Full wwPDB X-ray Structure Validation Report ⓘ

Sep 12, 2022 – 06:04 pm BST

PDB ID	:	7POC
Title	:	An Irreversible, Promiscuous and Highly Thermostable Claisen-Condensation Biocatalyst Drives the Synthesis of Substituted Pyrroles
Authors	:	Basle, A.; Ashley, B.; Campopiano, D.; Marles-Wright, J.
Deposited on	:	2021-09-08
Resolution	:	2.60 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

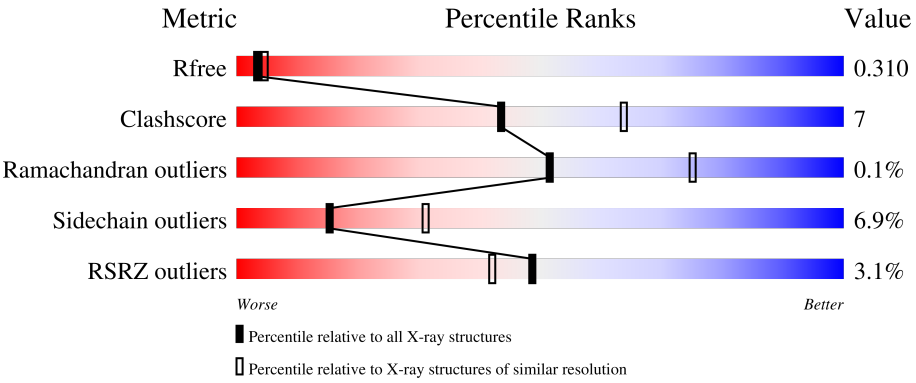
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.30
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.30

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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	421	% 75% 18% • 7%
1	B	421	7% 76% 16% • 7%
1	C	421	74% 18% • 7%
1	D	421	3% 76% 15% • 7%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 24484 atoms, of which 12197 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 8-amino-7-oxononanoate synthase/2-amino-3-ketobutyrate coenzyme A ligase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	392	Total	C	H	N	O	S	0	0	0
			6084	1945	3041	539	557	2			
1	B	393	Total	C	H	N	O	S	0	0	0
			6089	1948	3043	537	559	2			
1	C	392	Total	C	H	N	O	S	0	0	0
			6084	1945	3041	539	557	2			
1	D	393	Total	C	H	N	O	S	0	0	0
			6090	1948	3044	537	559	2			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	MET	-	initiating methionine	UNP Q5SHZ8
A	-23	SER	-	expression tag	UNP Q5SHZ8
A	-22	TYR	-	expression tag	UNP Q5SHZ8
A	-21	TYR	-	expression tag	UNP Q5SHZ8
A	-20	HIS	-	expression tag	UNP Q5SHZ8
A	-19	HIS	-	expression tag	UNP Q5SHZ8
A	-18	HIS	-	expression tag	UNP Q5SHZ8
A	-17	HIS	-	expression tag	UNP Q5SHZ8
A	-16	HIS	-	expression tag	UNP Q5SHZ8
A	-15	HIS	-	expression tag	UNP Q5SHZ8
A	-14	ASP	-	expression tag	UNP Q5SHZ8
A	-13	TYR	-	expression tag	UNP Q5SHZ8
A	-12	ASP	-	expression tag	UNP Q5SHZ8
A	-11	ILE	-	expression tag	UNP Q5SHZ8
A	-10	PRO	-	expression tag	UNP Q5SHZ8
A	-9	THR	-	expression tag	UNP Q5SHZ8
A	-8	THR	-	expression tag	UNP Q5SHZ8
A	-7	GLU	-	expression tag	UNP Q5SHZ8
A	-6	ASN	-	expression tag	UNP Q5SHZ8
A	-5	LEU	-	expression tag	UNP Q5SHZ8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	TYR	-	expression tag	UNP Q5SHZ8
A	-3	PHE	-	expression tag	UNP Q5SHZ8
A	-2	GLN	-	expression tag	UNP Q5SHZ8
A	-1	GLY	-	expression tag	UNP Q5SHZ8
A	0	ALA	-	expression tag	UNP Q5SHZ8
A	1	MET	-	expression tag	UNP Q5SHZ8
A	2	GLY	-	expression tag	UNP Q5SHZ8
B	-24	MET	-	initiating methionine	UNP Q5SHZ8
B	-23	SER	-	expression tag	UNP Q5SHZ8
B	-22	TYR	-	expression tag	UNP Q5SHZ8
B	-21	TYR	-	expression tag	UNP Q5SHZ8
B	-20	HIS	-	expression tag	UNP Q5SHZ8
B	-19	HIS	-	expression tag	UNP Q5SHZ8
B	-18	HIS	-	expression tag	UNP Q5SHZ8
B	-17	HIS	-	expression tag	UNP Q5SHZ8
B	-16	HIS	-	expression tag	UNP Q5SHZ8
B	-15	HIS	-	expression tag	UNP Q5SHZ8
B	-14	ASP	-	expression tag	UNP Q5SHZ8
B	-13	TYR	-	expression tag	UNP Q5SHZ8
B	-12	ASP	-	expression tag	UNP Q5SHZ8
B	-11	ILE	-	expression tag	UNP Q5SHZ8
B	-10	PRO	-	expression tag	UNP Q5SHZ8
B	-9	THR	-	expression tag	UNP Q5SHZ8
B	-8	THR	-	expression tag	UNP Q5SHZ8
B	-7	GLU	-	expression tag	UNP Q5SHZ8
B	-6	ASN	-	expression tag	UNP Q5SHZ8
B	-5	LEU	-	expression tag	UNP Q5SHZ8
B	-4	TYR	-	expression tag	UNP Q5SHZ8
B	-3	PHE	-	expression tag	UNP Q5SHZ8
B	-2	GLN	-	expression tag	UNP Q5SHZ8
B	-1	GLY	-	expression tag	UNP Q5SHZ8
B	0	ALA	-	expression tag	UNP Q5SHZ8
B	1	MET	-	expression tag	UNP Q5SHZ8
B	2	GLY	-	expression tag	UNP Q5SHZ8
C	-24	MET	-	initiating methionine	UNP Q5SHZ8
C	-23	SER	-	expression tag	UNP Q5SHZ8
C	-22	TYR	-	expression tag	UNP Q5SHZ8
C	-21	TYR	-	expression tag	UNP Q5SHZ8
C	-20	HIS	-	expression tag	UNP Q5SHZ8
C	-19	HIS	-	expression tag	UNP Q5SHZ8
C	-18	HIS	-	expression tag	UNP Q5SHZ8
C	-17	HIS	-	expression tag	UNP Q5SHZ8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-16	HIS	-	expression tag	UNP Q5SHZ8
C	-15	HIS	-	expression tag	UNP Q5SHZ8
C	-14	ASP	-	expression tag	UNP Q5SHZ8
C	-13	TYR	-	expression tag	UNP Q5SHZ8
C	-12	ASP	-	expression tag	UNP Q5SHZ8
C	-11	ILE	-	expression tag	UNP Q5SHZ8
C	-10	PRO	-	expression tag	UNP Q5SHZ8
C	-9	THR	-	expression tag	UNP Q5SHZ8
C	-8	THR	-	expression tag	UNP Q5SHZ8
C	-7	GLU	-	expression tag	UNP Q5SHZ8
C	-6	ASN	-	expression tag	UNP Q5SHZ8
C	-5	LEU	-	expression tag	UNP Q5SHZ8
C	-4	TYR	-	expression tag	UNP Q5SHZ8
C	-3	PHE	-	expression tag	UNP Q5SHZ8
C	-2	GLN	-	expression tag	UNP Q5SHZ8
C	-1	GLY	-	expression tag	UNP Q5SHZ8
C	0	ALA	-	expression tag	UNP Q5SHZ8
C	1	MET	-	expression tag	UNP Q5SHZ8
C	2	GLY	-	expression tag	UNP Q5SHZ8
D	-24	MET	-	initiating methionine	UNP Q5SHZ8
D	-23	SER	-	expression tag	UNP Q5SHZ8
D	-22	TYR	-	expression tag	UNP Q5SHZ8
D	-21	TYR	-	expression tag	UNP Q5SHZ8
D	-20	HIS	-	expression tag	UNP Q5SHZ8
D	-19	HIS	-	expression tag	UNP Q5SHZ8
D	-18	HIS	-	expression tag	UNP Q5SHZ8
D	-17	HIS	-	expression tag	UNP Q5SHZ8
D	-16	HIS	-	expression tag	UNP Q5SHZ8
D	-15	HIS	-	expression tag	UNP Q5SHZ8
D	-14	ASP	-	expression tag	UNP Q5SHZ8
D	-13	TYR	-	expression tag	UNP Q5SHZ8
D	-12	ASP	-	expression tag	UNP Q5SHZ8
D	-11	ILE	-	expression tag	UNP Q5SHZ8
D	-10	PRO	-	expression tag	UNP Q5SHZ8
D	-9	THR	-	expression tag	UNP Q5SHZ8
D	-8	THR	-	expression tag	UNP Q5SHZ8
D	-7	GLU	-	expression tag	UNP Q5SHZ8
D	-6	ASN	-	expression tag	UNP Q5SHZ8
D	-5	LEU	-	expression tag	UNP Q5SHZ8
D	-4	TYR	-	expression tag	UNP Q5SHZ8
D	-3	PHE	-	expression tag	UNP Q5SHZ8
D	-2	GLN	-	expression tag	UNP Q5SHZ8

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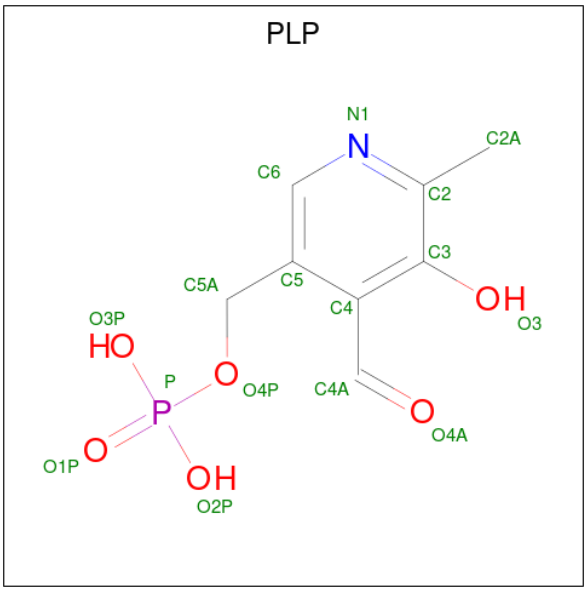
Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	GLY	-	expression tag	UNP Q5SHZ8
D	0	ALA	-	expression tag	UNP Q5SHZ8
D	1	MET	-	expression tag	UNP Q5SHZ8
D	2	GLY	-	expression tag	UNP Q5SHZ8

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C H N O P 22 8 7 1 5 1	0	0
2	B	1	Total C H N O P 22 8 7 1 5 1	0	0
2	C	1	Total C H N O P 22 8 7 1 5 1	0	0
2	D	1	Total C H N O P 22 8 7 1 5 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	15	Total O 15 15	0	0
3	B	11	Total O 11 11	0	0
3	C	15	Total O 15 15	0	0

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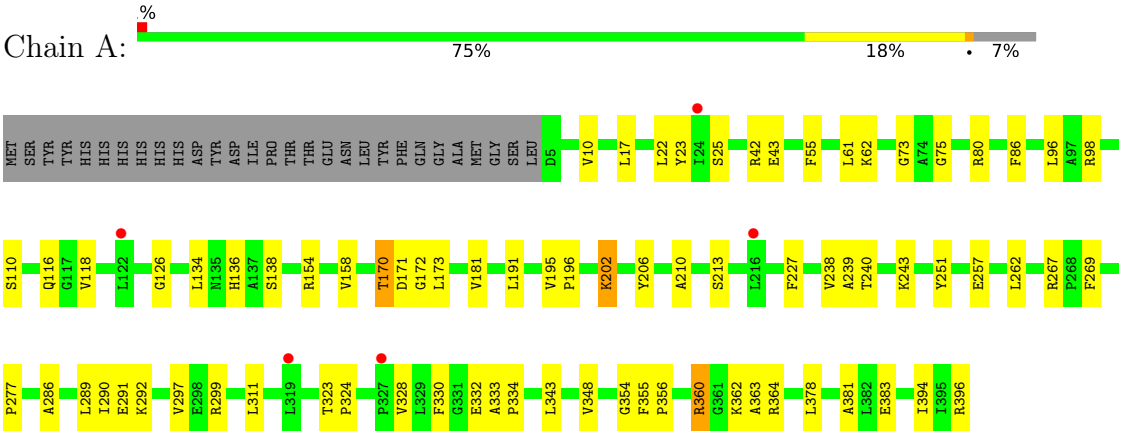
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	8	Total O 8 8	0	0

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.

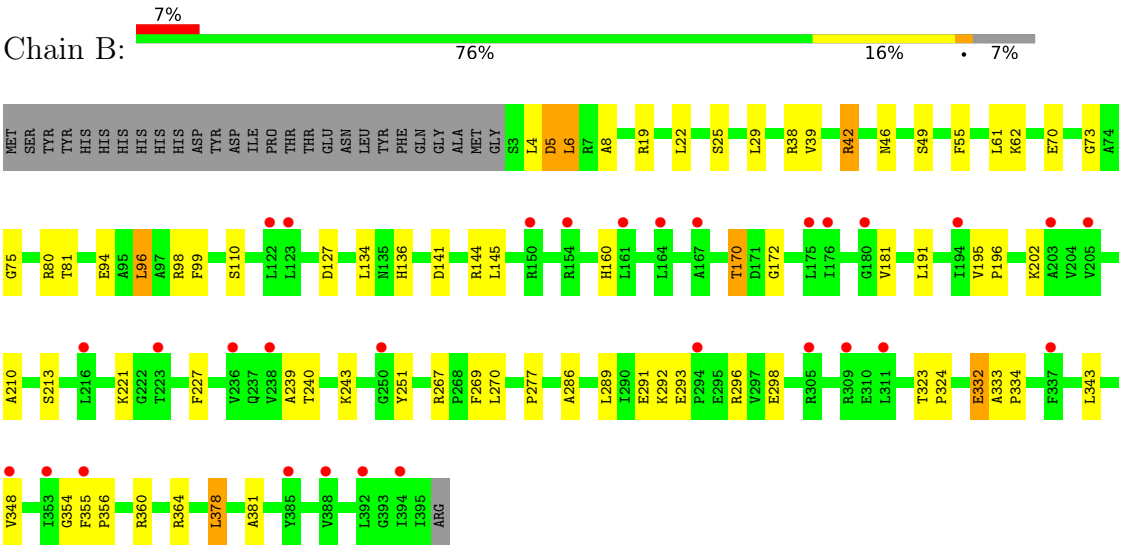
• Molecule 1: 8-amino-7-oxononanoate synthase/2-amino-3-ketobutyrate coenzyme A ligase

Chain A:



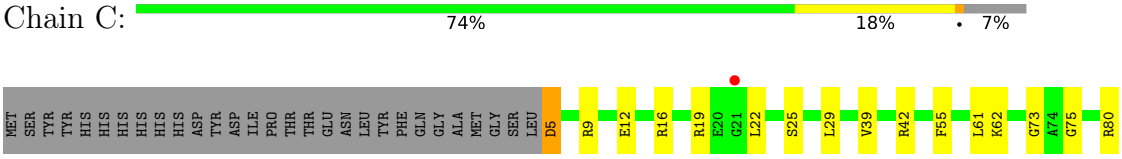
• Molecule 1: 8-amino-7-oxononanoate synthase/2-amino-3-ketobutyrate coenzyme A ligase

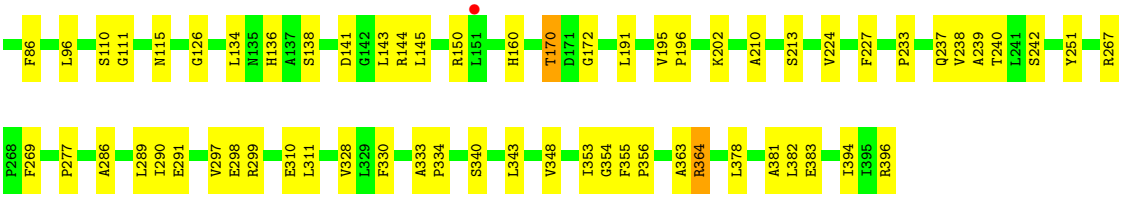
Chain B:



• Molecule 1: 8-amino-7-oxononanoate synthase/2-amino-3-ketobutyrate coenzyme A ligase

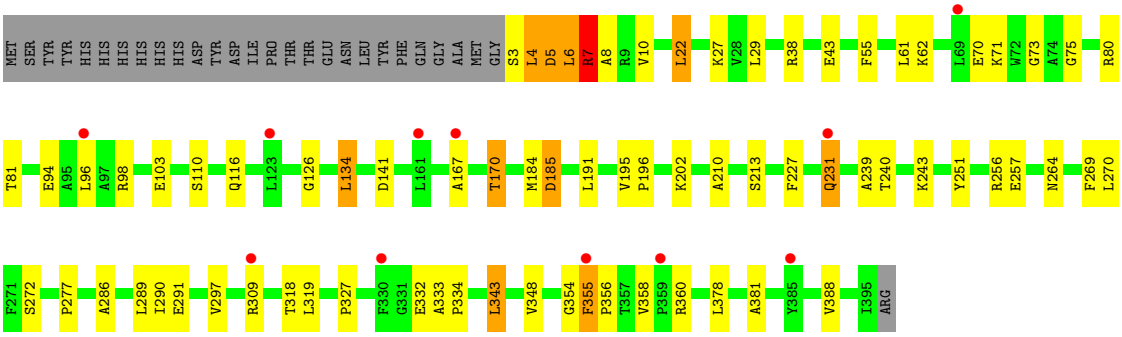
Chain C:





• Molecule 1: 8-amino-7-oxononanoate synthase/2-amino-3-ketobutyrate coenzyme A ligase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	57.04Å 134.79Å 184.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.48 – 2.60 54.48 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (54.48-2.60) 99.7 (54.48-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.05 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0267, REFMAC 5.8.0267	Depositor
R, R_{free}	0.242 , 0.311 0.240 , 0.310	Depositor DCC
R_{free} test set	2229 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	51.9	Xtriage
Anisotropy	0.486	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	24484	wwPDB-VP
Average B, all atoms (Å^2)	63.0	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 63.38 % 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 9.7519e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

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	0.71	0/3103	0.86	1/4197 (0.0%)
1	B	0.74	0/3106	0.87	0/4202
1	C	0.71	0/3103	0.89	0/4197
1	D	0.74	0/3106	0.89	2/4202 (0.0%)
All	All	0.73	0/12418	0.88	3/16798 (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	2
1	B	0	2
1	C	0	2
1	D	0	2
All	All	0	8

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	360	ARG	CG-CD-NE	5.76	123.89	111.80
1	D	7	ARG	N-CA-CB	5.42	120.36	110.60
1	D	355	PHE	CB-CA-C	5.25	120.89	110.40

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	354	GLY	Peptide
1	A	75	GLY	Peptide
1	B	354	GLY	Peptide
1	B	75	GLY	Peptide
1	C	354	GLY	Peptide
1	C	75	GLY	Peptide
1	D	354	GLY	Peptide
1	D	75	GLY	Peptide

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	3043	3041	3098	52	0
1	B	3046	3043	3100	44	0
1	C	3043	3041	3098	47	0
1	D	3046	3044	3101	51	0
2	A	15	7	6	4	0
2	B	15	7	6	2	0
2	C	15	7	6	3	0
2	D	15	7	6	1	0
3	A	15	0	0	2	0
3	B	11	0	0	0	0
3	C	15	0	0	0	0
3	D	8	0	0	1	0
All	All	12287	12197	12421	164	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 7.

All (164) 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:98:ARG:HD3	3:A:506:HOH:O	1.55	1.04
1:C:240:THR:HG22	1:C:242:SER:H	1.24	0.99
1:C:126:GLY:O	1:C:170:THR:HG21	1.74	0.88
1:A:126:GLY:O	1:A:170:THR:HG21	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:240:THR:HG22	1:C:242:SER:N	1.99	0.78
1:B:360:ARG:O	1:B:360:ARG:CZ	2.34	0.76
1:D:5:ASP:OD1	1:D:6:LEU:O	2.06	0.73
1:D:126:GLY:O	1:D:170:THR:HG21	1.89	0.71
1:A:118:VAL:HG13	1:A:206:TYR:HE2	1.57	0.69
1:A:172:GLY:O	1:D:4:LEU:HB2	1.93	0.69
1:C:55:PHE:CE1	1:C:289:LEU:HD23	2.28	0.69
1:B:267:ARG:NH1	1:C:141:ASP:OD1	2.26	0.67
1:A:55:PHE:CE1	1:A:289:LEU:HD23	2.30	0.67
1:C:39:VAL:O	1:C:42:ARG:HG2	1.95	0.65
1:A:240:THR:HG21	1:A:243:LYS:HG3	1.78	0.65
1:D:240:THR:HG21	1:D:243:LYS:HE2	1.78	0.65
1:B:55:PHE:CE1	1:B:289:LEU:HD23	2.34	0.62
1:B:240:THR:HG21	1:B:243:LYS:HG3	1.81	0.62
1:D:55:PHE:CE1	1:D:289:LEU:HD23	2.34	0.62
1:D:191:LEU:HB2	1:D:227:PHE:CD2	2.35	0.62
1:C:111:GLY:N	2:C:401:PLP:O2P	2.32	0.61
1:B:292:LYS:HE2	1:B:292:LYS:HA	1.83	0.61
1:D:240:THR:HG21	1:D:243:LYS:HG3	1.81	0.61
1:B:144:ARG:NH2	1:C:145:LEU:O	2.34	0.60
1:C:240:THR:HG21	1:C:242:SER:OG	2.02	0.60
1:B:94:GLU:HG3	1:B:98:ARG:HH21	1.67	0.60
1:D:355:PHE:HA	1:D:358:VAL:O	2.02	0.60
1:A:191:LEU:HB2	1:A:227:PHE:CD2	2.37	0.59
1:D:22:LEU:HD11	1:D:355:PHE:CD2	2.37	0.59
1:A:311:LEU:HD13	1:A:328:VAL:HG22	1.85	0.59
1:A:10:VAL:HG11	1:D:257:GLU:HB2	1.85	0.58
1:B:141:ASP:OD1	1:C:267:ARG:NH1	2.37	0.58
1:B:145:LEU:O	1:C:144:ARG:NH2	2.36	0.58
1:D:94:GLU:HG3	1:D:98:ARG:HH21	1.69	0.58
1:C:191:LEU:HB2	1:C:227:PHE:CD2	2.39	0.57
1:D:210:ALA:HA	1:D:240:THR:HG22	1.86	0.57
1:B:210:ALA:HA	1:B:240:THR:HG22	1.87	0.55
1:A:73:GLY:HA2	1:D:62:LYS:HD2	1.88	0.55
1:C:311:LEU:HD13	1:C:328:VAL:HG22	1.88	0.55
1:C:80:ARG:HG3	1:C:269:PHE:CE1	2.42	0.55
1:D:343:LEU:HD13	1:D:388:VAL:HG21	1.89	0.55
1:B:323:THR:CG2	1:B:324:PRO:HD2	2.37	0.54
1:A:118:VAL:CG1	1:A:206:TYR:HE2	2.20	0.54
1:A:202:LYS:HG2	1:D:3:SER:O	2.07	0.54
1:A:80:ARG:HG3	1:A:269:PHE:CE1	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:VAL:HG23	1:A:262:LEU:HD21	1.89	0.54
1:C:310:GLU:HB3	1:C:382:LEU:HD22	1.89	0.54
1:D:103:GLU:HB3	1:D:256:ARG:HG2	1.90	0.54
1:B:80:ARG:HG3	1:B:269:PHE:CE1	2.43	0.53
1:D:184:MET:HG3	1:D:358:VAL:HG12	1.91	0.53
1:B:160:HIS:CE1	1:D:167:ALA:HB1	2.43	0.53
1:B:195:VAL:HB	1:B:196:PRO:HD3	1.91	0.52
1:D:80:ARG:HG3	1:D:269:PHE:CE1	2.45	0.52
1:D:195:VAL:HB	1:D:196:PRO:HD3	1.91	0.52
1:C:195:VAL:HB	1:C:196:PRO:HD3	1.91	0.52
1:A:73:GLY:HA2	1:D:62:LYS:CD	2.41	0.51
1:A:195:VAL:HB	1:A:196:PRO:HD3	1.93	0.51
1:B:191:LEU:HB2	1:B:227:PHE:CD2	2.45	0.51
1:D:134:LEU:HD23	1:D:185:ASP:OD2	2.11	0.51
1:B:127:ASP:OD2	1:C:9:ARG:NH2	2.43	0.51
1:B:62:LYS:HD2	1:C:73:GLY:HA2	1.91	0.51
1:A:323:THR:CG2	1:A:324:PRO:HD2	2.41	0.50
1:A:239:ALA:HB3	1:A:251:TYR:CZ	2.46	0.50
1:B:239:ALA:HB3	1:B:251:TYR:CZ	2.46	0.50
1:A:118:VAL:CG1	1:A:206:TYR:CE2	2.95	0.50
1:C:311:LEU:HD13	1:C:328:VAL:CG2	2.42	0.50
1:A:98:ARG:CD	3:A:506:HOH:O	2.32	0.50
1:B:62:LYS:CD	1:C:73:GLY:HA2	2.42	0.50
1:B:73:GLY:HA2	1:C:62:LYS:HD2	1.93	0.50
1:A:171:ASP:O	1:D:4:LEU:HD13	2.12	0.49
1:A:126:GLY:O	1:A:170:THR:CG2	2.57	0.49
1:A:257:GLU:HB3	1:D:10:VAL:CG1	2.42	0.49
1:A:181:VAL:HG11	1:A:323:THR:HG21	1.94	0.49
1:C:239:ALA:HB3	1:C:251:TYR:CZ	2.47	0.49
1:C:355:PHE:O	1:C:356:PRO:C	2.50	0.49
1:D:319:LEU:HD13	1:D:327:PRO:HB2	1.94	0.49
1:A:118:VAL:HG13	1:A:206:TYR:CE2	2.43	0.49
1:A:311:LEU:HD13	1:A:328:VAL:CG2	2.42	0.49
1:D:5:ASP:OD2	1:D:8:ALA:HB2	2.12	0.48
1:B:355:PHE:O	1:B:356:PRO:C	2.51	0.48
1:B:181:VAL:HG11	1:B:323:THR:HG21	1.94	0.48
1:D:6:LEU:O	1:D:7:ARG:HG3	2.13	0.48
1:A:136:HIS:CB	2:A:401:PLP:H2A3	2.44	0.48
1:B:170:THR:HB	1:B:172:GLY:H	1.79	0.48
1:D:360:ARG:HD2	3:D:507:HOH:O	2.14	0.48
1:C:348:VAL:HG21	1:C:381:ALA:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:ASP:OD2	1:B:8:ALA:HB2	2.14	0.48
1:B:136:HIS:HB2	2:B:401:PLP:H2A3	1.95	0.47
1:A:116:GLN:HE22	1:D:116:GLN:HE22	1.63	0.47
1:A:355:PHE:O	1:A:356:PRO:C	2.52	0.47
1:A:118:VAL:HG11	1:A:238:VAL:HG11	1.96	0.47
1:A:257:GLU:HB3	1:D:10:VAL:HG11	1.96	0.47
1:A:257:GLU:CB	1:D:10:VAL:HG11	2.45	0.47
1:C:240:THR:HG23	2:C:401:PLP:O2P	2.15	0.47
1:D:239:ALA:HB3	1:D:251:TYR:CE1	2.51	0.46
1:B:323:THR:HG22	1:B:324:PRO:HD2	1.97	0.46
1:B:73:GLY:HA2	1:C:62:LYS:CD	2.46	0.46
1:B:29:LEU:O	1:C:86:PHE:HA	2.16	0.46
1:D:355:PHE:O	1:D:356:PRO:C	2.53	0.46
1:A:61:LEU:HD21	1:A:286:ALA:HB2	1.98	0.46
1:A:239:ALA:HB3	1:A:251:TYR:CE1	2.51	0.46
1:D:81:THR:HG21	1:D:270:LEU:HD23	1.98	0.46
1:A:210:ALA:CB	2:A:401:PLP:C3	2.93	0.46
1:C:353:ILE:HB	1:C:364:ARG:HD2	1.98	0.46
1:D:239:ALA:HB3	1:D:251:TYR:CZ	2.50	0.46
1:A:210:ALA:HA	1:A:240:THR:HG22	1.98	0.46
2:A:401:PLP:O3P	1:D:272:SER:HA	2.16	0.46
1:A:290:ILE:HD11	1:A:297:VAL:HG23	1.97	0.45
1:B:6:LEU:HD22	1:C:233:PRO:O	2.15	0.45
1:C:170:THR:HB	1:C:172:GLY:H	1.80	0.45
1:C:290:ILE:HD11	1:C:297:VAL:HG23	1.98	0.45
1:B:81:THR:HG21	1:B:270:LEU:HD23	1.99	0.45
1:C:290:ILE:HD12	1:C:290:ILE:HA	1.89	0.45
1:A:348:VAL:HG21	1:A:381:ALA:HA	1.99	0.45
1:A:23:TYR:HA	1:D:264:ASN:OD1	2.17	0.44
1:D:290:ILE:HD11	1:D:297:VAL:HG23	2.00	0.44
1:B:333:ALA:N	1:B:334:PRO:CD	2.81	0.44
1:B:99:PHE:O	1:B:221:LYS:HE2	2.18	0.44
1:C:29:LEU:HG	1:C:39:VAL:HG22	2.00	0.44
1:B:172:GLY:O	1:C:5:ASP:OD1	2.36	0.44
1:D:61:LEU:HD21	1:D:286:ALA:HB2	2.00	0.44
1:A:86:PHE:HA	1:D:29:LEU:O	2.18	0.43
1:A:333:ALA:N	1:A:334:PRO:CD	2.81	0.43
1:C:61:LEU:HD21	1:C:286:ALA:HB2	2.01	0.43
1:C:210:ALA:CB	2:C:401:PLP:C3	2.96	0.43
1:C:136:HIS:ND1	1:C:138:SER:HB3	2.33	0.43
1:B:136:HIS:CB	2:B:401:PLP:H2A3	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:333:ALA:N	1:D:334:PRO:CD	2.81	0.43
1:B:348:VAL:HG21	1:B:381:ALA:HA	2.00	0.43
1:C:239:ALA:HB3	1:C:251:TYR:CE1	2.53	0.43
1:D:355:PHE:HB3	1:D:360:ARG:HG3	2.01	0.43
1:B:61:LEU:HD21	1:B:286:ALA:HB2	2.01	0.43
1:B:332:GLU:HB3	1:B:334:PRO:HD2	2.00	0.43
1:C:115:ASN:OD1	1:C:238:VAL:HG21	2.19	0.43
1:A:136:HIS:HB2	2:A:401:PLP:H2A3	2.00	0.42
1:A:62:LYS:CD	1:D:73:GLY:HA2	2.50	0.42
1:C:143:LEU:HB3	1:C:150:ARG:HD3	2.02	0.42
1:D:231:GLN:HE21	1:D:231:GLN:HA	1.85	0.42
1:B:46:ASN:HD21	1:B:49:SER:HB3	1.84	0.42
1:B:39:VAL:O	1:B:42:ARG:HG3	2.20	0.42
1:B:293:GLU:OE1	1:B:296:ARG:NH1	2.52	0.41
1:D:38:ARG:HH11	1:D:38:ARG:HG3	1.85	0.41
1:A:10:VAL:HG11	1:D:257:GLU:CB	2.51	0.41
1:D:332:GLU:HB3	1:D:334:PRO:HD2	2.03	0.41
1:B:378:LEU:HD12	1:B:378:LEU:HA	1.91	0.41
1:A:333:ALA:HA	1:A:363:ALA:CB	2.51	0.41
1:C:333:ALA:HA	1:C:363:ALA:CB	2.50	0.41
1:A:136:HIS:ND1	1:A:138:SER:HB3	2.36	0.41
1:A:267:ARG:NH1	1:D:141:ASP:OD1	2.54	0.41
1:A:330:PHE:CE1	1:A:394:ILE:HD11	2.56	0.41
1:C:333:ALA:N	1:C:334:PRO:CD	2.83	0.41
1:D:348:VAL:HG21	1:D:381:ALA:HA	2.02	0.41
1:A:332:GLU:HB3	1:A:334:PRO:HD2	2.03	0.41
1:B:4:LEU:HB2	1:C:172:GLY:O	2.22	0.40
1:C:16:ARG:HA	1:C:19:ARG:CZ	2.51	0.40
1:D:318:THR:HG22	1:D:318:THR:O	2.21	0.40
1:A:323:THR:HG22	1:A:324:PRO:HD2	2.03	0.40
1:D:210:ALA:CB	2:D:401:PLP:C3	2.99	0.40
1:A:118:VAL:HA	1:A:262:LEU:HD21	2.03	0.40
1:A:154:ARG:HG3	1:C:160:HIS:NE2	2.35	0.40
1:B:96:LEU:HD23	1:B:96:LEU:HA	1.88	0.40
1:B:323:THR:HG23	1:B:324:PRO:HD2	2.03	0.40
1:C:224:VAL:HG11	1:C:237:GLN:OE1	2.21	0.40
1:C:330:PHE:CE2	1:C:394:ILE:HD11	2.57	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	390/421 (93%)	376 (96%)	14 (4%)	0	100	100
1	B	391/421 (93%)	376 (96%)	15 (4%)	0	100	100
1	C	390/421 (93%)	375 (96%)	15 (4%)	0	100	100
1	D	391/421 (93%)	376 (96%)	14 (4%)	1 (0%)	41	64
All	All	1562/1684 (93%)	1503 (96%)	58 (4%)	1 (0%)	51	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	7	ARG

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	313/339 (92%)	289 (92%)	24 (8%)	13	25
1	B	314/339 (93%)	293 (93%)	21 (7%)	16	33
1	C	313/339 (92%)	293 (94%)	20 (6%)	17	35
1	D	314/339 (93%)	293 (93%)	21 (7%)	16	33
All	All	1254/1356 (92%)	1168 (93%)	86 (7%)	15	31

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LEU
1	A	22	LEU
1	A	25	SER
1	A	42	ARG
1	A	43	GLU
1	A	96	LEU
1	A	110	SER
1	A	134	LEU
1	A	158	VAL
1	A	170	THR
1	A	173	LEU
1	A	202	LYS
1	A	213	SER
1	A	277	PRO
1	A	291	GLU
1	A	292	LYS
1	A	299	ARG
1	A	343	LEU
1	A	360	ARG
1	A	362	LYS
1	A	364	ARG
1	A	378	LEU
1	A	383	GLU
1	A	396	ARG
1	B	5	ASP
1	B	6	LEU
1	B	19	ARG
1	B	22	LEU
1	B	25	SER
1	B	38	ARG
1	B	42	ARG
1	B	70	GLU
1	B	96	LEU
1	B	110	SER
1	B	134	LEU
1	B	170	THR
1	B	202	LYS
1	B	213	SER
1	B	277	PRO
1	B	291	GLU
1	B	298	GLU
1	B	332	GLU
1	B	343	LEU

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Mol	Chain	Res	Type
1	B	364	ARG
1	B	378	LEU
1	C	5	ASP
1	C	12	GLU
1	C	22	LEU
1	C	25	SER
1	C	96	LEU
1	C	110	SER
1	C	134	LEU
1	C	170	THR
1	C	202	LYS
1	C	213	SER
1	C	277	PRO
1	C	291	GLU
1	C	298	GLU
1	C	299	ARG
1	C	340	SER
1	C	343	LEU
1	C	364	ARG
1	C	378	LEU
1	C	383	GLU
1	C	396	ARG
1	D	4	LEU
1	D	5	ASP
1	D	6	LEU
1	D	22	LEU
1	D	27	LYS
1	D	43	GLU
1	D	70	GLU
1	D	71	LYS
1	D	96	LEU
1	D	110	SER
1	D	134	LEU
1	D	170	THR
1	D	185	ASP
1	D	202	LYS
1	D	213	SER
1	D	231	GLN
1	D	277	PRO
1	D	291	GLU
1	D	309	ARG
1	D	343	LEU

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Mol	Chain	Res	Type
1	D	378	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	GLN
1	D	116	GLN
1	D	231	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no 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	0.71	1 (6%)	20,22,23	1.14	1 (5%)
2	PLP	D	401	1	15,15,16	0.73	0	20,22,23	1.19	1 (5%)
2	PLP	B	401	1	15,15,16	1.06	1 (6%)	20,22,23	1.85	3 (15%)
2	PLP	C	401	1	15,15,16	0.95	1 (6%)	20,22,23	1.25	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	A	401	1	-	0/6/6/8	0/1/1/1
2	PLP	D	401	1	-	3/6/6/8	0/1/1/1
2	PLP	B	401	1	-	3/6/6/8	0/1/1/1
2	PLP	C	401	1	-	3/6/6/8	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	PLP	C4A-C4	-3.25	1.44	1.51
2	C	401	PLP	C4A-C4	-2.34	1.46	1.51
2	A	401	PLP	C4A-C4	-2.25	1.47	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	PLP	C4A-C4-C5	5.40	126.50	120.94
2	B	401	PLP	O4P-C5A-C5	4.38	117.70	109.35
2	B	401	PLP	C4A-C4-C3	-3.63	114.34	120.50
2	A	401	PLP	C4A-C4-C5	3.32	124.36	120.94
2	D	401	PLP	C4A-C4-C5	3.29	124.32	120.94
2	C	401	PLP	C4A-C4-C5	3.22	124.25	120.94
2	C	401	PLP	O4P-C5A-C5	2.91	114.90	109.35

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	PLP	C5A-O4P-P-O2P
2	B	401	PLP	C5A-O4P-P-O3P
2	C	401	PLP	C5A-O4P-P-O1P
2	C	401	PLP	C5A-O4P-P-O2P
2	C	401	PLP	C5A-O4P-P-O3P
2	D	401	PLP	C5A-O4P-P-O1P
2	D	401	PLP	C5A-O4P-P-O2P
2	D	401	PLP	C5A-O4P-P-O3P
2	B	401	PLP	C5A-O4P-P-O1P

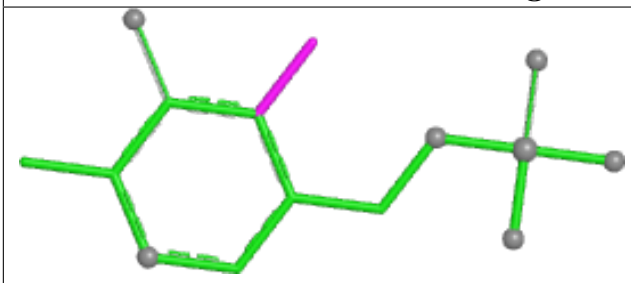
There are no ring outliers.

4 monomers are involved in 10 short contacts:

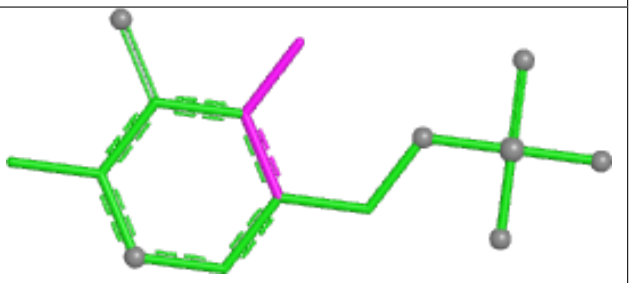
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	PLP	4	0
2	D	401	PLP	1	0
2	B	401	PLP	2	0
2	C	401	PLP	3	0

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.

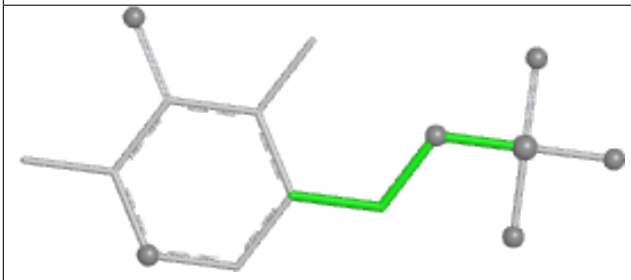
Ligand PLP A 401



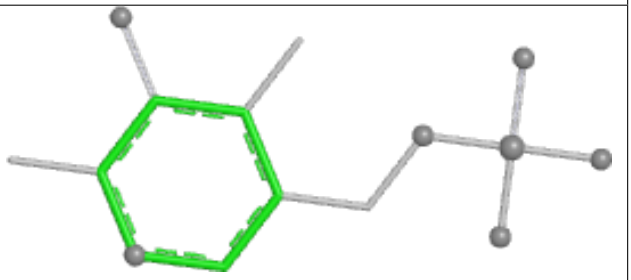
Bond lengths



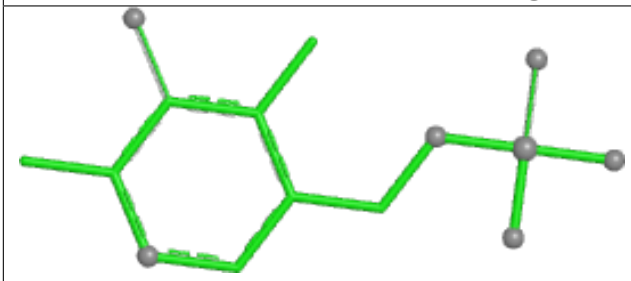
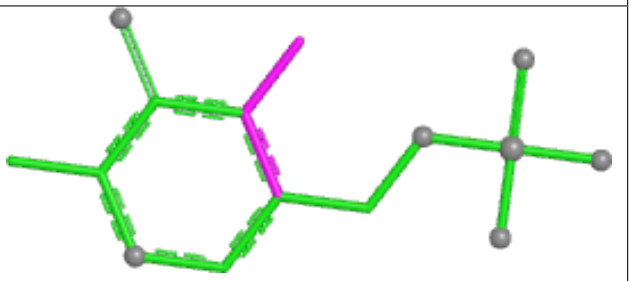
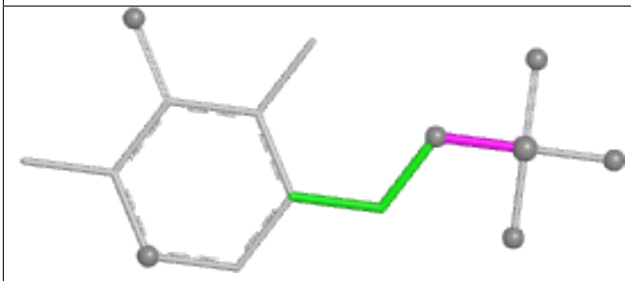
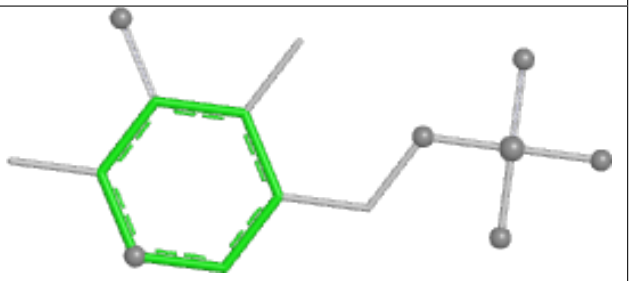
Bond angles

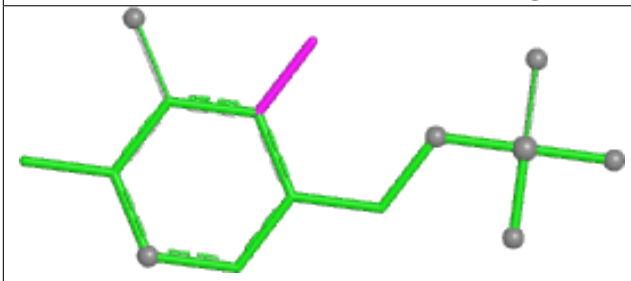
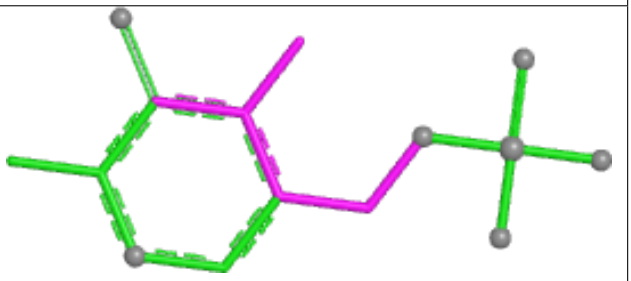
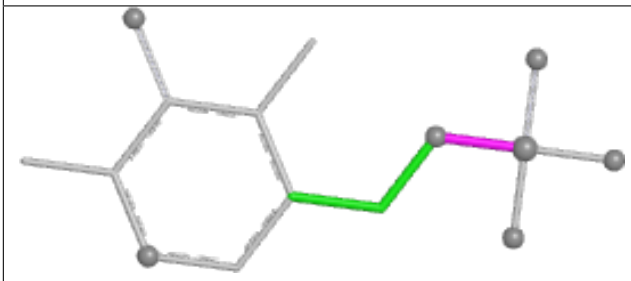
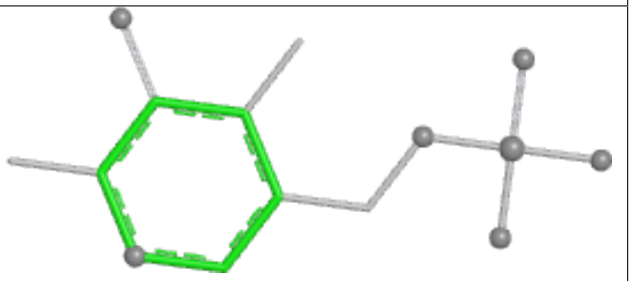


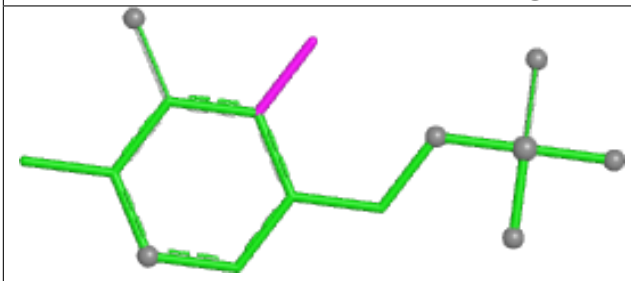
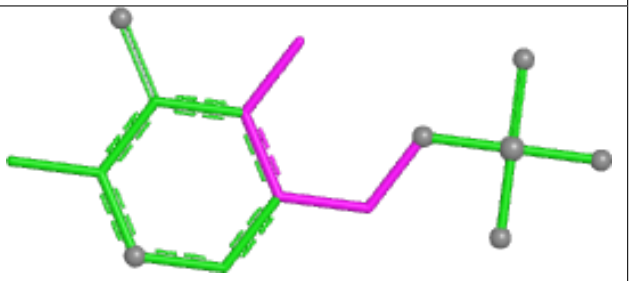
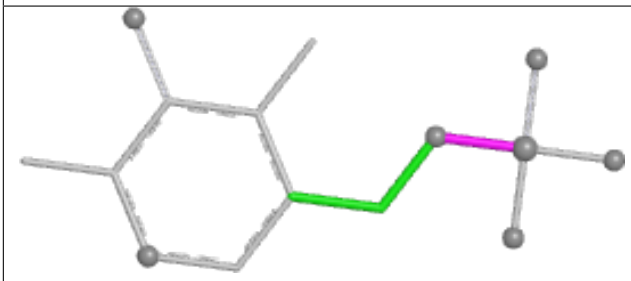
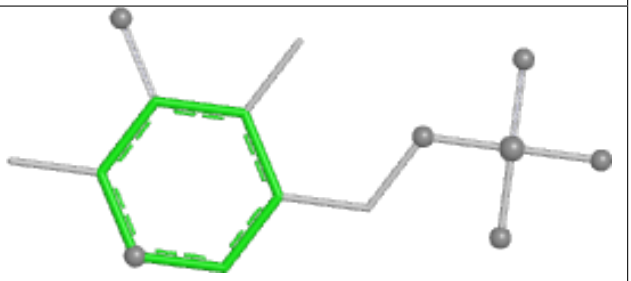
Torsions



Rings

Ligand PLP D 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PLP B 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PLP C 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	392/421 (93%)	0.00	5 (1%) 77 73	35, 53, 77, 102	0
1	B	393/421 (93%)	0.51	30 (7%) 13 10	42, 72, 112, 143	0
1	C	392/421 (93%)	0.05	2 (0%) 91 89	33, 55, 88, 123	0
1	D	393/421 (93%)	0.15	11 (2%) 53 46	36, 57, 96, 130	0
All	All	1570/1684 (93%)	0.18	48 (3%) 49 42	33, 58, 101, 143	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	194	ILE	5.0
1	B	203	ALA	4.4
1	B	355	PHE	4.2
1	B	180	GLY	3.5
1	B	205	VAL	3.4
1	D	355	PHE	3.4
1	B	154	ARG	3.4
1	B	167	ALA	3.3
1	B	238	VAL	3.2
1	B	353	ILE	3.1
1	B	175	LEU	3.1
1	B	311	LEU	3.1
1	D	96	LEU	3.0
1	B	161	LEU	2.9
1	D	359	PRO	2.9
1	B	123	LEU	2.8
1	D	309	ARG	2.8
1	D	231	GLN	2.7
1	B	250	GLY	2.6
1	D	167	ALA	2.6
1	C	151	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	388	VAL	2.5
1	B	236	VAL	2.5
1	B	392	LEU	2.5
1	B	309	ARG	2.5
1	D	330	PHE	2.4
1	B	385	TYR	2.4
1	D	123	LEU	2.4
1	D	69	LEU	2.3
1	C	21	GLY	2.3
1	A	319	LEU	2.3
1	A	24	ILE	2.3
1	B	164	LEU	2.3
1	D	161	LEU	2.3
1	B	294	PRO	2.2
1	B	394	ILE	2.2
1	A	216	LEU	2.2
1	B	216	LEU	2.2
1	B	150	ARG	2.2
1	B	223	THR	2.2
1	B	176	ILE	2.1
1	D	385	TYR	2.1
1	B	337	PHE	2.1
1	B	122	LEU	2.1
1	B	348	VAL	2.1
1	A	327	PRO	2.0
1	B	305	ARG	2.0
1	A	122	LEU	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,

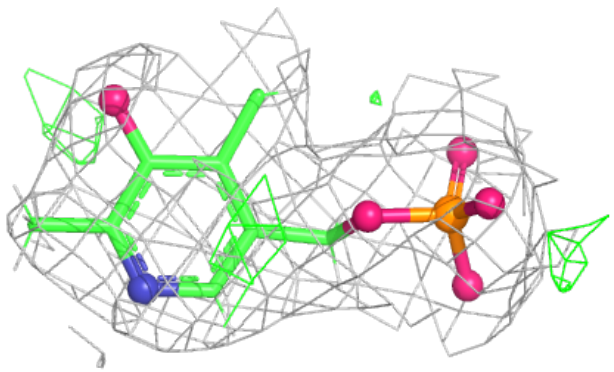
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

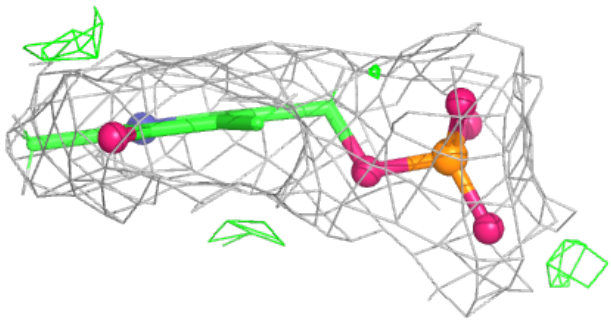
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PLP	A	401	15/16	0.94	0.14	40,47,50,52	0
2	PLP	C	401	15/16	0.94	0.15	35,42,50,62	0
2	PLP	B	401	15/16	0.95	0.16	53,63,69,71	0
2	PLP	D	401	15/16	0.95	0.16	41,46,53,57	0

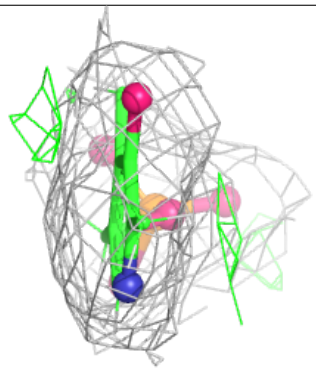
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PLP A 401:

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

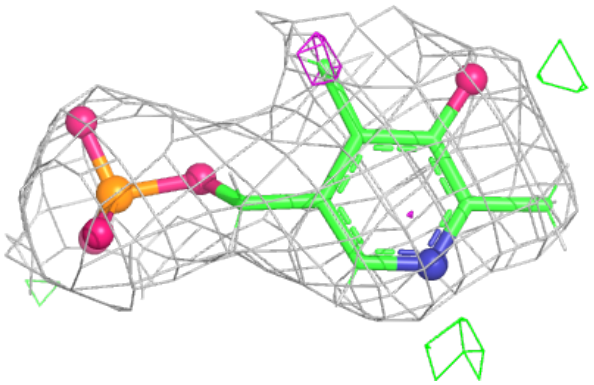


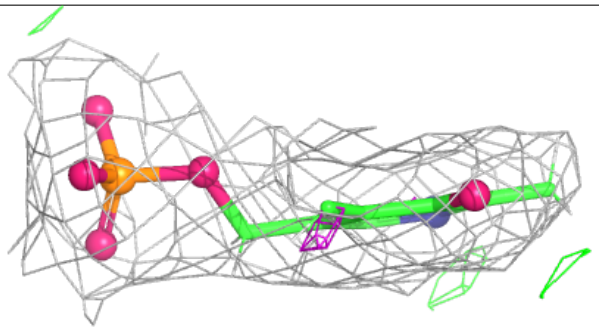


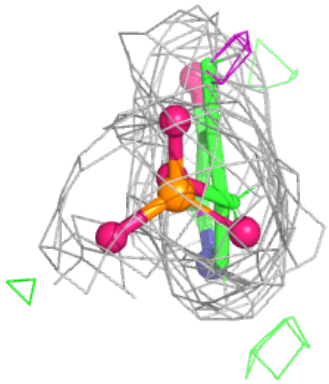


Electron density around PLP C 401:

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

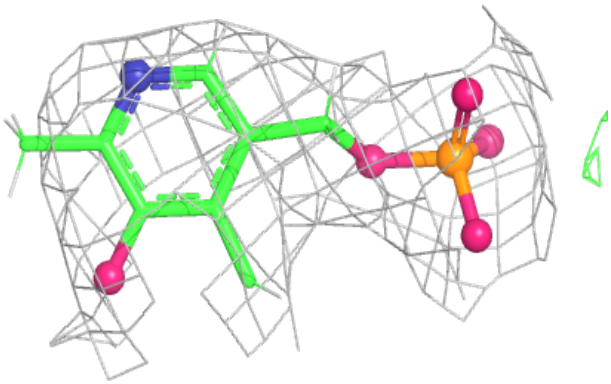


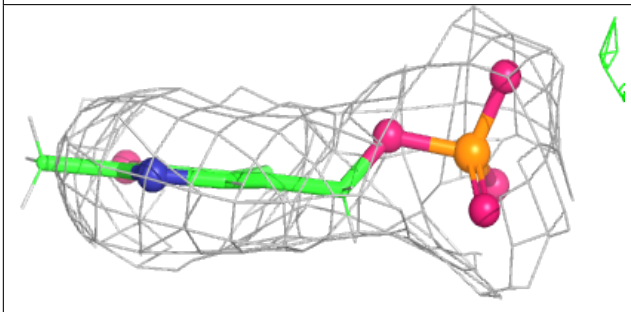


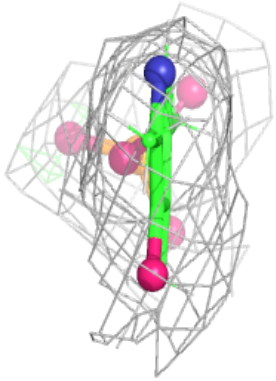


Electron density around PLP B 401:

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

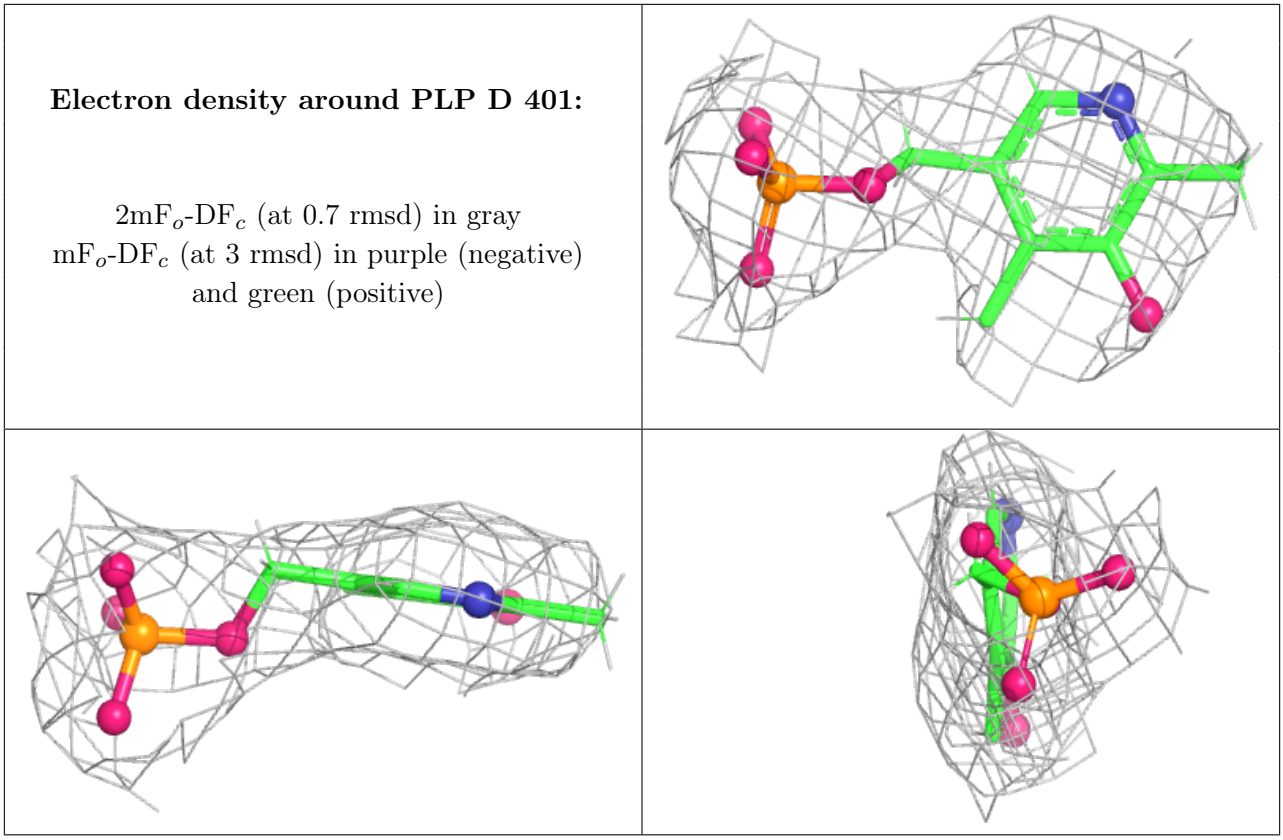






Electron density around PLP D 401:

$2mF_o$-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.