



Full wwPDB X-ray Structure Validation Report ⓘ

May 19, 2021 – 10:11 AM EDT

PDB ID : 7KZ6
Title : Crystal structure of KabA from Bacillus cereus UW85 with bound cofactor PMP
Authors : Prasertanan, T.; Palmer, D.R.J.; Sanders, D.A.R.
Deposited on : 2020-12-10
Resolution : 1.65 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 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 : 2.18
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) : 2.18

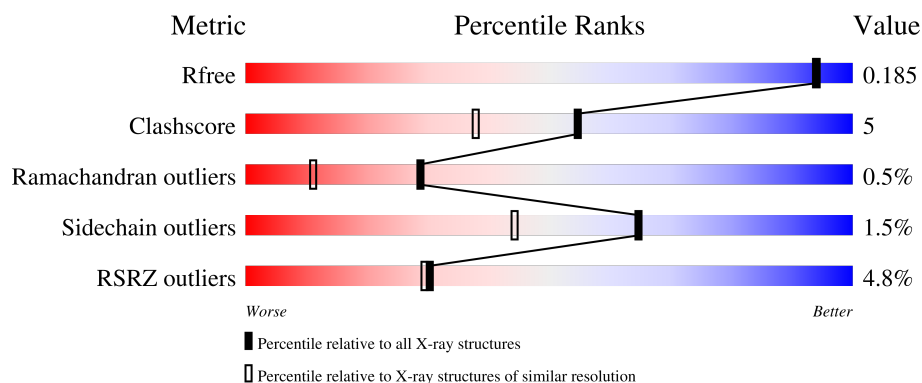
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (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 ≥ 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	445	 2% 84% 13% .
1	B	445	 5% 85% 13% .
1	C	445	 3% 90% 8% .
1	D	445	 9% 86% 13% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15631 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.

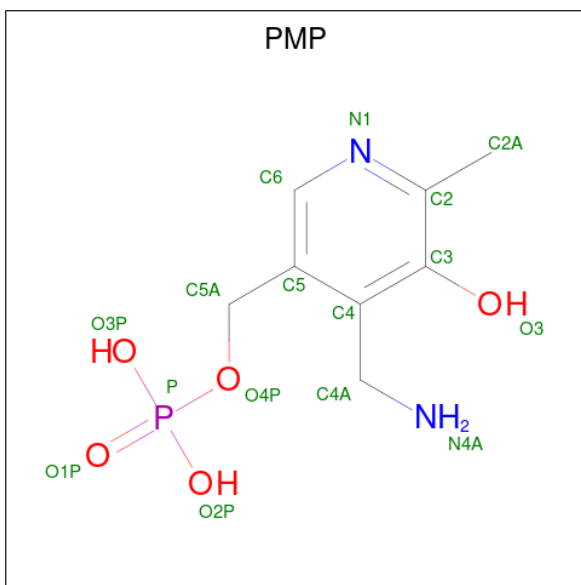
- Molecule 1 is a protein called Aminotransferase class I/II-fold pyridoxal phosphate-dependent enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	438	Total	C	N	O	S	0	3	0
			3558	2276	606	660	16			
1	B	438	Total	C	N	O	S	0	4	0
			3561	2275	607	663	16			
1	C	438	Total	C	N	O	S	0	7	0
			3585	2290	612	668	15			
1	D	439	Total	C	N	O	S	0	0	0
			3537	2262	603	657	15			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP C0JRF5
A	0	ALA	-	expression tag	UNP C0JRF5
A	1	MET	-	expression tag	UNP C0JRF5
A	2	ASP	-	expression tag	UNP C0JRF5
B	-1	GLY	-	expression tag	UNP C0JRF5
B	0	ALA	-	expression tag	UNP C0JRF5
B	1	MET	-	expression tag	UNP C0JRF5
B	2	ASP	-	expression tag	UNP C0JRF5
C	-1	GLY	-	expression tag	UNP C0JRF5
C	0	ALA	-	expression tag	UNP C0JRF5
C	1	MET	-	expression tag	UNP C0JRF5
C	2	ASP	-	expression tag	UNP C0JRF5
D	-1	GLY	-	expression tag	UNP C0JRF5
D	0	ALA	-	expression tag	UNP C0JRF5
D	1	MET	-	expression tag	UNP C0JRF5
D	2	ASP	-	expression tag	UNP C0JRF5

- Molecule 2 is 4'-DEOXY-4'-AMINOPYRIDOXAL-5'-PHOSPHATE (three-letter code: 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		
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: C₂H₆O₂).



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

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

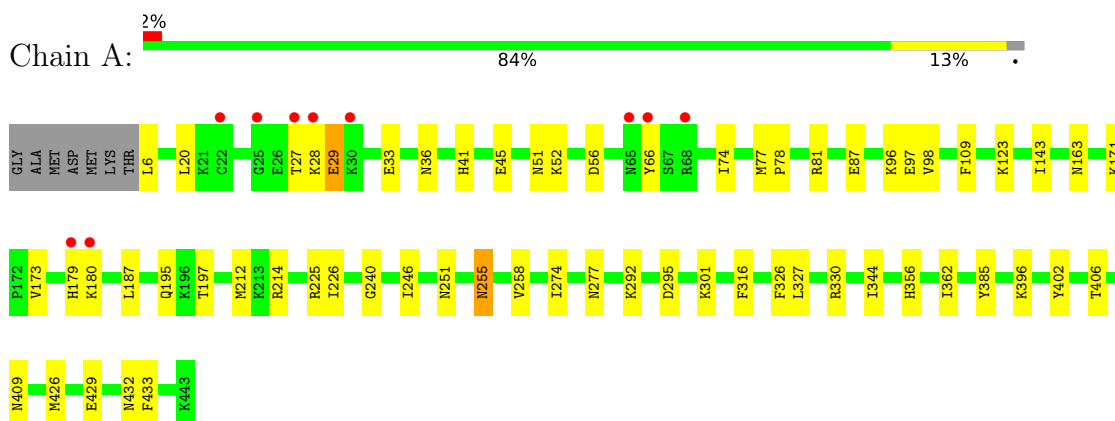
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	356	Total O 356 356	0	0
4	B	284	Total O 284 284	0	0
4	C	344	Total O 344 344	0	0
4	D	230	Total O 230 230	0	0

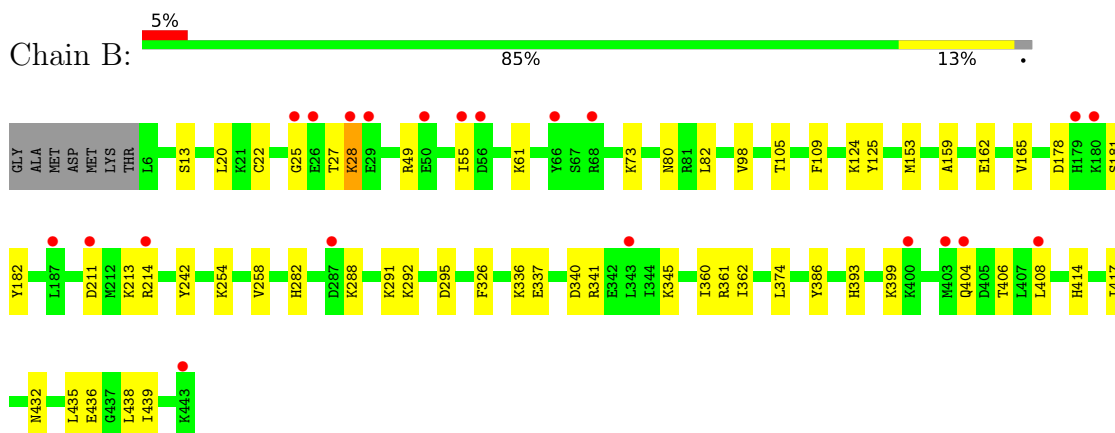
3 Residue-property plots [i](#)

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.

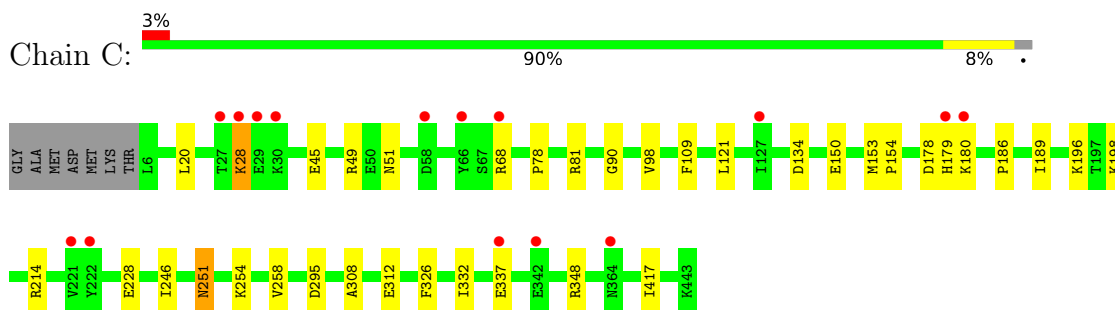
- Molecule 1: Aminotransferase class I/II-fold pyridoxal phosphate-dependent enzyme



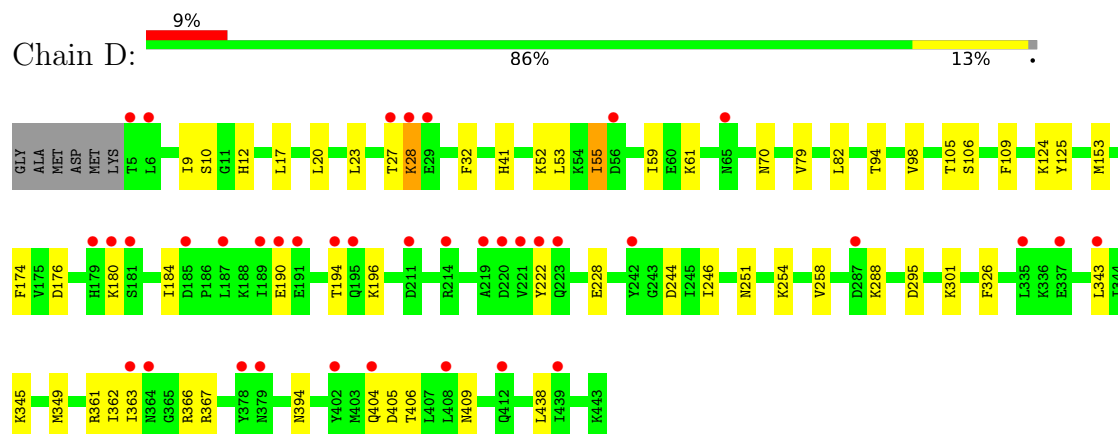
- Molecule 1: Aminotransferase class I/II-fold pyridoxal phosphate-dependent enzyme



- Molecule 1: Aminotransferase class I/II-fold pyridoxal phosphate-dependent enzyme



- Molecule 1: Aminotransferase class I/II-fold pyridoxal phosphate-dependent enzyme



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	66.53Å 66.64Å 112.22Å 77.42° 81.06° 88.34°	Depositor
Resolution (Å)	46.88 – 1.65 47.07 – 1.39	Depositor EDS
% Data completeness (in resolution range)	95.3 (46.88-1.65) 94.4 (47.07-1.39)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 1.39Å)	Xtriage
Refinement program	PHENIX dev_2398	Depositor
R, R_{free}	0.168 , 0.201 0.170 , 0.185	Depositor DCC
R_{free} test set	17659 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	22.8	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.019 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	15631	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.15% 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: 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	0.68	0/3620	0.75	0/4880
1	B	0.63	0/3622	0.74	0/4881
1	C	0.64	0/3651	0.74	0/4923
1	D	0.58	0/3598	0.70	0/4850
All	All	0.63	0/14491	0.73	0/19534

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3558	0	3642	45	0
1	B	3561	0	3642	40	0
1	C	3585	0	3658	25	0
1	D	3537	0	3627	40	0
2	A	16	0	11	0	0
2	B	16	0	11	1	0
2	C	16	0	11	1	0
2	D	16	0	10	1	0
3	A	52	0	78	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	12	0	18	4	0
3	C	28	0	42	6	0
3	D	20	0	30	7	0
4	A	356	0	0	10	0
4	B	284	0	0	5	0
4	C	344	0	0	6	0
4	D	230	0	0	5	0
All	All	15631	0	14780	152	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 5.

All (152) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:295:ASP:H	3:C:502:EDO:H22	1.33	0.93
4:C:609:HOH:O	1:D:105:THR:HG21	1.70	0.90
1:A:330:ARG:HH22	1:A:432:ASN:HD21	1.23	0.86
1:B:295:ASP:H	3:B:502:EDO:H11	1.43	0.81
1:A:51:ASN:HB3	3:A:505:EDO:H22	1.61	0.80
1:D:295:ASP:H	3:D:503:EDO:H11	1.48	0.76
1:A:295:ASP:HB2	3:A:502:EDO:H12	1.69	0.74
1:C:337:GLU:CD	1:C:337:GLU:H	1.93	0.72
1:D:194:THR:HG22	1:D:196:LYS:H	1.54	0.72
1:B:105:THR:HG21	4:B:863:HOH:O	1.89	0.71
1:C:178[B]:ASP:OD1	1:C:179[B]:HIS:N	2.25	0.69
1:A:225:ARG:HH21	3:A:509:EDO:H11	1.58	0.69
1:D:106:SER:HB3	1:D:301:LYS:NZ	2.08	0.69
1:D:105:THR:HB	3:D:502:EDO:H21	1.76	0.68
1:D:394:ASN:H	3:D:505:EDO:H22	1.60	0.66
1:A:77[B]:MET:SD	3:A:511:EDO:H21	2.36	0.66
1:A:225:ARG:NH2	3:A:509:EDO:H11	2.11	0.66
1:B:417:ILE:HG21	3:B:503:EDO:H22	1.78	0.65
1:C:348:ARG:NH1	4:C:603:HOH:O	2.29	0.64
1:A:6:LEU:N	4:A:607:HOH:O	2.31	0.64
1:A:385:TYR:HE2	3:A:506:EDO:H22	1.62	0.64
3:D:505:EDO:H11	4:D:914:HOH:O	1.97	0.64
1:B:374:LEU:HD11	1:B:438:LEU:HD13	1.80	0.64
1:B:153:MET:HE1	1:B:165:VAL:HG21	1.81	0.63
1:B:288:LYS:HG2	1:B:291:LYS:HD2	1.80	0.62
1:A:98:VAL:HG22	1:A:109:PHE:CE2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:514:EDO:H12	4:A:612:HOH:O	2.01	0.60
1:A:78:PRO:HG2	1:A:81:ARG:HG3	1.83	0.60
1:A:195:GLN:O	3:A:503:EDO:H22	2.02	0.60
1:C:98:VAL:HG22	1:C:109:PHE:CE2	2.36	0.60
1:B:153:MET:CE	1:B:165:VAL:HG21	2.32	0.59
1:A:173:VAL:HG22	3:A:512:EDO:H22	1.84	0.59
1:A:255:ASN:HD21	1:A:356:HIS:HA	1.67	0.59
1:A:402:TYR:CE1	3:A:512:EDO:H11	2.38	0.58
1:A:41:HIS:HD2	4:A:910:HOH:O	1.87	0.58
1:D:70:ASN:ND2	4:D:801:HOH:O	2.35	0.58
1:B:49:ARG:NH2	1:B:55:ILE:H	2.01	0.58
1:B:22:CYS:HA	1:B:27:THR:O	2.04	0.57
1:A:277:ASN:OD1	1:A:301:LYS:NZ	2.37	0.57
1:D:343:LEU:O	1:D:363:ILE:HG22	2.05	0.57
1:B:404:GLN:HB2	4:B:772:HOH:O	2.05	0.56
1:A:51:ASN:O	1:A:52:LYS:HE2	2.04	0.56
1:D:194:THR:HG21	4:D:859:HOH:O	2.05	0.56
1:D:254:LYS:HE2	2:D:501:PMP:N4A	2.20	0.55
1:B:399:LYS:HE2	4:B:855:HOH:O	2.06	0.54
1:A:163:ASN:HD21	1:B:292:LYS:NZ	2.04	0.54
1:B:213:LYS:HG2	1:B:242:TYR:CE2	2.42	0.54
1:D:9:ILE:HD11	1:D:32:PHE:CD2	2.43	0.54
1:A:123:LYS:HD3	4:A:604:HOH:O	2.07	0.54
1:C:134:ASP:OD2	3:C:503:EDO:H22	2.08	0.53
1:A:330:ARG:NH2	1:A:432:ASN:HD21	2.01	0.53
1:B:213:LYS:HG2	1:B:242:TYR:CZ	2.44	0.53
1:A:36:ASN:ND2	4:A:615:HOH:O	2.41	0.53
1:C:150:GLU:HG3	1:C:196:LYS:HB3	1.89	0.53
1:D:301:LYS:HB2	3:D:502:EDO:H11	1.90	0.53
1:B:393:HIS:HE1	4:B:614:HOH:O	1.92	0.53
1:D:98:VAL:HG22	1:D:109:PHE:CE2	2.44	0.53
1:B:182:TYR:CE1	1:B:417:ILE:HD12	2.44	0.52
1:D:124:LYS:HE3	1:D:125:TYR:OH	2.09	0.52
1:A:292:LYS:H	1:B:393:HIS:CD2	2.27	0.52
1:A:143:ILE:HA	3:A:509:EDO:H12	1.90	0.52
1:D:52:LYS:HD2	1:D:53:LEU:H	1.73	0.52
1:B:49:ARG:HH21	1:B:55:ILE:HD12	1.74	0.51
1:C:251[B]:ASN:ND2	4:C:609:HOH:O	2.38	0.51
1:D:176:ASP:OD2	1:D:409:ASN:HB3	2.10	0.51
1:A:187:LEU:HD23	1:A:214:ARG:NH1	2.26	0.51
1:B:124:LYS:HG2	1:B:125:TYR:CZ	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:LYS:NZ	4:A:620:HOH:O	2.44	0.50
1:B:211:ASP:OD2	1:B:214:ARG:NH1	2.39	0.49
1:B:336:LYS:NZ	1:B:340:ASP:OD2	2.45	0.49
1:D:32:PHE:H	1:D:52:LYS:HZ2	1.61	0.49
1:D:295:ASP:H	3:D:503:EDO:C1	2.21	0.49
1:A:171:LYS:HB3	3:A:512:EDO:O2	2.13	0.49
1:C:254:LYS:NZ	2:C:501:PMP:H4A2	2.28	0.48
1:A:327:LEU:HD13	1:A:426:MET:HE2	1.94	0.48
1:B:211:ASP:OD2	1:B:214:ARG:HD2	2.14	0.48
1:C:20:LEU:HD11	1:C:326:PHE:HD1	1.79	0.47
1:A:344:ILE:HG22	1:A:362:ILE:HD13	1.96	0.47
1:B:20:LEU:HD11	1:B:326:PHE:HD1	1.79	0.47
1:B:345:LYS:HB2	1:B:361:ARG:HB2	1.97	0.47
1:B:254:LYS:HE2	2:B:501:PMP:N4A	2.30	0.47
1:B:295:ASP:H	3:B:502:EDO:C1	2.19	0.46
1:D:55:ILE:H	1:D:55:ILE:HG13	1.43	0.46
1:D:124:LYS:HG2	1:D:125:TYR:CZ	2.50	0.46
4:A:769:HOH:O	1:B:282:HIS:HE1	1.99	0.46
1:D:345:LYS:HZ1	1:D:361:ARG:NH2	2.13	0.46
1:D:17:LEU:HD21	1:D:349:MET:HG3	1.97	0.46
1:D:366:ARG:HD3	4:D:855:HOH:O	2.16	0.46
1:C:332:ILE:HG23	1:C:348:ARG:HH22	1.80	0.46
1:C:178[B]:ASP:OD1	1:C:180:LYS:HG2	2.16	0.46
1:A:28:LYS:HE3	1:A:29:GLU:HB2	1.96	0.46
1:C:417:ILE:HD12	3:C:504:EDO:H22	1.98	0.45
1:D:10:SER:OG	1:D:12:HIS:HD2	2.00	0.45
1:D:23:LEU:HB3	1:D:59:ILE:HD11	1.97	0.45
1:D:228:GLU:HB2	1:D:246:ILE:HD12	1.98	0.45
1:A:197:THR:O	3:A:503:EDO:H21	2.17	0.45
1:C:150:GLU:HG3	1:C:196:LYS:CB	2.47	0.45
1:B:295:ASP:HB2	3:B:502:EDO:H22	1.99	0.44
1:C:90:GLY:HA3	1:C:312:GLU:OE2	2.17	0.44
1:D:20:LEU:HD11	1:D:326:PHE:HD1	1.82	0.44
1:D:41:HIS:HD2	4:D:1010:HOH:O	1.99	0.44
1:D:52:LYS:HD2	1:D:52:LYS:HA	1.84	0.44
1:C:78:PRO:HG2	1:C:81:ARG:HG3	1.98	0.44
3:A:502:EDO:H21	4:A:701:HOH:O	2.17	0.44
1:D:362:ILE:HD12	1:D:367:ARG:HG2	2.00	0.44
1:A:212:MET:HE1	1:A:226:ILE:HG21	1.99	0.44
3:C:504:EDO:H12	4:C:812:HOH:O	2.17	0.44
1:B:80[A]:ASN:ND2	1:C:49:ARG:HD3	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:ASP:OD2	1:B:181:SER:OG	2.33	0.44
1:A:385:TYR:CE2	3:A:506:EDO:H22	2.47	0.44
1:A:97:GLU:OE2	4:A:601:HOH:O	2.21	0.43
1:A:274:ILE:HG12	3:A:504:EDO:H22	2.00	0.43
3:C:507:EDO:H12	4:C:903:HOH:O	2.19	0.43
1:A:187:LEU:HD23	1:A:214:ARG:HH12	1.82	0.43
1:A:179:HIS:CE1	1:A:409:ASN:OD1	2.72	0.43
1:A:74:ILE:HG12	1:A:433:PHE:CD1	2.54	0.43
1:D:190:GLU:OE2	1:D:222:TYR:OH	2.35	0.43
1:A:327:LEU:HD22	1:A:426:MET:CE	2.49	0.43
1:D:79:VAL:HA	1:D:82:LEU:HG	2.00	0.43
1:A:6:LEU:HD11	1:A:33:GLU:HG3	2.00	0.43
1:B:98:VAL:HG22	1:B:109:PHE:CE2	2.54	0.42
1:D:438:LEU:HD23	1:D:438:LEU:HA	1.76	0.42
1:A:20:LEU:HD11	1:A:326:PHE:HD1	1.84	0.42
1:B:435:LEU:O	1:B:439:ILE:HG12	2.20	0.42
1:C:28:LYS:H	1:C:28:LYS:HG2	1.39	0.42
1:A:56:ASP:OD2	4:A:602:HOH:O	2.21	0.42
1:D:345:LYS:HZ1	1:D:361:ARG:CZ	2.33	0.42
1:D:32:PHE:H	1:D:52:LYS:NZ	2.18	0.41
1:D:61:LYS:N	1:D:61:LYS:HD2	2.35	0.41
1:A:240:GLY:HA2	1:A:246:ILE:HD11	2.01	0.41
1:A:396:LYS:HA	1:A:396:LYS:HD2	1.84	0.41
1:C:45:GLU:OE2	3:C:507:EDO:H22	2.20	0.41
1:A:87:GLU:HG3	1:A:316:PHE:CE1	2.55	0.41
1:B:82:LEU:HD22	4:B:848:HOH:O	2.21	0.41
1:D:153:MET:O	1:D:174:PHE:HA	2.20	0.41
1:B:360:ILE:CD1	1:B:362:ILE:HD11	2.50	0.41
1:B:432:ASN:O	1:B:436:GLU:HG2	2.21	0.41
1:C:198:LYS:NZ	4:C:613:HOH:O	2.43	0.41
1:B:337:GLU:O	1:B:341:ARG:HG3	2.21	0.41
1:B:25:GLY:HA2	1:B:28:LYS:HG3	2.01	0.40
1:C:98:VAL:HG21	1:C:308:ALA:CB	2.51	0.40
1:B:408:LEU:HD23	1:B:408:LEU:HA	1.93	0.40
1:C:68:ARG:HH11	1:C:68:ARG:HG3	1.86	0.40
1:B:386:TYR:O	1:B:414:HIS:HE1	2.03	0.40
1:D:94:THR:O	1:D:98:VAL:HG23	2.21	0.40
1:A:66:TYR:CE1	1:A:429:GLU:HG3	2.57	0.40
1:B:159:ALA:O	1:B:162[B]:GLU:HG2	2.22	0.40
1:C:153:MET:HB2	1:C:154:PRO:HD2	2.04	0.40
1:C:186:PRO:HA	1:C:189:ILE:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:244:ASP:HA	3:D:506:EDO:H22	2.03	0.40
1:C:228:GLU:HB2	1:C:246:ILE:HD12	2.01	0.40
1:D:52:LYS:CD	1:D:53:LEU:H	2.34	0.40

There are no symmetry-related clashes.

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	439/445 (99%)	425 (97%)	11 (2%)	3 (1%)	22	6
1	B	440/445 (99%)	424 (96%)	15 (3%)	1 (0%)	47	28
1	C	443/445 (100%)	429 (97%)	12 (3%)	2 (0%)	29	11
1	D	437/445 (98%)	419 (96%)	16 (4%)	2 (0%)	29	11
All	All	1759/1780 (99%)	1697 (96%)	54 (3%)	8 (0%)	29	11

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	51	ASN
1	A	29	GLU
1	A	180	LYS
1	D	28	LYS
1	B	258	VAL
1	C	258	VAL
1	D	258	VAL
1	A	258	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	399/401 (100%)	394 (99%)	5 (1%)	69	50
1	B	400/401 (100%)	395 (99%)	5 (1%)	69	50
1	C	403/401 (100%)	398 (99%)	5 (1%)	71	53
1	D	397/401 (99%)	387 (98%)	10 (2%)	47	22
All	All	1599/1604 (100%)	1574 (98%)	25 (2%)	65	41

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	THR
1	A	45	GLU
1	A	251	ASN
1	A	255	ASN
1	A	406	THR
1	B	13	SER
1	B	28	LYS
1	B	61	LYS
1	B	73	LYS
1	B	406	THR
1	C	28	LYS
1	C	121	LEU
1	C	214	ARG
1	C	251[A]	ASN
1	C	251[B]	ASN
1	D	27	THR
1	D	28	LYS
1	D	55	ILE
1	D	180	LYS
1	D	184	ILE
1	D	251	ASN
1	D	288	LYS
1	D	404	GLN
1	D	405	ASP
1	D	406	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	HIS
1	A	163	ASN
1	A	255	ASN
1	A	432	ASN
1	B	278	GLN
1	B	282	HIS
1	B	393	HIS
1	B	412	GLN
1	C	440	ASN
1	D	12	HIS
1	D	24	GLN
1	D	40	ASN
1	D	41	HIS
1	D	103	GLN
1	D	278	GLN
1	D	409	ASN
1	D	425	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

32 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	A	506	-	3,3,3	0.43	0	2,2,2	0.24	0
3	EDO	A	513	-	3,3,3	0.32	0	2,2,2	0.41	0
3	EDO	C	503	-	3,3,3	0.27	0	2,2,2	0.23	0
3	EDO	D	503	-	3,3,3	0.29	0	2,2,2	0.28	0
3	EDO	B	502	-	3,3,3	0.30	0	2,2,2	0.57	0
3	EDO	A	512	-	3,3,3	0.32	0	2,2,2	0.44	0
3	EDO	C	505	-	3,3,3	0.41	0	2,2,2	0.06	0
3	EDO	C	506	-	3,3,3	0.33	0	2,2,2	0.55	0
2	PMP	D	501	-	16,16,16	1.09	1 (6%)	17,23,23	1.59	2 (11%)
3	EDO	B	503	-	3,3,3	0.41	0	2,2,2	0.88	0
3	EDO	B	504	-	3,3,3	0.33	0	2,2,2	0.66	0
3	EDO	A	508	-	3,3,3	0.37	0	2,2,2	0.08	0
3	EDO	A	502	-	3,3,3	0.32	0	2,2,2	0.71	0
3	EDO	A	503	-	3,3,3	0.44	0	2,2,2	0.60	0
3	EDO	A	514	-	3,3,3	0.37	0	2,2,2	0.61	0
3	EDO	C	507	-	3,3,3	0.38	0	2,2,2	0.20	0
2	PMP	C	501	-	16,16,16	0.92	0	21,23,23	1.14	1 (4%)
3	EDO	D	504	-	3,3,3	0.26	0	2,2,2	0.68	0
3	EDO	A	510	-	3,3,3	0.33	0	2,2,2	0.46	0
3	EDO	D	502	-	3,3,3	0.34	0	2,2,2	0.84	0
3	EDO	C	504	-	3,3,3	0.35	0	2,2,2	1.13	0
3	EDO	C	502	-	3,3,3	0.37	0	2,2,2	0.15	0
3	EDO	D	506	-	3,3,3	0.30	0	2,2,2	0.37	0
3	EDO	C	508	-	3,3,3	0.35	0	2,2,2	0.23	0
3	EDO	D	505	-	3,3,3	0.38	0	2,2,2	0.65	0
2	PMP	B	501	-	16,16,16	1.40	2 (12%)	21,23,23	1.64	4 (19%)
3	EDO	A	507	-	3,3,3	0.34	0	2,2,2	0.38	0
2	PMP	A	501	-	16,16,16	1.08	1 (6%)	21,23,23	1.25	1 (4%)
3	EDO	A	504	-	3,3,3	0.37	0	2,2,2	0.23	0
3	EDO	A	509	-	3,3,3	0.48	0	2,2,2	0.33	0
3	EDO	A	505	-	3,3,3	0.36	0	2,2,2	0.69	0
3	EDO	A	511	-	3,3,3	0.27	0	2,2,2	0.85	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
3	EDO	A	506	-	-	0/1/1/1	-
3	EDO	A	513	-	-	1/1/1/1	-
3	EDO	C	503	-	-	0/1/1/1	-
3	EDO	D	503	-	-	0/1/1/1	-
3	EDO	B	502	-	-	0/1/1/1	-
3	EDO	A	512	-	-	1/1/1/1	-
3	EDO	C	505	-	-	1/1/1/1	-
3	EDO	C	506	-	-	0/1/1/1	-
3	EDO	B	503	-	-	1/1/1/1	-
3	EDO	B	504	-	-	1/1/1/1	-
3	EDO	A	508	-	-	0/1/1/1	-
3	EDO	A	502	-	-	1/1/1/1	-
3	EDO	A	503	-	-	0/1/1/1	-
3	EDO	A	514	-	-	1/1/1/1	-
3	EDO	C	507	-	-	1/1/1/1	-
2	PMP	C	501	-	-	2/8/8/8	0/1/1/1
3	EDO	D	504	-	-	0/1/1/1	-
3	EDO	A	510	-	-	1/1/1/1	-
3	EDO	D	502	-	-	0/1/1/1	-
3	EDO	C	504	-	-	1/1/1/1	-
3	EDO	C	502	-	-	1/1/1/1	-
3	EDO	D	506	-	-	1/1/1/1	-
3	EDO	C	508	-	-	0/1/1/1	-
3	EDO	D	505	-	-	1/1/1/1	-
2	PMP	B	501	-	-	3/8/8/8	0/1/1/1
3	EDO	A	507	-	-	0/1/1/1	-
2	PMP	A	501	-	-	2/8/8/8	0/1/1/1
3	EDO	A	504	-	-	0/1/1/1	-
3	EDO	A	509	-	-	1/1/1/1	-
3	EDO	A	505	-	-	0/1/1/1	-
3	EDO	A	511	-	-	0/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	PMP	C2A-C2	3.26	1.55	1.50
2	A	501	PMP	C5-C4	-2.40	1.37	1.40
2	D	501	PMP	C2A-C2	2.25	1.54	1.50
2	B	501	PMP	C2-N1	-2.15	1.29	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	PMP	C3-C4-C5	-3.46	115.40	118.72
2	B	501	PMP	C4A-C4-C3	-3.38	114.96	120.34
2	B	501	PMP	C4A-C4-C5	3.08	126.58	120.19
2	B	501	PMP	C5-C6-N1	-2.91	118.97	123.82
2	B	501	PMP	C6-N1-C2	2.83	124.41	119.17
2	C	501	PMP	C2A-C2-C3	2.37	123.82	120.89
2	D	501	PMP	O4P-P-O1P	2.24	112.77	106.47
2	A	501	PMP	C2A-C2-C3	2.01	123.38	120.89

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	PMP	C5-C4-C4A-N4A
2	B	501	PMP	C5-C4-C4A-N4A
2	C	501	PMP	C5-C4-C4A-N4A
3	A	514	EDO	O1-C1-C2-O2
3	B	503	EDO	O1-C1-C2-O2
3	B	504	EDO	O1-C1-C2-O2
3	C	505	EDO	O1-C1-C2-O2
3	D	505	EDO	O1-C1-C2-O2
3	D	506	EDO	O1-C1-C2-O2
3	A	509	EDO	O1-C1-C2-O2
3	C	504	EDO	O1-C1-C2-O2
2	A	501	PMP	C3-C4-C4A-N4A
2	B	501	PMP	C3-C4-C4A-N4A
2	B	501	PMP	C5A-O4P-P-O1P
3	C	502	EDO	O1-C1-C2-O2
3	A	512	EDO	O1-C1-C2-O2
3	A	513	EDO	O1-C1-C2-O2
3	A	502	EDO	O1-C1-C2-O2
3	A	510	EDO	O1-C1-C2-O2
3	C	507	EDO	O1-C1-C2-O2
2	C	501	PMP	C3-C4-C4A-N4A

There are no ring outliers.

22 monomers are involved in 36 short contacts:

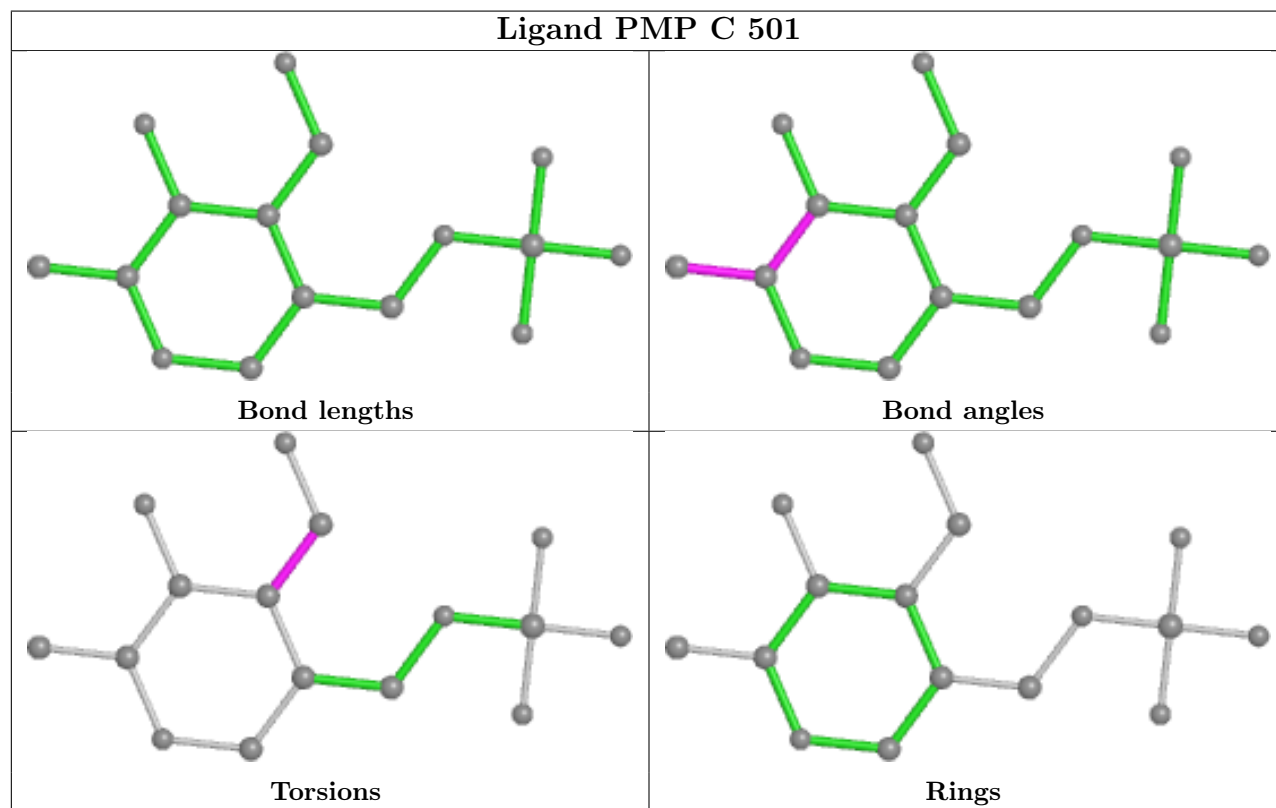
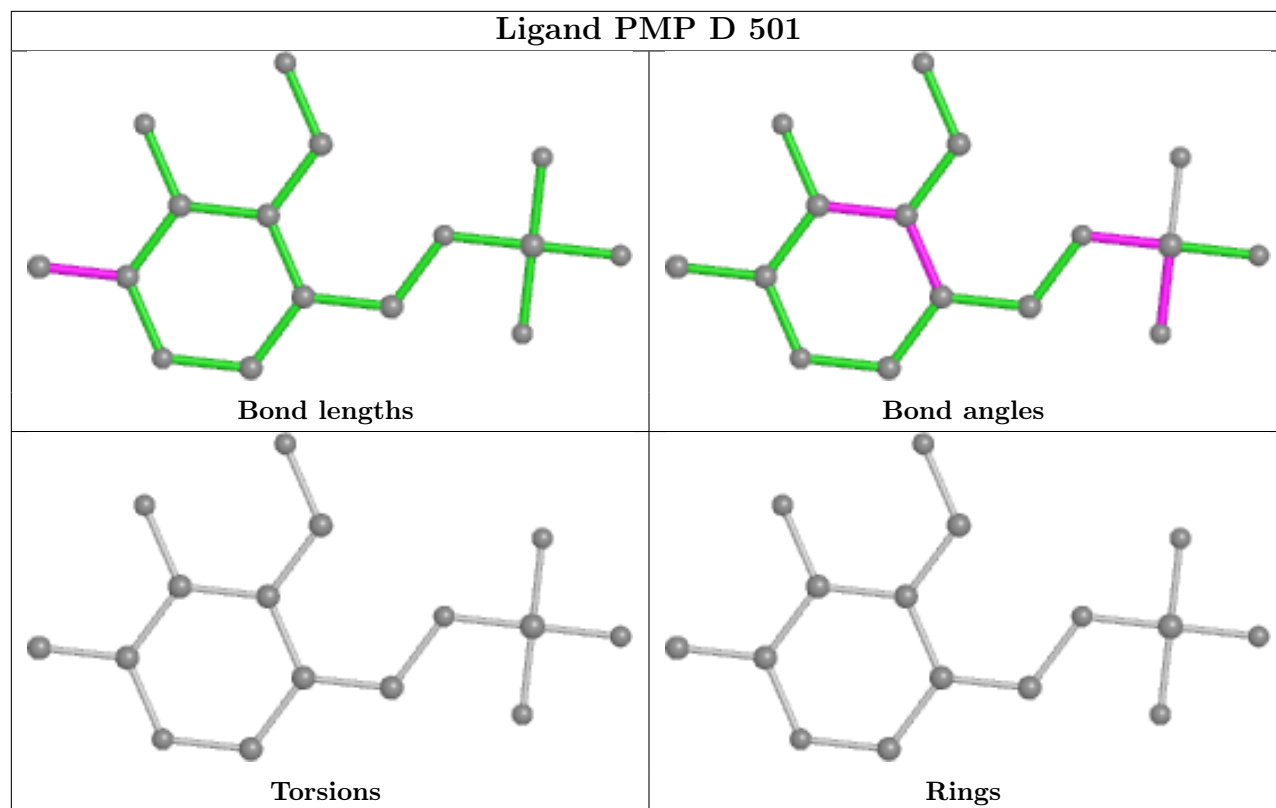
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	506	EDO	2	0
3	C	503	EDO	1	0
3	D	503	EDO	2	0

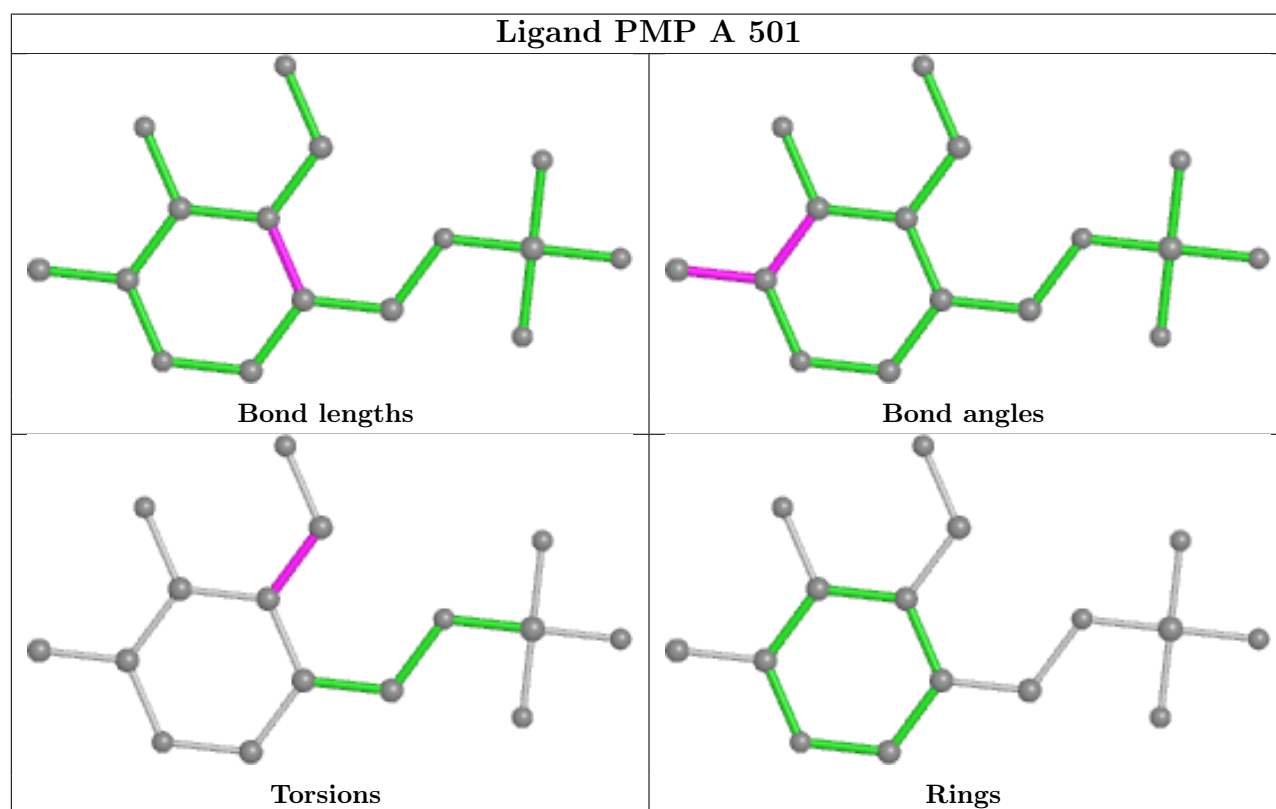
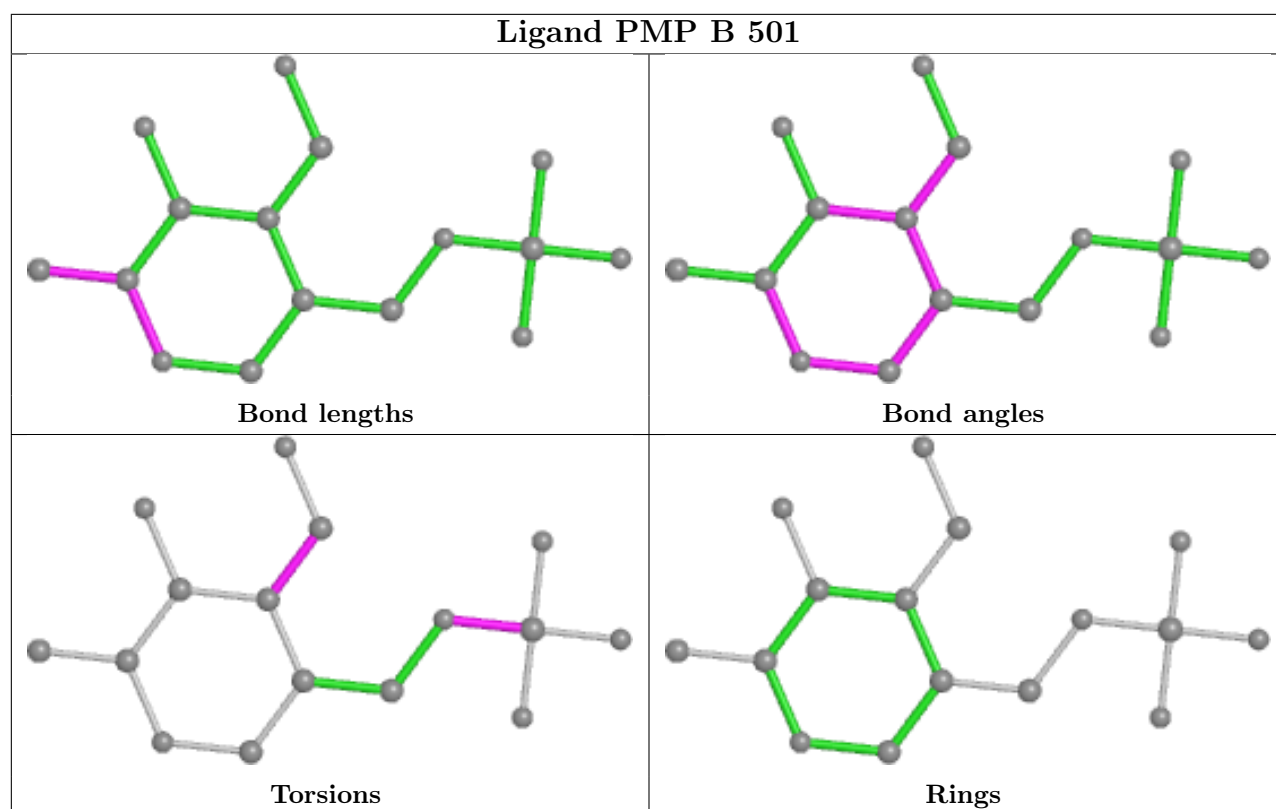
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	EDO	3	0
3	A	512	EDO	3	0
2	D	501	PMP	1	0
3	B	503	EDO	1	0
3	A	502	EDO	2	0
3	A	503	EDO	2	0
3	A	514	EDO	1	0
3	C	507	EDO	2	0
2	C	501	PMP	1	0
3	D	502	EDO	2	0
3	C	504	EDO	2	0
3	C	502	EDO	1	0
3	D	506	EDO	1	0
3	D	505	EDO	2	0
2	B	501	PMP	1	0
3	A	504	EDO	1	0
3	A	509	EDO	3	0
3	A	505	EDO	1	0
3	A	511	EDO	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, 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	438/445 (98%)	0.19	10 (2%) 60 61	14, 26, 49, 90	0
1	B	438/445 (98%)	0.36	21 (4%) 30 29	16, 32, 58, 108	0
1	C	438/445 (98%)	0.24	15 (3%) 45 45	16, 28, 51, 90	0
1	D	439/445 (98%)	0.55	38 (8%) 10 9	18, 38, 63, 104	0
All	All	1753/1780 (98%)	0.33	84 (4%) 30 29	14, 31, 58, 108	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	187	LEU	7.5
1	D	27	THR	6.7
1	C	27	THR	6.6
1	B	29	GLU	6.0
1	B	187	LEU	6.0
1	D	221	VAL	5.6
1	D	179	HIS	5.5
1	D	404	GLN	5.5
1	A	28	LYS	5.5
1	D	222	TYR	5.1
1	D	408	LEU	4.8
1	B	179	HIS	4.8
1	B	26	GLU	4.8
1	D	56	ASP	4.8
1	A	66	TYR	4.6
1	D	364	ASN	4.5
1	B	403[A]	MET	4.5
1	A	27	THR	4.4
1	B	28	LYS	4.4
1	D	29	GLU	4.3
1	A	179	HIS	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	363	ILE	4.1
1	D	223	GLN	4.0
1	D	28	LYS	3.9
1	C	179[A]	HIS	3.9
1	C	66	TYR	3.8
1	D	180	LYS	3.7
1	D	343	LEU	3.7
1	B	214	ARG	3.6
1	D	378	TYR	3.6
1	B	443	LYS	3.4
1	D	287	ASP	3.4
1	B	180	LYS	3.4
1	D	181	SER	3.3
1	B	287	ASP	3.2
1	C	221	VAL	3.2
1	B	55	ILE	3.2
1	B	404	GLN	3.2
1	B	343	LEU	3.1
1	B	408	LEU	3.1
1	B	50	GLU	3.1
1	D	195	GLN	3.1
1	D	5	THR	3.1
1	C	222	TYR	3.0
1	B	66	TYR	3.0
1	B	56	ASP	2.9
1	D	194	THR	2.9
1	D	214	ARG	2.8
1	B	211	ASP	2.8
1	A	68	ARG	2.8
1	C	28	LYS	2.8
1	C	337	GLU	2.8
1	A	180	LYS	2.8
1	D	439	ILE	2.7
1	D	219	ALA	2.7
1	C	180	LYS	2.7
1	D	335	LEU	2.6
1	C	342	GLU	2.5
1	D	189	ILE	2.5
1	D	379	ASN	2.5
1	C	127	ILE	2.4
1	D	412	GLN	2.4
1	D	65	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	29	GLU	2.4
1	C	30	LYS	2.3
1	D	220	ASP	2.3
1	A	65	ASN	2.3
1	C	364	ASN	2.3
1	D	337	GLU	2.2
1	D	185	ASP	2.2
1	D	211	ASP	2.2
1	A	22	CYS	2.2
1	D	402	TYR	2.2
1	D	191	GLU	2.2
1	B	25	GLY	2.2
1	D	242	TYR	2.1
1	D	6	LEU	2.1
1	A	30	LYS	2.1
1	A	25	GLY	2.1
1	C	68	ARG	2.1
1	B	68	ARG	2.1
1	D	190	GLU	2.1
1	C	58	ASP	2.0
1	B	400	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 [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	EDO	A	502	4/4	0.40	0.29	27,36,40,43	0
3	EDO	A	514	4/4	0.49	0.24	46,46,49,51	0

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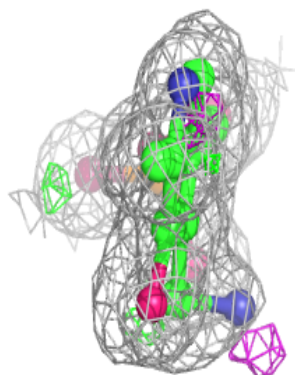
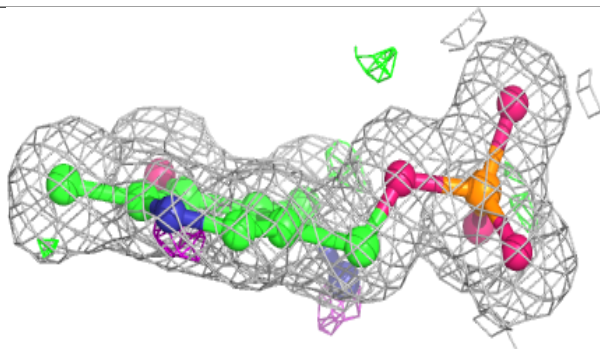
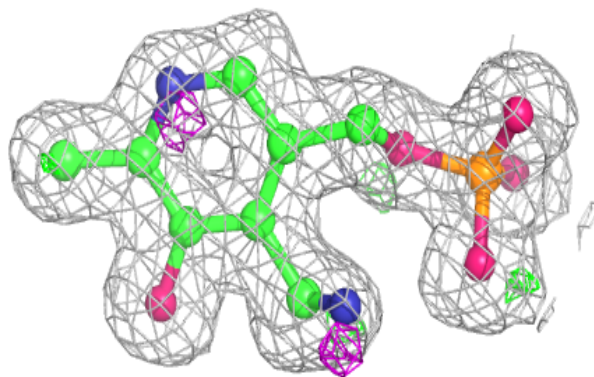
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	EDO	C	505	4/4	0.53	0.29	51,53,53,53	0
3	EDO	A	503	4/4	0.56	0.19	47,51,51,56	0
3	EDO	C	502	4/4	0.65	0.26	40,43,50,53	0
3	EDO	D	506	4/4	0.66	0.22	45,48,50,51	0
3	EDO	D	504	4/4	0.68	0.18	49,51,52,54	0
3	EDO	A	504	4/4	0.70	0.22	29,37,42,42	0
3	EDO	A	509	4/4	0.71	0.17	40,40,42,42	0
3	EDO	A	510	4/4	0.74	0.19	46,48,48,57	0
3	EDO	D	505	4/4	0.76	0.15	34,39,46,54	0
3	EDO	A	507	4/4	0.77	0.14	35,43,44,48	0
3	EDO	C	503	4/4	0.77	0.16	34,40,47,54	0
3	EDO	C	507	4/4	0.78	0.13	53,54,54,58	0
3	EDO	A	506	4/4	0.82	0.16	35,45,50,54	0
3	EDO	C	506	4/4	0.82	0.31	45,53,57,58	0
3	EDO	B	504	4/4	0.82	0.22	55,56,56,57	0
3	EDO	D	503	4/4	0.83	0.18	36,39,47,50	0
3	EDO	A	513	4/4	0.86	0.09	43,43,48,49	0
3	EDO	A	512	4/4	0.86	0.29	58,62,66,71	0
3	EDO	A	508	4/4	0.87	0.16	31,35,37,41	0
3	EDO	C	504	4/4	0.88	0.18	28,32,34,41	0
3	EDO	B	503	4/4	0.88	0.15	39,39,41,42	0
3	EDO	C	508	4/4	0.89	0.11	47,50,52,53	0
3	EDO	A	511	4/4	0.90	0.13	44,48,48,54	0
3	EDO	B	502	4/4	0.93	0.18	31,36,42,47	0
3	EDO	D	502	4/4	0.93	0.12	37,39,42,48	0
2	PMP	A	501	16/16	0.96	0.12	14,17,25,38	0
2	PMP	B	501	16/16	0.97	0.10	16,21,27,33	0
2	PMP	C	501	16/16	0.97	0.11	14,18,25,35	0
2	PMP	D	501	16/16	0.97	0.10	18,22,26,33	0
3	EDO	A	505	4/4	0.97	0.25	30,37,39,43	0

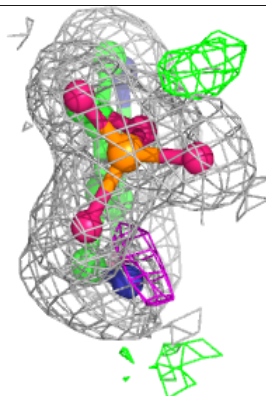
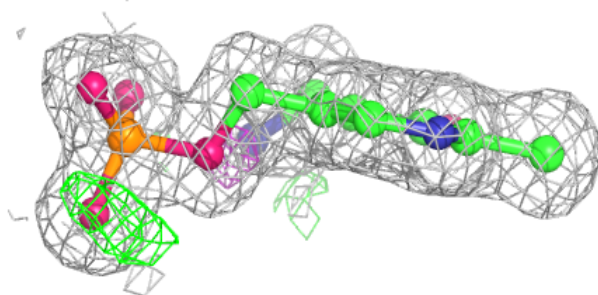
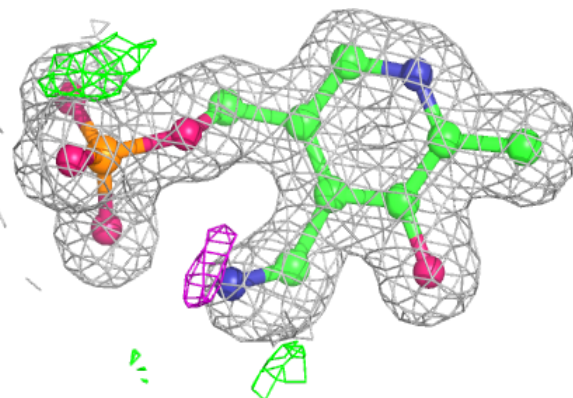
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation 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)

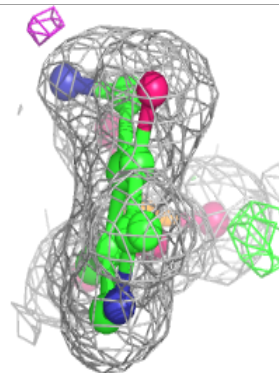
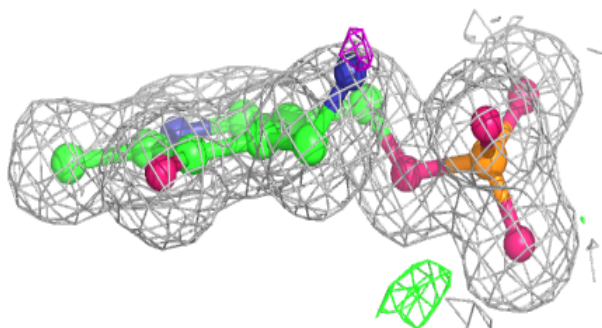
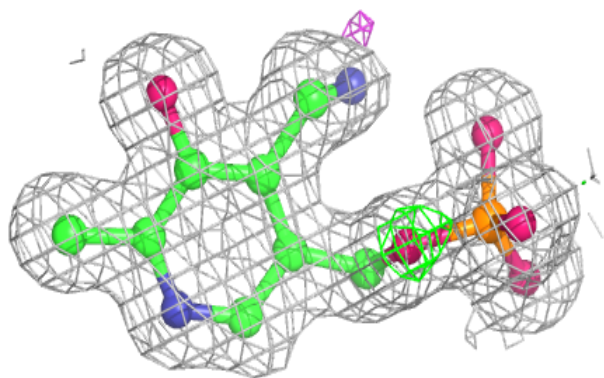
**Electron density around PMP B 501:**

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

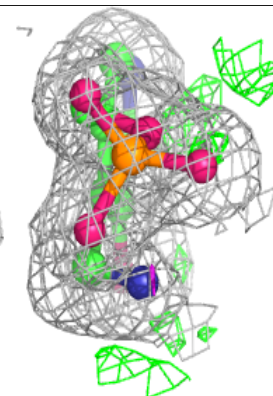
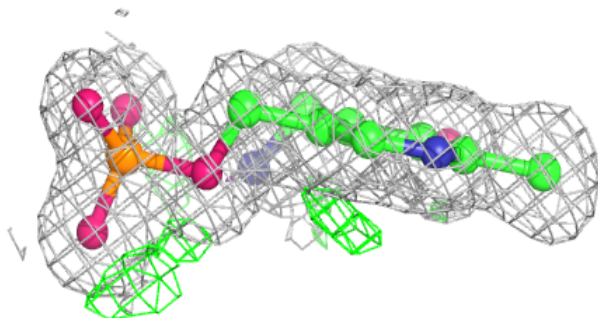
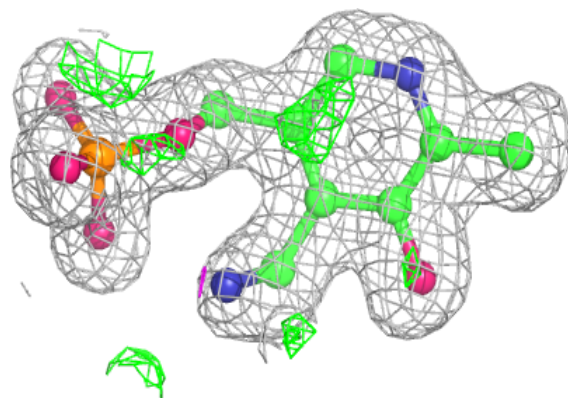


Electron density around PMP C 501:

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

**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 ⓘ

There are no such residues in this entry.