Full wwPDB X-ray Structure Validation Report ⓘ

Aug 17, 2023 – 12:05 AM EDT

PDB ID	:	2F2L
Title	:	Crystal structure of tracheal cytotoxin (TCT) bound to the ectodomain complex of peptidoglycan recognition proteins LCa (PGRP-LCa) and LCx (PGRP-LCx)
Authors	:	Chang, C.I.; Deisenhofer, J.
Deposited on	:	2005-11-17
Resolution	:	2.10 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:

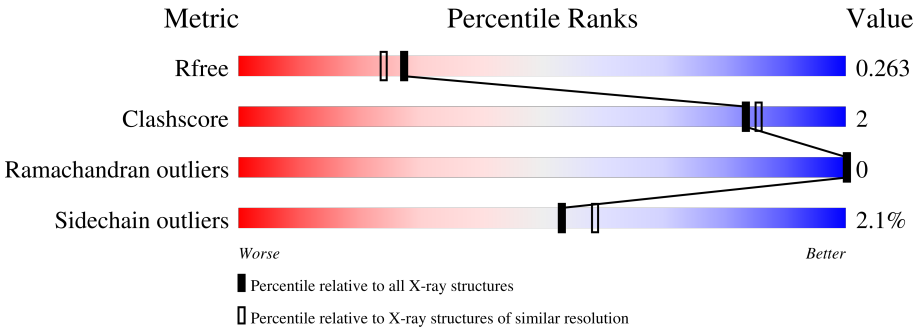
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	167	93% 7%
2	X	167	90% 8%

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	HSQ	A	999	X	-	-	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 2991 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 Peptidoglycan-recognition protein-LC isoform LCa.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	167	Total	C	N	O	S	0	3	0
			1346	857	231	252	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	354	ASP	-	cloning artifact	UNP Q9GNK5
A	414	CSO	CYS	modified residue	UNP Q9GNK5

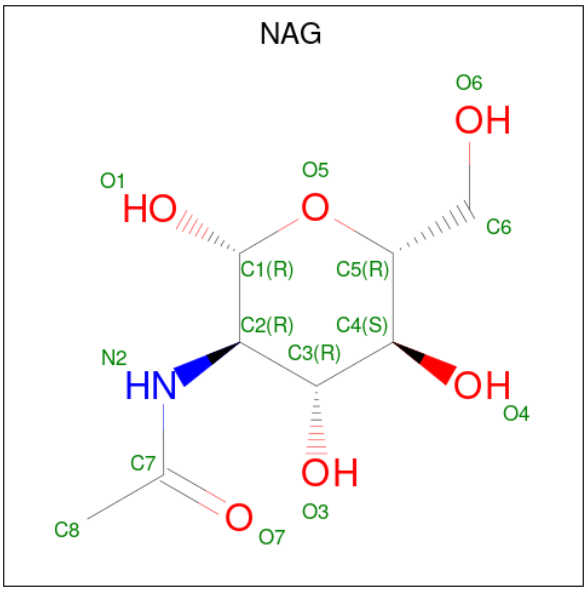
- Molecule 2 is a protein called Peptidoglycan recognition protein-LC isoform LCx.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	166	Total	C	N	O	S	0	0	0
			1335	844	247	238	6			

There is a discrepancy between the modelled and reference sequences:

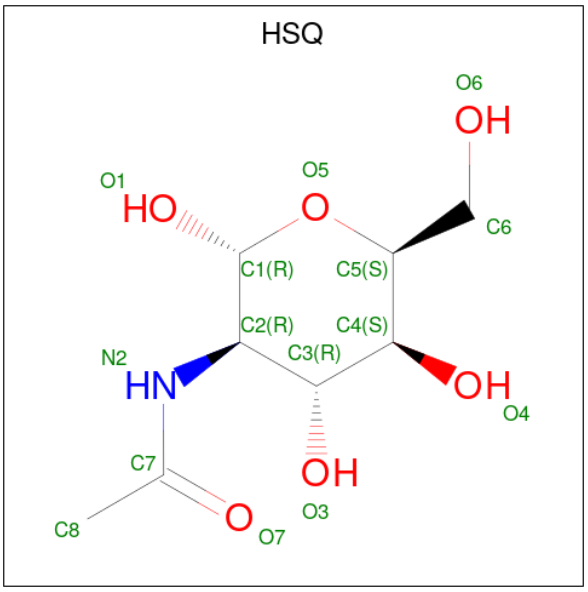
Chain	Residue	Modelled	Actual	Comment	Reference
X	334	MET	-	cloning artifact	GB 20271150

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



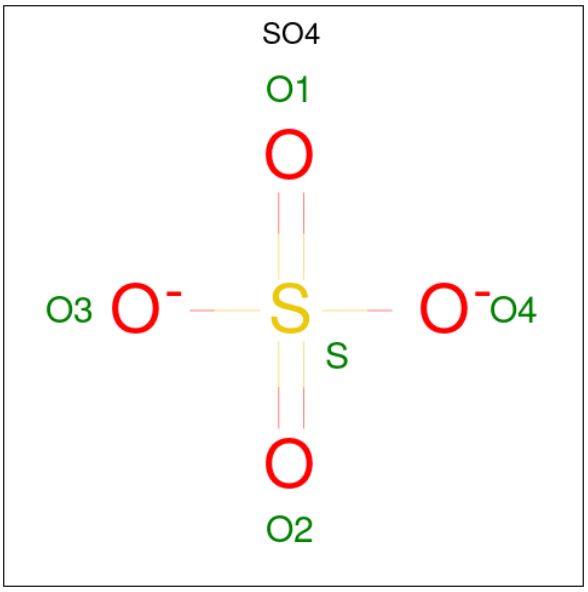
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is 2-acetylamino-2-deoxy-alpha-L-idopyranose (three-letter code: HSQ) (formula: $C_8H_{15}NO_6$).



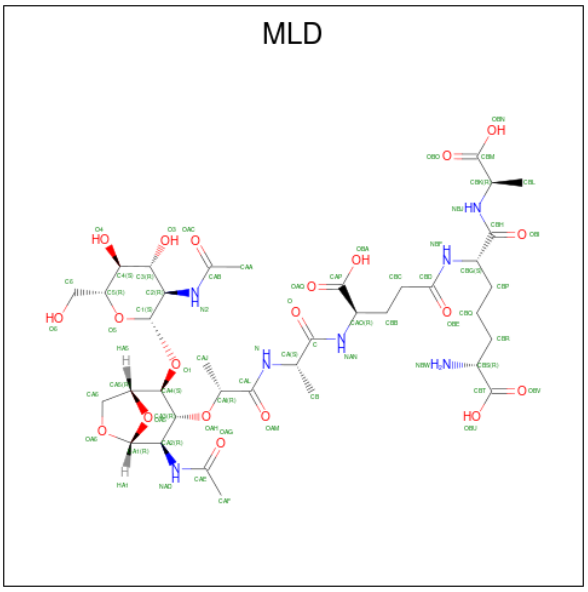
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



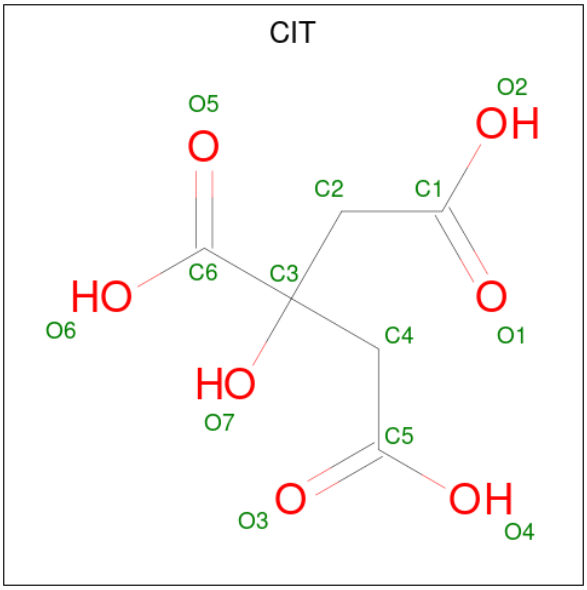
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	X	1	Total O S 5 4 1	0	0

- Molecule 6 is GLCNAC(BETA1-4)-MURNAC(1,6-ANHYDRO)-L-ALA-GAMMA-D-GLU-MESO-A2PM-D-ALA (three-letter code: MLD) (formula: $C_{37}H_{59}N_7O_{20}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	X	1	Total C N O 64 37 7 20	0	0

- Molecule 7 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	X	1	Total C O 13 6 7	0	0

- Molecule 8 is water.

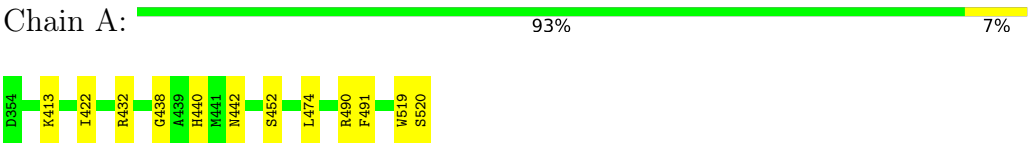
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	89	Total O 89 89	0	0
8	X	106	Total O 106 106	0	0

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. 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. 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.

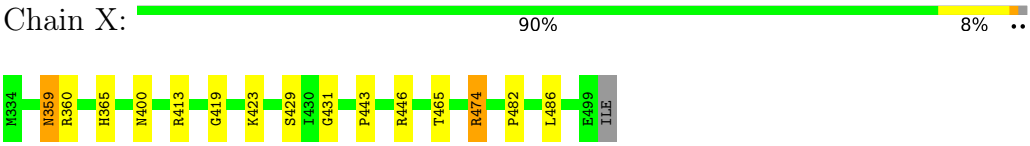
• Molecule 1: Peptidoglycan-recognition protein-LC isoform LCa

Chain A:



• Molecule 2: Peptidoglycan recognition protein-LC isoform LCx

Chain X:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	41.12Å 79.69Å 114.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10 28.60 – 2.06	Depositor EDS
% Data completeness (in resolution range)	98.5 (30.00-2.10) 98.0 (28.60-2.06)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.48 (at 2.06Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.166 , 0.214 0.219 , 0.263	Depositor DCC
R_{free} test set	1212 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	25.9	Xtriage
Anisotropy	0.606	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 53.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	2991	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.07% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MLD, CIT, HSQ, CSO, SO4, NAG

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	0.47	0/1369	0.62	0/1854
2	X	0.51	0/1369	0.69	3/1849 (0.2%)
All	All	0.49	0/2738	0.65	3/3703 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	X	474	ARG	NE-CZ-NH2	-6.88	116.86	120.30
2	X	474	ARG	NE-CZ-NH1	6.79	123.70	120.30
2	X	446	ARG	NE-CZ-NH1	5.07	122.84	120.30

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	1346	0	1326	5	0
2	X	1335	0	1307	7	0
3	A	14	0	13	1	0
4	A	14	0	13	0	0
5	A	5	0	0	0	0
5	X	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	X	64	0	56	0	0
7	X	13	0	5	0	0
8	A	89	0	0	1	0
8	X	106	0	0	0	0
All	All	2991	0	2720	13	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 (13) 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)
2:X:400:ASN:HD22	2:X:431:GLY:H	1.22	0.86
1:A:413:LYS:NZ	1:A:442:ASN:OD1	2.18	0.74
3:A:998:NAG:O4	8:A:185:HOH:O	2.11	0.69
1:A:490:ARG:HE	1:A:520:SER:HB2	1.67	0.59
2:X:413:ARG:HD2	2:X:419:GLY:HA2	1.88	0.56
2:X:360:ARG:HD2	2:X:429:SER:HB3	1.89	0.55
2:X:400:ASN:ND2	2:X:431:GLY:H	1.98	0.53
2:X:443:PRO:HG3	2:X:486:LEU:HD13	1.95	0.48
1:A:440:HIS:CG	1:A:452:SER:HB3	2.49	0.47
1:A:432:ARG:HD2	1:A:438:GLY:HA2	1.97	0.46
2:X:482:PRO:HB2	2:X:486:LEU:HD23	1.98	0.46
2:X:359:ASN:HB2	2:X:465:THR:OG1	2.18	0.42
1:A:491:PHE:O	1:A:519:TRP:HA	2.21	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	166/167 (99%)	163 (98%)	3 (2%)	0	100	100
2	X	164/167 (98%)	161 (98%)	3 (2%)	0	100	100
All	All	330/334 (99%)	324 (98%)	6 (2%)	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	146/143 (102%)	144 (99%)	2 (1%)	67	73
2	X	139/140 (99%)	135 (97%)	4 (3%)	42	46
All	All	285/283 (101%)	279 (98%)	6 (2%)	53	59

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	422	ILE
1	A	474	LEU
2	X	359	ASN
2	X	365	HIS
2	X	423	LYS
2	X	474	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	X	400	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\| > 2$
1	CSO	A	414	1	3,6,7	0.56	0	0,6,8	-	-

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
1	CSO	A	414	1	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

6 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	$\#\|Z\| > 2$
7	CIT	X	301	-	12,12,12	1.06	0	17,17,17	1.65	4 (23%)
3	NAG	A	998	1	14,14,15	0.56	0	17,19,21	1.01	1 (5%)
5	SO4	X	501	-	4,4,4	0.16	0	6,6,6	0.18	0
6	MLD	X	201	-	65,66,66	0.88	2 (3%)	90,93,93	1.29	7 (7%)
4	HSQ	A	999	1	14,14,15	0.62	0	17,19,21	1.73	3 (17%)
5	SO4	A	1000	-	4,4,4	0.17	0	6,6,6	0.11	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
6	MLD	X	201	-	-	2/69/114/114	0/4/3/3
7	CIT	X	301	-	-	4/16/16/16	-
4	HSQ	A	999	1	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	A	998	1	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	X	201	MLD	OA6-CA1	2.22	1.46	1.41
6	X	201	MLD	OBA-CAP	-2.05	1.23	1.30

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	X	201	MLD	CA6-CA5-CA4	-5.56	100.95	112.55
4	A	999	HSQ	C4-C3-C2	4.74	117.96	111.02
7	X	301	CIT	O6-C6-C3	3.96	119.92	113.05
6	X	201	MLD	OA5-CA5-CA4	3.66	114.13	108.67
4	A	999	HSQ	O5-C1-C2	-3.53	105.71	111.29
7	X	301	CIT	O5-C6-C3	-2.97	118.04	122.25
4	A	999	HSQ	C3-C4-C5	2.64	114.94	110.24
6	X	201	MLD	O1-CA4-CA5	2.49	116.27	109.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	X	201	MLD	C1-O1-CA4	-2.46	111.88	117.96
6	X	201	MLD	CB-CA-N	-2.44	105.80	110.38
3	A	998	NAG	C2-N2-C7	2.37	126.27	122.90
6	X	201	MLD	CBB-CAO-CAP	-2.36	104.67	110.35
6	X	201	MLD	OA6-CA1-CA2	-2.25	107.97	110.84
7	X	301	CIT	O2-C1-C2	2.25	121.57	114.35
7	X	301	CIT	O4-C5-C4	2.15	121.27	114.35

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	999	HSQ	C1

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	999	HSQ	C8-C7-N2-C2
4	A	999	HSQ	O7-C7-N2-C2
3	A	998	NAG	C8-C7-N2-C2
3	A	998	NAG	O7-C7-N2-C2
7	X	301	CIT	O1-C1-C2-C3
7	X	301	CIT	O2-C1-C2-C3
6	X	201	MLD	CA5-CA4-O1-C1
6	X	201	MLD	CA3-CA4-O1-C1
7	X	301	CIT	C3-C4-C5-O4
7	X	301	CIT	C3-C4-C5-O3

There are no ring outliers.

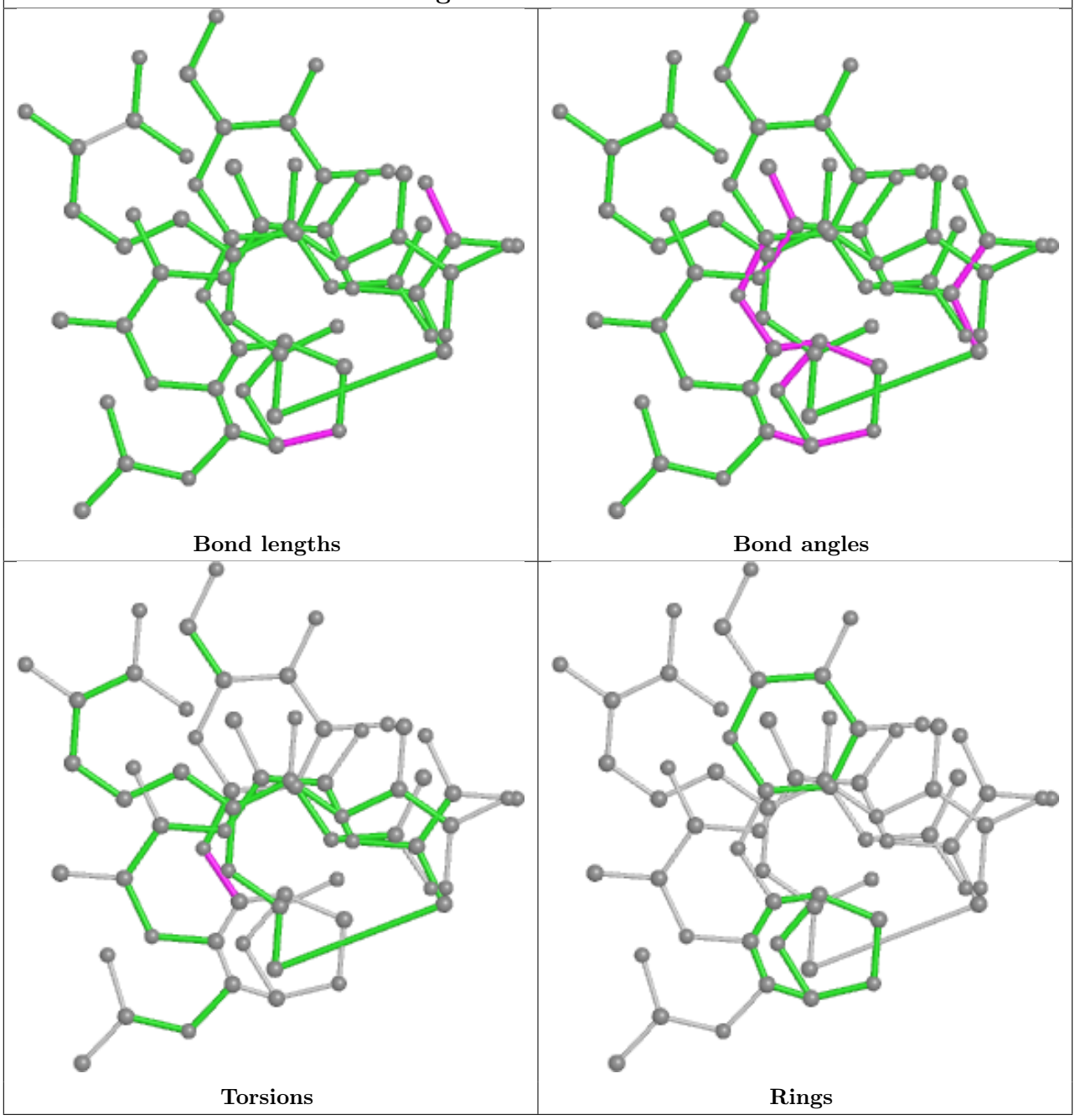
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	998	NAG	1	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 then 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 MLD X 201



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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

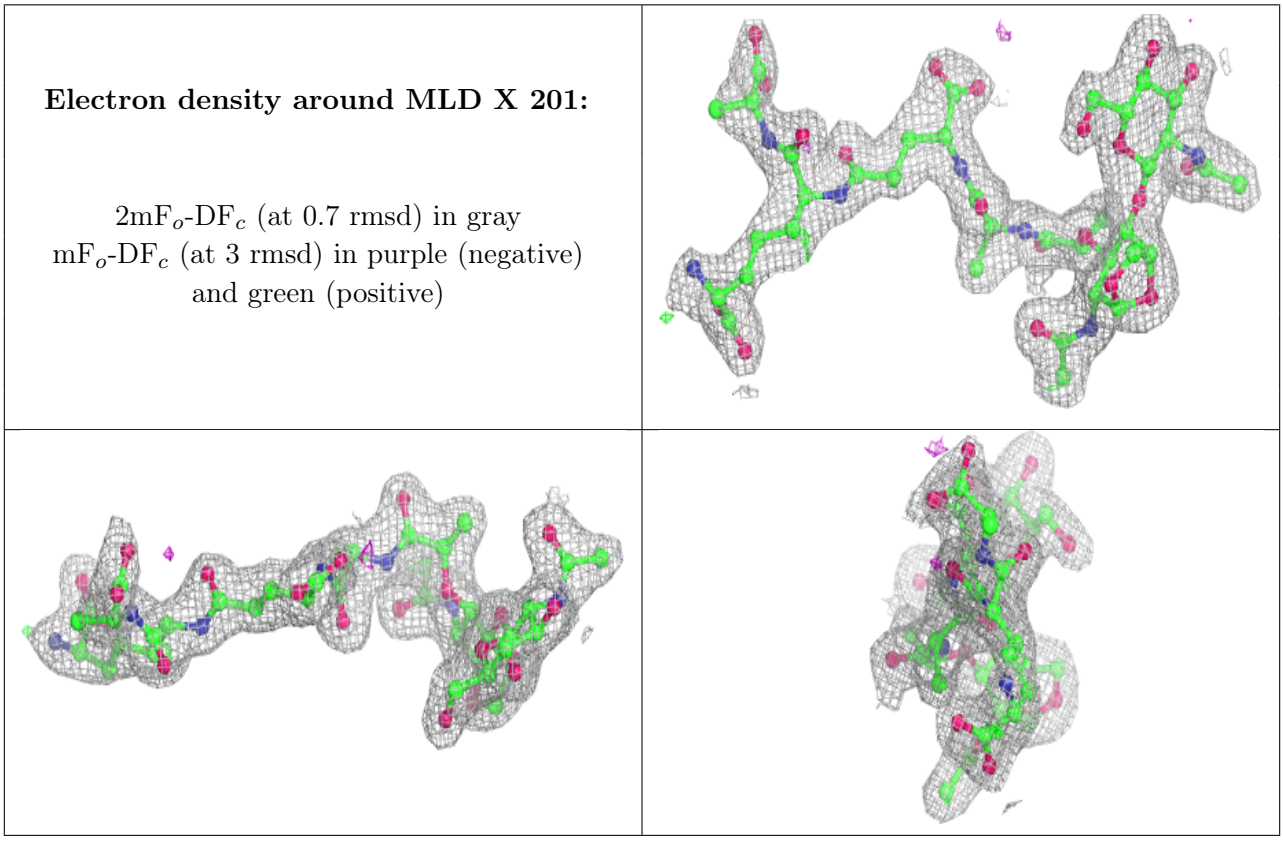
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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 MLD X 201:

$2mF_o$-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)

Unable to reproduce the depositors R factor - this section is therefore empty.