



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 07:03 AM UTC

PDB ID : 7OS5 / pdb_00007os5
Title : Crystal structure of Rhizobium etli inducible L-asparaginase ReAV (orthorhombic form OP)
Authors : Loch, J.I.; Imiolczyk, B.; Gilski, M.; Jaskolski, M.
Deposited on : 2021-06-07
Resolution : 1.29 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

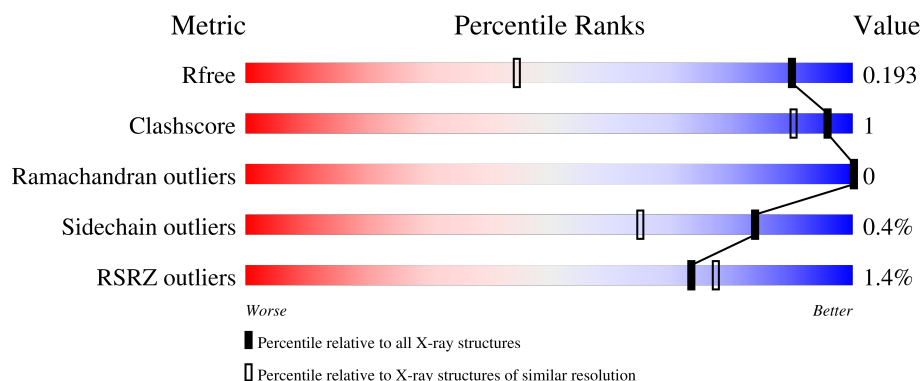
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.29 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}	180053	1553 (1.30-1.30)
Clashscore	190562	1595 (1.30-1.30)
Ramachandran outliers	187476	1551 (1.30-1.30)
Sidechain outliers	187428	1551 (1.30-1.30)
RSRZ outliers	180081	1549 (1.30-1.30)

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	% 94% • •
1	BBB	373	% 91% • 6%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6073 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	366	Total	C	N	O	S	0	11	0
			2767	1709	504	529	25			
1	BBB	349	Total	C	N	O	S	0	7	0
			2617	1617	479	498	23			

There are 12 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

- Molecule 2 is ZINC ION (CCD ID: 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		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).

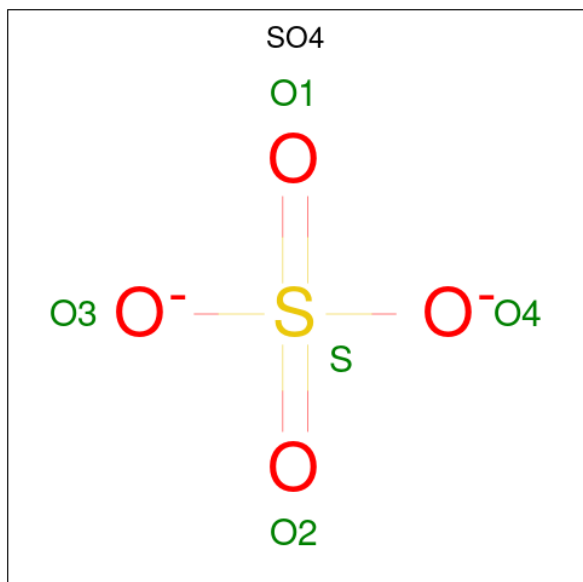


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	AAA	1	Total	C	O	0	0
			4	2	2		
3	BBB	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	1	Total	Cl	0	0
			1	1		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	1	Total O S 5 4 1	0	0
5	AAA	1	Total O S 5 4 1	0	0
5	AAA	1	Total O S 5 4 1	0	0
5	AAA	1	Total O S 5 4 1	0	0
5	BBB	1	Total O S 5 4 1	0	0
5	BBB	1	Total O S 5 4 1	0	0
5	BBB	1	Total O S 5 4 1	0	0
5	BBB	1	Total O S 5 4 1	0	0
5	BBB	1	Total O S 5 4 1	0	0
5	BBB	1	Total O S 5 4 1	0	0

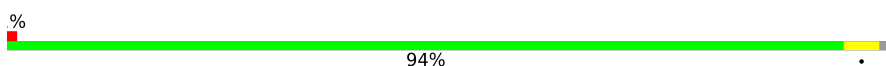
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	AAA	317	Total O 317 317	0	0
6	BBB	311	Total O 311 311	0	0

3 Residue-property plots [i](#)

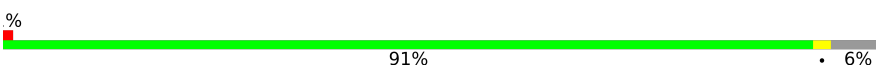
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

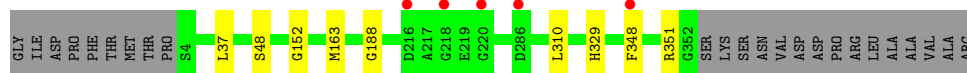
- Molecule 1: L-asparaginase

Chain AAA:  94%



- Molecule 1: L-asparaginase

Chain BBB:  91% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.23Å 91.14Å 106.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	69.11 – 1.29 69.11 – 1.29	Depositor EDS
% Data completeness (in resolution range)	68.6 (69.11-1.29) 68.6 (69.11-1.29)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 1.29Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.155 , 0.194 0.155 , 0.193	Depositor DCC
R_{free} test set	1000 reflections (0.77%)	wwPDB-VP
Wilson B-factor (Å ²)	6.4	Xtriage
Anisotropy	1.607	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6073	wwPDB-VP
Average B, all atoms (Å ²)	16.0	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 31.05 % 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 1.1798e-03. 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: SO4, EDO, ZN, CSO, CL

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	1.12	1/2826 (0.0%)	1.14	2/3816 (0.1%)
1	BBB	1.12	1/2664 (0.0%)	1.15	2/3596 (0.1%)
All	All	1.12	2/5490 (0.0%)	1.14	4/7412 (0.1%)

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	AAA	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BBB	329	HIS	CE1-NE2	7.03	1.39	1.32
1	AAA	329	HIS	CE1-NE2	5.43	1.38	1.32

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	348	PHE	CA-CB-CG	6.75	120.55	113.80
1	AAA	348	PHE	CA-CB-CG	6.29	120.09	113.80
1	AAA	193	THR	CB-CA-C	5.28	117.12	109.20
1	BBB	351	ARG	CB-CA-C	5.12	118.60	109.38

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AAA	79	ALA	Peptide

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	AAA	2767	0	2745	8	0
1	BBB	2617	0	2599	5	0
2	AAA	1	0	0	0	0
2	BBB	1	0	0	0	0
3	AAA	4	0	6	0	0
3	BBB	4	0	6	0	0
4	AAA	1	0	0	0	0
5	AAA	20	0	0	0	0
5	BBB	30	0	0	1	0
6	AAA	317	0	0	2	0
6	BBB	311	0	0	1	0
All	All	6073	0	5356	12	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.

The worst 5 of 12 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:163[B]:MET:HE2	1:BBB:163[B]:MET:HA	1.77	0.65
1:AAA:187[B]:ASP:OD1	1:AAA:189:CYS:SG	2.57	0.62
1:AAA:187[B]:ASP:OD2	1:AAA:189:CYS:SG	2.58	0.62
1:AAA:187[B]:ASP:CG	1:AAA:189:CYS:SG	2.83	0.62
1:AAA:-3:ASP:N	6:AAA:510:HOH:O	2.47	0.48

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	371/373 (100%)	363 (98%)	8 (2%)	0	100	100
1	BBB	352/373 (94%)	344 (98%)	8 (2%)	0	100	100
All	All	723/746 (97%)	707 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	286/282 (101%)	284 (99%)	2 (1%)	76	50
1	BBB	268/282 (95%)	268 (100%)	0	100	100
All	All	554/564 (98%)	552 (100%)	2 (0%)	84	65

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	147	ARG
1	AAA	289	LEU

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 ⓘ

4 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	BBB	249[A]	-	3,6,7	0.85	0	1,6,8	0.35	0
1	CSO	AAA	249[B]	-	3,6,7	0.79	0	1,6,8	0.72	0
1	CSO	BBB	249[B]	-	3,6,7	0.97	0	1,6,8	0.93	0
1	CSO	AAA	249[A]	-	3,6,7	0.81	0	1,6,8	0.69	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
1	CSO	BBB	249[A]	-	-	0/1/5/7	-
1	CSO	AAA	249[B]	-	-	0/1/5/7	-
1	CSO	BBB	249[B]	-	-	1/1/5/7	-
1	CSO	AAA	249[A]	-	-	1/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AAA	249[A]	CSO	N-CA-CB-SG
1	BBB	249[B]	CSO	N-CA-CB-SG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 3 are monoatomic - leaving 12 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	SO4	BBB	406	-	4,4,4	0.22	0	6,6,6	0.19	0
3	EDO	BBB	404	-	3,3,3	0.13	0	2,2,2	0.24	0
5	SO4	BBB	407	-	4,4,4	0.28	0	6,6,6	0.30	0
3	EDO	AAA	402	-	3,3,3	0.10	0	2,2,2	0.20	0
5	SO4	AAA	404	-	4,4,4	0.40	0	6,6,6	0.15	0
5	SO4	BBB	403	-	4,4,4	0.32	0	6,6,6	0.05	0
5	SO4	BBB	405	-	4,4,4	0.28	0	6,6,6	0.16	0
5	SO4	AAA	406	-	4,4,4	0.35	0	6,6,6	0.11	0
5	SO4	AAA	405	-	4,4,4	0.40	0	6,6,6	0.06	0
5	SO4	AAA	407	-	4,4,4	0.50	0	6,6,6	0.28	0
5	SO4	BBB	408	-	4,4,4	0.34	0	6,6,6	0.08	0
5	SO4	BBB	402	-	4,4,4	0.52	0	6,6,6	0.11	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
3	EDO	AAA	402	-	-	0/1/1/1	-
3	EDO	BBB	404	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	BBB	404	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	BBB	405	SO4	1	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	365/373 (97%)	-0.15	5 (1%) 73 77	4, 11, 31, 68	10 (2%)
1	BBB	348/373 (93%)	-0.09	5 (1%) 73 77	5, 12, 29, 68	6 (1%)
All	All	713/746 (95%)	-0.12	10 (1%) 73 77	4, 11, 31, 68	16 (2%)

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	348	PHE	5.8
1	BBB	216	ASP	3.3
1	BBB	220	GLY	3.1
1	BBB	218	GLY	3.1
1	AAA	321	VAL	2.7

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	BBB	249[A]	7/8	0.98	0.05	8,8,10,15	4
1	CSO	BBB	249[B]	7/8	0.98	0.05	8,8,16,17	4
1	CSO	AAA	249[A]	7/8	0.99	0.04	8,8,14,14	4
1	CSO	AAA	249[B]	7/8	0.99	0.04	8,8,11,18	4

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

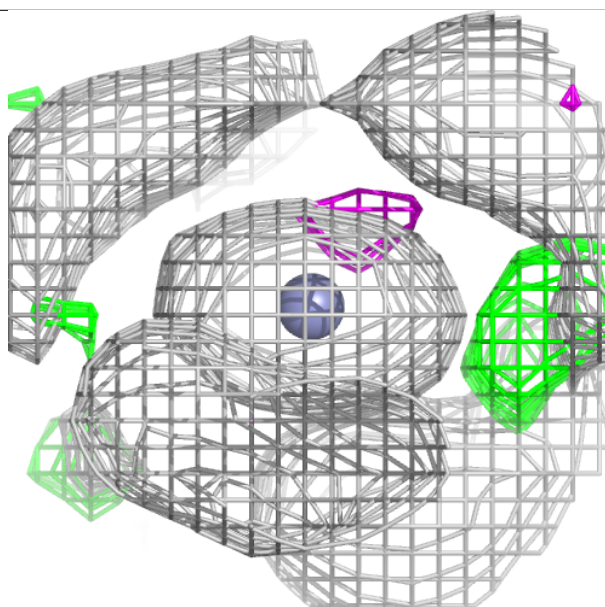
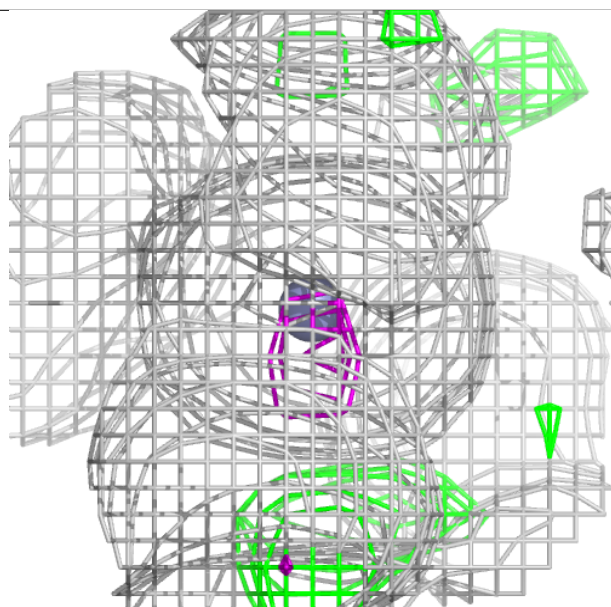
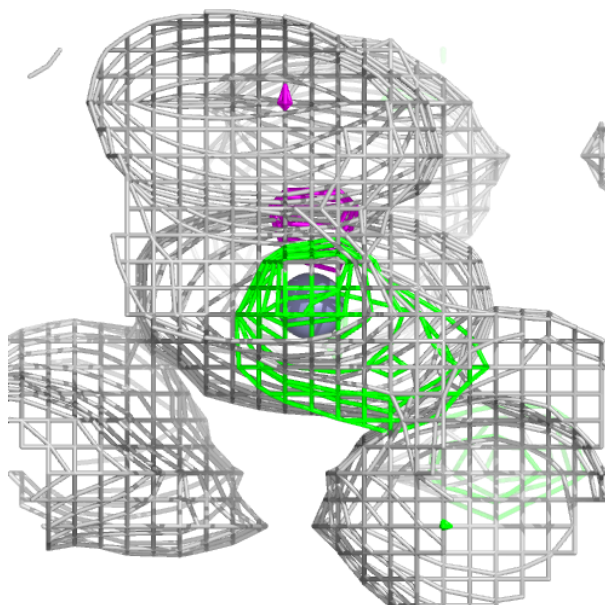
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	SO4	BBB	407	5/5	0.87	0.12	26,39,47,65	5
3	EDO	AAA	402	4/4	0.90	0.13	53,57,57,60	0
5	SO4	AAA	405	5/5	0.91	0.11	35,36,39,40	5
3	EDO	BBB	404	4/4	0.91	0.15	23,24,29,33	0
5	SO4	BBB	408	5/5	0.91	0.10	37,40,44,46	5
5	SO4	BBB	403	5/5	0.92	0.11	27,34,39,42	5
5	SO4	AAA	407	5/5	0.93	0.11	13,23,32,35	5
5	SO4	AAA	404	5/5	0.93	0.11	16,24,27,28	5
5	SO4	BBB	406	5/5	0.94	0.09	19,26,28,31	5
5	SO4	AAA	406	5/5	0.95	0.09	25,27,28,36	5
4	CL	AAA	403	1/1	0.95	0.09	46,46,46,46	0
5	SO4	BBB	405	5/5	0.97	0.07	30,35,42,43	5
5	SO4	BBB	402	5/5	0.97	0.06	11,12,15,15	5
2	ZN	BBB	401	1/1	1.00	0.02	8,8,8,8	1
2	ZN	AAA	401	1/1	1.00	0.04	8,8,8,8	1

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.

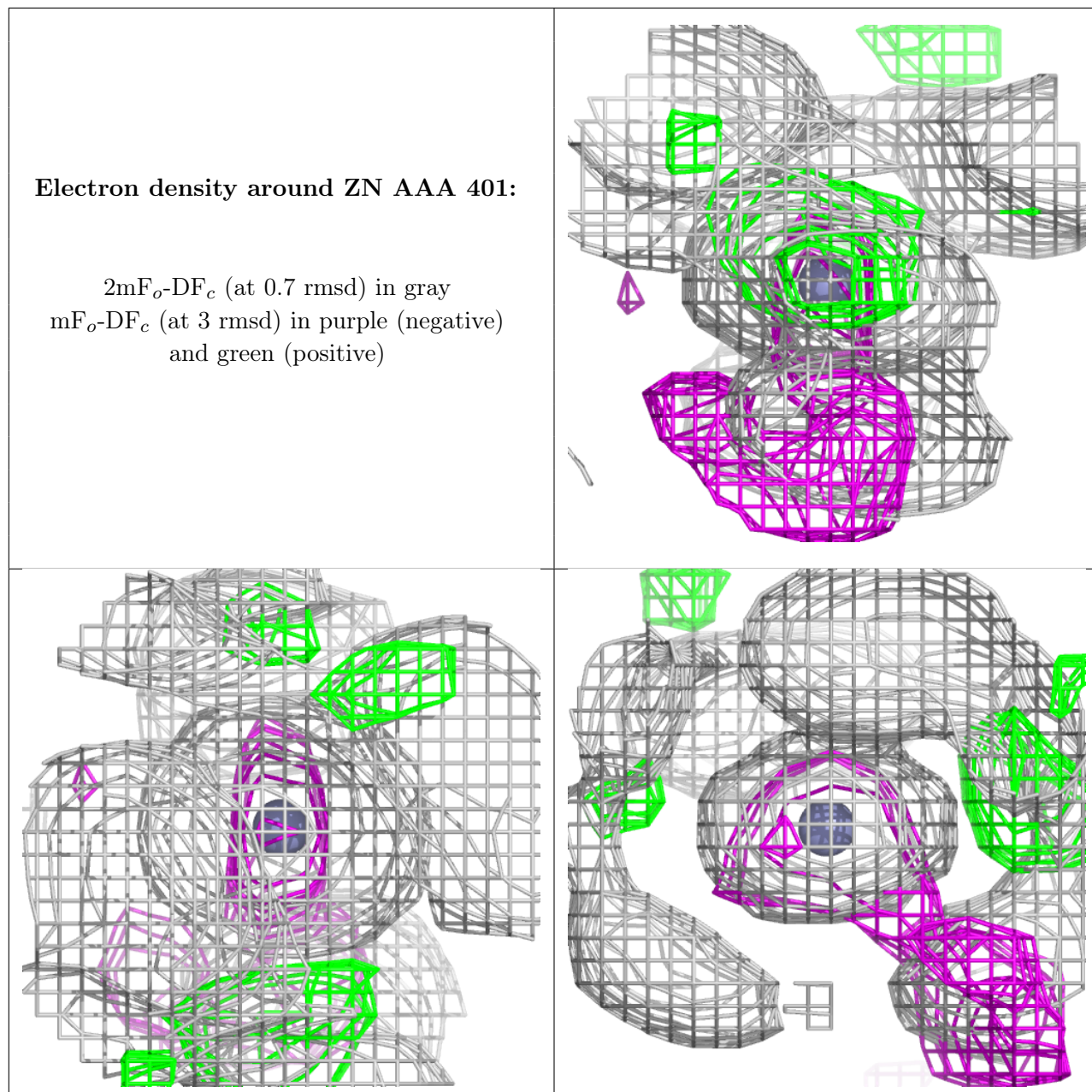
Electron density around ZN BBB 401:

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



Electron density around ZN 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.