



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 20, 2025 – 12:56 PM EDT

PDB ID : 9MKE / pdb\_00009mke  
Title : Crystal structure of MALT1 in complex with an allosteric inhibitor  
Authors : Bell, J.A.  
Deposited on : 2024-12-17  
Resolution : 2.34 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 : 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

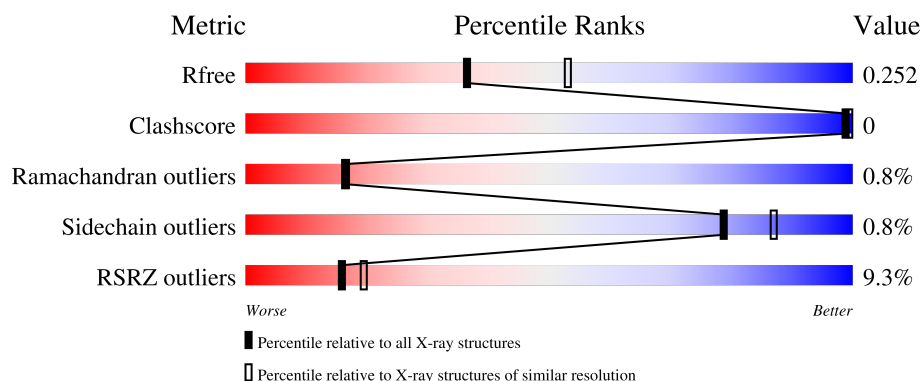
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.34 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	2747 (2.36-2.32)
Clashscore	180529	2936 (2.36-2.32)
Ramachandran outliers	177936	2912 (2.36-2.32)
Sidechain outliers	177891	2912 (2.36-2.32)
RSRZ outliers	164620	2747 (2.36-2.32)

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	386	<div> <div>8%</div> <div>91%</div> <div>5%</div> <div>• • •</div> </div>
1	B	386	<div> <div>10%</div> <div>91%</div> <div>5%</div> <div>•</div> </div>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 13126 atoms, of which 6726 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.

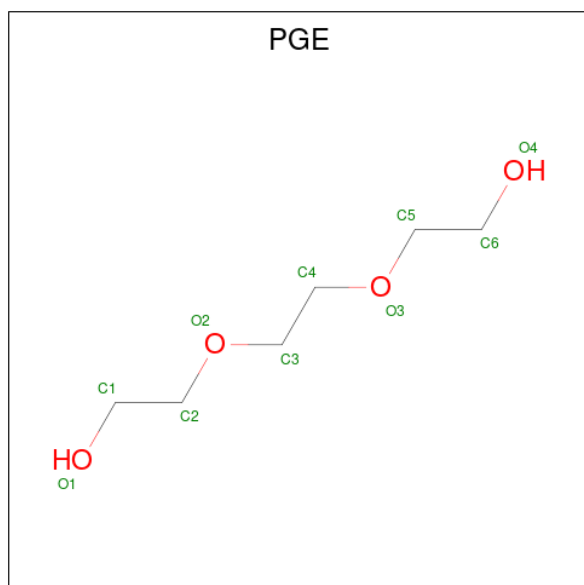
- Molecule 1 is a protein called Mucosa-associated lymphoid tissue lymphoma translocation protein 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	373	Total	C	H	N	O	S	0	0	0
			5972	1903	2998	487	564	20			
1	B	371	Total	C	H	N	O	S	0	0	0
			5933	1891	2976	485	561	20			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

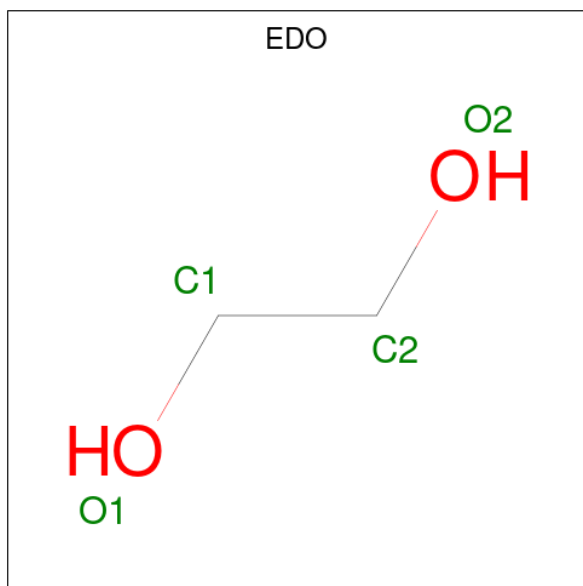
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	7	Total	Ca	0	0
			7	7		
2	B	5	Total	Ca	0	0
			5	5		

- Molecule 3 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			24	6	14	4		
3	A	1	Total	C	H	O	0	0
			24	6	14	4		
3	B	1	Total	C	H	O	0	0
			24	6	14	4		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



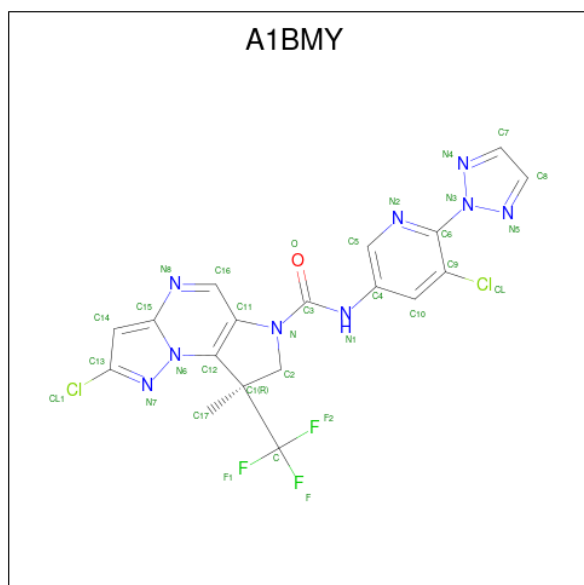
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 5 is (8R,9R)-2-chloro-N-[5-chloro-6-(2H-1,2,3-triazol-2-yl)pyridin-3-yl]-8-methyl-8-(trifluoromethyl)-7,8-dihydro-6H-pyrazolo[1,5-a]pyrrolo[2,3-e]pyrimidine-6-carboxamide (CCD ID: A1BMY) (formula: C<sub>18</sub>H<sub>12</sub>Cl<sub>2</sub>F<sub>3</sub>N<sub>9</sub>O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
5	A	1	Total	C	Cl	F	H	N	O	0	0
			45	18	2	3	12	9	1		

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Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
5	B	1	Total	C	Cl	F	H	N	O	0	0
			45	18	2	3	12	9	1		

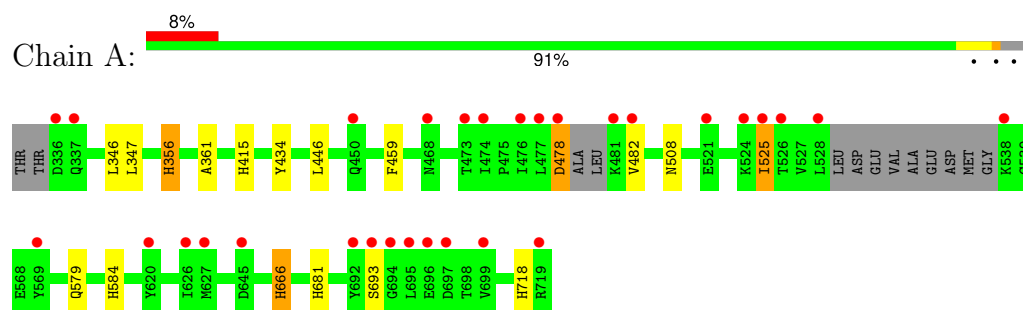
- Molecule 6 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	145	Total	H	O	0	0
			435	290	145		
6	B	144	Total	H	O	0	0
			432	288	144		

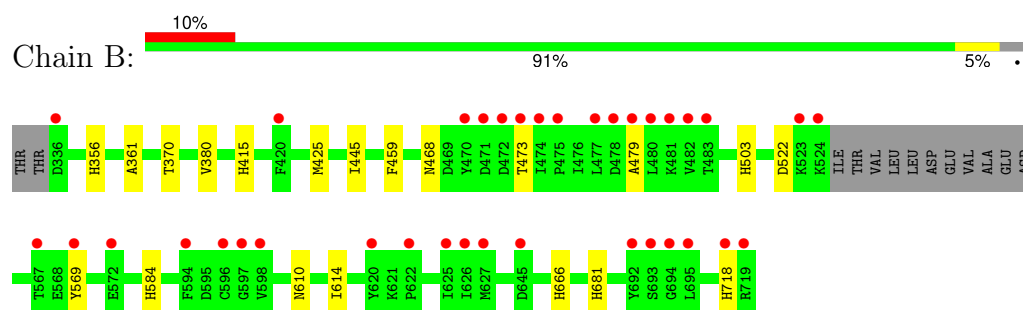
### 3 Residue-property plots [i](#)

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: Mucosa-associated lymphoid tissue lymphoma translocation protein 1



- Molecule 1: Mucosa-associated lymphoid tissue lymphoma translocation protein 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.26Å 77.87Å 93.22Å 90.00° 93.00° 90.00°	Depositor
Resolution (Å)	56.11 – 2.34 56.11 – 2.34	Depositor EDS
% Data completeness (in resolution range)	98.6 (56.11-2.34) 98.5 (56.11-2.34)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.48 (at 2.34Å)	Xtriage
Refinement program	PRIME-X	Depositor
R, $R_{free}$	0.204 , 0.258 0.202 , 0.252	Depositor DCC
$R_{free}$ test set	2059 reflections (4.32%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.7	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 55.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13126	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.65% 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: A1BMY, CA, EDO, PGE

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	0.60	0/3029	1.09	11/4092 (0.3%)
1	B	0.61	1/3013 (0.0%)	1.09	12/4071 (0.3%)
All	All	0.60	1/6042 (0.0%)	1.09	23/8163 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	503	HIS	CG-CD2	5.25	1.41	1.35

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	459	PHE	CA-CB-CG	6.02	119.82	113.80
1	B	459	PHE	CA-CB-CG	6.00	119.81	113.80
1	B	584	HIS	ND1-CE1-NE2	5.96	114.36	108.40
1	A	584	HIS	ND1-CE1-NE2	5.94	114.34	108.40
1	B	356	HIS	ND1-CE1-NE2	5.88	114.28	108.40
1	A	356	HIS	ND1-CE1-NE2	5.85	114.25	108.40
1	B	718	HIS	ND1-CE1-NE2	5.85	114.25	108.40
1	A	681	HIS	ND1-CE1-NE2	5.82	114.22	108.40
1	A	540	HIS	ND1-CE1-NE2	5.78	114.18	108.40
1	A	718	HIS	ND1-CE1-NE2	5.78	114.18	108.40
1	B	540	HIS	ND1-CE1-NE2	5.78	114.18	108.40
1	B	666	HIS	ND1-CE1-NE2	5.77	114.17	108.40
1	B	415	HIS	ND1-CE1-NE2	5.76	114.16	108.40
1	A	666	HIS	ND1-CE1-NE2	5.75	114.15	108.40
1	B	681	HIS	ND1-CE1-NE2	5.74	114.14	108.40
1	B	468	ASN	CA-CB-CG	5.73	118.33	112.60
1	A	415	HIS	ND1-CE1-NE2	5.71	114.11	108.40
1	B	522	ASP	CA-CB-CG	5.41	118.01	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	478	ASP	CA-CB-CG	5.37	117.97	112.60
1	B	610	ASN	CA-CB-CG	5.30	117.90	112.60
1	A	508	ASN	CA-CB-CG	5.26	117.86	112.60
1	B	361	ALA	N-CA-C	5.22	120.71	113.45
1	A	361	ALA	N-CA-C	5.05	120.47	113.45

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	2974	2998	2993	3	0
1	B	2957	2976	2972	2	0
2	A	7	0	0	0	0
2	B	5	0	0	0	0
3	A	20	28	28	0	0
3	B	10	14	14	0	0
4	A	32	48	48	0	0
4	B	40	60	60	0	0
5	A	33	12	0	0	0
5	B	33	12	0	0	0
6	A	145	290	0	0	0
6	B	144	288	0	0	0
All	All	6400	6726	6115	5	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 0.

All (5) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:MET:HE1	1:B:445:ILE:CD1	2.41	0.50
1:A:346:LEU:C	1:A:347:LEU:HD12	2.40	0.47
1:A:525:ILE:HD12	1:A:561:THR:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:HIS:CE1	1:A:434:TYR:CE1	3.08	0.40
1:B:370:THR:HG23	1:B:380:VAL:HG11	2.04	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	367/386 (95%)	351 (96%)	13 (4%)	3 (1%)	16	16
1	B	367/386 (95%)	347 (95%)	17 (5%)	3 (1%)	16	16
All	All	734/772 (95%)	698 (95%)	30 (4%)	6 (1%)	16	16

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	666	HIS
1	B	479	ALA
1	B	473	THR
1	B	569	TYR
1	A	693	SER
1	A	482	VAL

### 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	333/343 (97%)	329 (99%)	4 (1%)	67	79
1	B	330/343 (96%)	329 (100%)	1 (0%)	91	95
All	All	663/686 (97%)	658 (99%)	5 (1%)	79	87

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	446	LEU
1	A	478	ASP
1	A	525	ILE
1	A	579	GLN
1	B	614	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	337	GLN
1	A	371	ASN
1	A	393	ASN
1	A	601	GLN
1	A	666	HIS
1	B	579	GLN
1	B	666	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 35 ligands modelled in this entry, 12 are monoatomic - leaving 23 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	EDO	A	1015	-	3,3,3	0.46	0	2,2,2	0.30	0
4	EDO	A	1011	-	3,3,3	0.50	0	2,2,2	0.38	0
3	PGE	A	1008	-	9,9,9	0.52	0	8,8,8	0.45	0
4	EDO	A	1018	-	3,3,3	0.46	0	2,2,2	0.66	0
4	EDO	B	812	-	3,3,3	0.41	0	2,2,2	0.50	0
4	EDO	B	809	-	3,3,3	0.43	0	2,2,2	0.77	0
4	EDO	B	816	-	3,3,3	0.45	0	2,2,2	0.28	0
4	EDO	B	808	-	3,3,3	0.40	0	2,2,2	0.78	0
4	EDO	B	814	-	3,3,3	0.46	0	2,2,2	0.18	0
4	EDO	B	815	-	3,3,3	0.46	0	2,2,2	0.35	0
4	EDO	B	810	-	3,3,3	0.40	0	2,2,2	0.76	0
4	EDO	A	1013	-	3,3,3	0.47	0	2,2,2	0.60	0
3	PGE	A	1009	-	9,9,9	0.57	0	8,8,8	0.22	0
4	EDO	A	1010	-	3,3,3	0.46	0	2,2,2	0.77	0
4	EDO	A	1012	-	3,3,3	0.42	0	2,2,2	0.89	0
4	EDO	A	1017	-	3,3,3	0.43	0	2,2,2	0.35	0
4	EDO	B	811	-	3,3,3	0.38	0	2,2,2	0.81	0
4	EDO	B	813	-	3,3,3	0.43	0	2,2,2	0.77	0
3	PGE	B	807	-	9,9,9	0.56	0	8,8,8	0.38	0
5	A1BMY	B	817	-	33,37,37	2.34	9 (27%)	33,58,58	2.05	9 (27%)
5	A1BMY	A	1016	-	33,37,37	2.34	9 (27%)	33,58,58	2.04	8 (24%)
4	EDO	A	1014	-	3,3,3	0.48	0	2,2,2	0.31	0
4	EDO	B	801	-	3,3,3	0.38	0	2,2,2	0.33	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	EDO	A	1015	-	-	0/1/1/1	-
4	EDO	A	1011	-	-	0/1/1/1	-
3	PGE	A	1008	-	-	3/7/7/7	-
4	EDO	A	1018	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	B	812	-	-	0/1/1/1	-
4	EDO	B	809	-	-	1/1/1/1	-
4	EDO	B	816	-	-	0/1/1/1	-
4	EDO	B	808	-	-	0/1/1/1	-
4	EDO	B	814	-	-	0/1/1/1	-
4	EDO	B	815	-	-	0/1/1/1	-
4	EDO	B	810	-	-	0/1/1/1	-
4	EDO	A	1013	-	-	0/1/1/1	-
3	PGE	A	1009	-	-	0/7/7/7	-
4	EDO	A	1010	-	-	1/1/1/1	-
4	EDO	A	1012	-	-	0/1/1/1	-
4	EDO	A	1017	-	-	0/1/1/1	-
4	EDO	B	811	-	-	0/1/1/1	-
4	EDO	B	813	-	-	0/1/1/1	-
3	PGE	B	807	-	-	0/7/7/7	-
5	A1BMY	B	817	-	-	2/17/36/36	0/5/5/5
5	A1BMY	A	1016	-	-	2/17/36/36	0/5/5/5
4	EDO	A	1014	-	-	1/1/1/1	-
4	EDO	B	801	-	-	0/1/1/1	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1016	A1BMY	C2-C1	6.76	1.65	1.53
5	B	817	A1BMY	C2-C1	6.73	1.65	1.53
5	B	817	A1BMY	C11-C12	-5.47	1.28	1.39
5	A	1016	A1BMY	C11-C12	-5.42	1.28	1.39
5	B	817	A1BMY	N4-N3	4.90	1.39	1.32
5	A	1016	A1BMY	N4-N3	4.52	1.39	1.32
5	B	817	A1BMY	N5-N3	4.00	1.38	1.32
5	A	1016	A1BMY	N5-N3	3.99	1.38	1.32
5	A	1016	A1BMY	C14-C13	3.41	1.44	1.39
5	B	817	A1BMY	C14-C13	3.29	1.44	1.39
5	A	1016	A1BMY	C15-N8	2.97	1.38	1.34
5	B	817	A1BMY	C9-C6	2.96	1.43	1.39
5	B	817	A1BMY	C15-N8	2.95	1.38	1.34
5	A	1016	A1BMY	C9-C6	2.79	1.43	1.39
5	A	1016	A1BMY	C13-CL1	-2.57	1.68	1.74
5	B	817	A1BMY	C11-N	-2.53	1.35	1.39
5	A	1016	A1BMY	C11-N	-2.44	1.35	1.39
5	B	817	A1BMY	C13-CL1	-2.21	1.69	1.74

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1016	A1BMY	C12-C11-N	6.24	112.58	108.91
5	B	817	A1BMY	C12-C11-N	6.10	112.50	108.91
5	B	817	A1BMY	C1-C12-C11	5.24	114.22	109.18
5	A	1016	A1BMY	C1-C12-C11	5.11	114.10	109.18
5	A	1016	A1BMY	F-C-C1	-3.82	108.87	112.28
5	B	817	A1BMY	F2-C-C1	-3.45	109.19	112.28
5	B	817	A1BMY	N1-C3-N	-3.43	112.47	115.94
5	A	1016	A1BMY	N1-C3-N	-3.39	112.51	115.94
5	A	1016	A1BMY	C14-C13-N7	3.13	115.73	111.34
5	B	817	A1BMY	C14-C13-N7	3.07	115.64	111.34
5	B	817	A1BMY	C2-N-C11	2.89	111.49	109.36
5	A	1016	A1BMY	C2-N-C11	2.69	111.34	109.36
5	A	1016	A1BMY	C7-C8-N5	2.17	111.74	107.23
5	B	817	A1BMY	C8-C7-N4	2.15	111.71	107.23
5	A	1016	A1BMY	C8-C7-N4	2.12	111.65	107.23
5	B	817	A1BMY	C7-C8-N5	2.11	111.62	107.23
5	B	817	A1BMY	C5-N2-C6	2.01	118.58	116.66

There are no chirality outliers.

All (11) torsion outliers are listed below:

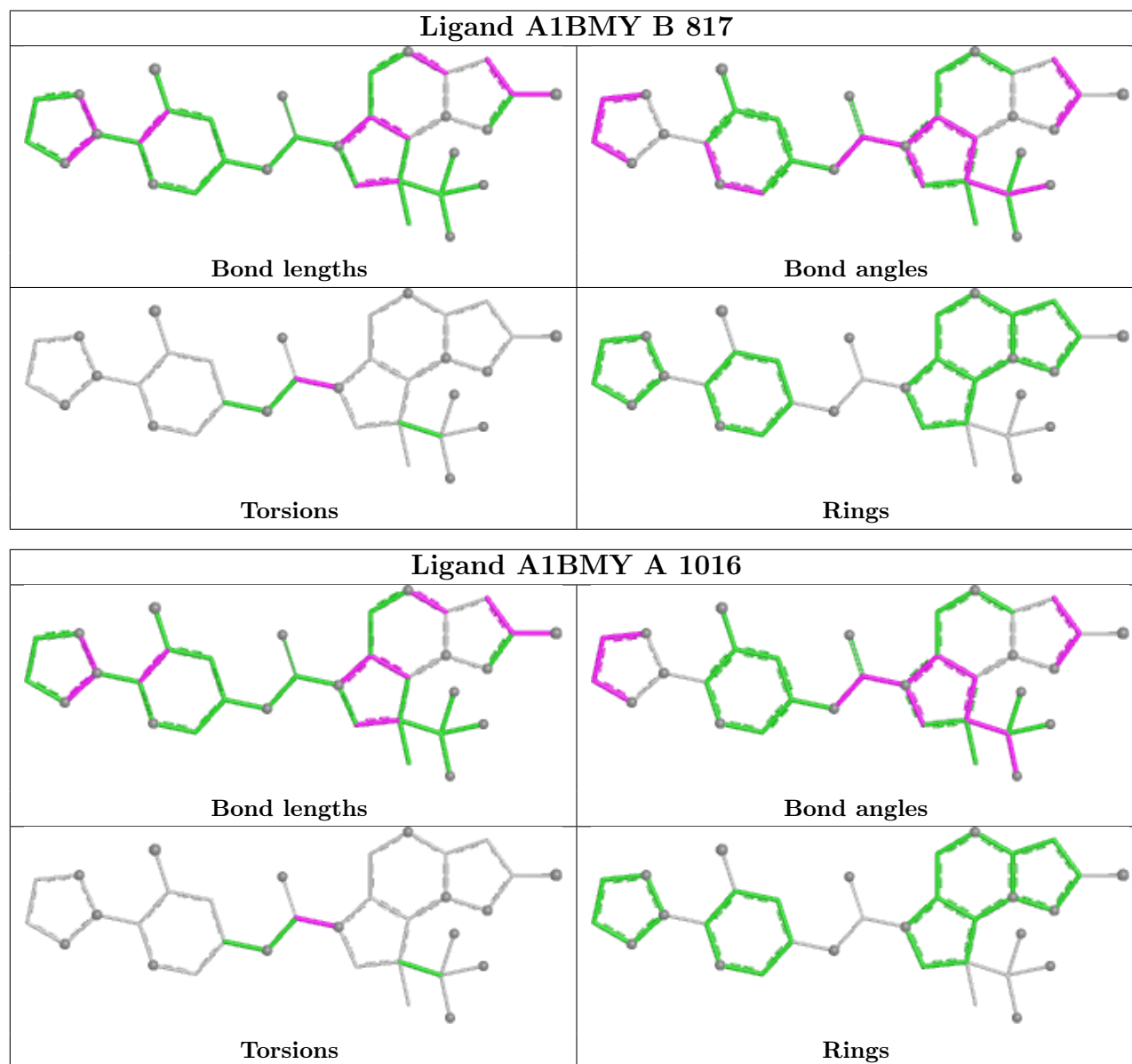
Mol	Chain	Res	Type	Atoms
5	A	1016	A1BMY	O-C3-N-C2
5	B	817	A1BMY	O-C3-N-C2
3	A	1008	PGE	C3-C4-O3-C5
4	A	1014	EDO	O1-C1-C2-O2
4	A	1010	EDO	O1-C1-C2-O2
4	A	1018	EDO	O1-C1-C2-O2
5	A	1016	A1BMY	N1-C3-N-C2
5	B	817	A1BMY	N1-C3-N-C2
3	A	1008	PGE	C6-C5-O3-C4
4	B	809	EDO	O1-C1-C2-O2
3	A	1008	PGE	O3-C5-C6-O4

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

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	373/386 (96%)	0.37	31 (8%) 19 23	25, 50, 99, 130	0
1	B	371/386 (96%)	0.49	38 (10%) 13 17	22, 51, 104, 128	0
All	All	744/772 (96%)	0.43	69 (9%) 16 19	22, 50, 101, 130	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	473	THR	5.4
1	A	525	ILE	4.8
1	A	478	ASP	4.6
1	A	695	LEU	4.5
1	A	482	VAL	4.1
1	B	477	LEU	4.0
1	A	477	LEU	4.0
1	A	476	ILE	4.0
1	B	524	LYS	3.8
1	A	528	LEU	3.8
1	A	569	TYR	3.7
1	A	626	ILE	3.7
1	B	692	TYR	3.6
1	B	695	LEU	3.5
1	B	472	ASP	3.5
1	A	524	LYS	3.3
1	B	420	PHE	3.3
1	B	718	HIS	3.2
1	A	473	THR	3.2
1	A	692	TYR	3.1
1	B	470	TYR	3.1
1	A	567	THR	3.1
1	B	478	ASP	3.0
1	B	471	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	694	GLY	2.9
1	B	598	VAL	2.9
1	B	597	GLY	2.9
1	B	694	GLY	2.8
1	A	627	MET	2.8
1	A	481	LYS	2.8
1	B	481	LYS	2.7
1	A	693	SER	2.7
1	A	474	ILE	2.7
1	B	474	ILE	2.7
1	B	336	ASP	2.7
1	A	620	TYR	2.6
1	A	538	LYS	2.6
1	B	482	VAL	2.5
1	B	626	ILE	2.5
1	A	645	ASP	2.5
1	B	569	TYR	2.5
1	A	336	ASP	2.5
1	B	719	ARG	2.5
1	B	625	ILE	2.4
1	B	567	THR	2.4
1	A	699	VAL	2.4
1	B	596	CYS	2.3
1	A	697	ASP	2.3
1	A	696	GLU	2.3
1	A	468	ASN	2.3
1	B	594	PHE	2.3
1	A	450	GLN	2.3
1	B	620	TYR	2.2
1	A	719	ARG	2.2
1	A	526	THR	2.2
1	B	627	MET	2.2
1	B	479	ALA	2.2
1	B	480	LEU	2.1
1	B	483	THR	2.1
1	B	523	LYS	2.1
1	B	693	SER	2.1
1	A	521	GLU	2.1
1	B	645	ASP	2.1
1	B	539	CYS	2.1
1	B	572	GLU	2.0
1	B	475	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	622	PRO	2.0
1	B	538	LYS	2.0
1	A	337	GLN	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(Å <sup>2</sup> )	Q<0.9
4	EDO	B	814	4/4	0.66	0.26	66,95,110,110	0
4	EDO	B	812	4/4	0.68	0.33	93,128,134,134	0
4	EDO	B	813	4/4	0.69	0.28	98,104,113,113	0
4	EDO	A	1017	4/4	0.71	0.38	45,78,99,101	0
4	EDO	B	816	4/4	0.72	0.27	102,111,120,122	0
4	EDO	A	1015	4/4	0.74	0.28	53,72,88,88	0
3	PGE	A	1009	10/10	0.76	0.29	74,93,111,113	0
4	EDO	B	810	4/4	0.76	0.18	101,103,109,111	0
2	CA	B	803	1/1	0.76	0.24	108,108,108,108	0
4	EDO	A	1018	4/4	0.77	0.28	84,96,108,108	0
4	EDO	B	809	4/4	0.78	0.24	75,99,101,101	0
4	EDO	A	1011	4/4	0.79	0.23	28,54,88,88	0
3	PGE	A	1008	10/10	0.79	0.20	88,112,120,132	0
3	PGE	B	807	10/10	0.81	0.20	58,73,109,124	0
4	EDO	A	1010	4/4	0.86	0.24	76,96,112,113	0
2	CA	A	1001	1/1	0.87	0.17	90,90,90,90	0
2	CA	A	1002	1/1	0.87	0.13	80,80,80,80	0
4	EDO	A	1012	4/4	0.87	0.20	45,83,99,99	0
2	CA	B	806	1/1	0.88	0.19	68,68,68,68	0
4	EDO	B	811	4/4	0.88	0.27	40,43,93,93	0

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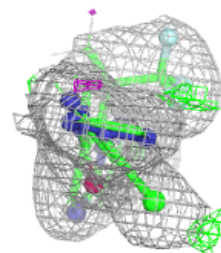
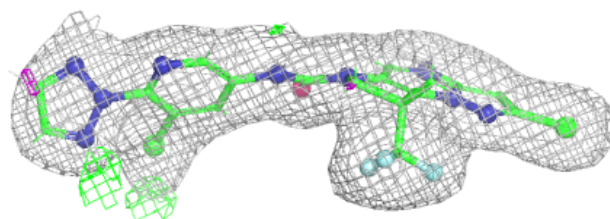
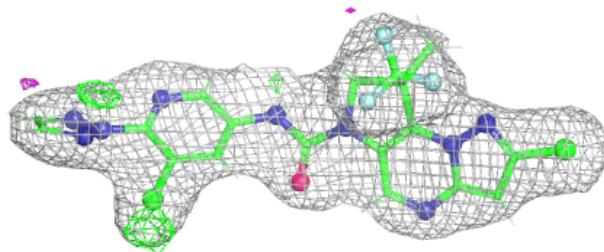
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	CA	A	1006	1/1	0.89	0.08	73,73,73,73	1
4	EDO	A	1013	4/4	0.89	0.17	40,56,105,107	0
2	CA	B	805	1/1	0.89	0.13	85,85,85,85	0
2	CA	A	1005	1/1	0.90	0.19	100,100,100,100	0
2	CA	B	804	1/1	0.91	0.10	72,72,72,72	0
4	EDO	A	1014	4/4	0.91	0.14	48,66,77,79	0
4	EDO	B	808	4/4	0.93	0.22	55,65,87,89	0
2	CA	A	1003	1/1	0.93	0.07	53,53,53,53	0
4	EDO	B	815	4/4	0.94	0.22	40,45,123,125	0
2	CA	A	1007	1/1	0.94	0.11	73,73,73,73	0
4	EDO	B	801	4/4	0.95	0.13	47,58,83,85	0
5	A1BMY	B	817	33/33	0.95	0.08	26,38,51,59	0
2	CA	B	802	1/1	0.96	0.20	54,54,54,54	0
5	A1BMY	A	1016	33/33	0.97	0.07	22,32,42,49	0
2	CA	A	1004	1/1	0.97	0.20	59,59,59,59	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.

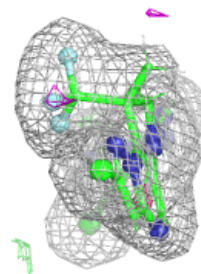
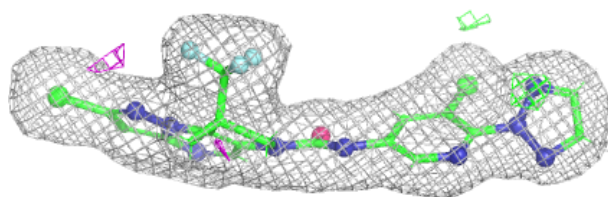
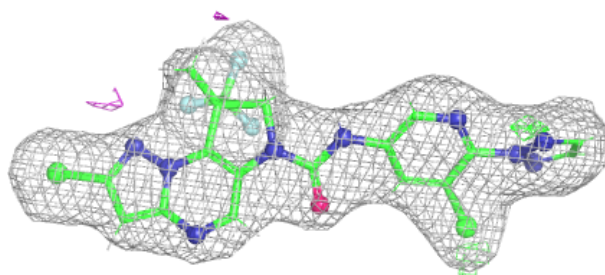
**Electron density around A1BMY B 817:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around A1BMY A 1016:**

$2mF_o-DF_c$  (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.