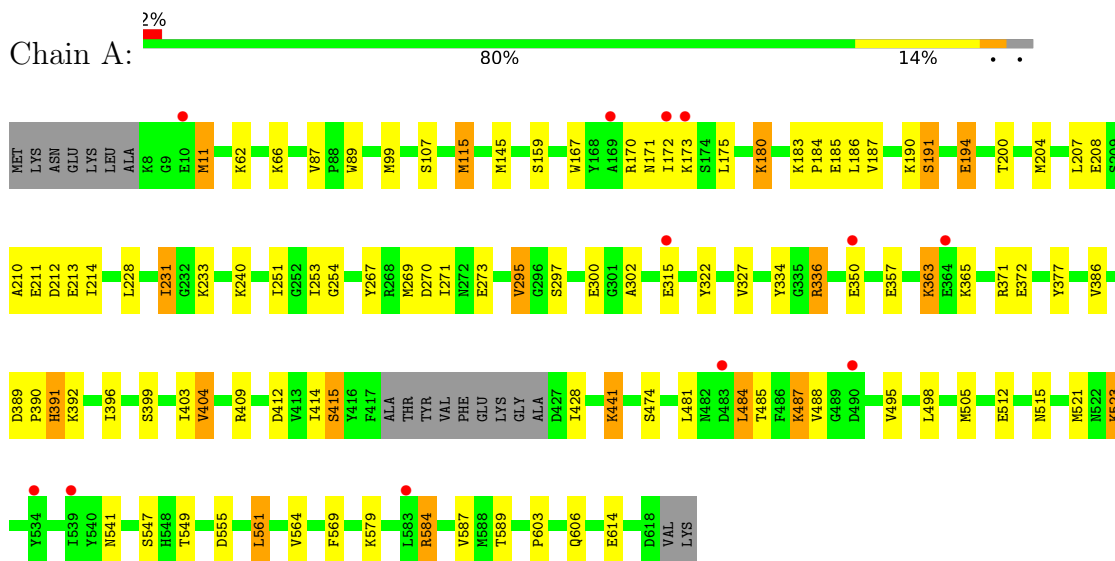
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	14	Total	O		
			14	14	0	0
4	B	10	Total	O		
			10	10	0	0
4	C	9	Total	O		
			9	9	0	0

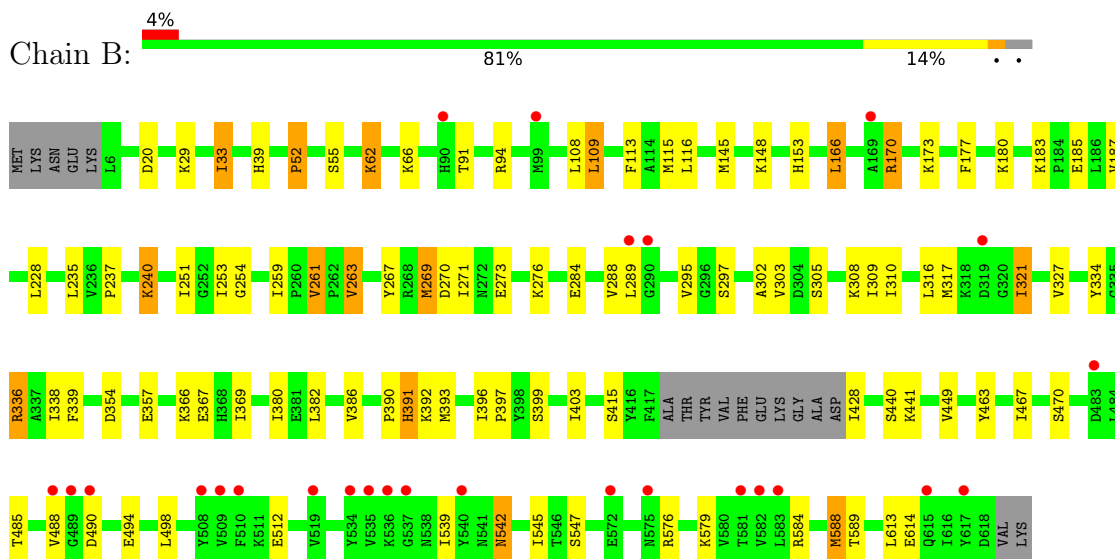
3 Residue-property plots

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.

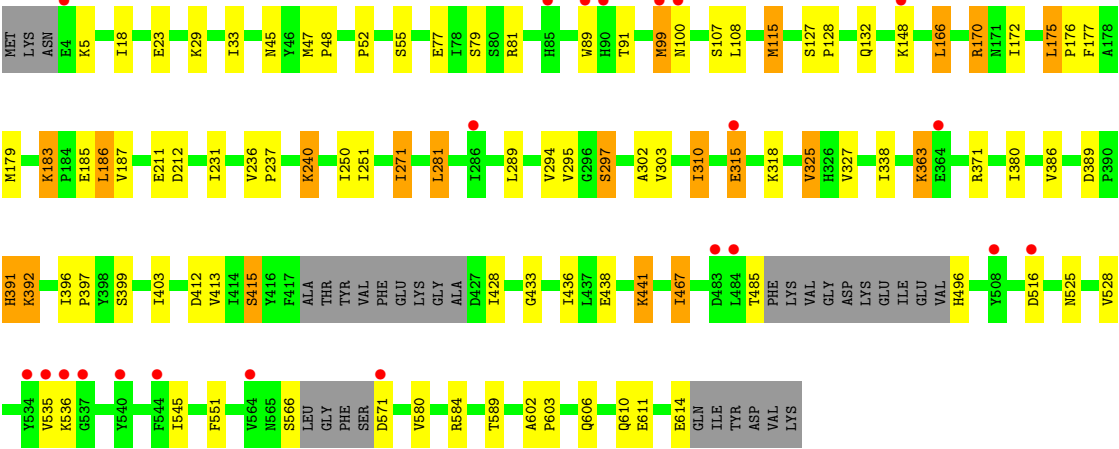
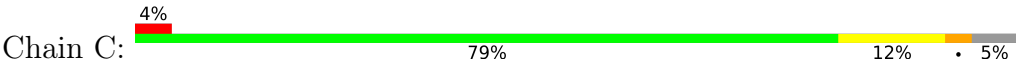
• Molecule 1: Decarboxylase



• Molecule 1: Decarboxylase



• 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	131.70Å 131.70Å 390.01Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.89 – 2.66 24.89 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.4 (24.89-2.66) 93.6 (24.89-2.65)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 2.64Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.215 , 0.268 0.237 , 0.254	Depositor DCC
R_{free} test set	2920 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	61.2	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 36.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14273	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 142, PLP

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	0.59	0/4874	0.76	0/6616
1	B	0.58	0/4863	0.75	0/6604
1	C	0.59	0/4697	0.78	0/6385
All	All	0.59	0/14434	0.77	0/19605

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	4757	0	4552	50	0
1	B	4747	0	4520	44	0
1	C	4586	0	4322	45	0
2	A	15	8	7	0	0
2	B	15	8	7	0	0
2	C	15	8	7	0	0
3	A	16	11	11	0	0
3	B	16	11	11	0	0
3	C	16	11	11	0	0
4	A	14	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	10	0	0	0	0
4	C	9	0	0	0	0
All	All	14216	57	13448	132	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 5.

All (132) 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:C:297:SER:HB3	1:C:302:ALA:H	1.39	0.88
1:A:267:TYR:CE2	1:A:498:LEU:HD21	2.19	0.78
1:C:295:VAL:HG13	1:C:303:VAL:HG13	1.66	0.77
1:B:263:VAL:HG13	1:B:267:TYR:HA	1.77	0.67
1:B:270:ASP:HB3	1:B:273:GLU:HB2	1.77	0.64
1:B:145:MET:HA	1:B:336:ARG:HE	1.64	0.63
1:A:208:GLU:HG3	1:A:409:ARG:HD2	1.81	0.62
1:A:145:MET:HA	1:A:336:ARG:HE	1.64	0.62
1:A:267:TYR:CE2	1:A:498:LEU:CD2	2.83	0.61
1:B:488:VAL:HG11	1:B:613:LEU:HB3	1.82	0.61
1:A:167:TRP:CZ3	1:A:414:ILE:HG23	2.39	0.57
1:A:180:LYS:HA	1:A:184:PRO:HA	1.87	0.57
1:B:263:VAL:CG1	1:B:267:TYR:HA	2.35	0.57
1:A:386:VAL:HB	1:A:404:VAL:HG13	1.88	0.55
1:C:237:PRO:O	1:C:240:LYS:HB3	2.07	0.55
1:C:389:ASP:HB2	1:C:392:LYS:HD3	1.89	0.54
1:A:170:ARG:HD3	1:A:228:LEU:HD22	1.88	0.54
1:A:412:ASP:HA	1:A:415:SER:HB3	1.91	0.53
1:C:179:MET:HB3	1:C:186:LEU:HD11	1.90	0.53
1:A:270:ASP:HB3	1:A:273:GLU:HB2	1.91	0.53
1:A:183:LYS:HB3	1:A:186:LEU:HD12	1.90	0.53
1:A:170:ARG:HG2	1:A:231:ILE:HD12	1.91	0.52
1:C:389:ASP:CB	1:C:392:LYS:HD3	2.41	0.51
1:C:297:SER:HB3	1:C:302:ALA:N	2.19	0.51
1:C:327:VAL:HB	1:C:386:VAL:HG13	1.93	0.51
1:A:172:ILE:HG12	1:A:204:MET:HE3	1.92	0.51
1:A:505:MET:SD	1:A:584:ARG:HD2	2.51	0.51
1:C:310:ILE:HD13	1:C:325:VAL:HG11	1.93	0.51
1:B:297:SER:HB3	1:B:302:ALA:H	1.76	0.50
1:C:412:ASP:HA	1:C:415:SER:HB3	1.93	0.50
1:C:391:HIS:HA	1:C:396:ILE:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:THR:HG21	1:B:94:ARG:HB2	1.94	0.49
1:B:547:SER:HB2	1:B:584:ARG:HB3	1.94	0.49
1:A:170:ARG:HG2	1:A:231:ILE:CD1	2.43	0.49
1:B:339:PHE:HE1	1:B:369:ILE:HG21	1.77	0.49
1:C:327:VAL:HG21	1:C:380:ILE:HG23	1.94	0.48
1:A:145:MET:C	1:A:336:ARG:HH21	2.16	0.48
1:B:52:PRO:HB3	1:C:23:GLU:HG2	1.96	0.48
1:A:207:LEU:HD11	1:A:214:ILE:HG23	1.95	0.48
1:A:210:ALA:HB1	1:A:213:GLU:HB2	1.96	0.48
1:B:166:LEU:HG	1:B:251:ILE:HG21	1.95	0.48
1:B:251:ILE:HA	1:C:250:ILE:O	2.14	0.48
1:B:316:LEU:HB3	1:B:321:ILE:HB	1.95	0.47
1:A:171:ASN:O	1:A:175:LEU:HG	2.14	0.47
1:C:170:ARG:HG2	1:C:231:ILE:HD12	1.95	0.47
1:B:253:ILE:HG13	1:B:254:GLY:N	2.30	0.47
1:B:295:VAL:HG13	1:B:303:VAL:HG13	1.95	0.47
1:B:396:ILE:HG21	1:B:449:VAL:HG22	1.96	0.47
1:C:170:ARG:HE	1:C:170:ARG:HB3	1.52	0.47
1:A:389:ASP:CB	1:A:392:LYS:HD2	2.45	0.46
1:C:237:PRO:HG2	1:C:294:VAL:HG23	1.97	0.46
1:B:273:GLU:HA	1:B:276:LYS:HD3	1.97	0.46
1:B:539:ILE:HA	1:B:542:ASN:HB2	1.98	0.46
1:C:115:MET:HE3	1:C:115:MET:HB3	1.75	0.46
1:B:295:VAL:HG21	1:B:380:ILE:HD11	1.98	0.46
1:A:512:GLU:HB3	1:A:515:ASN:HB2	1.98	0.46
1:C:281:LEU:HD12	1:C:281:LEU:HA	1.82	0.46
1:A:474:SER:HA	1:A:587:VAL:HG21	1.98	0.46
1:C:396:ILE:HG23	1:C:397:PRO:HD2	1.97	0.45
1:B:261:VAL:CG2	1:B:269:MET:HG2	2.46	0.45
1:A:267:TYR:HE2	1:A:498:LEU:CD2	2.30	0.45
1:C:441:LYS:HB3	1:C:441:LYS:HE3	1.40	0.45
1:B:235:LEU:HG	1:B:288:VAL:HG13	1.99	0.45
1:B:271:ILE:HG12	1:B:308:LYS:HE3	1.98	0.45
1:C:99:MET:HE2	1:C:99:MET:HB2	1.68	0.45
1:C:175:LEU:O	1:C:179:MET:HG3	2.16	0.45
1:A:295:VAL:HG13	1:A:327:VAL:HG12	1.97	0.45
1:A:487:LYS:HD2	1:A:487:LYS:HA	1.56	0.45
1:A:336:ARG:NH1	1:A:377:TYR:O	2.50	0.44
1:C:77:GLU:HG3	1:C:81:ARG:HD2	1.98	0.44
1:B:113:PHE:CE2	1:C:79:SER:HA	2.52	0.44
1:A:11:MET:HB3	1:A:11:MET:HE3	1.27	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:LEU:HD22	1:A:495:VAL:HG11	2.00	0.44
1:A:170:ARG:HE	1:A:251:ILE:HG13	1.82	0.44
1:B:94:ARG:HD3	1:C:47:MET:HG3	2.00	0.44
1:B:170:ARG:HA	1:B:289:LEU:HD11	1.98	0.44
1:C:231:ILE:HB	1:C:289:LEU:HD13	1.99	0.44
1:B:327:VAL:HB	1:B:386:VAL:HG22	2.00	0.44
1:B:235:LEU:HD22	1:B:259:ILE:HB	2.00	0.44
1:C:551:PHE:HB2	1:C:580:VAL:HG13	2.00	0.43
1:A:488:VAL:HG13	1:A:614:GLU:HG2	2.00	0.43
1:C:525:ASN:HA	1:C:528:VAL:HG22	2.01	0.43
1:A:208:GLU:HG3	1:A:409:ARG:HH11	1.83	0.43
1:B:396:ILE:HG23	1:B:397:PRO:HD2	2.00	0.43
1:B:39:His:CD2	1:B:116:LEU:HB3	2.53	0.43
1:B:391:His:HA	1:B:396:ILE:O	2.18	0.43
1:C:315:GLU:HA	1:C:318:LYS:HE3	2.00	0.43
1:C:338:ILE:HD12	1:C:467:ILE:HG22	2.01	0.43
1:B:109:LEU:HD12	1:B:109:LEU:HA	1.87	0.43
1:A:561:LEU:HD23	1:A:561:LEU:HA	1.84	0.43
1:B:29:LYS:HG2	1:C:33:ILE:HD12	2.01	0.43
1:B:271:ILE:CG1	1:B:308:LYS:HE3	2.48	0.43
1:C:166:LEU:HG	1:C:251:ILE:HG21	2.00	0.43
1:C:363:LYS:HE3	1:C:363:LYS:HB3	1.50	0.42
1:A:297:SER:HB3	1:A:302:ALA:H	1.83	0.42
1:A:363:LYS:HB3	1:A:363:LYS:HE3	1.46	0.42
1:C:183:LYS:HE3	1:C:183:LYS:HB2	1.56	0.42
1:A:334:TYR:CE1	1:A:390:PRO:HA	2.54	0.42
1:A:391:His:HA	1:A:396:ILE:O	2.19	0.42
1:A:441:LYS:HB3	1:A:441:LYS:HE3	1.72	0.42
1:B:115:MET:HE1	1:C:108:LEU:HA	2.01	0.42
1:A:564:VAL:HG13	1:A:569:PHE:HB2	2.02	0.42
1:B:588:MET:HE3	1:B:588:MET:HB3	1.78	0.42
1:A:523:LYS:HD3	1:A:523:LYS:HA	1.42	0.42
1:B:33:ILE:HD12	1:C:29:LYS:HG2	2.01	0.42
1:B:441:LYS:HE3	1:B:441:LYS:HB3	1.51	0.42
1:A:200:THR:HG23	1:A:322:TYR:HE2	1.85	0.42
1:B:62:LYS:HA	1:B:62:LYS:HD3	1.56	0.42
1:B:463:TYR:O	1:B:467:ILE:HG12	2.19	0.42
1:B:237:PRO:O	1:B:240:LYS:HB3	2.20	0.41
1:C:310:ILE:CD1	1:C:325:VAL:HG11	2.48	0.41
1:C:433:GLY:HA2	1:C:436:ILE:HG12	2.02	0.41
1:A:271:ILE:H	1:A:271:ILE:HG12	1.71	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:603:PRO:HA	1:A:606:GLN:HG3	2.01	0.41
1:C:175:LEU:HD13	1:C:175:LEU:HA	1.86	0.41
1:C:392:LYS:HZ3	1:C:392:LYS:HG2	1.74	0.41
1:A:167:TRP:CD2	1:A:414:ILE:HD12	2.55	0.41
1:A:253:ILE:HG13	1:A:254:GLY:N	2.35	0.41
1:C:436:ILE:HG13	1:C:438:GLU:O	2.19	0.41
1:A:186:LEU:HD11	1:A:210:ALA:HB2	2.01	0.41
1:B:392:LYS:O	1:B:393:MET:HB2	2.21	0.41
1:C:271:ILE:H	1:C:271:ILE:HG12	1.42	0.41
1:A:115:MET:HE3	1:A:115:MET:HB3	1.88	0.41
1:B:170:ARG:NE	1:B:251:ILE:HG13	2.36	0.41
1:A:389:ASP:HB2	1:A:392:LYS:HD2	2.03	0.40
1:A:484:LEU:HD23	1:A:484:LEU:HA	1.75	0.40
1:B:271:ILE:CD1	1:B:309:ILE:HG13	2.52	0.40
1:A:295:VAL:HG13	1:A:327:VAL:CG1	2.52	0.40
1:A:191:SER:OG	1:A:194:GLU:HB2	2.21	0.40
1:C:45:ASN:HA	1:C:48:PRO:HG3	2.03	0.40
1:B:334:TYR:CE1	1:B:390:PRO:HA	2.56	0.40
1:C:602:ALA:HB3	1:C:603:PRO:HD3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	598/620 (96%)	563 (94%)	35 (6%)	0	100	100
1	B	599/620 (97%)	574 (96%)	25 (4%)	0	100	100
1	C	580/620 (94%)	543 (94%)	37 (6%)	0	100	100
All	All	1777/1860 (96%)	1680 (94%)	97 (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	501/525 (95%)	449 (90%)	52 (10%)	7	10
1	B	497/525 (95%)	443 (89%)	54 (11%)	6	9
1	C	473/525 (90%)	414 (88%)	59 (12%)	4	6
All	All	1471/1575 (93%)	1306 (89%)	165 (11%)	6	8

All (165) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	MET
1	A	62	LYS
1	A	66	LYS
1	A	87	VAL
1	A	89	TRP
1	A	99	MET
1	A	107	SER
1	A	115	MET
1	A	159	SER
1	A	173	LYS
1	A	180	LYS
1	A	185	GLU
1	A	187	VAL
1	A	190	LYS
1	A	191	SER
1	A	194	GLU
1	A	211	GLU
1	A	212	ASP
1	A	231	ILE
1	A	233	LYS
1	A	240	LYS
1	A	269	MET
1	A	295	VAL
1	A	300	GLU
1	A	315	GLU
1	A	336	ARG

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Mol	Chain	Res	Type
1	A	350	GLU
1	A	357	GLU
1	A	363	LYS
1	A	365	LYS
1	A	371	ARG
1	A	372	GLU
1	A	391	HIS
1	A	399	SER
1	A	403	ILE
1	A	404	VAL
1	A	415	SER
1	A	428	ILE
1	A	441	LYS
1	A	484	LEU
1	A	485	THR
1	A	487	LYS
1	A	521	MET
1	A	523	LYS
1	A	541	ASN
1	A	547	SER
1	A	549	THR
1	A	555	ASP
1	A	561	LEU
1	A	579	LYS
1	A	584	ARG
1	A	589	THR
1	B	20	ASP
1	B	33	ILE
1	B	52	PRO
1	B	55	SER
1	B	62	LYS
1	B	66	LYS
1	B	108	LEU
1	B	109	LEU
1	B	148	LYS
1	B	153	HIS
1	B	166	LEU
1	B	170	ARG
1	B	173	LYS
1	B	177	PHE
1	B	180	LYS
1	B	183	LYS

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Mol	Chain	Res	Type
1	B	185	GLU
1	B	187	VAL
1	B	228	LEU
1	B	240	LYS
1	B	261	VAL
1	B	263	VAL
1	B	269	MET
1	B	284	GLU
1	B	305	SER
1	B	310	ILE
1	B	317	MET
1	B	321	ILE
1	B	336	ARG
1	B	338	ILE
1	B	354	ASP
1	B	357	GLU
1	B	366	LYS
1	B	367	GLU
1	B	382	LEU
1	B	391	HIS
1	B	399	SER
1	B	403	ILE
1	B	415	SER
1	B	428	ILE
1	B	440	SER
1	B	470	SER
1	B	485	THR
1	B	490	ASP
1	B	494	GLU
1	B	498	LEU
1	B	512	GLU
1	B	542	ASN
1	B	545	ILE
1	B	576	ARG
1	B	579	LYS
1	B	588	MET
1	B	589	THR
1	B	614	GLU
1	C	5	LYS
1	C	18	ILE
1	C	52	PRO
1	C	55	SER

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Mol	Chain	Res	Type
1	C	89	TRP
1	C	91	THR
1	C	99	MET
1	C	100	ASN
1	C	107	SER
1	C	115	MET
1	C	127	SER
1	C	128	PRO
1	C	132	GLN
1	C	148	LYS
1	C	166	LEU
1	C	170	ARG
1	C	172	ILE
1	C	175	LEU
1	C	176	PRO
1	C	177	PHE
1	C	183	LYS
1	C	185	GLU
1	C	186	LEU
1	C	187	VAL
1	C	211	GLU
1	C	212	ASP
1	C	236	VAL
1	C	240	LYS
1	C	271	ILE
1	C	281	LEU
1	C	297	SER
1	C	310	ILE
1	C	315	GLU
1	C	325	VAL
1	C	363	LYS
1	C	371	ARG
1	C	391	HIS
1	C	392	LYS
1	C	399	SER
1	C	403	ILE
1	C	413	VAL
1	C	415	SER
1	C	428	ILE
1	C	441	LYS
1	C	467	ILE
1	C	485	THR

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Mol	Chain	Res	Type
1	C	496	HIS
1	C	516	ASP
1	C	535	VAL
1	C	536	LYS
1	C	545	ILE
1	C	566	SER
1	C	571	ASP
1	C	584	ARG
1	C	589	THR
1	C	606	GLN
1	C	610	GLN
1	C	611	GLU
1	C	614	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	565	ASN
1	B	45	ASN
1	B	238	GLN
1	B	482	ASN
1	B	496	HIS
1	C	76	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

6 ligands 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	$\# Z > 2$
3	142	A	702	2	11,16,16	1.01	0	17,23,23	2.03	3 (17%)
3	142	C	702	2	11,16,16	1.06	0	17,23,23	2.03	3 (17%)
2	PLP	B	701	3	15,15,16	1.37	1 (6%)	20,22,23	1.12	0
2	PLP	C	701	3	15,15,16	1.22	0	20,22,23	1.19	1 (5%)
3	142	B	702	2	11,16,16	1.07	0	17,23,23	1.57	2 (11%)
2	PLP	A	701	3	15,15,16	1.41	1 (6%)	20,22,23	1.45	4 (20%)

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	142	A	702	2	-	0/5/14/14	0/1/1/1
3	142	C	702	2	-	0/5/14/14	0/1/1/1
2	PLP	B	701	3	-	0/6/6/8	0/1/1/1
2	PLP	C	701	3	-	0/6/6/8	0/1/1/1
3	142	B	702	2	-	2/5/14/14	0/1/1/1
2	PLP	A	701	3	-	1/6/6/8	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	PLP	C3-C2	-3.06	1.37	1.40
2	A	701	PLP	C3-C2	-3.01	1.37	1.40

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	702	142	CA-NN-N	7.46	125.69	113.73
3	A	702	142	CA-NN-N	6.45	124.07	113.73
3	B	702	142	CA-NN-N	4.74	121.32	113.73
3	A	702	142	CA-CB-CG	3.56	121.89	114.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	702	142	CA-CB-CG	3.33	121.43	114.85
3	A	702	142	CB-CA-NN	-3.04	101.69	110.23
3	C	702	142	CA-CB-CG	2.50	119.79	114.85
2	A	701	PLP	C3-C4-C5	2.42	121.35	118.74
2	A	701	PLP	C6-N1-C2	2.21	123.26	119.17
3	C	702	142	CB-CA-NN	-2.16	104.17	110.23
2	A	701	PLP	O3-C3-C2	2.16	122.19	117.49
2	A	701	PLP	C4A-C4-C5	-2.11	118.77	120.94
2	C	701	PLP	O3-C3-C2	2.02	121.90	117.49

There are no chirality outliers.

All (3) torsion outliers are listed below:

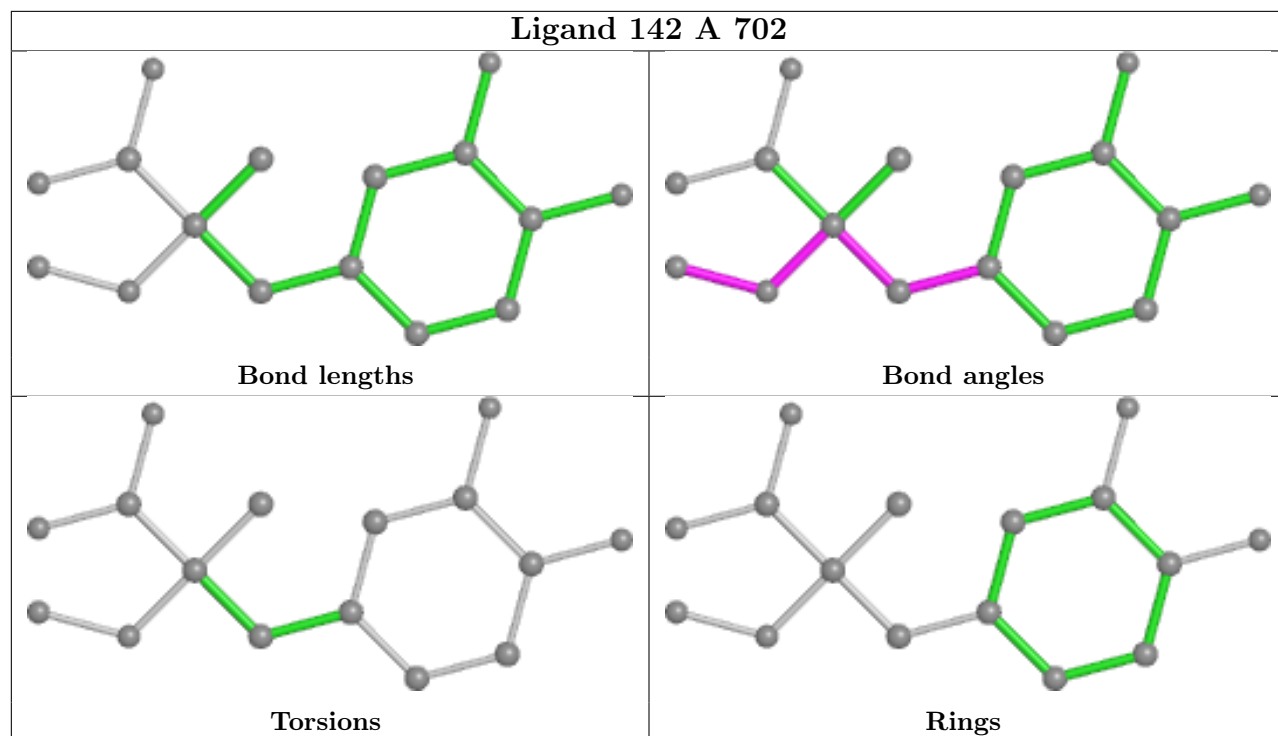
Mol	Chain	Res	Type	Atoms
3	B	702	142	CA-CB-CG-CD2
3	B	702	142	CA-CB-CG-CD1
2	A	701	PLP	C5A-O4P-P-O2P

There are no ring outliers.

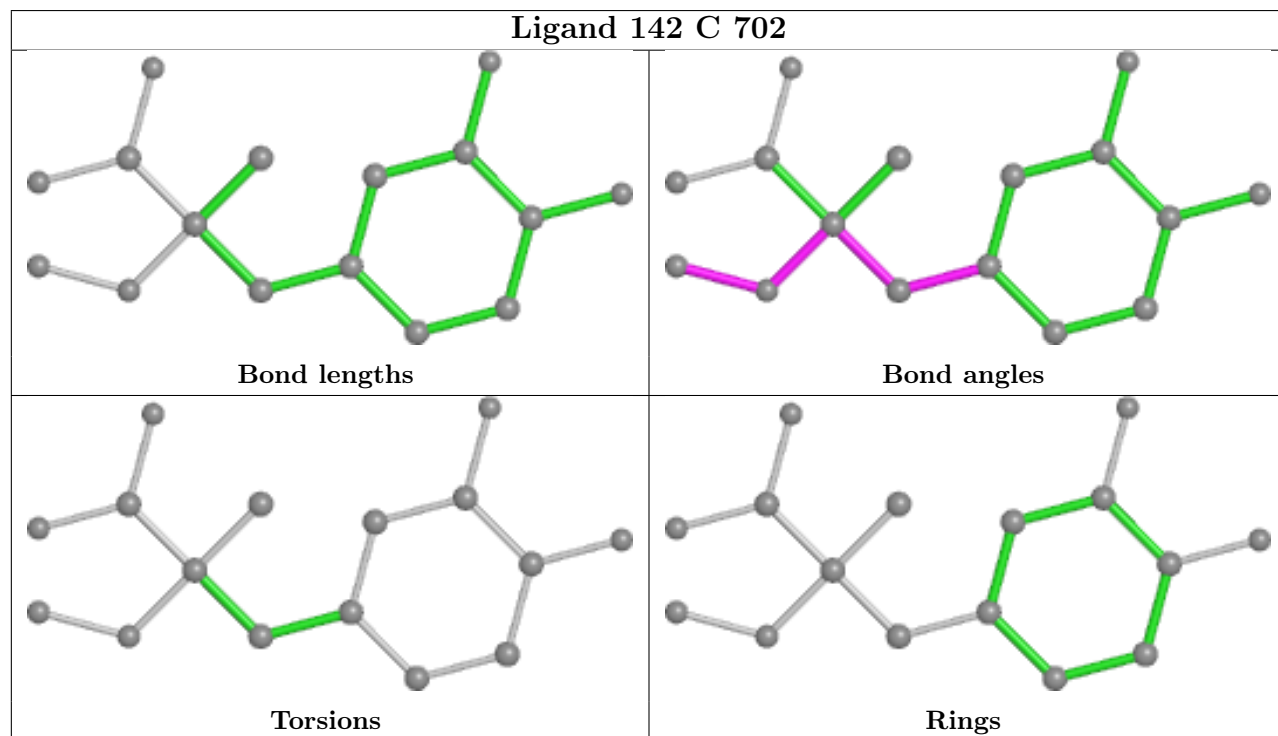
No monomer is involved in short contacts.

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.

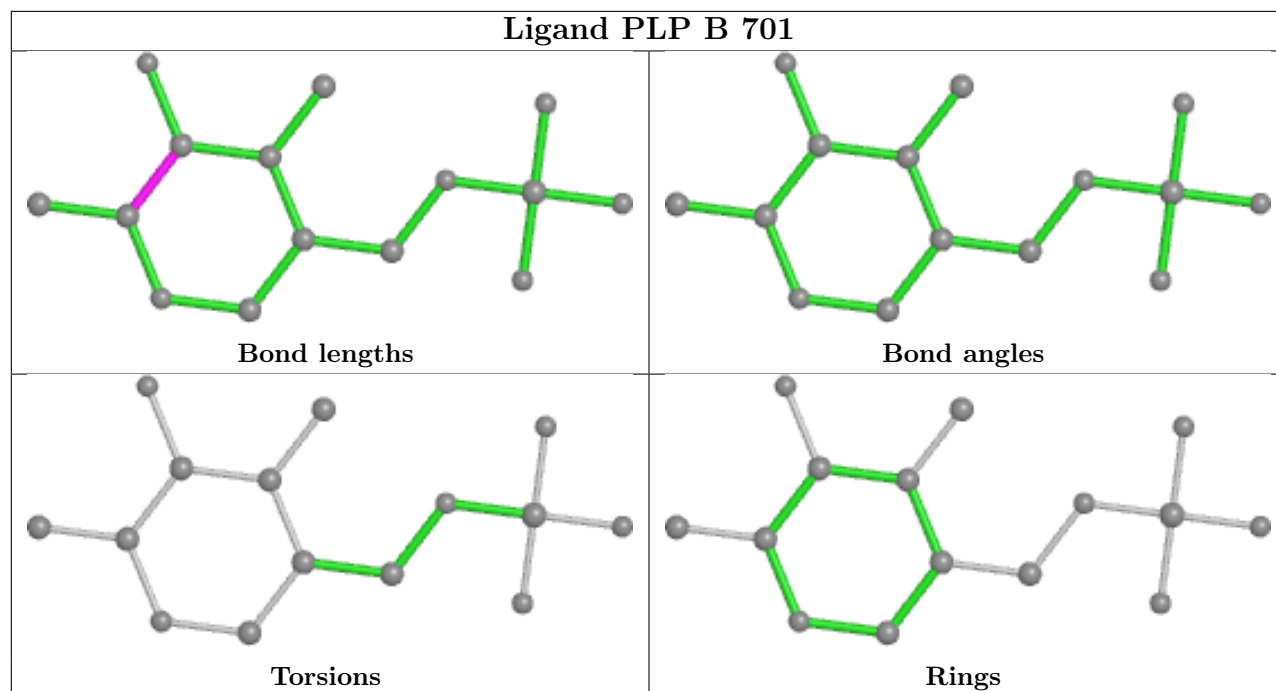
Ligand 142 A 702



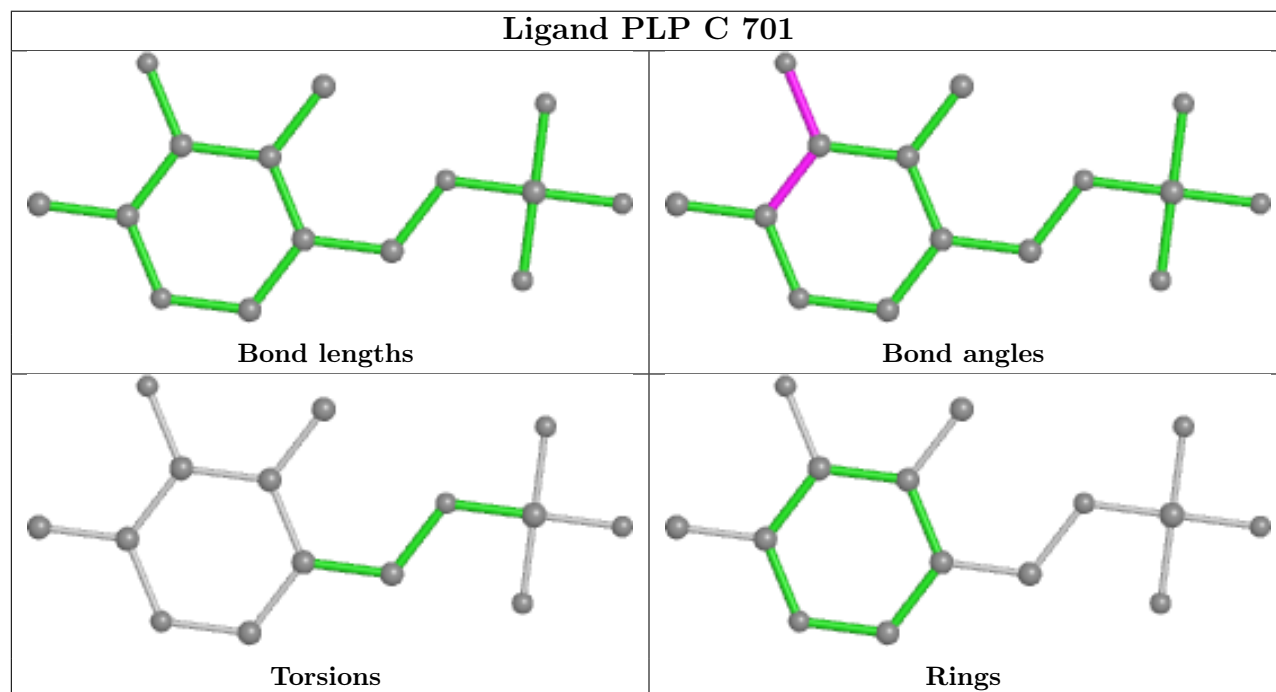
Ligand 142 C 702

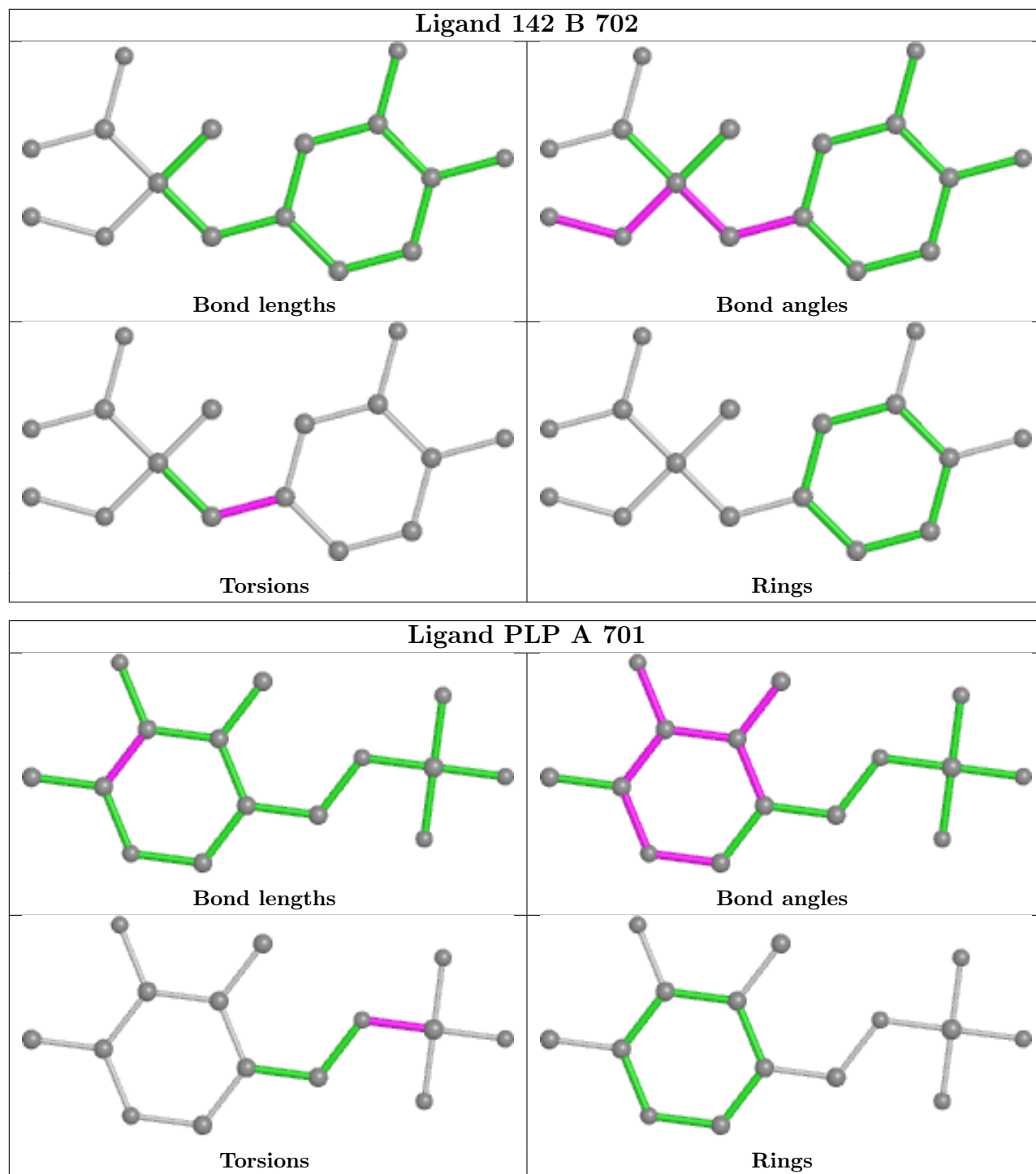


Ligand PLP B 701



Ligand PLP C 701





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, 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	602/620 (97%)	0.02	12 (1%) 65 60	30, 66, 94, 112	0
1	B	603/620 (97%)	0.21	26 (4%) 35 31	30, 71, 99, 118	0
1	C	588/620 (94%)	0.09	22 (3%) 41 38	39, 67, 109, 129	0
All	All	1793/1860 (96%)	0.11	60 (3%) 46 43	30, 68, 102, 129	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	537	GLY	5.4
1	C	535	VAL	4.9
1	B	540	TYR	4.6
1	A	490	ASP	4.3
1	B	519	VAL	4.2
1	A	169	ALA	3.5
1	B	536	LYS	3.5
1	B	289	LEU	3.5
1	C	516	ASP	3.3
1	B	535	VAL	3.2
1	C	534	TYR	3.2
1	A	483	ASP	3.1
1	B	583	LEU	3.1
1	C	90	HIS	3.1
1	C	148	LYS	3.0
1	B	483	ASP	2.9
1	B	290	GLY	2.9
1	C	315	GLU	2.8
1	A	10	GLU	2.8
1	B	572	GLU	2.8
1	C	536	LYS	2.8
1	C	364	GLU	2.8
1	C	540	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	489	GLY	2.8
1	B	534	TYR	2.7
1	C	483	ASP	2.7
1	A	173	LYS	2.7
1	C	4	GLU	2.7
1	A	534	TYR	2.5
1	A	539	ILE	2.5
1	C	99	MET	2.5
1	C	508	TYR	2.5
1	C	484	LEU	2.4
1	B	615	GLN	2.3
1	C	544	PHE	2.3
1	B	575	ASN	2.3
1	B	581	THR	2.2
1	B	509	VAL	2.2
1	B	99	MET	2.2
1	B	510	PHE	2.2
1	A	315	GLU	2.2
1	A	172	ILE	2.2
1	B	169	ALA	2.2
1	C	571	ASP	2.2
1	A	583	LEU	2.2
1	B	582	VAL	2.1
1	C	100	ASN	2.1
1	A	350	GLU	2.1
1	B	319	ASP	2.1
1	C	286	ILE	2.1
1	A	364	GLU	2.1
1	B	537	GLY	2.1
1	B	508	TYR	2.1
1	B	488	VAL	2.1
1	C	89	TRP	2.1
1	C	564	VAL	2.0
1	B	90	HIS	2.0
1	C	85	HIS	2.0
1	B	490	ASP	2.0
1	B	617	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

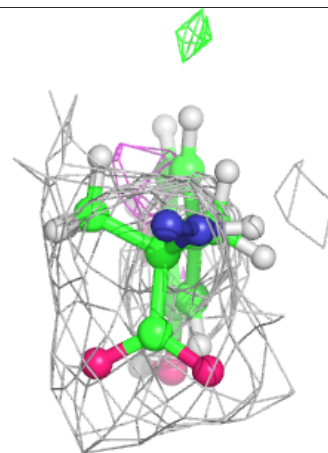
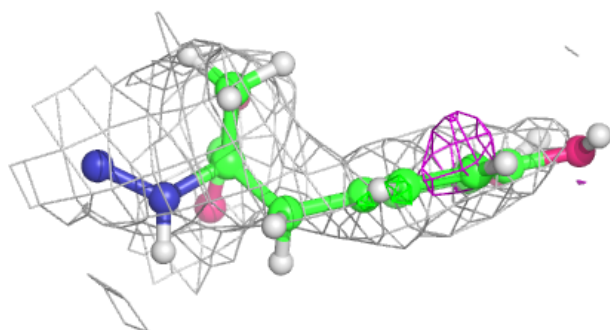
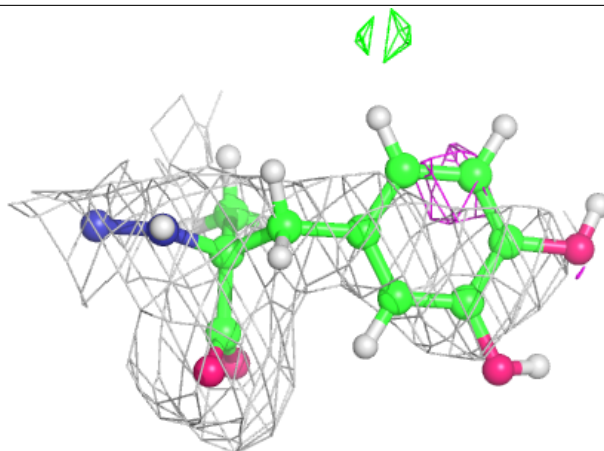
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	142	A	702	16/16	0.80	0.37	65,79,93,106	0
3	142	B	702	16/16	0.81	0.32	68,82,98,101	0
3	142	C	702	16/16	0.87	0.34	62,70,84,97	0
2	PLP	B	701	15/16	0.94	0.13	54,60,75,79	0
2	PLP	A	701	15/16	0.95	0.12	46,57,70,70	0
2	PLP	C	701	15/16	0.96	0.13	50,57,67,76	0

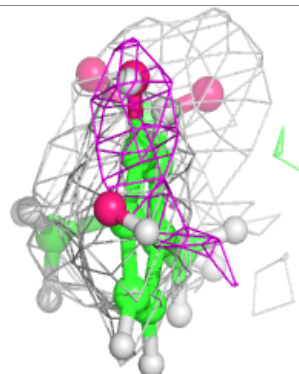
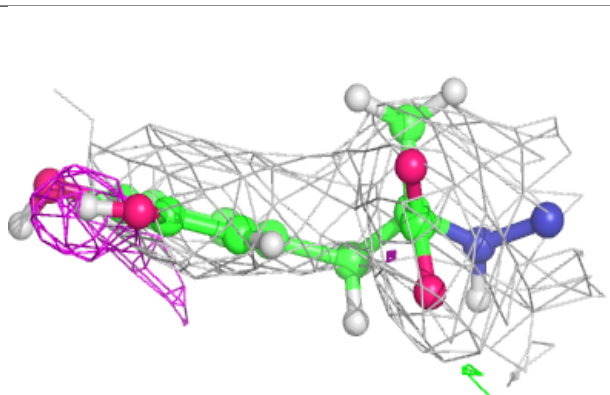
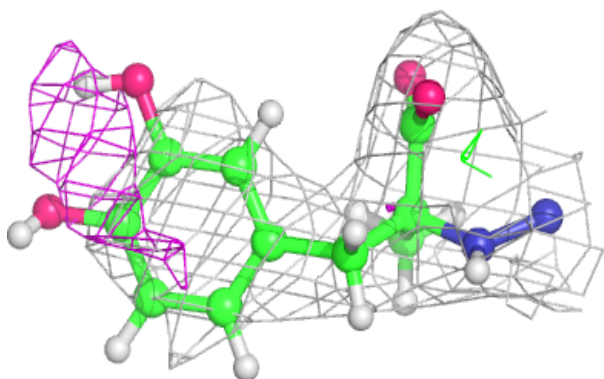
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 142 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)

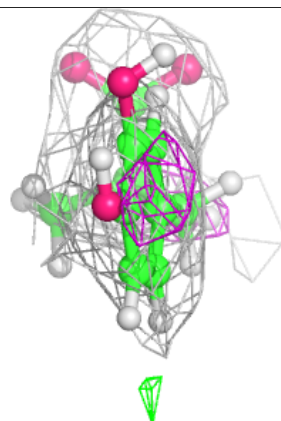
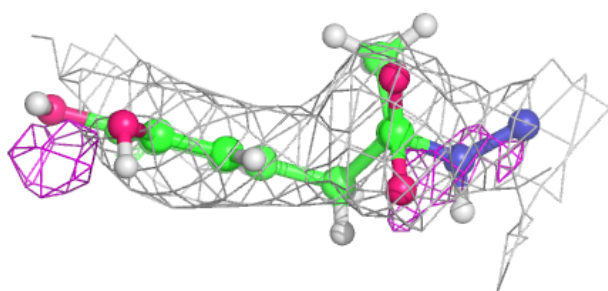
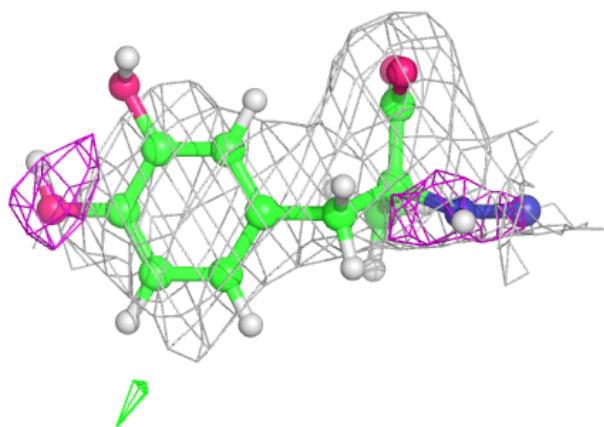
**Electron density around 142 B 702:**

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



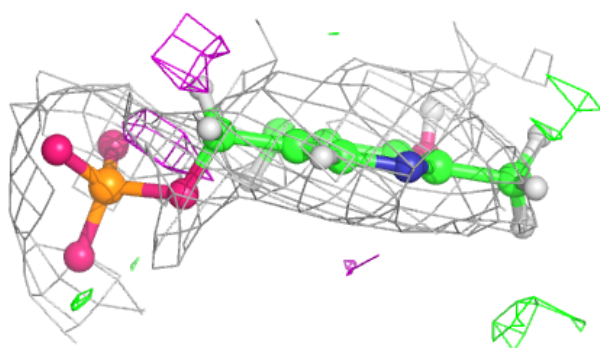
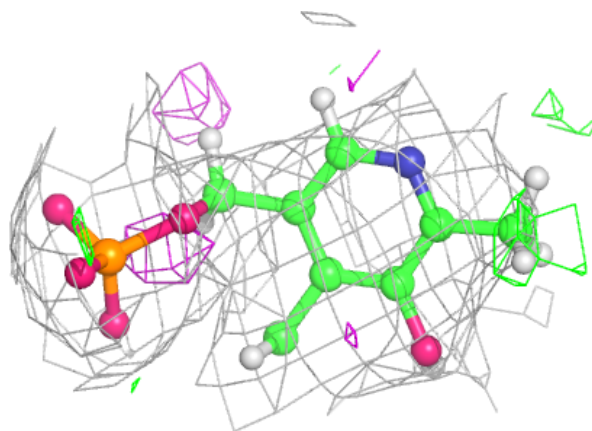
Electron density around 142 C 702:

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

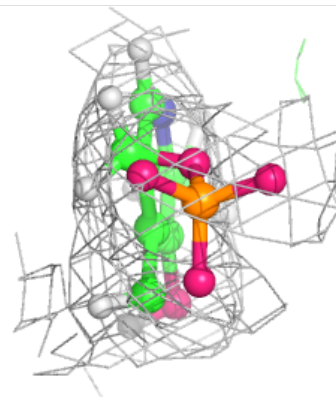
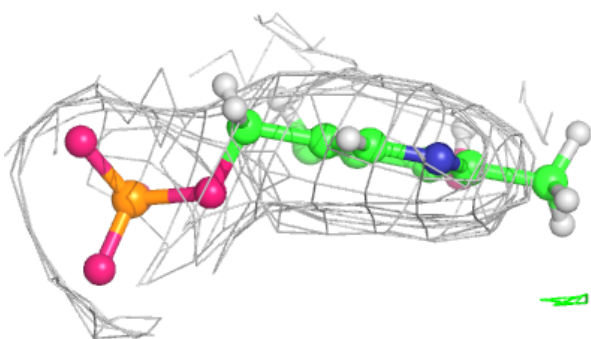
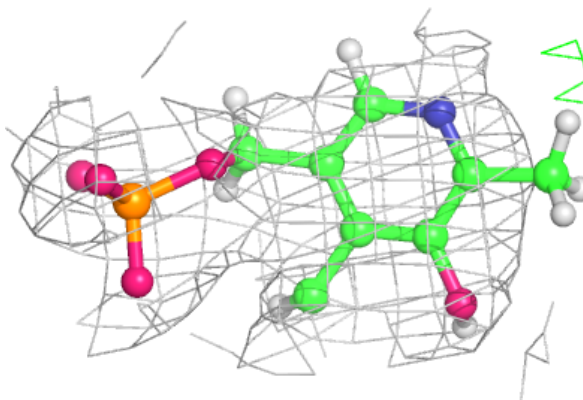


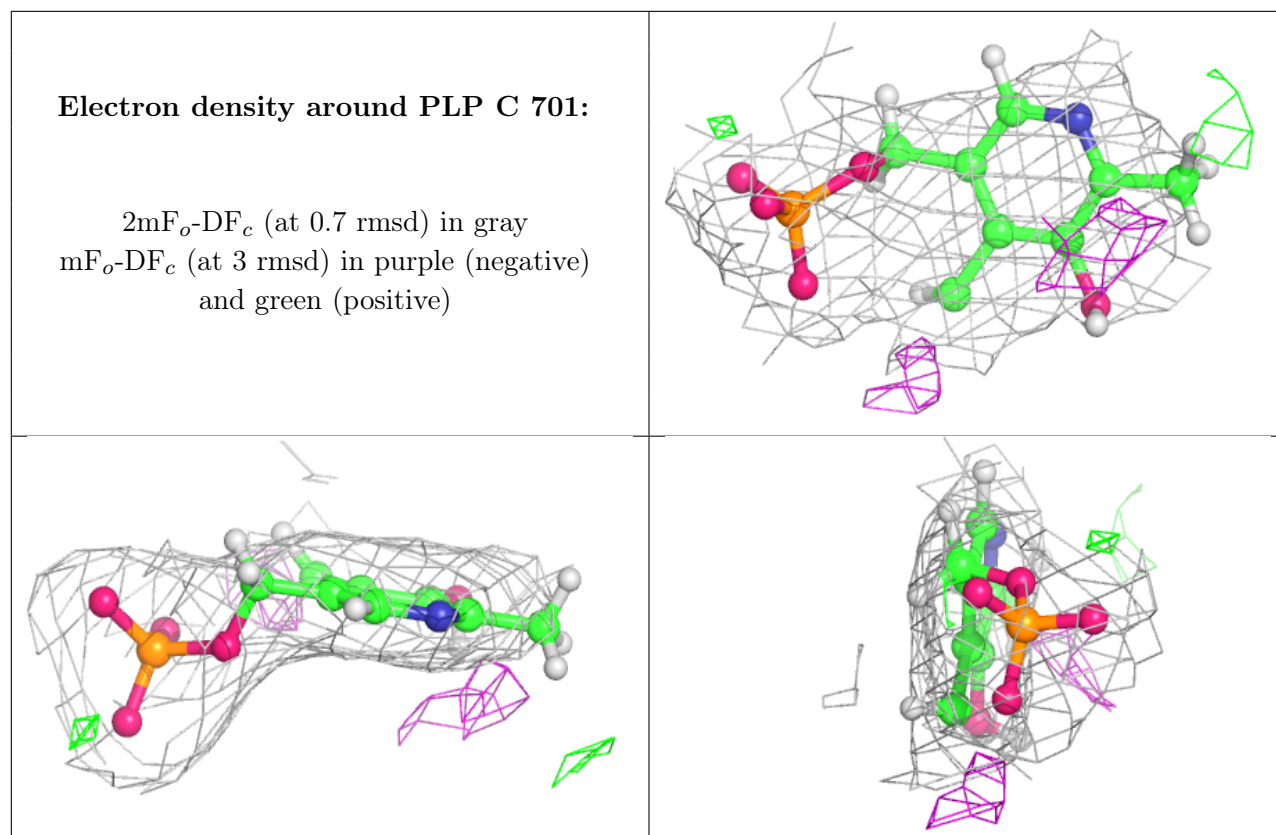
Electron density around PLP B 701:

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

**Electron density around PLP 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.