



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:36 AM UTC

PDB ID : 8B9Y / pdb_00008b9y
Title : Cysteine Synthase from Trypanosoma cruzi with PLP and OAS
Authors : Sowerby, K.V.; Pohl, E.
Deposited on : 2022-10-10
Resolution : 1.80 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

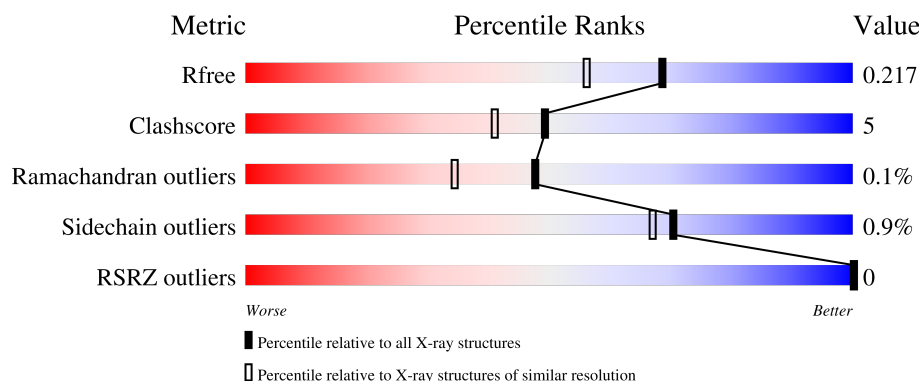
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	344	 84% 7% 9%
1	B	344	 84% 8% 8%
1	C	344	 87% 8% . .
1	D	344	 85% 8% . 7%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 19553 atoms, of which 9519 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 Cysteine synthase, putative.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	313	Total	C	H	N	O	S	134	2	0
			4575	1450	2293	384	435	13			
1	B	316	Total	C	H	N	O	S	128	4	0
			4710	1483	2368	397	448	14			
1	C	330	Total	C	H	N	O	S	136	3	0
			4814	1524	2407	405	463	15			
1	D	321	Total	C	H	N	O	S	139	5	0
			4747	1494	2384	402	451	16			

There are 52 discrepancies between the modelled and reference sequences:

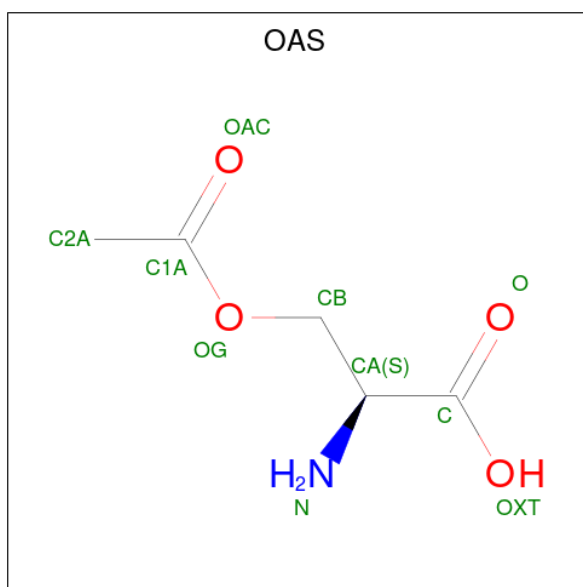
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q4CST7
A	2	THR	-	expression tag	UNP Q4CST7
A	3	MET	-	expression tag	UNP Q4CST7
A	4	ILE	-	expression tag	UNP Q4CST7
A	5	THR	-	expression tag	UNP Q4CST7
A	6	HIS	-	expression tag	UNP Q4CST7
A	7	HIS	-	expression tag	UNP Q4CST7
A	8	HIS	-	expression tag	UNP Q4CST7
A	9	HIS	-	expression tag	UNP Q4CST7
A	10	HIS	-	expression tag	UNP Q4CST7
A	11	HIS	-	expression tag	UNP Q4CST7
A	12	GLY	-	expression tag	UNP Q4CST7
A	13	SER	-	expression tag	UNP Q4CST7
B	1	MET	-	initiating methionine	UNP Q4CST7
B	2	THR	-	expression tag	UNP Q4CST7
B	3	MET	-	expression tag	UNP Q4CST7
B	4	ILE	-	expression tag	UNP Q4CST7
B	5	THR	-	expression tag	UNP Q4CST7
B	6	HIS	-	expression tag	UNP Q4CST7
B	7	HIS	-	expression tag	UNP Q4CST7
B	8	HIS	-	expression tag	UNP Q4CST7

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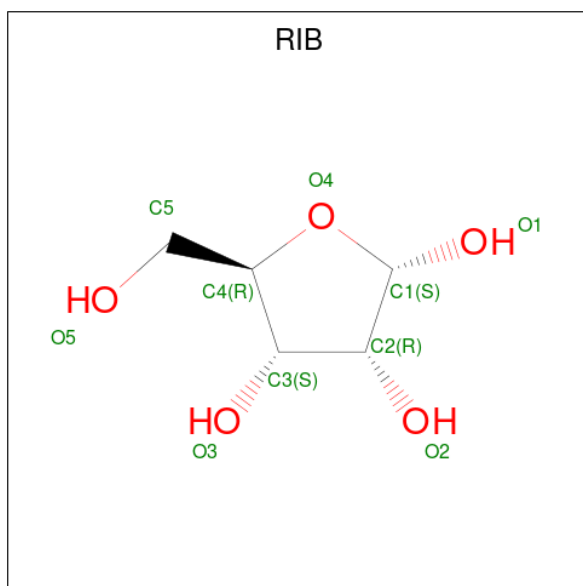
Chain	Residue	Modelled	Actual	Comment	Reference
B	9	HIS	-	expression tag	UNP Q4CST7
B	10	HIS	-	expression tag	UNP Q4CST7
B	11	HIS	-	expression tag	UNP Q4CST7
B	12	GLY	-	expression tag	UNP Q4CST7
B	13	SER	-	expression tag	UNP Q4CST7
C	1	MET	-	initiating methionine	UNP Q4CST7
C	2	THR	-	expression tag	UNP Q4CST7
C	3	MET	-	expression tag	UNP Q4CST7
C	4	ILE	-	expression tag	UNP Q4CST7
C	5	THR	-	expression tag	UNP Q4CST7
C	6	HIS	-	expression tag	UNP Q4CST7
C	7	HIS	-	expression tag	UNP Q4CST7
C	8	HIS	-	expression tag	UNP Q4CST7
C	9	HIS	-	expression tag	UNP Q4CST7
C	10	HIS	-	expression tag	UNP Q4CST7
C	11	HIS	-	expression tag	UNP Q4CST7
C	12	GLY	-	expression tag	UNP Q4CST7
C	13	SER	-	expression tag	UNP Q4CST7
D	1	MET	-	initiating methionine	UNP Q4CST7
D	2	THR	-	expression tag	UNP Q4CST7
D	3	MET	-	expression tag	UNP Q4CST7
D	4	ILE	-	expression tag	UNP Q4CST7
D	5	THR	-	expression tag	UNP Q4CST7
D	6	HIS	-	expression tag	UNP Q4CST7
D	7	HIS	-	expression tag	UNP Q4CST7
D	8	HIS	-	expression tag	UNP Q4CST7
D	9	HIS	-	expression tag	UNP Q4CST7
D	10	HIS	-	expression tag	UNP Q4CST7
D	11	HIS	-	expression tag	UNP Q4CST7
D	12	GLY	-	expression tag	UNP Q4CST7
D	13	SER	-	expression tag	UNP Q4CST7

- Molecule 2 is O-ACETYLSELINE (CCD ID: OAS) (formula: C₅H₉NO₄) (labeled as "Ligand of Interest" by depositor).



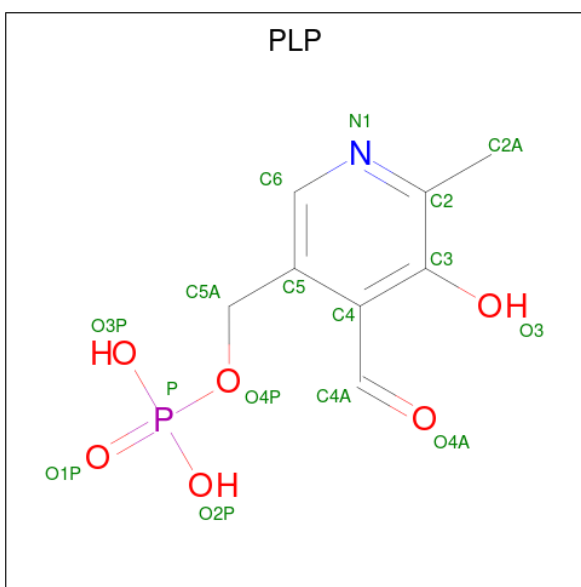
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			19	5	9	1	4		

- Molecule 3 is alpha-D-ribofuranose (CCD ID: RIB) (formula: C₅H₁₀O₅).



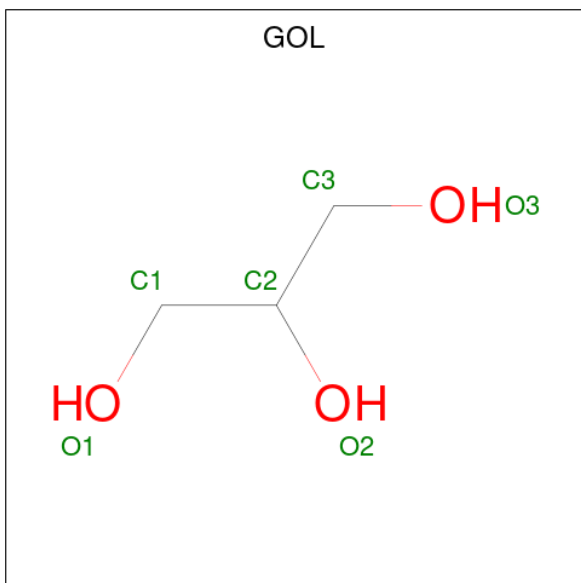
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	3	0
			20	5	10	5		

- Molecule 4 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total 23	C 8	H 8	N 1	O 5	P 1	1	0
4	B	1	Total 23	C 8	H 8	N 1	O 5	P 1	1	0
4	C	1	Total 23	C 8	H 8	N 1	O 5	P 1	1	0
4	D	1	Total 23	C 8	H 8	N 1	O 5	P 1	1	0

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	H	O	2	0
			14	3	8	3		
5	D	1	Total	C	H	O	2	0
			14	3	8	3		

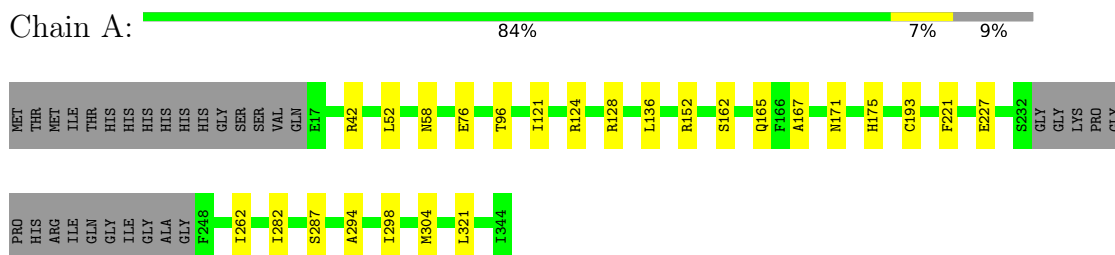
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	123	Total	O	0	0
			123	123		
6	B	143	Total	O	0	0
			143	143		
6	C	141	Total	O	0	0
			141	141		
6	D	141	Total	O	0	0
			141	141		

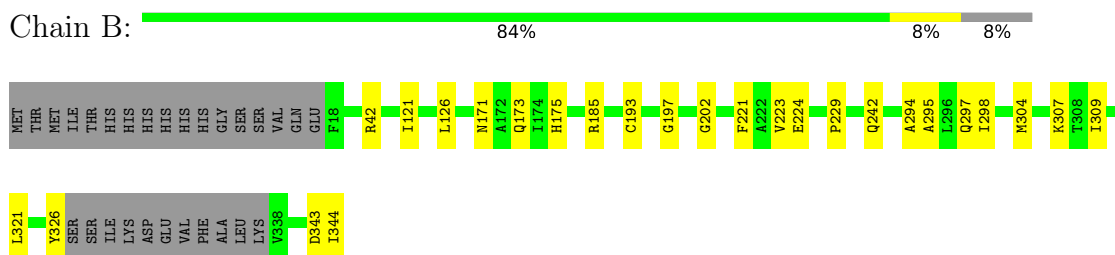
3 Residue-property plots

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.

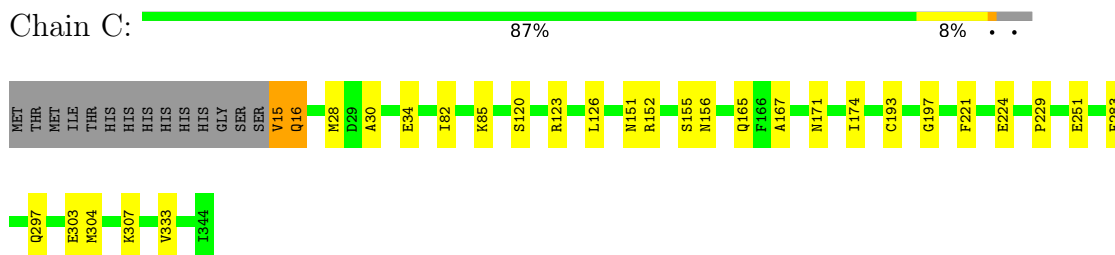
- Molecule 1: Cysteine synthase, putative



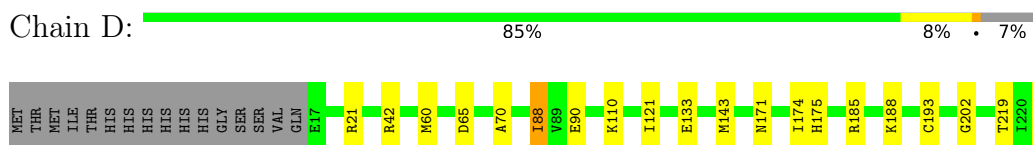
- Molecule 1: Cysteine synthase, putative



- Molecule 1: Cysteine synthase, putative



- Molecule 1: Cysteine synthase, putative





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	55.01Å 66.67Å 167.52Å 90.00° 90.47° 90.00°	Depositor
Resolution (Å)	54.94 – 1.80 54.94 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.9 (54.94-1.80) 95.5 (54.94-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.70 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.191 , 0.217 0.191 , 0.217	Depositor DCC
R_{free} test set	5483 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	22.4	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 37.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.167 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	19553	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.04% 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: GOL, RIB, OAS, PLP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.62	1/2326 (0.0%)	0.91	0/3170
1	B	0.66	1/2391 (0.0%)	0.90	1/3249 (0.0%)
1	C	0.63	0/2458	0.90	0/3347
1	D	0.65	1/2415 (0.0%)	0.92	1/3282 (0.0%)
All	All	0.64	3/9590 (0.0%)	0.91	2/13048 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
1	C	0	1
1	D	0	3
All	All	0	7

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	175	HIS	CE1-NE2	6.45	1.39	1.32
1	D	175	HIS	CE1-NE2	5.88	1.38	1.32
1	A	175	HIS	CE1-NE2	5.72	1.38	1.32

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	90	GLU	CB-CG-CD	5.21	121.45	112.60
1	B	343	ASP	CB-CA-C	-5.15	101.90	110.81

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	128	ARG	Sidechain
1	A	152	ARG	Sidechain
1	B	185	ARG	Sidechain
1	C	152	ARG	Sidechain
1	D	185	ARG	Sidechain
1	D	278	ARG	Sidechain
1	D	42	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	2282	2293	2253	20	0
1	B	2342	2368	2355	28	0
1	C	2407	2407	2376	30	0
1	D	2363	2384	2361	27	0
2	A	10	9	8	2	0
3	A	10	10	0	1	0
4	A	15	8	7	0	0
4	B	15	8	7	0	0
4	C	15	8	7	0	0
4	D	15	8	6	0	0
5	C	6	8	8	0	0
5	D	6	8	8	1	0
6	A	123	0	0	4	0
6	B	143	0	0	6	0
6	C	141	0	0	11	0
6	D	141	0	0	4	1
All	All	10034	9519	9396	101	1

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 5.

All (101) 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:143[B]:MET:HA	1:D:143[B]:MET:HE3	1.35	1.05
1:C:156:ASN:ND2	6:C:501:HOH:O	2.08	0.85
1:D:143[B]:MET:HA	1:D:143[B]:MET:CE	2.06	0.85
1:D:143[B]:MET:HE3	1:D:143[B]:MET:CA	2.06	0.85
1:A:76:GLU:OE1	6:A:801:HOH:O	1.98	0.80
1:C:151:ASN:HB3	6:C:612:HOH:O	1.83	0.78
1:C:126:LEU:HD21	1:D:321:LEU:HD21	1.68	0.75
1:B:326:TYR:OH	6:B:601:HOH:O	2.05	0.73
1:B:193[A]:CYS:SG	1:B:298:ILE:CD1	2.77	0.73
1:B:295:ALA:O	1:B:298:ILE:CG2	2.41	0.69
1:B:193[A]:CYS:SG	1:B:298:ILE:HD11	2.32	0.69
1:A:58:ASN:O	3:A:702:RIB:O2	2.09	0.68
1:D:193[B]:CYS:SG	1:D:304:MET:HE1	2.33	0.68
1:B:295:ALA:O	1:B:298:ILE:HG23	1.94	0.67
1:C:151:ASN:HB3	6:C:606:HOH:O	1.95	0.66
1:A:287:SER:OG	6:A:802:HOH:O	2.14	0.66
1:D:193[B]:CYS:SG	1:D:304:MET:CE	2.86	0.65
1:C:82:ILE:HD12	1:C:85:LYS:HE2	1.80	0.64
1:C:193[B]:CYS:SG	1:C:221:PHE:CE1	2.91	0.63
1:D:344:ILE:OXT	6:D:502:HOH:O	2.16	0.61
1:D:110:LYS:HE3	1:D:133:GLU:HG2	1.82	0.60
1:C:15:VAL:O	1:C:16:GLN:CB	2.50	0.58
1:C:193[A]:CYS:SG	1:C:304:MET:HE1	2.44	0.57
1:B:344:ILE:HG13	6:B:681:HOH:O	2.04	0.57
1:D:262:ILE:HD11	1:D:298:ILE:HD11	1.86	0.57
1:A:52:LEU:HD12	1:A:282:ILE:HD13	1.86	0.57
1:D:219[A]:THR:HG23	1:D:221:PHE:HE1	1.70	0.57
1:C:297:GLN:HG2	6:C:515:HOH:O	2.03	0.56
1:A:193[A]:CYS:SG	1:A:304:MET:HE1	2.45	0.56
1:B:193[B]:CYS:SG	1:B:304:MET:CE	2.93	0.56
1:B:193[A]:CYS:SG	1:B:298:ILE:HD13	2.46	0.55
1:B:193[B]:CYS:SG	1:B:304:MET:SD	3.04	0.55
1:A:227:GLU:CB	6:A:856:HOH:O	2.53	0.55
1:B:304:MET:HE3	1:B:307:LYS:HB2	1.89	0.55
1:C:193[B]:CYS:HG	1:C:221:PHE:HE1	1.50	0.55
1:A:52:LEU:CD1	1:A:282:ILE:HD13	2.36	0.55
1:A:193[B]:CYS:SG	1:A:221:PHE:CE1	3.00	0.55
1:B:344:ILE:CG1	6:B:681:HOH:O	2.56	0.54
1:C:167:ALA:O	1:C:171:ASN:HB2	2.08	0.54
1:B:242:GLN:NE2	6:B:602:HOH:O	2.31	0.54
1:B:221:PHE:CE1	1:B:298:ILE:CD1	2.91	0.53
1:B:193[B]:CYS:SG	1:B:304:MET:HE1	2.49	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:143[B]:MET:CE	1:D:143[B]:MET:CA	2.79	0.53
1:B:221:PHE:CE1	1:B:298:ILE:HD12	2.44	0.53
1:C:15:VAL:HB	1:C:30:ALA:O	2.09	0.52
1:A:167:ALA:O	1:A:171:ASN:HB2	2.08	0.52
1:B:297:GLN:NE2	6:B:605:HOH:O	2.43	0.52
1:B:173:GLN:HG3	6:B:707:HOH:O	2.10	0.52
1:C:28:MET:HE2	6:D:517:HOH:O	2.09	0.52
1:C:193[B]:CYS:SG	1:C:221:PHE:CD1	3.03	0.52
1:C:333:VAL:HG23	1:D:121:ILE:HD11	1.90	0.52
1:C:193[A]:CYS:SG	1:C:304:MET:CE	2.99	0.51
1:A:52:LEU:HD12	1:A:282:ILE:CD1	2.41	0.50
1:C:82:ILE:HD12	1:C:85:LYS:CE	2.42	0.50
1:D:304:MET:HE3	1:D:307:LYS:HB2	1.94	0.50
1:B:295:ALA:O	1:B:298:ILE:HG22	2.11	0.49
1:C:304:MET:HE3	1:C:307:LYS:HB2	1.95	0.49
1:A:193[A]:CYS:SG	1:A:304:MET:CE	3.01	0.49
1:C:156:ASN:CG	6:C:501:HOH:O	2.49	0.47
1:A:124:ARG:HD3	1:A:136:LEU:HD11	1.96	0.47
1:B:295:ALA:HA	1:B:298:ILE:CG2	2.45	0.47
1:A:193[B]:CYS:SG	1:A:221:PHE:CD1	3.08	0.47
1:C:165:GLN:CB	6:C:618:HOH:O	2.63	0.47
1:C:197:GLY:HA3	6:C:533:HOH:O	2.15	0.46
1:B:294:ALA:O	1:B:298:ILE:HG22	2.17	0.45
1:D:193[A]:CYS:SG	1:D:221:PHE:CE1	3.10	0.45
5:D:402:GOL:H32	6:D:525:HOH:O	2.16	0.45
1:C:229:PRO:HG3	6:C:562:HOH:O	2.15	0.45
1:D:193[B]:CYS:SG	1:D:304:MET:SD	3.15	0.45
1:D:171:ASN:OD1	1:D:202:GLY:HA3	2.17	0.44
1:A:96:THR:CB	2:A:701:OAS:H	2.30	0.44
1:C:120:SER:OG	1:C:123:ARG:HG3	2.17	0.44
1:D:88:ILE:HD12	1:D:88:ILE:N	2.32	0.44
1:D:224:GLU:CD	1:D:229:PRO:HA	2.43	0.44
1:B:295:ALA:C	1:B:298:ILE:HG22	2.43	0.44
1:D:60[A]:MET:HB2	1:D:65:ASP:OD1	2.18	0.44
1:B:224:GLU:CD	1:B:229:PRO:HA	2.43	0.43
1:D:219[A]:THR:CG2	1:D:221:PHE:HE1	2.31	0.43
1:A:96:THR:HB	2:A:701:OAS:H	1.83	0.43
1:D:193[A]:CYS:SG	1:D:221:PHE:CD1	3.11	0.43
1:C:224:GLU:CD	1:C:229:PRO:HA	2.44	0.43
1:B:193[A]:CYS:SG	1:B:221:PHE:CE1	3.12	0.43
1:C:155:SER:HB2	6:C:501:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:ARG:NH2	6:A:804:HOH:O	2.52	0.42
1:C:229:PRO:CG	6:C:562:HOH:O	2.68	0.42
1:B:221:PHE:CE1	1:B:298:ILE:HD11	2.54	0.42
1:C:151:ASN:CB	6:C:612:HOH:O	2.55	0.42
1:D:70:ALA:HB2	1:D:174:ILE:HB	2.02	0.41
1:A:162:SER:O	1:A:165:GLN:HG2	2.21	0.41
1:C:34:GLU:OE1	1:D:21:ARG:HB3	2.20	0.41
1:D:188:LYS:NZ	6:D:508:HOH:O	2.51	0.41
1:C:283:PHE:CD2	1:D:60[B]:MET:HE1	2.55	0.41
1:A:321[B]:LEU:HD11	1:B:126:LEU:HD21	2.03	0.41
1:B:304:MET:HE2	1:B:309:ILE:CG1	2.50	0.41
1:A:262:ILE:HD12	1:A:294:ALA:HB1	2.03	0.41
1:D:193[B]:CYS:HG	1:D:304:MET:CE	2.33	0.40
1:D:174:ILE:HD12	1:D:174:ILE:HA	1.99	0.40
1:A:262:ILE:HD11	1:A:298:ILE:HD11	2.03	0.40
1:C:174:ILE:HD12	1:C:174:ILE:HA	2.00	0.40
1:B:171:ASN:OD1	1:B:202:GLY:HA3	2.22	0.40
1:B:197:GLY:HA2	1:B:223:VAL:HB	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:502:HOH:O	6:D:606:HOH:O[2_546]	1.70	0.50

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	311/344 (90%)	305 (98%)	6 (2%)	0	100	100
1	B	316/344 (92%)	309 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	331/344 (96%)	324 (98%)	6 (2%)	1 (0%)	36	25
1	D	322/344 (94%)	315 (98%)	7 (2%)	0	100	100
All	All	1280/1376 (93%)	1253 (98%)	26 (2%)	1 (0%)	48	34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	16	GLN

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	231/271 (85%)	230 (100%)	1 (0%)	84	83
1	B	244/271 (90%)	241 (99%)	3 (1%)	63	57
1	C	245/271 (90%)	242 (99%)	3 (1%)	63	57
1	D	244/271 (90%)	242 (99%)	2 (1%)	73	70
All	All	964/1084 (89%)	955 (99%)	9 (1%)	70	67

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	121	ILE
1	B	42	ARG
1	B	121	ILE
1	B	321	LEU
1	C	15	VAL
1	C	251	GLU
1	C	303	GLU
1	D	88	ILE
1	D	321	LEU

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	297	GLN
1	B	173	GLN
1	B	242	GLN
1	C	22	ASN
1	C	242	GLN
1	D	242	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 ⓘ

8 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	$\# Z > 2$
4	PLP	C	401	1	15,15,16	0.73	0	21,22,23	0.89	1 (4%)
4	PLP	A	703	1	15,15,16	0.76	0	21,22,23	1.12	1 (4%)
5	GOL	D	402	-	5,5,5	0.15	0	5,5,5	0.49	0
4	PLP	B	500	1	15,15,16	1.22	2 (13%)	21,22,23	0.96	0
4	PLP	D	401	1	15,15,16	0.94	1 (6%)	21,22,23	1.02	0
3	RIB	A	702	-	10,10,10	1.02	1 (10%)	13,14,14	1.22	1 (7%)
2	OAS	A	701	-	8,9,9	0.68	0	7,11,11	0.60	0
5	GOL	C	402	-	5,5,5	0.11	0	5,5,5	0.26	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
4	PLP	C	401	1	-	0/6/6/8	0/1/1/1
4	PLP	A	703	1	-	1/6/6/8	0/1/1/1
5	GOL	D	402	-	-	2/4/4/4	-
4	PLP	B	500	1	-	0/6/6/8	0/1/1/1
4	PLP	D	401	1	-	0/6/6/8	0/1/1/1
3	RIB	A	702	-	-	2/2/18/18	0/1/1/1
2	OAS	A	701	-	-	7/9/9/9	-
5	GOL	C	402	-	-	2/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	500	PLP	C4A-C4	-3.25	1.45	1.51
4	D	401	PLP	C4A-C4	-3.02	1.45	1.51
3	A	702	RIB	O4-C1	2.68	1.46	1.43
4	B	500	PLP	C5-C4	2.34	1.43	1.40

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	703	PLP	O4P-C5A-C5	3.08	115.13	109.36
3	A	702	RIB	C1-C2-C3	2.88	105.83	102.29
4	C	401	PLP	O4P-C5A-C5	2.27	113.61	109.36

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	OAS	N-CA-CB-OG
2	A	701	OAS	C-CA-CB-OG
2	A	701	OAS	O-C-CA-CB
2	A	701	OAS	OXT-C-CA-CB
4	A	703	PLP	C6-C5-C5A-O4P
5	C	402	GOL	C1-C2-C3-O3
3	A	702	RIB	O4-C4-C5-O5
2	A	701	OAS	OAC-C1A-OG-CB
2	A	701	OAS	C2A-C1A-OG-CB

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Mol	Chain	Res	Type	Atoms
5	D	402	GOL	O1-C1-C2-C3
5	D	402	GOL	O1-C1-C2-O2
5	C	402	GOL	O2-C2-C3-O3
3	A	702	RIB	C3-C4-C5-O5
2	A	701	OAS	OXT-C-CA-N

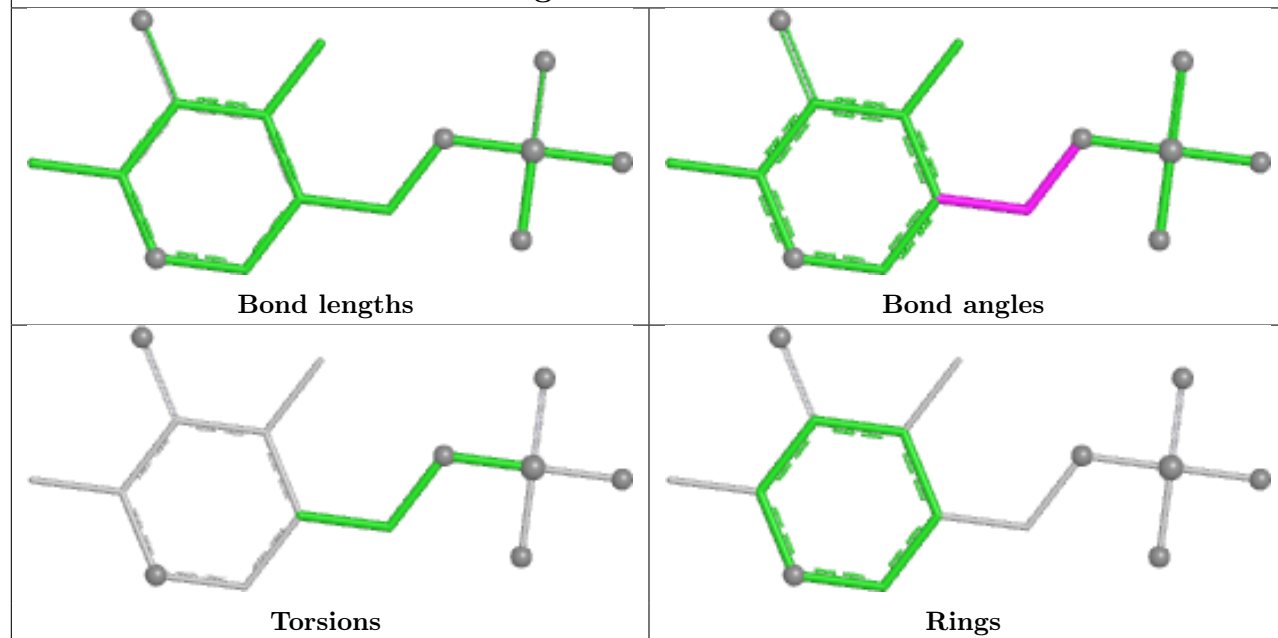
There are no ring outliers.

3 monomers are involved in 4 short contacts:

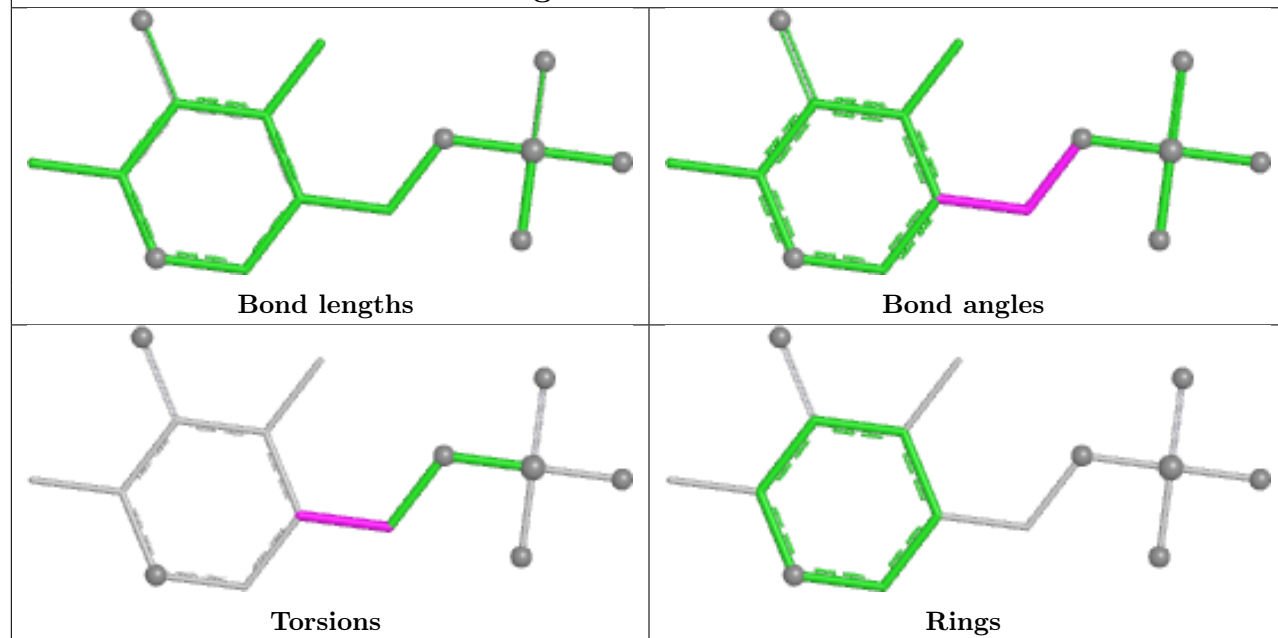
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	402	GOL	1	0
3	A	702	RIB	1	0
2	A	701	OAS	2	0

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

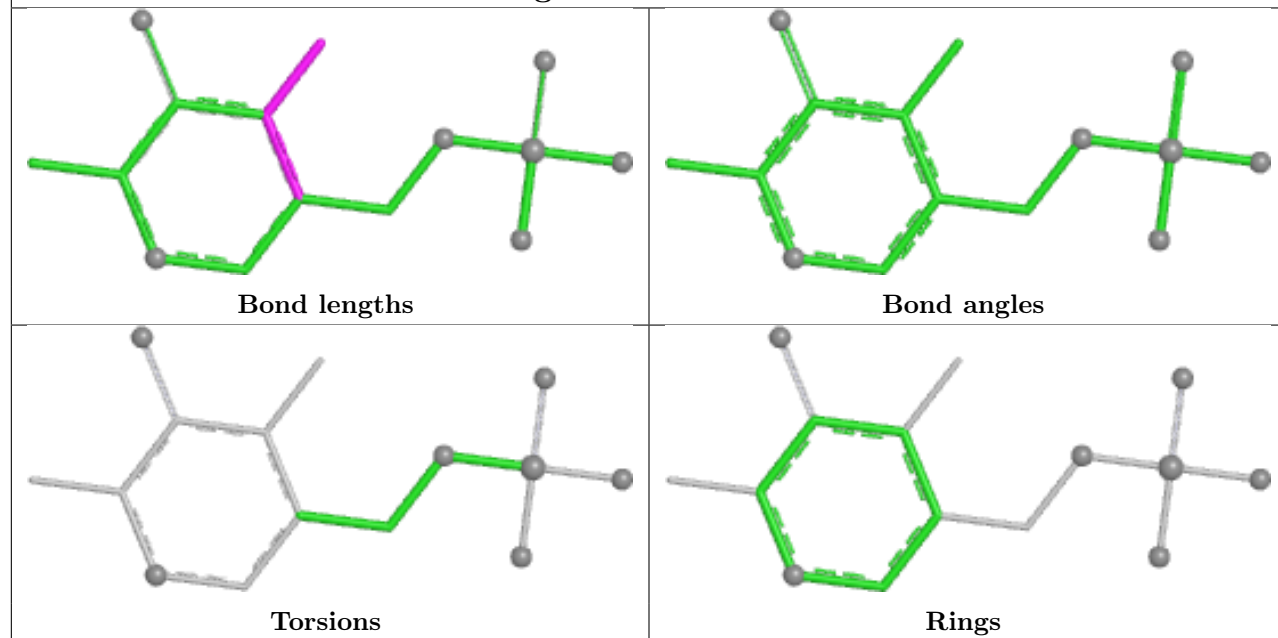
Ligand PLP C 401



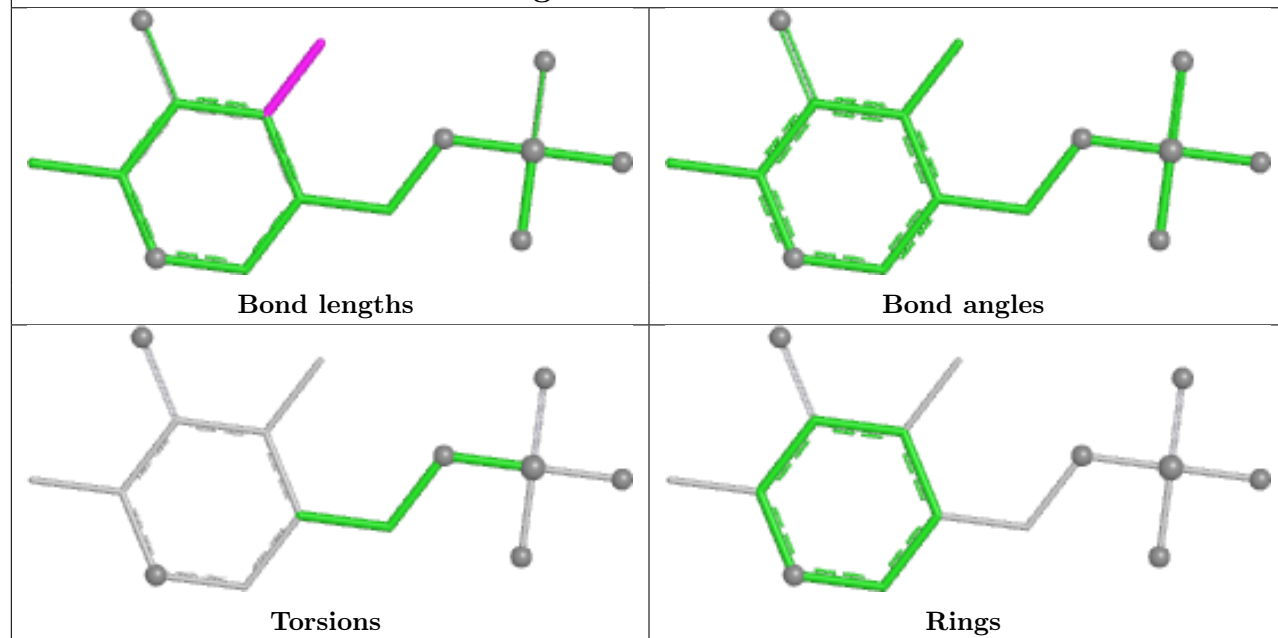
Ligand PLP A 703

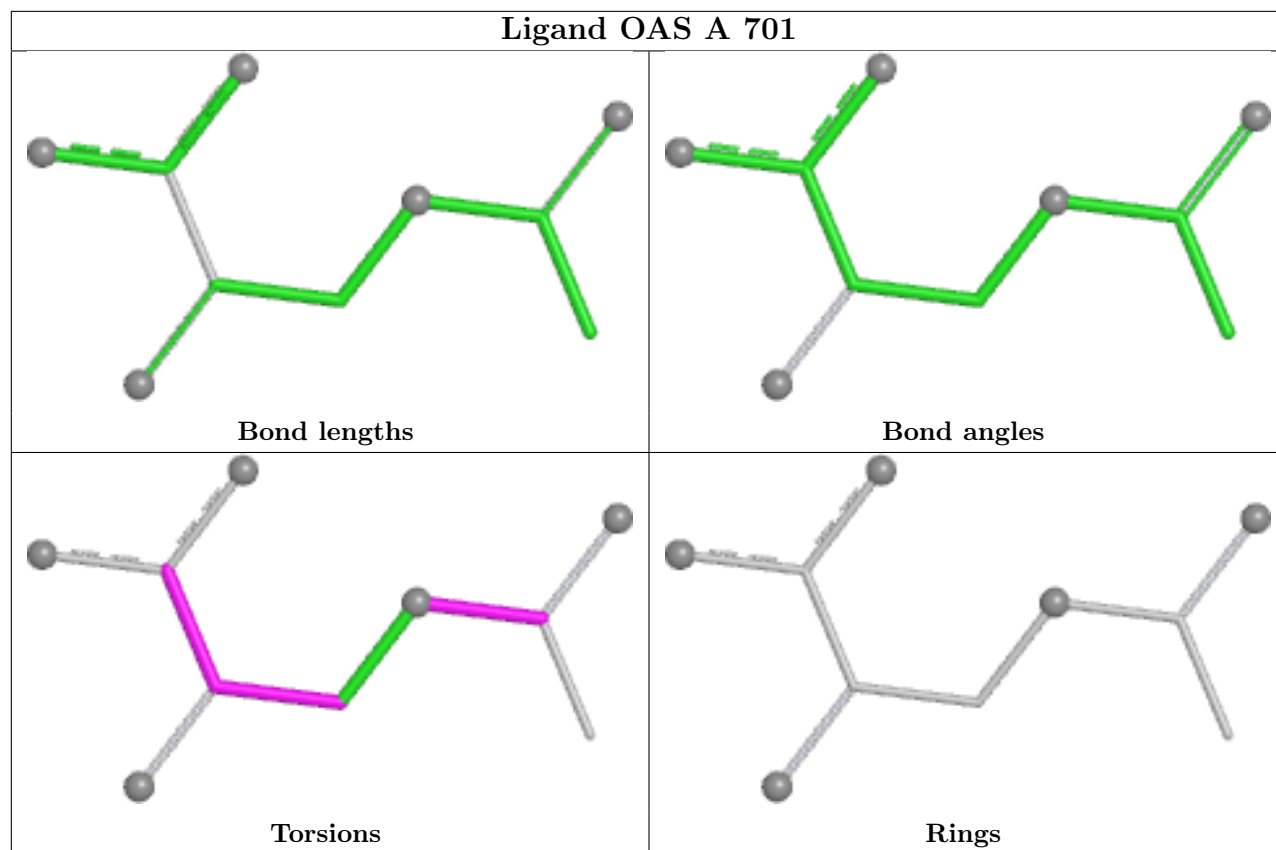


Ligand PLP B 500



Ligand PLP D 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 [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	313/344 (90%)	-1.05	0 100 100	13, 26, 47, 66	2 (0%)
1	B	316/344 (91%)	-1.19	0 100 100	11, 21, 38, 59	4 (1%)
1	C	330/344 (95%)	-1.03	0 100 100	10, 25, 57, 79	3 (0%)
1	D	321/344 (93%)	-1.18	0 100 100	12, 21, 37, 70	5 (1%)
All	All	1280/1376 (93%)	-1.11	0 100 100	10, 24, 46, 79	14 (1%)

There are no RSRZ outliers to report.

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 [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.

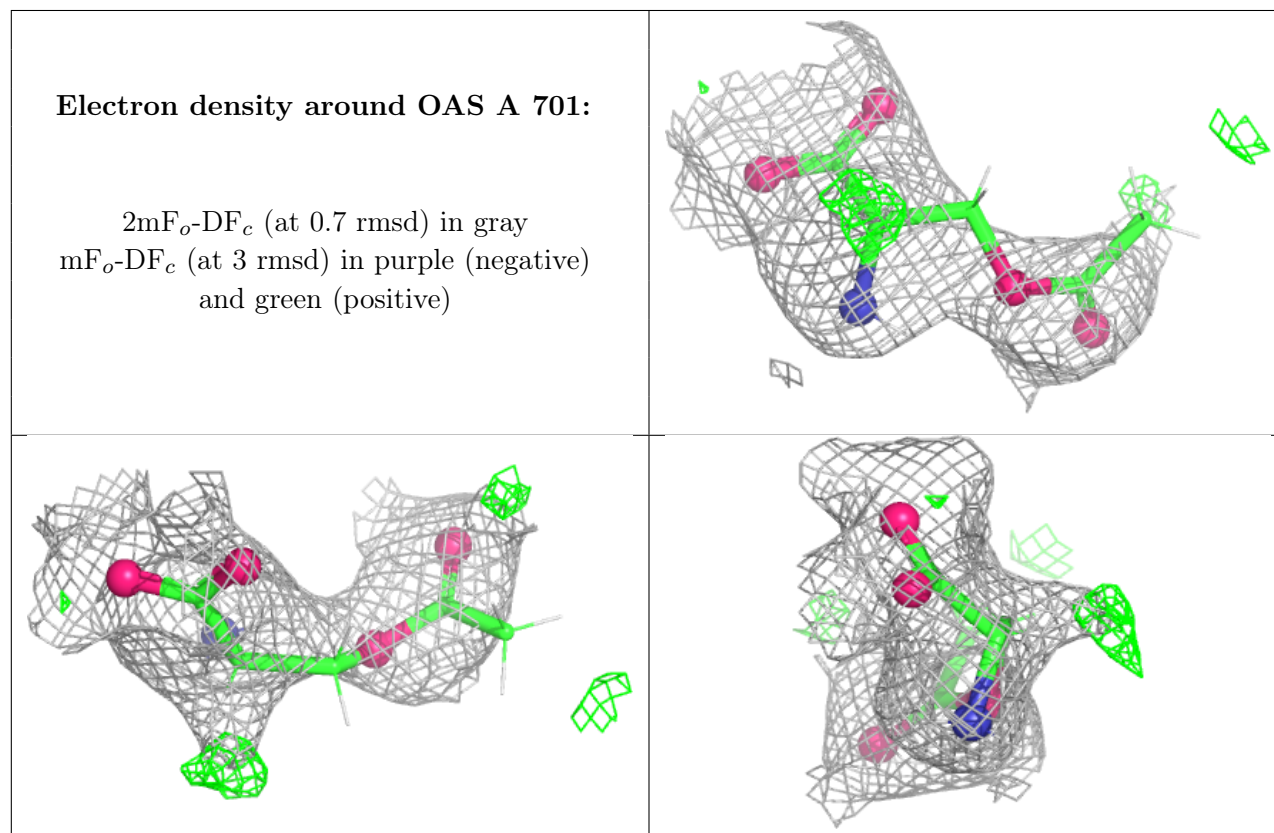
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GOL	C	402	6/6	0.97	0.08	45,51,55,55	2
3	RIB	A	702	10/10	0.98	0.07	36,43,62,62	3
2	OAS	A	701	10/10	0.98	0.07	47,52,57,57	0
5	GOL	D	402	6/6	0.98	0.05	28,31,40,40	2

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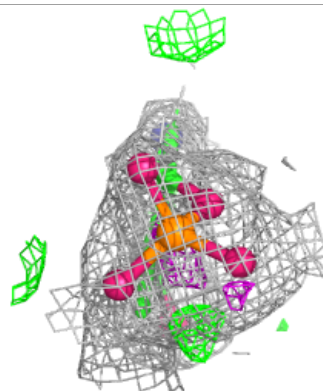
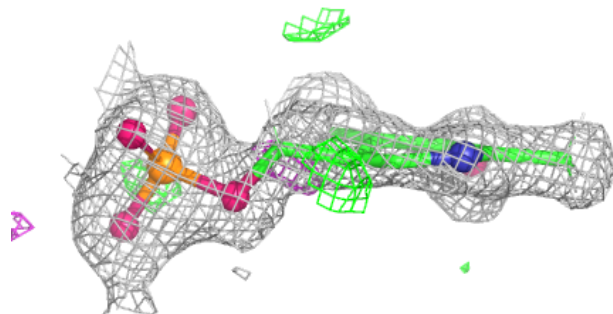
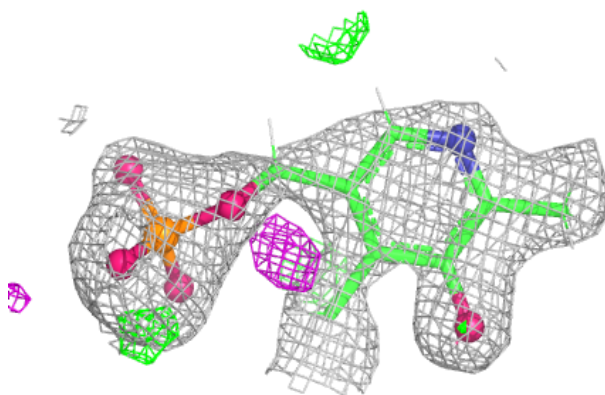
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PLP	C	401	15/16	0.99	0.06	30,36,38,40	1
4	PLP	A	703	15/16	0.99	0.05	32,41,43,44	1
4	PLP	B	500	15/16	0.99	0.03	14,16,18,18	1
4	PLP	D	401	15/16	1.00	0.02	15,17,18,20	1

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.

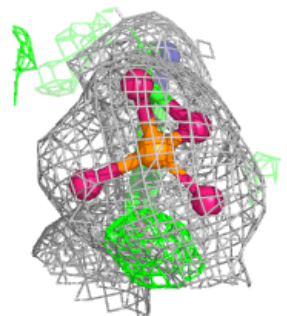
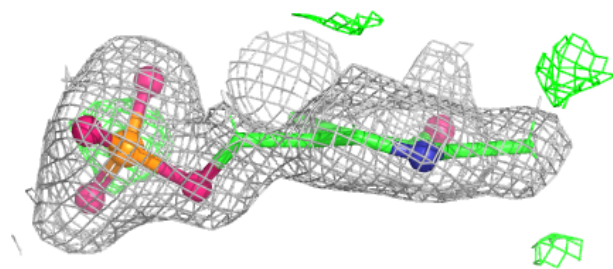
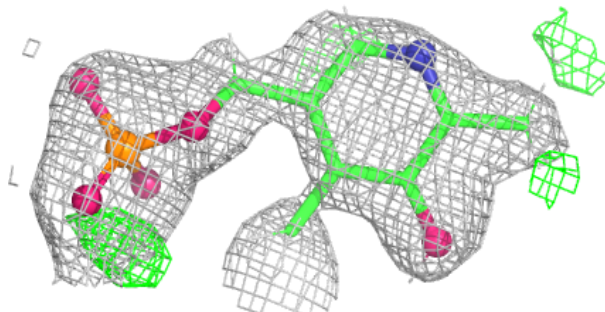


Electron density around PLP C 401:

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

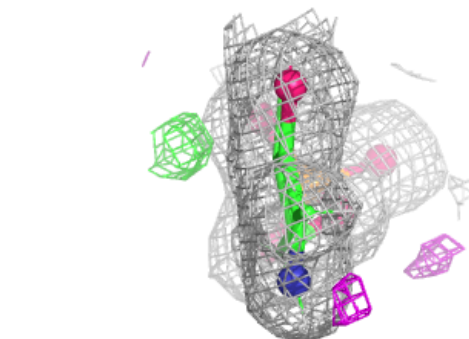
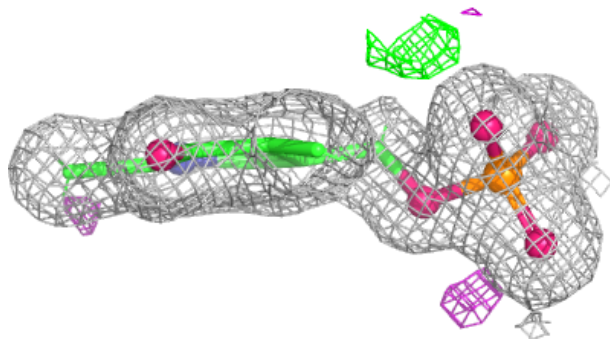
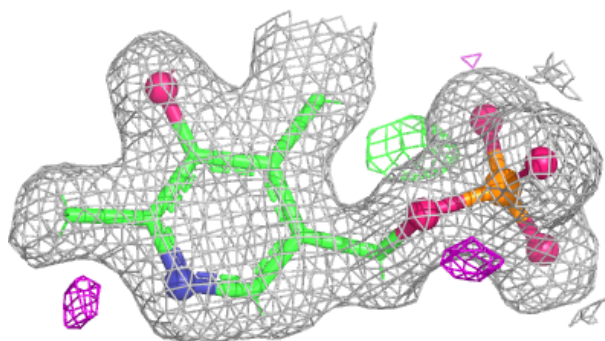
**Electron density around PLP A 703:**

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

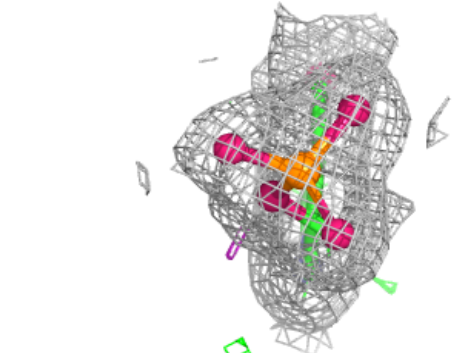
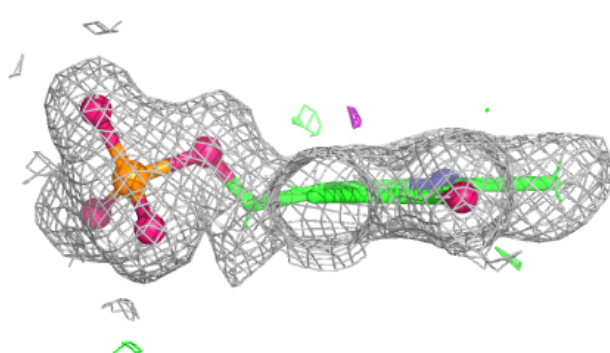
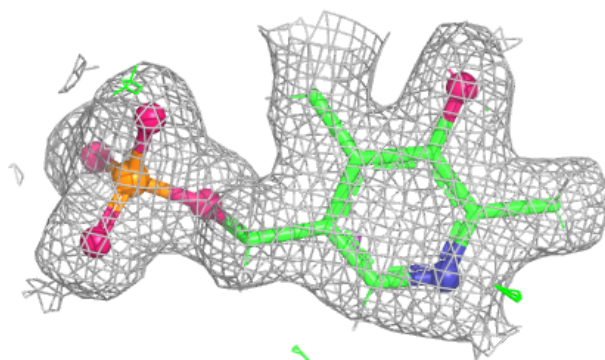


Electron density around PLP B 500:

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

**Electron density around PLP D 401:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.