



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:06 PM UTC

PDB ID : 7XIN / pdb_00007xin
Title : Crystal structure of DODC from Pseudomonas
Authors : Li, X.; Zhou, Y.L.; Liao, L.J.; Liu, X.K.; Liu, B.; Guo, Y.; Feng, Z.; Sun, D.Y.; Zeng, Z.X.
Deposited on : 2022-04-13
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

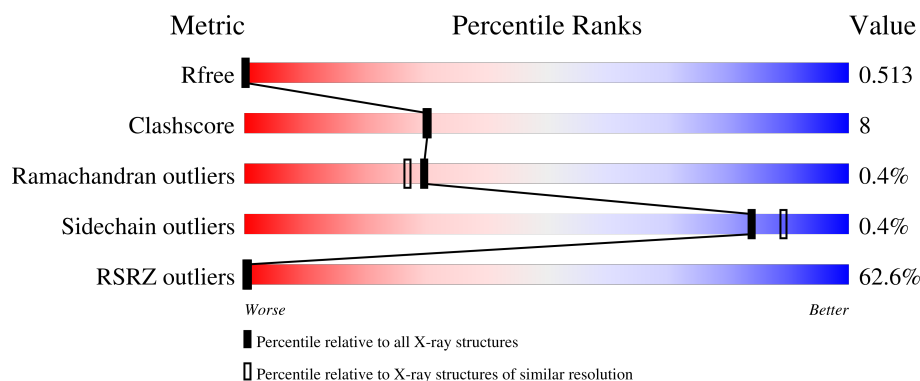
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	476	62% 80% 18%
1	C	476	61% 78% 21%
1	E	476	63% 78% 20%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10953 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 DOPA decarboxylase.

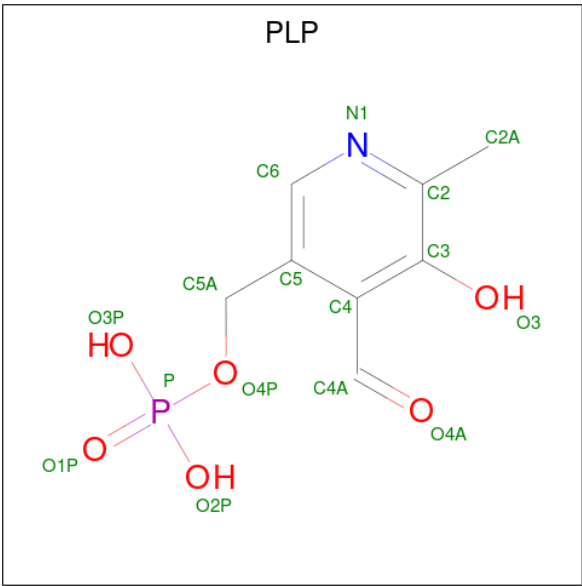
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	470	Total	C	N	O	S	0	0	0
			3636	2302	649	673	12			
1	C	470	Total	C	N	O	S	0	0	0
			3636	2302	649	673	12			
1	E	470	Total	C	N	O	S	0	0	0
			3636	2302	649	673	12			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	expression tag	UNP Q88JU5
A	1	ALA	-	expression tag	UNP Q88JU5
A	471	LEU	-	expression tag	UNP Q88JU5
A	472	GLU	-	expression tag	UNP Q88JU5
A	473	HIS	-	expression tag	UNP Q88JU5
A	474	HIS	-	expression tag	UNP Q88JU5
A	475	HIS	-	expression tag	UNP Q88JU5
C	0	MET	-	expression tag	UNP Q88JU5
C	1	ALA	-	expression tag	UNP Q88JU5
C	471	LEU	-	expression tag	UNP Q88JU5
C	472	GLU	-	expression tag	UNP Q88JU5
C	473	HIS	-	expression tag	UNP Q88JU5
C	474	HIS	-	expression tag	UNP Q88JU5
C	475	HIS	-	expression tag	UNP Q88JU5
E	0	MET	-	expression tag	UNP Q88JU5
E	1	ALA	-	expression tag	UNP Q88JU5
E	471	LEU	-	expression tag	UNP Q88JU5
E	472	GLU	-	expression tag	UNP Q88JU5
E	473	HIS	-	expression tag	UNP Q88JU5
E	474	HIS	-	expression tag	UNP Q88JU5
E	475	HIS	-	expression tag	UNP Q88JU5

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$)

(labeled as "Ligand of Interest" by depositor).

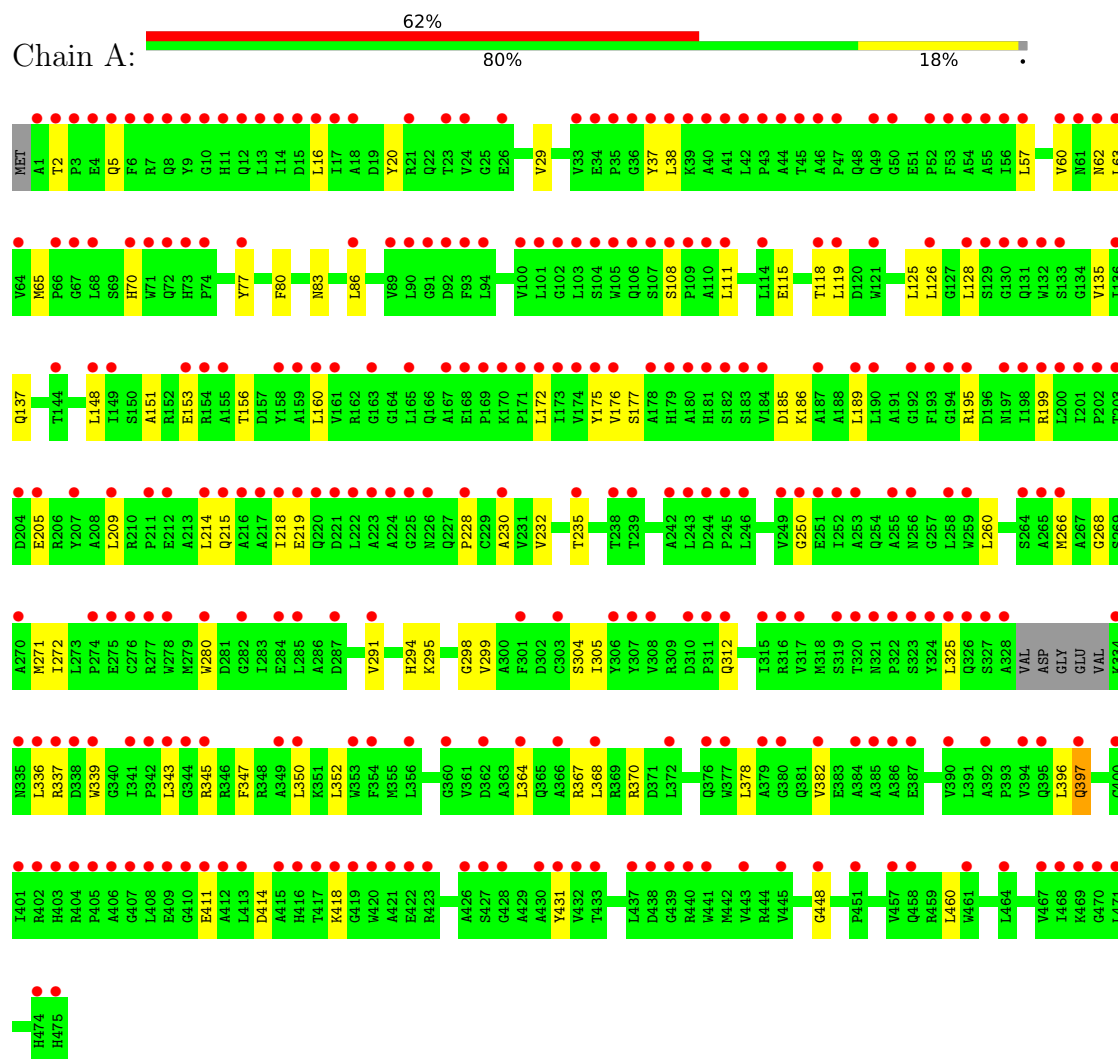


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	15	0
			15	8	1	5	1		
2	C	1	Total	C	N	O	P	15	0
			15	8	1	5	1		
2	E	1	Total	C	N	O	P	15	0
			15	8	1	5	1		

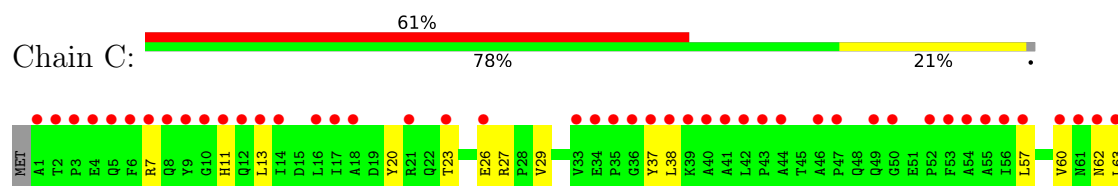
3 Residue-property plots

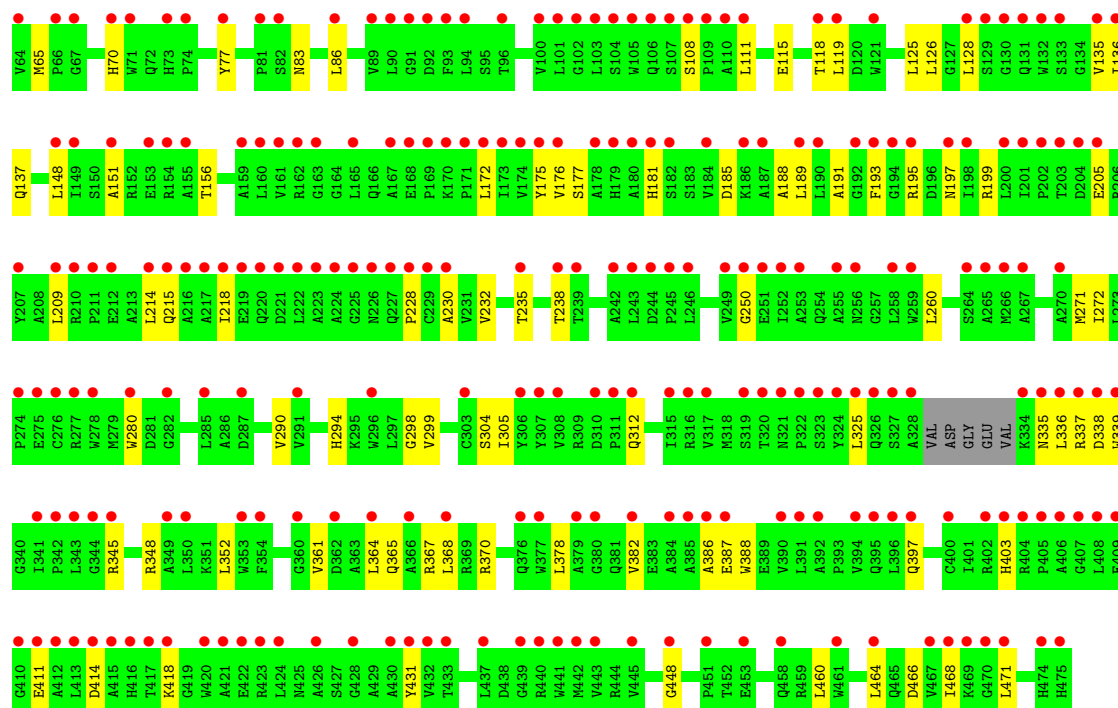
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: DOPA decarboxylase

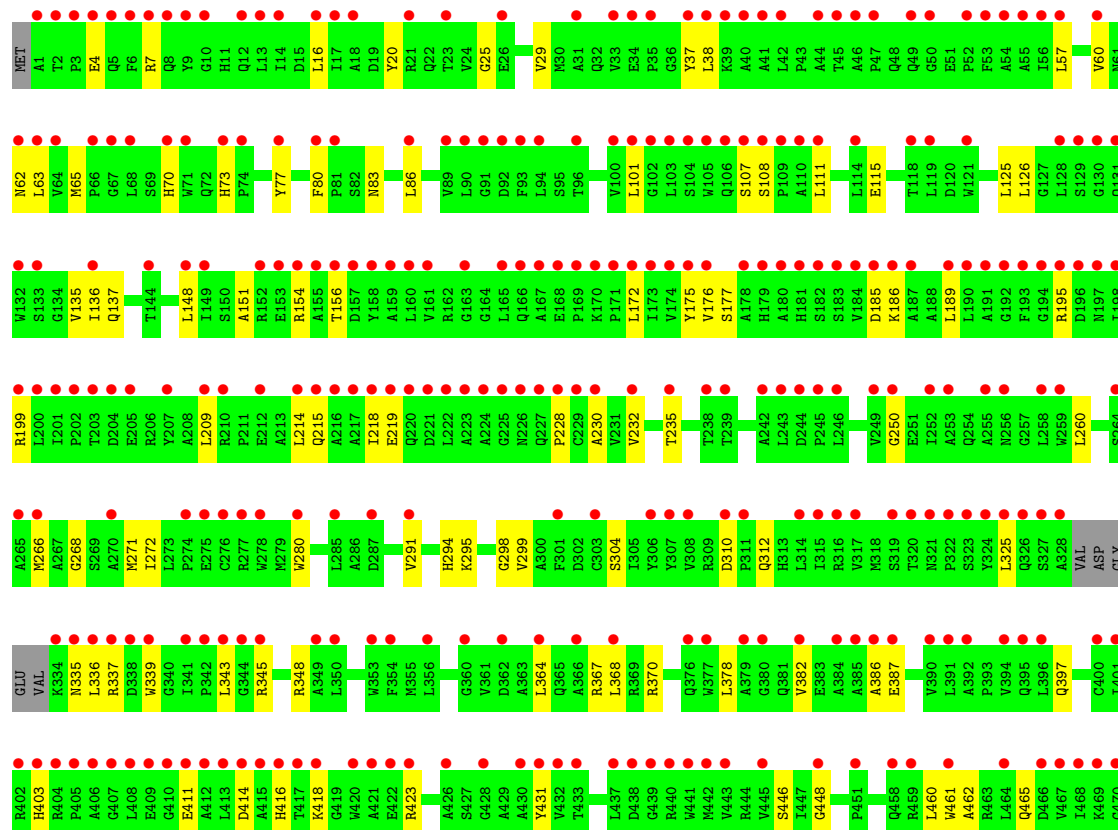
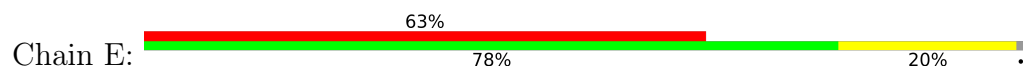


• Molecule 1: DOPA decarboxylase





● Molecule 1: DOPA decarboxylase



L471	E472	H473	H474
		H475	

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	57.77Å 67.01Å 168.58Å 90.27° 92.38° 90.36°	Depositor
Resolution (Å)	43.59 – 2.00 43.59 – 2.00	Depositor EDS
% Data completeness (in resolution range)	70.0 (43.59-2.00) 70.0 (43.59-2.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.96 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0123	Depositor
R, R_{free}	0.473 , 0.521 0.469 , 0.513	Depositor DCC
R_{free} test set	5861 reflections (3.43%)	wwPDB-VP
Wilson B-factor (Å ²)	21.6	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 17.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-l 0.000 for -h,k,-l 0.000 for -h,-k,l	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	10953	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 96.32 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.0910e-10. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

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	0.44	0/3723	0.66	0/5081
1	C	0.44	0/3723	0.65	0/5081
1	E	0.43	0/3723	0.64	0/5081
All	All	0.44	0/11169	0.65	0/15243

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

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	3636	0	3586	59	0
1	C	3636	0	3586	64	0
1	E	3636	0	3586	58	0
2	A	15	0	7	0	0
2	C	15	0	7	0	0
2	E	15	0	7	0	0
All	All	10953	0	10779	181	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 8.

All (181) 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:A:80:PHE:HB3	1:A:266:MET:HE3	1.42	1.01
1:A:199:ARG:HG2	1:A:199:ARG:HH11	1.37	0.89
1:E:80:PHE:HB3	1:E:266:MET:HE3	1.55	0.88
1:E:423:ARG:CZ	1:E:472:GLU:OE2	2.29	0.81
1:C:388:TRP:CZ2	1:C:468:ILE:HD11	2.19	0.77
1:E:115:GLU:OE2	1:E:345:ARG:NH2	2.22	0.69
1:A:115:GLU:OE2	1:A:345:ARG:NH2	2.23	0.67
1:C:388:TRP:HZ2	1:C:468:ILE:CD1	2.07	0.66
1:E:185:ASP:OD1	1:E:195:ARG:NH1	2.29	0.65
1:A:294:HIS:HA	1:A:299:VAL:O	1.96	0.65
1:C:115:GLU:OE2	1:C:345:ARG:NH2	2.26	0.65
1:C:294:HIS:HA	1:C:299:VAL:O	1.97	0.65
1:C:176:VAL:HG12	1:C:232:VAL:HB	1.78	0.65
1:C:388:TRP:HZ2	1:C:468:ILE:HD11	1.63	0.64
1:A:199:ARG:HH11	1:A:199:ARG:CG	2.10	0.64
1:C:388:TRP:CZ2	1:C:468:ILE:CD1	2.81	0.64
1:E:294:HIS:HA	1:E:299:VAL:O	1.98	0.64
1:A:20:TYR:OH	1:A:70:HIS:HD2	1.82	0.63
1:C:199:ARG:HG3	1:C:199:ARG:HH11	1.64	0.62
1:C:20:TYR:OH	1:C:70:HIS:HD2	1.83	0.62
1:A:176:VAL:HG12	1:A:232:VAL:HB	1.81	0.61
1:A:266:MET:HE2	1:A:295:LYS:HD3	1.82	0.61
1:E:268:GLY:HA3	1:E:291:VAL:HG22	1.83	0.60
1:E:423:ARG:NH2	1:E:472:GLU:OE2	2.35	0.60
1:E:176:VAL:HG12	1:E:232:VAL:HB	1.82	0.60
1:E:20:TYR:OH	1:E:70:HIS:HD2	1.85	0.59
1:E:136:ILE:O	1:E:348:ARG:NH2	2.36	0.58
1:E:125:LEU:O	1:E:272:ILE:HA	2.03	0.58
1:A:266:MET:CE	1:A:295:LYS:HB3	2.34	0.58
1:C:271:MET:HG3	1:C:280:TRP:CE2	2.39	0.57
1:A:125:LEU:O	1:A:272:ILE:HA	2.04	0.57
1:E:266:MET:CE	1:E:295:LYS:HB3	2.34	0.57
1:E:135:VAL:HG23	1:E:336:LEU:HD22	1.88	0.56
1:A:205:GLU:H	1:A:205:GLU:CD	2.14	0.54
1:C:125:LEU:O	1:C:272:ILE:HA	2.08	0.54
1:C:185:ASP:O	1:C:189:LEU:HG	2.06	0.53
1:A:199:ARG:CG	1:A:199:ARG:NH1	2.71	0.53
1:C:361:VAL:O	1:C:365:GLN:HG3	2.08	0.53
1:C:205:GLU:H	1:C:205:GLU:CD	2.16	0.53
1:E:154:ARG:NH2	1:E:310:ASP:OD2	2.27	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ASP:O	1:A:189:LEU:HG	2.09	0.53
1:A:268:GLY:HA3	1:A:291:VAL:HG12	1.90	0.53
1:E:185:ASP:O	1:E:189:LEU:HG	2.09	0.53
1:E:250:GLY:HA2	1:E:260:LEU:HD22	1.91	0.53
1:A:111:LEU:HD21	1:A:345:ARG:HG3	1.91	0.52
1:C:135:VAL:HG23	1:C:336:LEU:HD22	1.92	0.52
1:A:199:ARG:HG2	1:A:199:ARG:NH1	2.15	0.52
1:E:111:LEU:HD21	1:E:345:ARG:HG3	1.90	0.52
1:C:271:MET:HG3	1:C:280:TRP:CZ2	2.44	0.52
1:C:235:THR:HG21	1:C:280:TRP:CD1	2.44	0.52
1:C:62:ASN:C	1:C:63:LEU:HD23	2.34	0.52
1:A:414:ASP:O	1:A:418:LYS:HG2	2.10	0.52
1:C:137:GLN:N	1:C:304:SER:O	2.41	0.51
1:E:62:ASN:C	1:E:63:LEU:HD23	2.35	0.51
1:C:367:ARG:O	1:C:370:ARG:HB3	2.11	0.51
1:C:199:ARG:HG3	1:C:199:ARG:NH1	2.25	0.51
1:C:335:ASN:HB3	1:C:338:ASP:OD1	2.12	0.50
1:A:83:ASN:HB3	1:A:298:GLY:HA2	1.94	0.50
1:C:111:LEU:HD21	1:C:345:ARG:HG3	1.93	0.50
1:A:62:ASN:C	1:A:63:LEU:HD23	2.36	0.50
1:E:403:HIS:HD2	1:E:416:HIS:NE2	2.10	0.50
1:A:80:PHE:CB	1:A:266:MET:HE3	2.29	0.50
1:C:136:ILE:O	1:C:348:ARG:NH2	2.45	0.50
1:A:266:MET:HE2	1:A:295:LYS:HB3	1.93	0.50
1:A:118:THR:HB	1:A:352:LEU:HD23	1.94	0.49
1:E:126:LEU:HD22	1:E:271:MET:HB2	1.93	0.49
1:A:135:VAL:HG23	1:A:336:LEU:HD22	1.95	0.49
1:C:135:VAL:HG11	1:C:339:TRP:HB3	1.94	0.49
1:C:386:ALA:O	1:C:387:GLU:HB2	2.10	0.49
1:A:185:ASP:OD1	1:A:195:ARG:NH1	2.45	0.49
1:C:466:ASP:HB3	1:C:471:LEU:HB2	1.95	0.49
1:A:137:GLN:N	1:A:304:SER:O	2.43	0.49
1:C:250:GLY:HA2	1:C:260:LEU:HD22	1.94	0.48
1:A:2:THR:H	1:A:5:GLN:HE21	1.60	0.48
1:C:335:ASN:HD21	1:C:337:ARG:CZ	2.25	0.48
1:A:126:LEU:HD22	1:A:271:MET:HB2	1.96	0.48
1:E:266:MET:HE1	1:E:295:LYS:HB3	1.95	0.48
1:A:151:ALA:HB1	1:A:230:ALA:HB2	1.96	0.48
1:C:214:LEU:O	1:C:218:ILE:HG13	2.14	0.47
1:E:186:LYS:HA	1:E:189:LEU:HD12	1.96	0.47
1:A:250:GLY:HA2	1:A:260:LEU:HD22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:414:ASP:O	1:E:418:LYS:HG2	2.14	0.47
1:A:135:VAL:HG11	1:A:339:TRP:HB3	1.97	0.47
1:A:128:LEU:HD21	1:A:280:TRP:CZ3	2.49	0.47
1:A:266:MET:CE	1:A:295:LYS:HD3	2.44	0.47
1:C:378:LEU:O	1:C:382:VAL:HG23	2.15	0.47
1:C:118:THR:HB	1:C:352:LEU:HD23	1.97	0.47
1:A:364:LEU:O	1:A:368:LEU:HG	2.15	0.47
1:C:215:GLN:O	1:C:215:GLN:HG3	2.15	0.47
1:E:77:TYR:CE2	1:E:460:LEU:HD22	2.50	0.46
1:E:337:ARG:HD3	1:E:343:LEU:HD23	1.97	0.46
1:C:151:ALA:HB1	1:C:230:ALA:HB2	1.98	0.46
1:C:83:ASN:HB3	1:C:298:GLY:HA2	1.98	0.46
1:E:83:ASN:HB3	1:E:298:GLY:HA2	1.98	0.46
1:C:290:VAL:HG23	1:C:305:ILE:O	2.16	0.46
1:A:378:LEU:O	1:A:382:VAL:HG23	2.16	0.46
1:E:86:LEU:HD23	1:E:86:LEU:HA	1.68	0.46
1:E:364:LEU:O	1:E:368:LEU:HG	2.16	0.46
1:A:214:LEU:O	1:A:218:ILE:HG13	2.16	0.45
1:A:235:THR:HG21	1:A:280:TRP:CD1	2.51	0.45
1:A:367:ARG:O	1:A:370:ARG:HB3	2.16	0.45
1:C:29:VAL:CG1	1:C:431:TYR:HB2	2.47	0.45
1:E:137:GLN:N	1:E:304:SER:O	2.46	0.45
1:E:148:LEU:HD23	1:E:148:LEU:HA	1.78	0.45
1:A:312:GLN:OE1	1:A:325:LEU:HA	2.16	0.45
1:A:186:LYS:HA	1:A:189:LEU:HD12	1.98	0.45
1:C:77:TYR:CE2	1:C:460:LEU:HD22	2.52	0.45
1:E:60:VAL:O	1:E:65:MET:HG2	2.17	0.45
1:E:335:ASN:HD21	1:E:337:ARG:CZ	2.29	0.45
1:A:86:LEU:HD23	1:A:86:LEU:HA	1.71	0.45
1:C:188:ALA:O	1:C:193:PHE:HD1	1.98	0.45
1:E:151:ALA:HB1	1:E:230:ALA:HB2	1.99	0.45
1:E:367:ARG:O	1:E:370:ARG:HB3	2.17	0.45
1:E:235:THR:HG21	1:E:280:TRP:CD1	2.52	0.44
1:C:126:LEU:HD22	1:C:271:MET:HB2	1.99	0.44
1:E:135:VAL:HG11	1:E:339:TRP:HB3	1.99	0.44
1:E:177:SER:HB2	1:E:209:LEU:HB3	2.00	0.44
1:C:156:THR:CG2	1:C:172:LEU:HD11	2.47	0.44
1:C:364:LEU:O	1:C:368:LEU:HG	2.17	0.44
1:E:199:ARG:HH11	1:E:199:ARG:HG3	1.81	0.44
1:A:77:TYR:CE2	1:A:460:LEU:HD22	2.53	0.44
1:A:153:GLU:OE1	1:A:160:LEU:HD22	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:VAL:HG11	1:A:339:TRP:O	2.18	0.44
1:E:135:VAL:HG11	1:E:339:TRP:O	2.18	0.44
1:E:266:MET:HE2	1:E:295:LYS:HB3	1.98	0.44
1:C:460:LEU:O	1:C:464:LEU:HD12	2.17	0.44
1:E:266:MET:HE2	1:E:295:LYS:HD3	2.00	0.44
1:A:60:VAL:O	1:A:65:MET:HG2	2.18	0.44
1:C:175:TYR:HE2	1:C:228:PRO:HB3	1.82	0.44
1:A:177:SER:HB2	1:A:209:LEU:HB3	2.00	0.44
1:C:7:ARG:HG2	1:C:11:HIS:CE1	2.53	0.43
1:A:266:MET:HE1	1:A:295:LYS:HB3	1.98	0.43
1:C:148:LEU:HD23	1:C:148:LEU:HA	1.79	0.43
1:A:29:VAL:CG1	1:A:431:TYR:HB2	2.49	0.43
1:A:37:TYR:CG	1:A:38:LEU:N	2.87	0.43
1:A:396:LEU:HD23	1:A:397:GLN:OE1	2.17	0.43
1:A:175:TYR:HE2	1:A:228:PRO:HB3	1.82	0.43
1:A:337:ARG:CG	1:A:343:LEU:HD23	2.49	0.43
1:C:37:TYR:CG	1:C:38:LEU:N	2.87	0.43
1:E:37:TYR:CG	1:E:38:LEU:N	2.87	0.43
1:E:215:GLN:HG3	1:E:219:GLU:OE2	2.18	0.43
1:E:29:VAL:CG1	1:E:431:TYR:HB2	2.49	0.43
1:A:148:LEU:HD23	1:A:148:LEU:HA	1.82	0.43
1:C:414:ASP:O	1:C:418:LYS:HG2	2.19	0.43
1:E:312:GLN:OE1	1:E:325:LEU:HA	2.19	0.43
1:A:156:THR:CG2	1:A:172:LEU:HD11	2.48	0.43
1:C:185:ASP:OD1	1:C:195:ARG:NH2	2.51	0.43
1:E:378:LEU:O	1:E:382:VAL:HG23	2.19	0.43
1:A:215:GLN:O	1:A:215:GLN:HG3	2.18	0.42
1:C:411:GLU:H	1:C:411:GLU:HG2	1.57	0.42
1:E:175:TYR:HE2	1:E:228:PRO:HB3	1.84	0.42
1:A:411:GLU:H	1:A:411:GLU:HG2	1.56	0.42
1:E:386:ALA:O	1:E:387:GLU:HB2	2.20	0.42
1:A:119:LEU:CD2	1:A:305:ILE:HD12	2.49	0.42
1:C:119:LEU:CD2	1:C:305:ILE:HD12	2.49	0.42
1:C:23:THR:HB	1:C:26:GLU:OE2	2.20	0.42
1:C:37:TYR:OH	1:C:63:LEU:O	2.34	0.42
1:A:215:GLN:HG3	1:A:219:GLU:OE2	2.19	0.41
1:C:135:VAL:HG11	1:C:339:TRP:O	2.20	0.41
1:C:193:PHE:O	1:C:197:ASN:ND2	2.38	0.41
1:A:16:LEU:HD13	1:A:57:LEU:HD22	2.02	0.41
1:C:177:SER:HB2	1:C:209:LEU:HB3	2.03	0.41
1:C:387:GLU:HB3	1:C:403:HIS:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:VAL:O	1:C:65:MET:HG2	2.20	0.41
1:C:312:GLN:OE1	1:C:325:LEU:HA	2.21	0.41
1:E:77:TYR:HA	1:E:446:SER:O	2.21	0.41
1:E:461:TRP:O	1:E:465:GLN:HG3	2.19	0.41
1:E:214:LEU:O	1:E:218:ILE:HG13	2.19	0.41
1:E:16:LEU:HD13	1:E:57:LEU:HD22	2.02	0.41
1:C:86:LEU:HD23	1:C:86:LEU:HA	1.78	0.41
1:E:4:GLU:OE2	1:E:7:ARG:NE	2.54	0.41
1:E:101:LEU:O	1:E:107:SER:OG	2.39	0.41
1:E:411:GLU:H	1:E:411:GLU:HG2	1.57	0.41
1:E:156:THR:CG2	1:E:172:LEU:HD11	2.51	0.41
1:E:462:ALA:HA	1:E:465:GLN:HE21	1.86	0.40
1:C:181:HIS:CD2	1:C:238:THR:HG21	2.57	0.40
1:C:191:ALA:HB3	1:C:193:PHE:CE1	2.56	0.40
1:A:347:PHE:CD1	1:A:350:LEU:HG	2.56	0.40
1:C:27:ARG:CZ	1:C:65:MET:HE2	2.52	0.40
1:C:13:LEU:HD13	1:C:57:LEU:HD21	2.04	0.40
1:E:25:GLY:HA2	1:E:73:HIS:NE2	2.37	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	466/476 (98%)	440 (94%)	24 (5%)	2 (0%)	30	27
1	C	466/476 (98%)	438 (94%)	26 (6%)	2 (0%)	30	27
1	E	466/476 (98%)	441 (95%)	23 (5%)	2 (0%)	30	27
All	All	1398/1428 (98%)	1319 (94%)	73 (5%)	6 (0%)	30	27

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	108	SER
1	C	108	SER
1	E	108	SER
1	E	448	GLY
1	A	448	GLY
1	C	448	GLY

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	375/380 (99%)	374 (100%)	1 (0%)	86	91
1	C	375/380 (99%)	373 (100%)	2 (0%)	81	87
1	E	375/380 (99%)	374 (100%)	1 (0%)	86	91
All	All	1125/1140 (99%)	1121 (100%)	4 (0%)	84	89

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	397	GLN
1	C	128	LEU
1	C	397	GLN
1	E	397	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	12	GLN
1	A	32	GLN
1	A	70	HIS
1	A	106	GLN
1	A	131	GLN
1	A	220	GLN
1	A	381	GLN

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Mol	Chain	Res	Type
1	A	475	HIS
1	C	12	GLN
1	C	49	GLN
1	C	70	HIS
1	C	106	GLN
1	C	226	ASN
1	C	381	GLN
1	C	458	GLN
1	C	475	HIS
1	E	12	GLN
1	E	70	HIS
1	E	106	GLN
1	E	124	GLN
1	E	381	GLN
1	E	403	HIS
1	E	465	GLN
1	E	475	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	C	501	1	15,15,16	1.12	2 (13%)	21,22,23	1.10	2 (9%)
2	PLP	E	501	1	15,15,16	1.08	1 (6%)	21,22,23	1.31	2 (9%)
2	PLP	A	501	1	15,15,16	1.12	1 (6%)	21,22,23	1.15	2 (9%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLP	C	501	1	-	0/6/6/8	0/1/1/1
2	PLP	E	501	1	-	1/6/6/8	0/1/1/1
2	PLP	A	501	1	-	0/6/6/8	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	PLP	C2-N1	2.63	1.38	1.33
2	C	501	PLP	C2-N1	2.59	1.38	1.33
2	E	501	PLP	C6-N1	2.17	1.38	1.34
2	C	501	PLP	C6-N1	2.02	1.38	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	501	PLP	C5-C6-N1	-3.28	118.49	123.83
2	E	501	PLP	C6-C5-C4	2.50	120.15	118.10
2	A	501	PLP	C6-C5-C4	2.45	120.11	118.10
2	A	501	PLP	C5-C6-N1	-2.40	119.92	123.83
2	C	501	PLP	C5-C6-N1	-2.34	120.02	123.83
2	C	501	PLP	C6-C5-C4	2.31	119.99	118.10

There are no chirality outliers.

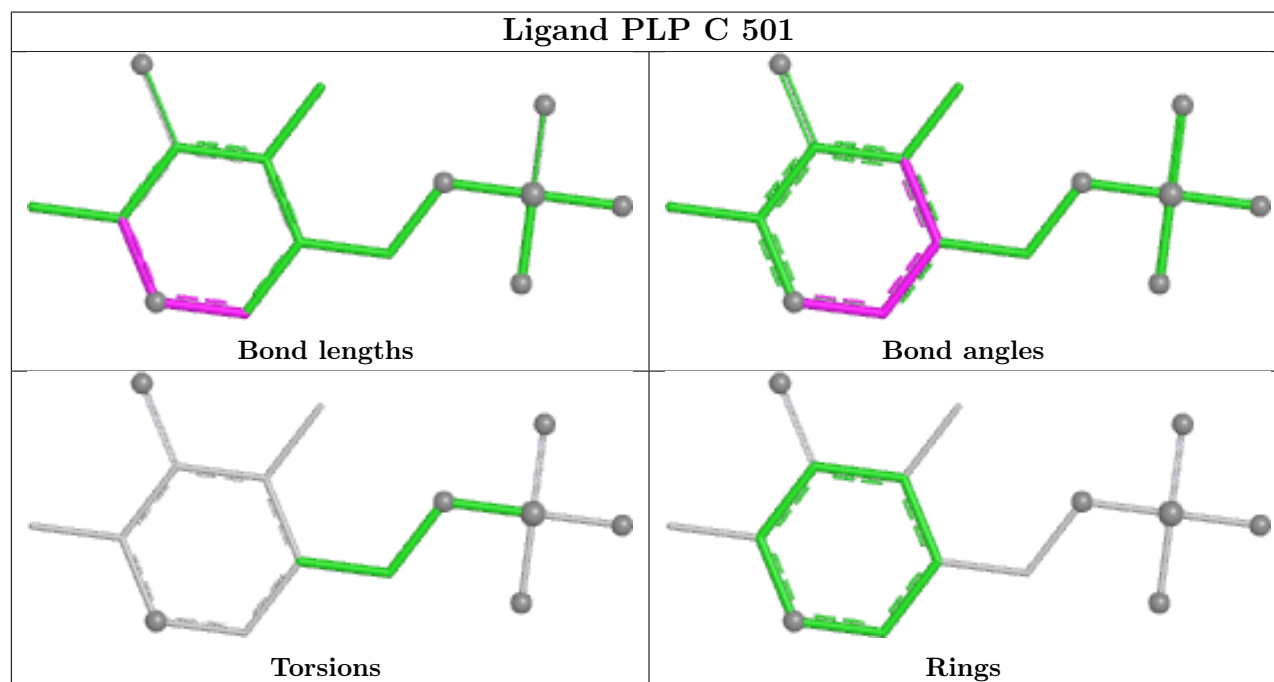
All (1) torsion outliers are listed below:

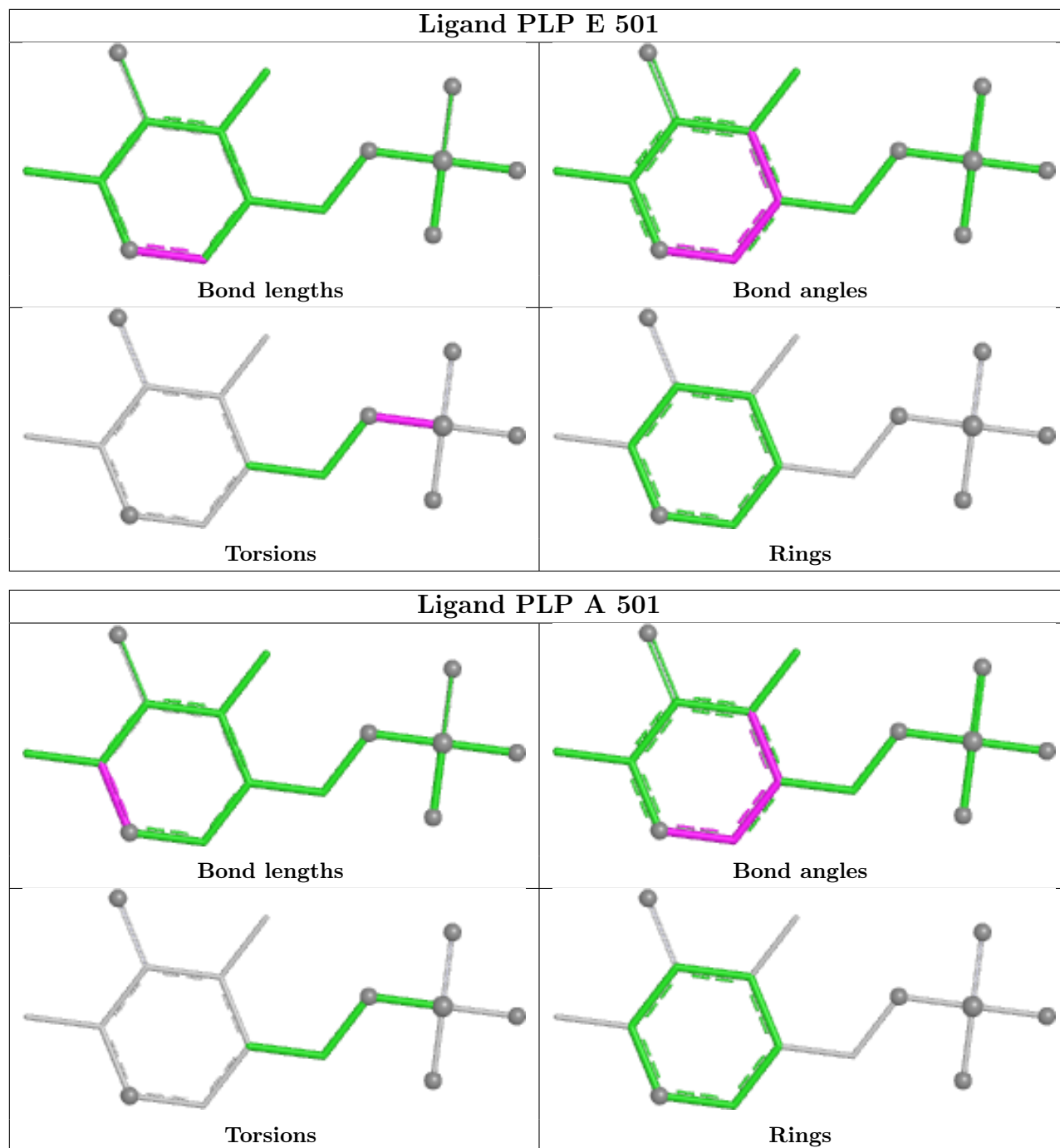
Mol	Chain	Res	Type	Atoms
2	E	501	PLP	C5A-O4P-P-O1P

There are no ring outliers.

No monomer is involved in short contacts.

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





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	470/476 (98%)	2.54	293 (62%) 0 0	17, 30, 41, 51	0
1	C	470/476 (98%)	2.53	291 (61%) 0 0	17, 30, 42, 51	0
1	E	470/476 (98%)	2.57	299 (63%) 0 0	17, 30, 42, 52	0
All	All	1410/1428 (98%)	2.55	883 (62%) 0 0	17, 30, 42, 52	0

All (883) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	328	ALA	9.3
1	E	328	ALA	9.2
1	C	328	ALA	9.0
1	A	39	LYS	7.4
1	C	280	TRP	7.3
1	A	2	THR	6.7
1	E	224	ALA	6.7
1	E	34	GLU	6.7
1	C	224	ALA	6.6
1	C	39	LYS	6.5
1	E	343	LEU	6.5
1	A	224	ALA	6.3
1	E	413	LEU	6.3
1	E	387	GLU	6.2
1	E	468	ILE	6.2
1	A	411	GLU	6.1
1	C	266	MET	6.1
1	E	406	ALA	6.1
1	E	408	LEU	6.0
1	A	408	LEU	6.0
1	E	2	THR	6.0
1	C	411	GLU	6.0
1	C	408	LEU	5.9

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Mol	Chain	Res	Type	RSRZ
1	C	343	LEU	5.9
1	A	445	VAL	5.9
1	E	159	ALA	5.8
1	E	101	LEU	5.8
1	C	2	THR	5.8
1	A	426	ALA	5.8
1	E	39	LYS	5.8
1	A	406	ALA	5.7
1	C	406	ALA	5.7
1	C	413	LEU	5.7
1	C	303	CYS	5.7
1	C	410	GLY	5.6
1	E	411	GLU	5.6
1	A	413	LEU	5.6
1	C	169	PRO	5.6
1	A	159	ALA	5.6
1	C	159	ALA	5.6
1	E	426	ALA	5.5
1	A	343	LEU	5.5
1	E	26	GLU	5.4
1	A	169	PRO	5.4
1	C	426	ALA	5.4
1	C	6	PHE	5.4
1	A	6	PHE	5.4
1	E	169	PRO	5.3
1	E	404	ARG	5.3
1	C	101	LEU	5.3
1	E	4	GLU	5.3
1	C	405	PRO	5.3
1	E	198	ILE	5.3
1	A	55	ALA	5.2
1	C	404	ARG	5.2
1	E	405	PRO	5.2
1	C	55	ALA	5.2
1	E	445	VAL	5.2
1	A	410	GLY	5.1
1	A	107	SER	5.1
1	E	6	PHE	5.1
1	A	423	ARG	5.0
1	A	198	ILE	5.0
1	E	415	ALA	5.0
1	C	38	LEU	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	405	PRO	5.0
1	E	410	GLY	5.0
1	A	258	LEU	5.0
1	A	280	TRP	4.9
1	C	5	GLN	4.9
1	A	128	LEU	4.9
1	A	5	GLN	4.9
1	A	101	LEU	4.8
1	C	198	ILE	4.8
1	E	258	LEU	4.8
1	E	193	PHE	4.8
1	E	202	PRO	4.8
1	A	26	GLU	4.8
1	A	193	PHE	4.8
1	A	202	PRO	4.8
1	E	5	GLN	4.8
1	A	199	ARG	4.8
1	C	26	GLU	4.7
1	C	258	LEU	4.7
1	E	325	LEU	4.7
1	A	178	ALA	4.7
1	A	415	ALA	4.7
1	E	55	ALA	4.7
1	C	468	ILE	4.7
1	E	205	GLU	4.7
1	E	324	TYR	4.6
1	C	202	PRO	4.6
1	C	415	ALA	4.6
1	E	475	HIS	4.6
1	A	379	ALA	4.6
1	A	285	LEU	4.6
1	C	107	SER	4.6
1	A	325	LEU	4.5
1	A	205	GLU	4.5
1	E	338	ASP	4.5
1	A	18	ALA	4.5
1	E	63	LEU	4.5
1	A	324	TYR	4.4
1	E	105	TRP	4.4
1	E	407	GLY	4.4
1	A	317	VAL	4.4
1	C	128	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	218	ILE	4.4
1	C	474	HIS	4.4
1	E	173	ILE	4.4
1	E	317	VAL	4.4
1	C	119	LEU	4.4
1	E	128	LEU	4.4
1	E	280	TRP	4.3
1	C	53	PHE	4.3
1	A	255	ALA	4.3
1	E	100	VAL	4.3
1	E	107	SER	4.3
1	C	325	LEU	4.3
1	E	379	ALA	4.3
1	A	63	LEU	4.3
1	E	103	LEU	4.3
1	C	423	ARG	4.3
1	A	220	GLN	4.3
1	C	105	TRP	4.3
1	A	53	PHE	4.3
1	C	220	GLN	4.3
1	A	412	ALA	4.2
1	C	63	LEU	4.2
1	E	326	GLN	4.2
1	E	327	SER	4.2
1	A	195	ARG	4.2
1	E	18	ALA	4.2
1	A	475	HIS	4.2
1	E	220	GLN	4.2
1	A	407	GLY	4.2
1	A	173	ILE	4.2
1	A	404	ARG	4.2
1	C	379	ALA	4.2
1	A	38	LEU	4.2
1	C	317	VAL	4.2
1	C	205	GLU	4.2
1	A	468	ILE	4.2
1	E	178	ALA	4.2
1	A	57	LEU	4.2
1	A	119	LEU	4.2
1	C	103	LEU	4.2
1	C	182	SER	4.1
1	E	255	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
1	E	38	LEU	4.1
1	C	193	PHE	4.1
1	A	161	VAL	4.1
1	C	195	ARG	4.1
1	E	53	PHE	4.1
1	A	17	ILE	4.1
1	C	17	ILE	4.1
1	C	173	ILE	4.1
1	C	35	PRO	4.1
1	E	474	HIS	4.1
1	A	167	ALA	4.1
1	C	18	ALA	4.1
1	A	103	LEU	4.1
1	A	437	LEU	4.1
1	A	326	GLN	4.1
1	C	475	HIS	4.1
1	A	4	GLU	4.1
1	A	105	TRP	4.1
1	E	423	ARG	4.1
1	C	1	ALA	4.1
1	C	336	LEU	4.1
1	E	161	VAL	4.1
1	A	182	SER	4.1
1	A	327	SER	4.1
1	E	353	TRP	4.0
1	A	1	ALA	4.0
1	C	255	ALA	4.0
1	C	407	GLY	4.0
1	E	119	LEU	4.0
1	C	4	GLU	4.0
1	C	445	VAL	4.0
1	E	432	VAL	4.0
1	C	327	SER	4.0
1	E	17	ILE	4.0
1	E	102	GLY	4.0
1	A	165	LEU	4.0
1	A	336	LEU	4.0
1	C	57	LEU	4.0
1	E	336	LEU	4.0
1	E	409	GLU	4.0
1	C	218	ILE	4.0
1	E	181	HIS	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	64	VAL	4.0
1	C	409	GLU	4.0
1	A	353	TRP	3.9
1	E	222	LEU	3.9
1	C	326	GLN	3.9
1	C	7	ARG	3.9
1	A	102	GLY	3.9
1	E	1	ALA	3.9
1	C	165	LEU	3.9
1	E	13	LEU	3.9
1	A	249	VAL	3.9
1	A	52	PRO	3.9
1	E	149	ILE	3.9
1	C	219	GLU	3.9
1	C	353	TRP	3.9
1	C	100	VAL	3.9
1	E	57	LEU	3.9
1	E	52	PRO	3.9
1	A	100	VAL	3.8
1	A	474	HIS	3.8
1	E	64	VAL	3.8
1	C	324	TYR	3.8
1	A	8	GLN	3.8
1	A	46	ALA	3.8
1	E	218	ILE	3.8
1	E	385	ALA	3.8
1	E	170	LYS	3.8
1	A	149	ILE	3.8
1	C	149	ILE	3.8
1	E	14	ILE	3.8
1	C	385	ALA	3.8
1	C	412	ALA	3.8
1	A	432	VAL	3.8
1	C	161	VAL	3.8
1	C	275	GLU	3.8
1	E	129	SER	3.7
1	A	37	TYR	3.7
1	C	37	TYR	3.7
1	A	181	HIS	3.7
1	A	392	ALA	3.7
1	C	178	ALA	3.7
1	E	94	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	E	285	LEU	3.7
1	E	3	PRO	3.7
1	C	8	GLN	3.7
1	E	195	ARG	3.7
1	C	67	GLY	3.7
1	A	16	LEU	3.7
1	A	35	PRO	3.7
1	C	14	ILE	3.7
1	C	320	THR	3.7
1	E	223	ALA	3.7
1	C	16	LEU	3.7
1	E	8	GLN	3.7
1	A	225	GLY	3.7
1	A	337	ARG	3.7
1	C	384	ALA	3.7
1	E	412	ALA	3.7
1	C	285	LEU	3.6
1	C	437	LEU	3.6
1	E	16	LEU	3.6
1	E	209	LEU	3.6
1	C	52	PRO	3.6
1	E	182	SER	3.6
1	C	337	ARG	3.6
1	C	167	ALA	3.6
1	A	94	LEU	3.6
1	A	342	PRO	3.6
1	E	165	LEU	3.6
1	C	94	LEU	3.6
1	E	437	LEU	3.6
1	C	276	CYS	3.6
1	A	409	GLU	3.6
1	A	129	SER	3.6
1	A	170	LYS	3.6
1	E	337	ARG	3.6
1	A	60	VAL	3.6
1	A	64	VAL	3.6
1	A	253	ALA	3.6
1	E	335	ASN	3.6
1	C	129	SER	3.6
1	C	60	VAL	3.5
1	E	308	VAL	3.5
1	E	7	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	111	LEU	3.5
1	E	200	LEU	3.5
1	C	102	GLY	3.5
1	E	37	TYR	3.5
1	A	339	TRP	3.5
1	C	432	VAL	3.5
1	A	422	GLU	3.5
1	A	3	PRO	3.5
1	E	35	PRO	3.5
1	E	253	ALA	3.5
1	E	342	PRO	3.5
1	E	392	ALA	3.5
1	C	86	LEU	3.5
1	E	464	LEU	3.5
1	E	264	SER	3.5
1	E	219	GLU	3.5
1	A	33	VAL	3.5
1	C	334	LYS	3.5
1	A	14	ILE	3.5
1	A	385	ALA	3.5
1	C	3	PRO	3.5
1	E	384	ALA	3.5
1	A	214	LEU	3.5
1	E	469	LYS	3.5
1	C	308	VAL	3.5
1	C	382	VAL	3.5
1	E	249	VAL	3.5
1	E	167	ALA	3.4
1	E	90	LEU	3.4
1	A	387	GLU	3.4
1	E	207	TYR	3.4
1	A	315	ILE	3.4
1	E	10	GLY	3.4
1	E	46	ALA	3.4
1	E	67	GLY	3.4
1	A	7	ARG	3.4
1	E	189	LEU	3.4
1	E	275	GLU	3.4
1	C	181	HIS	3.4
1	E	33	VAL	3.4
1	A	311	PRO	3.4
1	C	66	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	50	GLY	3.4
1	C	392	ALA	3.4
1	C	90	LEU	3.4
1	C	189	LEU	3.4
1	A	376	GLN	3.4
1	C	376	GLN	3.4
1	C	62	ASN	3.4
1	C	238	THR	3.4
1	C	387	GLU	3.4
1	A	344	GLY	3.4
1	C	46	ALA	3.4
1	C	201	ILE	3.4
1	A	172	LEU	3.4
1	C	13	LEU	3.4
1	C	200	LEU	3.4
1	E	62	ASN	3.3
1	E	320	THR	3.3
1	C	170	LYS	3.3
1	A	319	SER	3.3
1	A	382	VAL	3.3
1	E	382	VAL	3.3
1	A	222	LEU	3.3
1	A	62	ASN	3.3
1	E	238	THR	3.3
1	A	171	PRO	3.3
1	E	228	PRO	3.3
1	A	308	VAL	3.3
1	E	179	HIS	3.3
1	E	226	ASN	3.3
1	E	339	TRP	3.3
1	C	49	GLN	3.3
1	A	264	SER	3.3
1	C	431	TYR	3.3
1	E	60	VAL	3.3
1	A	90	LEU	3.3
1	E	422	GLU	3.3
1	C	469	LYS	3.3
1	A	66	PRO	3.2
1	C	225	GLY	3.2
1	C	249	VAL	3.2
1	E	40	ALA	3.2
1	A	200	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	334	LYS	3.2
1	C	264	SER	3.2
1	E	104	SER	3.2
1	A	380	GLY	3.2
1	C	342	PRO	3.2
1	E	311	PRO	3.2
1	E	291	VAL	3.2
1	E	394	VAL	3.2
1	C	207	TYR	3.2
1	C	148	LEU	3.2
1	E	201	ILE	3.2
1	A	49	GLN	3.2
1	E	131	GLN	3.2
1	A	92	ASP	3.2
1	A	133	SER	3.2
1	C	21	ARG	3.2
1	E	316	ARG	3.2
1	E	163	GLY	3.2
1	E	194	GLY	3.2
1	C	89	VAL	3.2
1	A	223	ALA	3.2
1	E	41	ALA	3.2
1	E	431	TYR	3.2
1	A	320	THR	3.2
1	C	130	GLY	3.2
1	A	384	ALA	3.1
1	C	33	VAL	3.1
1	C	174	VAL	3.1
1	C	111	LEU	3.1
1	A	21	ARG	3.1
1	A	207	TYR	3.1
1	A	431	TYR	3.1
1	E	175	TYR	3.1
1	E	239	THR	3.1
1	A	395	GLN	3.1
1	E	400	CYS	3.1
1	A	40	ALA	3.1
1	C	40	ALA	3.1
1	E	176	VAL	3.1
1	C	339	TRP	3.1
1	A	219	GLU	3.1
1	A	252	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	252	ILE	3.1
1	E	160	LEU	3.1
1	A	175	TYR	3.1
1	A	226	ASN	3.1
1	E	47	PRO	3.1
1	E	21	ARG	3.1
1	A	244	ASP	3.1
1	C	214	LEU	3.1
1	E	252	ILE	3.1
1	A	71	TRP	3.1
1	E	278	TRP	3.1
1	A	323	SER	3.1
1	E	417	THR	3.1
1	E	244	ASP	3.1
1	A	394	VAL	3.1
1	E	443	VAL	3.1
1	A	13	LEU	3.1
1	A	160	LEU	3.1
1	C	222	LEU	3.1
1	A	201	ILE	3.1
1	C	104	SER	3.1
1	A	163	GLY	3.0
1	C	439	GLY	3.0
1	E	225	GLY	3.0
1	E	306	TYR	3.0
1	E	344	GLY	3.0
1	C	321	ASN	3.0
1	E	93	PHE	3.0
1	C	244	ASP	3.0
1	A	179	HIS	3.0
1	C	464	LEU	3.0
1	E	376	GLN	3.0
1	A	67	GLY	3.0
1	C	226	ASN	3.0
1	C	306	TYR	3.0
1	E	212	GLU	3.0
1	C	179	HIS	3.0
1	C	253	ALA	3.0
1	A	89	VAL	3.0
1	A	104	SER	3.0
1	A	464	LEU	3.0
1	C	467	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	275	GLU	3.0
1	A	420	TRP	3.0
1	A	469	LYS	3.0
1	E	155	ALA	3.0
1	A	400	CYS	3.0
1	E	174	VAL	3.0
1	C	34	GLU	3.0
1	A	132	TRP	3.0
1	E	441	TRP	3.0
1	A	212	GLU	2.9
1	A	349	ALA	2.9
1	A	421	ALA	2.9
1	C	422	GLU	2.9
1	E	44	ALA	2.9
1	E	54	ALA	2.9
1	C	368	LEU	2.9
1	E	89	VAL	2.9
1	E	334	LYS	2.9
1	A	338	ASP	2.9
1	A	362	ASP	2.9
1	A	416	HIS	2.9
1	E	66	PRO	2.9
1	C	316	ARG	2.9
1	C	132	TRP	2.9
1	C	133	SER	2.9
1	E	214	LEU	2.9
1	A	10	GLY	2.9
1	A	194	GLY	2.9
1	C	10	GLY	2.9
1	C	394	VAL	2.9
1	C	417	THR	2.9
1	A	131	GLN	2.9
1	A	228	PRO	2.9
1	C	131	GLN	2.9
1	A	306	TYR	2.9
1	A	321	ASN	2.9
1	A	377	TRP	2.9
1	C	259	TRP	2.9
1	C	441	TRP	2.9
1	E	71	TRP	2.9
1	C	110	ALA	2.9
1	C	160	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	243	LEU	2.9
1	C	448	GLY	2.9
1	E	439	GLY	2.9
1	A	287	ASP	2.9
1	C	338	ASP	2.9
1	A	239	THR	2.9
1	A	335	ASN	2.9
1	C	155	ALA	2.9
1	C	180	ALA	2.9
1	E	50	GLY	2.9
1	A	86	LEU	2.8
1	C	172	LEU	2.8
1	C	47	PRO	2.8
1	A	155	ALA	2.8
1	E	470	GLY	2.8
1	E	368	LEU	2.8
1	C	451	PRO	2.8
1	E	274	PRO	2.8
1	E	92	ASP	2.8
1	C	344	GLY	2.8
1	A	180	ALA	2.8
1	E	180	ALA	2.8
1	A	189	LEU	2.8
1	A	238	THR	2.8
1	C	171	PRO	2.8
1	C	377	TRP	2.8
1	E	420	TRP	2.8
1	C	315	ILE	2.8
1	E	315	ILE	2.8
1	C	335	ASN	2.8
1	C	380	GLY	2.8
1	A	44	ALA	2.8
1	C	44	ALA	2.8
1	E	187	ALA	2.8
1	E	111	LEU	2.8
1	E	148	LEU	2.8
1	E	235	THR	2.8
1	A	47	PRO	2.8
1	A	390	VAL	2.8
1	A	467	VAL	2.8
1	A	316	ARG	2.7
1	A	345	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	420	TRP	2.8
1	E	121	TRP	2.8
1	A	41	ALA	2.7
1	C	41	ALA	2.7
1	C	386	ALA	2.7
1	A	243	LEU	2.7
1	C	77	TYR	2.7
1	C	228	PRO	2.7
1	C	176	VAL	2.7
1	A	341	ILE	2.7
1	E	256	ASN	2.7
1	C	323	SER	2.7
1	E	377	TRP	2.7
1	C	92	ASP	2.7
1	A	130	GLY	2.7
1	A	439	GLY	2.7
1	C	223	ALA	2.7
1	A	148	LEU	2.7
1	A	417	THR	2.7
1	C	209	LEU	2.7
1	A	307	TYR	2.7
1	C	322	PRO	2.7
1	C	395	GLN	2.7
1	E	322	PRO	2.7
1	A	291	VAL	2.7
1	C	212	GLU	2.7
1	E	467	VAL	2.7
1	C	319	SER	2.7
1	E	133	SER	2.7
1	A	204	ASP	2.7
1	E	221	ASP	2.7
1	C	71	TRP	2.7
1	E	345	ARG	2.7
1	E	395	GLN	2.7
1	C	311	PRO	2.7
1	C	9	TYR	2.7
1	C	175	TYR	2.7
1	E	321	ASN	2.7
1	E	403	HIS	2.7
1	C	278	TRP	2.7
1	E	49	GLN	2.6
1	A	168	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	168	GLU	2.6
1	A	266	MET	2.6
1	E	172	LEU	2.6
1	A	109	PRO	2.6
1	C	274	PRO	2.6
1	A	174	VAL	2.6
1	C	291	VAL	2.6
1	A	470	GLY	2.6
1	E	458	GLN	2.6
1	A	121	TRP	2.6
1	A	187	ALA	2.6
1	C	187	ALA	2.6
1	C	256	ASN	2.6
1	E	70	HIS	2.6
1	C	235	THR	2.6
1	E	341	ILE	2.6
1	C	400	CYS	2.6
1	E	303	CYS	2.6
1	A	441	TRP	2.6
1	C	239	THR	2.6
1	C	349	ALA	2.6
1	C	421	ALA	2.6
1	A	209	LEU	2.6
1	C	246	LEU	2.6
1	E	86	LEU	2.6
1	E	243	LEU	2.6
1	A	9	TYR	2.6
1	A	176	VAL	2.6
1	A	215	GLN	2.6
1	E	77	TYR	2.6
1	E	130	GLY	2.6
1	E	266	MET	2.6
1	A	217	ALA	2.6
1	A	430	ALA	2.6
1	C	287	ASP	2.6
1	E	171	PRO	2.6
1	E	362	ASP	2.6
1	E	414	ASP	2.6
1	A	278	TRP	2.6
1	C	364	LEU	2.6
1	A	93	PHE	2.5
1	A	301	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	341	ILE	2.5
1	C	192	GLY	2.5
1	C	194	GLY	2.5
1	C	470	GLY	2.5
1	E	380	GLY	2.5
1	A	418	LYS	2.5
1	E	204	ASP	2.5
1	C	74	PRO	2.5
1	A	246	LEU	2.5
1	E	471	LEU	2.5
1	C	251	GLU	2.5
1	A	259	TRP	2.5
1	C	121	TRP	2.5
1	C	50	GLY	2.5
1	A	73	HIS	2.5
1	E	73	HIS	2.5
1	A	77	TYR	2.5
1	C	418	LYS	2.5
1	A	303	CYS	2.5
1	C	440	ARG	2.5
1	A	118	THR	2.5
1	A	322	PRO	2.5
1	A	458	GLN	2.5
1	E	215	GLN	2.5
1	E	421	ALA	2.5
1	C	93	PHE	2.5
1	E	132	TRP	2.5
1	A	360	GLY	2.5
1	A	158	TYR	2.5
1	C	221	ASP	2.5
1	C	362	ASP	2.5
1	C	215	GLN	2.5
1	C	458	GLN	2.5
1	A	203	THR	2.5
1	C	118	THR	2.5
1	C	109	PRO	2.5
1	C	217	ALA	2.5
1	E	430	ALA	2.5
1	A	356	LEU	2.5
1	E	197	ASN	2.5
1	E	136	ILE	2.5
1	A	23	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	109	PRO	2.4
1	A	110	ALA	2.4
1	C	430	ALA	2.4
1	E	110	ALA	2.4
1	E	349	ALA	2.4
1	E	114	LEU	2.4
1	C	345	ARG	2.4
1	A	250	GLY	2.4
1	A	153	GLU	2.4
1	C	307	TYR	2.4
1	E	307	TYR	2.4
1	E	323	SER	2.4
1	A	270	ALA	2.4
1	C	402	ARG	2.4
1	A	372	LEU	2.4
1	C	190	LEU	2.4
1	E	473	HIS	2.4
1	A	36	GLY	2.4
1	E	168	GLU	2.4
1	A	154	ARG	2.4
1	C	277	ARG	2.4
1	E	9	TYR	2.4
1	E	203	THR	2.4
1	A	451	PRO	2.4
1	A	242	ALA	2.4
1	A	265	ALA	2.4
1	E	242	ALA	2.4
1	A	471	LEU	2.4
1	E	364	LEU	2.4
1	A	197	ASN	2.4
1	A	256	ASN	2.4
1	C	197	ASN	2.4
1	C	312	GLN	2.4
1	E	448	GLY	2.4
1	A	221	ASP	2.4
1	E	199	ARG	2.4
1	E	402	ARG	2.4
1	E	319	SER	2.4
1	E	418	LYS	2.4
1	C	73	HIS	2.4
1	C	96	THR	2.4
1	E	229	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	416	HIS	2.4
1	E	451	PRO	2.4
1	A	230	ALA	2.3
1	C	242	ALA	2.3
1	E	230	ALA	2.3
1	A	114	LEU	2.3
1	A	364	LEU	2.3
1	A	368	LEU	2.3
1	C	61	ASN	2.3
1	C	391	LEU	2.3
1	E	350	LEU	2.3
1	A	428	GLY	2.3
1	A	448	GLY	2.3
1	E	428	GLY	2.3
1	C	204	ASP	2.3
1	C	186	LYS	2.3
1	C	354	PHE	2.3
1	C	390	VAL	2.3
1	E	390	VAL	2.3
1	A	235	THR	2.3
1	A	433	THR	2.3
1	C	43	PRO	2.3
1	C	453	GLU	2.3
1	E	74	PRO	2.3
1	E	118	THR	2.3
1	E	433	THR	2.3
1	C	216	ALA	2.3
1	E	158	TYR	2.3
1	E	386	ALA	2.3
1	A	91	GLY	2.3
1	C	42	LEU	2.3
1	C	154	ARG	2.3
1	E	442	MET	2.3
1	C	416	HIS	2.3
1	C	184	VAL	2.3
1	A	43	PRO	2.3
1	A	211	PRO	2.3
1	A	386	ALA	2.3
1	E	31	ALA	2.3
1	E	190	LEU	2.3
1	A	183	SER	2.3
1	E	108	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	12	GLN	2.3
1	C	245	PRO	2.3
1	E	440	ARG	2.3
1	E	459	ARG	2.3
1	A	310	ASP	2.3
1	C	54	ALA	2.3
1	E	191	ALA	2.3
1	E	217	ALA	2.3
1	E	310	ASP	2.3
1	C	442	MET	2.3
1	A	12	GLN	2.2
1	C	56	ILE	2.2
1	E	401	ILE	2.2
1	C	81	PRO	2.2
1	C	203	THR	2.2
1	E	232	VAL	2.2
1	A	282	GLY	2.2
1	E	366	ALA	2.2
1	A	350	LEU	2.2
1	E	153	GLU	2.2
1	E	227	GLN	2.2
1	A	354	PHE	2.2
1	E	354	PHE	2.2
1	C	23	THR	2.2
1	C	136	ILE	2.2
1	C	211	PRO	2.2
1	C	310	ASP	2.2
1	C	414	ASP	2.2
1	A	192	GLY	2.2
1	C	36	GLY	2.2
1	C	428	GLY	2.2
1	E	192	GLY	2.2
1	A	34	GLU	2.2
1	E	216	ALA	2.2
1	E	68	LEU	2.2
1	A	70	HIS	2.2
1	E	106	GLN	2.2
1	A	108	SER	2.2
1	A	402	ARG	2.2
1	E	154	ARG	2.2
1	A	61	ASN	2.2
1	A	15	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	136	ILE	2.2
1	A	144	THR	2.2
1	E	438	ASP	2.2
1	E	466	ASP	2.2
1	A	443	VAL	2.2
1	C	443	VAL	2.2
1	E	184	VAL	2.2
1	C	360	GLY	2.2
1	A	216	ALA	2.2
1	C	227	GLN	2.2
1	C	350	LEU	2.2
1	C	471	LEU	2.2
1	E	276	CYS	2.2
1	E	391	LEU	2.2
1	C	461	TRP	2.2
1	A	438	ASP	2.2
1	E	96	THR	2.2
1	E	245	PRO	2.1
1	E	287	ASP	2.2
1	A	251	GLU	2.1
1	C	153	GLU	2.1
1	C	163	GLY	2.1
1	E	91	GLY	2.1
1	A	403	HIS	2.1
1	C	267	ALA	2.1
1	C	270	ALA	2.1
1	A	427	SER	2.1
1	C	82	SER	2.1
1	A	45	THR	2.1
1	A	74	PRO	2.1
1	A	245	PRO	2.1
1	C	433	THR	2.1
1	E	259	TRP	2.1
1	A	401	ILE	2.1
1	E	12	GLN	2.1
1	E	56	ILE	2.1
1	C	70	HIS	2.1
1	C	135	VAL	2.1
1	C	250	GLY	2.1
1	E	250	GLY	2.1
1	A	277	ARG	2.1
1	A	440	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	277	ARG	2.1
1	A	54	ALA	2.1
1	E	265	ALA	2.1
1	E	270	ALA	2.1
1	C	396	LEU	2.1
1	E	157	ASP	2.1
1	A	72	GLN	2.1
1	A	312	GLN	2.1
1	C	106	GLN	2.1
1	C	397	GLN	2.1
1	A	11	HIS	2.1
1	A	419	GLY	2.1
1	E	360	GLY	2.1
1	E	80	PHE	2.1
1	E	301	PHE	2.1
1	A	366	ALA	2.1
1	C	151	ALA	2.1
1	C	265	ALA	2.1
1	A	42	LEU	2.1
1	E	183	SER	2.1
1	E	246	LEU	2.1
1	E	396	LEU	2.1
1	A	276	CYS	2.1
1	E	185	ASP	2.1
1	E	166	GLN	2.1
1	A	461	TRP	2.1
1	C	296	TRP	2.1
1	A	284	GLU	2.0
1	C	230	ALA	2.1
1	A	126	LEU	2.0
1	A	190	LEU	2.0
1	C	424	LEU	2.0
1	E	314	LEU	2.0
1	A	106	GLN	2.0
1	A	397	GLN	2.0
1	C	229	CYS	2.0
1	E	196	ASP	2.0
1	C	210	ARG	2.0
1	C	11	HIS	2.0
1	C	403	HIS	2.0
1	A	274	PRO	2.0
1	E	23	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	144	THR	2.0
1	E	156	THR	2.0
1	E	186	LYS	2.0
1	C	282	GLY	2.0
1	A	56	ILE	2.0
1	A	24	VAL	2.0
1	A	184	VAL	2.0
1	A	457	VAL	2.0
1	C	108	SER	2.0
1	C	366	ALA	2.0
1	E	461	TRP	2.0
1	A	68	LEU	2.0
1	E	42	LEU	2.0
1	E	356	LEU	2.0
1	C	162	ARG	2.0
1	E	152	ARG	2.0
1	E	210	ARG	2.0
1	E	45	THR	2.0
1	E	81	PRO	2.0
1	C	91	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

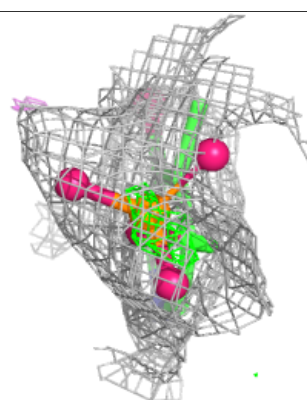
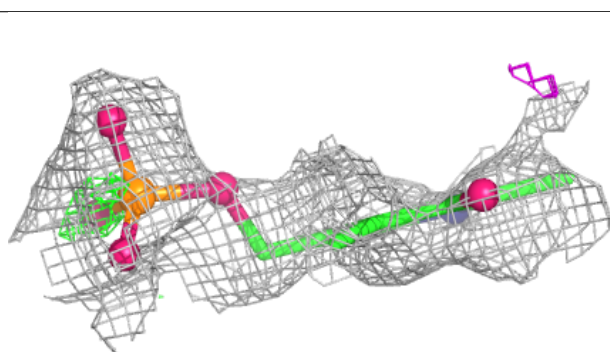
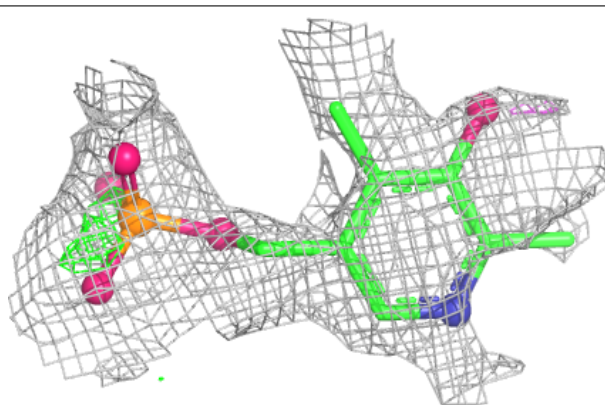
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	PLP	A	501	15/16	-	-	25,27,28,28	15
2	PLP	C	501	15/16	-	-	25,27,28,28	15
2	PLP	E	501	15/16	-	-	25,27,28,28	15

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.

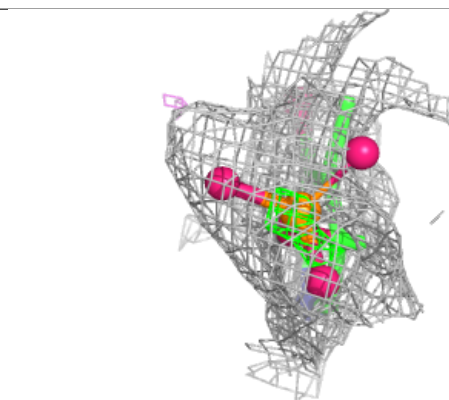
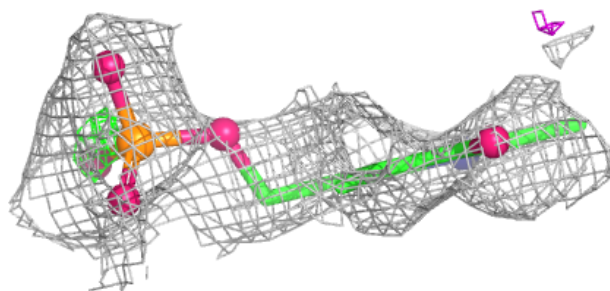
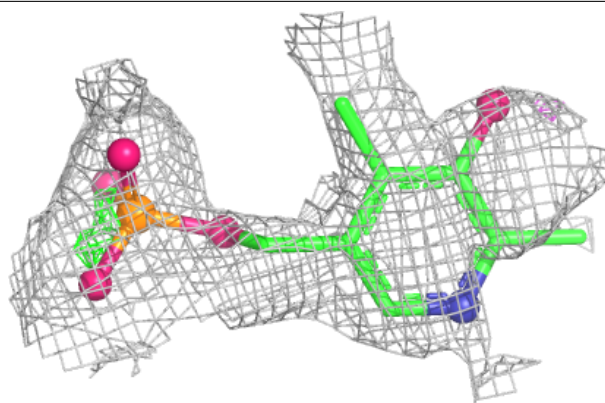
Electron density around PLP A 501:

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

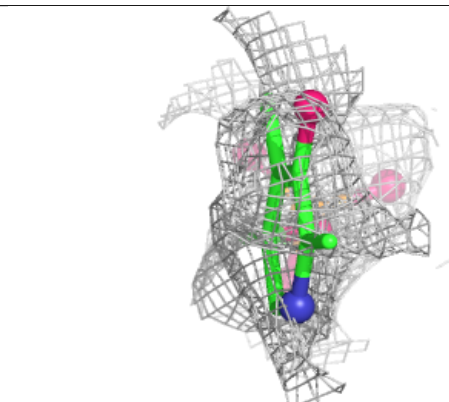
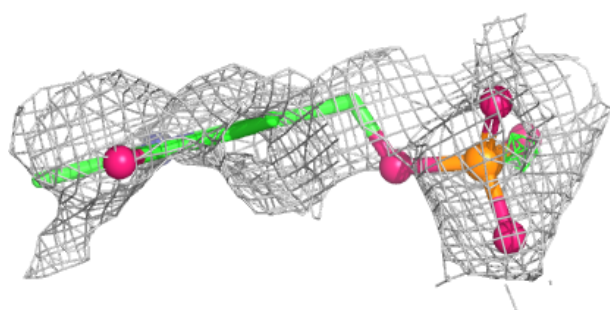
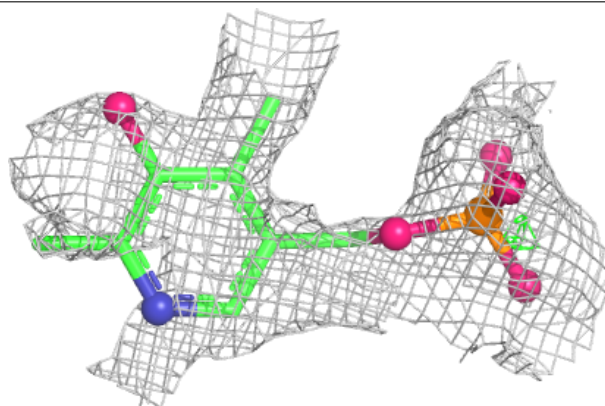


Electron density around PLP C 501:

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

**Electron density around PLP E 501:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.