



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:53 AM UTC

PDB ID : 9MKD / pdb_00009mkd
Title : Crystal structure of MALT1 in complex with an allosteric inhibitor
Authors : Bell, J.A.
Deposited on : 2024-12-17
Resolution : 2.45 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 types of validation reports are described at

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

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

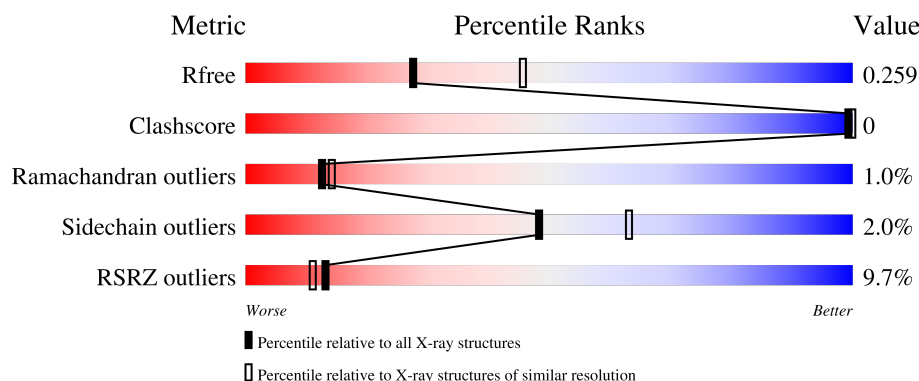
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	386	 10% 85% 9% • 5%
1	B	386	 9% 86% 8% • •

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 12564 atoms, of which 6403 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.

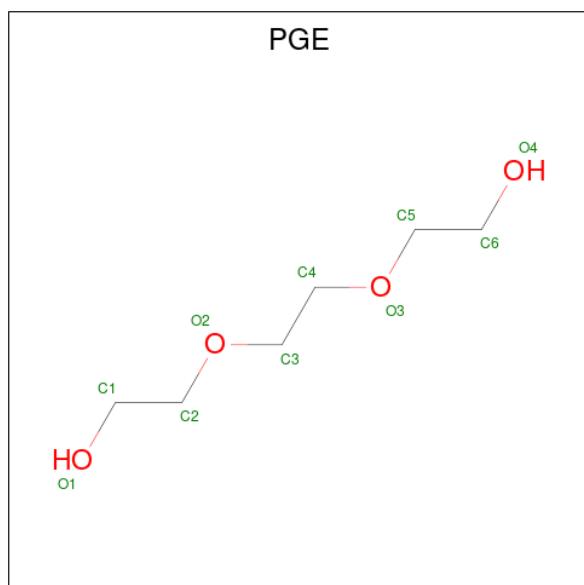
- Molecule 1 is a protein called Mucosa-associated lymphoid tissue lymphoma translocation protein 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	365	Total	C	H	N	O	S	0	0	0
			5819	1859	2917	473	550	20			
1	B	369	Total	C	H	N	O	S	0	0	0
			5882	1877	2950	479	556	20			

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

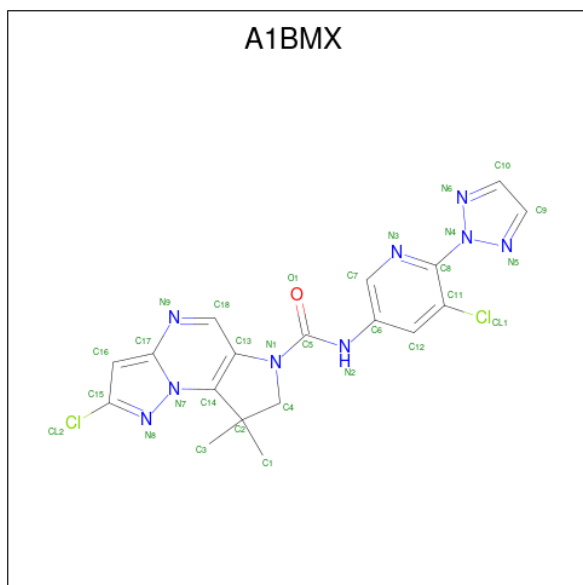
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	6	Total	Ca	0	0
			6	6		
2	B	5	Total	Ca	0	0
			5	5		

- Molecule 3 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



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

- Molecule 4 is (9R)-2-chloro-N-[5-chloro-6-(2H-1,2,3-triazol-2-yl)pyridin-3-yl]-8,8-dimethyl-7,8-dihydro-6H-pyrazolo[1,5-a]pyrrolo[2,3-e]pyrimidine-6-carboxamide (CCD ID: A1BMX) (formula: C₁₈H₁₅Cl₂N₉O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	Cl	H	N	O	0	0
			45	18	2	15	9	1		
4	B	1	Total	C	Cl	H	N	O	0	0
			45	18	2	15	9	1		

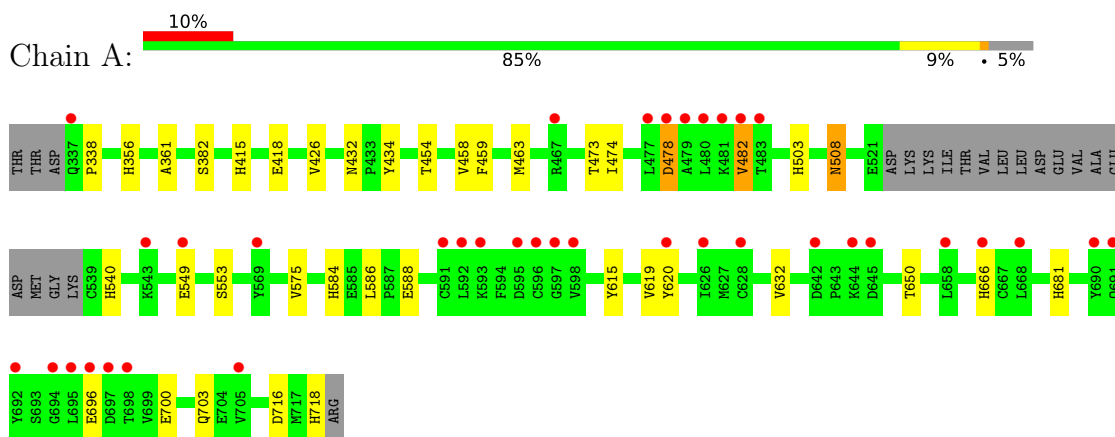
- Molecule 5 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	123	Total	H	O	0	0
			369	246	123		
5	B	123	Total	H	O	0	0
			369	246	123		

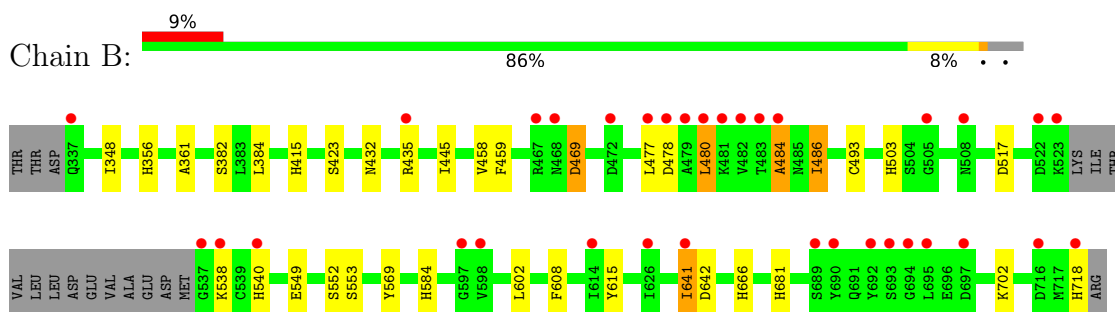
3 Residue-property plots [i](#)

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, α , β , γ	72.91Å 76.97Å 92.27Å 90.00° 93.42° 90.00°	Depositor
Resolution (Å)	34.56 – 2.45 34.56 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.9 (34.56-2.45) 99.9 (34.56-2.45)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 2.45Å)	Xtriage
Refinement program	PRIME-X	Depositor
R, R_{free}	0.211 , 0.268 0.211 , 0.259	Depositor DCC
R_{free} test set	1768 reflections (4.69%)	wwPDB-VP
Wilson B-factor (Å ²)	45.7	Xtriage
Anisotropy	0.461	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 56.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12564	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, A1BMX, 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	0.61	1/2958 (0.0%)	1.36	31/4002 (0.8%)
1	B	0.60	2/2988 (0.1%)	1.39	29/4040 (0.7%)
All	All	0.61	3/5946 (0.1%)	1.38	60/8042 (0.7%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	718	HIS	CG-CD2	5.24	1.41	1.35
1	B	503	HIS	CG-CD2	5.14	1.41	1.35
1	A	503	HIS	CG-CD2	5.02	1.41	1.35

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	703	GLN	CB-CA-C	6.42	120.31	110.62
1	A	382	SER	CB-CA-C	6.29	120.20	110.14
1	B	382	SER	CB-CA-C	6.20	120.06	110.14
1	A	586	LEU	CB-CA-C	6.18	118.15	108.63
1	A	459	PHE	CB-CA-C	6.04	119.80	110.14
1	A	584	HIS	ND1-CE1-NE2	6.00	114.40	108.40
1	B	459	PHE	CB-CA-C	5.98	119.35	110.62
1	B	584	HIS	ND1-CE1-NE2	5.93	114.33	108.40
1	A	718	HIS	ND1-CE1-NE2	5.92	114.32	108.40
1	B	553	SER	CB-CA-C	5.90	119.22	110.14
1	B	356	HIS	ND1-CE1-NE2	5.88	114.28	108.40
1	A	356	HIS	ND1-CE1-NE2	5.84	114.25	108.40
1	A	540	HIS	ND1-CE1-NE2	5.84	114.24	108.40
1	B	540	HIS	ND1-CE1-NE2	5.84	114.24	108.40
1	A	681	HIS	ND1-CE1-NE2	5.83	114.23	108.40
1	A	418	GLU	CB-CA-C	5.82	120.87	109.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	681	HIS	ND1-CE1-NE2	5.78	114.17	108.40
1	B	666	HIS	ND1-CE1-NE2	5.77	114.17	108.40
1	A	478	ASP	CB-CA-C	5.76	121.08	109.68
1	B	415	HIS	ND1-CE1-NE2	5.76	114.16	108.40
1	A	666	HIS	ND1-CE1-NE2	5.71	114.11	108.40
1	A	508	ASN	CA-CB-CG	5.66	118.26	112.60
1	A	415	HIS	ND1-CE1-NE2	5.65	114.05	108.40
1	B	423	SER	CB-CA-C	5.58	121.04	109.38
1	B	549	GLU	CB-CA-C	5.55	118.69	110.14
1	A	356	HIS	CB-CA-C	5.51	117.59	109.22
1	B	702	LYS	CB-CA-C	5.48	120.53	109.68
1	B	361	ALA	N-CA-C	5.46	120.98	113.77
1	A	473	THR	CB-CA-C	5.45	118.72	109.84
1	B	469	ASP	CA-CB-CG	5.45	118.05	112.60
1	A	361	ALA	N-CA-C	5.42	120.92	113.77
1	A	432	ASN	CB-CA-C	5.42	115.86	109.47
1	B	602	LEU	CB-CA-C	5.40	118.78	110.62
1	B	435	ARG	CB-CA-C	5.40	120.04	109.35
1	B	615	TYR	CB-CA-C	5.40	120.34	109.38
1	B	569	TYR	CB-CA-C	5.38	118.95	111.63
1	B	484	ALA	CB-CA-C	5.38	121.12	110.42
1	A	615	TYR	CB-CA-C	5.37	120.28	109.38
1	A	619	VAL	CB-CA-C	5.32	116.68	110.88
1	B	486	ILE	CB-CA-C	5.32	119.91	110.71
1	B	517	ASP	CA-CB-CG	5.30	117.90	112.60
1	B	477	LEU	CB-CA-C	5.29	121.22	109.94
1	A	716	ASP	CB-CA-C	5.29	118.82	111.63
1	A	458	VAL	CB-CA-C	5.29	118.05	110.33
1	A	459	PHE	CA-CB-CG	5.25	119.05	113.80
1	B	356	HIS	CB-CA-C	5.25	118.30	109.32
1	B	445	ILE	CB-CA-C	5.22	119.19	112.14
1	B	458	VAL	CB-CA-C	5.22	118.36	110.63
1	B	552	SER	CB-CA-C	5.22	119.69	109.35
1	A	620	TYR	CB-CA-C	5.19	118.74	109.65
1	B	348	ILE	CB-CA-C	5.17	118.28	110.63
1	A	553	SER	CB-CA-C	5.11	118.08	110.62
1	B	642	ASP	CA-CB-CG	5.08	117.69	112.60
1	A	482	VAL	CB-CA-C	5.07	119.61	111.29
1	A	549	GLU	CB-CA-C	5.06	118.86	109.70
1	A	474	ILE	CB-CA-C	5.05	114.28	109.33
1	A	650	THR	CB-CA-C	5.03	116.67	108.87
1	B	718	HIS	ND1-CE1-NE2	5.02	113.42	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	338	PRO	CB-CA-C	5.01	117.02	111.56
1	A	575	VAL	CB-CA-C	5.00	118.29	111.88

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	A	2902	2917	2912	1	0
1	B	2932	2950	2945	1	0
2	A	6	0	0	0	0
2	B	5	0	0	0	0
3	A	10	14	14	0	0
4	A	30	15	0	0	0
4	B	30	15	0	0	0
5	A	123	246	0	0	0
5	B	123	246	0	0	0
All	All	6161	6403	5871	2	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 (2) 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:384:LEU:HD11	1:B:608:PHE:CE1	2.54	0.42
1:A:426:VAL:HG11	1:A:434:TYR:CE1	2.55	0.41

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	361/386 (94%)	345 (96%)	14 (4%)	2 (1%)	21	27
1	B	365/386 (95%)	335 (92%)	25 (7%)	5 (1%)	9	8
All	All	726/772 (94%)	680 (94%)	39 (5%)	7 (1%)	12	14

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	478	ASP
1	B	484	ALA
1	A	454	THR
1	B	641	ILE
1	B	538	LYS
1	B	480	LEU
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	324/343 (94%)	317 (98%)	7 (2%)	45	60
1	B	327/343 (95%)	321 (98%)	6 (2%)	51	65
All	All	651/686 (95%)	638 (98%)	13 (2%)	48	63

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	463	MET
1	A	478	ASP
1	A	508	ASN
1	A	588	GLU
1	A	632	VAL
1	A	696	GLU
1	A	700	GLU
1	B	432	ASN
1	B	469	ASP
1	B	480	LEU
1	B	486	ILE
1	B	493	CYS
1	B	641	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	371	ASN
1	A	393	ASN
1	A	508	ASN
1	A	599	GLN
1	B	393	ASN
1	B	432	ASN
1	B	450	GLN
1	B	508	ASN
1	B	666	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 14 ligands modelled in this entry, 11 are monoatomic - leaving 3 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	A1BMX	A	807	-	34,34,34	2.67	14 (41%)	42,52,52	2.47	14 (33%)
4	A1BMX	B	1006	-	34,34,34	2.75	12 (35%)	42,52,52	2.30	13 (30%)
3	PGE	A	806	-	9,9,9	0.52	0	8,8,8	0.22	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	A1BMX	A	807	-	-	4/12/27/27	0/5/5/5
4	A1BMX	B	1006	-	-	5/12/27/27	0/5/5/5
3	PGE	A	806	-	-	1/7/7/7	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1006	A1BMX	C4-C2	9.44	1.65	1.54
4	A	807	A1BMX	C4-C2	8.70	1.64	1.54
4	A	807	A1BMX	C16-C17	-4.94	1.33	1.38
4	B	1006	A1BMX	C13-C14	-4.79	1.28	1.40
4	B	1006	A1BMX	C16-C17	-4.62	1.33	1.38
4	B	1006	A1BMX	N4-N6	4.32	1.39	1.33
4	A	807	A1BMX	C13-C14	-4.32	1.29	1.40
4	A	807	A1BMX	N4-N6	4.08	1.38	1.33
4	A	807	A1BMX	C17-N9	3.91	1.39	1.36
4	A	807	A1BMX	C18-C13	-3.88	1.38	1.43
4	A	807	A1BMX	N4-N5	3.68	1.38	1.33
4	B	1006	A1BMX	C11-C8	3.68	1.44	1.39
4	B	1006	A1BMX	N4-N5	3.68	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1006	A1BMX	C18-C13	-3.38	1.38	1.43
4	A	807	A1BMX	C11-C8	3.36	1.43	1.39
4	B	1006	A1BMX	C17-N9	3.30	1.38	1.36
4	B	1006	A1BMX	C5-N1	-3.23	1.36	1.41
4	B	1006	A1BMX	C15-N8	2.80	1.35	1.32
4	A	807	A1BMX	C5-N1	-2.75	1.36	1.41
4	B	1006	A1BMX	C13-N1	-2.71	1.35	1.39
4	A	807	A1BMX	C15-N8	2.66	1.35	1.32
4	A	807	A1BMX	C16-C15	2.57	1.44	1.39
4	A	807	A1BMX	C13-N1	-2.51	1.35	1.39
4	B	1006	A1BMX	C16-C15	2.50	1.44	1.39
4	A	807	A1BMX	C15-CL2	-2.05	1.68	1.73
4	A	807	A1BMX	C17-N7	-2.05	1.36	1.39

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	807	A1BMX	C17-C16-C15	-9.66	102.63	105.61
4	B	1006	A1BMX	C17-C16-C15	-8.39	103.02	105.61
4	A	807	A1BMX	C15-N8-N7	-5.90	97.84	104.66
4	B	1006	A1BMX	C15-N8-N7	-5.71	98.06	104.66
4	B	1006	A1BMX	C14-N7-C17	-4.39	116.93	121.08
4	A	807	A1BMX	O1-C5-N1	4.04	124.26	119.59
4	A	807	A1BMX	N2-C5-N1	-3.99	111.55	115.23
4	A	807	A1BMX	C14-N7-C17	-3.49	117.77	121.08
4	B	1006	A1BMX	O1-C5-N1	3.33	123.43	119.59
4	B	1006	A1BMX	C17-N7-N8	3.22	116.57	111.96
4	A	807	A1BMX	C17-N7-N8	3.21	116.54	111.96
4	B	1006	A1BMX	C14-C13-N1	3.01	112.52	106.57
4	B	1006	A1BMX	N2-C5-N1	-2.86	112.59	115.23
4	A	807	A1BMX	C2-C14-C13	2.71	114.97	109.89
4	A	807	A1BMX	C14-C13-N1	2.52	111.55	106.57
4	B	1006	A1BMX	C3-C2-C1	2.50	112.90	109.51
4	B	1006	A1BMX	C2-C14-C13	2.43	114.43	109.89
4	B	1006	A1BMX	C1-C2-C4	-2.38	108.09	111.83
4	A	807	A1BMX	C16-C17-N7	2.33	107.04	105.65
4	A	807	A1BMX	C10-N6-N4	-2.31	100.25	103.42
4	B	1006	A1BMX	C16-C15-CL2	-2.27	123.44	126.64
4	A	807	A1BMX	C16-C15-CL2	-2.26	123.45	126.64
4	A	807	A1BMX	C4-N1-C5	2.17	123.09	119.46
4	B	1006	A1BMX	C10-N6-N4	-2.16	100.46	103.42
4	A	807	A1BMX	C9-N5-N4	-2.08	100.57	103.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1006	A1BMX	C4-N1-C5	2.07	122.93	119.46
4	A	807	A1BMX	C9-C10-N6	2.03	111.77	109.06

There are no chirality outliers.

All (10) torsion outliers are listed below:

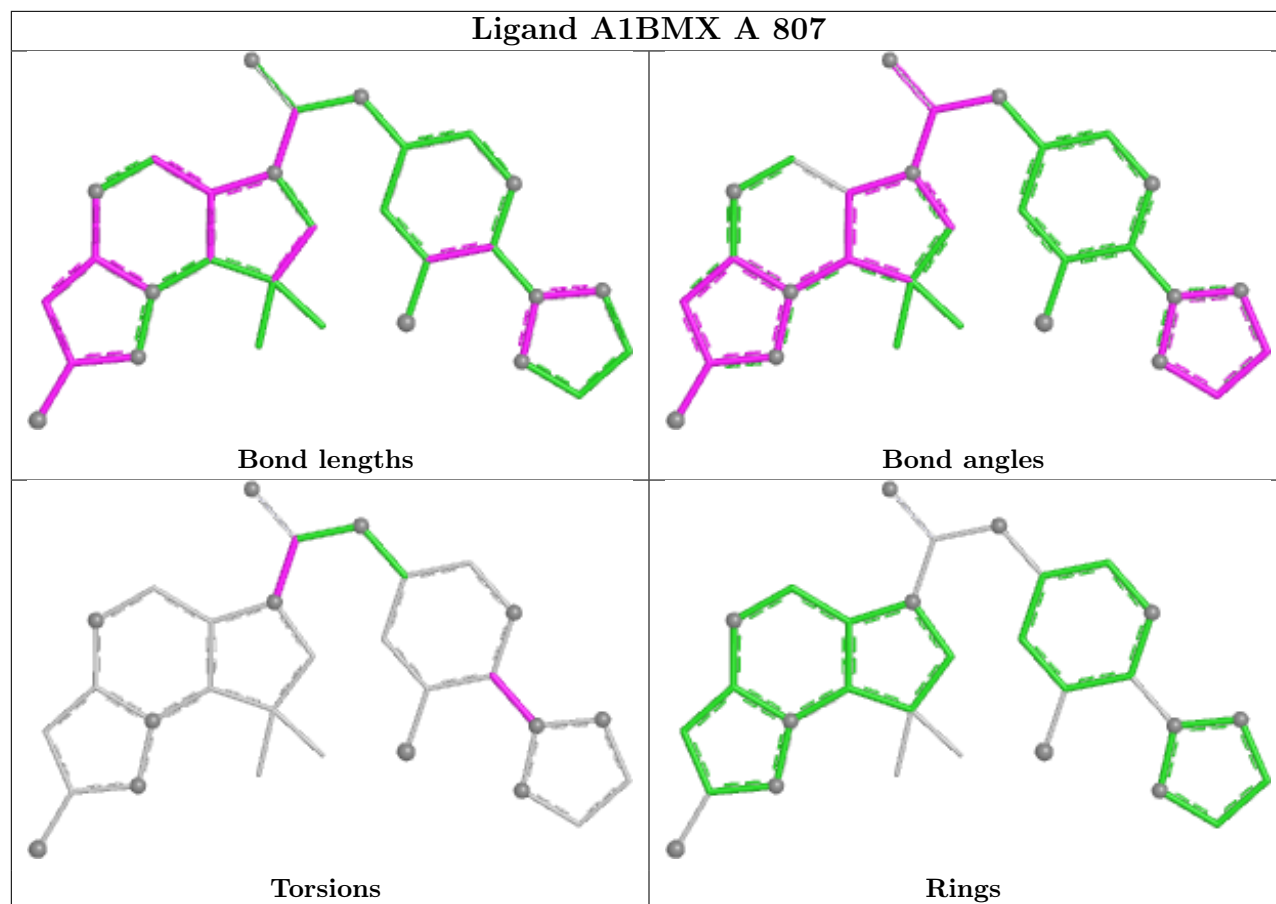
Mol	Chain	Res	Type	Atoms
4	A	807	A1BMX	O1-C5-N1-C4
4	A	807	A1BMX	O1-C5-N1-C13
4	A	807	A1BMX	C11-C8-N4-N6
4	B	1006	A1BMX	O1-C5-N1-C4
4	B	1006	A1BMX	O1-C5-N1-C13
4	B	1006	A1BMX	C11-C8-N4-N6
3	A	806	PGE	C3-C4-O3-C5
4	A	807	A1BMX	N3-C8-N4-N6
4	B	1006	A1BMX	N3-C8-N4-N6
4	B	1006	A1BMX	N2-C5-N1-C4

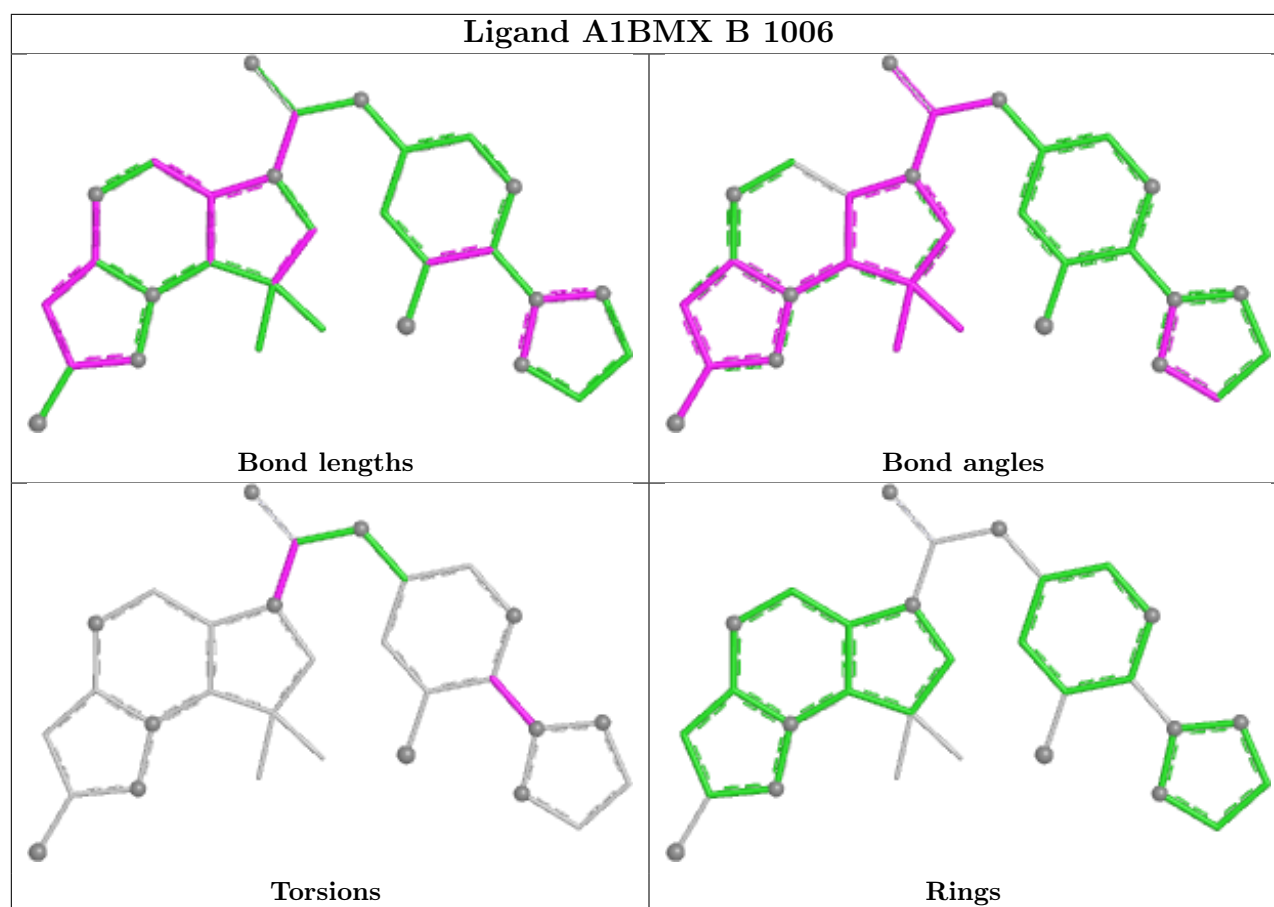
There are no ring outliers.

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.

Ligand A1BMX A 807





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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	365/386 (94%)	0.55	37 (10%)	12 10	23, 49, 107, 141	0
1	B	369/386 (95%)	0.56	34 (9%)	14 12	25, 51, 97, 140	0
All	All	734/772 (95%)	0.56	71 (9%)	13 11	23, 51, 103, 141	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	480	LEU	7.0
1	B	537	GLY	5.9
1	B	482	VAL	4.9
1	B	477	LEU	4.6
1	A	481	LYS	4.6
1	A	477	LEU	4.5
1	B	523	LYS	4.4
1	B	479	ALA	4.3
1	A	482	VAL	4.1
1	A	483	THR	3.7
1	B	718	HIS	3.6
1	B	483	THR	3.5
1	A	695	LEU	3.5
1	A	696	GLU	3.5
1	A	479	ALA	3.5
1	A	697	ASP	3.4
1	B	478	ASP	3.4
1	B	694	GLY	3.4
1	A	692	TYR	3.3
1	B	626	ILE	3.2
1	B	480	LEU	3.1
1	B	484	ALA	2.9
1	A	626	ILE	2.9
1	A	666	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	668	LEU	2.9
1	A	597	GLY	2.9
1	A	337	GLN	2.9
1	A	691	GLN	2.9
1	B	693	SER	2.8
1	A	478	ASP	2.8
1	A	690	TYR	2.7
1	B	522	ASP	2.7
1	A	698	THR	2.7
1	B	641	ILE	2.7
1	A	658	LEU	2.6
1	A	549	GLU	2.6
1	B	695	LEU	2.6
1	B	690	TYR	2.6
1	A	593	LYS	2.6
1	B	467	ARG	2.5
1	B	716	ASP	2.5
1	B	538	LYS	2.5
1	B	472	ASP	2.5
1	A	628	CYS	2.4
1	A	644	LYS	2.4
1	B	597	GLY	2.4
1	A	592	LEU	2.4
1	B	540	HIS	2.4
1	A	705	VAL	2.4
1	B	435	ARG	2.4
1	B	505	GLY	2.3
1	A	596	CYS	2.3
1	A	569	TYR	2.3
1	A	591	CYS	2.3
1	B	692	TYR	2.3
1	A	543	LYS	2.3
1	B	468	ASN	2.2
1	B	689	SER	2.2
1	A	595	ASP	2.2
1	B	697	ASP	2.2
1	A	694	GLY	2.2
1	A	642	ASP	2.2
1	B	614	ILE	2.2
1	A	620	TYR	2.1
1	A	598	VAL	2.1
1	A	645	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	337	GLN	2.1
1	B	598	VAL	2.1
1	B	481	LYS	2.1
1	A	467	ARG	2.0
1	B	508	ASN	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](#)

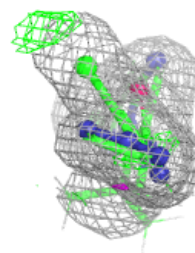
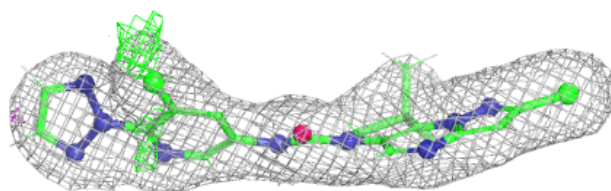
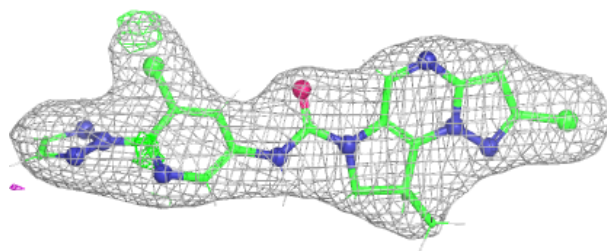
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CA	A	808	1/1	0.34	0.23	89,89,89,89	0
2	CA	B	1005	1/1	0.68	0.31	114,114,114,114	0
2	CA	A	804	1/1	0.79	0.27	115,115,115,115	0
3	PGE	A	806	10/10	0.84	0.18	46,69,90,103	0
2	CA	A	803	1/1	0.86	0.21	63,63,63,63	0
2	CA	B	1002	1/1	0.89	0.13	74,74,74,74	0
2	CA	B	1001	1/1	0.90	0.15	71,71,71,71	0
2	CA	B	1004	1/1	0.94	0.18	57,57,57,57	0
2	CA	A	805	1/1	0.94	0.10	62,62,62,62	0
2	CA	A	802	1/1	0.94	0.14	56,56,56,56	0
4	A1BMX	B	1006	30/30	0.94	0.09	27,40,61,63	0
4	A1BMX	A	807	30/30	0.95	0.09	25,36,47,54	0
2	CA	A	801	1/1	0.95	0.14	70,70,70,70	0
2	CA	B	1003	1/1	0.96	0.12	57,57,57,57	0

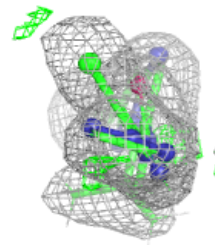
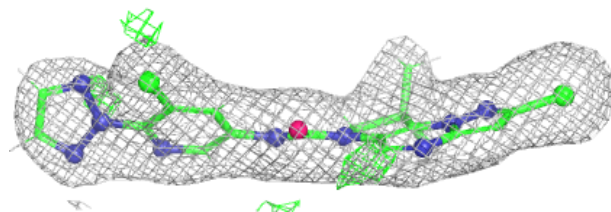
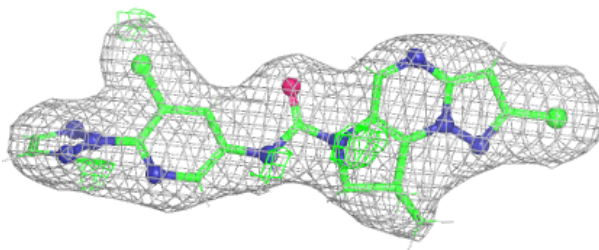
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1BMX B 1006:

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

**Electron density around A1BMX A 807:**

$2mF_o-DF_c$ (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.