



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 30, 2025 – 06:28 PM JST

PDB ID : 9M6P / pdb\_00009m6p  
Title : Discovery of a bifunctional PKMYT1-targeting PROTAC empowered by AI-generation  
Authors : Yazhou, W.; Chao, W.  
Deposited on : 2025-03-07  
Resolution : 2.38 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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
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)	:	2.46

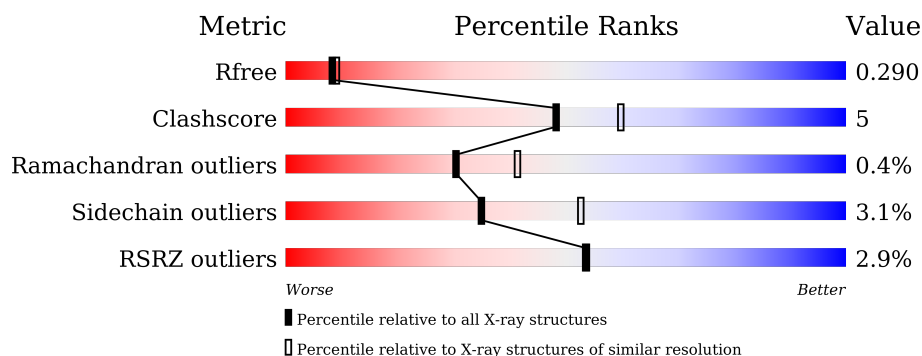
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.38 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))
$R_{free}$	164625	6699 (2.40-2.36)
Clashscore	180529	7414 (2.40-2.36)
Ramachandran outliers	177936	7337 (2.40-2.36)
Sidechain outliers	177891	7338 (2.40-2.36)
RSRZ outliers	164620	6699 (2.40-2.36)

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	AAA	311	<div> <div>2%</div> <div> <div></div> <div>74%</div> <div>14%</div> <div>12%</div> </div> </div>
1	BBB	311	<div> <div>3%</div> <div> <div></div> <div>78%</div> <div>13%</div> <div>9%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PO4	AAA	402	-	-	X	-
4	CL	BBB	403	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4433 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 Membrane-associated tyrosine- and threonine-specific cdc2-inhibitory kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	274	Total	C	N	O	S	0	0	0
			2139	1353	385	390	11			
1	BBB	284	Total	C	N	O	S	0	0	0
			2202	1389	396	406	11			

There are 46 discrepancies between the modelled and reference sequences:

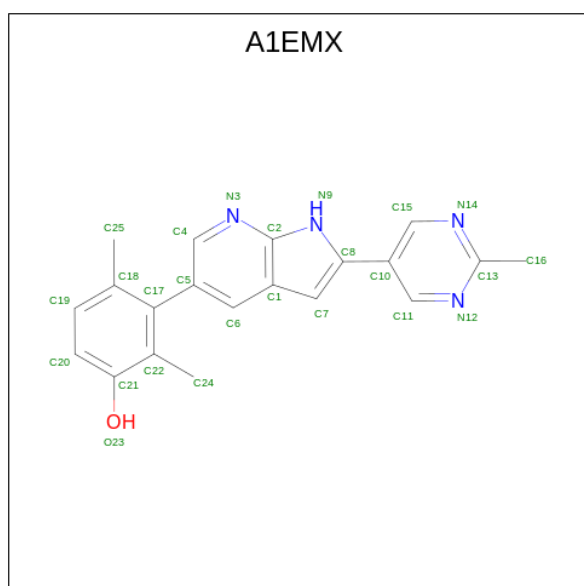
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	52	MET	-	initiating methionine	UNP Q99640
AAA	53	HIS	-	expression tag	UNP Q99640
AAA	54	HIS	-	expression tag	UNP Q99640
AAA	55	HIS	-	expression tag	UNP Q99640
AAA	56	HIS	-	expression tag	UNP Q99640
AAA	57	HIS	-	expression tag	UNP Q99640
AAA	58	HIS	-	expression tag	UNP Q99640
AAA	59	SER	-	expression tag	UNP Q99640
AAA	60	SER	-	expression tag	UNP Q99640
AAA	61	GLY	-	expression tag	UNP Q99640
AAA	62	VAL	-	expression tag	UNP Q99640
AAA	63	ASP	-	expression tag	UNP Q99640
AAA	64	LEU	-	expression tag	UNP Q99640
AAA	65	GLY	-	expression tag	UNP Q99640
AAA	66	THR	-	expression tag	UNP Q99640
AAA	67	GLU	-	expression tag	UNP Q99640
AAA	68	ASN	-	expression tag	UNP Q99640
AAA	69	LEU	-	expression tag	UNP Q99640
AAA	70	TYR	-	expression tag	UNP Q99640
AAA	71	PHE	-	expression tag	UNP Q99640
AAA	72	GLN	-	expression tag	UNP Q99640
AAA	73	SER	-	expression tag	UNP Q99640
AAA	74	MET	-	expression tag	UNP Q99640
BBB	52	MET	-	initiating methionine	UNP Q99640

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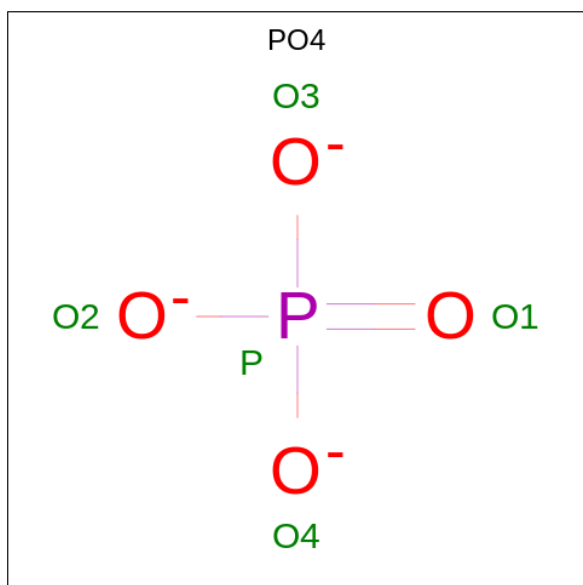
Chain	Residue	Modelled	Actual	Comment	Reference
BBB	53	HIS	-	expression tag	UNP Q99640
BBB	54	HIS	-	expression tag	UNP Q99640
BBB	55	HIS	-	expression tag	UNP Q99640
BBB	56	HIS	-	expression tag	UNP Q99640
BBB	57	HIS	-	expression tag	UNP Q99640
BBB	58	HIS	-	expression tag	UNP Q99640
BBB	59	SER	-	expression tag	UNP Q99640
BBB	60	SER	-	expression tag	UNP Q99640
BBB	61	GLY	-	expression tag	UNP Q99640
BBB	62	VAL	-	expression tag	UNP Q99640
BBB	63	ASP	-	expression tag	UNP Q99640
BBB	64	LEU	-	expression tag	UNP Q99640
BBB	65	GLY	-	expression tag	UNP Q99640
BBB	66	THR	-	expression tag	UNP Q99640
BBB	67	GLU	-	expression tag	UNP Q99640
BBB	68	ASN	-	expression tag	UNP Q99640
BBB	69	LEU	-	expression tag	UNP Q99640
BBB	70	TYR	-	expression tag	UNP Q99640
BBB	71	PHE	-	expression tag	UNP Q99640
BBB	72	GLN	-	expression tag	UNP Q99640
BBB	73	SER	-	expression tag	UNP Q99640
BBB	74	MET	-	expression tag	UNP Q99640

- Molecule 2 is 2,4-dimethyl-3-[2-(2-methylpyrimidin-5-yl)-1 {H}-pyrrolo[2,3-b]pyridin-5-yl]phenol (CCD ID: A1EMX) (formula: C<sub>20</sub>H<sub>18</sub>N<sub>4</sub>O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	AAA	1	Total	C	N	O	0	0
			25	20	4	1		
2	BBB	1	Total	C	N	O	0	0
			25	20	4	1		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula:  $O_4P$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	AAA	1	Total	O	P	0	0
			5	4	1		
3	BBB	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	BBB	1	Total	Cl	0	0
			1	1		

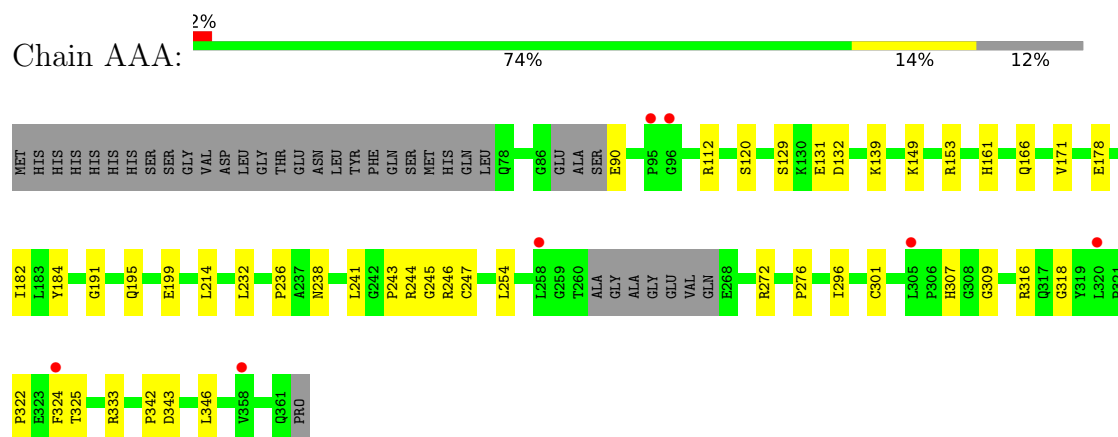
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	18	Total	O	0	0
			18	18		
5	BBB	13	Total	O	0	0
			13	13		

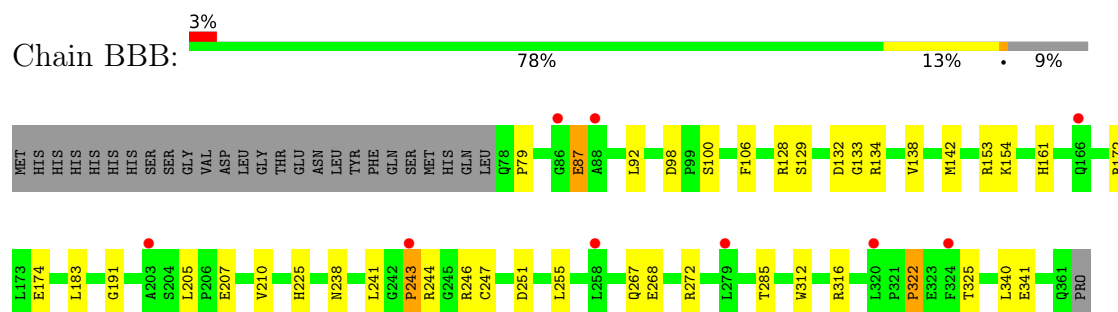
### 3 Residue-property plots [i](#)

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: Membrane-associated tyrosine- and threonine-specific cdc2-inhibitory kinase



- Molecule 1: Membrane-associated tyrosine- and threonine-specific cdc2-inhibitory kinase



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	127.93Å 127.93Å 184.66Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	95.00 – 2.38 95.00 – 2.38	Depositor EDS
% Data completeness (in resolution range)	54.7 (95.00-2.38) 54.7 (95.00-2.38)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.44 (at 2.37Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.203 , 0.290 0.206 , 0.290	Depositor DCC
$R_{free}$ test set	652 reflections (2.78%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	57.9	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 47.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4433	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.24% of the height of the origin peak. No significant pseudotranslation is detected.*

<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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1EMX, PO4, CL

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	AAA	0.96	0/2189	1.40	0/2958
1	BBB	0.93	0/2254	1.40	0/3049
All	All	0.95	0/4443	1.40	0/6007

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

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	AAA	2139	0	2119	25	0
1	BBB	2202	0	2176	23	0
2	AAA	25	0	0	0	0
2	BBB	25	0	0	0	0
3	AAA	5	0	0	2	0
3	BBB	5	0	0	1	0
4	BBB	1	0	0	2	0
5	AAA	18	0	0	3	0
5	BBB	13	0	0	0	0
All	All	4433	0	4295	47	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 (47) 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:BBB:238:ASN:OD1	4:BBB:403:CL:CL	2.31	0.86
1:AAA:243:PRO:O	5:AAA:501:HOH:O	1.98	0.81
1:BBB:251:ASP:OD2	4:BBB:403:CL:CL	2.37	0.79
1:AAA:301:CYS:SG	1:AAA:324:PHE:O	2.51	0.68
1:AAA:322:PRO:HA	1:AAA:325:THR:HG22	1.77	0.66
1:BBB:322:PRO:HA	1:BBB:325:THR:CG2	2.26	0.65
1:AAA:238:ASN:OD1	5:AAA:502:HOH:O	2.15	0.61
1:AAA:309:GLY:HA3	3:BBB:402:PO4:O1	2.06	0.55
1:AAA:246:ARG:HB2	5:AAA:501:HOH:O	2.07	0.55
1:BBB:129:SER:O	1:BBB:133:GLY:HA2	2.07	0.54
1:BBB:322:PRO:HA	1:BBB:325:THR:HG22	1.89	0.53
1:AAA:178:GLU:HA	1:AAA:182:ILE:O	2.09	0.53
1:AAA:276:PRO:HB3	1:AAA:316:ARG:HB3	1.91	0.52
1:AAA:318:GLY:N	1:AAA:342:PRO:HG3	2.24	0.51
1:BBB:255:LEU:C	1:BBB:255:LEU:HD23	2.36	0.51
1:AAA:245:GLY:O	1:AAA:246:ARG:C	2.54	0.50
1:BBB:106:PHE:CE1	1:BBB:138:VAL:HG11	2.46	0.50
1:BBB:87:GLU:N	1:BBB:87:GLU:CD	2.70	0.49
1:BBB:225:HIS:CG	1:BBB:285:THR:HB	2.48	0.49
1:AAA:112:ARG:HH12	3:AAA:402:PO4:P	2.36	0.48
1:BBB:191:GLY:N	1:BBB:241:LEU:O	2.45	0.48
1:BBB:172:ARG:HH12	1:BBB:174:GLU:HG2	1.79	0.47
1:AAA:129:SER:HB3	1:AAA:132:ASP:OD1	2.14	0.47
1:AAA:112:ARG:NH1	3:AAA:402:PO4:O2	2.42	0.47
1:AAA:195:GLN:O	1:AAA:199:GLU:HB2	2.15	0.47
1:AAA:343:ASP:HB3	1:AAA:346:LEU:HB2	1.96	0.47
1:AAA:139:LYS:O	1:AAA:184:TYR:HA	2.15	0.46
1:BBB:132:ASP:OD1	1:BBB:134:ARG:HB2	2.17	0.44
1:AAA:195:GLN:HB2	1:AAA:236:PRO:HB2	2.00	0.44
1:AAA:232:LEU:HD12	1:AAA:254:LEU:O	2.18	0.44
1:AAA:149:LYS:HD2	1:BBB:267:GLN:HE21	1.83	0.43
1:BBB:340:LEU:O	1:BBB:341:GLU:C	2.61	0.43
1:BBB:207:GLU:O	1:BBB:210:VAL:HB	2.18	0.43
1:AAA:214:LEU:HD13	1:AAA:296:ILE:HG13	2.01	0.43
1:BBB:241:LEU:HD23	1:BBB:247:CYS:HB3	2.00	0.42
1:AAA:191:GLY:N	1:AAA:241:LEU:O	2.52	0.42
1:AAA:161:HIS:NE2	1:AAA:171:VAL:O	2.51	0.42
1:AAA:272:ARG:HD3	1:AAA:307:HIS:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:129:SER:OG	1:AAA:131:GLU:HB3	2.20	0.41
1:BBB:154:LYS:HB3	1:BBB:183:LEU:HD22	2.02	0.41
1:BBB:79:PRO:HB2	1:BBB:92:LEU:HB2	2.03	0.41
1:BBB:243:PRO:HD2	1:BBB:246:ARG:HB2	2.03	0.41
1:BBB:312:TRP:CH2	1:BBB:316:ARG:HD2	2.56	0.41
1:AAA:166:GLN:OE1	1:AAA:166:GLN:N	2.53	0.40
1:BBB:98:ASP:OD1	1:BBB:100:SER:OG	2.40	0.40
1:BBB:128:ARG:NH1	1:BBB:133:GLY:O	2.54	0.40
1:BBB:129:SER:O	1:BBB:133:GLY:CA	2.69	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	AAA	268/311 (86%)	243 (91%)	25 (9%)	0	100	100
1	BBB	282/311 (91%)	252 (89%)	28 (10%)	2 (1%)	19	26
All	All	550/622 (88%)	495 (90%)	53 (10%)	2 (0%)	30	41

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BBB	243	PRO
1	BBB	322	PRO

### 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	AAA	226/256 (88%)	220 (97%)	6 (3%)	40	58
1	BBB	231/256 (90%)	223 (96%)	8 (4%)	31	48
All	All	457/512 (89%)	443 (97%)	14 (3%)	35	53

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

Mol	Chain	Res	Type
1	AAA	90	GLU
1	AAA	120	SER
1	AAA	153	ARG
1	AAA	244	ARG
1	AAA	247	CYS
1	AAA	333	ARG
1	BBB	87	GLU
1	BBB	142	MET
1	BBB	153	ARG
1	BBB	161	HIS
1	BBB	205	LEU
1	BBB	244	ARG
1	BBB	268	GLU
1	BBB	272	ARG

Sometimes 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 oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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$
3	PO4	AAA	402	-	4,4,4	0.69	0	6,6,6	0.47	0
3	PO4	BBB	402	-	4,4,4	0.75	0	6,6,6	0.40	0
2	A1EMX	AAA	401	-	28,28,28	1.17	4 (14%)	35,41,41	1.90	10 (28%)
2	A1EMX	BBB	401	-	28,28,28	1.46	4 (14%)	35,41,41	2.02	14 (40%)

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	A1EMX	AAA	401	-	-	0/8/8/8	0/4/4/4
2	A1EMX	BBB	401	-	-	0/8/8/8	0/4/4/4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	BBB	401	A1EMX	O23-C21	3.64	1.43	1.36
2	BBB	401	A1EMX	C10-C8	3.47	1.54	1.48
2	AAA	401	A1EMX	O23-C21	2.66	1.41	1.36
2	BBB	401	A1EMX	C2-N9	2.64	1.39	1.34
2	AAA	401	A1EMX	C10-C8	2.63	1.53	1.48
2	BBB	401	A1EMX	C17-C5	2.34	1.54	1.50
2	AAA	401	A1EMX	C17-C5	2.30	1.54	1.50
2	AAA	401	A1EMX	C1-C2	-2.19	1.37	1.43

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AAA	401	A1EMX	C4-N3-C2	4.18	120.89	116.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AAA	401	A1EMX	C15-N14-C13	3.84	122.49	115.96
2	AAA	401	A1EMX	C5-C4-N3	-3.80	122.03	125.55
2	BBB	401	A1EMX	C5-C4-N3	-3.74	122.09	125.55
2	BBB	401	A1EMX	C10-C8-N9	3.70	127.00	120.78
2	AAA	401	A1EMX	C10-C15-N14	-3.59	118.41	124.32
2	BBB	401	A1EMX	C11-N12-C13	3.30	121.58	115.96
2	BBB	401	A1EMX	C4-N3-C2	3.25	119.96	116.69
2	BBB	401	A1EMX	C7-C8-C10	-3.17	125.04	129.44
2	AAA	401	A1EMX	C16-C13-N12	3.05	120.49	117.14
2	BBB	401	A1EMX	C20-C21-C22	-3.01	118.51	121.61
2	BBB	401	A1EMX	C15-N14-C13	2.94	120.96	115.96
2	BBB	401	A1EMX	N14-C13-N12	-2.90	120.62	125.51
2	AAA	401	A1EMX	C10-C8-N9	2.88	125.62	120.78
2	AAA	401	A1EMX	N14-C13-N12	-2.83	120.73	125.51
2	BBB	401	A1EMX	C10-C11-N12	-2.72	119.84	124.32
2	BBB	401	A1EMX	C10-C15-N14	-2.46	120.27	124.32
2	AAA	401	A1EMX	C20-C21-C22	-2.38	119.15	121.61
2	BBB	401	A1EMX	C16-C13-N14	2.38	119.75	117.14
2	AAA	401	A1EMX	C7-C8-C10	-2.31	126.23	129.44
2	BBB	401	A1EMX	C16-C13-N12	2.27	119.63	117.14
2	BBB	401	A1EMX	C5-C6-C1	-2.24	117.64	121.53
2	AAA	401	A1EMX	C11-N12-C13	2.14	119.61	115.96
2	BBB	401	A1EMX	C6-C5-C4	2.11	119.18	116.24

There are no chirality outliers.

There are no torsion outliers.

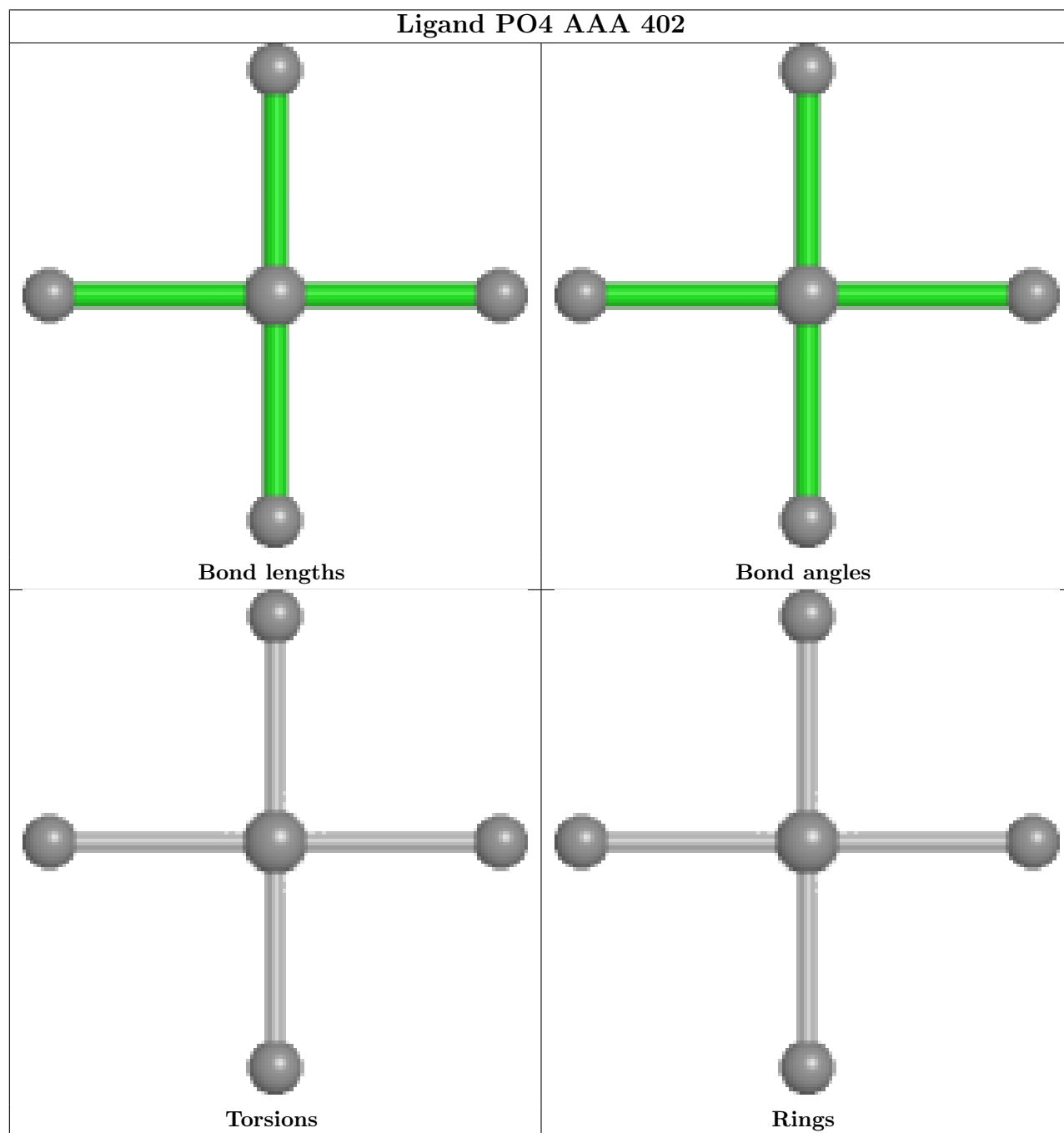
There are no ring outliers.

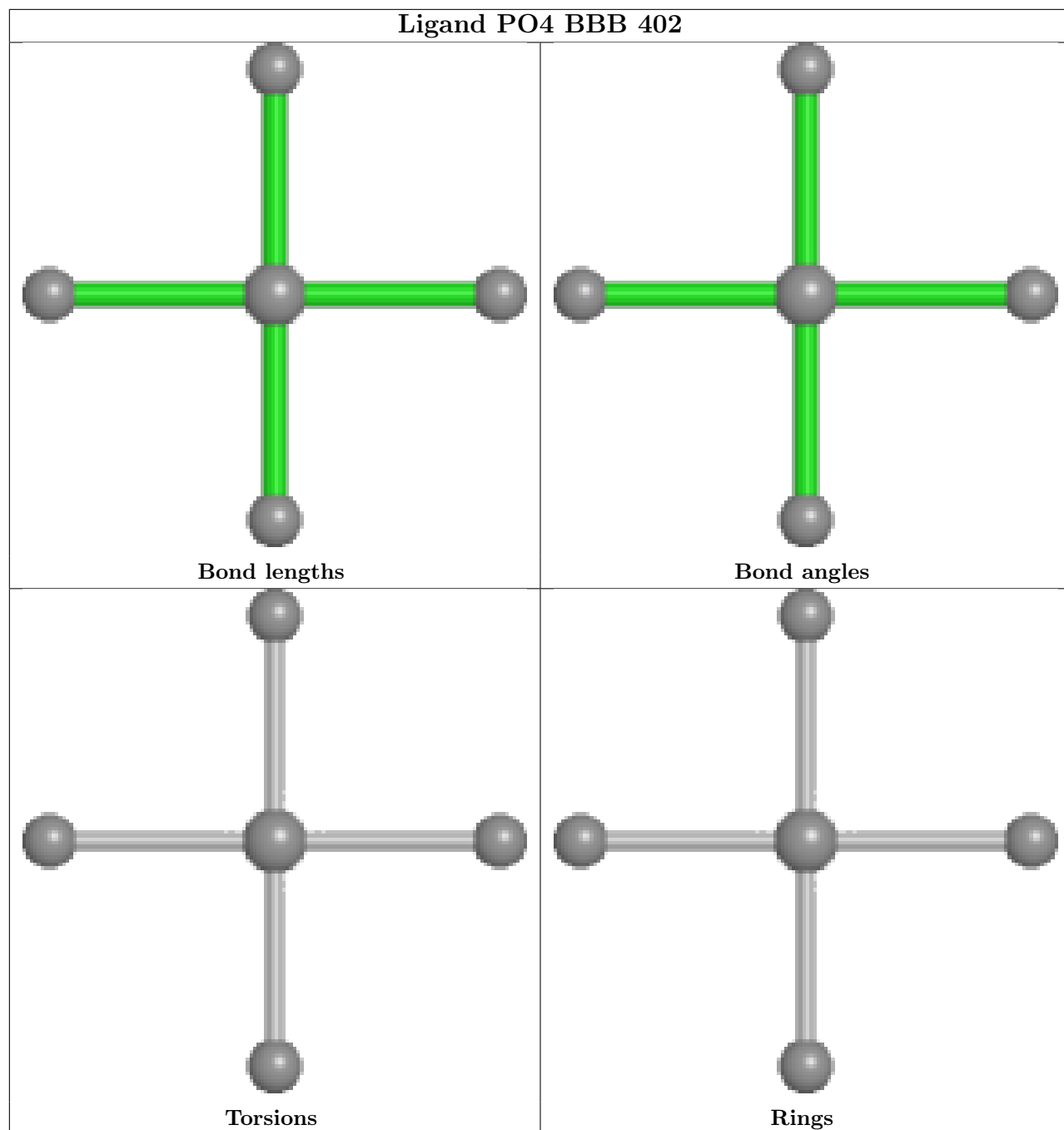
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AAA	402	PO4	2	0
3	BBB	402	PO4	1	0

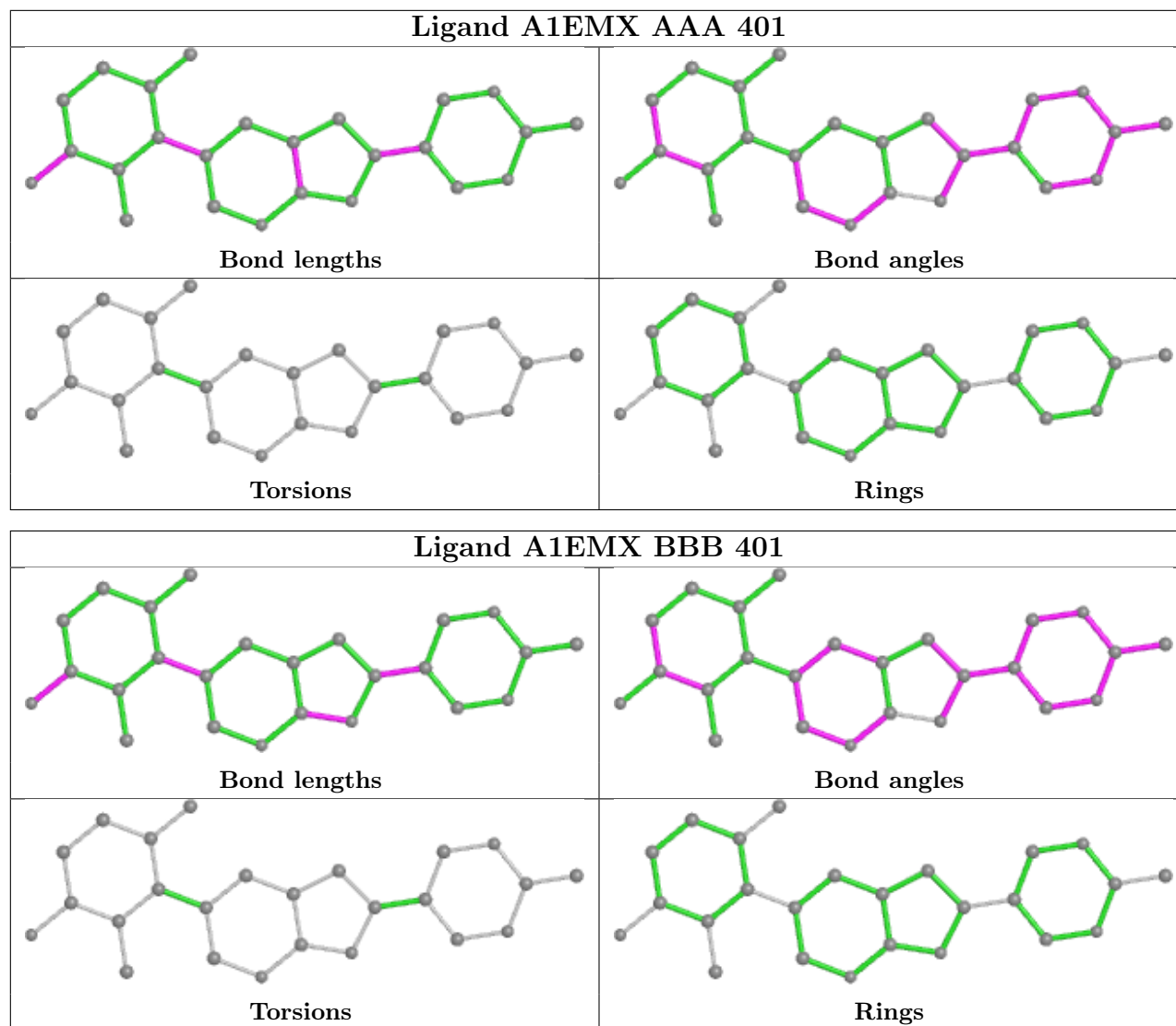
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	AAA	274/311 (88%)	0.16	7 (2%) 57 56	45, 66, 108, 126	0
1	BBB	284/311 (91%)	0.08	9 (3%) 50 50	40, 58, 93, 136	0
All	All	558/622 (89%)	0.12	16 (2%) 54 53	40, 61, 104, 136	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	324	PHE	5.0
1	BBB	320	LEU	3.2
1	AAA	305	LEU	3.1
1	BBB	203	ALA	2.7
1	BBB	88	ALA	2.7
1	AAA	320	LEU	2.6
1	AAA	95	PRO	2.4
1	BBB	86	GLY	2.4
1	BBB	324	PHE	2.2
1	BBB	258	LEU	2.2
1	AAA	358	VAL	2.2
1	AAA	96	GLY	2.1
1	BBB	166	GLN	2.1
1	AAA	258	LEU	2.1
1	BBB	243	PRO	2.1
1	BBB	279	LEU	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](#)

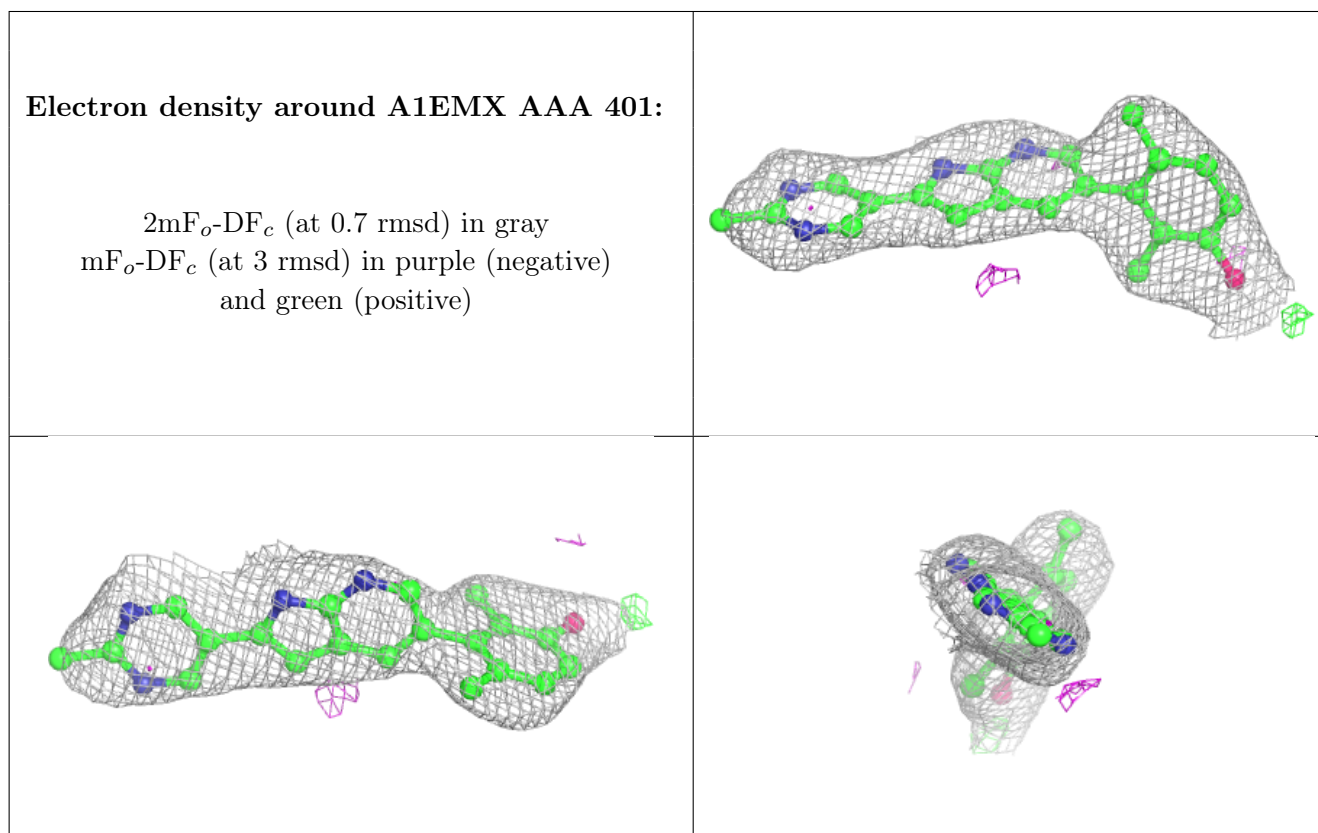
There are no oligosaccharides in this entry.

## 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.

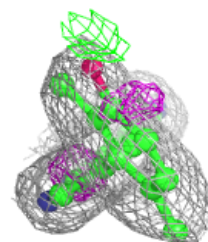
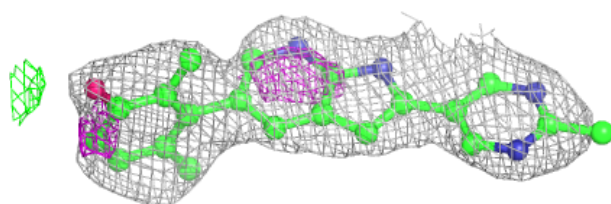
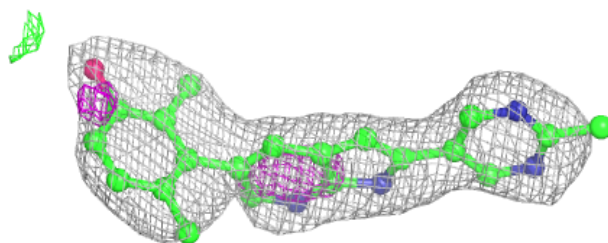
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	A1EMX	AAA	401	25/25	0.93	0.07	37,41,46,49	0
2	A1EMX	BBB	401	25/25	0.93	0.08	39,41,45,46	0
4	CL	BBB	403	1/1	0.93	0.10	75,75,75,75	0
3	PO4	BBB	402	5/5	0.95	0.14	52,55,56,61	0
3	PO4	AAA	402	5/5	0.97	0.07	55,56,62,63	0

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.



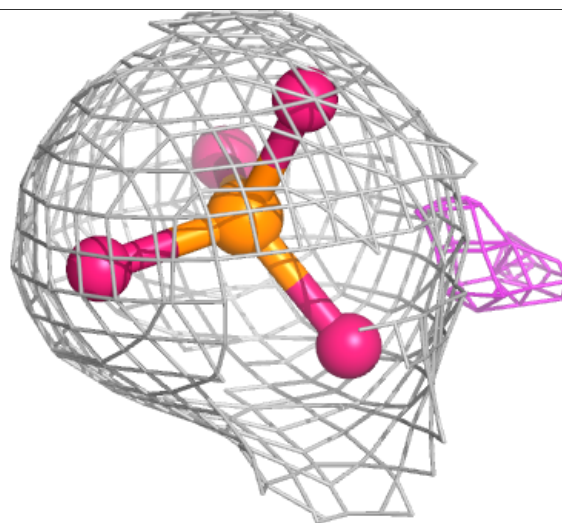
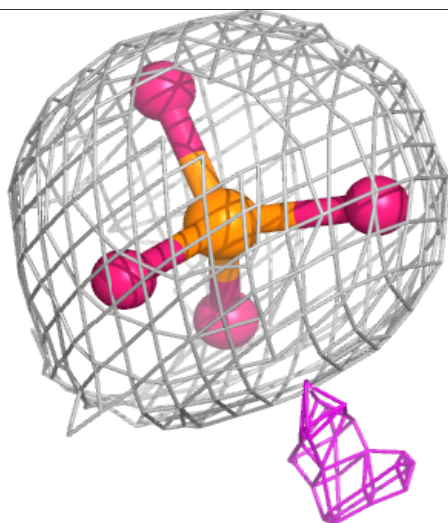
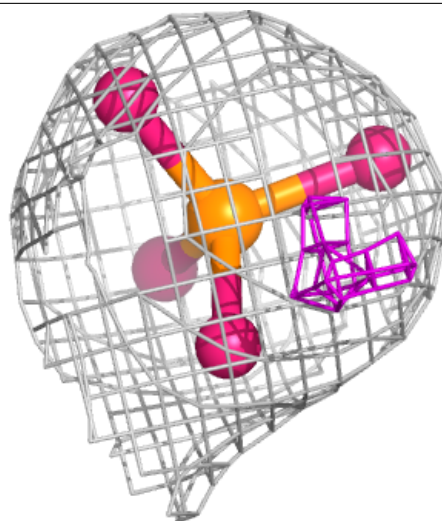
**Electron density around A1EMX BBB 401:**

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



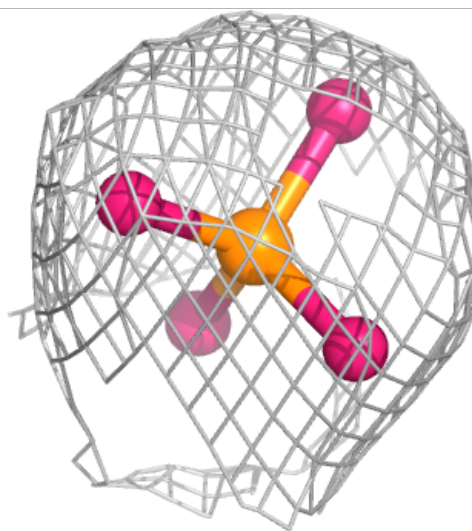
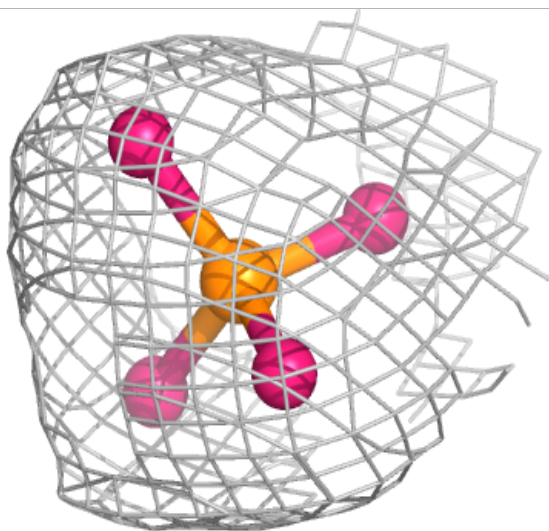
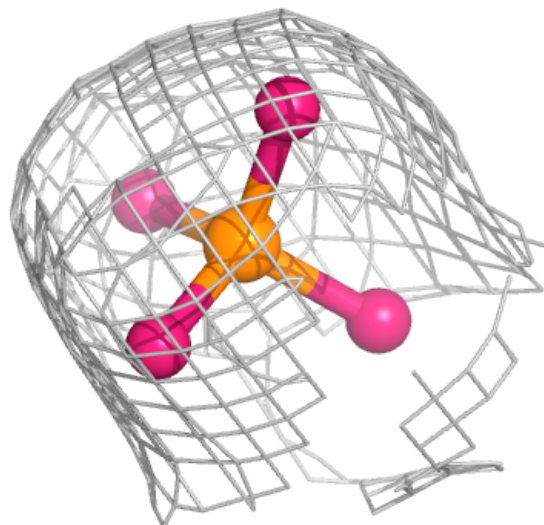
**Electron density around PO4 BBB 402:**

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



**Electron density around PO4 AAA 402:**

$2mF_o-DF_c$  (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.