wwPDB X-ray Structure Validation Summary Report (i)

Mar 17, 2026 – 11:44 PM UTC

PDB ID	:	7TLP / pdb_00007tlp
Title	:	Structure of Atopobium parvulum SufS K235R
Authors	:	Karunakaran, G.; Couture, J.F.
Deposited on	:	2022-01-18
Resolution	:	2.99 Å(reported)

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

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

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

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

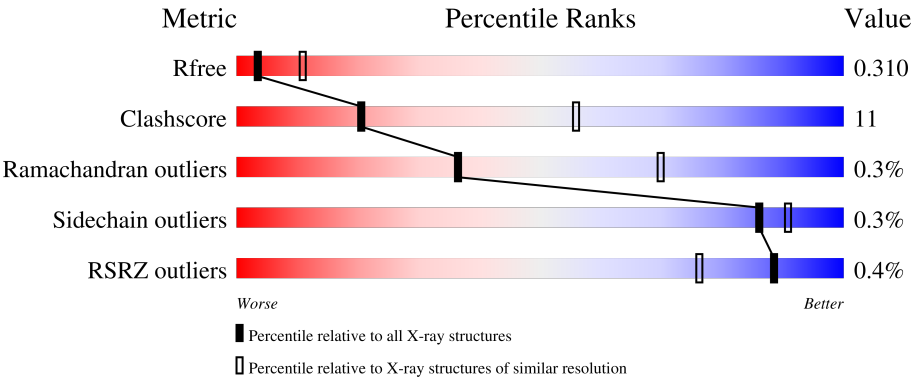
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

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

The reported resolution of this entry is 2.99 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	447	70% 17% 13%
1	B	447	70% 18% 12%
1	C	447	67% 21% 12%
1	D	447	74% 15% 11%
1	E	447	67% 21% 12%

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Mol	Chain	Length	Quality of chain
1	F	447	73% 15% 11%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PLG	A	501	-	-	X	-
2	PLG	D	501	-	X	-	-

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 16670 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 Cysteine desulfurase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	391	Total	C	N	O	S	0	3	0
			2708	1708	475	507	18			
1	B	393	Total	C	N	O	S	0	3	0
			2748	1743	477	511	17			
1	C	392	Total	C	N	O	S	0	3	0
			2741	1730	475	518	18			
1	D	398	Total	C	N	O	S	0	3	0
			2813	1787	491	517	18			
1	E	395	Total	C	N	O	S	0	2	0
			2785	1763	488	516	18			
1	F	396	Total	C	N	O	S	0	3	0
			2755	1748	478	512	17			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	initiating methionine	UNP C8W9P2
A	-16	ALA	-	expression tag	UNP C8W9P2
A	-15	SER	-	expression tag	UNP C8W9P2
A	-14	SER	-	expression tag	UNP C8W9P2
A	-13	HIS	-	expression tag	UNP C8W9P2
A	-12	HIS	-	expression tag	UNP C8W9P2
A	-11	HIS	-	expression tag	UNP C8W9P2
A	-10	HIS	-	expression tag	UNP C8W9P2
A	-9	HIS	-	expression tag	UNP C8W9P2
A	-8	HIS	-	expression tag	UNP C8W9P2
A	-7	HIS	-	expression tag	UNP C8W9P2
A	-6	GLU	-	expression tag	UNP C8W9P2
A	-5	ASN	-	expression tag	UNP C8W9P2
A	-4	LEU	-	expression tag	UNP C8W9P2
A	-3	TYR	-	expression tag	UNP C8W9P2
A	-2	PHE	-	expression tag	UNP C8W9P2
A	-1	GLN	-	expression tag	UNP C8W9P2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP C8W9P2
A	90	ALA	ASP	conflict	UNP C8W9P2
A	235	ARG	LYS	engineered mutation	UNP C8W9P2
B	-17	MET	-	initiating methionine	UNP C8W9P2
B	-16	ALA	-	expression tag	UNP C8W9P2
B	-15	SER	-	expression tag	UNP C8W9P2
B	-14	SER	-	expression tag	UNP C8W9P2
B	-13	HIS	-	expression tag	UNP C8W9P2
B	-12	HIS	-	expression tag	UNP C8W9P2
B	-11	HIS	-	expression tag	UNP C8W9P2
B	-10	HIS	-	expression tag	UNP C8W9P2
B	-9	HIS	-	expression tag	UNP C8W9P2
B	-8	HIS	-	expression tag	UNP C8W9P2
B	-7	HIS	-	expression tag	UNP C8W9P2
B	-6	GLU	-	expression tag	UNP C8W9P2
B	-5	ASN	-	expression tag	UNP C8W9P2
B	-4	LEU	-	expression tag	UNP C8W9P2
B	-3	TYR	-	expression tag	UNP C8W9P2
B	-2	PHE	-	expression tag	UNP C8W9P2
B	-1	GLN	-	expression tag	UNP C8W9P2
B	0	GLY	-	expression tag	UNP C8W9P2
B	90	ALA	ASP	conflict	UNP C8W9P2
B	235	ARG	LYS	engineered mutation	UNP C8W9P2
C	-17	MET	-	initiating methionine	UNP C8W9P2
C	-16	ALA	-	expression tag	UNP C8W9P2
C	-15	SER	-	expression tag	UNP C8W9P2
C	-14	SER	-	expression tag	UNP C8W9P2
C	-13	HIS	-	expression tag	UNP C8W9P2
C	-12	HIS	-	expression tag	UNP C8W9P2
C	-11	HIS	-	expression tag	UNP C8W9P2
C	-10	HIS	-	expression tag	UNP C8W9P2
C	-9	HIS	-	expression tag	UNP C8W9P2
C	-8	HIS	-	expression tag	UNP C8W9P2
C	-7	HIS	-	expression tag	UNP C8W9P2
C	-6	GLU	-	expression tag	UNP C8W9P2
C	-5	ASN	-	expression tag	UNP C8W9P2
C	-4	LEU	-	expression tag	UNP C8W9P2
C	-3	TYR	-	expression tag	UNP C8W9P2
C	-2	PHE	-	expression tag	UNP C8W9P2
C	-1	GLN	-	expression tag	UNP C8W9P2
C	0	GLY	-	expression tag	UNP C8W9P2
C	90	ALA	ASP	conflict	UNP C8W9P2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	235	ARG	LYS	engineered mutation	UNP C8W9P2
D	-17	MET	-	initiating methionine	UNP C8W9P2
D	-16	ALA	-	expression tag	UNP C8W9P2
D	-15	SER	-	expression tag	UNP C8W9P2
D	-14	SER	-	expression tag	UNP C8W9P2
D	-13	HIS	-	expression tag	UNP C8W9P2
D	-12	HIS	-	expression tag	UNP C8W9P2
D	-11	HIS	-	expression tag	UNP C8W9P2
D	-10	HIS	-	expression tag	UNP C8W9P2
D	-9	HIS	-	expression tag	UNP C8W9P2
D	-8	HIS	-	expression tag	UNP C8W9P2
D	-7	HIS	-	expression tag	UNP C8W9P2
D	-6	GLU	-	expression tag	UNP C8W9P2
D	-5	ASN	-	expression tag	UNP C8W9P2
D	-4	LEU	-	expression tag	UNP C8W9P2
D	-3	TYR	-	expression tag	UNP C8W9P2
D	-2	PHE	-	expression tag	UNP C8W9P2
D	-1	GLN	-	expression tag	UNP C8W9P2
D	0	GLY	-	expression tag	UNP C8W9P2
D	90	ALA	ASP	conflict	UNP C8W9P2
D	235	ARG	LYS	engineered mutation	UNP C8W9P2
E	-17	MET	-	initiating methionine	UNP C8W9P2
E	-16	ALA	-	expression tag	UNP C8W9P2
E	-15	SER	-	expression tag	UNP C8W9P2
E	-14	SER	-	expression tag	UNP C8W9P2
E	-13	HIS	-	expression tag	UNP C8W9P2
E	-12	HIS	-	expression tag	UNP C8W9P2
E	-11	HIS	-	expression tag	UNP C8W9P2
E	-10	HIS	-	expression tag	UNP C8W9P2
E	-9	HIS	-	expression tag	UNP C8W9P2
E	-8	HIS	-	expression tag	UNP C8W9P2
E	-7	HIS	-	expression tag	UNP C8W9P2
E	-6	GLU	-	expression tag	UNP C8W9P2
E	-5	ASN	-	expression tag	UNP C8W9P2
E	-4	LEU	-	expression tag	UNP C8W9P2
E	-3	TYR	-	expression tag	UNP C8W9P2
E	-2	PHE	-	expression tag	UNP C8W9P2
E	-1	GLN	-	expression tag	UNP C8W9P2
E	0	GLY	-	expression tag	UNP C8W9P2
E	90	ALA	ASP	conflict	UNP C8W9P2
E	235	ARG	LYS	engineered mutation	UNP C8W9P2
F	-17	MET	-	initiating methionine	UNP C8W9P2

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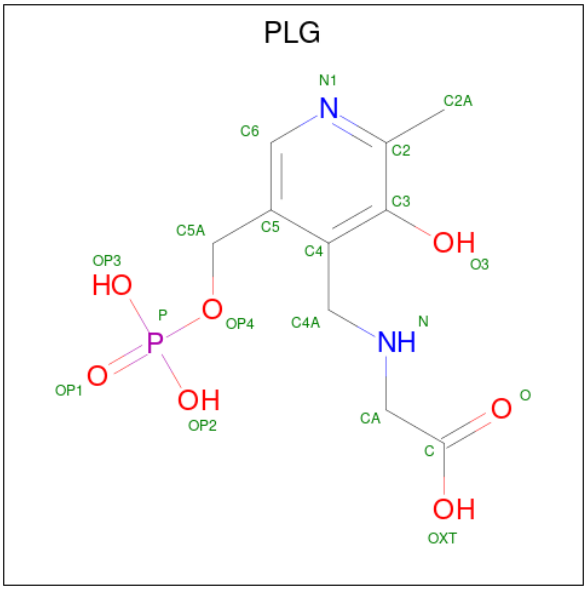
Chain	Residue	Modelled	Actual	Comment	Reference
F	-16	ALA	-	expression tag	UNP C8W9P2
F	-15	SER	-	expression tag	UNP C8W9P2
F	-14	SER	-	expression tag	UNP C8W9P2
F	-13	HIS	-	expression tag	UNP C8W9P2
F	-12	HIS	-	expression tag	UNP C8W9P2
F	-11	HIS	-	expression tag	UNP C8W9P2
F	-10	HIS	-	expression tag	UNP C8W9P2
F	-9	HIS	-	expression tag	UNP C8W9P2
F	-8	HIS	-	expression tag	UNP C8W9P2
F	-7	HIS	-	expression tag	UNP C8W9P2
F	-6	GLU	-	expression tag	UNP C8W9P2
F	-5	ASN	-	expression tag	UNP C8W9P2
F	-4	LEU	-	expression tag	UNP C8W9P2
F	-3	TYR	-	expression tag	UNP C8W9P2
F	-2	PHE	-	expression tag	UNP C8W9P2
F	-1	GLN	-	expression tag	UNP C8W9P2
F	0	GLY	-	expression tag	UNP C8W9P2
F	90	ALA	ASP	conflict	UNP C8W9P2
F	235	ARG	LYS	engineered mutation	UNP C8W9P2

- Molecule 2 is N-GLYCINE-[3-HYDROXY-2-METHYL-5-PHOSPHONOOXYMETHYL-PYRIDIN-4-YL-METHANE] (CCD ID: PLG) (formula: $C_{10}H_{15}N_2O_7P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	20	10	2	7	1	0	0

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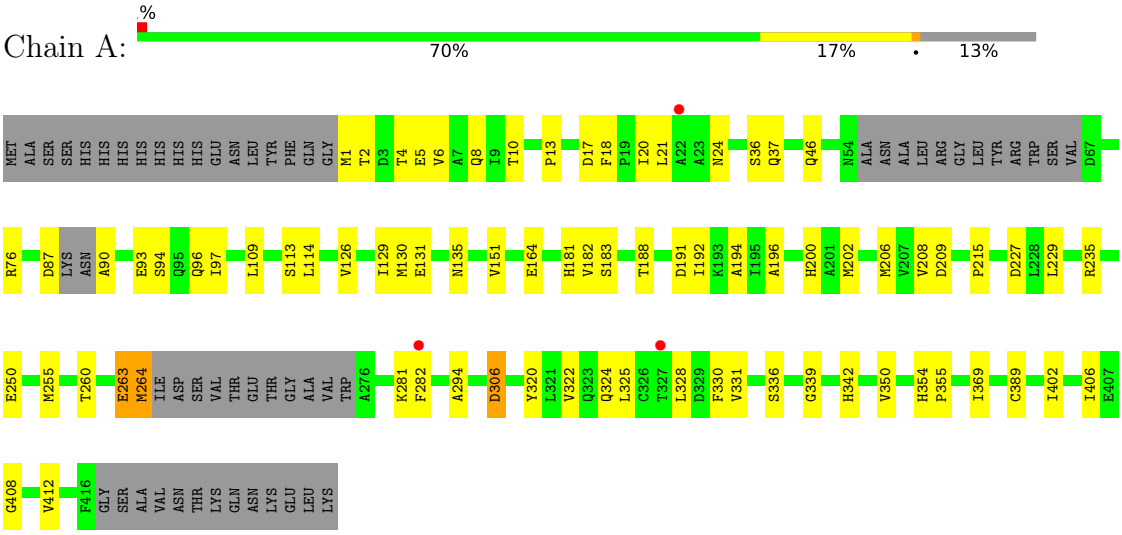
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			20	10	2	7	1		
2	C	1	Total	C	N	O	P	0	0
			20	10	2	7	1		
2	D	1	Total	C	N	O	P	0	0
			20	10	2	7	1		
2	E	1	Total	C	N	O	P	0	0
			20	10	2	7	1		
2	F	1	Total	C	N	O	P	0	0
			20	10	2	7	1		

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.

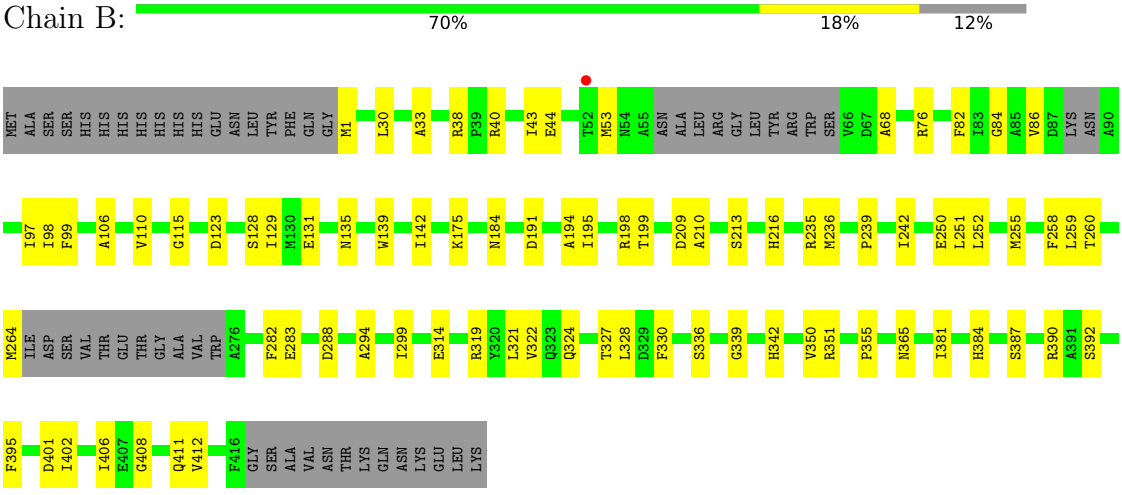
• Molecule 1: Cysteine desulfurase

Chain A:



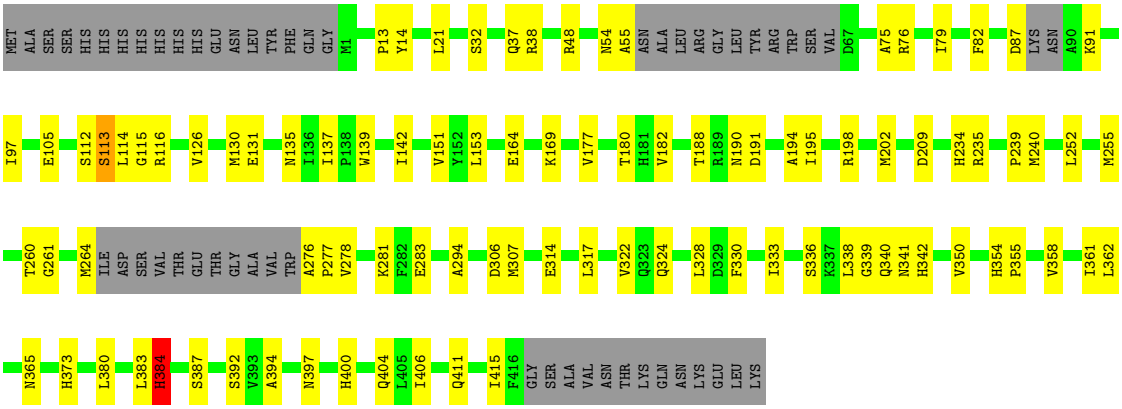
• Molecule 1: Cysteine desulfurase

Chain B:



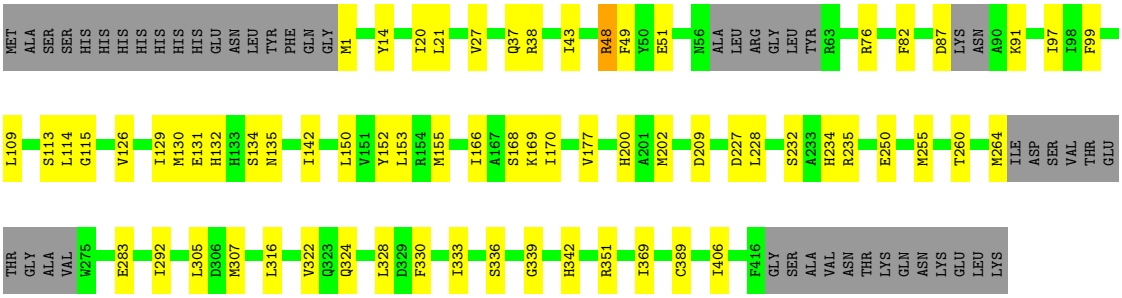
• Molecule 1: Cysteine desulfurase

Chain C:



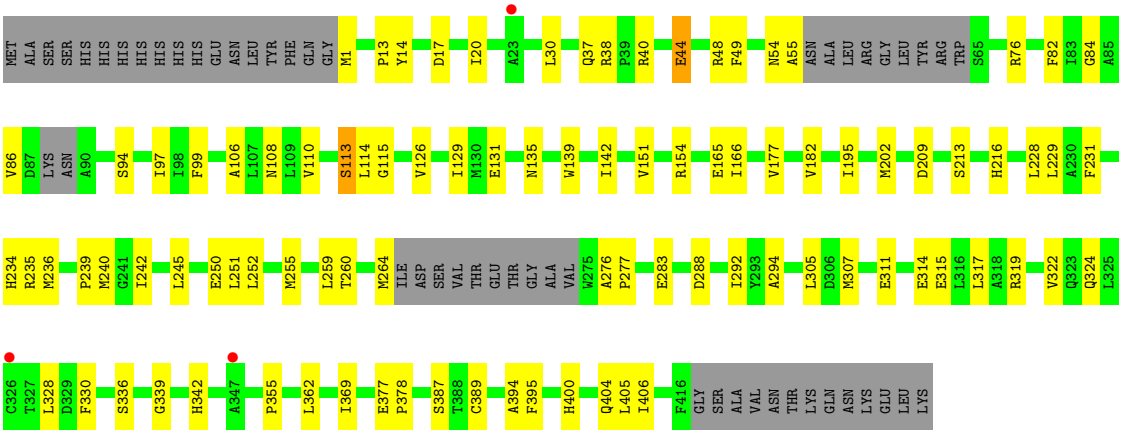
• Molecule 1: Cysteine desulfurase

Chain D:



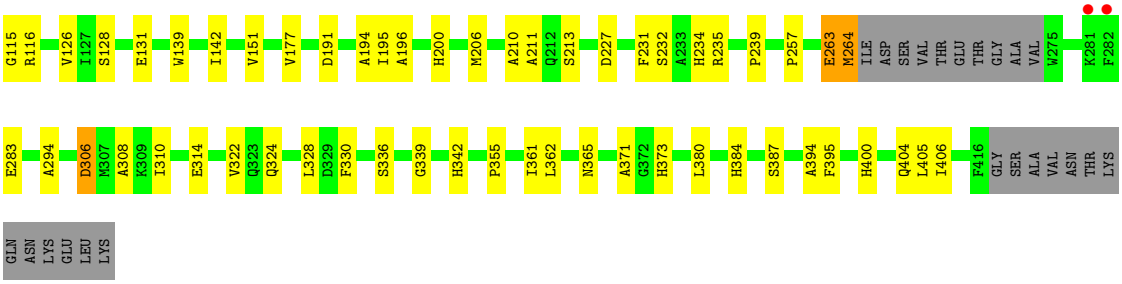
• Molecule 1: Cysteine desulfurase

Chain E:



• Molecule 1: Cysteine desulfurase

Chain F:


G115 R116 V126 I127 S128 E131 W139 I142 V151 V177 D191 A194 I195 A196 H200 M206 A210 A211 Q212 S213 D227 F231 S232 A233 H234 R235 P239 P257 E263 M264 ILE ASP SER VAL THR GLU THR GLY ALA VAL W275 K281 F282

E283 A294 D306 M307 A308 K309 I310 E314 V322 Q323 Q324 L328 D329 F330 S336 G339 H342 P355 I361 L362 N365 A371 G372 H373 L380 H384 S387 A394 F395 H400 Q404 L405 I406 F416 GLY SER ALA VAL ASN THR LYS

GLN ASN LYS GLU LEU LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	91.74Å 159.26Å 178.07Å 90.00° 90.16° 90.00°	Depositor
Resolution (Å)	38.86 – 2.99 38.86 – 2.99	Depositor EDS
% Data completeness (in resolution range)	96.3 (38.86-2.99) 95.6 (38.86-2.99)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.69 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.237 , 0.309 0.241 , 0.310	Depositor DCC
R_{free} test set	2009 reflections (3.89%)	wwPDB-VP
Wilson B-factor (Å^2)	68.8	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 84.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.55$, $< L^2 > = 0.39$	Xtriage
Estimated twinning fraction	0.448 for -1/2*h-1/2*k,-3/2*h+1/2*k,-l 0.450 for -1/2*h+1/2*k,3/2*h+1/2*k,-l 0.449 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.440 for 1/2*h+1/2*k,3/2*h-1/2*k,-l 0.457 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	16670	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.71% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: PLG

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	0.57	2/2769 (0.1%)	0.79	4/3797 (0.1%)
1	B	0.52	0/2810	0.71	0/3853
1	C	0.54	0/2801	0.75	3/3840 (0.1%)
1	D	0.53	0/2878	0.73	2/3944 (0.1%)
1	E	0.54	0/2844	0.76	3/3892 (0.1%)
1	F	0.52	0/2819	0.76	2/3870 (0.1%)
All	All	0.54	2/16921 (0.0%)	0.75	14/23196 (0.1%)

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	1
1	C	0	1
1	F	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	264	MET	CG-SD	5.84	1.95	1.80
1	A	264	MET	SD-CE	5.16	1.92	1.79

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	264	MET	N-CA-C	-11.75	78.09	111.00
1	A	264	MET	CA-CB-CG	-9.59	94.93	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	44	GLU	CB-CG-CD	-7.75	99.42	112.60
1	C	384	HIS	N-CA-CB	-7.43	100.91	112.13
1	A	264	MET	CG-SD-CE	-7.26	84.93	100.90

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	263	GLU	Peptide
1	C	384	HIS	Sidechain
1	F	263	GLU	Peptide

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	2708	0	2413	64	0
1	B	2748	0	2495	60	0
1	C	2741	0	2465	72	0
1	D	2813	0	2575	46	0
1	E	2785	0	2550	78	0
1	F	2755	0	2485	54	0
2	A	20	0	12	7	0
2	B	20	0	12	4	0
2	C	20	0	12	3	0
2	D	20	0	12	4	0
2	E	20	0	12	4	0
2	F	20	0	12	3	0
All	All	16670	0	15055	356	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 11.

The worst 5 of 356 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:E:40:ARG:NH1	1:E:44:GLU:OE2	1.88	1.07
1:A:260:THR:HG22	1:A:264:MET:HE1	1.37	1.06
1:E:1:MET:HG2	1:E:319:ARG:HH21	1.36	0.88
1:A:235:ARG:NH2	2:A:501:PLG:H4A2	1.90	0.87
1:E:324:GLN:HG2	1:E:406:ILE:HG13	1.56	0.86

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	386/447 (86%)	362 (94%)	22 (6%)	2 (0%)	24 60
1	B	388/447 (87%)	375 (97%)	13 (3%)	0	100 100
1	C	387/447 (87%)	376 (97%)	10 (3%)	1 (0%)	36 70
1	D	393/447 (88%)	377 (96%)	16 (4%)	0	100 100
1	E	389/447 (87%)	375 (96%)	14 (4%)	0	100 100
1	F	391/447 (88%)	377 (96%)	11 (3%)	3 (1%)	16 50
All	All	2334/2682 (87%)	2242 (96%)	86 (4%)	6 (0%)	36 70

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	65	SER
1	F	54	ASN
1	A	263	GLU
1	F	306	ASP
1	A	306	ASP

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	236/367 (64%)	236 (100%)	0	100 100
1	B	246/367 (67%)	246 (100%)	0	100 100
1	C	245/367 (67%)	243 (99%)	2 (1%)	73 86
1	D	254/367 (69%)	250 (98%)	4 (2%)	55 79
1	E	251/367 (68%)	249 (99%)	2 (1%)	73 86
1	F	246/367 (67%)	246 (100%)	0	100 100
All	All	1478/2202 (67%)	1470 (100%)	8 (0%)	86 89

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	113[B]	SER
1	E	113[A]	SER
1	D	168[A]	SER
1	D	113[B]	SER
1	D	168[B]	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	24	ASN
1	F	341	ASN
1	F	200	HIS
1	C	140	GLN
1	D	404	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	PLG	B	501	-	20,20,20	4.03	9 (45%)	26,28,28	1.96	9 (34%)
2	PLG	F	501	-	20,20,20	4.10	9 (45%)	26,28,28	1.76	5 (19%)
2	PLG	C	501	-	20,20,20	4.03	9 (45%)	26,28,28	1.81	7 (26%)
2	PLG	E	501	-	20,20,20	4.08	8 (40%)	26,28,28	2.03	8 (30%)
2	PLG	D	501	-	20,20,20	4.22	10 (50%)	26,28,28	1.97	10 (38%)
2	PLG	A	501	-	20,20,20	4.14	8 (40%)	26,28,28	1.66	7 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLG	B	501	-	-	5/12/12/12	0/1/1/1
2	PLG	F	501	-	-	4/12/12/12	0/1/1/1
2	PLG	C	501	-	-	5/12/12/12	0/1/1/1
2	PLG	E	501	-	-	4/12/12/12	0/1/1/1
2	PLG	D	501	-	-	5/12/12/12	0/1/1/1
2	PLG	A	501	-	-	5/12/12/12	0/1/1/1

The worst 5 of 53 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	PLG	C2-N1	9.14	1.50	1.33
2	D	501	PLG	C2-N1	8.92	1.49	1.33
2	A	501	PLG	C3-C2	-8.89	1.31	1.41
2	E	501	PLG	C3-C2	-8.73	1.31	1.41
2	D	501	PLG	C3-C2	-8.61	1.32	1.41

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	PLG	OP3-P-OP4	5.35	120.61	106.67
2	E	501	PLG	C4A-N-CA	-5.10	106.78	112.72
2	C	501	PLG	OP4-P-OP1	5.01	119.98	106.44
2	D	501	PLG	OP4-P-OP1	4.68	119.08	106.44
2	E	501	PLG	OP2-P-OP4	4.63	118.74	106.67

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	PLG	C5-C4-C4A-N
2	B	501	PLG	C5-C4-C4A-N
2	C	501	PLG	C5-C4-C4A-N
2	D	501	PLG	C5-C4-C4A-N
2	E	501	PLG	C5-C4-C4A-N

There are no ring outliers.

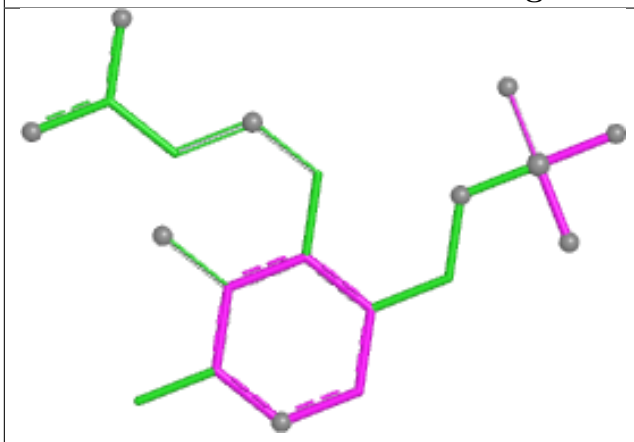
6 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	PLG	4	0
2	F	501	PLG	3	0
2	C	501	PLG	3	0
2	E	501	PLG	4	0
2	D	501	PLG	4	0
2	A	501	PLG	7	0

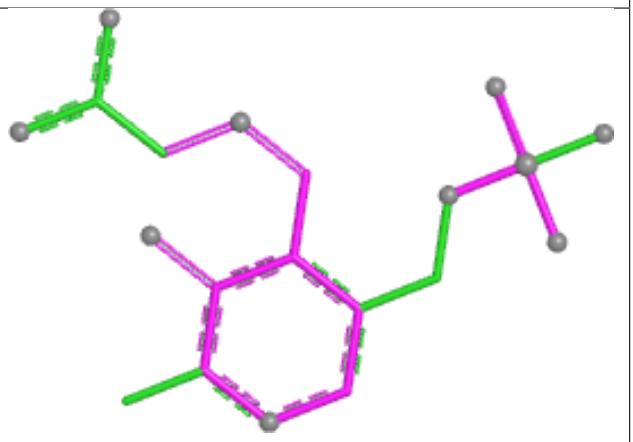
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

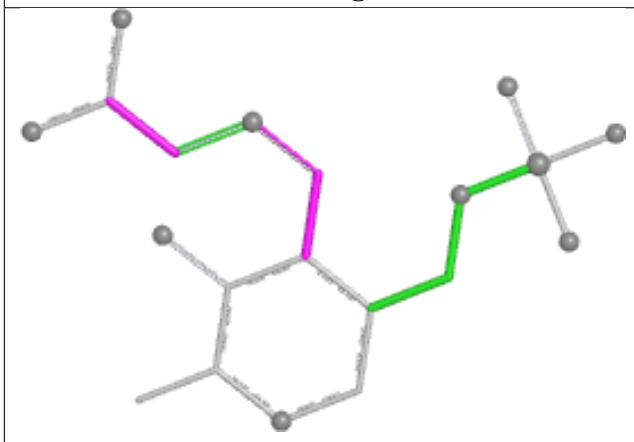
Ligand PLG B 501



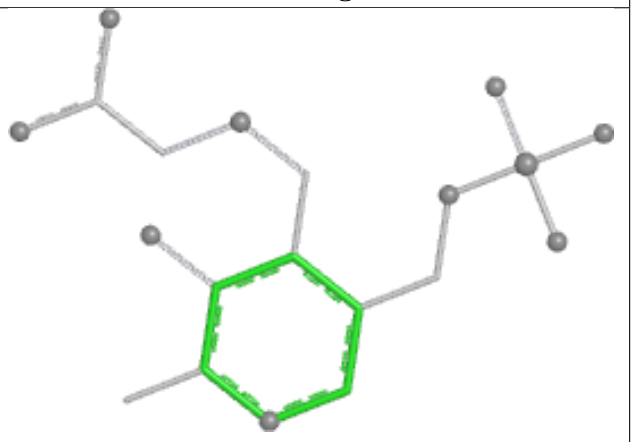
Bond lengths



Bond angles

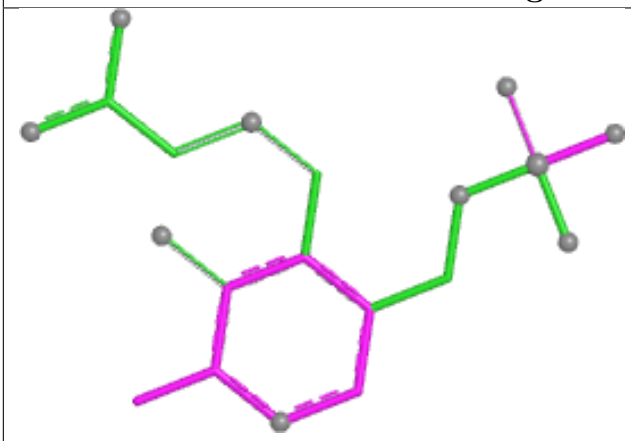


Torsions

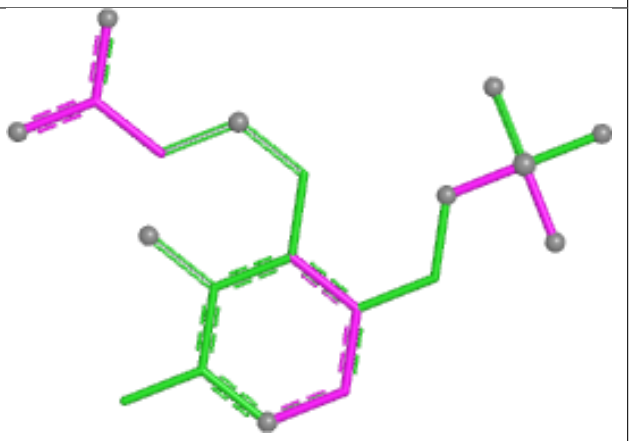


Rings

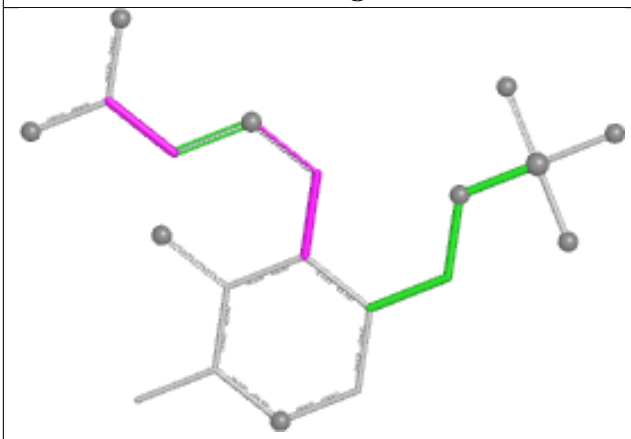
Ligand PLG F 501



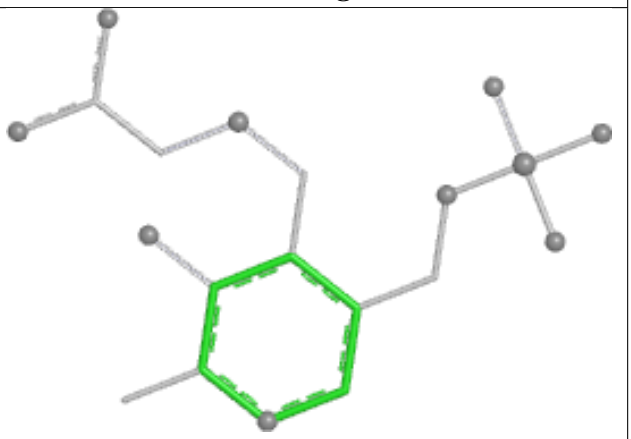
Bond lengths



Bond angles

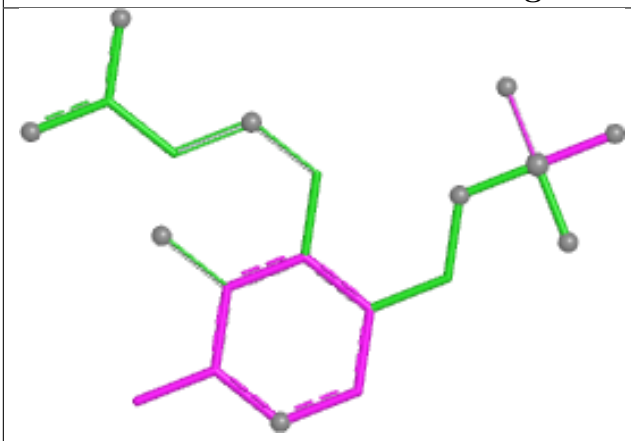


Torsions

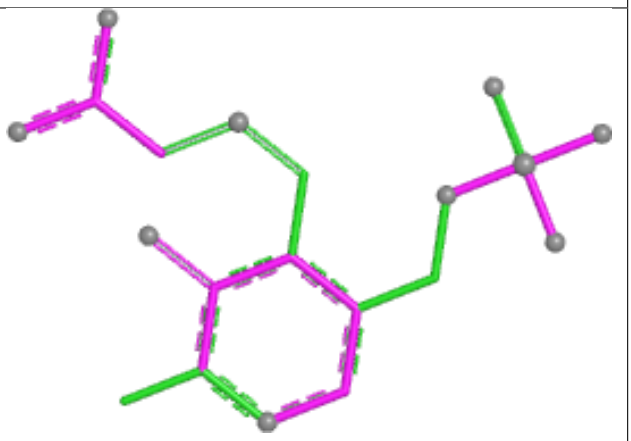


Rings

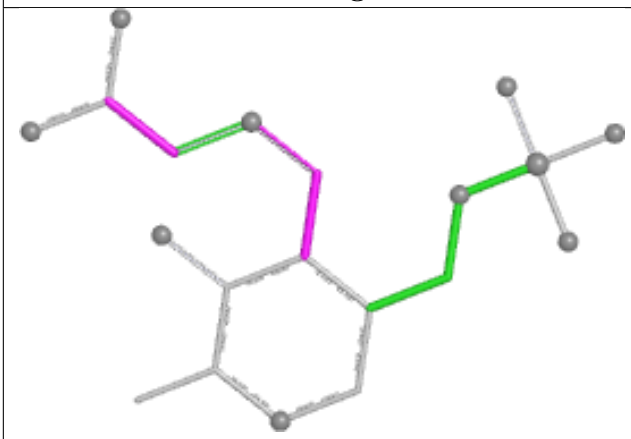
Ligand PLG C 501



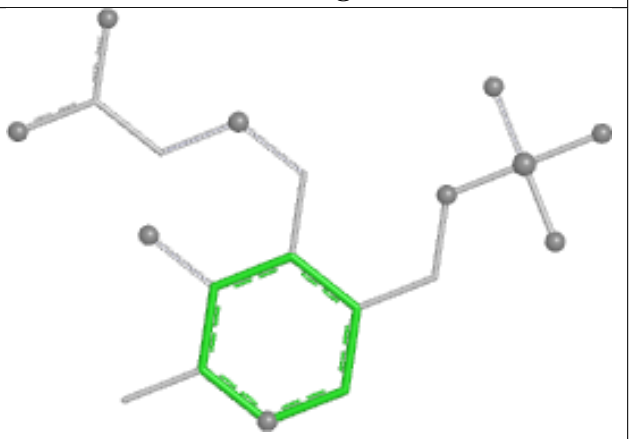
Bond lengths



Bond angles

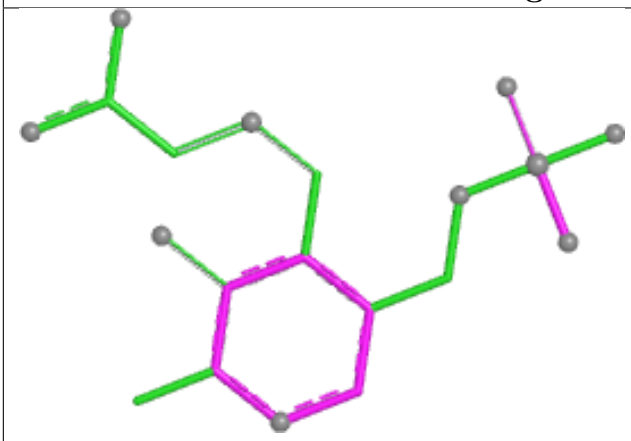


Torsions

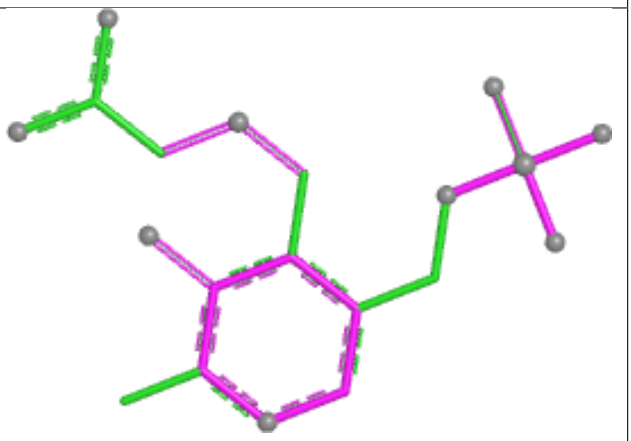


Rings

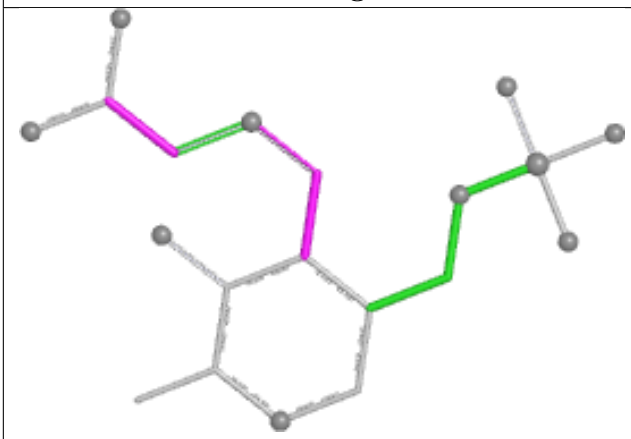
Ligand PLG E 501



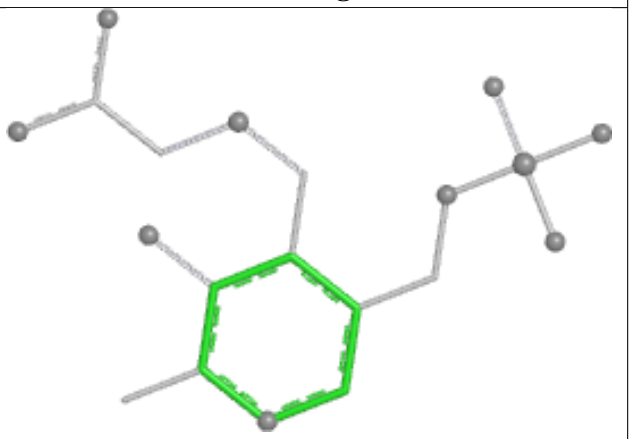
Bond lengths



Bond angles

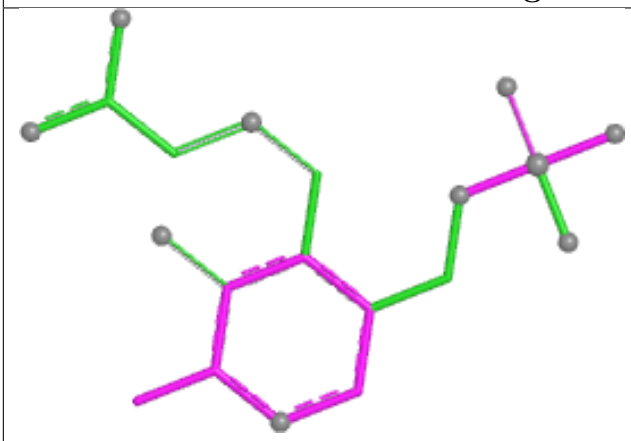


Torsions

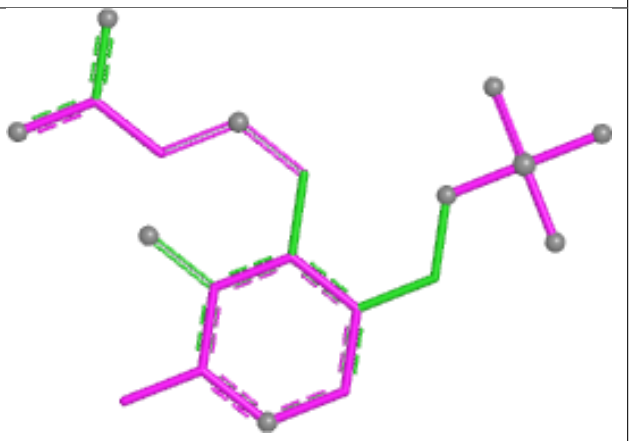


Rings

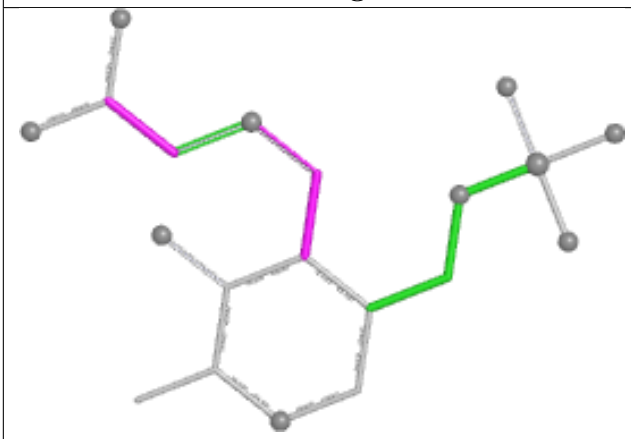
Ligand PLG D 501



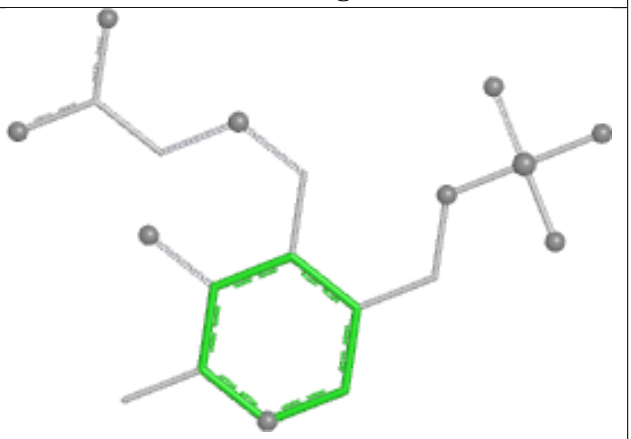
Bond lengths



Bond angles

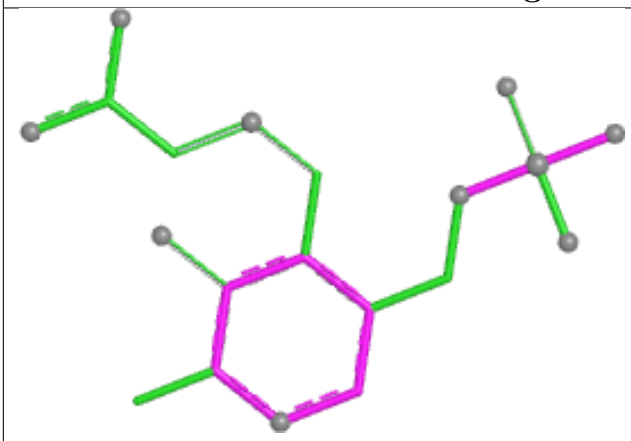


Torsions

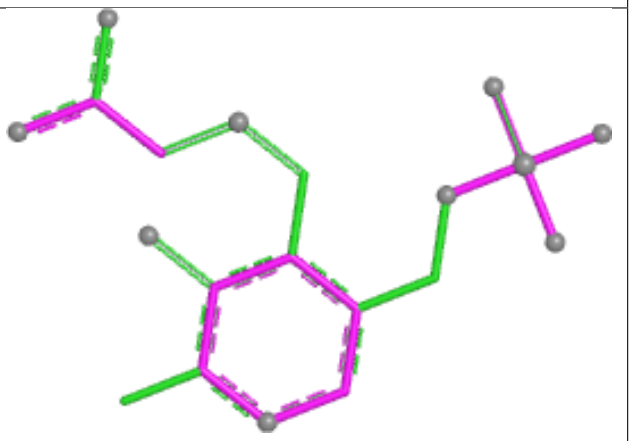


Rings

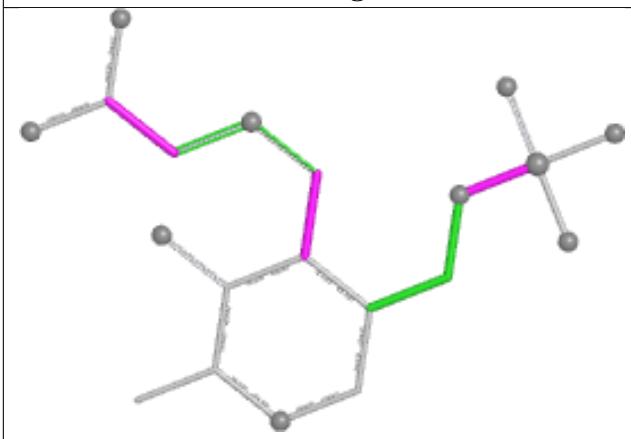
Ligand PLG A 501



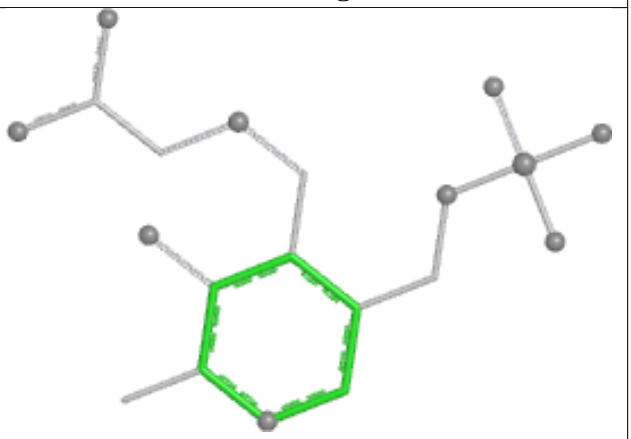
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	391/447 (87%)	-0.50	3 (0%)	82	64	36, 59, 73, 96	3 (0%)
1	B	393/447 (87%)	-0.57	1 (0%)	90	79	38, 58, 77, 101	3 (0%)
1	C	392/447 (87%)	-0.50	0	100	100	38, 61, 78, 104	3 (0%)
1	D	398/447 (89%)	-0.56	0	100	100	38, 61, 78, 92	3 (0%)
1	E	395/447 (88%)	-0.52	3 (0%)	82	64	38, 60, 74, 93	2 (0%)
1	F	396/447 (88%)	-0.50	2 (0%)	87	72	39, 61, 80, 118	3 (0%)
All	All	2365/2682 (88%)	-0.53	9 (0%)	88	76	36, 60, 77, 118	17 (0%)

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	326	CYS	3.4
1	E	347	ALA	2.9
1	F	282	PHE	2.8
1	F	281	LYS	2.7
1	A	22	ALA	2.6

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 (i)

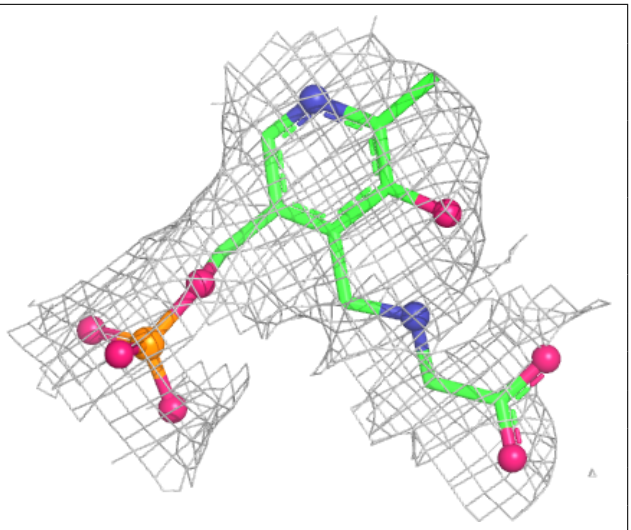
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

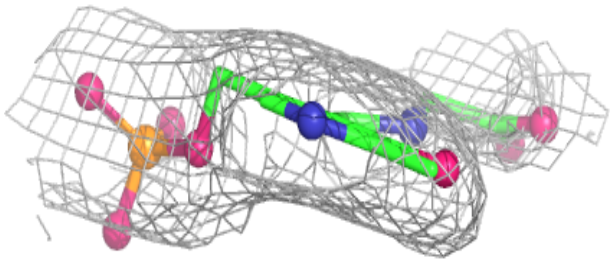
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PLG	A	501	20/20	0.98	0.06	51,53,54,56	0
2	PLG	B	501	20/20	0.98	0.07	50,53,54,54	0
2	PLG	D	501	20/20	0.98	0.07	53,54,55,56	0
2	PLG	E	501	20/20	0.98	0.06	54,55,57,57	0
2	PLG	F	501	20/20	0.98	0.06	55,57,60,62	0
2	PLG	C	501	20/20	0.99	0.05	54,56,58,60	0

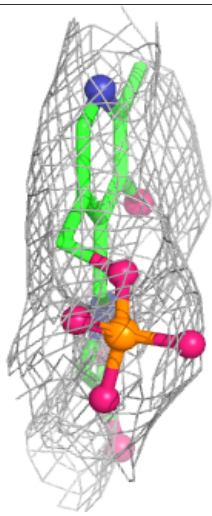
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PLG A 501:

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

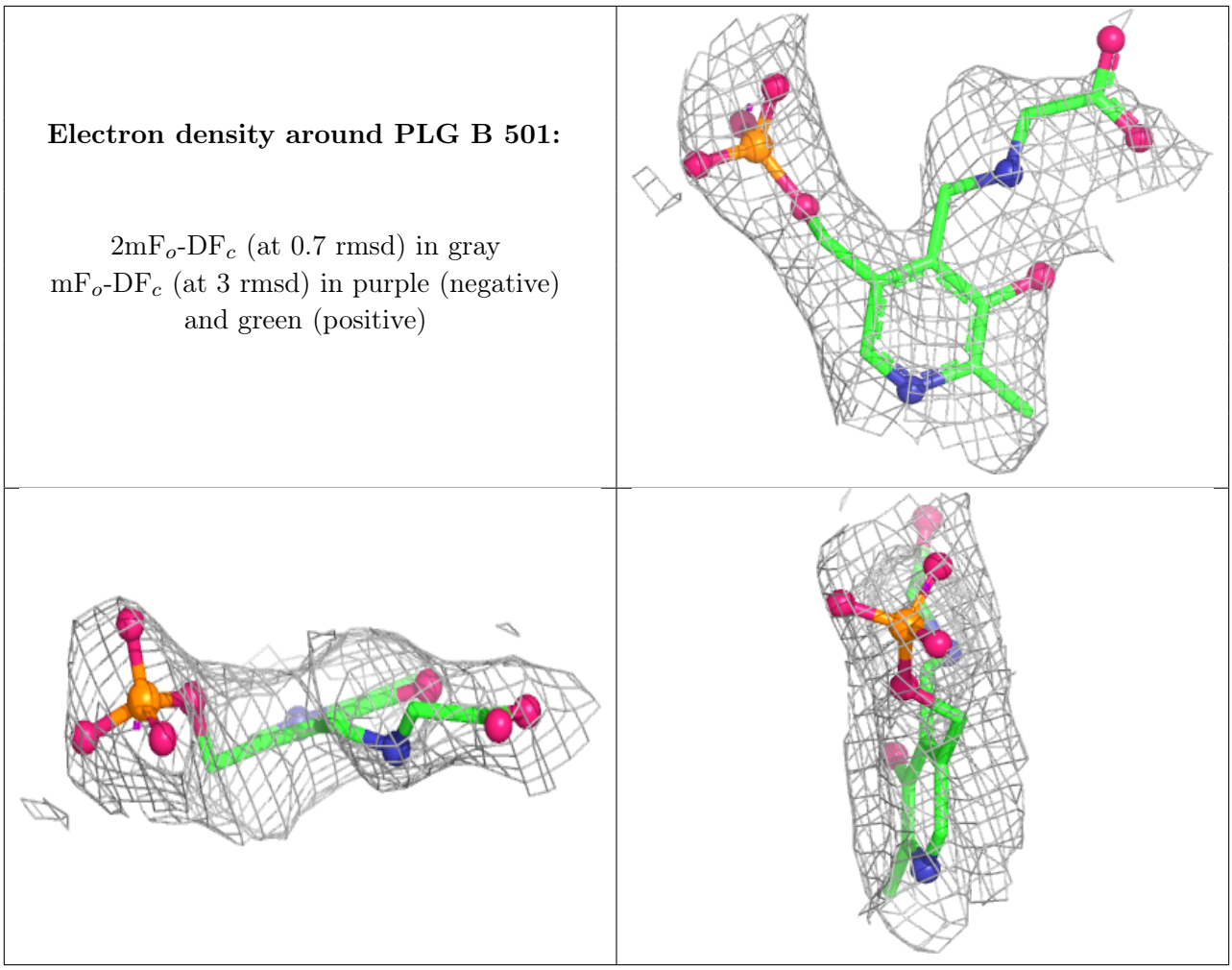






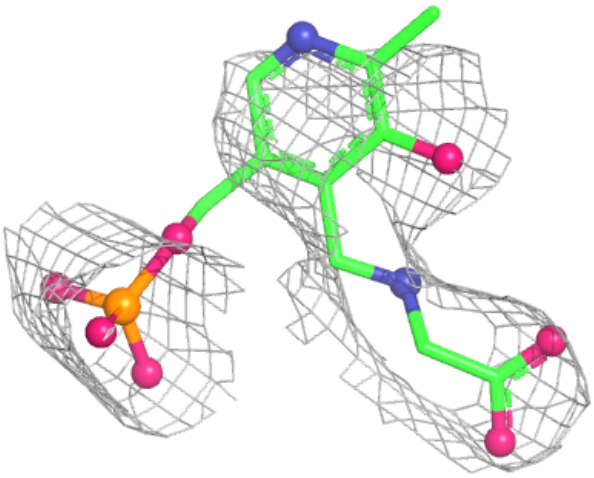
Electron density around PLG B 501:

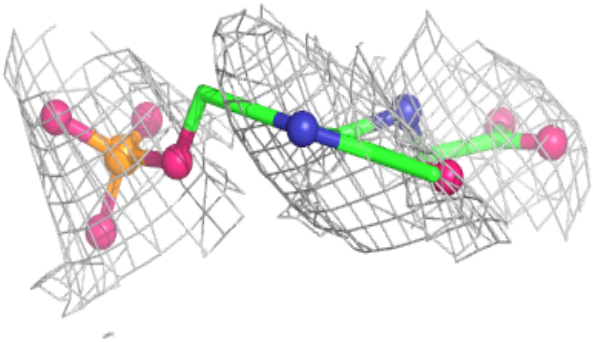
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around PLG D 501:

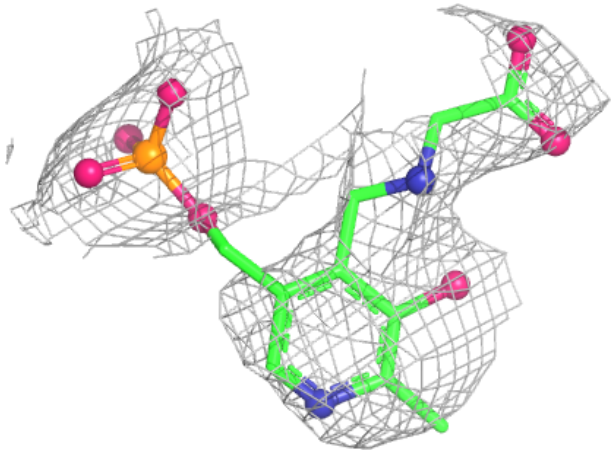
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

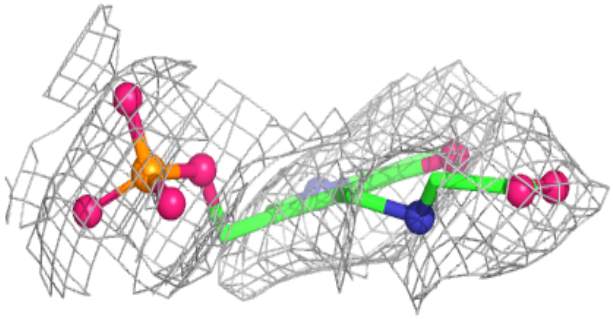


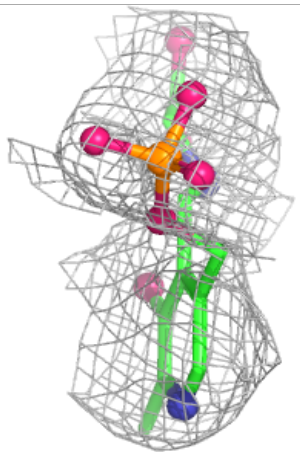


Electron density around PLG E 501:

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

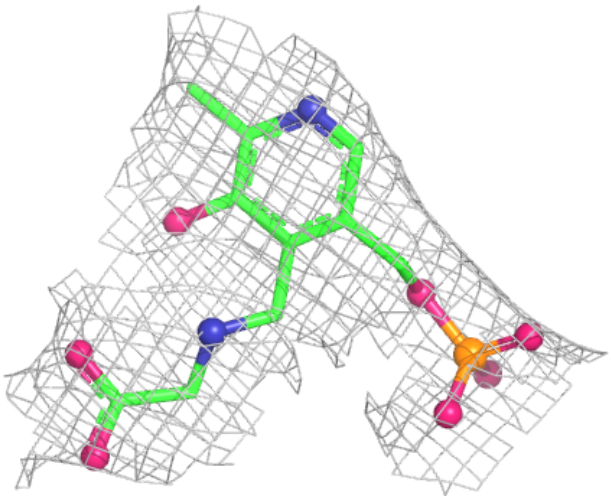


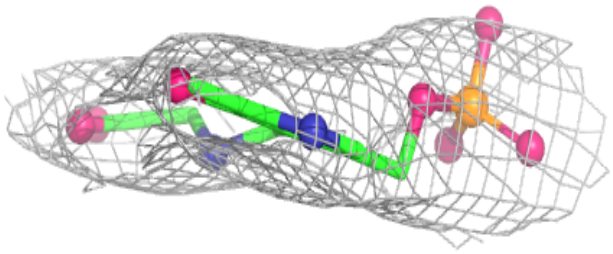


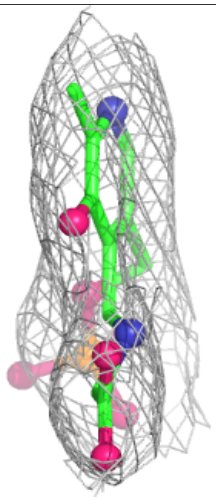


Electron density around PLG F 501:

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

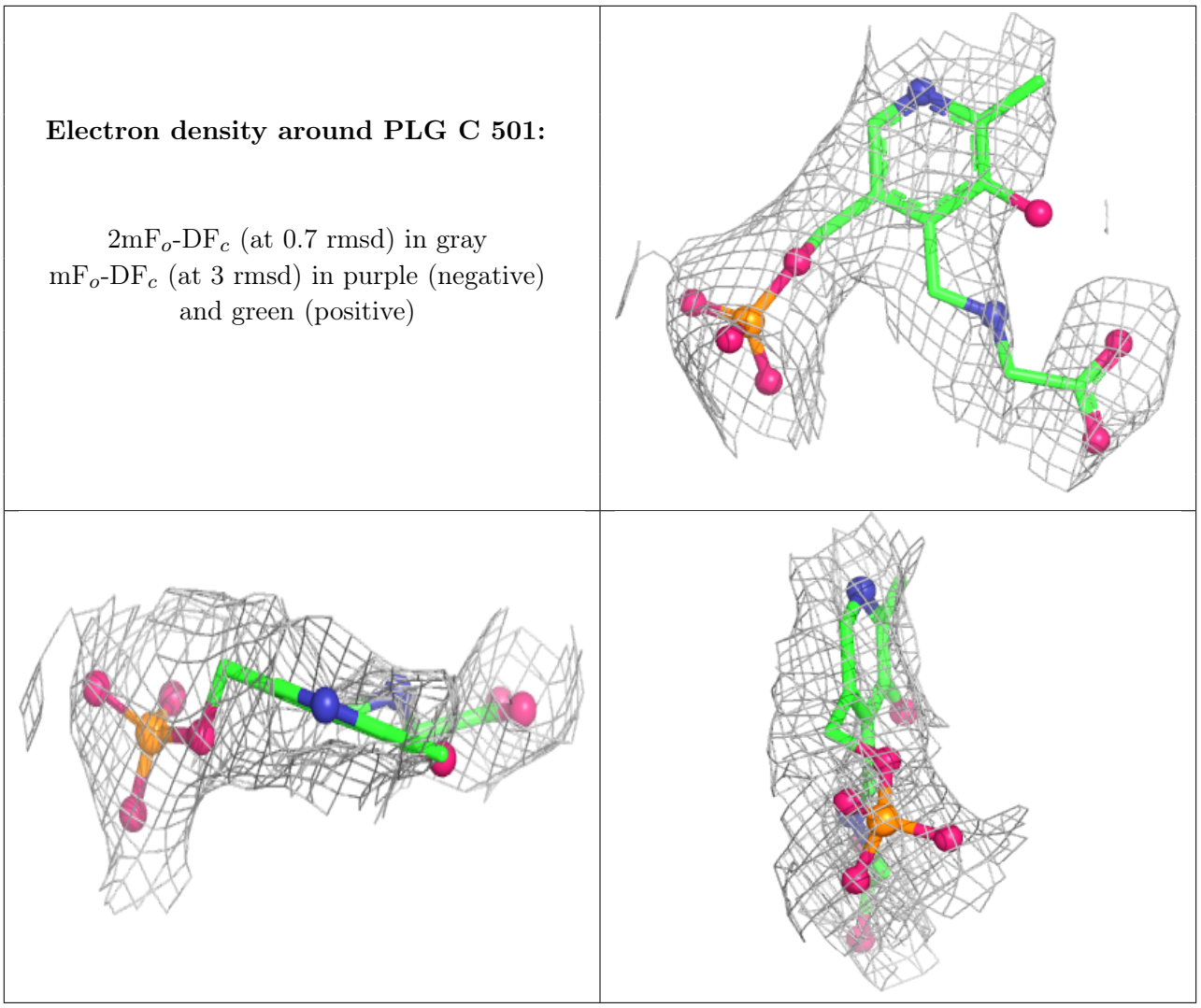






Electron density around PLG C 501:

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



6.5 Other polymers

There are no such residues in this entry.