



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:24 AM UTC

PDB ID : 6F7I / pdb_00006f7i
Title : human MALT1(329-728) IN COMPLEX WITH MLT-747
Authors : Renatus, M.; Renatus, M.
Deposited on : 2017-12-09
Resolution : 2.43 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

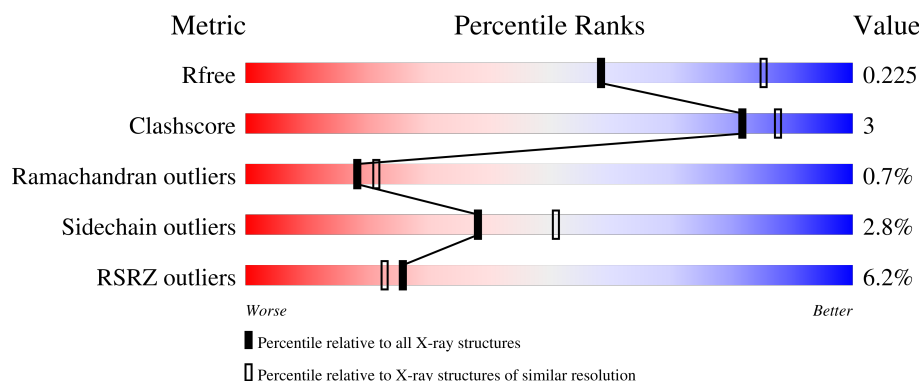
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.43 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	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (2.46-2.42)

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	404	
1	B	404	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5872 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.

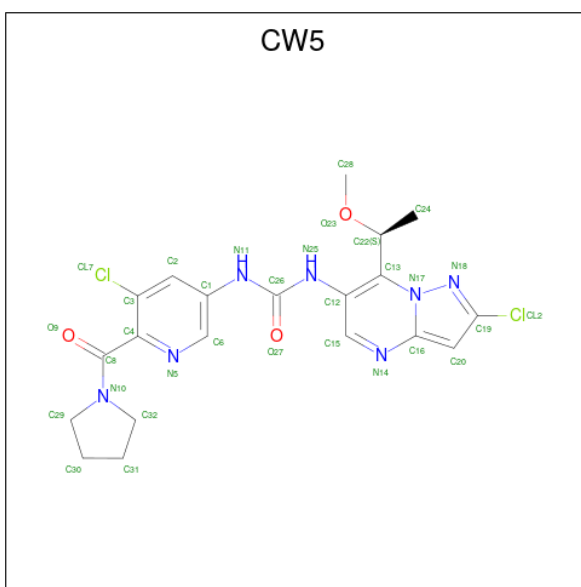
- Molecule 1 is a protein called Mucosa-associated lymphoid tissue lymphoma translocation protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	355	Total	C	N	O	S	0	0	0
			2813	1803	455	535	20			
1	B	365	Total	C	N	O	S	0	0	0
			2892	1851	468	552	21			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	325	GLY	-	expression tag	UNP Q9UDY8
A	326	PRO	-	expression tag	UNP Q9UDY8
A	327	GLY	-	expression tag	UNP Q9UDY8
A	328	SER	-	expression tag	UNP Q9UDY8
B	325	GLY	-	expression tag	UNP Q9UDY8
B	326	PRO	-	expression tag	UNP Q9UDY8
B	327	GLY	-	expression tag	UNP Q9UDY8
B	328	SER	-	expression tag	UNP Q9UDY8

- Molecule 2 is 1-[2-chloranyl-7-[(1 {S})-1-methoxyethyl]pyrazolo[1,5-a]pyrimidin-6-yl]-3-(5-chloranyl-6-pyrrolidin-1-ylcarbonyl-pyridin-3-yl)urea (CCD ID: CW5) (formula: C₂₀H₂₁Cl₂N₇O₃).

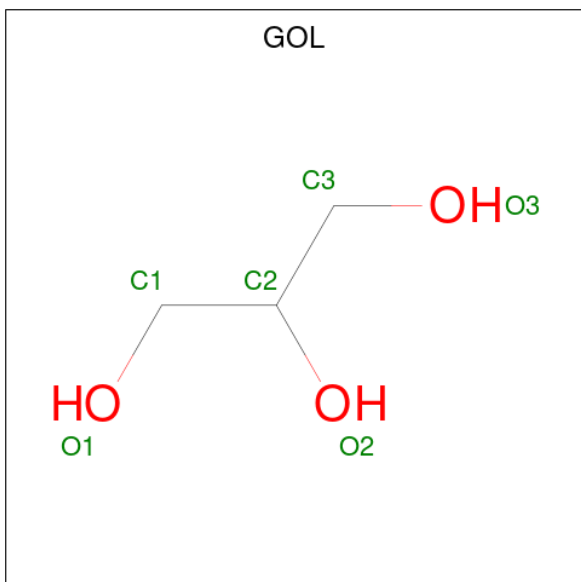


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0
			32	20	2	7	3	
2	B	1	Total	C	Cl	N	O	0
			32	20	2	7	3	

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg	0	0
			2	2		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

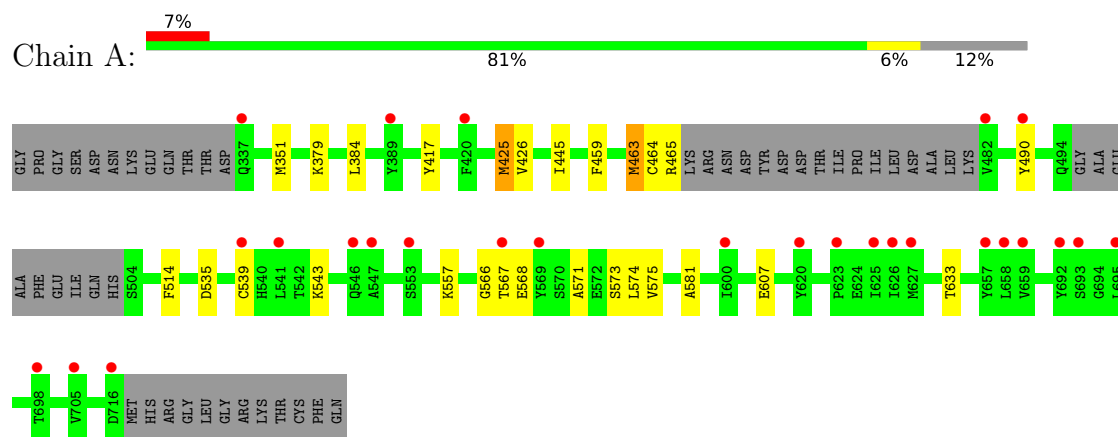
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	46	Total	O	0	0
			46	46		
5	B	43	Total	O	0	0
			43	43		

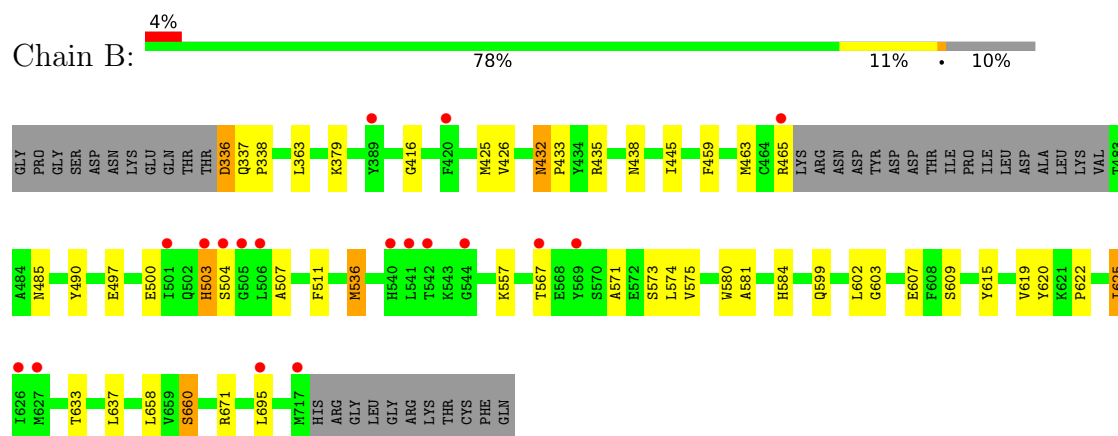
3 Residue-property plots

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	64.20Å 108.97Å 73.51Å 90.00° 111.79° 90.00°	Depositor
Resolution (Å)	68.26 – 2.43 68.26 – 2.43	Depositor EDS
% Data completeness (in resolution range)	99.6 (68.26-2.43) 99.6 (68.26-2.43)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 2.42Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.190 , 0.218 0.194 , 0.225	Depositor DCC
R_{free} test set	1749 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	55.4	Xtriage
Anisotropy	0.338	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 44.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5872	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, CW5

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	0.84	1/2863 (0.0%)	1.24	11/3870 (0.3%)
1	B	0.84	1/2945 (0.0%)	1.24	11/3981 (0.3%)
All	All	0.84	2/5808 (0.0%)	1.24	22/7851 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	536	MET	SD-CE	-6.18	1.64	1.79
1	A	425	MET	SD-CE	-5.32	1.66	1.79

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	426	VAL	N-CA-C	6.34	113.33	107.56
1	A	581	ALA	CA-C-N	6.32	129.61	120.38
1	A	581	ALA	C-N-CA	6.32	129.61	120.38
1	B	581	ALA	CA-C-N	6.01	129.16	120.38
1	B	581	ALA	C-N-CA	6.01	129.16	120.38
1	A	426	VAL	N-CA-C	5.91	112.94	107.56
1	A	379	LYS	N-CA-C	-5.82	99.80	109.46
1	B	379	LYS	N-CA-C	-5.70	99.99	109.46
1	A	535	ASP	CA-C-N	5.55	128.27	120.28
1	A	535	ASP	C-N-CA	5.55	128.27	120.28
1	A	464	CYS	CA-C-N	5.41	131.44	121.70
1	A	464	CYS	C-N-CA	5.41	131.44	121.70
1	B	459	PHE	CA-CB-CG	5.37	119.17	113.80
1	B	485	ASN	CA-CB-CG	5.32	117.92	112.60
1	A	607	GLU	N-CA-C	-5.27	106.54	113.12
1	B	660	SER	CA-C-N	5.25	127.74	120.29
1	B	660	SER	C-N-CA	5.25	127.74	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	336	ASP	CA-C-N	5.24	127.77	120.65
1	B	336	ASP	C-N-CA	5.24	127.77	120.65
1	A	459	PHE	CA-CB-CG	5.18	118.98	113.80
1	B	432	ASN	CA-CB-CG	5.14	117.74	112.60
1	A	463	MET	N-CA-C	5.03	117.94	109.95

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	2813	0	2840	8	0
1	B	2892	0	2905	21	0
2	A	32	0	0	0	0
2	B	32	0	0	0	0
3	A	2	0	0	0	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
5	A	46	0	0	0	0
5	B	43	0	0	0	0
All	All	5872	0	5761	29	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 (29) 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:497:GLU:HG2	1:B:500:GLU:HB2	1.75	0.67
1:B:580:TRP:O	1:B:584:HIS:HD2	1.83	0.62
1:A:351:MET:HE1	1:A:384:LEU:HD13	1.83	0.61
1:A:514:PHE:HZ	1:A:539:CYS:HB2	1.67	0.59
1:B:435:ARG:HB2	1:B:438:ASN:ND2	2.18	0.58
1:B:571:ALA:O	1:B:575:VAL:HG23	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:MET:HE1	1:A:445:ILE:CD1	2.36	0.55
1:A:571:ALA:O	1:A:575:VAL:HG23	2.07	0.55
1:B:463:MET:HE2	1:B:490:TYR:HE1	1.71	0.54
1:B:607:GLU:CD	1:B:671:ARG:HH12	2.14	0.54
1:A:514:PHE:CZ	1:A:539:CYS:HB2	2.42	0.54
1:B:584:HIS:HE1	1:B:609:SER:OG	1.90	0.53
1:B:425:MET:HE1	1:B:445:ILE:CD1	2.39	0.53
1:B:463:MET:HE2	1:B:490:TYR:CE1	2.45	0.51
1:B:363:LEU:HG	1:B:658:LEU:HD11	1.93	0.49
1:B:416:GLY:HA3	1:B:463:MET:SD	2.53	0.48
1:B:622:PRO:HD2	1:B:625:ILE:HG13	1.96	0.48
1:A:417:TYR:HA	1:A:465:ARG:NH2	2.29	0.47
1:B:432:ASN:HD22	1:B:433:PRO:HA	1.79	0.47
1:A:463:MET:HE2	1:A:490:TYR:HE1	1.79	0.47
1:A:463:MET:HE2	1:A:490:TYR:CE1	2.52	0.44
1:B:511:PHE:HA	1:B:536:MET:CE	2.49	0.43
1:B:504:SER:HB2	1:B:507:ALA:HB2	2.00	0.43
1:B:584:HIS:CE1	1:B:609:SER:OG	2.72	0.42
1:B:603:GLY:HA3	1:B:615:TYR:CE1	2.54	0.42
1:B:435:ARG:HB2	1:B:438:ASN:HD22	1.83	0.42
1:B:337:GLN:HA	1:B:338:PRO:HD3	1.98	0.42
1:B:511:PHE:HA	1:B:536:MET:HE1	2.03	0.41
1:B:599:GLN:HB2	1:B:620:TYR:HB3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	349/404 (86%)	337 (97%)	10 (3%)	2 (1%)	21	25
1	B	361/404 (89%)	345 (96%)	13 (4%)	3 (1%)	16	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	710/808 (88%)	682 (96%)	23 (3%)	5 (1%)	18 21

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	566	GLY
1	A	567	THR
1	B	503	HIS
1	B	567	THR
1	B	660	SER

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	316/357 (88%)	310 (98%)	6 (2%)	50 63
1	B	323/357 (90%)	311 (96%)	12 (4%)	30 41
All	All	639/714 (90%)	621 (97%)	18 (3%)	38 51

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	543	LYS
1	A	557	LYS
1	A	568	GLU
1	A	573	SER
1	A	574	LEU
1	A	633	THR
1	B	336	ASP
1	B	465	ARG
1	B	503	HIS
1	B	557	LYS
1	B	573	SER
1	B	574	LEU
1	B	602	LEU

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Mol	Chain	Res	Type
1	B	619	VAL
1	B	625	ILE
1	B	633	THR
1	B	637	LEU
1	B	695	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	457	ASN
1	A	579	GLN
1	A	599	GLN
1	A	681	HIS
1	B	432	ASN
1	B	438	ASN
1	B	444	ASN
1	B	457	ASN
1	B	485	ASN
1	B	508	ASN
1	B	546	GLN
1	B	577	ASN
1	B	579	GLN
1	B	584	HIS
1	B	599	GLN
1	B	681	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 6 ligands modelled in this entry, 2 are 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
4	GOL	A	804	-	5,5,5	0.10	0	5,5,5	0.35	0
2	CW5	B	801	-	33,35,35	2.72	11 (33%)	38,50,50	4.50	15 (39%)
4	GOL	B	802	-	5,5,5	0.06	0	5,5,5	0.15	0
2	CW5	A	801	-	33,35,35	2.91	9 (27%)	38,50,50	4.24	15 (39%)

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	GOL	A	804	-	-	0/4/4/4	-
2	CW5	B	801	-	-	3/17/29/29	0/4/4/4
4	GOL	B	802	-	-	2/4/4/4	-
2	CW5	A	801	-	-	1/17/29/29	0/4/4/4

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	CW5	C16-N14	9.91	1.43	1.36
2	B	801	CW5	C16-N14	9.62	1.43	1.36
2	A	801	CW5	C15-C12	5.57	1.50	1.43
2	B	801	CW5	C15-C12	5.06	1.49	1.43
2	A	801	CW5	C19-N18	-4.98	1.26	1.32
2	B	801	CW5	C20-C16	-4.90	1.33	1.38
2	A	801	CW5	C16-N17	-4.88	1.32	1.39
2	A	801	CW5	C20-C19	4.38	1.47	1.39
2	B	801	CW5	C16-N17	-4.28	1.33	1.39
2	A	801	CW5	C20-C16	-4.21	1.33	1.38
2	A	801	CW5	C22-C13	4.19	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	CW5	C13-N17	-3.86	1.33	1.37
2	B	801	CW5	C20-C19	3.84	1.46	1.39
2	B	801	CW5	C19-N18	-3.72	1.28	1.32
2	B	801	CW5	C13-N17	-3.62	1.33	1.37
2	A	801	CW5	C15-N14	-2.94	1.26	1.32
2	B	801	CW5	C26-N25	-2.75	1.33	1.39
2	B	801	CW5	C15-N14	-2.72	1.27	1.32
2	B	801	CW5	C22-C13	2.48	1.54	1.51
2	B	801	CW5	C12-N25	-2.33	1.35	1.41

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	CW5	C16-C20-C19	-15.41	100.86	105.61
2	B	801	CW5	C16-C20-C19	-15.15	100.94	105.61
2	B	801	CW5	C20-C16-N17	13.90	113.91	105.65
2	A	801	CW5	C20-C16-N17	13.11	113.44	105.65
2	B	801	CW5	C20-C16-N14	-9.79	124.17	132.87
2	A	801	CW5	C20-C16-N14	-8.52	125.30	132.87
2	A	801	CW5	C1-C6-N5	-5.86	119.22	124.07
2	B	801	CW5	C13-N17-N18	5.64	133.41	124.59
2	B	801	CW5	C1-C6-N5	-5.60	119.44	124.07
2	B	801	CW5	C15-N14-C16	5.44	120.01	116.39
2	A	801	CW5	C19-N18-N17	5.29	110.77	104.66
2	B	801	CW5	CL2-C19-N18	5.12	127.73	120.18
2	B	801	CW5	C19-N18-N17	5.09	110.53	104.66
2	A	801	CW5	C15-N14-C16	4.73	119.54	116.39
2	B	801	CW5	C16-N17-N18	-4.48	105.57	111.96
2	A	801	CW5	C13-N17-N18	4.20	131.16	124.59
2	B	801	CW5	C12-N25-C26	4.15	128.14	124.85
2	A	801	CW5	C16-N17-N18	-4.14	106.05	111.96
2	B	801	CW5	C32-N10-C29	3.62	116.17	111.37
2	A	801	CW5	CL2-C19-N18	3.50	125.33	120.18
2	B	801	CW5	C6-N5-C4	3.30	123.60	117.92
2	A	801	CW5	C32-N10-C29	2.96	115.29	111.37
2	B	801	CW5	C30-C29-N10	-2.95	98.47	103.44
2	B	801	CW5	C2-C3-C4	-2.95	118.90	121.88
2	A	801	CW5	C2-C3-C4	-2.93	118.91	121.88
2	A	801	CW5	C6-N5-C4	2.83	122.79	117.92
2	A	801	CW5	C30-C29-N10	-2.76	98.78	103.44
2	A	801	CW5	C12-N25-C26	2.70	126.99	124.85
2	A	801	CW5	C2-C1-C6	2.65	120.00	118.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	CW5	C20-C19-CL2	-2.34	123.33	126.64

There are no chirality outliers.

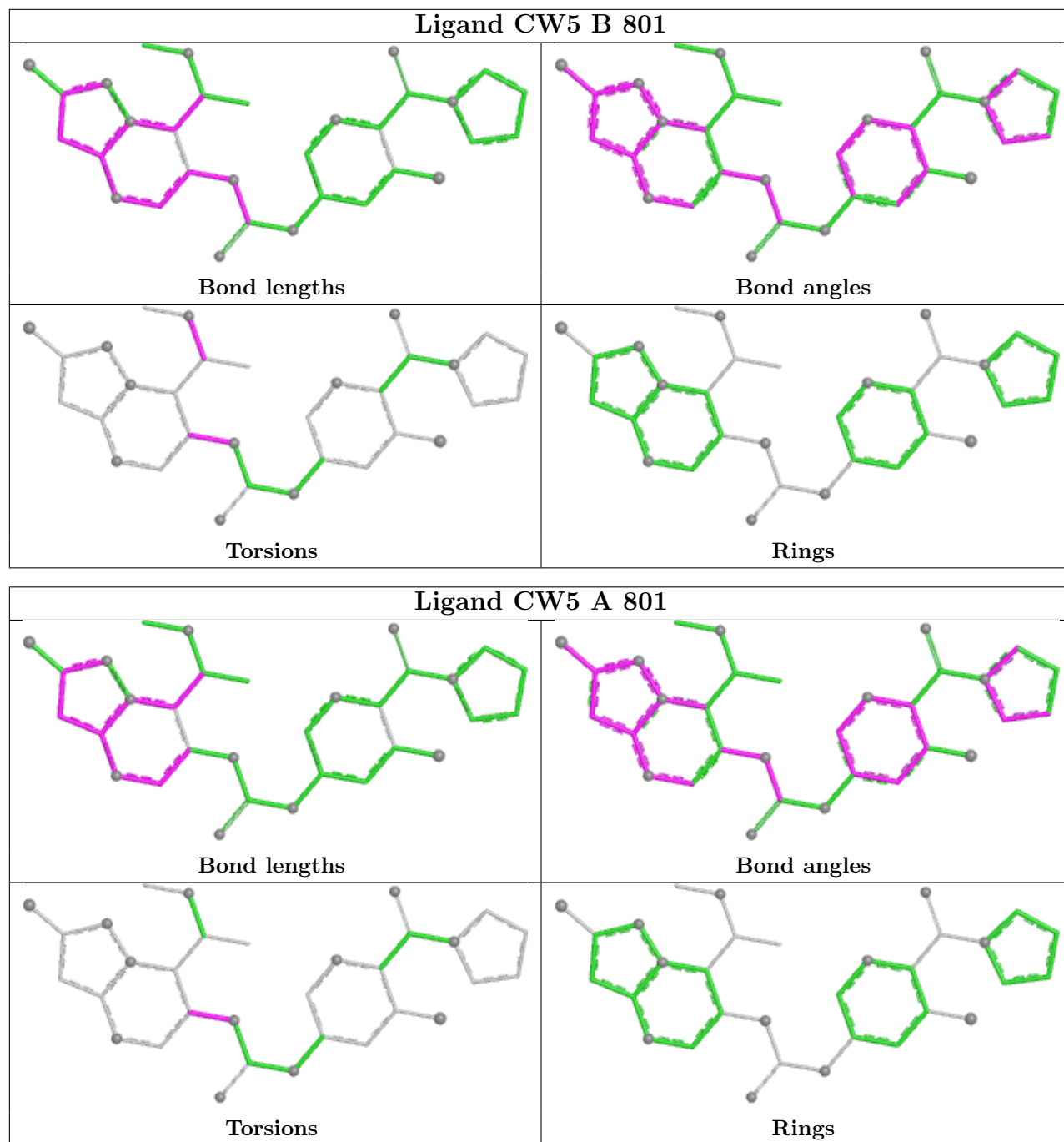
All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	801	CW5	C13-C22-O23-C28
4	B	802	GOL	O1-C1-C2-C3
4	B	802	GOL	O1-C1-C2-O2
2	B	801	CW5	C13-C12-N25-C26
2	A	801	CW5	C13-C12-N25-C26
2	B	801	CW5	C24-C22-O23-C28

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 [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	355/404 (87%)	0.34	27 (7%)	20 17	38, 61, 107, 140	0
1	B	365/404 (90%)	0.27	18 (4%)	35 32	41, 60, 100, 119	0
All	All	720/808 (89%)	0.30	45 (6%)	26 23	38, 60, 105, 140	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	717	MET	4.2
1	B	567	THR	3.8
1	B	503	HIS	3.2
1	A	695	LEU	3.2
1	A	692	TYR	3.1
1	B	420	PHE	3.1
1	B	626	ILE	3.1
1	A	658	LEU	3.0
1	A	546	GLN	3.0
1	A	567	THR	3.0
1	B	540	HIS	3.0
1	A	569	TYR	3.0
1	A	626	ILE	2.9
1	A	698	THR	2.9
1	B	569	TYR	2.8
1	A	716	ASP	2.7
1	A	541	LEU	2.6
1	A	620	TYR	2.6
1	A	600	ILE	2.6
1	A	623	PRO	2.5
1	B	501	ILE	2.5
1	B	541	LEU	2.5
1	A	705	VAL	2.5
1	B	506	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	504	SER	2.3
1	B	544	GLY	2.3
1	B	695	LEU	2.3
1	B	389	TYR	2.2
1	A	490	TYR	2.2
1	A	625	ILE	2.1
1	A	482	VAL	2.1
1	A	547	ALA	2.1
1	B	465	ARG	2.1
1	A	693	SER	2.1
1	A	659	VAL	2.1
1	A	539	CYS	2.1
1	A	627	MET	2.1
1	A	420	PHE	2.1
1	A	553	SER	2.1
1	B	627	MET	2.1
1	A	337	GLN	2.0
1	B	505	GLY	2.0
1	B	542	THR	2.0
1	A	389	TYR	2.0
1	A	657	TYR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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.

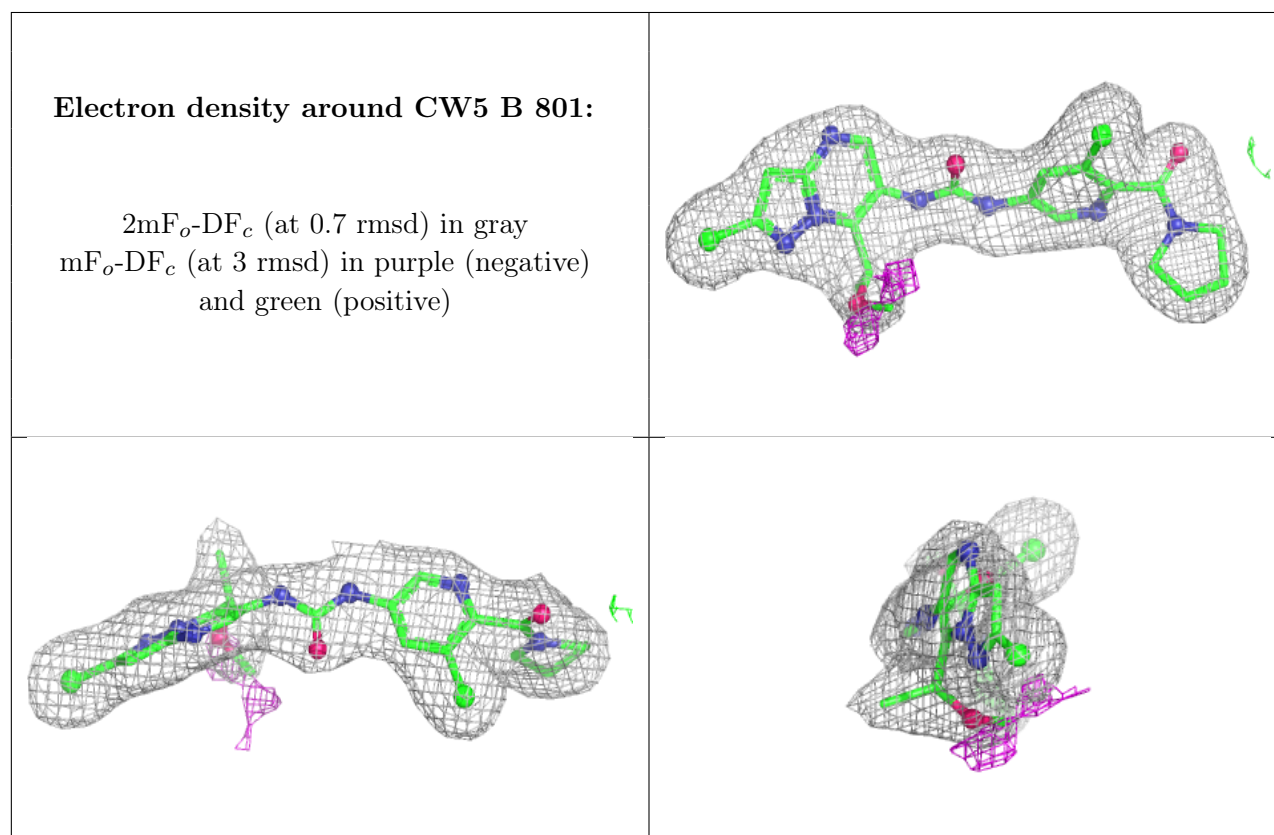
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	A	803	1/1	0.81	0.23	82,82,82,82	0
3	MG	A	802	1/1	0.92	0.17	69,69,69,69	0

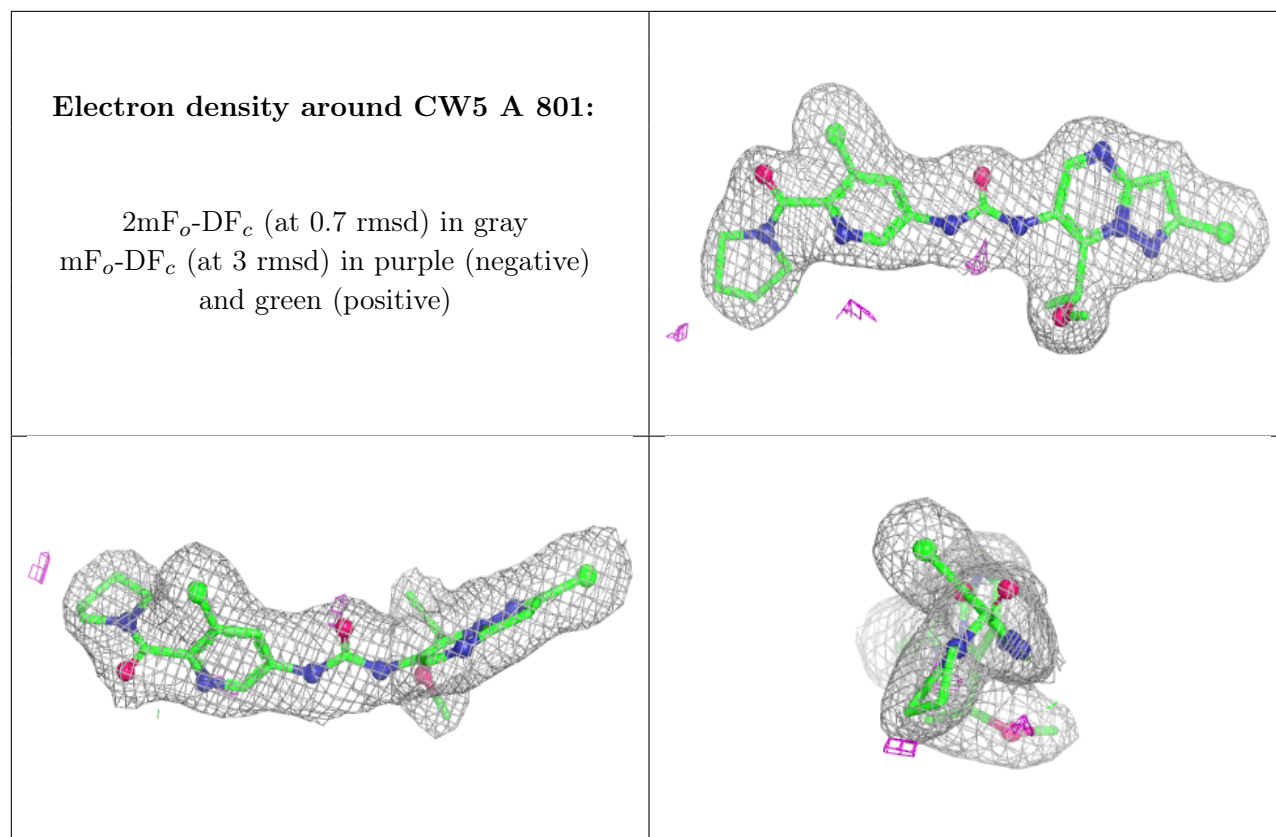
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	A	804	6/6	0.93	0.12	55,65,67,70	0
4	GOL	B	802	6/6	0.94	0.12	78,82,83,84	0
2	CW5	B	801	32/32	0.96	0.07	43,48,52,53	0
2	CW5	A	801	32/32	0.98	0.05	38,45,50,52	0

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.





6.5 Other polymers [i](#)

There are no such residues in this entry.