



# Full wwPDB X-ray Structure Validation Report ⓘ

May 5, 2025 – 01:45 pm BST

PDB ID : 9F3L / pdb\_00009f3l  
Title : Crystal structure of Kluyveromyces lactis glucokinase mutant H304Q in complex with mannose  
Authors : Weisse, R.H.; Strater, N.  
Deposited on : 2024-04-25  
Resolution : 2.48 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 Phenix2.0rc1
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

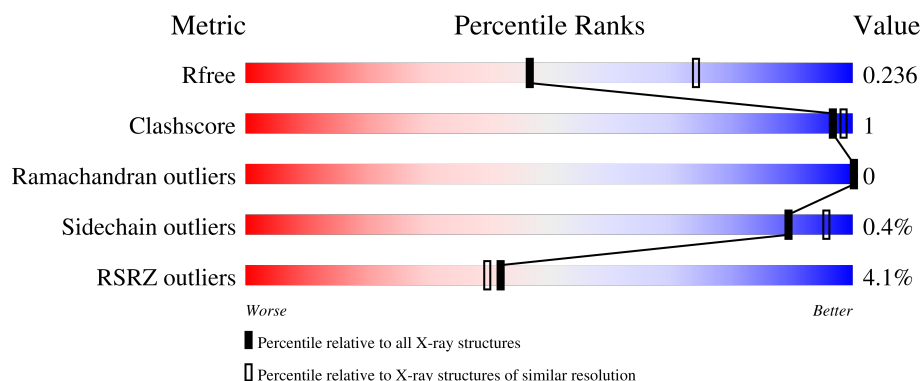
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.48 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	7106 (2.50-2.46)
Clashscore	180529	7991 (2.50-2.46)
Ramachandran outliers	177936	7888 (2.50-2.46)
Sidechain outliers	177891	7890 (2.50-2.46)
RSRZ outliers	164620	7106 (2.50-2.46)

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  $\geq 3$ , 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	481	<div> <div>4%</div> <div>99%</div> </div>
1	B	481	<div> <div>5%</div> <div>96%</div> </div>
1	C	481	<div> <div>5%</div> <div>96%</div> </div>
1	D	481	<div> <div>3%</div> <div>98%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 30430 atoms, of which 15031 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.

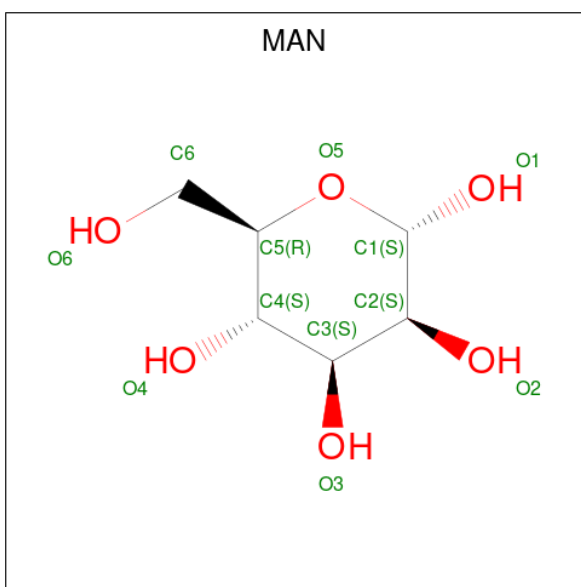
- Molecule 1 is a protein called Glucokinase-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	480	Total	C	H	N	O	S	0	1	0
			7507	2383	3734	641	729	20			
1	B	480	Total	C	H	N	O	S	0	1	0
			7510	2385	3735	642	728	20			
1	C	480	Total	C	H	N	O	S	0	0	0
			7497	2380	3729	640	728	20			
1	D	480	Total	C	H	N	O	S	0	3	0
			7529	2389	3747	642	730	21			

There are 4 discrepancies between the modelled and reference sequences:

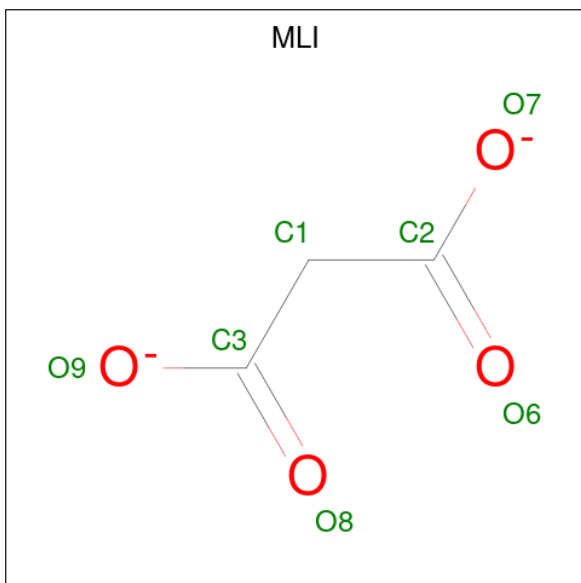
Chain	Residue	Modelled	Actual	Comment	Reference
A	304	GLN	HIS	engineered mutation	UNP Q6CUZ3
B	304	GLN	HIS	engineered mutation	UNP Q6CUZ3
C	304	GLN	HIS	engineered mutation	UNP Q6CUZ3
D	304	GLN	HIS	engineered mutation	UNP Q6CUZ3

- Molecule 2 is alpha-D-mannopyranose (CCD ID: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			24	6	12	6		
2	B	1	Total	C	H	O	0	0
			24	6	12	6		
2	C	1	Total	C	H	O	0	0
			24	6	12	6		
2	D	1	Total	C	H	O	0	0
			24	6	12	6		

- Molecule 3 is MALONATE ION (CCD ID: MLI) (formula:  $C_3H_2O_4$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C H O 9 3 2 4	0	0
3	A	1	Total C H O 9 3 2 4	0	0
3	A	1	Total C H O 9 3 2 4	0	0
3	B	1	Total C H O 9 3 2 4	0	0
3	B	1	Total C H O 9 3 2 4	0	0
3	B	1	Total C H O 9 3 2 4	0	0
3	B	1	Total C H O 9 3 2 4	0	0
3	B	1	Total C H O 9 3 2 4	0	0
3	C	1	Total C H O 9 3 2 4	0	0
3	C	1	Total C H O 9 3 2 4	0	0
3	C	1	Total C H O 9 3 2 4	0	0
3	C	1	Total C H O 9 3 2 4	0	0
3	C	1	Total C H O 9 3 2 4	0	0
3	C	1	Total C H O 9 3 2 4	0	0
3	C	1	Total C H O 9 3 2 4	0	0
3	D	1	Total C H O 9 3 2 4	0	0
3	D	1	Total C H O 9 3 2 4	0	0
3	D	1	Total C H O 9 3 2 4	0	0
3	D	1	Total C H O 9 3 2 4	0	0
3	D	1	Total C H O 9 3 2 4	0	0
3	D	1	Total C H O 9 3 2 4	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	13	Total O 13 13	0	0

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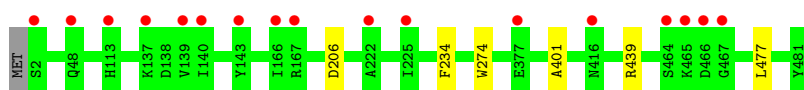
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	20	Total 20	O 20	0	0
4	C	23	Total 23	O 23	0	0
4	D	64	Total 64	O 64	0	1

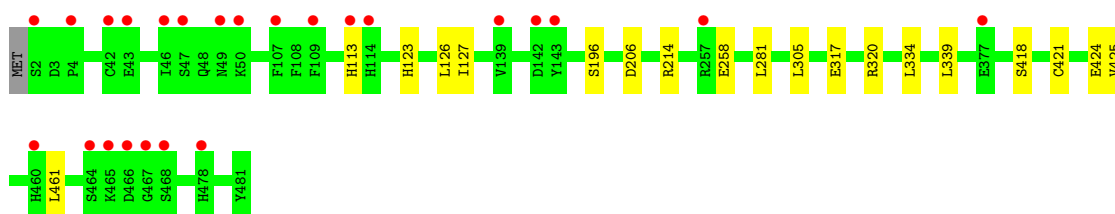
### 3 Residue-property plots [i](#)

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.

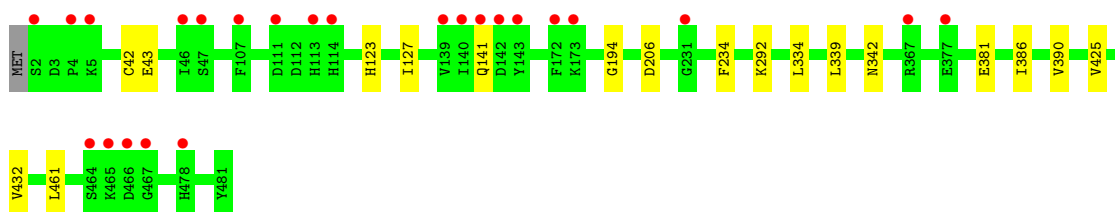
- Molecule 1: Glucokinase-1



- Molecule 1: Glucokinase-1



- Molecule 1: Glucokinase-1



- Molecule 1: Glucokinase-1



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	202.41Å 88.34Å 212.45Å 90.00° 89.92° 90.00°	Depositor
Resolution (Å)	64.28 – 2.48 64.28 – 2.48	Depositor EDS
% Data completeness (in resolution range)	97.5 (64.28-2.48) 97.6 (64.28-2.48)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.25 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.211 , 0.237 0.210 , 0.236	Depositor DCC
$R_{free}$ test set	6627 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	66.1	Xtriage
Anisotropy	0.327	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 62.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for -l,k,h 0.000 for -l,-k,-h 0.000 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	30430	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MLI, MAN

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	0.18	0/3849	0.34	0/5207
1	B	0.17	0/3852	0.34	0/5211
1	C	0.16	0/3841	0.32	0/5196
1	D	0.24	0/3864	0.39	0/5227
All	All	0.19	0/15406	0.35	0/20841

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [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	3773	3734	3733	4	0
1	B	3775	3735	3734	9	0
1	C	3768	3729	3727	9	0
1	D	3782	3747	3746	5	0
2	A	12	12	12	0	0
2	B	12	12	12	0	0
2	C	12	12	12	0	0
2	D	12	12	12	0	0
3	A	21	6	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	28	8	8	0	0
3	C	42	12	12	0	0
3	D	42	12	12	0	0
4	A	13	0	0	0	0
4	B	20	0	0	0	0
4	C	23	0	0	0	0
4	D	64	0	0	0	0
All	All	15399	15031	15026	26	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 1.

All (26) 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:D:74:ALA:HB3	1:D:85[A]:CYS:SG	2.38	0.63
1:B:418:SER:HG	1:B:421:CYS:HG	1.41	0.62
1:B:317:GLU:OE2	1:B:320:ARG:NH1	2.39	0.56
1:C:334:LEU:HD22	1:C:339:LEU:HD12	1.87	0.55
1:C:425:VAL:HB	1:C:461:LEU:HD23	1.89	0.54
1:C:141:GLN:NE2	1:C:194:GLY:O	2.35	0.53
1:C:42:CYS:O	1:C:43:GLU:HB2	2.09	0.53
1:D:53:PRO:O	1:D:251:LYS:NZ	2.43	0.52
1:D:74:ALA:HB3	1:D:85[A]:CYS:HG	1.76	0.50
1:B:334:LEU:HD22	1:B:339:LEU:HD12	1.95	0.49
1:B:123:HIS:NE2	1:B:127:ILE:HD11	2.30	0.47
1:B:126:LEU:HD13	1:C:381:GLU:HG3	1.97	0.46
1:B:214:ARG:NE	1:B:424:GLU:OE2	2.42	0.45
1:D:425:VAL:HB	1:D:461:LEU:HD23	1.99	0.44
1:A:477:LEU:C	1:A:477:LEU:HD23	2.43	0.44
1:B:206:ASP:OD1	1:B:206:ASP:N	2.50	0.43
1:A:234:PHE:CE1	1:A:401:ALA:HB1	2.55	0.42
1:B:425:VAL:HB	1:B:461:LEU:HD23	2.01	0.42
1:B:281:LEU:HD21	1:B:305:LEU:HD22	2.01	0.42
1:D:63:PRO:HD3	1:D:212:LEU:HD22	2.01	0.41
1:A:274:TRP:C	1:A:274:TRP:CD1	2.99	0.41
1:C:234:PHE:HB2	1:C:432:VAL:HB	2.02	0.41
1:C:123:HIS:NE2	1:C:127:ILE:HD11	2.36	0.40
1:C:386:ILE:O	1:C:390:VAL:HG23	2.21	0.40
1:C:206:ASP:OD1	1:C:206:ASP:N	2.54	0.40
1:A:206:ASP:N	1:A:206:ASP:OD1	2.54	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	479/481 (100%)	463 (97%)	16 (3%)	0	100	100
1	B	479/481 (100%)	463 (97%)	16 (3%)	0	100	100
1	C	478/481 (99%)	459 (96%)	19 (4%)	0	100	100
1	D	481/481 (100%)	465 (97%)	16 (3%)	0	100	100
All	All	1917/1924 (100%)	1850 (96%)	67 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	422/422 (100%)	421 (100%)	1 (0%)	92	97
1	B	422/422 (100%)	419 (99%)	3 (1%)	81	92
1	C	421/422 (100%)	419 (100%)	2 (0%)	86	94
1	D	424/422 (100%)	423 (100%)	1 (0%)	92	97
All	All	1689/1688 (100%)	1682 (100%)	7 (0%)	89	95

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	439	ARG
1	B	113	HIS
1	B	196	SER
1	B	258	GLU
1	C	292	LYS
1	C	342	ASN
1	D	305	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	B	16	GLN
1	B	114	HIS
1	B	141	GLN
1	B	188	GLN
1	B	283	HIS
1	B	434	HIS
1	C	16	GLN
1	C	48	GLN
1	C	49	ASN
1	C	129	HIS
1	C	283	HIS
1	D	66	GLN
1	D	114	HIS
1	D	141	GLN
1	D	180	GLN
1	D	283	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

23 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	MLI	D	506	-	6,6,6	1.36	0	7,7,7	0.95	0
3	MLI	C	506	-	6,6,6	1.28	0	7,7,7	0.96	0
3	MLI	C	502	-	6,6,6	1.30	0	7,7,7	0.96	0
2	MAN	B	501	-	12,12,12	0.21	0	17,17,17	0.76	0
3	MLI	A	504	-	6,6,6	1.31	0	7,7,7	1.00	0
2	MAN	D	501	-	12,12,12	0.32	0	17,17,17	0.73	0
3	MLI	D	502	-	6,6,6	1.37	0	7,7,7	1.00	0
3	MLI	D	505	-	6,6,6	1.39	0	7,7,7	0.92	0
3	MLI	C	503	-	6,6,6	1.29	0	7,7,7	1.02	0
3	MLI	B	504	-	6,6,6	1.35	0	7,7,7	0.94	0
3	MLI	B	503	-	6,6,6	1.25	0	7,7,7	1.01	0
3	MLI	D	504	-	6,6,6	1.39	0	7,7,7	0.93	0
2	MAN	C	501	-	12,12,12	0.25	0	17,17,17	0.66	0
3	MLI	D	503	-	6,6,6	1.38	0	7,7,7	0.92	0
3	MLI	B	502	-	6,6,6	1.36	0	7,7,7	0.91	0
3	MLI	C	507	-	6,6,6	1.32	0	7,7,7	0.92	0
3	MLI	B	505	-	6,6,6	1.26	0	7,7,7	0.97	0
3	MLI	D	507	-	6,6,6	1.24	0	7,7,7	1.02	0
2	MAN	A	501	-	12,12,12	0.35	0	17,17,17	0.67	0
3	MLI	A	503	-	6,6,6	1.40	0	7,7,7	0.95	0
3	MLI	C	505	-	6,6,6	1.40	0	7,7,7	0.91	0
3	MLI	C	504	-	6,6,6	1.33	0	7,7,7	0.95	0
3	MLI	A	502	-	6,6,6	1.35	0	7,7,7	0.99	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
3	MLI	D	506	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MLI	C	506	-	-	2/4/4/4	-
3	MLI	C	502	-	-	2/4/4/4	-
2	MAN	B	501	-	-	0/2/22/22	0/1/1/1
3	MLI	A	504	-	-	4/4/4/4	-
2	MAN	D	501	-	-	0/2/22/22	0/1/1/1
3	MLI	D	502	-	-	3/4/4/4	-
3	MLI	D	505	-	-	2/4/4/4	-
3	MLI	C	503	-	-	0/4/4/4	-
3	MLI	B	504	-	-	4/4/4/4	-
3	MLI	B	503	-	-	0/4/4/4	-
3	MLI	D	504	-	-	2/4/4/4	-
2	MAN	C	501	-	-	0/2/22/22	0/1/1/1
3	MLI	D	503	-	-	2/4/4/4	-
3	MLI	B	502	-	-	2/4/4/4	-
3	MLI	C	507	-	-	0/4/4/4	-
3	MLI	B	505	-	-	2/4/4/4	-
3	MLI	D	507	-	-	3/4/4/4	-
2	MAN	A	501	-	-	0/2/22/22	0/1/1/1
3	MLI	A	503	-	-	2/4/4/4	-
3	MLI	C	505	-	-	2/4/4/4	-
3	MLI	C	504	-	-	4/4/4/4	-
3	MLI	A	502	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	504	MLI	C2-C1-C3-O8
3	B	504	MLI	C2-C1-C3-O9
3	D	505	MLI	C3-C1-C2-O7
3	B	502	MLI	C3-C1-C2-O7
3	C	502	MLI	C2-C1-C3-O9
3	C	504	MLI	C2-C1-C3-O8
3	C	504	MLI	C2-C1-C3-O9
3	A	504	MLI	C3-C1-C2-O7
3	C	504	MLI	C3-C1-C2-O7

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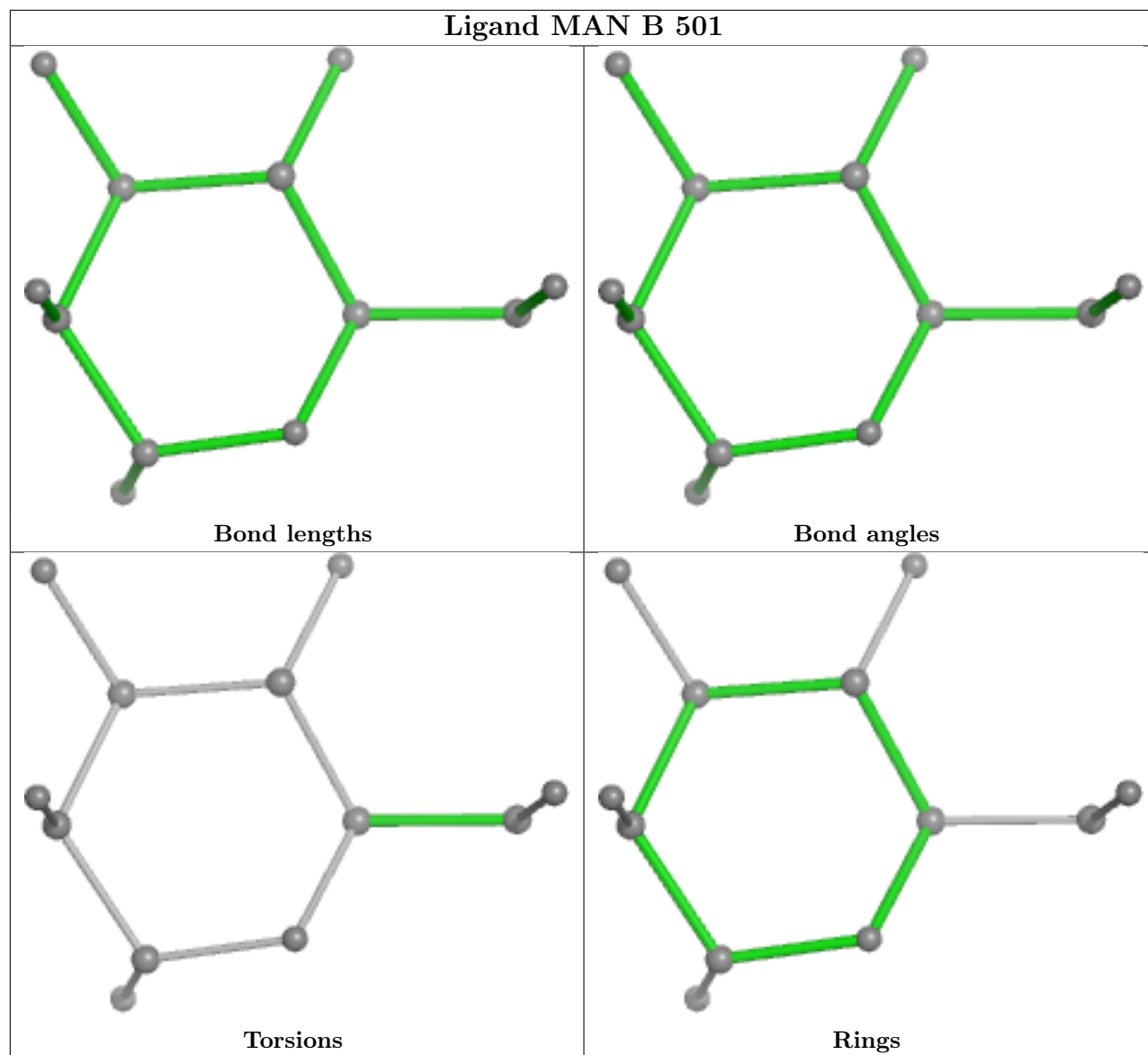
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Mol	Chain	Res	Type	Atoms
3	C	505	MLI	C2-C1-C3-O9
3	C	506	MLI	C2-C1-C3-O9
3	D	502	MLI	C3-C1-C2-O6
3	D	502	MLI	C3-C1-C2-O7
3	D	503	MLI	C3-C1-C2-O7
3	D	504	MLI	C2-C1-C3-O9
3	B	502	MLI	C3-C1-C2-O6
3	C	502	MLI	C2-C1-C3-O8
3	C	504	MLI	C3-C1-C2-O6
3	C	505	MLI	C2-C1-C3-O8
3	C	506	MLI	C2-C1-C3-O8
3	D	507	MLI	C3-C1-C2-O7
3	A	504	MLI	C3-C1-C2-O6
3	D	504	MLI	C2-C1-C3-O8
3	D	505	MLI	C3-C1-C2-O6
3	D	507	MLI	C3-C1-C2-O6
3	B	505	MLI	C2-C1-C3-O8
3	D	503	MLI	C3-C1-C2-O6
3	B	504	MLI	C3-C1-C2-O6
3	B	505	MLI	C2-C1-C3-O9
3	A	503	MLI	C3-C1-C2-O6
3	A	503	MLI	C3-C1-C2-O7
3	B	504	MLI	C3-C1-C2-O7
3	A	504	MLI	C2-C1-C3-O8
3	A	504	MLI	C2-C1-C3-O9
3	D	502	MLI	C2-C1-C3-O9
3	D	507	MLI	C2-C1-C3-O8

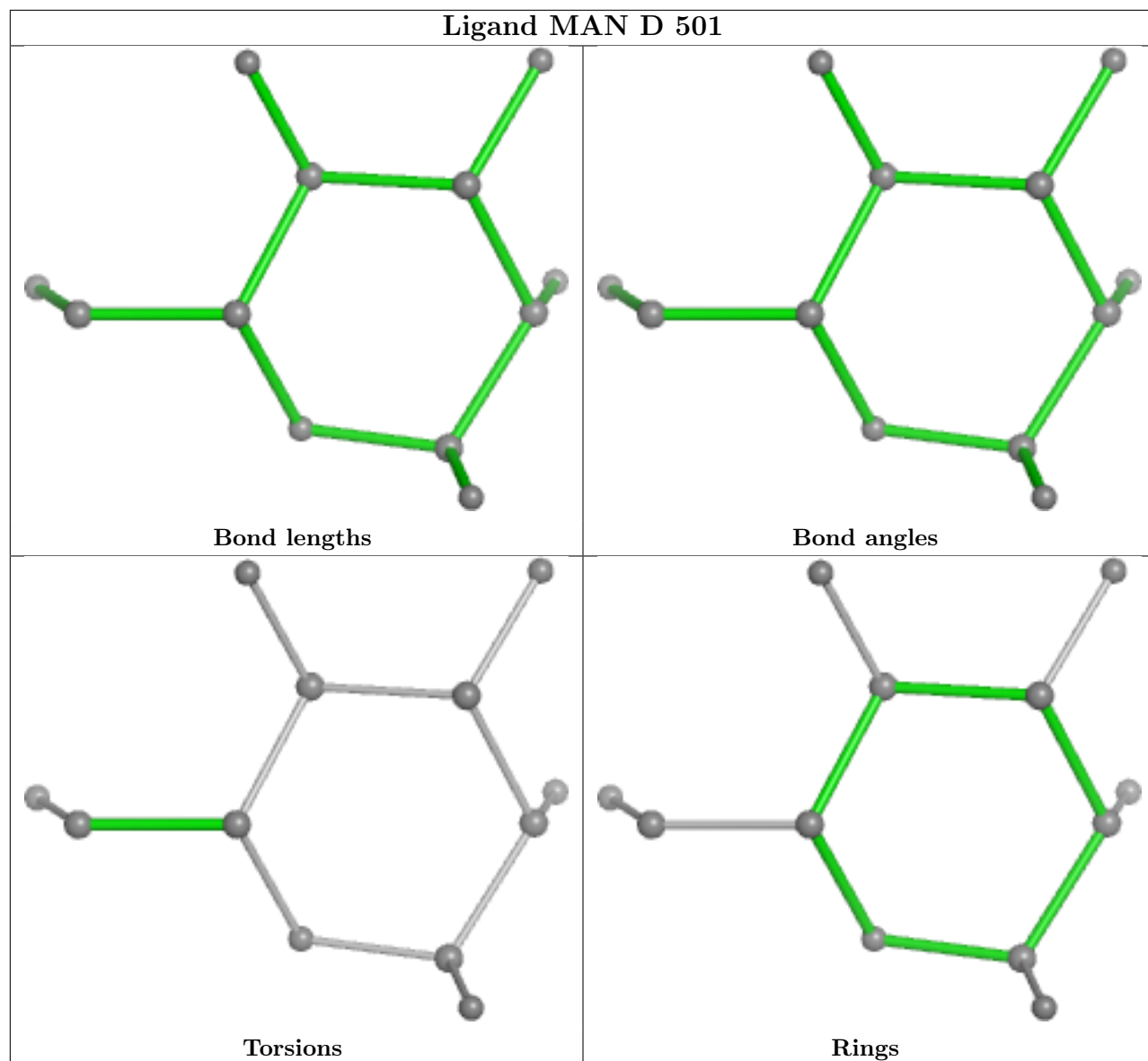
There are no ring outliers.

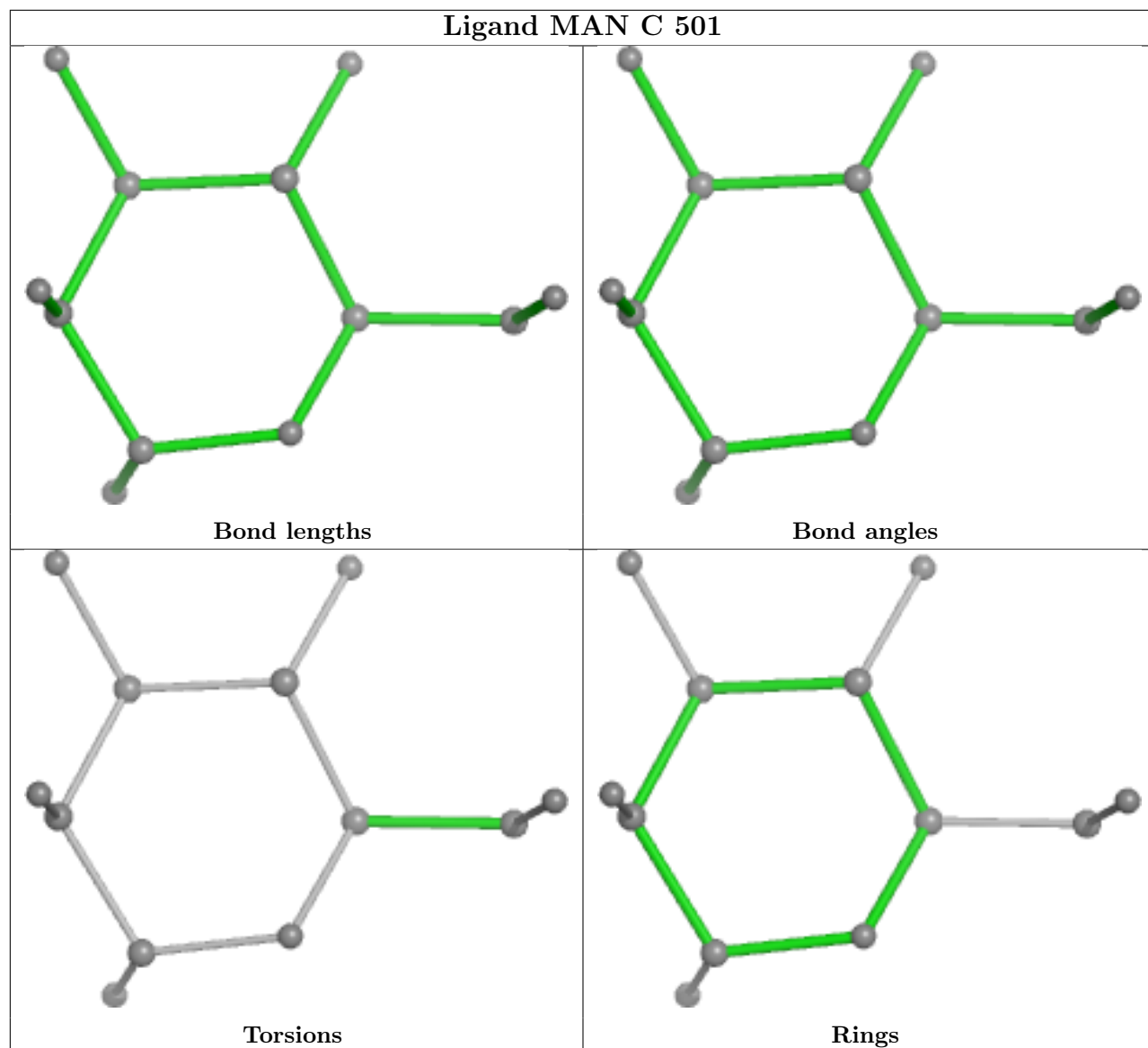
No monomer is involved in short contacts.

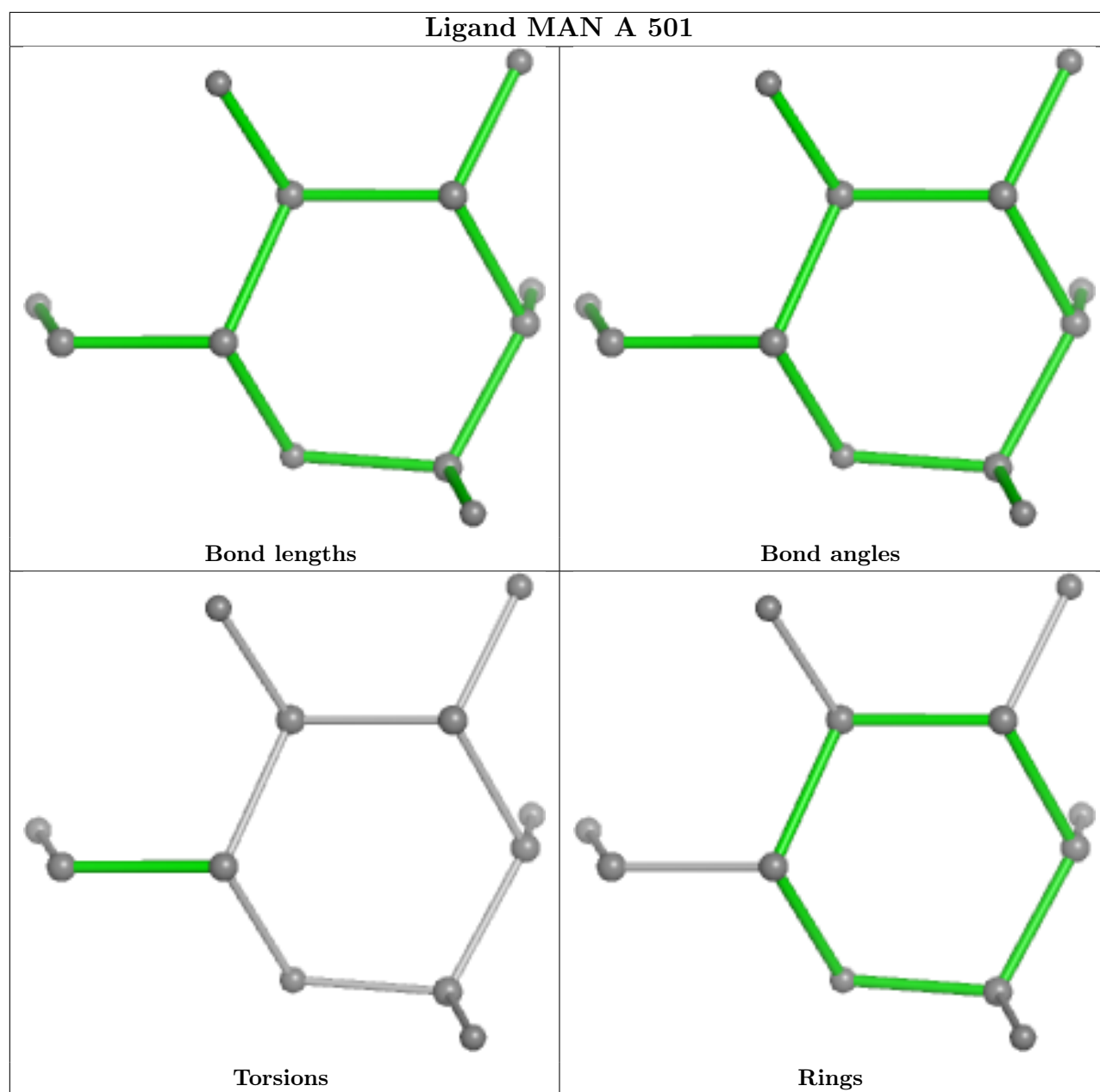
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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, 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	480/481 (99%)	0.24	17 (3%)	47 45	51, 90, 133, 157	1 (0%)
1	B	480/481 (99%)	0.38	24 (5%)	35 33	45, 102, 147, 191	1 (0%)
1	C	480/481 (99%)	0.38	24 (5%)	35 33	76, 108, 152, 206	0
1	D	480/481 (99%)	0.03	13 (2%)	56 54	42, 81, 120, 155	3 (0%)
All	All	1920/1924 (99%)	0.26	78 (4%)	42 40	42, 96, 140, 206	5 (0%)

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	466	ASP	5.5
1	B	460[A]	HIS	5.1
1	B	467	GLY	4.8
1	C	113	HIS	4.6
1	C	467	GLY	4.6
1	D	466	ASP	4.5
1	C	143	TYR	4.5
1	C	139	VAL	4.4
1	B	139	VAL	4.4
1	B	47	SER	4.3
1	B	113	HIS	4.1
1	C	107	PHE	4.1
1	C	114	HIS	4.1
1	A	139	VAL	4.1
1	C	141	GLN	4.0
1	A	464	SER	4.0
1	A	467	GLY	3.9
1	D	467	GLY	3.9
1	C	172	PHE	3.7
1	C	140	ILE	3.6
1	A	466	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	225	ILE	3.5
1	D	2	SER	3.5
1	A	465	LYS	3.4
1	B	114	HIS	3.3
1	D	47	SER	3.0
1	B	109	PHE	3.0
1	B	143	TYR	3.0
1	C	465	LYS	2.9
1	B	43	GLU	2.9
1	B	46	ILE	2.9
1	C	466	ASP	2.9
1	D	143	TYR	2.8
1	B	50	LYS	2.8
1	A	143	TYR	2.8
1	D	356	ILE	2.7
1	D	465	LYS	2.7
1	D	173	LYS	2.7
1	A	113	HIS	2.7
1	A	166	ILE	2.7
1	B	2	SER	2.7
1	C	2	SER	2.6
1	B	142	ASP	2.6
1	C	142	ASP	2.6
1	B	464	SER	2.5
1	B	42	CYS	2.5
1	A	48	GLN	2.5
1	D	377	GLU	2.5
1	C	377	GLU	2.5
1	B	478	HIS	2.4
1	B	377	GLU	2.4
1	C	4	PRO	2.4
1	C	173	LYS	2.4
1	A	222	ALA	2.4
1	A	2	SER	2.4
1	C	111	ASP	2.3
1	D	468	SER	2.3
1	A	140	ILE	2.3
1	B	465	LYS	2.2
1	C	5	LYS	2.2
1	C	464	SER	2.2
1	B	107	PHE	2.2
1	B	49	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	367	ARG	2.2
1	B	468	SER	2.2
1	C	47	SER	2.2
1	A	377	GLU	2.2
1	A	416	ASN	2.2
1	B	257	ARG	2.1
1	D	464	SER	2.1
1	C	478	HIS	2.1
1	A	167	ARG	2.1
1	C	231	GLY	2.1
1	A	137	LYS	2.0
1	C	46	ILE	2.0
1	B	4	PRO	2.0
1	D	48	GLN	2.0
1	D	46	ILE	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 monosaccharides 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
3	MLI	D	506	7/7	0.64	0.17	76,81,98,98	0
3	MLI	D	504	7/7	0.77	0.22	78,80,94,94	0
3	MLI	B	505	7/7	0.78	0.21	75,79,90,90	0
3	MLI	C	505	7/7	0.80	0.19	78,79,94,94	0
3	MLI	D	507	7/7	0.80	0.20	71,74,91,91	0
3	MLI	C	506	7/7	0.81	0.20	76,79,95,95	0
3	MLI	D	505	7/7	0.82	0.22	72,76,90,90	0
3	MLI	B	504	7/7	0.83	0.14	90,92,111,111	0

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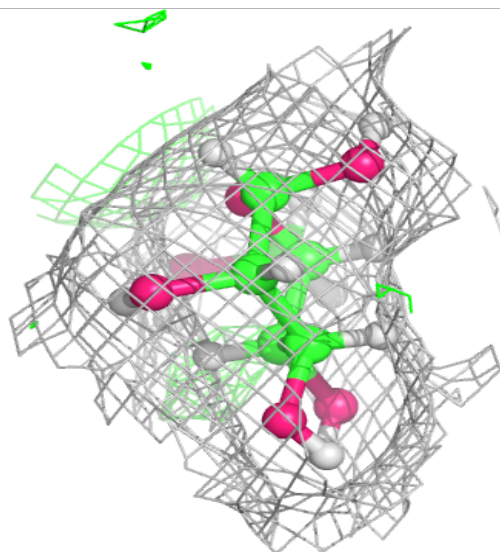
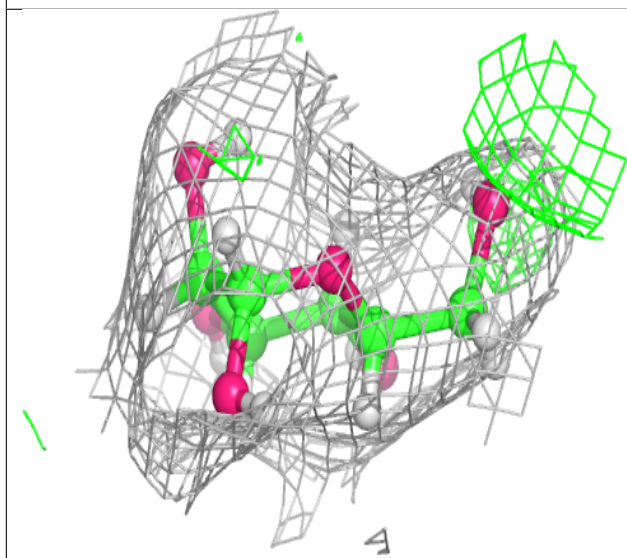
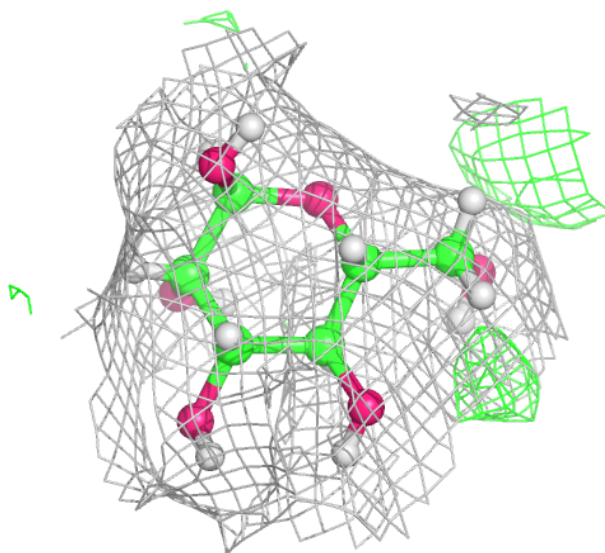
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MLI	C	502	7/7	0.84	0.15	85,88,105,105	0
3	MLI	C	504	7/7	0.84	0.12	99,100,120,120	0
3	MLI	A	503	7/7	0.85	0.21	84,85,102,102	0
3	MLI	D	503	7/7	0.85	0.14	84,87,101,101	0
3	MLI	D	502	7/7	0.86	0.13	66,71,86,86	0
3	MLI	A	502	7/7	0.86	0.13	69,72,85,85	0
3	MLI	A	504	7/7	0.92	0.11	74,78,94,94	0
3	MLI	B	503	7/7	0.92	0.10	73,77,92,92	0
3	MLI	C	507	7/7	0.93	0.11	72,73,86,86	0
2	MAN	C	501	12/12	0.94	0.09	80,87,104,105	0
3	MLI	B	502	7/7	0.94	0.09	71,72,85,85	0
2	MAN	D	501	12/12	0.95	0.09	56,61,74,74	0
3	MLI	C	503	7/7	0.95	0.09	66,68,82,82	0
2	MAN	B	501	12/12	0.96	0.07	69,75,89,90	0
2	MAN	A	501	12/12	0.97	0.06	64,69,81,83	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 MAN C 501:**

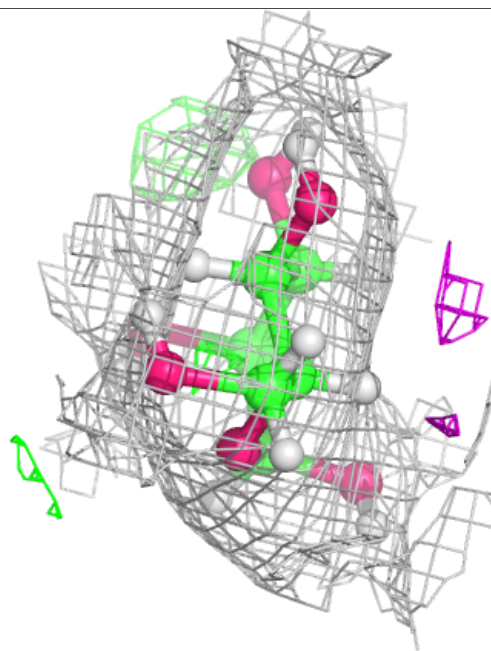
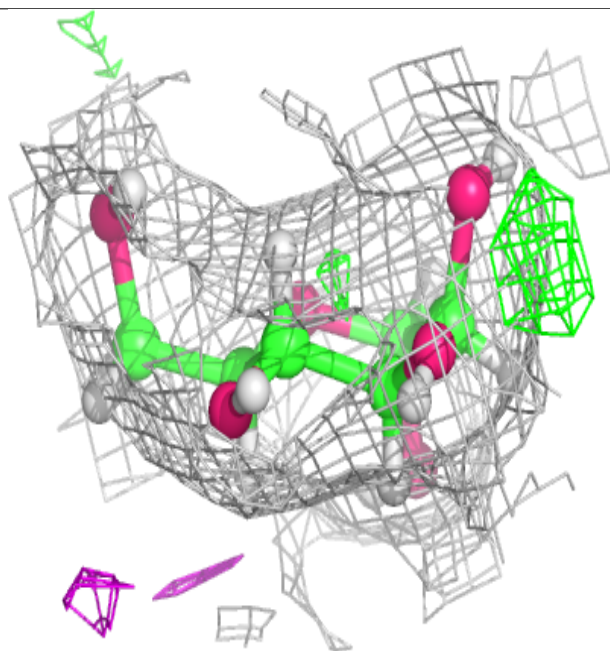
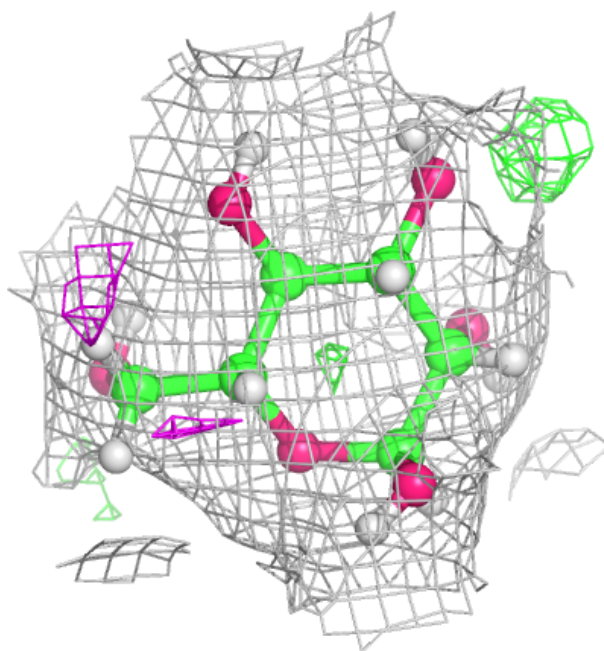
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





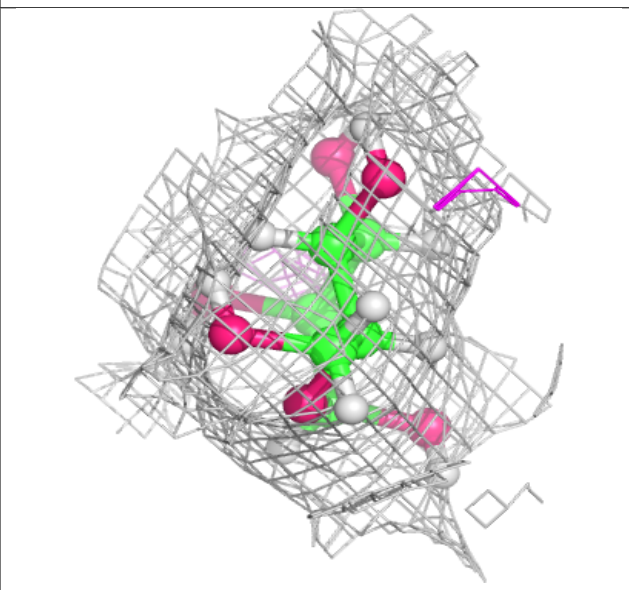
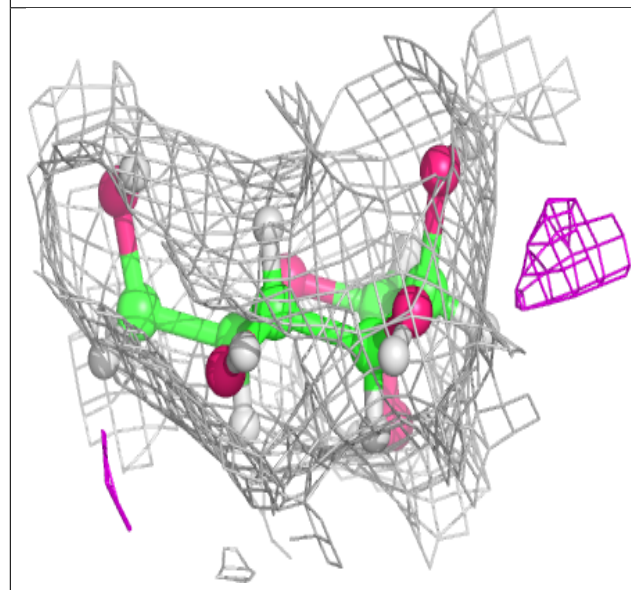
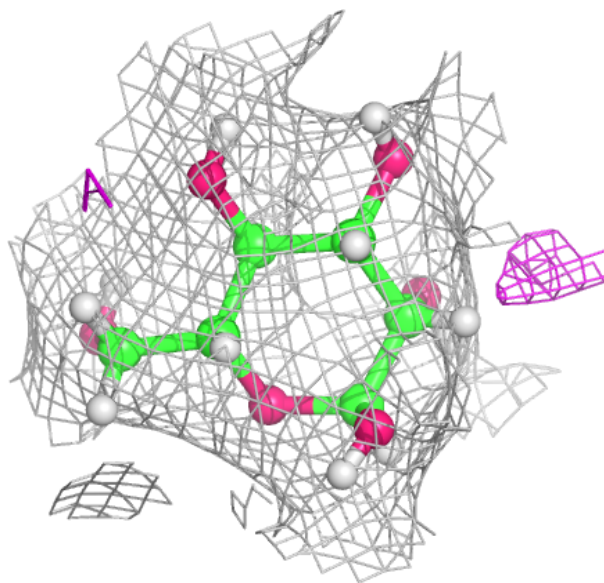
**Electron density around MAN D 501:**

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



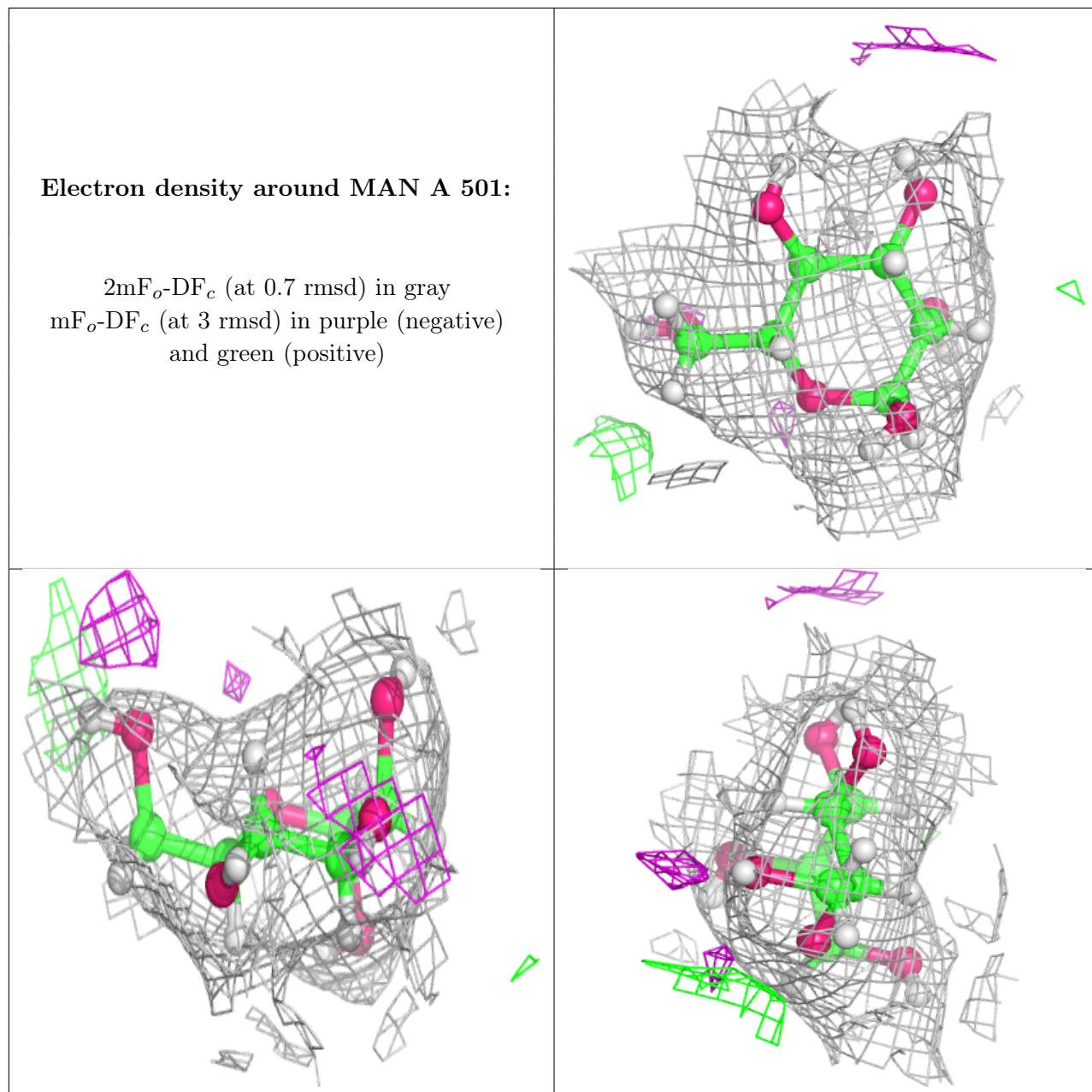
**Electron density around MAN B 501:**

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



**Electron density around MAN A 501:**

$2mF_o-DF_c$  (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.