WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Dec 8, 2021 – 02:08 pm GMT

PDB ID	:	7P3T
Title	:	Transaminase of gamma-proteobacterium
Authors	:	Ermler, U.
Deposited on	:	2021-07-08
Resolution	:	1.60 Å(reported)

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

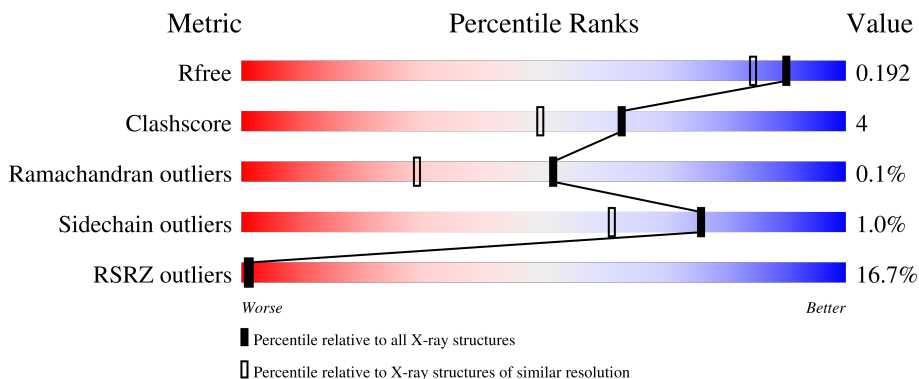|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4 (270009), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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.
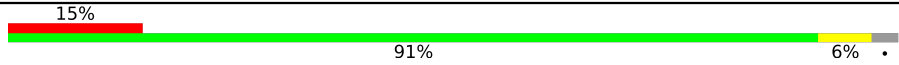
Metric	Percentile Ranks	Value
Rfree		0.192
Clashscore		4
Ramachandran outliers		0.1%
Sidechain outliers		1.0%
RSRZ outliers		16.7%

Worse *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (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 <=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	16% / 90% / 8% ·
1	B	302	24% / 88% / 10% ·
1	C	302	11% / 87% / 11% ·
1	D	302	19% / 88% / 10% ·
1	E	302	15% / 89% / 8% ·

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Mol	Chain	Length	Quality of chain
1	F	302	

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

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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 (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$) (labeled as "Ligand of Interest" by depositor).

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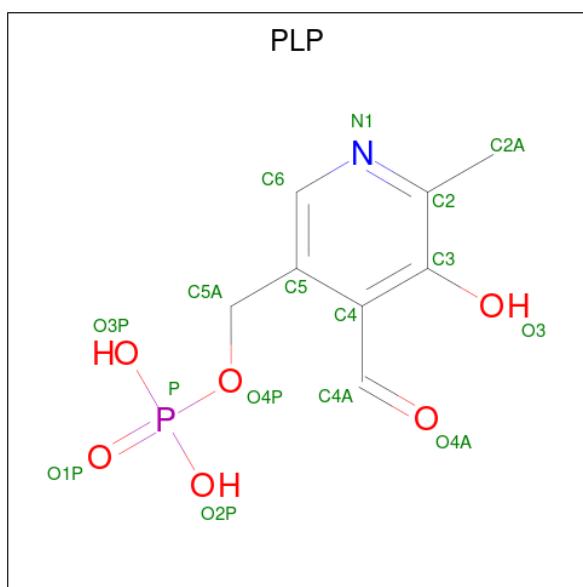
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	E	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	F	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL

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

- Molecule 4 is water.

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

3 Residue-property plots ⓘ

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

- Molecule 1: Branched-chain amino acid aminotransferase

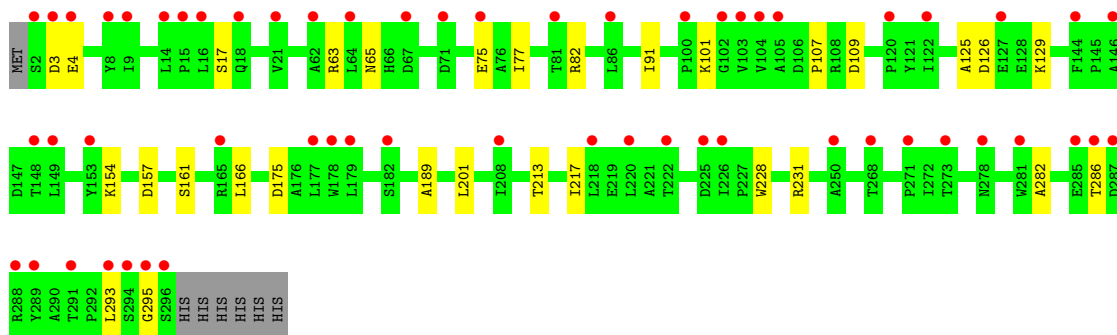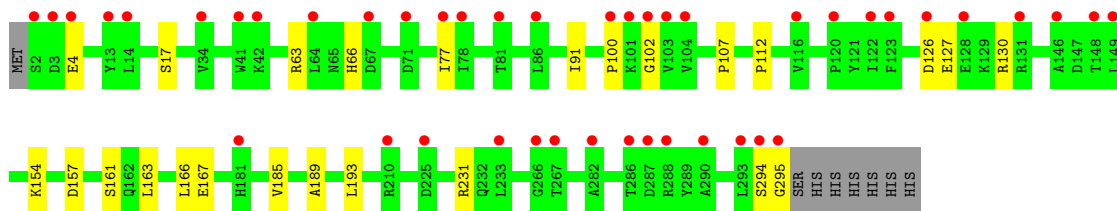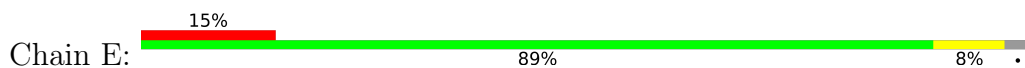Chain A:

- Molecule 1: Branched-chain amino acid aminotransferase

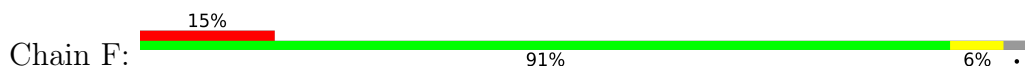Chain B:

- Molecule 1: Branched-chain amino acid aminotransferase

Chain C:

- Molecule 1: Branched-chain amino acid aminotransferase

Chain D:

MET S2 D3 E4 Y8 I9 L14 P15 L16 S17 Q18 V21 A62 R63 L64 N65 H66 D67 D71 E75 A76 I77 T81 R82 L86 I91 P100 K101 G102 V103 V104 A105 D106 P107 R108 D109 P120 Y121 I122 A125 D126 E127 E128 K129 F144 P145 A146

D147 T148 L149 Y153 K154 D157 S161 R165 L166 D175 A176 L177 W178 L179 S182 A189 L201 I208 T213 I217 L218 E219 L220 A221 T222 D225 I226 P227 W228 R231 A250 T268 P271 I272 T273 N278 W281 A282 E285 T286 D287

R288 Y289 A290 T291 P292 L293 S294 G295 S296 HIS HIS HIS HIS HIS HIS

• Molecule 1: Branched-chain amino acid aminotransferase

Chain E:

15%

89%　　　　8%　　•

MET S2 D3 E4 Y13 L14 S17 V34 W41 K42 R63 L64 N65 H66 D67 D71 I77 I78 T81 L86 I91 P100 K101 G102 V103 V104 P107 P112 V116 P120 Y121 I122 F123 D126 E127 E128 K129 R130 R131 A146 D147 T148 L149

K154 D157 S161 Q162 L163 L166 E167 H181 V185 A189 L193 R210 D225 R231 Q232 L233 G266 T267 A282 T286 D287 R288 Y289 A290 L293 S294 G295 SER HIS HIS HIS HIS HIS HIS

• Molecule 1: Branched-chain amino acid aminotransferase

Chain F:

15%

91%　　　　6%　•

MET S2 D3 E4 P5 I6 I7 Y8 Y13 L14 Q18 V38 I59 D67 M68 S69 I77 L86 I91 P100 K101 G102 V103 V104 A105 D106 P107 R108 D109 C114 I115 P120 E127 L136 F144 P145 A146 L149 Y153 K154 C155 L156 D157 R158

L159 L163 I164 R165 L166 E167 L177 W178 L179 V185 L193 I208 L209 R210 T213 I217 T222 D225 R231 G261 I264 L293 S294 G295 SER HIS HIS HIS HIS HIS HIS

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
$< I/\sigma(I) >$ [1]	1.45 (at 1.60Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.169 , 0.185 0.176 , 0.192	Depositor DCC
R_{free} test set	12305 reflections (4.92%)	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)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o,F_c correlation	0.97	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.*

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[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, 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	0.46	0/2412	0.66	0/3278
1	B	0.38	0/2487	0.64	0/3379
1	C	0.43	0/2479	0.66	0/3367
1	D	0.40	0/2435	0.64	0/3308
1	E	0.38	0/2451	0.62	0/3329
1	F	0.41	0/2420	0.63	0/3289
All	All	0.41	0/14684	0.64	0/19950

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2359	0	2322	28	0
1	B	2429	0	2373	27	0
1	C	2426	0	2369	33	0
1	D	2382	0	2339	22	0
1	E	2397	0	2353	17	0
1	F	2367	0	2321	18	0
2	A	15	0	7	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	2	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	124	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.

The worst 5 of 124 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

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%)	41	21
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%)	51	29

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%)	247 (99%)	2 (1%)	81	70
1	B	256/252 (102%)	253 (99%)	3 (1%)	71	54
1	C	256/252 (102%)	252 (98%)	4 (2%)	62	41
1	D	251/252 (100%)	247 (98%)	4 (2%)	62	41
1	E	252/252 (100%)	249 (99%)	3 (1%)	71	54
1	F	250/252 (99%)	248 (99%)	2 (1%)	81	70
All	All	1514/1512 (100%)	1496 (99%)	18 (1%)	76	54

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	231[A]	ARG
1	F	231	ARG

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Mol	Chain	Res	Type
1	F	157	ASP
1	C	175[B]	ASP
1	E	157	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	18	GLN
1	D	65	ASN

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 ⓘ

12 ligands are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 B 401

Bond lengths

Bond angles

Torsions

Rings

Ligand PLP C 401

Bond lengths

Bond angles

Torsions

Rings

Ligand PLP D 401

Bond lengths

Bond angles

Torsions

Rings

Ligand PLP E 401

Bond lengths

Bond angles

Torsions

Rings

Ligand PLP F 401

Bond lengths

Bond angles

Torsions

Rings
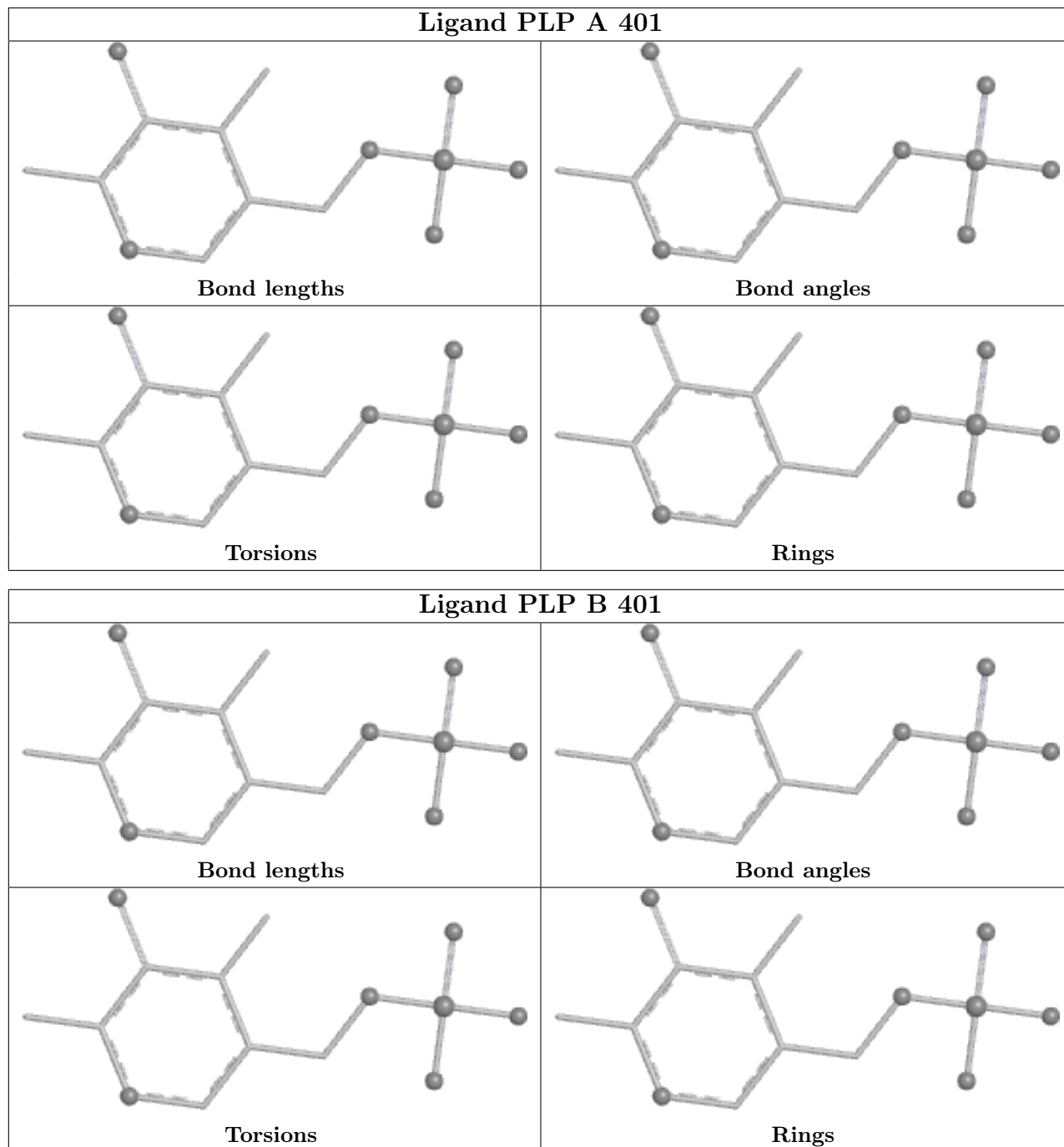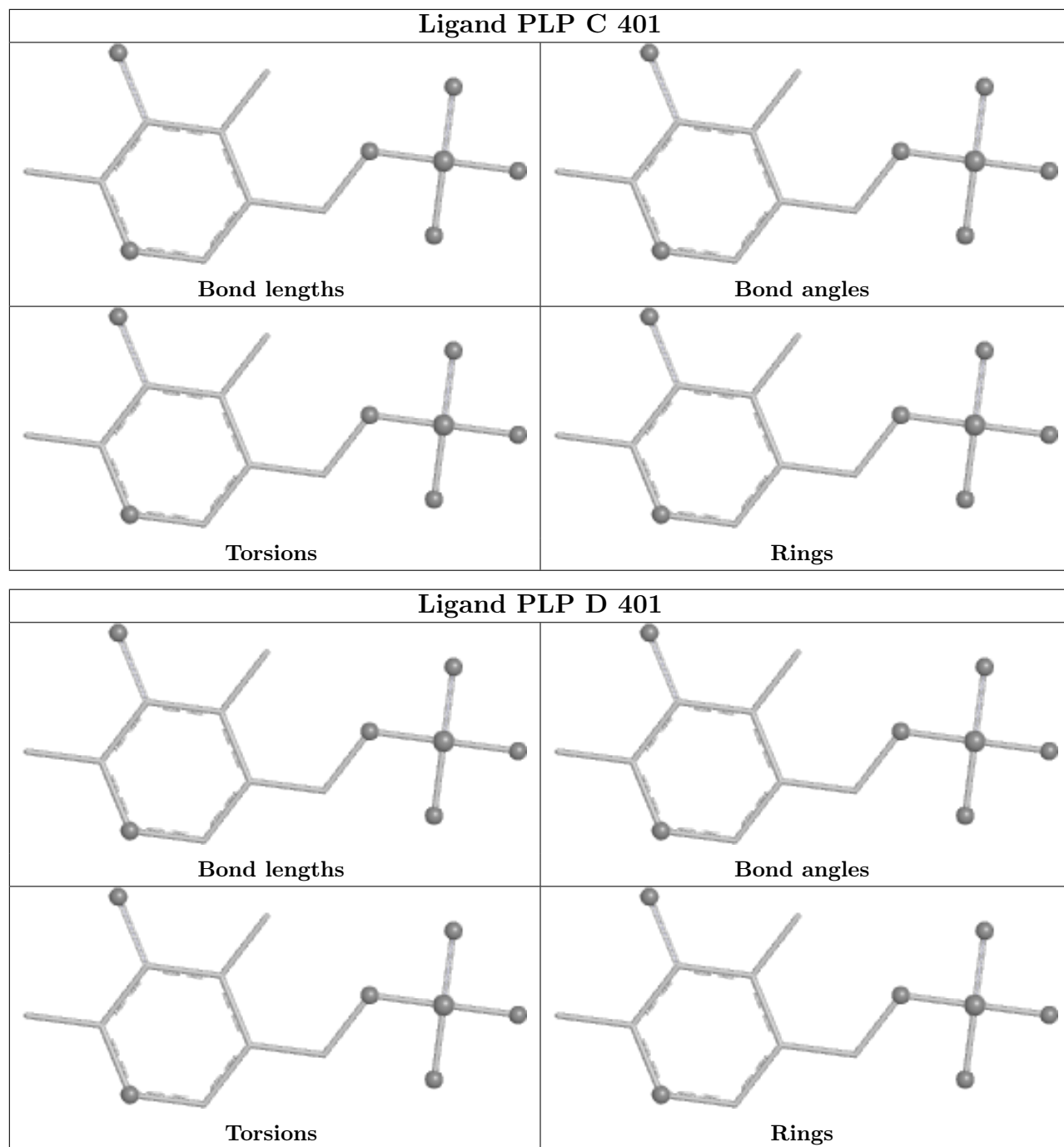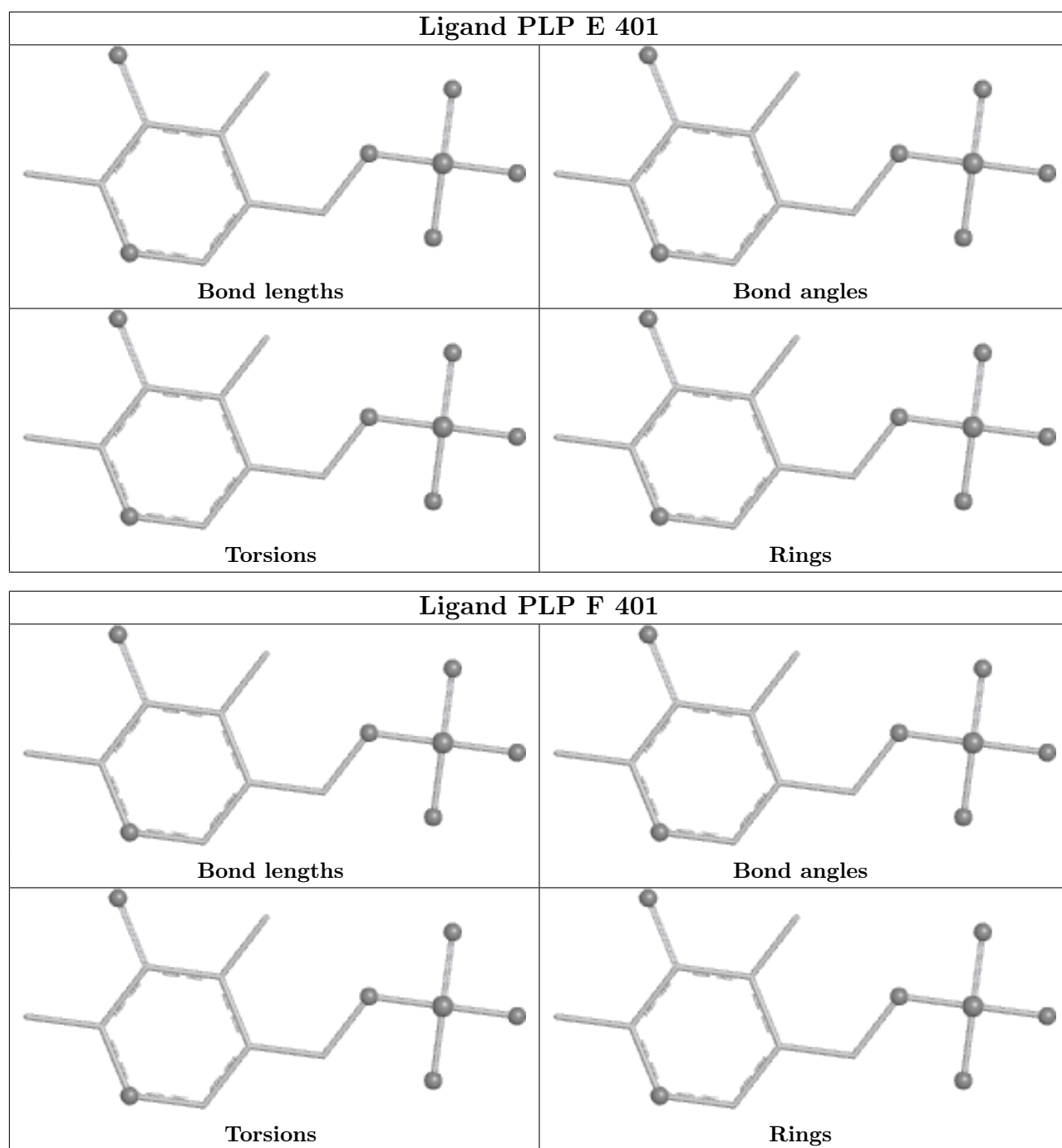
5.7 Other polymers ⓘ

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, 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(Å²)	Q<0.9
1	A	296/302 (98%)	1.22	48 (16%)	1	1	20, 28, 50, 73	0
1	B	299/302 (99%)	1.46	71 (23%)	0	0	20, 30, 53, 79	0
1	C	294/302 (97%)	1.15	32 (10%)	5	4	20, 27, 43, 84	0
1	D	295/302 (97%)	1.35	57 (19%)	1	1	21, 32, 55, 101	0
1	E	294/302 (97%)	1.25	44 (14%)	2	1	21, 32, 55, 80	0
1	F	294/302 (97%)	1.31	44 (14%)	2	1	20, 29, 51, 84	0
All	All	1772/1812 (97%)	1.29	296 (16%)	1	1	20, 30, 52, 101	0

The worst 5 of 296 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	103	VAL	18.5
1	F	2	SER	15.0
1	C	2	SER	14.9
1	B	103	VAL	13.6
1	F	103	VAL	13.2

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 monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
3	GOL	E	402	6/6	0.70	0.19	49,58,66,67	0
3	GOL	D	402	6/6	0.75	0.14	40,44,49,50	0
3	GOL	C	402	6/6	0.79	0.15	43,48,53,54	0
3	GOL	F	402	6/6	0.80	0.11	38,39,42,43	0
3	GOL	B	402	6/6	0.81	0.16	34,35,36,37	0
3	GOL	A	402	6/6	0.83	0.16	44,52,61,62	0
2	PLP	F	401	15/16	0.89	0.13	22,24,25,25	0
2	PLP	D	401	15/16	0.90	0.13	25,26,27,27	0
2	PLP	A	401	15/16	0.90	0.12	21,23,25,26	0
2	PLP	B	401	15/16	0.91	0.13	23,24,25,26	0
2	PLP	E	401	15/16	0.93	0.10	23,25,26,27	0
2	PLP	C	401	15/16	0.94	0.10	19,22,23,26	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 F 401:

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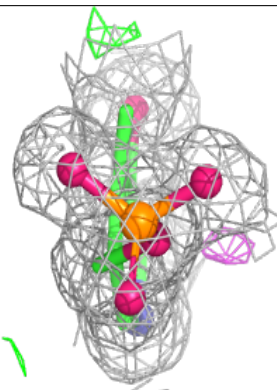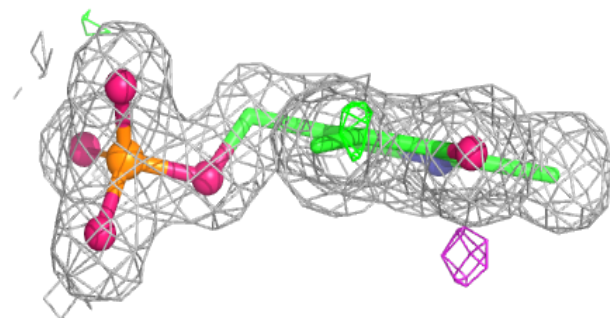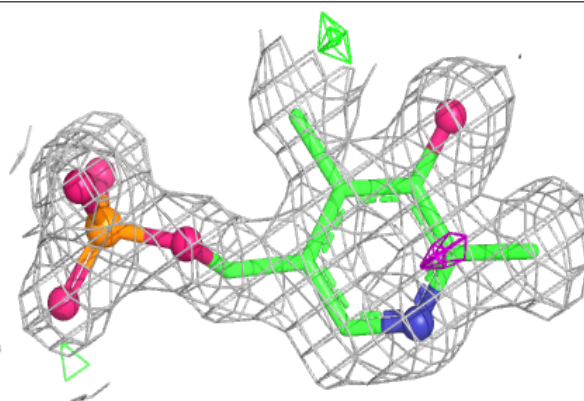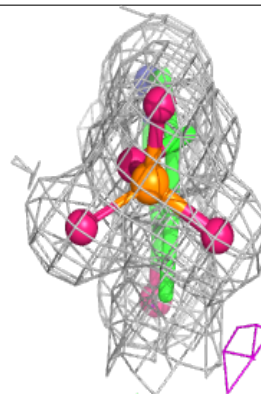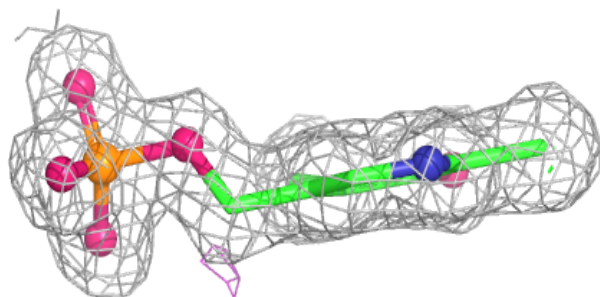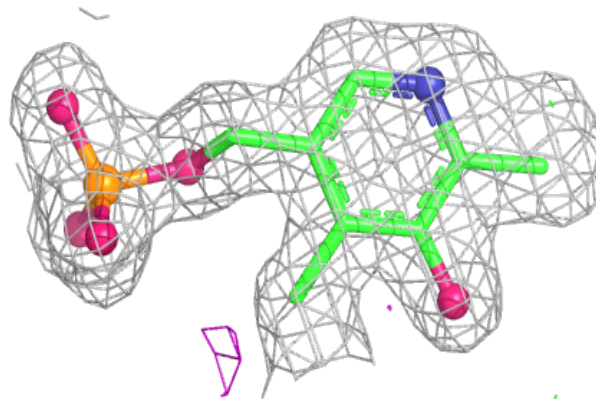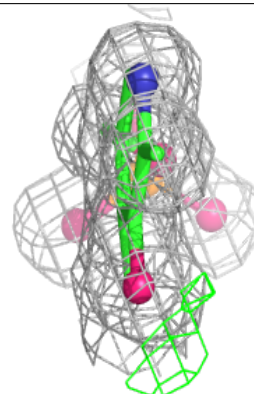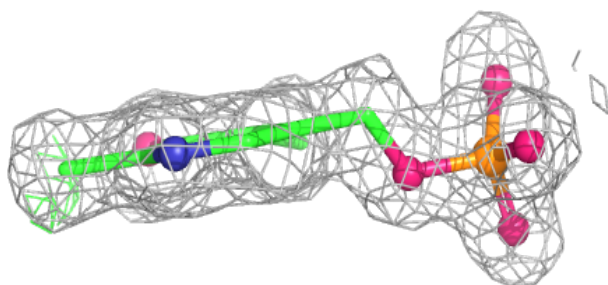mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
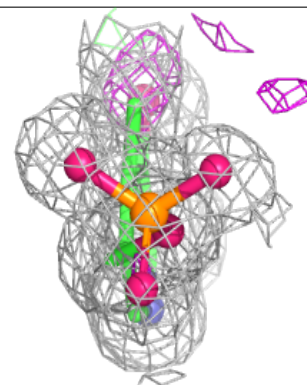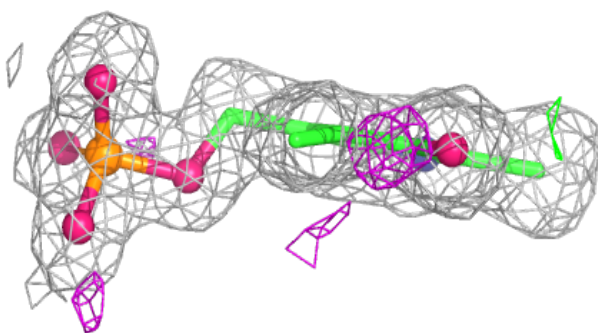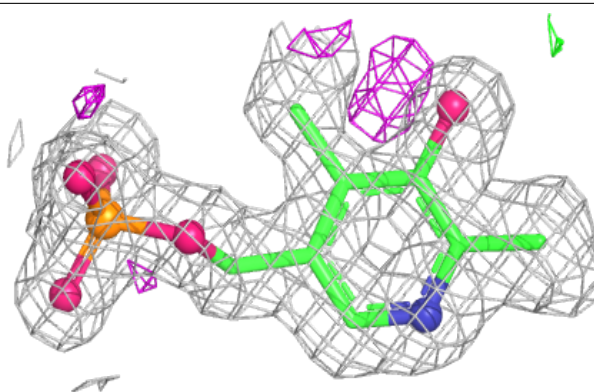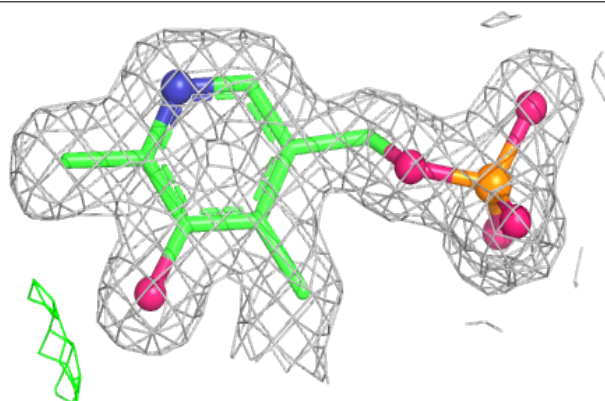

Electron density around PLP D 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
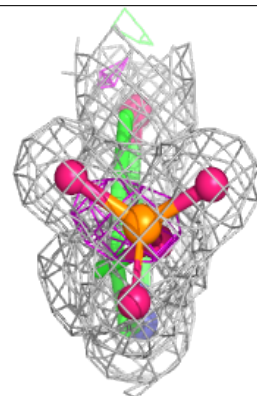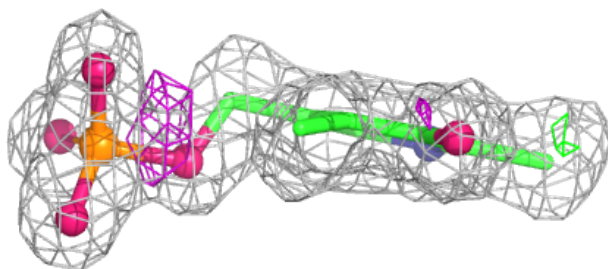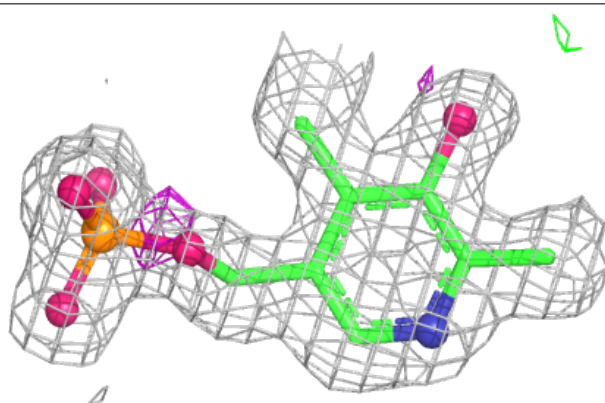
Electron density around PLP A 401:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
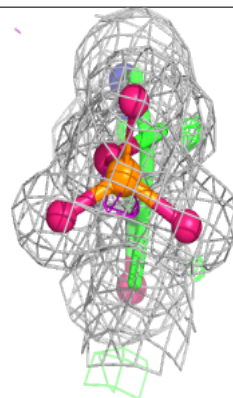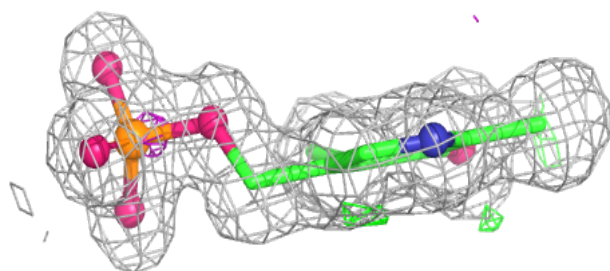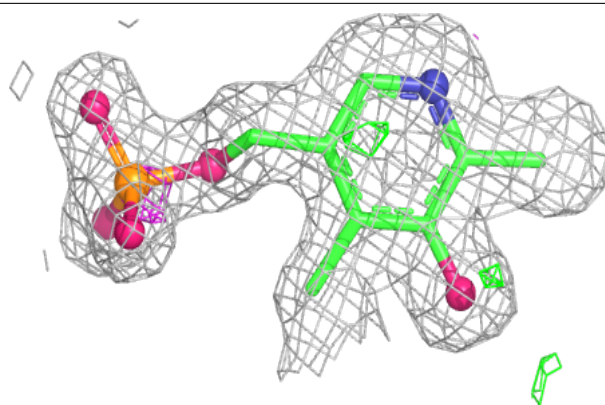
Electron density around PLP B 401:

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

Electron density around PLP E 401:

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

Electron density around PLP C 401:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.