



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 08:36 PM UTC

PDB ID : 8B9W / pdb_00008b9w
Title : Cysteine Synthase from Trypanosoma theileri with PLP bound
Authors : Sowerby, K.V.; Pohl, E.
Deposited on : 2022-10-10
Resolution : 2.75 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

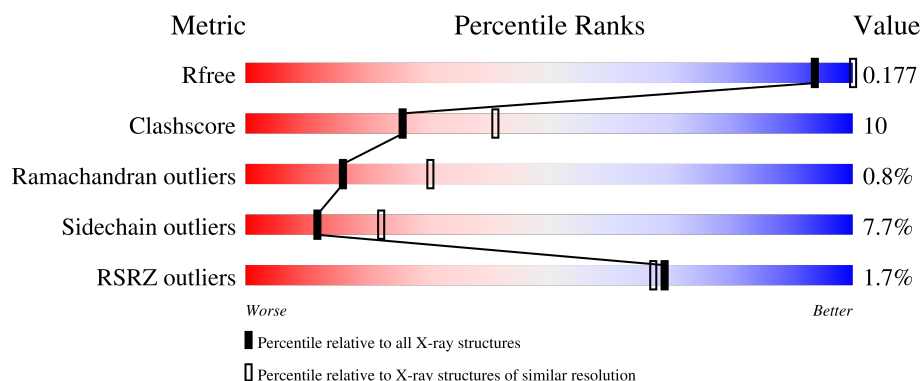
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	354	2% 74% 15% • • 7%
1	B	354	% 63% 23% 5% • 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10044 atoms, of which 4985 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 Putative cysteine synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	329	Total	C	H	N	O	S	146	4	0
			4981	1551	2520	430	468	12			
1	B	327	Total	C	H	N	O	S	149	2	0
			4805	1507	2409	413	465	11			

There are 38 discrepancies between the modelled and reference sequences:

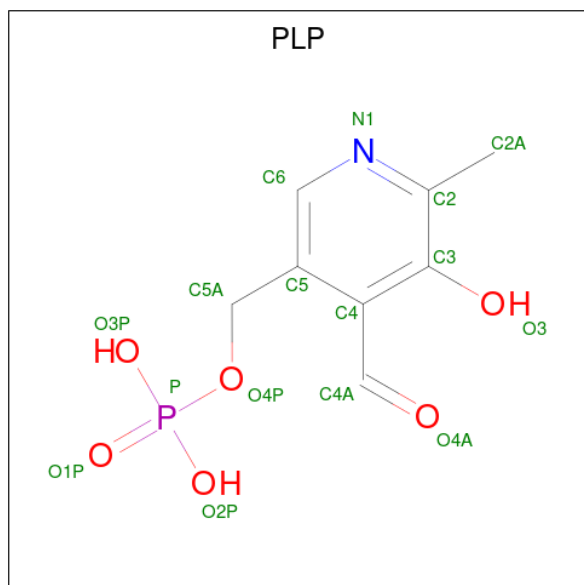
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A1X0P4R1
A	2	GLY	-	expression tag	UNP A0A1X0P4R1
A	3	SER	-	expression tag	UNP A0A1X0P4R1
A	4	SER	-	expression tag	UNP A0A1X0P4R1
A	5	HIS	-	expression tag	UNP A0A1X0P4R1
A	6	HIS	-	expression tag	UNP A0A1X0P4R1
A	7	HIS	-	expression tag	UNP A0A1X0P4R1
A	8	HIS	-	expression tag	UNP A0A1X0P4R1
A	9	HIS	-	expression tag	UNP A0A1X0P4R1
A	10	HIS	-	expression tag	UNP A0A1X0P4R1
A	11	SER	-	expression tag	UNP A0A1X0P4R1
A	12	SER	-	expression tag	UNP A0A1X0P4R1
A	13	GLY	-	expression tag	UNP A0A1X0P4R1
A	14	LEU	-	expression tag	UNP A0A1X0P4R1
A	15	VAL	-	expression tag	UNP A0A1X0P4R1
A	16	PRO	-	expression tag	UNP A0A1X0P4R1
A	17	ARG	-	expression tag	UNP A0A1X0P4R1
A	18	GLY	-	expression tag	UNP A0A1X0P4R1
A	19	SER	-	expression tag	UNP A0A1X0P4R1
B	1	MET	-	initiating methionine	UNP A0A1X0P4R1
B	2	GLY	-	expression tag	UNP A0A1X0P4R1
B	3	SER	-	expression tag	UNP A0A1X0P4R1
B	4	SER	-	expression tag	UNP A0A1X0P4R1
B	5	HIS	-	expression tag	UNP A0A1X0P4R1
B	6	HIS	-	expression tag	UNP A0A1X0P4R1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	7	HIS	-	expression tag	UNP A0A1X0P4R1
B	8	HIS	-	expression tag	UNP A0A1X0P4R1
B	9	HIS	-	expression tag	UNP A0A1X0P4R1
B	10	HIS	-	expression tag	UNP A0A1X0P4R1
B	11	SER	-	expression tag	UNP A0A1X0P4R1
B	12	SER	-	expression tag	UNP A0A1X0P4R1
B	13	GLY	-	expression tag	UNP A0A1X0P4R1
B	14	LEU	-	expression tag	UNP A0A1X0P4R1
B	15	VAL	-	expression tag	UNP A0A1X0P4R1
B	16	PRO	-	expression tag	UNP A0A1X0P4R1
B	17	ARG	-	expression tag	UNP A0A1X0P4R1
B	18	GLY	-	expression tag	UNP A0A1X0P4R1
B	19	SER	-	expression tag	UNP A0A1X0P4R1

- 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	H	N	O	P	1	0
			23	8	8	1	5	1		
2	B	1	Total	C	H	N	O	P	1	0
			23	8	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	H	O	2	0
			14	3	8	3		
3	A	1	Total	C	H	O	2	0
			14	3	8	3		
3	A	1	Total	C	H	O	2	0
			14	3	8	3		
3	A	1	Total	C	H	O	2	0
			14	3	8	3		
3	B	1	Total	C	H	O	2	0
			14	3	8	3		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		

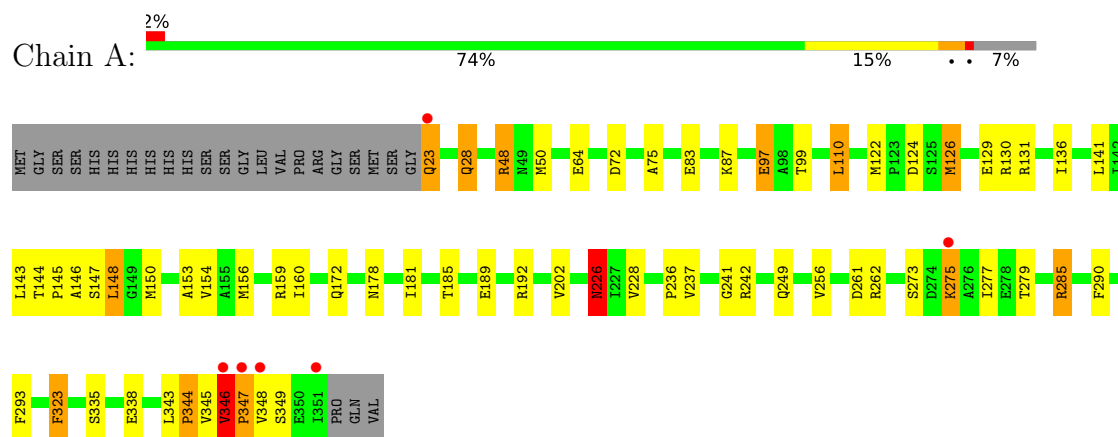
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	81	Total	O	0	0
			81	81		
5	B	60	Total	O	0	0
			60	60		

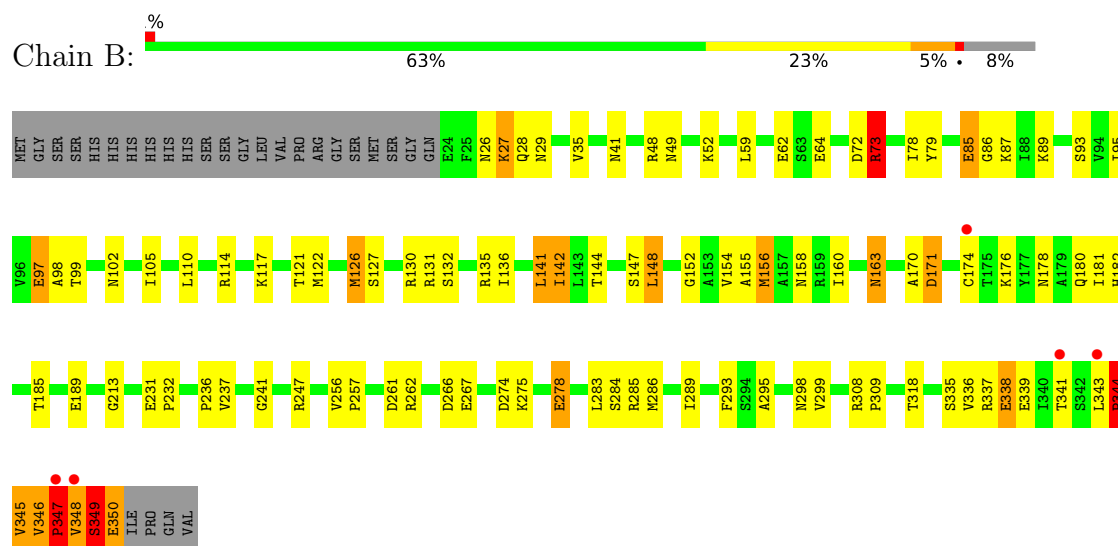
3 Residue-property plots [i](#)

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: Putative cysteine synthase



• Molecule 1: Putative cysteine synthase



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	187.30Å 187.30Å 187.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	76.47 – 2.75 76.47 – 2.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (76.47-2.75) 100.0 (76.47-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.148 , 0.208 (Not available) , 0.177	Depositor DCC
R_{free} test set	1448 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	64.1	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 58.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.021 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10044	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, 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	0.99	2/2510 (0.1%)	1.44	13/3404 (0.4%)
1	B	0.92	1/2439 (0.0%)	1.49	20/3317 (0.6%)
All	All	0.95	3/4949 (0.1%)	1.46	33/6721 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	11
1	B	0	10
All	All	0	21

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	83	GLU	CD-OE1	7.39	1.39	1.25
1	B	284	SER	CA-CB	-5.43	1.44	1.53
1	A	261	ASP	CG-OD1	5.00	1.34	1.25

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	347	PRO	N-CA-CB	-9.98	92.77	103.25
1	B	347	PRO	N-CD-CG	-8.54	90.39	103.20
1	A	72	ASP	CA-CB-CG	8.11	120.71	112.60
1	B	171	ASP	CA-CB-CG	7.57	120.17	112.60
1	B	72	ASP	CA-CB-CG	7.44	120.04	112.60
1	B	275	LYS	CB-CA-C	7.27	125.51	110.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	293	PHE	CA-CB-CG	7.25	121.05	113.80
1	B	347	PRO	N-CA-C	7.18	127.26	112.47
1	B	266	ASP	CA-CB-CG	6.99	119.59	112.60
1	B	261	ASP	CA-CB-CG	6.41	119.01	112.60
1	A	344	PRO	CB-CA-C	-6.18	103.80	111.64
1	B	142	ILE	CB-CA-C	6.09	118.40	110.12
1	A	275	LYS	CB-CA-C	5.90	122.63	110.31
1	A	293	PHE	CA-CB-CG	5.83	119.63	113.80
1	A	275	LYS	N-CA-C	-5.71	105.58	112.54
1	A	64	GLU	CB-CG-CD	5.64	122.18	112.60
1	B	344	PRO	CB-CA-C	-5.56	104.58	111.64
1	B	275	LYS	N-CA-C	-5.51	105.81	112.54
1	B	27	LYS	CB-CA-C	-5.49	100.47	110.63
1	B	174	CYS	CB-CA-C	5.49	118.28	109.07
1	A	97	GLU	CB-CG-CD	5.44	121.84	112.60
1	A	256	VAL	O-C-N	-5.42	117.70	121.55
1	A	28	GLN	CB-CA-C	-5.42	100.61	110.63
1	A	23	GLN	CB-CA-C	5.33	120.24	110.10
1	B	85	GLU	CB-CA-C	-5.29	104.72	111.22
1	A	226[A]	ASN	CB-CA-C	5.27	118.32	109.89
1	A	226[B]	ASN	CB-CA-C	5.27	118.32	109.89
1	A	323	PHE	CA-CB-CG	5.21	119.01	113.80
1	B	256	VAL	O-C-N	-5.14	118.13	121.37
1	B	117	LYS	N-CA-CB	5.10	117.45	109.85
1	B	27	LYS	N-CA-CB	5.08	118.05	110.22
1	B	257	PRO	CB-CA-C	5.07	117.63	110.98
1	B	64	GLU	CB-CG-CD	5.02	121.14	112.60

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	130	ARG	Sidechain
1	A	131	ARG	Sidechain
1	A	159	ARG	Sidechain
1	A	23	GLN	Peptide
1	A	242[A]	ARG	Sidechain
1	A	242[B]	ARG	Sidechain
1	A	285	ARG	Sidechain
1	A	344	PRO	Peptide
1	A	346	VAL	Peptide
1	A	348	VAL	Peptide

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Mol	Chain	Res	Type	Group
1	A	48	ARG	Sidechain
1	B	114	ARG	Sidechain
1	B	130	ARG	Sidechain
1	B	131	ARG	Sidechain
1	B	135	ARG	Sidechain
1	B	247	ARG	Sidechain
1	B	285	ARG	Sidechain
1	B	337	ARG	Sidechain
1	B	344	PRO	Peptide
1	B	349	SER	Peptide
1	B	73	ARG	Sidechain

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	2461	2520	2510	39	0
1	B	2396	2409	2380	60	0
2	A	15	8	7	0	0
2	B	15	8	7	1	0
3	A	24	32	32	4	0
3	B	6	8	8	1	0
4	A	1	0	0	0	0
5	A	81	0	0	6	0
5	B	60	0	0	18	0
All	All	5059	4985	4944	94	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 10.

All (94) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226[A]:ASN:OD1	5:A:501:HOH:O	1.88	0.92
1:B:348:VAL:HG23	1:B:348:VAL:O	1.81	0.81
1:B:89:LYS:HA	5:B:539:HOH:O	1.82	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:VAL:HA	5:B:512:HOH:O	1.82	0.78
1:B:350:GLU:C	1:B:350:GLU:OE2	2.29	0.75
1:B:122:MET:SD	1:B:126:MET:HE2	2.29	0.72
1:A:122:MET:SD	1:A:126:MET:HE2	2.31	0.70
1:B:163:ASN:CB	5:B:519:HOH:O	2.40	0.70
1:B:97:GLU:HG2	1:B:170:ALA:HB3	1.74	0.69
1:A:262:ARG:HG3	5:A:578:HOH:O	1.90	0.69
1:A:346:VAL:HG13	1:A:347:PRO:HD2	1.73	0.69
1:B:99:THR:OG1	3:B:402:GOL:H31	1.93	0.69
1:B:26:ASN:HD21	1:B:28:GLN:HG2	1.59	0.68
1:B:97:GLU:CG	1:B:170:ALA:HB3	2.23	0.68
1:B:144:THR:HG22	5:B:509:HOH:O	1.95	0.65
1:B:348:VAL:O	1:B:348:VAL:CG2	2.45	0.62
1:B:132:SER:O	1:B:136:ILE:HG23	2.00	0.61
1:B:127:SER:HB2	5:B:542:HOH:O	2.01	0.61
1:A:136:ILE:HG13	1:B:336:VAL:HG11	1.83	0.60
1:B:121:THR:HG22	1:B:142:ILE:HD11	1.83	0.60
1:A:48:ARG:HH22	3:A:403:GOL:H31	1.67	0.59
1:A:346:VAL:HG13	1:A:347:PRO:CD	2.33	0.59
1:A:150:MET:O	1:A:154:VAL:HG23	2.03	0.58
1:B:335:SER:HB3	5:B:516:HOH:O	2.04	0.58
1:B:152:GLY:O	1:B:155:ALA:HB3	2.03	0.58
1:B:295:ALA:O	1:B:299:VAL:HG23	2.03	0.58
1:B:122:MET:HE1	1:B:141:LEU:HD12	1.86	0.58
1:A:290:PHE:H	3:A:404:GOL:H12	1.71	0.55
1:A:323:PHE:HE1	3:A:404:GOL:H11	1.71	0.55
1:B:274:ASP:O	1:B:278:GLU:HG2	2.06	0.55
1:B:121:THR:CG2	1:B:142:ILE:HD11	2.36	0.55
1:B:283:LEU:HD11	1:B:299:VAL:HG21	1.89	0.55
2:B:401:PLP:H2A3	5:B:518:HOH:O	2.07	0.55
1:B:163:ASN:HB2	5:B:519:HOH:O	2.05	0.54
1:B:148:LEU:HD23	1:B:148:LEU:N	2.23	0.54
1:B:49:ASN:ND2	5:B:503:HOH:O	2.42	0.53
1:B:338:GLU:O	1:B:341:THR:O	2.27	0.53
1:B:85:GLU:O	1:B:87:LYS:N	2.42	0.52
1:A:156:MET:O	1:A:160:ILE:HG13	2.08	0.52
1:B:231:GLU:HB2	1:B:232:PRO:HD2	1.91	0.52
1:B:349:SER:O	5:B:501:HOH:O	2.19	0.52
1:A:185:THR:O	1:A:189:GLU:HG3	2.09	0.52
1:B:286:MET:HE1	5:B:556:HOH:O	2.09	0.51
1:A:346:VAL:HG11	1:B:156:MET:HE2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:PRO:HB2	1:B:348:VAL:HG13	1.93	0.50
1:A:28:GLN:HG3	5:B:550:HOH:O	2.11	0.50
1:A:145:PRO:HG3	1:B:346:VAL:O	2.13	0.49
1:B:97:GLU:HG3	1:B:170:ALA:HB3	1.94	0.49
1:B:178:ASN:O	1:B:181:ILE:HG22	2.13	0.49
1:A:122:MET:HE1	1:A:141:LEU:HG	1.93	0.48
1:A:178:ASN:O	1:A:181:ILE:HG22	2.13	0.48
1:A:347:PRO:HG2	1:A:349:SER:HB2	1.96	0.48
1:B:59:LEU:HD12	1:B:289:ILE:HD13	1.96	0.47
1:B:73:ARG:HH22	1:B:189:GLU:CD	2.22	0.47
1:B:185:THR:O	1:B:189:GLU:HG3	2.14	0.47
1:A:347:PRO:HD2	1:A:349:SER:HB3	1.97	0.47
1:A:226[B]:ASN:HB3	5:A:501:HOH:O	2.14	0.47
1:B:236:PRO:HG2	1:B:241:GLY:HA3	1.97	0.47
1:B:154:VAL:O	1:B:158:ASN:ND2	2.48	0.47
1:A:148:LEU:N	1:A:148:LEU:HD23	2.30	0.46
1:A:202[A]:VAL:HG23	1:A:228:VAL:CG1	2.45	0.46
1:A:249:GLN:HB3	5:A:563:HOH:O	2.16	0.46
1:B:27:LYS:HE2	1:B:41:ASN:HB2	1.98	0.46
1:A:236:PRO:HG2	1:A:241:GLY:HA3	1.98	0.45
1:A:136:ILE:CG2	5:A:561:HOH:O	2.64	0.45
1:B:62:GLU:CD	1:B:73:ARG:HH11	2.24	0.45
1:B:298:ASN:HB3	1:B:318:THR:OG1	2.17	0.45
1:B:343:LEU:HA	1:B:344:PRO:HD2	1.67	0.45
1:B:48:ARG:HD3	1:B:48:ARG:HA	1.70	0.44
1:A:126:MET:HE3	1:A:126:MET:HB3	1.57	0.44
1:B:171:ASP:HA	5:B:507:HOH:O	2.18	0.44
1:B:102:ASN:HA	1:B:105:ILE:HD12	2.00	0.43
1:A:273:SER:O	1:A:277:ILE:HG13	2.18	0.43
1:A:75:ALA:HB3	1:A:110:LEU:HD13	2.01	0.43
1:B:163:ASN:CA	5:B:519:HOH:O	2.66	0.43
1:A:136:ILE:HG21	5:A:561:HOH:O	2.18	0.43
1:A:124[B]:ASP:OD1	1:A:146:ALA:HB2	2.18	0.43
1:B:78:ILE:HG22	1:B:79:TYR:N	2.33	0.43
1:A:323:PHE:CE1	3:A:404:GOL:H11	2.51	0.42
1:B:308:ARG:HA	1:B:309:PRO:HD3	1.90	0.42
1:A:345:VAL:HG12	1:A:346:VAL:H	1.84	0.42
1:B:93:SER:CB	5:B:505:HOH:O	2.67	0.42
1:A:144:THR:HG21	1:A:153:ALA:HA	2.01	0.41
1:B:93:SER:HB3	5:B:505:HOH:O	2.20	0.41
1:A:97:GLU:OE2	1:A:172:GLN:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:ALA:HA	1:B:121:THR:O	2.20	0.41
1:B:27:LYS:NZ	5:B:508:HOH:O	2.54	0.41
1:A:50:MET:HE2	1:A:50:MET:HB3	1.92	0.41
1:B:339:GLU:HB3	5:B:512:HOH:O	2.20	0.41
1:A:346:VAL:HG11	1:B:156:MET:CE	2.52	0.41
1:A:192:ARG:NE	1:B:29:ASN:HD22	2.19	0.40
1:A:124[A]:ASP:HB2	1:B:345:VAL:HG23	2.03	0.40
1:B:182:HIS:HB2	1:B:213:GLY:HA3	2.03	0.40
1:A:50:MET:HE1	1:A:279:THR:HG23	2.03	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	331/354 (94%)	316 (96%)	14 (4%)	1 (0%)	36	56
1	B	327/354 (92%)	304 (93%)	19 (6%)	4 (1%)	10	20
All	All	658/708 (93%)	620 (94%)	33 (5%)	5 (1%)	16	30

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	347	PRO
1	B	347	PRO
1	B	86	GLY
1	B	267	GLU
1	B	348	VAL

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	262/285 (92%)	245 (94%)	17 (6%)	15	29
1	B	249/285 (87%)	226 (91%)	23 (9%)	8	17
All	All	511/570 (90%)	471 (92%)	40 (8%)	12	21

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	LYS
1	A	99	THR
1	A	110	LEU
1	A	126	MET
1	A	129	GLU
1	A	143	LEU
1	A	147	SER
1	A	148	LEU
1	A	226[A]	ASN
1	A	226[B]	ASN
1	A	237	VAL
1	A	275	LYS
1	A	285	ARG
1	A	335	SER
1	A	338	GLU
1	A	343	LEU
1	A	346	VAL
1	B	35	VAL
1	B	52	LYS
1	B	73	ARG
1	B	95	ILE
1	B	97	GLU
1	B	110	LEU
1	B	126	MET
1	B	141	LEU
1	B	147	SER
1	B	148	LEU

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Mol	Chain	Res	Type
1	B	156	MET
1	B	160	ILE
1	B	163	ASN
1	B	176	LYS
1	B	180	GLN
1	B	237	VAL
1	B	262	ARG
1	B	278	GLU
1	B	338	GLU
1	B	345	VAL
1	B	346	VAL
1	B	349	SER
1	B	350	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	233	GLN
1	B	26	ASN
1	B	29	ASN
1	B	158	ASN
1	B	233	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 ⓘ

Of 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 for Mogul analysis.

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	A	404	-	5,5,5	0.47	0	5,5,5	1.01	0
3	GOL	A	403	-	5,5,5	0.10	0	5,5,5	0.30	0
2	PLP	A	401	1	15,15,16	1.50	3 (20%)	21,22,23	1.56	3 (14%)
2	PLP	B	401	1	15,15,16	2.19	5 (33%)	21,22,23	2.39	10 (47%)
3	GOL	A	405	-	5,5,5	0.24	0	5,5,5	0.54	0
3	GOL	A	402	-	5,5,5	0.29	0	5,5,5	1.09	1 (20%)
3	GOL	B	402	-	5,5,5	0.25	0	5,5,5	0.51	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	A	404	-	-	4/4/4/4	-
3	GOL	A	403	-	-	2/4/4/4	-
2	PLP	A	401	1	-	0/6/6/8	0/1/1/1
2	PLP	B	401	1	-	2/6/6/8	0/1/1/1
3	GOL	A	405	-	-	2/4/4/4	-
3	GOL	A	402	-	-	0/4/4/4	-
3	GOL	B	402	-	-	4/4/4/4	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	PLP	P-O1P	5.18	1.66	1.50
2	B	401	PLP	O3-C3	3.64	1.45	1.36
2	B	401	PLP	C5-C4	2.97	1.43	1.40
2	A	401	PLP	C5-C4	2.88	1.43	1.40
2	B	401	PLP	P-O4P	2.74	1.69	1.60
2	B	401	PLP	C3-C4	2.72	1.45	1.40
2	A	401	PLP	C4A-C4	-2.69	1.46	1.51
2	A	401	PLP	O3-C3	2.03	1.41	1.36

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	PLP	O3-C3-C4	5.05	131.28	118.10
2	B	401	PLP	O3P-P-O4P	-4.87	93.97	106.67
2	B	401	PLP	O4P-C5A-C5	4.21	117.24	109.36
2	A	401	PLP	O3-C3-C4	3.89	128.24	118.10
2	B	401	PLP	O4P-P-O1P	3.40	115.62	106.44
2	B	401	PLP	O3-C3-C2	-2.80	111.78	117.58
2	B	401	PLP	C4-C3-C2	-2.57	116.05	119.89
2	A	401	PLP	O3-C3-C2	-2.48	112.44	117.58
2	A	401	PLP	O4P-C5A-C5	2.41	113.87	109.36
2	B	401	PLP	C6-C5-C4	-2.27	116.23	118.10
3	A	402	GOL	C3-C2-C1	2.18	119.79	111.80
2	B	401	PLP	C4A-C4-C5	-2.06	118.82	120.94
2	B	401	PLP	O3P-P-O1P	2.05	118.82	110.83
2	B	401	PLP	C5A-C5-C6	-2.00	116.10	119.36

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	404	GOL	O1-C1-C2-C3
3	A	405	GOL	C1-C2-C3-O3
3	B	402	GOL	O1-C1-C2-C3
3	B	402	GOL	C1-C2-C3-O3
3	A	403	GOL	O1-C1-C2-C3
3	A	404	GOL	C1-C2-C3-O3
3	A	404	GOL	O1-C1-C2-O2
3	A	404	GOL	O2-C2-C3-O3
3	A	405	GOL	O2-C2-C3-O3
3	B	402	GOL	O2-C2-C3-O3
3	B	402	GOL	O1-C1-C2-O2
3	A	403	GOL	O1-C1-C2-O2
2	B	401	PLP	C5A-O4P-P-O2P
2	B	401	PLP	C5A-O4P-P-O1P

There are no ring outliers.

4 monomers are involved in 6 short contacts:

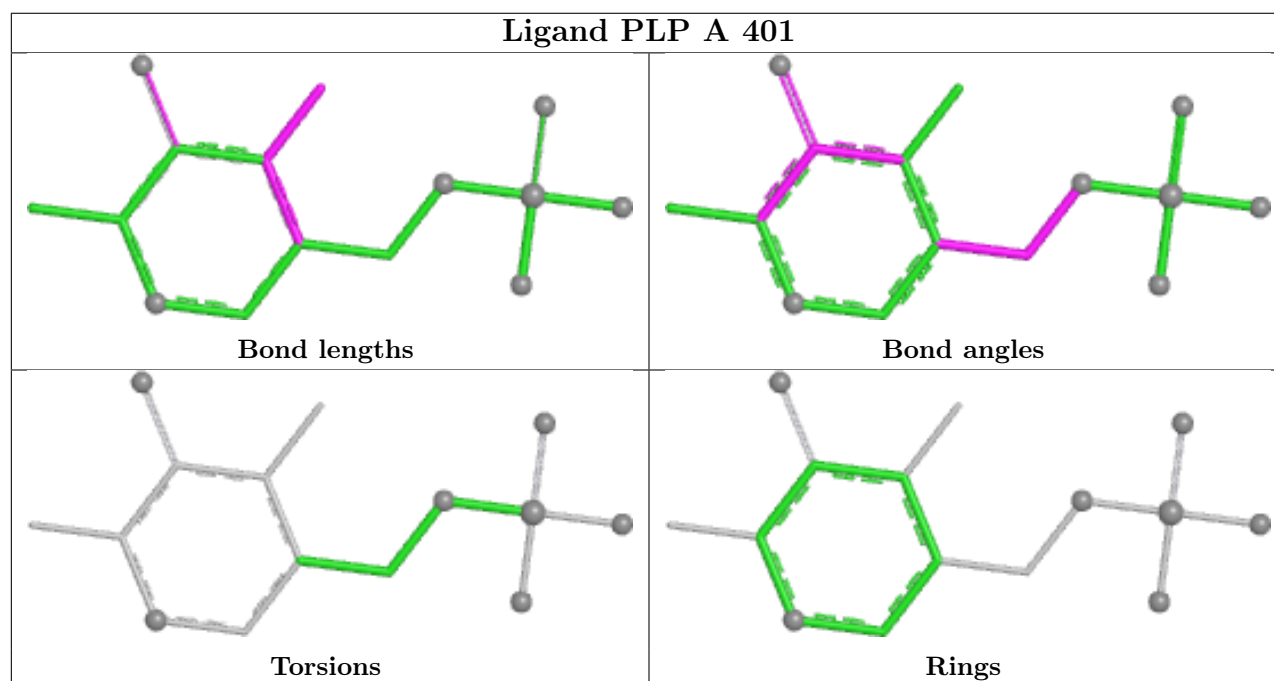
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	404	GOL	3	0
3	A	403	GOL	1	0

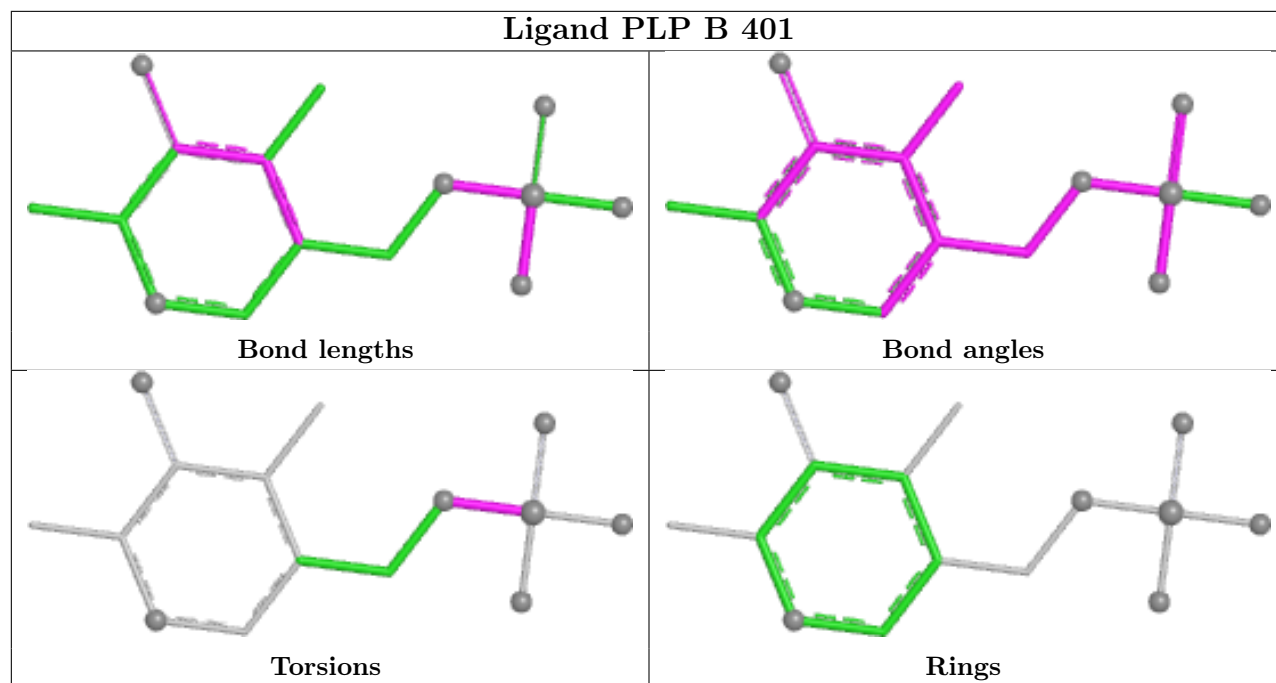
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	PLP	1	0
3	B	402	GOL	1	0

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.





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	329/354 (92%)	-0.80	6 (1%) 67 65	24, 53, 92, 168	4 (1%)
1	B	327/354 (92%)	-0.28	5 (1%) 72 71	29, 74, 126, 171	3 (0%)
All	All	656/708 (92%)	-0.54	11 (1%) 69 67	24, 61, 119, 171	7 (1%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	351	ILE	4.8
1	A	275	LYS	2.9
1	A	348	VAL	2.7
1	A	346	VAL	2.6
1	A	347	PRO	2.5
1	B	174	CYS	2.2
1	B	343	LEU	2.2
1	A	23	GLN	2.1
1	B	341	THR	2.1
1	B	348	VAL	2.1
1	B	347	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

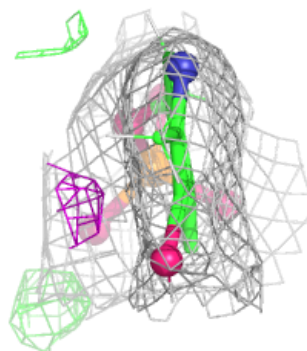
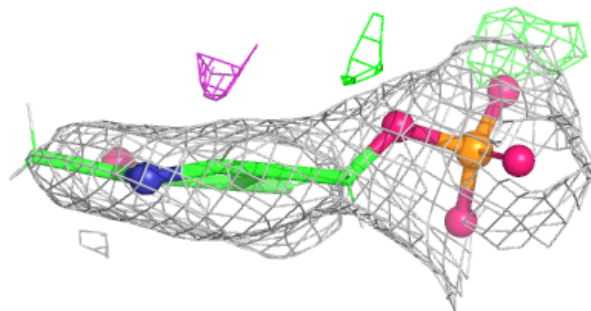
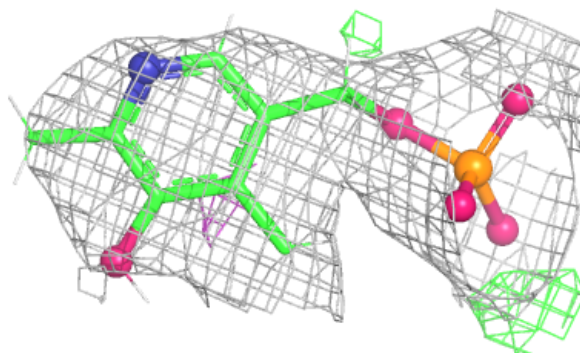
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	A	402	6/6	0.88	0.20	61,91,116,129	2
3	GOL	B	402	6/6	0.90	0.11	91,107,129,141	2
3	GOL	A	403	6/6	0.92	0.11	85,92,96,101	2
2	PLP	B	401	15/16	0.95	0.09	66,85,94,107	1
3	GOL	A	405	6/6	0.96	0.12	77,99,103,105	2
3	GOL	A	404	6/6	0.98	0.14	62,110,117,118	2
4	CL	A	406	1/1	0.98	0.15	76,76,76,76	0
2	PLP	A	401	15/16	0.99	0.06	36,53,64,72	1

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.

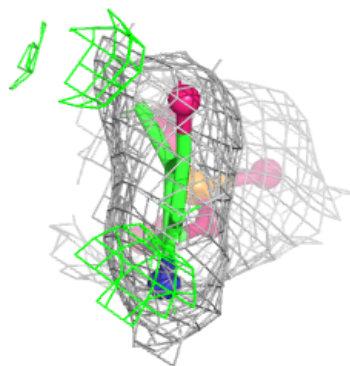
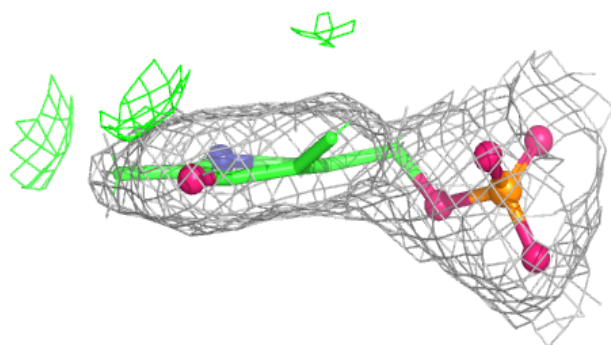
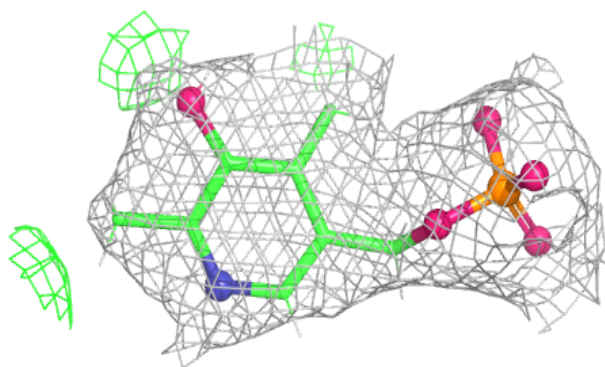
Electron density around PLP B 401:

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)



6.5 Other polymers [i](#)

There are no such residues in this entry.