wwPDB X-ray Structure Validation Summary Report (i)

Apr 10, 2024 – 01:24 pm BST

PDB ID	:	8RUE
Title	:	Crystal structure of Rhizobium etli L-asparaginase ReAV H139A mutant
Authors	:	Pokrywka, K.; Grzechowiak, M.; Sliwiak, J.; Worsztynowicz, P.; Loch, J.I.; Ruszkowski, M.; Gilski, M.; Jaskolski, M.
Deposited on	:	2024-01-30
Resolution	:	1.40 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 (i) 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 (i)) were used in the production of this report:

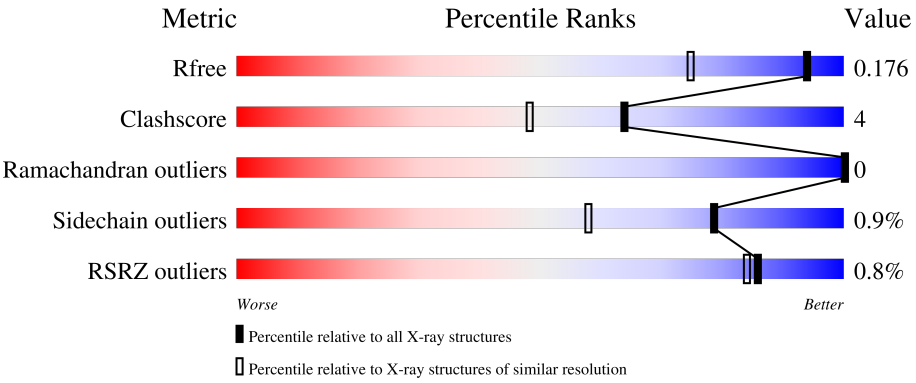
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.40 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	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (1.40-1.40)

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	A	373	87% 6% · 6%
1	B	373	85% 8% 6%
1	C	373	88% 6% 6%
1	D	373	88% 5% 6%

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
2	EDO	B	409	-	-	X	-
4	IPA	C	404	-	-	X	-
7	PEG	B	404	-	-	X	-
8	TRS	D	405	-	-	X	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 12352 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 II protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	350	Total	C	N	O	S	0	20	0
			2686	1670	489	504	23			
1	B	349	Total	C	N	O	S	0	23	0
			2701	1680	490	508	23			
1	C	349	Total	C	N	O	S	0	19	0
			2673	1662	486	501	24			
1	D	349	Total	C	N	O	S	0	17	0
			2665	1655	484	503	23			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP Q2K0Z2
A	-4	ILE	-	expression tag	UNP Q2K0Z2
A	-3	ASP	-	expression tag	UNP Q2K0Z2
A	-2	PRO	-	expression tag	UNP Q2K0Z2
A	-1	PHE	-	expression tag	UNP Q2K0Z2
A	0	THR	-	expression tag	UNP Q2K0Z2
A	139	ALA	HIS	engineered mutation	UNP Q2K0Z2
B	-5	GLY	-	expression tag	UNP Q2K0Z2
B	-4	ILE	-	expression tag	UNP Q2K0Z2
B	-3	ASP	-	expression tag	UNP Q2K0Z2
B	-2	PRO	-	expression tag	UNP Q2K0Z2
B	-1	PHE	-	expression tag	UNP Q2K0Z2
B	0	THR	-	expression tag	UNP Q2K0Z2
B	139	ALA	HIS	engineered mutation	UNP Q2K0Z2
C	-5	GLY	-	expression tag	UNP Q2K0Z2
C	-4	ILE	-	expression tag	UNP Q2K0Z2
C	-3	ASP	-	expression tag	UNP Q2K0Z2
C	-2	PRO	-	expression tag	UNP Q2K0Z2
C	-1	PHE	-	expression tag	UNP Q2K0Z2
C	0	THR	-	expression tag	UNP Q2K0Z2
C	139	ALA	HIS	engineered mutation	UNP Q2K0Z2

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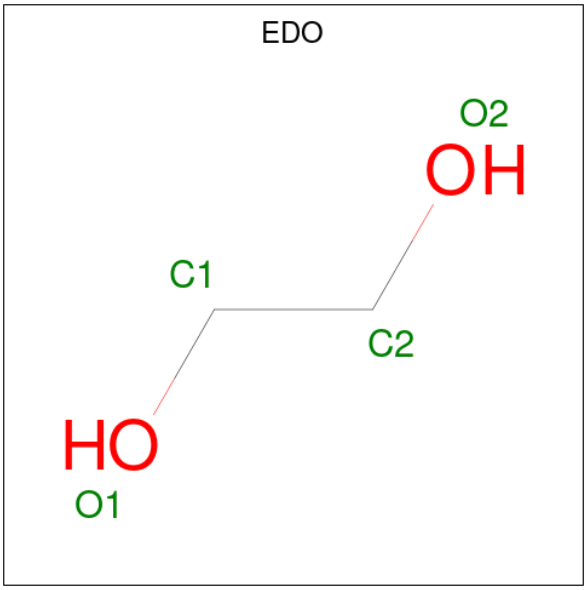
Chain	Residue	Modelled	Actual	Comment	Reference
D	-5	GLY	-	expression tag	UNP Q2K0Z2
D	-4	ILE	-	expression tag	UNP Q2K0Z2
D	-3	ASP	-	expression tag	UNP Q2K0Z2
D	-2	PRO	-	expression tag	UNP Q2K0Z2
D	-1	PHE	-	expression tag	UNP Q2K0Z2
D	0	THR	-	expression tag	UNP Q2K0Z2
D	139	ALA	HIS	engineered mutation	UNP Q2K0Z2

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



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

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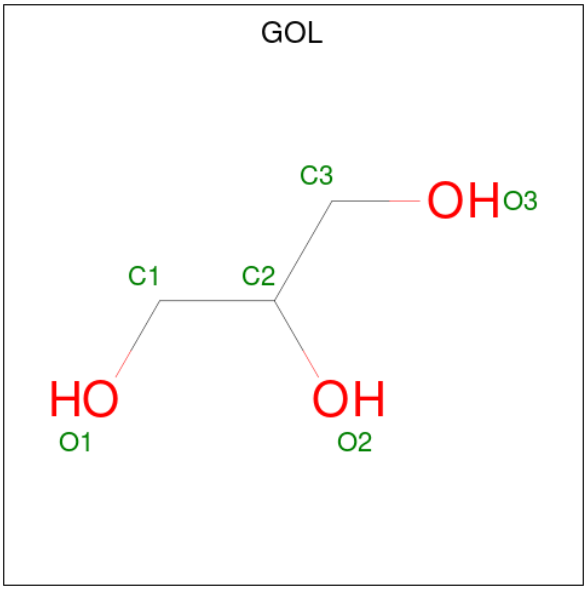
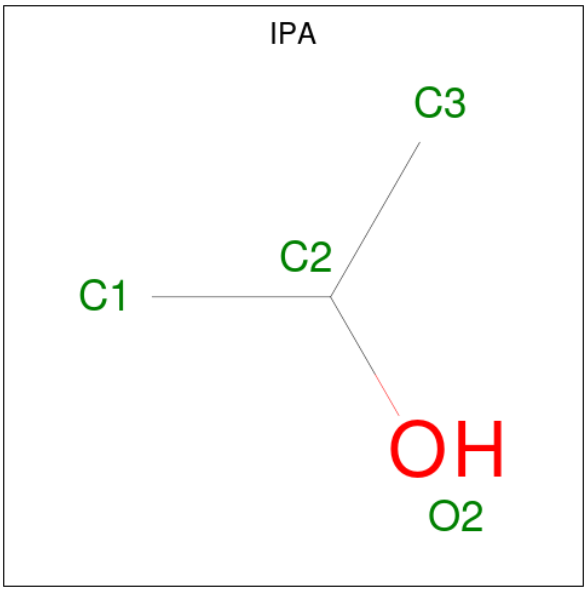
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0

- Molecule 4 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C_3H_8O).



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

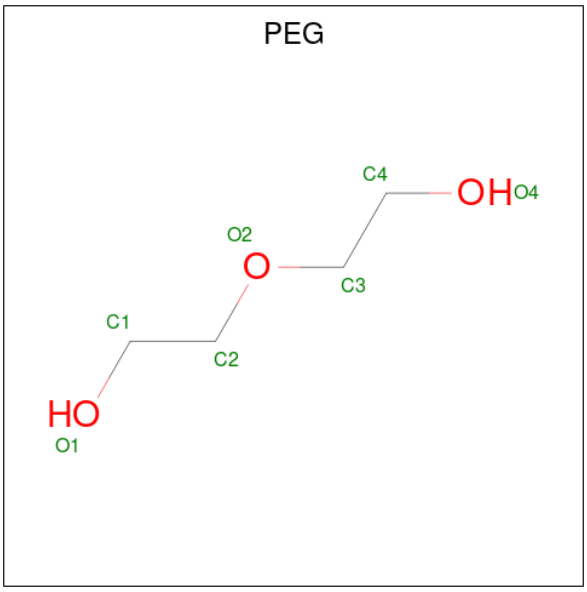
- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Zn 1 1	0	0
5	B	1	Total Zn 1 1	0	0
5	C	1	Total Zn 1 1	0	0
5	D	1	Total Zn 1 1	0	0

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

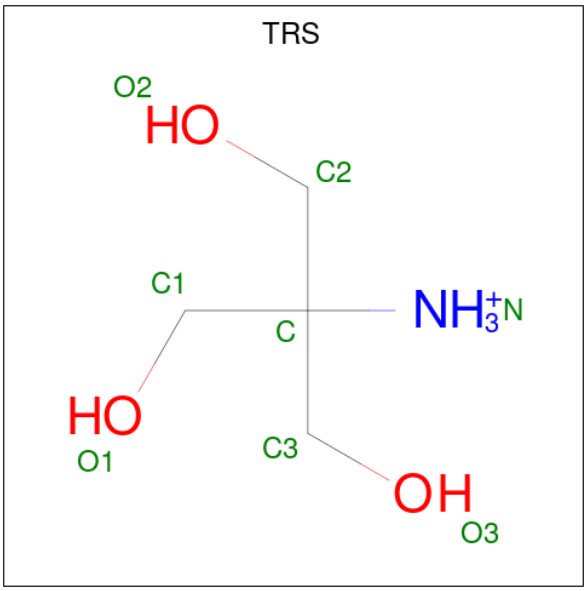
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Cl 1 1	0	0

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C O 7 4 3	0	0
7	B	1	Total C O 7 4 3	0	0
7	D	1	Total C O 7 4 3	0	0

- Molecule 8 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C N O 8 4 1 3	0	0
8	D	1	Total C N O 8 4 1 3	0	0

- Molecule 9 is water.

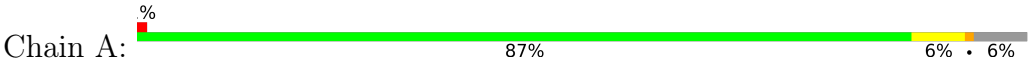
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	378	Total O 378 378	0	0
9	B	375	Total O 375 375	0	0
9	C	365	Total O 365 365	0	0
9	D	361	Total O 361 361	0	0

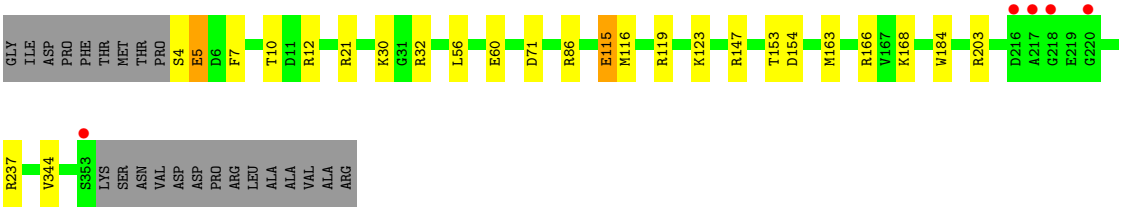
3 Residue-property plots (i)

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 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 II protein

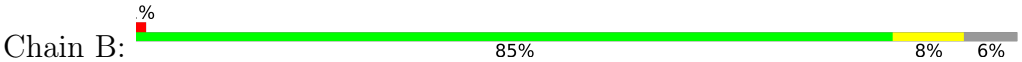
Chain A:

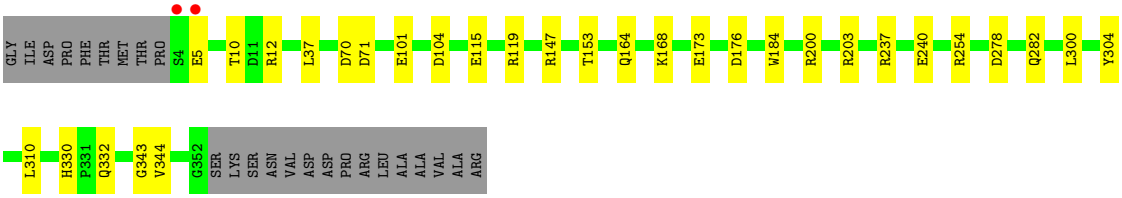




• Molecule 1: L-asparaginase II protein

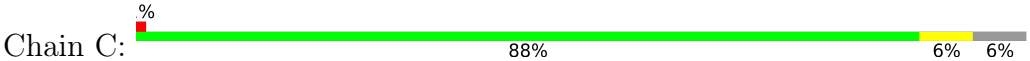
Chain B:

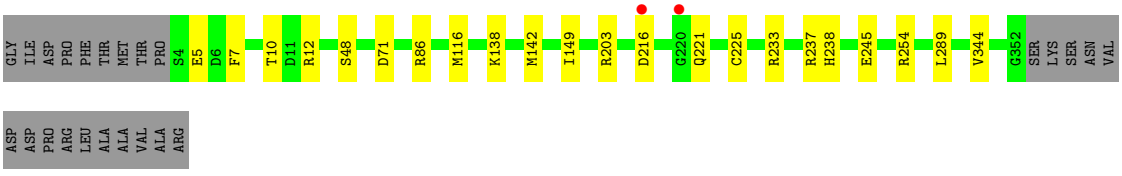




• Molecule 1: L-asparaginase II protein

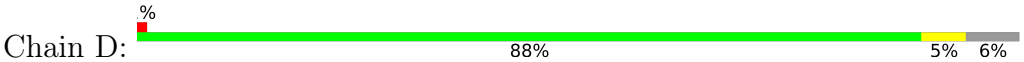
Chain C:

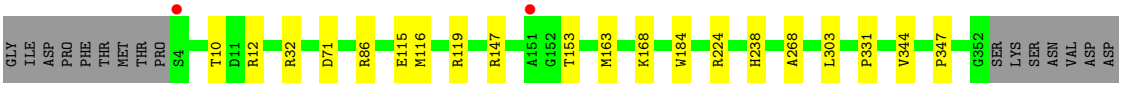




• Molecule 1: L-asparaginase II protein

Chain D:





PRO
ARG
LEU
ALA
ALA
VAL
ALA
ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	77.91Å 91.47Å 114.47Å 90.00° 96.98° 90.00°	Depositor
Resolution (Å)	37.87 – 1.40 77.33 – 1.40	Depositor EDS
% Data completeness (in resolution range)	99.2 (37.87-1.40) 99.2 (77.33-1.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.35 (at 1.40Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.141 , 0.176 0.141 , 0.176	Depositor DCC
R_{free} test set	1547 reflections (0.50%)	wwPDB-VP
Wilson B-factor (Å^2)	15.3	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 46.4	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	12352	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 38.50 % 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 3.6500e-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: TRS, PEG, GOL, IPA, EDO, CL, 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	0.49	0/2790	0.72	0/3765
1	B	0.48	0/2813	0.72	0/3794
1	C	0.46	0/2773	0.70	0/3741
1	D	0.47	0/2759	0.72	0/3723
All	All	0.47	0/11135	0.71	0/15023

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

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	2686	0	2721	21	0
1	B	2701	0	2742	28	0
1	C	2673	0	2710	16	0
1	D	2665	0	2688	24	0
2	A	16	0	24	5	0
2	B	16	0	24	6	0
2	C	8	0	12	0	0
2	D	20	0	30	1	0
3	A	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	6	0	7	2	0
3	D	6	0	8	2	0
4	A	12	0	24	3	0
4	B	4	0	8	2	0
4	C	8	0	16	6	0
4	D	4	0	8	2	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	1	0	0	0	0
7	B	14	0	20	4	0
7	D	7	0	10	3	0
8	B	8	0	12	1	0
8	D	8	0	12	6	0
9	A	378	0	0	3	0
9	B	375	0	0	3	0
9	C	365	0	0	4	0
9	D	361	0	0	4	0
All	All	12352	0	11084	92	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 4.

The worst 5 of 92 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)
4:C:404:IPA:H11	9:D:787:HOH:O	1.63	0.95
1:C:12:ARG:HH22	4:C:404:IPA:H12	1.29	0.94
1:A:154:ASP:H	2:A:402:EDO:H21	1.36	0.91
1:B:12:ARG:HH22	4:B:410:IPA:H32	1.37	0.90
1:D:12:ARG:HH22	4:D:408:IPA:H12	1.41	0.86

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	367/373 (98%)	356 (97%)	11 (3%)	0	100	100
1	B	370/373 (99%)	361 (98%)	9 (2%)	0	100	100
1	C	366/373 (98%)	356 (97%)	10 (3%)	0	100	100
1	D	364/373 (98%)	355 (98%)	9 (2%)	0	100	100
All	All	1467/1492 (98%)	1428 (97%)	39 (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	A	283/282 (100%)	278 (98%)	5 (2%)	59	28
1	B	285/282 (101%)	282 (99%)	3 (1%)	73	50
1	C	281/282 (100%)	279 (99%)	2 (1%)	84	66
1	D	279/282 (99%)	278 (100%)	1 (0%)	91	78
All	All	1128/1128 (100%)	1117 (99%)	11 (1%)	78	53

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	332[B]	GLN
1	C	216	ASP
1	D	116	MET

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Mol	Chain	Res	Type
1	C	289	LEU
1	A	123	LYS

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

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 35 ligands modelled in this entry, 5 are monoatomic - leaving 30 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	$\#\|Z\| > 2$
2	EDO	B	405	-	3,3,3	0.44	0	2,2,2	0.40	0
7	PEG	B	402	-	6,6,6	0.09	0	5,5,5	0.07	0
2	EDO	D	406	-	3,3,3	0.46	0	2,2,2	0.33	0
4	IPA	D	408	-	3,3,3	0.61	0	3,3,3	0.60	0
8	TRS	D	405	-	7,7,7	0.57	0	9,9,9	1.10	1 (11%)
3	GOL	A	403	-	5,5,5	1.17	1 (20%)	5,5,5	0.91	0
2	EDO	A	405	-	3,3,3	0.54	0	2,2,2	0.23	0
4	IPA	A	408	-	3,3,3	0.58	0	3,3,3	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	EDO	B	409	-	3,3,3	0.50	0	2,2,2	0.13	0
4	IPA	A	406	-	3,3,3	0.65	0	3,3,3	0.39	0
2	EDO	D	409	-	3,3,3	0.51	0	2,2,2	0.18	0
2	EDO	C	402	-	3,3,3	0.45	0	2,2,2	0.37	0
2	EDO	C	403	-	3,3,3	0.47	0	2,2,2	0.25	0
2	EDO	B	406	-	3,3,3	0.21	0	2,2,2	0.21	0
4	IPA	C	404	-	3,3,3	0.67	0	3,3,3	0.62	0
3	GOL	B	408	-	5,5,5	1.34	1 (20%)	5,5,5	1.05	0
2	EDO	D	410	-	3,3,3	0.42	0	2,2,2	0.58	0
7	PEG	D	407	-	6,6,6	0.09	0	5,5,5	0.15	0
4	IPA	B	410	-	3,3,3	0.56	0	3,3,3	0.80	0
2	EDO	D	403	-	3,3,3	0.32	0	2,2,2	0.51	0
2	EDO	A	401	-	3,3,3	0.41	0	2,2,2	0.58	0
8	TRS	B	407	-	7,7,7	0.30	0	9,9,9	0.47	0
2	EDO	A	404	-	3,3,3	0.56	0	2,2,2	0.16	0
3	GOL	D	404	-	5,5,5	0.90	0	5,5,5	1.11	0
7	PEG	B	404	-	6,6,6	0.08	0	5,5,5	0.15	0
4	IPA	C	405	-	3,3,3	0.50	0	3,3,3	0.44	0
4	IPA	A	407	-	3,3,3	0.50	0	3,3,3	0.31	0
2	EDO	D	402	-	3,3,3	0.37	0	2,2,2	0.78	0
2	EDO	B	403	-	3,3,3	0.47	0	2,2,2	0.13	0
2	EDO	A	402	-	3,3,3	0.46	0	2,2,2	0.30	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
2	EDO	B	405	-	-	0/1/1/1	-
7	PEG	B	402	-	-	0/4/4/4	-
2	EDO	D	406	-	-	1/1/1/1	-
8	TRS	D	405	-	-	3/9/9/9	-
3	GOL	A	403	-	-	4/4/4/4	-
2	EDO	A	405	-	-	1/1/1/1	-
2	EDO	B	409	-	-	1/1/1/1	-
2	EDO	D	409	-	-	0/1/1/1	-
2	EDO	C	402	-	-	0/1/1/1	-
2	EDO	C	403	-	-	0/1/1/1	-
2	EDO	B	406	-	-	1/1/1/1	-
3	GOL	B	408	-	-	4/4/4/4	-
2	EDO	D	410	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PEG	D	407	-	-	2/4/4/4	-
2	EDO	D	403	-	-	0/1/1/1	-
2	EDO	A	401	-	-	0/1/1/1	-
8	TRS	B	407	-	-	9/9/9/9	-
2	EDO	A	404	-	-	1/1/1/1	-
3	GOL	D	404	-	-	2/4/4/4	-
7	PEG	B	404	-	-	1/4/4/4	-
2	EDO	D	402	-	-	0/1/1/1	-
2	EDO	B	403	-	-	0/1/1/1	-
2	EDO	A	402	-	-	1/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	408	GOL	O2-C2	-2.12	1.37	1.43
3	A	403	GOL	O2-C2	-2.11	1.37	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	D	405	TRS	O1-C1-C	2.71	119.58	111.00

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	403	GOL	O1-C1-C2-C3
3	B	408	GOL	O1-C1-C2-C3
3	B	408	GOL	C1-C2-C3-O3
8	B	407	TRS	N-C-C1-O1
8	B	407	TRS	C1-C-C2-O2

There are no ring outliers.

18 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	408	IPA	2	0
8	D	405	TRS	6	0
2	A	405	EDO	1	0
4	A	408	IPA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	409	EDO	6	0
4	A	406	IPA	1	0
2	D	409	EDO	1	0
4	C	404	IPA	4	0
3	B	408	GOL	2	0
7	D	407	PEG	3	0
4	B	410	IPA	2	0
8	B	407	TRS	1	0
2	A	404	EDO	2	0
3	D	404	GOL	2	0
7	B	404	PEG	4	0
4	C	405	IPA	2	0
4	A	407	IPA	1	0
2	A	402	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	A	350/373 (93%)	-0.47	5 (1%)	75	74	11, 17, 36, 63	0
1	B	349/373 (93%)	-0.51	2 (0%)	89	88	11, 16, 30, 52	0
1	C	349/373 (93%)	-0.49	2 (0%)	89	88	12, 17, 34, 51	0
1	D	349/373 (93%)	-0.52	2 (0%)	89	88	11, 16, 30, 53	0
All	All	1397/1492 (93%)	-0.50	11 (0%)	86	84	11, 17, 33, 63	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	353	SER	4.8
1	D	4	SER	4.4
1	A	216	ASP	3.2
1	B	4	SER	3.2
1	A	220	GLY	3.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

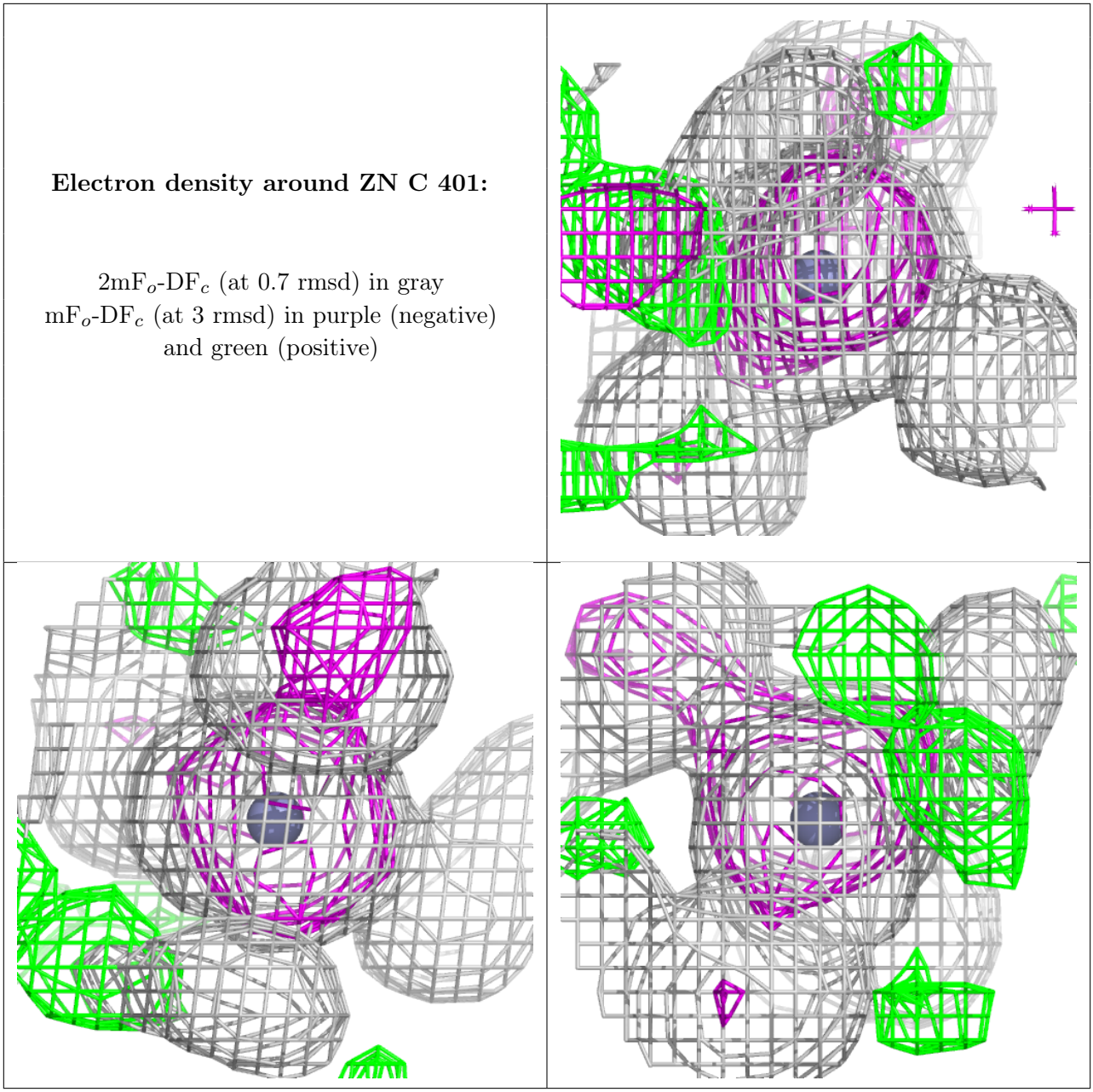
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	EDO	A	404	4/4	0.70	0.15	42,42,43,43	0
7	PEG	D	407	7/7	0.72	0.27	52,53,54,54	0
7	PEG	B	404	7/7	0.78	0.14	60,61,61,61	0
2	EDO	D	409	4/4	0.78	0.22	47,49,49,50	0
2	EDO	A	402	4/4	0.80	0.16	45,46,46,46	0
2	EDO	D	406	4/4	0.81	0.15	56,57,57,58	0
2	EDO	B	406	4/4	0.82	0.29	57,57,57,58	0
2	EDO	B	409	4/4	0.83	0.21	56,57,58,59	0
8	TRS	D	405	8/8	0.83	0.21	26,29,31,31	8
3	GOL	D	404	6/6	0.85	0.14	47,47,48,49	0
2	EDO	C	403	4/4	0.85	0.11	44,44,44,44	0
2	EDO	A	405	4/4	0.86	0.15	30,34,35,35	0
2	EDO	D	403	4/4	0.86	0.18	42,44,45,45	0
8	TRS	B	407	8/8	0.87	0.18	50,52,52,52	0
2	EDO	B	405	4/4	0.87	0.12	53,53,53,54	0
2	EDO	C	402	4/4	0.88	0.14	56,56,56,57	0
4	IPA	A	408	4/4	0.88	0.17	50,50,50,50	0
2	EDO	D	410	4/4	0.89	0.13	55,56,56,56	0
3	GOL	B	408	6/6	0.89	0.19	38,43,45,47	0
7	PEG	B	402	7/7	0.90	0.16	44,46,48,48	0
2	EDO	A	401	4/4	0.90	0.10	53,54,54,54	0
2	EDO	D	402	4/4	0.90	0.09	29,30,31,34	0
3	GOL	A	403	6/6	0.90	0.18	35,39,40,41	0
4	IPA	C	405	4/4	0.90	0.16	47,47,47,48	0
4	IPA	A	407	4/4	0.91	0.07	47,48,48,49	0
4	IPA	A	406	4/4	0.92	0.14	28,30,32,32	0
6	CL	A	410	1/1	0.93	0.06	60,60,60,60	0
2	EDO	B	403	4/4	0.93	0.09	27,28,31,33	0
4	IPA	C	404	4/4	0.94	0.12	25,26,28,29	0
4	IPA	B	410	4/4	0.95	0.15	36,37,38,39	0
4	IPA	D	408	4/4	0.95	0.11	28,30,31,31	0
5	ZN	C	401	1/1	1.00	0.04	19,19,19,19	0
5	ZN	D	401	1/1	1.00	0.04	19,19,19,19	0
5	ZN	A	409	1/1	1.00	0.03	18,18,18,18	0
5	ZN	B	401	1/1	1.00	0.03	19,19,19,19	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.

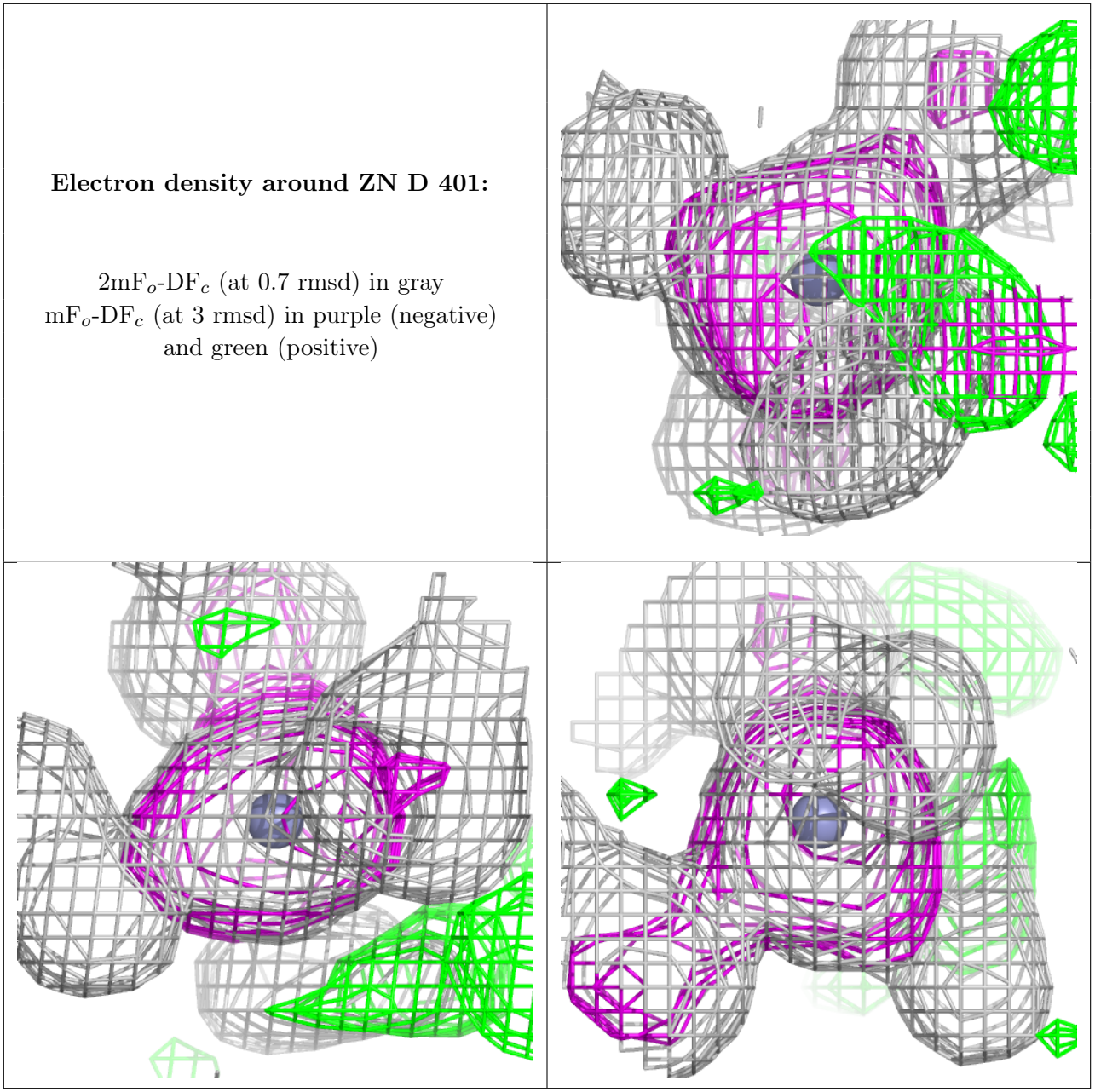
Electron density around ZN C 401:

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



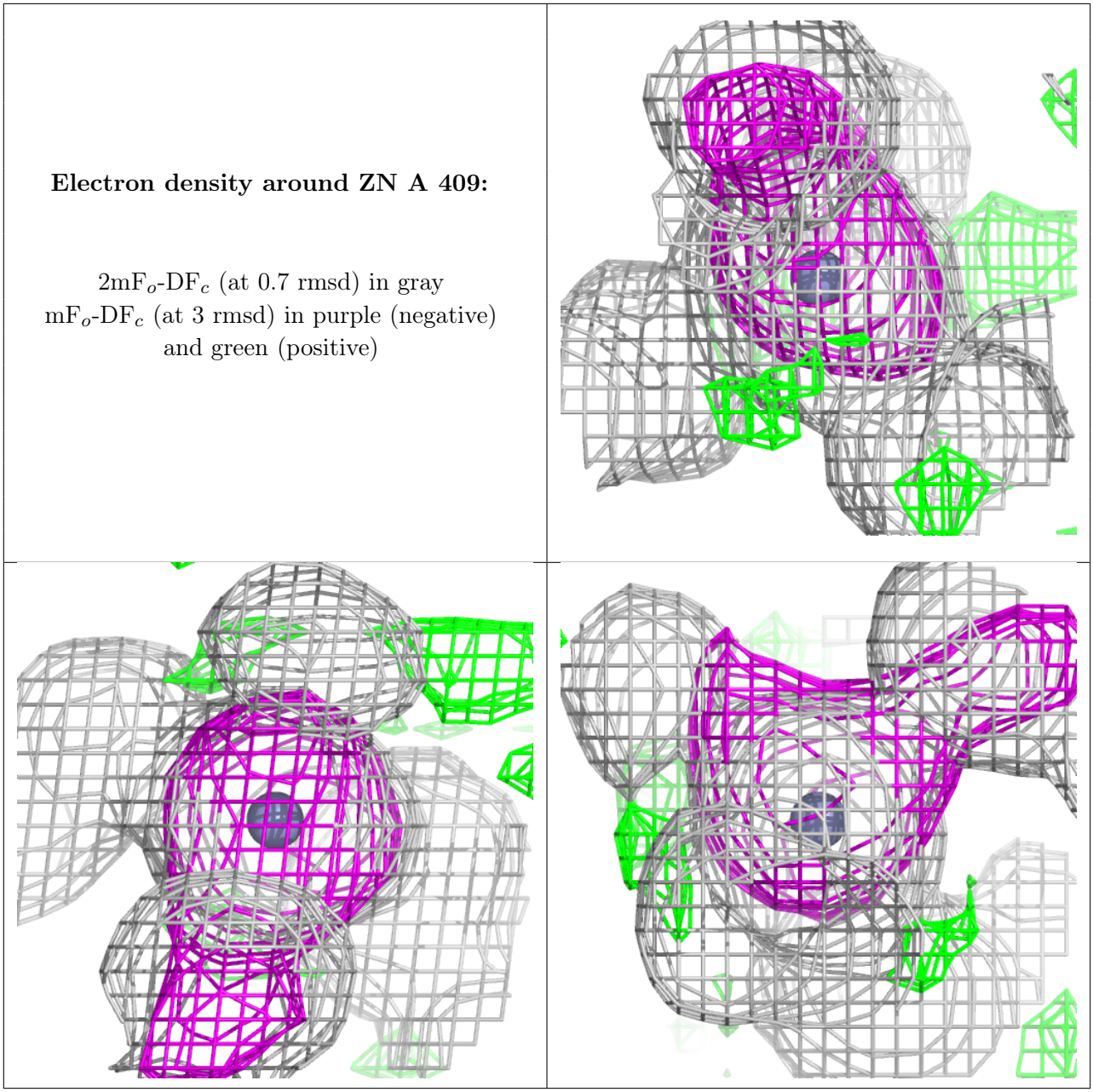
Electron density around ZN D 401:

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



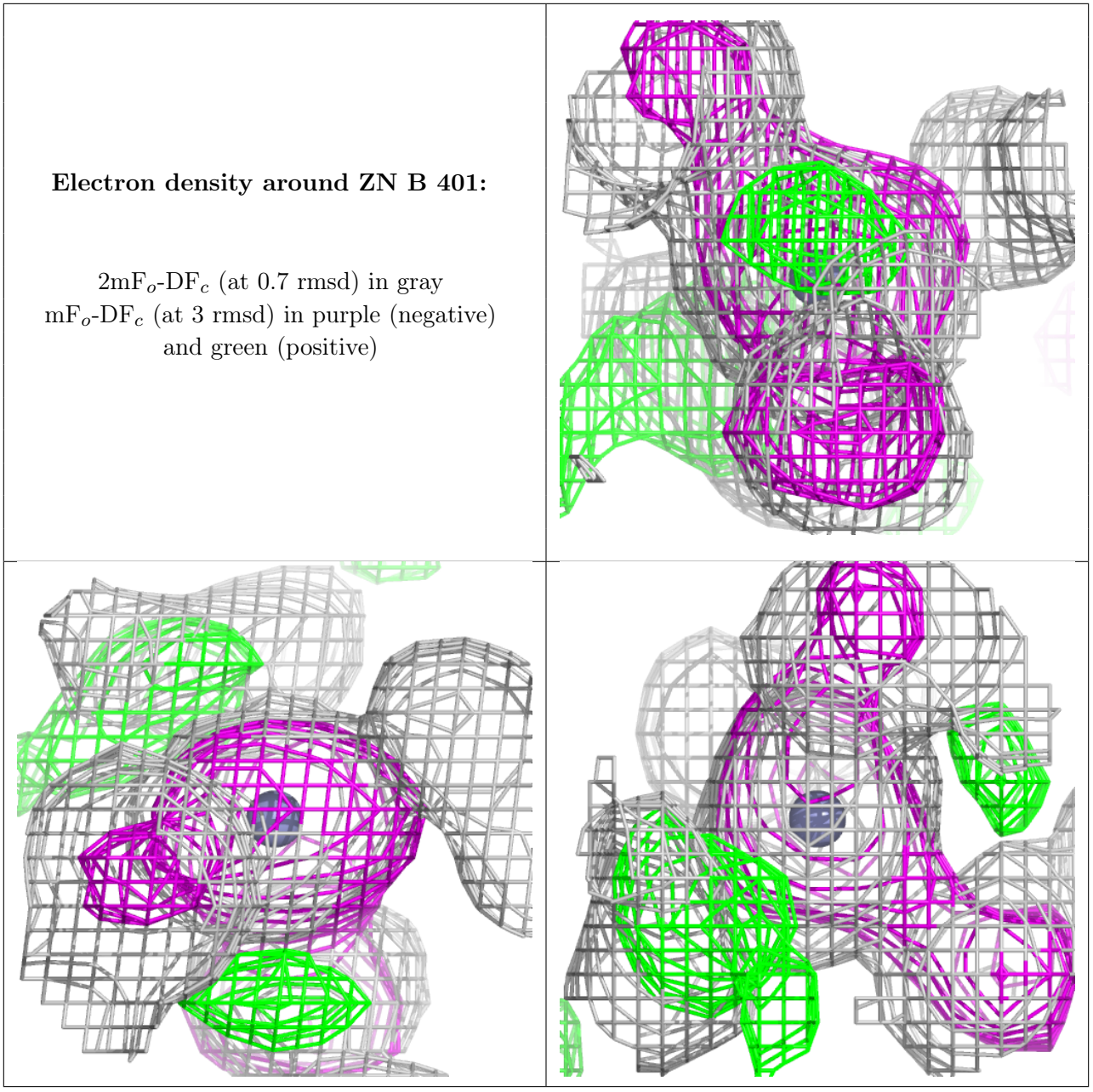
Electron density around ZN A 409:

$2mF_o$-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 B 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.