Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 07:59 AM BST

PDB ID	:	6EWR
Title	:	Putative sugar aminotransferase Spr1654 from Streptococcus pneumoniae, PMP-form
Authors	:	Achour, A.; Sun, R.; Sandalova, T.; Han, X.
Deposited on	:	2017-11-06
Resolution	:	2.40 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:

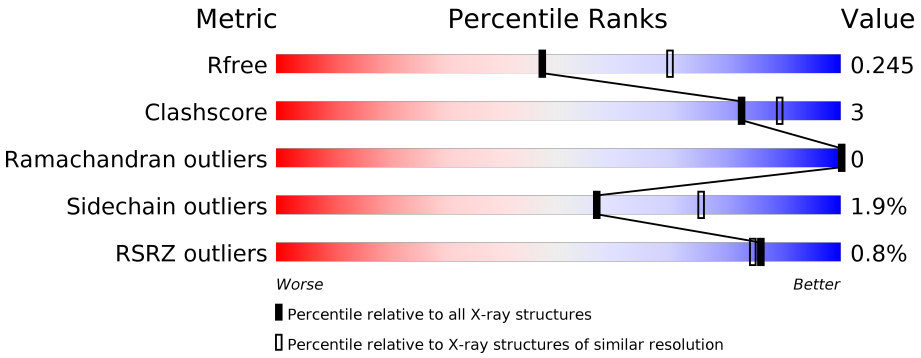
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	427	86% 7% • 7%
1	B	427	85% 7% 7%
1	C	427	2% 86% 7% 6%
1	D	427	85% 7% 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12804 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 Putative capsular polysaccharide biosynthesis protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	399	Total	C	N	O	S	0	0	0
			3136	2002	514	608	12			
1	B	396	Total	C	N	O	S	0	0	0
			3123	1996	511	605	11			
1	C	400	Total	C	N	O	S	0	0	0
			3143	2006	515	610	12			
1	D	397	Total	C	N	O	S	0	0	0
			3131	2000	512	608	11			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	initiating methionine	UNP A0A0H2URM1
A	-4	ALA	-	expression tag	UNP A0A0H2URM1
A	-3	SER	-	expression tag	UNP A0A0H2URM1
A	-2	MET	-	expression tag	UNP A0A0H2URM1
A	-1	THR	-	expression tag	UNP A0A0H2URM1
A	0	GLY	-	expression tag	UNP A0A0H2URM1
A	178	THR	ILE	conflict	UNP A0A0H2URM1
A	409	LYS	-	expression tag	UNP A0A0H2URM1
A	410	LEU	-	expression tag	UNP A0A0H2URM1
A	411	ALA	-	expression tag	UNP A0A0H2URM1
A	412	ALA	-	expression tag	UNP A0A0H2URM1
A	413	ALA	-	expression tag	UNP A0A0H2URM1
A	414	LEU	-	expression tag	UNP A0A0H2URM1
A	415	GLU	-	expression tag	UNP A0A0H2URM1
A	416	HIS	-	expression tag	UNP A0A0H2URM1
A	417	HIS	-	expression tag	UNP A0A0H2URM1
A	418	HIS	-	expression tag	UNP A0A0H2URM1
A	419	HIS	-	expression tag	UNP A0A0H2URM1
A	420	HIS	-	expression tag	UNP A0A0H2URM1
A	421	HIS	-	expression tag	UNP A0A0H2URM1
B	-5	MET	-	initiating methionine	UNP A0A0H2URM1

Continued on next page...

Continued from previous page...

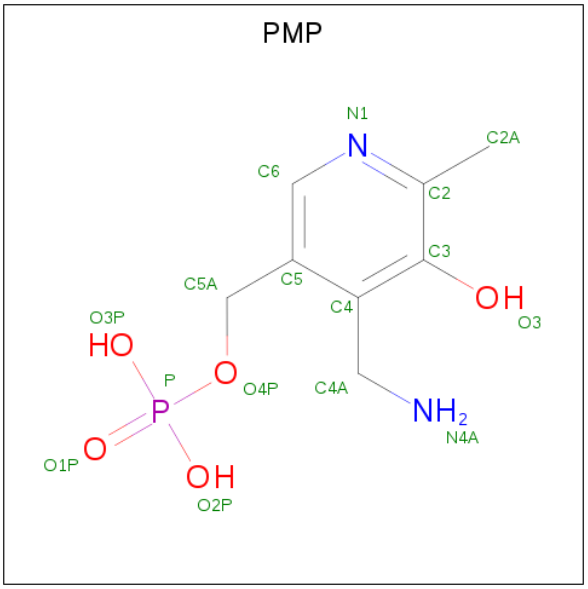
Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	ALA	-	expression tag	UNP A0A0H2URM1
B	-3	SER	-	expression tag	UNP A0A0H2URM1
B	-2	MET	-	expression tag	UNP A0A0H2URM1
B	-1	THR	-	expression tag	UNP A0A0H2URM1
B	0	GLY	-	expression tag	UNP A0A0H2URM1
B	178	THR	ILE	conflict	UNP A0A0H2URM1
B	409	LYS	-	expression tag	UNP A0A0H2URM1
B	410	LEU	-	expression tag	UNP A0A0H2URM1
B	411	ALA	-	expression tag	UNP A0A0H2URM1
B	412	ALA	-	expression tag	UNP A0A0H2URM1
B	413	ALA	-	expression tag	UNP A0A0H2URM1
B	414	LEU	-	expression tag	UNP A0A0H2URM1
B	415	GLU	-	expression tag	UNP A0A0H2URM1
B	416	HIS	-	expression tag	UNP A0A0H2URM1
B	417	HIS	-	expression tag	UNP A0A0H2URM1
B	418	HIS	-	expression tag	UNP A0A0H2URM1
B	419	HIS	-	expression tag	UNP A0A0H2URM1
B	420	HIS	-	expression tag	UNP A0A0H2URM1
B	421	HIS	-	expression tag	UNP A0A0H2URM1
C	-5	MET	-	initiating methionine	UNP A0A0H2URM1
C	-4	ALA	-	expression tag	UNP A0A0H2URM1
C	-3	SER	-	expression tag	UNP A0A0H2URM1
C	-2	MET	-	expression tag	UNP A0A0H2URM1
C	-1	THR	-	expression tag	UNP A0A0H2URM1
C	0	GLY	-	expression tag	UNP A0A0H2URM1
C	178	THR	ILE	conflict	UNP A0A0H2URM1
C	409	LYS	-	expression tag	UNP A0A0H2URM1
C	410	LEU	-	expression tag	UNP A0A0H2URM1
C	411	ALA	-	expression tag	UNP A0A0H2URM1
C	412	ALA	-	expression tag	UNP A0A0H2URM1
C	413	ALA	-	expression tag	UNP A0A0H2URM1
C	414	LEU	-	expression tag	UNP A0A0H2URM1
C	415	GLU	-	expression tag	UNP A0A0H2URM1
C	416	HIS	-	expression tag	UNP A0A0H2URM1
C	417	HIS	-	expression tag	UNP A0A0H2URM1
C	418	HIS	-	expression tag	UNP A0A0H2URM1
C	419	HIS	-	expression tag	UNP A0A0H2URM1
C	420	HIS	-	expression tag	UNP A0A0H2URM1
C	421	HIS	-	expression tag	UNP A0A0H2URM1
D	-5	MET	-	initiating methionine	UNP A0A0H2URM1
D	-4	ALA	-	expression tag	UNP A0A0H2URM1
D	-3	SER	-	expression tag	UNP A0A0H2URM1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	MET	-	expression tag	UNP A0A0H2URM1
D	-1	THR	-	expression tag	UNP A0A0H2URM1
D	0	GLY	-	expression tag	UNP A0A0H2URM1
D	178	THR	ILE	conflict	UNP A0A0H2URM1
D	409	LYS	-	expression tag	UNP A0A0H2URM1
D	410	LEU	-	expression tag	UNP A0A0H2URM1
D	411	ALA	-	expression tag	UNP A0A0H2URM1
D	412	ALA	-	expression tag	UNP A0A0H2URM1
D	413	ALA	-	expression tag	UNP A0A0H2URM1
D	414	LEU	-	expression tag	UNP A0A0H2URM1
D	415	GLU	-	expression tag	UNP A0A0H2URM1
D	416	HIS	-	expression tag	UNP A0A0H2URM1
D	417	HIS	-	expression tag	UNP A0A0H2URM1
D	418	HIS	-	expression tag	UNP A0A0H2URM1
D	419	HIS	-	expression tag	UNP A0A0H2URM1
D	420	HIS	-	expression tag	UNP A0A0H2URM1
D	421	HIS	-	expression tag	UNP A0A0H2URM1

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



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

Continued on next page...

Continued from previous page...

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 water.

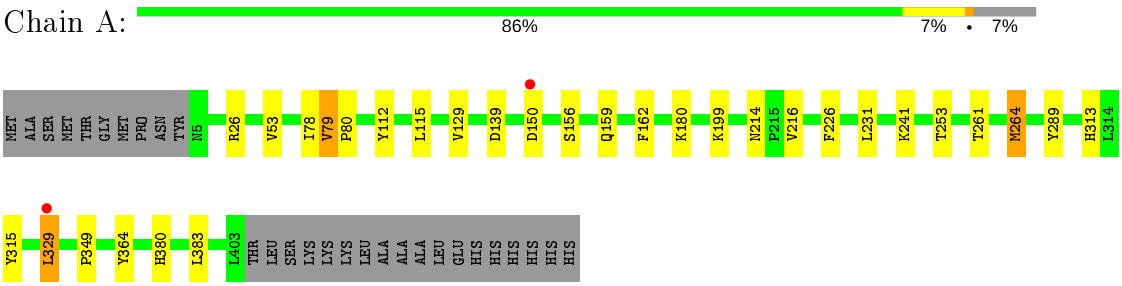
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	47	Total	O	0	0
			47	47		
3	B	47	Total	O	0	0
			47	47		
3	C	55	Total	O	0	0
			55	55		
3	D	58	Total	O	0	0
			58	58		

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.

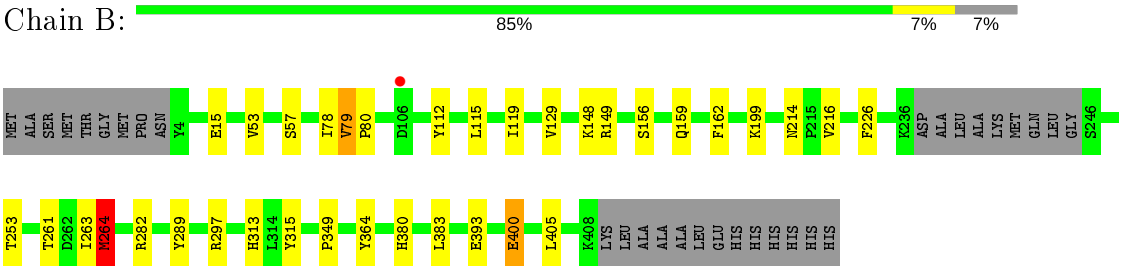
- Molecule 1: Putative capsular polysaccharide biosynthesis protein

Chain A:



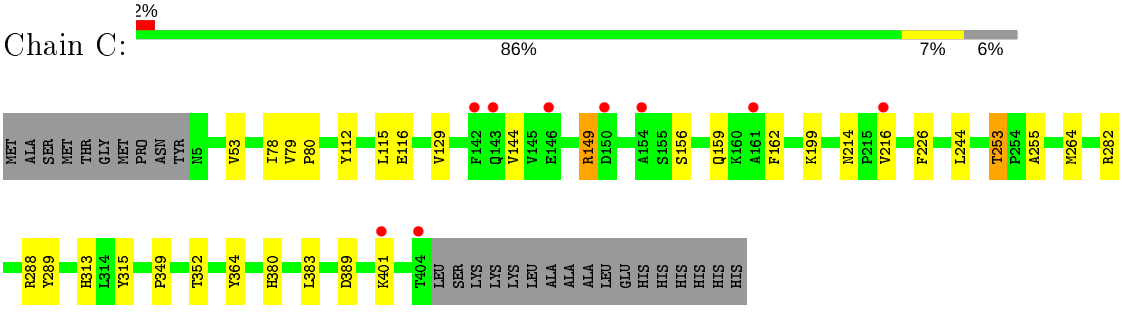
- Molecule 1: Putative capsular polysaccharide biosynthesis protein

Chain B:



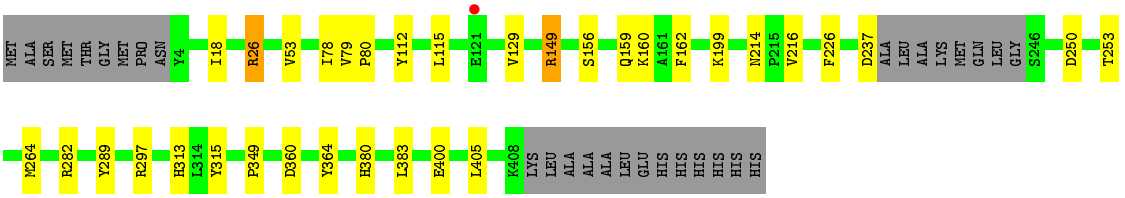
- Molecule 1: Putative capsular polysaccharide biosynthesis protein

Chain C:



- Molecule 1: Putative capsular polysaccharide biosynthesis protein

Chain D:


MET ALA SER MET THR GLY MET PRO ASN Y4 I18 R26 V53 I78 V79 P80 Y112 L115 E121 V129 R149 S156 Q159 K160 A161 F162 K199 N214 P215 V216 F226 D237 ALA LEU ALA LYS MET GLN LEU GLY S246 D250 T253

M264 R282 Y289 R297 H313 L314 Y315 P349 D360 Y364 H380 L383 E400 L405 K408 LYS LEU ALA ALA ALA LEU GLU HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	78.90Å 99.56Å 108.09Å 90.00° 97.53° 90.00°	Depositor
Resolution (Å)	29.80 – 2.40 47.18 – 2.38	Depositor EDS
% Data completeness (in resolution range)	99.0 (29.80-2.40) 98.9 (47.18-2.38)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.13 (at 2.37Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.242 , 0.285 0.248 , 0.245	Depositor DCC
R_{free} test set	3233 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	21.0	Xtriage
Anisotropy	0.852	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 29.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	12804	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.95% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.58	0/3202	0.79	4/4351 (0.1%)
1	B	0.64	0/3189	0.78	4/4332 (0.1%)
1	C	0.58	0/3209	0.77	2/4361 (0.0%)
1	D	0.58	0/3197	0.78	5/4343 (0.1%)
All	All	0.60	0/12797	0.78	15/17387 (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	A	0	1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	264	MET	CG-SD-CE	8.06	113.10	100.20
1	B	149	ARG	NE-CZ-NH1	7.61	124.10	120.30
1	D	360	ASP	CB-CG-OD2	6.80	124.42	118.30
1	A	329	LEU	CA-CB-CG	6.62	130.52	115.30
1	C	149	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	A	139	ASP	CB-CG-OD2	-6.57	112.39	118.30
1	D	282	ARG	NE-CZ-NH2	-5.97	117.32	120.30
1	B	149	ARG	NE-CZ-NH2	-5.87	117.36	120.30
1	A	180	LYS	CD-CE-NZ	5.83	125.11	111.70
1	C	282	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	B	282	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	D	149	ARG	NE-CZ-NH2	-5.46	117.57	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	231	LEU	CA-CB-CG	5.17	127.19	115.30
1	D	149	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	D	26	ARG	NE-CZ-NH1	5.14	122.87	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	150	ASP	Peptide

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	3136	0	3121	15	0
1	B	3123	0	3109	19	0
1	C	3143	0	3128	15	0
1	D	3131	0	3113	16	0
2	A	16	0	11	0	0
2	B	16	0	10	2	0
2	C	16	0	10	1	0
2	D	16	0	11	1	0
3	A	47	0	0	1	0
3	B	47	0	0	0	0
3	C	55	0	0	0	0
3	D	58	0	0	1	0
All	All	12804	0	12513	63	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 (63) 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:199:LYS:NZ	3:D:601:HOH:O	2.13	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:THR:OG1	1:B:264:MET:HE2	1.87	0.73
1:B:297:ARG:NH1	1:B:400:GLU:OE2	2.28	0.65
1:B:119:ILE:HB	1:B:148:LYS:HD2	1.83	0.61
1:D:297:ARG:HH12	1:D:400:GLU:HG3	1.69	0.57
1:B:199:LYS:HE2	2:B:500:PMP:N4A	2.21	0.56
1:C:78:ILE:HG21	1:C:115:LEU:HD13	1.86	0.56
1:C:352:THR:OG1	1:D:250:ASP:OD2	2.15	0.56
1:B:78:ILE:HG21	1:B:115:LEU:HD13	1.88	0.56
1:D:78:ILE:HG21	1:D:115:LEU:HD13	1.88	0.56
1:A:78:ILE:HG21	1:A:115:LEU:HD13	1.87	0.56
1:C:288:ARG:NH1	1:C:389:ASP:OD1	2.40	0.54
1:B:261:THR:OG1	1:B:264:MET:CE	2.57	0.52
1:A:264:MET:HE2	3:A:635:HOH:O	2.10	0.52
1:A:79:VAL:HG12	1:A:80:PRO:HD2	1.93	0.50
1:A:159:GLN:O	1:A:162:PHE:O	2.30	0.50
1:C:159:GLN:O	1:C:162:PHE:O	2.30	0.50
1:C:79:VAL:HG22	1:C:80:PRO:HD2	1.95	0.49
1:B:79:VAL:HG12	1:B:80:PRO:HD2	1.93	0.49
1:A:261:THR:OG1	1:A:264:MET:HE2	2.13	0.49
1:B:159:GLN:O	1:B:162:PHE:O	2.30	0.49
1:D:159:GLN:O	1:D:162:PHE:O	2.30	0.49
1:B:57:SER:HB2	2:B:500:PMP:O1P	2.13	0.48
1:B:15:GLU:HG3	1:D:18:ILE:HG22	1.95	0.48
1:B:199:LYS:HA	1:B:313:HIS:CE1	2.49	0.48
1:D:199:LYS:HE2	2:D:500:PMP:N4A	2.29	0.47
1:D:199:LYS:HA	1:D:313:HIS:CE1	2.50	0.47
1:A:199:LYS:HA	1:A:313:HIS:CE1	2.50	0.47
1:B:214:ASN:OD1	1:B:216:VAL:HG22	2.15	0.46
1:D:214:ASN:OD1	1:D:216:VAL:HG22	2.15	0.46
1:C:214:ASN:OD1	1:C:216:VAL:HG22	2.16	0.46
1:C:199:LYS:HA	1:C:313:HIS:CE1	2.50	0.46
1:D:349:PRO:HG2	1:D:364:TYR:CD1	2.51	0.45
1:B:263:ILE:HB	1:B:264:MET:HE2	1.99	0.45
2:C:500:PMP:O3	2:C:500:PMP:N4A	2.49	0.45
1:A:214:ASN:OD1	1:A:216:VAL:HG22	2.17	0.45
1:B:349:PRO:HG2	1:B:364:TYR:CD2	2.52	0.45
1:C:112:TYR:HD1	1:C:115:LEU:HD23	1.82	0.44
1:A:112:TYR:HD1	1:A:115:LEU:HD23	1.83	0.44
1:C:349:PRO:HG2	1:C:364:TYR:CD2	2.53	0.44
1:B:380:HIS:CE1	1:B:383:LEU:HG	2.53	0.43
1:C:380:HIS:CE1	1:C:383:LEU:HG	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:HIS:CE1	1:A:383:LEU:HG	2.53	0.43
1:D:380:HIS:CE1	1:D:383:LEU:HG	2.54	0.43
1:D:53:VAL:HG11	1:D:226:PHE:HB3	2.00	0.43
1:A:53:VAL:HG11	1:A:226:PHE:HB3	2.01	0.42
1:C:116:GLU:HG2	1:C:144:VAL:HG13	2.01	0.42
1:C:53:VAL:HG11	1:C:226:PHE:HB3	2.02	0.42
1:D:80:PRO:HG2	1:D:129:VAL:HG12	2.01	0.42
1:A:349:PRO:HG2	1:A:364:TYR:CD2	2.55	0.42
1:B:53:VAL:HG11	1:B:226:PHE:HB3	2.00	0.42
1:B:80:PRO:HG2	1:B:129:VAL:HG12	2.02	0.42
1:D:289:TYR:HB3	1:D:315:TYR:CZ	2.55	0.42
1:C:80:PRO:HG2	1:C:129:VAL:HG12	2.01	0.41
1:C:253:THR:HG22	1:C:255:ALA:HB2	2.02	0.41
1:B:112:TYR:HD1	1:B:115:LEU:HD23	1.83	0.41
1:D:112:TYR:HD1	1:D:115:LEU:HD23	1.84	0.41
1:A:80:PRO:HG2	1:A:129:VAL:HG12	2.02	0.41
1:C:289:TYR:HB3	1:C:315:TYR:CZ	2.56	0.41
1:A:289:TYR:HB3	1:A:315:TYR:CZ	2.56	0.41
1:A:26:ARG:NH1	1:D:26:ARG:HD3	2.35	0.40
1:B:289:TYR:HB3	1:B:315:TYR:CZ	2.56	0.40
1:A:261:THR:OG1	1:A:264:MET:CE	2.70	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	397/427 (93%)	384 (97%)	13 (3%)	0	100	100
1	B	392/427 (92%)	379 (97%)	13 (3%)	0	100	100
1	C	398/427 (93%)	386 (97%)	12 (3%)	0	100	100
1	D	393/427 (92%)	381 (97%)	12 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1580/1708 (92%)	1530 (97%)	50 (3%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	346/371 (93%)	340 (98%)	6 (2%)	60 78
1	B	346/371 (93%)	339 (98%)	7 (2%)	55 74
1	C	347/371 (94%)	341 (98%)	6 (2%)	60 78
1	D	347/371 (94%)	339 (98%)	8 (2%)	50 70
All	All	1386/1484 (93%)	1359 (98%)	27 (2%)	57 75

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	VAL
1	A	156	SER
1	A	241	LYS
1	A	253	THR
1	A	264	MET
1	A	329	LEU
1	B	79	VAL
1	B	156	SER
1	B	253	THR
1	B	264	MET
1	B	393	GLU
1	B	400	GLU
1	B	405	LEU
1	C	149	ARG
1	C	156	SER
1	C	244	LEU
1	C	253	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	264	MET
1	C	401	LYS
1	D	79	VAL
1	D	149	ARG
1	D	156	SER
1	D	160	LYS
1	D	237	ASP
1	D	253	THR
1	D	264	MET
1	D	405	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

4 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	C	500	-	16,16,16	2.89	3 (18%)	21,23,23	1.51	2 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	PMP	A	500	-	16,16,16	3.07	3 (18%)	21,23,23	1.36	3 (14%)
2	PMP	D	500	-	16,16,16	3.31	4 (25%)	21,23,23	1.86	8 (38%)
2	PMP	B	500	-	16,16,16	3.31	5 (31%)	21,23,23	1.60	5 (23%)

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	C	500	-	-	7/8/8/8	0/1/1/1
2	PMP	A	500	-	-	7/8/8/8	0/1/1/1
2	PMP	D	500	-	-	0/8/8/8	0/1/1/1
2	PMP	B	500	-	-	1/8/8/8	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	PMP	C5-C4	8.43	1.52	1.40
2	D	500	PMP	C5-C4	7.98	1.51	1.40
2	B	500	PMP	C3-C2	7.56	1.48	1.40
2	A	500	PMP	C5-C4	7.54	1.51	1.40
2	A	500	PMP	C3-C2	7.46	1.48	1.40
2	C	500	PMP	C3-C2	7.36	1.48	1.40
2	D	500	PMP	C3-C2	7.24	1.48	1.40
2	C	500	PMP	C5-C4	6.73	1.49	1.40
2	D	500	PMP	C3-C4	6.58	1.50	1.40
2	B	500	PMP	C3-C4	5.63	1.48	1.40
2	A	500	PMP	C3-C4	5.55	1.48	1.40
2	C	500	PMP	C3-C4	5.24	1.48	1.40
2	B	500	PMP	C2-N1	2.36	1.38	1.33
2	D	500	PMP	C2-N1	2.34	1.38	1.33
2	B	500	PMP	C6-C5	2.23	1.42	1.37

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	500	PMP	C6-N1-C2	3.87	126.33	119.17
2	D	500	PMP	C2A-C2-C3	-3.52	116.53	120.89
2	D	500	PMP	C6-N1-C2	3.22	125.14	119.17
2	D	500	PMP	C6-C5-C4	3.08	120.30	118.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	500	PMP	C6-N1-C2	3.00	124.72	119.17
2	D	500	PMP	O4P-P-O1P	2.84	114.43	106.47
2	B	500	PMP	C2A-C2-C3	-2.82	117.40	120.89
2	B	500	PMP	C6-N1-C2	2.80	124.34	119.17
2	D	500	PMP	C2A-C2-N1	2.77	123.09	117.67
2	A	500	PMP	C4-C3-C2	-2.68	115.95	120.06
2	A	500	PMP	O3-C3-C2	2.56	123.08	117.49
2	B	500	PMP	O3-C3-C2	2.52	122.99	117.49
2	C	500	PMP	C2A-C2-N1	2.15	121.86	117.67
2	B	500	PMP	C4-C3-C2	-2.14	116.78	120.06
2	D	500	PMP	C4-C3-C2	-2.13	116.80	120.06
2	D	500	PMP	O3-C3-C4	2.10	124.30	118.13
2	B	500	PMP	C2A-C2-N1	2.02	121.62	117.67
2	D	500	PMP	C5-C6-N1	-2.01	120.47	123.82

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	500	PMP	C4-C5-C5A-O4P
2	C	500	PMP	C5A-O4P-P-O1P
2	C	500	PMP	C5A-O4P-P-O3P
2	A	500	PMP	C5-C4-C4A-N4A
2	A	500	PMP	C4-C5-C5A-O4P
2	A	500	PMP	C6-C5-C5A-O4P
2	A	500	PMP	C5A-O4P-P-O1P
2	A	500	PMP	C5A-O4P-P-O2P
2	A	500	PMP	C5A-O4P-P-O3P
2	C	500	PMP	C3-C4-C4A-N4A
2	A	500	PMP	C3-C4-C4A-N4A
2	C	500	PMP	C5-C4-C4A-N4A
2	C	500	PMP	C5A-O4P-P-O2P
2	C	500	PMP	C6-C5-C5A-O4P
2	B	500	PMP	C5A-O4P-P-O2P

There are no ring outliers.

3 monomers are involved in 4 short contacts:

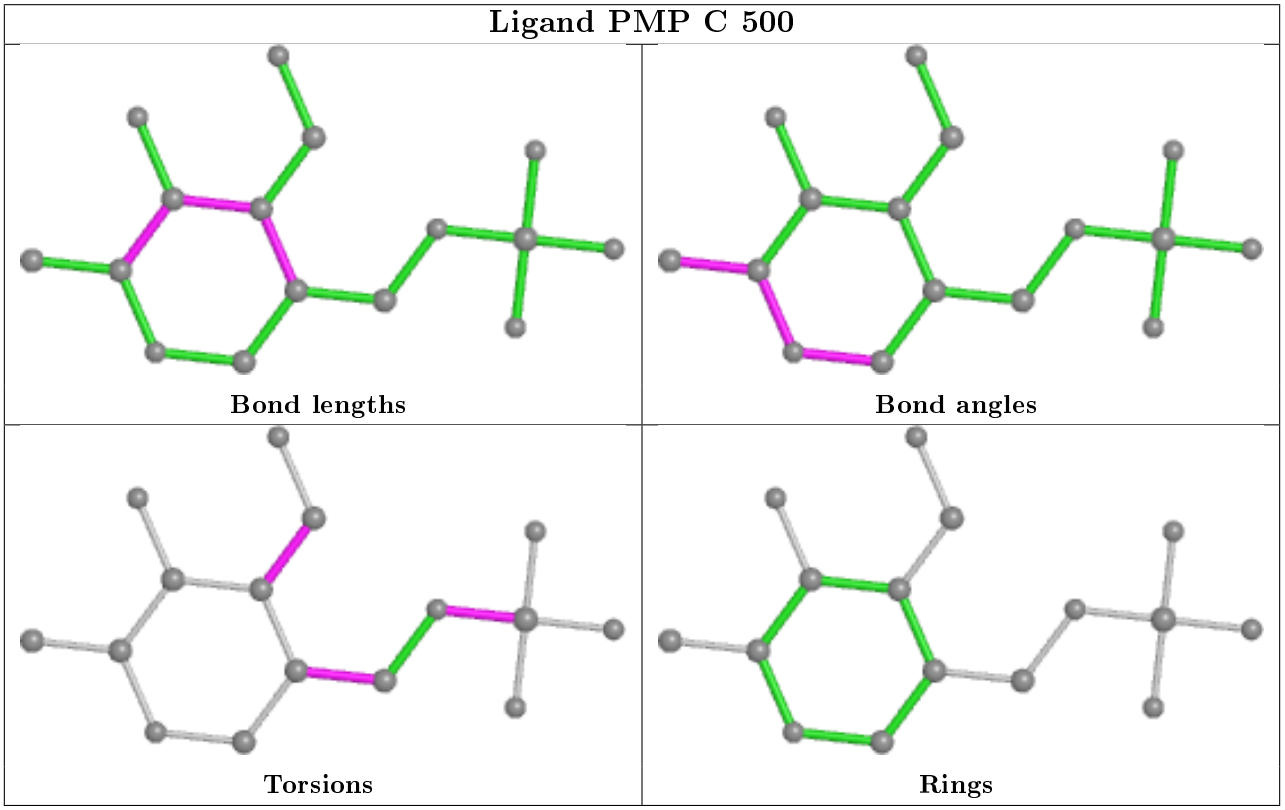
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	500	PMP	1	0
2	D	500	PMP	1	0

Continued on next page...

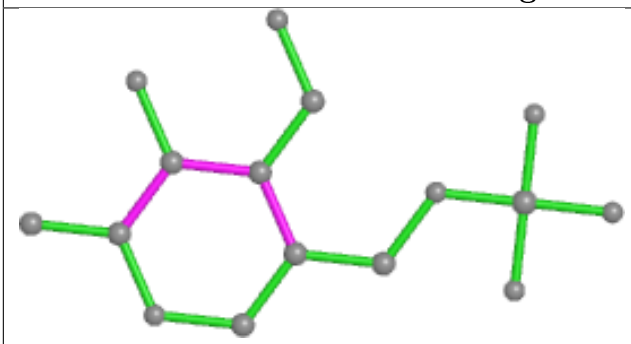
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	500	PMP	2	0

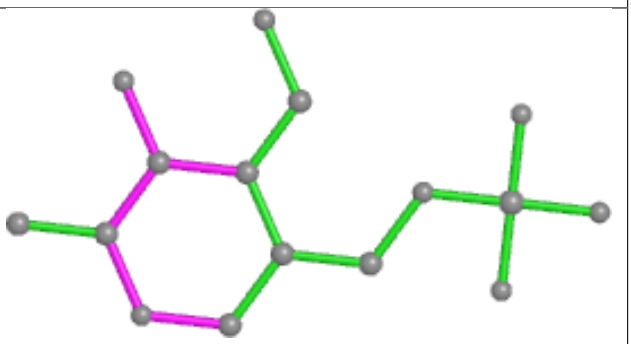
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.



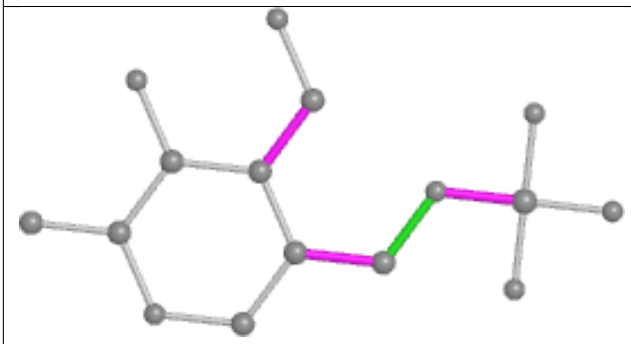
Ligand PMP A 500



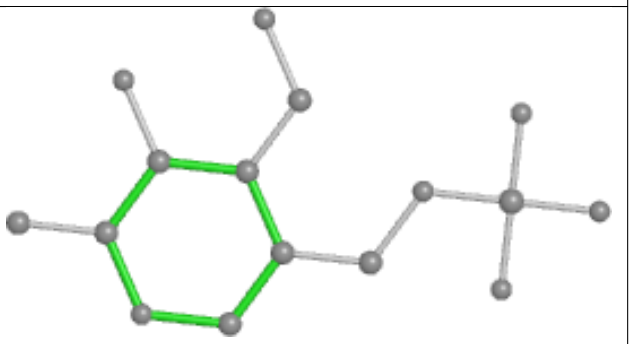
Bond lengths



Bond angles

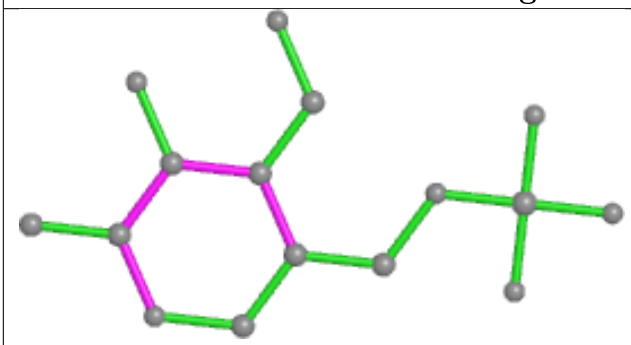


Torsions

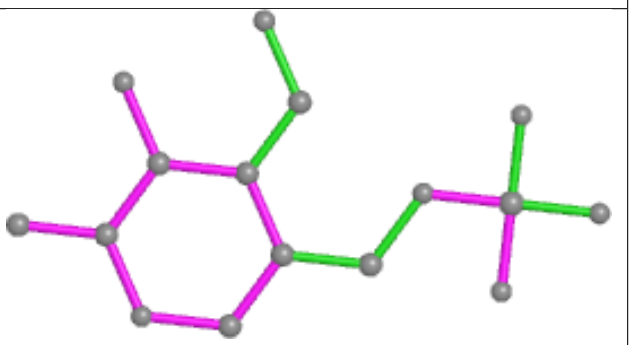


Rings

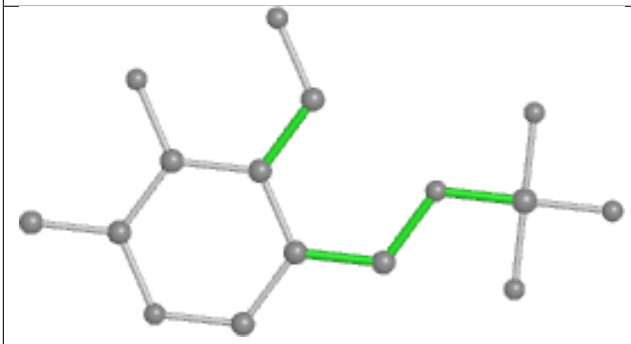
Ligand PMP D 500



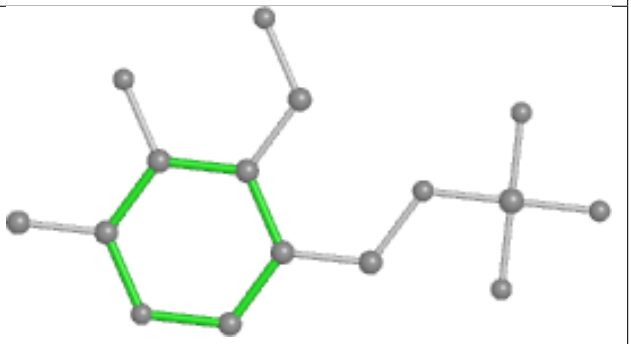
Bond lengths



Bond angles

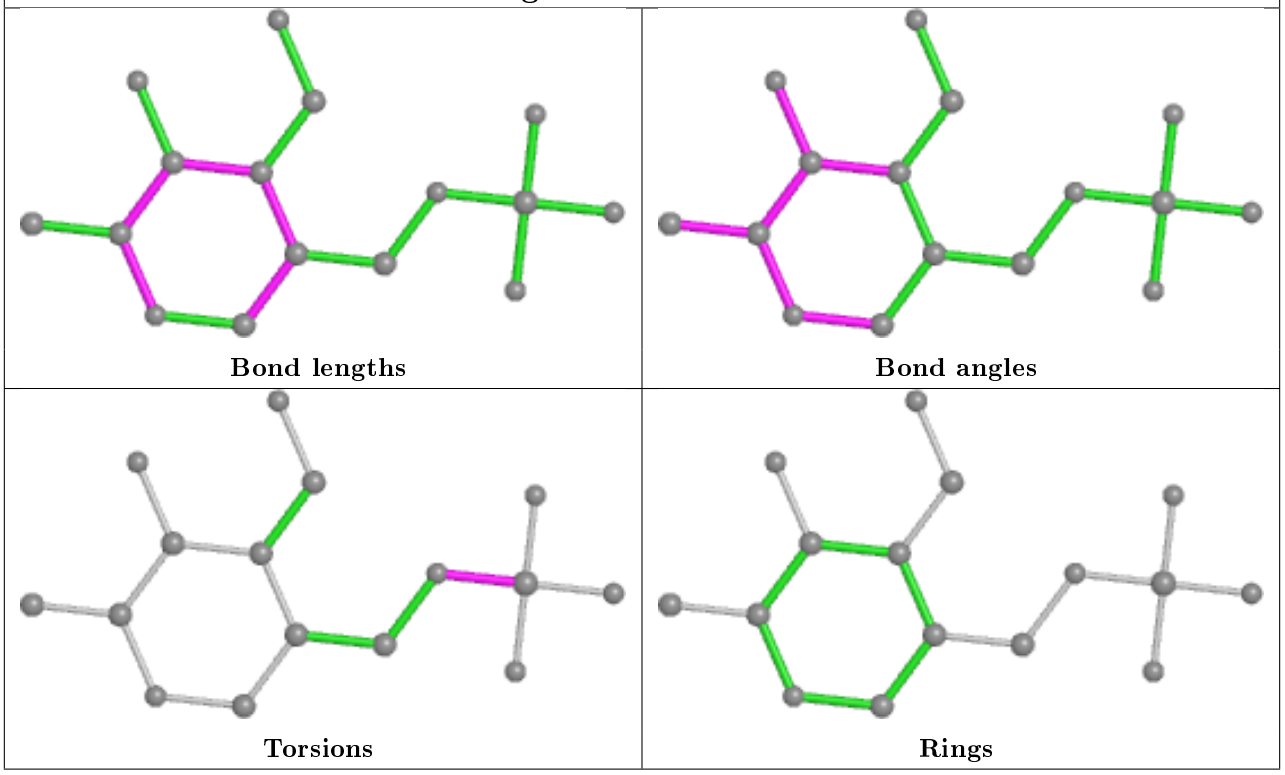


Torsions



Rings

Ligand PMP B 500



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	399/427 (93%)	0.02	2 (0%)	91	89	13, 24, 40, 58	0
1	B	396/427 (92%)	-0.05	1 (0%)	94	93	13, 23, 37, 54	0
1	C	400/427 (93%)	0.05	9 (2%)	60	58	14, 23, 42, 67	0
1	D	397/427 (92%)	-0.00	1 (0%)	94	93	14, 24, 39, 70	0
All	All	1592/1708 (93%)	0.01	13 (0%)	86	84	13, 23, 40, 70	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	150	ASP	3.5
1	C	154	ALA	3.1
1	C	143	GLN	3.1
1	C	216	VAL	2.8
1	A	150	ASP	2.8
1	A	329	LEU	2.6
1	B	106	ASP	2.3
1	C	401	LYS	2.3
1	D	121	GLU	2.1
1	C	404	THR	2.1
1	C	146	GLU	2.1
1	C	161	ALA	2.1
1	C	142	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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)

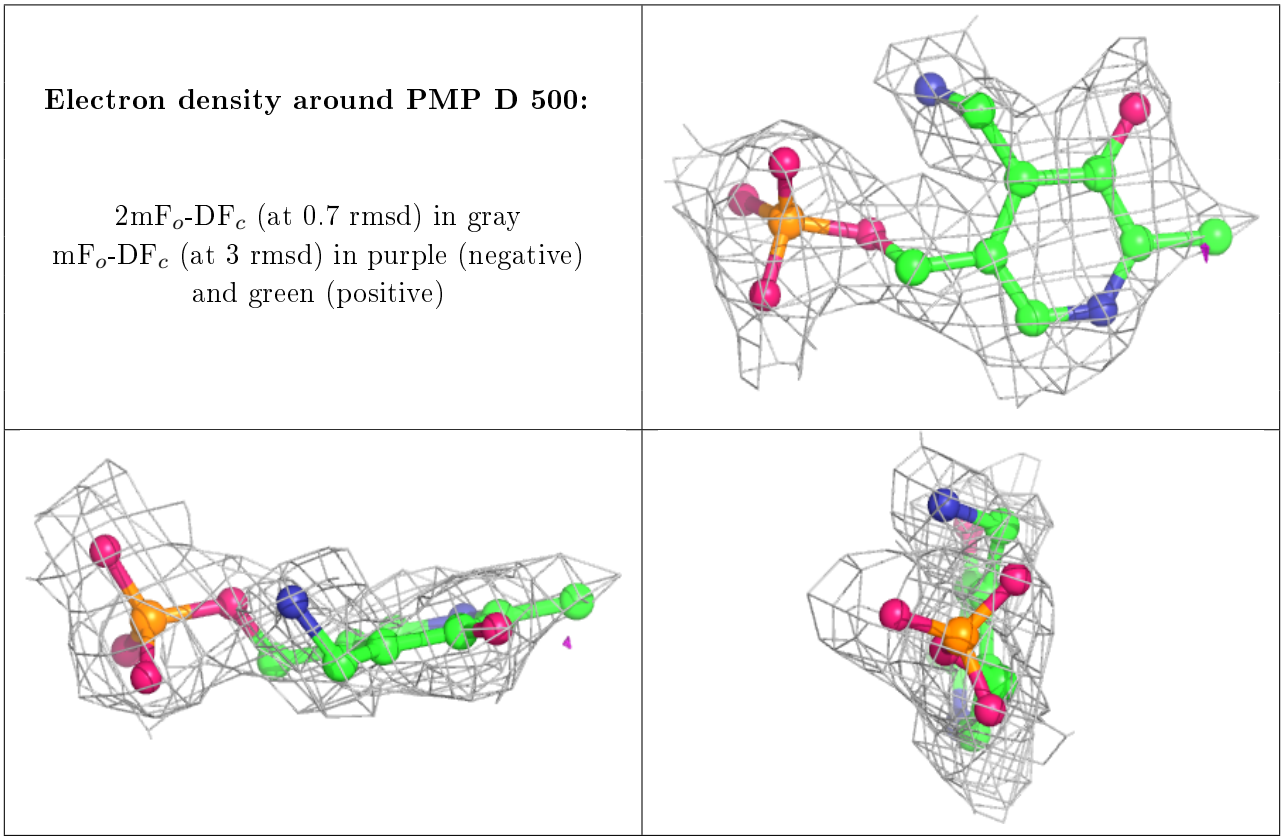
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	PMP	D	500	16/16	0.92	0.16	25,32,37,38	0
2	PMP	B	500	16/16	0.93	0.16	19,22,25,27	0
2	PMP	C	500	16/16	0.94	0.17	17,22,25,27	0
2	PMP	A	500	16/16	0.95	0.16	21,24,30,32	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.

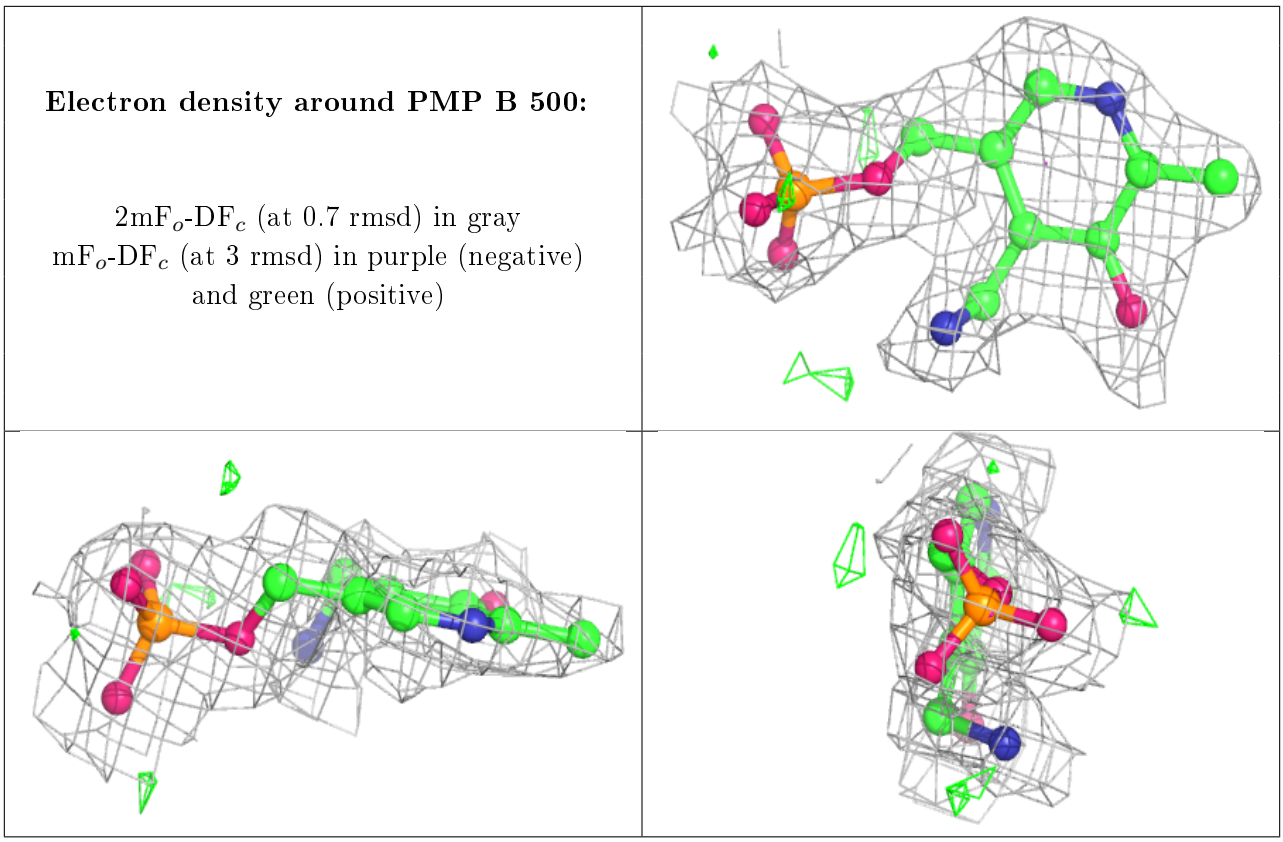
Electron density around PMP D 500:

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



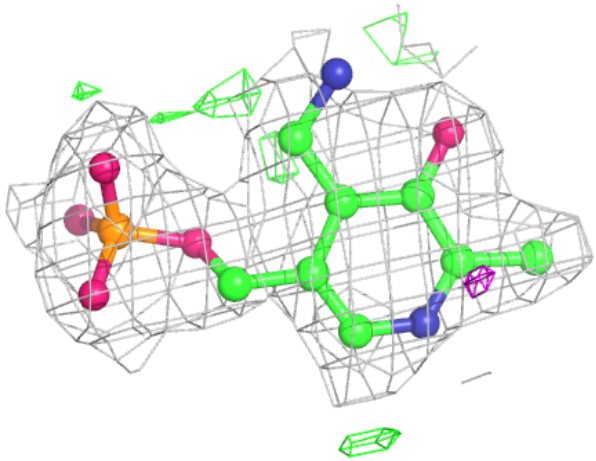
Electron density around PMP B 500:

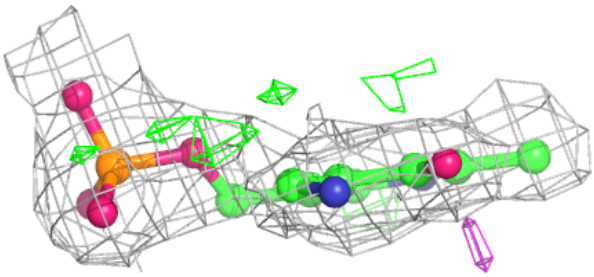
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

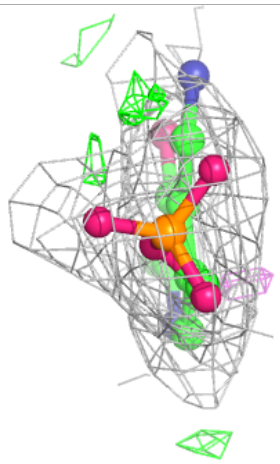


Electron density around PMP C 500:

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

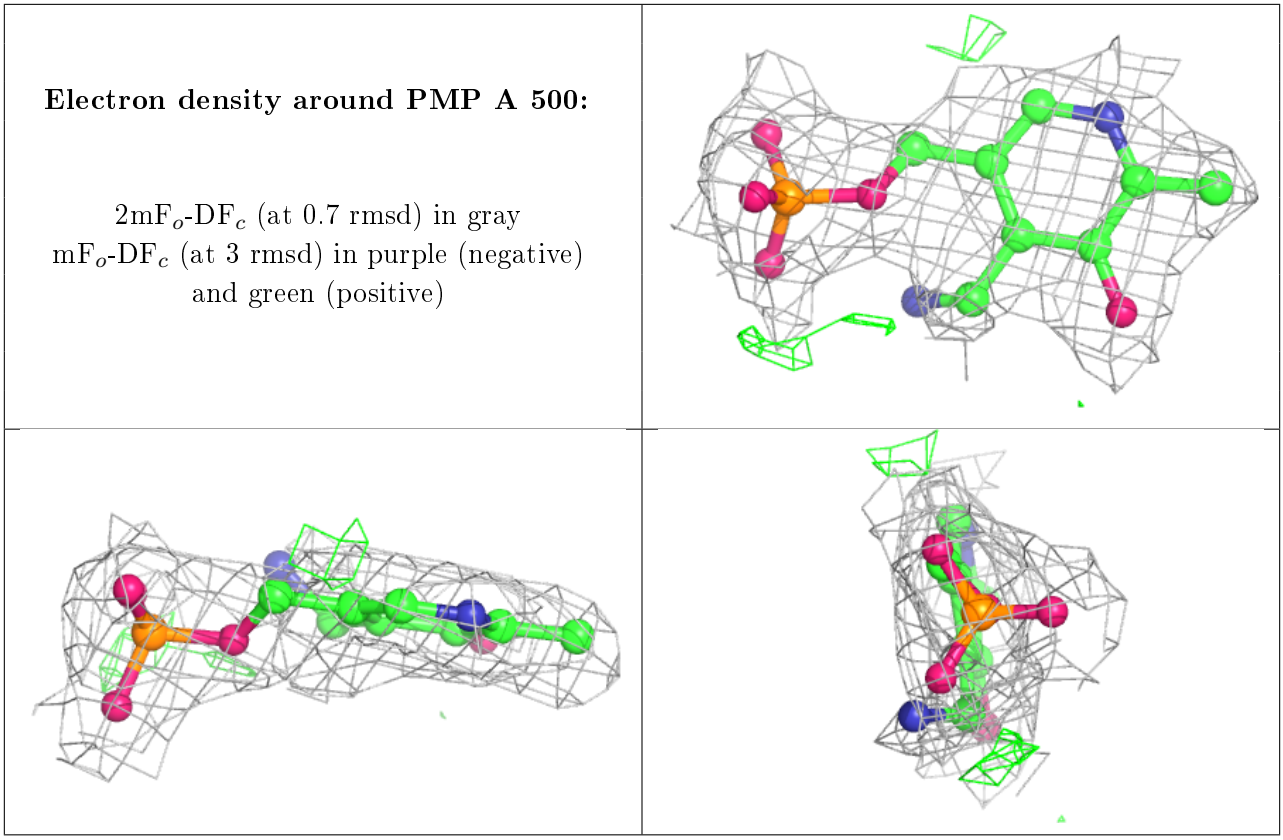






Electron density around PMP A 500:

$2mF_o$-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.