



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:00 PM UTC

PDB ID : 7P3T / pdb_00007p3t
Title : Transaminase of gamma-proteobacterium
Authors : Ermler, U.
Deposited on : 2021-07-08
Resolution : 1.60 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 : 4-5-2 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

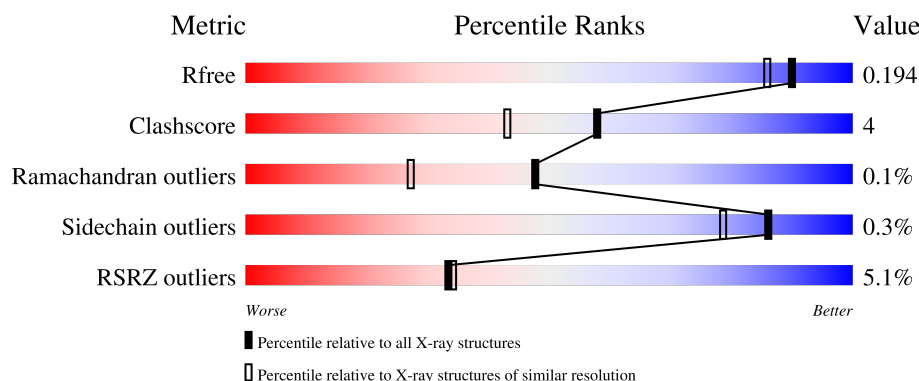
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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}	180053	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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 $\leq 5\%$. 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	302	4% 91% 7%
1	B	302	7% 89% 10%
1	C	302	3% 87% 10%
1	D	302	4% 87% 10%
1	E	302	6% 89% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	302	 A horizontal bar chart showing the quality of chain F. The bar is divided into three segments: a red segment at the beginning labeled '5%', a long green segment in the middle labeled '90%', and a yellow segment at the end labeled '7%'. A small grey dot is located at the far right end of the bar.

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15759 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 Branched-chain amino acid aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	3	0
			2359	1493	416	443	7			
1	B	299	Total	C	N	O	S	0	7	0
			2429	1533	439	451	6			
1	C	294	Total	C	N	O	S	0	12	0
			2426	1529	432	459	6			
1	D	295	Total	C	N	O	S	0	6	0
			2382	1505	424	447	6			
1	E	294	Total	C	N	O	S	0	8	0
			2397	1514	430	447	6			
1	F	294	Total	C	N	O	S	0	6	0
			2367	1498	416	447	6			

There are 54 discrepancies between the modelled and reference sequences:

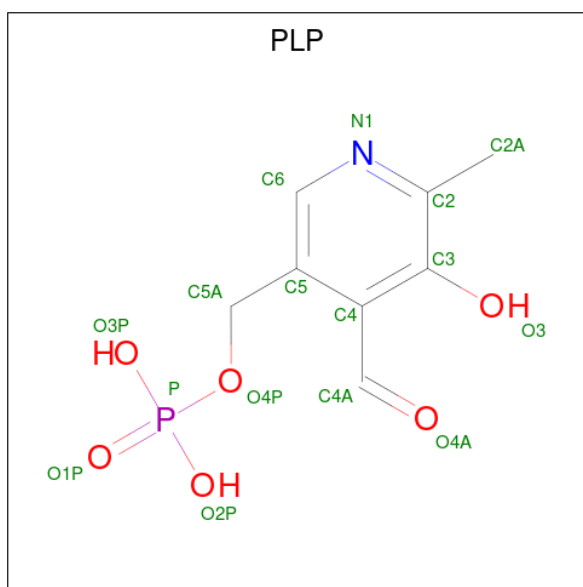
Chain	Residue	Modelled	Actual	Comment	Reference
A	294	SER	-	expression tag	UNP B8KQT8
A	295	GLY	-	expression tag	UNP B8KQT8
A	296	SER	-	expression tag	UNP B8KQT8
A	297	HIS	-	expression tag	UNP B8KQT8
A	298	HIS	-	expression tag	UNP B8KQT8
A	299	HIS	-	expression tag	UNP B8KQT8
A	300	HIS	-	expression tag	UNP B8KQT8
A	301	HIS	-	expression tag	UNP B8KQT8
A	302	HIS	-	expression tag	UNP B8KQT8
B	294	SER	-	expression tag	UNP B8KQT8
B	295	GLY	-	expression tag	UNP B8KQT8
B	296	SER	-	expression tag	UNP B8KQT8
B	297	HIS	-	expression tag	UNP B8KQT8
B	298	HIS	-	expression tag	UNP B8KQT8
B	299	HIS	-	expression tag	UNP B8KQT8
B	300	HIS	-	expression tag	UNP B8KQT8
B	301	HIS	-	expression tag	UNP B8KQT8

Continued on next page...

Continued from previous page...

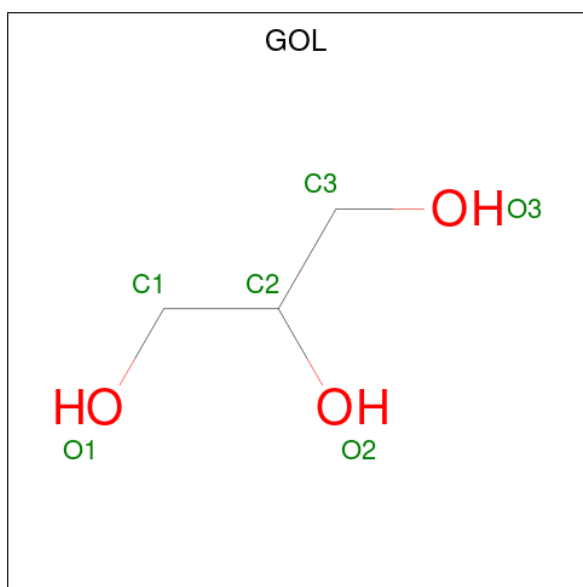
Chain	Residue	Modelled	Actual	Comment	Reference
B	302	HIS	-	expression tag	UNP B8KQT8
C	294	SER	-	expression tag	UNP B8KQT8
C	295	GLY	-	expression tag	UNP B8KQT8
C	296	SER	-	expression tag	UNP B8KQT8
C	297	HIS	-	expression tag	UNP B8KQT8
C	298	HIS	-	expression tag	UNP B8KQT8
C	299	HIS	-	expression tag	UNP B8KQT8
C	300	HIS	-	expression tag	UNP B8KQT8
C	301	HIS	-	expression tag	UNP B8KQT8
C	302	HIS	-	expression tag	UNP B8KQT8
D	294	SER	-	expression tag	UNP B8KQT8
D	295	GLY	-	expression tag	UNP B8KQT8
D	296	SER	-	expression tag	UNP B8KQT8
D	297	HIS	-	expression tag	UNP B8KQT8
D	298	HIS	-	expression tag	UNP B8KQT8
D	299	HIS	-	expression tag	UNP B8KQT8
D	300	HIS	-	expression tag	UNP B8KQT8
D	301	HIS	-	expression tag	UNP B8KQT8
D	302	HIS	-	expression tag	UNP B8KQT8
E	294	SER	-	expression tag	UNP B8KQT8
E	295	GLY	-	expression tag	UNP B8KQT8
E	296	SER	-	expression tag	UNP B8KQT8
E	297	HIS	-	expression tag	UNP B8KQT8
E	298	HIS	-	expression tag	UNP B8KQT8
E	299	HIS	-	expression tag	UNP B8KQT8
E	300	HIS	-	expression tag	UNP B8KQT8
E	301	HIS	-	expression tag	UNP B8KQT8
E	302	HIS	-	expression tag	UNP B8KQT8
F	294	SER	-	expression tag	UNP B8KQT8
F	295	GLY	-	expression tag	UNP B8KQT8
F	296	SER	-	expression tag	UNP B8KQT8
F	297	HIS	-	expression tag	UNP B8KQT8
F	298	HIS	-	expression tag	UNP B8KQT8
F	299	HIS	-	expression tag	UNP B8KQT8
F	300	HIS	-	expression tag	UNP B8KQT8
F	301	HIS	-	expression tag	UNP B8KQT8
F	302	HIS	-	expression tag	UNP B8KQT8

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

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		

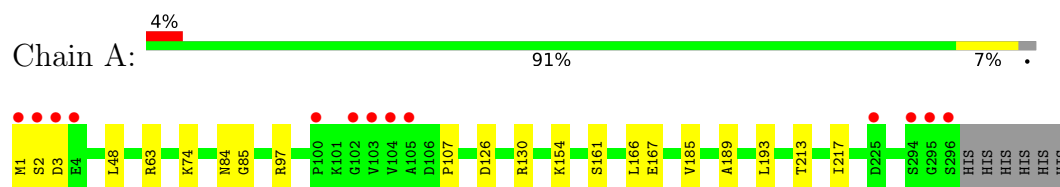
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	221	Total	O	0	2
			223	223		
4	B	210	Total	O	0	2
			212	212		
4	C	253	Total	O	0	1
			254	254		
4	D	183	Total	O	0	3
			186	186		
4	E	181	Total	O	0	1
			182	182		
4	F	215	Total	O	0	1
			216	216		

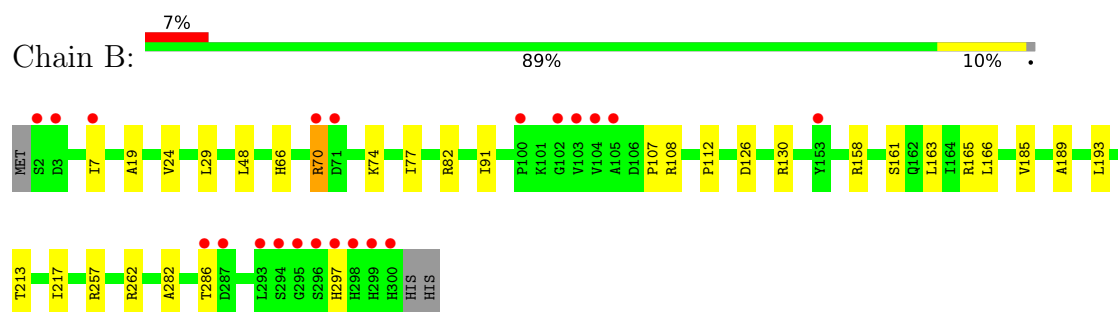
3 Residue-property plots [i](#)

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.

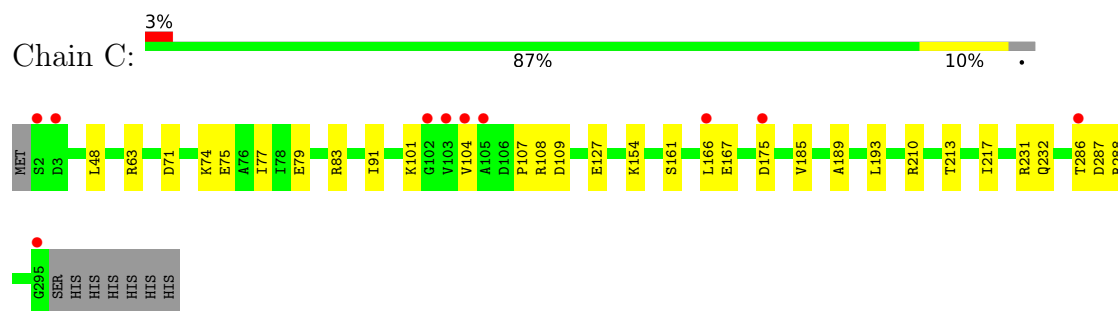
- Molecule 1: Branched-chain amino acid aminotransferase



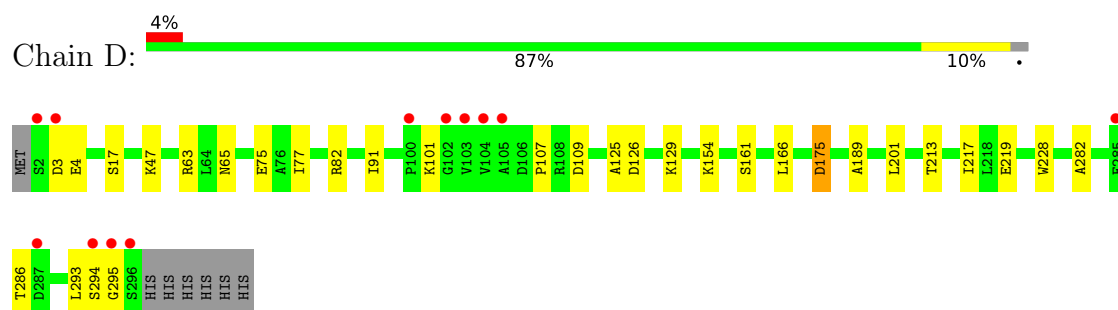
- Molecule 1: Branched-chain amino acid aminotransferase



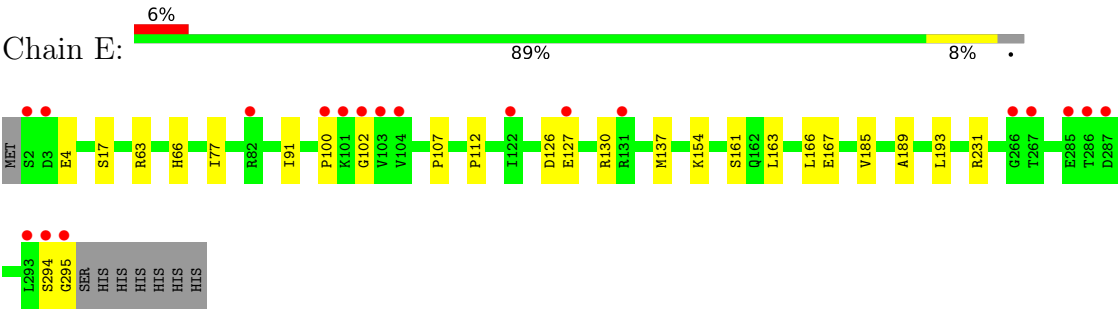
- Molecule 1: Branched-chain amino acid aminotransferase



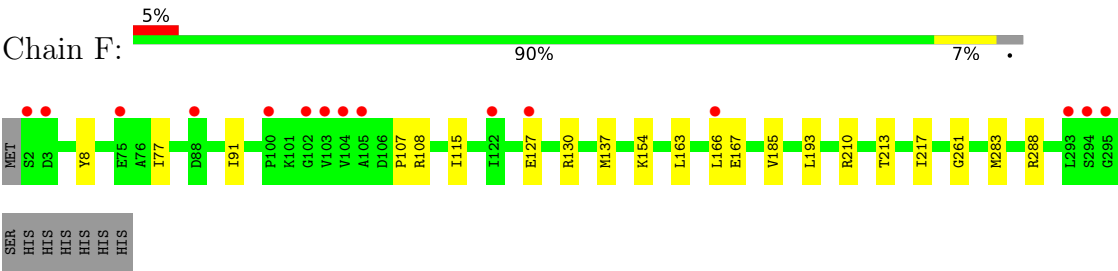
- Molecule 1: Branched-chain amino acid aminotransferase



● Molecule 1: Branched-chain amino acid aminotransferase



● Molecule 1: Branched-chain amino acid aminotransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.81Å 144.58Å 151.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.93 – 1.60 45.93 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (45.93-1.60) 99.7 (45.93-1.60)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 1.60Å)	Xtriage
Refinement program	PHENIX 1.14 _3260	Depositor
R, R_{free}	0.169 , 0.185 0.178 , 0.194	Depositor DCC
R_{free} test set	12305 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	26.8	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 35.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15759	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PLP, GOL

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	0.39	0/2412	0.66	0/3278
1	B	0.34	0/2487	0.60	0/3379
1	C	0.38	0/2479	0.64	0/3367
1	D	0.34	0/2435	0.62	3/3308 (0.1%)
1	E	0.30	0/2451	0.60	0/3329
1	F	0.35	0/2420	0.59	0/3289
All	All	0.35	0/14684	0.62	3/19950 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	294	SER	CA-C-N	5.49	132.17	121.41
1	D	294	SER	C-N-CA	5.49	132.17	121.41
1	D	175	ASP	CA-CB-CG	-5.37	107.23	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2359	0	2322	29	0
1	B	2429	0	2373	27	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2426	0	2369	33	0
1	D	2382	0	2339	23	0
1	E	2397	0	2353	18	0
1	F	2367	0	2321	20	0
2	A	15	0	7	1	0
2	B	15	0	7	1	0
2	C	15	0	7	1	0
2	D	15	0	7	1	0
2	E	15	0	6	1	0
2	F	15	0	7	1	0
3	A	6	0	8	0	0
3	B	6	0	8	0	0
3	C	6	0	8	0	0
3	D	6	0	8	0	0
3	E	6	0	7	1	0
3	F	6	0	8	0	0
4	A	223	0	0	1	0
4	B	212	0	0	1	0
4	C	254	0	0	4	0
4	D	186	0	0	1	0
4	E	182	0	0	2	0
4	F	216	0	0	2	0
All	All	15759	0	14165	129	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (129) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:75:GLU:OE2	4:D:501:HOH:O	1.68	1.10
1:D:63[B]:ARG:HH21	1:D:63[B]:ARG:HG3	1.31	0.91
1:D:63[A]:ARG:HD3	1:F:166:LEU:HD22	1.60	0.83
1:A:166:LEU:HG	1:C:107:PRO:HG2	1.60	0.83
1:E:167[A]:GLU:OE1	4:E:501:HOH:O	2.00	0.79
1:B:166:LEU:HD22	1:E:63:ARG:HD3	1.66	0.78
1:D:166:LEU:HG	1:F:107:PRO:HG2	1.66	0.77
1:B:257[B]:ARG:NH1	4:B:501:HOH:O	2.20	0.74
1:A:167:GLU:OE1	4:A:501:HOH:O	2.07	0.71
1:F:167[A]:GLU:OE1	4:F:501:HOH:O	2.09	0.69
1:A:63[A]:ARG:HD3	1:C:166:LEU:CD2	2.23	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:LEU:HD23	1:C:108:ARG:HG3	1.73	0.68
1:A:1:MET:N	1:A:84:ASN:O	2.26	0.67
1:C:167:GLU:OE1	4:C:501:HOH:O	2.13	0.67
1:A:63[A]:ARG:HH11	1:C:166:LEU:HD11	1.61	0.66
1:A:1:MET:HE2	1:A:85:GLY:O	1.97	0.65
1:C:63[B]:ARG:HH21	1:C:63[B]:ARG:HG2	1.60	0.65
1:C:286[B]:THR:HG21	1:C:288:ARG:HG3	1.79	0.64
1:D:4:GLU:OE2	1:D:17:SER:HB3	1.97	0.64
1:C:101:LYS:HE2	1:C:109:ASP:OD1	1.99	0.63
1:F:163:LEU:HA	1:F:166:LEU:HD12	1.80	0.62
1:B:7:ILE:HD11	1:B:19:ALA:HB1	1.81	0.62
1:E:137:MET:HE1	1:E:167[B]:GLU:HG2	1.82	0.62
1:D:63[B]:ARG:HG3	1:D:63[B]:ARG:NH2	2.07	0.62
1:A:63[B]:ARG:HH21	1:A:63[B]:ARG:HG3	1.64	0.61
1:D:82:ARG:HD3	1:D:293:LEU:O	2.01	0.61
1:B:163:LEU:HD23	1:B:166:LEU:HD12	1.81	0.61
1:A:166:LEU:CD2	1:C:108:ARG:HG3	2.31	0.60
1:A:63[A]:ARG:NH1	1:C:166:LEU:HD11	2.17	0.59
1:E:294:SER:OG	1:E:295:GLY:N	2.36	0.59
1:C:286[B]:THR:HG22	1:C:287:ASP:N	2.16	0.59
1:B:158:ARG:NH2	2:B:401:PLP:O3	2.30	0.58
1:D:101:LYS:NZ	1:D:109:ASP:OD1	2.36	0.58
1:A:63[A]:ARG:HD3	1:C:166:LEU:HD21	1.85	0.58
1:B:7:ILE:HD11	1:B:19:ALA:CB	2.34	0.58
1:B:165:ARG:HH21	1:B:165:ARG:HG3	1.69	0.57
1:C:63[B]:ARG:HH21	1:C:63[B]:ARG:CG	2.17	0.57
1:B:82[A]:ARG:HH11	1:B:297:HIS:CE1	2.23	0.57
1:B:107:PRO:HG2	1:E:166:LEU:HG	1.87	0.56
1:D:107:PRO:HG2	1:F:166:LEU:HG	1.88	0.56
1:D:166:LEU:HD23	1:F:108:ARG:HG3	1.88	0.55
1:A:63[B]:ARG:HG3	1:A:63[B]:ARG:NH2	2.21	0.54
1:E:126:ASP:O	1:E:130[B]:ARG:HG3	2.06	0.54
1:A:63[A]:ARG:HD3	1:C:166:LEU:CD1	2.37	0.54
1:F:185:VAL:HG11	1:F:193:LEU:HD22	1.90	0.54
1:F:210[B]:ARG:NH1	4:F:505:HOH:O	2.40	0.54
1:B:163:LEU:HD23	1:B:166:LEU:CD1	2.37	0.54
1:D:3:ASP:N	1:D:3:ASP:OD1	2.41	0.54
1:A:2:SER:OG	1:A:3:ASP:N	2.41	0.53
1:B:163:LEU:HA	1:B:166:LEU:HD12	1.90	0.53
1:C:286[B]:THR:CG2	1:C:288:ARG:HG3	2.38	0.53
1:B:166:LEU:HG	1:E:107:PRO:HG2	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:161:SER:HB2	1:E:189:ALA:HB2	1.91	0.52
1:A:63[B]:ARG:NH2	1:F:261:GLY:O	2.43	0.51
1:B:282:ALA:O	1:B:286:THR:HG23	2.11	0.51
1:E:154:LYS:NZ	2:E:401:PLP:O3	2.44	0.50
1:C:77:ILE:HG23	1:C:91:ILE:HG21	1.94	0.50
1:A:63[A]:ARG:CD	1:C:166:LEU:HD21	2.41	0.50
1:B:185:VAL:HG11	1:B:193:LEU:HD22	1.94	0.50
1:B:70[B]:ARG:HG2	1:B:70[B]:ARG:HH21	1.77	0.49
1:F:154:LYS:NZ	2:F:401:PLP:O3	2.43	0.49
1:E:4:GLU:OE2	1:E:17:SER:HB3	2.12	0.49
1:F:185:VAL:HG11	1:F:193:LEU:CD2	2.43	0.48
1:A:167:GLU:CD	1:B:262:ARG:HH22	2.21	0.48
1:C:79:GLU:O	1:C:83:ARG:HG2	2.14	0.48
1:A:166:LEU:HD11	1:C:107:PRO:HB2	1.96	0.48
1:B:185:VAL:HG11	1:B:193:LEU:CD2	2.44	0.48
1:A:1:MET:HE3	1:A:85:GLY:HA3	1.94	0.48
1:A:213:THR:O	1:A:217:ILE:HG12	2.14	0.48
1:B:126:ASP:O	1:B:130:ARG:HG3	2.14	0.47
1:C:71:ASP:O	1:C:75[A]:GLU:HG2	2.15	0.47
1:E:4:GLU:OE2	1:E:17:SER:CB	2.62	0.47
1:B:48:LEU:HD21	1:B:74:LYS:HG3	1.97	0.47
1:E:163:LEU:HD23	1:E:166:LEU:HD12	1.96	0.47
1:C:63[B]:ARG:HG2	1:C:63[B]:ARG:NH2	2.26	0.47
1:A:161:SER:HB2	1:A:189:ALA:HB2	1.96	0.46
1:D:126:ASP:OD1	1:D:129:LYS:HG2	2.14	0.46
1:C:210[B]:ARG:HG2	1:C:210[B]:ARG:HH21	1.80	0.46
1:C:210[B]:ARG:NH1	4:C:505:HOH:O	2.48	0.46
1:F:283:MET:HE2	1:F:288:ARG:CZ	2.46	0.46
1:D:161:SER:HB2	1:D:189:ALA:HB2	1.97	0.46
3:E:402:GOL:H2	4:E:572:HOH:O	2.16	0.45
1:D:154:LYS:NZ	2:D:401:PLP:O3	2.48	0.45
1:A:63[B]:ARG:HH21	1:A:63[B]:ARG:CG	2.30	0.45
1:B:108:ARG:HG3	1:E:166:LEU:HD23	1.98	0.45
1:F:163:LEU:HD23	1:F:166:LEU:HD12	1.99	0.44
1:C:231[A]:ARG:HG2	1:C:232:GLN:O	2.17	0.44
1:B:66:HIS:HB2	1:B:112:PRO:HG3	1.99	0.44
1:B:70[B]:ARG:HG2	1:B:70[B]:ARG:NH2	2.33	0.44
1:B:77:ILE:HG23	1:B:91:ILE:HG21	1.99	0.44
1:A:1:MET:CE	1:A:85:GLY:O	2.64	0.44
1:F:213:THR:O	1:F:217:ILE:HG12	2.18	0.44
1:B:213:THR:O	1:B:217:ILE:HG12	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:282:ALA:O	1:D:286:THR:HG23	2.18	0.43
1:A:185:VAL:HG11	1:A:193:LEU:HD22	2.00	0.43
1:C:185:VAL:HG11	1:C:193:LEU:HD22	2.00	0.43
1:D:166:LEU:HG	1:F:107:PRO:CG	2.40	0.43
1:C:213:THR:O	1:C:217:ILE:HG12	2.19	0.43
1:F:137:MET:HE1	1:F:167[B]:GLU:HG2	2.01	0.43
1:A:63[A]:ARG:HD3	1:C:166:LEU:HD11	2.00	0.43
1:D:65:ASN:HD22	1:D:65:ASN:H	1.67	0.43
1:D:213:THR:O	1:D:217:ILE:HG12	2.18	0.43
1:D:65:ASN:H	1:D:65:ASN:ND2	2.18	0.42
1:C:154:LYS:NZ	2:C:401:PLP:O3	2.52	0.42
1:F:8:TYR:O	1:F:115:ILE:HA	2.20	0.42
1:E:185:VAL:HG11	1:E:193:LEU:HD22	2.02	0.42
1:C:48:LEU:HD21	1:C:74:LYS:HG3	2.00	0.42
1:D:125:ALA:HB1	1:D:129:LYS:HB2	2.02	0.42
1:B:161:SER:HB2	1:B:189:ALA:HB2	2.02	0.42
1:C:286[B]:THR:HG22	1:C:288:ARG:H	1.83	0.41
1:E:66:HIS:HB2	1:E:112:PRO:HG3	2.01	0.41
1:E:100:PRO:HB2	1:E:102:GLY:O	2.20	0.41
1:B:24:VAL:HA	1:B:29:LEU:HD11	2.02	0.41
1:C:161:SER:HB2	1:C:189:ALA:HB2	2.02	0.41
1:A:48:LEU:HD21	1:A:74:LYS:HG3	2.02	0.41
1:C:127[B]:GLU:HG3	4:C:717:HOH:O	2.21	0.41
1:F:127:GLU:CD	1:F:130:ARG:HH21	2.27	0.41
1:E:127:GLU:OE2	1:E:130[B]:ARG:NH1	2.54	0.41
1:D:47:LYS:NZ	1:D:219:GLU:OE2	2.49	0.41
1:E:77:ILE:HG23	1:E:91:ILE:HG21	2.03	0.41
1:F:163:LEU:HD23	1:F:166:LEU:CD1	2.50	0.41
1:A:154:LYS:NZ	2:A:401:PLP:O3	2.54	0.40
1:F:77:ILE:HG23	1:F:91:ILE:HG21	2.03	0.40
1:C:231[B]:ARG:NH1	4:C:512:HOH:O	2.54	0.40
1:A:126:ASP:O	1:A:130[A]:ARG:HG3	2.21	0.40
1:B:82[A]:ARG:NH1	1:B:297:HIS:CE1	2.88	0.40
1:A:97:ARG:HD2	1:A:107:PRO:HA	2.03	0.40
1:D:77:ILE:HG23	1:D:91:ILE:HG21	2.04	0.40
1:D:201:LEU:O	1:D:228:TRP:HA	2.22	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	297/302 (98%)	292 (98%)	5 (2%)	0	100	100
1	B	304/302 (101%)	300 (99%)	4 (1%)	0	100	100
1	C	304/302 (101%)	298 (98%)	6 (2%)	0	100	100
1	D	299/302 (99%)	294 (98%)	4 (1%)	1 (0%)	36	20
1	E	300/302 (99%)	293 (98%)	7 (2%)	0	100	100
1	F	298/302 (99%)	293 (98%)	5 (2%)	0	100	100
All	All	1802/1812 (99%)	1770 (98%)	31 (2%)	1 (0%)	48	27

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	295	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	249/252 (99%)	249 (100%)	0	100	100
1	B	256/252 (102%)	254 (99%)	2 (1%)	73	59
1	C	256/252 (102%)	253 (99%)	3 (1%)	63	43
1	D	251/252 (100%)	250 (100%)	1 (0%)	84	75
1	E	252/252 (100%)	250 (99%)	2 (1%)	73	59
1	F	250/252 (99%)	250 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1514/1512 (100%)	1506 (100%)	8 (0%)	86 70

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	70[A]	ARG
1	B	70[B]	ARG
1	C	104	VAL
1	C	175[A]	ASP
1	C	175[B]	ASP
1	D	175	ASP
1	E	231[A]	ARG
1	E	231[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	274	GLN
1	D	18	GLN
1	D	65	ASN
1	D	274	GLN
1	E	274	GLN
1	F	162	GLN
1	F	232	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry

12 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
3	GOL	C	402	-	5,5,5	1.14	0	5,5,5	1.28	1 (20%)
3	GOL	E	402	-	5,5,5	1.33	1 (20%)	5,5,5	1.44	1 (20%)
2	PLP	F	401	1	15,15,16	0.85	0	21,22,23	1.11	1 (4%)
2	PLP	C	401	1	15,15,16	1.05	1 (6%)	21,22,23	1.00	2 (9%)
2	PLP	A	401	1	15,15,16	1.02	1 (6%)	21,22,23	1.31	3 (14%)
2	PLP	B	401	1	15,15,16	0.91	1 (6%)	21,22,23	1.27	2 (9%)
3	GOL	A	402	-	5,5,5	1.08	0	5,5,5	1.01	1 (20%)
3	GOL	F	402	-	5,5,5	0.84	0	5,5,5	0.93	0
2	PLP	D	401	1	15,15,16	0.98	0	21,22,23	1.22	2 (9%)
2	PLP	E	401	1	15,15,16	1.04	1 (6%)	21,22,23	1.22	3 (14%)
3	GOL	D	402	-	5,5,5	0.82	0	5,5,5	0.70	0
3	GOL	B	402	-	5,5,5	0.64	0	5,5,5	0.99	0

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
3	GOL	C	402	-	-	2/4/4/4	-
3	GOL	E	402	-	-	2/4/4/4	-
2	PLP	F	401	1	-	0/6/6/8	0/1/1/1
2	PLP	C	401	1	-	0/6/6/8	0/1/1/1
2	PLP	A	401	1	-	0/6/6/8	0/1/1/1
2	PLP	B	401	1	-	0/6/6/8	0/1/1/1
3	GOL	A	402	-	-	2/4/4/4	-
3	GOL	F	402	-	-	0/4/4/4	-
2	PLP	D	401	1	-	0/6/6/8	0/1/1/1
2	PLP	E	401	1	-	0/6/6/8	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	D	402	-	-	0/4/4/4	-
3	GOL	B	402	-	-	1/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	402	GOL	O2-C2	-2.81	1.35	1.43
2	A	401	PLP	C2-N1	2.38	1.38	1.33
2	C	401	PLP	C6-N1	2.28	1.39	1.34
2	B	401	PLP	C2-N1	2.10	1.37	1.33
2	E	401	PLP	C6-N1	2.05	1.38	1.34

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	PLP	C6-C5-C4	3.69	121.12	118.10
2	D	401	PLP	C5-C6-N1	-2.77	119.33	123.83
2	A	401	PLP	C5-C6-N1	-2.59	119.62	123.83
2	E	401	PLP	C6-C5-C4	2.51	120.16	118.10
2	B	401	PLP	C4A-C4-C5	-2.45	118.41	120.94
2	C	401	PLP	O3P-P-O2P	2.44	116.94	107.80
3	C	402	GOL	C3-C2-C1	-2.42	102.92	111.80
2	A	401	PLP	C4A-C4-C5	-2.30	118.57	120.94
2	E	401	PLP	C5-C6-N1	-2.29	120.10	123.83
2	F	401	PLP	C6-C5-C4	2.25	119.94	118.10
2	D	401	PLP	C4A-C4-C5	-2.20	118.67	120.94
2	B	401	PLP	C5-C6-N1	-2.12	120.38	123.83
3	E	402	GOL	O3-C3-C2	-2.12	100.84	110.38
2	E	401	PLP	O3P-P-O4P	-2.02	101.41	106.67
2	C	401	PLP	O3P-P-O4P	-2.01	101.43	106.67
3	A	402	GOL	C3-C2-C1	-2.01	104.43	111.80

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	GOL	C1-C2-C3-O3
3	C	402	GOL	O1-C1-C2-C3
3	A	402	GOL	O2-C2-C3-O3
3	E	402	GOL	C1-C2-C3-O3
3	C	402	GOL	C1-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	E	402	GOL	O2-C2-C3-O3
3	B	402	GOL	C1-C2-C3-O3

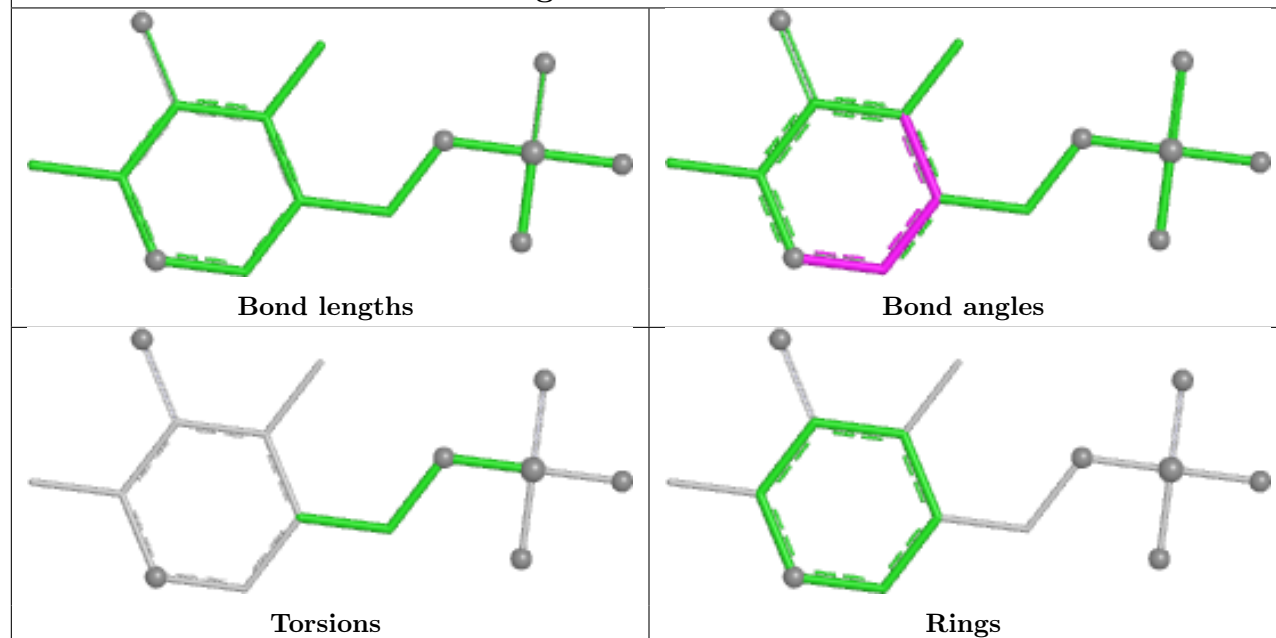
There are no ring outliers.

7 monomers are involved in 7 short contacts:

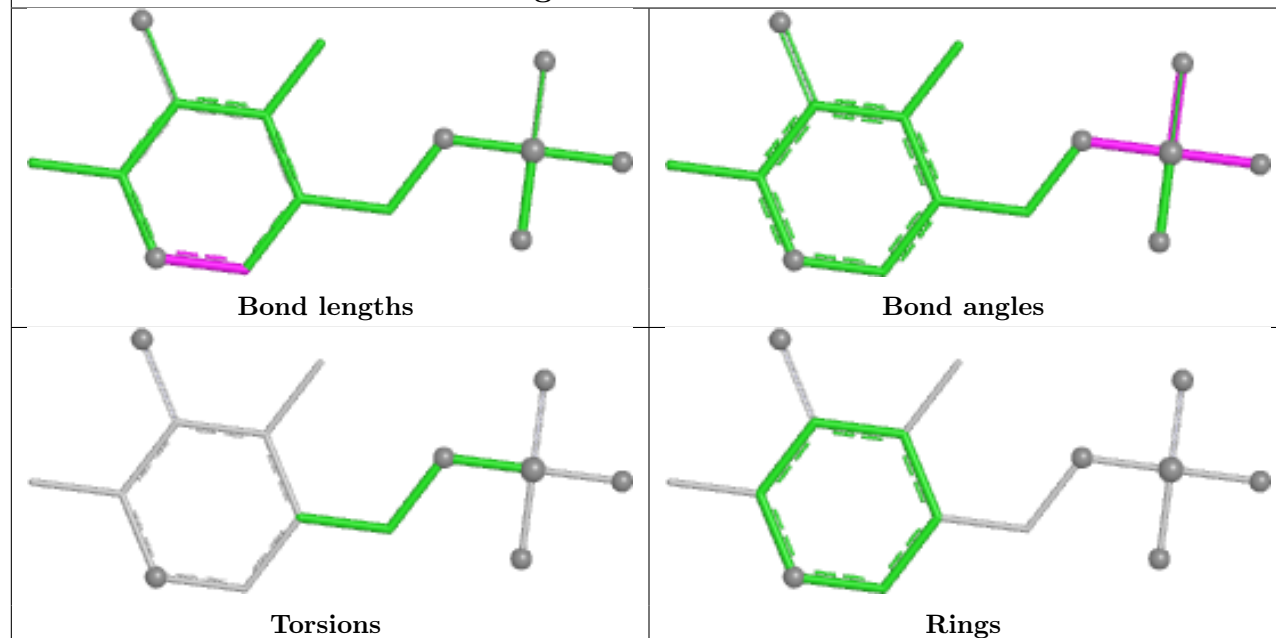
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	402	GOL	1	0
2	F	401	PLP	1	0
2	C	401	PLP	1	0
2	A	401	PLP	1	0
2	B	401	PLP	1	0
2	D	401	PLP	1	0
2	E	401	PLP	1	0

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

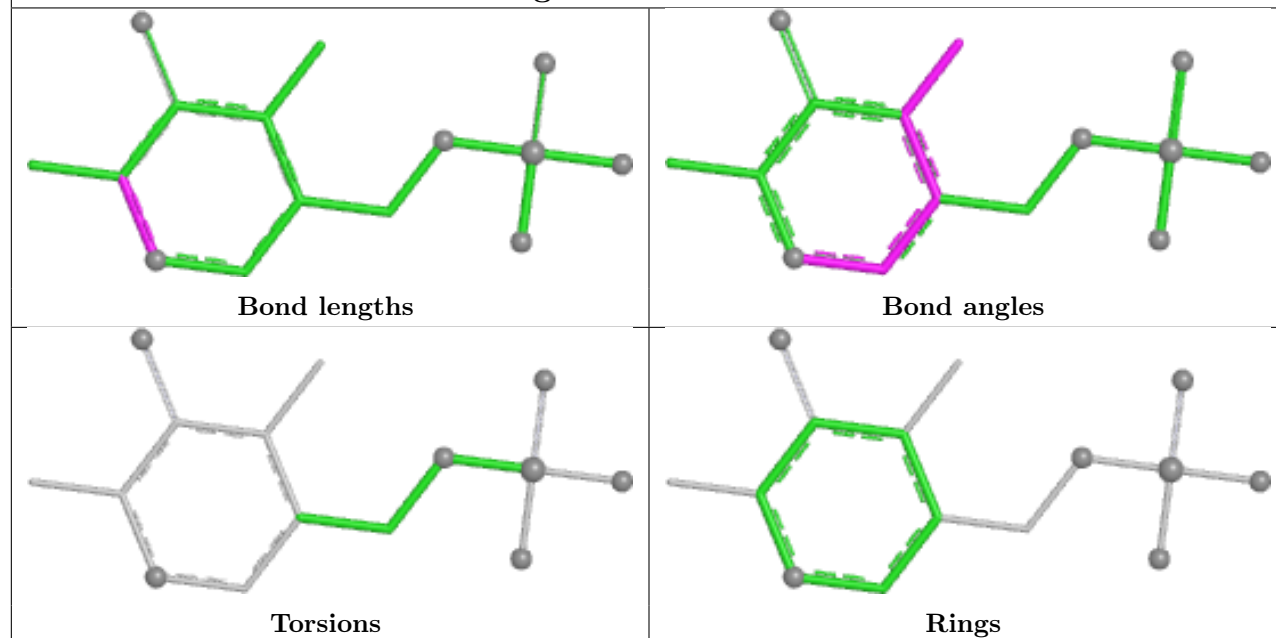
Ligand PLP F 401



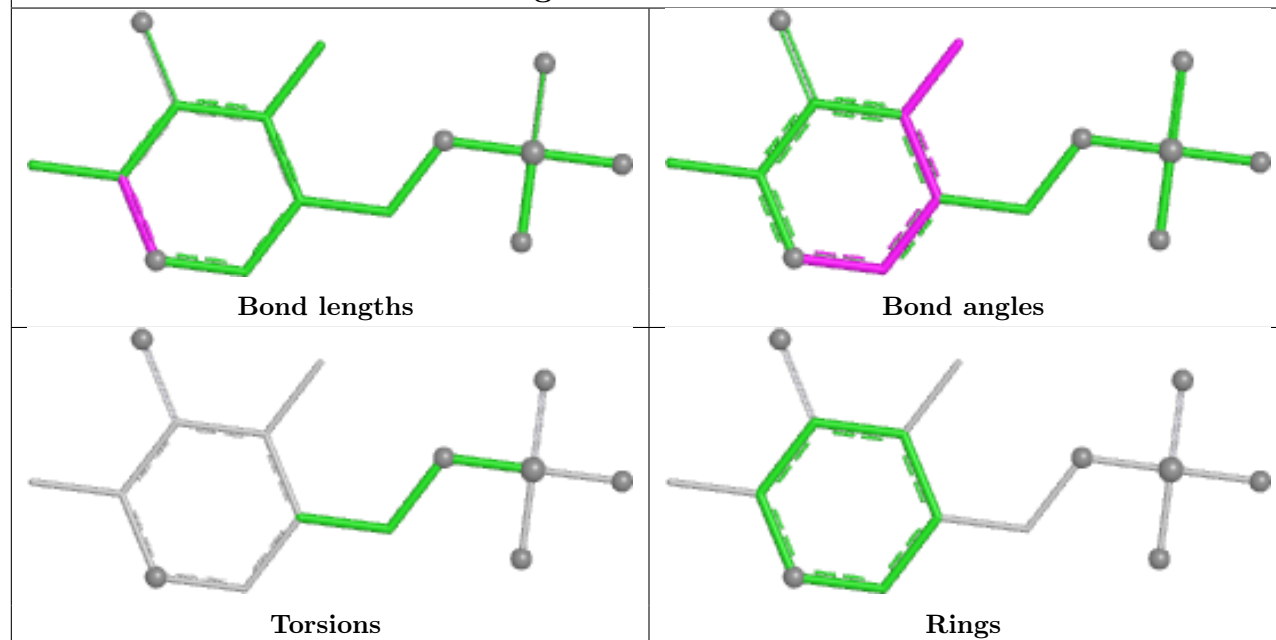
Ligand PLP C 401

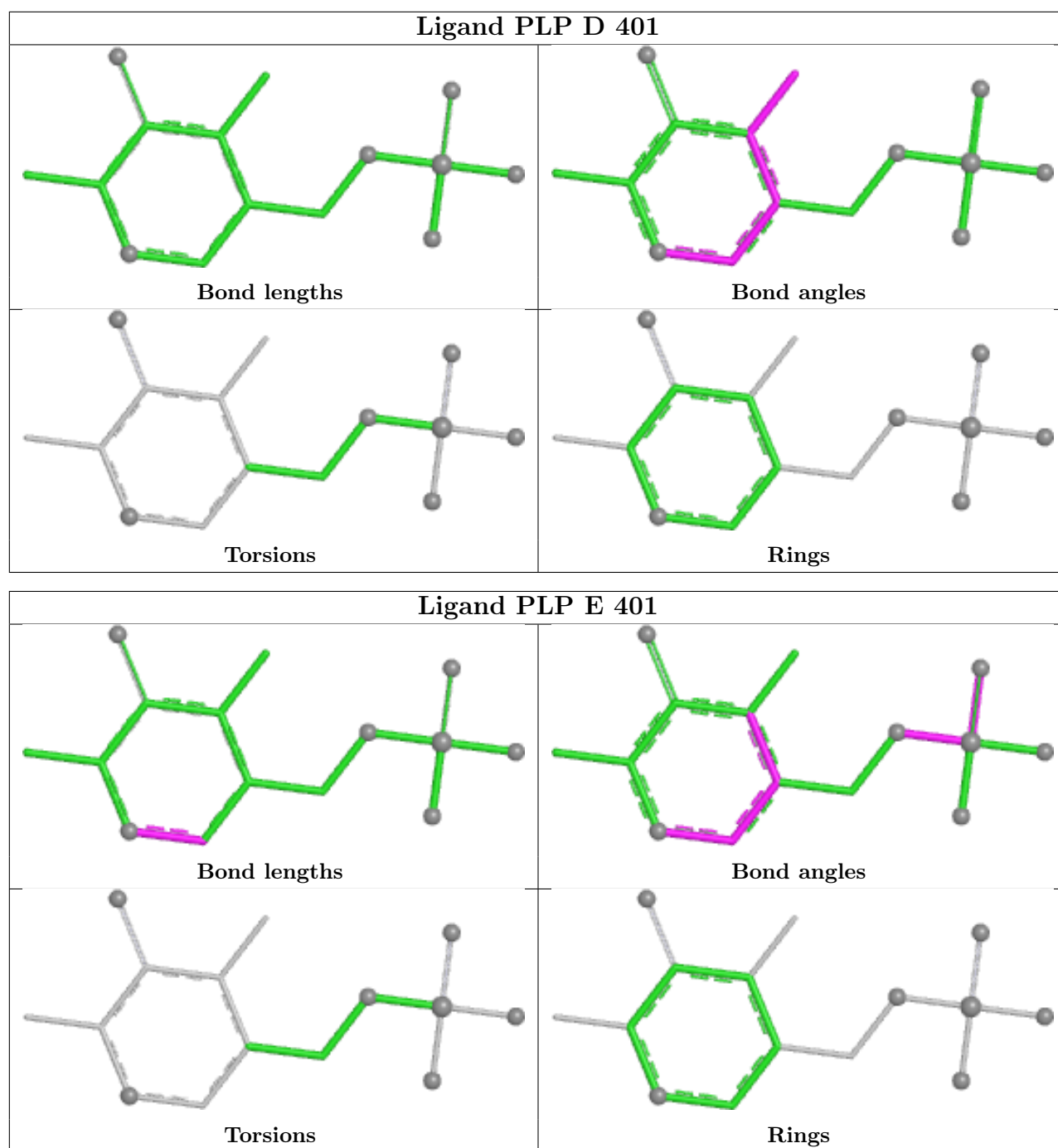


Ligand PLP A 401



Ligand PLP B 401





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	296/302 (98%)	0.26	13 (4%)	39 40	13, 27, 50, 73	3 (1%)
1	B	299/302 (99%)	0.39	21 (7%)	22 23	12, 30, 53, 79	7 (2%)
1	C	294/302 (97%)	0.14	10 (3%)	48 50	11, 26, 43, 84	12 (4%)
1	D	295/302 (97%)	0.43	12 (4%)	41 43	14, 32, 55, 101	6 (2%)
1	E	294/302 (97%)	0.47	19 (6%)	25 25	11, 31, 55, 80	8 (2%)
1	F	294/302 (97%)	0.31	15 (5%)	33 34	14, 29, 51, 84	6 (2%)
All	All	1772/1812 (97%)	0.33	90 (5%)	33 34	11, 29, 52, 101	42 (2%)

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	104	VAL	7.2
1	D	103	VAL	7.0
1	E	103	VAL	5.7
1	D	104	VAL	5.6
1	A	295	GLY	5.6
1	C	105	ALA	5.5
1	C	103	VAL	5.3
1	E	102	GLY	5.0
1	F	104	VAL	5.0
1	F	2	SER	5.0
1	C	104	VAL	4.9
1	B	104	VAL	4.8
1	E	295	GLY	4.7
1	A	1	MET	4.7
1	C	295	GLY	4.6
1	F	103	VAL	4.5
1	B	297	HIS	4.4
1	D	296	SER	4.3
1	A	103	VAL	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	102	GLY	4.2
1	A	296	SER	4.2
1	F	88	ASP	4.2
1	A	104	VAL	4.2
1	B	295	GLY	4.1
1	B	103	VAL	4.0
1	D	2	SER	3.9
1	F	105	ALA	3.9
1	D	3	ASP	3.9
1	F	295	GLY	3.9
1	D	287	ASP	3.8
1	E	294	SER	3.8
1	D	295	GLY	3.7
1	B	105	ALA	3.7
1	E	2	SER	3.7
1	E	287	ASP	3.6
1	B	300	HIS	3.3
1	A	105	ALA	3.3
1	C	286[A]	THR	3.2
1	D	100	PRO	3.2
1	F	122	ILE	3.2
1	A	100	PRO	3.1
1	A	2	SER	3.1
1	B	287	ASP	3.0
1	D	105	ALA	3.0
1	B	299	HIS	3.0
1	C	166	LEU	3.0
1	F	293	LEU	3.0
1	B	70[A]	ARG	2.9
1	E	82[A]	ARG	2.9
1	B	100	PRO	2.9
1	B	3	ASP	2.9
1	F	3	ASP	2.9
1	B	2	SER	2.9
1	F	166	LEU	2.8
1	F	294	SER	2.8
1	A	294	SER	2.8
1	B	298	HIS	2.8
1	D	294	SER	2.8
1	E	100	PRO	2.7
1	E	267	THR	2.7
1	F	102	GLY	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	153[A]	TYR	2.7
1	C	175[A]	ASP	2.7
1	A	3	ASP	2.6
1	E	285	GLU	2.6
1	C	2	SER	2.6
1	E	266	GLY	2.6
1	E	286	THR	2.6
1	F	100	PRO	2.6
1	E	293	LEU	2.5
1	A	225	ASP	2.5
1	B	71	ASP	2.5
1	E	122	ILE	2.5
1	E	101	LYS	2.4
1	B	102	GLY	2.4
1	B	296	SER	2.4
1	E	3	ASP	2.4
1	D	285	GLU	2.4
1	B	7	ILE	2.4
1	C	3	ASP	2.3
1	A	4	GLU	2.3
1	A	102	GLY	2.3
1	F	127	GLU	2.2
1	C	102	GLY	2.2
1	E	131[A]	ARG	2.2
1	F	75	GLU	2.1
1	B	293	LEU	2.1
1	B	286	THR	2.1
1	E	127	GLU	2.1
1	B	294	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands

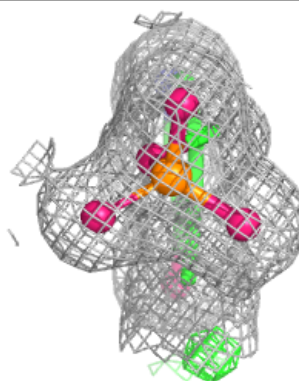
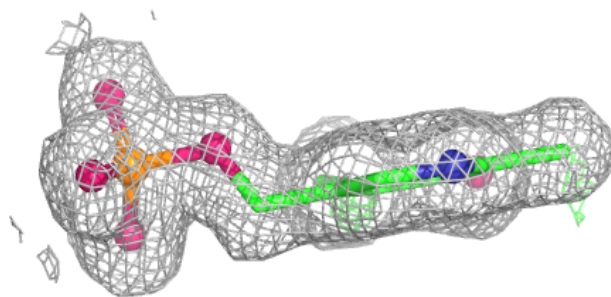
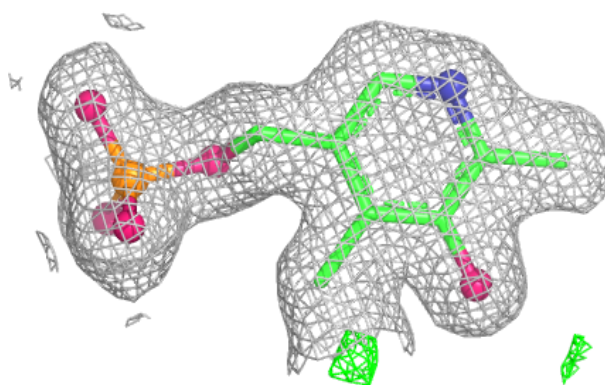
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	E	402	6/6	0.88	0.21	49,58,66,67	0
3	GOL	A	402	6/6	0.89	0.15	44,52,61,62	0
3	GOL	F	402	6/6	0.90	0.13	38,39,42,43	0
3	GOL	D	402	6/6	0.91	0.13	40,44,49,50	0
3	GOL	C	402	6/6	0.92	0.13	43,48,53,54	0
3	GOL	B	402	6/6	0.94	0.09	34,35,36,37	0
2	PLP	E	401	15/16	0.98	0.05	23,25,26,27	0
2	PLP	F	401	15/16	0.98	0.05	22,24,25,25	0
2	PLP	A	401	15/16	0.98	0.06	21,23,25,26	0
2	PLP	D	401	15/16	0.98	0.06	25,26,27,27	0
2	PLP	C	401	15/16	0.99	0.04	19,22,23,26	0
2	PLP	B	401	15/16	0.99	0.04	23,24,25,26	0

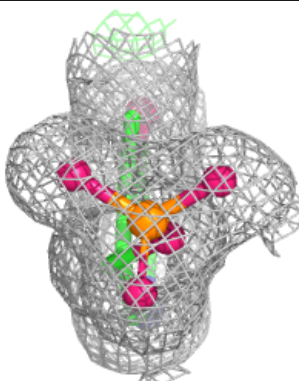
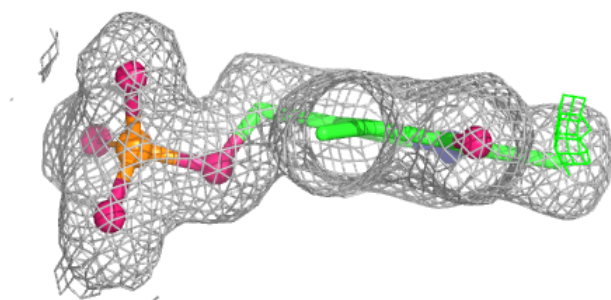
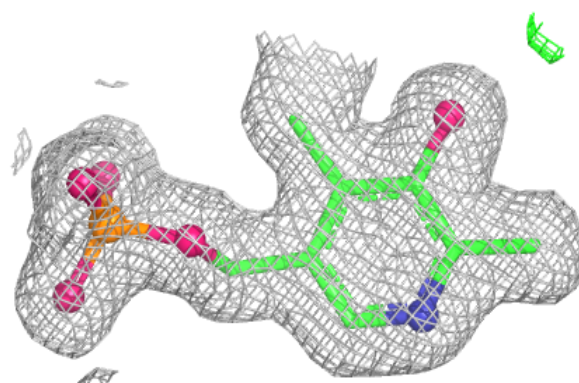
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PLP E 401:

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

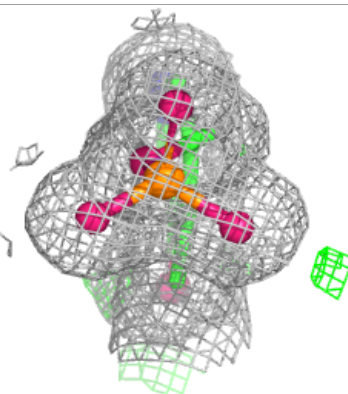
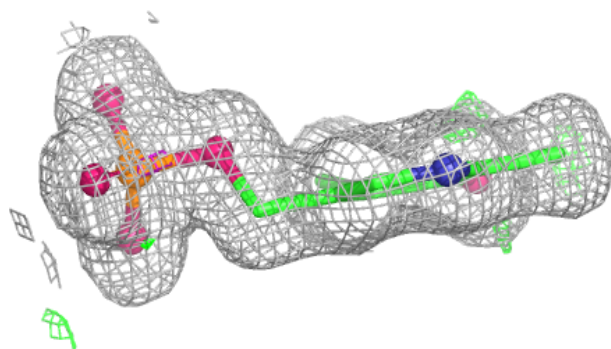
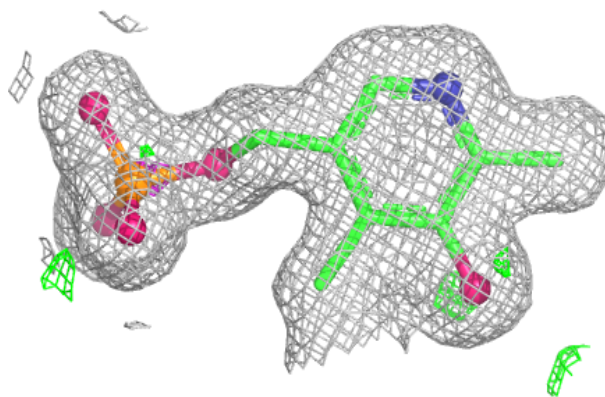
**Electron density around PLP F 401:**

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

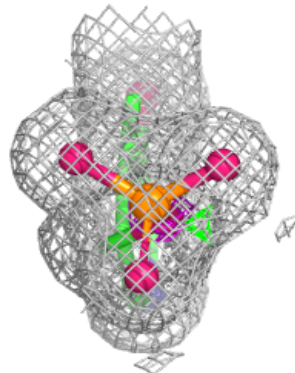
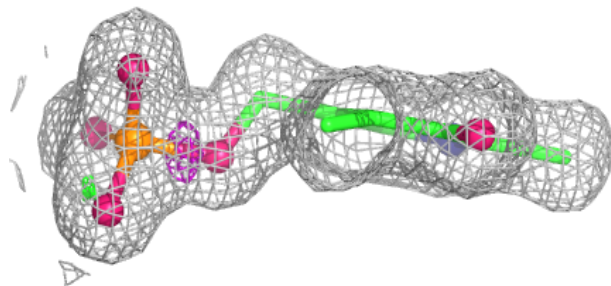
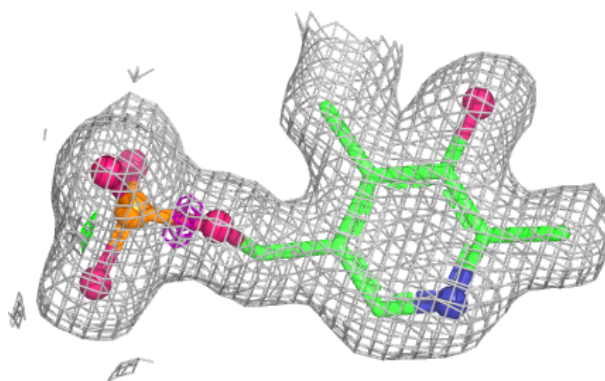


Electron density around PLP A 401:

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

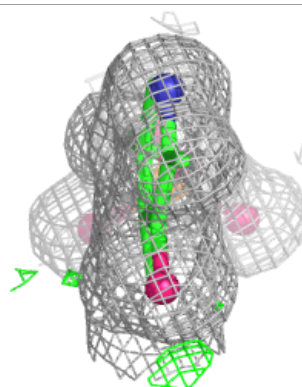
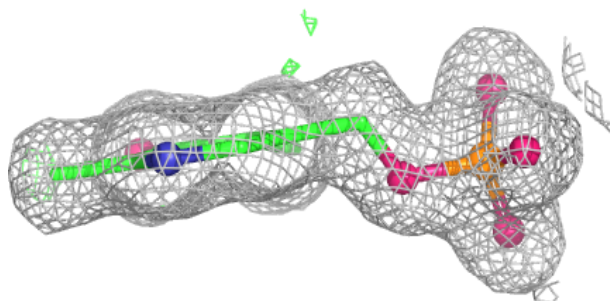
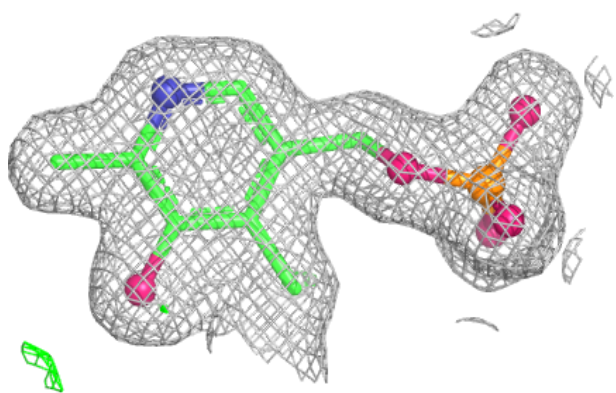
**Electron density around PLP D 401:**

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

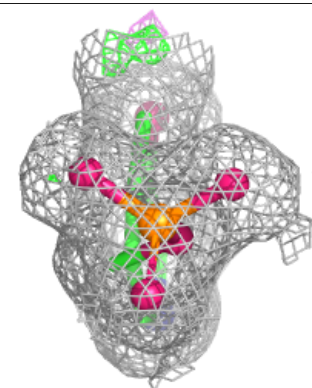
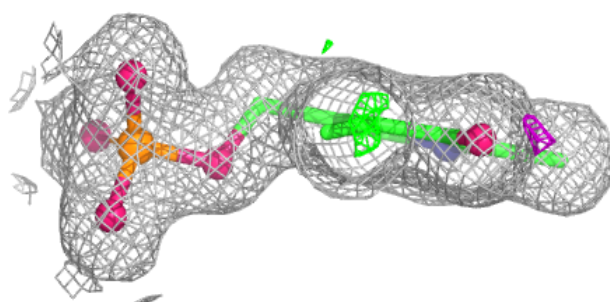
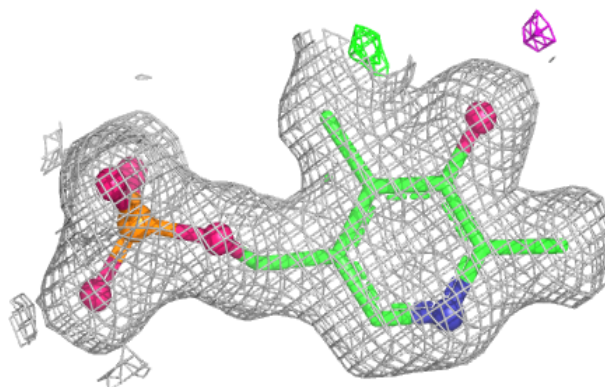


Electron density around PLP C 401:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.