Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2023 – 12:19 pm GMT

PDB ID	:	8BYK
Title	:	The structure of MadC from Clostridium maddingley reveals new insights into class I lanthipeptide cyclases
Authors	:	Knospe, C.V.; Kamel, M.; Spitz, O.; Hoeppner, A.; Galle, S.; Reiners, J.; Kedrov, A.; Smits, S.H.; Schmitt, L.
Deposited on	:	2022-12-13
Resolution	:	1.70 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:

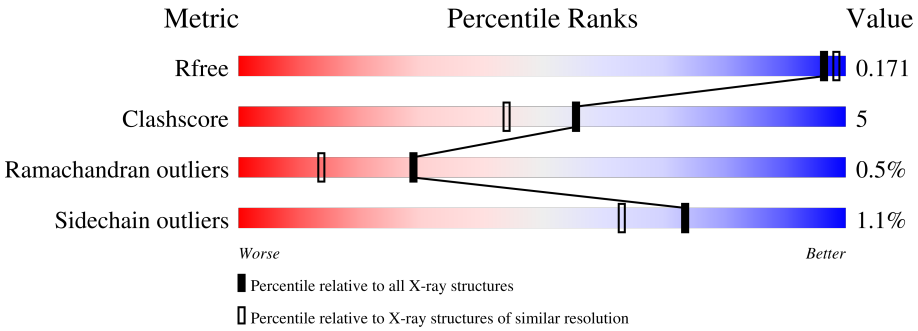
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

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 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)

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	449	84% 12%

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	MPD	A	605	-	X	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 3886 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 Lanthionine synthetase C-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	21	0
			3560	2268	585	681	26			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP K6THC9
A	-1	HIS	-	expression tag	UNP K6THC9
A	0	MET	-	expression tag	UNP K6THC9
A	498	ALA	-	expression tag	UNP K6THC9
A	499	ALA	-	expression tag	UNP K6THC9
A	500	ALA	-	expression tag	UNP K6THC9
A	501	HIS	-	expression tag	UNP K6THC9
A	502	HIS	-	expression tag	UNP K6THC9
A	503	ALA	-	expression tag	UNP K6THC9
A	504	ALA	-	expression tag	UNP K6THC9
A	505	ALA	-	expression tag	UNP K6THC9

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

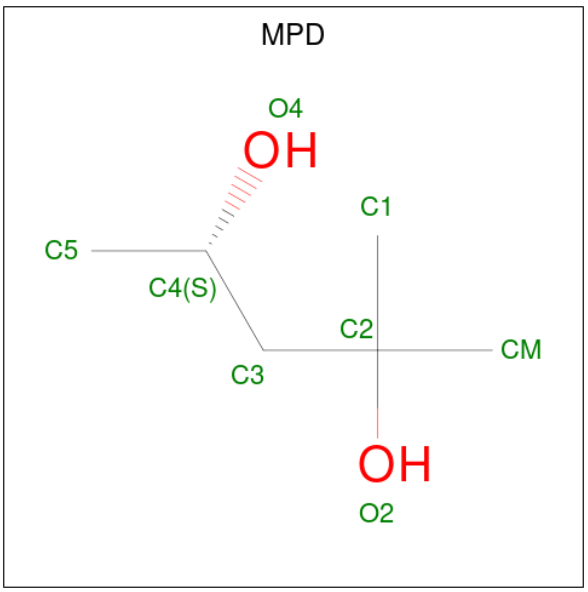
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

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

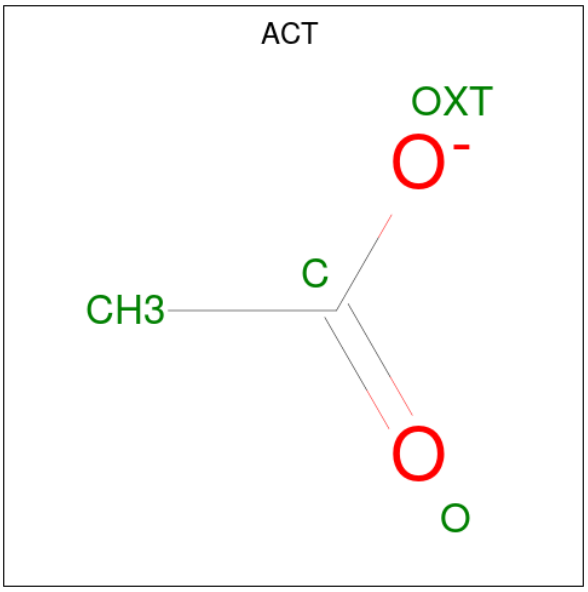
- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:

$C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 8 6 2	0	0
4	A	1	Total C O 8 6 2	0	0
4	A	1	Total C O 8 6 2	0	0

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Cl 1 1	0	0

- Molecule 7 is water.

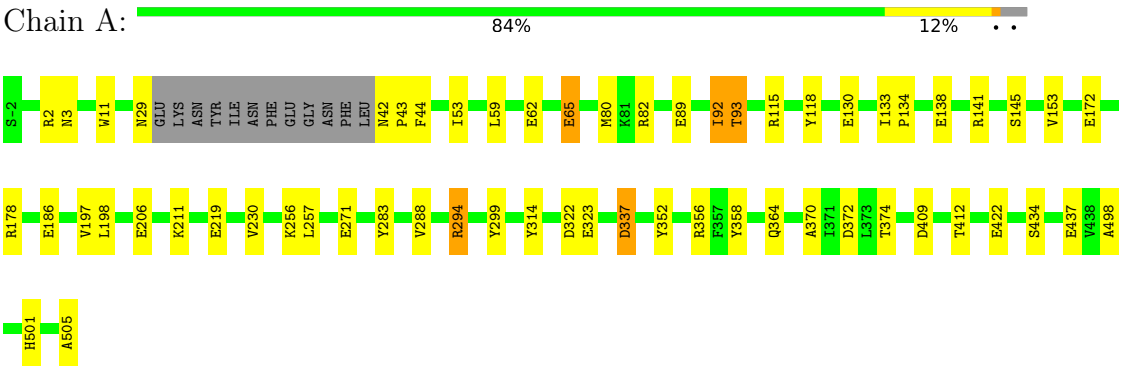
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	294	Total O 294 294	0	0

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: Lanthionine synthetase C-like protein

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	54.14Å 66.12Å 117.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.89 – 1.70 57.59 – 1.14	Depositor EDS
% Data completeness (in resolution range)	99.0 (41.89-1.70) 59.3 (57.59-1.14)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.47 (at 1.14Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.190 , 0.220 0.126 , 0.171	Depositor DCC
R_{free} test set	4589 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	9.4	Xtriage
Anisotropy	0.935	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 54.6	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	0.98	EDS
Total number of atoms	3886	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.03% 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: NA, ZN, ACT, CL, MPD

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	1.39	22/3661 (0.6%)	1.25	20/4948 (0.4%)

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	186	GLU	CG-CD	13.04	1.71	1.51
1	A	172	GLU	CD-OE2	11.73	1.38	1.25
1	A	271	GLU	CD-OE1	-8.90	1.15	1.25
1	A	271	GLU	CB-CG	-8.54	1.35	1.52
1	A	288	VAL	CB-CG2	-7.84	1.36	1.52
1	A	138	GLU	CD-OE2	7.58	1.33	1.25
1	A	437	GLU	CD-OE1	-7.17	1.17	1.25
1	A	65	GLU	CD-OE2	7.13	1.33	1.25
1	A	172	GLU	CD-OE1	7.09	1.33	1.25
1	A	323	GLU	CD-OE1	-6.82	1.18	1.25
1	A	358	TYR	CE1-CZ	-6.35	1.30	1.38
1	A	219	GLU	CD-OE2	6.24	1.32	1.25
1	A	206	GLU	CG-CD	6.12	1.61	1.51
1	A	62	GLU	CD-OE2	5.99	1.32	1.25
1	A	271	GLU	CA-CB	-5.66	1.41	1.53
1	A	138	GLU	CG-CD	5.31	1.59	1.51
1	A	314	TYR	CB-CG	5.19	1.59	1.51
1	A	153	VAL	CB-CG2	-5.16	1.42	1.52
1	A	145	SER	CB-OG	-5.14	1.35	1.42
1	A	89	GLU	CG-CD	5.09	1.59	1.51
1	A	130	GLU	CD-OE2	5.08	1.31	1.25
1	A	11	TRP	CG-CD1	-5.08	1.29	1.36

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	115	ARG	NE-CZ-NH1	13.14	126.87	120.30
1	A	186	GLU	OE1-CD-OE2	11.39	136.97	123.30
1	A	294[A]	ARG	NE-CZ-NH2	-9.53	115.54	120.30
1	A	294[B]	ARG	NE-CZ-NH2	-9.53	115.54	120.30
1	A	178	ARG	NE-CZ-NH1	-8.64	115.98	120.30
1	A	178	ARG	NE-CZ-NH2	8.08	124.34	120.30
1	A	372	ASP	CB-CG-OD2	-7.34	111.69	118.30
1	A	294[A]	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	A	294[B]	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	A	299	TYR	CD1-CE1-CZ	-6.52	113.93	119.80
1	A	141	ARG	NE-CZ-NH2	6.52	123.56	120.30
1	A	92	ILE	C-N-CA	6.11	136.96	121.70
1	A	283	TYR	CZ-CE2-CD2	5.82	125.04	119.80
1	A	356	ARG	CD-NE-CZ	5.82	131.75	123.60
1	A	322	ASP	CB-CG-OD2	-5.57	113.29	118.30
1	A	2	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	92	ILE	CA-C-N	5.42	129.11	117.20
1	A	352	TYR	CB-CG-CD2	5.25	124.15	121.00
1	A	409	ASP	CB-CG-OD2	-5.25	113.58	118.30
1	A	206	GLU	OE1-CD-OE2	-5.06	117.23	123.30

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	3560	0	3453	29	0
2	A	1	0	0	0	0
3	A	2	0	0	0	0
4	A	24	0	42	8	0
5	A	4	0	3	0	0
6	A	1	0	0	0	0
7	A	294	0	0	6	0
All	All	3886	0	3498	36	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 5.

All (36) 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:A:92:ILE:HA	1:A:93:THR:HG22	1.64	0.79
4:A:604:MPD:H53	7:A:705:HOH:O	1.85	0.75
1:A:92:ILE:CG1	1:A:93:THR:HG22	2.22	0.69
4:A:605:MPD:C1	4:A:605:MPD:H52	2.25	0.66
1:A:294[B]:ARG:NH1	1:A:501:HIS:O	2.29	0.64
1:A:92:ILE:HG13	1:A:93:THR:HG22	1.78	0.64
1:A:92:ILE:CA	1:A:93:THR:HG22	2.28	0.63
4:A:605:MPD:H52	4:A:605:MPD:H11	1.81	0.62
4:A:606:MPD:H53	7:A:964:HOH:O	1.99	0.62
4:A:605:MPD:H11	4:A:605:MPD:C5	2.33	0.59
1:A:92:ILE:HD12	1:A:93:THR:CG2	2.35	0.57
1:A:197[B]:VAL:HG12	4:A:605:MPD:HM1	1.87	0.56
4:A:605:MPD:C1	4:A:605:MPD:C5	2.83	0.56
1:A:42:ASN:HB2	1:A:43:PRO:HD2	1.91	0.52
1:A:92:ILE:HA	1:A:93:THR:CG2	2.38	0.51
1:A:53:ILE:HD13	1:A:82:ARG:HG2	1.93	0.50
1:A:370:ALA:O	1:A:374:THR:HG23	2.14	0.48
1:A:133[A]:ILE:HG22	1:A:134:PRO:HD3	1.95	0.48
1:A:65:GLU:OE1	7:A:701:HOH:O	2.20	0.47
1:A:92:ILE:CD1	1:A:93:THR:HG22	2.45	0.47
1:A:3:ASN:OD1	1:A:422:GLU:HG3	2.15	0.47
1:A:505:ALA:HB1	7:A:879:HOH:O	2.14	0.46
1:A:92:ILE:HD12	1:A:93:THR:HG22	1.98	0.46
1:A:133[A]:ILE:CG2	1:A:134:PRO:HD3	2.45	0.46
1:A:29:ASN:OD1	1:A:29:ASN:C	2.54	0.45
1:A:82:ARG:NH2	7:A:709:HOH:O	2.48	0.45
1:A:198:LEU:HD23	1:A:198:LEU:N	2.32	0.45
1:A:80:MET:HG2	1:A:118:TYR:CE1	2.52	0.44
1:A:230:VAL:HG13	1:A:257:LEU:HD22	1.99	0.44
1:A:92:ILE:CD1	1:A:93:THR:CG2	2.96	0.44
1:A:59:LEU:HD22	1:A:412[B]:THR:HG22	1.99	0.44
1:A:294[B]:ARG:HD3	1:A:337:ASP:HB3	1.99	0.44
1:A:498:ALA:HB1	7:A:750:HOH:O	2.18	0.42
4:A:604:MPD:HM1	4:A:604:MPD:H52	2.01	0.42
1:A:92:ILE:HG13	1:A:93:THR:CG2	2.49	0.41

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	453/449 (101%)	440 (97%)	11 (2%)	2 (0%)	34 18

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	93	THR
1	A	44	PHE

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	388/388 (100%)	384 (99%)	4 (1%)	76 67

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	211	LYS
1	A	337	ASP
1	A	364	GLN
1	A	434	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 4 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	$\#\|Z\| > 2$
5	ACT	A	607	-	3,3,3	1.85	1 (33%)	3,3,3	0.31	0
4	MPD	A	606	-	7,7,7	2.65	2 (28%)	9,10,10	3.74	2 (22%)
4	MPD	A	604	-	7,7,7	0.79	0	9,10,10	1.32	0
4	MPD	A	605	-	7,7,7	1.05	1 (14%)	9,10,10	2.17	3 (33%)

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	MPD	A	606	-	-	3/5/5/5	-
4	MPD	A	604	-	-	2/5/5/5	-
4	MPD	A	605	-	-	5/5/5/5	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	606	MPD	CM-C2	5.24	1.68	1.52
4	A	606	MPD	O2-C2	4.45	1.55	1.44
5	A	607	ACT	O-C	2.94	1.35	1.22
4	A	605	MPD	O2-C2	2.32	1.50	1.44

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	606	MPD	CM-C2-C1	-9.08	91.65	110.57
4	A	606	MPD	O2-C2-CM	5.90	127.02	108.08
4	A	605	MPD	CM-C2-C1	-3.91	102.42	110.57
4	A	605	MPD	CM-C2-C3	3.86	127.92	109.96
4	A	605	MPD	O2-C2-C3	-2.43	100.67	109.80

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	605	MPD	C1-C2-C3-C4
4	A	605	MPD	O2-C2-C3-C4
4	A	605	MPD	C2-C3-C4-C5
4	A	604	MPD	CM-C2-C3-C4
4	A	605	MPD	CM-C2-C3-C4
4	A	606	MPD	O2-C2-C3-C4
4	A	604	MPD	C2-C3-C4-C5
4	A	606	MPD	C2-C3-C4-C5
4	A	605	MPD	C2-C3-C4-O4
4	A	606	MPD	C2-C3-C4-O4

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	606	MPD	1	0
4	A	604	MPD	2	0
4	A	605	MPD	5	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	438[B]:VAL	C	498:ALA	N	31.46
1	A	438[A]:VAL	C	498:ALA	N	31.36

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.

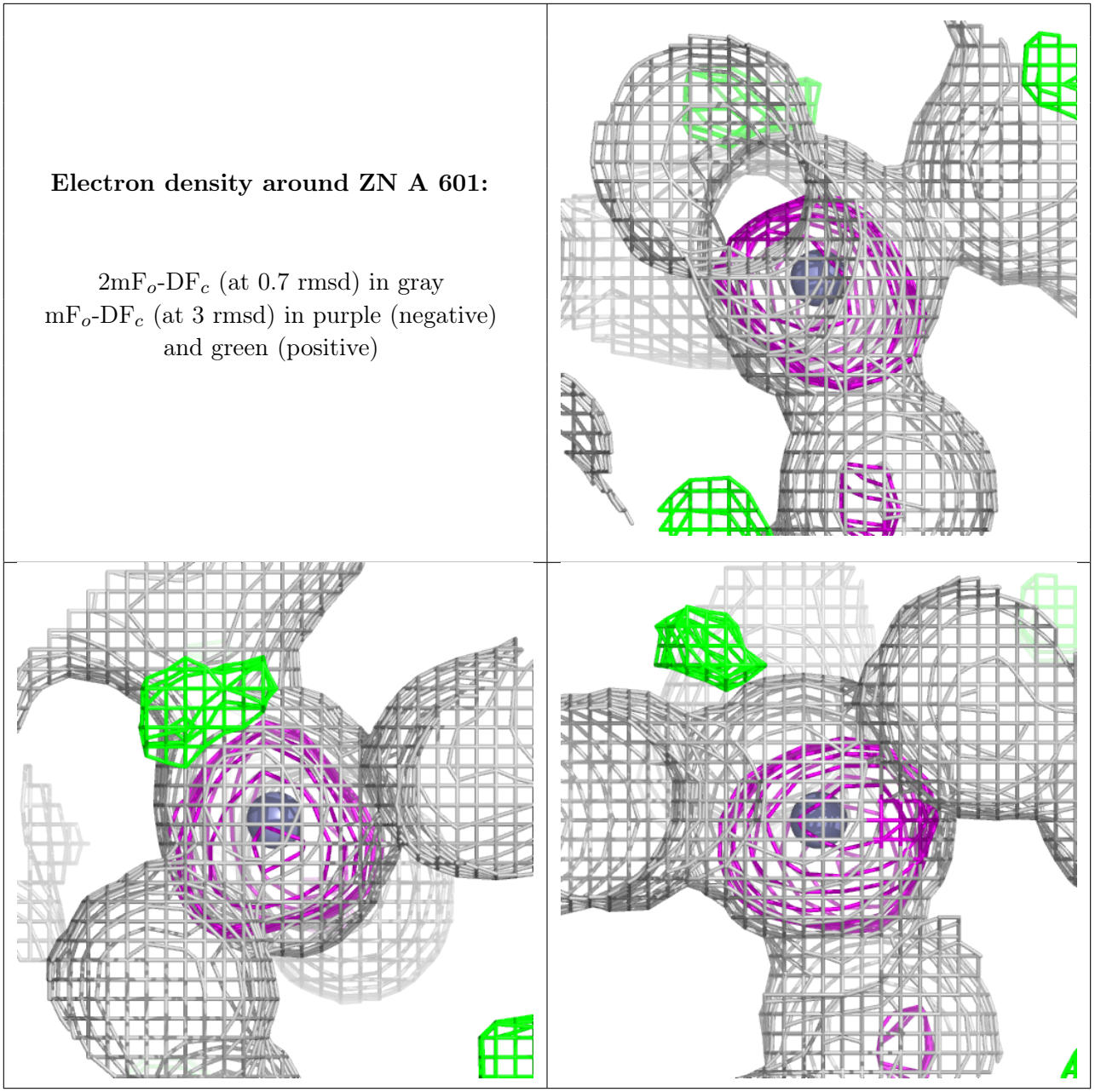
6.4 Ligands

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 ZN A 601:

$2mF_o$-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.