



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 10:31 am BST

PDB ID : 6S4G  
Title : Crystal structure of the omega transaminase from *Chromobacterium violaceum* in complex with PMP  
Authors : Ruggieri, F.; Campillo Brocal, J.C.; Humble, M.S.; Walse, B.; Logan, D.T.; Berglund, P.  
Deposited on : 2019-06-27  
Resolution : 1.67 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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

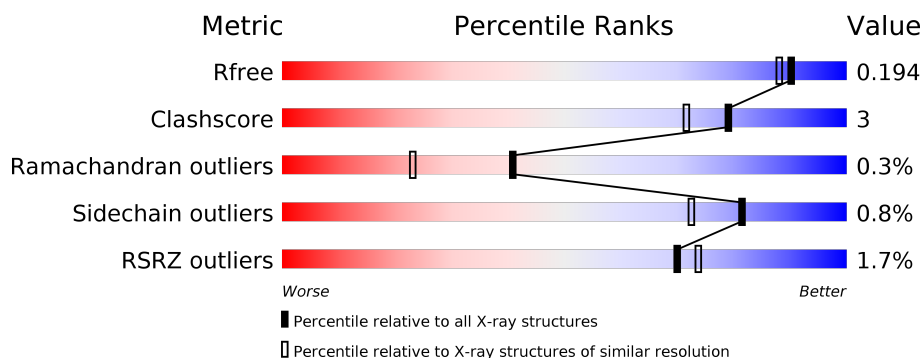
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.67 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))
$R_{free}$	130704	6780 (1.70-1.66)
Clashscore	141614	7310 (1.70-1.66)
Ramachandran outliers	138981	7173 (1.70-1.66)
Sidechain outliers	138945	7172 (1.70-1.66)
RSRZ outliers	127900	6661 (1.70-1.66)

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 on 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	465	<div> <div>3%</div> <div>91%</div> <div>6%</div> <div>•</div> </div>
1	B	465	<div> <div>3%</div> <div>88%</div> <div>9%</div> <div>• •</div> </div>
1	C	465	<div> <div>93%</div> <div>5%</div> <div>•</div> </div>
1	D	465	<div> <div>%</div> <div>91%</div> <div>7%</div> <div>•</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14848 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 Probable aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	453	Total	C	N	O	S	0	0	0
			3557	2267	625	644	21			
1	B	453	Total	C	N	O	S	0	0	0
			3557	2267	625	644	21			
1	C	455	Total	C	N	O	S	0	1	0
			3581	2281	631	647	22			
1	D	454	Total	C	N	O	S	0	1	0
			3576	2279	630	646	21			

There are 24 discrepancies between the modelled and reference sequences:

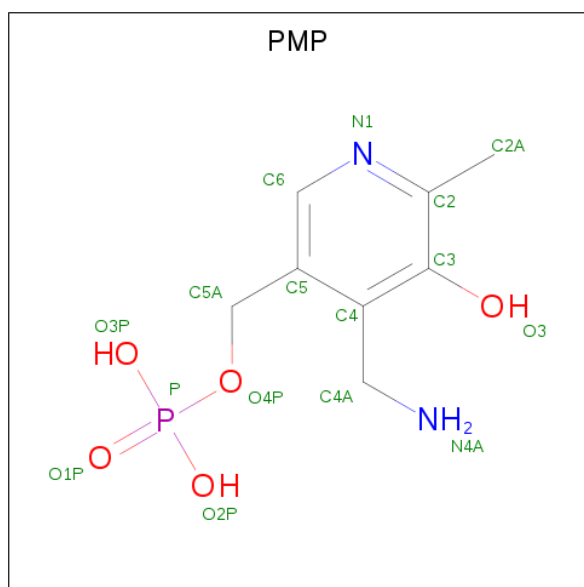
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP Q7NWXG4
A	-4	HIS	-	expression tag	UNP Q7NWXG4
A	-3	HIS	-	expression tag	UNP Q7NWXG4
A	-2	HIS	-	expression tag	UNP Q7NWXG4
A	-1	HIS	-	expression tag	UNP Q7NWXG4
A	0	HIS	-	expression tag	UNP Q7NWXG4
B	-5	HIS	-	expression tag	UNP Q7NWXG4
B	-4	HIS	-	expression tag	UNP Q7NWXG4
B	-3	HIS	-	expression tag	UNP Q7NWXG4
B	-2	HIS	-	expression tag	UNP Q7NWXG4
B	-1	HIS	-	expression tag	UNP Q7NWXG4
B	0	HIS	-	expression tag	UNP Q7NWXG4
C	-5	HIS	-	expression tag	UNP Q7NWXG4
C	-4	HIS	-	expression tag	UNP Q7NWXG4
C	-3	HIS	-	expression tag	UNP Q7NWXG4
C	-2	HIS	-	expression tag	UNP Q7NWXG4
C	-1	HIS	-	expression tag	UNP Q7NWXG4
C	0	HIS	-	expression tag	UNP Q7NWXG4
D	-5	HIS	-	expression tag	UNP Q7NWXG4
D	-4	HIS	-	expression tag	UNP Q7NWXG4
D	-3	HIS	-	expression tag	UNP Q7NWXG4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	HIS	-	expression tag	UNP Q7NWX4
D	-1	HIS	-	expression tag	UNP Q7NWX4
D	0	HIS	-	expression tag	UNP Q7NWX4

- Molecule 2 is 4'-DEOXY-4'-AMINOPYRIDOXAL-5'-PHOSPHATE (three-letter code: PMP) (formula:  $C_8H_{13}N_2O_5P$ ) (labeled as "Ligand of Interest" by author).



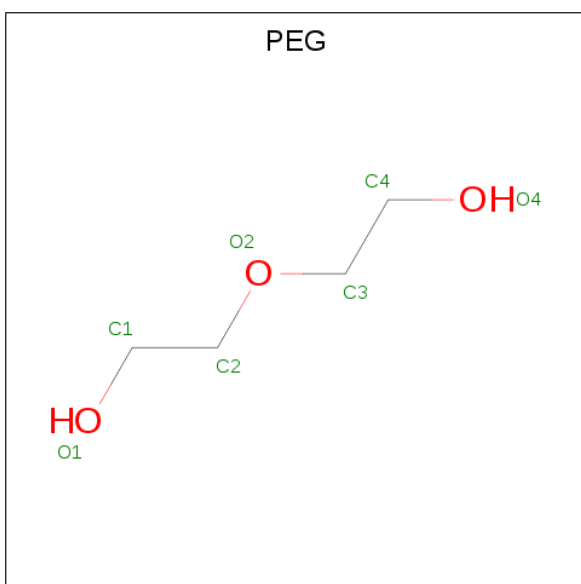
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			16	8	2	5	1		
2	B	1	Total	C	N	O	P	0	0
			16	8	2	5	1		
2	C	1	Total	C	N	O	P	0	0
			16	8	2	5	1		
2	D	1	Total	C	N	O	P	0	0
			16	8	2	5	1		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			7	4	3		

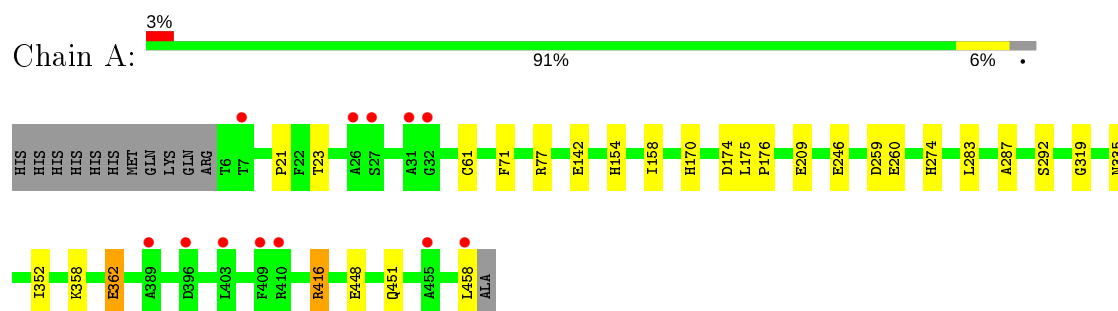
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	91	Total	O	0	0
			91	91		
5	B	123	Total	O	0	0
			123	123		
5	C	155	Total	O	0	0
			155	155		
5	D	110	Total	O	0	0
			110	110		

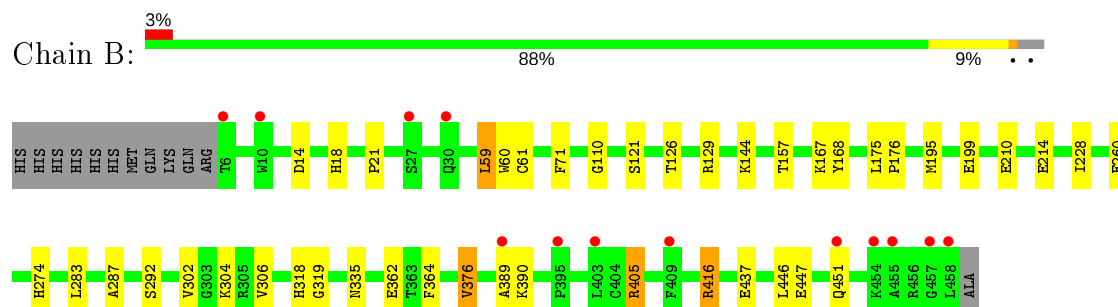
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

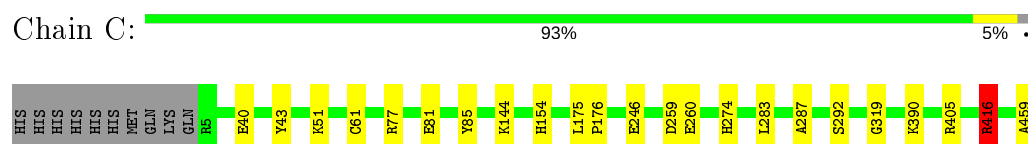
- Molecule 1: Probable aminotransferase



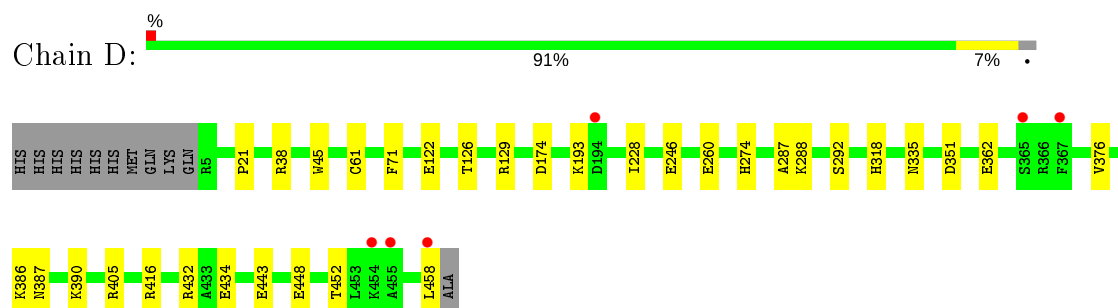
- Molecule 1: Probable aminotransferase



- Molecule 1: Probable aminotransferase



- Molecule 1: Probable aminotransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.91Å 61.97Å 118.81Å 75.07° 81.31° 75.30°	Depositor
Resolution (Å)	48.09 – 1.67 48.04 – 1.67	Depositor EDS
% Data completeness (in resolution range)	91.9 (48.09-1.67) 91.9 (48.04-1.67)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.71 (at 1.67Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.161 , 0.185 0.173 , 0.194	Depositor DCC
$R_{free}$ test set	8608 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.3	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 46.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	14848	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.40% 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: PEG, PMP, EDO

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	0.87	5/3651 (0.1%)	0.88	1/4943 (0.0%)
1	B	0.87	5/3651 (0.1%)	0.91	2/4943 (0.0%)
1	C	0.91	1/3675 (0.0%)	0.94	2/4974 (0.0%)
1	D	0.91	7/3670 (0.2%)	0.90	2/4968 (0.0%)
All	All	0.89	18/14647 (0.1%)	0.91	7/19828 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	434	GLU	CD-OE2	12.00	1.38	1.25
1	B	362	GLU	CD-OE1	-11.04	1.13	1.25
1	A	362	GLU	CD-OE1	-11.03	1.13	1.25
1	D	246	GLU	CD-OE2	-9.83	1.14	1.25
1	D	362	GLU	CD-OE1	-8.52	1.16	1.25
1	A	246	GLU	CD-OE2	-8.29	1.16	1.25
1	C	246	GLU	CD-OE1	-7.74	1.17	1.25
1	D	434	GLU	CD-OE1	-7.72	1.17	1.25
1	D	362	GLU	CD-OE2	7.26	1.33	1.25
1	A	142	GLU	CD-OE1	6.58	1.32	1.25
1	A	362	GLU	CD-OE2	6.32	1.32	1.25
1	B	214	GLU	CD-OE1	5.97	1.32	1.25
1	D	122	GLU	CD-OE1	-5.89	1.19	1.25
1	B	437	GLU	CD-OE2	-5.75	1.19	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	210	GLU	CD-OE1	5.74	1.31	1.25
1	A	209	GLU	CD-OE1	-5.34	1.19	1.25
1	D	443	GLU	CD-OE2	-5.33	1.19	1.25
1	B	389	ALA	C-O	5.07	1.32	1.23

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	416	ARG	NE-CZ-NH2	7.89	124.25	120.30
1	D	362	GLU	OE1-CD-OE2	7.08	131.80	123.30
1	C	459	ALA	CA-C-O	-6.69	106.05	120.10
1	B	416	ARG	CG-CD-NE	5.61	123.58	111.80
1	D	362	GLU	CG-CD-OE2	-5.40	107.51	118.30
1	C	416	ARG	CG-CD-NE	5.30	122.94	111.80
1	B	405	ARG	CG-CD-NE	-5.22	100.83	111.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	85	TYR	Sidechain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3557	0	3455	18	0
1	B	3557	0	3455	31	0
1	C	3581	0	3481	12	0
1	D	3576	0	3478	25	0
2	A	16	0	11	0	0
2	B	16	0	11	1	0
2	C	16	0	10	0	0
2	D	16	0	11	0	0
3	A	4	0	6	1	0
3	B	4	0	6	0	0
3	D	12	0	18	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	7	0	10	1	0
4	C	7	0	10	0	0
5	A	91	0	0	1	0
5	B	123	0	0	1	0
5	C	155	0	0	1	0
5	D	110	0	0	2	0
All	All	14848	0	13962	80	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 (80) 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:351:ASP:OD1	1:D:432:ARG:NH1	2.00	0.95
1:A:21:PRO:O	1:A:23:THR:HG23	1.72	0.88
1:D:416:ARG:NH1	5:D:601:HOH:O	2.07	0.85
1:B:129:ARG:HH11	1:B:318:HIS:HD2	1.26	0.81
1:D:129:ARG:HH11	1:D:318:HIS:HD2	1.26	0.80
1:D:228:ILE:HD11	1:D:376:VAL:HG11	1.70	0.72
1:C:416:ARG:HG3	1:C:416:ARG:HH11	1.58	0.67
1:A:158:ILE:HD11	1:B:129:ARG:HG3	1.81	0.63
1:B:447:GLU:O	1:B:451:GLN:HG3	2.00	0.62
1:B:168:TYR:OH	4:B:503:PEG:H22	2.01	0.61
1:C:154:HIS:HD2	1:C:259:ASP:OD2	1.85	0.59
1:A:154:HIS:HD2	1:A:259:ASP:OD2	1.85	0.59
1:B:110:GLY:HA2	1:B:304:LYS:HE2	1.83	0.59
2:B:501:PMP:N4A	2:B:501:PMP:O3	2.36	0.58
1:A:319:GLY:HA3	1:B:21:PRO:HB3	1.87	0.57
1:D:129:ARG:HH11	1:D:318:HIS:CD2	2.16	0.57
1:B:416:ARG:HG3	1:B:416:ARG:HH11	1.70	0.57
1:C:405:ARG:HD3	5:C:739:HOH:O	2.05	0.56
1:B:14:ASP:OD1	1:B:18:HIS:HD2	1.88	0.56
1:C:77:ARG:NH1	1:C:81:GLU:OE1	2.40	0.55
1:A:260:GLU:OE2	1:A:274:HIS:HD2	1.91	0.54
1:D:126:THR:OG1	1:D:318:HIS:HE1	1.91	0.54
1:B:129:ARG:HH11	1:B:318:HIS:CD2	2.17	0.53
1:D:386:LYS:NZ	1:D:458:LEU:HD11	2.23	0.53
1:B:228:ILE:HD11	1:B:376:VAL:HG11	1.90	0.52
1:D:38:ARG:HG3	1:D:45:TRP:HB2	1.92	0.52
1:B:260:GLU:OE2	1:B:274:HIS:HD2	1.93	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:THR:OG1	1:B:318:HIS:HE1	1.93	0.51
1:D:228:ILE:HD11	1:D:376:VAL:CG1	2.40	0.50
1:D:351:ASP:OD1	1:D:432:ARG:CZ	2.60	0.50
1:C:260:GLU:OE2	1:C:274:HIS:HD2	1.95	0.50
1:D:260:GLU:OE2	1:D:274:HIS:HD2	1.95	0.49
1:D:448:GLU:O	1:D:452:THR:HG23	2.12	0.49
1:D:387:ASN:ND2	1:D:390:LYS:HE2	2.28	0.48
1:B:283:LEU:CD2	1:B:302:VAL:HG13	2.44	0.48
1:A:358:LYS:HE2	1:A:362:GLU:OE2	2.15	0.47
1:D:405:ARG:HD3	5:D:704:HOH:O	2.14	0.47
1:A:158:ILE:HD11	1:B:129:ARG:CG	2.45	0.47
5:A:637:HOH:O	1:B:18:HIS:HE1	1.97	0.47
1:A:448:GLU:O	1:A:451:GLN:HG2	2.15	0.47
1:D:129:ARG:NH1	1:D:318:HIS:HD2	2.03	0.46
1:C:40:GLU:HG3	1:C:40:GLU:O	2.16	0.45
1:C:61:CYS:O	1:C:292:SER:HA	2.16	0.45
1:A:23:THR:HG21	5:B:666:HOH:O	2.16	0.45
1:B:390:LYS:O	1:B:390:LYS:HG2	2.17	0.45
1:B:364:PHE:CD1	1:B:446:LEU:HD22	2.52	0.44
1:B:260:GLU:OE2	1:B:274:HIS:CD2	2.70	0.44
1:B:175:LEU:HB3	1:B:176:PRO:HA	2.00	0.44
1:D:61:CYS:O	1:D:292:SER:HA	2.18	0.44
1:C:319:GLY:HA3	1:D:21:PRO:HB3	2.00	0.44
1:D:260:GLU:OE2	1:D:274:HIS:CD2	2.71	0.43
1:B:129:ARG:NH1	1:B:318:HIS:HD2	2.05	0.43
1:D:351:ASP:CG	1:D:432:ARG:HH12	2.21	0.43
1:C:175:LEU:HB3	1:C:176:PRO:HA	2.01	0.43
1:A:260:GLU:OE2	1:A:274:HIS:CD2	2.69	0.43
1:C:260:GLU:OE2	1:C:274:HIS:CD2	2.71	0.43
1:D:129:ARG:HD3	1:D:318:HIS:CD2	2.53	0.43
1:A:175:LEU:HB3	1:A:176:PRO:HA	2.01	0.42
1:B:71:PHE:CZ	1:B:335:ASN:HA	2.54	0.42
1:B:59:LEU:CD2	1:B:60:TRP:CD1	3.02	0.42
1:B:129:ARG:HD3	1:B:318:HIS:CD2	2.54	0.42
1:B:283:LEU:HD21	1:B:306:VAL:HG11	2.01	0.42
1:A:352:ILE:HD12	1:A:352:ILE:HA	1.97	0.41
1:B:61:CYS:O	1:B:292:SER:HA	2.20	0.41
1:D:387:ASN:HD21	1:D:390:LYS:HE2	1.84	0.41
1:A:61:CYS:O	1:A:292:SER:HA	2.19	0.41
1:B:195:MET:HE2	1:B:199:GLU:HB3	2.01	0.41
1:C:43:TYR:CG	1:C:51:LYS:HE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:ASP:OD2	1:B:144:LYS:HG3	2.20	0.41
1:A:416:ARG:HH12	3:A:502:EDO:C2	2.34	0.41
1:D:71:PHE:CZ	1:D:335:ASN:HA	2.56	0.41
1:A:170:HIS:HA	1:A:175:LEU:HB2	2.02	0.41
1:A:21:PRO:HB3	1:B:319:GLY:HA3	2.02	0.41
1:B:126:THR:OG1	1:B:318:HIS:CE1	2.73	0.41
1:C:144:LYS:HG3	1:D:174:ASP:OD2	2.21	0.40
1:D:228:ILE:CD1	1:D:376:VAL:CG1	2.99	0.40
1:D:386:LYS:HZ1	1:D:458:LEU:HD11	1.84	0.40
1:A:71:PHE:CZ	1:A:335:ASN:HA	2.57	0.40
1:B:110:GLY:HA2	1:B:304:LYS:CE	2.51	0.40
1:B:121:SER:HB3	1:B:157:THR:HG23	2.02	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	451/465 (97%)	437 (97%)	13 (3%)	1 (0%)	47	29
1	B	451/465 (97%)	437 (97%)	13 (3%)	1 (0%)	47	29
1	C	454/465 (98%)	440 (97%)	13 (3%)	1 (0%)	47	29
1	D	453/465 (97%)	436 (96%)	15 (3%)	2 (0%)	34	17
All	All	1809/1860 (97%)	1750 (97%)	54 (3%)	5 (0%)	41	23

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	287	ALA
1	B	287	ALA
1	C	287	ALA

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Mol	Chain	Res	Type
1	D	287	ALA
1	D	288	LYS

### 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	363/374 (97%)	360 (99%)	3 (1%)	81	72
1	B	363/374 (97%)	359 (99%)	4 (1%)	73	61
1	C	365/374 (98%)	362 (99%)	3 (1%)	81	72
1	D	365/374 (98%)	364 (100%)	1 (0%)	92	89
All	All	1456/1496 (97%)	1445 (99%)	11 (1%)	81	72

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	ARG
1	A	283	LEU
1	A	458	LEU
1	B	59	LEU
1	B	167	LYS
1	B	376	VAL
1	B	405	ARG
1	C	283	LEU
1	C	390	LYS
1	C	416	ARG
1	D	193	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	154	HIS
1	A	274	HIS
1	A	451	GLN

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Mol	Chain	Res	Type
1	B	18	HIS
1	B	274	HIS
1	B	318	HIS
1	C	154	HIS
1	C	274	HIS
1	C	369	HIS
1	D	274	HIS
1	D	318	HIS

### 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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

11 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	PMP	D	501	-	16,16,16	1.01	1 (6%)	21,23,23	1.15	0
3	EDO	D	504	-	3,3,3	0.21	0	2,2,2	0.37	0
4	PEG	C	502	-	6,6,6	0.44	0	5,5,5	0.30	0
2	PMP	A	501	-	16,16,16	1.00	1 (6%)	21,23,23	1.36	3 (14%)
2	PMP	C	501	-	16,16,16	0.60	0	21,23,23	1.06	2 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	EDO	A	502	-	3,3,3	0.13	0	2,2,2	0.26	0
3	EDO	D	502	-	3,3,3	0.19	0	2,2,2	0.28	0
3	EDO	B	502	-	3,3,3	0.18	0	2,2,2	0.26	0
3	EDO	D	503	-	3,3,3	0.24	0	2,2,2	0.29	0
2	PMP	B	501	-	16,16,16	1.12	1 (6%)	21,23,23	1.09	2 (9%)
4	PEG	B	503	-	6,6,6	0.15	0	5,5,5	0.09	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PMP	D	501	-	-	2/8/8/8	0/1/1/1
3	EDO	D	504	-	-	1/1/1/1	-
4	PEG	C	502	-	-	4/4/4/4	-
2	PMP	A	501	-	-	2/8/8/8	0/1/1/1
2	PMP	C	501	-	-	2/8/8/8	0/1/1/1
3	EDO	A	502	-	-	1/1/1/1	-
3	EDO	D	502	-	-	0/1/1/1	-
3	EDO	B	502	-	-	1/1/1/1	-
3	EDO	D	503	-	-	1/1/1/1	-
2	PMP	B	501	-	-	2/8/8/8	0/1/1/1
4	PEG	B	503	-	-	2/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	PMP	P-O1P	2.94	1.60	1.50
2	A	501	PMP	C3-C2	2.83	1.43	1.40
2	D	501	PMP	P-O3P	-2.21	1.46	1.54

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	PMP	O4P-P-O1P	2.79	114.29	106.47
2	A	501	PMP	O3-C3-C2	2.57	123.10	117.49
2	A	501	PMP	O3P-P-O4P	-2.57	99.89	106.73
2	B	501	PMP	O3-C3-C2	2.43	122.80	117.49
2	B	501	PMP	O2P-P-O4P	2.20	112.58	106.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	PMP	O3P-P-O2P	2.17	115.92	107.64
2	C	501	PMP	C4A-C4-C3	2.15	123.76	120.34

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	501	PMP	C3-C4-C4A-N4A
2	A	501	PMP	C3-C4-C4A-N4A
2	C	501	PMP	C3-C4-C4A-N4A
2	B	501	PMP	C3-C4-C4A-N4A
2	C	501	PMP	C5-C4-C4A-N4A
3	D	504	EDO	O1-C1-C2-O2
3	B	502	EDO	O1-C1-C2-O2
4	C	502	PEG	O2-C3-C4-O4
4	B	503	PEG	O2-C3-C4-O4
2	D	501	PMP	C5-C4-C4A-N4A
2	A	501	PMP	C5-C4-C4A-N4A
2	B	501	PMP	C5-C4-C4A-N4A
4	C	502	PEG	O1-C1-C2-O2
4	C	502	PEG	C4-C3-O2-C2
4	C	502	PEG	C1-C2-O2-C3
3	A	502	EDO	O1-C1-C2-O2
3	D	503	EDO	O1-C1-C2-O2
4	B	503	PEG	C4-C3-O2-C2

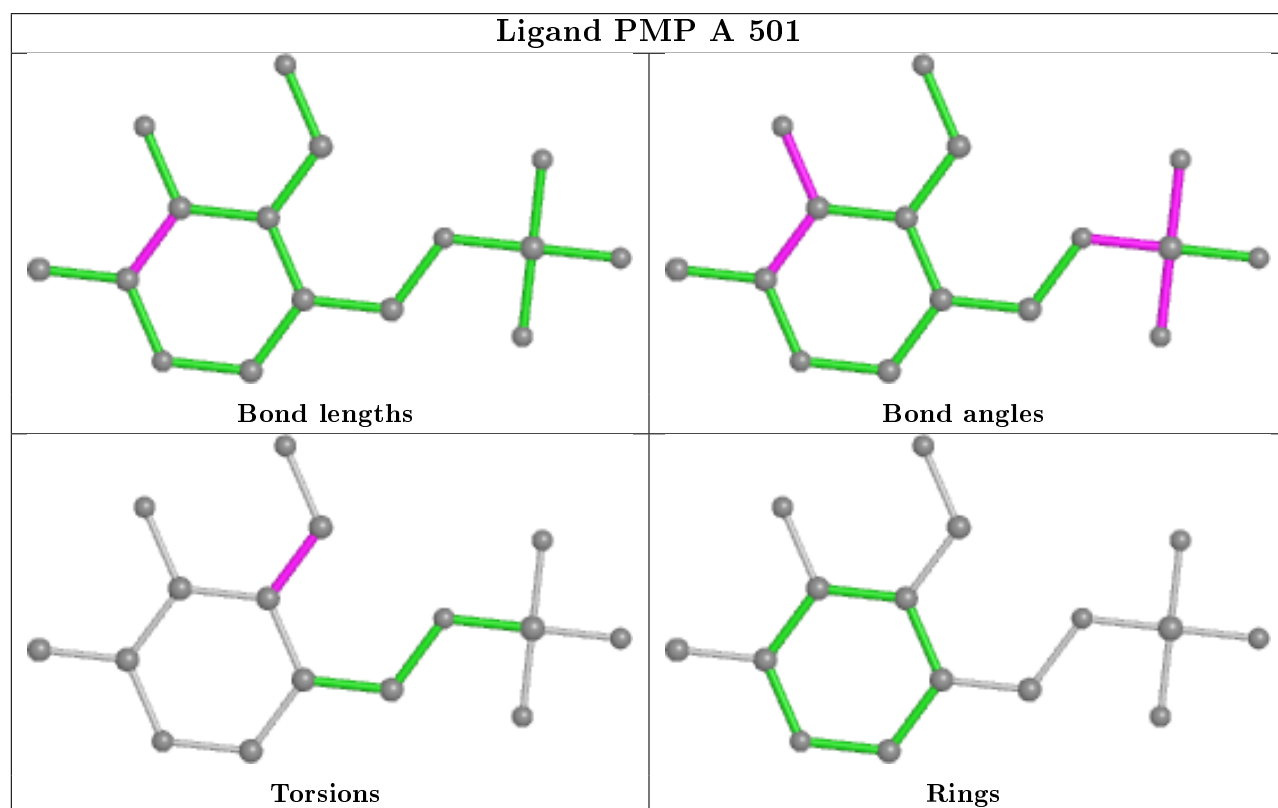
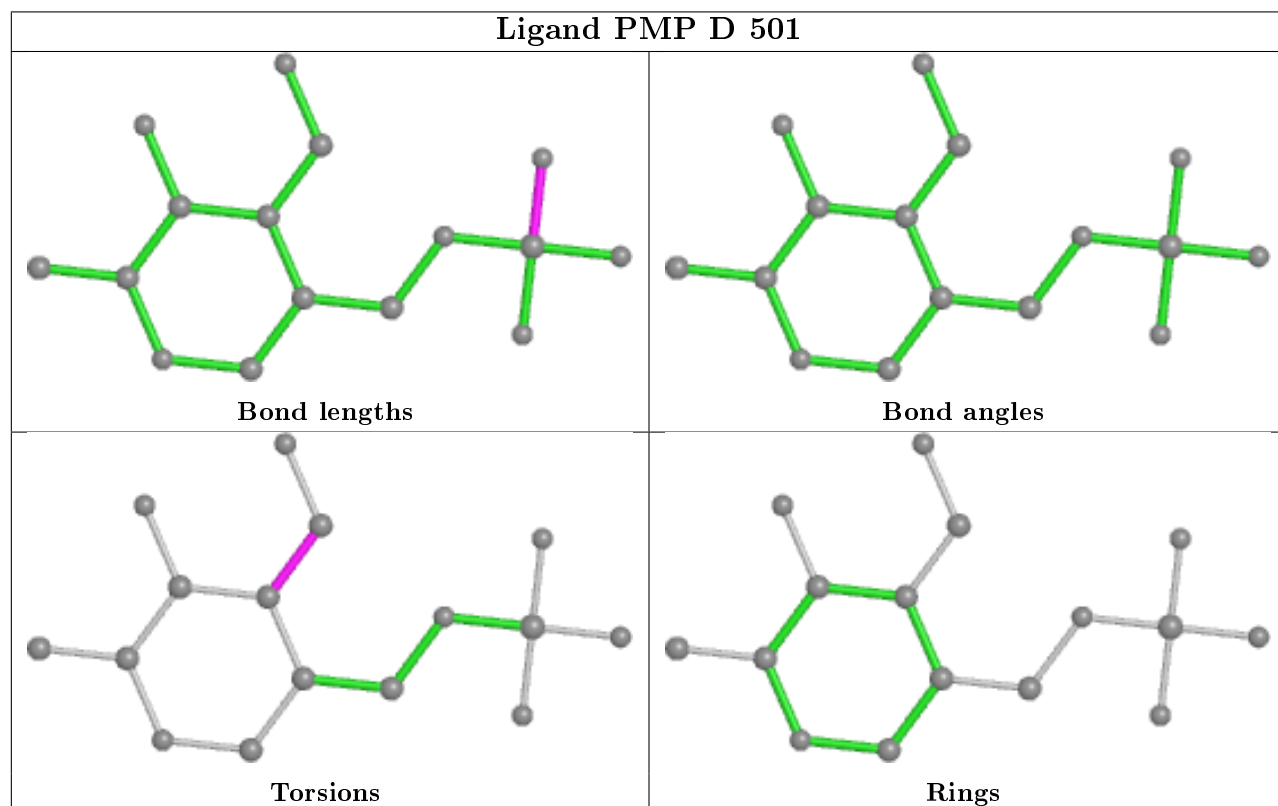
There are no ring outliers.

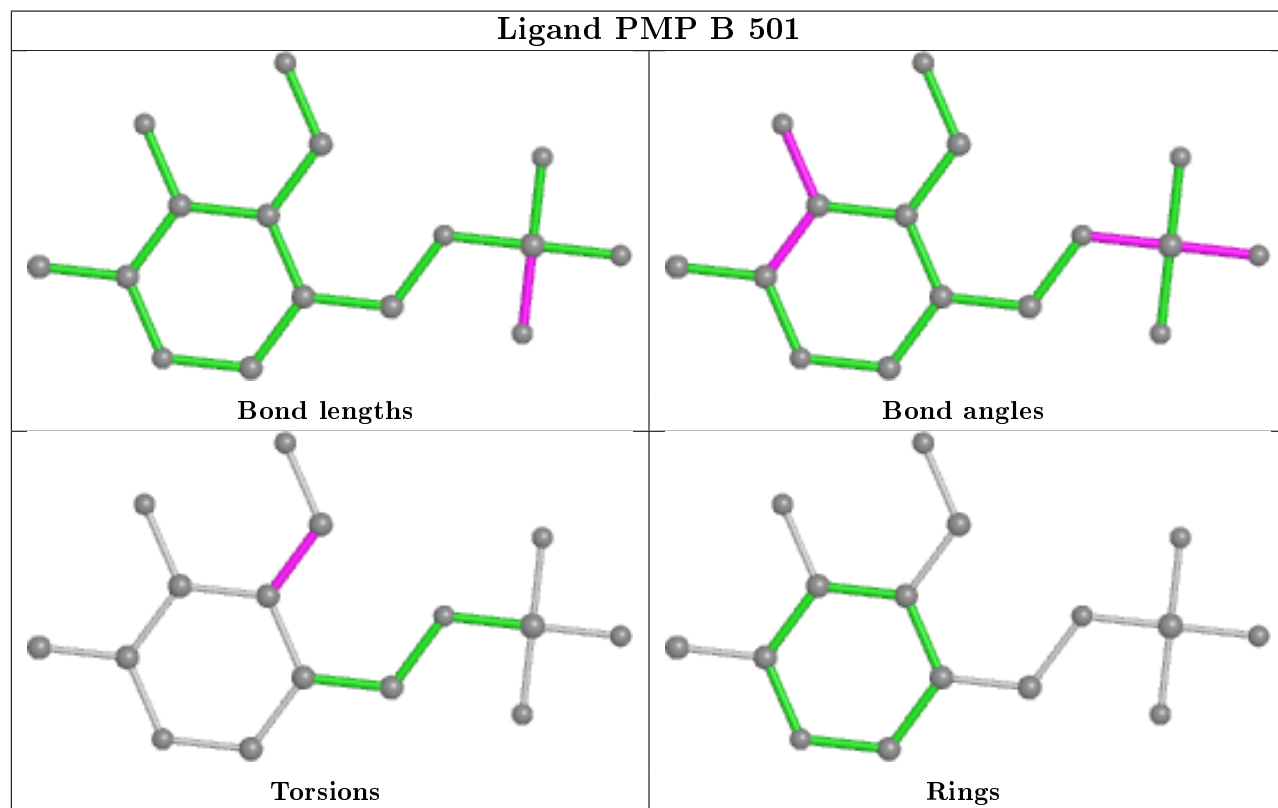
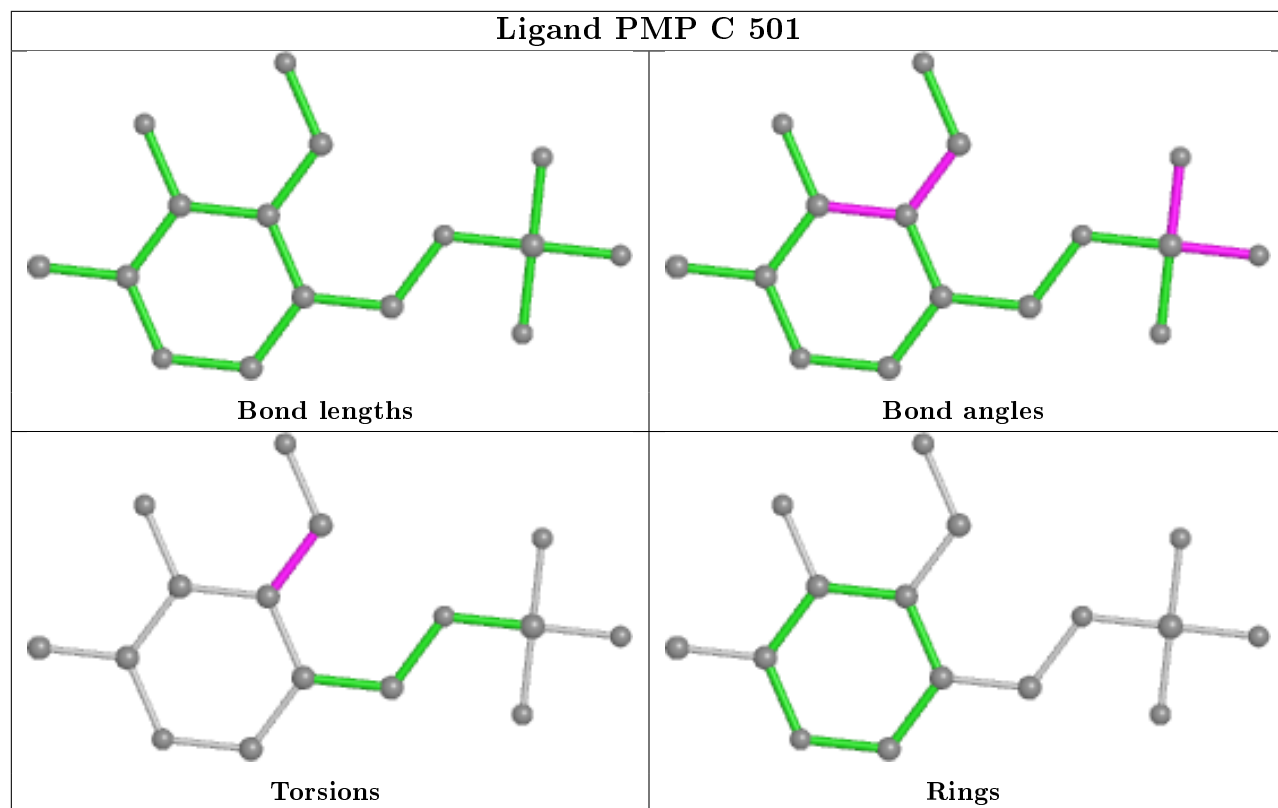
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	EDO	1	0
2	B	501	PMP	1	0
4	B	503	PEG	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 ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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<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	453/465 (97%)	-0.05	12 (2%) 56 58	17, 29, 51, 74	0
1	B	453/465 (97%)	-0.18	13 (2%) 51 54	15, 26, 47, 66	0
1	C	455/465 (97%)	-0.40	0 100 100	12, 20, 36, 49	0
1	D	454/465 (97%)	-0.28	6 (1%) 77 80	14, 26, 46, 69	0
All	All	1815/1860 (97%)	-0.23	31 (1%) 70 74	12, 25, 46, 74	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	458	LEU	6.0
1	D	194	ASP	4.3
1	D	455	ALA	3.5
1	A	409	PHE	3.2
1	A	403	LEU	3.1
1	B	451	GLN	3.0
1	B	6	THR	2.9
1	D	365	SER	2.8
1	B	30	GLN	2.8
1	D	454	LYS	2.8
1	B	403	LEU	2.7
1	D	458	LEU	2.7
1	A	455	ALA	2.6
1	B	395	PRO	2.6
1	A	396	ASP	2.5
1	B	10	TRP	2.5
1	D	367	PHE	2.5
1	B	455	ALA	2.4
1	B	457	GLY	2.4
1	A	32	GLY	2.4
1	B	389	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	26	ALA	2.4
1	B	454	LYS	2.3
1	B	27	SER	2.3
1	A	458	LEU	2.3
1	A	410	ARG	2.2
1	A	389	ALA	2.2
1	B	409	PHE	2.1
1	A	31	ALA	2.1
1	A	27	SER	2.1
1	A	7	THR	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 carbohydrates in this entry.

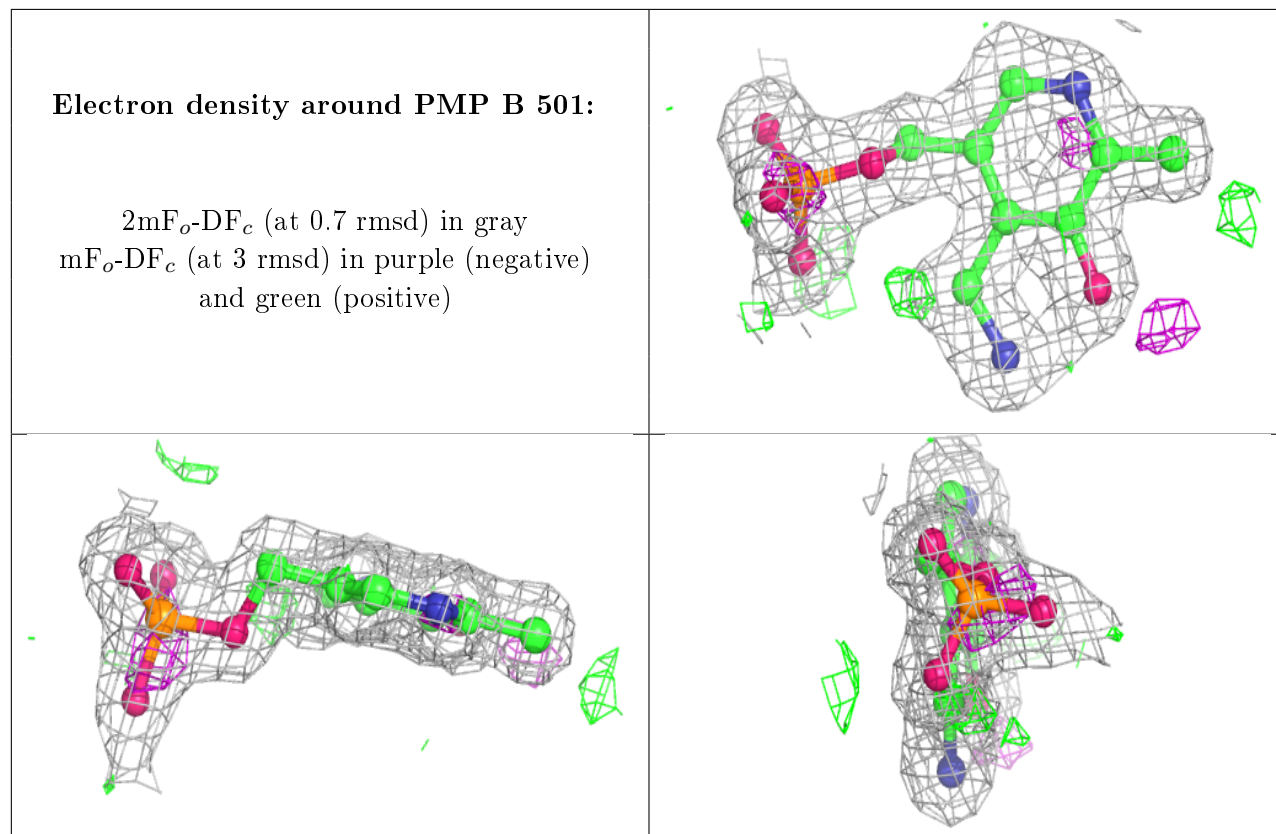
## 6.4 Ligands [i](#)

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<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
3	EDO	D	504	4/4	0.82	0.13	33,37,41,41	0
4	PEG	C	502	7/7	0.84	0.14	26,39,48,53	0
3	EDO	B	502	4/4	0.84	0.12	48,50,54,55	0
3	EDO	D	503	4/4	0.85	0.11	42,45,45,51	0
4	PEG	B	503	7/7	0.85	0.17	43,45,50,52	0
3	EDO	D	502	4/4	0.91	0.10	49,51,53,54	0
3	EDO	A	502	4/4	0.93	0.14	45,46,46,49	0
2	PMP	B	501	16/16	0.96	0.09	20,24,26,28	0
2	PMP	A	501	16/16	0.97	0.07	20,22,27,29	0
2	PMP	C	501	16/16	0.97	0.07	13,15,18,20	0
2	PMP	D	501	16/16	0.98	0.06	15,17,20,24	0

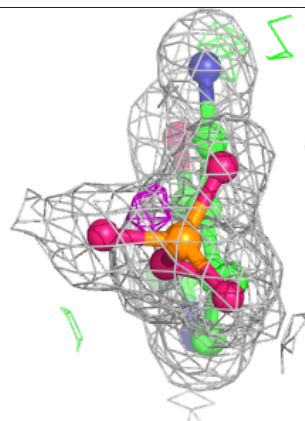
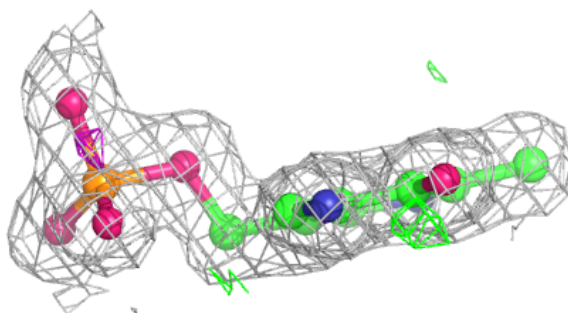
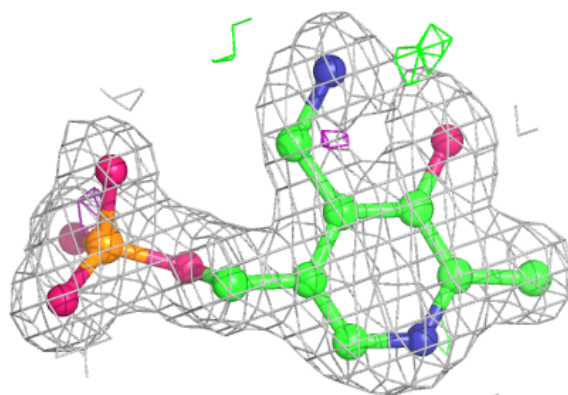
The following is a graphical depiction of the model fit to experimental electron density of all

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.

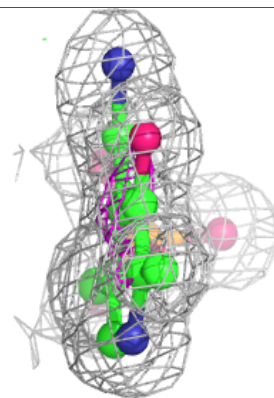
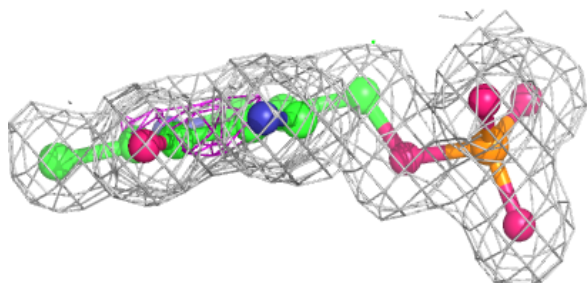
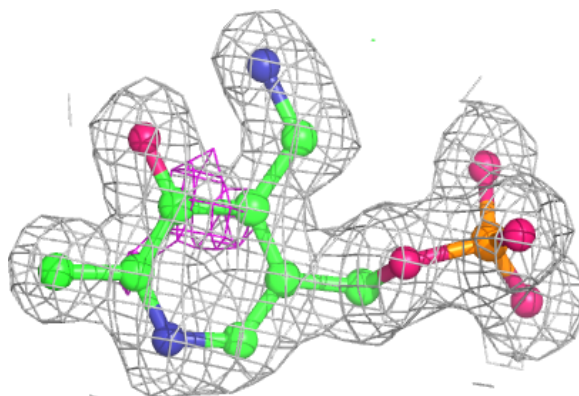


**Electron density around PMP A 501:**

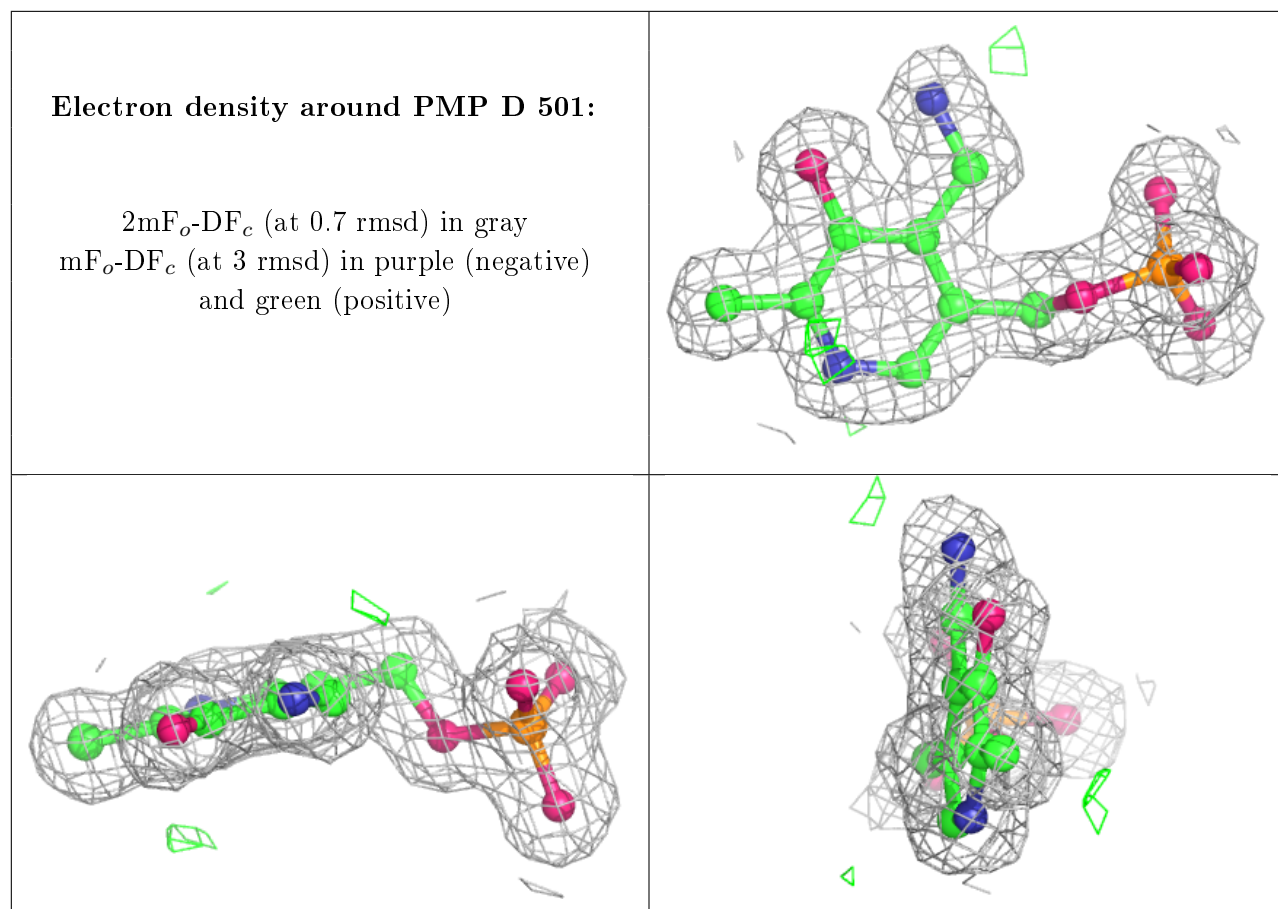
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around PMP 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.