



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 23, 2021 – 12:25 PM JST

PDB ID : 7V5I
Title : Structural insights into the substrate selectivity of acyl-CoA transferase
Authors : Chang, H.Y.; Ko, T.P.
Deposited on : 2021-08-17
Resolution : 3.08 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.25
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) : 2.25

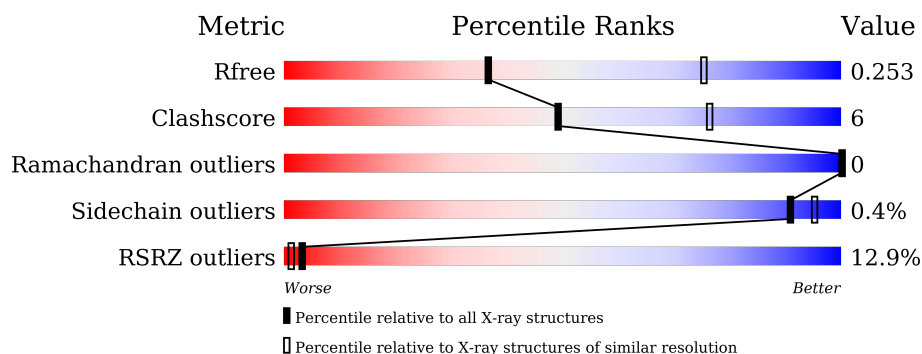
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.08 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	1447 (3.10-3.06)
Clashscore	141614	1546 (3.10-3.06)
Ramachandran outliers	138981	1487 (3.10-3.06)
Sidechain outliers	138945	1486 (3.10-3.06)
RSRZ outliers	127900	1416 (3.10-3.06)

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	400	<div> <div>87%</div> <div>13%</div> </div>
1	B	400	<div> <div>88%</div> <div>12%</div> </div>
1	C	400	<div> <div>18%</div> <div>83%</div> <div>17%</div> </div>
1	D	400	<div> <div>34%</div> <div>82%</div> <div>17%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PLP	D	500	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12369 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.

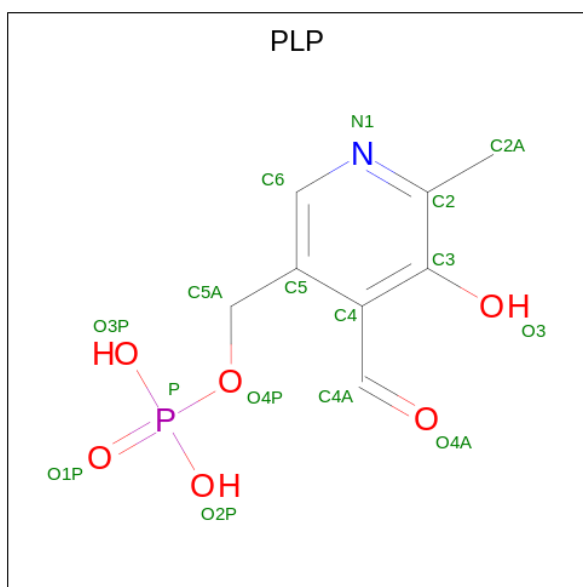
- Molecule 1 is a protein called 2-amino-3-ketobutyrate coenzyme A ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	400	Total	C	N	O	S	0	0	0
			3064	1923	532	591	18			
1	B	400	Total	C	N	O	S	0	0	0
			3064	1923	532	591	18			
1	C	400	Total	C	N	O	S	0	0	0
			3064	1923	532	591	18			
1	D	400	Total	C	N	O	S	0	0	0
			3064	1923	532	591	18			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ASN	-	expression tag	UNP U3BPN5
A	2	ILE	-	expression tag	UNP U3BPN5
B	1	ASN	-	expression tag	UNP U3BPN5
B	2	ILE	-	expression tag	UNP U3BPN5
C	1	ASN	-	expression tag	UNP U3BPN5
C	2	ILE	-	expression tag	UNP U3BPN5
D	1	ASN	-	expression tag	UNP U3BPN5
D	2	ILE	-	expression tag	UNP U3BPN5

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C₈H₁₀NO₆P) (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		

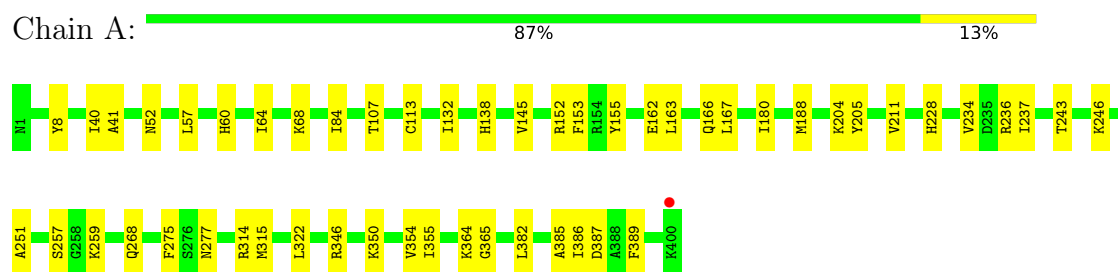
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	24	Total	O	0	0
			24	24		
3	B	29	Total	O	0	0
			29	29		

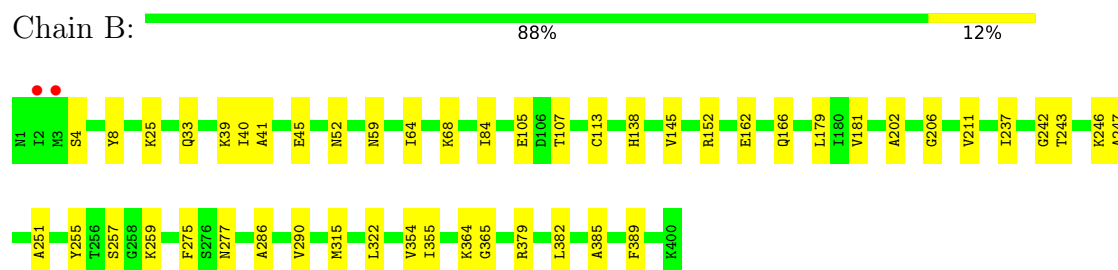
3 Residue-property plots [i](#)

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.

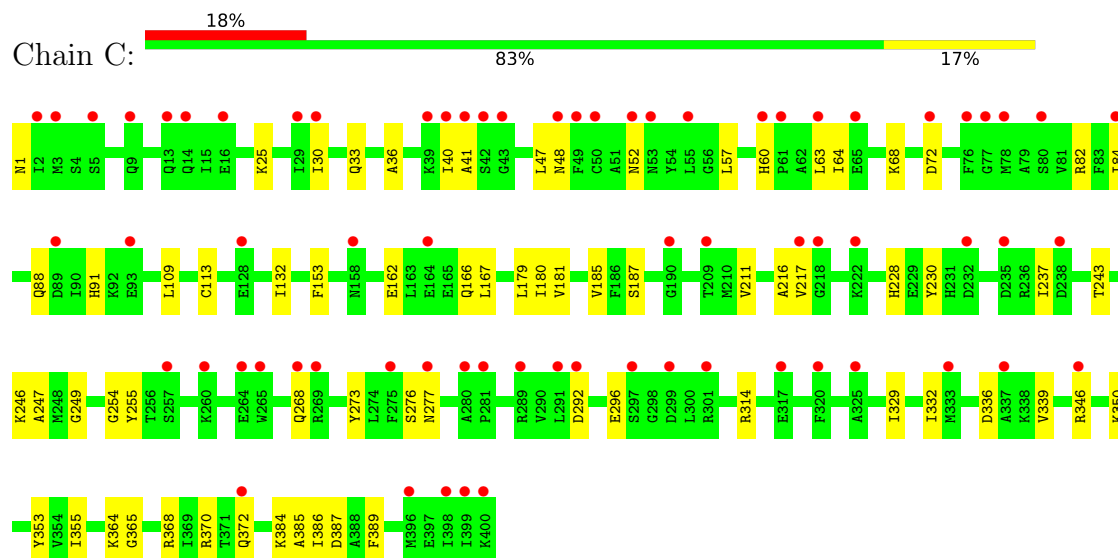
- Molecule 1: 2-amino-3-ketobutyrate coenzyme A ligase



- Molecule 1: 2-amino-3-ketobutyrate coenzyme A ligase

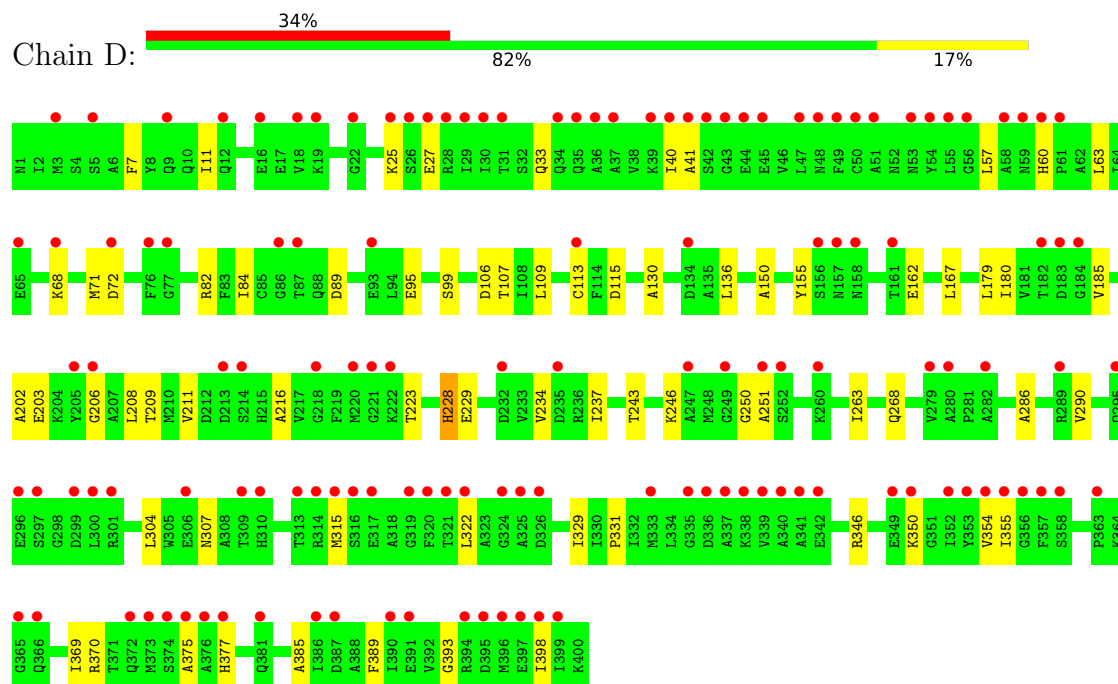


- Molecule 1: 2-amino-3-ketobutyrate coenzyme A ligase



● Molecule 1: 2-amino-3-ketobutyrate coenzyme A ligase

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.12Å 136.24Å 219.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.41 – 3.08 27.41 – 3.08	Depositor EDS
% Data completeness (in resolution range)	88.5 (27.41-3.08) 88.4 (27.41-3.08)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 3.05Å)	Xtriage
Refinement program	REFMAC 1.17.1_3660	Depositor
R, R_{free}	0.204 , 0.249 0.210 , 0.253	Depositor DCC
R_{free} test set	1594 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	59.1	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 82.1	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	0.91	EDS
Total number of atoms	12369	wwPDB-VP
Average B, all atoms (Å ²)	126.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% 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	0.26	0/3111	0.43	0/4193
1	B	0.25	0/3111	0.43	0/4193
1	C	0.25	0/3111	0.42	0/4193
1	D	0.24	0/3111	0.43	0/4193
All	All	0.25	0/12444	0.43	0/16772

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	3064	0	3044	35	0
1	B	3064	0	3044	35	0
1	C	3064	0	3044	49	0
1	D	3064	0	3044	47	0
2	A	15	0	7	3	0
2	B	15	0	7	3	0
2	C	15	0	7	5	0
2	D	15	0	7	4	0
3	A	24	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	29	0	0	0	0
All	All	12369	0	12204	144	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 6.

All (144) 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:246:LYS:NZ	2:D:500:PLP:C4A	2.25	0.99
1:A:246:LYS:NZ	2:A:500:PLP:C4A	2.27	0.98
1:B:246:LYS:NZ	2:B:500:PLP:C4A	2.29	0.95
1:A:246:LYS:HZ1	2:A:500:PLP:C4A	1.81	0.94
1:D:246:LYS:HZ3	2:D:500:PLP:C4A	1.81	0.92
1:B:246:LYS:HZ3	2:B:500:PLP:C4A	1.91	0.83
1:C:246:LYS:NZ	2:C:500:PLP:C4A	2.41	0.83
1:B:246:LYS:HZ1	2:B:500:PLP:C4A	1.93	0.78
1:D:246:LYS:HZ1	2:D:500:PLP:C4A	1.95	0.77
1:C:1:ASN:HD21	1:D:203:GLU:HA	1.53	0.74
1:A:246:LYS:HZ3	2:A:500:PLP:C4A	2.00	0.73
1:D:82:ARG:HH12	1:D:109:LEU:HB2	1.56	0.69
1:C:246:LYS:HE2	2:C:500:PLP:C4A	2.24	0.68
1:C:246:LYS:CE	2:C:500:PLP:C4A	2.72	0.67
1:D:329:ILE:HG23	1:D:370:ARG:HG3	1.76	0.66
1:C:355:ILE:HD12	1:D:84:ILE:HG23	1.76	0.66
1:C:277:ASN:ND2	1:D:250:GLY:O	2.29	0.65
1:A:84:ILE:HG23	1:B:355:ILE:HD12	1.79	0.65
1:C:246:LYS:HZ1	2:C:500:PLP:C4A	2.08	0.64
1:A:355:ILE:HD12	1:B:84:ILE:HG23	1.82	0.61
1:C:25:LYS:O	1:D:268:GLN:NE2	2.32	0.61
1:C:84:ILE:HG23	1:D:355:ILE:HD12	1.84	0.60
1:C:187:SER:O	1:C:370:ARG:NH1	2.29	0.60
1:D:113:CYS:HB2	1:D:243:THR:HB	1.85	0.59
1:C:57:LEU:HA	1:C:60:HIS:HB2	1.86	0.58
1:C:72:ASP:O	1:D:33:GLN:NE2	2.37	0.58
1:C:113:CYS:HB2	1:C:243:THR:HB	1.86	0.57
1:A:314:ARG:NH2	1:A:387:ASP:OD1	2.38	0.57
1:C:277:ASN:ND2	1:D:251:ALA:O	2.27	0.56
1:B:4:SER:HB3	1:B:8:TYR:CE2	2.40	0.56
1:C:314:ARG:NH2	1:C:387:ASP:OD1	2.38	0.56
1:C:64:ILE:HG23	1:D:71:MET:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:385:ALA:O	1:B:389:PHE:HD1	1.90	0.55
1:D:82:ARG:NH2	1:D:95:GLU:OE2	2.39	0.55
1:A:52:ASN:HB3	1:A:246:LYS:HG3	1.89	0.55
1:C:273:TYR:OH	1:D:27:GLU:OE2	2.21	0.55
1:D:307:ASN:ND2	1:D:377:HIS:O	2.39	0.55
1:A:132:ILE:HG12	1:A:153:PHE:HB2	1.90	0.54
1:A:277:ASN:ND2	1:B:251:ALA:O	2.39	0.54
1:C:52:ASN:OD1	1:C:372:GLN:NE2	2.41	0.54
1:C:167:LEU:HD21	1:C:180:ILE:HD11	1.91	0.53
1:D:304:LEU:HB2	1:D:375:ALA:HB2	1.90	0.53
1:A:8:TYR:CE2	1:B:259:LYS:HD2	2.44	0.52
1:A:315:MET:HB2	1:A:322:LEU:HD11	1.91	0.52
1:C:346:ARG:O	1:C:350:LYS:HG2	2.08	0.52
1:A:113:CYS:HB2	1:A:243:THR:HB	1.90	0.52
1:C:33:GLN:NE2	1:D:72:ASP:O	2.43	0.52
1:C:385:ALA:O	1:C:389:PHE:HD1	1.92	0.52
1:D:202:ALA:O	1:D:206:GLY:N	2.43	0.51
1:A:385:ALA:O	1:A:389:PHE:HD1	1.94	0.51
1:B:33:GLN:OE1	1:B:59:ASN:ND2	2.43	0.51
1:A:145:VAL:HG12	1:A:152:ARG:HD3	1.93	0.51
1:B:145:VAL:HG12	1:B:152:ARG:HD3	1.92	0.51
1:D:346:ARG:O	1:D:350:LYS:HG2	2.11	0.51
1:B:354:VAL:HG11	1:B:389:PHE:HZ	1.77	0.50
1:C:185:VAL:HG23	1:C:216:ALA:HB2	1.92	0.50
1:C:276:SER:OG	2:D:500:PLP:O1P	2.24	0.50
1:A:354:VAL:HG11	1:A:389:PHE:HZ	1.77	0.49
1:B:52:ASN:HB3	1:B:246:LYS:HG3	1.95	0.49
1:C:329:ILE:HG23	1:C:370:ARG:HG3	1.93	0.49
1:B:107:THR:HG22	1:B:257:SER:HB3	1.94	0.49
1:D:393:GLY:HA2	1:D:398:ILE:HD12	1.95	0.49
1:A:40:ILE:HG22	1:A:41:ALA:H	1.78	0.48
1:A:138:HIS:CE1	1:B:275:PHE:HB3	2.48	0.48
1:A:167:LEU:HD21	1:A:180:ILE:HD11	1.94	0.48
1:C:36:ALA:O	1:C:47:LEU:HA	2.14	0.48
1:B:379:ARG:HA	1:B:382:LEU:HB2	1.95	0.48
1:A:251:ALA:O	1:B:277:ASN:ND2	2.45	0.47
1:B:40:ILE:HG22	1:B:41:ALA:H	1.79	0.47
1:D:60:HIS:HB3	1:D:63:LEU:HG	1.96	0.47
1:D:209:THR:HG21	1:D:237:ILE:HG12	1.97	0.47
1:B:179:LEU:HD22	1:B:181:VAL:HG22	1.95	0.47
1:A:314:ARG:HD3	1:A:386:ILE:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:LEU:HD11	1:C:384:LYS:HD3	1.97	0.47
1:B:64:ILE:HG22	1:B:68:LYS:HE3	1.96	0.47
1:D:385:ALA:O	1:D:389:PHE:HD1	1.97	0.47
1:D:223:THR:OG1	1:D:229:GLU:OE1	2.30	0.47
1:D:331:PRO:HA	1:D:369:ILE:O	2.15	0.47
1:B:242:GLY:HA3	1:B:255:TYR:CZ	2.51	0.46
1:D:211:VAL:HG21	1:D:237:ILE:HD13	1.96	0.46
1:C:82:ARG:HH12	1:C:109:LEU:HB2	1.80	0.46
1:A:346:ARG:O	1:A:350:LYS:HG2	2.16	0.46
1:A:107:THR:HG22	1:A:257:SER:HB3	1.97	0.46
1:A:211:VAL:HG21	1:A:237:ILE:HD13	1.98	0.46
1:A:64:ILE:HG22	1:A:68:LYS:HE3	1.97	0.45
1:B:113:CYS:HB2	1:B:243:THR:HB	1.98	0.45
1:B:286:ALA:O	1:B:290:VAL:HG23	2.15	0.45
1:B:315:MET:HB2	1:B:322:LEU:HD11	1.98	0.45
1:C:48:ASN:HA	1:C:353:TYR:HB3	1.99	0.45
1:B:211:VAL:HG21	1:B:237:ILE:HD13	1.98	0.44
1:C:57:LEU:HB2	1:C:249:GLY:HA2	1.98	0.44
1:C:336:ASP:HB3	1:C:339:VAL:HG23	2.00	0.44
1:D:167:LEU:HD21	1:D:180:ILE:HD11	1.99	0.44
1:C:40:ILE:HG22	1:C:41:ALA:H	1.82	0.44
1:A:259:LYS:HD2	1:B:8:TYR:CE2	2.53	0.44
1:C:30:ILE:O	1:D:89:ASP:N	2.50	0.44
1:C:88:GLN:HB2	1:C:91:HIS:ND1	2.33	0.43
1:A:275:PHE:HB3	1:B:138:HIS:CE1	2.53	0.43
1:C:314:ARG:HD3	1:C:386:ILE:HG21	2.00	0.43
1:C:68:LYS:HG2	1:D:68:LYS:HG2	2.01	0.43
1:D:40:ILE:HG22	1:D:41:ALA:H	1.83	0.43
1:B:107:THR:HG22	1:B:257:SER:CB	2.49	0.43
1:C:332:ILE:O	1:C:368:ARG:HA	2.19	0.43
1:D:286:ALA:O	1:D:290:VAL:HG23	2.19	0.42
1:C:243:THR:HA	1:C:254:GLY:HA2	2.01	0.42
1:D:179:LEU:HG	1:D:208:LEU:HB2	2.00	0.42
1:A:268:GLN:NE2	1:B:25:LYS:O	2.46	0.42
1:C:364:LYS:HA	1:C:365:GLY:HA2	1.68	0.42
1:C:292:ASP:O	1:C:296:GLU:HG3	2.20	0.42
1:D:106:ASP:HB3	1:D:263:ILE:HG13	2.01	0.42
1:C:179:LEU:HD22	1:C:181:VAL:HG22	2.02	0.42
1:A:107:THR:HG22	1:A:257:SER:CB	2.50	0.42
1:A:204:LYS:HD2	1:A:205:TYR:CE2	2.55	0.42
1:B:202:ALA:O	1:B:206:GLY:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:LYS:HB3	1:B:247:ALA:H	1.64	0.41
1:C:162:GLU:O	1:C:166:GLN:HG2	2.19	0.41
1:D:7:PHE:CZ	1:D:11:ILE:HD11	2.54	0.41
1:A:162:GLU:O	1:A:166:GLN:HG2	2.19	0.41
1:A:57:LEU:HA	1:A:60:HIS:HB2	2.03	0.41
1:A:188:MET:HB3	1:A:188:MET:HE3	1.92	0.41
1:C:217:VAL:HG11	1:C:255:TYR:OH	2.19	0.41
1:D:115:ASP:N	1:D:115:ASP:OD1	2.53	0.41
1:D:130:ALA:HA	1:D:150:ALA:HB1	2.02	0.41
1:A:364:LYS:HA	1:A:365:GLY:HA2	1.69	0.41
1:B:364:LYS:HA	1:B:365:GLY:HA2	1.67	0.41
1:D:136:LEU:HD12	1:D:136:LEU:HA	1.88	0.41
1:D:99:SER:HB3	1:D:107:THR:HG23	2.03	0.41
1:C:268:GLN:HE22	1:D:25:LYS:N	2.19	0.41
1:A:155:TYR:CE2	1:A:163:LEU:HD13	2.55	0.41
1:D:57:LEU:HA	1:D:60:HIS:HB2	2.02	0.41
1:D:185:VAL:HG23	1:D:216:ALA:HB2	2.03	0.41
1:B:39:LYS:HG2	1:B:45:GLU:HG2	2.02	0.41
1:C:57:LEU:HB3	1:C:63:LEU:HD12	2.01	0.41
1:D:354:VAL:HG11	1:D:389:PHE:HZ	1.85	0.41
1:C:246:LYS:HZ3	2:C:500:PLP:C4A	2.27	0.41
1:D:155:TYR:HB2	1:D:162:GLU:HB3	2.02	0.41
1:C:211:VAL:HG21	1:C:237:ILE:HD13	2.03	0.40
1:B:105:GLU:HB2	1:B:259:LYS:HA	2.03	0.40
1:C:132:ILE:HG12	1:C:153:PHE:HB2	2.02	0.40
1:D:315:MET:HB2	1:D:322:LEU:HD11	2.02	0.40
1:A:234:VAL:C	1:A:236:ARG:H	2.25	0.40
1:C:246:LYS:HB3	1:C:247:ALA:H	1.67	0.40
1:D:228:HIS:CD2	1:D:234:VAL:HG13	2.56	0.40
1:B:162:GLU:O	1:B:166:GLN:HG2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	398/400 (100%)	374 (94%)	24 (6%)	0	100	100
1	B	398/400 (100%)	374 (94%)	24 (6%)	0	100	100
1	C	398/400 (100%)	372 (94%)	26 (6%)	0	100	100
1	D	398/400 (100%)	374 (94%)	24 (6%)	0	100	100
All	All	1592/1600 (100%)	1494 (94%)	98 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	319/319 (100%)	317 (99%)	2 (1%)	86	93
1	B	319/319 (100%)	319 (100%)	0	100	100
1	C	319/319 (100%)	317 (99%)	2 (1%)	86	93
1	D	319/319 (100%)	318 (100%)	1 (0%)	92	96
All	All	1276/1276 (100%)	1271 (100%)	5 (0%)	91	95

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	228	HIS
1	A	382	LEU
1	C	228	HIS
1	C	230	TYR
1	D	228	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	1	ASN

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	B	500	-	15,15,16	1.07	1 (6%)	20,22,23	0.97	2 (10%)
2	PLP	D	500	-	15,15,16	1.08	1 (6%)	20,22,23	1.01	2 (10%)
2	PLP	A	500	-	15,15,16	1.06	1 (6%)	20,22,23	1.01	1 (5%)
2	PLP	C	500	-	15,15,16	1.09	2 (13%)	20,22,23	1.13	2 (10%)

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	B	500	-	-	0/6/6/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLP	D	500	-	-	0/6/6/8	0/1/1/1
2	PLP	A	500	-	-	2/6/6/8	0/1/1/1
2	PLP	C	500	-	-	1/6/6/8	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	PLP	C2-N1	2.59	1.38	1.33
2	B	500	PLP	C2-N1	2.56	1.38	1.33
2	D	500	PLP	C2-N1	2.44	1.38	1.33
2	C	500	PLP	C2-N1	2.22	1.38	1.33
2	C	500	PLP	C6-N1	2.12	1.38	1.34

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	500	PLP	C6-C5-C4	2.55	120.17	118.16
2	C	500	PLP	C5-C6-N1	-2.36	119.89	123.82
2	A	500	PLP	C6-C5-C4	2.26	119.93	118.16
2	D	500	PLP	C6-C5-C4	2.20	119.89	118.16
2	D	500	PLP	C5-C6-N1	-2.17	120.20	123.82
2	B	500	PLP	C6-C5-C4	2.15	119.85	118.16
2	B	500	PLP	C5-C6-N1	-2.11	120.31	123.82

There are no chirality outliers.

All (3) torsion outliers are listed below:

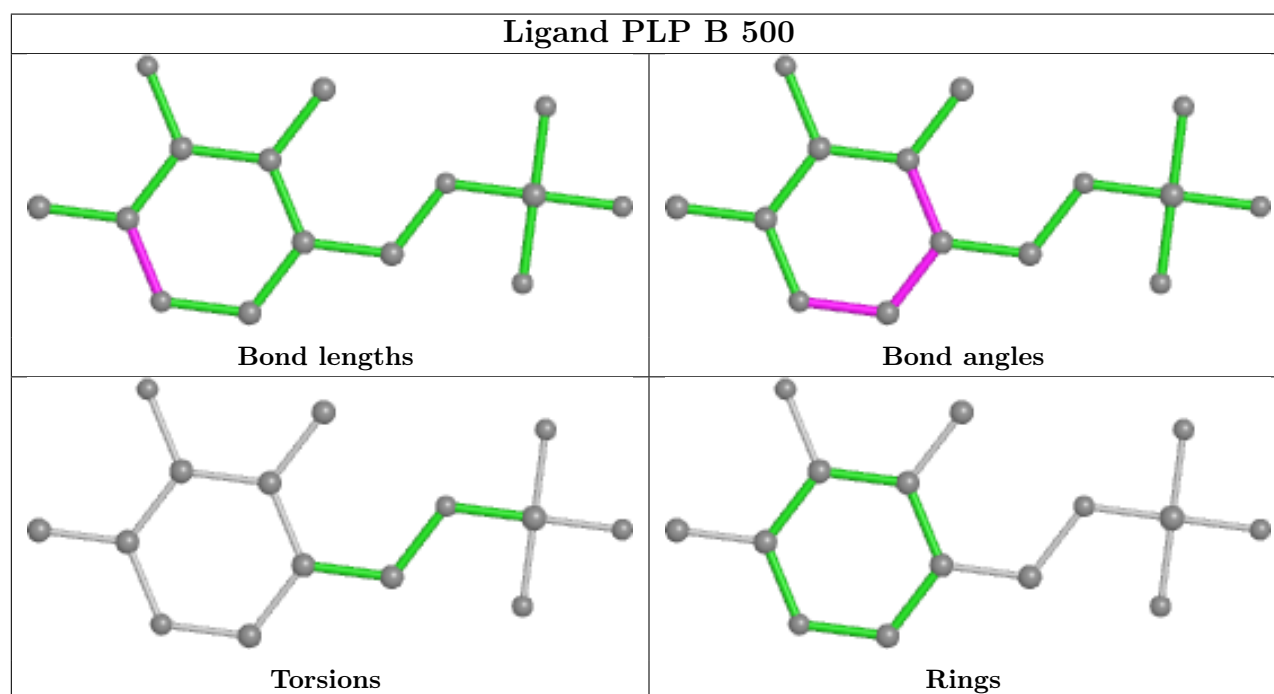
Mol	Chain	Res	Type	Atoms
2	A	500	PLP	C6-C5-C5A-O4P
2	C	500	PLP	C6-C5-C5A-O4P
2	A	500	PLP	C4-C5-C5A-O4P

There are no ring outliers.

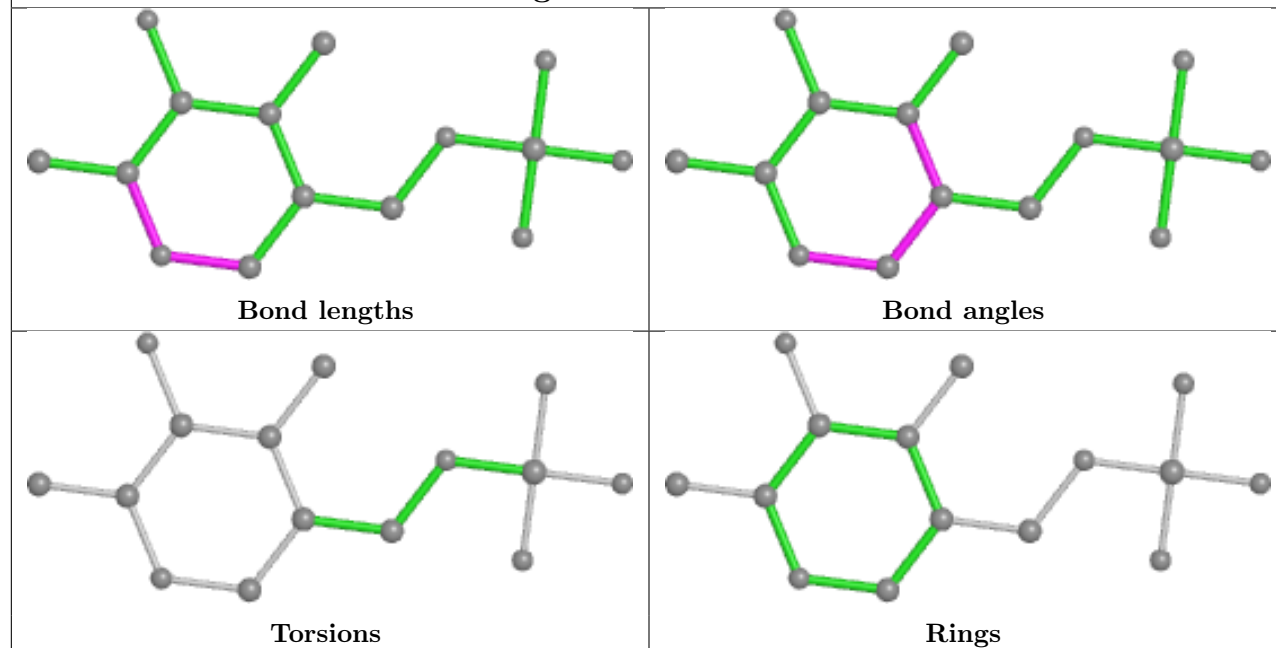
4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	500	PLP	3	0
2	D	500	PLP	4	0
2	A	500	PLP	3	0
2	C	500	PLP	5	0

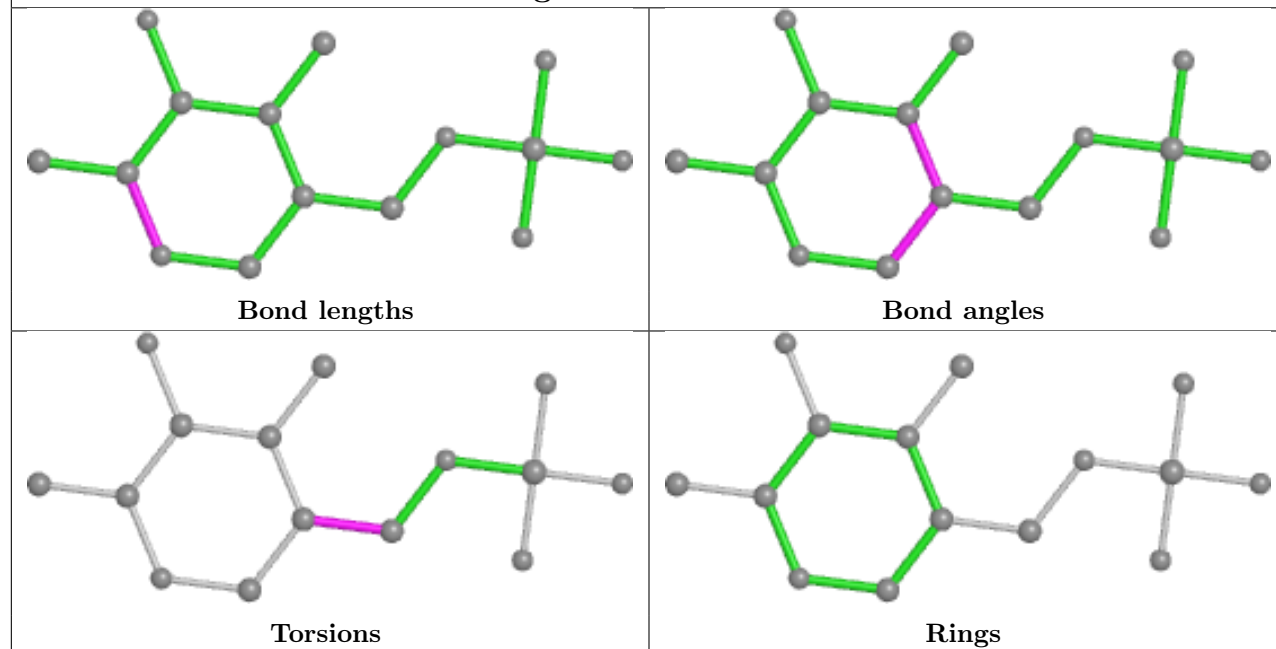
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

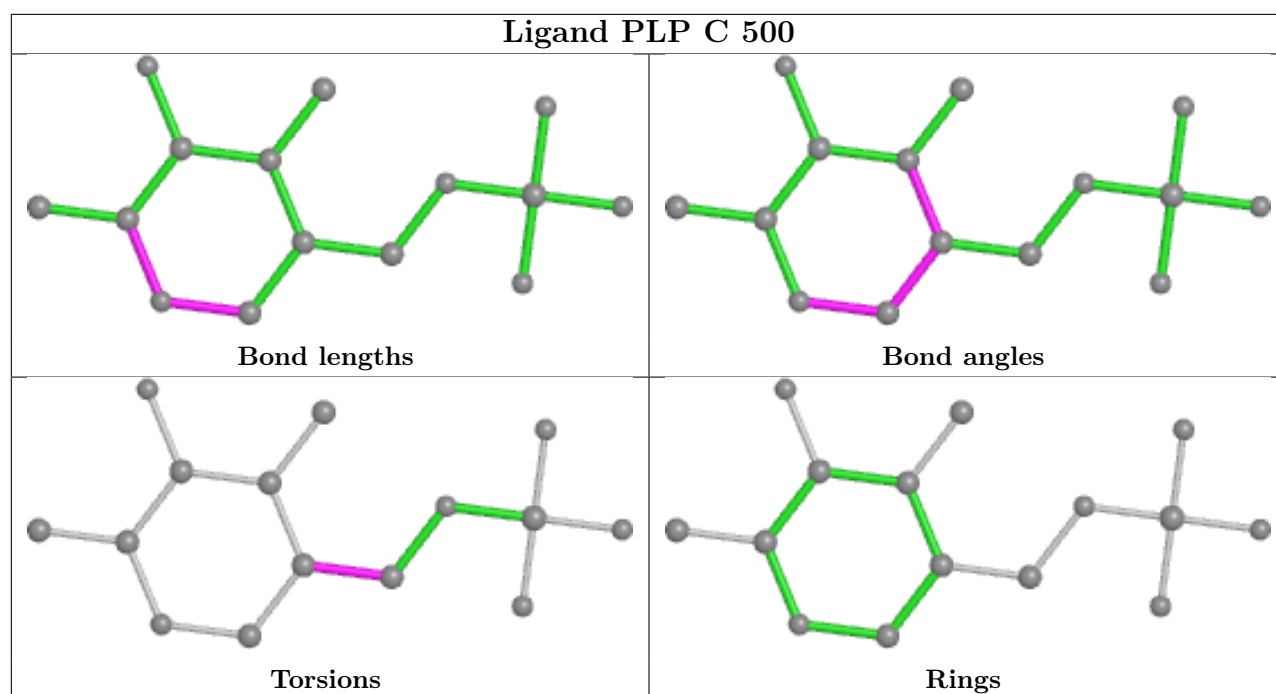


Ligand PLP D 500



Ligand PLP A 500





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	400/400 (100%)	-0.56	1 (0%) 94 87	18, 48, 87, 113	0
1	B	400/400 (100%)	-0.49	2 (0%) 91 80	14, 52, 94, 197	0
1	C	400/400 (100%)	0.96	70 (17%) 1 0	104, 183, 246, 300	0
1	D	400/400 (100%)	1.64	134 (33%) 0 0	130, 218, 288, 329	0
All	All	1600/1600 (100%)	0.39	207 (12%) 3 1	14, 115, 258, 329	0

All (207) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	37	ALA	14.4
1	D	321	THR	8.1
1	D	325	ALA	7.9
1	C	89	ASP	7.2
1	D	55	LEU	6.9
1	D	35	GLN	6.7
1	D	320	PHE	6.2
1	D	27	GLU	6.1
1	D	48	ASN	6.1
1	D	252	SER	6.0
1	C	260	LYS	5.6
1	D	41	ALA	5.6
1	D	28	ARG	5.6
1	C	41	ALA	5.4
1	C	3	MET	5.4
1	D	56	GLY	5.4
1	D	72	ASP	5.4
1	D	206	GLY	5.2
1	D	29	ILE	5.2
1	D	357	PHE	5.2
1	D	356	GLY	5.1

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Mol	Chain	Res	Type	RSRZ
1	D	386	ILE	5.1
1	D	352	ILE	4.9
1	D	42	SER	4.9
1	C	9	GLN	4.9
1	C	77	GLY	4.8
1	D	396	MET	4.8
1	D	5	SER	4.7
1	D	54	TYR	4.7
1	D	398	ILE	4.7
1	C	400	LYS	4.6
1	D	376	ALA	4.6
1	D	40	ILE	4.5
1	D	315	MET	4.5
1	D	324	GLY	4.4
1	C	61	PRO	4.2
1	D	375	ALA	4.2
1	D	355	ILE	4.1
1	D	353	TYR	4.1
1	C	65	GLU	4.1
1	C	2	ILE	4.1
1	C	42	SER	4.1
1	D	60	HIS	4.0
1	D	316	SER	4.0
1	C	235	ASP	4.0
1	D	339	VAL	3.9
1	D	322	LEU	3.9
1	D	394	ARG	3.9
1	D	391	GLU	3.9
1	C	43	GLY	3.8
1	D	222	LYS	3.8
1	D	50	CYS	3.8
1	D	36	ALA	3.8
1	C	5	SER	3.8
1	D	39	LYS	3.7
1	D	232	ASP	3.7
1	D	349	GLU	3.7
1	D	26	SER	3.7
1	C	78	MET	3.7
1	C	29	ILE	3.7
1	D	337	ALA	3.6
1	D	25	LYS	3.6
1	D	390	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	358	SER	3.5
1	D	156	SER	3.5
1	C	280	ALA	3.5
1	D	354	VAL	3.5
1	C	265	TRP	3.5
1	D	30	ILE	3.5
1	C	93	GLU	3.4
1	D	65	GLU	3.4
1	C	372	GLN	3.4
1	D	218	GLY	3.4
1	C	268	GLN	3.4
1	C	238	ASP	3.3
1	D	336	ASP	3.3
1	C	76	PHE	3.3
1	D	299	ASP	3.3
1	D	301	ARG	3.3
1	D	31	THR	3.3
1	D	235	ASP	3.3
1	C	317	GLU	3.3
1	D	306	GLU	3.3
1	D	319	GLY	3.3
1	C	13	GLN	3.2
1	D	338	LYS	3.2
1	D	45	GLU	3.2
1	C	269	ARG	3.2
1	D	297	SER	3.2
1	D	377	HIS	3.2
1	C	277	ASN	3.1
1	D	310	HIS	3.1
1	D	3	MET	3.1
1	D	399	ILE	3.1
1	C	72	ASP	3.1
1	C	218	GLY	3.1
1	D	205	TYR	3.1
1	C	281	PRO	3.0
1	C	299	ASP	3.0
1	D	314	ARG	3.0
1	C	399	ILE	3.0
1	D	58	ALA	2.9
1	D	251	ALA	2.9
1	D	43	GLY	2.9
1	D	59	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	2	ILE	2.9
1	D	381	GLN	2.9
1	D	68	LYS	2.9
1	D	296	GLU	2.9
1	D	220	MET	2.9
1	D	373	MET	2.9
1	D	300	LEU	2.9
1	D	61	PRO	2.9
1	C	30	ILE	2.8
1	C	297	SER	2.8
1	C	53	ASN	2.8
1	C	264	GLU	2.8
1	C	40	ILE	2.8
1	D	16	GLU	2.8
1	D	247	ALA	2.8
1	C	14	GLN	2.8
1	C	301	ARG	2.8
1	C	333	MET	2.8
1	D	372	GLN	2.8
1	C	292	ASP	2.7
1	C	49	PHE	2.7
1	C	289	ARG	2.7
1	C	222	LYS	2.7
1	D	161	THR	2.7
1	D	9	GLN	2.7
1	B	3	MET	2.7
1	D	363	PRO	2.7
1	D	184	GLY	2.6
1	D	221	GLY	2.6
1	C	325	ALA	2.6
1	D	157	ASN	2.6
1	A	400	LYS	2.6
1	D	34	GLN	2.6
1	D	387	ASP	2.6
1	D	49	PHE	2.6
1	D	280	ALA	2.6
1	D	214	SER	2.6
1	C	84	ILE	2.6
1	D	53	ASN	2.5
1	D	19	LYS	2.5
1	D	342	GLU	2.5
1	D	134	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	396	MET	2.5
1	C	291	LEU	2.5
1	D	77	GLY	2.5
1	C	39	LYS	2.4
1	C	190	GLY	2.4
1	D	374	SER	2.4
1	D	12	GLN	2.4
1	C	346	ARG	2.4
1	D	333	MET	2.4
1	C	164	GLU	2.4
1	C	232	ASP	2.4
1	D	260	LYS	2.4
1	D	395	ASP	2.4
1	D	326	ASP	2.4
1	C	16	GLU	2.4
1	D	51	ALA	2.4
1	D	350	LYS	2.4
1	D	93	GLU	2.4
1	C	275	PHE	2.3
1	D	22	GLY	2.3
1	D	183	ASP	2.3
1	D	295	GLN	2.3
1	D	18	VAL	2.3
1	D	182	THR	2.3
1	C	158	ASN	2.2
1	C	60	HIS	2.2
1	D	87	THR	2.2
1	D	282	ALA	2.2
1	D	76	PHE	2.2
1	D	335	GLY	2.2
1	C	209	THR	2.2
1	D	397	GLU	2.2
1	C	48	ASN	2.2
1	D	317	GLU	2.2
1	C	337	ALA	2.2
1	D	309	THR	2.2
1	C	80	SER	2.2
1	C	50	CYS	2.2
1	D	86	GLY	2.2
1	D	340	ALA	2.2
1	D	47	LEU	2.2
1	C	55	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	213	ASP	2.2
1	D	249	GLY	2.2
1	C	63	LEU	2.1
1	C	257	SER	2.1
1	D	44	GLU	2.1
1	D	289	ARG	2.1
1	C	320	PHE	2.1
1	D	366	GLN	2.1
1	D	365	GLY	2.1
1	C	217	VAL	2.1
1	D	158	ASN	2.1
1	C	128	GLU	2.1
1	D	341	ALA	2.1
1	C	398	ILE	2.1
1	D	279	VAL	2.1
1	D	113	CYS	2.0
1	D	313	THR	2.0
1	C	52	ASN	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](#)

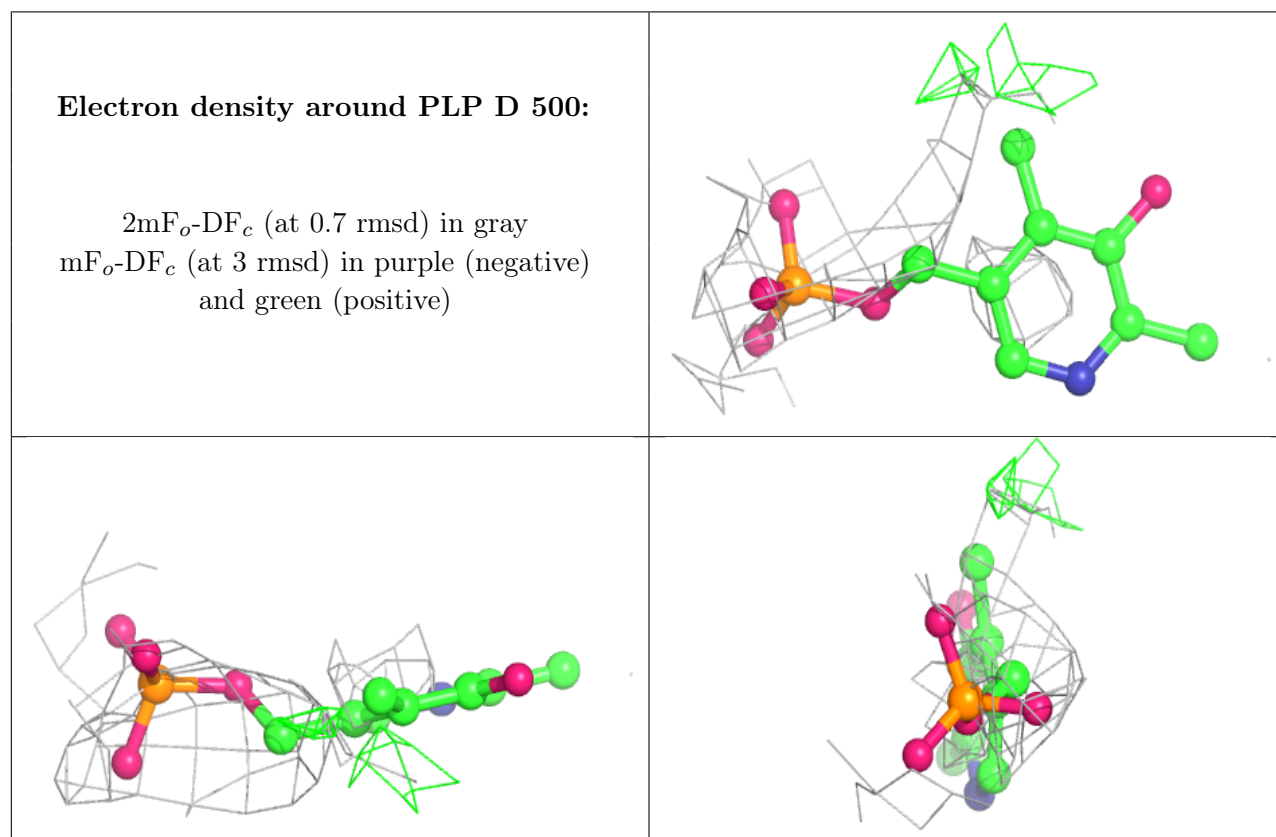
There are no monosaccharides in this entry.

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.

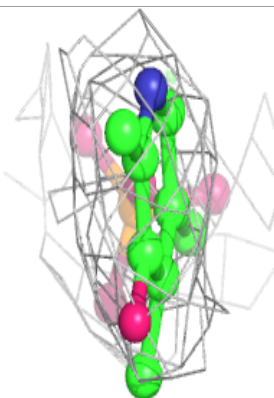
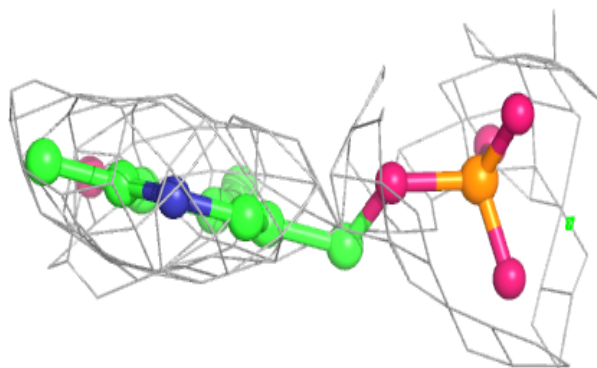
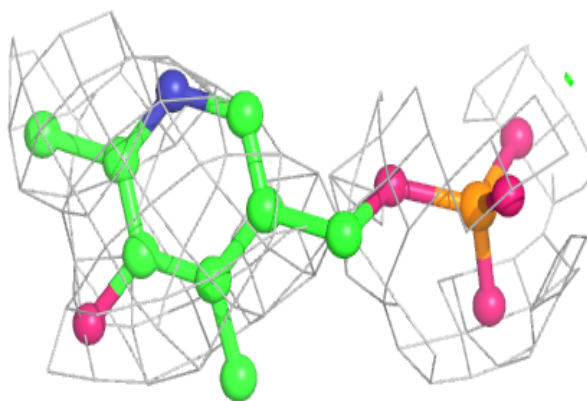
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	PLP	D	500	15/16	0.40	0.47	203,228,245,245	0
2	PLP	C	500	15/16	0.84	0.20	81,123,161,161	0
2	PLP	A	500	15/16	0.94	0.20	46,75,87,89	0
2	PLP	B	500	15/16	0.95	0.18	52,82,120,128	0

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.

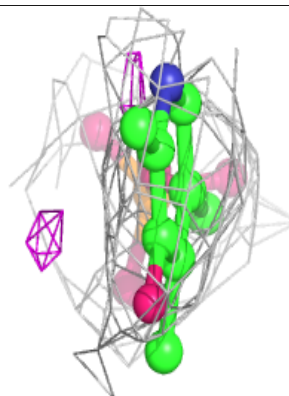
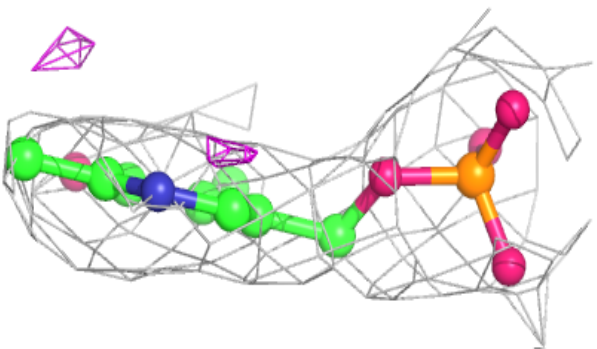
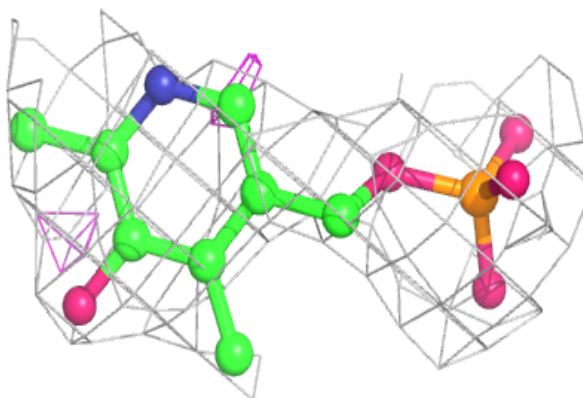


Electron density around PLP C 500:

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

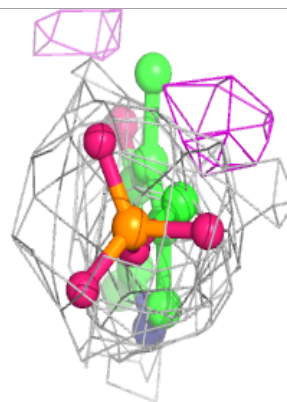
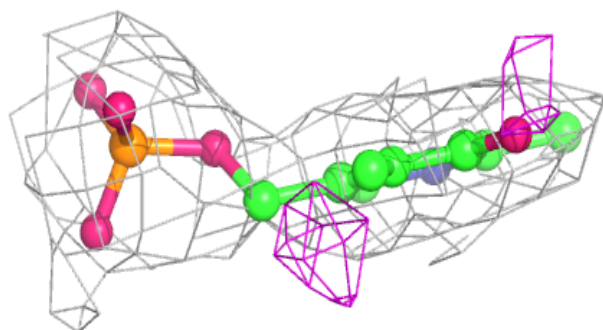
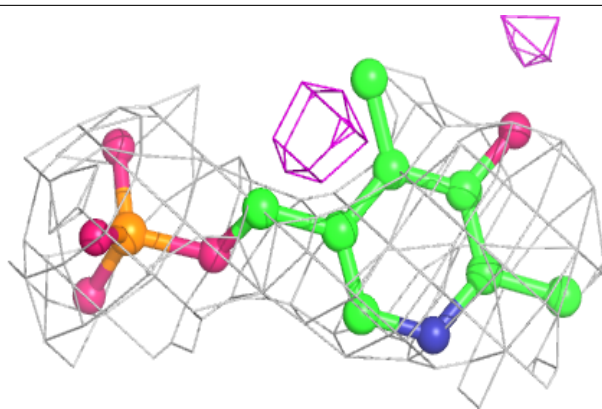
**Electron density around PLP A 500:**

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



Electron density around PLP B 500:

$2mF_o - DF_c$ (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.