



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:03 PM UTC

PDB ID : 7X4L / pdb_00007x4l
Title : Crystal structure of Bacteroides thetaiotaomicron glutamate decarboxylase mutant Y303F-PLP complex
Authors : Liu, S.; Guoming, D.; Yulu, W.; Boting, W.; Xin, F.
Deposited on : 2022-03-02
Resolution : 2.59 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 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 (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

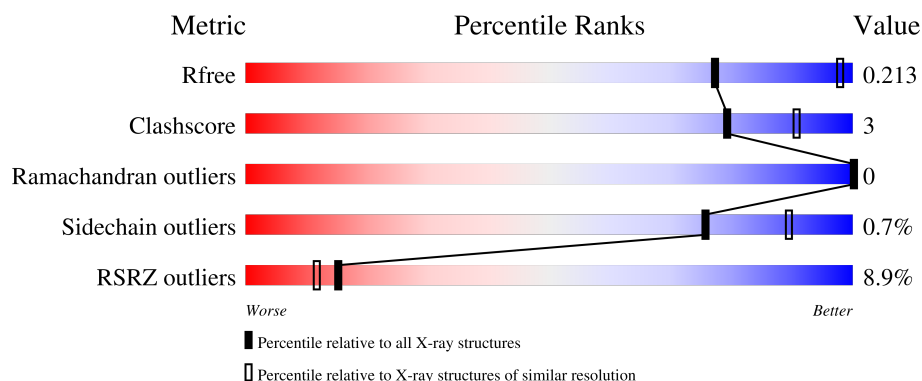
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	481	10% 88% 5% 7%
1	B	481	7% 87% 6% 6%
1	C	481	7% 86% 7% 7%
1	D	481	11% 86% 7% 6%
1	E	481	6% 88% • 8%

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Mol	Chain	Length	Quality of chain
1	F	481	9% 86% 7% 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21530 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 Glutamate decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	448	Total	C	N	O	S	4	0	0
			3542	2294	586	642	20			
1	B	450	Total	C	N	O	S	4	0	0
			3551	2301	585	645	20			
1	C	446	Total	C	N	O	S	4	0	0
			3514	2282	580	632	20			
1	D	450	Total	C	N	O	S	4	0	0
			3523	2285	581	637	20			
1	E	444	Total	C	N	O	S	4	0	0
			3514	2283	579	632	20			
1	F	450	Total	C	N	O	S	4	0	0
			3547	2301	586	640	20			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	303	PHE	TYR	engineered mutation	UNP Q8A4M9
B	303	PHE	TYR	engineered mutation	UNP Q8A4M9
C	303	PHE	TYR	engineered mutation	UNP Q8A4M9
D	303	PHE	TYR	engineered mutation	UNP Q8A4M9
E	303	PHE	TYR	engineered mutation	UNP Q8A4M9
F	303	PHE	TYR	engineered mutation	UNP Q8A4M9

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: 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	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	E	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	F	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

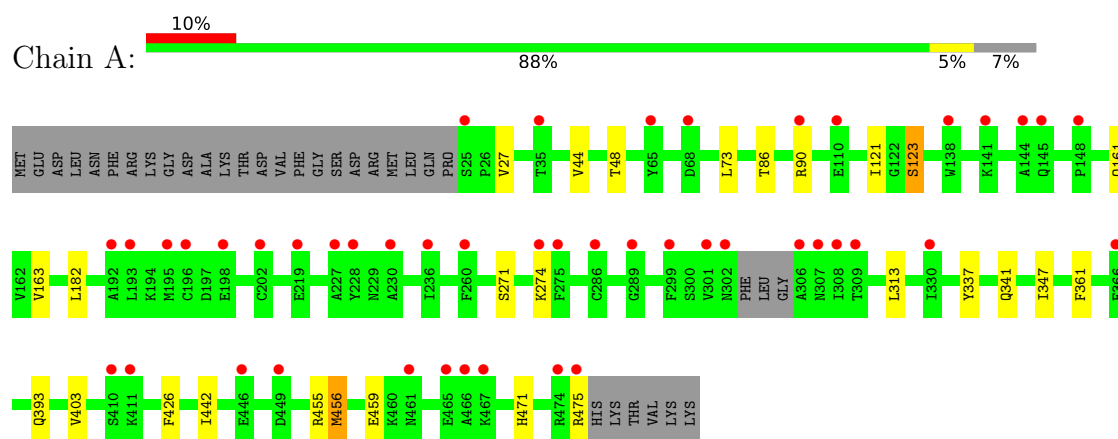
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	44	Total	O	0	0
			44	44		
3	B	64	Total	O	0	0
			64	64		
3	C	24	Total	O	0	0
			24	24		
3	D	31	Total	O	0	0
			31	31		
3	E	40	Total	O	0	0
			40	40		
3	F	46	Total	O	0	0
			46	46		

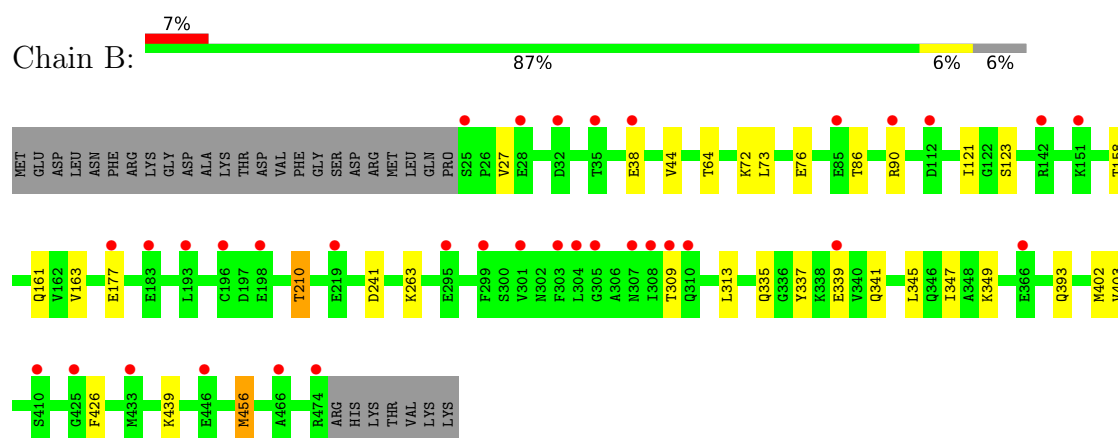
3 Residue-property plots [i](#)

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.

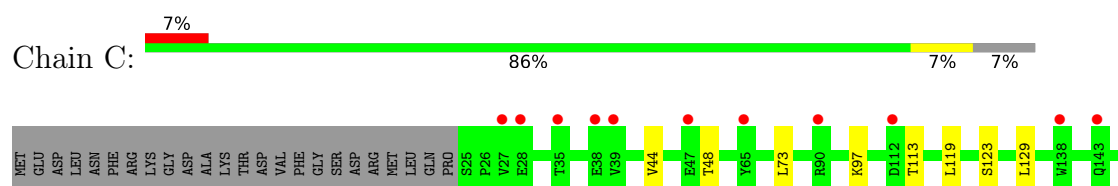
• Molecule 1: Glutamate decarboxylase

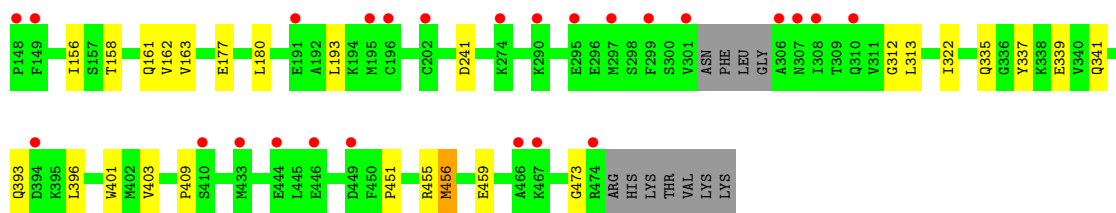


• Molecule 1: Glutamate decarboxylase

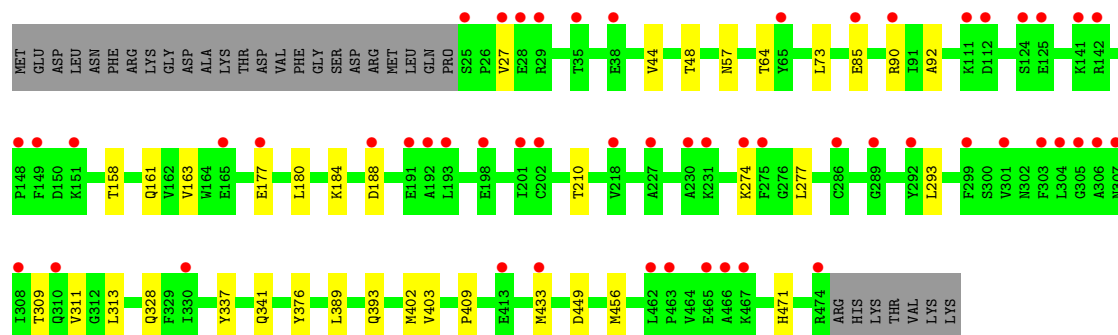
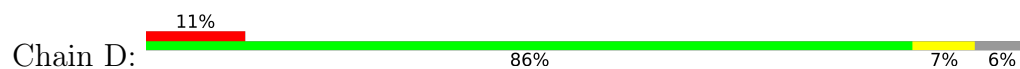


• Molecule 1: Glutamate decarboxylase

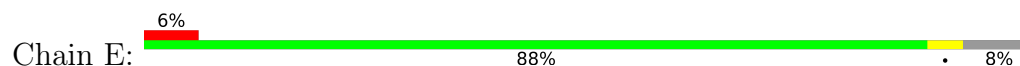




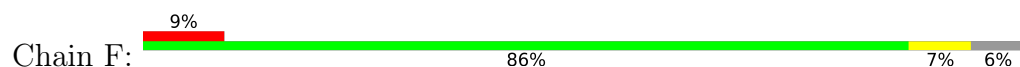
● Molecule 1: Glutamate decarboxylase



● Molecule 1: Glutamate decarboxylase



● Molecule 1: Glutamate decarboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	155.45Å 176.38Å 176.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.40 – 2.59 29.40 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.3 (29.40-2.59) 99.5 (29.40-2.59)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.57Å)	Xtriage
Refinement program	PHENIX (1.19.1_4122: ???)	Depositor
R, R_{free}	0.203 , 0.214 0.203 , 0.213	Depositor DCC
R_{free} test set	7440 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	59.4	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 29.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.017 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	21530	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.78% 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: 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	0.15	0/3639	0.36	0/4957
1	B	0.11	0/3649	0.33	0/4971
1	C	0.11	0/3611	0.33	0/4919
1	D	0.20	0/3621	0.38	0/4940
1	E	0.11	0/3611	0.32	0/4917
1	F	0.16	0/3645	0.35	0/4965
All	All	0.14	0/21776	0.35	0/29669

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	3542	0	3454	22	0
1	B	3551	0	3465	23	0
1	C	3514	0	3438	24	0
1	D	3523	0	3416	24	0
1	E	3514	0	3452	15	0
1	F	3547	0	3468	26	0
2	A	15	0	6	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	15	0	6	3	0
2	C	15	0	6	4	0
2	D	15	0	6	2	0
2	E	15	0	6	0	0
2	F	15	0	6	4	0
3	A	44	0	0	0	0
3	B	64	0	0	2	0
3	C	24	0	0	0	0
3	D	31	0	0	0	0
3	E	40	0	0	0	0
3	F	46	0	0	0	0
All	All	21530	0	20729	113	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 3.

All (113) 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:274:LYS:NZ	1:D:471:HIS:NE2	2.20	0.89
1:F:274:LYS:NZ	2:F:501:PLP:C5A	2.37	0.86
1:A:274:LYS:NZ	2:A:501:PLP:C5A	2.38	0.84
1:D:274:LYS:NZ	1:D:471:HIS:CD2	2.58	0.71
1:A:274:LYS:NZ	2:A:501:PLP:H5A1	2.11	0.66
1:F:274:LYS:NZ	2:F:501:PLP:H5A2	2.11	0.65
1:F:274:LYS:NZ	2:F:501:PLP:H5A1	2.11	0.64
1:C:241:ASP:OD2	2:C:501:PLP:H2A2	1.99	0.63
1:C:241:ASP:OD2	2:C:501:PLP:C2A	2.47	0.62
1:D:293:LEU:HD21	1:D:311:VAL:HG21	1.85	0.59
1:C:313:LEU:HD13	1:D:313:LEU:HD13	1.85	0.58
1:B:90:ARG:NH2	1:E:46:ASP:O	2.37	0.58
1:C:335:GLN:O	1:C:339:GLU:HG2	2.04	0.57
1:B:72:LYS:NZ	1:B:76:GLU:OE2	2.38	0.56
1:B:241:ASP:OD2	2:B:501:PLP:C2A	2.54	0.56
1:A:274:LYS:NZ	2:A:501:PLP:H5A2	2.18	0.55
1:A:123:SER:HB2	1:A:271:SER:OG	2.07	0.54
1:C:97:LYS:HD2	1:D:27:VAL:HA	1.88	0.54
1:B:241:ASP:OD2	2:B:501:PLP:H2A2	2.09	0.53
1:C:180:LEU:HD12	1:C:409:PRO:HG2	1.90	0.53
1:F:241:ASP:OD2	2:F:501:PLP:C2A	2.57	0.53
1:B:345:LEU:HG	1:B:349:LYS:HE2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:LEU:HD11	1:C:312:GLY:HA2	1.91	0.53
1:D:180:LEU:HD12	1:D:409:PRO:HG2	1.90	0.53
1:B:402:MET:HE2	1:E:86:THR:HG22	1.90	0.52
1:B:44:VAL:HG11	1:E:73:LEU:HD21	1.92	0.52
1:F:158:THR:HG22	1:F:177:GLU:HB3	1.92	0.52
1:A:313:LEU:HD13	1:F:313:LEU:HD13	1.92	0.51
1:B:86:THR:HG22	1:E:402:MET:HE2	1.94	0.51
1:B:161:GLN:OE1	1:B:163:VAL:HG13	2.11	0.51
1:C:123:SER:HB2	2:C:501:PLP:C5A	2.41	0.50
1:B:73:LEU:HD21	1:E:44:VAL:HG11	1.94	0.50
1:C:123:SER:HB2	2:C:501:PLP:H5A1	1.93	0.50
1:F:158:THR:O	1:F:474:ARG:NH2	2.44	0.49
1:D:161:GLN:OE1	1:D:163:VAL:HG13	2.12	0.49
1:A:86:THR:HG22	1:F:402:MET:HE2	1.95	0.49
1:B:335:GLN:O	1:B:339:GLU:HG2	2.13	0.49
1:F:161:GLN:OE1	1:F:163:VAL:HG13	2.13	0.49
1:C:161:GLN:OE1	1:C:163:VAL:HG13	2.12	0.48
1:E:337:TYR:O	1:E:341:GLN:HG2	2.13	0.48
1:B:27:VAL:HA	1:E:97:LYS:HD2	1.96	0.48
1:D:85:GLU:HG2	1:D:92:ALA:HB2	1.96	0.48
1:A:161:GLN:OE1	1:A:163:VAL:HG13	2.14	0.47
1:C:73:LEU:HD21	1:D:44:VAL:HG11	1.95	0.47
1:A:456:MET:HE3	1:A:456:MET:HB3	1.73	0.47
1:E:158:THR:HG22	1:E:177:GLU:HB3	1.97	0.46
1:B:439:LYS:NZ	3:B:607:HOH:O	2.48	0.46
1:D:337:TYR:O	1:D:341:GLN:HG2	2.15	0.46
1:D:376:TYR:HA	1:D:389:LEU:HD11	1.97	0.46
1:A:44:VAL:HG11	1:F:73:LEU:HD21	1.98	0.46
1:B:263:LYS:NZ	3:B:603:HOH:O	2.40	0.46
1:B:456:MET:HE3	1:B:456:MET:HB3	1.71	0.45
1:B:337:TYR:O	1:B:341:GLN:HG2	2.16	0.45
1:E:161:GLN:OE1	1:E:163:VAL:HG13	2.16	0.45
1:C:456:MET:HE3	1:C:456:MET:HB3	1.75	0.45
1:D:456:MET:HE3	1:D:456:MET:HB3	1.86	0.45
1:A:337:TYR:O	1:A:341:GLN:HG2	2.16	0.45
1:A:471:HIS:CD2	2:A:501:PLP:C4A	3.00	0.45
1:C:44:VAL:HG11	1:D:73:LEU:HD21	1.99	0.45
1:C:337:TYR:O	1:C:341:GLN:HG2	2.17	0.45
1:C:396:LEU:HB3	1:C:401:TRP:HB2	1.99	0.45
1:F:393:GLN:HG3	1:F:403:VAL:O	2.17	0.45
1:A:44:VAL:O	1:A:48:THR:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:ILE:HG13	1:E:121:ILE:HG13	1.99	0.45
1:D:44:VAL:O	1:D:48:THR:HG23	2.17	0.45
1:A:73:LEU:HD21	1:F:44:VAL:HG11	2.00	0.44
1:F:90:ARG:HE	1:F:90:ARG:HB2	1.59	0.44
1:A:475:ARG:C	1:F:299:PHE:HE1	2.25	0.44
1:A:456:MET:HE2	1:D:449:ASP:OD2	2.17	0.43
1:C:455:ARG:NH1	1:C:459:GLU:HG2	2.34	0.43
1:A:27:VAL:HA	1:F:97:LYS:HD2	2.01	0.43
1:C:193:LEU:HD23	1:C:193:LEU:HA	1.82	0.43
1:E:112:ASP:OD1	1:E:113:THR:N	2.51	0.43
1:F:293:LEU:HD21	1:F:311:VAL:HG21	1.99	0.43
1:D:158:THR:HG22	1:D:177:GLU:HB3	2.00	0.43
1:F:347:ILE:HD13	1:F:426:PHE:O	2.19	0.43
1:F:180:LEU:HD12	1:F:409:PRO:HG2	2.01	0.43
1:A:347:ILE:HD13	1:A:426:PHE:O	2.19	0.43
1:D:90:ARG:HE	1:D:90:ARG:HB2	1.46	0.43
1:E:44:VAL:O	1:E:48:THR:HG23	2.19	0.43
1:F:193:LEU:HA	1:F:193:LEU:HD13	1.82	0.43
1:C:44:VAL:O	1:C:48:THR:HG23	2.19	0.43
1:E:52:THR:OG1	1:E:402:MET:HE3	2.18	0.43
1:C:393:GLN:HG3	1:C:403:VAL:O	2.19	0.42
1:F:129:LEU:HD11	1:F:312:GLY:HA2	2.01	0.42
1:C:158:THR:HG22	1:C:177:GLU:HB3	2.01	0.42
1:B:393:GLN:HG3	1:B:403:VAL:O	2.19	0.42
1:D:57:ASN:HA	1:D:402:MET:HB2	2.02	0.42
1:F:337:TYR:O	1:F:341:GLN:HG2	2.19	0.42
1:B:158:THR:HG22	1:B:177:GLU:HB3	2.00	0.42
1:B:210:THR:HG22	2:B:501:PLP:O3	2.19	0.42
1:A:121:ILE:HG13	1:F:121:ILE:HG13	2.00	0.42
1:C:162:VAL:HB	1:C:473:GLY:HA3	2.00	0.42
1:D:393:GLN:HG3	1:D:403:VAL:O	2.20	0.42
1:A:393:GLN:HG3	1:A:403:VAL:O	2.20	0.41
1:B:38:GLU:H	1:B:38:GLU:CD	2.28	0.41
1:A:455:ARG:NH1	1:A:459:GLU:HG2	2.35	0.41
1:D:277:LEU:HB2	1:D:328:GLN:HE21	1.85	0.41
1:B:347:ILE:HD13	1:B:426:PHE:O	2.21	0.41
1:F:376:TYR:HA	1:F:389:LEU:HD11	2.02	0.41
1:D:210:THR:OG1	2:D:501:PLP:O3	2.37	0.41
1:F:179:PRO:HB2	1:F:411:LYS:HD2	2.02	0.41
1:B:313:LEU:HD13	1:E:313:LEU:HD13	2.02	0.41
1:A:361:PHE:CE2	1:A:442:ILE:HD11	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:433:MET:SD	1:F:90:ARG:HD3	2.61	0.41
1:E:225:LEU:HD12	1:E:225:LEU:HA	1.85	0.41
1:F:265:VAL:O	1:F:288:LYS:HE3	2.21	0.41
1:A:182:LEU:HD23	1:A:182:LEU:HA	1.90	0.40
1:D:274:LYS:HE3	2:D:501:PLP:C5A	2.52	0.40
1:C:119:LEU:HD22	1:C:322:ILE:HD11	2.03	0.40
1:C:156:ILE:O	1:C:177:GLU:HA	2.21	0.40
1:C:451:PRO:HB2	1:C:456:MET:HG2	2.04	0.40
1:D:184:LYS:HD2	1:D:188:ASP:HB2	2.02	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	444/481 (92%)	429 (97%)	15 (3%)	0	100	100
1	B	448/481 (93%)	432 (96%)	16 (4%)	0	100	100
1	C	442/481 (92%)	427 (97%)	15 (3%)	0	100	100
1	D	448/481 (93%)	434 (97%)	14 (3%)	0	100	100
1	E	440/481 (92%)	425 (97%)	15 (3%)	0	100	100
1	F	448/481 (93%)	430 (96%)	18 (4%)	0	100	100
All	All	2670/2886 (92%)	2577 (96%)	93 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	370/414 (89%)	367 (99%)	3 (1%)	73	88
1	B	371/414 (90%)	366 (99%)	5 (1%)	61	82
1	C	366/414 (88%)	364 (100%)	2 (0%)	81	92
1	D	364/414 (88%)	362 (100%)	2 (0%)	81	92
1	E	369/414 (89%)	368 (100%)	1 (0%)	86	94
1	F	369/414 (89%)	367 (100%)	2 (0%)	81	92
All	All	2209/2484 (89%)	2194 (99%)	15 (1%)	76	89

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	ARG
1	A	123	SER
1	A	456	MET
1	B	64	THR
1	B	123	SER
1	B	210	THR
1	B	309	THR
1	B	456	MET
1	C	113	THR
1	C	456	MET
1	D	64	THR
1	D	309	THR
1	E	113	THR
1	F	113	THR
1	F	210	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	363	ASN
1	A	370	ASN
1	A	398	GLN
1	B	172	GLN
1	B	363	ASN
1	B	398	GLN
1	C	172	GLN

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Mol	Chain	Res	Type
1	C	363	ASN
1	C	370	ASN
1	D	370	ASN
1	D	398	GLN
1	E	81	ASN
1	E	169	GLN
1	E	363	ASN
1	E	370	ASN
1	F	107	ASN
1	F	172	GLN
1	F	307	ASN
1	F	310	GLN
1	F	398	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
2	PLP	A	501	1	15,15,16	1.14	2 (13%)	21,22,23	1.46	2 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PLP	E	501	1	15,15,16	1.14	2 (13%)	21,22,23	1.47	2 (9%)
2	PLP	D	501	1	15,15,16	1.13	2 (13%)	21,22,23	1.47	2 (9%)
2	PLP	C	501	1	15,15,16	1.14	2 (13%)	21,22,23	1.46	2 (9%)
2	PLP	B	501	1	15,15,16	1.15	2 (13%)	21,22,23	1.46	2 (9%)
2	PLP	F	501	1	15,15,16	1.13	2 (13%)	21,22,23	1.47	2 (9%)

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
2	PLP	A	501	1	-	0/6/6/8	0/1/1/1
2	PLP	E	501	1	-	0/6/6/8	0/1/1/1
2	PLP	D	501	1	-	0/6/6/8	0/1/1/1
2	PLP	C	501	1	-	0/6/6/8	0/1/1/1
2	PLP	B	501	1	-	0/6/6/8	0/1/1/1
2	PLP	F	501	1	-	0/6/6/8	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	PLP	C4A-C4	-2.81	1.46	1.51
2	B	501	PLP	C4A-C4	-2.81	1.46	1.51
2	D	501	PLP	C4A-C4	-2.81	1.46	1.51
2	F	501	PLP	C4A-C4	-2.81	1.46	1.51
2	E	501	PLP	C4A-C4	-2.80	1.46	1.51
2	C	501	PLP	C4A-C4	-2.79	1.46	1.51
2	B	501	PLP	C3-C2	-2.57	1.38	1.41
2	C	501	PLP	C3-C2	-2.52	1.38	1.41
2	A	501	PLP	C3-C2	-2.50	1.38	1.41
2	E	501	PLP	C3-C2	-2.48	1.38	1.41
2	D	501	PLP	C3-C2	-2.47	1.38	1.41
2	F	501	PLP	C3-C2	-2.46	1.38	1.41

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	PLP	O4P-C5A-C5	4.86	118.46	109.36
2	F	501	PLP	O4P-C5A-C5	4.85	118.45	109.36
2	E	501	PLP	O4P-C5A-C5	4.85	118.45	109.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	PLP	O4P-C5A-C5	4.84	118.43	109.36
2	A	501	PLP	O4P-C5A-C5	4.84	118.43	109.36
2	B	501	PLP	O4P-C5A-C5	4.84	118.42	109.36
2	B	501	PLP	C4A-C4-C5	2.47	123.49	120.94
2	D	501	PLP	C4A-C4-C5	2.46	123.47	120.94
2	A	501	PLP	C4A-C4-C5	2.45	123.47	120.94
2	F	501	PLP	C4A-C4-C5	2.44	123.46	120.94
2	E	501	PLP	C4A-C4-C5	2.43	123.44	120.94
2	C	501	PLP	C4A-C4-C5	2.41	123.42	120.94

There are no chirality outliers.

There are no torsion outliers.

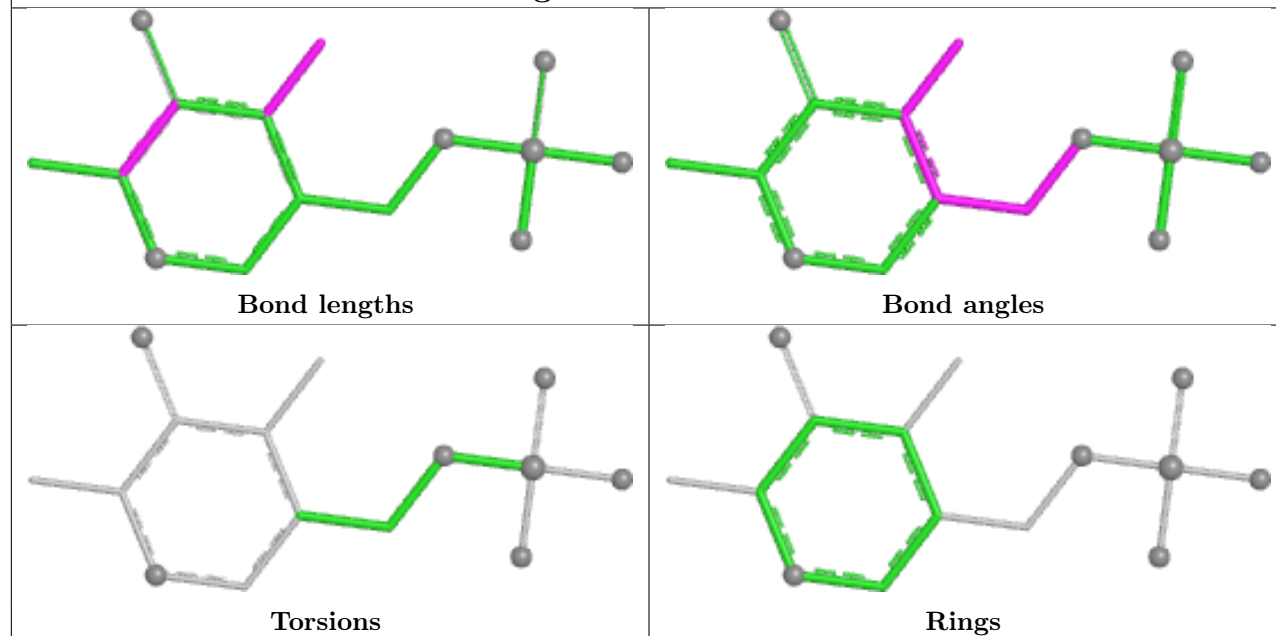
There are no ring outliers.

5 monomers are involved in 17 short contacts:

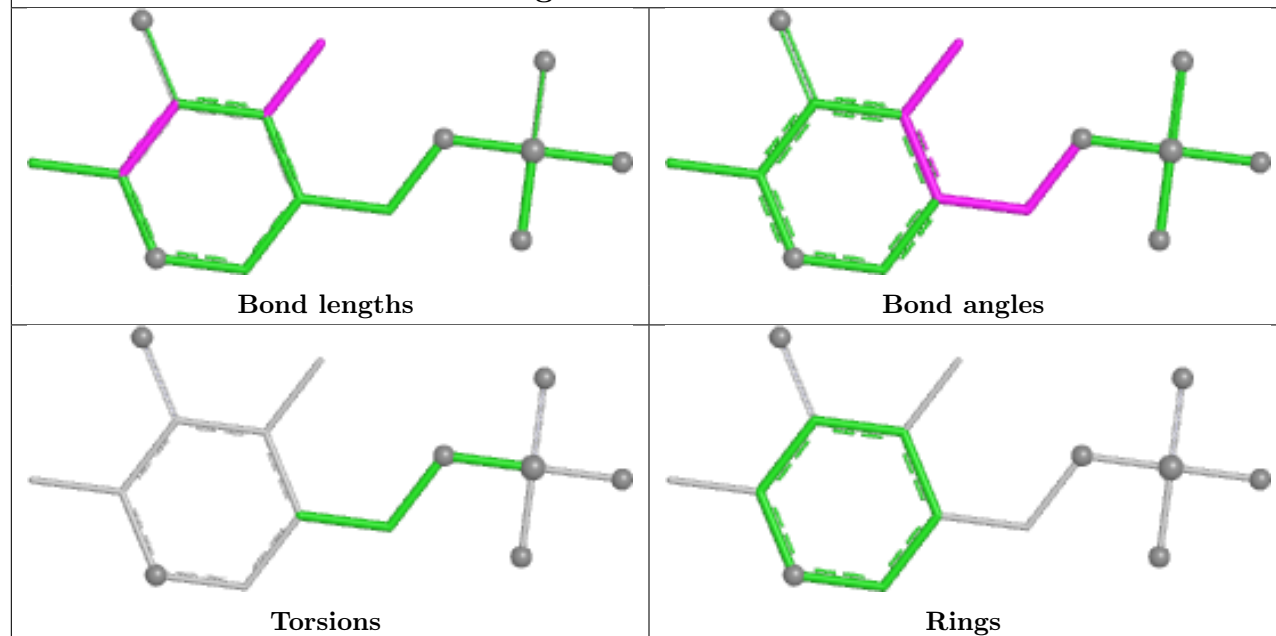
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	PLP	4	0
2	D	501	PLP	2	0
2	C	501	PLP	4	0
2	B	501	PLP	3	0
2	F	501	PLP	4	0

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

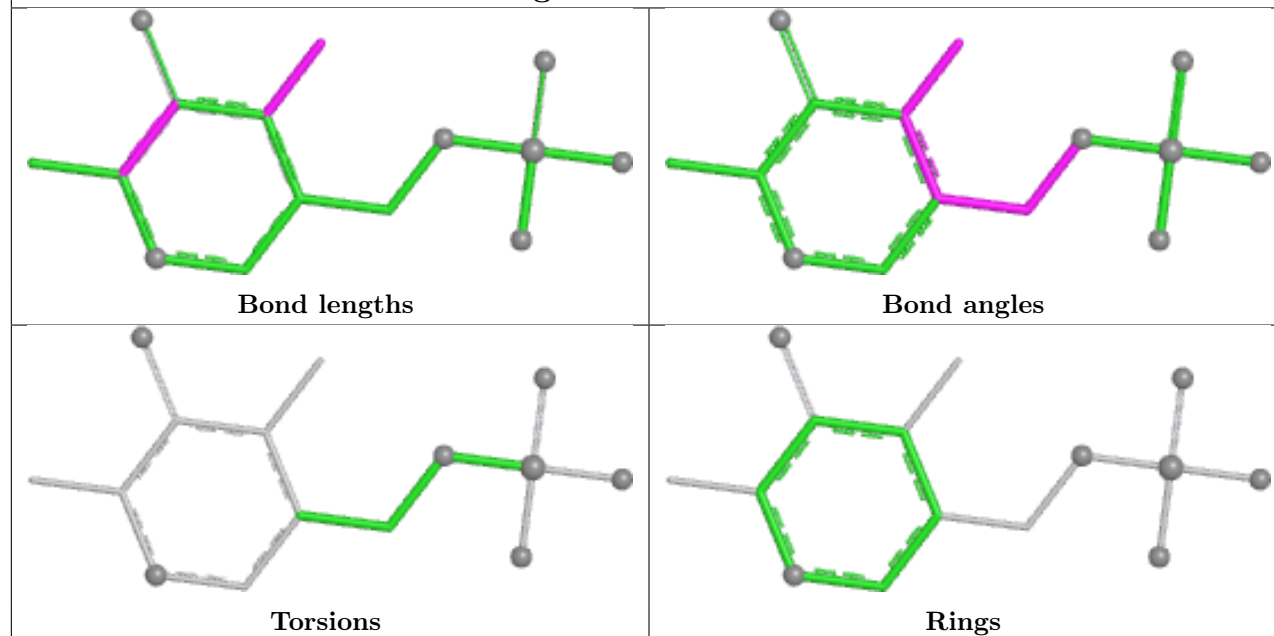
Ligand PLP A 501



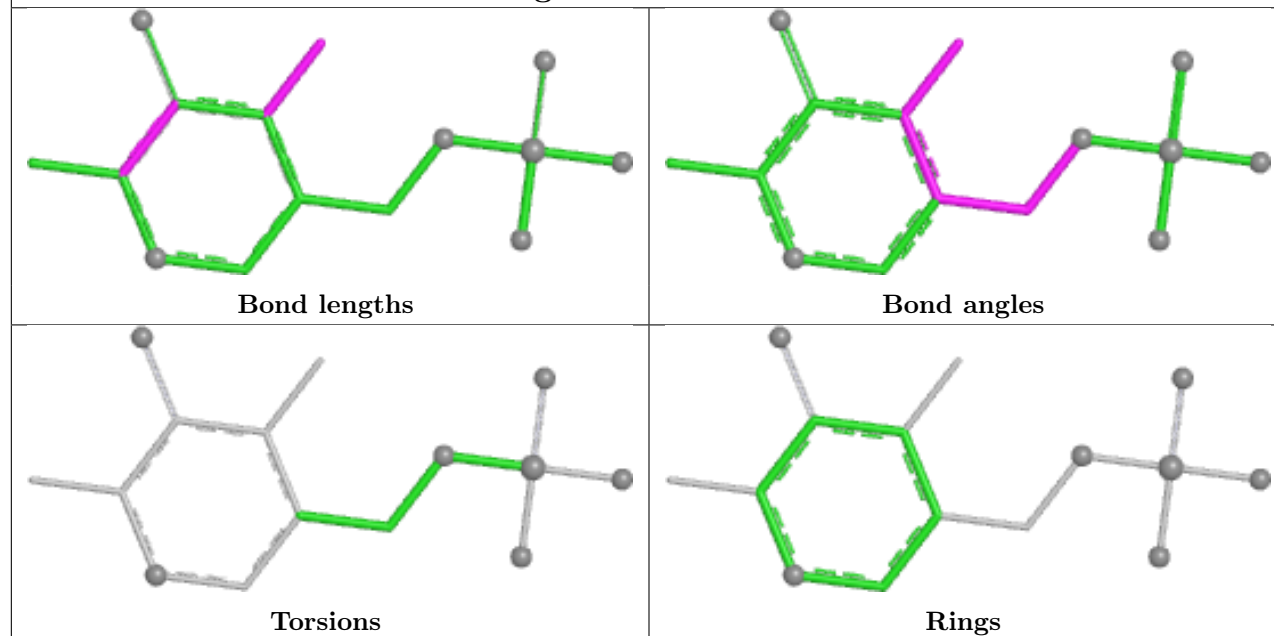
Ligand PLP E 501

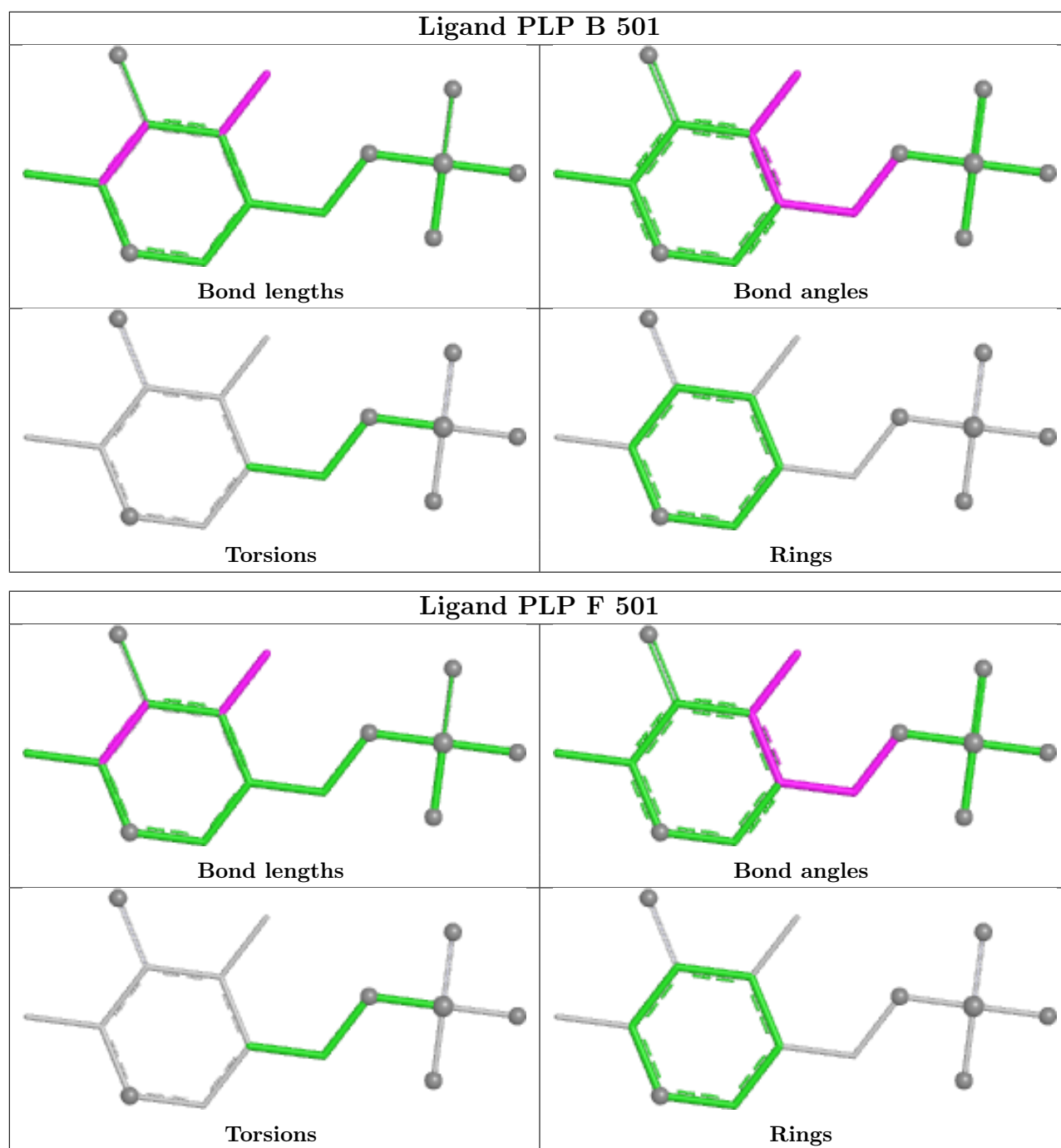


Ligand PLP D 501



Ligand PLP C 501





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	448/481 (93%)	0.82	46 (10%) 12 9	35, 62, 104, 148	1 (0%)
1	B	450/481 (93%)	0.44	34 (7%) 20 16	25, 54, 88, 113	1 (0%)
1	C	446/481 (92%)	0.74	36 (8%) 18 14	31, 66, 108, 141	1 (0%)
1	D	450/481 (93%)	0.97	54 (12%) 9 7	32, 69, 112, 150	1 (0%)
1	E	444/481 (92%)	0.63	27 (6%) 27 22	30, 61, 97, 133	1 (0%)
1	F	450/481 (93%)	0.69	42 (9%) 14 11	30, 61, 99, 142	1 (0%)
All	All	2688/2886 (93%)	0.72	239 (8%) 15 12	25, 62, 104, 150	6 (0%)

All (239) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	274	LYS	5.9
1	B	303	PHE	5.9
1	F	274	LYS	5.6
1	D	299	PHE	5.6
1	B	308	ILE	5.3
1	D	274	LYS	5.3
1	A	299	PHE	5.1
1	E	299	PHE	5.1
1	D	303	PHE	5.0
1	E	301	VAL	5.0
1	D	466	ALA	4.8
1	D	85	GLU	4.6
1	E	308	ILE	4.6
1	C	301	VAL	4.5
1	A	307	ASN	4.4
1	E	466	ALA	4.3
1	A	302	ASN	4.3
1	B	299	PHE	4.2
1	D	192	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
1	F	303	PHE	4.0
1	D	310	GLN	4.0
1	A	198	GLU	4.0
1	D	149	PHE	3.9
1	B	466	ALA	3.9
1	A	475	ARG	3.9
1	A	466	ALA	3.8
1	C	299	PHE	3.8
1	C	307	ASN	3.8
1	B	304	LEU	3.7
1	A	196	CYS	3.7
1	F	299	PHE	3.7
1	B	309	THR	3.6
1	F	25	SER	3.6
1	C	306	ALA	3.6
1	E	235	ASP	3.6
1	E	190	GLU	3.5
1	C	35	THR	3.5
1	F	35	THR	3.5
1	A	306	ALA	3.5
1	C	274	LYS	3.5
1	D	467	LYS	3.5
1	C	149	PHE	3.5
1	D	148	PRO	3.4
1	D	112	ASP	3.4
1	A	35	THR	3.4
1	A	366	GLU	3.4
1	A	446	GLU	3.4
1	C	195	MET	3.4
1	F	310	GLN	3.3
1	A	308	ILE	3.3
1	B	198	GLU	3.3
1	E	85	GLU	3.3
1	F	28	GLU	3.3
1	D	462	LEU	3.2
1	C	28	GLU	3.2
1	C	449	ASP	3.2
1	F	300	SER	3.2
1	D	177	GLU	3.1
1	B	307	ASN	3.1
1	D	230	ALA	3.1
1	F	198	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	474	ARG	3.1
1	A	110	GLU	3.1
1	E	474	ARG	3.1
1	A	467	LYS	3.0
1	C	65	TYR	3.0
1	A	192	ALA	3.0
1	C	394	ASP	3.0
1	C	90	ARG	3.0
1	A	25	SER	3.0
1	D	25	SER	3.0
1	E	274	LYS	3.0
1	F	394	ASP	3.0
1	D	90	ARG	2.9
1	E	309	THR	2.9
1	F	462	LEU	2.9
1	A	301	VAL	2.9
1	B	90	ARG	2.9
1	F	459	GLU	2.9
1	F	233	GLY	2.9
1	B	446	GLU	2.8
1	C	308	ILE	2.8
1	A	219	GLU	2.8
1	C	310	GLN	2.8
1	B	35	THR	2.8
1	E	462	LEU	2.8
1	B	339	GLU	2.8
1	F	290	LYS	2.8
1	F	302	ASN	2.8
1	D	193	LEU	2.8
1	D	304	LEU	2.8
1	E	196	CYS	2.8
1	D	289	GLY	2.7
1	D	151	LYS	2.7
1	C	444	GLU	2.7
1	B	112	ASP	2.7
1	F	469	PHE	2.7
1	C	466	ALA	2.7
1	D	28	GLU	2.7
1	D	35	THR	2.6
1	F	309	THR	2.6
1	E	286	CYS	2.6
1	B	366	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	65	TYR	2.6
1	A	286	CYS	2.6
1	F	301	VAL	2.6
1	F	144	ALA	2.6
1	C	148	PRO	2.6
1	A	145	GLN	2.6
1	D	465	GLU	2.5
1	D	202	CYS	2.5
1	E	144	ALA	2.5
1	D	29	ARG	2.5
1	D	307	ASN	2.5
1	A	202	CYS	2.5
1	B	474	ARG	2.5
1	C	202	CYS	2.5
1	A	465	GLU	2.5
1	D	308	ILE	2.5
1	B	301	VAL	2.5
1	D	218	VAL	2.5
1	E	25	SER	2.5
1	E	295	GLU	2.5
1	B	310	GLN	2.5
1	D	301	VAL	2.5
1	D	38	GLU	2.4
1	D	191	GLU	2.4
1	F	295	GLU	2.4
1	F	275	PHE	2.4
1	C	191	GLU	2.4
1	B	196	CYS	2.4
1	B	295	GLU	2.4
1	F	193	LEU	2.4
1	A	260	PHE	2.4
1	B	28	GLU	2.4
1	F	29	ARG	2.4
1	E	464	VAL	2.4
1	F	413	GLU	2.4
1	F	425	GLY	2.3
1	F	304	LEU	2.3
1	C	297	MET	2.3
1	A	141	LYS	2.3
1	C	38	GLU	2.3
1	E	467	LYS	2.3
1	E	463	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	463	PRO	2.3
1	E	310	GLN	2.3
1	F	235	ASP	2.3
1	C	467	LYS	2.3
1	B	38	GLU	2.3
1	B	85	GLU	2.3
1	C	196	CYS	2.3
1	C	295	GLU	2.3
1	A	230	ALA	2.3
1	F	466	ALA	2.3
1	B	183	GLU	2.3
1	E	198	GLU	2.3
1	A	195	MET	2.2
1	F	110	GLU	2.2
1	F	149	PHE	2.2
1	C	39	VAL	2.2
1	D	286	CYS	2.2
1	A	309	THR	2.2
1	A	411	LYS	2.2
1	C	290	LYS	2.2
1	D	124	SER	2.2
1	D	330	ILE	2.2
1	D	198	GLU	2.2
1	D	413	GLU	2.2
1	A	144	ALA	2.2
1	F	141	LYS	2.2
1	A	289	GLY	2.2
1	B	410	SER	2.2
1	E	32	ASP	2.2
1	E	465	GLU	2.2
1	D	142	ARG	2.2
1	A	275	PHE	2.2
1	D	27	VAL	2.2
1	C	433	MET	2.2
1	C	410	SER	2.2
1	F	165	GLU	2.2
1	B	151	LYS	2.2
1	D	111	LYS	2.2
1	D	306	ALA	2.1
1	F	70	ALA	2.1
1	B	177	GLU	2.1
1	D	125	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	165	GLU	2.1
1	A	449	ASP	2.1
1	B	193	LEU	2.1
1	A	90	ARG	2.1
1	A	474	ARG	2.1
1	C	446	GLU	2.1
1	B	32	ASP	2.1
1	C	112	ASP	2.1
1	D	188	ASP	2.1
1	D	141	LYS	2.1
1	F	145	GLN	2.1
1	B	305	GLY	2.1
1	F	232	THR	2.1
1	A	236	ILE	2.1
1	B	219	GLU	2.1
1	D	201	ILE	2.1
1	D	292	TYR	2.1
1	F	231	LYS	2.1
1	F	433	MET	2.1
1	D	275	PHE	2.1
1	A	227	ALA	2.1
1	A	138	TRP	2.1
1	B	425	GLY	2.1
1	C	47	GLU	2.1
1	A	68	ASP	2.1
1	A	410	SER	2.1
1	F	410	SER	2.1
1	B	433	MET	2.1
1	D	433	MET	2.1
1	C	27	VAL	2.0
1	B	142	ARG	2.0
1	D	227	ALA	2.0
1	A	193	LEU	2.0
1	D	231	LYS	2.0
1	F	411	LYS	2.0
1	A	65	TYR	2.0
1	A	148	PRO	2.0
1	A	228	TYR	2.0
1	B	25	SER	2.0
1	D	463	PRO	2.0
1	C	143	GLN	2.0
1	F	458	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	474	ARG	2.0
1	E	38	GLU	2.0
1	A	461	ASN	2.0
1	D	305	GLY	2.0
1	A	330	ILE	2.0
1	C	138	TRP	2.0
1	E	112	ASP	2.0
1	E	414	ASP	2.0
1	F	150	ASP	2.0
1	E	410	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

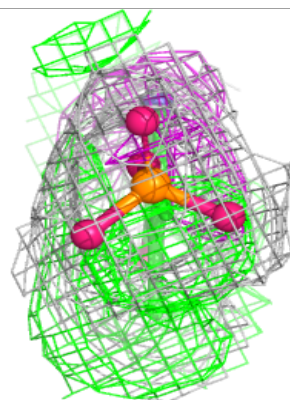
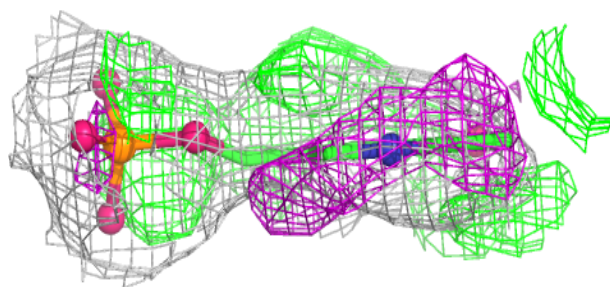
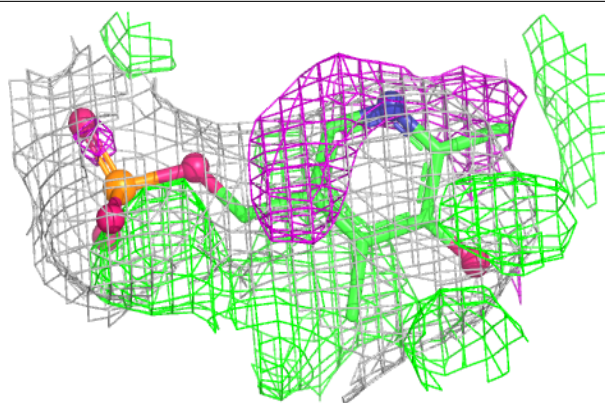
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	PLP	C	501	15/16	0.84	0.17	41,46,48,53	0
2	PLP	B	501	15/16	0.85	0.17	41,46,48,53	0
2	PLP	D	501	15/16	0.88	0.13	41,46,48,53	0
2	PLP	F	501	15/16	0.88	0.15	41,46,48,53	0
2	PLP	E	501	15/16	0.89	0.13	41,46,48,53	0
2	PLP	A	501	15/16	0.89	0.13	41,46,48,53	0

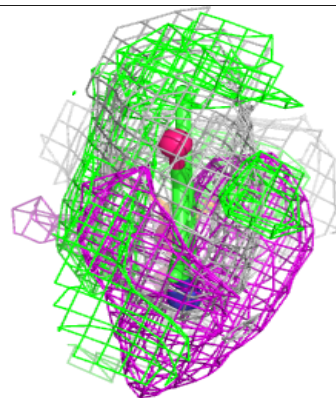
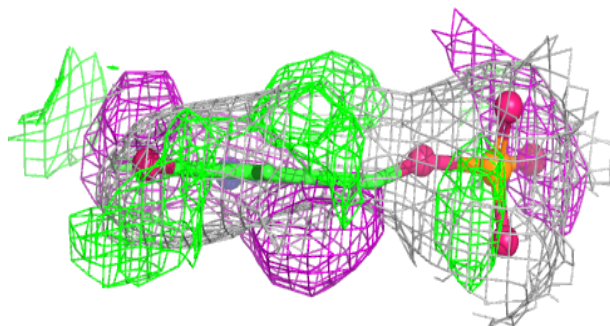
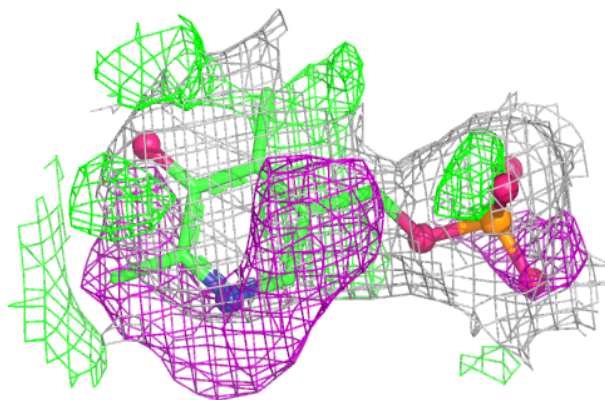
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PLP C 501:

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

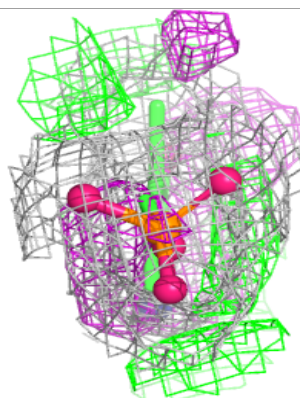
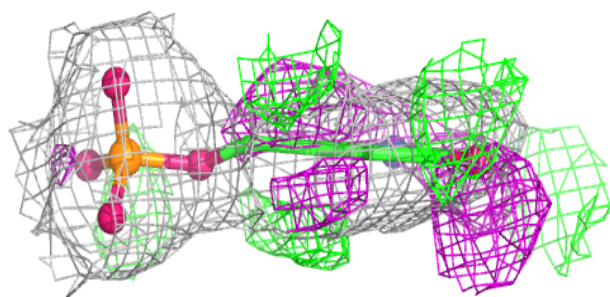
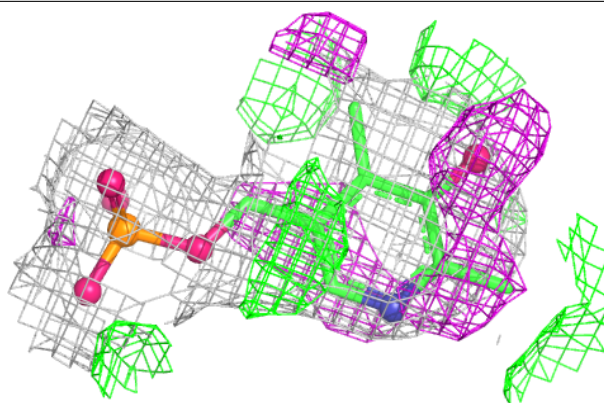
**Electron density around PLP B 501:**

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

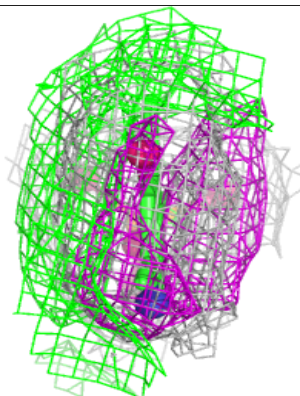
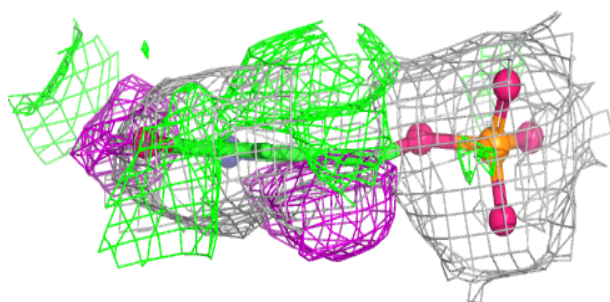
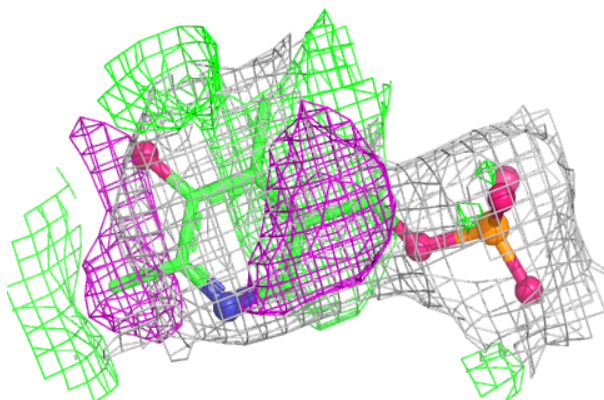


Electron density around PLP D 501:

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

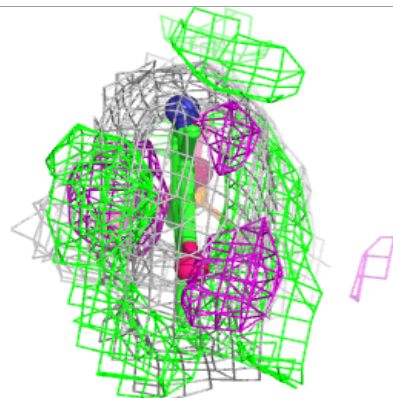
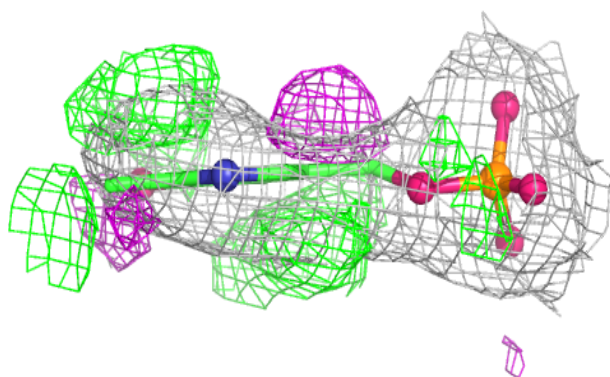
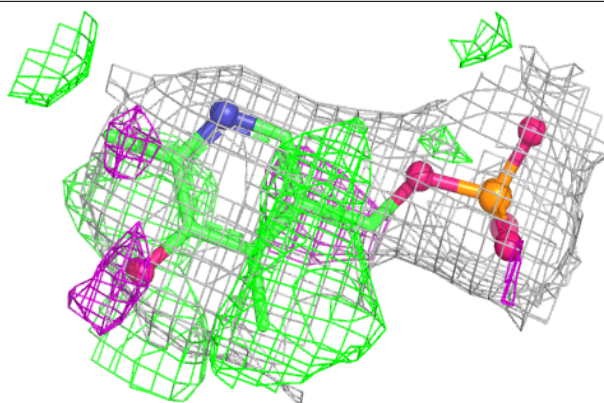
**Electron density around PLP F 501:**

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

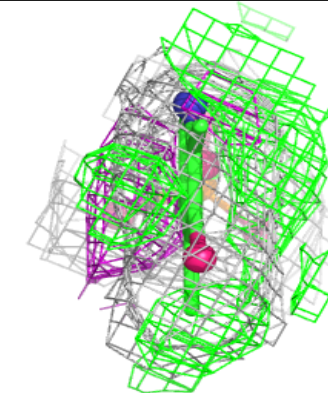
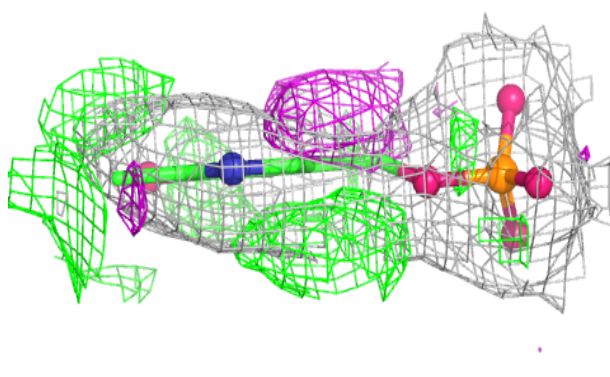
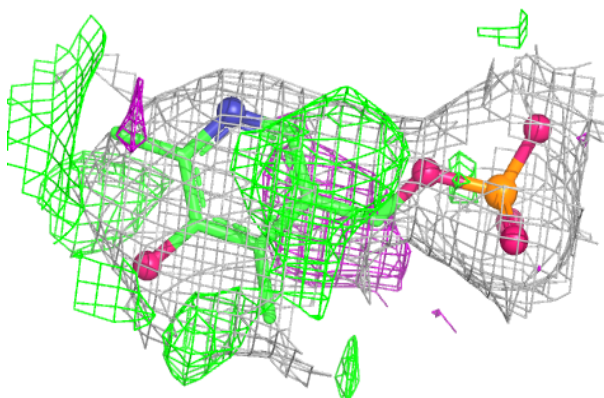


Electron density around PLP E 501:

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

**Electron density around PLP A 501:**

$2mF_o-DF_c$ (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.