



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:34 PM UTC

PDB ID : 9S1Q / pdb_00009s1q
Title : Crystal structure of the DABA transaminase EctB from the halophilic and cold-adapted *Marinobacter* sp. CK1
Authors : Erlandsen, H.; Skogvold, A.; Leiros, I.
Deposited on : 2025-07-18
Resolution : 2.00 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

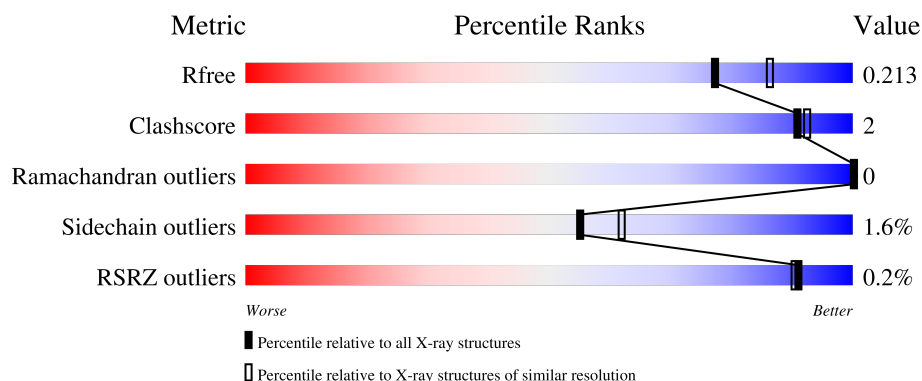
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION




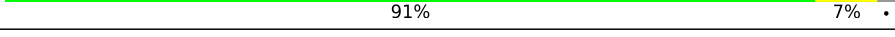
The reported resolution of this entry is 2.00 Å.

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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	428	 91% 6% ..
1	B	428	 90% 6% ..
1	C	428	 89% 8% .
1	D	428	 91% 7% .

2 Entry composition [i](#)

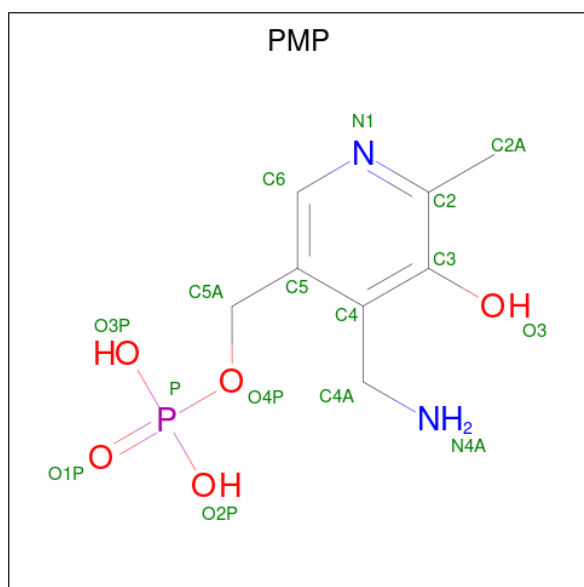
There are 4 unique types of molecules in this entry. The entry contains 13487 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Diaminobutyrate-2-oxoglutarate transaminase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	418	Total	C	N	O	S	0	0	0
			3191	2019	537	616	19			
1	B	418	Total	C	N	O	S	0	0	0
			3191	2019	537	616	19			
1	C	418	Total	C	N	O	S	0	0	0
			3191	2019	537	616	19			
1	D	418	Total	C	N	O	S	0	0	0
			3191	2019	537	616	19			

- Molecule 2 is 4'-DEOXY-4'-AMINOPYRIDOXAL-5'-PHOSPHATE (CCD ID: PMP) (formula: C₈H₁₃N₂O₅P) (labeled as "Ligand of Interest" by depositor).



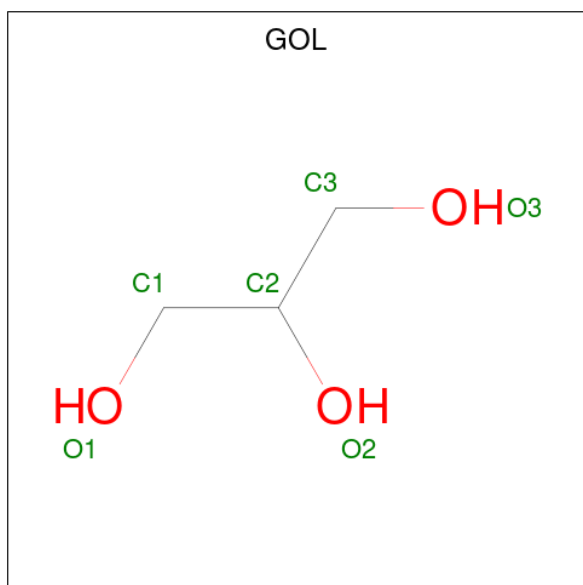
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			16	8	2	5	1		
2	B	1	Total	C	N	O	P	0	0
			16	8	2	5	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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 GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

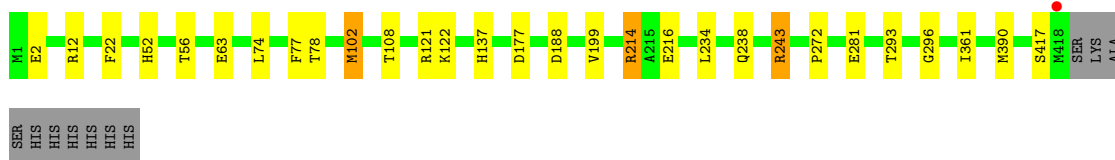
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	154	Total	O	0	0
			154	154		
4	B	134	Total	O	0	0
			134	134		
4	C	182	Total	O	0	0
			182	182		
4	D	171	Total	O	0	0
			171	171		

3 Residue-property plots


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.

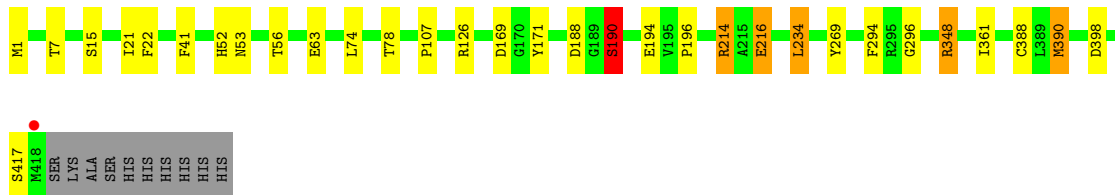
- Molecule 1: Diaminobutyrate-2-oxoglutarate transaminase

Chain A: 




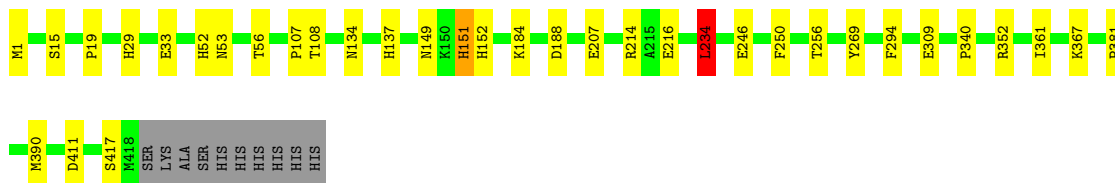
- Molecule 1: Diaminobutyrate-2-oxoglutarate transaminase

Chain B: 



- Molecule 1: Diaminobutyrate-2-oxoglutarate transaminase

Chain C: 



- Molecule 1: Diaminobutyrate-2-oxoglutarate transaminase

Chain D: 



ALA
SER
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.65Å 99.33Å 112.70Å 90.00° 104.82° 90.00°	Depositor
Resolution (Å)	40.13 – 2.00 40.13 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (40.13-2.00) 99.5 (40.13-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.165 , 0.208 (Not available) , 0.213	Depositor DCC
R_{free} test set	5736 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	30.3	Xtriage
Anisotropy	0.627	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 32.1	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	13487	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% 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: GOL, 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	0.92	2/3250 (0.1%)	1.25	11/4380 (0.3%)
1	B	0.90	1/3250 (0.0%)	1.26	11/4380 (0.3%)
1	C	1.02	6/3250 (0.2%)	1.28	20/4380 (0.5%)
1	D	0.96	0/3250	1.29	18/4380 (0.4%)
All	All	0.95	9/13000 (0.1%)	1.27	60/17520 (0.3%)

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	3
1	B	0	2
1	C	0	1
All	All	0	6

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	352	ARG	NE-CZ	-7.71	1.24	1.33
1	C	152	HIS	CG-CD2	-7.11	1.28	1.35
1	A	214	ARG	NE-CZ	6.29	1.40	1.33
1	C	137	HIS	CE1-NE2	6.29	1.38	1.32
1	C	152	HIS	CE1-NE2	-6.04	1.26	1.32
1	C	19	PRO	CA-CB	5.62	1.59	1.53
1	C	216	GLU	CD-OE1	5.55	1.35	1.25
1	B	348	ARG	NE-CZ	5.53	1.39	1.33
1	A	137	HIS	ND1-CE1	5.04	1.37	1.32

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	126	ARG	CD-NE-CZ	12.79	142.30	124.40
1	B	126	ARG	CB-CG-CD	10.10	134.54	111.30
1	D	378	THR	OG1-CB-CG2	8.75	126.79	109.30
1	A	243	ARG	CB-CG-CD	-8.34	92.12	111.30
1	D	66	GLU	CB-CG-CD	7.93	126.08	112.60
1	A	188	ASP	CA-CB-CG	7.19	119.79	112.60
1	B	390	MET	CG-SD-CE	-7.18	85.09	100.90
1	D	188	ASP	CA-CB-CG	7.17	119.78	112.60
1	A	102	MET	CG-SD-CE	-6.97	85.57	100.90
1	B	188	ASP	CA-CB-CG	6.90	119.50	112.60
1	C	340	PRO	CA-C-N	-6.89	112.49	123.31
1	C	340	PRO	C-N-CA	-6.89	112.49	123.31
1	C	188	ASP	CA-CB-CG	6.77	119.37	112.60
1	D	2	GLU	N-CA-CB	6.50	119.68	110.12
1	A	63	GLU	CB-CG-CD	6.49	123.63	112.60
1	A	56	THR	CA-CB-OG1	-6.49	99.87	109.60
1	C	216	GLU	CG-CD-OE2	-6.43	103.61	118.40
1	C	151	HIS	CA-CB-CG	6.39	120.19	113.80
1	C	246	GLU	CG-CD-OE2	-6.39	103.70	118.40
1	D	216	GLU	CB-CG-CD	6.34	123.38	112.60
1	A	52	HIS	CA-CB-CG	6.31	120.11	113.80
1	D	52	HIS	CA-CB-CG	6.26	120.06	113.80
1	C	340	PRO	N-CA-C	-6.25	101.37	111.19
1	A	216	GLU	CB-CG-CD	5.86	122.56	112.60
1	D	216	GLU	CG-CD-OE2	-5.84	104.96	118.40
1	C	216	GLU	CB-CG-CD	5.74	122.36	112.60
1	D	216	GLU	CG-CD-OE1	5.60	131.29	118.40
1	B	63	GLU	CB-CG-CD	5.59	122.11	112.60
1	D	207	GLU	CG-CD-OE2	-5.56	105.61	118.40
1	D	5	LYS	CB-CG-CD	5.53	124.02	111.30
1	D	24	ARG	CG-CD-NE	-5.52	99.85	112.00
1	C	234	LEU	CD1-CG-CD2	5.50	122.91	110.80
1	D	194	GLU	CB-CG-CD	5.49	121.92	112.60
1	D	236	ASP	CA-CB-CG	5.46	118.06	112.60
1	A	293	THR	OG1-CB-CG2	5.43	120.16	109.30
1	C	33	GLU	CB-CA-C	-5.42	100.61	110.63
1	B	52	HIS	CA-CB-CG	5.40	119.20	113.80
1	C	246	GLU	CG-CD-OE1	5.39	130.81	118.40
1	B	194	GLU	CB-CG-CD	5.38	121.75	112.60
1	D	378	THR	N-CA-CB	-5.37	102.21	111.55
1	D	207	GLU	CG-CD-OE1	5.31	130.61	118.40
1	B	398	ASP	CA-CB-CG	5.29	117.89	112.60
1	C	367	LYS	CA-CB-CG	5.23	124.56	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	190	SER	CA-CB-OG	-5.22	100.66	111.10
1	B	56	THR	CA-CB-OG1	-5.21	101.79	109.60
1	B	216	GLU	CB-CG-CD	5.20	121.44	112.60
1	D	63	GLU	CB-CG-CD	5.18	121.40	112.60
1	C	56	THR	CA-CB-OG1	-5.17	101.84	109.60
1	C	1	MET	CG-SD-CE	5.16	112.25	100.90
1	D	8	GLU	CB-CG-CD	5.16	121.37	112.60
1	D	56	THR	CA-CB-OG1	-5.15	101.87	109.60
1	C	256	THR	CA-CB-OG1	-5.14	101.89	109.60
1	C	309	GLU	CB-CG-CD	5.11	121.28	112.60
1	C	411	ASP	CA-CB-CG	5.09	117.69	112.60
1	A	281	GLU	CB-CG-CD	5.09	121.25	112.60
1	A	121	ARG	CD-NE-CZ	5.08	131.52	124.40
1	A	243	ARG	NE-CZ-NH2	-5.08	114.63	119.20
1	C	52	HIS	CA-CB-CG	5.08	118.88	113.80
1	C	207	GLU	CG-CD-OE1	5.03	129.96	118.40
1	C	216	GLU	CG-CD-OE1	5.00	129.90	118.40

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	12	ARG	Sidechain
1	A	214	ARG	Sidechain
1	A	243	ARG	Sidechain
1	B	214	ARG	Sidechain
1	B	348	ARG	Sidechain
1	C	214	ARG	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	3191	0	3159	11	0
1	B	3191	0	3159	20	0
1	C	3191	0	3159	13	0
1	D	3191	0	3159	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	16	0	11	0	0
2	B	16	0	10	0	0
2	C	16	0	11	1	0
2	D	16	0	11	0	0
3	A	6	0	8	0	0
3	C	6	0	8	0	0
3	D	6	0	8	0	0
4	A	154	0	0	2	1
4	B	134	0	0	0	1
4	C	182	0	0	2	0
4	D	171	0	0	1	0
All	All	13487	0	12703	43	1

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 2.

All (43) 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:B:388:CYS:HB3	1:B:390:MET:HE1	1.56	0.87
1:D:378:THR:HG23	1:D:383:ASP:OD1	1.87	0.75
1:A:177:ASP:OD1	4:A:601:HOH:O	2.10	0.69
1:C:29:HIS:HD2	4:C:741:HOH:O	1.76	0.68
1:C:234:LEU:HD22	1:C:250:PHE:HD2	1.66	0.61
1:D:378:THR:CG2	1:D:383:ASP:OD1	2.48	0.60
1:B:169:ASP:OD2	1:B:214:ARG:HD3	2.02	0.59
1:B:41:PHE:CE2	1:B:390:MET:CE	2.88	0.57
1:B:171:TYR:CE2	1:C:184:LYS:HE3	2.41	0.55
1:B:190:SER:HB2	1:C:381:PRO:HB3	1.89	0.55
1:B:1:MET:HE2	1:B:21:ILE:HG13	1.88	0.54
1:C:29:HIS:HE1	4:C:625:HOH:O	1.90	0.53
1:A:122:LYS:HB2	4:A:644:HOH:O	2.09	0.53
1:B:41:PHE:CD2	1:B:390:MET:CE	2.94	0.51
1:A:22:PHE:O	1:B:78:THR:HA	2.12	0.50
1:A:102:MET:HE3	1:B:7:THR:HG21	1.95	0.48
1:A:234:LEU:C	1:A:234:LEU:HD13	2.38	0.47
1:B:41:PHE:CE2	1:B:390:MET:HE2	2.49	0.47
1:D:234:LEU:HD13	1:D:234:LEU:C	2.39	0.47
1:B:190:SER:HB3	1:C:134:ASN:HD22	1.80	0.46
1:D:29:HIS:HE1	4:D:749:HOH:O	1.97	0.46
1:B:41:PHE:CD2	1:B:390:MET:HE3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:LEU:C	1:B:234:LEU:HD13	2.41	0.46
1:A:272:PRO:HG3	1:B:294:PHE:HB3	1.98	0.45
1:A:77:PHE:CZ	1:B:15:SER:HB2	2.52	0.45
1:A:108:THR:HG22	1:B:107:PRO:HD2	1.97	0.45
1:C:107:PRO:HD2	1:D:108:THR:HG22	1.98	0.45
1:C:108:THR:HG22	1:D:107:PRO:HD2	1.98	0.45
1:B:74:LEU:O	1:B:296:GLY:HA3	2.16	0.45
1:C:15:SER:HB2	1:D:77:PHE:CZ	2.52	0.44
1:D:378:THR:HA	1:D:385:VAL:O	2.19	0.43
1:C:149:ASN:OD1	1:C:151:HIS:HB3	2.19	0.42
1:A:74:LEU:O	1:A:296:GLY:HA3	2.21	0.41
1:D:205:GLN:O	1:D:210:LEU:HA	2.20	0.41
2:C:501:PMP:O3	2:C:501:PMP:N4A	2.52	0.41
1:B:390:MET:HE3	1:B:390:MET:HB3	1.90	0.41
1:A:78:THR:HA	1:B:22:PHE:O	2.21	0.41
1:C:53:ASN:HA	1:C:269:TYR:CZ	2.56	0.41
1:C:234:LEU:HD22	1:C:250:PHE:CD2	2.51	0.41
1:B:53:ASN:HA	1:B:269:TYR:CZ	2.56	0.40
1:C:294:PHE:HB3	1:D:272:PRO:HG3	2.03	0.40
1:A:238:GLN:HE21	1:A:238:GLN:HB2	1.72	0.40
1:D:74:LEU:O	1:D:296:GLY:HA3	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:607:HOH:O	4:B:719:HOH:O[1_655]	1.29	0.91

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	416/428 (97%)	401 (96%)	15 (4%)	0	100	100
1	B	416/428 (97%)	402 (97%)	14 (3%)	0	100	100
1	C	416/428 (97%)	402 (97%)	14 (3%)	0	100	100
1	D	416/428 (97%)	403 (97%)	13 (3%)	0	100	100
All	All	1664/1712 (97%)	1608 (97%)	56 (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	335/344 (97%)	330 (98%)	5 (2%)	57	64
1	B	335/344 (97%)	329 (98%)	6 (2%)	51	58
1	C	335/344 (97%)	331 (99%)	4 (1%)	63	70
1	D	335/344 (97%)	329 (98%)	6 (2%)	51	58
All	All	1340/1376 (97%)	1319 (98%)	21 (2%)	55	62

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	199	VAL
1	A	361	ILE
1	A	390	MET
1	A	417	SER
1	B	190	SER
1	B	196	PRO
1	B	216	GLU
1	B	234	LEU
1	B	361	ILE
1	B	417	SER
1	C	234	LEU
1	C	361	ILE

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Mol	Chain	Res	Type
1	C	390	MET
1	C	417	SER
1	D	2	GLU
1	D	361	ILE
1	D	378	THR
1	D	390	MET
1	D	417	SER
1	D	418	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	HIS
1	A	134	ASN
1	A	238	GLN
1	A	241	ASN
1	B	37	GLN
1	B	91	HIS
1	B	134	ASN
1	B	241	ASN
1	B	382	ASN
1	C	91	HIS
1	C	134	ASN
1	C	151	HIS
1	C	241	ASN
1	C	326	GLN
1	D	91	HIS
1	D	134	ASN
1	D	241	ASN
1	D	415	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 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	A	501	-	16,16,16	1.52	3 (18%)	22,23,23	1.22	3 (13%)
3	GOL	A	502	-	5,5,5	0.42	0	5,5,5	1.13	0
2	PMP	C	501	-	16,16,16	0.43	0	22,23,23	1.20	2 (9%)
3	GOL	D	502	-	5,5,5	0.41	0	5,5,5	0.64	0
2	PMP	D	501	-	16,16,16	1.52	2 (12%)	22,23,23	0.91	1 (4%)
2	PMP	B	501	-	16,16,16	0.97	1 (6%)	22,23,23	1.28	1 (4%)
3	GOL	C	502	-	5,5,5	0.25	0	5,5,5	0.45	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	A	501	-	-	3/8/8/8	0/1/1/1
3	GOL	A	502	-	-	2/4/4/4	-
2	PMP	C	501	-	-	2/8/8/8	0/1/1/1
3	GOL	D	502	-	-	2/4/4/4	-
2	PMP	D	501	-	-	2/8/8/8	0/1/1/1
2	PMP	B	501	-	-	5/8/8/8	0/1/1/1
3	GOL	C	502	-	-	4/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	PMP	C3-C2	4.45	1.45	1.41
2	D	501	PMP	C3-C2	4.09	1.45	1.41
2	B	501	PMP	P-O4P	2.59	1.68	1.60
2	D	501	PMP	P-O4P	2.55	1.68	1.60
2	A	501	PMP	P-O4P	2.28	1.67	1.60
2	A	501	PMP	P-O1P	2.18	1.57	1.50

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	PMP	O3-C3-C2	3.60	125.03	117.58
2	A	501	PMP	C2A-C2-C3	2.48	123.70	120.80
2	A	501	PMP	O3-C3-C2	2.43	122.62	117.58
2	D	501	PMP	O3P-P-O2P	2.41	116.83	107.80
2	C	501	PMP	O4P-C5A-C5	2.40	113.85	109.36
2	C	501	PMP	O3P-P-O2P	2.37	116.68	107.80
2	A	501	PMP	O4P-C5A-C5	2.09	113.27	109.36

There are no chirality outliers.

All (20) torsion outliers are listed below:

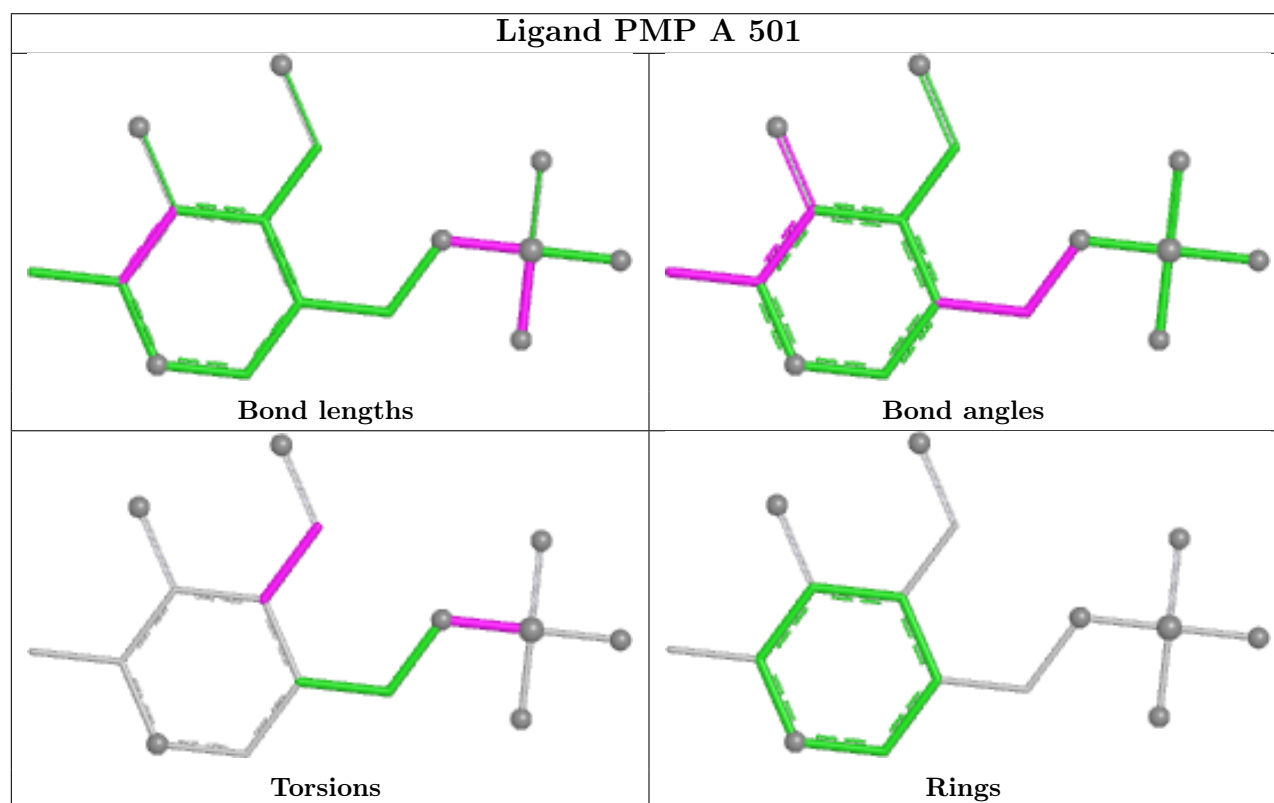
Mol	Chain	Res	Type	Atoms
2	B	501	PMP	C3-C4-C4A-N4A
2	B	501	PMP	C5-C4-C4A-N4A
2	B	501	PMP	C5A-O4P-P-O1P
2	B	501	PMP	C5A-O4P-P-O3P
2	C	501	PMP	C3-C4-C4A-N4A
2	C	501	PMP	C5-C4-C4A-N4A
2	D	501	PMP	C3-C4-C4A-N4A
2	D	501	PMP	C5-C4-C4A-N4A
3	C	502	GOL	O1-C1-C2-O2
3	C	502	GOL	O1-C1-C2-C3
3	D	502	GOL	C1-C2-C3-O3
2	A	501	PMP	C3-C4-C4A-N4A
3	A	502	GOL	O1-C1-C2-C3
3	C	502	GOL	C1-C2-C3-O3
3	A	502	GOL	O1-C1-C2-O2
3	D	502	GOL	O2-C2-C3-O3
2	A	501	PMP	C5-C4-C4A-N4A
3	C	502	GOL	O2-C2-C3-O3
2	A	501	PMP	C5A-O4P-P-O2P
2	B	501	PMP	C5A-O4P-P-O2P

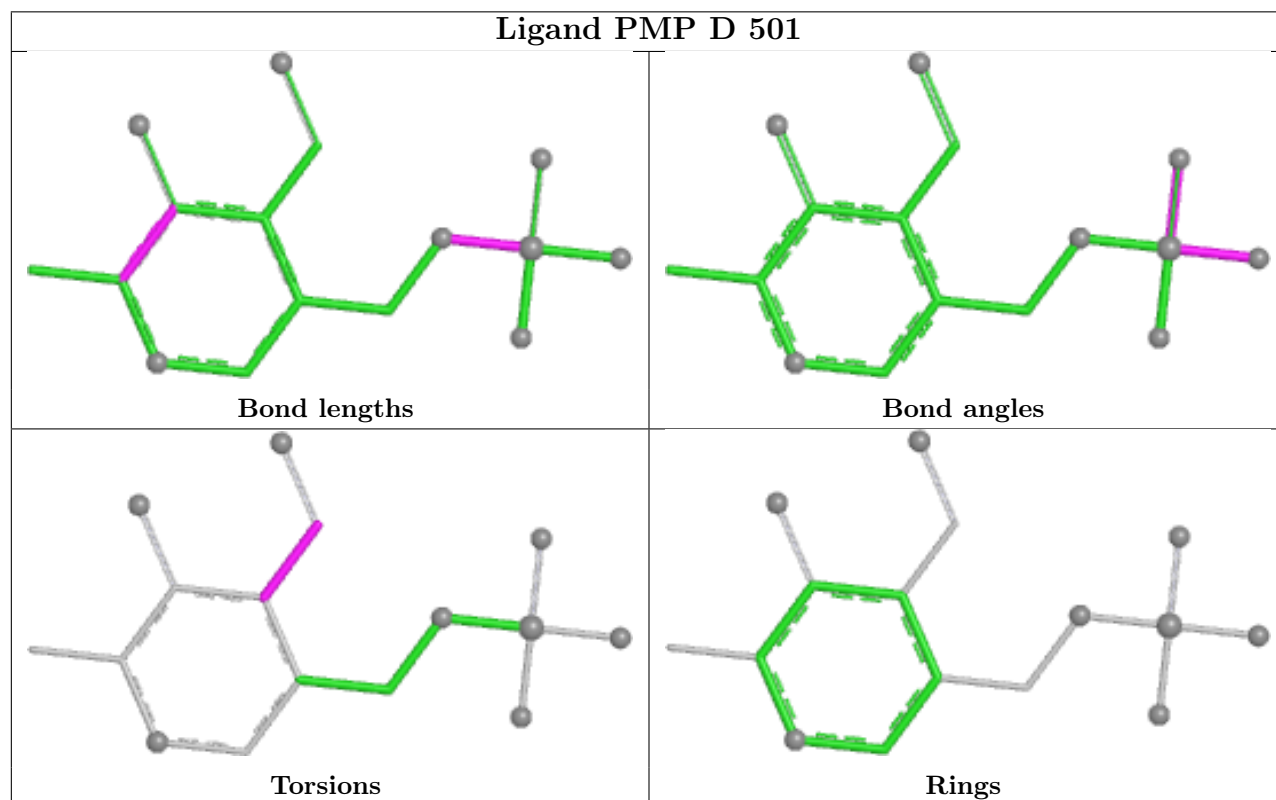
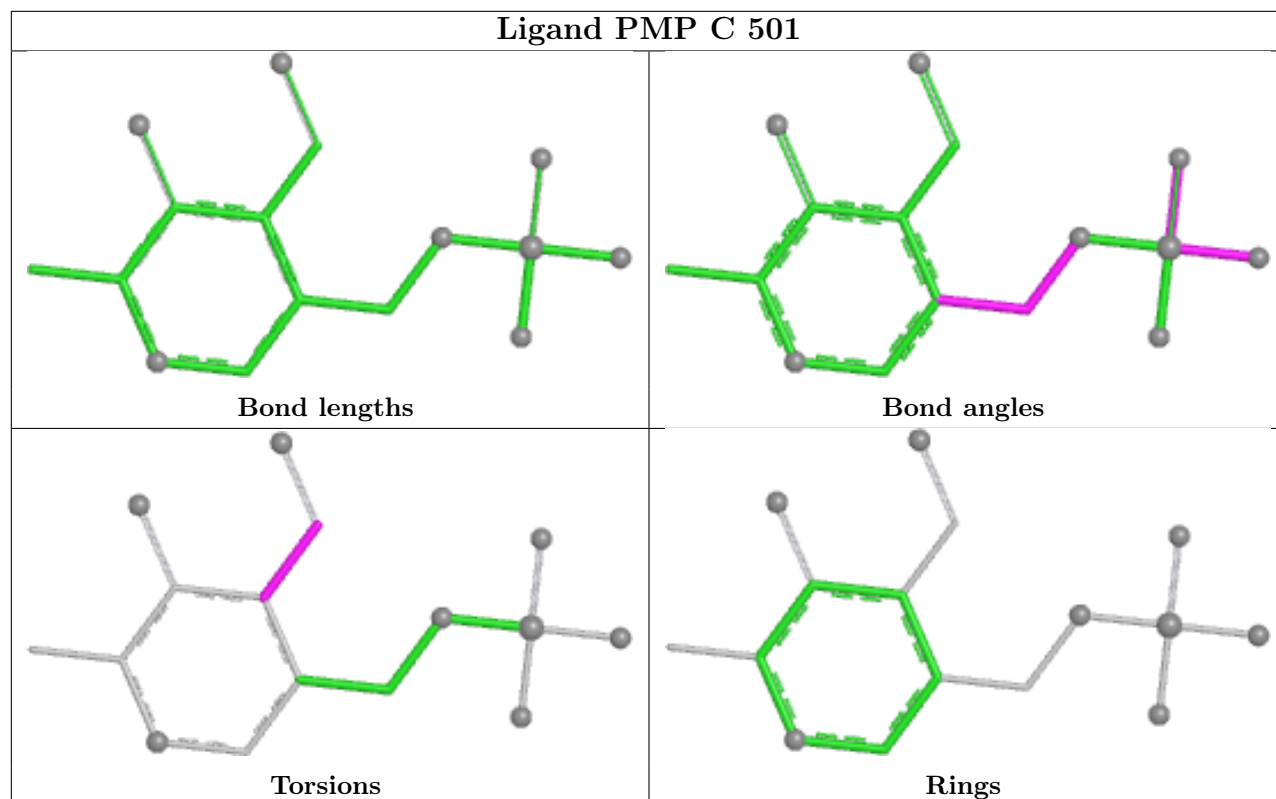
There are no ring outliers.

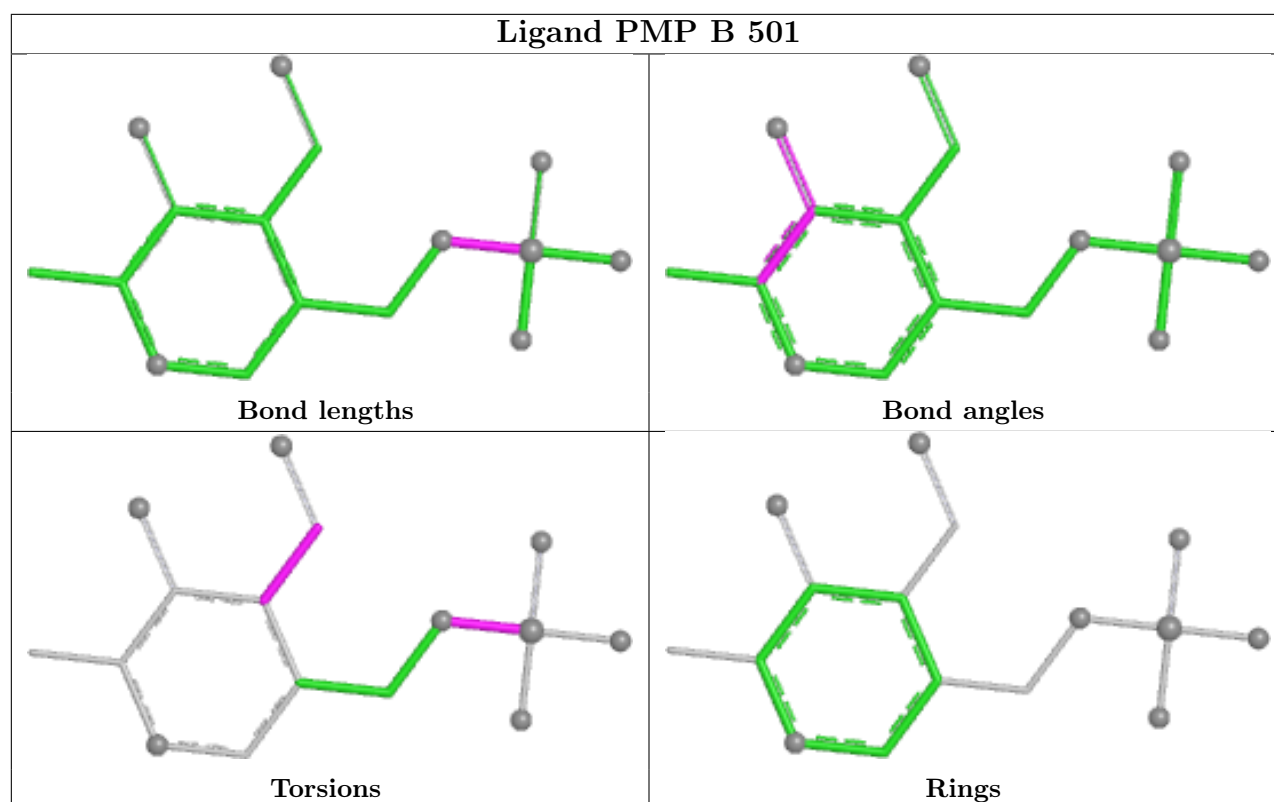
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	PMP	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, 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	418/428 (97%)	-0.32	1 (0%) 91 90	25, 39, 58, 98	0
1	B	418/428 (97%)	-0.19	1 (0%) 91 90	25, 43, 64, 102	0
1	C	418/428 (97%)	-0.52	0 100 100	20, 32, 51, 101	0
1	D	418/428 (97%)	-0.52	1 (0%) 91 90	21, 32, 49, 86	0
All	All	1672/1712 (97%)	-0.39	3 (0%) 91 90	20, 36, 58, 102	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	418	MET	3.2
1	B	418	MET	2.8
1	D	418	MET	2.2

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](#)

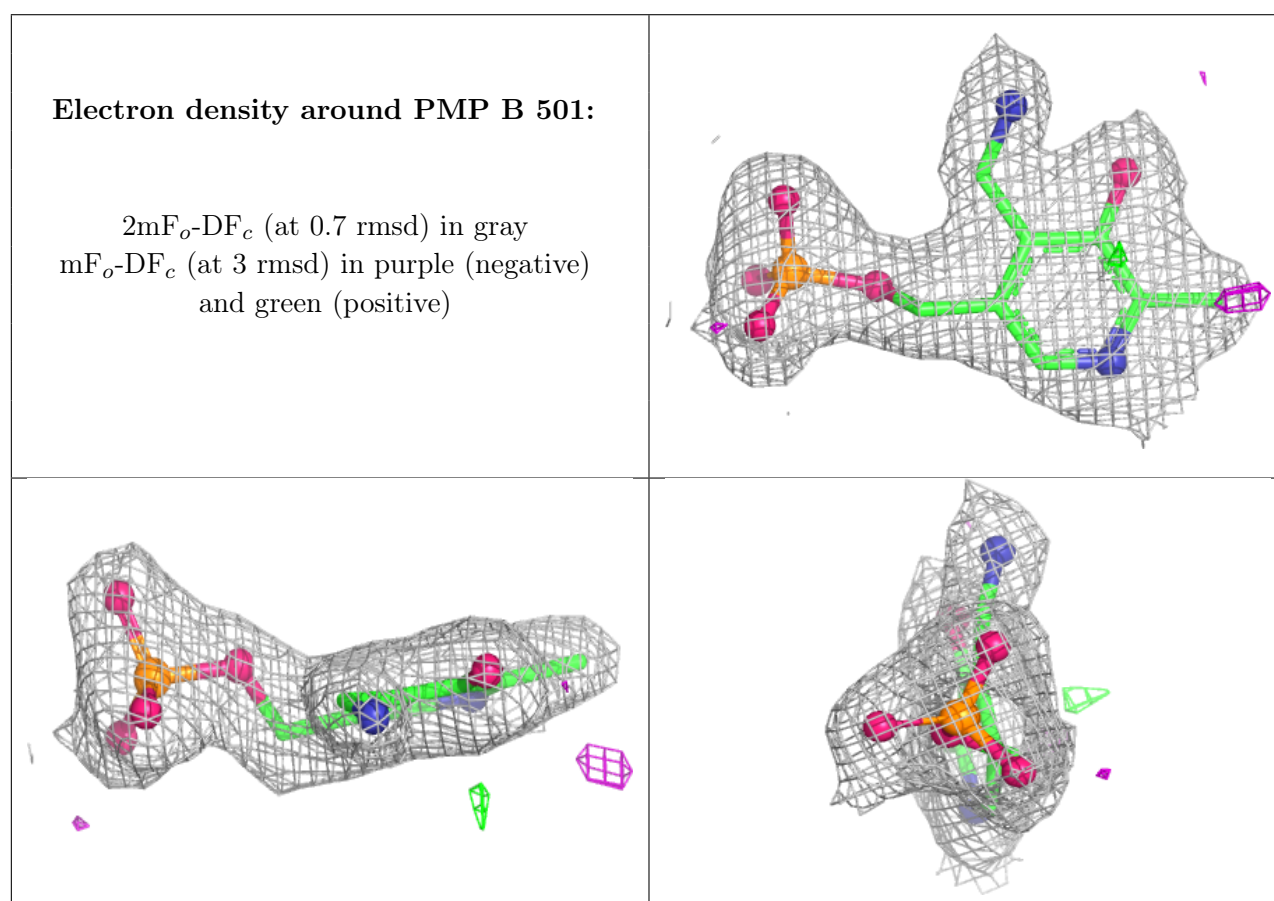
There are no oligosaccharides in this entry.

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.

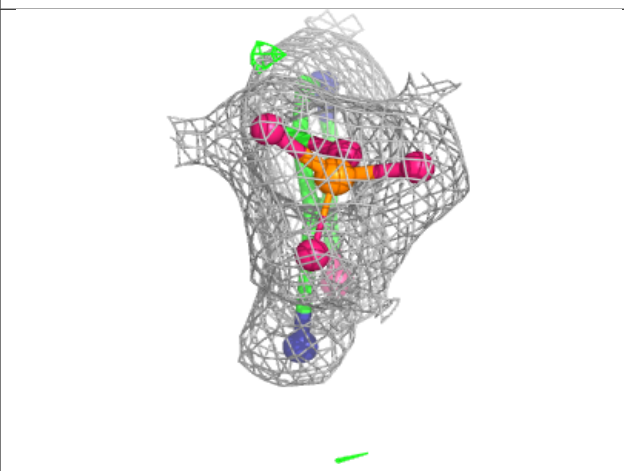
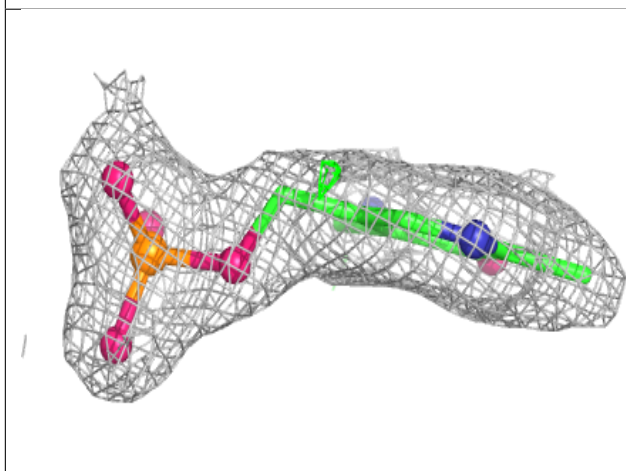
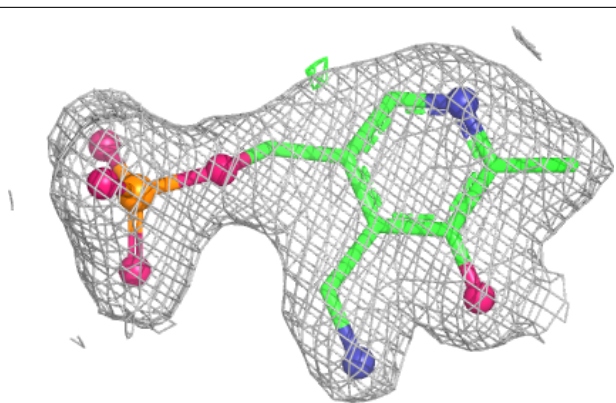
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GOL	C	502	6/6	0.87	0.13	46,60,61,67	0
3	GOL	A	502	6/6	0.90	0.12	59,64,76,76	0
3	GOL	D	502	6/6	0.91	0.10	40,54,63,79	0
2	PMP	B	501	16/16	0.97	0.06	28,36,39,39	0
2	PMP	A	501	16/16	0.97	0.06	30,38,46,48	0
2	PMP	D	501	16/16	0.98	0.05	21,26,32,32	0
2	PMP	C	501	16/16	0.98	0.05	23,28,37,39	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.



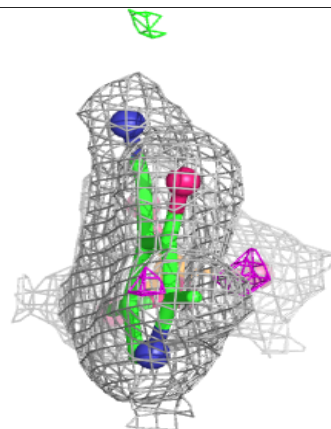
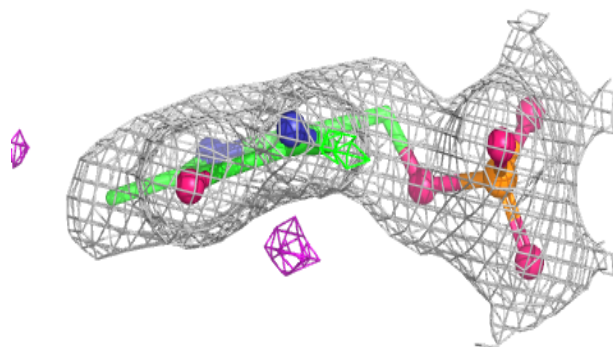
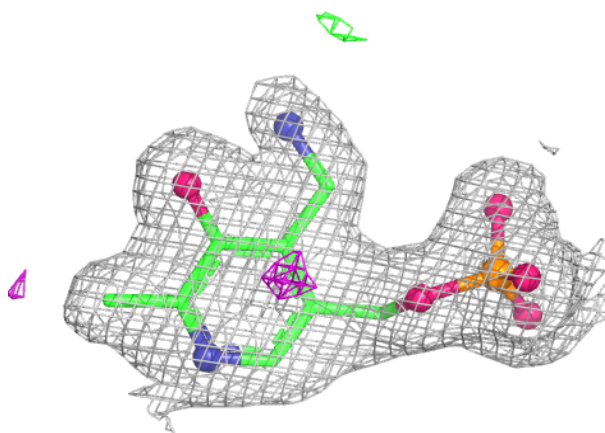
Electron density around PMP A 501:

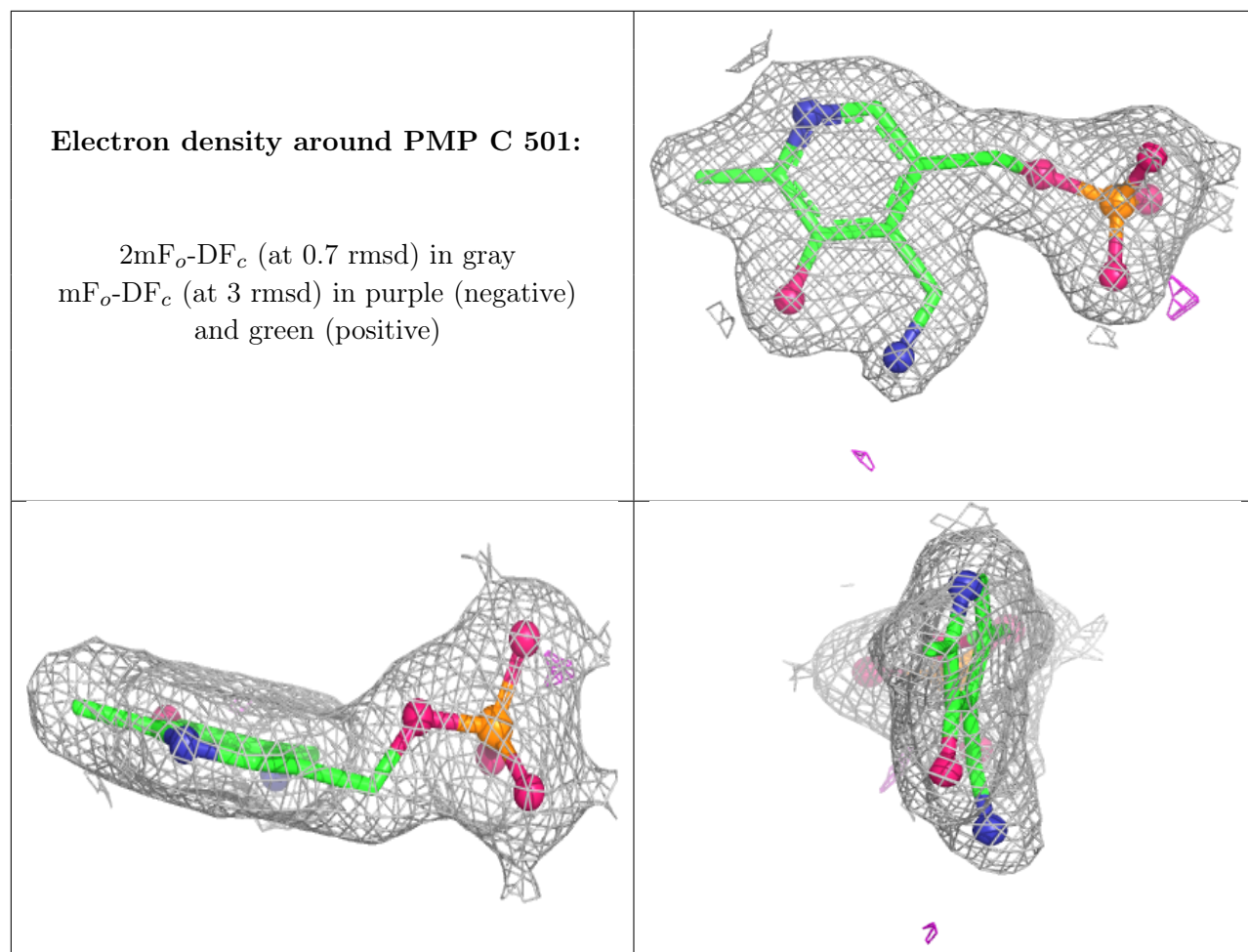
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers [i](#)

There are no such residues in this entry.