



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 09:56 AM EDT

PDB ID : 6AMH / pdb_00006amh
Title : Engineered tryptophan synthase b-subunit from *Pyrococcus furiosus*, PfTrpB4D11 with Ser bound as E(Aex1)
Authors : Buller, A.R.
Deposited on : 2017-08-09
Resolution : 1.63 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

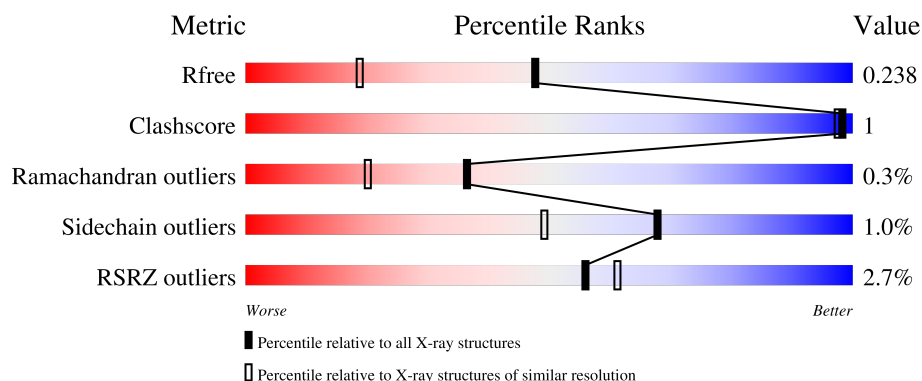
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.63 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	1141 (1.64-1.64)
Clashscore	190562	1171 (1.64-1.64)
Ramachandran outliers	187476	1151 (1.64-1.64)
Sidechain outliers	187428	1150 (1.64-1.64)
RSRZ outliers	180081	1141 (1.64-1.64)

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	396	2% 94% ..
1	B	396	5% 96% ..
1	C	396	3% 96% ..
1	D	396	0% 95% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12380 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 Tryptophan synthase beta chain 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	388	Total	C	N	O	S	0	1	0
			2930	1868	507	543	12			
1	B	391	Total	C	N	O	S	0	0	0
			2948	1880	515	541	12			
1	C	385	Total	C	N	O	S	0	1	0
			2915	1859	503	541	12			
1	D	385	Total	C	N	O	S	0	1	0
			2918	1862	505	539	12			

There are 52 discrepancies between the modelled and reference sequences:

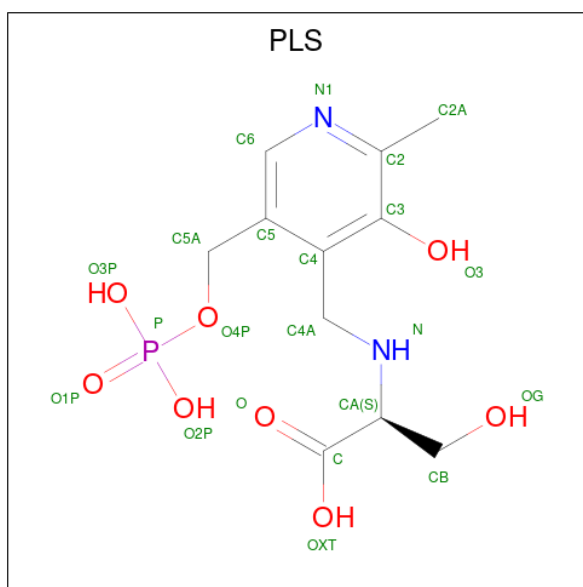
Chain	Residue	Modelled	Actual	Comment	Reference
A	17	GLY	GLU	engineered mutation	UNP Q8U093
A	68	VAL	ILE	engineered mutation	UNP Q8U093
A	274	SER	PHE	engineered mutation	UNP Q8U093
A	292	SER	THR	engineered mutation	UNP Q8U093
A	321	ALA	THR	engineered mutation	UNP Q8U093
A	389	LEU	-	expression tag	UNP Q8U093
A	390	GLU	-	expression tag	UNP Q8U093
A	391	HIS	-	expression tag	UNP Q8U093
A	392	HIS	-	expression tag	UNP Q8U093
A	393	HIS	-	expression tag	UNP Q8U093
A	394	HIS	-	expression tag	UNP Q8U093
A	395	HIS	-	expression tag	UNP Q8U093
A	396	HIS	-	expression tag	UNP Q8U093
B	17	GLY	GLU	engineered mutation	UNP Q8U093
B	68	VAL	ILE	engineered mutation	UNP Q8U093
B	274	SER	PHE	engineered mutation	UNP Q8U093
B	292	SER	THR	engineered mutation	UNP Q8U093
B	321	ALA	THR	engineered mutation	UNP Q8U093
B	389	LEU	-	expression tag	UNP Q8U093
B	390	GLU	-	expression tag	UNP Q8U093
B	391	HIS	-	expression tag	UNP Q8U093

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Chain	Residue	Modelled	Actual	Comment	Reference
B	392	HIS	-	expression tag	UNP Q8U093
B	393	HIS	-	expression tag	UNP Q8U093
B	394	HIS	-	expression tag	UNP Q8U093
B	395	HIS	-	expression tag	UNP Q8U093
B	396	HIS	-	expression tag	UNP Q8U093
C	17	GLY	GLU	engineered mutation	UNP Q8U093
C	68	VAL	ILE	engineered mutation	UNP Q8U093
C	274	SER	PHE	engineered mutation	UNP Q8U093
C	292	SER	THR	engineered mutation	UNP Q8U093
C	321	ALA	THR	engineered mutation	UNP Q8U093
C	389	LEU	-	expression tag	UNP Q8U093
C	390	GLU	-	expression tag	UNP Q8U093
C	391	HIS	-	expression tag	UNP Q8U093
C	392	HIS	-	expression tag	UNP Q8U093
C	393	HIS	-	expression tag	UNP Q8U093
C	394	HIS	-	expression tag	UNP Q8U093
C	395	HIS	-	expression tag	UNP Q8U093
C	396	HIS	-	expression tag	UNP Q8U093
D	17	GLY	GLU	engineered mutation	UNP Q8U093
D	68	VAL	ILE	engineered mutation	UNP Q8U093
D	274	SER	PHE	engineered mutation	UNP Q8U093
D	292	SER	THR	engineered mutation	UNP Q8U093
D	321	ALA	THR	engineered mutation	UNP Q8U093
D	389	LEU	-	expression tag	UNP Q8U093
D	390	GLU	-	expression tag	UNP Q8U093
D	391	HIS	-	expression tag	UNP Q8U093
D	392	HIS	-	expression tag	UNP Q8U093
D	393	HIS	-	expression tag	UNP Q8U093
D	394	HIS	-	expression tag	UNP Q8U093
D	395	HIS	-	expression tag	UNP Q8U093
D	396	HIS	-	expression tag	UNP Q8U093

- Molecule 2 is [3-HYDROXY-2-METHYL-5-PHOSPHONOXYMETHYL-PYRIDIN-4-YLMETHYL]-SERINE (CCD ID: PLS) (formula: C₁₁H₁₇N₂O₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			22	11	2	8	1		
2	B	1	Total	C	N	O	P	0	0
			22	11	2	8	1		
2	C	1	Total	C	N	O	P	0	0
			22	11	2	8	1		
2	D	1	Total	C	N	O	P	0	0
			22	11	2	8	1		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		
3	B	1	Total	Na	0	0
			1	1		
3	C	1	Total	Na	0	0
			1	1		
3	D	1	Total	Na	0	0
			1	1		

- Molecule 4 is water.

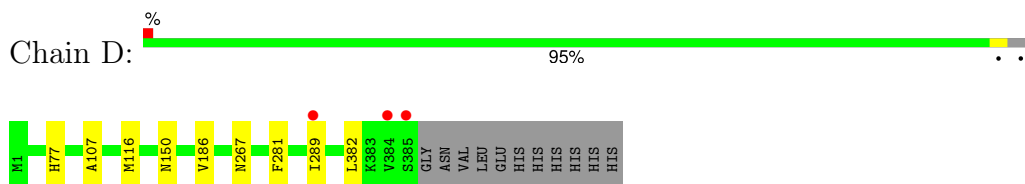
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	163	Total	O	0	0
			163	163		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	130	Total 130	O 130	0	0
4	C	142	Total 142	O 142	0	0
4	D	142	Total 142	O 142	0	0

- Molecule 1: Tryptophan synthase beta chain 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.76Å 109.60Å 160.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.63 40.00 – 1.63	Depositor EDS
% Data completeness (in resolution range)	99.2 (40.00-1.63) 99.2 (40.00-1.63)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 1.63Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.207 , 0.233 0.214 , 0.238	Depositor DCC
R_{free} test set	9239 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	26.0	Xtriage
Anisotropy	0.335	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 27.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12380	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.51	0/2991	0.80	1/4050 (0.0%)
1	B	0.51	0/3011	0.80	0/4078
1	C	0.52	0/2976	0.80	0/4029
1	D	0.51	0/2979	0.79	0/4032
All	All	0.51	0/11957	0.80	1/16189 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	SER	N-CA-C	5.72	117.32	111.14

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2930	0	2887	5	0
1	B	2948	0	2893	3	0
1	C	2915	0	2873	4	0
1	D	2918	0	2883	4	0
2	A	22	0	13	1	0
2	B	22	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	22	0	13	1	0
2	D	22	0	13	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	163	0	0	0	0
4	B	130	0	0	0	0
4	C	142	0	0	0	0
4	D	142	0	0	0	0
All	All	12380	0	11588	15	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 1.

All (15) 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:C:77:HIS:NE2	1:C:116:MET:HE3	2.28	0.48
1:D:281:PHE:HB3	1:D:289:ILE:HD12	1.95	0.47
1:C:77:HIS:CD2	1:C:116:MET:CE	2.98	0.46
1:B:77:HIS:NE2	1:B:116:MET:HE3	2.30	0.46
1:C:139:MET:HE1	1:D:382:LEU:HD22	1.98	0.46
1:A:77:HIS:NE2	1:A:116:MET:HE2	2.30	0.46
1:A:298:GLY:O	2:A:401:PLS:H4A2	2.16	0.45
1:C:298:GLY:O	2:C:401:PLS:H4A2	2.16	0.45
1:B:77:HIS:CD2	1:B:116:MET:HE3	2.51	0.45
1:D:107:ALA:H	2:D:401:PLS:HOG	1.65	0.44
1:A:170:ARG:O	1:A:173:VAL:HG12	2.19	0.42
1:A:264:ALA:HB1	1:A:267:ASN:HB2	2.01	0.42
1:A:351:ALA:HA	1:A:354:MET:HE2	2.02	0.41
1:D:77:HIS:NE2	1:D:116:MET:HE3	2.35	0.41
1:B:211:ILE:HG21	1:B:219:PRO:HD3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	387/396 (98%)	379 (98%)	7 (2%)	1 (0%)	36	20
1	B	387/396 (98%)	379 (98%)	7 (2%)	1 (0%)	36	20
1	C	384/396 (97%)	374 (97%)	9 (2%)	1 (0%)	36	20
1	D	384/396 (97%)	378 (98%)	5 (1%)	1 (0%)	36	20
All	All	1542/1584 (97%)	1510 (98%)	28 (2%)	4 (0%)	36	20

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	186	VAL
1	C	186	VAL
1	D	186	VAL
1	A	186	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	292/314 (93%)	287 (98%)	5 (2%)	53	27
1	B	292/314 (93%)	288 (99%)	4 (1%)	59	35
1	C	291/314 (93%)	290 (100%)	1 (0%)	86	79
1	D	291/314 (93%)	289 (99%)	2 (1%)	76	62
All	All	1166/1256 (93%)	1154 (99%)	12 (1%)	68	49

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ARG
1	A	139	MET
1	A	145	LYS
1	A	170	ARG
1	A	322	VAL
1	B	28	ARG
1	B	267	ASN
1	B	322	VAL
1	B	361	SER
1	C	267	ASN
1	D	150	ASN
1	D	267	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	217	GLN
1	B	283	GLN
1	C	89	GLN
1	C	155	ASN
1	C	231	ASN
1	C	369	ASN
1	D	89	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

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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
2	PLS	D	401	-	22,22,22	2.69	3 (13%)	28,31,31	1.39	6 (21%)
2	PLS	B	401	-	22,22,22	2.61	3 (13%)	28,31,31	1.34	4 (14%)
2	PLS	A	401	-	22,22,22	2.63	3 (13%)	28,31,31	1.30	3 (10%)
2	PLS	C	401	-	22,22,22	2.58	3 (13%)	28,31,31	1.28	3 (10%)

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	PLS	D	401	-	-	4/17/17/17	0/1/1/1
2	PLS	B	401	-	-	4/17/17/17	0/1/1/1
2	PLS	A	401	-	-	4/17/17/17	0/1/1/1
2	PLS	C	401	-	-	4/17/17/17	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	PLS	C3-C2	8.17	1.49	1.41
2	B	401	PLS	C3-C2	7.97	1.49	1.41
2	A	401	PLS	C3-C2	7.96	1.49	1.41
2	C	401	PLS	C3-C2	7.65	1.48	1.41
2	D	401	PLS	C5-C4	6.62	1.49	1.40
2	C	401	PLS	C5-C4	6.54	1.49	1.40
2	A	401	PLS	C5-C4	6.48	1.49	1.40
2	B	401	PLS	C5-C4	6.34	1.49	1.40
2	D	401	PLS	C3-C4	6.13	1.49	1.40
2	A	401	PLS	C3-C4	5.98	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	PLS	C3-C4	5.95	1.48	1.40
2	C	401	PLS	C3-C4	5.94	1.48	1.40

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	PLS	C4A-C4-C3	3.08	124.07	119.98
2	C	401	PLS	C4A-C4-C3	3.02	124.00	119.98
2	A	401	PLS	C4A-C4-C3	2.93	123.88	119.98
2	B	401	PLS	C4A-C4-C3	2.81	123.72	119.98
2	A	401	PLS	C6-N1-C2	2.48	123.69	119.20
2	B	401	PLS	C6-N1-C2	2.47	123.68	119.20
2	D	401	PLS	C4A-N-CA	2.45	118.45	113.84
2	C	401	PLS	C6-N1-C2	2.42	123.59	119.20
2	D	401	PLS	C6-N1-C2	2.36	123.47	119.20
2	D	401	PLS	C3-C4-C5	-2.35	116.60	118.73
2	B	401	PLS	C4A-N-CA	2.34	118.24	113.84
2	D	401	PLS	C6-C5-C4	2.28	119.79	118.06
2	C	401	PLS	C4A-N-CA	2.28	118.12	113.84
2	A	401	PLS	C4A-N-CA	2.26	118.09	113.84
2	D	401	PLS	O3-C3-C2	2.00	121.73	117.58
2	B	401	PLS	C6-C5-C4	2.00	119.57	118.06

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	PLS	C-CA-N-C4A
2	A	401	PLS	C5-C4-C4A-N
2	B	401	PLS	C-CA-N-C4A
2	B	401	PLS	C5-C4-C4A-N
2	C	401	PLS	C-CA-N-C4A
2	C	401	PLS	C5-C4-C4A-N
2	D	401	PLS	C-CA-N-C4A
2	D	401	PLS	C5-C4-C4A-N
2	A	401	PLS	C3-C4-C4A-N
2	B	401	PLS	C3-C4-C4A-N
2	C	401	PLS	C3-C4-C4A-N
2	D	401	PLS	C3-C4-C4A-N
2	A	401	PLS	CB-CA-N-C4A
2	B	401	PLS	CB-CA-N-C4A
2	C	401	PLS	CB-CA-N-C4A

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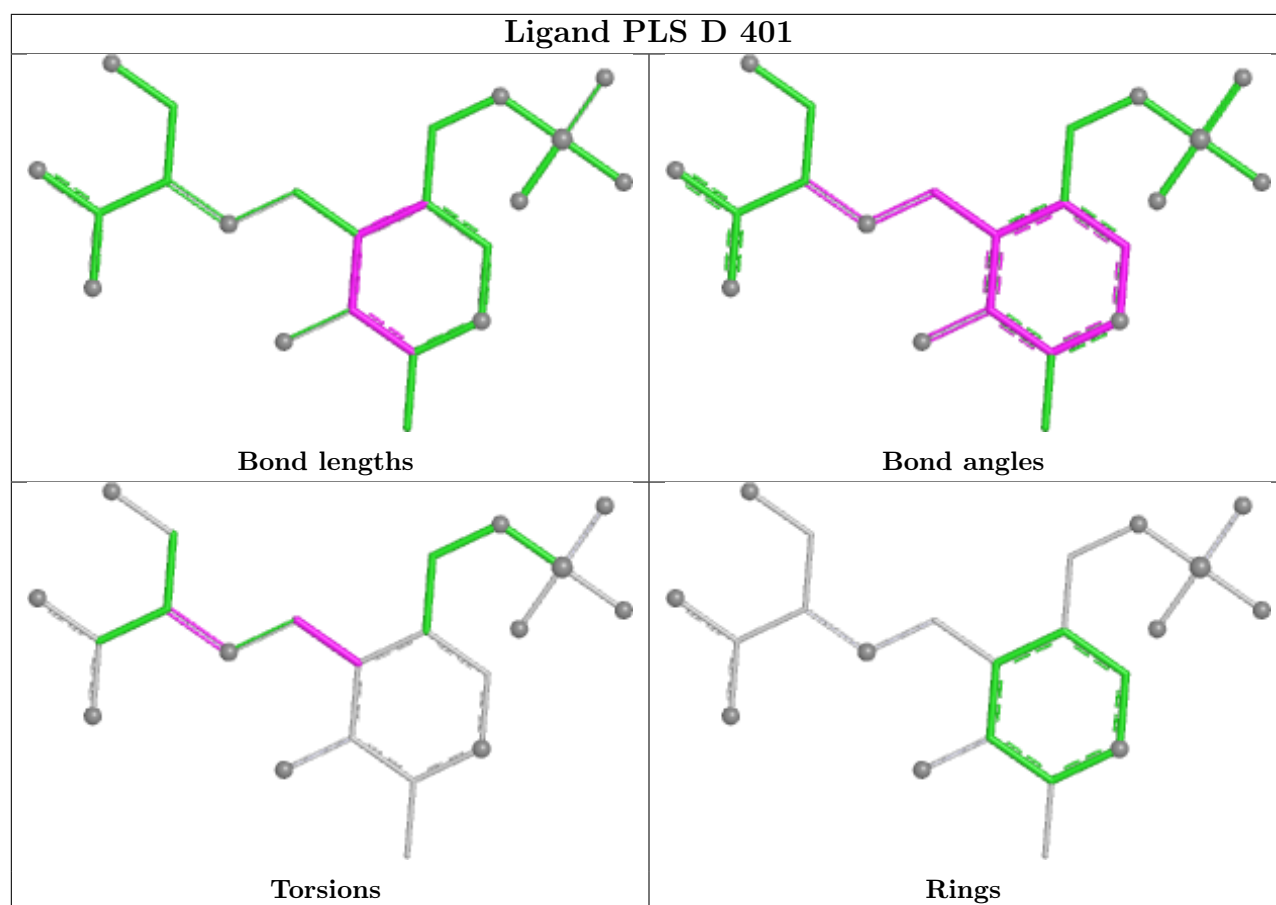
Mol	Chain	Res	Type	Atoms
2	D	401	PLS	CB-CA-N-C4A

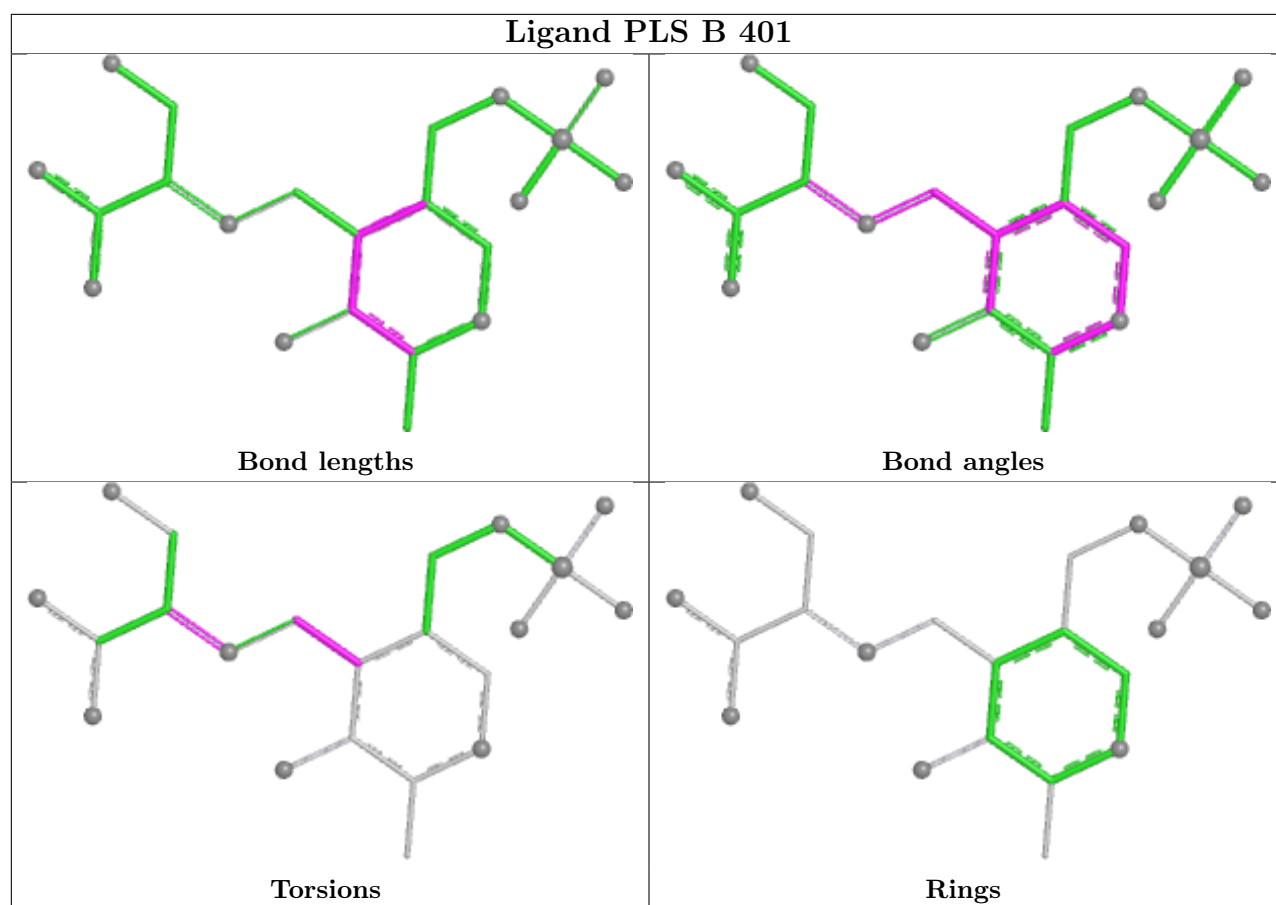
There are no ring outliers.

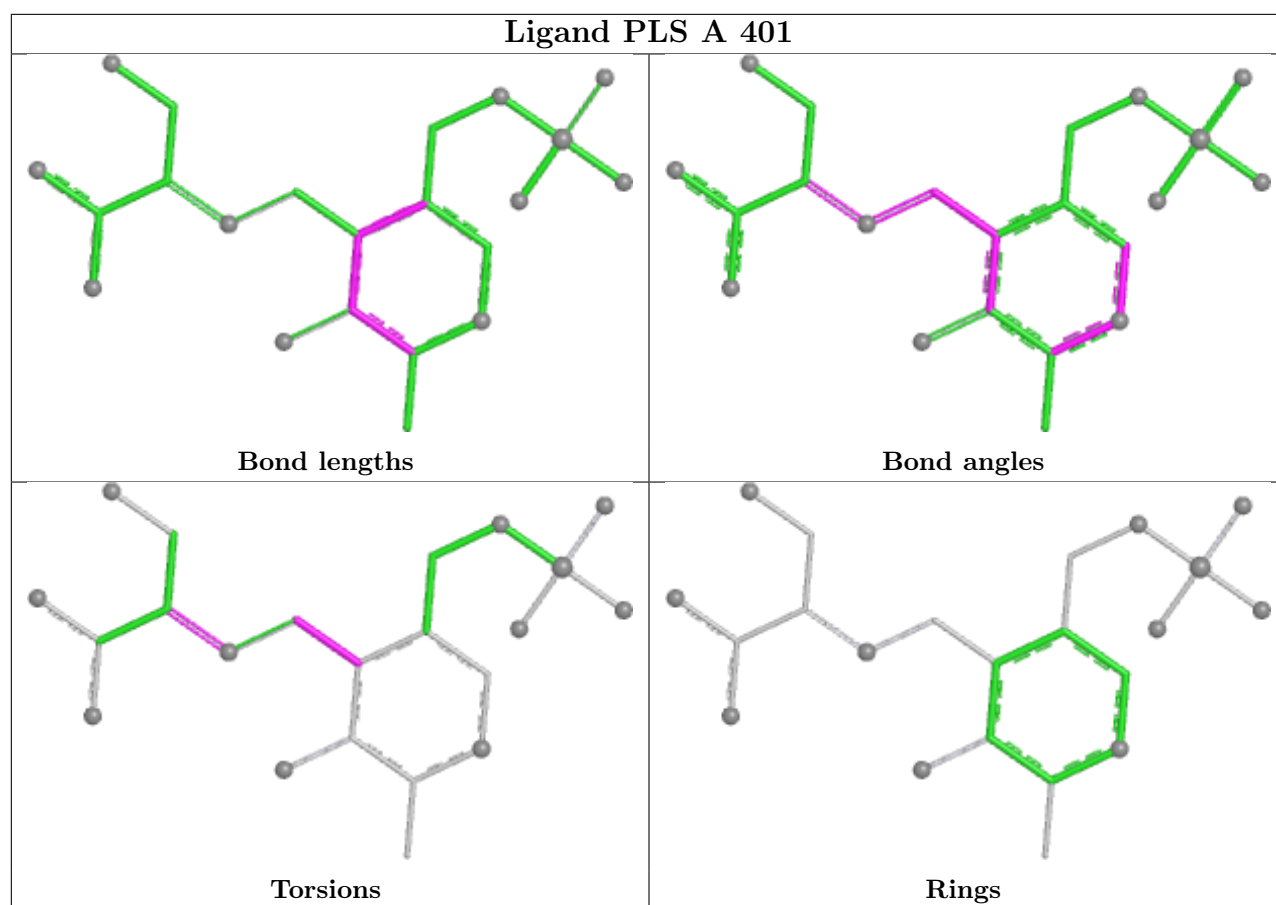
3 monomers are involved in 3 short contacts:

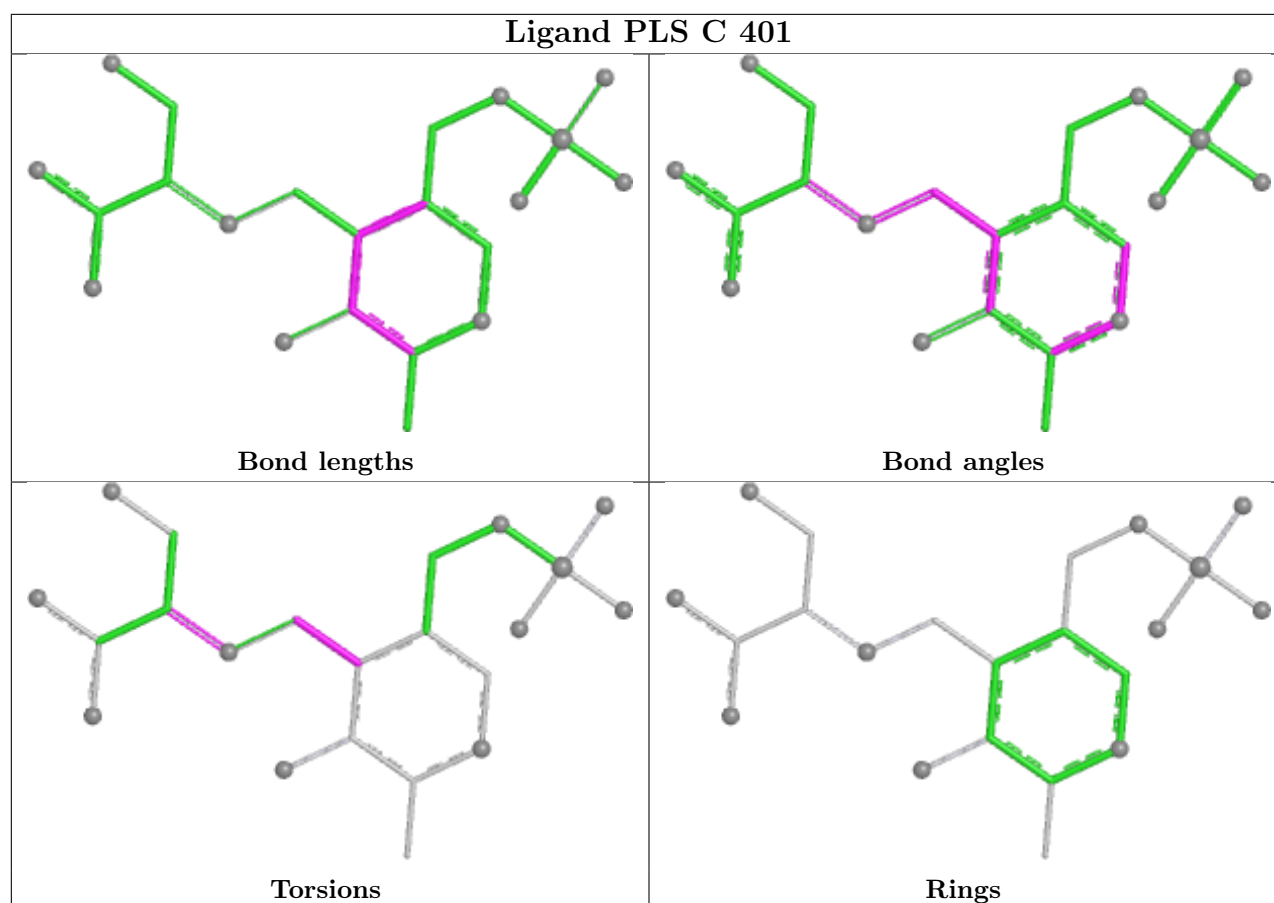
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	PLS	1	0
2	A	401	PLS	1	0
2	C	401	PLS	1	0

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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	388/396 (97%)	0.19	8 (2%) 63 70	17, 31, 49, 71	1 (0%)
1	B	391/396 (98%)	0.52	20 (5%) 33 38	20, 34, 61, 82	0
1	C	385/396 (97%)	0.35	11 (2%) 53 59	16, 31, 50, 78	1 (0%)
1	D	385/396 (97%)	0.32	3 (0%) 82 86	17, 34, 53, 66	1 (0%)
All	All	1549/1584 (97%)	0.35	42 (2%) 56 61	16, 32, 53, 82	3 (0%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	388	VAL	6.3
1	B	389	LEU	4.6
1	B	391	HIS	3.9
1	B	289	ILE	3.8
1	B	293	HIS	3.4
1	B	394	HIS	3.4
1	A	289	ILE	3.1
1	B	287	GLY	3.0
1	B	384	VAL	2.9
1	B	392	HIS	2.9
1	C	359	GLU	2.9
1	B	385	SER	2.9
1	C	289	ILE	2.8
1	B	393	HIS	2.8
1	A	388	VAL	2.7
1	B	291	PRO	2.7
1	D	384	VAL	2.7
1	C	212	LEU	2.6
1	B	282	LEU	2.5
1	C	385	SER	2.4
1	C	282	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	271	VAL	2.4
1	C	286	GLU	2.3
1	A	270	GLN	2.3
1	B	268	ALA	2.3
1	C	355	LYS	2.3
1	A	288	GLN	2.2
1	A	293[A]	HIS	2.2
1	C	292	SER	2.2
1	B	11	VAL	2.2
1	C	287	GLY	2.2
1	A	302	PRO	2.2
1	A	292	SER	2.2
1	A	285	GLU	2.1
1	B	17	GLY	2.1
1	C	269	GLY	2.1
1	B	13	GLU	2.1
1	B	390	GLU	2.1
1	B	14	THR	2.1
1	D	289	ILE	2.1
1	D	385	SER	2.1
1	C	384	VAL	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 [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($\text{\AA}^2$)	Q<0.9
3	NA	A	402	1/1	0.78	0.14	36,36,36,36	0
3	NA	C	402	1/1	0.84	0.12	31,31,31,31	0

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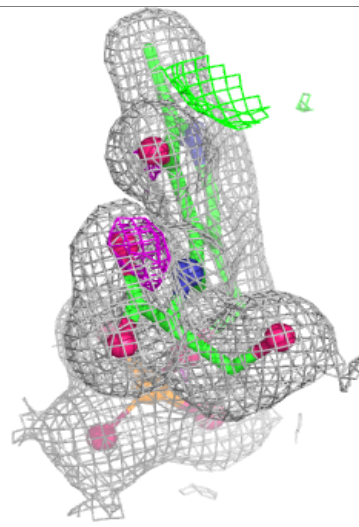
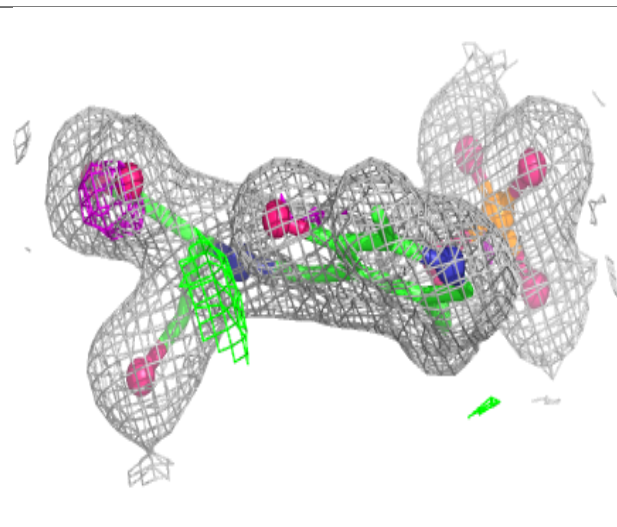
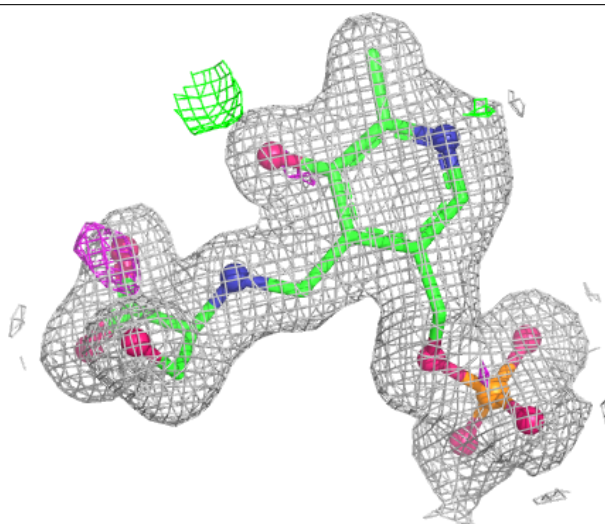
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NA	B	402	1/1	0.87	0.12	33,33,33,33	0
3	NA	D	402	1/1	0.93	0.09	29,29,29,29	0
2	PLS	D	401	22/22	0.96	0.07	23,24,25,25	0
2	PLS	C	401	22/22	0.97	0.05	18,18,19,19	0
2	PLS	B	401	22/22	0.97	0.06	23,24,24,24	0
2	PLS	A	401	22/22	0.98	0.05	18,19,19,20	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.

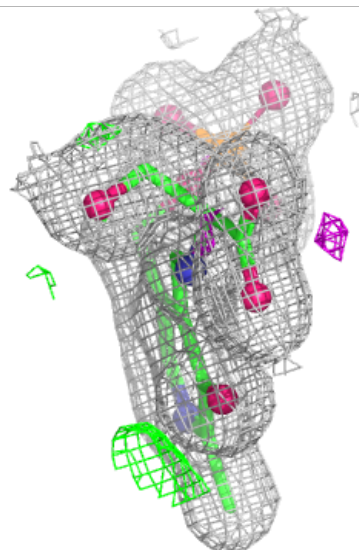
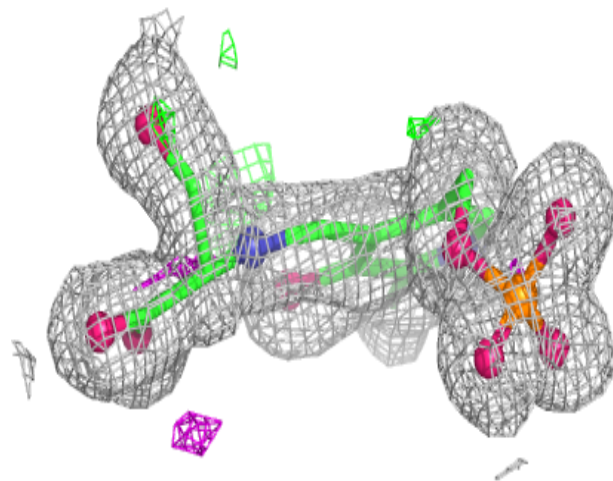
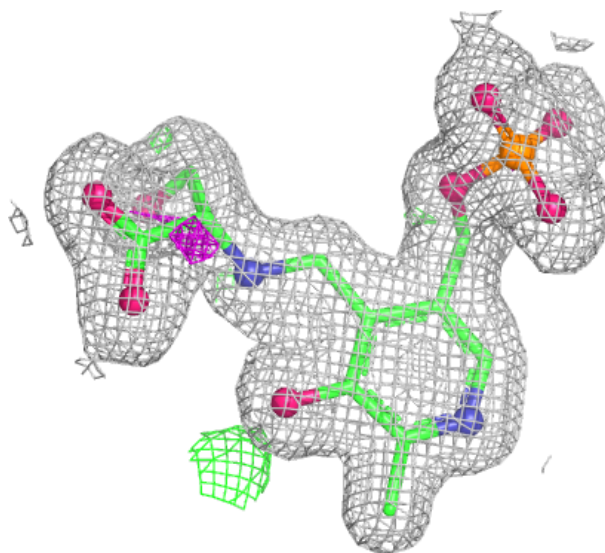
Electron density around PLS D 401:

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



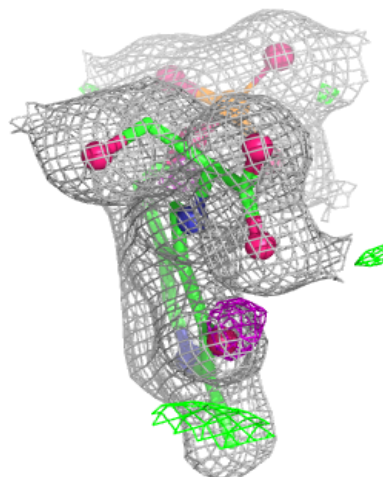
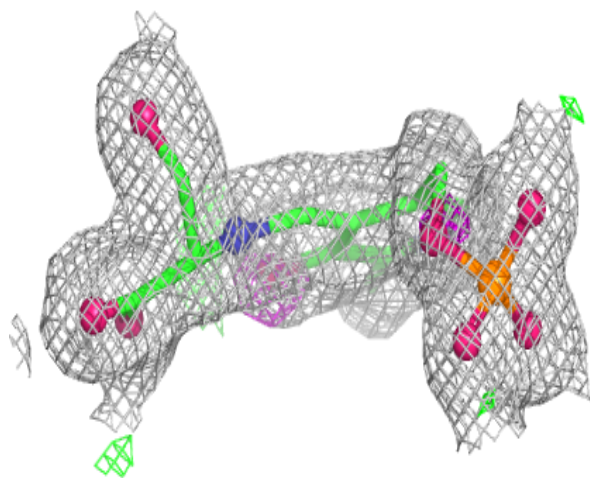
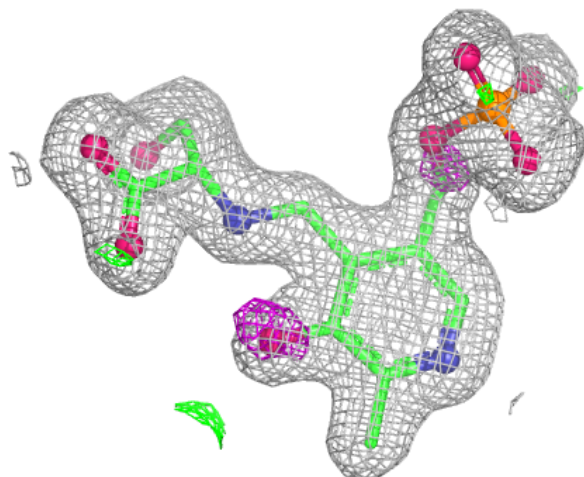
Electron density around PLS C 401:

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



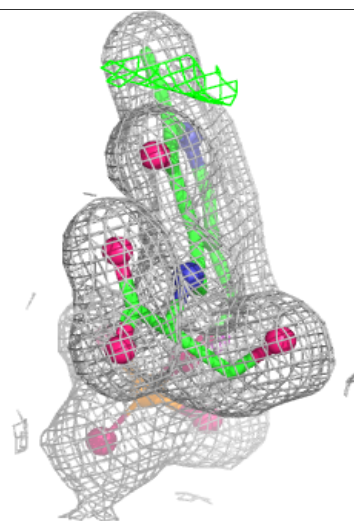
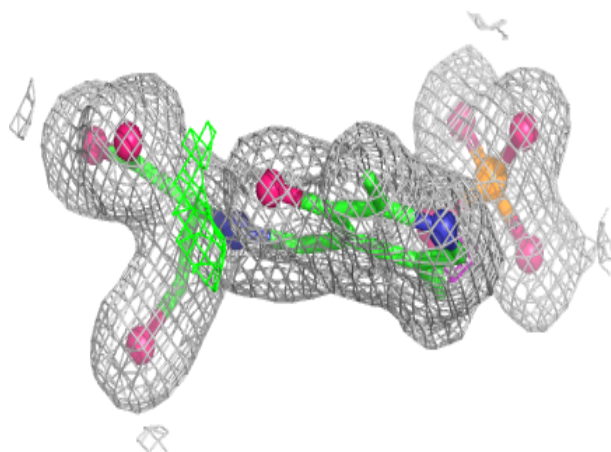
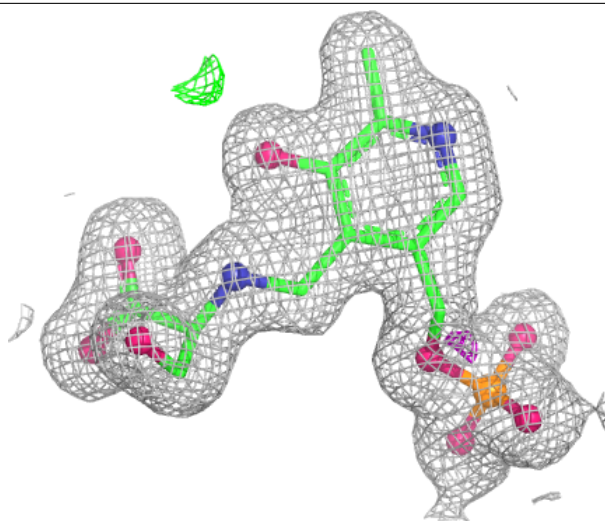
Electron density around PLS B 401:

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



Electron density around PLS 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.