



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2025 – 06:08 PM EDT

PDB ID : 3B1D  
Title : Crystal structure of betaC-S lyase from Streptococcus anginosus in complex with L-serine: External aldimine form  
Authors : Kezuka, Y.; Yoshida, Y.; Nonaka, T.  
Deposited on : 2011-06-29  
Resolution : 1.66 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](mailto: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>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

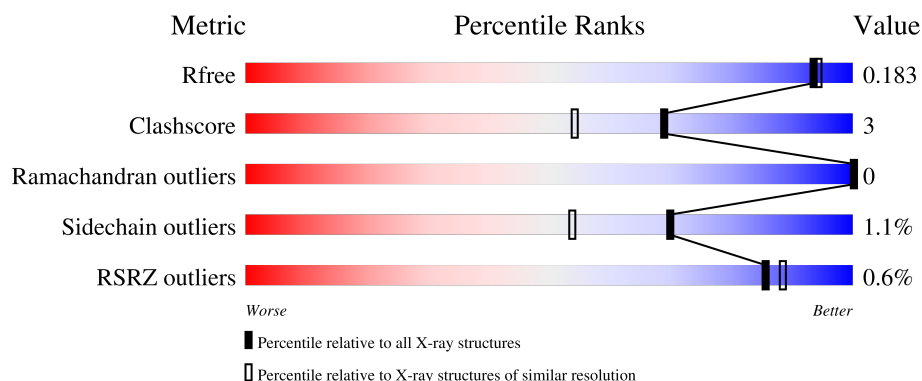
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.66 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))
$R_{free}$	164625	2328 (1.66-1.66)
Clashscore	180529	2515 (1.66-1.66)
Ramachandran outliers	177936	2475 (1.66-1.66)
Sidechain outliers	177891	2475 (1.66-1.66)
RSRZ outliers	164620	2328 (1.66-1.66)

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  $\geq 3$ , 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	392	 92% 7% .
1	B	392	 92% 7% ..
1	C	392	 92% 6% ..
1	D	392	 92% 6% .

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14658 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.

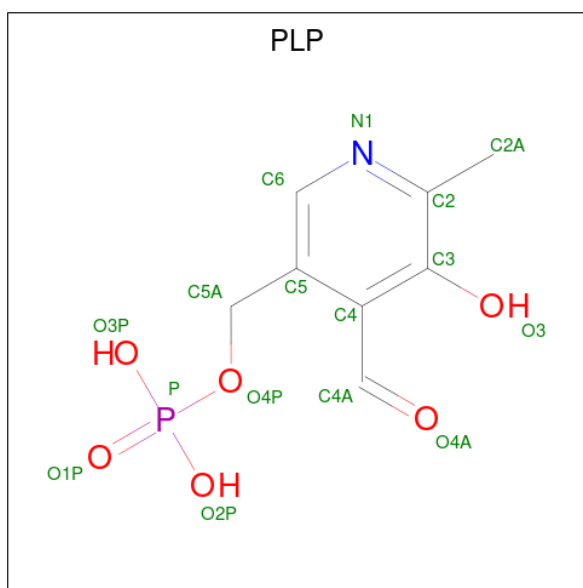
- Molecule 1 is a protein called BetaC-S lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	387	Total	C	N	O	S	0	12	0
			3189	2052	528	598	11			
1	B	387	Total	C	N	O	S	0	13	0
			3189	2051	528	598	12			
1	C	386	Total	C	N	O	S	0	16	0
			3202	2060	527	605	10			
1	D	386	Total	C	N	O	S	0	11	0
			3175	2045	522	598	10			

There are 20 discrepancies between the modelled and reference sequences:

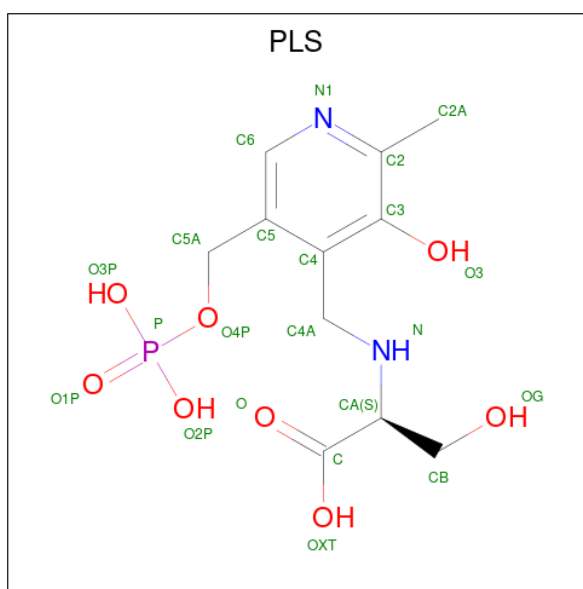
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP A6BMJ3
A	-2	PRO	-	expression tag	UNP A6BMJ3
A	-1	LEU	-	expression tag	UNP A6BMJ3
A	0	GLY	-	expression tag	UNP A6BMJ3
A	1	SER	-	expression tag	UNP A6BMJ3
B	-3	GLY	-	expression tag	UNP A6BMJ3
B	-2	PRO	-	expression tag	UNP A6BMJ3
B	-1	LEU	-	expression tag	UNP A6BMJ3
B	0	GLY	-	expression tag	UNP A6BMJ3
B	1	SER	-	expression tag	UNP A6BMJ3
C	-3	GLY	-	expression tag	UNP A6BMJ3
C	-2	PRO	-	expression tag	UNP A6BMJ3
C	-1	LEU	-	expression tag	UNP A6BMJ3
C	0	GLY	-	expression tag	UNP A6BMJ3
C	1	SER	-	expression tag	UNP A6BMJ3
D	-3	GLY	-	expression tag	UNP A6BMJ3
D	-2	PRO	-	expression tag	UNP A6BMJ3
D	-1	LEU	-	expression tag	UNP A6BMJ3
D	0	GLY	-	expression tag	UNP A6BMJ3
D	1	SER	-	expression tag	UNP A6BMJ3

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula:  $C_8H_{10}NO_6P$ ).



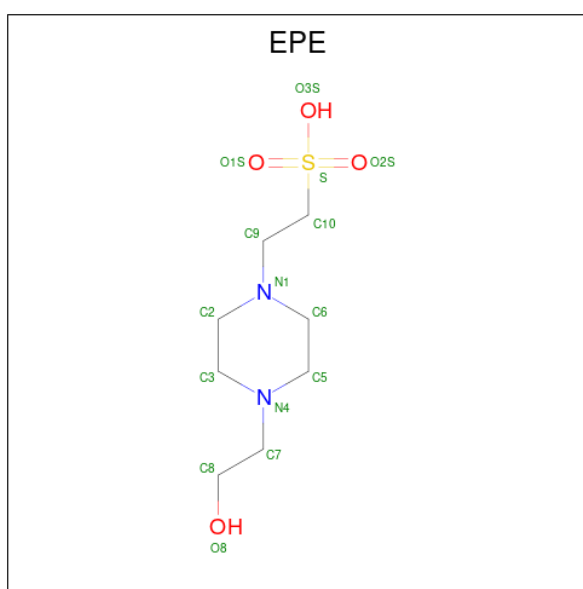
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	1
			15	8	1	5	1		
2	C	1	Total	C	N	O	P	0	1
			15	8	1	5	1		

- Molecule 3 is [3-HYDROXY-2-METHYL-5-PHOSPHONOOXYMETHYL-PYRIDIN-4-YL METHYL]-SERINE (three-letter code: PLS) (formula:  $C_{11}H_{17}N_2O_8P$ ).



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

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	B	1	Total	C	N	O	S	11	0
			15	8	2	4	1		
4	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	C	1	Total	C	N	O	S	11	0
			15	8	2	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	N	O	S	11	0
			15	8	2	4	1		
4	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	D	1	Total	C	N	O	S	11	0
			15	8	2	4	1		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

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

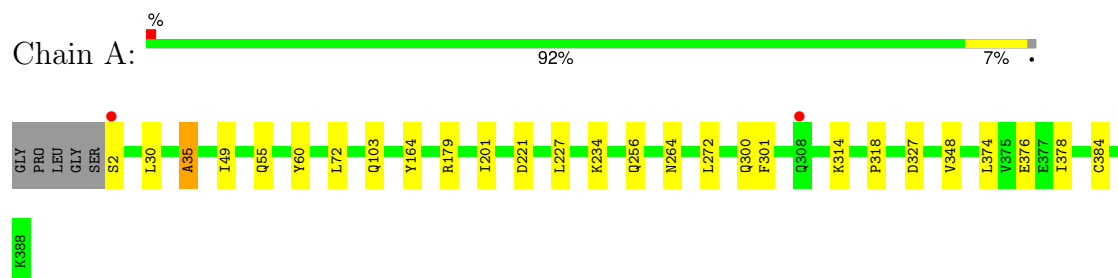
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	421	Total	O	0	8
			421	421		
6	B	433	Total	O	0	12
			433	433		
6	C	374	Total	O	0	8
			374	374		
6	D	388	Total	O	0	7
			388	388		

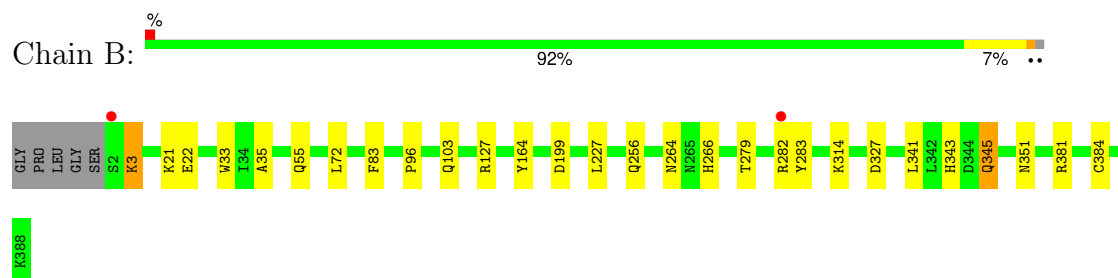
### 3 Residue-property plots [i](#)

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.

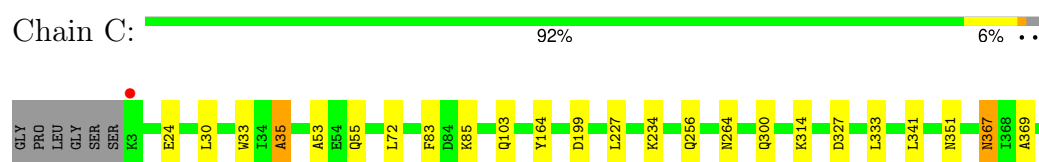
- Molecule 1: BetaC-S lyase



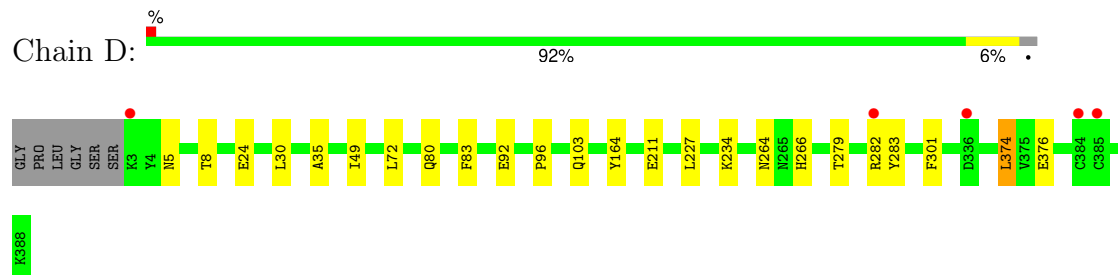
- Molecule 1: BetaC-S lyase



- Molecule 1: BetaC-S lyase



- Molecule 1: BetaC-S lyase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.97Å 111.30Å 217.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.84 – 1.66 36.84 – 1.66	Depositor EDS
% Data completeness (in resolution range)	100.0 (36.84-1.66) 98.7 (36.84-1.66)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	9.10 (at 1.66Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.151 , 0.177 0.160 , 0.183	Depositor DCC
$R_{free}$ test set	9529 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	11.0	Xtriage
Anisotropy	0.480	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 38.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	14658	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: EPE, PLP, 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	0/3301	0.62	0/4486
1	B	0.50	0/3307	0.63	0/4496
1	C	0.49	0/3326	0.62	0/4520
1	D	0.49	0/3287	0.61	0/4469
All	All	0.50	0/13221	0.62	0/17971

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
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	35	ALA	Peptide
1	C	35	ALA	Peptide

## 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	3189	0	3143	21	0
1	B	3189	0	3143	23	0
1	C	3202	0	3158	21	0
1	D	3175	0	3127	24	0
2	A	15	0	6	2	0
2	C	15	0	6	0	0
3	A	22	0	13	1	0
3	B	22	0	13	2	0
3	C	22	0	13	3	0
3	D	22	0	13	6	0
4	A	45	0	51	1	0
4	B	30	0	34	0	0
4	C	45	0	51	0	0
4	D	45	0	51	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	421	0	0	8	0
6	B	433	0	0	3	0
6	C	374	0	0	5	0
6	D	388	0	0	3	0
All	All	14658	0	12822	88	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 3.

All (88) 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:234:LYS:HE2	3:D:501:PLS:H4A1	1.38	1.02
1:D:234:LYS:CE	3:D:501:PLS:H4A1	1.96	0.95
1:D:5:ASN:HD21	1:D:8:THR:HG23	1.35	0.90
1:D:5:ASN:HD21	1:D:8:THR:CG2	1.91	0.82
1:A:234[B]:LYS:NZ	6:A:831:HOH:O	2.20	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:234:LYS:HE2	3:D:501:PLS:C4A	2.18	0.72
1:A:2:SER:HA	6:A:1166:HOH:O	1.89	0.72
1:D:282:ARG:HG3	1:D:283:TYR:CD2	2.25	0.71
1:B:282:ARG:HG3	1:B:283:TYR:CD2	2.27	0.70
1:B:72:LEU:HD23	1:B:83:PHE:CE1	2.28	0.69
1:C:35:ALA:HB3	3:C:501[D]:PLS:HA	1.73	0.68
1:C:55:GLN:NE2	6:C:917:HOH:O	2.27	0.68
1:A:103:GLN:NE2	1:A:264:ASN:HD21	1.95	0.64
1:D:72:LEU:HD12	1:D:83:PHE:CE1	2.31	0.64
1:A:35:ALA:HB3	3:A:501[D]:PLS:HA	1.80	0.64
1:C:300:GLN:HG3	6:C:1165:HOH:O	2.00	0.62
1:D:5:ASN:ND2	1:D:8:THR:CG2	2.63	0.61
1:D:35:ALA:HB3	3:D:501:PLS:HA	1.81	0.61
1:D:103:GLN:NE2	1:D:264:ASN:HD21	1.98	0.61
1:D:234:LYS:CE	3:D:501:PLS:C4A	2.76	0.60
1:C:30:LEU:HD22	1:C:374:LEU:HD21	1.82	0.59
1:A:55:GLN:NE2	6:A:823:HOH:O	2.33	0.59
1:B:103:GLN:NE2	1:B:264:ASN:HD21	2.00	0.59
1:D:103:GLN:HE22	1:D:264:ASN:HD21	1.48	0.59
1:C:103:GLN:HE22	1:C:264:ASN:HD21	1.49	0.59
1:C:367:ASN:ND2	1:C:369:ALA:H	2.01	0.59
1:D:279:THR:HA	1:D:282:ARG:HE	1.69	0.58
1:C:199:ASP:OD2	3:C:501[D]:PLS:N1	2.38	0.57
1:C:103:GLN:NE2	1:C:264:ASN:HD21	2.02	0.56
1:C:72:LEU:HD23	1:C:83:PHE:CE1	2.40	0.56
1:B:35:ALA:HB3	3:B:501:PLS:HA	1.88	0.55
1:A:103:GLN:HE22	1:A:264:ASN:HD21	1.52	0.55
1:B:3:LYS:NZ	1:B:3:LYS:HB3	2.22	0.54
1:B:103:GLN:HE22	1:B:264:ASN:HD21	1.57	0.53
1:D:211:GLU:HG3	6:D:1054:HOH:O	2.08	0.52
1:D:282:ARG:HG3	1:D:283:TYR:CE2	2.44	0.52
1:C:367:ASN:C	1:C:367:ASN:HD22	2.13	0.51
1:C:367:ASN:HD22	1:C:369:ALA:H	1.58	0.50
1:C:234[B]:LYS:HB2	6:C:813:HOH:O	2.11	0.49
1:D:234:LYS:HE3	3:D:501:PLS:H4A1	1.87	0.49
1:A:60:TYR:CD1	4:A:601:EPE:H32	2.48	0.48
1:B:22:GLU:OE1	1:B:343:HIS:HE1	1.95	0.48
1:B:381:ARG:O	1:B:384[B]:CYS:SG	2.71	0.48
1:A:179:ARG:HD3	6:A:1010:HOH:O	2.13	0.48
1:C:314:LYS:HB2	1:C:327:ASP:HB3	1.95	0.48
1:A:256[B]:GLN:NE2	6:A:1059:HOH:O	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:501[D]:PLS:H4A2	3:C:501[D]:PLS:H5A1	1.61	0.47
1:A:30:LEU:HD22	1:A:374[A]:LEU:HD11	1.97	0.46
1:B:279:THR:HA	1:B:282:ARG:HE	1.81	0.46
1:B:256:GLN:HG3	6:B:1139:HOH:O	2.16	0.45
1:D:301:PHE:CZ	1:D:376[A]:GLU:HG2	2.51	0.45
1:A:256[A]:GLN:HG3	6:A:1174:HOH:O	2.16	0.45
1:C:72:LEU:HD11	1:C:85:LYS:CG	2.46	0.45
1:A:348[B]:VAL:HG21	1:A:378:ILE:HG23	1.97	0.45
1:B:55:GLN:NE2	6:B:1178:HOH:O	2.41	0.45
1:B:72:LEU:CD2	1:B:83:PHE:CE1	2.98	0.45
1:D:5:ASN:ND2	1:D:8:THR:HG23	2.18	0.44
1:B:22:GLU:OE1	1:B:343:HIS:CE1	2.71	0.44
1:B:282:ARG:HG3	1:B:283:TYR:CE2	2.52	0.44
1:B:33:TRP:C	1:B:351:ASN:HD21	2.20	0.43
1:B:314:LYS:HB2	1:B:327:ASP:HB3	1.99	0.43
1:A:301:PHE:CZ	1:A:376:GLU:HG2	2.53	0.43
1:D:24:GLU:OE2	6:D:1171:HOH:O	2.21	0.43
1:C:33:TRP:C	1:C:351:ASN:HD21	2.21	0.43
1:B:96:PRO:HB3	1:B:266:HIS:CE1	2.54	0.43
1:A:300:GLN:NE2	6:A:1013:HOH:O	2.51	0.43
1:D:30:LEU:HD22	1:D:374:LEU:HD21	2.01	0.43
1:D:5:ASN:ND2	1:D:8:THR:HG22	2.33	0.42
1:C:24:GLU:OE2	6:C:1118:HOH:O	2.22	0.42
1:A:201:ILE:CD1	2:A:401[C]:PLP:H5A1	2.49	0.42
1:A:221[B]:ASP:CG	6:A:1162:HOH:O	2.58	0.42
1:D:96:PRO:HB3	1:D:266:HIS:CE1	2.55	0.42
1:B:21:LYS:NZ	6:B:1231:HOH:O	2.49	0.42
1:A:314:LYS:HB2	1:A:327:ASP:HB3	2.01	0.41
1:C:53:ALA:HB2	1:D:49:ILE:CG2	2.50	0.41
1:B:127[A]:ARG:HG2	1:C:333:LEU:O	2.21	0.41
1:B:199:ASP:OD2	3:B:501:PLS:N1	2.54	0.41
1:D:80:GLN:HG3	6:D:1026:HOH:O	2.19	0.41
1:A:49:ILE:HG12	1:A:272:LEU:HD11	2.03	0.41
1:A:72:LEU:C	1:A:72:LEU:HD23	2.40	0.41
1:B:3:LYS:HB3	1:B:3:LYS:HZ2	1.86	0.40
1:B:341[B]:LEU:HD22	1:B:345:GLN:HB2	2.03	0.40
1:A:201:ILE:HD13	2:A:401[C]:PLP:H5A1	2.04	0.40
1:C:256[B]:GLN:NE2	6:C:1081:HOH:O	2.54	0.40
1:C:367:ASN:HD21	1:C:369:ALA:HB3	1.86	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	397/392 (101%)	386 (97%)	11 (3%)	0	100	100
1	B	398/392 (102%)	387 (97%)	11 (3%)	0	100	100
1	C	400/392 (102%)	390 (98%)	10 (2%)	0	100	100
1	D	395/392 (101%)	385 (98%)	10 (2%)	0	100	100
All	All	1590/1568 (101%)	1548 (97%)	42 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	354/345 (103%)	351 (99%)	3 (1%)	79	68
1	B	355/345 (103%)	351 (99%)	4 (1%)	70	54
1	C	357/345 (104%)	353 (99%)	4 (1%)	70	54
1	D	352/345 (102%)	348 (99%)	4 (1%)	70	54
All	All	1418/1380 (103%)	1403 (99%)	15 (1%)	70	54

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	164	TYR
1	A	227	LEU

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Mol	Chain	Res	Type
1	A	318	PRO
1	B	3	LYS
1	B	164	TYR
1	B	227	LEU
1	B	345	GLN
1	C	164	TYR
1	C	227	LEU
1	C	367	ASN
1	C	374	LEU
1	D	92	GLU
1	D	164	TYR
1	D	227	LEU
1	D	374	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	55	GLN
1	A	103	GLN
1	A	261	GLN
1	A	351	ASN
1	B	103	GLN
1	B	260	GLN
1	B	261	GLN
1	B	308	GLN
1	B	343	HIS
1	B	351	ASN
1	C	16	HIS
1	C	55	GLN
1	C	103	GLN
1	C	151	GLN
1	C	190	GLN
1	C	261	GLN
1	C	298	ASN
1	C	351	ASN
1	C	367	ASN
1	D	7	GLN
1	D	80	GLN
1	D	103	GLN
1	D	159	ASN
1	D	261	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 21 ligands modelled in this entry, 4 are monoatomic - leaving 17 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	PLS	C	501[D]	-	22,22,22	1.69	3 (13%)	28,31,31	1.50	3 (10%)
4	EPE	B	601	-	15,15,15	0.77	1 (6%)	19,20,20	1.30	2 (10%)
3	PLS	D	501	-	22,22,22	1.81	7 (31%)	28,31,31	1.50	7 (25%)
4	EPE	C	601	-	15,15,15	0.70	1 (6%)	19,20,20	1.02	1 (5%)
4	EPE	C	602	-	15,15,15	1.73	1 (6%)	19,20,20	1.89	2 (10%)
3	PLS	A	501[D]	-	22,22,22	1.73	4 (18%)	28,31,31	1.25	3 (10%)
2	PLP	C	401[C]	1	15,15,16	1.14	2 (13%)	21,22,23	1.31	3 (14%)
4	EPE	A	603	-	15,15,15	0.81	1 (6%)	19,20,20	0.97	2 (10%)
4	EPE	B	602	-	15,15,15	1.78	1 (6%)	19,20,20	1.84	4 (21%)
4	EPE	C	603	-	15,15,15	0.86	1 (6%)	19,20,20	1.01	1 (5%)
4	EPE	D	601	-	15,15,15	0.81	1 (6%)	19,20,20	1.14	2 (10%)
2	PLP	A	401[C]	1	15,15,16	1.14	2 (13%)	21,22,23	1.49	3 (14%)
4	EPE	A	602	-	15,15,15	0.96	1 (6%)	19,20,20	1.20	1 (5%)
4	EPE	D	602	-	15,15,15	0.90	1 (6%)	19,20,20	1.15	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PLS	B	501	-	22,22,22	1.93	5 (22%)	28,31,31	1.43	5 (17%)
4	EPE	D	603	-	15,15,15	1.98	1 (6%)	19,20,20	2.45	3 (15%)
4	EPE	A	601	-	15,15,15	0.65	1 (6%)	19,20,20	1.34	3 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PLS	C	501[D]	-	-	5/17/17/17	0/1/1/1
4	EPE	B	601	-	-	0/9/19/19	0/1/1/1
3	PLS	D	501	-	-	9/17/17/17	0/1/1/1
4	EPE	C	601	-	-	0/9/19/19	0/1/1/1
4	EPE	C	602	-	-	2/9/19/19	0/1/1/1
3	PLS	A	501[D]	-	-	7/17/17/17	0/1/1/1
2	PLP	C	401[C]	1	-	3/6/6/8	0/1/1/1
4	EPE	A	603	-	-	0/9/19/19	0/1/1/1
4	EPE	B	602	-	-	2/9/19/19	0/1/1/1
4	EPE	C	603	-	-	3/9/19/19	0/1/1/1
4	EPE	D	601	-	-	0/9/19/19	0/1/1/1
2	PLP	A	401[C]	1	-	0/6/6/8	0/1/1/1
4	EPE	A	602	-	-	1/9/19/19	0/1/1/1
4	EPE	D	602	-	-	0/9/19/19	0/1/1/1
3	PLS	B	501	-	-	6/17/17/17	0/1/1/1
4	EPE	D	603	-	-	1/9/19/19	0/1/1/1
4	EPE	A	601	-	-	4/9/19/19	0/1/1/1

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	603	EPE	C10-S	-7.23	1.67	1.77
4	B	602	EPE	C10-S	6.74	1.87	1.77
4	C	602	EPE	C10-S	6.39	1.86	1.77
3	D	501	PLS	C4A-N	-5.13	1.31	1.46
3	B	501	PLS	C4A-N	-5.08	1.31	1.46
3	A	501[D]	PLS	C4A-N	-5.00	1.32	1.46
3	C	501[D]	PLS	C4A-N	-4.68	1.33	1.46
3	B	501	PLS	P-O2P	-3.82	1.40	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	501[D]	PLS	P-O2P	-3.58	1.41	1.54
3	A	501[D]	PLS	P-O3P	-3.37	1.42	1.54
3	B	501	PLS	C2A-C2	3.32	1.55	1.50
4	A	602	EPE	C10-S	3.28	1.82	1.77
3	B	501	PLS	O4P-C5A	-3.24	1.32	1.44
3	C	501[D]	PLS	P-O3P	-3.19	1.43	1.54
4	D	602	EPE	C10-S	2.95	1.81	1.77
3	D	501	PLS	P-O2P	-2.86	1.44	1.54
3	A	501[D]	PLS	P-O2P	-2.86	1.44	1.54
4	C	603	EPE	C10-S	2.81	1.81	1.77
4	D	601	EPE	C10-S	2.77	1.81	1.77
3	D	501	PLS	P-O3P	-2.74	1.44	1.54
3	D	501	PLS	C2A-C2	2.74	1.54	1.50
4	A	603	EPE	C10-S	2.74	1.81	1.77
4	B	601	EPE	C10-S	2.71	1.81	1.77
3	B	501	PLS	P-O3P	-2.64	1.45	1.54
2	A	401[C]	PLP	C2-N1	2.61	1.38	1.33
3	D	501	PLS	O4P-C5A	-2.45	1.35	1.44
3	A	501[D]	PLS	C2A-C2	2.44	1.54	1.50
2	C	401[C]	PLP	C2-N1	2.40	1.38	1.33
4	C	601	EPE	C10-S	2.34	1.80	1.77
4	A	601	EPE	C10-S	2.25	1.80	1.77
3	D	501	PLS	C3-C2	-2.13	1.38	1.41
2	C	401[C]	PLP	C6-N1	2.13	1.38	1.34
2	A	401[C]	PLP	C6-N1	2.07	1.38	1.34
3	D	501	PLS	P-O1P	-2.02	1.44	1.50

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	603	EPE	O3S-S-C10	7.37	120.42	106.00
4	B	602	EPE	O2S-S-C10	6.80	117.00	106.73
4	C	602	EPE	O2S-S-C10	6.68	116.82	106.73
4	D	603	EPE	O1S-S-C10	-6.06	97.57	106.73
2	A	401[C]	PLP	O4P-C5A-C5	4.61	117.99	109.36
3	D	501	PLS	C4A-N-CA	3.69	120.76	113.84
3	C	501[D]	PLS	C4A-C4-C3	3.59	124.76	119.98
3	B	501	PLS	C4A-N-CA	3.15	119.75	113.84
3	B	501	PLS	CB-CA-C	3.03	120.44	107.55
3	C	501[D]	PLS	C4A-N-CA	3.00	119.46	113.84
2	A	401[C]	PLP	C6-C5-C4	2.83	120.42	118.10
4	B	601	EPE	O2S-S-C10	2.79	110.95	106.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	603	EPE	O2S-S-C10	2.78	110.94	106.73
4	A	601	EPE	C7-N4-C5	-2.62	104.25	111.24
2	C	401[C]	PLP	O3P-P-O2P	2.61	117.58	107.80
4	D	603	EPE	C5-N4-C3	-2.54	103.36	108.84
4	B	601	EPE	C2-C3-N4	2.52	115.74	110.65
2	A	401[C]	PLP	C5-C6-N1	-2.44	119.86	123.83
2	C	401[C]	PLP	O4P-C5A-C5	2.43	113.92	109.36
3	A	501[D]	PLS	CB-CA-C	2.43	117.87	107.55
3	D	501	PLS	C6-C5-C4	2.42	119.89	118.06
3	A	501[D]	PLS	C4A-N-CA	2.41	118.37	113.84
3	D	501	PLS	C5-C6-N1	-2.39	119.94	123.83
3	D	501	PLS	CB-CA-C	2.37	117.63	107.55
4	C	602	EPE	C8-C7-N4	2.37	121.77	113.44
2	C	401[C]	PLP	C6-C5-C4	2.36	120.03	118.10
4	A	603	EPE	C7-N4-C5	-2.34	104.99	111.24
4	A	601	EPE	O1S-S-C10	2.34	110.27	106.73
4	C	601	EPE	C2-C3-N4	2.29	115.27	110.65
4	D	601	EPE	C2-C3-N4	2.26	115.21	110.65
4	D	602	EPE	O3S-S-C10	2.26	110.43	106.00
4	B	602	EPE	O3S-S-C10	-2.26	101.58	106.00
4	D	602	EPE	C5-N4-C3	-2.24	104.01	108.84
3	C	501[D]	PLS	CB-CA-C	2.23	117.03	107.55
4	A	601	EPE	O2S-S-C10	2.22	110.09	106.73
4	A	603	EPE	C5-N4-C3	-2.20	104.10	108.84
3	B	501	PLS	C6-C5-C4	2.18	119.71	118.06
3	D	501	PLS	O-C-CA	-2.17	115.24	122.26
3	D	501	PLS	C5A-C5-C4	-2.14	118.16	122.67
4	B	602	EPE	C5-N4-C3	-2.14	104.23	108.84
4	A	602	EPE	O2S-S-C10	2.12	109.94	106.73
4	D	601	EPE	O2S-S-C10	2.09	109.89	106.73
3	A	501[D]	PLS	O3P-P-O2P	2.05	115.48	107.80
4	B	602	EPE	C7-N4-C5	-2.04	105.80	111.24
3	B	501	PLS	O-C-CA	-2.03	115.72	122.26
3	B	501	PLS	C5A-C5-C4	-2.01	118.43	122.67
3	D	501	PLS	O3-C3-C2	2.00	121.73	117.58

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	401[C]	PLP	C5A-O4P-P-O2P
3	A	501[D]	PLS	C-CA-N-C4A

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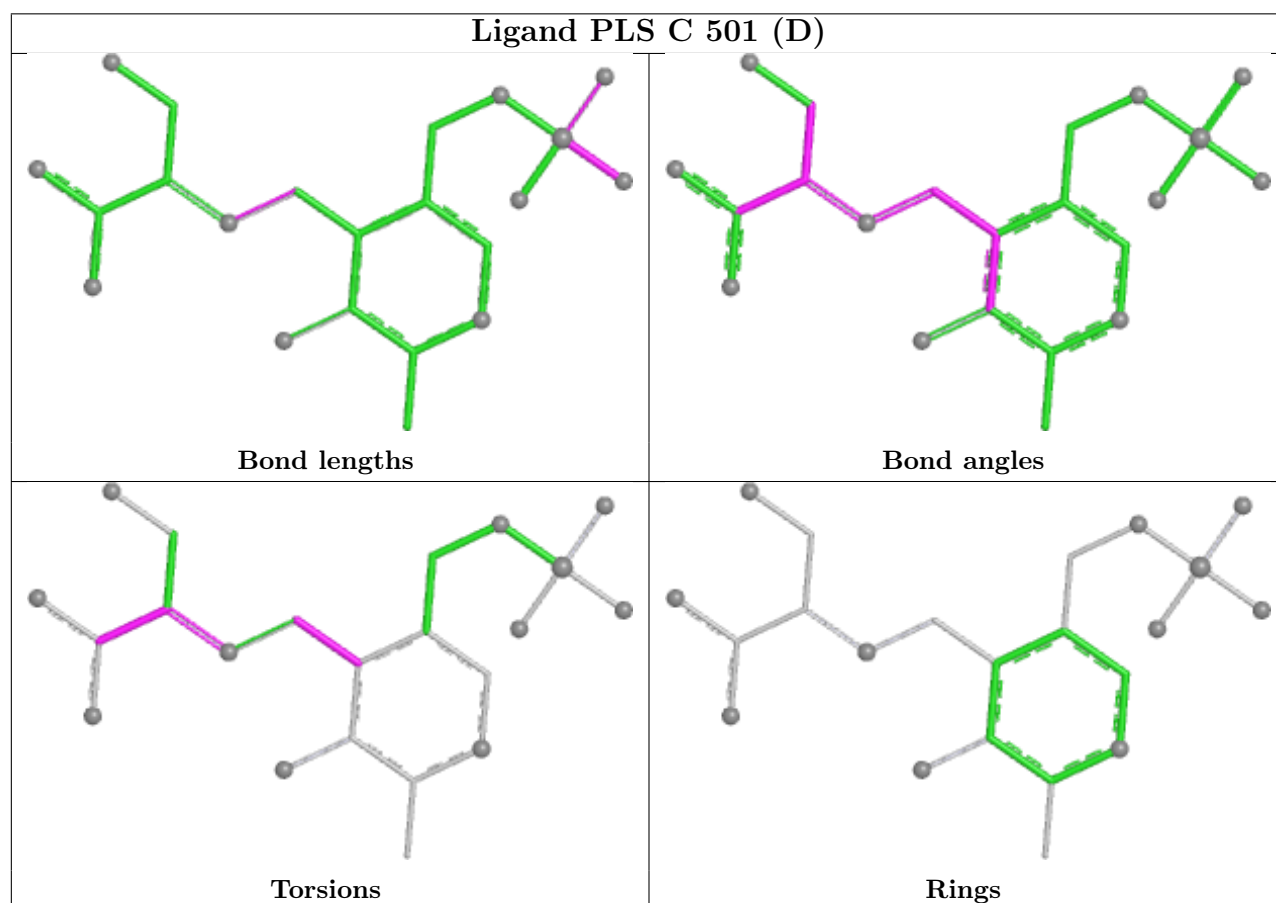
Mol	Chain	Res	Type	Atoms
3	A	501[D]	PLS	C5A-O4P-P-O2P
3	A	501[D]	PLS	C5A-O4P-P-O3P
3	B	501	PLS	C-CA-N-C4A
3	B	501	PLS	C5A-O4P-P-O2P
3	B	501	PLS	C5A-O4P-P-O3P
3	C	501[D]	PLS	C-CA-N-C4A
3	D	501	PLS	C-CA-N-C4A
3	D	501	PLS	C5A-O4P-P-O1P
3	D	501	PLS	C5A-O4P-P-O2P
3	D	501	PLS	C5A-O4P-P-O3P
4	C	603	EPE	C9-C10-S-O2S
4	C	603	EPE	C9-C10-S-O3S
4	C	602	EPE	C8-C7-N4-C5
4	A	601	EPE	C8-C7-N4-C5
3	A	501[D]	PLS	O-C-CA-CB
3	C	501[D]	PLS	O-C-CA-CB
4	A	602	EPE	N4-C7-C8-O8
3	A	501[D]	PLS	C5A-O4P-P-O1P
3	B	501	PLS	C5A-O4P-P-O1P
3	C	501[D]	PLS	C5-C4-C4A-N
4	A	601	EPE	C8-C7-N4-C3
4	C	602	EPE	C8-C7-N4-C3
4	C	603	EPE	C9-C10-S-O1S
4	B	602	EPE	C8-C7-N4-C3
3	B	501	PLS	CB-CA-N-C4A
3	C	501[D]	PLS	CB-CA-N-C4A
2	C	401[C]	PLP	C5A-O4P-P-O1P
4	A	601	EPE	C10-C9-N1-C6
3	D	501	PLS	C5-C4-C4A-N
4	D	603	EPE	C8-C7-N4-C5
2	C	401[C]	PLP	C5A-O4P-P-O3P
4	A	601	EPE	C10-C9-N1-C2
3	B	501	PLS	O-C-CA-CB
3	D	501	PLS	O-C-CA-CB
3	D	501	PLS	OXT-C-CA-CB
3	A	501[D]	PLS	CB-CA-N-C4A
3	D	501	PLS	CB-CA-N-C4A
3	C	501[D]	PLS	C3-C4-C4A-N
3	D	501	PLS	C3-C4-C4A-N
4	B	602	EPE	C8-C7-N4-C5
3	A	501[D]	PLS	C5-C4-C4A-N

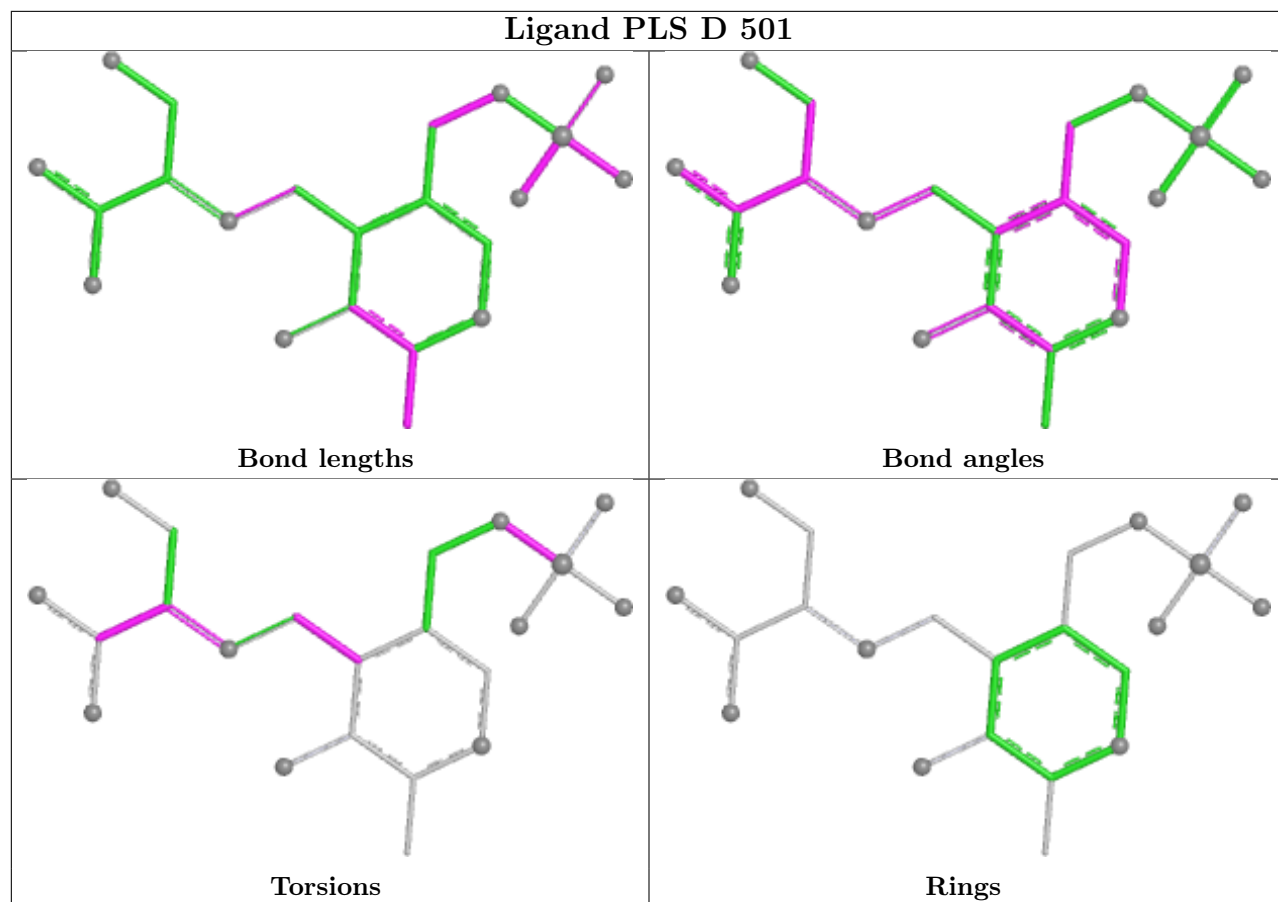
There are no ring outliers.

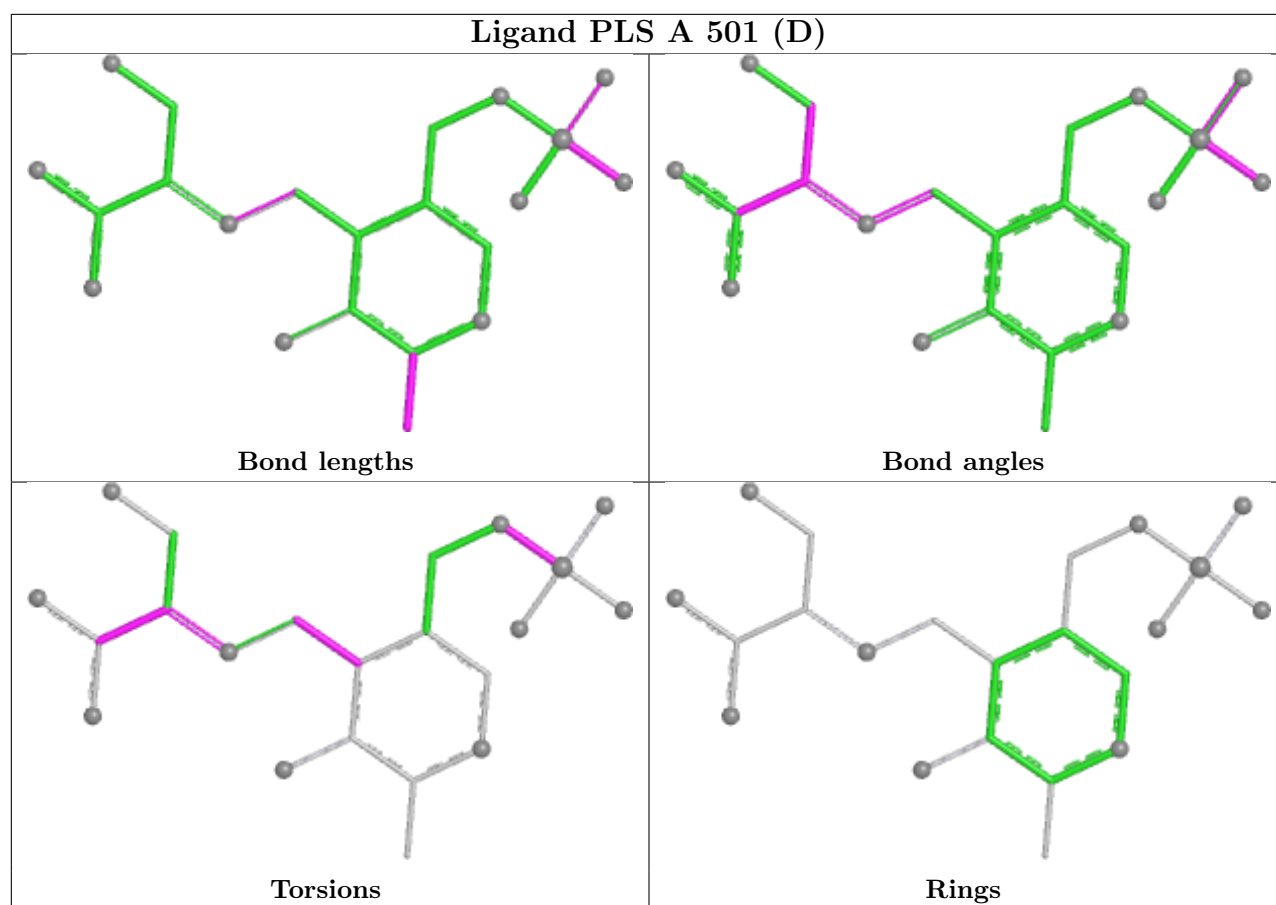
6 monomers are involved in 15 short contacts:

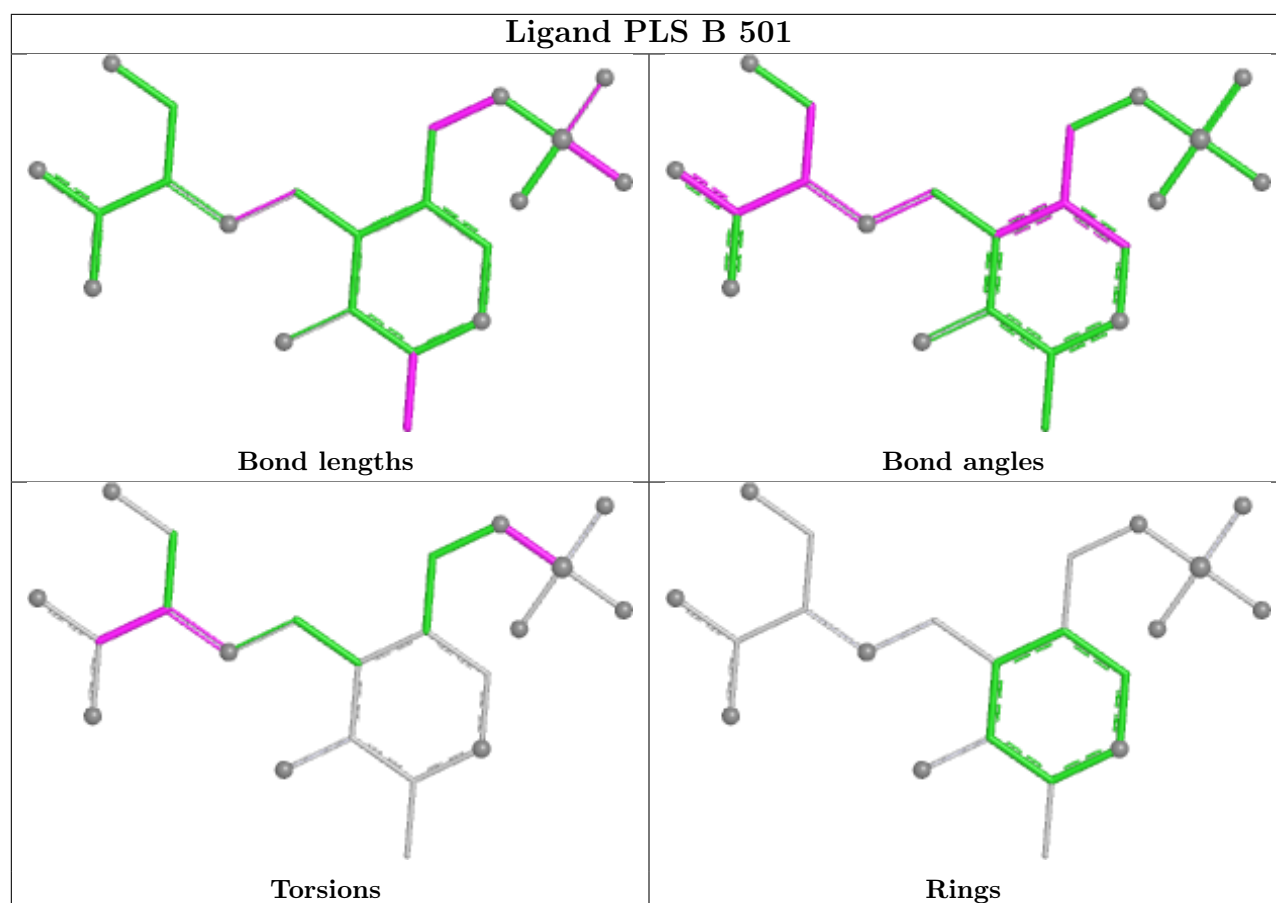
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	501[D]	PLS	3	0
3	D	501	PLS	6	0
3	A	501[D]	PLS	1	0
2	A	401[C]	PLP	2	0
3	B	501	PLS	2	0
4	A	601	EPE	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	387/392 (98%)	-0.58	2 (0%) 87 90	3, 8, 17, 26	12 (3%)
1	B	387/392 (98%)	-0.51	2 (0%) 87 90	4, 9, 17, 28	13 (3%)
1	C	386/392 (98%)	-0.33	1 (0%) 90 93	5, 11, 20, 30	16 (4%)
1	D	386/392 (98%)	-0.43	5 (1%) 74 79	4, 10, 19, 31	11 (2%)
All	All	1546/1568 (98%)	-0.46	10 (0%) 85 88	3, 10, 19, 31	52 (3%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	SER	3.8
1	B	282	ARG	3.3
1	D	282	ARG	3.2
1	D	3	LYS	3.1
1	D	385	CYS	2.4
1	A	308	GLN	2.4
1	A	2	SER	2.2
1	D	336	ASP	2.2
1	D	384	CYS	2.1
1	C	3	LYS	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 monosaccharides in this entry.



## 6.4 Ligands ⓘ

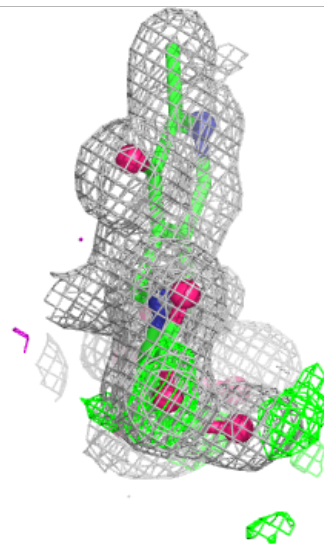
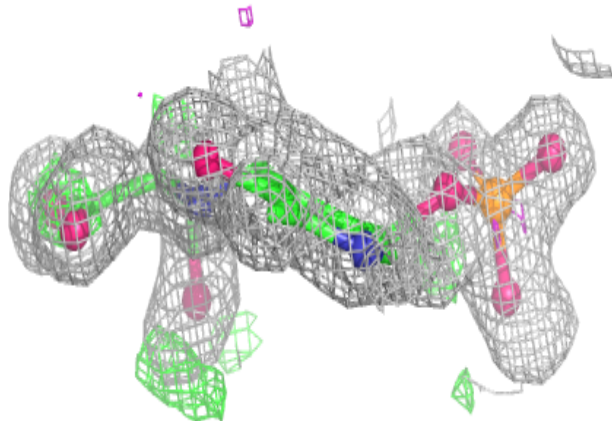
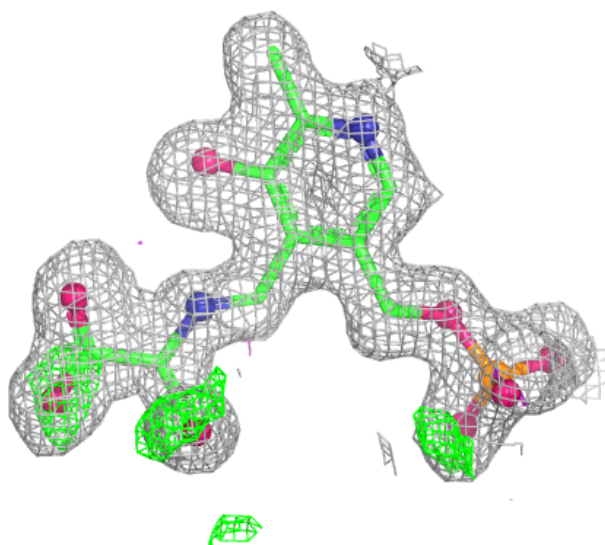
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	EPE	A	601	15/15	0.80	0.15	33,34,41,41	0
4	EPE	A	602	15/15	0.82	0.17	29,36,42,43	0
4	EPE	D	601	15/15	0.82	0.14	33,35,41,42	0
4	EPE	C	602	15/15	0.86	0.21	19,27,34,36	11
4	EPE	B	601	15/15	0.87	0.12	24,25,34,35	0
4	EPE	C	603	15/15	0.88	0.20	24,30,36,37	11
4	EPE	D	603	15/15	0.89	0.14	37,41,46,47	11
4	EPE	B	602	15/15	0.90	0.16	30,33,40,42	11
4	EPE	C	601	15/15	0.90	0.10	19,20,28,30	0
4	EPE	D	602	15/15	0.90	0.14	21,29,35,37	0
4	EPE	A	603	15/15	0.90	0.12	25,31,37,39	0
3	PLS	C	501[D]	22/22	0.93	0.08	5,7,11,14	22
3	PLS	D	501	22/22	0.97	0.06	5,9,15,16	0
3	PLS	A	501[D]	22/22	0.97	0.05	3,6,9,10	22
3	PLS	B	501	22/22	0.97	0.06	6,10,14,17	0
2	PLP	C	401[C]	15/16	0.97	0.06	2,5,7,9	15
2	PLP	A	401[C]	15/16	0.98	0.05	5,7,10,10	15
5	NA	A	701	1/1	0.98	0.08	14,14,14,14	0
5	NA	B	701	1/1	0.98	0.07	20,20,20,20	0
5	NA	C	701	1/1	0.98	0.09	20,20,20,20	0
5	NA	D	701	1/1	0.99	0.08	15,15,15,15	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.

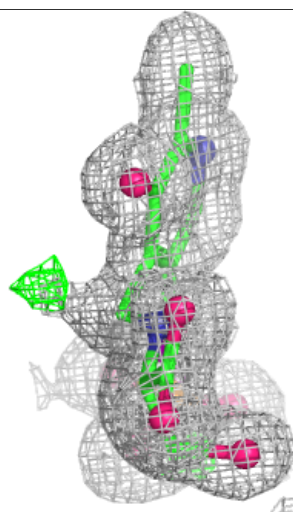
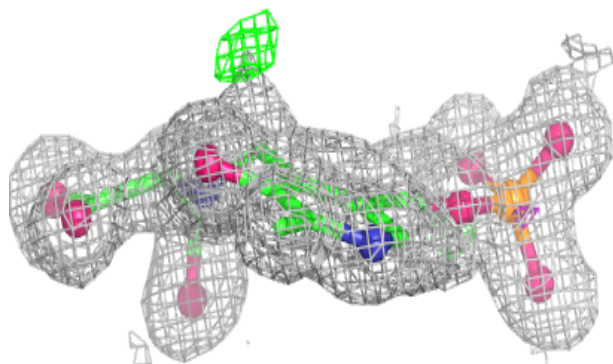
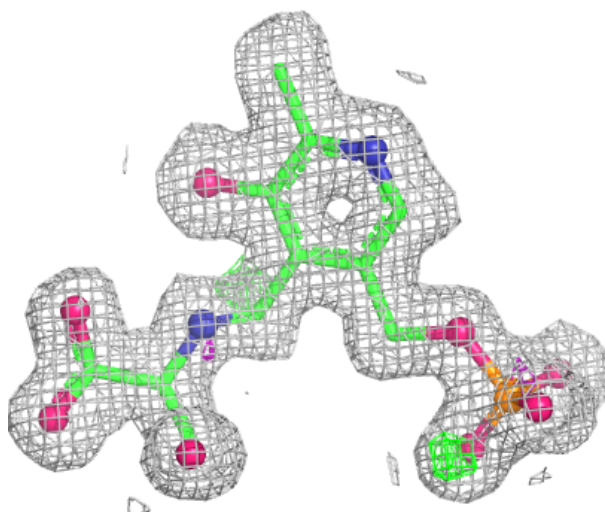
**Electron density around PLS C 501 (D):**

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



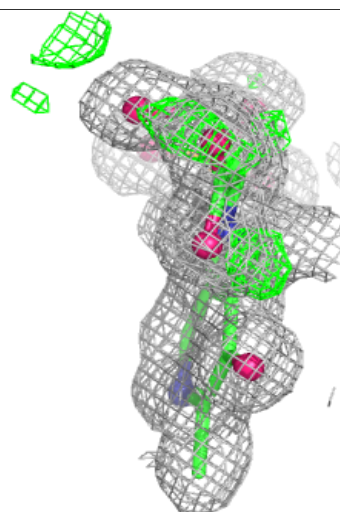
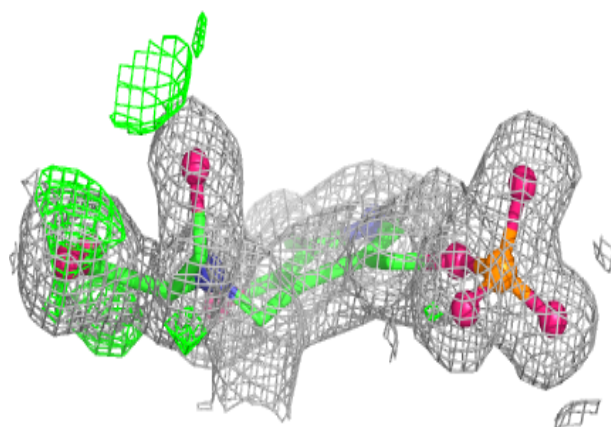
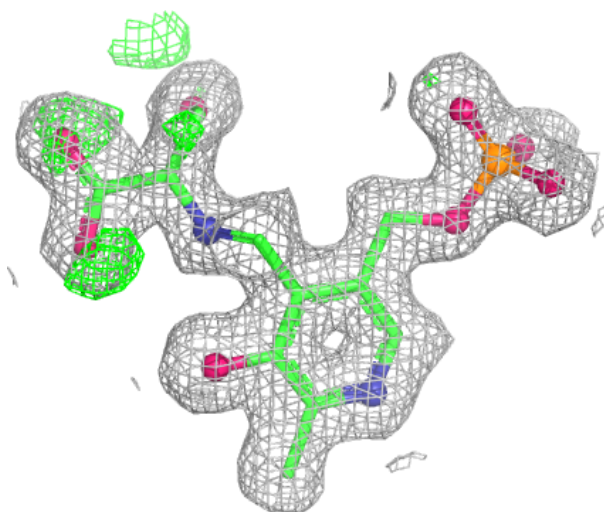
**Electron density around PLS D 501:**

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



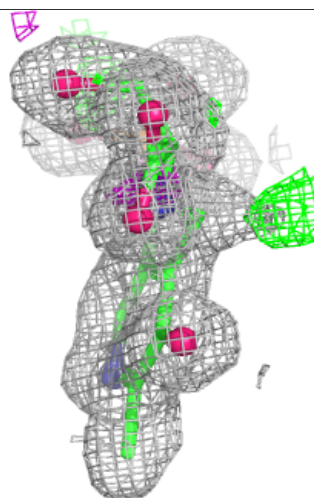
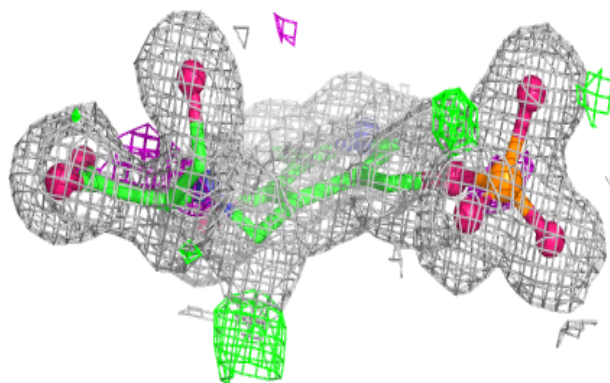
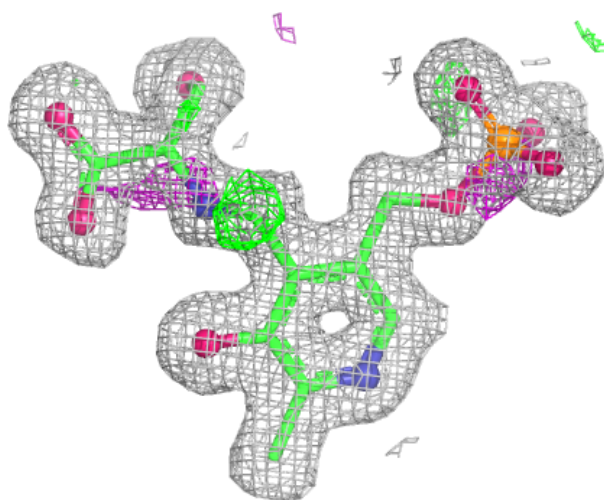
**Electron density around PLS A 501 (D):**

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



**Electron density around PLS B 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.