



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 22, 2023 – 06:34 PM JST

PDB ID : 7WI7
Title : Crystal structure of human MCM8/9 complex
Authors : Li, J.; Liu, Y.
Deposited on : 2022-01-03
Resolution : 6.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

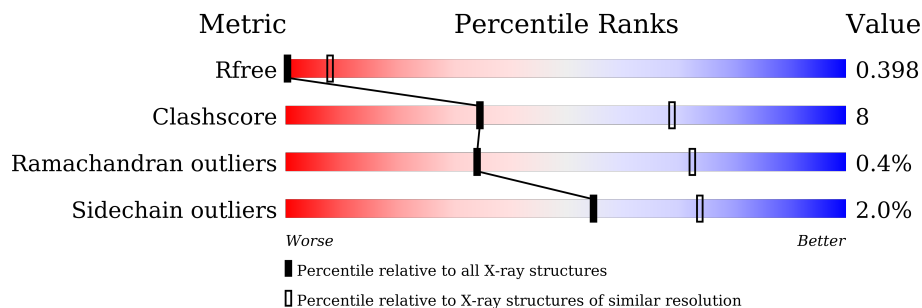
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.60 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	1000 (9.00-3.90)
Clashscore	141614	1064 (9.00-3.90)
Ramachandran outliers	138981	1012 (9.00-3.88)
Sidechain outliers	138945	1010 (9.00-3.84)

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	787	
2	B	684	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8839 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 DNA helicase MCM8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	565	4406	2791	758	831	26	0	1	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	MET	-	initiating methionine	UNP Q9UJA3
A	841	HIS	-	expression tag	UNP Q9UJA3
A	842	HIS	-	expression tag	UNP Q9UJA3
A	843	HIS	-	expression tag	UNP Q9UJA3
A	844	HIS	-	expression tag	UNP Q9UJA3
A	845	HIS	-	expression tag	UNP Q9UJA3
A	846	HIS	-	expression tag	UNP Q9UJA3

- Molecule 2 is a protein called DNA helicase MCM9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	566	4431	2800	758	840	33	0	0	0

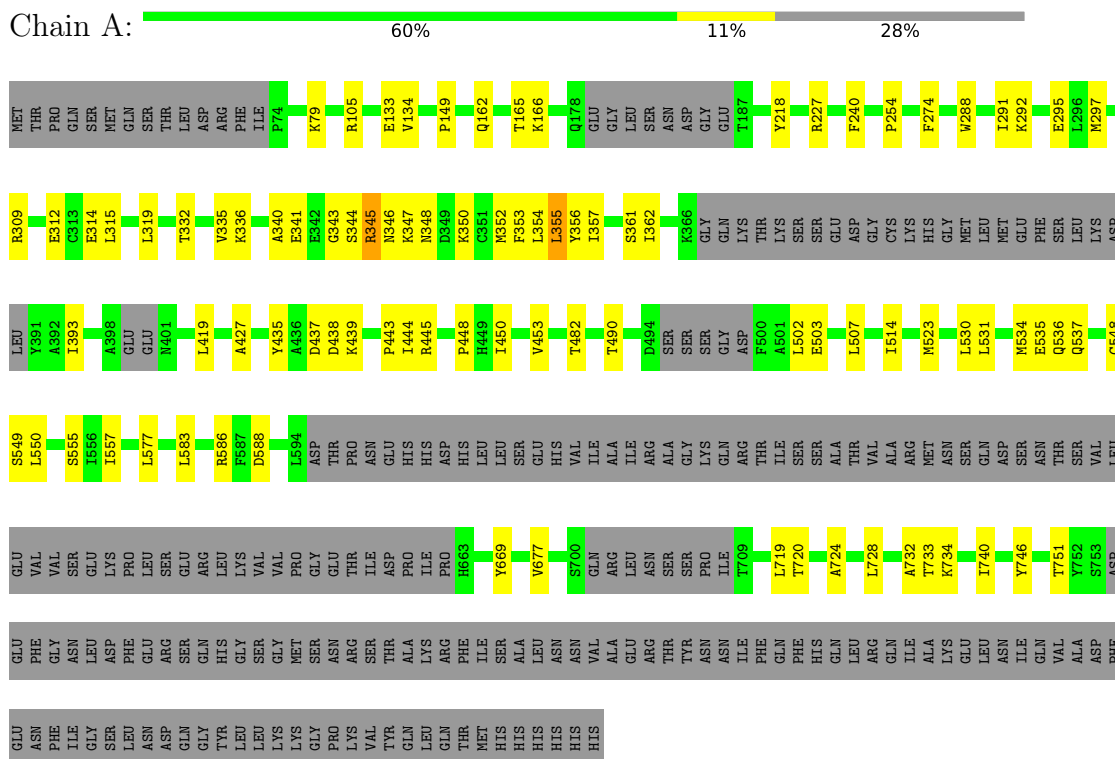
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		

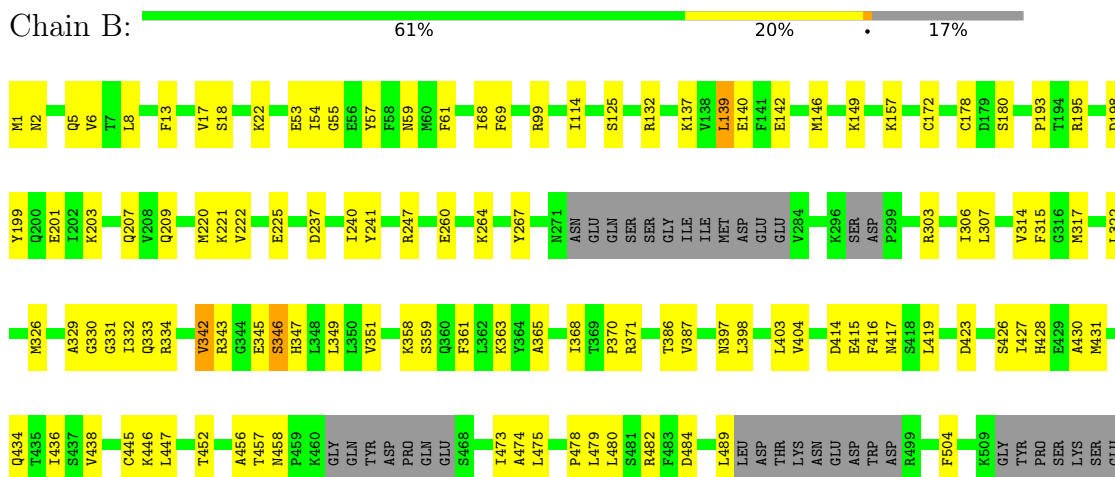
3 Residue-property plots [i](#)

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. 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: DNA helicase MCM8



- Molecule 2: DNA helicase MCM9



LYS	GLY	GLU
LEU	GLY	THR
TRP	VAL	THR
S520	ASN	PRO
M521	ALA	GLY
M524	LEU	SER
K525	HIS	LEU
I526	THR	ARG
Y527	SER	ASN
	PHE	GLY
	PRO	PRO
I531	GLU	GLY
R532	ASN	GLU
M533	PRO	GLU
L534	GLY	GLU
	GLN	GLU
PRO	GLN	GLN
THR	TYR	THR
LEU	GLN	GLN
S539	ARG	ARG
	GLN	GLN
V545	CYS	GLU
L546	GLU	LEU
	LEU	LEU
Y549	ILE	LEU
Y550	LEU	LEU
	GLU	GLU
R554	LYS	LEU
	GLU	LEU
R559	LEU	LEU
	GLN	GLN
T565	SER	SER
S566	LEU	LEU
R567	LEU	LEU
L568	LEU	LEU
L569	SER	SER
E570	GLU	GLU
S571	GLU	GLU
L572	LEU	LEU
I573	ARG	ARG
R574	ARG	ARG
L575	LEU	LEU
A576	GLU	GLU
E577	ARG	ARG
A578	LEU	LEU
H579	GLN	GLN
A580	ASN	ASN
R581	GLN	GLN
L582	SER	SER
M583	VAL	VAL
F584	HIS	HIS
R585	GLN	GLN
	SER	SER
V588	GLN	GLN
	PRO	PRO
A593	ARG	ARG
	VAL	VAL
M604	LEU	LEU
	GLU	GLU
L610	VAL	VAL

GLU
THR
THR
PRO
GLY
SER
LEU
ARG
ASN
GLY
PRO
GLY
GLU
GLU

4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	185.62Å 185.62Å 185.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.50 – 6.60 49.61 – 6.60	Depositor EDS
% Data completeness (in resolution range)	98.4 (41.50-6.60) 92.9 (49.61-6.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.28 (at 6.68Å)	Xtrriage
Refinement program	PHENIX 1.17_3644	Depositor
R, R_{free}	0.321 , 0.398 0.322 , 0.398	Depositor DCC
R_{free} test set	415 reflections (9.96%)	wwPDB-VP
Wilson B-factor (Å ²)	404.8	Xtrriage
Anisotropy	0.000	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 641.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.055 for l,-k,h	Xtrriage
F_o, F_c correlation	0.75	EDS
Total number of atoms	8839	wwPDB-VP
Average B, all atoms (Å ²)	627.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.24	0/4479	0.43	0/6049
2	B	0.24	0/4496	0.43	0/6069
All	All	0.24	0/8975	0.43	0/12118

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	4406	0	4472	54	0
2	B	4431	0	4494	96	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
All	All	8839	0	8966	147	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 8.

The worst 5 of 147 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:B:571:SER:HA	2:B:574:ARG:HD2	1.63	0.79
2:B:546:LEU:HD22	2:B:572:LEU:HD22	1.66	0.76
2:B:580:ALA:HB1	2:B:585:ARG:HB2	1.69	0.74
2:B:209:GLN:HB3	2:B:371:ARG:HG2	1.71	0.73
2:B:531:ILE:HG22	2:B:581:ARG:HG2	1.71	0.73

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	552/787 (70%)	524 (95%)	26 (5%)	2 (0%)	34 72
2	B	552/684 (81%)	505 (92%)	45 (8%)	2 (0%)	34 72
All	All	1104/1471 (75%)	1029 (93%)	71 (6%)	4 (0%)	34 72

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	254	PRO
1	A	444	ILE
2	B	566	ILE
2	B	527	TYR

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	483/681 (71%)	477 (99%)	6 (1%)	71	83
2	B	502/610 (82%)	488 (97%)	14 (3%)	43	65
All	All	985/1291 (76%)	965 (98%)	20 (2%)	55	74

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	546	LEU
2	B	566	ILE
2	B	581	ARG
2	B	574	ARG
2	B	137	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	162	GLN
2	B	246	GLN
2	B	458	ASN
1	A	537	GLN
1	A	348	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](#)

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 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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.

5.7 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.

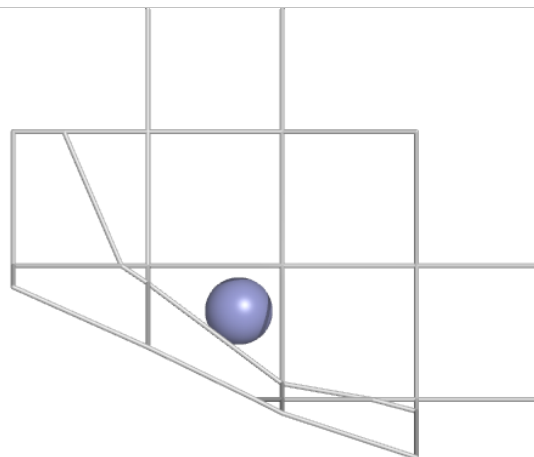
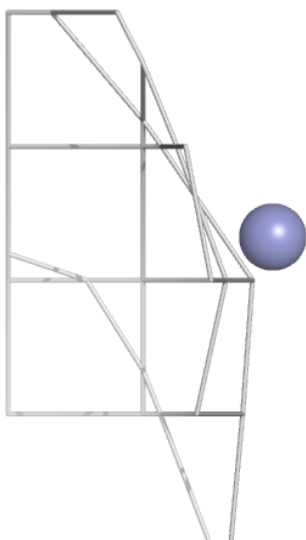
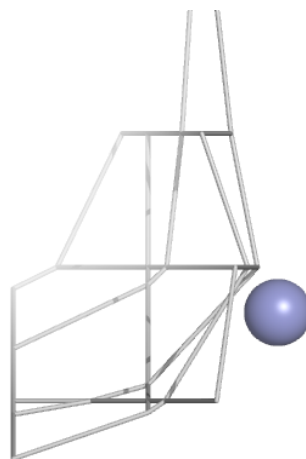
6.4 Ligands

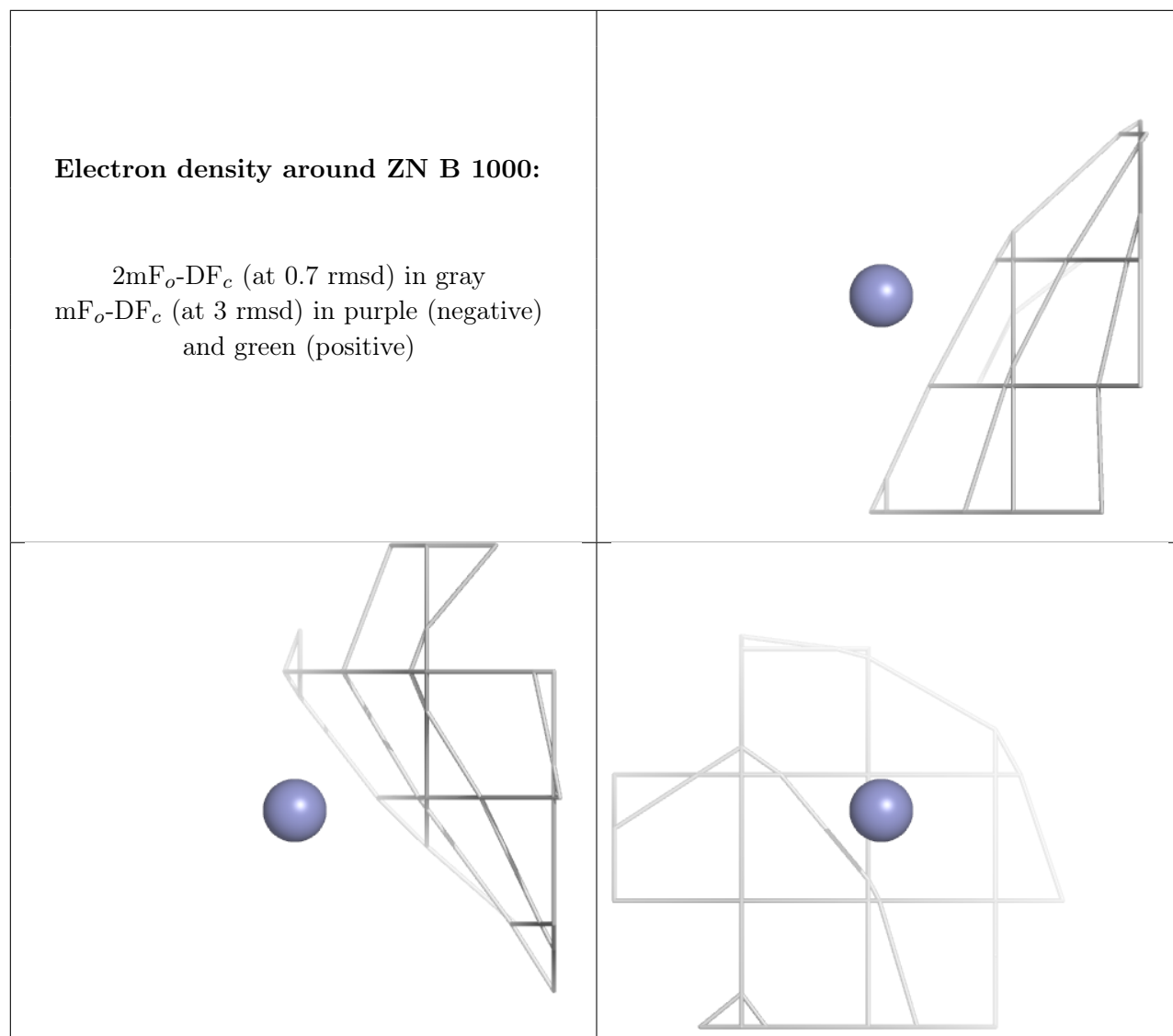
Unable to reproduce the depositors R factor - this section is therefore empty.

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 ZN A 1000:

$2mF_o-DF_c$ (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 depositor's R factor - this section is therefore empty.