



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:58 PM UTC

PDB ID : 9CPZ / pdb\_00009cpz  
Title : C387S variant of D-ornithine/D-lysine decarboxylase complexed with PMP  
and 4-guanidinobutanol  
Authors : Phillips, R.S.; Blankenship, S.  
Deposited on : 2024-07-18  
Resolution : 1.54 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

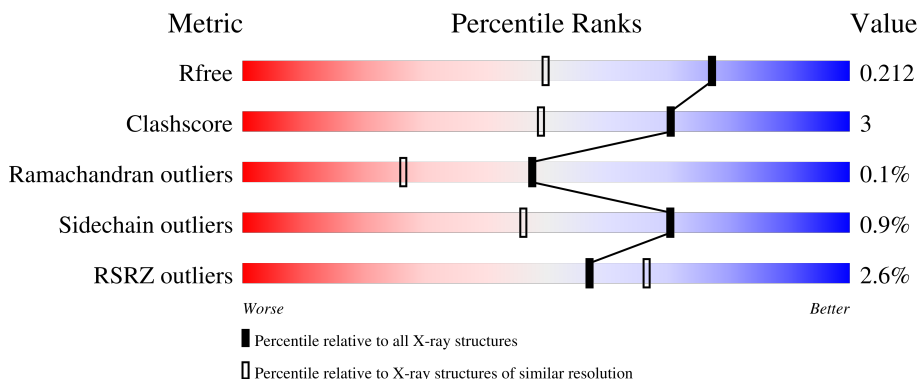
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.54 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	1003 (1.54-1.54)
Clashscore	190562	1025 (1.54-1.54)
Ramachandran outliers	187476	1007 (1.54-1.54)
Sidechain outliers	187428	1007 (1.54-1.54)
RSRZ outliers	180081	1002 (1.54-1.54)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	478	<div> <div>3%</div> <div> <div></div> <div>89%</div> <div>9%</div> <div></div> </div> </div>
1	B	478	<div> <div>2%</div> <div> <div></div> <div>90%</div> <div>7%</div> <div></div> </div> </div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8784 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 D-ornithine/D-lysine decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	470	Total	C	N	O	S	0	28	0
			3925	2486	679	738	22			
1	B	465	Total	C	N	O	S	0	29	0
			3895	2470	674	731	20			

There are 28 discrepancies between the modelled and reference sequences:

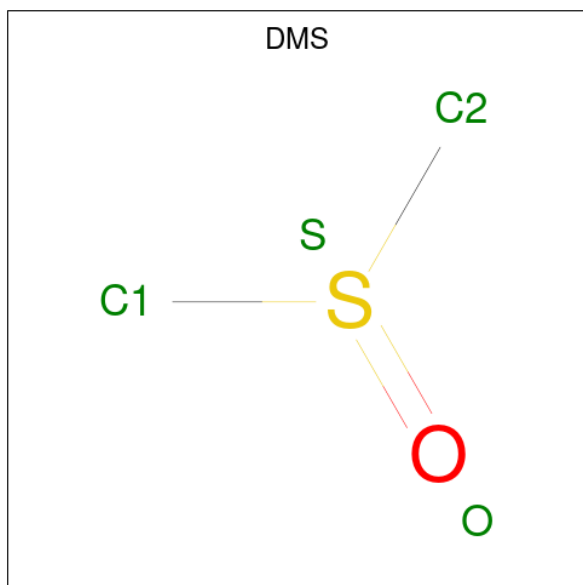
Chain	Residue	Modelled	Actual	Comment	Reference
A	387	SER	CYS	engineered mutation	UNP Q8ZNC4
A	466	LEU	-	expression tag	UNP Q8ZNC4
A	467	LEU	-	expression tag	UNP Q8ZNC4
A	478	ALA	-	expression tag	UNP Q8ZNC4
A	479	ALA	-	expression tag	UNP Q8ZNC4
A	480	ALA	-	expression tag	UNP Q8ZNC4
A	481	LEU	-	expression tag	UNP Q8ZNC4
A	482	GLU	-	expression tag	UNP Q8ZNC4
A	483	HIS	-	expression tag	UNP Q8ZNC4
A	484	HIS	-	expression tag	UNP Q8ZNC4
A	485	HIS	-	expression tag	UNP Q8ZNC4
A	486	HIS	-	expression tag	UNP Q8ZNC4
A	487	HIS	-	expression tag	UNP Q8ZNC4
A	488	HIS	-	expression tag	UNP Q8ZNC4
B	387	SER	CYS	engineered mutation	UNP Q8ZNC4
B	466	LEU	-	expression tag	UNP Q8ZNC4
B	467	LEU	-	expression tag	UNP Q8ZNC4
B	468	ALA	-	expression tag	UNP Q8ZNC4
B	469	ALA	-	expression tag	UNP Q8ZNC4
B	470	ALA	-	expression tag	UNP Q8ZNC4
B	471	LEU	-	expression tag	UNP Q8ZNC4
B	472	GLU	-	expression tag	UNP Q8ZNC4
B	473	HIS	-	expression tag	UNP Q8ZNC4
B	474	HIS	-	expression tag	UNP Q8ZNC4
B	475	HIS	-	expression tag	UNP Q8ZNC4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	476	HIS	-	expression tag	UNP Q8ZNC4
B	477	HIS	-	expression tag	UNP Q8ZNC4
B	478	HIS	-	expression tag	UNP Q8ZNC4

- Molecule 2 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C<sub>2</sub>H<sub>6</sub>OS).

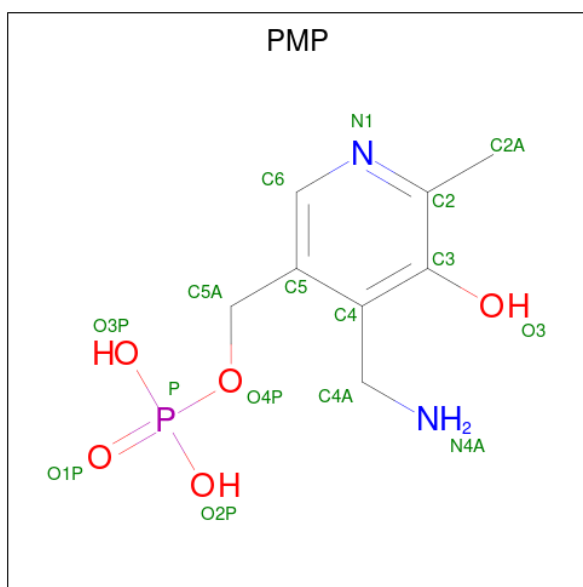


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	B	1	Total	C	O	S	0	0
			4	2	1	1		
2	B	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

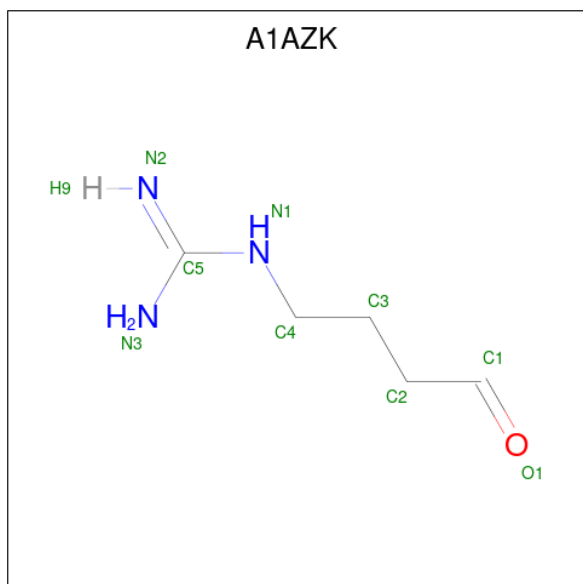
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		
3	B	1	Total	Na	0	0
			1	1		

- Molecule 4 is 4'-DEOXY-4'-AMINOPYRIDOXAL-5'-PHOSPHATE (CCD ID: PMP) (formula: C<sub>8</sub>H<sub>13</sub>N<sub>2</sub>O<sub>5</sub>P) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is N-(4-oxobutyl)guanidine (CCD ID: A1AZK) (formula:  $C_5H_{11}N_3O$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			9	5	3	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			9	5	3	1		

- Molecule 6 is ACETATE ION (CCD ID: ACT) (formula:  $C_2H_3O_2$ ).



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

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Cl	0	0
			1	1		

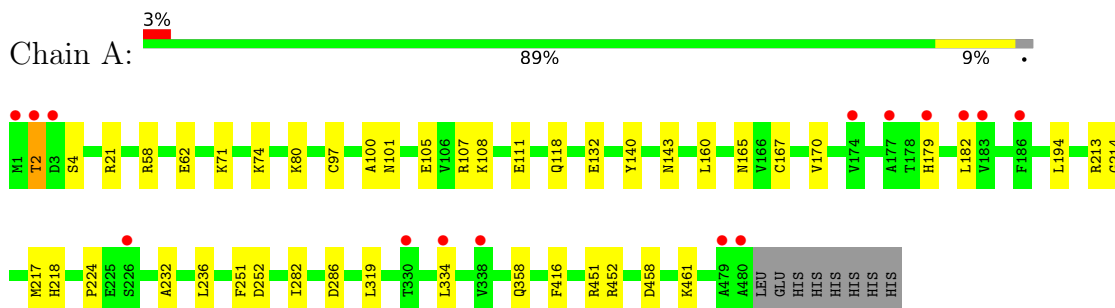
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	436	Total	O	0	28
			436	436		
8	B	455	Total	O	0	35
			455	455		

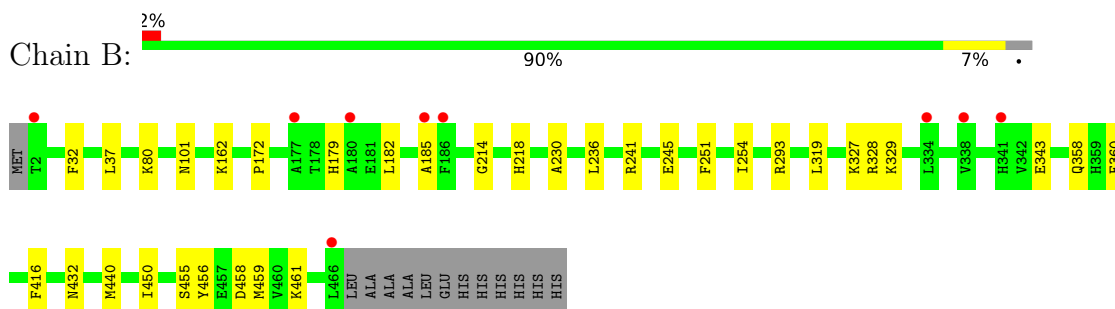
### 3 Residue-property plots [i](#)

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: D-ornithine/D-lysine decarboxylase



- Molecule 1: D-ornithine/D-lysine decarboxylase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	141.59Å 49.11Å 139.81Å 90.00° 115.80° 90.00°	Depositor
Resolution (Å)	48.92 – 1.54 48.92 – 1.54	Depositor EDS
% Data completeness (in resolution range)	64.6 (48.92-1.54) 64.7 (48.92-1.54)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.57 (at 1.54Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, $R_{free}$	0.168 , 0.213 0.168 , 0.212	Depositor DCC
$R_{free}$ test set	2005 reflections (1.56%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.4	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 44.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	8784	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 33.76 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.6010e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, DMS, ACT, A1AZK, CL, 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	0.27	0/4052	0.46	0/5480
1	B	0.29	0/4031	0.48	0/5451
All	All	0.28	0/8083	0.47	0/10931

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	3925	0	3876	33	0
1	B	3895	0	3849	24	0
2	A	8	0	12	0	0
2	B	8	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	16	0	11	3	0
4	B	16	0	10	1	0
5	A	9	0	0	0	0
5	B	9	0	0	1	0
6	B	4	0	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	1	0	0	0	0
8	A	436	0	0	6	0
8	B	455	0	0	2	0
All	All	8784	0	7773	54	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 (54) 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)
4:A:504:PMP:N4A	8:A:601:HOH:O	2.21	0.73
1:A:213[B]:ARG:NH1	8:A:605[B]:HOH:O	2.30	0.65
1:A:217[B]:MET:HG2	1:A:236:LEU:HD22	1.81	0.63
1:A:71:LYS:NZ	8:A:608:HOH:O	2.32	0.62
1:A:458[A]:ASP:HA	1:A:461[A]:LYS:HE3	1.82	0.60
1:B:218:HIS:HE2	4:B:505:PMP:HNA1	1.51	0.59
1:A:105:GLU:HG3	1:B:432[A]:ASN:HD22	1.67	0.59
1:B:458[A]:ASP:HA	1:B:461[A]:LYS:HD2	1.85	0.58
1:A:100:ALA:HB1	1:A:105:GLU:HB3	1.86	0.58
1:A:451[A]:ARG:NH1	1:A:452:ARG:O	2.37	0.57
1:A:170[A]:VAL:HG11	1:A:194:LEU:HD13	1.91	0.53
1:A:143:ASN:OD1	1:A:167:CYS:HB2	2.09	0.52
1:A:140:TYR:CZ	1:A:213[A]:ARG:NH2	2.77	0.52
1:B:230:ALA:HB1	1:B:293[B]:ARG:HH12	1.75	0.51
1:A:214:GLY:HA2	1:A:251:PHE:CD1	2.46	0.51
1:B:327:LYS:HD2	1:B:329[A]:LYS:HD2	1.91	0.51
1:A:179:HIS:HB2	1:A:182:LEU:HD22	1.91	0.51
1:B:236:LEU:HB3	1:B:254:ILE:HD11	1.92	0.50
1:B:328[B]:ARG:NH1	1:B:343:GLU:OE2	2.43	0.50
1:B:172:PRO:HG2	1:B:185:ALA:HB1	1.95	0.49
1:A:21:ARG:NH1	1:A:62[A]:GLU:OE2	2.36	0.49
1:A:458[A]:ASP:O	1:A:461[A]:LYS:HG2	2.13	0.49
1:B:179:HIS:HB2	1:B:182:LEU:HD13	1.95	0.49
1:B:214:GLY:HA2	1:B:251:PHE:CD1	2.48	0.48
1:A:461[B]:LYS:HE2	1:B:461[B]:LYS:HE2	1.96	0.47
1:A:213[B]:ARG:HD3	1:A:252:ASP:OD2	2.14	0.47
1:A:319:LEU:HB3	1:A:416:PHE:HB2	1.96	0.47
1:A:213[A]:ARG:NH2	8:A:629:HOH:O	2.48	0.46
1:B:319:LEU:HB3	1:B:416:PHE:HB2	1.97	0.46
1:A:458[B]:ASP:HA	1:A:461[B]:LYS:HD3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:GLU:HG3	1:B:432[A]:ASN:ND2	2.29	0.46
1:A:217[B]:MET:SD	1:A:232:ALA:HB1	2.56	0.46
1:A:132:GLU:HG3	1:A:160:LEU:HD11	1.98	0.46
1:B:241:ARG:O	1:B:245:GLU:HG3	2.16	0.45
1:B:455:SER:O	1:B:458[B]:ASP:HB2	2.17	0.45
4:A:504:PMP:HNA2	5:B:503:A1AZK:C1	2.29	0.45
1:A:74[B]:LYS:HE2	1:A:74[B]:LYS:HB3	1.84	0.44
1:A:108[B]:LYS:HG3	1:B:456:TYR:CE1	2.53	0.44
1:A:358:GLN:NE2	8:A:631:HOH:O	2.49	0.43
1:A:2:THR:HG22	8:A:971:HOH:O	2.18	0.43
1:A:108[B]:LYS:HG3	1:B:456:TYR:HE1	1.82	0.43
1:B:179:HIS:HE1	1:B:360:PHE:O	2.02	0.43
1:B:358:GLN:NE2	8:B:638[A]:HOH:O	2.52	0.42
1:A:97:CYS:HB3	1:A:118:GLN:O	2.20	0.42
1:A:282:ILE:HB	1:A:286:ASP:HB2	2.01	0.42
1:A:218:HIS:HE2	4:A:504:PMP:HNA1	1.68	0.42
1:B:461[B]:LYS:HD2	8:B:972:HOH:O	2.20	0.42
1:B:440[A]:MET:HB2	1:B:450:ILE:HD13	2.02	0.41
1:B:162[A]:LYS:HE3	1:B:162[A]:LYS:HB3	1.89	0.41
1:A:58:ARG:O	1:A:62[A]:GLU:HG3	2.19	0.41
1:B:456:TYR:O	1:B:459[B]:MET:N	2.53	0.41
1:A:165:ASN:HB3	1:A:213[A]:ARG:HH11	1.84	0.41
1:B:32:PHE:HB2	1:B:37:LEU:HD11	2.02	0.40
1:A:107:ARG:O	1:A:111[B]:GLU:HG3	2.19	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	496/478 (104%)	487 (98%)	8 (2%)	1 (0%)	43 25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	492/478 (103%)	480 (98%)	12 (2%)	0	100	100
All	All	988/956 (103%)	967 (98%)	20 (2%)	1 (0%)	48	26

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	224	PRO

### 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	427/407 (105%)	422 (99%)	5 (1%)	63	34
1	B	425/407 (104%)	423 (100%)	2 (0%)	81	64
All	All	852/814 (105%)	845 (99%)	7 (1%)	70	51

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	4	SER
1	A	80	LYS
1	A	101	ASN
1	A	334	LEU
1	B	80	LYS
1	B	101	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	ASN
1	A	196	GLN
1	B	152	HIS

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Mol	Chain	Res	Type
1	B	179	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 3 are monoatomic - leaving 9 for Mogul analysis.

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	$\# Z  > 2$
4	PMP	A	504	-	16,16,16	0.88	1 (6%)	22,23,23	0.86	0
2	DMS	A	501	-	3,3,3	0.60	0	3,3,3	0.19	0
2	DMS	B	501	-	3,3,3	0.52	0	3,3,3	0.52	0
2	DMS	B	504	-	3,3,3	0.61	0	3,3,3	0.17	0
5	A1AZK	A	505	-	7,8,8	0.35	0	6,8,8	1.31	1 (16%)
2	DMS	A	502	-	3,3,3	0.54	0	3,3,3	0.32	0
5	A1AZK	B	503	-	7,8,8	0.28	0	6,8,8	0.36	0
4	PMP	B	505	-	16,16,16	0.97	1 (6%)	22,23,23	1.17	2 (9%)
6	ACT	B	506	-	3,3,3	1.20	0	3,3,3	1.13	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
4	PMP	A	504	-	-	0/8/8/8	0/1/1/1
5	A1AZK	B	503	-	-	2/6/6/6	-
4	PMP	B	505	-	-	0/8/8/8	0/1/1/1
5	A1AZK	A	505	-	-	0/6/6/6	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	505	PMP	C2-N1	2.80	1.38	1.33
4	A	504	PMP	C2-N1	2.33	1.38	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	505	A1AZK	C3-C4-N1	2.73	119.85	112.20
4	B	505	PMP	C6-C5-C4	2.60	120.03	118.06
4	B	505	PMP	C5-C6-N1	-2.59	119.61	123.83

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	503	A1AZK	C2-C3-C4-N1
5	B	503	A1AZK	C3-C4-N1-C5

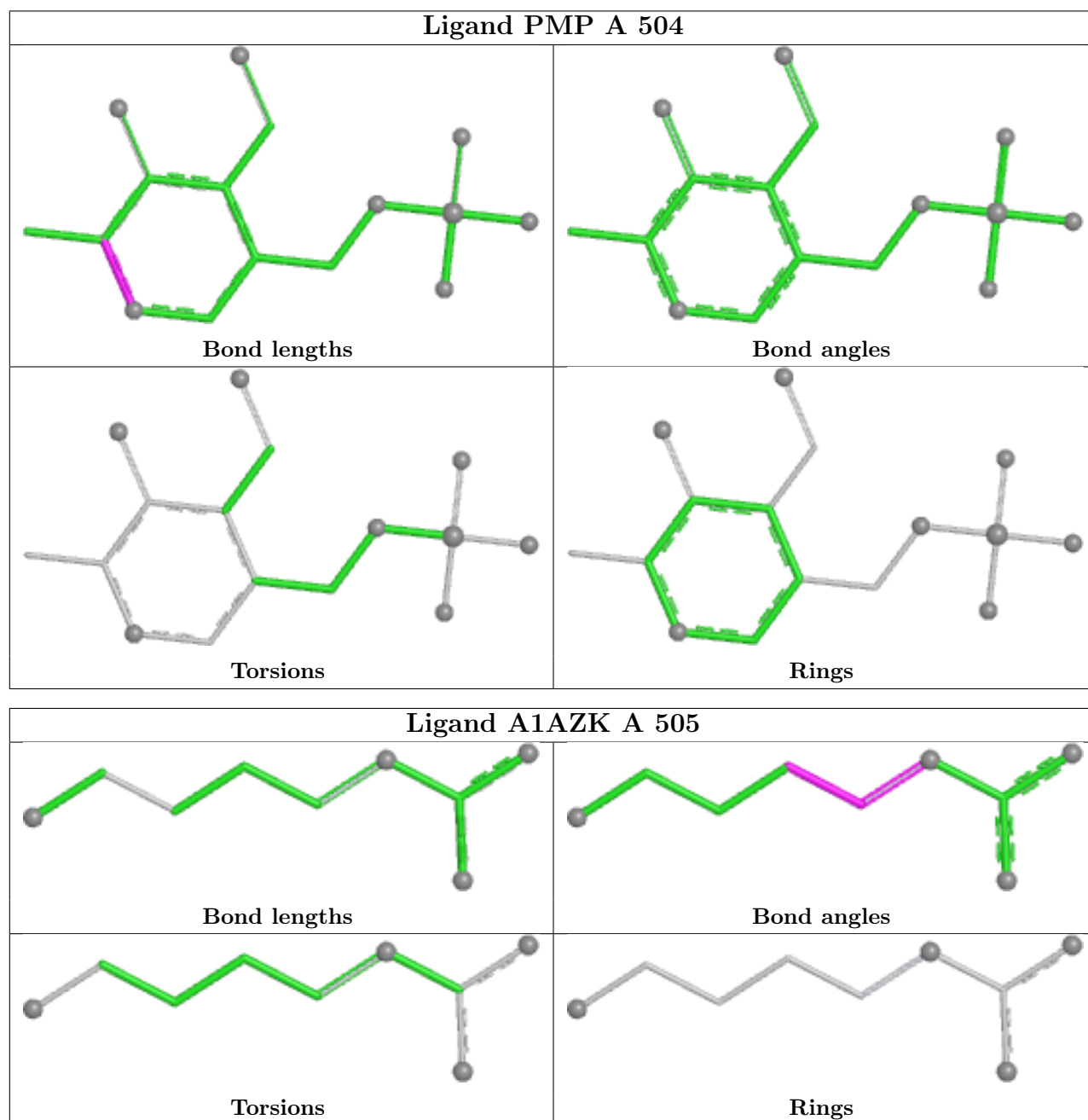
There are no ring outliers.

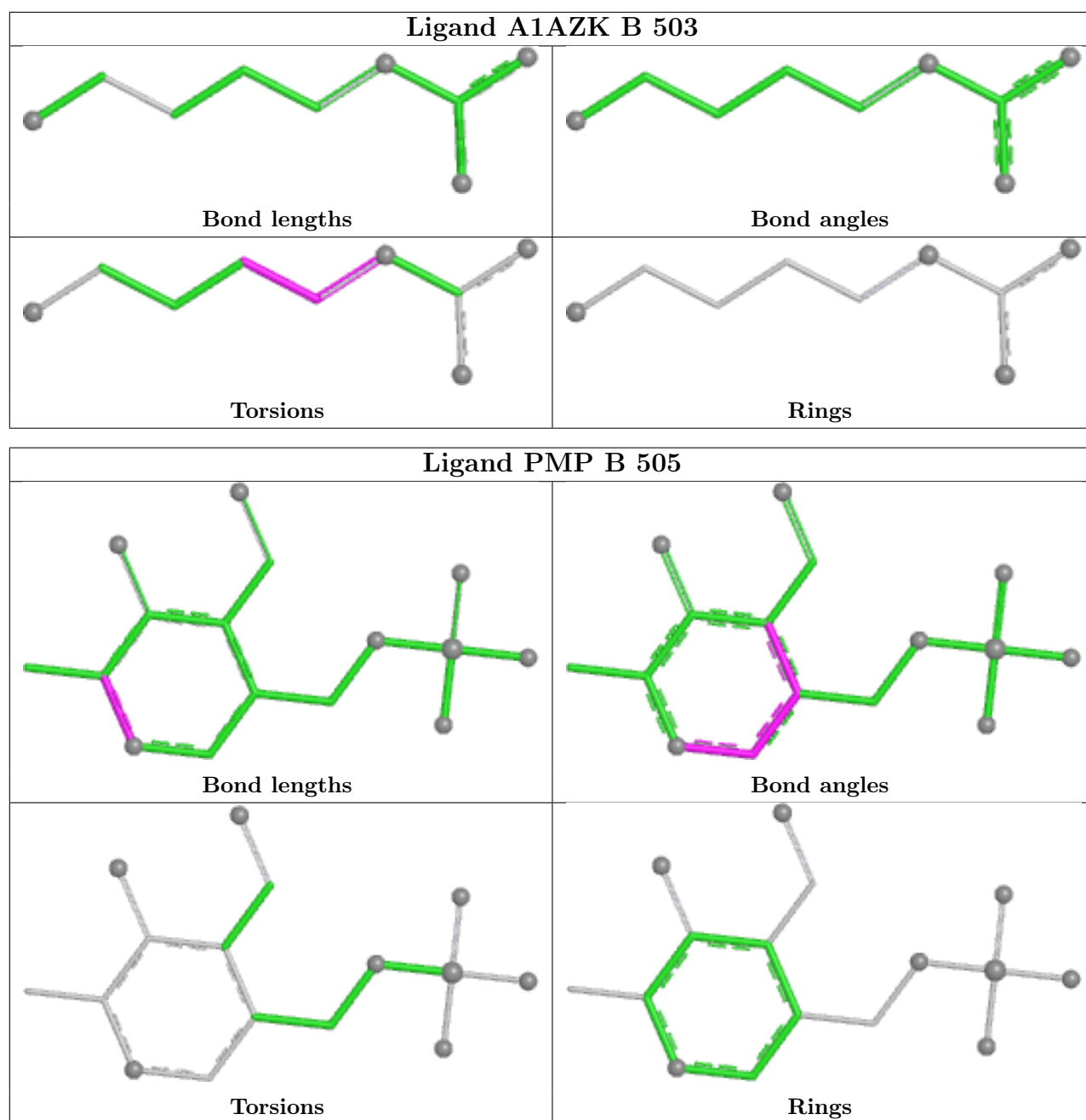
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	504	PMP	3	0
5	B	503	A1AZK	1	0
4	B	505	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

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	470/478 (98%)	-0.06	15 (3%) 50 59	10, 28, 51, 87	28 (5%)
1	B	465/478 (97%)	-0.18	9 (1%) 66 76	7, 26, 48, 82	29 (6%)
All	All	935/956 (97%)	-0.12	24 (2%) 57 66	7, 27, 50, 87	57 (6%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	186	PHE	4.4
1	B	186	PHE	4.2
1	A	480	ALA	3.6
1	B	466	LEU	3.6
1	B	334	LEU	3.4
1	A	334	LEU	3.2
1	A	177	ALA	2.9
1	A	226[A]	SER	2.8
1	B	338	VAL	2.8
1	A	182	LEU	2.8
1	A	2	THR	2.6
1	A	174	VAL	2.6
1	A	338	VAL	2.5
1	A	479	ALA	2.5
1	B	341[A]	HIS	2.5
1	A	330	THR	2.5
1	B	2	THR	2.4
1	A	179	HIS	2.4
1	A	1	MET	2.3
1	B	180	ALA	2.3
1	B	177	ALA	2.2
1	A	183	VAL	2.2
1	B	185	ALA	2.1
1	A	3[A]	ASP	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

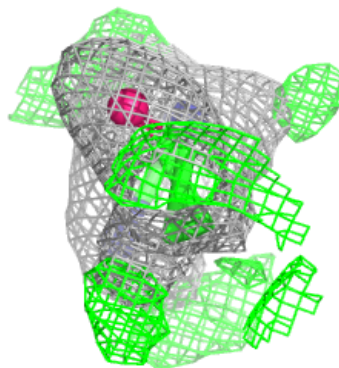
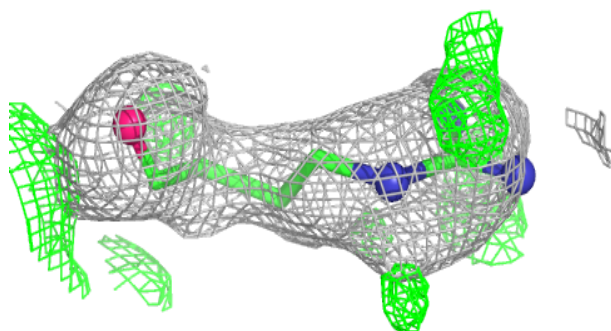
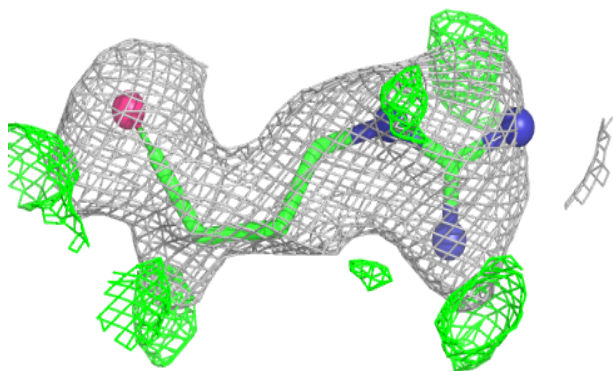
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	ACT	B	506	4/4	0.64	0.16	44,47,48,50	0
5	A1AZK	A	505	9/9	0.83	0.11	34,39,45,49	0
5	A1AZK	B	503	9/9	0.84	0.11	33,42,45,46	0
2	DMS	B	501	4/4	0.85	0.12	26,37,38,56	4
2	DMS	A	502	4/4	0.86	0.14	41,50,58,70	0
2	DMS	A	501	4/4	0.88	0.11	43,54,56,64	0
2	DMS	B	504	4/4	0.89	0.12	43,46,56,66	0
3	NA	B	502	1/1	0.93	0.06	35,35,35,35	0
7	CL	B	507	1/1	0.96	0.08	35,35,35,35	0
3	NA	A	503	1/1	0.97	0.04	26,26,26,26	0
4	PMP	B	505	16/16	0.97	0.06	19,23,30,37	0
4	PMP	A	504	16/16	0.98	0.04	18,21,23,39	0

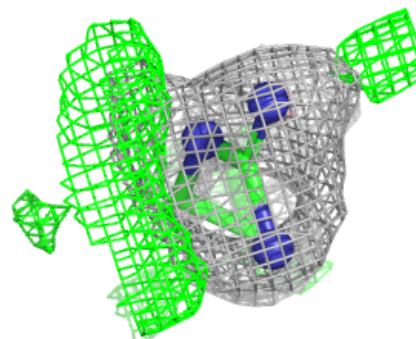
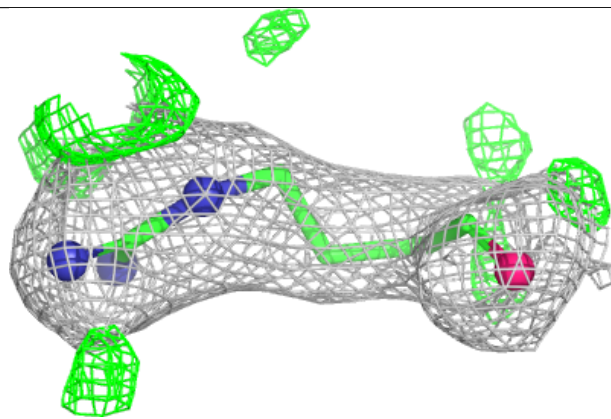
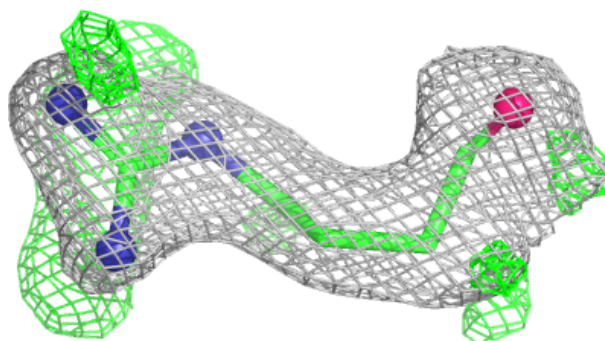
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around A1AZK A 505:**

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

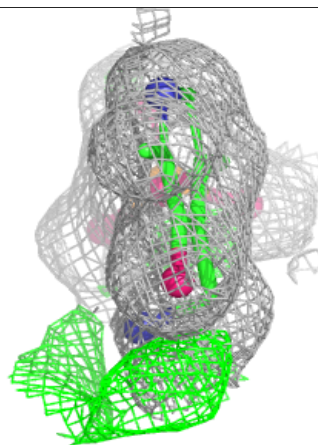
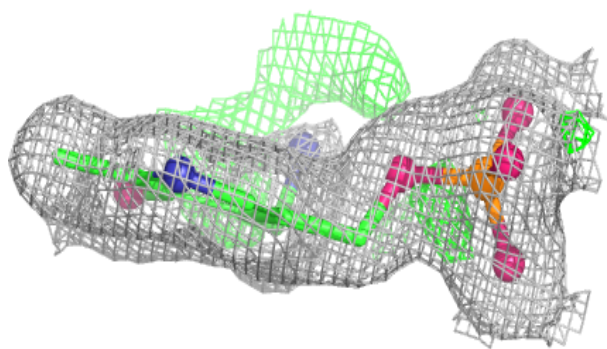
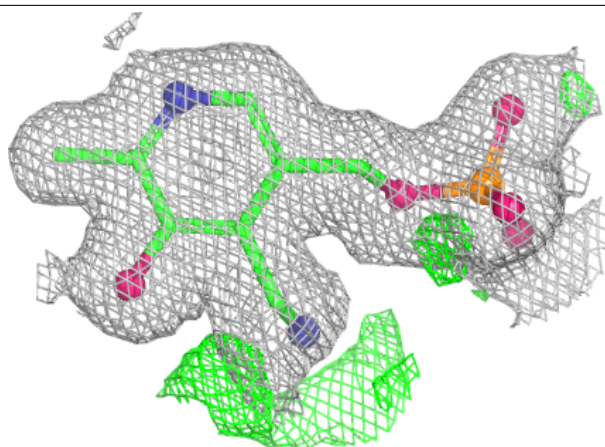
**Electron density around A1AZK B 503:**

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



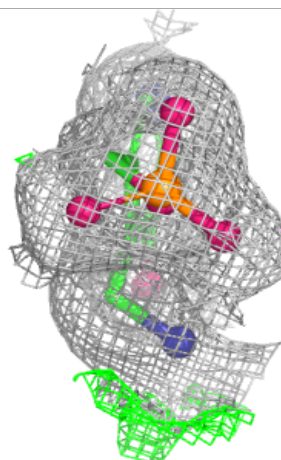
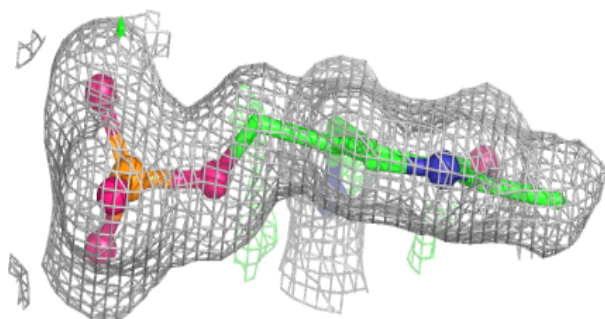
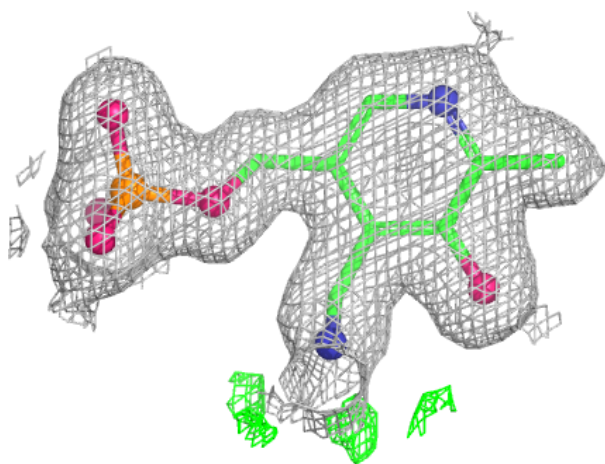
**Electron density around PMP B 505:**

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



**Electron density around PMP A 504:**

$2mF_o-DF_c$  (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.