



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:03 PM UTC

PDB ID : 7V9N / pdb_00007v9n
Title : Crystal structure of the lanthipeptide zinc-metallopeptidase EryP from
saccharopolyspora erythraea in closed state
Authors : Zhao, C.; Zhao, N.L.; Bao, R.
Deposited on : 2021-08-26
Resolution : 1.90 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 : 4-5-2 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

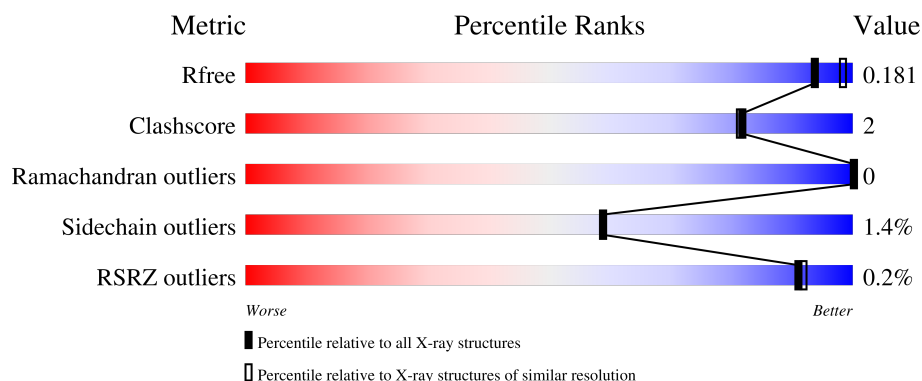
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	A	884	 89% 7% .

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
5	ACT	A	906	-	X	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7628 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 Alanine aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	859	6808	4287	1196	1308	17	0	9	0

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	initiating methionine	UNP A4F9D7
A	-22	GLY	-	expression tag	UNP A4F9D7
A	-21	SER	-	expression tag	UNP A4F9D7
A	-20	SER	-	expression tag	UNP A4F9D7
A	-19	HIS	-	expression tag	UNP A4F9D7
A	-18	HIS	-	expression tag	UNP A4F9D7
A	-17	HIS	-	expression tag	UNP A4F9D7
A	-16	HIS	-	expression tag	UNP A4F9D7
A	-15	HIS	-	expression tag	UNP A4F9D7
A	-14	HIS	-	expression tag	UNP A4F9D7
A	-13	HIS	-	expression tag	UNP A4F9D7
A	-12	HIS	-	expression tag	UNP A4F9D7
A	-11	HIS	-	expression tag	UNP A4F9D7
A	-10	HIS	-	expression tag	UNP A4F9D7
A	-9	SER	-	expression tag	UNP A4F9D7
A	-8	SER	-	expression tag	UNP A4F9D7
A	-7	GLY	-	expression tag	UNP A4F9D7
A	-6	LEU	-	expression tag	UNP A4F9D7
A	-5	VAL	-	expression tag	UNP A4F9D7
A	-4	PRO	-	expression tag	UNP A4F9D7
A	-3	ARG	-	expression tag	UNP A4F9D7
A	-2	GLY	-	expression tag	UNP A4F9D7
A	-1	SER	-	expression tag	UNP A4F9D7
A	0	HIS	-	expression tag	UNP A4F9D7
A	1	VAL	-	expression tag	UNP A4F9D7

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by

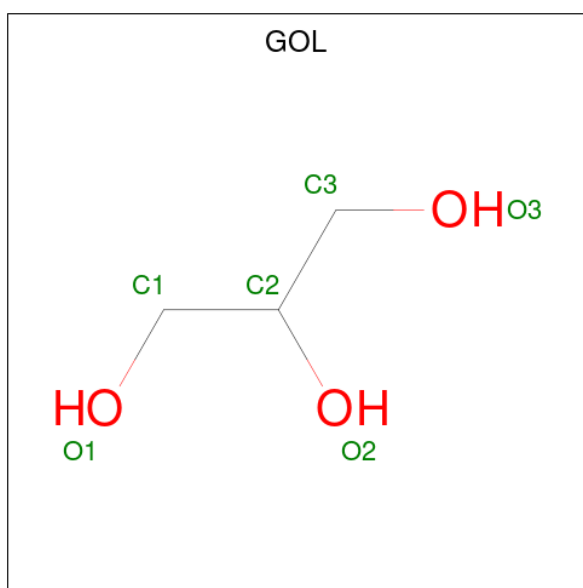
depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

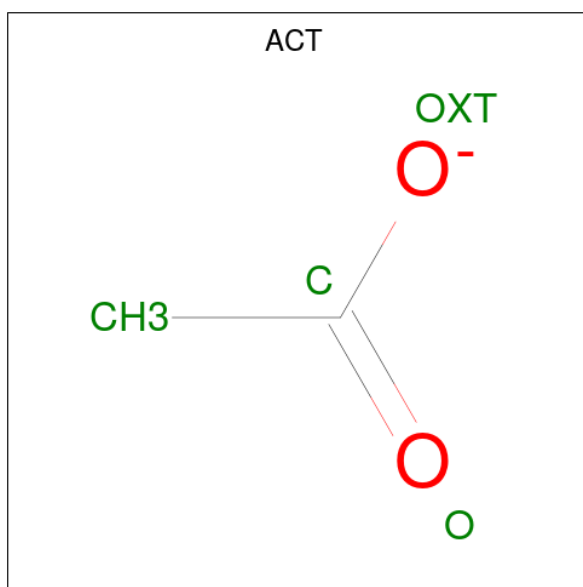
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

- Molecule 6 is water.

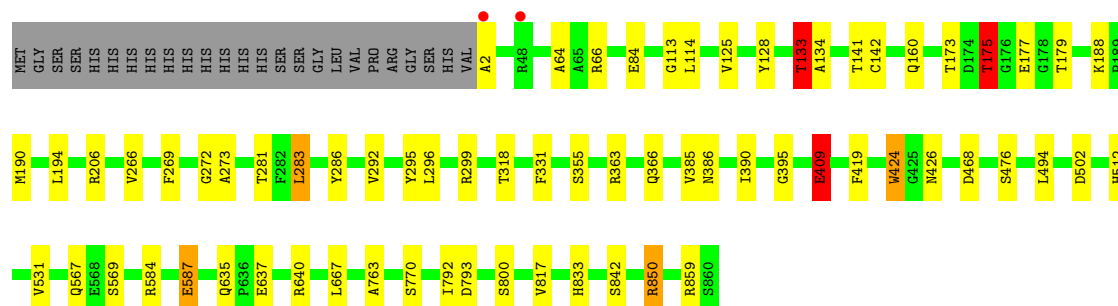
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	796	Total	O	0	0
			796	796		

3 Residue-property plots

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: Alanine aminopeptidase

Chain A:  89% 7% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	153.58Å 153.58Å 98.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.08 – 1.90 32.08 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (32.08-1.90) 99.9 (32.08-1.90)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.10 (at 1.89Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.154 , 0.181 0.155 , 0.181	Depositor DCC
R_{free} test set	2000 reflections (2.16%)	wwPDB-VP
Wilson B-factor (Å ²)	26.1	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 38.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7628	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	1.39	25/6972 (0.4%)	1.14	12/9500 (0.1%)

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	409	GLU	CD-OE1	8.98	1.42	1.25
1	A	266	VAL	CA-C	6.12	1.59	1.52
1	A	419	PHE	CA-CB	-5.96	1.44	1.53
1	A	272	GLY	CA-C	5.91	1.60	1.51
1	A	141	THR	N-CA	-5.90	1.38	1.46
1	A	424	TRP	CA-CB	5.81	1.61	1.53
1	A	113	GLY	CA-C	-5.77	1.46	1.52
1	A	269	PHE	C-O	-5.76	1.17	1.24
1	A	587	GLU	C-O	-5.70	1.16	1.24
1	A	850	ARG	CZ-NH2	5.63	1.40	1.33
1	A	128	TYR	CA-C	-5.53	1.45	1.52
1	A	569	SER	CB-OG	-5.47	1.31	1.42
1	A	635	GLN	C-O	-5.47	1.19	1.24
1	A	842	SER	CA-C	-5.17	1.46	1.52
1	A	770	SER	C-O	-5.17	1.17	1.24
1	A	667	LEU	CA-C	-5.16	1.46	1.52
1	A	395	GLY	CA-C	5.14	1.57	1.51
1	A	763	ALA	CA-C	5.11	1.59	1.52
1	A	502	ASP	CA-C	5.11	1.58	1.52
1	A	64	ALA	CA-C	5.07	1.58	1.52
1	A	125	VAL	CA-CB	-5.06	1.48	1.54
1	A	142	CYS	CA-C	-5.03	1.46	1.52
1	A	206	ARG	N-CA	5.02	1.52	1.45
1	A	114	LEU	N-CA	-5.01	1.40	1.46
1	A	175	THR	CA-C	5.01	1.59	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	850	ARG	NE-CZ-NH2	8.91	127.22	119.20
1	A	409	GLU	CB-CG-CD	7.14	124.75	112.60
1	A	850	ARG	NE-CZ-NH1	-6.87	114.63	121.50
1	A	175	THR	OG1-CB-CG2	6.79	122.88	109.30
1	A	133	THR	N-CA-CB	-6.27	100.84	111.50
1	A	175	THR	N-CA-CB	-6.22	100.73	110.44
1	A	859	ARG	NE-CZ-NH2	6.06	124.66	119.20
1	A	160	GLN	N-CA-C	6.00	118.61	111.71
1	A	859	ARG	NE-CZ-NH1	-5.69	115.81	121.50
1	A	800	SER	N-CA-C	-5.58	103.17	110.53
1	A	133	THR	OG1-CB-CG2	5.35	120.00	109.30
1	A	792	ILE	CB-CA-C	-5.12	105.23	112.14

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	6808	0	6550	32	0
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	18	0	24	1	0
5	A	4	0	3	3	0
6	A	796	0	0	6	0
All	All	7628	0	6577	33	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 (33) 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:A:409:GLU:HG2	6:A:1147:HOH:O	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:THR:HG21	1:A:179:THR:OG1	1.92	0.68
1:A:175:THR:HG22	1:A:177:GLU:H	1.59	0.68
1:A:188:LYS:H	5:A:906:ACT:H1	1.61	0.65
1:A:173:THR:HG23	6:A:1520:HOH:O	1.96	0.64
1:A:133:THR:HG21	6:A:1026:HOH:O	1.97	0.63
5:A:906:ACT:H3	6:A:1452:HOH:O	2.00	0.61
1:A:567:GLN:NE2	6:A:1005:HOH:O	2.36	0.58
1:A:188:LYS:H	5:A:906:ACT:CH3	2.17	0.57
1:A:584:ARG:NH1	6:A:1001:HOH:O	2.27	0.54
1:A:295:TYR:CE1	1:A:299:ARG:HD3	2.44	0.51
1:A:175:THR:CG2	1:A:177:GLU:H	2.22	0.50
1:A:295:TYR:CZ	1:A:299:ARG:HD3	2.46	0.50
1:A:494:LEU:C	1:A:494:LEU:HD12	2.37	0.49
1:A:188:LYS:HD3	1:A:424:TRP:CH2	2.48	0.47
1:A:292:VAL:HB	1:A:296:LEU:HD12	1.97	0.47
1:A:318:THR:O	1:A:426:ASN:HA	2.14	0.47
1:A:637:GLU:OE1	1:A:640[A]:ARG:NH1	2.48	0.47
1:A:175:THR:HG21	1:A:179:THR:HG1	1.81	0.45
1:A:133:THR:CG2	1:A:134:ALA:N	2.80	0.44
1:A:385:VAL:HG23	1:A:386:ASN:OD1	2.18	0.44
1:A:512[B]:HIS:CD2	1:A:531:VAL:HG13	2.53	0.44
1:A:793:ASP:OD2	1:A:833:HIS:CE1	2.71	0.43
1:A:817:VAL:O	4:A:905:GOL:H2	2.19	0.42
1:A:366:GLN:OE1	1:A:584:ARG:NH2	2.46	0.42
1:A:363:ARG:O	1:A:850:ARG:NH1	2.50	0.42
1:A:2:ALA:N	1:A:84:GLU:OE1	2.52	0.42
1:A:190:MET:HE3	1:A:194:LEU:HB2	2.02	0.42
1:A:273:ALA:HA	1:A:281:THR:O	2.20	0.41
1:A:190:MET:CE	1:A:194:LEU:HB2	2.49	0.41
1:A:133:THR:HG23	1:A:134:ALA:N	2.35	0.41
1:A:331:PHE:CD1	1:A:331:PHE:C	2.98	0.41
1:A:283:LEU:HD23	1:A:286:TYR:CD2	2.56	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	A	866/884 (98%)	846 (98%)	20 (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	A	704/717 (98%)	694 (99%)	10 (1%)	59	59

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	ARG
1	A	133	THR
1	A	175	THR
1	A	283	LEU
1	A	355	SER
1	A	390	ILE
1	A	409	GLU
1	A	468	ASP
1	A	476	SER
1	A	587	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	231	HIS
1	A	243	GLN
1	A	249	HIS
1	A	263	GLN

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Mol	Chain	Res	Type
1	A	345	GLN
1	A	381	GLN
1	A	554	GLN
1	A	726	GLN
1	A	752	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	GOL	A	903	-	5,5,5	0.94	0	5,5,5	0.98	0
5	ACT	A	906	-	3,3,3	1.72	1 (33%)	3,3,3	2.20	2 (66%)
4	GOL	A	905	-	5,5,5	0.73	0	5,5,5	0.72	0
4	GOL	A	904	-	5,5,5	0.37	0	5,5,5	0.94	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	GOL	A	903	-	-	0/4/4/4	-
4	GOL	A	905	-	-	4/4/4/4	-
4	GOL	A	904	-	-	1/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	906	ACT	CH3-C	-2.53	1.39	1.49

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	906	ACT	OXT-C-O	2.74	132.18	122.03
5	A	906	ACT	O-C-CH3	-2.63	111.74	122.53

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	905	GOL	C1-C2-C3-O3
4	A	904	GOL	O1-C1-C2-C3
4	A	905	GOL	O1-C1-C2-C3
4	A	905	GOL	O2-C2-C3-O3
4	A	905	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	906	ACT	3	0
4	A	905	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	A	859/884 (97%)	-0.37	2 (0%) 91 92	7, 24, 44, 71	9 (1%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	ALA	2.3
1	A	48[A]	ARG	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

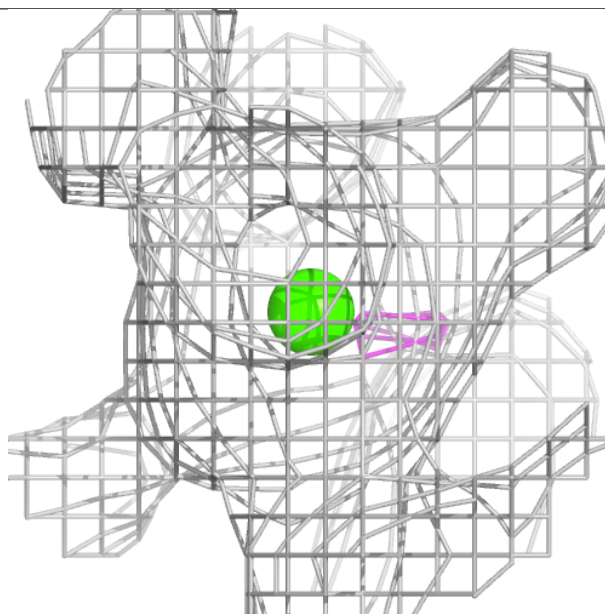
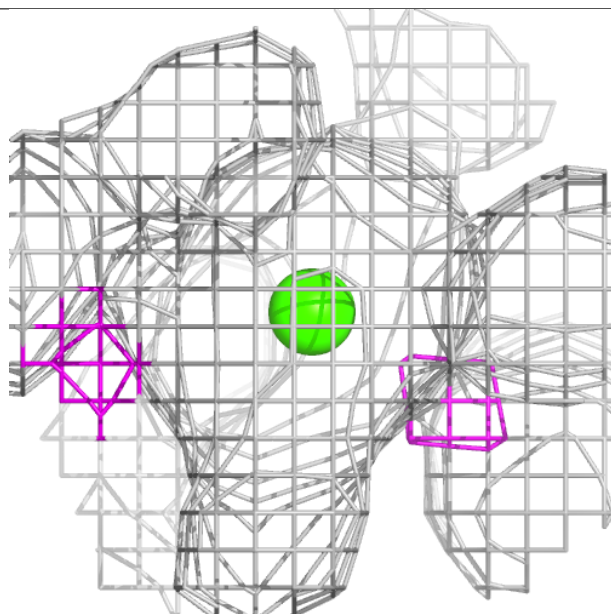
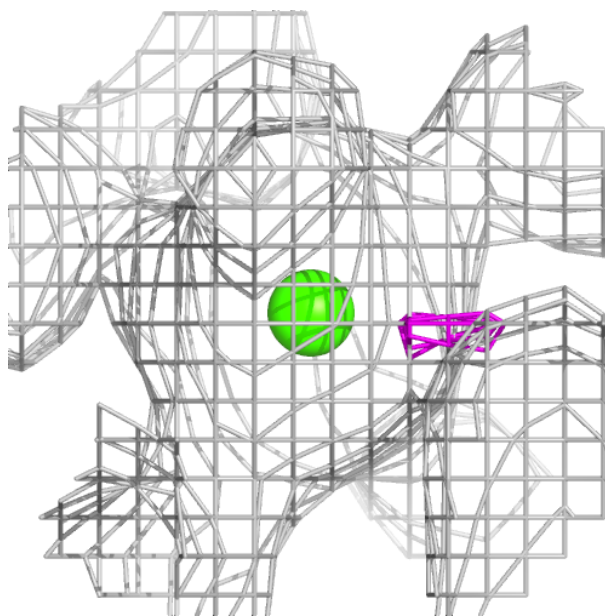
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

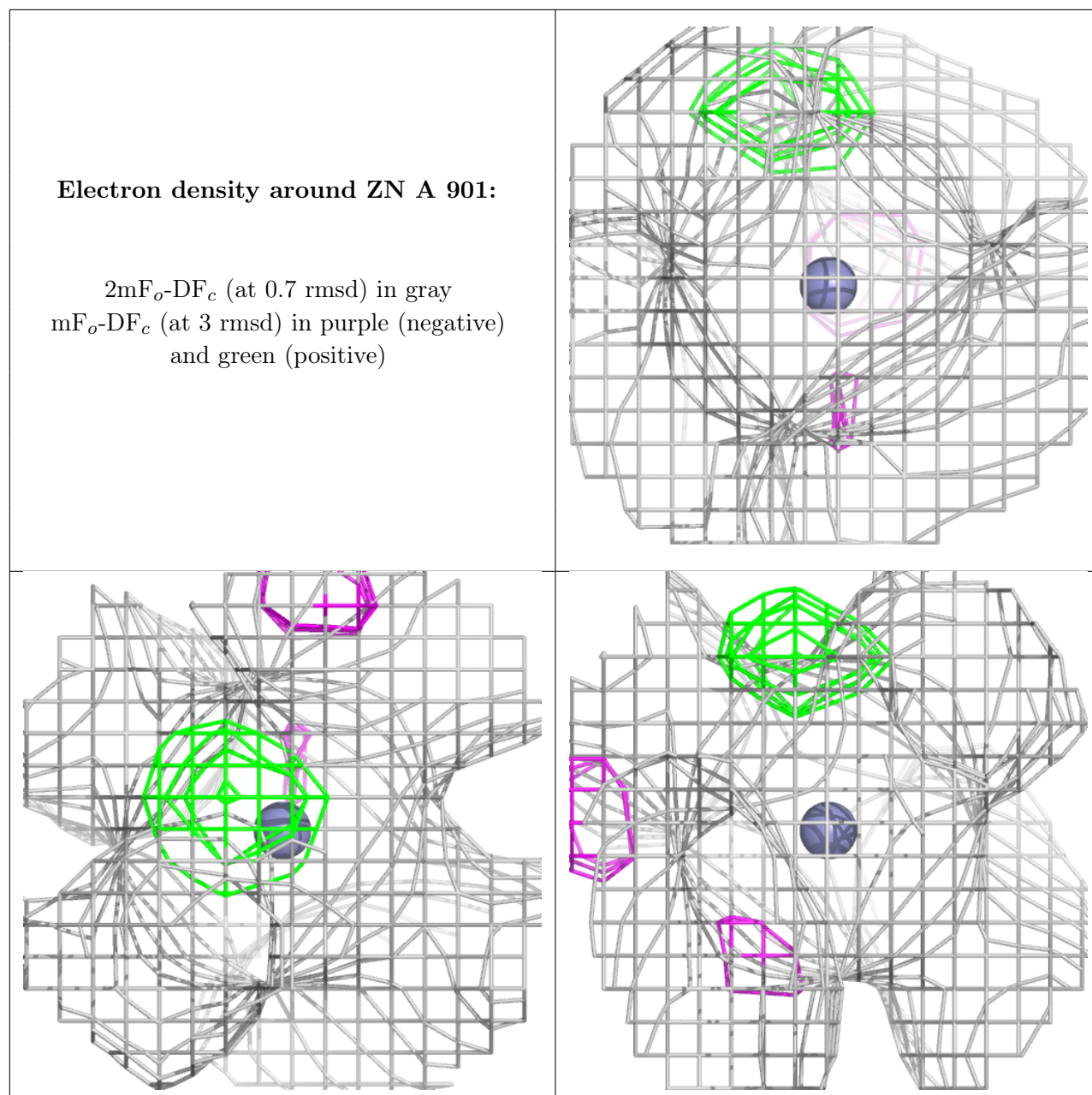
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	A	905	6/6	0.73	0.17	39,49,52,56	0
4	GOL	A	904	6/6	0.90	0.10	29,39,41,52	0
5	ACT	A	906	4/4	0.91	0.10	15,26,32,34	0
4	GOL	A	903	6/6	0.97	0.07	20,28,35,44	0
3	CA	A	902	1/1	0.98	0.04	26,26,26,26	1
2	ZN	A	901	1/1	1.00	0.01	19,19,19,19	0

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 CA A 902:

$2mF_o-DF_c$ (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.