



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 05:04 PM UTC

PDB ID : 4JL1 / pdb_00004jl1
Title : Crystal structure of a bacterial fucosidase with a multivalent iminocyclitol inhibitor
Authors : Wright, D.W.; Davies, G.J.
Deposited on : 2013-03-12
Resolution : 1.68 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

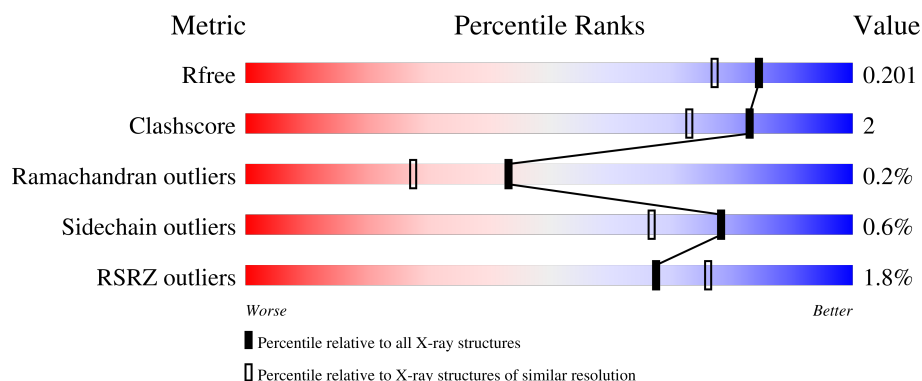
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.68 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	1054 (1.68-1.68)
Clashscore	190562	1078 (1.68-1.68)
Ramachandran outliers	187476	1068 (1.68-1.68)
Sidechain outliers	187428	1067 (1.68-1.68)
RSRZ outliers	180081	1055 (1.68-1.68)

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	450	 91% 6% ..
1	B	450	 92% 6% .

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
4	IMD	B	507	-	-	X	-

2 Entry composition [i](#)

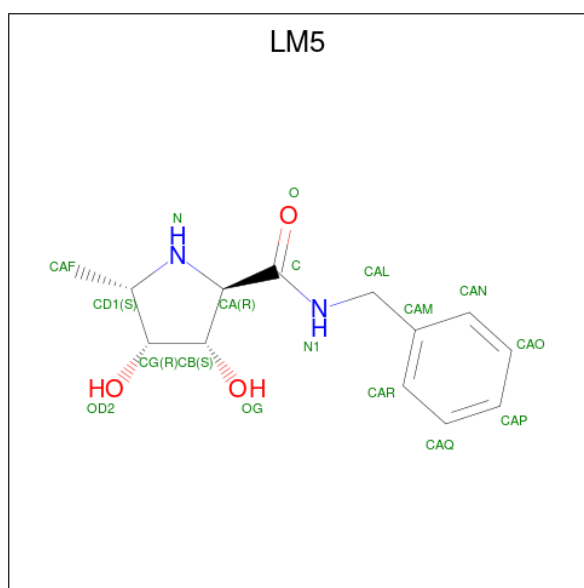
There are 6 unique types of molecules in this entry. The entry contains 8378 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 alpha-L-fucosidase.

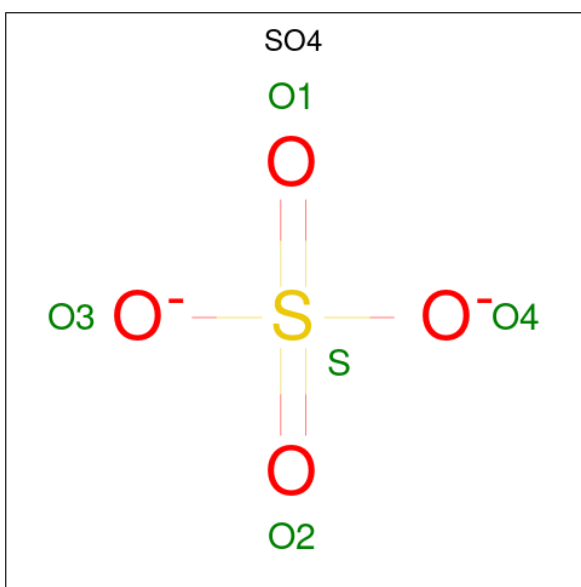
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	439	Total	C	N	O	S	0	13	0
			3609	2326	600	665	18			
1	B	439	Total	C	N	O	S	0	11	0
			3578	2313	587	659	19			

- Molecule 2 is (3S,4R,5S)-N-benzyl-3,4-dihydroxy-5-methyl-D-prolinamide (CCD ID: LM5) (formula: C₁₃H₁₈N₂O₃).



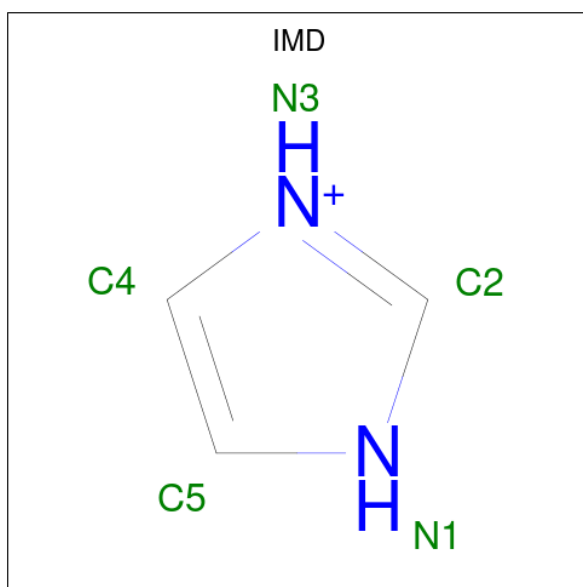
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	1
			36	26	4	6		
2	B	1	Total	C	N	O	0	1
			22	12	4	6		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is IMIDAZOLE (CCD ID: IMD) (formula: C₃H₅N₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			5	3	2		
4	A	1	Total	C	N	0	0
			5	3	2		
4	A	1	Total	C	N	0	0
			5	3	2		
4	B	1	Total	C	N	0	0
			5	3	2		
4	B	1	Total	C	N	0	0
			5	3	2		
4	B	1	Total	C	N	0	0
			5	3	2		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

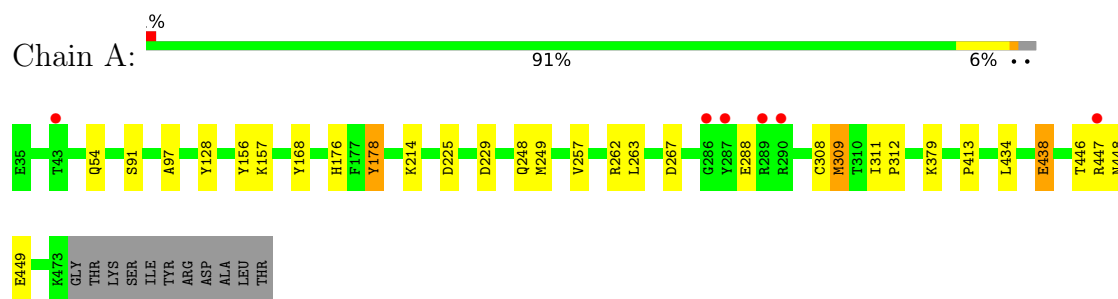
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	564	Total	O	0	0
			564	564		
6	B	491	Total	O	0	0
			491	491		

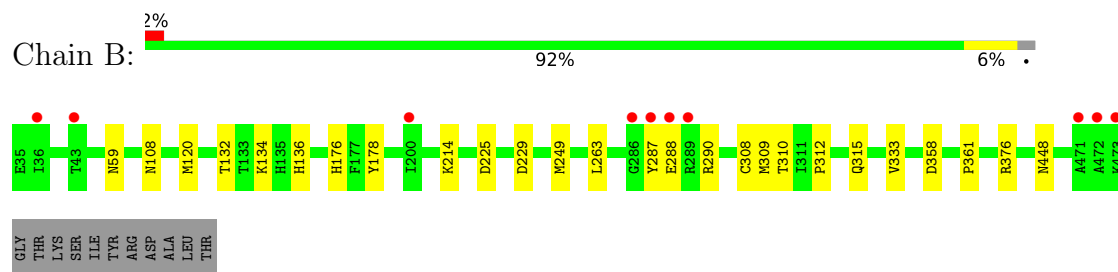
3 Residue-property plots [i](#)

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: alpha-L-fucosidase



• Molecule 1: alpha-L-fucosidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.38Å 96.05Å 97.20Å 90.00° 91.29° 90.00°	Depositor
Resolution (Å)	48.71 – 1.68 48.71 – 1.68	Depositor EDS
% Data completeness (in resolution range)	98.8 (48.71-1.68) 98.8 (48.71-1.68)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 1.68Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.165 , 0.192 0.175 , 0.201	Depositor DCC
R_{free} test set	7032 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	20.0	Xtriage
Anisotropy	0.669	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.020 for -h,l,k 0.027 for -h,-l,-k 0.036 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8378	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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: SO4, LM5, IMD, GOL

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	1.18	3/3749 (0.1%)	0.98	3/5089 (0.1%)
1	B	1.16	4/3719 (0.1%)	0.97	1/5055 (0.0%)
All	All	1.17	7/7468 (0.1%)	0.98	4/10144 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	134	LYS	CA-C	5.45	1.58	1.52
1	A	438	GLU	N-CA	5.43	1.53	1.46
1	B	310	THR	C-O	5.40	1.30	1.23
1	B	59	ASN	CA-C	5.34	1.59	1.52
1	A	257	VAL	N-CA	5.27	1.52	1.46
1	B	108	ASN	N-CA	-5.08	1.41	1.46
1	A	413	PRO	CA-C	-5.02	1.46	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	156	TYR	N-CA-C	5.54	117.39	111.36
1	A	97	ALA	N-CA-C	5.18	117.32	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	376	ARG	CG-CD-NE	-5.14	100.69	112.00
1	A	168	TYR	N-CA-C	-5.13	105.77	111.36

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	263	LEU	Peptide
1	B	263	LEU	Peptide

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	3609	0	3447	18	0
1	B	3578	0	3394	16	0
2	A	36	0	36	1	0
2	B	22	0	20	2	0
3	A	15	0	0	0	0
3	B	15	0	0	0	0
4	A	15	0	15	2	0
4	B	15	0	15	5	0
5	A	12	0	16	0	0
5	B	6	0	8	0	0
6	A	564	0	0	3	0
6	B	491	0	0	0	0
All	All	8378	0	6951	34	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 2.

All (34) 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:309[B]:MET:HE1	1:B:333:VAL:HG13	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288[B]:GLU:HG3	1:A:308[B]:CYS:SG	2.31	0.70
1:A:54[B]:GLN:NE2	6:A:678:HOH:O	2.18	0.63
1:A:157:LYS:HE2	6:A:1019:HOH:O	1.98	0.63
1:B:136:HIS:NE2	2:B:501[A]:LM5:O	2.25	0.63
1:B:361:PRO:HD3	4:B:507:IMD:H4	1.86	0.58
1:B:176:HIS:CG	1:B:225:ASP:HB3	2.39	0.58
1:A:214:LYS:HE3	1:A:249:MET:SD	2.48	0.53
1:B:120:MET:SD	4:B:505:IMD:H5	2.49	0.52
1:B:361:PRO:CD	4:B:507:IMD:H4	2.39	0.52
1:B:287[B]:TYR:HD1	1:B:290:ARG:O	1.92	0.52
1:B:361:PRO:HD3	4:B:507:IMD:C4	2.40	0.52
1:A:176:HIS:CG	1:A:225:ASP:HB3	2.44	0.52
1:B:214:LYS:HE3	1:B:249:MET:SD	2.50	0.51
1:A:446:THR:HG22	1:A:449:GLU:HB3	1.92	0.50
1:A:229:ASP:OD2	2:A:501[A]:LM5:H9	2.11	0.50
1:A:91:SER:HA	4:A:506:IMD:H5	1.93	0.50
1:A:288[B]:GLU:CG	1:A:308[B]:CYS:SG	2.99	0.49
1:B:178:TYR:C	1:B:178:TYR:CD1	2.91	0.48
1:A:178:TYR:C	1:A:178:TYR:CD1	2.92	0.48
1:B:288:GLU:HG2	1:B:308[A]:CYS:SG	2.54	0.48
1:A:379:LYS:HE2	1:A:434:LEU:HD11	1.96	0.47
1:A:288[B]:GLU:HG3	1:A:308[B]:CYS:HG	1.82	0.45
1:A:91:SER:CB	4:A:506:IMD:H5	2.49	0.43
1:A:309[A]:MET:HB3	1:A:309[A]:MET:HE3	1.72	0.43
1:A:311:ILE:HB	1:A:312:PRO:HD3	2.01	0.42
1:A:262[B]:ARG:NH1	1:A:288[B]:GLU:OE2	2.53	0.42
1:A:128:TYR:CD2	1:A:176:HIS:CE1	3.08	0.42
1:B:229:ASP:OD2	2:B:501[A]:LM5:H9	2.20	0.42
1:B:358:ASP:OD2	4:B:507:IMD:H2	2.21	0.41
1:B:312:PRO:HG2	1:B:315:GLN:HB2	2.02	0.41
1:B:132:THR:HA	1:B:178:TYR:HB3	2.02	0.41
1:A:248:GLN:NE2	6:A:1118:HOH:O	2.47	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	450/450 (100%)	438 (97%)	9 (2%)	3 (1%)	18	5
1	B	448/450 (100%)	441 (98%)	7 (2%)	0	100	100
All	All	898/900 (100%)	879 (98%)	16 (2%)	3 (0%)	43	21

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	447[A]	ARG
1	A	447[B]	ARG
1	A	448	ASN

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	370/383 (97%)	365 (99%)	5 (1%)	59	36
1	B	363/383 (95%)	363 (100%)	0	100	100
All	All	733/766 (96%)	728 (99%)	5 (1%)	78	62

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

Mol	Chain	Res	Type
1	A	178	TYR
1	A	267	ASP
1	A	309[A]	MET
1	A	309[B]	MET
1	A	438	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	354	GLN
1	A	411	ASN
1	B	411	ASN

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 ⓘ

19 ligands are modelled in this entry.

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	SO4	B	503	-	4,4,4	0.47	0	6,6,6	0.51	0
3	SO4	B	502	-	4,4,4	0.65	0	6,6,6	0.54	0
5	GOL	A	509	-	5,5,5	0.51	0	5,5,5	0.86	0
5	GOL	A	508	-	5,5,5	0.55	0	5,5,5	0.80	0
2	LM5	B	501[B]	-	10,11,19	2.59	6 (60%)	11,16,26	1.26	2 (18%)
3	SO4	B	504	-	4,4,4	0.46	0	6,6,6	0.27	0
4	IMD	A	505	-	5,5,5	1.14	1 (20%)	5,5,5	0.19	0
4	IMD	B	507	-	5,5,5	0.85	0	5,5,5	0.05	0
5	GOL	B	508	-	5,5,5	0.38	0	5,5,5	0.71	0
4	IMD	A	507	-	5,5,5	0.47	0	5,5,5	0.68	0
2	LM5	A	501[A]	-	18,19,19	1.75	4 (22%)	21,26,26	1.30	3 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	A	504	-	4,4,4	0.24	0	6,6,6	0.59	0
4	IMD	B	506	-	5,5,5	0.75	0	5,5,5	0.24	0
4	IMD	B	505	-	5,5,5	1.14	0	5,5,5	0.59	0
3	SO4	A	503	-	4,4,4	0.50	0	6,6,6	0.49	0
2	LM5	B	501[A]	-	10,11,19	1.62	2 (20%)	11,16,26	1.18	1 (9%)
2	LM5	A	501[B]	-	18,19,19	1.82	3 (16%)	21,26,26	1.05	1 (4%)
3	SO4	A	502	-	4,4,4	0.55	0	6,6,6	0.39	0
4	IMD	A	506	-	5,5,5	0.66	0	5,5,5	0.91	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
2	LM5	A	501[B]	-	-	4/9/25/25	0/2/2/2
5	GOL	A	509	-	-	0/4/4/4	-
4	IMD	B	506	-	-	-	0/1/1/1
5	GOL	A	508	-	-	2/4/4/4	-
2	LM5	B	501[B]	-	-	2/3/20/25	0/1/1/2
4	IMD	A	505	-	-	-	0/1/1/1
4	IMD	B	507	-	-	-	0/1/1/1
5	GOL	B	508	-	-	4/4/4/4	-
4	IMD	B	505	-	-	-	0/1/1/1
4	IMD	A	507	-	-	-	0/1/1/1
2	LM5	A	501[A]	-	-	2/9/25/25	0/2/2/2
4	IMD	A	506	-	-	-	0/1/1/1
2	LM5	B	501[A]	-	-	2/3/20/25	0/1/1/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501[A]	LM5	CAL-CAM	-5.24	1.39	1.51
2	A	501[B]	LM5	CAL-CAM	-4.45	1.41	1.51
2	B	501[B]	LM5	CA-C	4.29	1.59	1.52
2	B	501[B]	LM5	OD2-CG	4.17	1.53	1.43
2	A	501[B]	LM5	CAL-N1	3.59	1.53	1.46
2	B	501[A]	LM5	CA-C	3.41	1.57	1.52
2	A	501[B]	LM5	CA-C	3.31	1.61	1.52
2	B	501[B]	LM5	OG-CB	3.18	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501[B]	LM5	CA-N	2.99	1.50	1.46
2	A	501[A]	LM5	CAL-N1	2.58	1.51	1.46
2	A	501[A]	LM5	CA-C	2.42	1.59	1.52
2	B	501[B]	LM5	C-N1	2.40	1.38	1.32
2	B	501[A]	LM5	OD2-CG	2.35	1.48	1.43
2	A	501[A]	LM5	CA-N	2.14	1.49	1.46
4	A	505	IMD	C2-N1	2.09	1.42	1.34
2	B	501[B]	LM5	CG-CD1	2.07	1.56	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501[A]	LM5	CAM-CAL-N1	3.23	119.89	113.07
2	B	501[A]	LM5	CA-C-N1	2.89	121.57	117.02
2	B	501[B]	LM5	O-C-CA	2.73	124.03	119.94
2	A	501[A]	LM5	CAL-CAM-CAN	2.58	126.20	120.94
2	A	501[A]	LM5	CAL-CAM-CAR	-2.52	115.79	120.94
2	A	501[B]	LM5	CA-C-N1	2.09	119.83	116.38
2	B	501[B]	LM5	O-C-N1	-2.04	119.44	123.04

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501[B]	LM5	N1-C-CA-N
2	A	501[B]	LM5	N1-C-CA-CB
2	A	501[B]	LM5	O-C-CA-N
2	B	501[A]	LM5	O-C-CA-N
2	B	501[B]	LM5	N1-C-CA-CB
2	B	501[B]	LM5	O-C-CA-CB
5	A	508	GOL	C1-C2-C3-O3
5	A	508	GOL	O2-C2-C3-O3
5	B	508	GOL	O1-C1-C2-O2
5	B	508	GOL	O1-C1-C2-C3
5	B	508	GOL	C1-C2-C3-O3
2	B	501[A]	LM5	O-C-CA-CB
2	A	501[B]	LM5	O-C-CA-CB
2	A	501[A]	LM5	N1-C-CA-N
5	B	508	GOL	O2-C2-C3-O3
2	A	501[A]	LM5	O-C-CA-N

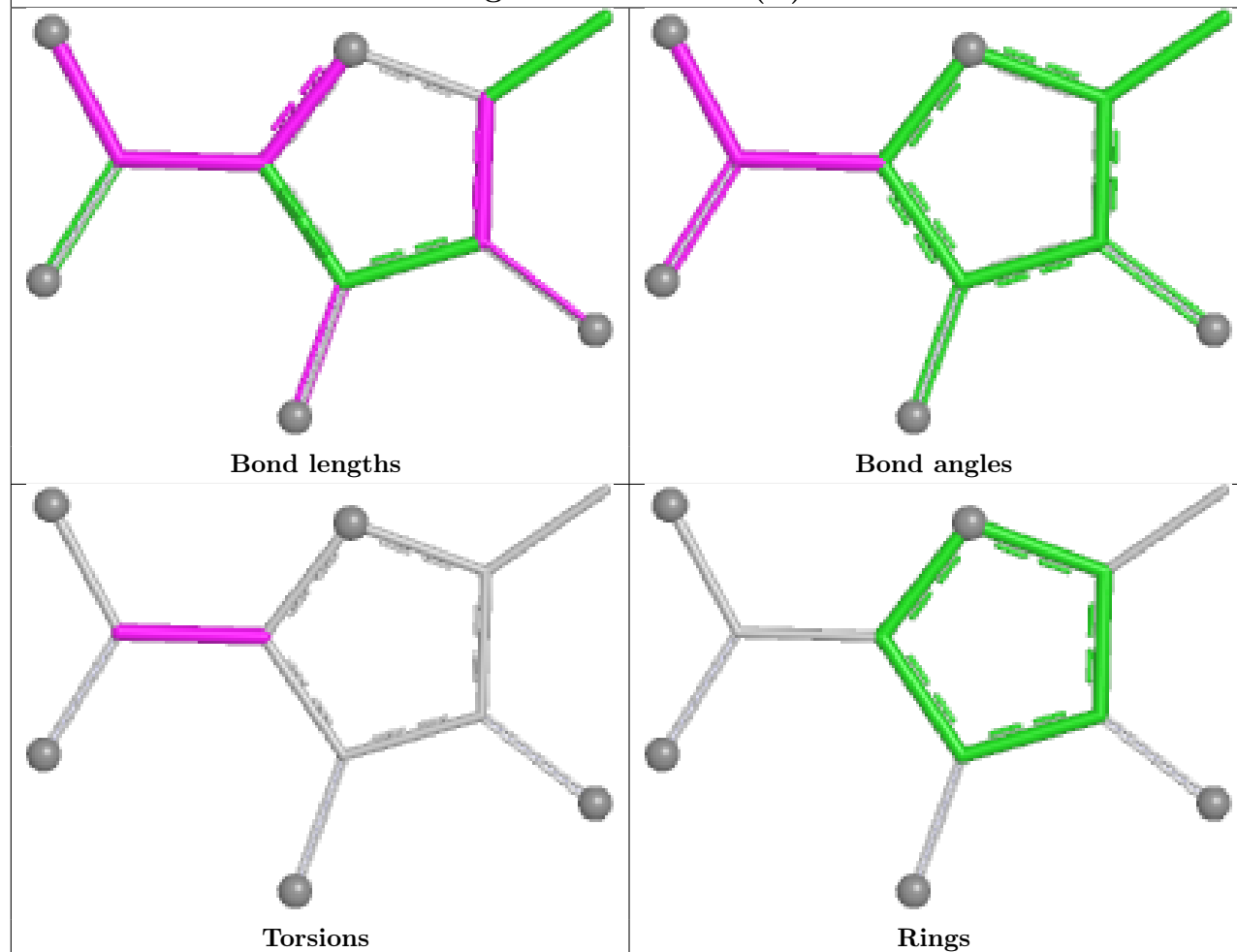
There are no ring outliers.

5 monomers are involved in 10 short contacts:

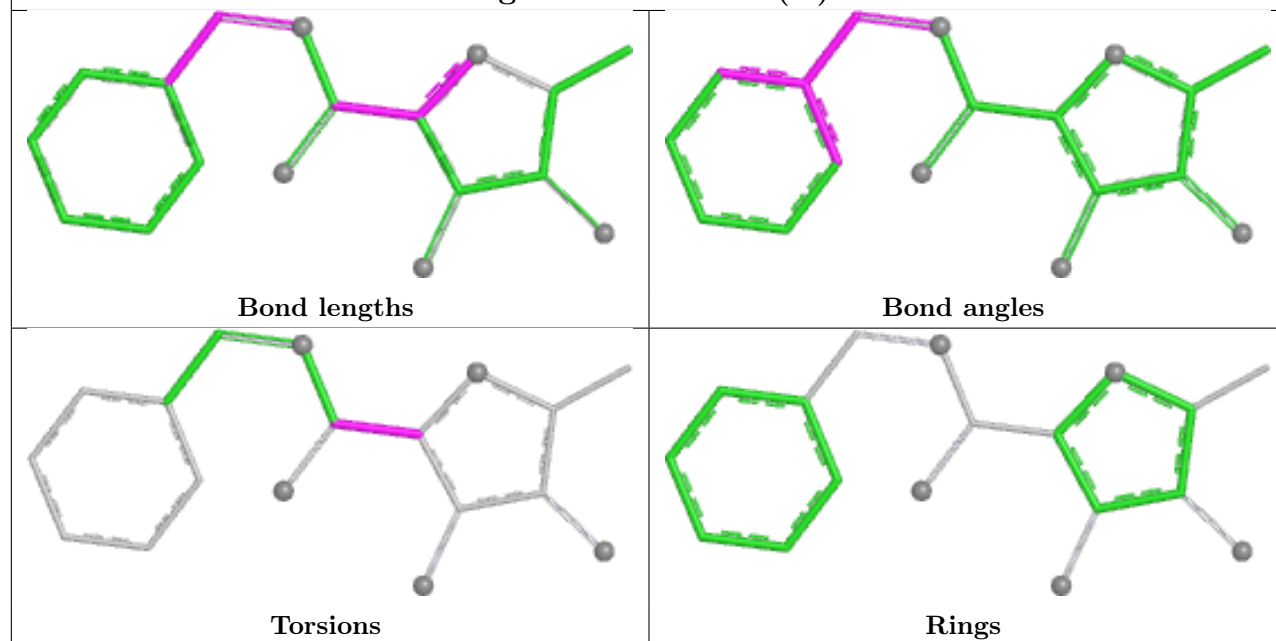
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	507	IMD	4	0
2	A	501[A]	LM5	1	0
4	B	505	IMD	1	0
2	B	501[A]	LM5	2	0
4	A	506	IMD	2	0

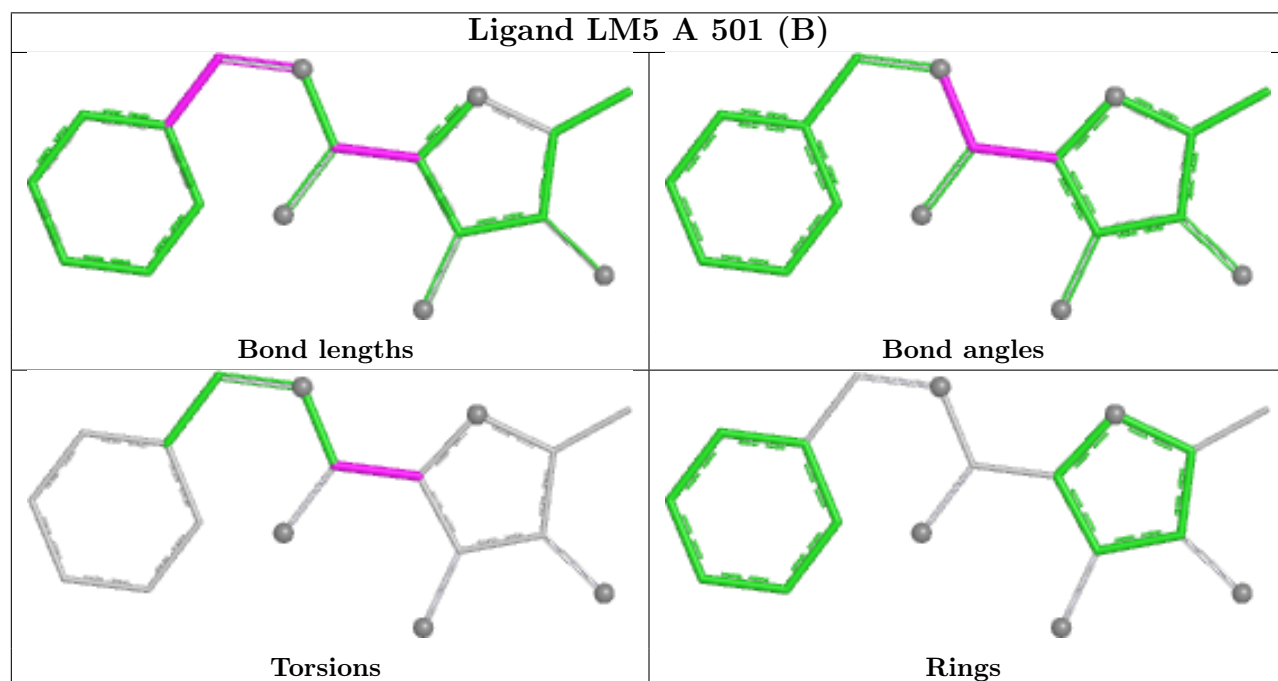
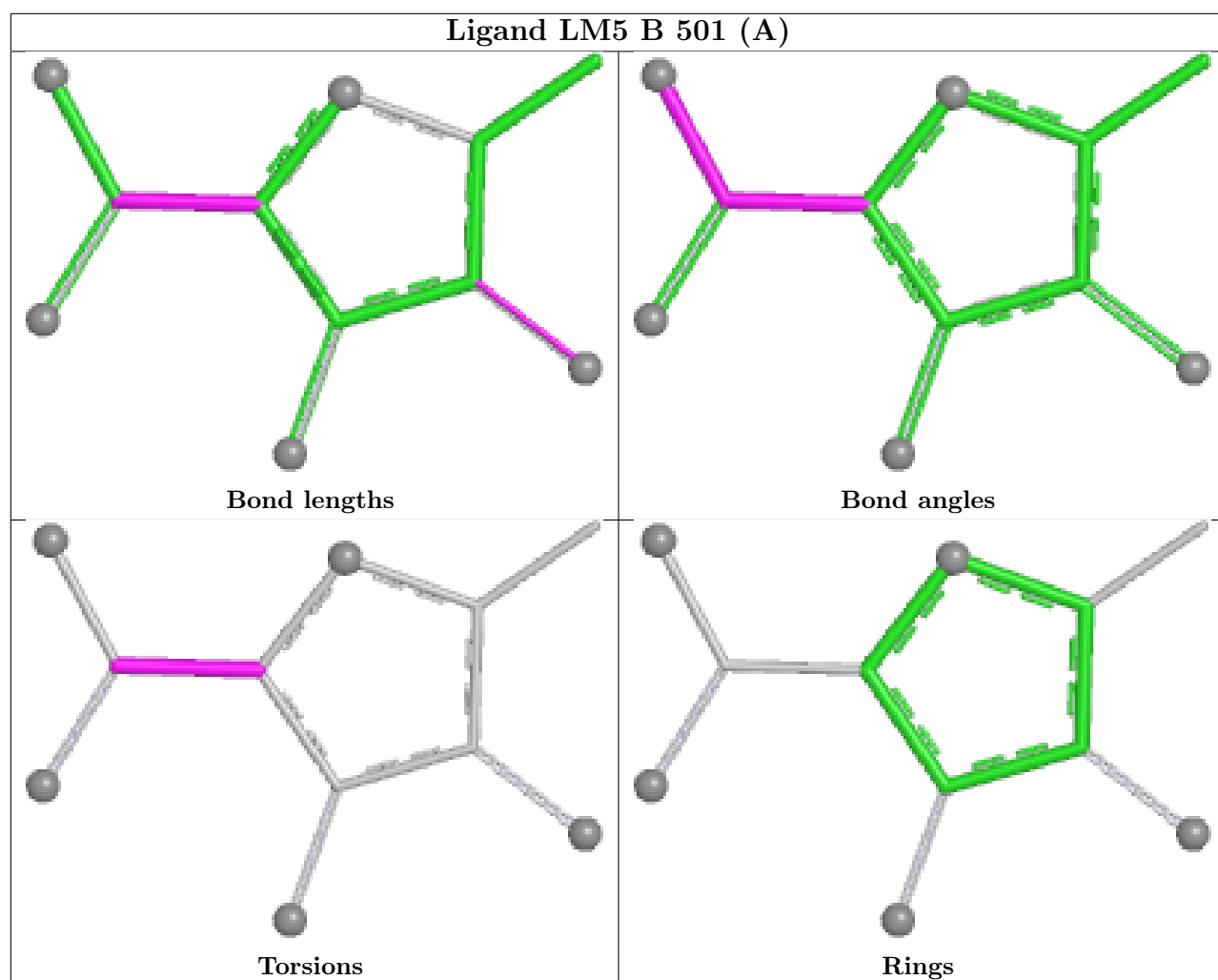
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

Ligand LM5 B 501 (B)



Ligand LM5 A 501 (A)





5.7 Other polymers

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 [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, 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	439/450 (97%)	-0.19	6 (1%) 73 81	10, 20, 37, 66	13 (2%)
1	B	439/450 (97%)	-0.06	10 (2%) 61 68	12, 22, 40, 66	11 (2%)
All	All	878/900 (97%)	-0.13	16 (1%) 67 76	10, 21, 39, 66	24 (2%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	472	ALA	4.5
1	B	287[A]	TYR	3.7
1	A	447[A]	ARG	3.7
1	B	473	LYS	3.6
1	A	43	THR	3.5
1	B	289	ARG	3.3
1	B	43	THR	3.2
1	B	286	GLY	2.9
1	A	286	GLY	2.9
1	B	36	ILE	2.9
1	B	471	ALA	2.8
1	B	288	GLU	2.8
1	A	287	TYR	2.7
1	B	200	ILE	2.4
1	A	289	ARG	2.2
1	A	290	ARG	2.1

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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

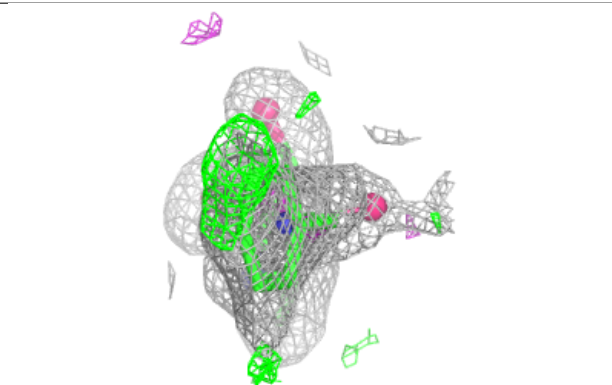
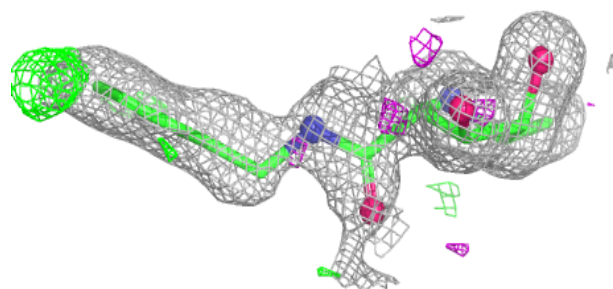
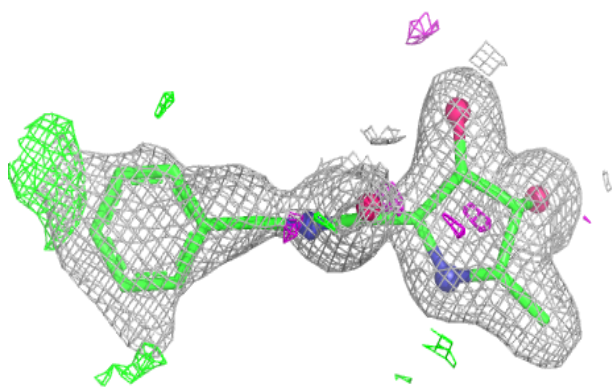
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	IMD	A	507	5/5	0.56	0.25	70,71,73,74	0
4	IMD	B	507	5/5	0.66	0.24	55,56,62,63	0
4	IMD	A	506	5/5	0.71	0.24	55,58,60,61	0
4	IMD	B	506	5/5	0.79	0.21	54,59,61,61	0
5	GOL	B	508	6/6	0.83	0.14	60,64,66,69	0
5	GOL	A	509	6/6	0.86	0.16	32,50,56,58	0
3	SO4	A	504	5/5	0.88	0.19	41,42,45,46	5
5	GOL	A	508	6/6	0.89	0.16	24,43,52,56	0
2	LM5	A	501[B]	18/18	0.89	0.15	23,33,49,51	18
2	LM5	A	501[A]	18/18	0.89	0.15	23,32,59,60	18
2	LM5	B	501[A]	11/18	0.90	0.11	26,29,35,39	11
3	SO4	B	504	5/5	0.90	0.10	70,81,82,85	0
2	LM5	B	501[B]	11/18	0.90	0.11	17,19,21,24	11
3	SO4	B	503	5/5	0.91	0.14	22,26,36,37	5
3	SO4	A	503	5/5	0.91	0.09	52,61,69,70	0
3	SO4	A	502	5/5	0.91	0.11	48,49,59,65	0
3	SO4	B	502	5/5	0.94	0.11	30,45,53,54	0
4	IMD	A	505	5/5	0.95	0.08	21,21,25,26	0
4	IMD	B	505	5/5	0.98	0.07	18,20,23,26	0

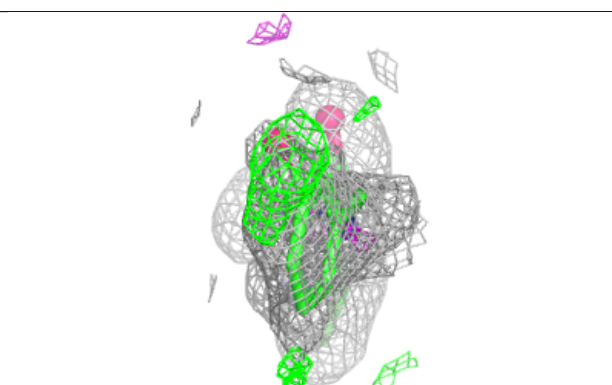
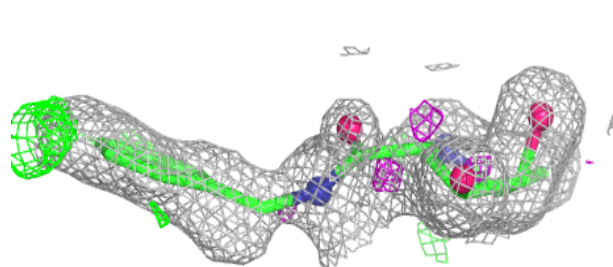
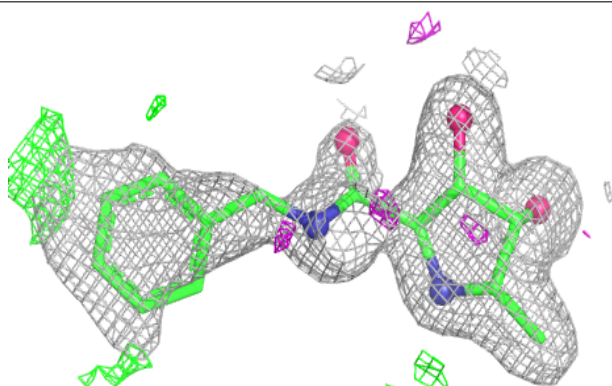
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LM5 A 501 (B):

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

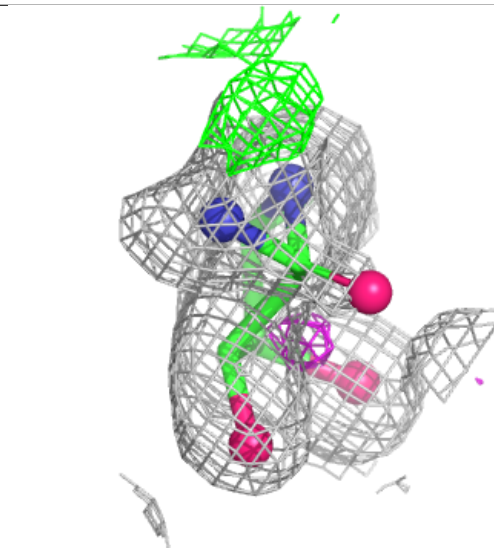
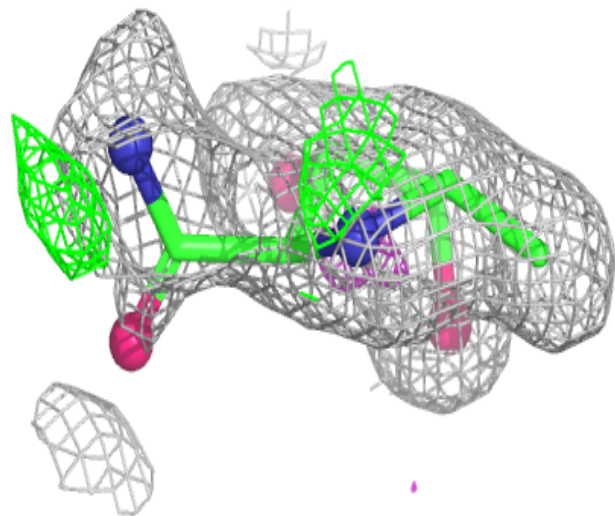
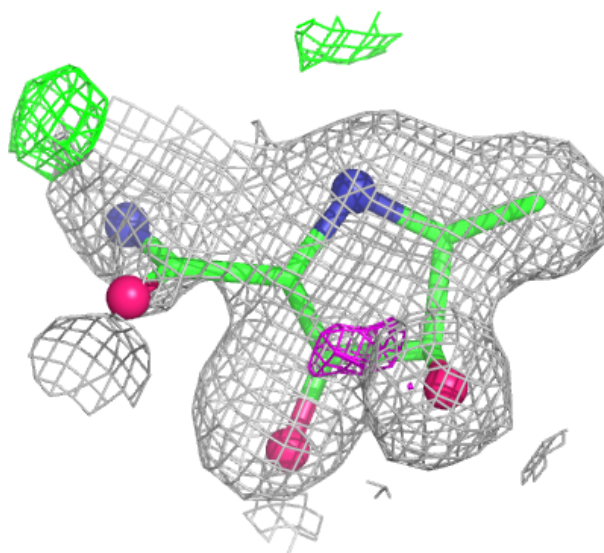
**Electron density around LM5 A 501 (A):**

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



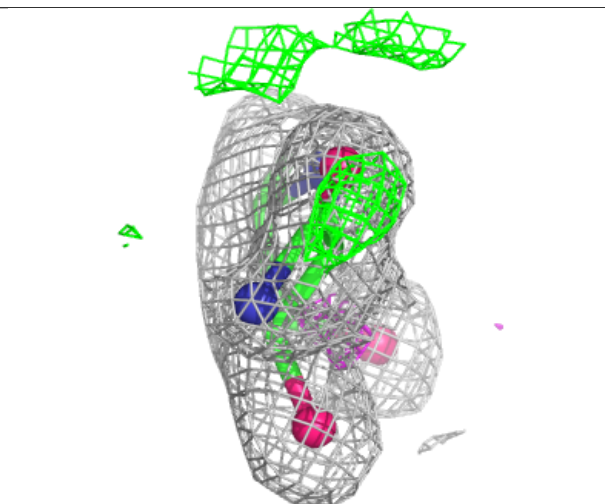
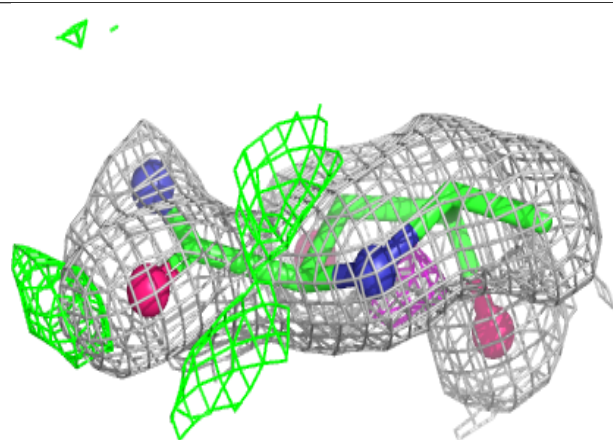
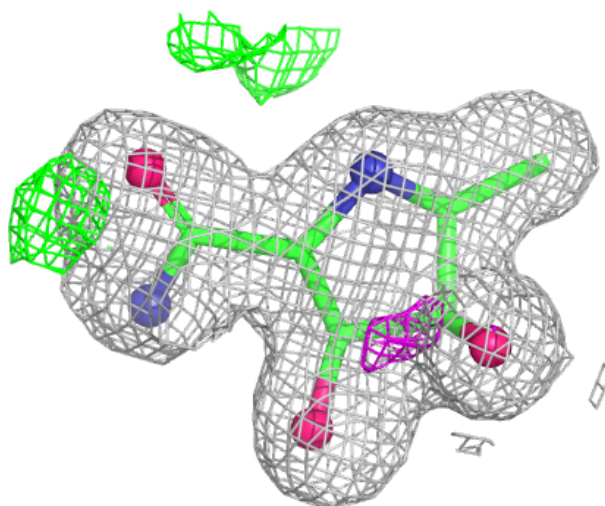
Electron density around LM5 B 501 (A):

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



Electron density around LM5 B 501 (B):

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



6.5 Other polymers ⓘ

There are no such residues in this entry.