



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 30, 2026 – 10:49 AM UTC

PDB ID : 6S4G / pdb_00006s4g
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

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

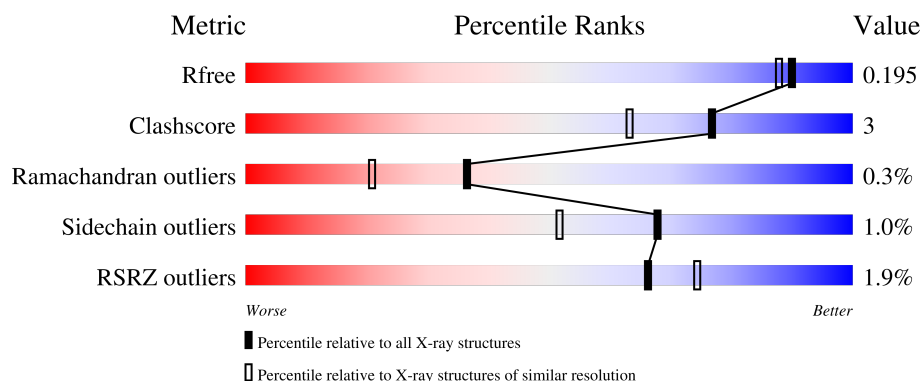
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.67 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}	180053	1054 (1.68-1.68)
Clashscore	190562	1078 (1.68-1.68)
Ramachandran outliers	187476	1068 (1.68-1.68)
Sidechain outliers	187428	1067 (1.68-1.68)
RSRZ outliers	180081	1055 (1.68-1.68)

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	465	3% 90% 7%
1	B	465	2% 87% 10%
1	C	465	91% 7%
1	D	465	% 89% 8%

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:

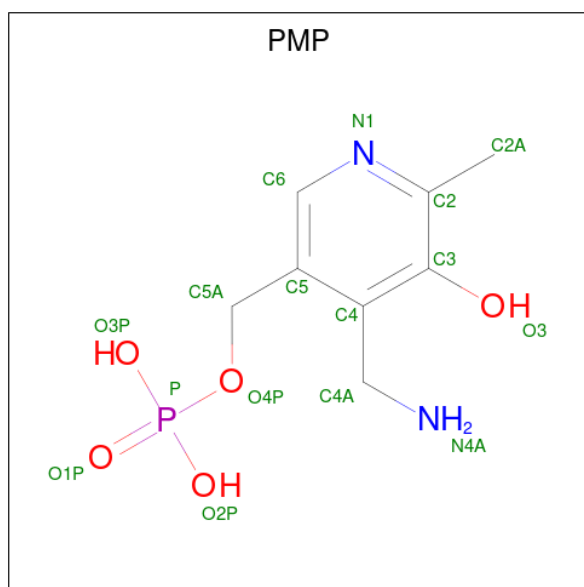
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP Q7NWX4
A	-4	HIS	-	expression tag	UNP Q7NWX4
A	-3	HIS	-	expression tag	UNP Q7NWX4
A	-2	HIS	-	expression tag	UNP Q7NWX4
A	-1	HIS	-	expression tag	UNP Q7NWX4
A	0	HIS	-	expression tag	UNP Q7NWX4
B	-5	HIS	-	expression tag	UNP Q7NWX4
B	-4	HIS	-	expression tag	UNP Q7NWX4
B	-3	HIS	-	expression tag	UNP Q7NWX4
B	-2	HIS	-	expression tag	UNP Q7NWX4
B	-1	HIS	-	expression tag	UNP Q7NWX4
B	0	HIS	-	expression tag	UNP Q7NWX4
C	-5	HIS	-	expression tag	UNP Q7NWX4
C	-4	HIS	-	expression tag	UNP Q7NWX4
C	-3	HIS	-	expression tag	UNP Q7NWX4
C	-2	HIS	-	expression tag	UNP Q7NWX4
C	-1	HIS	-	expression tag	UNP Q7NWX4
C	0	HIS	-	expression tag	UNP Q7NWX4
D	-5	HIS	-	expression tag	UNP Q7NWX4
D	-4	HIS	-	expression tag	UNP Q7NWX4
D	-3	HIS	-	expression tag	UNP Q7NWX4

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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 (CCD ID: PMP) (formula: $C_8H_{13}N_2O_5P$) (labeled as "Ligand of Interest" by depositor).



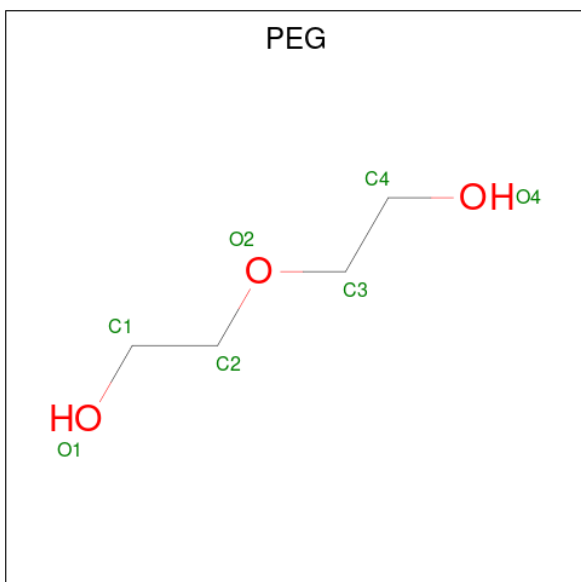
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			16	8	2	5	1		
2	B	1	Total	C	N	O	P	0	0
			16	8	2	5	1		
2	C	1	Total	C	N	O	P	0	0
			16	8	2	5	1		
2	D	1	Total	C	N	O	P	0	0
			16	8	2	5	1		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: 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 (CCD ID: 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		

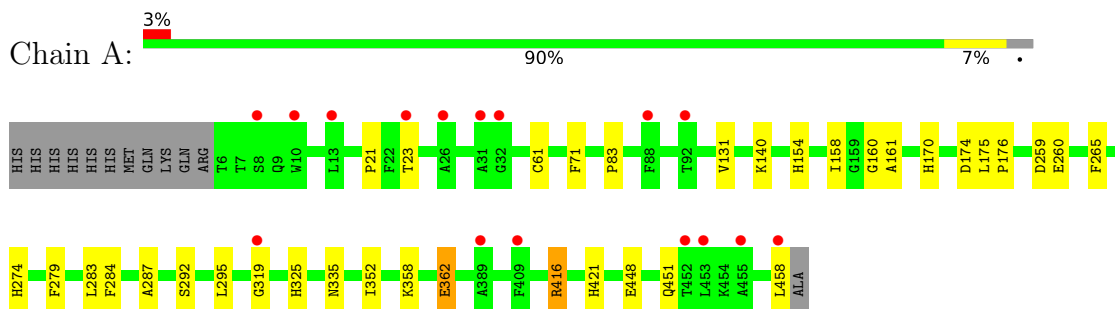
- Molecule 5 is water.

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		

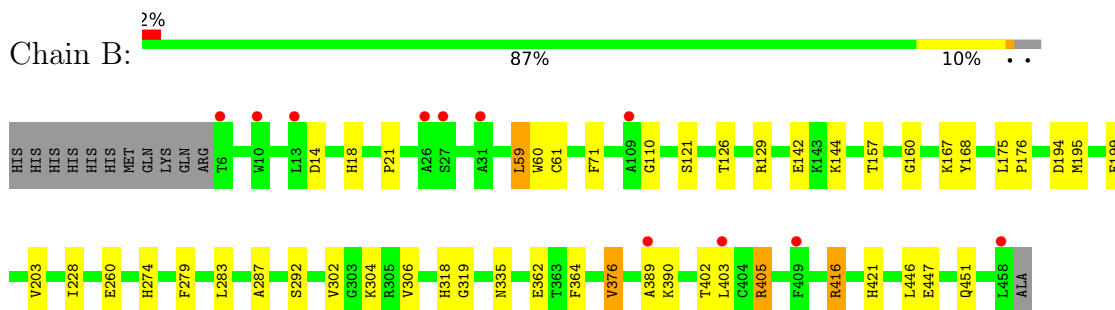
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

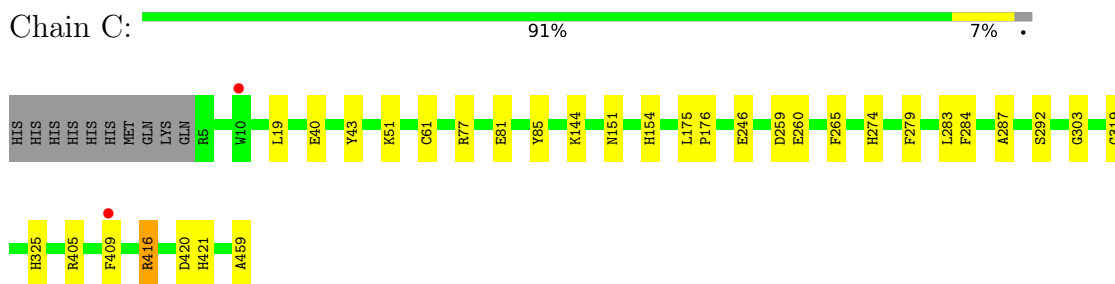
- Molecule 1: Probable aminotransferase



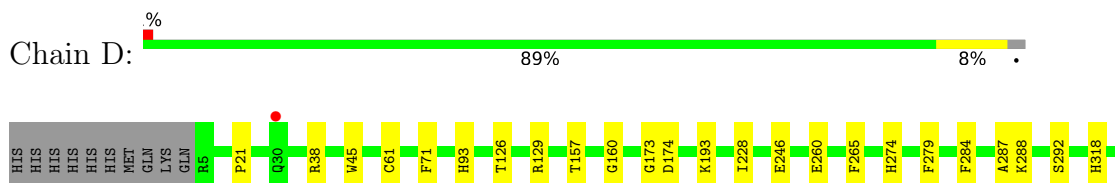
- Molecule 1: Probable aminotransferase

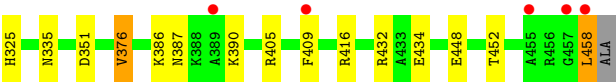


- Molecule 1: Probable aminotransferase



- Molecule 1: Probable aminotransferase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	60.91Å 61.97Å 118.81Å 75.07° 81.31° 75.30°	Depositor
Resolution (Å)	48.09 – 1.67 48.09 – 1.67	Depositor EDS
% Data completeness (in resolution range)	91.9 (48.09-1.67) 91.9 (48.09-1.67)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 1.67Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.161 , 0.185 0.173 , 0.195	Depositor DCC
R_{free} test set	8608 reflections (4.59%)	wwPDB-VP
Wilson B-factor (Å ²)	21.3	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 33.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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 ²)	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.*

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: EDO, PEG, PMP

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	1.15	7/3651 (0.2%)	1.22	5/4943 (0.1%)
1	B	1.15	4/3651 (0.1%)	1.25	5/4943 (0.1%)
1	C	1.21	5/3675 (0.1%)	1.28	8/4974 (0.2%)
1	D	1.16	6/3670 (0.2%)	1.24	5/4968 (0.1%)
All	All	1.17	22/14647 (0.2%)	1.25	23/19828 (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	C	0	1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	325	HIS	CE1-NE2	8.87	1.41	1.32
1	B	389	ALA	C-O	7.75	1.32	1.24
1	D	434	GLU	CD-OE2	7.10	1.38	1.25
1	C	325	HIS	CE1-NE2	6.90	1.39	1.32
1	D	160	GLY	C-O	6.52	1.31	1.23
1	B	421	HIS	CE1-NE2	6.27	1.38	1.32
1	A	161	ALA	C-O	6.24	1.31	1.24
1	B	362	GLU	CD-OE1	-6.24	1.13	1.25
1	A	362	GLU	CD-OE1	-6.23	1.13	1.25
1	C	421	HIS	CG-ND1	6.00	1.44	1.38
1	C	420	ASP	C-O	5.88	1.31	1.24
1	A	83	PRO	C-O	-5.72	1.17	1.24
1	A	421	HIS	CE1-NE2	5.60	1.38	1.32
1	D	93	HIS	CE1-NE2	5.59	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	295	LEU	N-CA	5.56	1.51	1.45
1	D	246	GLU	CD-OE2	-5.53	1.14	1.25
1	C	19	LEU	C-O	5.49	1.30	1.24
1	A	325	HIS	CE1-NE2	5.20	1.37	1.32
1	B	160	GLY	C-O	5.18	1.30	1.23
1	D	173	GLY	C-O	5.10	1.29	1.24
1	C	303	GLY	C-O	5.09	1.29	1.23
1	A	160	GLY	C-O	5.00	1.29	1.23

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	459	ALA	CA-C-O	-8.68	106.05	120.80
1	A	284	PHE	CA-CB-CG	7.03	120.83	113.80
1	B	194	ASP	CA-CB-CG	-6.30	106.30	112.60
1	C	409	PHE	CA-CB-CG	6.03	119.83	113.80
1	C	265	PHE	CA-CB-CG	-6.03	107.77	113.80
1	B	279	PHE	CA-CB-CG	5.87	119.67	113.80
1	D	265	PHE	CA-CB-CG	-5.65	108.15	113.80
1	A	416	ARG	NE-CZ-NH2	5.61	124.25	119.20
1	C	151	ASN	CA-C-N	5.54	125.60	120.34
1	C	151	ASN	C-N-CA	5.54	125.60	120.34
1	C	246	GLU	CB-CG-CD	5.50	121.96	112.60
1	A	265	PHE	CA-CB-CG	-5.41	108.39	113.80
1	C	284	PHE	CA-CB-CG	5.39	119.19	113.80
1	B	402	THR	CA-CB-OG1	-5.33	101.60	109.60
1	D	279	PHE	CA-CB-CG	5.32	119.12	113.80
1	B	416	ARG	CG-CD-NE	5.26	123.58	112.00
1	D	157	THR	N-CA-C	-5.25	103.96	110.41
1	A	131	VAL	N-CA-CB	5.20	118.38	110.58
1	D	284	PHE	CA-CB-CG	5.16	118.96	113.80
1	B	405	ARG	CG-CD-NE	-5.08	100.83	112.00
1	C	279	PHE	CA-CB-CG	5.07	118.87	113.80
1	A	279	PHE	CA-CB-CG	5.03	118.83	113.80
1	D	409	PHE	CA-CB-CG	5.02	118.82	113.80

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	33	0
1	C	3581	0	3481	12	0
1	D	3576	0	3478	26	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
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	83	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 (83) 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:B:195:MET:HE2	1:B:199:GLU:HB3	1.64	0.79
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O3	2:B:501:PMP:N4A	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:HH11	1:B:416:ARG:HG3	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
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:B:195:MET:HE1	1:B:203:VAL:CG2	2.43	0.49
1:D:351:ASP:CG	1:D:432:ARG:HH12	2.21	0.48
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:O	1:C:40:GLU:HG3	2.16	0.45
1:D:386:LYS:HZ1	1:D:458:LEU:HD11	1.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:195:MET:HE1	1:B:203:VAL:HG21	2.00	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:351:ASP:CG	1:D:432:ARG:NH1	2.76	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:C:43:TYR:CG	1:C:51:LYS:HE2	2.56	0.41
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: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%)	43	27
1	B	451/465 (97%)	437 (97%)	13 (3%)	1 (0%)	43	27
1	C	454/465 (98%)	440 (97%)	13 (3%)	1 (0%)	43	27
1	D	453/465 (97%)	436 (96%)	15 (3%)	2 (0%)	30	13
All	All	1809/1860 (97%)	1750 (97%)	54 (3%)	5 (0%)	36	21

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	287	ALA
1	B	287	ALA
1	C	287	ALA
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%)	73	59
1	B	363/374 (97%)	357 (98%)	6 (2%)	53	29
1	C	365/374 (98%)	363 (100%)	2 (0%)	81	72
1	D	365/374 (98%)	362 (99%)	3 (1%)	73	59
All	All	1456/1496 (97%)	1442 (99%)	14 (1%)	68	52

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	140	LYS

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Mol	Chain	Res	Type
1	A	283	LEU
1	A	458	LEU
1	B	59	LEU
1	B	142	GLU
1	B	167	LYS
1	B	376	VAL
1	B	403	LEU
1	B	405	ARG
1	C	283	LEU
1	C	416	ARG
1	D	193	LYS
1	D	376	VAL
1	D	458	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	ASN
1	A	154	HIS
1	A	274	HIS
1	B	18	HIS
1	B	151	ASN
1	B	274	HIS
1	B	318	HIS
1	C	151	ASN
1	C	154	HIS
1	C	274	HIS
1	C	276	HIS
1	C	369	HIS
1	D	274	HIS
1	D	318	HIS

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 [i](#)

There are no oligosaccharides 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	$\# Z > 2$
3	EDO	B	502	-	3,3,3	0.18	0	2,2,2	0.18	0
2	PMP	D	501	-	16,16,16	1.04	1 (6%)	22,23,23	1.17	0
3	EDO	D	504	-	3,3,3	0.21	0	2,2,2	0.29	0
2	PMP	A	501	-	16,16,16	1.00	1 (6%)	22,23,23	1.41	3 (13%)
2	PMP	B	501	-	16,16,16	1.15	1 (6%)	22,23,23	1.13	2 (9%)
3	EDO	D	502	-	3,3,3	0.19	0	2,2,2	0.21	0
3	EDO	A	502	-	3,3,3	0.13	0	2,2,2	0.19	0
4	PEG	B	503	-	6,6,6	0.14	0	5,5,5	0.08	0
3	EDO	D	503	-	3,3,3	0.24	0	2,2,2	0.21	0
4	PEG	C	502	-	6,6,6	0.44	0	5,5,5	0.29	0
2	PMP	C	501	-	16,16,16	0.62	0	22,23,23	1.06	2 (9%)

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	EDO	B	502	-	-	1/1/1/1	-
2	PMP	D	501	-	-	1/8/8/8	0/1/1/1
3	EDO	D	504	-	-	1/1/1/1	-
2	PMP	A	501	-	-	1/8/8/8	0/1/1/1
2	PMP	B	501	-	-	1/8/8/8	0/1/1/1
3	EDO	D	502	-	-	0/1/1/1	-
3	EDO	A	502	-	-	1/1/1/1	-
4	PEG	B	503	-	-	3/4/4/4	-

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	PMP	P-O1P	3.07	1.60	1.50
2	A	501	PMP	C3-C2	2.66	1.43	1.41
2	D	501	PMP	P-O3P	-2.28	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	2.91	114.29	106.44
2	A	501	PMP	O3-C3-C2	2.66	123.10	117.58
2	A	501	PMP	O3P-P-O4P	-2.60	99.89	106.67
2	B	501	PMP	O3-C3-C2	2.52	122.80	117.58
2	B	501	PMP	O2P-P-O4P	2.27	112.58	106.67
2	C	501	PMP	O3P-P-O2P	2.16	115.92	107.80
2	C	501	PMP	C4A-C4-C3	2.09	123.76	120.22

There are no chirality outliers.

All (16) torsion outliers are listed below:

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

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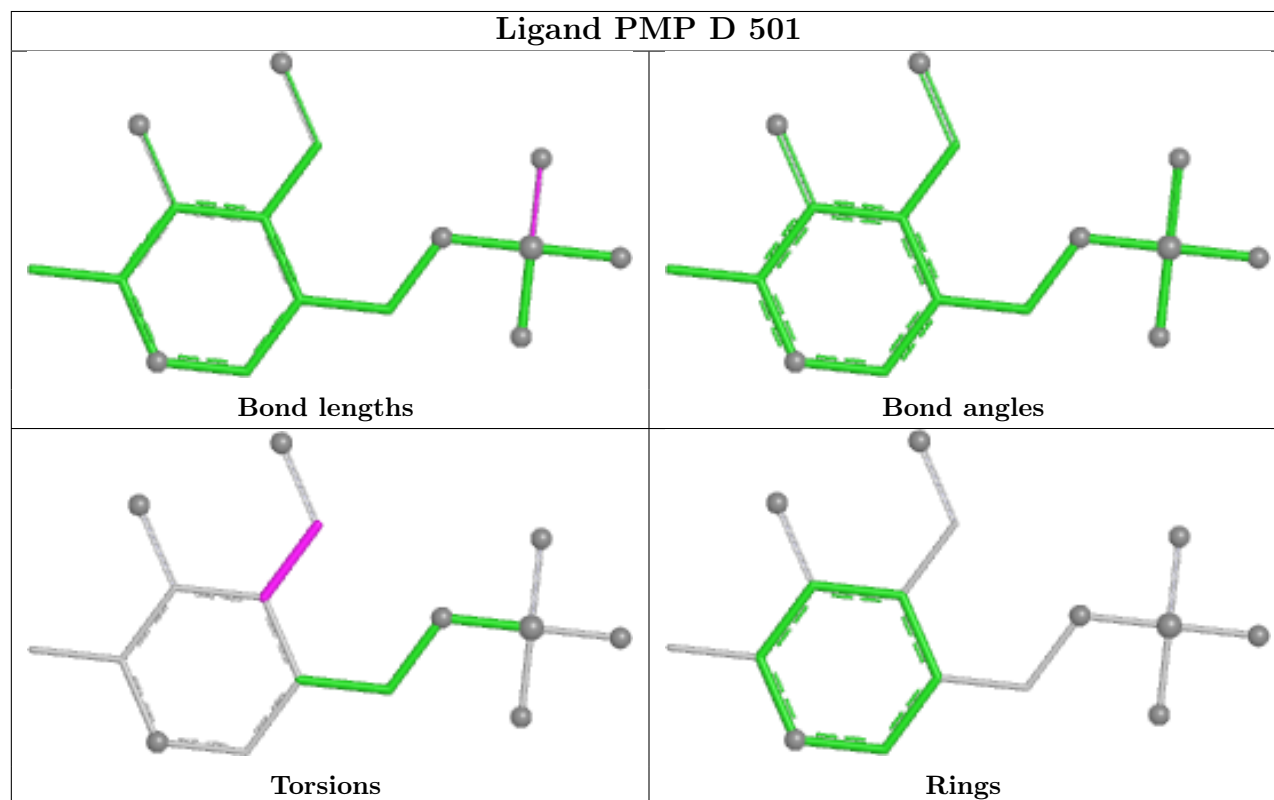
Mol	Chain	Res	Type	Atoms
4	B	503	PEG	C1-C2-O2-C3

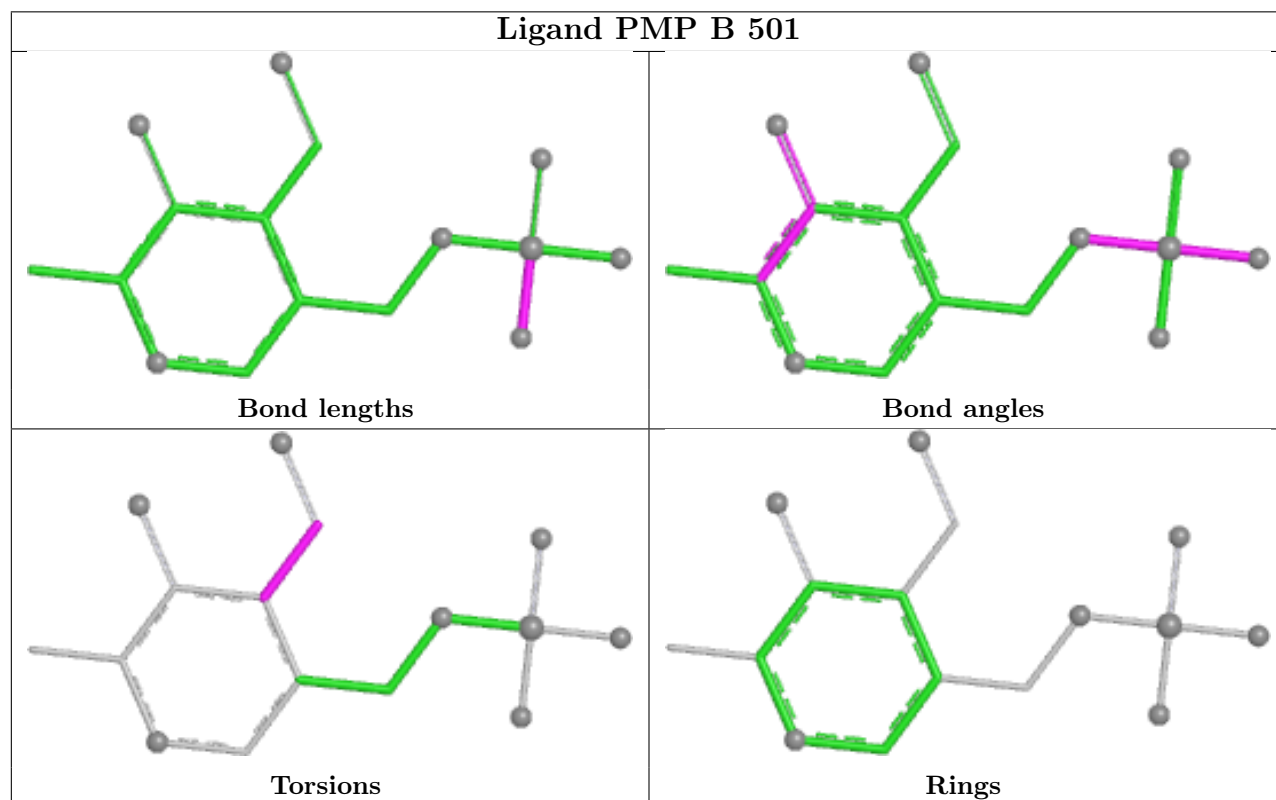
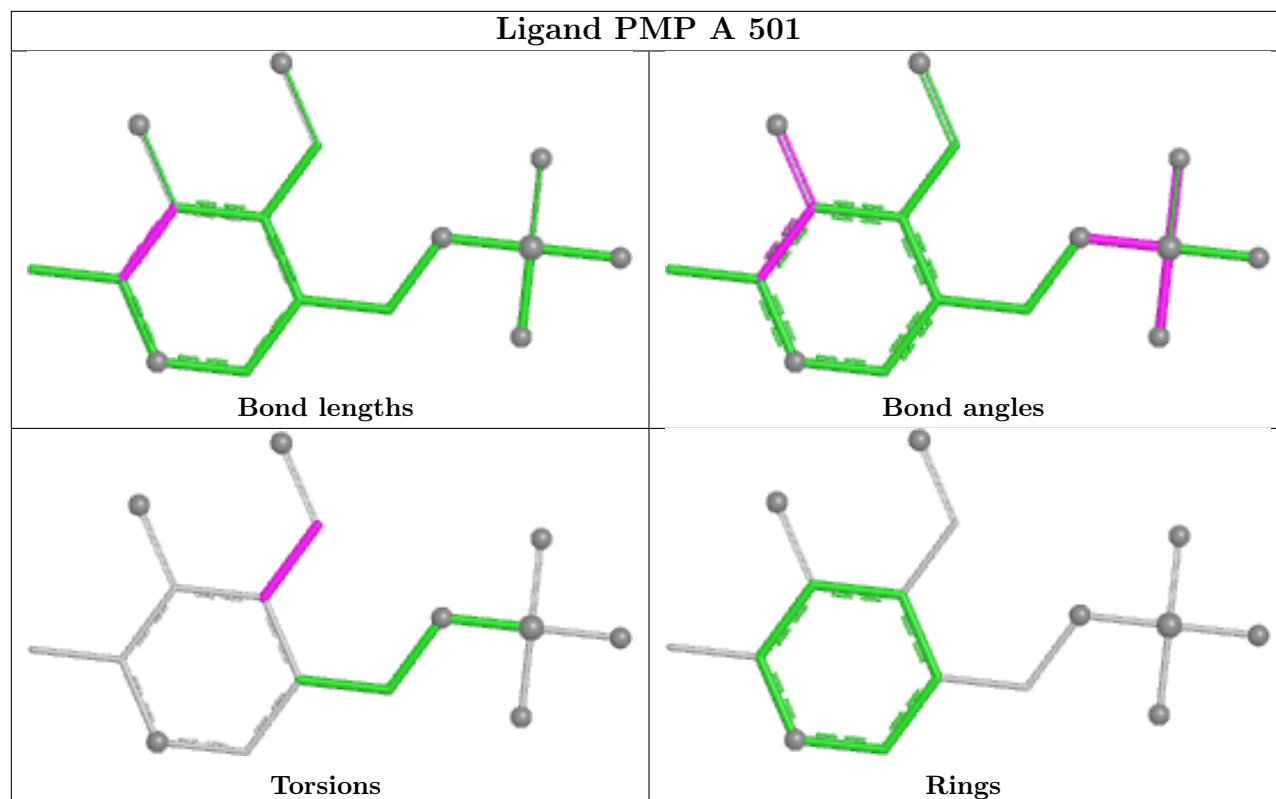
There are no ring outliers.

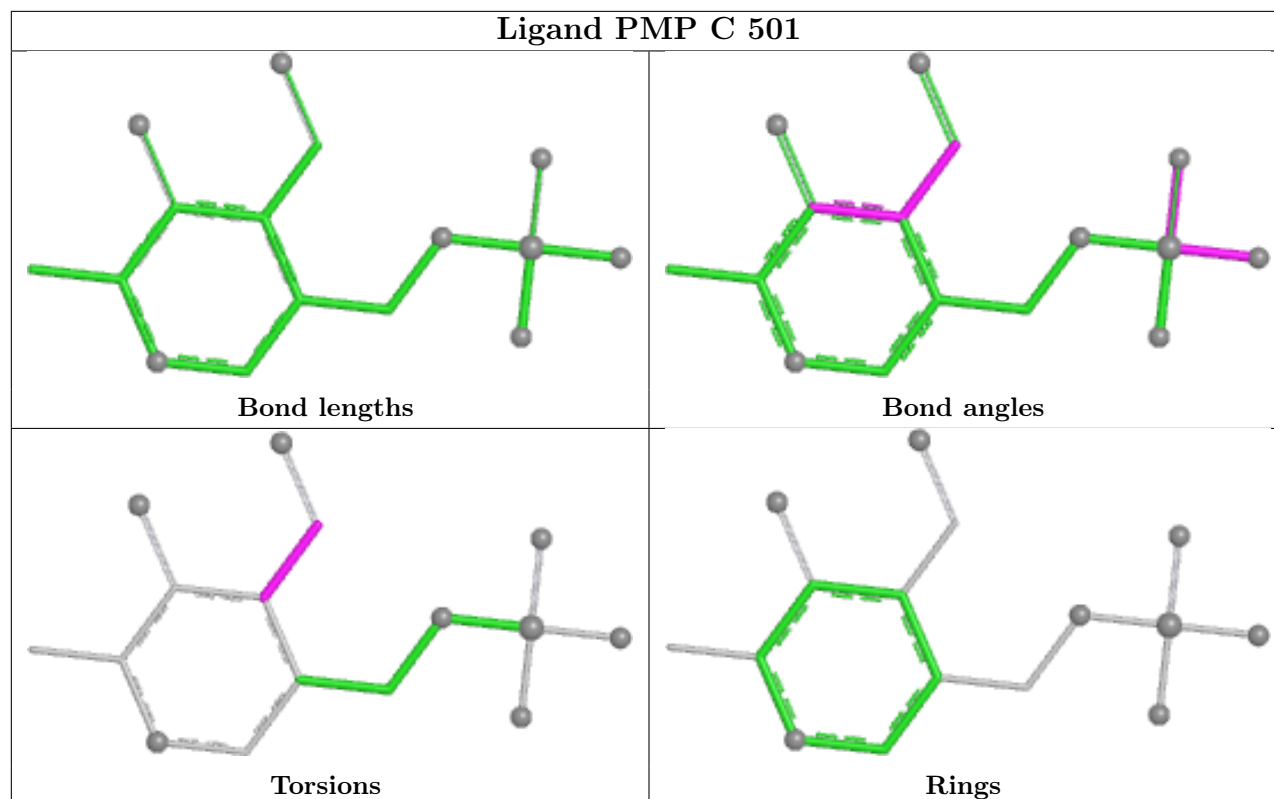
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	PMP	1	0
3	A	502	EDO	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 [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	453/465 (97%)	0.20	16 (3%) 47 55	17, 29, 51, 74	0
1	B	453/465 (97%)	0.07	11 (2%) 59 67	15, 26, 47, 66	0
1	C	455/465 (97%)	-0.27	2 (0%) 88 93	9, 20, 36, 49	1 (0%)
1	D	454/465 (97%)	-0.04	6 (1%) 75 83	13, 26, 46, 69	1 (0%)
All	All	1815/1860 (97%)	-0.01	35 (1%) 66 74	9, 25, 46, 74	2 (0%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	458	LEU	5.0
1	D	458	LEU	4.8
1	D	389	ALA	3.4
1	A	455	ALA	3.3
1	B	10	TRP	3.2
1	B	409	PHE	3.1
1	A	31	ALA	2.9
1	B	389	ALA	2.9
1	D	457	GLY	2.8
1	B	26	ALA	2.7
1	B	6	THR	2.7
1	C	10	TRP	2.7
1	A	458	LEU	2.7
1	D	30	GLN	2.6
1	A	23	THR	2.6
1	B	109	ALA	2.6
1	A	26	ALA	2.5
1	A	13	LEU	2.5
1	B	403	LEU	2.5
1	A	389	ALA	2.4
1	D	455	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	27	SER	2.3
1	A	32	GLY	2.3
1	A	319	GLY	2.3
1	A	10	TRP	2.2
1	B	13	LEU	2.2
1	A	88	PHE	2.2
1	C	409	PHE	2.2
1	D	409	PHE	2.2
1	A	453	LEU	2.1
1	B	31	ALA	2.1
1	A	92	THR	2.1
1	A	409	PHE	2.1
1	A	8	SER	2.0
1	A	452	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

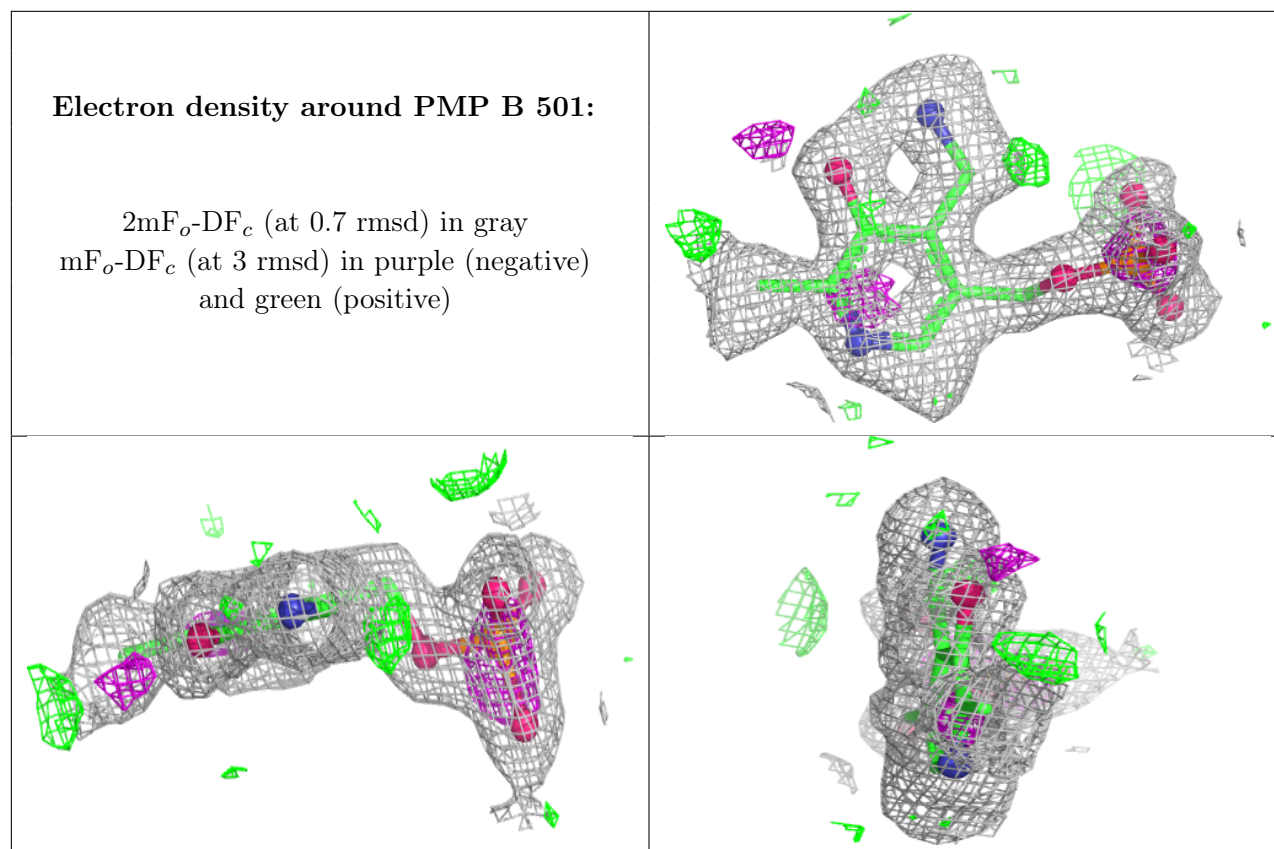
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	EDO	D	502	4/4	0.84	0.13	49,51,53,54	0
3	EDO	D	503	4/4	0.84	0.14	42,45,45,51	0
3	EDO	A	502	4/4	0.85	0.13	45,46,46,49	0
4	PEG	C	502	7/7	0.85	0.15	26,39,48,53	0
3	EDO	B	502	4/4	0.88	0.14	48,50,54,55	0
4	PEG	B	503	7/7	0.91	0.12	43,45,50,52	0
3	EDO	D	504	4/4	0.91	0.11	33,37,41,41	0
2	PMP	B	501	16/16	0.94	0.08	20,24,26,28	0
2	PMP	A	501	16/16	0.97	0.06	20,22,27,29	0

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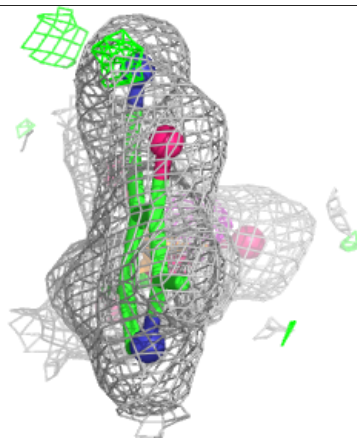
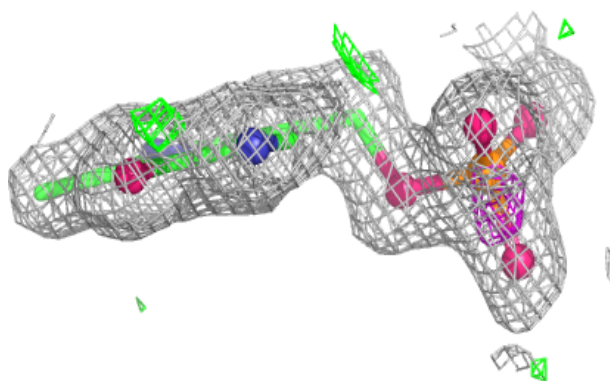
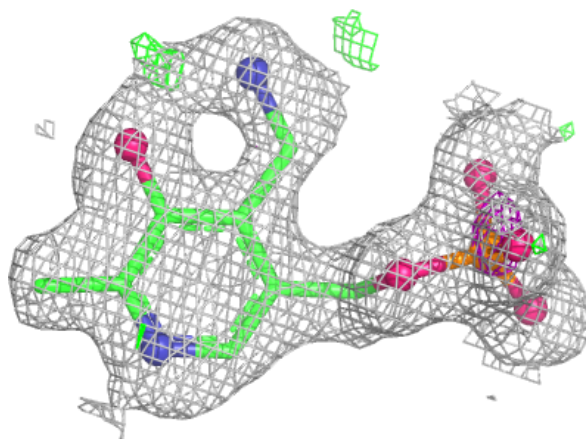
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PMP	D	501	16/16	0.98	0.05	15,17,20,24	0
2	PMP	C	501	16/16	0.98	0.06	13,15,18,20	0

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.



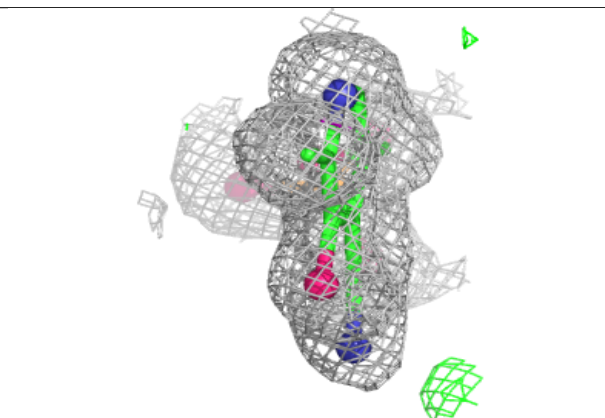
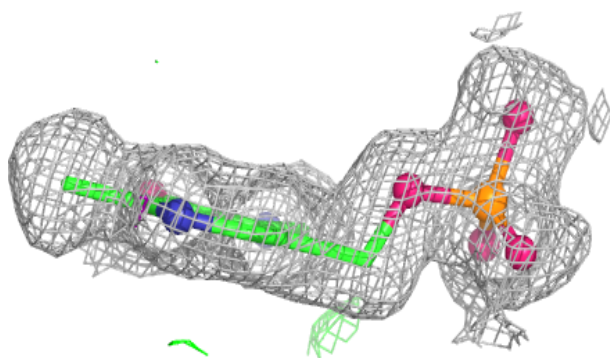
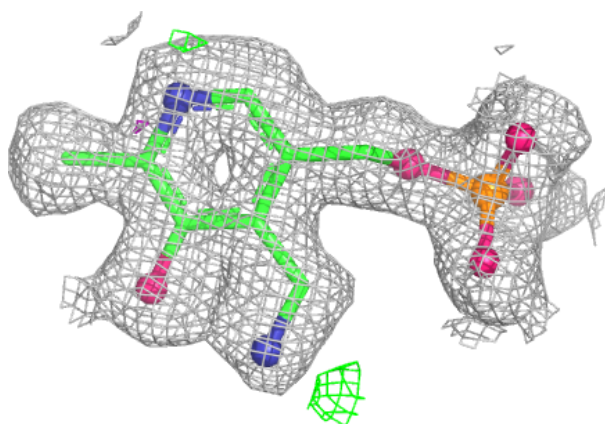
Electron density around PMP A 501:

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

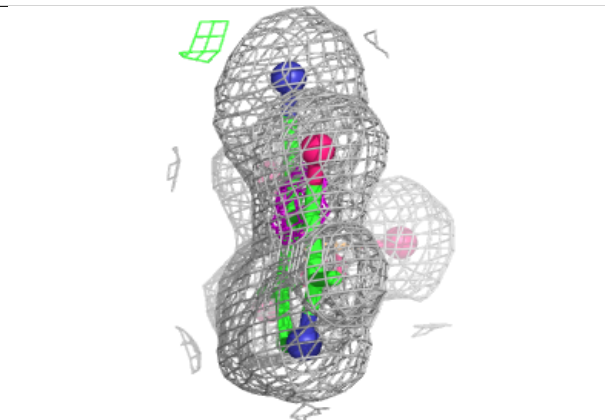
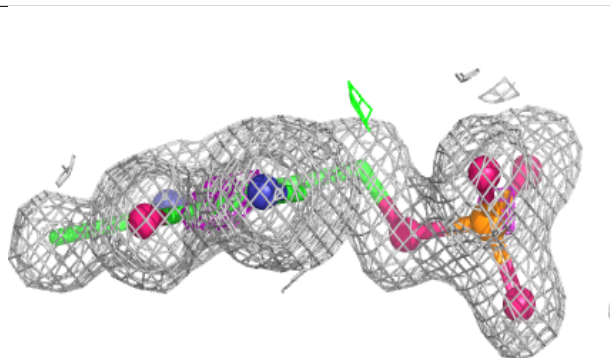
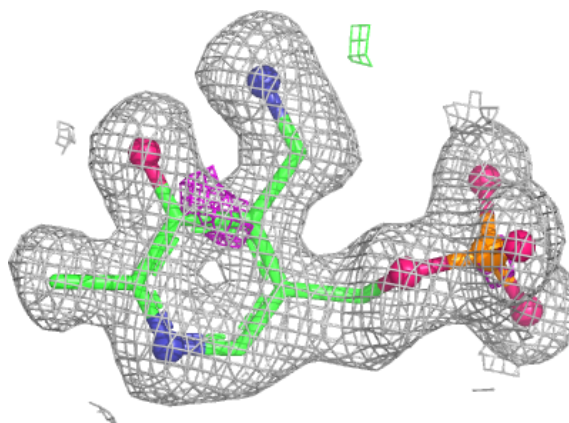


Electron density around PMP D 501:

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

**Electron density around 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 [i](#)

There are no such residues in this entry.