Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2023 – 01:31 pm BST

PDB ID	:	7OS6
Title	:	Crystal structure of Rhizobium etli inducible L-asparaginase ReAV (monoclinic form MP1)
Authors	:	Loch, J.I.; Imiolczyk, B.; Gilski, M.; Jaskolski, M.
Deposited on	:	2021-06-07
Resolution	:	1.43 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:

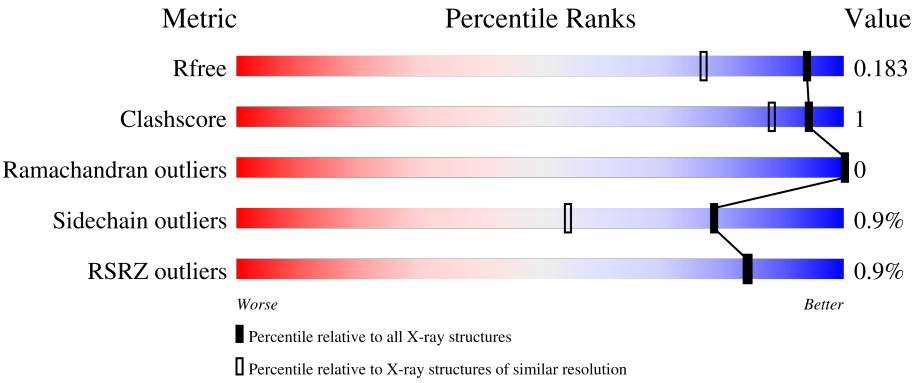
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

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 1.43 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	2021 (1.46-1.42)
Clashscore	141614	2086 (1.46-1.42)
Ramachandran outliers	138981	2047 (1.46-1.42)
Sidechain outliers	138945	2047 (1.46-1.42)
RSRZ outliers	127900	1993 (1.46-1.42)

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% 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	AAA	373	90% · 7%
1	BBB	373	90% · · 6%
1	CCC	373	91% · 6%
1	DDD	373	90% · 6%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 12194 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 L-asparaginase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	347	Total	C	N	O	S	0	14	0
			2644	1639	482	498	25			
1	DDD	350	Total	C	N	O	S	0	12	0
			2655	1646	484	502	23			
1	BBB	350	Total	C	N	O	S	0	12	0
			2655	1644	485	503	23			
1	CCC	350	Total	C	N	O	S	0	9	0
			2638	1630	484	501	23			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-5	GLY	-	expression tag	UNP Q2K0Z2
AAA	-4	ILE	-	expression tag	UNP Q2K0Z2
AAA	-3	ASP	-	expression tag	UNP Q2K0Z2
AAA	-2	PRO	-	expression tag	UNP Q2K0Z2
AAA	-1	PHE	-	expression tag	UNP Q2K0Z2
AAA	0	THR	-	expression tag	UNP Q2K0Z2
DDD	-5	GLY	-	expression tag	UNP Q2K0Z2
DDD	-4	ILE	-	expression tag	UNP Q2K0Z2
DDD	-3	ASP	-	expression tag	UNP Q2K0Z2
DDD	-2	PRO	-	expression tag	UNP Q2K0Z2
DDD	-1	PHE	-	expression tag	UNP Q2K0Z2
DDD	0	THR	-	expression tag	UNP Q2K0Z2
BBB	-5	GLY	-	expression tag	UNP Q2K0Z2
BBB	-4	ILE	-	expression tag	UNP Q2K0Z2
BBB	-3	ASP	-	expression tag	UNP Q2K0Z2
BBB	-2	PRO	-	expression tag	UNP Q2K0Z2
BBB	-1	PHE	-	expression tag	UNP Q2K0Z2
BBB	0	THR	-	expression tag	UNP Q2K0Z2
CCC	-5	GLY	-	expression tag	UNP Q2K0Z2
CCC	-4	ILE	-	expression tag	UNP Q2K0Z2
CCC	-3	ASP	-	expression tag	UNP Q2K0Z2

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Chain	Residue	Modelled	Actual	Comment	Reference
CCC	-2	PRO	-	expression tag	UNP Q2K0Z2
CCC	-1	PHE	-	expression tag	UNP Q2K0Z2
CCC	0	THR	-	expression tag	UNP Q2K0Z2

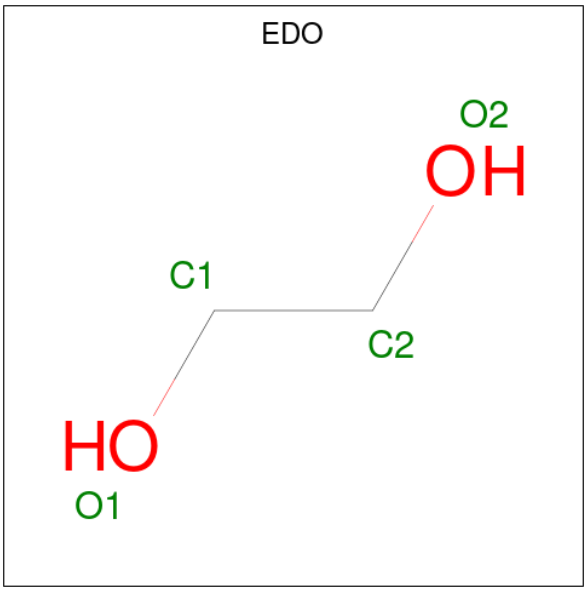
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AAA	1	Total Zn 1 1	0	0
2	DDD	1	Total Zn 1 1	0	0
2	BBB	1	Total Zn 1 1	0	0
2	CCC	1	Total Zn 1 1	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

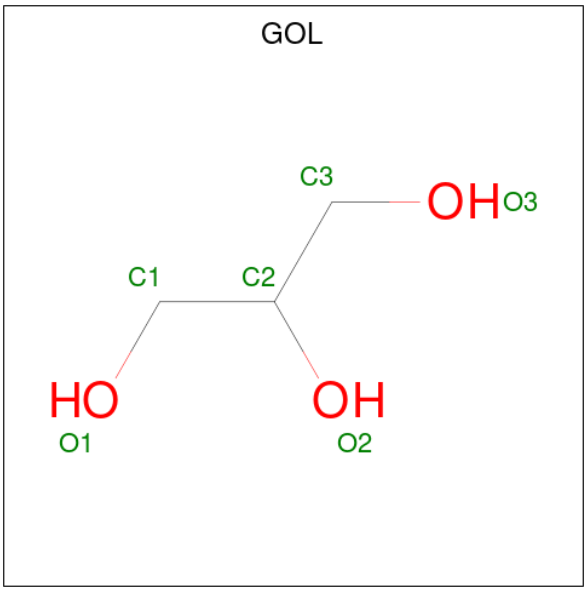
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total Cl 1 1	0	0
3	DDD	2	Total Cl 2 2	0	0
3	BBB	1	Total Cl 1 1	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



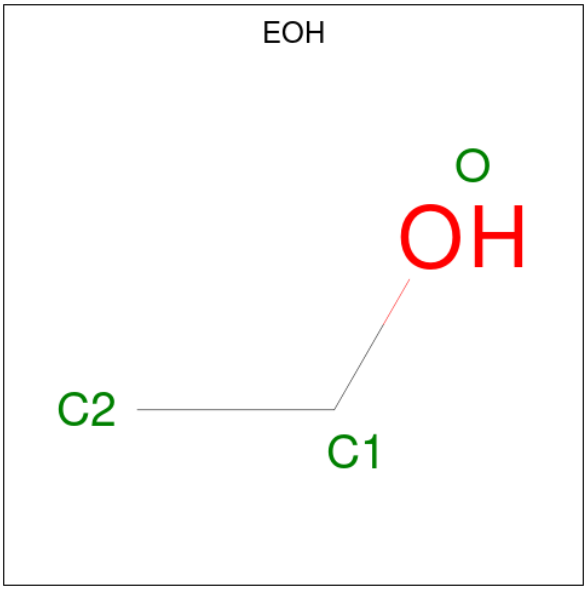
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	AAA	1	Total	C	O	0	0
			4	2	2		
4	DDD	1	Total	C	O	0	0
			4	2	2		
4	DDD	1	Total	C	O	0	0
			4	2	2		
4	BBB	1	Total	C	O	0	0
			4	2	2		
4	CCC	1	Total	C	O	0	0
			4	2	2		
4	CCC	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is ETHANOL (three-letter code: EOH) (formula: C_2H_6O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	DDD	1	Total	C	O	0	0
			3	2	1		

- Molecule 7 is water.

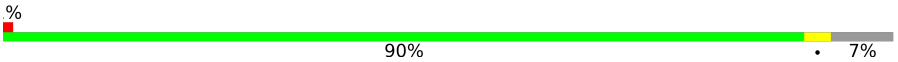
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	AAA	369	Total O 371 371	0	2
7	DDD	399	Total O 400 400	0	1
7	BBB	380	Total O 382 382	0	2
7	CCC	395	Total O 402 402	0	7

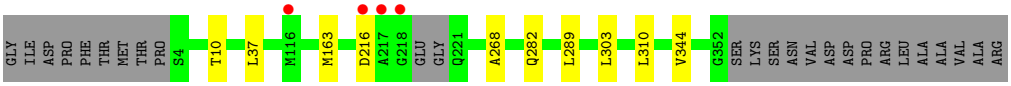
3 Residue-property plots (i)

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: L-asparaginase

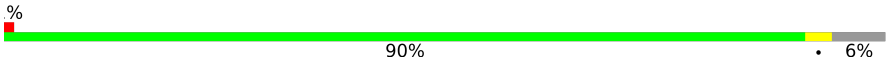
Chain AAA:





- Molecule 1: L-asparaginase

Chain DDD:

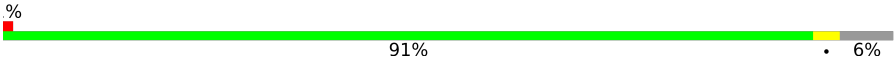


- Molecule 1: L-asparaginase

Chain BBB:

- Molecule 1: L-asparaginase

Chain CCC:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	77.81Å 91.04Å 113.66Å 90.00° 97.08° 90.00°	Depositor
Resolution (Å)	77.22 – 1.43 77.22 – 1.43	Depositor EDS
% Data completeness (in resolution range)	99.3 (77.22-1.43) 99.3 (77.22-1.43)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.16 (at 1.43Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.159 , 0.179 0.161 , 0.183	Depositor DCC
R_{free} test set	1000 reflections (0.35%)	wwPDB-VP
Wilson B-factor (Å^2)	16.2	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 46.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	12194	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.63 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.5799e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: ZN, EDO, CL, CSO, EOH, 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	AAA	0.80	0/2709	0.79	0/3655
1	BBB	0.82	1/2715 (0.0%)	0.80	0/3665
1	CCC	0.83	0/2689	0.79	0/3629
1	DDD	0.81	0/2716	0.78	0/3667
All	All	0.81	1/10829 (0.0%)	0.79	0/14616

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	BBB	0	1
1	CCC	0	1
1	DDD	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BBB	17	GLU	CD-OE2	5.51	1.31	1.25

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	BBB	79	ALA	Peptide
1	CCC	79	ALA	Peptide

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Mol	Chain	Res	Type	Group
1	DDD	79	ALA	Peptide

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	AAA	2644	0	2644	5	0
1	BBB	2655	0	2651	9	0
1	CCC	2638	0	2624	5	0
1	DDD	2655	0	2652	9	0
2	AAA	1	0	0	0	0
2	BBB	1	0	0	0	0
2	CCC	1	0	0	0	0
2	DDD	1	0	0	0	0
3	AAA	1	0	0	0	0
3	BBB	1	0	0	0	0
3	DDD	2	0	0	1	0
4	AAA	4	0	6	0	0
4	BBB	4	0	6	0	0
4	CCC	8	0	12	0	0
4	DDD	8	0	12	2	0
5	DDD	12	0	16	0	0
6	DDD	3	0	6	0	0
7	AAA	371	0	0	1	0
7	BBB	382	0	0	5	0
7	CCC	402	0	0	2	0
7	DDD	400	0	0	2	0
All	All	12194	0	10629	28	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 (28) 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:BBB:115:GLU:O	1:BBB:119:ARG:HD2	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:163[A]:MET:HA	1:AAA:163[A]:MET:HE2	1.71	0.70
1:DDD:113:LEU:HD22	4:DDD:408:EDO:H12	1.75	0.68
1:DDD:264:LEU:HD21	4:DDD:408:EDO:H22	1.81	0.61
1:BBB:10:THR:HB	7:BBB:743:HOH:O	2.06	0.56
1:BBB:37:LEU:HD11	1:BBB:310[B]:LEU:HD21	1.89	0.54
1:BBB:10:THR:HG22	1:BBB:344[B]:VAL:HG22	1.89	0.54
1:CCC:10:THR:HG22	1:CCC:344:VAL:HG22	1.89	0.52
1:CCC:178:ASP:HB3	7:CCC:726:HOH:O	2.10	0.51
1:DDD:10:THR:HB	7:DDD:693:HOH:O	2.09	0.51
1:BBB:187:ASP:OD1	7:BBB:501:HOH:O	2.19	0.51
1:AAA:10:THR:HG22	1:AAA:344:VAL:HG22	1.94	0.50
1:BBB:32:ARG:NH2	7:BBB:502:HOH:O	2.24	0.50
1:BBB:282:GLN:HG3	7:BBB:586:HOH:O	2.12	0.48
1:AAA:282:GLN:HG3	7:AAA:565:HOH:O	2.15	0.46
1:CCC:80:SER:HA	1:CCC:134:ASN:HD22	1.81	0.46
1:CCC:178:ASP:HB3	7:CCC:636:HOH:O	2.15	0.46
1:CCC:268:ALA:HA	1:CCC:303:LEU:HD22	1.99	0.45
1:AAA:268:ALA:HA	1:AAA:303:LEU:HD22	1.99	0.44
1:AAA:37:LEU:HD11	1:AAA:310[A]:LEU:HD21	2.00	0.44
1:DDD:268:ALA:HA	1:DDD:303:LEU:HD22	2.00	0.44
1:DDD:37:LEU:HD11	1:DDD:310[A]:LEU:HD21	2.00	0.43
1:DDD:10:THR:HG22	1:DDD:344[B]:VAL:HG22	1.99	0.43
1:DDD:99:LYS:NZ	7:DDD:518:HOH:O	2.52	0.42
1:DDD:331:PRO:HD2	1:DDD:344[A]:VAL:HG11	2.01	0.42
1:DDD:81:HIS:O	3:DDD:407:CL:CL	2.76	0.41
1:BBB:220:GLY:HA2	7:BBB:549:HOH:O	2.20	0.41
1:BBB:268:ALA:HA	1:BBB:303:LEU:HD22	2.02	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	AAA	355/373 (95%)	345 (97%)	10 (3%)	0	100	100
1	BBB	358/373 (96%)	349 (98%)	9 (2%)	0	100	100
1	CCC	355/373 (95%)	347 (98%)	8 (2%)	0	100	100
1	DDD	358/373 (96%)	348 (97%)	10 (3%)	0	100	100
All	All	1426/1492 (96%)	1389 (97%)	37 (3%)	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	AAA	274/282 (97%)	272 (99%)	2 (1%)	84	64
1	BBB	274/282 (97%)	271 (99%)	3 (1%)	73	47
1	CCC	271/282 (96%)	268 (99%)	3 (1%)	73	47
1	DDD	274/282 (97%)	273 (100%)	1 (0%)	91	80
All	All	1093/1128 (97%)	1084 (99%)	9 (1%)	78	61

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	216	ASP
1	AAA	289	LEU
1	DDD	289	LEU
1	BBB	119	ARG
1	BBB	187	ASP
1	BBB	289	LEU
1	CCC	187	ASP
1	CCC	237	ARG
1	CCC	289	LEU

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)

8 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	CSO	DDD	249[A]	-	3,6,7	0.97	0	0,6,8	-	-
1	CSO	CCC	249[B]	-	3,6,7	0.93	0	0,6,8	-	-
1	CSO	BBB	249[A]	-	3,6,7	0.81	0	0,6,8	-	-
1	CSO	AAA	249[A]	-	3,6,7	0.92	0	0,6,8	-	-
1	CSO	DDD	249[B]	-	3,6,7	0.95	0	0,6,8	-	-
1	CSO	BBB	249[B]	-	3,6,7	0.85	0	0,6,8	-	-
1	CSO	CCC	249[A]	-	3,6,7	0.85	0	0,6,8	-	-
1	CSO	AAA	249[B]	-	3,6,7	0.84	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	DDD	249[A]	-	-	0/1/5/7	-
1	CSO	CCC	249[B]	-	-	0/1/5/7	-
1	CSO	BBB	249[A]	-	-	0/1/5/7	-
1	CSO	AAA	249[A]	-	-	0/1/5/7	-
1	CSO	DDD	249[B]	-	-	0/1/5/7	-
1	CSO	BBB	249[B]	-	-	0/1/5/7	-
1	CSO	CCC	249[A]	-	-	0/1/5/7	-
1	CSO	AAA	249[B]	-	-	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)

Of 17 ligands modelled in this entry, 8 are monoatomic - leaving 9 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	$\#\|Z\| > 2$
4	EDO	DDD	408	-	3,3,3	0.14	0	2,2,2	0.43	0
4	EDO	AAA	403	-	3,3,3	0.16	0	2,2,2	0.19	0
5	GOL	DDD	405	-	5,5,5	0.08	0	5,5,5	0.32	0
4	EDO	CCC	402	-	3,3,3	0.07	0	2,2,2	0.20	0
4	EDO	BBB	402	-	3,3,3	0.32	0	2,2,2	0.35	0
6	EOH	DDD	406	-	2,2,2	0.08	0	1,1,1	0.09	0
4	EDO	DDD	402	-	3,3,3	0.19	0	2,2,2	0.38	0
5	GOL	DDD	401	-	5,5,5	0.07	0	5,5,5	0.26	0
4	EDO	CCC	403	-	3,3,3	0.36	0	2,2,2	0.08	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
4	EDO	DDD	408	-	-	1/1/1/1	-
4	EDO	AAA	403	-	-	1/1/1/1	-
5	GOL	DDD	405	-	-	0/4/4/4	-
4	EDO	CCC	402	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	BBB	402	-	-	0/1/1/1	-
4	EDO	DDD	402	-	-	1/1/1/1	-
5	GOL	DDD	401	-	-	0/4/4/4	-
4	EDO	CCC	403	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	DDD	402	EDO	O1-C1-C2-O2
4	AAA	403	EDO	O1-C1-C2-O2
4	CCC	402	EDO	O1-C1-C2-O2
4	DDD	408	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	DDD	408	EDO	2	0

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^{th} 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	AAA	346/373 (92%)	-0.29	4 (1%)	79	79	12, 18, 36, 64	0
1	BBB	349/373 (93%)	-0.34	1 (0%)	94	95	11, 16, 31, 45	0
1	CCC	349/373 (93%)	-0.29	4 (1%)	80	81	11, 16, 32, 53	0
1	DDD	349/373 (93%)	-0.32	4 (1%)	80	81	12, 18, 35, 48	0
All	All	1393/1492 (93%)	-0.31	13 (0%)	84	84	11, 17, 34, 64	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CCC	3	PRO	3.8
1	CCC	220	GLY	3.0
1	CCC	217	ALA	3.0
1	AAA	216	ASP	2.9
1	DDD	220	GLY	2.8
1	AAA	218	GLY	2.4
1	DDD	154	ASP	2.3
1	AAA	217	ALA	2.2
1	CCC	124	GLN	2.2
1	DDD	319	PRO	2.2
1	DDD	317	GLY	2.1
1	BBB	3	PRO	2.1
1	AAA	116	MET	2.0

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

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^{th} 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
1	CSO	AAA	249[A]	7/8	0.97	0.09	14,15,15,17	4
1	CSO	AAA	249[B]	7/8	0.97	0.09	14,15,18,20	4
1	CSO	DDD	249[A]	7/8	0.98	0.08	14,15,17,20	4
1	CSO	DDD	249[B]	7/8	0.98	0.08	14,15,16,17	4
1	CSO	BBB	249[A]	7/8	0.98	0.07	13,13,15,16	4
1	CSO	BBB	249[B]	7/8	0.98	0.07	13,13,14,17	4
1	CSO	CCC	249[A]	7/8	0.98	0.06	12,13,14,16	4
1	CSO	CCC	249[B]	7/8	0.98	0.06	12,13,16,18	4

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^{th} 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.

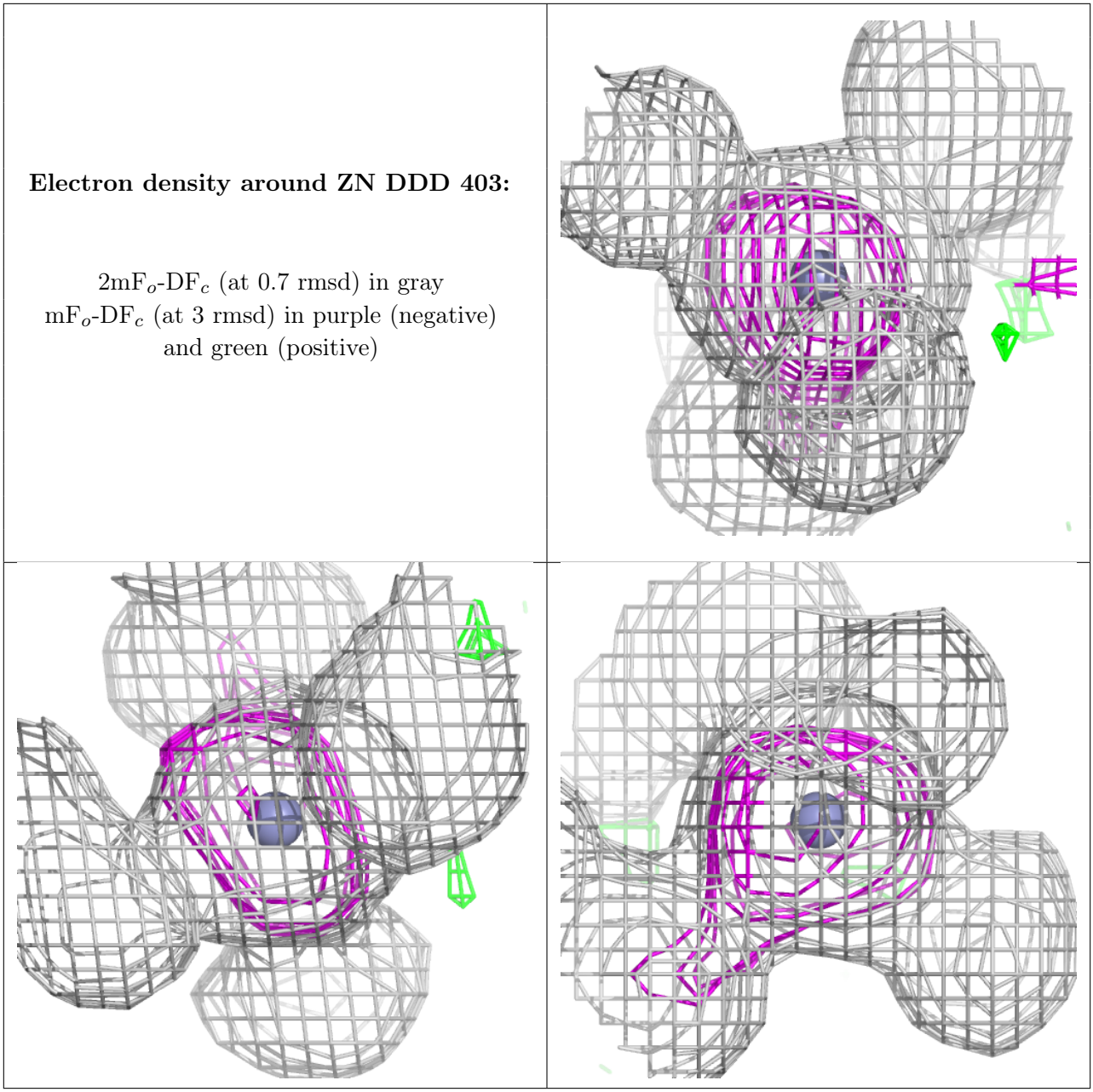
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	GOL	DDD	401	6/6	0.73	0.12	59,61,62,63	0
4	EDO	AAA	403	4/4	0.75	0.17	41,46,48,54	0
4	EDO	DDD	402	4/4	0.77	0.18	44,45,45,48	0
4	EDO	DDD	408	4/4	0.81	0.17	39,43,43,44	0
5	GOL	DDD	405	6/6	0.81	0.28	57,59,60,62	0
6	EOH	DDD	406	3/3	0.81	0.12	41,41,42,45	0
4	EDO	CCC	402	4/4	0.83	0.13	51,52,52,53	0
4	EDO	BBB	402	4/4	0.83	0.12	32,33,36,37	0
4	EDO	CCC	403	4/4	0.88	0.10	30,32,33,34	0
3	CL	BBB	403	1/1	0.97	0.07	35,35,35,35	0
3	CL	DDD	404	1/1	0.97	0.05	32,32,32,32	0
3	CL	AAA	402	1/1	0.98	0.06	33,33,33,33	0
3	CL	DDD	407	1/1	0.99	0.08	28,28,28,28	0
2	ZN	DDD	403	1/1	1.00	0.04	18,18,18,18	0
2	ZN	BBB	401	1/1	1.00	0.04	17,17,17,17	0
2	ZN	CCC	401	1/1	1.00	0.03	17,17,17,17	0
2	ZN	AAA	401	1/1	1.00	0.03	18,18,18,18	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.

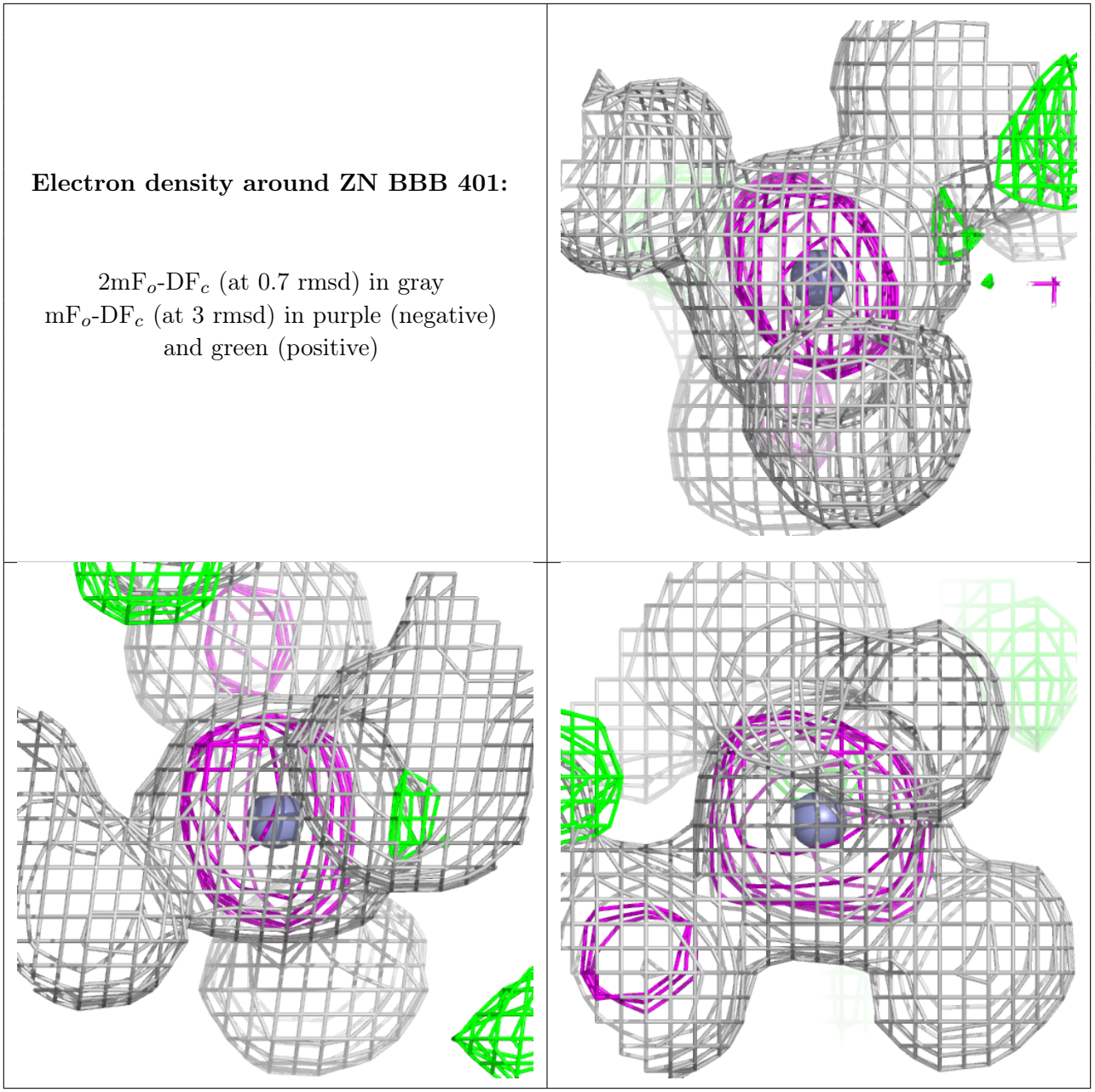
Electron density around ZN DDD 403:

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



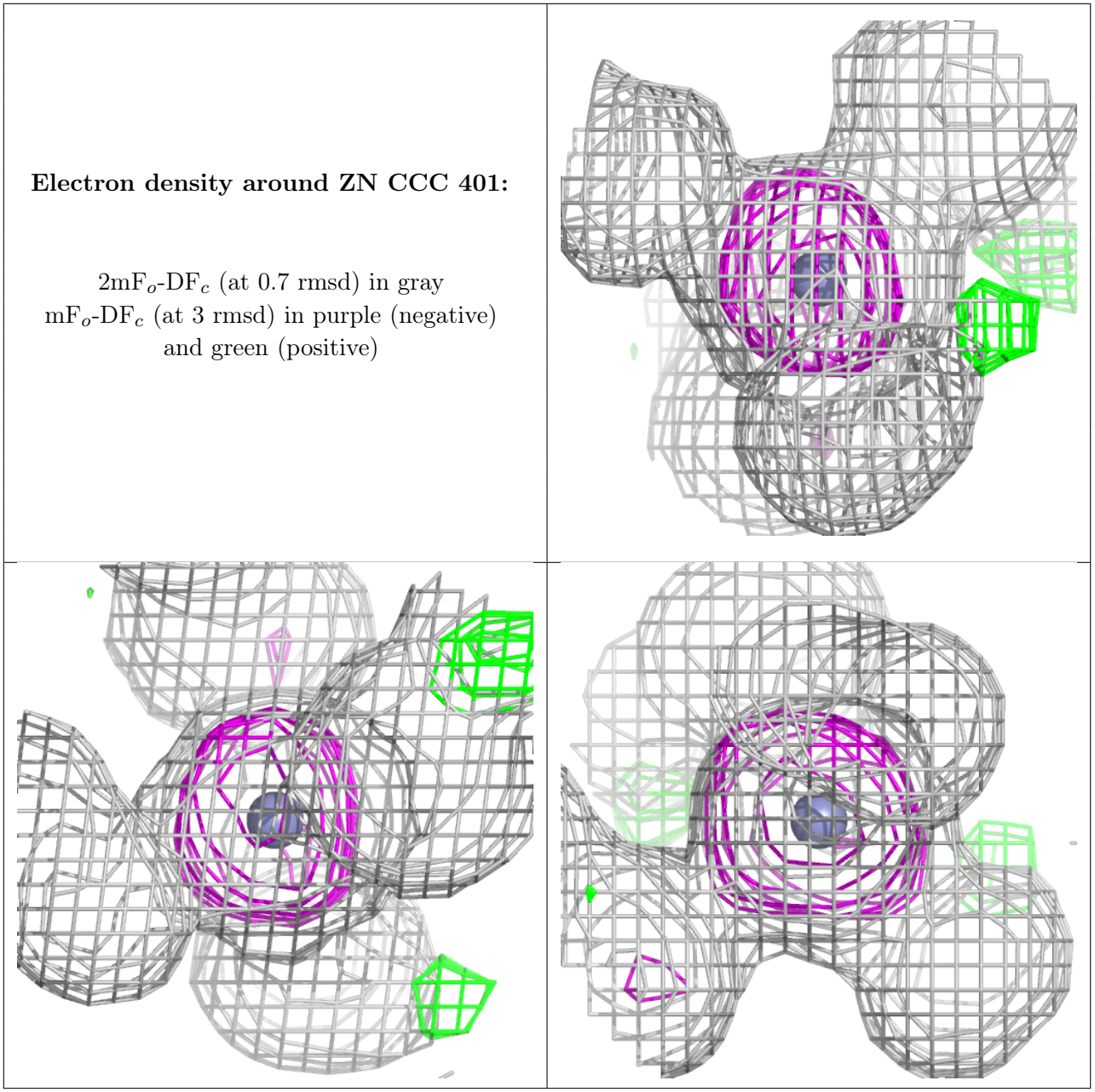
Electron density around ZN BBB 401:

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



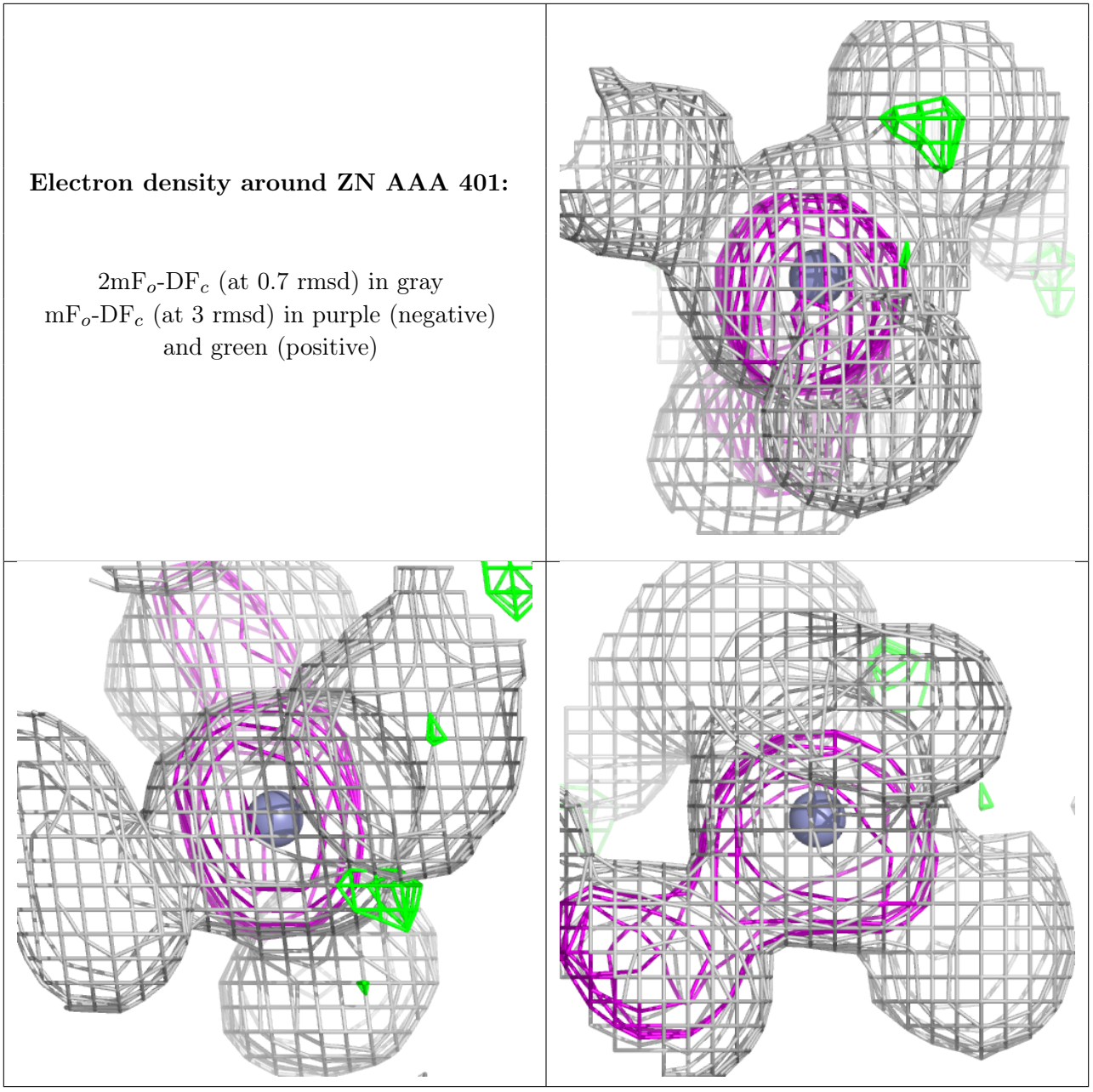
Electron density around ZN CCC 401:

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



Electron density around ZN AAA 401:

$2mF_o$-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.