



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 15, 2021 – 12:05 pm GMT

PDB ID : 7OU1
Title : Crystal structure of Rhizobium etli inducible L-asparaginase ReAV (monoclinic form MP2)
Authors : Imiolczyk, B.; Loch, J.I.; Gilski, M.; Jaskolski, M.
Deposited on : 2021-06-10
Resolution : 1.65 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.4 (270009), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

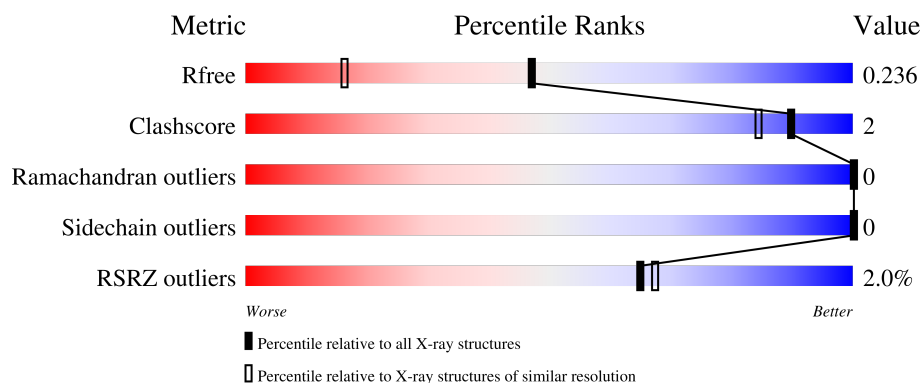
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

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 $\leq 5\%$. 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	<div> <div>%</div> <div>91% 6%</div> </div>
1	BBB	373	<div> <div>2%</div> <div>91% 6%</div> </div>
1	CCC	373	<div> <div>%</div> <div>89% 5% 6%</div> </div>
1	DDD	373	<div> <div>3%</div> <div>92% 6%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11942 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	350	Total	C	N	O	S	0	5	0
			2619	1617	481	499	22			
1	BBB	350	Total	C	N	O	S	0	8	0
			2635	1626	484	503	22			
1	CCC	350	Total	C	N	O	S	0	9	0
			2641	1632	483	503	23			
1	DDD	350	Total	C	N	O	S	0	8	0
			2636	1627	485	502	22			

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
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
CCC	-2	PRO	-	expression tag	UNP Q2K0Z2
CCC	-1	PHE	-	expression tag	UNP Q2K0Z2
CCC	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

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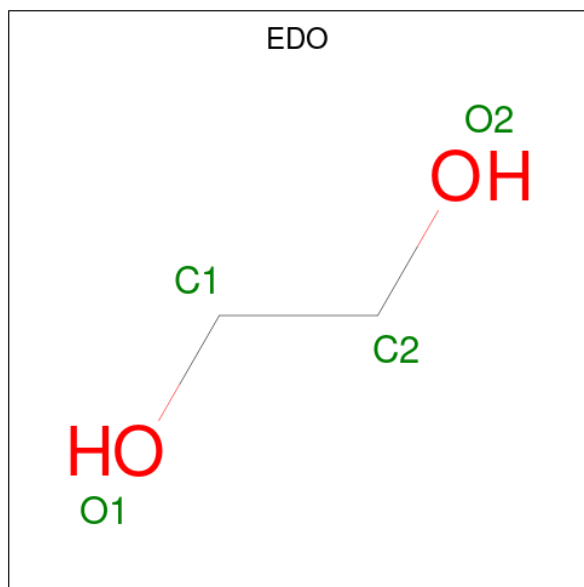
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Chain	Residue	Modelled	Actual	Comment	Reference
DDD	-2	PRO	-	expression tag	UNP Q2K0Z2
DDD	-1	PHE	-	expression tag	UNP Q2K0Z2
DDD	0	THR	-	expression tag	UNP Q2K0Z2

- 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	0	0
			1	1		
2	BBB	1	Total	Zn	0	0
			1	1		
2	CCC	1	Total	Zn	0	0
			1	1		
2	DDD	1	Total	Zn	0	0
			1	1		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	336	Total 336	O 336	0	0
4	BBB	364	Total 364	O 364	0	0
4	CCC	373	Total 373	O 373	0	0
4	DDD	330	Total 330	O 330	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.

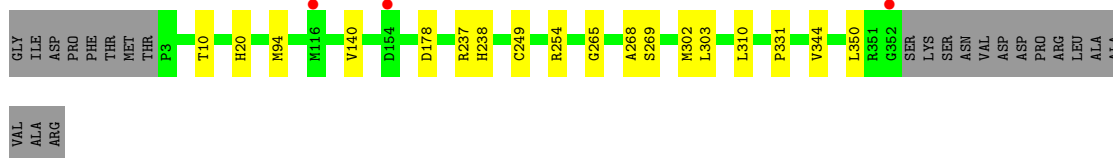
- Molecule 1: L-asparaginase



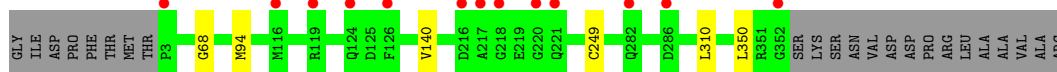
- Molecule 1: L-asparaginase



- Molecule 1: L-asparaginase



- Molecule 1: L-asparaginase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	77.92Å 91.31Å 114.16Å 90.00° 97.11° 90.00°	Depositor
Resolution (Å)	45.65 – 1.65 45.65 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.0 (45.65-1.65) 99.1 (45.65-1.65)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.06 (at 1.64Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.190 , 0.222 0.202 , 0.236	Depositor DCC
R_{free} test set	1000 reflections (0.53%)	wwPDB-VP
Wilson B-factor (Å ²)	14.4	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11942	wwPDB-VP
Average B, all atoms (Å ²)	18.0	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 36.45 % 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 4.9855e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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, CSO, EDO

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	0.84	0/2658	0.83	0/3589
1	BBB	0.87	0/2683	0.84	0/3622
1	CCC	0.86	0/2686	0.82	0/3627
1	DDD	0.83	0/2681	0.82	0/3619
All	All	0.85	0/10708	0.83	0/14457

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	AAA	2619	0	2592	9	0
1	BBB	2635	0	2612	9	0
1	CCC	2641	0	2620	14	0
1	DDD	2636	0	2614	5	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	DDD	4	0	6	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	AAA	336	0	0	5	0
4	BBB	364	0	0	6	0
4	CCC	373	0	0	5	0
4	DDD	330	0	0	2	0
All	All	11942	0	10444	37	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 (37) 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:AAA:249[A]:CSO:OD	4:AAA:501:HOH:O	1.62	1.15
1:BBB:249[A]:CSO:OD	4:BBB:501:HOH:O	1.80	0.97
1:DDD:249[A]:CSO:OD	4:DDD:501:HOH:O	1.80	0.96
1:AAA:249[B]:CSO:OD	4:AAA:502:HOH:O	1.98	0.82
1:CCC:249[A]:CSO:OD	4:CCC:501:HOH:O	1.98	0.82
1:CCC:249[B]:CSO:OD	4:CCC:502:HOH:O	2.07	0.71
1:BBB:249[B]:CSO:OD	4:BBB:502:HOH:O	2.11	0.68
1:DDD:249[B]:CSO:OD	4:DDD:502:HOH:O	2.13	0.65
1:CCC:331:PRO:HD2	1:CCC:344[A]:VAL:HG11	1.80	0.63
1:DDD:310:LEU:HD11	1:DDD:350:LEU:HD21	1.81	0.61
1:DDD:68:GLY:HA3	3:DDD:402:EDO:H22	1.88	0.56
1:CCC:10:THR:HB	4:CCC:718:HOH:O	2.06	0.56
1:AAA:37:LEU:HD11	1:AAA:310:LEU:HD21	1.90	0.54
1:CCC:310:LEU:HD11	1:CCC:350:LEU:HD21	1.90	0.53
1:BBB:330:HIS:HE1	4:BBB:644:HOH:O	1.91	0.52
1:CCC:237:ARG:HG2	1:CCC:238:HIS:CE1	2.45	0.51
1:CCC:10:THR:HG22	1:CCC:344[B]:VAL:HG22	1.96	0.47
1:AAA:10:THR:HB	4:AAA:675:HOH:O	2.14	0.47
1:BBB:268:ALA:HA	1:BBB:303:LEU:HD22	1.97	0.46
1:BBB:223[B]:THR:HG22	4:BBB:541:HOH:O	2.16	0.45
1:CCC:331:PRO:HD2	1:CCC:344[A]:VAL:CG1	2.46	0.45
1:CCC:20:HIS:CD2	1:CCC:302:MET:HG3	2.54	0.43
1:CCC:265:GLY:HA3	1:CCC:269[B]:SER:OG	2.19	0.43
1:CCC:268:ALA:HA	1:CCC:303:LEU:HD22	2.01	0.43
1:AAA:43:MET:HE1	4:AAA:567:HOH:O	2.19	0.42
1:AAA:20:HIS:CD2	1:AAA:302:MET:HG3	2.55	0.42
1:AAA:322:ARG:HB3	4:AAA:753:HOH:O	2.20	0.42
1:DDD:94:MET:HB3	1:DDD:140:VAL:HG11	2.02	0.42
1:BBB:223[B]:THR:CG2	4:BBB:541:HOH:O	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:230:HIS:HA	1:BBB:233:ARG:NH2	2.34	0.41
1:CCC:94:MET:HB3	1:CCC:140:VAL:HG11	2.01	0.41
1:BBB:221:GLN:HA	4:BBB:702:HOH:O	2.21	0.41
1:CCC:254:ARG:NH1	4:CCC:503:HOH:O	2.26	0.41
1:AAA:138:LYS:O	1:AAA:142[B]:MET:HG2	2.21	0.41
1:AAA:268:ALA:HA	1:AAA:303:LEU:HD22	2.03	0.41
1:CCC:178:ASP:HB3	4:CCC:686:HOH:O	2.21	0.40
1:BBB:10:THR:HG22	1:BBB:344:VAL:HG22	2.04	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	AAA	351/373 (94%)	343 (98%)	8 (2%)	0	100	100
1	BBB	354/373 (95%)	344 (97%)	10 (3%)	0	100	100
1	CCC	355/373 (95%)	347 (98%)	8 (2%)	0	100	100
1	DDD	354/373 (95%)	345 (98%)	9 (2%)	0	100	100
All	All	1414/1492 (95%)	1379 (98%)	35 (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	AAA	267/282 (95%)	267 (100%)	0	100	100
1	BBB	270/282 (96%)	270 (100%)	0	100	100
1	CCC	271/282 (96%)	271 (100%)	0	100	100
1	DDD	270/282 (96%)	270 (100%)	0	100	100
All	All	1078/1128 (96%)	1078 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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.

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 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 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

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, 95th 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	349/373 (93%)	-0.05	5 (1%) 75 79	9, 16, 33, 48	0
1	BBB	349/373 (93%)	-0.13	7 (2%) 65 67	8, 13, 29, 39	0
1	CCC	349/373 (93%)	-0.16	3 (0%) 84 86	8, 13, 28, 41	0
1	DDD	349/373 (93%)	0.04	13 (3%) 41 41	9, 16, 35, 65	0
All	All	1396/1492 (93%)	-0.07	28 (2%) 65 67	8, 15, 32, 65	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	3	PRO	4.1
1	DDD	220	GLY	3.7
1	DDD	124	GLN	3.2
1	DDD	3	PRO	3.2
1	DDD	116	MET	3.1
1	DDD	126	PHE	3.0
1	AAA	286	ASP	2.8
1	CCC	154	ASP	2.8
1	DDD	216	ASP	2.8
1	DDD	218	GLY	2.8
1	AAA	220	GLY	2.7
1	CCC	352	GLY	2.7
1	BBB	3	PRO	2.7
1	DDD	217	ALA	2.6
1	AAA	122	ILE	2.6
1	DDD	352	GLY	2.6
1	DDD	119	ARG	2.6
1	BBB	151	ALA	2.4
1	DDD	221	GLN	2.4
1	CCC	116	MET	2.3
1	BBB	119	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	BBB	116	MET	2.2
1	DDD	282	GLN	2.2
1	BBB	154	ASP	2.1
1	BBB	220	GLY	2.1
1	AAA	127	ILE	2.0
1	BBB	122	ILE	2.0
1	DDD	286	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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, 95th 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	DDD	249[A]	7/8	0.96	0.10	12,14,17,17	4
1	CSO	DDD	249[B]	7/8	0.96	0.10	12,13,15,16	4
1	CSO	BBB	249[A]	7/8	0.98	0.08	11,11,13,13	4
1	CSO	BBB	249[B]	7/8	0.98	0.08	11,11,14,15	4
1	CSO	CCC	249[A]	7/8	0.98	0.09	12,12,15,17	7
1	CSO	CCC	249[B]	7/8	0.98	0.09	12,12,13,14	7
1	CSO	AAA	249[A]	7/8	0.98	0.10	13,14,15,17	4
1	CSO	AAA	249[B]	7/8	0.98	0.10	13,13,14,15	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, 95th 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
3	EDO	DDD	402	4/4	0.80	0.14	43,43,44,45	0
2	ZN	AAA	401	1/1	0.99	0.04	22,22,22,22	0
2	ZN	CCC	401	1/1	1.00	0.03	18,18,18,18	0

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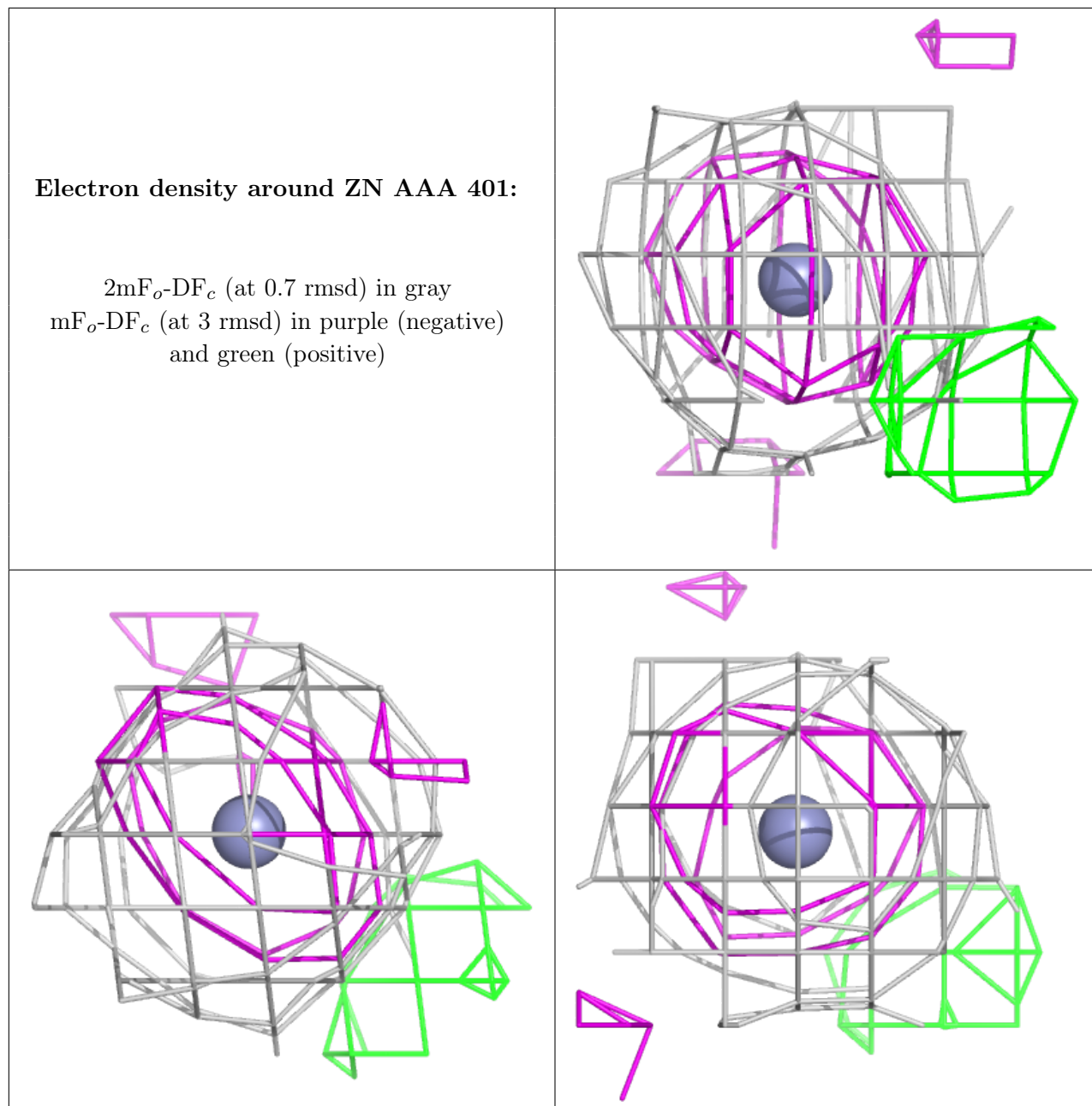
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ZN	DDD	401	1/1	1.00	0.04	16,16,16,16	1
2	ZN	BBB	401	1/1	1.00	0.03	20,20,20,20	0

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.

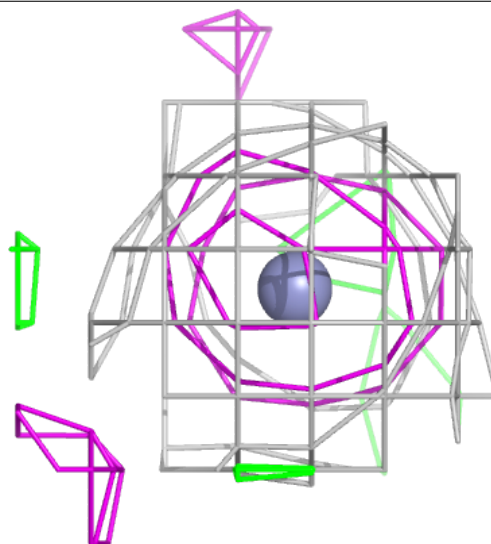
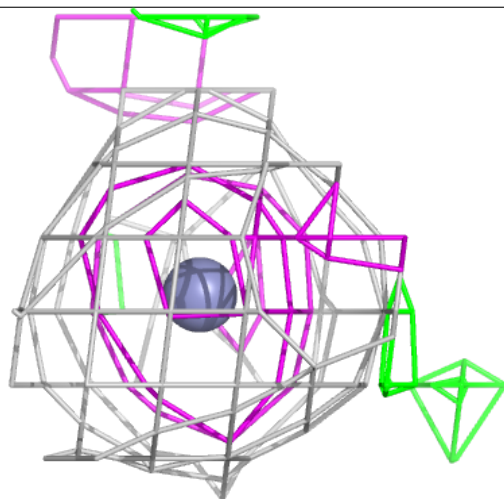
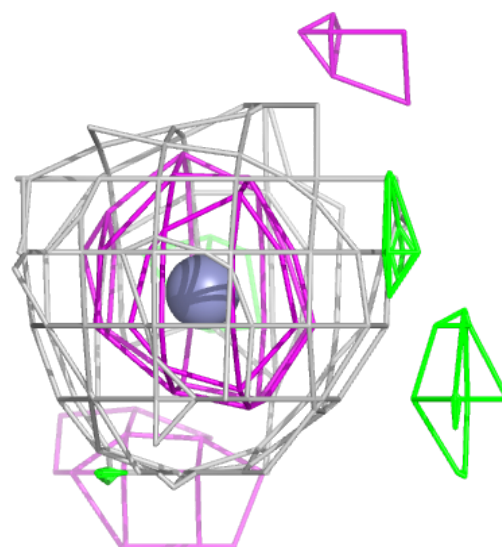
Electron density around ZN AAA 401:

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



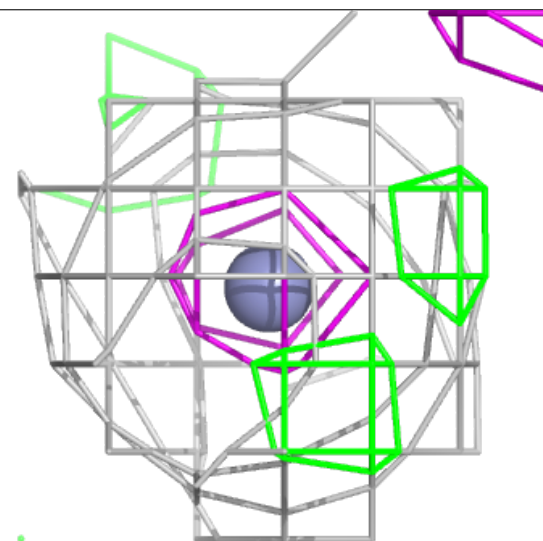
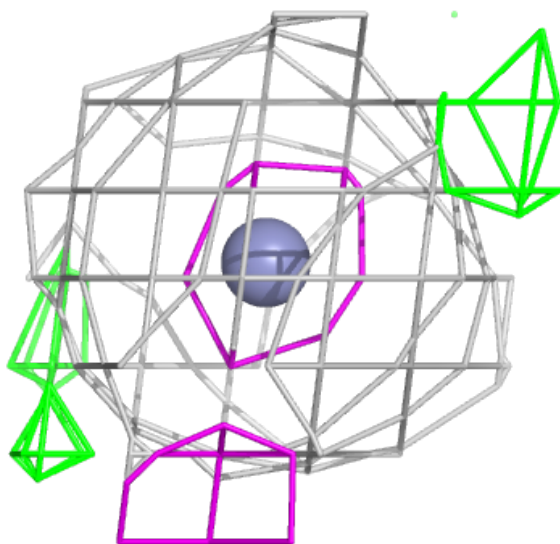
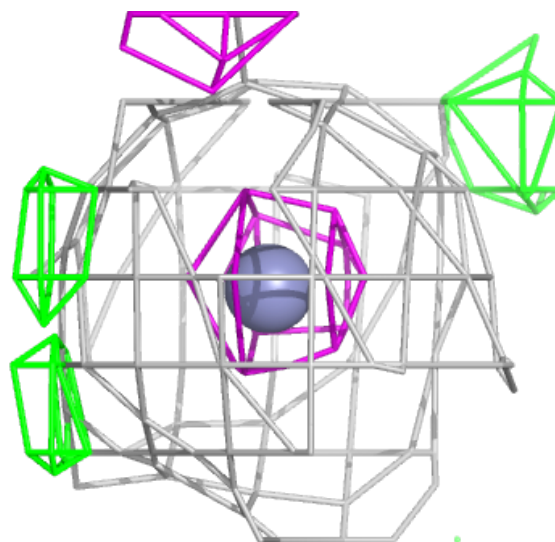
Electron density around ZN CCC 401:

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



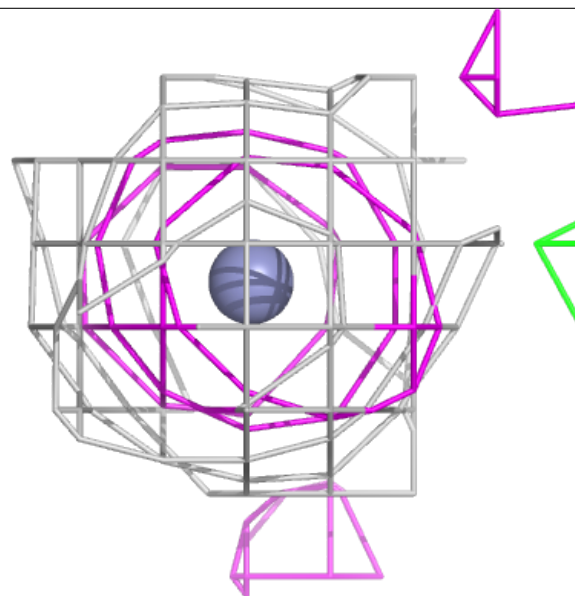
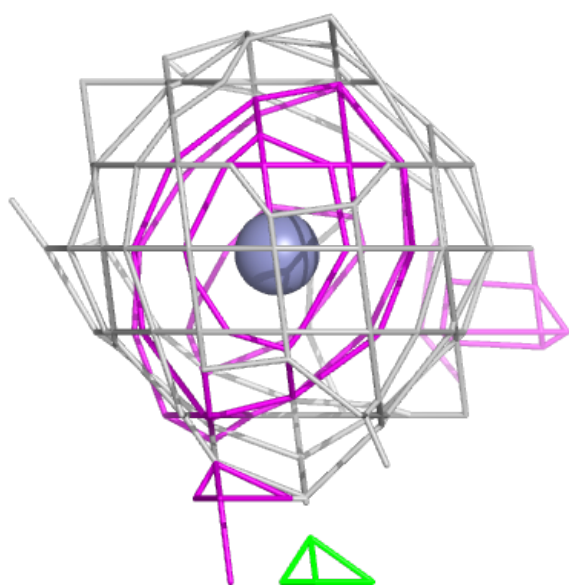
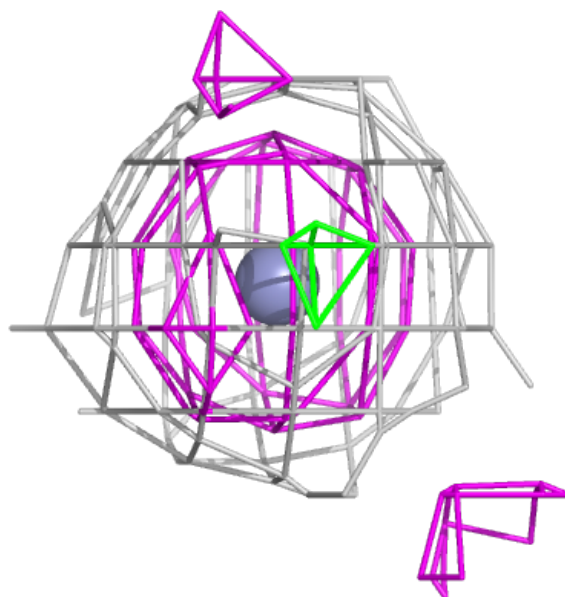
Electron density around ZN DDD 401:

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



Electron density around ZN 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.