



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 26, 2024 – 07:16 AM EDT

PDB ID : 7KH2
Title : Structure of N-citrylornithine decarboxylase bound with PLP
Authors : Deng, X.; Tomchick, D.; Phillips, M.; Michael, A.
Deposited on : 2020-10-19
Resolution : 2.05 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.37.1
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) : 2.37.1

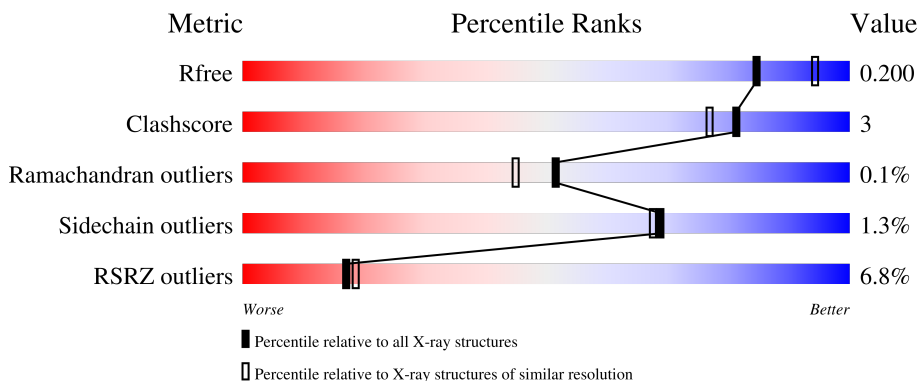
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	436	 10% 85% 9% 6%
1	B	436	 2% 86% 7% 6%
1	C	436	 11% 87% 7% 6%
1	D	436	 2% 91% 5% 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 27519 atoms, of which 13535 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 N-citrylornithine decarboxylase.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	409	Total	C	H	N	O	S	Se	0	0	0
			6625	2104	3346	556	611	5	3			
1	B	409	Total	C	H	N	O	S	Se	0	2	0
			6651	2111	3362	557	613	5	3			
1	C	409	Total	C	H	N	O	S	Se	0	2	0
			6644	2108	3360	556	611	5	4			
1	D	415	Total	C	H	N	O	S	Se	0	3	0
			6748	2140	3411	564	624	5	4			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MSE	-	initiating methionine	UNP Q15EG8
A	-17	GLY	-	expression tag	UNP Q15EG8
A	-16	HIS	-	expression tag	UNP Q15EG8
A	-15	HIS	-	expression tag	UNP Q15EG8
A	-14	HIS	-	expression tag	UNP Q15EG8
A	-13	HIS	-	expression tag	UNP Q15EG8
A	-12	HIS	-	expression tag	UNP Q15EG8
A	-11	HIS	-	expression tag	UNP Q15EG8
A	-10	ALA	-	expression tag	UNP Q15EG8
A	-9	GLU	-	expression tag	UNP Q15EG8
A	-8	ASN	-	expression tag	UNP Q15EG8
A	-7	LEU	-	expression tag	UNP Q15EG8
A	-6	TYR	-	expression tag	UNP Q15EG8
A	-5	PHE	-	expression tag	UNP Q15EG8
A	-4	GLN	-	expression tag	UNP Q15EG8
A	-3	GLY	-	expression tag	UNP Q15EG8
A	-2	ALA	-	expression tag	UNP Q15EG8
A	-1	ASP	-	expression tag	UNP Q15EG8
A	0	PRO	-	expression tag	UNP Q15EG8
B	-18	MSE	-	initiating methionine	UNP Q15EG8
B	-17	GLY	-	expression tag	UNP Q15EG8

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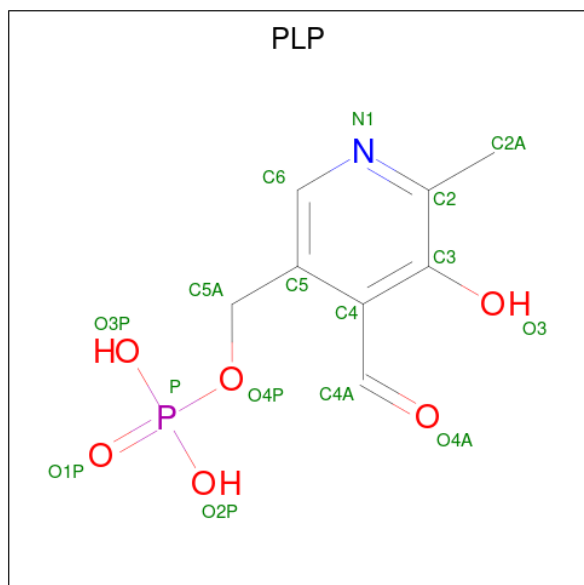
Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	HIS	-	expression tag	UNP Q15EG8
B	-15	HIS	-	expression tag	UNP Q15EG8
B	-14	HIS	-	expression tag	UNP Q15EG8
B	-13	HIS	-	expression tag	UNP Q15EG8
B	-12	HIS	-	expression tag	UNP Q15EG8
B	-11	HIS	-	expression tag	UNP Q15EG8
B	-10	ALA	-	expression tag	UNP Q15EG8
B	-9	GLU	-	expression tag	UNP Q15EG8
B	-8	ASN	-	expression tag	UNP Q15EG8
B	-7	LEU	-	expression tag	UNP Q15EG8
B	-6	TYR	-	expression tag	UNP Q15EG8
B	-5	PHE	-	expression tag	UNP Q15EG8
B	-4	GLN	-	expression tag	UNP Q15EG8
B	-3	GLY	-	expression tag	UNP Q15EG8
B	-2	ALA	-	expression tag	UNP Q15EG8
B	-1	ASP	-	expression tag	UNP Q15EG8
B	0	PRO	-	expression tag	UNP Q15EG8
C	-18	MSE	-	initiating methionine	UNP Q15EG8
C	-17	GLY	-	expression tag	UNP Q15EG8
C	-16	HIS	-	expression tag	UNP Q15EG8
C	-15	HIS	-	expression tag	UNP Q15EG8
C	-14	HIS	-	expression tag	UNP Q15EG8
C	-13	HIS	-	expression tag	UNP Q15EG8
C	-12	HIS	-	expression tag	UNP Q15EG8
C	-11	HIS	-	expression tag	UNP Q15EG8
C	-10	ALA	-	expression tag	UNP Q15EG8
C	-9	GLU	-	expression tag	UNP Q15EG8
C	-8	ASN	-	expression tag	UNP Q15EG8
C	-7	LEU	-	expression tag	UNP Q15EG8
C	-6	TYR	-	expression tag	UNP Q15EG8
C	-5	PHE	-	expression tag	UNP Q15EG8
C	-4	GLN	-	expression tag	UNP Q15EG8
C	-3	GLY	-	expression tag	UNP Q15EG8
C	-2	ALA	-	expression tag	UNP Q15EG8
C	-1	ASP	-	expression tag	UNP Q15EG8
C	0	PRO	-	expression tag	UNP Q15EG8
D	-18	MSE	-	initiating methionine	UNP Q15EG8
D	-17	GLY	-	expression tag	UNP Q15EG8
D	-16	HIS	-	expression tag	UNP Q15EG8
D	-15	HIS	-	expression tag	UNP Q15EG8
D	-14	HIS	-	expression tag	UNP Q15EG8
D	-13	HIS	-	expression tag	UNP Q15EG8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-12	HIS	-	expression tag	UNP Q15EG8
D	-11	HIS	-	expression tag	UNP Q15EG8
D	-10	ALA	-	expression tag	UNP Q15EG8
D	-9	GLU	-	expression tag	UNP Q15EG8
D	-8	ASN	-	expression tag	UNP Q15EG8
D	-7	LEU	-	expression tag	UNP Q15EG8
D	-6	TYR	-	expression tag	UNP Q15EG8
D	-5	PHE	-	expression tag	UNP Q15EG8
D	-4	GLN	-	expression tag	UNP Q15EG8
D	-3	GLY	-	expression tag	UNP Q15EG8
D	-2	ALA	-	expression tag	UNP Q15EG8
D	-1	ASP	-	expression tag	UNP Q15EG8
D	0	PRO	-	expression tag	UNP Q15EG8

- 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	0	0
			25	8	10	1	5	1		
2	B	1	Total	C	H	N	O	P	0	0
			25	8	10	1	5	1		
2	C	1	Total	C	H	N	O	P	0	0
			25	8	10	1	5	1		
2	D	1	Total	C	H	N	O	P	0	0
			25	8	10	1	5	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	H	O	0	0
			14	3	8	3		
4	B	1	Total	C	H	O	0	0
			14	3	8	3		

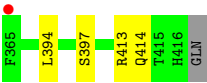
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	103	Total	O	0	0
			103	103		
5	B	195	Total	O	0	0
			195	195		
5	C	141	Total	O	0	0
			141	141		
5	D	244	Total	O	0	0
			244	244		

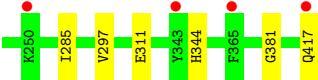
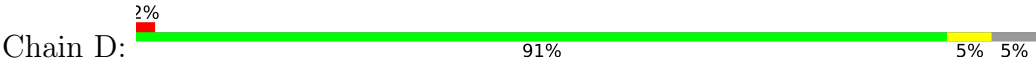
i

- Molecule 1: N-citrylornithine decarboxylase





● Molecule 1: N-citrylornithine decarboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	70.84Å 279.06Å 108.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.65 – 2.05 40.65 – 2.05	Depositor EDS
% Data completeness (in resolution range)	90.9 (40.65-2.05) 98.9 (40.65-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 2.05Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.174 , 0.199 0.174 , 0.200	Depositor DCC
R_{free} test set	2065 reflections (1.54%)	wwPDB-VP
Wilson B-factor (Å ²)	23.6	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 50.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	27519	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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: GOL, SO4, 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	0.30	0/3336	0.50	0/4509
1	B	0.31	1/3352 (0.0%)	0.48	0/4530
1	C	0.30	0/3347	0.48	0/4521
1	D	0.27	0/3403	0.47	0/4597
All	All	0.30	1/13438 (0.0%)	0.48	0/18157

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	256	ASN	CB-CG	-5.85	1.37	1.51

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	3279	3346	3347	19	0
1	B	3289	3362	3363	22	0
1	C	3284	3360	3362	17	0
1	D	3337	3411	3413	12	0
2	A	15	10	7	0	0
2	B	15	10	7	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	15	10	7	0	0
2	D	15	10	7	0	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0
3	C	10	0	0	0	0
3	D	10	0	0	0	0
4	B	12	16	16	0	0
5	A	103	0	0	0	0
5	B	195	0	0	6	0
5	C	141	0	0	0	0
5	D	244	0	0	1	0
All	All	13984	13535	13529	69	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 (69) 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:B:94:LYS:HE2	1:D:417:GLN:HA	1.51	0.93
1:B:356:GLN:NE2	5:B:1101:HOH:O	2.12	0.82
1:D:123:MSE:HE2	1:D:233:TRP:CD2	2.23	0.74
1:B:57:ILE:HG21	1:B:80:ILE:HD12	1.74	0.69
1:D:123:MSE:HE2	1:D:233:TRP:CE3	2.27	0.69
1:B:97:LEU:O	5:B:1102:HOH:O	2.14	0.64
1:D:185:GLN:NE2	5:D:1102:HOH:O	2.33	0.61
1:B:228:LYS:N	1:B:228:LYS:HD2	2.18	0.58
1:C:138:ILE:HG22	1:C:142:LEU:HD12	1.87	0.56
1:C:394:LEU:HB3	1:C:414:GLN:HB3	1.90	0.53
1:C:115:ILE:HG23	1:C:142:LEU:HD11	1.90	0.53
1:C:202:ASN:HA	1:C:241:ALA:HA	1.91	0.53
1:D:123:MSE:HE2	1:D:233:TRP:CG	2.44	0.53
1:D:123:MSE:HE1	1:D:285:ILE:HD11	1.94	0.50
1:B:303:ILE:HD13	1:B:318:THR:HG22	1.93	0.50
1:D:202:ASN:HA	1:D:241:ALA:HA	1.94	0.50
1:D:132:ILE:HG23	1:D:190:ILE:HD13	1.93	0.49
1:A:355:MSE:HE3	1:A:357:HIS:CE1	2.48	0.49
1:A:69:THR:O	1:A:73:LYS:HG2	2.12	0.49
1:C:225:THR:OG1	1:C:226:LYS:HD3	2.13	0.49
1:B:18:GLN:HG2	5:B:1235:HOH:O	2.13	0.49
1:A:156:LYS:HE2	1:A:169:THR:C	2.33	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:LYS:HD2	1:A:339:LYS:O	2.12	0.48
1:A:202:ASN:HA	1:A:241:ALA:HA	1.96	0.48
1:C:180:THR:O	1:C:184:ILE:HG13	2.14	0.47
1:C:142:LEU:O	1:C:144:ILE:N	2.47	0.47
1:B:141:LYS:HD2	5:B:1281:HOH:O	2.15	0.47
1:A:54:GLN:OE1	1:A:54:GLN:HA	2.15	0.46
1:A:100:LYS:HA	1:A:100:LYS:HD2	1.80	0.46
1:A:274:TYR:O	1:A:278:THR:HG23	2.15	0.46
1:B:297:VAL:HB	1:B:381:GLY:CA	2.47	0.45
1:B:202:ASN:HA	1:B:241:ALA:HA	1.97	0.45
1:B:43:ARG:NH1	5:B:1111:HOH:O	2.49	0.45
1:C:114:LEU:HD22	1:C:135:ILE:HG12	1.98	0.45
1:C:94:LYS:HB3	1:C:94:LYS:HE2	1.82	0.44
1:C:144:ILE:HG13	1:C:145:THR:N	2.32	0.44
1:C:356:GLN:NE2	1:C:356:GLN:HA	2.32	0.44
1:C:26:TYR:O	1:C:27:ALA:HB3	2.18	0.44
1:A:323:HIS:NE2	1:A:355:MSE:HE1	2.33	0.44
1:A:128:HIS:HD2	1:A:130:ASP:OD2	2.01	0.44
1:B:89:PHE:O	1:B:93:GLN:HG2	2.18	0.43
1:B:228:LYS:N	1:B:228:LYS:CD	2.81	0.43
1:B:274:TYR:O	1:B:278:THR:HG23	2.19	0.43
1:C:110:ASN:O	1:C:114:LEU:HD12	2.18	0.43
1:C:356:GLN:HA	1:C:356:GLN:HE21	1.83	0.43
1:B:116:LYS:HE2	5:B:1218:HOH:O	2.17	0.43
1:A:89:PHE:O	1:A:93:GLN:HG2	2.19	0.43
1:A:156:LYS:HE2	1:A:169:THR:O	2.18	0.43
1:B:26:TYR:O	1:B:27:ALA:HB3	2.18	0.43
1:D:26:TYR:O	1:D:27:ALA:HB3	2.19	0.42
1:B:94:LYS:HD2	1:B:94:LYS:HA	1.90	0.42
1:A:339:LYS:HE3	1:A:369:LEU:HD23	2.02	0.42
1:A:325:ILE:O	1:A:328:ILE:HG22	2.19	0.42
1:D:179:THR:O	1:D:183:LYS:HG3	2.19	0.42
1:A:57:ILE:HG21	1:A:80:ILE:HD12	2.02	0.42
1:D:123:MSE:CE	1:D:233:TRP:HB3	2.50	0.41
1:A:229:LEU:HD23	1:A:230:THR:N	2.36	0.41
1:A:224:LEU:O	1:A:228:LYS:HA	2.21	0.41
1:A:297:VAL:HB	1:A:381:GLY:CA	2.51	0.41
1:C:168:LEU:HD21	1:C:215:ASN:HB3	2.03	0.41
1:A:346:LYS:HE3	1:A:363:ASP:OD1	2.22	0.40
1:B:311:GLU:H	1:B:311:GLU:CD	2.24	0.40
1:B:287:GLU:O	2:B:1001:PLP:H6	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:397:SER:OG	1:C:413:ARG:HB2	2.21	0.40
1:B:93:GLN:OE1	1:B:120:LEU:HD11	2.21	0.40
1:C:183:LYS:O	1:C:187:ILE:HG13	2.21	0.40
1:B:102:ILE:HG12	1:B:103:ILE:N	2.36	0.40
1:B:278:THR:O	1:B:281:LYS:HG2	2.22	0.40
1:D:297:VAL:HB	1:D:381:GLY:CA	2.52	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	405/436 (93%)	390 (96%)	15 (4%)	0	100	100
1	B	407/436 (93%)	397 (98%)	10 (2%)	0	100	100
1	C	407/436 (93%)	389 (96%)	17 (4%)	1 (0%)	47	39
1	D	414/436 (95%)	401 (97%)	13 (3%)	0	100	100
All	All	1633/1744 (94%)	1577 (97%)	55 (3%)	1 (0%)	51	45

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	143	ASN

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	365/383 (95%)	359 (98%)	6 (2%)	62	59
1	B	367/383 (96%)	362 (99%)	5 (1%)	67	65
1	C	367/383 (96%)	364 (99%)	3 (1%)	81	82
1	D	374/383 (98%)	369 (99%)	5 (1%)	69	67
All	All	1473/1532 (96%)	1454 (99%)	19 (1%)	69	67

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LYS
1	A	24	GLN
1	A	104	PHE
1	A	137	LYS
1	A	250	LYS
1	A	374	LYS
1	B	100	LYS
1	B	104	PHE
1	B	130	ASP
1	B	228	LYS
1	B	279	ASN
1	C	104	PHE
1	C	129	PHE
1	C	250	LYS
1	D	17	LYS
1	D	24	GLN
1	D	104	PHE
1	D	311	GLU
1	D	344	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	215	ASN
1	A	405	GLN
1	B	143	ASN
1	B	256	ASN
1	C	279	ASN
1	C	356	GLN
1	D	143	ASN

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Mol	Chain	Res	Type
1	D	276	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 ⓘ

14 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	D	1001	1	15,15,16	4.55	8 (53%)	20,22,23	1.58	5 (25%)
3	SO4	B	1002	-	4,4,4	0.15	0	6,6,6	0.07	0
3	SO4	C	1002	-	4,4,4	0.16	0	6,6,6	0.08	0
3	SO4	C	1003	-	4,4,4	0.14	0	6,6,6	0.05	0
4	GOL	B	1004	-	5,5,5	0.81	0	5,5,5	1.21	1 (20%)
2	PLP	A	1001	1	15,15,16	4.70	8 (53%)	20,22,23	1.51	4 (20%)
2	PLP	C	1001	1	15,15,16	4.69	8 (53%)	20,22,23	1.48	5 (25%)
3	SO4	D	1002	-	4,4,4	0.13	0	6,6,6	0.05	0
3	SO4	D	1003	-	4,4,4	0.14	0	6,6,6	0.05	0
4	GOL	B	1005	-	5,5,5	0.84	0	5,5,5	1.17	1 (20%)
3	SO4	B	1003	-	4,4,4	0.15	0	6,6,6	0.05	0
3	SO4	A	1002	-	4,4,4	0.11	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PLP	B	1001	1	15,15,16	4.71	8 (53%)	20,22,23	1.59	5 (25%)
3	SO4	A	1003	-	4,4,4	0.13	0	6,6,6	0.05	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
2	PLP	D	1001	1	-	0/6/6/8	0/1/1/1
4	GOL	B	1004	-	-	2/4/4/4	-
2	PLP	A	1001	1	-	0/6/6/8	0/1/1/1
2	PLP	C	1001	1	-	0/6/6/8	0/1/1/1
4	GOL	B	1005	-	-	2/4/4/4	-
2	PLP	B	1001	1	-	0/6/6/8	0/1/1/1

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1001	PLP	C5-C4	-10.07	1.29	1.40
2	C	1001	PLP	C5-C4	-10.05	1.29	1.40
2	A	1001	PLP	C5-C4	-9.86	1.29	1.40
2	D	1001	PLP	C5-C4	-9.40	1.30	1.40
2	A	1001	PLP	C3-C2	-8.40	1.32	1.40
2	C	1001	PLP	C3-C2	-8.35	1.32	1.40
2	B	1001	PLP	C3-C2	-8.35	1.32	1.40
2	D	1001	PLP	C3-C2	-8.02	1.32	1.40
2	A	1001	PLP	C2-N1	7.91	1.48	1.33
2	B	1001	PLP	C2-N1	7.86	1.48	1.33
2	C	1001	PLP	C2-N1	7.83	1.48	1.33
2	D	1001	PLP	C2-N1	7.82	1.48	1.33
2	B	1001	PLP	C6-C5	7.10	1.52	1.37
2	A	1001	PLP	C6-C5	7.08	1.52	1.37
2	D	1001	PLP	C6-C5	6.95	1.52	1.37
2	C	1001	PLP	C6-C5	6.92	1.52	1.37
2	C	1001	PLP	C3-C4	4.61	1.49	1.40
2	A	1001	PLP	C3-C4	4.61	1.49	1.40
2	D	1001	PLP	C3-C4	4.55	1.49	1.40
2	B	1001	PLP	C3-C4	4.33	1.49	1.40
2	B	1001	PLP	C6-N1	-2.83	1.28	1.34
2	C	1001	PLP	C6-N1	-2.76	1.28	1.34
2	A	1001	PLP	C6-N1	-2.72	1.28	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1001	PLP	C6-N1	-2.58	1.29	1.34
2	B	1001	PLP	P-O2P	-2.57	1.45	1.54
2	B	1001	PLP	P-O3P	-2.37	1.45	1.54
2	A	1001	PLP	P-O2P	-2.35	1.45	1.54
2	D	1001	PLP	P-O3P	-2.29	1.46	1.54
2	C	1001	PLP	P-O2P	-2.26	1.46	1.54
2	C	1001	PLP	P-O3P	-2.22	1.46	1.54
2	A	1001	PLP	P-O3P	-2.18	1.46	1.54
2	D	1001	PLP	P-O2P	-2.02	1.47	1.54

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	PLP	O2P-P-O4P	3.38	115.72	106.73
2	B	1001	PLP	O2P-P-O4P	2.98	114.67	106.73
2	D	1001	PLP	O3P-P-O4P	2.91	114.49	106.73
2	D	1001	PLP	O4P-P-O1P	2.90	114.61	106.47
2	D	1001	PLP	C6-C5-C4	2.88	120.43	118.16
2	C	1001	PLP	O4P-P-O1P	2.86	114.51	106.47
2	A	1001	PLP	O4P-P-O1P	2.82	114.37	106.47
2	B	1001	PLP	C6-C5-C4	2.68	120.27	118.16
2	C	1001	PLP	O3P-P-O4P	2.67	113.83	106.73
2	B	1001	PLP	O3P-P-O4P	2.66	113.81	106.73
2	D	1001	PLP	O2P-P-O4P	2.60	113.66	106.73
2	C	1001	PLP	O2P-P-O4P	2.58	113.59	106.73
2	C	1001	PLP	C6-C5-C4	2.57	120.18	118.16
2	B	1001	PLP	O4P-P-O1P	2.52	113.53	106.47
2	B	1001	PLP	C5-C6-N1	-2.38	119.86	123.82
4	B	1004	GOL	C3-C2-C1	-2.26	102.94	111.70
2	C	1001	PLP	C5-C6-N1	-2.24	120.09	123.82
2	D	1001	PLP	C5-C6-N1	-2.23	120.11	123.82
2	A	1001	PLP	O3P-P-O4P	2.21	112.61	106.73
4	B	1005	GOL	C3-C2-C1	-2.17	103.27	111.70
2	A	1001	PLP	C5-C6-N1	-2.16	120.22	123.82

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1004	GOL	O1-C1-C2-C3
4	B	1004	GOL	O1-C1-C2-O2
4	B	1005	GOL	O1-C1-C2-O2

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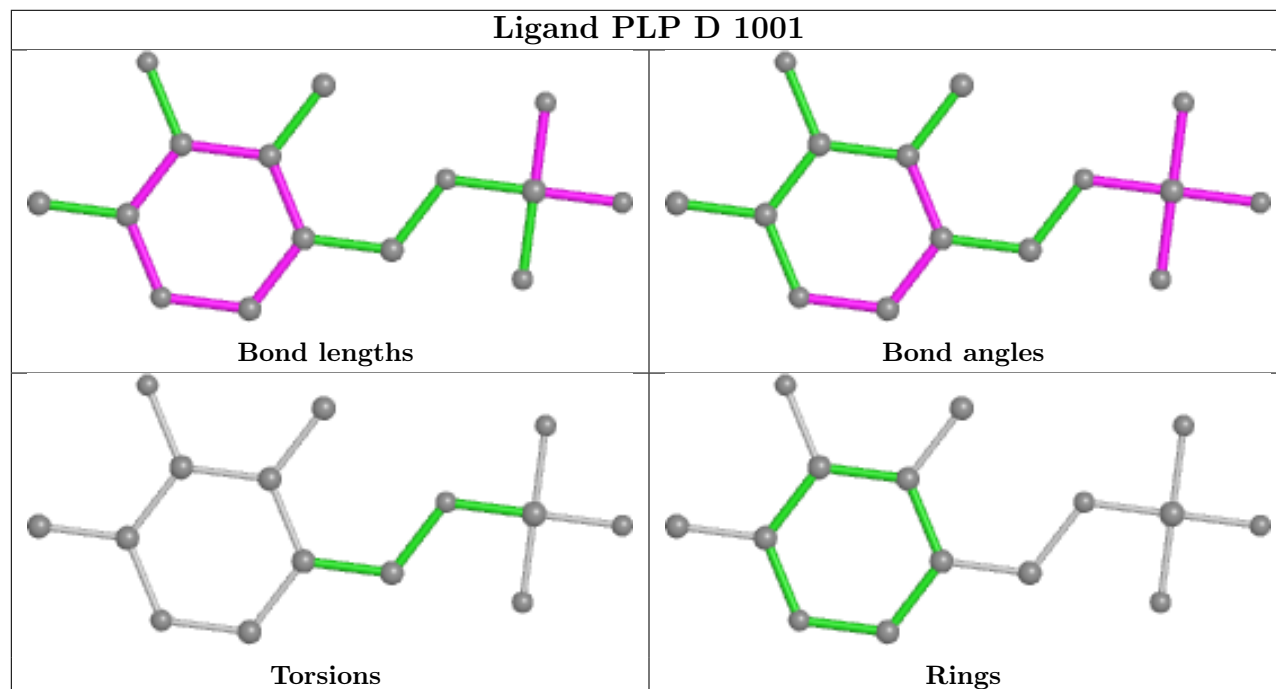
Mol	Chain	Res	Type	Atoms
4	B	1005	GOL	O1-C1-C2-C3

There are no ring outliers.

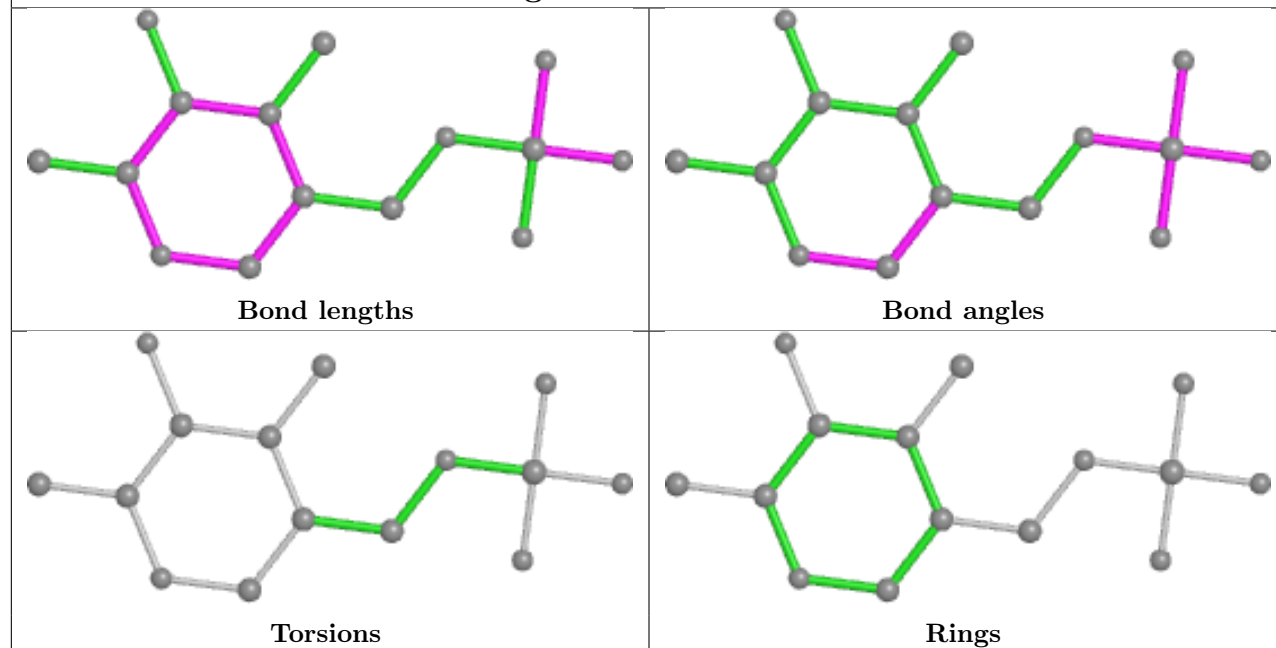
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1001	PLP	1	0

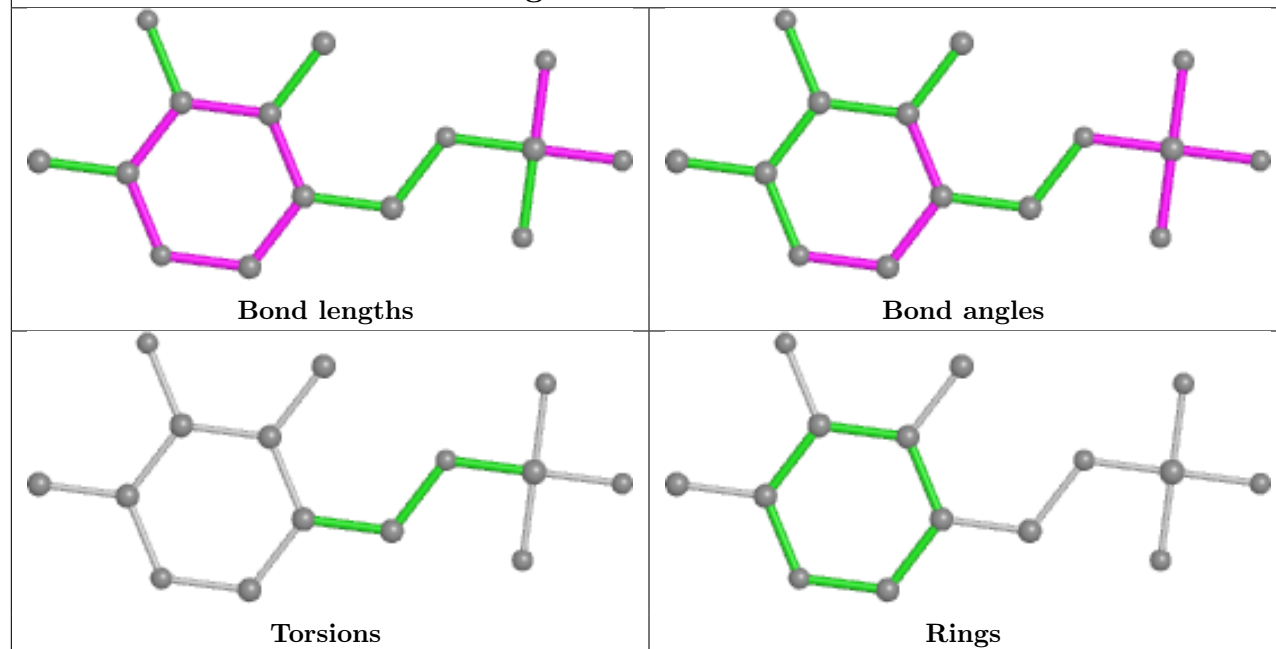
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

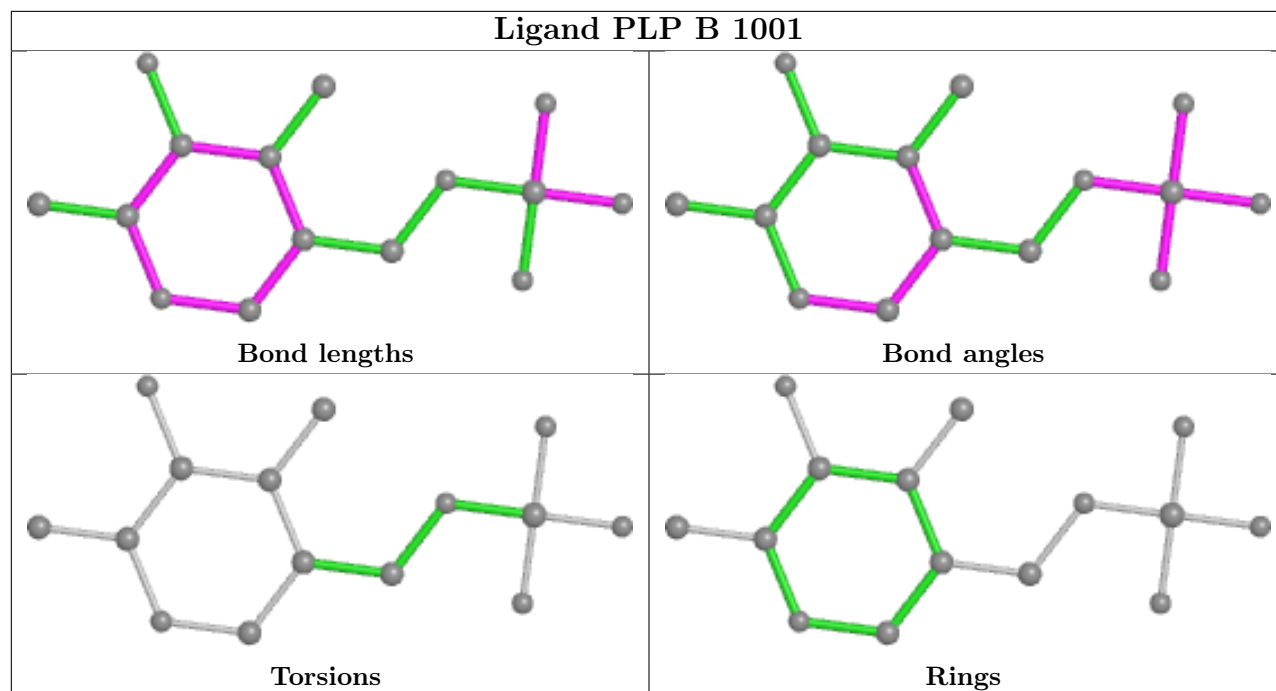


Ligand PLP A 1001



Ligand PLP C 1001





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	406/436 (93%)	0.55	44 (10%) 5 6	23, 41, 72, 110	0
1	B	406/436 (93%)	0.09	9 (2%) 62 66	12, 26, 56, 76	0
1	C	405/436 (92%)	0.56	48 (11%) 4 4	13, 35, 75, 112	0
1	D	411/436 (94%)	0.03	10 (2%) 59 63	11, 23, 49, 81	0
All	All	1628/1744 (93%)	0.30	111 (6%) 17 18	11, 31, 67, 112	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	142	LEU	9.5
1	C	98	CYS	5.8
1	C	188	ALA	5.6
1	C	144	ILE	4.9
1	C	343	TYR	4.7
1	A	343	TYR	4.5
1	C	190	ILE	4.4
1	C	181	ILE	4.4
1	A	54	GLN	4.2
1	C	129	PHE	4.1
1	A	313	PHE	4.1
1	A	408	GLN	4.0
1	A	178	PHE	4.0
1	B	356	GLN	3.9
1	D	343	TYR	3.8
1	A	121	ASN	3.7
1	C	187	ILE	3.6
1	D	417	GLN	3.6
1	A	365	PHE	3.5
1	A	363	ASP	3.5
1	A	342	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	184	ILE	3.5
1	A	406	GLN	3.5
1	C	189	ASN	3.5
1	C	139	ALA	3.4
1	A	404	ASN	3.4
1	C	140	LYS	3.4
1	C	186	GLN	3.3
1	C	141	LYS	3.3
1	A	346	LYS	3.3
1	C	146	ALA	3.3
1	C	356	GLN	3.3
1	A	312	ASP	3.2
1	A	176	ASP	3.2
1	B	178	PHE	3.2
1	A	120	LEU	3.2
1	C	342	SER	3.2
1	A	356	GLN	3.1
1	C	229	LEU	3.1
1	C	143	ASN	3.1
1	D	143	ASN	3.1
1	C	276	ASN	3.0
1	C	183	LYS	3.0
1	A	24	GLN	3.0
1	A	179	THR	3.0
1	C	137	LYS	2.9
1	C	226	LYS	2.9
1	A	405	GLN	2.9
1	A	311	GLU	2.9
1	C	161	TRP	2.9
1	C	250	LYS	2.9
1	C	178	PHE	2.8
1	A	98	CYS	2.8
1	A	403	LYS	2.8
1	C	222	THR	2.8
1	C	158	PRO	2.8
1	C	311	GLU	2.8
1	A	13	LYS	2.8
1	D	142	LEU	2.7
1	A	17	LYS	2.7
1	C	119	GLN	2.7
1	D	140	LYS	2.7
1	C	168	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	353	SER	2.7
1	A	22	ILE	2.6
1	D	144	ILE	2.6
1	A	15	SER	2.6
1	A	279	ASN	2.6
1	C	97	LEU	2.6
1	C	227	TYR	2.5
1	A	281	LYS	2.5
1	C	312	ASP	2.5
1	B	179	THR	2.5
1	A	354	CYS	2.5
1	C	362	ASP	2.5
1	C	225	THR	2.4
1	C	96	GLN	2.4
1	A	183	LYS	2.4
1	C	279	ASN	2.4
1	B	101	SER	2.3
1	A	362	ASP	2.3
1	A	25	ARG	2.3
1	A	224	LEU	2.3
1	D	175	SER	2.3
1	C	365	PHE	2.3
1	C	228	LYS	2.2
1	D	365	PHE	2.2
1	A	51	ASN	2.2
1	D	250	LYS	2.2
1	A	97	LEU	2.2
1	A	5	SER	2.2
1	C	169	THR	2.2
1	C	138	ILE	2.2
1	A	402	ASP	2.2
1	A	18	GLN	2.1
1	A	229	LEU	2.1
1	C	357	HIS	2.1
1	A	43	ARG	2.1
1	B	353	SER	2.1
1	A	225	THR	2.1
1	B	250	LYS	2.1
1	A	400	LEU	2.1
1	B	228	LYS	2.1
1	C	281	LYS	2.1
1	D	188	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	156	LYS	2.1
1	B	227	TYR	2.0
1	A	8	LYS	2.0
1	A	401	ILE	2.0
1	C	252	LEU	2.0
1	B	100	LYS	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 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.

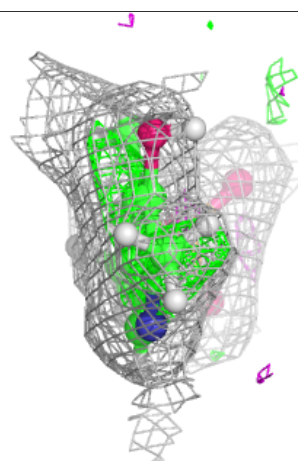
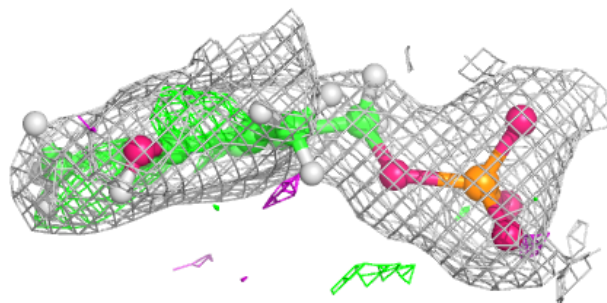
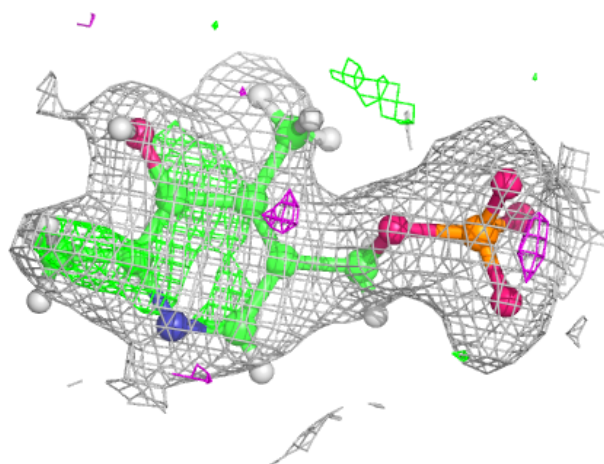
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	B	1005	6/6	0.67	0.24	90,108,113,115	0
4	GOL	B	1004	6/6	0.81	0.22	45,55,66,66	0
3	SO4	C	1003	5/5	0.83	0.23	96,96,102,102	0
3	SO4	B	1003	5/5	0.87	0.26	94,98,103,107	0
3	SO4	D	1003	5/5	0.90	0.15	69,70,72,76	0
2	PLP	A	1001	15/16	0.94	0.25	23,42,73,73	0
3	SO4	A	1003	5/5	0.96	0.24	70,73,75,79	0
2	PLP	C	1001	15/16	0.97	0.24	19,42,67,67	0
2	PLP	B	1001	15/16	0.98	0.16	12,20,28,28	0
2	PLP	D	1001	15/16	0.98	0.18	9,15,21,22	0
3	SO4	D	1002	5/5	0.99	0.18	36,38,45,48	0
3	SO4	A	1002	5/5	0.99	0.10	30,33,38,39	0
3	SO4	C	1002	5/5	0.99	0.17	42,45,48,52	0
3	SO4	B	1002	5/5	0.99	0.09	29,31,35,38	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.

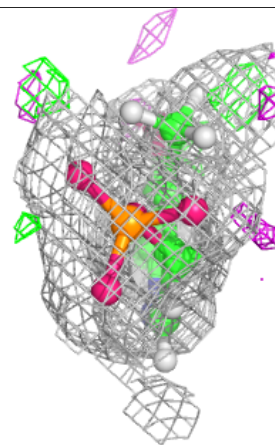
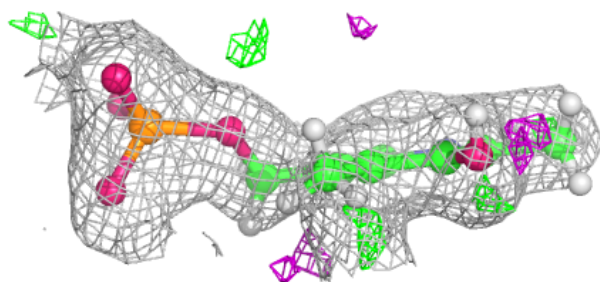
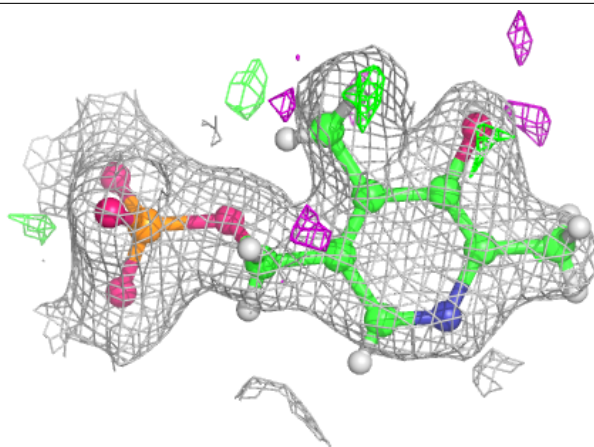
Electron density around PLP A 1001:

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

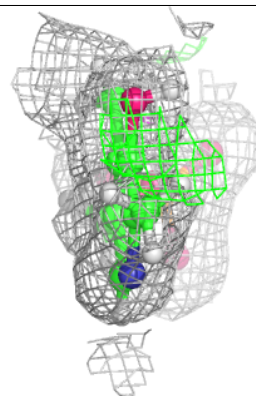
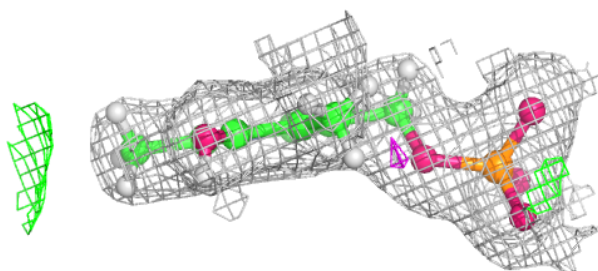
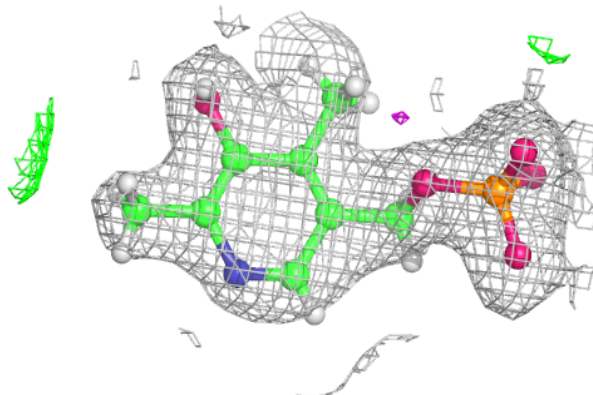


Electron density around PLP C 1001:

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

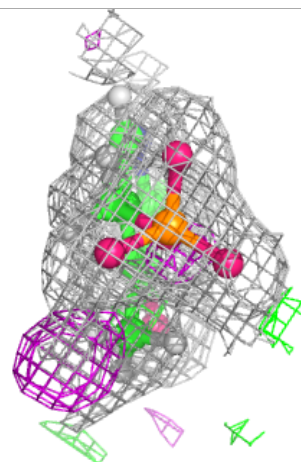
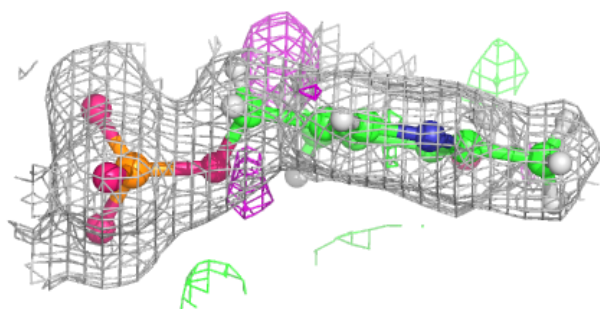
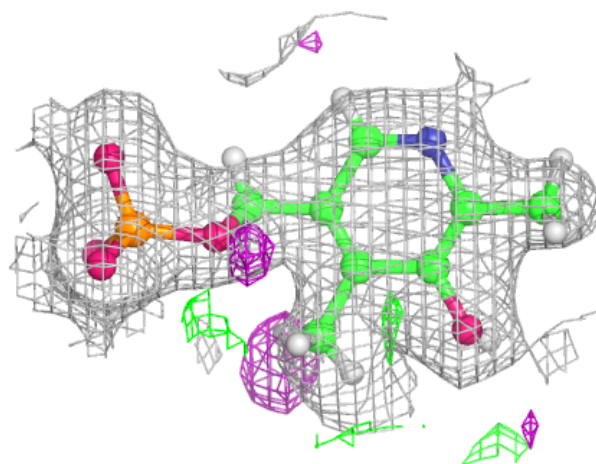
**Electron density around PLP B 1001:**

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



Electron density around PLP D 1001:

$2mF_o-DF_c$ (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.