Full wwPDB X-ray Structure Validation Report (i)

Apr 22, 2024 – 06:58 PM JST

PDB ID	:	8I7U
Title	:	Crystal structure of alpha-Oxoamine Synthase Alb29 with PLP cofactor
Authors	:	Xu, M.J.; Zhang, D.K.
Deposited on	:	2023-02-02
Resolution	:	2.49 Å(reported)

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

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

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

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

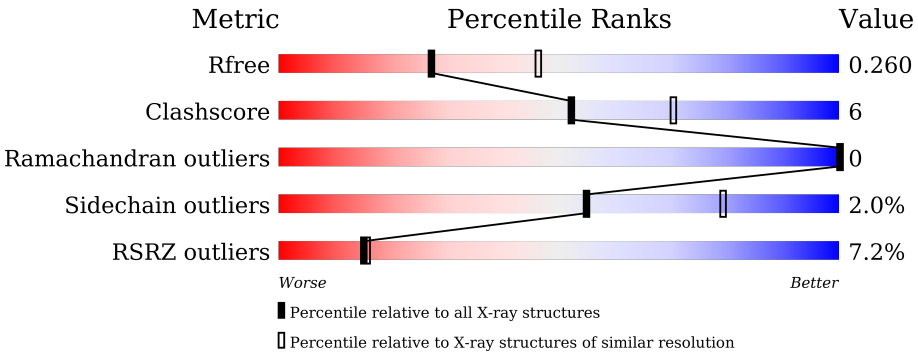
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh &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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.49 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	394	7% 85% 15%
1	B	394	10% 84% 13%
1	C	394	6% 90% 9%
1	D	394	7% 84% 14%
1	E	394	8% 83% 16%
1	F	394	5% 85% 14%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 17998 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.

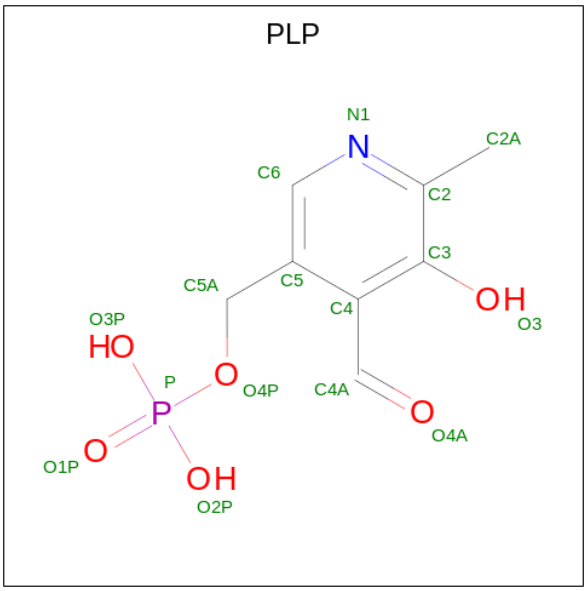
- Molecule 1 is a protein called 8-amino-7-oxononanoate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	393	Total	C	N	O	S	0	0	0
			2976	1873	528	559	16			
1	A	394	Total	C	N	O	S	0	0	0
			2983	1878	529	560	16			
1	B	386	Total	C	N	O	S	0	0	0
			2915	1834	514	551	16			
1	D	391	Total	C	N	O	S	0	0	0
			2958	1861	524	557	16			
1	E	391	Total	C	N	O	S	0	0	0
			2958	1861	524	557	16			
1	F	390	Total	C	N	O	S	0	0	0
			2950	1855	523	556	16			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	87	GLY	SER	engineered mutation	UNP A0A6B9KSL0
A	87	GLY	SER	engineered mutation	UNP A0A6B9KSL0
B	87	GLY	SER	engineered mutation	UNP A0A6B9KSL0
D	87	GLY	SER	engineered mutation	UNP A0A6B9KSL0
E	87	GLY	SER	engineered mutation	UNP A0A6B9KSL0
F	87	GLY	SER	engineered mutation	UNP A0A6B9KSL0

- 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	C	1	Total C N O P 15 8 1 5 1	0	0
2	A	1	Total C N O P 15 8 1 5 1	0	0
2	B	1	Total C N O P 15 8 1 5 1	0	0
2	D	1	Total C N O P 15 8 1 5 1	0	0
2	E	1	Total C N O P 15 8 1 5 1	0	0
2	F	1	Total C N O P 15 8 1 5 1	0	0

- Molecule 3 is water.

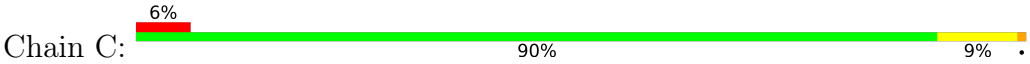
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	35	Total O 35 35	0	0
3	A	24	Total O 24 24	0	0
3	B	29	Total O 29 29	0	0
3	D	25	Total O 25 25	0	0
3	E	19	Total O 19 19	0	0
3	F	36	Total O 36 36	0	0

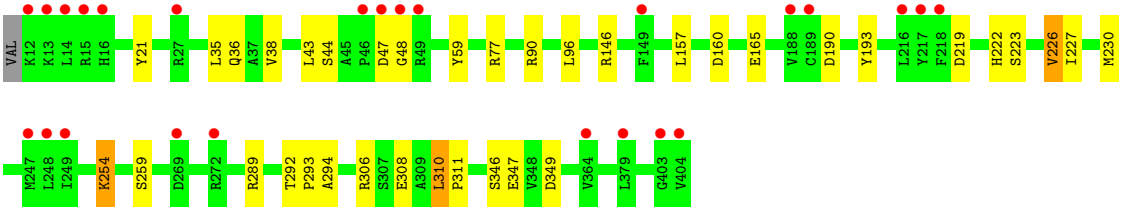
3 Residue-property plots (i)

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

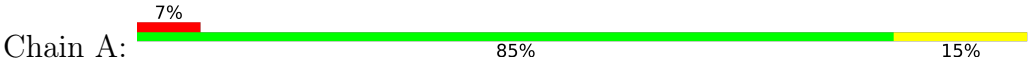
Chain C:

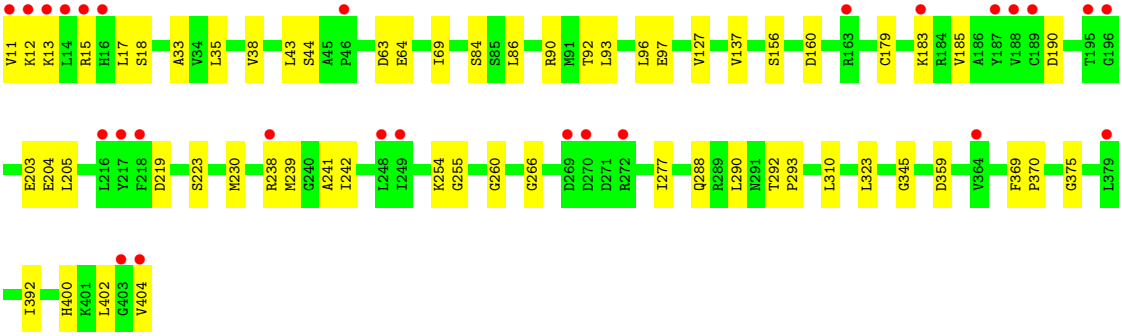




• Molecule 1: 8-amino-7-oxononanoate synthase

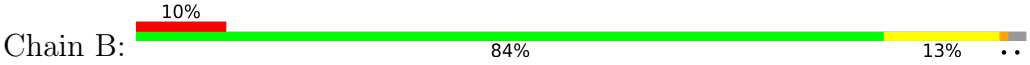
Chain A:

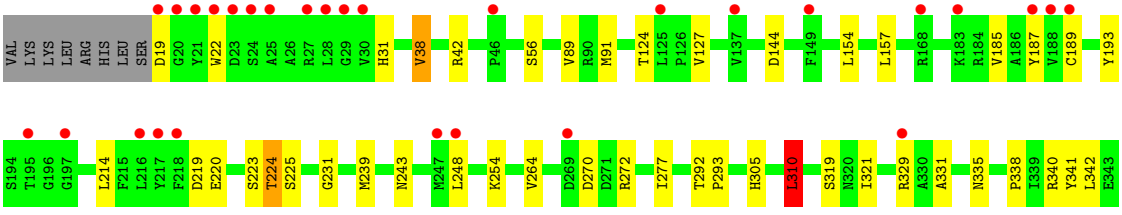


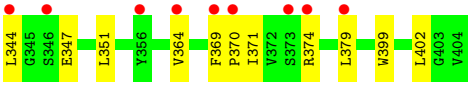


• Molecule 1: 8-amino-7-oxononanoate synthase

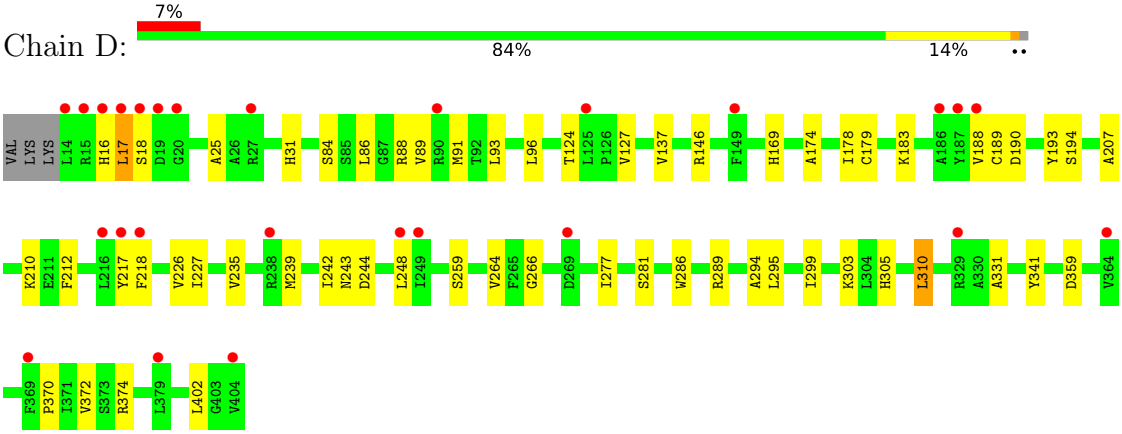
Chain B:



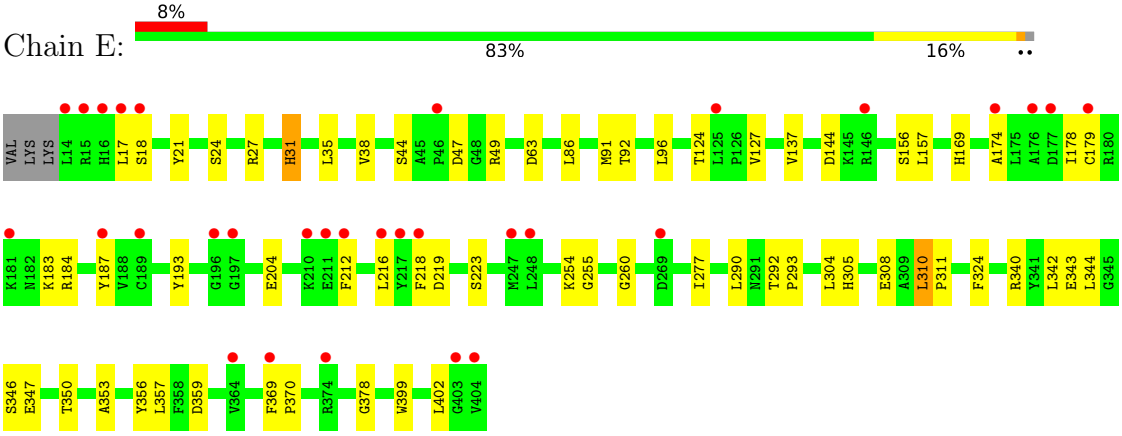




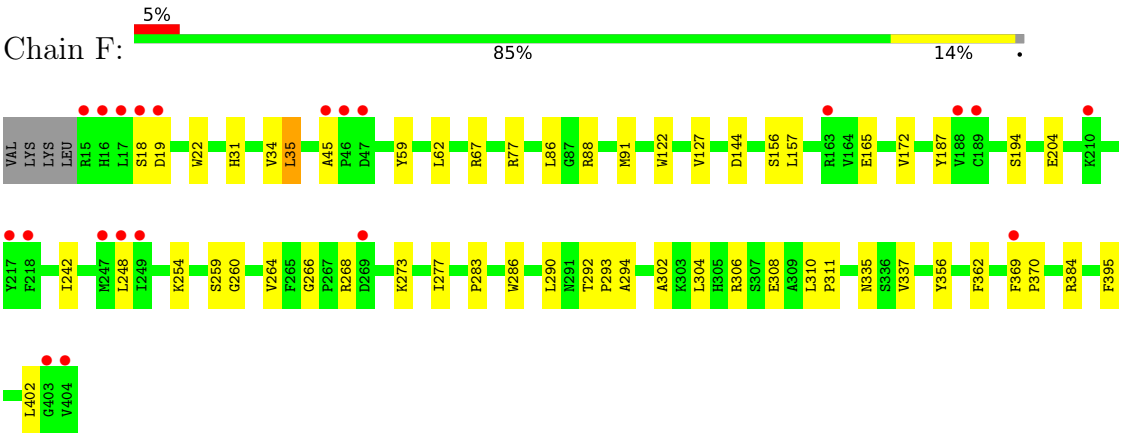
• Molecule 1: 8-amino-7-oxononanoate synthase



• Molecule 1: 8-amino-7-oxononanoate synthase



• Molecule 1: 8-amino-7-oxononanoate synthase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	65.47Å 110.46Å 353.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.18 – 2.49 25.18 – 2.49	Depositor EDS
% Data completeness (in resolution range)	98.3 (25.18-2.49) 98.3 (25.18-2.49)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.35 (at 2.50Å)	Xtriage
Refinement program	REFMAC 7.1.018, PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.197 , 0.251 0.208 , 0.260	Depositor DCC
R_{free} test set	4536 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	48.1	Xtriage
Anisotropy	0.544	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 46.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	17998	wwPDB-VP
Average B, all atoms (Å^2)	52.0	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 28.46 % 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 1.8347e-03. 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	0.42	0/3038	0.62	0/4113
1	B	0.38	0/2969	0.63	1/4022 (0.0%)
1	C	0.42	0/3031	0.65	2/4103 (0.0%)
1	D	0.40	0/3013	0.64	0/4081
1	E	0.39	0/3013	0.62	0/4081
1	F	0.40	0/3005	0.64	0/4070
All	All	0.40	0/18069	0.63	3/24470 (0.0%)

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	B	310	LEU	CA-CB-CG	-6.11	101.24	115.30
1	C	310	LEU	CA-CB-CG	-5.64	102.32	115.30
1	C	254	LYS	C-N-CA	-5.19	111.40	122.30

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	2983	0	2980	39	0
1	B	2915	0	2898	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2976	0	2971	25	0
1	D	2958	0	2945	31	0
1	E	2958	0	2946	48	0
1	F	2950	0	2934	42	0
2	A	15	0	6	2	0
2	B	15	0	6	2	0
2	C	15	0	7	2	0
2	D	15	0	7	0	0
2	E	15	0	7	3	0
2	F	15	0	6	1	0
3	A	24	0	0	1	0
3	B	29	0	0	0	0
3	C	35	0	0	0	0
3	D	25	0	0	1	0
3	E	19	0	0	2	0
3	F	36	0	0	1	0
All	All	17998	0	17713	197	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 (197) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:ARG:HH22	1:F:77:ARG:HH22	1.27	0.83
1:E:86:LEU:HD12	1:E:91:MET:HB2	1.62	0.81
1:C:226:VAL:HG22	1:C:227:ILE:HG13	1.61	0.81
1:D:84:SER:HA	1:D:93:LEU:HD12	1.71	0.73
1:C:43:LEU:HD22	1:F:86:LEU:HD13	1.72	0.72
1:D:18:SER:HB2	1:D:370:PRO:HD3	1.72	0.72
1:D:127:VAL:HG21	1:D:277:ILE:HG12	1.72	0.70
1:A:35:LEU:HB2	1:E:86:LEU:HD11	1.74	0.69
1:D:226:VAL:HG23	1:D:227:ILE:HG13	1.75	0.69
1:D:17:LEU:HG	1:D:374:ARG:HH12	1.57	0.69
1:F:18:SER:HB2	1:F:370:PRO:HD3	1.75	0.68
1:F:35:LEU:HD12	1:F:45:ALA:HA	1.74	0.67
1:B:19:ASP:HA	1:B:22:TRP:HD1	1.59	0.67
1:A:43:LEU:HD22	1:E:86:LEU:HD13	1.75	0.67
1:C:157:LEU:HD11	1:F:157:LEU:HD11	1.76	0.66
1:F:127:VAL:HG21	1:F:277:ILE:HD12	1.79	0.65
1:F:86:LEU:HD12	1:F:91:MET:HB2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:289:ARG:NH1	3:D:601:HOH:O	2.27	0.64
1:C:59:TYR:HH	1:C:222:HIS:CE1	2.16	0.64
1:E:124:THR:HG22	1:E:277:ILE:HD13	1.79	0.64
1:B:225:SER:OG	1:B:305:HIS:NE2	2.30	0.63
1:B:321:ILE:HD11	1:B:338:PRO:HB3	1.82	0.62
1:C:254:LYS:NZ	2:C:501:PLP:O3	2.31	0.62
1:F:19:ASP:HA	1:F:22:TRP:HD1	1.65	0.61
1:E:342:LEU:HD23	1:E:399:TRP:CE2	2.35	0.61
1:B:369:PHE:CD1	1:B:370:PRO:HA	2.35	0.61
1:E:204:GLU:N	1:E:204:GLU:OE1	2.33	0.61
1:B:335:ASN:HB2	1:B:340:ARG:HH12	1.67	0.59
1:D:331:ALA:HB3	1:D:341:TYR:HB3	1.85	0.59
1:F:144:ASP:OD2	1:F:187:TYR:OH	2.19	0.58
1:D:189:CYS:HB2	1:D:193:TYR:OH	2.04	0.58
1:F:248:LEU:HB2	1:F:264:VAL:HB	1.86	0.58
1:A:90:ARG:HD2	1:E:31:HIS:NE2	2.19	0.57
1:A:255:GLY:HA2	3:A:603:HOH:O	2.04	0.57
1:E:344:LEU:HD12	1:E:350:THR:HA	1.85	0.57
1:A:13:LYS:HG2	1:A:17:LEU:HD23	1.87	0.56
1:B:22:TRP:HZ3	1:B:31:HIS:CE1	2.23	0.56
1:A:13:LYS:HG2	1:A:13:LYS:O	2.04	0.56
1:B:254:LYS:NZ	2:B:501:PLP:O3	2.38	0.56
1:E:219:ASP:OD2	2:E:501:PLP:N1	2.39	0.56
1:C:90:ARG:HD2	1:F:31:HIS:CE1	2.41	0.56
1:F:254:LYS:NZ	2:F:501:PLP:O3	2.39	0.55
1:B:220:GLU:OE1	1:B:223:SER:OG	2.16	0.55
1:A:92:THR:HG21	1:A:97:GLU:OE2	2.06	0.54
1:A:260:GLY:HA3	1:A:290:LEU:HD21	1.88	0.54
1:F:273:LYS:O	1:F:277:ILE:HG12	2.08	0.54
1:A:179:CYS:HA	1:A:185:VAL:HG21	1.90	0.54
1:A:92:THR:HG23	1:A:96:LEU:HB3	1.89	0.53
1:B:224:THR:O	1:B:231:GLY:O	2.26	0.53
1:F:268:ARG:NH1	3:F:605:HOH:O	2.41	0.53
1:A:204:GLU:OE1	1:A:204:GLU:N	2.38	0.53
1:A:242:ILE:HD13	1:A:266:GLY:HA2	1.89	0.53
1:E:260:GLY:HA3	1:E:290:LEU:HD21	1.90	0.53
1:F:259:SER:HB3	1:F:294:ALA:HB1	1.88	0.53
1:D:248:LEU:HB2	1:D:264:VAL:HB	1.90	0.53
1:C:346:SER:HB3	1:C:349:ASP:HB2	1.90	0.52
1:A:400:HIS:O	1:A:404:VAL:HG13	2.09	0.52
1:F:127:VAL:HG21	1:F:277:ILE:CD1	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:17:LEU:CG	1:D:374:ARG:HH12	2.22	0.52
1:E:21:TYR:CE2	1:E:347:GLU:HG2	2.45	0.52
1:E:344:LEU:HD21	1:E:399:TRP:HH2	1.74	0.52
1:A:254:LYS:NZ	2:A:501:PLP:O3	2.42	0.52
1:D:89:VAL:HG12	1:D:91:MET:HG2	1.90	0.52
1:E:47:ASP:OD2	1:E:49:ARG:NH2	2.43	0.52
1:A:203:GLU:HA	1:A:238:ARG:HH12	1.75	0.52
1:D:239:MET:HE1	1:D:243:ASN:H	1.74	0.52
1:C:219:ASP:OD2	2:C:501:PLP:N1	2.43	0.51
1:B:270:ASP:OD2	1:B:272:ARG:NH1	2.43	0.51
1:C:77:ARG:HH21	1:F:77:ARG:HH12	1.57	0.51
1:A:18:SER:HB2	1:A:370:PRO:HD3	1.92	0.51
1:A:345:GLY:HA2	1:A:375:GLY:O	2.10	0.51
1:B:331:ALA:HB3	1:B:341:TYR:HB3	1.93	0.51
1:A:33:ALA:H	1:E:91:MET:HE2	1.75	0.51
1:D:239:MET:CE	1:D:243:ASN:H	2.24	0.51
1:E:216:LEU:HB3	1:E:218:PHE:CE2	2.46	0.51
1:F:18:SER:HB3	1:F:369:PHE:CE2	2.46	0.50
1:D:146:ARG:HH21	1:D:169:HIS:CD2	2.30	0.50
1:B:154:LEU:HD22	1:B:157:LEU:HD12	1.93	0.50
1:A:230:MET:HA	1:A:310:LEU:HD22	1.94	0.50
1:D:299:ILE:O	1:D:303:LYS:HG3	2.11	0.50
1:F:172:VAL:HG21	1:F:204:GLU:HG2	1.94	0.50
1:E:369:PHE:CD1	1:E:370:PRO:HA	2.47	0.50
1:B:144:ASP:OD2	1:B:187:TYR:OH	2.29	0.49
1:C:259:SER:HB2	1:C:294:ALA:HB1	1.94	0.49
1:A:35:LEU:HB2	1:E:86:LEU:CD1	2.42	0.49
1:E:346:SER:O	1:E:350:THR:HG23	2.12	0.49
1:E:92:THR:OG1	1:E:96:LEU:HB3	2.13	0.49
1:F:259:SER:HB3	1:F:294:ALA:CB	2.43	0.49
1:D:218:PHE:CG	1:D:235:VAL:HG21	2.48	0.48
1:C:254:LYS:HE3	1:F:88:ARG:NH1	2.28	0.48
1:B:219:ASP:OD2	2:B:501:PLP:N1	2.46	0.48
1:F:67:ARG:CZ	1:F:304:LEU:HD13	2.42	0.48
1:C:35:LEU:HB2	1:F:86:LEU:HD11	1.94	0.48
1:B:38:VAL:HG12	1:B:42:ARG:HB2	1.96	0.48
1:B:342:LEU:HD22	1:B:399:TRP:CZ2	2.48	0.47
1:E:174:ALA:O	1:E:178:ILE:HG13	2.14	0.47
1:F:18:SER:HB2	1:F:370:PRO:CD	2.44	0.47
1:C:38:VAL:CG2	1:C:44:SER:HB3	2.45	0.47
1:B:347:GLU:O	1:B:351:LEU:HG	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:254:LYS:NZ	2:E:501:PLP:O3	2.48	0.47
1:F:122:TRP:HB3	1:F:283:PRO:HG2	1.96	0.47
1:A:11:VAL:HA	1:A:15:ARG:HD3	1.97	0.47
1:E:18:SER:HB2	1:E:370:PRO:HD3	1.96	0.47
1:C:77:ARG:NH2	1:F:77:ARG:HH12	2.13	0.46
1:C:59:TYR:OH	1:C:222:HIS:CE1	2.66	0.46
1:C:190:ASP:HB2	1:C:193:TYR:CE2	2.50	0.46
1:A:323:LEU:HB2	1:B:319:SER:HB2	1.96	0.46
1:E:137:VAL:HG11	1:E:183:LYS:HD2	1.97	0.46
1:E:343:GLU:HA	1:E:378:GLY:HA3	1.95	0.46
1:C:292:THR:N	1:C:293:PRO:HD2	2.31	0.46
1:E:38:VAL:HG21	1:E:44:SER:HB3	1.96	0.46
1:C:36:GLN:HB3	1:C:44:SER:OG	2.14	0.46
1:A:63:ASP:OD1	1:A:64:GLU:HG3	2.15	0.46
1:A:33:ALA:H	1:E:91:MET:CE	2.27	0.46
1:A:137:VAL:HG11	1:A:183:LYS:HD2	1.97	0.46
1:B:124:THR:HG22	1:B:277:ILE:HD13	1.98	0.45
1:D:25:ALA:HB1	1:D:31:HIS:HB2	1.99	0.45
1:D:242:ILE:HD13	1:D:266:GLY:HA2	1.98	0.45
1:B:22:TRP:CZ3	1:B:31:HIS:CE1	3.03	0.45
1:A:292:THR:N	1:A:293:PRO:HD2	2.32	0.45
1:F:369:PHE:CD1	1:F:370:PRO:HA	2.51	0.45
1:F:286:TRP:CD1	1:F:286:TRP:C	2.90	0.45
1:C:21:TYR:CE2	1:C:347:GLU:HG2	2.52	0.44
1:D:188:VAL:HG13	1:D:217:TYR:CD1	2.52	0.44
1:E:356:TYR:CD2	1:E:402:LEU:HD12	2.51	0.44
1:C:47:ASP:OD1	1:C:48:GLY:N	2.51	0.44
1:D:305:HIS:HA	1:D:310:LEU:HD23	1.99	0.44
1:F:302:ALA:O	1:F:306:ARG:HG3	2.18	0.44
1:A:160:ASP:OD2	1:E:156:SER:OG	2.24	0.44
1:D:190:ASP:HB2	1:D:193:TYR:CE1	2.52	0.44
1:A:219:ASP:OD2	2:A:501:PLP:N1	2.51	0.44
1:E:63:ASP:HA	3:E:618:HOH:O	2.18	0.44
1:E:255:GLY:HA2	3:E:603:HOH:O	2.17	0.44
1:C:230:MET:HG2	1:C:306:ARG:HA	1.99	0.44
1:C:308:GLU:O	1:C:311:PRO:HD2	2.18	0.43
1:F:356:TYR:CD2	1:F:402:LEU:HD13	2.53	0.43
1:B:305:HIS:CG	1:B:310:LEU:HD13	2.54	0.43
1:D:86:LEU:HD13	1:D:86:LEU:HA	1.66	0.43
1:F:62:LEU:HD23	1:F:62:LEU:HA	1.89	0.43
1:E:305:HIS:HA	1:E:310:LEU:HD23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:67:ARG:NH1	1:F:304:LEU:HD13	2.33	0.43
1:E:324:PHE:CE1	1:E:340:ARG:HG3	2.54	0.43
1:F:157:LEU:H	1:F:157:LEU:HD12	1.84	0.43
1:E:21:TYR:CZ	1:E:347:GLU:HG2	2.53	0.42
1:A:38:VAL:HG21	1:A:44:SER:HB3	2.01	0.42
1:A:84:SER:HA	1:A:93:LEU:HD12	2.00	0.42
1:B:185:VAL:O	1:B:214:LEU:HD12	2.18	0.42
1:B:335:ASN:HB2	1:B:340:ARG:NH1	2.31	0.42
1:D:137:VAL:HG11	1:D:183:LYS:HD2	2.02	0.42
1:F:34:VAL:O	1:F:35:LEU:HD13	2.19	0.42
1:E:169:HIS:HE1	1:E:193:TYR:CE1	2.36	0.42
1:F:292:THR:N	1:F:293:PRO:HD2	2.34	0.42
1:D:124:THR:HG22	1:D:277:ILE:HD13	2.01	0.42
1:E:344:LEU:HD12	1:E:350:THR:HG22	2.00	0.42
1:E:179:CYS:HB3	1:E:212:PHE:CG	2.54	0.42
1:A:369:PHE:CD1	1:A:370:PRO:HA	2.55	0.42
1:B:239:MET:HE1	1:B:243:ASN:H	1.83	0.42
1:E:144:ASP:OD2	1:E:187:TYR:OH	2.37	0.42
1:E:86:LEU:HD12	1:E:91:MET:CB	2.40	0.42
1:E:137:VAL:HB	1:E:184:ARG:HG3	2.01	0.42
1:F:242:ILE:HD13	1:F:266:GLY:HA2	2.02	0.42
1:F:335:ASN:HB3	1:F:337:VAL:H	1.84	0.42
1:B:248:LEU:HB2	1:B:264:VAL:HB	2.02	0.42
1:D:174:ALA:O	1:D:178:ILE:HG13	2.20	0.41
1:D:259:SER:HB2	1:D:294:ALA:HB1	2.01	0.41
1:E:17:LEU:HG	1:E:21:TYR:CE2	2.54	0.41
1:D:124:THR:O	1:D:127:VAL:HG22	2.20	0.41
1:B:22:TRP:CH2	1:B:371:ILE:HD11	2.55	0.41
1:E:342:LEU:HD23	1:E:399:TRP:CZ2	2.55	0.41
1:F:362:PHE:CE1	1:F:395:PHE:HB2	2.56	0.41
1:B:89:VAL:HG23	1:B:91:MET:HG2	2.02	0.41
1:C:96:LEU:HD11	1:C:289:ARG:HD2	2.01	0.41
1:A:156:SER:HB2	1:E:157:LEU:HD23	2.03	0.41
1:F:59:TYR:O	1:F:384:ARG:HA	2.21	0.41
1:A:12:LYS:HE3	1:A:12:LYS:HB2	1.79	0.41
1:A:127:VAL:HG21	1:A:277:ILE:HG12	2.03	0.41
1:A:288:GLN:N	2:E:501:PLP:O1P	2.51	0.41
1:D:96:LEU:HA	1:D:295:LEU:HD13	2.03	0.41
1:D:179:CYS:HB3	1:D:212:PHE:CG	2.56	0.41
1:E:24:SER:HA	1:E:27:ARG:HH11	1.86	0.41
1:E:292:THR:N	1:E:293:PRO:HD2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:308:GLU:O	1:E:311:PRO:HD2	2.21	0.41
1:F:308:GLU:O	1:F:311:PRO:HD2	2.21	0.41
1:B:364:VAL:HG12	1:B:379:LEU:HB3	2.03	0.41
1:B:402:LEU:HA	1:B:402:LEU:HD12	1.80	0.41
1:C:160:ASP:OD2	1:F:156:SER:OG	2.35	0.40
1:A:323:LEU:HD23	1:A:392:ILE:HB	2.03	0.40
1:B:344:LEU:HD23	1:B:379:LEU:HG	2.03	0.40
1:D:207:ALA:HA	1:D:210:LYS:HD2	2.04	0.40
1:E:353:ALA:O	1:E:357:LEU:HG	2.21	0.40
1:A:86:LEU:CD1	1:E:35:LEU:HB2	2.51	0.40
1:A:86:LEU:HD13	1:E:35:LEU:HB2	2.04	0.40
1:B:189:CYS:HB2	1:B:193:TYR:OH	2.22	0.40
1:F:260:GLY:HA3	1:F:290:LEU:HD21	2.02	0.40
1:D:281:SER:OG	1:D:286:TRP:HZ3	2.05	0.40
1:A:239:MET:HG2	1:A:241:ALA:O	2.22	0.40
1:B:292:THR:N	1:B:293:PRO:HD2	2.37	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	392/394 (100%)	379 (97%)	13 (3%)	0	100	100
1	B	384/394 (98%)	367 (96%)	17 (4%)	0	100	100
1	C	391/394 (99%)	382 (98%)	9 (2%)	0	100	100
1	D	389/394 (99%)	380 (98%)	9 (2%)	0	100	100
1	E	389/394 (99%)	377 (97%)	12 (3%)	0	100	100
1	F	388/394 (98%)	371 (96%)	17 (4%)	0	100	100
All	All	2333/2364 (99%)	2256 (97%)	77 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	313/313 (100%)	307 (98%)	6 (2%)	57	80
1	B	305/313 (97%)	298 (98%)	7 (2%)	50	76
1	C	312/313 (100%)	307 (98%)	5 (2%)	62	84
1	D	310/313 (99%)	301 (97%)	9 (3%)	42	69
1	E	310/313 (99%)	304 (98%)	6 (2%)	57	80
1	F	309/313 (99%)	305 (99%)	4 (1%)	69	87
All	All	1859/1878 (99%)	1822 (98%)	37 (2%)	55	79

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	146	ARG
1	C	165	GLU
1	C	223	SER
1	C	226	VAL
1	C	310	LEU
1	A	69	ILE
1	A	190	ASP
1	A	205	LEU
1	A	223	SER
1	A	359	ASP
1	A	402	LEU
1	B	38	VAL
1	B	56	SER
1	B	127	VAL
1	B	224	THR
1	B	310	LEU
1	B	329	ARG
1	B	374	ARG
1	D	16	HIS

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Mol	Chain	Res	Type
1	D	17	LEU
1	D	88	ARG
1	D	194	SER
1	D	244	ASP
1	D	310	LEU
1	D	359	ASP
1	D	372	VAL
1	D	402	LEU
1	E	31	HIS
1	E	127	VAL
1	E	223	SER
1	E	304	LEU
1	E	310	LEU
1	E	359	ASP
1	F	35	LEU
1	F	165	GLU
1	F	194	SER
1	F	310	LEU

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

Mol	Chain	Res	Type
1	B	31	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

6 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	E	501	1	15,15,16	1.62	3 (20%)	20,22,23	1.41	5 (25%)
2	PLP	B	501	1	15,15,16	1.27	2 (13%)	20,22,23	1.38	1 (5%)
2	PLP	F	501	1	15,15,16	1.42	3 (20%)	20,22,23	1.17	0
2	PLP	D	501	1	15,15,16	1.23	2 (13%)	20,22,23	1.25	2 (10%)
2	PLP	A	501	1	15,15,16	1.60	3 (20%)	20,22,23	1.46	5 (25%)
2	PLP	C	501	1	15,15,16	1.07	1 (6%)	20,22,23	1.52	4 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLP	E	501	1	-	1/6/6/8	0/1/1/1
2	PLP	B	501	1	-	2/6/6/8	0/1/1/1
2	PLP	F	501	1	-	3/6/6/8	0/1/1/1
2	PLP	D	501	1	-	1/6/6/8	0/1/1/1
2	PLP	A	501	1	-	2/6/6/8	0/1/1/1
2	PLP	C	501	1	-	0/6/6/8	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	501	PLP	C5-C4	-3.86	1.36	1.40
2	F	501	PLP	C3-C2	-3.75	1.37	1.40
2	A	501	PLP	C3-C2	-3.54	1.37	1.40
2	A	501	PLP	C5-C4	-3.19	1.37	1.40
2	E	501	PLP	C3-C2	-3.18	1.37	1.40
2	B	501	PLP	C5-C4	-3.15	1.37	1.40
2	D	501	PLP	C5-C4	-2.87	1.37	1.40
2	C	501	PLP	C2-N1	2.72	1.39	1.33
2	D	501	PLP	C3-C2	-2.24	1.38	1.40
2	F	501	PLP	C5-C4	-2.24	1.38	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	501	PLP	C2-N1	2.11	1.37	1.33
2	B	501	PLP	C2-N1	2.10	1.37	1.33
2	F	501	PLP	C2-N1	2.03	1.37	1.33
2	A	501	PLP	C2-N1	2.00	1.37	1.33

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	501	PLP	C4A-C4-C5	-4.28	116.53	120.94
2	D	501	PLP	C4A-C4-C5	-4.19	116.61	120.94
2	B	501	PLP	C4A-C4-C5	-4.17	116.64	120.94
2	A	501	PLP	C2A-C2-C3	-2.98	117.21	120.89
2	E	501	PLP	C5A-C5-C6	2.72	123.85	119.37
2	A	501	PLP	C4A-C4-C5	-2.65	118.20	120.94
2	C	501	PLP	C4A-C4-C3	-2.57	116.14	120.50
2	A	501	PLP	C2A-C2-N1	2.48	122.52	117.67
2	A	501	PLP	C5A-C5-C6	2.48	123.45	119.37
2	E	501	PLP	C2A-C2-C3	-2.44	117.88	120.89
2	E	501	PLP	O4P-P-O1P	2.42	113.27	106.47
2	C	501	PLP	C6-C5-C4	2.40	120.05	118.16
2	E	501	PLP	C2A-C2-N1	2.18	121.93	117.67
2	A	501	PLP	O4P-C5A-C5	2.03	113.22	109.35
2	C	501	PLP	O3P-P-O4P	2.02	112.10	106.73
2	E	501	PLP	C4A-C4-C5	-2.01	118.87	120.94
2	D	501	PLP	C6-C5-C4	2.00	119.73	118.16

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	PLP	C4-C5-C5A-O4P
2	B	501	PLP	C4-C5-C5A-O4P
2	F	501	PLP	C5A-O4P-P-O1P
2	F	501	PLP	C5A-O4P-P-O3P
2	D	501	PLP	C4-C5-C5A-O4P
2	E	501	PLP	C4-C5-C5A-O4P
2	A	501	PLP	C6-C5-C5A-O4P
2	B	501	PLP	C6-C5-C5A-O4P
2	F	501	PLP	C5A-O4P-P-O2P

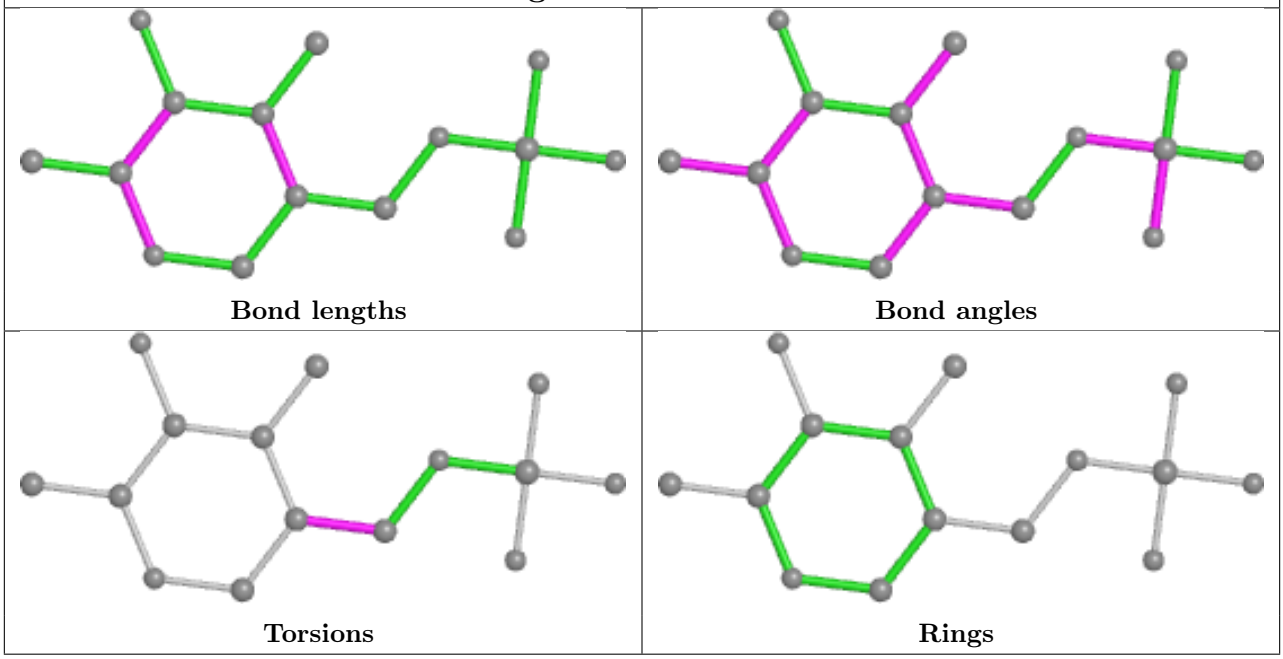
There are no ring outliers.

5 monomers are involved in 10 short contacts:

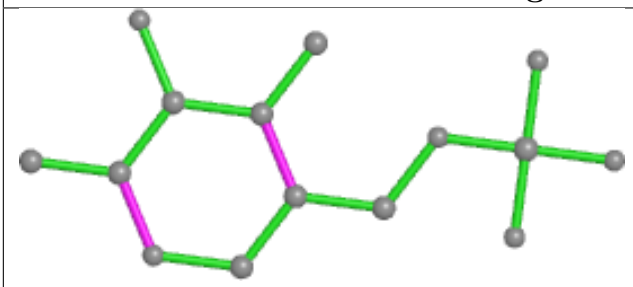
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	501	PLP	3	0
2	B	501	PLP	2	0
2	F	501	PLP	1	0
2	A	501	PLP	2	0
2	C	501	PLP	2	0

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.

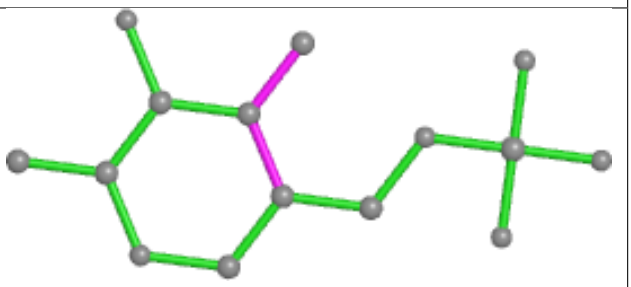
Ligand PLP E 501



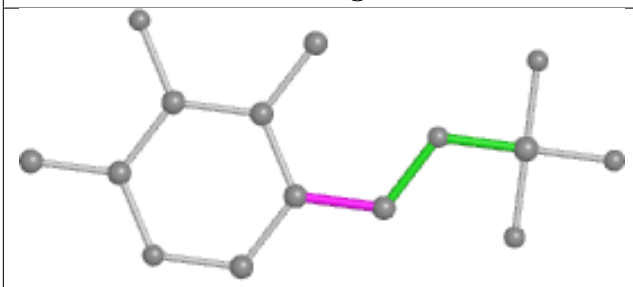
Ligand PLP B 501



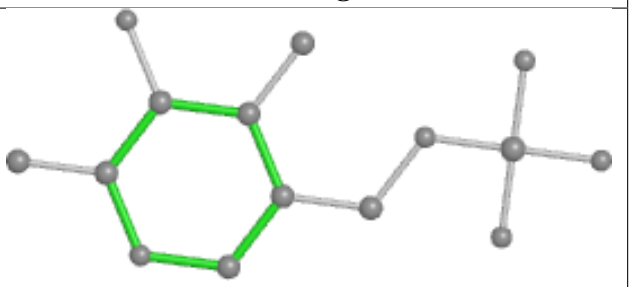
Bond lengths



Bond angles

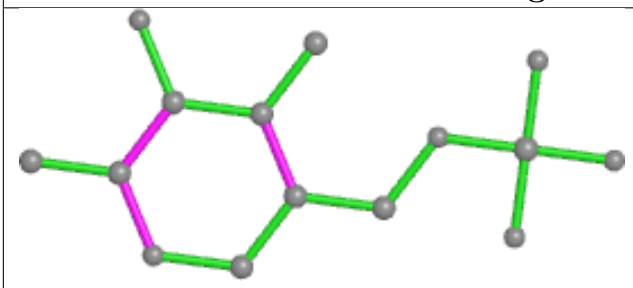


Torsions

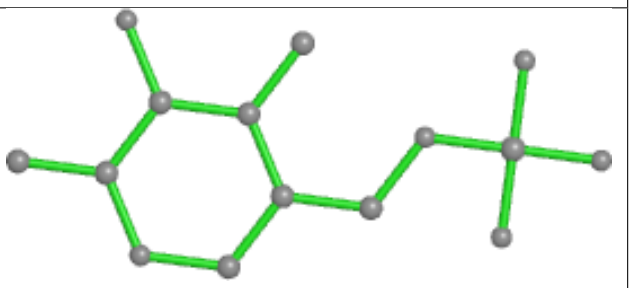


Rings

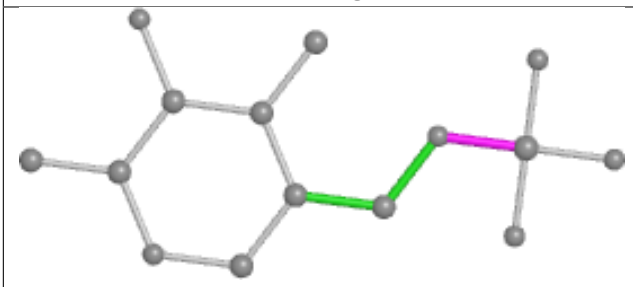
Ligand PLP F 501



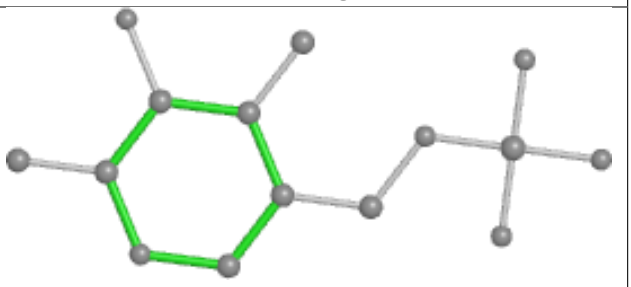
Bond lengths



Bond angles

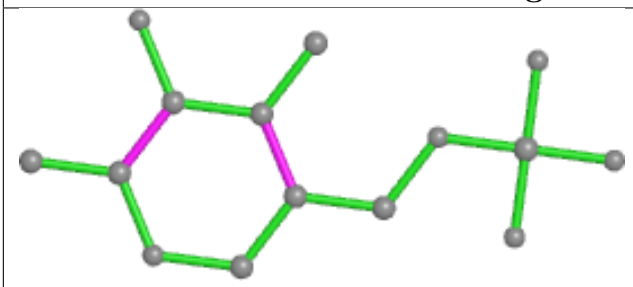


Torsions

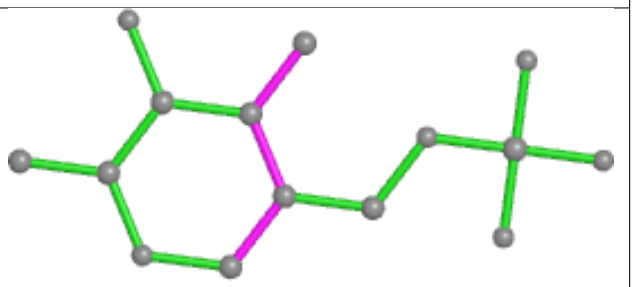


Rings

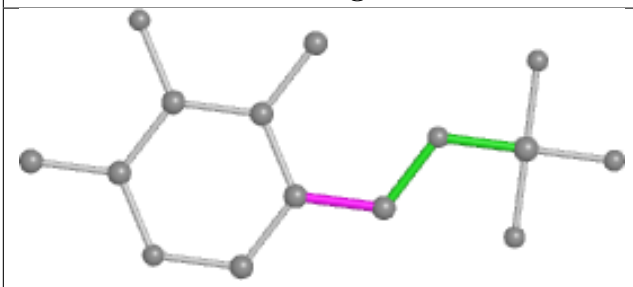
Ligand PLP D 501



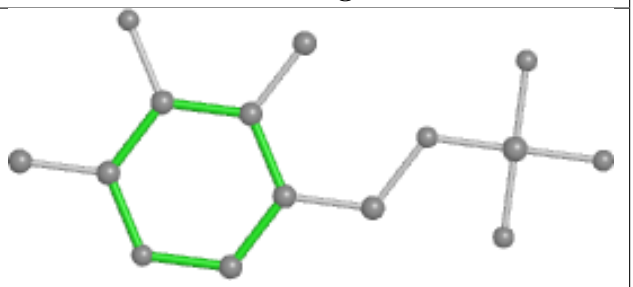
Bond lengths



Bond angles

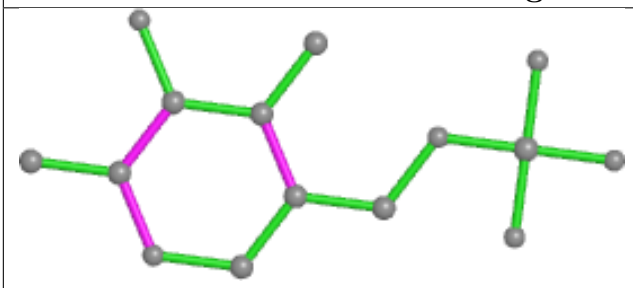


Torsions

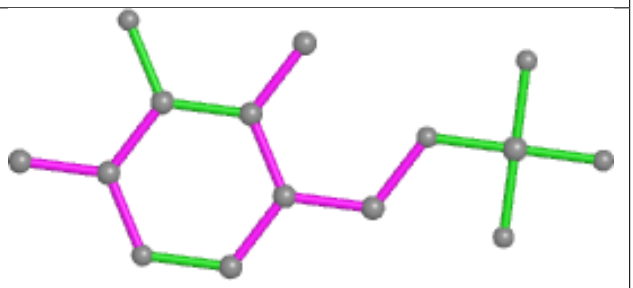


Rings

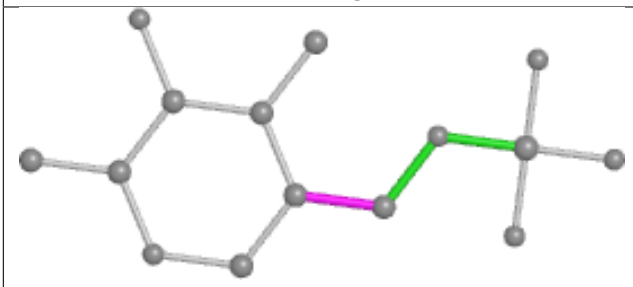
Ligand PLP A 501



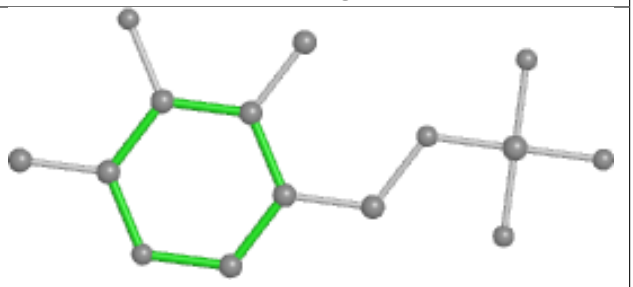
Bond lengths



Bond angles

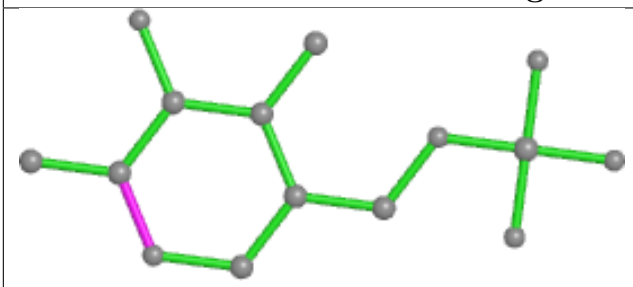


Torsions

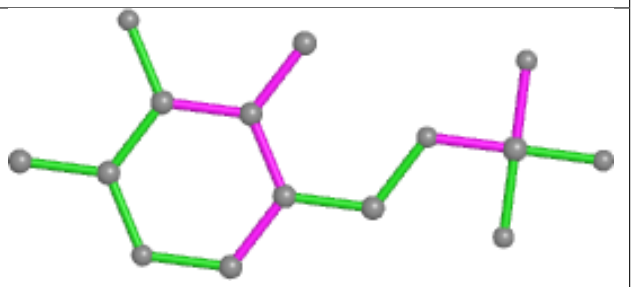


Rings

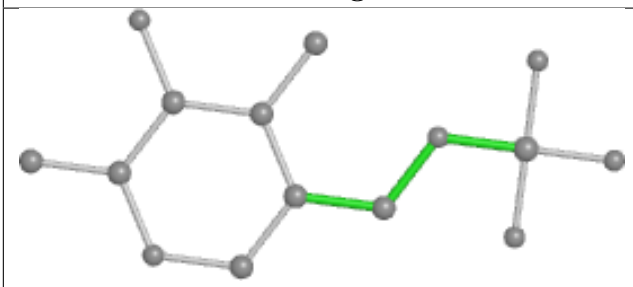
Ligand PLP C 501



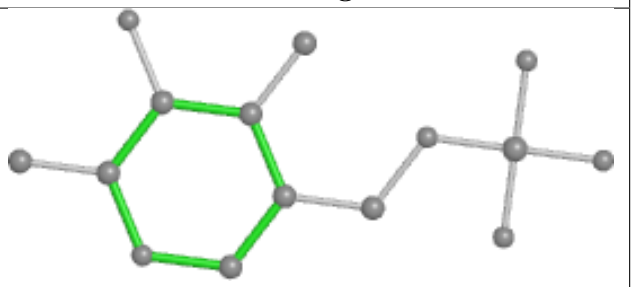
Bond lengths



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	394/394 (100%)	0.26	27 (6%)	16	17	35, 49, 71, 88	0
1	B	386/394 (97%)	0.39	38 (9%)	7	7	34, 51, 90, 104	0
1	C	393/394 (99%)	0.17	25 (6%)	19	20	36, 47, 63, 87	0
1	D	391/394 (99%)	0.28	26 (6%)	18	19	33, 50, 70, 102	0
1	E	391/394 (99%)	0.32	31 (7%)	12	12	35, 51, 77, 99	0
1	F	390/394 (98%)	0.28	21 (5%)	25	27	36, 49, 68, 100	0
All	All	2345/2364 (99%)	0.28	168 (7%)	15	16	33, 49, 73, 104	0

All (168) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	14	LEU	8.4
1	D	16	HIS	7.6
1	A	14	LEU	7.4
1	F	17	LEU	7.3
1	F	15	ARG	6.9
1	E	14	LEU	6.7
1	B	374	ARG	6.6
1	F	46	PRO	6.3
1	F	18	SER	6.3
1	E	404	VAL	6.2
1	E	16	HIS	6.0
1	F	404	VAL	6.0
1	D	15	ARG	5.8
1	A	13	LYS	5.2
1	C	14	LEU	5.2
1	A	404	VAL	5.1
1	C	13	LYS	4.9
1	E	217	TYR	4.8
1	B	19	ASP	4.8

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Mol	Chain	Res	Type	RSRZ
1	B	217	TYR	4.7
1	C	16	HIS	4.7
1	E	15	ARG	4.6
1	B	24	SER	4.5
1	E	197	GLY	4.5
1	F	217	TYR	4.5
1	F	16	HIS	4.4
1	A	183	LYS	4.3
1	B	28	LEU	4.3
1	D	217	TYR	4.2
1	E	218	PHE	4.1
1	B	369	PHE	4.1
1	E	17	LEU	4.0
1	A	16	HIS	4.0
1	E	212	PHE	3.9
1	B	20	GLY	3.9
1	B	344	LEU	3.9
1	B	27	ARG	3.8
1	E	46	PRO	3.8
1	A	196	GLY	3.8
1	C	46	PRO	3.8
1	C	404	VAL	3.7
1	B	370	PRO	3.7
1	F	403	GLY	3.7
1	B	216	LEU	3.6
1	A	11	VAL	3.6
1	D	17	LEU	3.6
1	D	18	SER	3.6
1	C	217	TYR	3.5
1	D	404	VAL	3.5
1	A	217	TYR	3.5
1	B	346	SER	3.5
1	B	195	THR	3.4
1	C	15	ARG	3.4
1	A	269	ASP	3.4
1	D	188	VAL	3.4
1	D	218	PHE	3.3
1	E	403	GLY	3.2
1	F	369	PHE	3.2
1	C	249	ILE	3.2
1	E	210	LYS	3.2
1	E	196	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	30	VAL	3.2
1	D	248	LEU	3.2
1	C	269	ASP	3.1
1	A	248	LEU	3.1
1	E	18	SER	3.1
1	D	216	LEU	3.1
1	B	364	VAL	3.1
1	B	21	TYR	3.0
1	A	188	VAL	3.0
1	B	269	ASP	3.0
1	E	369	PHE	3.0
1	B	188	VAL	2.9
1	C	403	GLY	2.9
1	C	47	ASP	2.9
1	B	218	PHE	2.9
1	C	149	PHE	2.9
1	C	216	LEU	2.8
1	C	48	GLY	2.8
1	A	218	PHE	2.8
1	E	181	LYS	2.8
1	B	189	CYS	2.8
1	F	249	ILE	2.8
1	E	248	LEU	2.8
1	C	188	VAL	2.7
1	C	218	PHE	2.7
1	C	248	LEU	2.7
1	A	189	CYS	2.7
1	B	248	LEU	2.7
1	A	364	VAL	2.7
1	B	22	TRP	2.7
1	F	47	ASP	2.7
1	F	45	ALA	2.7
1	F	218	PHE	2.7
1	E	189	CYS	2.7
1	D	19	ASP	2.7
1	E	125	LEU	2.7
1	B	25	ALA	2.6
1	C	364	VAL	2.6
1	B	46	PRO	2.6
1	D	187	TYR	2.6
1	E	216	LEU	2.6
1	F	189	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	19	ASP	2.6
1	A	46	PRO	2.6
1	A	163	ARG	2.6
1	B	329	ARG	2.6
1	D	186	ALA	2.6
1	C	12	LYS	2.5
1	A	12	LYS	2.5
1	A	216	LEU	2.5
1	B	247	MET	2.5
1	C	27	ARG	2.5
1	A	238	ARG	2.5
1	D	269	ASP	2.5
1	B	149	PHE	2.5
1	B	168	ARG	2.5
1	E	247	MET	2.5
1	B	379	LEU	2.5
1	D	125	LEU	2.4
1	F	269	ASP	2.4
1	C	49	ARG	2.4
1	B	23	ASP	2.4
1	D	238	ARG	2.4
1	A	403	GLY	2.4
1	D	20	GLY	2.4
1	B	187	TYR	2.4
1	F	188	VAL	2.3
1	F	248	LEU	2.3
1	E	269	ASP	2.3
1	D	249	ILE	2.3
1	E	146	ARG	2.3
1	E	374	ARG	2.3
1	D	369	PHE	2.3
1	A	187	TYR	2.3
1	A	195	THR	2.3
1	D	90	ARG	2.3
1	A	15	ARG	2.3
1	B	373	SER	2.3
1	B	183	LYS	2.2
1	D	329	ARG	2.2
1	F	163	ARG	2.2
1	B	137	VAL	2.2
1	A	272	ARG	2.2
1	D	27	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	189	CYS	2.2
1	F	210	LYS	2.2
1	C	247	MET	2.2
1	D	149	PHE	2.2
1	E	211	GLU	2.2
1	C	379	LEU	2.2
1	B	125	LEU	2.2
1	E	176	ALA	2.2
1	B	356	TYR	2.1
1	C	272	ARG	2.1
1	E	187	TYR	2.1
1	E	177	ASP	2.1
1	B	197	GLY	2.1
1	A	270	ASP	2.1
1	D	364	VAL	2.1
1	A	249	ILE	2.1
1	D	379	LEU	2.1
1	E	179	CYS	2.1
1	F	247	MET	2.1
1	E	174	ALA	2.1
1	E	364	VAL	2.0
1	B	29	GLY	2.0
1	A	379	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.

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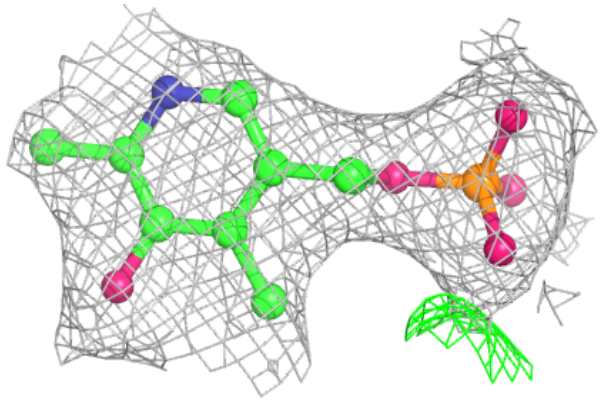
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

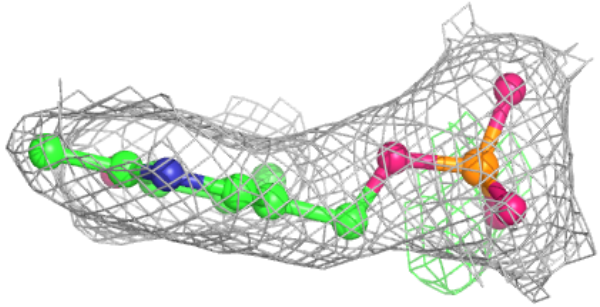
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PLP	B	501	15/16	0.97	0.11	38,43,51,51	0
2	PLP	E	501	15/16	0.97	0.14	39,45,49,49	0
2	PLP	C	501	15/16	0.98	0.10	35,39,42,43	0
2	PLP	D	501	15/16	0.98	0.11	36,42,47,47	0
2	PLP	A	501	15/16	0.98	0.12	41,44,49,51	0
2	PLP	F	501	15/16	0.98	0.12	38,41,44,46	0

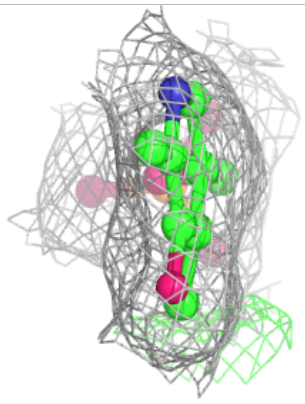
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PLP B 501:

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

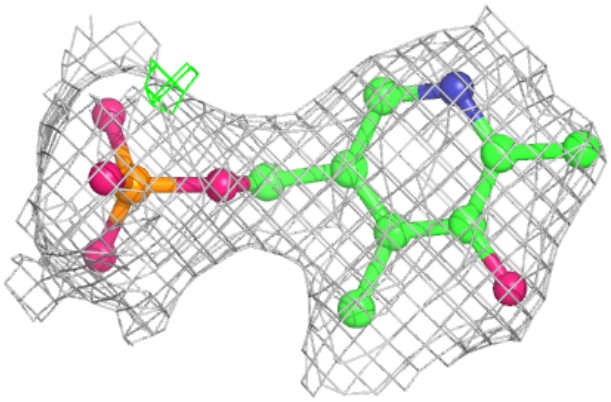


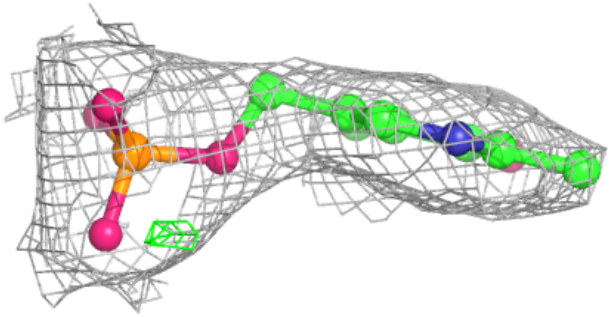


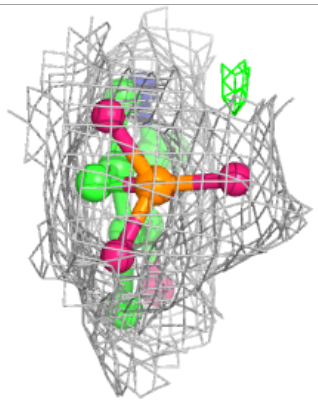


Electron density around PLP E 501:

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

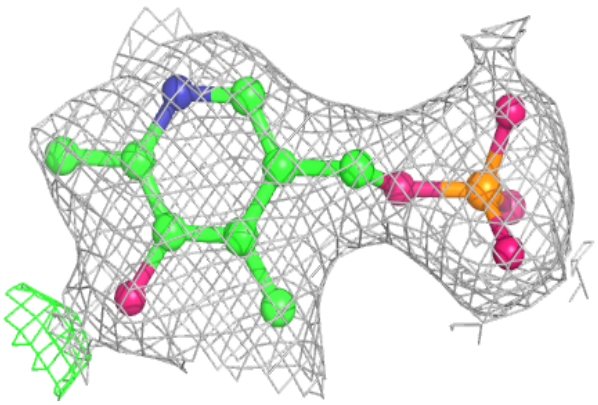


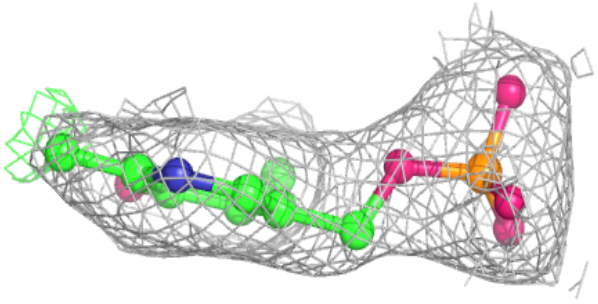




Electron density around PLP C 501:

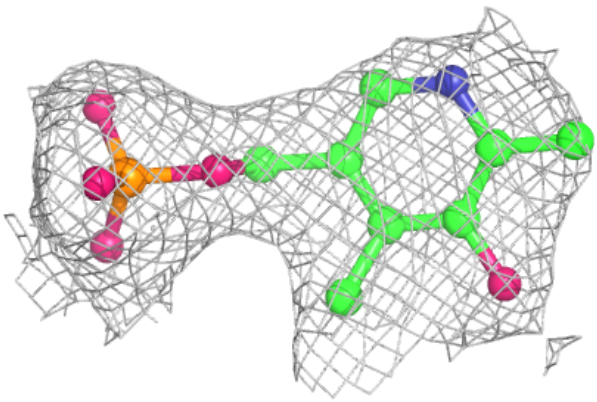
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

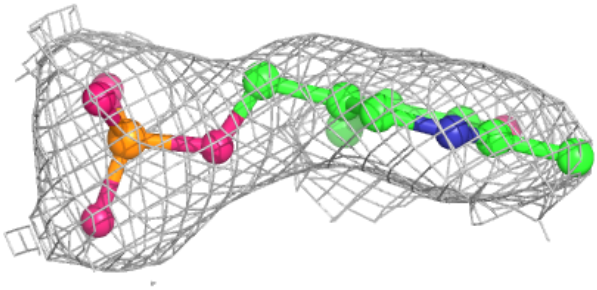


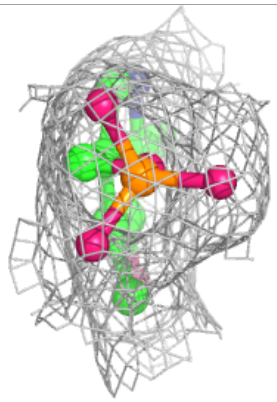


Electron density around PLP D 501:

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

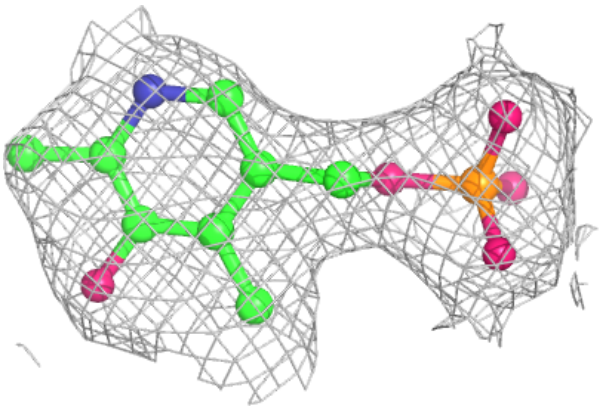


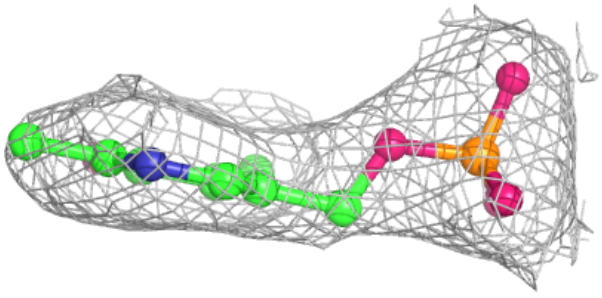


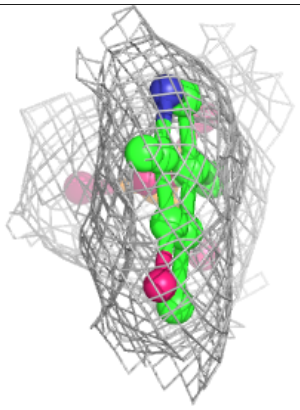


Electron density around PLP A 501:

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

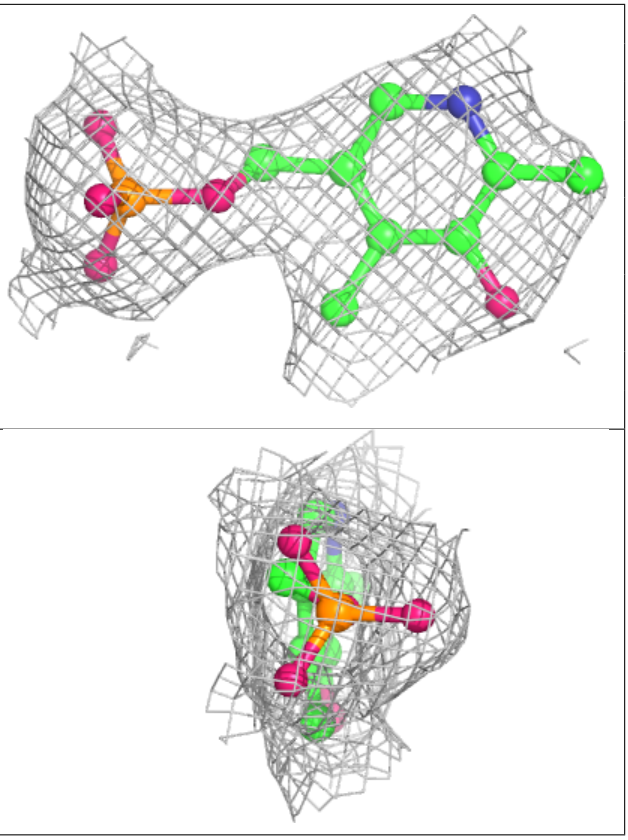


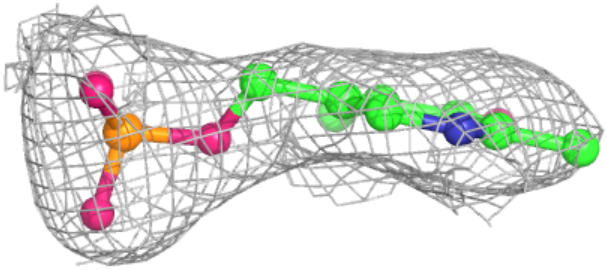




Electron density around PLP F 501:

$2mF_o$-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

There are no such residues in this entry.