Full wwPDB X-ray Structure Validation Report (i)

May 27, 2024 – 09:19 PM EDT

PDB ID	:	6MFB
Title	:	Crystal structure of 3-hydroxykynurenine transaminase from Aedes aegypti
Authors	:	Maciel, L.G.; Oliveira, A.A.; Romao, T.P.; Silva Filha, M.H.N.L.; dos Anjos, J.V.; Soares, T.A.; Guido, R.V.C.
Deposited on	:	2018-09-10
Resolution	:	2.50 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 (i) 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 (i)) were used in the production of this report:

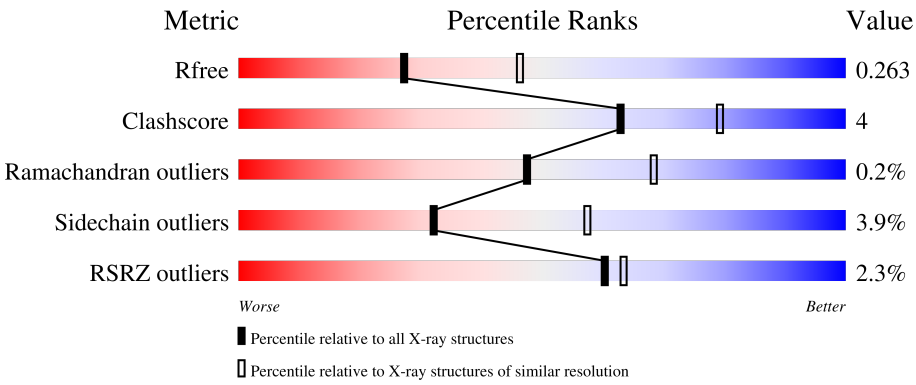
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

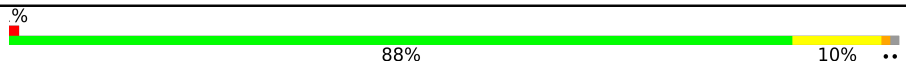
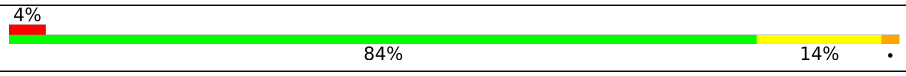
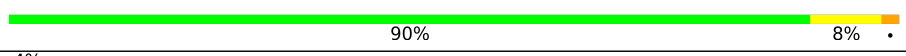
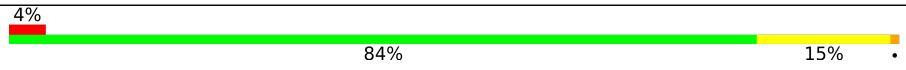
The reported resolution of this entry is 2.50 Å.

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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 <=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	386	
1	B	386	
1	C	386	
1	D	386	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 12510 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.

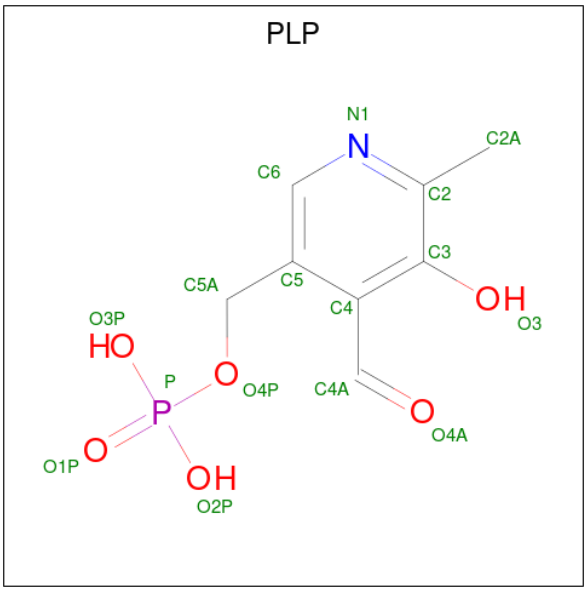
- Molecule 1 is a protein called Serine–pyruvate aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	384	3012	1928	511	549	24	0	0	0
1	C	385	3020	1933	512	550	25	0	0	0
1	B	385	3020	1933	512	550	25	0	0	0
1	D	386	3028	1937	513	553	25	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	123	GLU	GLY	conflict	UNP Q0IG34
C	123	GLU	GLY	conflict	UNP Q0IG34
B	123	GLU	GLY	conflict	UNP Q0IG34
D	123	GLU	GLY	conflict	UNP Q0IG34

- 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	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	B	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		

- Molecule 3 is water.

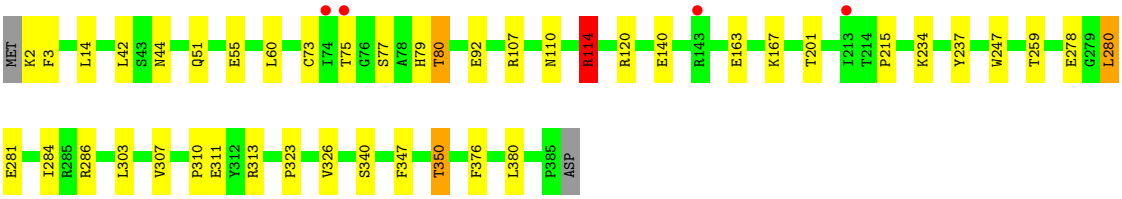
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	128	Total	O	0	0
			128	128		
3	C	82	Total	O	0	0
			82	82		
3	B	82	Total	O	0	0
			82	82		
3	D	78	Total	O	0	0
			78	78		

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.

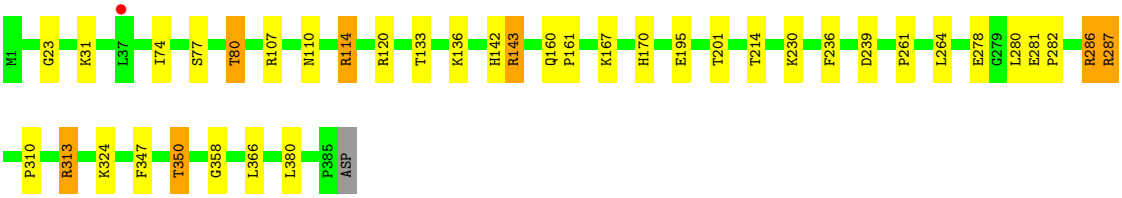
• Molecule 1: Serine–pyruvate aminotransferase

Chain A:



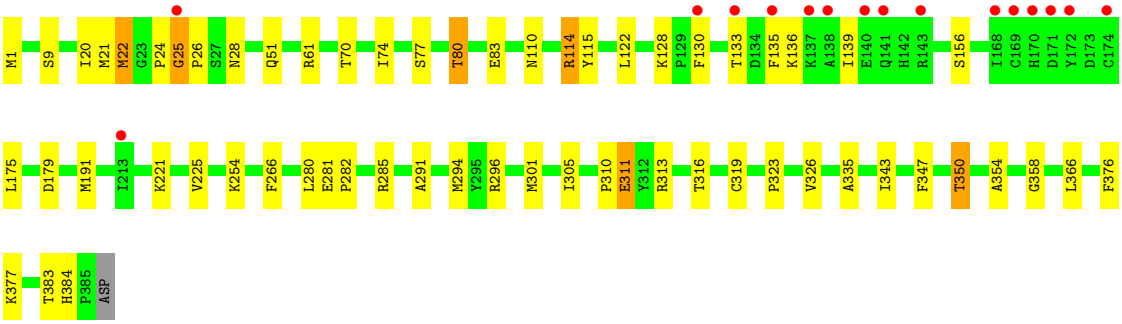
• Molecule 1: Serine–pyruvate aminotransferase

Chain C:



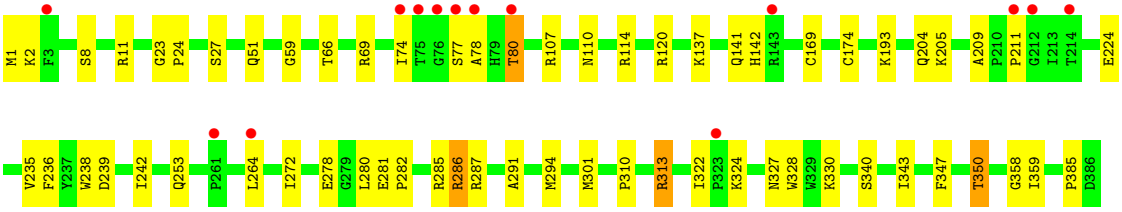
• Molecule 1: Serine–pyruvate aminotransferase

Chain B:



• Molecule 1: Serine–pyruvate aminotransferase

Chain D:


M1
K2
F3
S8
R11
G23
P24
S27
Q51
G59
T66
R69
I74
T75
G76
S77
A78
H79
T80
R107
N110
R114
R120
K137
Q141
H142
R143
C169
C174
K193
Q204
K205
A209
P210
P211
G212
I213
T214
E224
V235
F236
Y237
W238
D239
I242
Q253
P261
L264
I272
E278
G279
L280
E281
P282
R285
R286
R287
A291
M294
M301
P310
R313
I322
P323
K324
M327
W328
W329
K330
S340
I343
F347
T350
G358
I359
P385
D386

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	86.71Å 115.73Å 172.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.85 – 2.50 48.02 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.85-2.50) 99.8 (48.02-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.86 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.187 , 0.261 0.194 , 0.263	Depositor DCC
R_{free} test set	2946 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å^2)	49.7	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 35.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12510	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.56	0/3086	0.73	1/4185 (0.0%)
1	B	0.59	0/3094	0.72	0/4195
1	C	0.57	0/3094	0.71	0/4195
1	D	0.55	0/3102	0.68	0/4206
All	All	0.57	0/12376	0.71	1/16781 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	6
1	C	0	6
1	D	0	5
All	All	0	20

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	114	ARG	NE-CZ-NH2	-5.27	117.66	120.30

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	114	ARG	Sidechain
1	A	120	ARG	Sidechain
1	B	114	ARG	Sidechain
1	B	22	MET	Peptide
1	B	24	PRO	Peptide
1	B	25	GLY	Peptide
1	B	296	ARG	Sidechain
1	B	354	ALA	Peptide
1	C	107	ARG	Sidechain
1	C	114	ARG	Sidechain
1	C	143	ARG	Sidechain
1	C	286	ARG	Sidechain
1	C	287	ARG	Sidechain
1	C	313	ARG	Sidechain
1	D	107	ARG	Sidechain
1	D	24	PRO	Peptide
1	D	286	ARG	Sidechain
1	D	313	ARG	Sidechain
1	D	69	ARG	Sidechain

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	3012	0	3004	23	0
1	B	3020	0	3017	39	0
1	C	3020	0	3016	23	0
1	D	3028	0	3020	30	0
2	A	15	0	6	0	0
2	B	15	0	6	1	0
2	C	15	0	6	1	0
2	D	15	0	7	1	0
3	A	128	0	0	1	0
3	B	82	0	0	2	0
3	C	82	0	0	1	0
3	D	78	0	0	1	0
All	All	12510	0	12082	105	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 4.

All (105) 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:347:PHE:H	1:C:350:THR:HG22	1.49	0.77
1:A:77:SER:O	1:A:80:THR:HB	1.85	0.77
1:C:77:SER:O	1:C:80:THR:HB	1.83	0.76
1:A:307:VAL:O	1:A:313:ARG:HD3	1.93	0.69
1:C:120:ARG:HH11	1:C:142:HIS:HD2	1.37	0.69
1:B:21:MET:H	1:B:28:ASN:HD21	1.42	0.68
1:D:120:ARG:HH11	1:D:142:HIS:HD2	1.39	0.68
1:C:110:ASN:OD1	1:C:114:ARG:HD2	1.94	0.66
1:A:347:PHE:H	1:A:350:THR:HG22	1.60	0.66
1:B:254:LYS:NZ	3:B:501:HOH:O	2.20	0.66
1:B:74:ILE:HG21	1:B:80:THR:HG23	1.79	0.64
1:B:305:ILE:HD12	1:B:313:ARG:NH1	2.12	0.64
1:A:110:ASN:OD1	1:A:114:ARG:HD2	1.98	0.64
1:C:74:ILE:HG21	1:C:80:THR:HG23	1.80	0.64
1:A:310:PRO:HA	1:A:313:ARG:HG3	1.80	0.62
1:B:110:ASN:OD1	1:B:114:ARG:HD2	2.00	0.62
1:C:281:GLU:HB3	1:C:282:PRO:HD3	1.83	0.60
1:B:311:GLU:O	1:B:311:GLU:HG3	2.01	0.60
1:B:77:SER:O	1:B:80:THR:HB	2.02	0.59
1:A:347:PHE:O	1:A:350:THR:HG22	2.04	0.58
1:C:114:ARG:NH2	1:D:239:ASP:OD2	2.36	0.58
1:B:74:ILE:CG2	1:B:80:THR:HG23	2.33	0.57
1:D:74:ILE:HG21	1:D:80:THR:HG23	1.87	0.57
1:C:74:ILE:CG2	1:C:80:THR:HG23	2.33	0.57
1:D:110:ASN:OD1	1:D:114:ARG:HD2	2.05	0.56
1:C:278:GLU:OE1	1:C:286:ARG:NH2	2.39	0.56
1:D:285:ARG:HG2	1:D:285:ARG:HH11	1.71	0.55
1:D:281:GLU:HB3	1:D:282:PRO:HD3	1.88	0.55
1:B:326:VAL:HG22	1:B:384:HIS:CD2	2.43	0.54
1:D:77:SER:O	1:D:80:THR:HB	2.07	0.54
1:B:347:PHE:H	1:B:350:THR:HG22	1.72	0.53
1:A:347:PHE:H	1:A:350:THR:CG2	2.22	0.53
1:A:278:GLU:OE1	1:A:286:ARG:NH2	2.40	0.52
1:A:14:LEU:HD21	1:B:266:PHE:HB3	1.92	0.52
1:D:137:LYS:O	1:D:141:GLN:HG3	2.09	0.51
1:D:59:GLY:HA3	1:D:272:ILE:HG21	1.92	0.51
1:C:264:LEU:HD11	1:D:264:LEU:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:239:ASP:OD2	1:D:114:ARG:NH2	2.42	0.51
1:C:23:GLY:O	1:C:358:GLY:HA3	2.11	0.50
1:B:383:THR:O	1:B:384:HIS:ND1	2.44	0.50
1:A:163:GLU:HG3	3:A:607:HOH:O	2.11	0.50
1:D:291:ALA:O	1:D:294:MET:HB3	2.12	0.49
1:B:310:PRO:HA	1:B:313:ARG:HG3	1.95	0.49
1:B:323:PRO:HG2	1:B:326:VAL:HG21	1.94	0.49
1:B:383:THR:C	1:B:384:HIS:HD1	2.16	0.49
1:D:23:GLY:O	1:D:358:GLY:HA3	2.13	0.49
1:A:60:LEU:HD22	1:A:215:PRO:HB3	1.94	0.49
1:B:175:LEU:HD11	1:B:225:VAL:HG21	1.94	0.48
1:A:280:LEU:HD22	1:A:284:ILE:HD11	1.95	0.48
1:C:167:LYS:NZ	3:C:504:HOH:O	2.46	0.48
1:A:44:ASN:HD21	1:A:259:THR:HA	1.78	0.48
1:D:327:ASN:ND2	1:D:330:LYS:HE2	2.29	0.48
1:D:285:ARG:HH11	1:D:285:ARG:CG	2.27	0.47
1:B:305:ILE:HD12	1:B:313:ARG:HH12	1.80	0.47
1:A:281:GLU:OE2	1:B:1:MET:HB2	2.15	0.47
1:B:301:MET:CE	1:B:377:LYS:HG3	2.45	0.47
1:B:21:MET:H	1:B:28:ASN:ND2	2.11	0.46
1:B:291:ALA:O	1:B:294:MET:HB3	2.15	0.46
1:D:74:ILE:CG2	1:D:80:THR:HG23	2.45	0.46
1:C:170:HIS:CE1	1:C:195:GLU:HB3	2.50	0.46
1:D:78:ALA:HB3	2:D:401:PLP:O4P	2.15	0.46
1:B:310:PRO:HG3	1:B:313:ARG:NH2	2.31	0.46
1:A:110:ASN:OD1	1:A:114:ARG:CD	2.63	0.45
1:A:42:LEU:O	1:B:26:PRO:HG2	2.16	0.45
1:B:179:ASP:OD1	2:B:401:PLP:H2A2	2.16	0.45
1:A:55:GLU:HG2	1:B:9:SER:HB2	1.97	0.45
1:D:343:ILE:HA	3:D:522:HOH:O	2.16	0.45
1:C:347:PHE:N	1:C:350:THR:HG22	2.25	0.45
1:C:310:PRO:HA	1:C:313:ARG:HG3	1.98	0.45
1:D:310:PRO:HA	1:D:313:ARG:HE	1.82	0.45
1:B:74:ILE:CG2	1:B:80:THR:CG2	2.95	0.44
1:D:359:ILE:HG22	1:D:359:ILE:O	2.18	0.44
1:B:316:THR:O	1:B:358:GLY:HA2	2.18	0.44
1:D:235:VAL:HG11	1:D:238:TRP:CE2	2.53	0.44
1:D:278:GLU:OE1	1:D:286:ARG:NH2	2.51	0.44
1:C:261:PRO:HA	1:D:211:PRO:HG2	2.00	0.43
1:A:323:PRO:HG2	1:A:326:VAL:HG21	1.99	0.43
1:B:20:ILE:HG22	1:B:22:MET:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:347:PHE:O	1:D:350:THR:HG22	2.18	0.43
1:B:61:ARG:NH2	3:B:508:HOH:O	2.41	0.43
1:B:335:ALA:HB2	1:B:343:ILE:HD12	2.01	0.43
1:D:8:SER:HA	1:D:11:ARG:HG3	2.01	0.43
1:A:303:LEU:HD13	1:A:376:PHE:HE2	1.84	0.43
1:C:77:SER:HB2	2:C:401:PLP:O2P	2.19	0.43
1:B:281:GLU:OE1	1:B:285:ARG:NH2	2.52	0.42
1:D:322:ILE:HD13	1:D:328:TRP:HB3	1.99	0.42
1:B:281:GLU:CB	1:B:282:PRO:HD3	2.50	0.42
1:C:281:GLU:OE2	1:D:1:MET:HB2	2.20	0.42
1:D:204:GLN:HA	1:D:209:ALA:O	2.19	0.42
1:D:236:PHE:CE2	1:D:242:ILE:HD12	2.54	0.42
1:A:3:PHE:CE2	1:B:281:GLU:HG3	2.55	0.42
1:C:160:GLN:NE2	1:C:161:PRO:HD2	2.34	0.42
1:A:201:THR:HG22	1:A:215:PRO:HB2	2.01	0.42
1:C:236:PHE:CD1	1:C:236:PHE:C	2.93	0.42
1:A:75:THR:HB	1:A:237:TYR:OH	2.20	0.41
1:B:122:LEU:HG	1:B:130:PHE:CE1	2.55	0.41
1:B:135:PHE:O	1:B:139:ILE:HG13	2.20	0.41
1:C:143:ARG:HD2	1:C:143:ARG:HA	1.87	0.41
1:A:73:CYS:HB2	1:A:247:TRP:CZ2	2.56	0.41
1:B:383:THR:C	1:B:384:HIS:ND1	2.74	0.41
1:D:169:CYS:HB3	1:D:174:CYS:O	2.21	0.41
1:C:201:THR:O	1:C:214:THR:HG23	2.20	0.40
1:B:156:SER:O	1:B:319:CYS:SG	2.79	0.40
1:B:83:GLU:OE1	1:B:115:TYR:OH	2.33	0.40
1:B:305:ILE:CD1	1:B:313:ARG:NH1	2.81	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	382/386 (99%)	374 (98%)	8 (2%)	0	100	100
1	B	383/386 (99%)	365 (95%)	17 (4%)	1 (0%)	41	61
1	C	383/386 (99%)	368 (96%)	15 (4%)	0	100	100
1	D	384/386 (100%)	367 (96%)	15 (4%)	2 (0%)	29	48
All	All	1532/1544 (99%)	1474 (96%)	55 (4%)	3 (0%)	47	68

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	25	GLY
1	D	2	LYS
1	D	385	PRO

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	327/329 (99%)	314 (96%)	13 (4%)	31	56
1	B	328/329 (100%)	315 (96%)	13 (4%)	31	56
1	C	328/329 (100%)	317 (97%)	11 (3%)	37	63
1	D	329/329 (100%)	315 (96%)	14 (4%)	29	53
All	All	1312/1316 (100%)	1261 (96%)	51 (4%)	32	57

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	51	GLN
1	A	79	HIS
1	A	80	THR
1	A	92	GLU
1	A	140	GLU
1	A	167	LYS
1	A	234	LYS

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Mol	Chain	Res	Type
1	A	280	LEU
1	A	311	GLU
1	A	340	SER
1	A	350	THR
1	A	380	LEU
1	C	31	LYS
1	C	80	THR
1	C	133	THR
1	C	136	LYS
1	C	230	LYS
1	C	280	LEU
1	C	287	ARG
1	C	324	LYS
1	C	350	THR
1	C	366	LEU
1	C	380	LEU
1	B	51	GLN
1	B	70	THR
1	B	80	THR
1	B	128	LYS
1	B	133	THR
1	B	136	LYS
1	B	191	MET
1	B	221	LYS
1	B	280	LEU
1	B	311	GLU
1	B	350	THR
1	B	366	LEU
1	B	376	PHE
1	D	27	SER
1	D	51	GLN
1	D	66	THR
1	D	80	THR
1	D	193	LYS
1	D	205	LYS
1	D	224	GLU
1	D	253	GLN
1	D	280	LEU
1	D	287	ARG
1	D	301	MET
1	D	324	LYS
1	D	340	SER

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Mol	Chain	Res	Type
1	D	350	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	C	142	HIS
1	B	28	ASN
1	D	51	GLN
1	D	142	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

4 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	401	1	15,15,16	3.14	5 (33%)	20,22,23	2.57	7 (35%)
2	PLP	D	401	1	15,15,16	3.42	3 (20%)	20,22,23	1.64	3 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	PLP	C	401	1	15,15,16	3.42	4 (26%)	20,22,23	2.07	8 (40%)
2	PLP	B	401	1	15,15,16	3.45	4 (26%)	20,22,23	2.27	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
2	PLP	A	401	1	-	0/6/6/8	0/1/1/1
2	PLP	D	401	1	-	0/6/6/8	0/1/1/1
2	PLP	C	401	1	-	0/6/6/8	0/1/1/1
2	PLP	B	401	1	-	0/6/6/8	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	PLP	C5-C4	10.14	1.51	1.40
2	D	401	PLP	C5-C4	9.28	1.50	1.40
2	B	401	PLP	C5-C4	8.80	1.50	1.40
2	A	401	PLP	C5-C4	8.18	1.49	1.40
2	B	401	PLP	C3-C2	8.16	1.49	1.40
2	D	401	PLP	C3-C2	7.94	1.48	1.40
2	C	401	PLP	C3-C2	6.23	1.47	1.40
2	A	401	PLP	C3-C2	6.17	1.47	1.40
2	C	401	PLP	C3-C4	4.82	1.50	1.40
2	B	401	PLP	C3-C4	4.63	1.49	1.40
2	A	401	PLP	C3-C4	4.07	1.48	1.40
2	D	401	PLP	C3-C4	4.07	1.48	1.40
2	A	401	PLP	C2-N1	3.13	1.39	1.33
2	A	401	PLP	C6-C5	2.64	1.43	1.37
2	C	401	PLP	C2-N1	2.30	1.38	1.33
2	B	401	PLP	C2-N1	2.19	1.38	1.33

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	PLP	C2A-C2-C3	-6.94	112.32	120.89
2	B	401	PLP	C4A-C4-C5	5.18	126.27	120.94
2	B	401	PLP	C3-C4-C5	-4.76	113.60	118.74
2	B	401	PLP	C6-C5-C4	4.72	121.87	118.16
2	A	401	PLP	C2A-C2-N1	4.42	126.30	117.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	PLP	C4A-C4-C5	4.40	125.47	120.94
2	D	401	PLP	C4A-C4-C5	4.35	125.41	120.94
2	C	401	PLP	C4A-C4-C5	4.14	125.20	120.94
2	A	401	PLP	C3-C4-C5	-3.76	114.67	118.74
2	B	401	PLP	O3P-P-O4P	-3.21	98.20	106.73
2	C	401	PLP	C2A-C2-C3	-3.11	117.04	120.89
2	C	401	PLP	C3-C4-C5	-3.09	115.40	118.74
2	D	401	PLP	C3-C4-C5	-3.08	115.41	118.74
2	A	401	PLP	O4P-C5A-C5	3.06	115.19	109.35
2	C	401	PLP	C2A-C2-N1	2.90	123.33	117.67
2	A	401	PLP	C6-C5-C4	2.84	120.39	118.16
2	C	401	PLP	C6-C5-C4	2.69	120.28	118.16
2	C	401	PLP	C6-N1-C2	2.67	124.12	119.17
2	D	401	PLP	O2P-P-O4P	-2.64	99.71	106.73
2	C	401	PLP	O3P-P-O2P	2.46	117.04	107.64
2	A	401	PLP	O3-C3-C4	2.37	124.35	118.10
2	C	401	PLP	O3-C3-C4	2.07	123.55	118.10

There are no chirality outliers.

There are no torsion outliers.

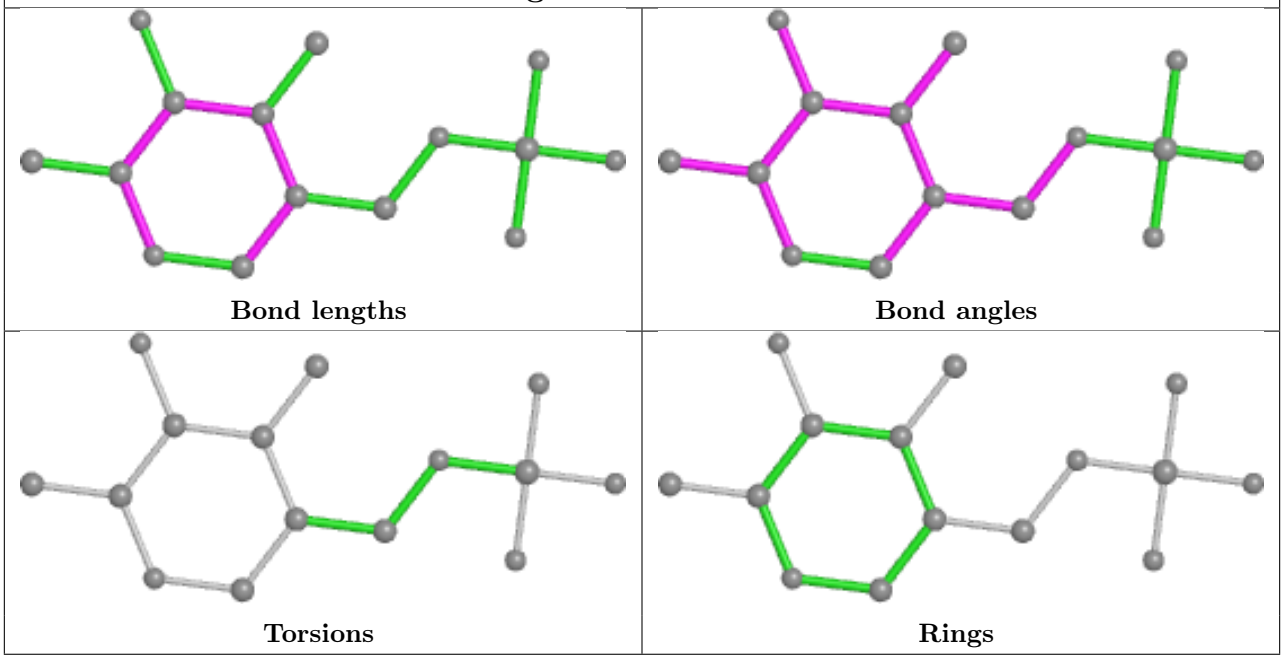
There are no ring outliers.

3 monomers are involved in 3 short contacts:

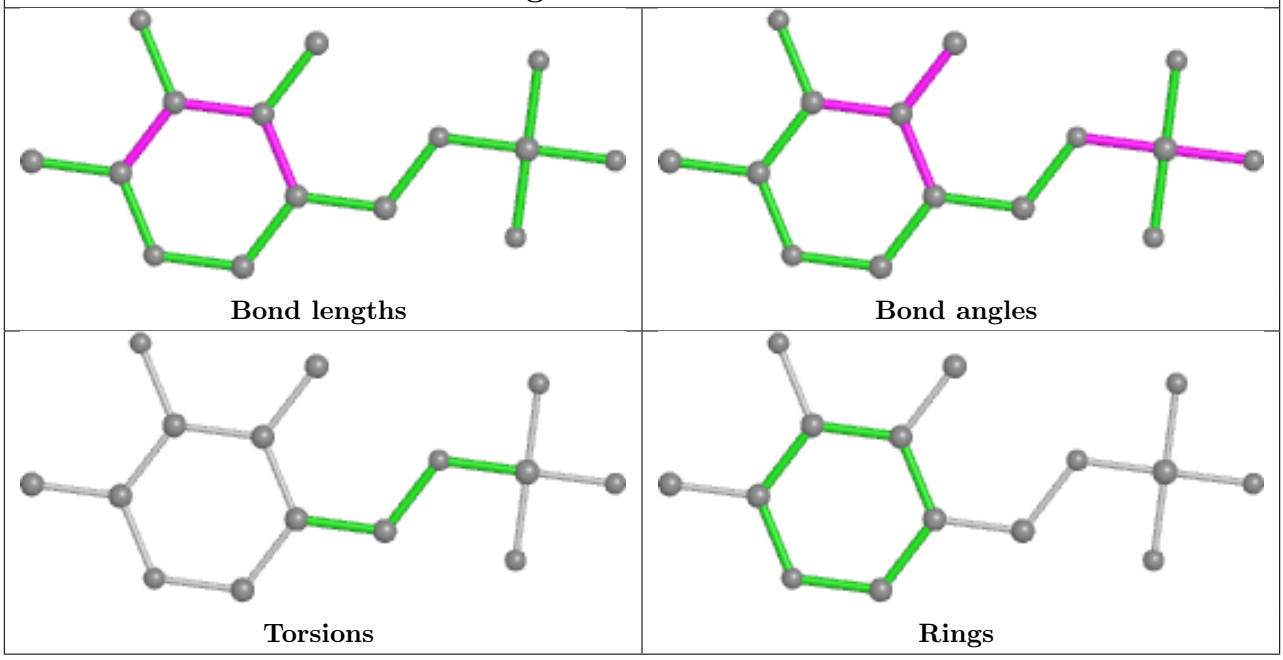
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	PLP	1	0
2	C	401	PLP	1	0
2	B	401	PLP	1	0

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 then 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.

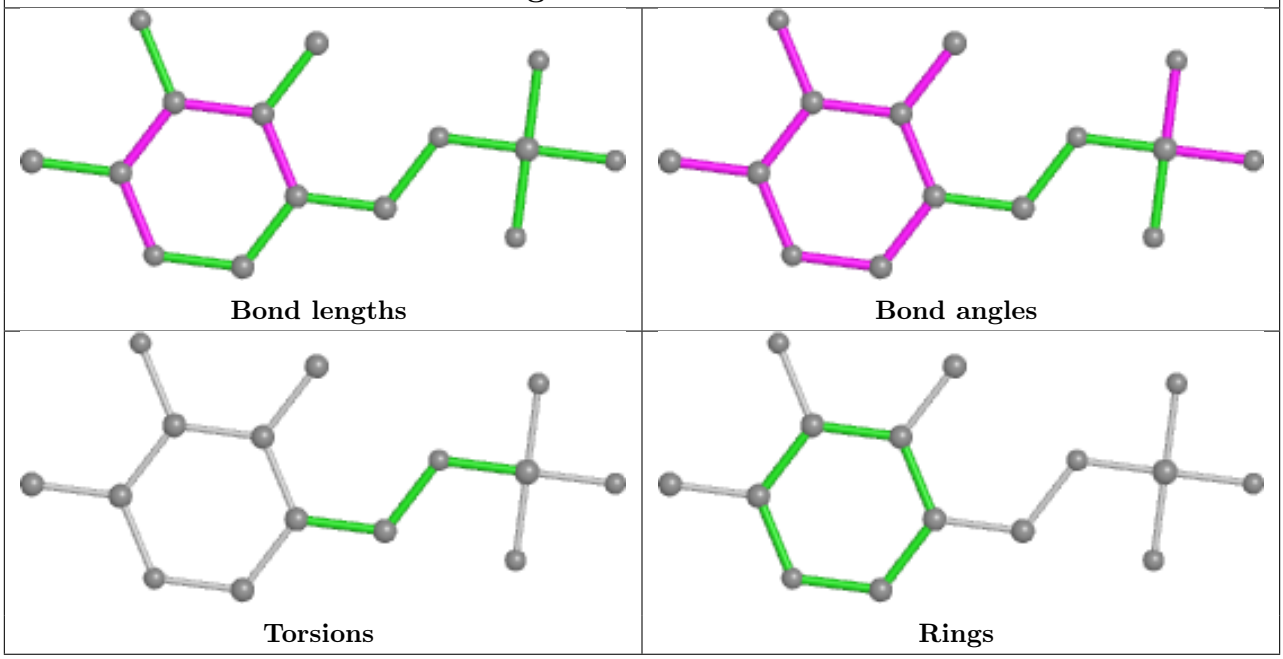
Ligand PLP A 401



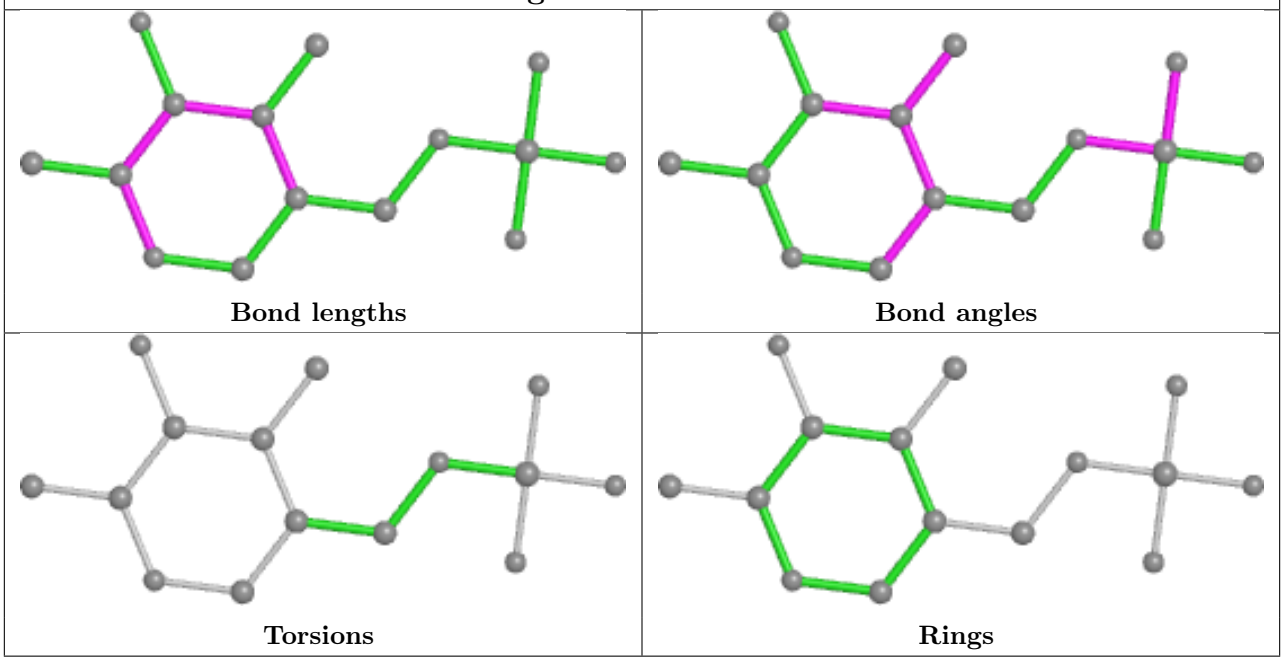
Ligand PLP D 401



Ligand PLP C 401



Ligand PLP B 401



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	384/386 (99%)	-0.24	4 (1%)	82	84	31, 44, 65, 92	0
1	B	385/386 (99%)	0.08	16 (4%)	36	39	31, 52, 76, 97	0
1	C	385/386 (99%)	-0.16	1 (0%)	94	94	33, 48, 68, 87	0
1	D	386/386 (100%)	0.11	14 (3%)	42	46	30, 52, 74, 98	0
All	All	1540/1544 (99%)	-0.05	35 (2%)	60	63	30, 49, 72, 98	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	172	TYR	5.0
1	B	140	GLU	4.2
1	B	143	ARG	3.5
1	B	133	THR	3.5
1	B	138	ALA	3.4
1	B	174	CYS	3.3
1	D	143	ARG	3.1
1	D	212	GLY	2.9
1	B	130	PHE	2.8
1	D	76	GLY	2.6
1	B	137	LYS	2.6
1	B	168	ILE	2.5
1	A	143	ARG	2.5
1	D	264	LEU	2.4
1	B	213	ILE	2.4
1	B	25	GLY	2.4
1	D	74	ILE	2.4
1	B	171	ASP	2.4
1	C	37	LEU	2.3
1	B	170	HIS	2.3
1	D	214	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	169	CYS	2.3
1	D	77	SER	2.2
1	D	80	THR	2.2
1	A	74	ILE	2.2
1	B	135	PHE	2.2
1	D	323	PRO	2.2
1	D	211	PRO	2.1
1	A	213	ILE	2.1
1	B	141	GLN	2.1
1	D	3	PHE	2.1
1	D	78	ALA	2.0
1	A	75	THR	2.0
1	D	75	THR	2.0
1	D	261	PRO	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)

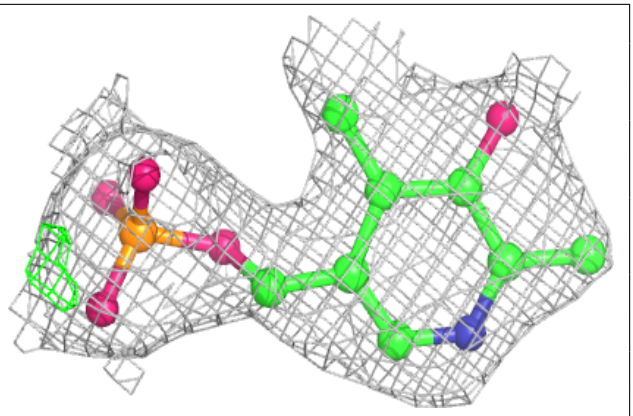
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

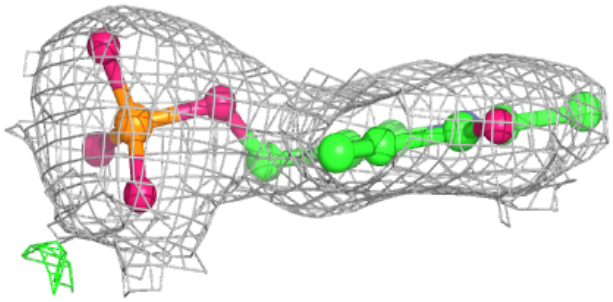
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PLP	C	401	15/16	0.97	0.15	43,45,51,53	0
2	PLP	B	401	15/16	0.97	0.19	43,56,60,61	0
2	PLP	D	401	15/16	0.97	0.18	46,49,55,58	0
2	PLP	A	401	15/16	0.98	0.13	37,43,46,49	0

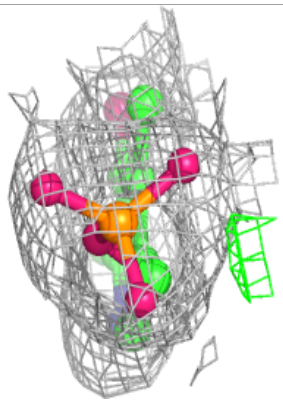
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PLP C 401:

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

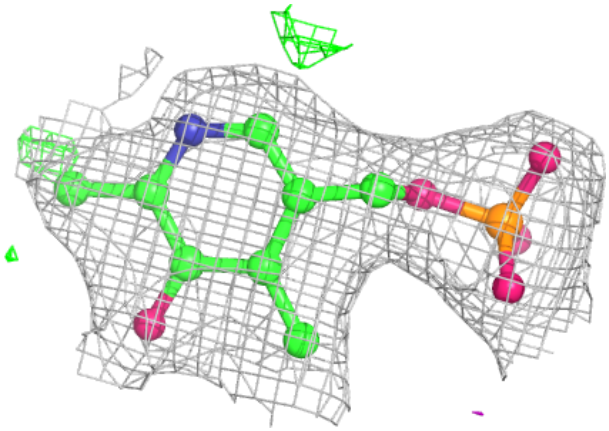


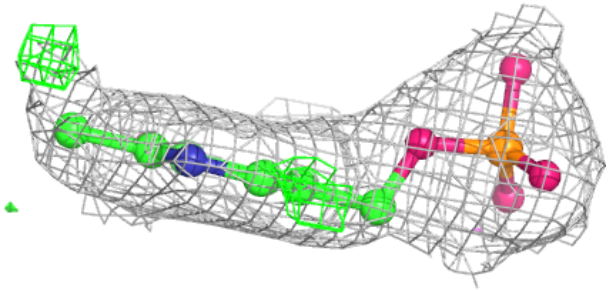


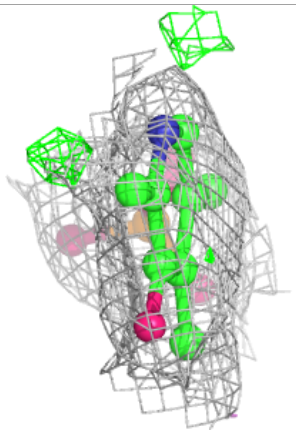


Electron density around PLP B 401:

$2mF_o$-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 401:

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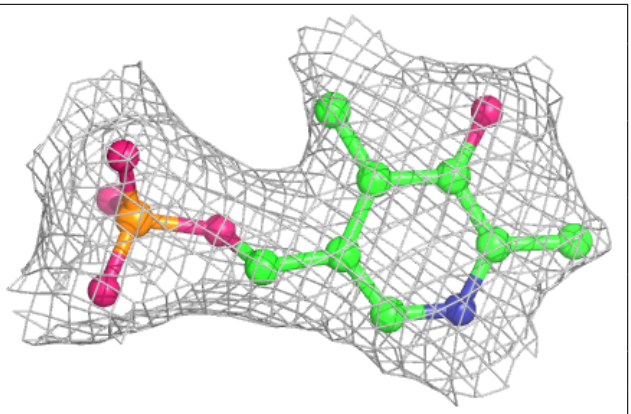
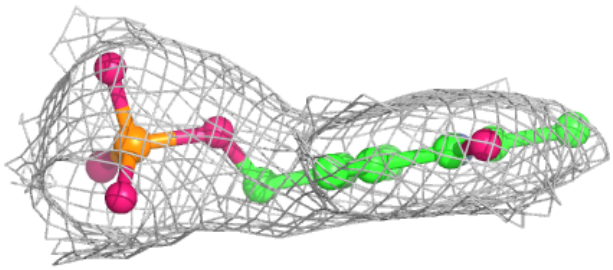
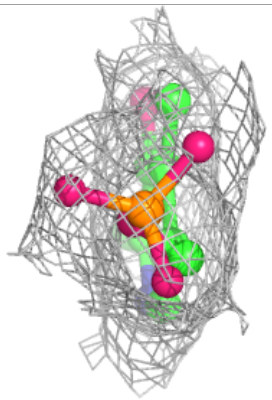
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

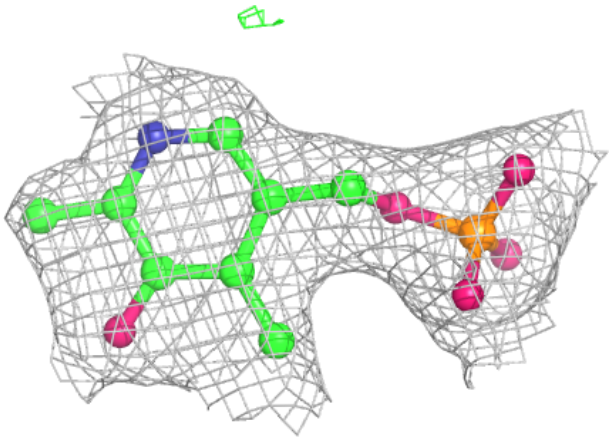


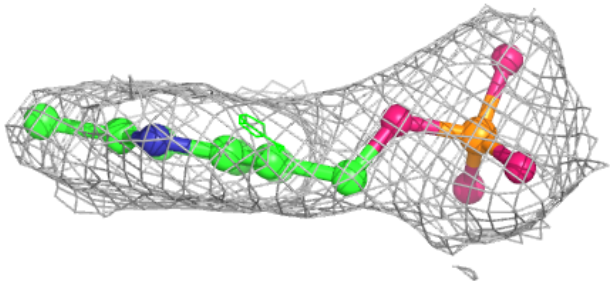


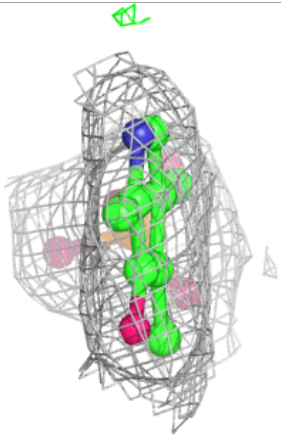


Electron density around PLP A 401:

$2mF_o$-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.