Full wwPDB X-ray Structure Validation Report ⓘ

Nov 28, 2024 – 09:06 am GMT

PDB ID	:	9F26
Title	:	Crystal structure of the PriS_PriL-Rpa2WH ternary complex from P. abyssi
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Deposited on	:	2024-04-22
Resolution	:	3.50 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:

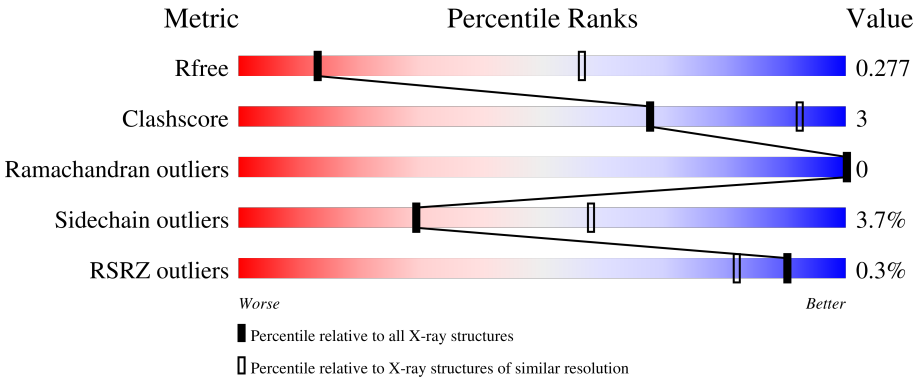
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 3.50 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}	164625	1094 (3.56-3.44)
Clashscore	180529	1045 (3.54-3.46)
Ramachandran outliers	177936	1032 (3.54-3.46)
Sidechain outliers	177891	1033 (3.54-3.46)
RSRZ outliers	164620	1093 (3.56-3.44)

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	346	87% 12% ·
2	B	393	49% 5% 46%
3	C	272	25% · 71%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5290 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 DNA primase small subunit PriS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	346	Total	C	N	O	S	0	0	0
			2871	1843	506	514	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP Q9V292

- Molecule 2 is a protein called DNA primase large subunit PriL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	211	Total	C	N	O	S	0	0	0
			1753	1140	284	326	3			

- Molecule 3 is a protein called RPA32 subunit of the hetero-oligomeric complex involved in homologous recombination.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	80	Total	C	N	O	S	0	0	0
			665	422	102	140	1			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

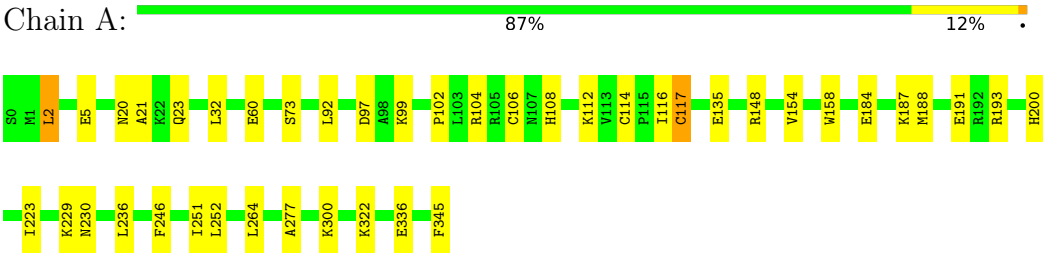
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		

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.

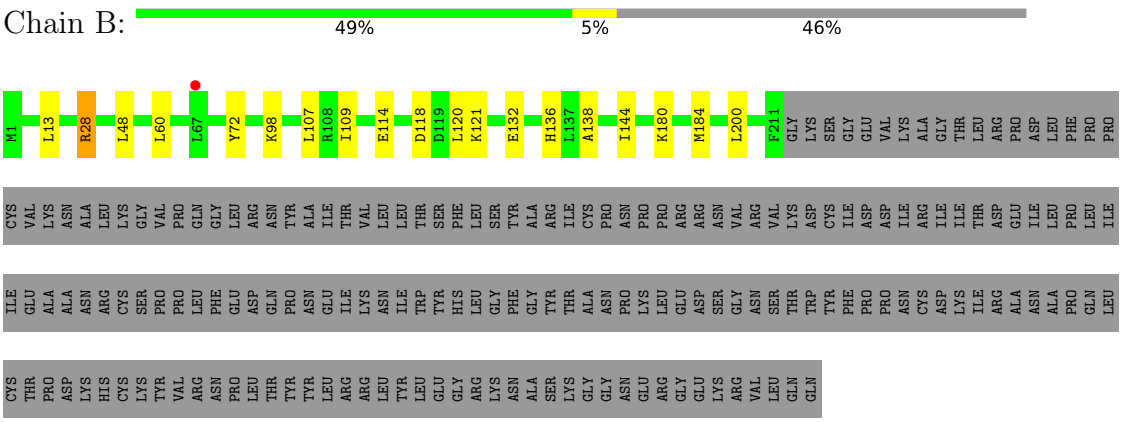
• Molecule 1: DNA primase small subunit PriS

Chain A:



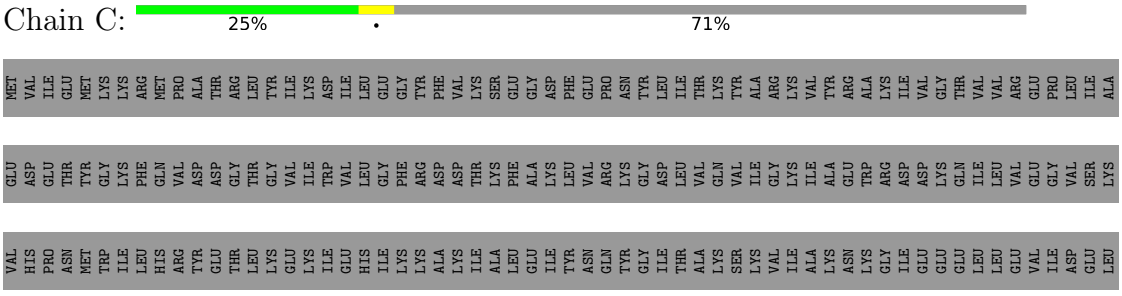
• Molecule 2: DNA primase large subunit PriL

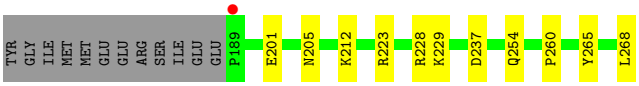
Chain B:



• Molecule 3: RPA32 subunit of the hetero-oligomeric complex involved in homologous recombination

Chain C:




TYR
GLY
ILE
MET
MET
GLU
GLU
ARG
SER
ILE
GLU
GLU
P189
E201
N205
K212
R223
R228
K229
D237
Q254
P260
Y265
L268

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	63.81Å 101.50Å 177.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.80 – 3.50 48.80 – 3.50	Depositor EDS
% Data completeness (in resolution range)	58.5 (48.80-3.50) 58.5 (48.80-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	2.45 (at 3.48Å)	Xtriage
Refinement program	BUSTER 2.10.4	Depositor
R, R_{free}	0.234 , 0.256 0.240 , 0.277	Depositor DCC
R_{free} test set	473 reflections (5.33%)	wwPDB-VP
Wilson B-factor (Å^2)	149.2	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 91.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5290	wwPDB-VP
Average B, all atoms (Å^2)	184.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

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	0.26	0/2937	0.50	0/3947
2	B	0.25	0/1785	0.46	0/2400
3	C	0.23	0/672	0.37	0/901
All	All	0.25	0/5394	0.48	0/7248

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	2871	0	2870	23	0
2	B	1753	0	1792	11	0
3	C	665	0	669	9	0
4	A	1	0	0	0	0
All	All	5290	0	5331	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 3.

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:A:345:PHE:HE2	3:C:228:ARG:HH11	1.33	0.74
1:A:158:TRP:CE3	2:B:138:ALA:HB2	2.25	0.70
1:A:219:VAL:O	1:A:223:ILE:HG12	1.93	0.69
1:A:135:GLU:OE2	1:A:200:HIS:HD2	1.82	0.62
2:B:28:ARG:NE	2:B:28:ARG:HA	2.20	0.56
1:A:106:CYS:HB3	1:A:116:ILE:HB	1.88	0.55
1:A:223:ILE:HD12	1:A:229:LYS:HG3	1.88	0.55
2:B:13:LEU:CD1	2:B:60:LEU:HD13	2.38	0.54
3:C:212:LYS:HZ2	3:C:254:GLN:HE22	1.59	0.51
2:B:28:ARG:HA	2:B:28:ARG:CZ	2.41	0.51
1:A:2:LEU:HG	1:A:336:GLU:HB3	1.94	0.50
1:A:112:LYS:HE3	1:A:148:ARG:HH11	1.76	0.49
1:A:104:ARG:HD3	1:A:117:CYS:HB3	1.96	0.47
1:A:219:VAL:HG13	1:A:236:LEU:HD12	1.96	0.47
2:B:180:LYS:O	2:B:184:MET:HG3	2.15	0.46
1:A:102:PRO:HG3	1:A:277:ALA:HB3	1.97	0.46
2:B:107:LEU:HB3	2:B:109:ILE:HG23	1.98	0.45
1:A:345:PHE:CE2	3:C:228:ARG:NH1	2.84	0.45
1:A:345:PHE:CZ	3:C:228:ARG:HB3	2.52	0.45
2:B:136:HIS:CD2	2:B:138:ALA:H	2.34	0.45
1:A:184:GLU:O	1:A:188:MET:HG3	2.18	0.44
3:C:228:ARG:HB2	3:C:265:TYR:HE2	1.82	0.44
2:B:72:TYR:HB2	2:B:200:LEU:HD22	1.98	0.44
1:A:21:ALA:HB2	1:A:60:GLU:HB2	2.00	0.43
3:C:212:LYS:NZ	3:C:254:GLN:HE22	2.17	0.42
1:A:20:ASN:ND2	1:A:23:GLN:NE2	2.67	0.42
1:A:92:LEU:HB3	1:A:154:VAL:HB	2.00	0.42
1:A:215:LEU:HD22	3:C:260:PRO:HA	2.01	0.41
1:A:187:LYS:O	1:A:191:GLU:HG2	2.20	0.41
1:A:193:ARG:HG2	1:A:252:LEU:HD23	2.01	0.41
2:B:13:LEU:HD12	2:B:60:LEU:HD13	2.02	0.41
2:B:136:HIS:HD2	2:B:138:ALA:H	1.69	0.41
1:A:246:PHE:HA	1:A:251:ILE:H	1.86	0.41
1:A:97:ASP:CG	1:A:99:LYS:HZ3	2.25	0.41
1:A:345:PHE:HB3	3:C:229:LYS:HD2	2.02	0.41
2:B:120:LEU:HB3	2:B:121:LYS:HZ2	1.86	0.41
3:C:201:GLU:O	3:C:205:ASN:OD1	2.39	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	344/346 (99%)	337 (98%)	7 (2%)	0	100	100
2	B	209/393 (53%)	207 (99%)	2 (1%)	0	100	100
3	C	78/272 (29%)	74 (95%)	4 (5%)	0	100	100
All	All	631/1011 (62%)	618 (98%)	13 (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	A	307/307 (100%)	296 (96%)	11 (4%)	30	59
2	B	191/351 (54%)	184 (96%)	7 (4%)	29	58
3	C	73/242 (30%)	70 (96%)	3 (4%)	26	55
All	All	571/900 (63%)	550 (96%)	21 (4%)	29	58

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	5	GLU
1	A	32	LEU
1	A	73	SER
1	A	108	HIS

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Mol	Chain	Res	Type
1	A	114	CYS
1	A	117	CYS
1	A	230	ASN
1	A	264	LEU
1	A	300	LYS
1	A	322	LYS
2	B	28	ARG
2	B	48	LEU
2	B	98	LYS
2	B	114	GLU
2	B	118	ASP
2	B	132	GLU
2	B	144	ILE
3	C	223	ARG
3	C	237	ASP
3	C	268	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	200	HIS
1	A	221	HIS
3	C	205	ASN
3	C	254	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

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 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

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

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	346/346 (100%)	-0.49	0 100 100	141, 175, 194, 208	0
2	B	211/393 (53%)	-0.43	1 (0%) 87 75	177, 201, 238, 261	0
3	C	80/272 (29%)	-0.56	1 (1%) 74 56	152, 170, 230, 232	0
All	All	637/1011 (63%)	-0.48	2 (0%) 90 82	141, 184, 227, 261	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	67	LEU	3.0
3	C	189	PRO	2.3

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

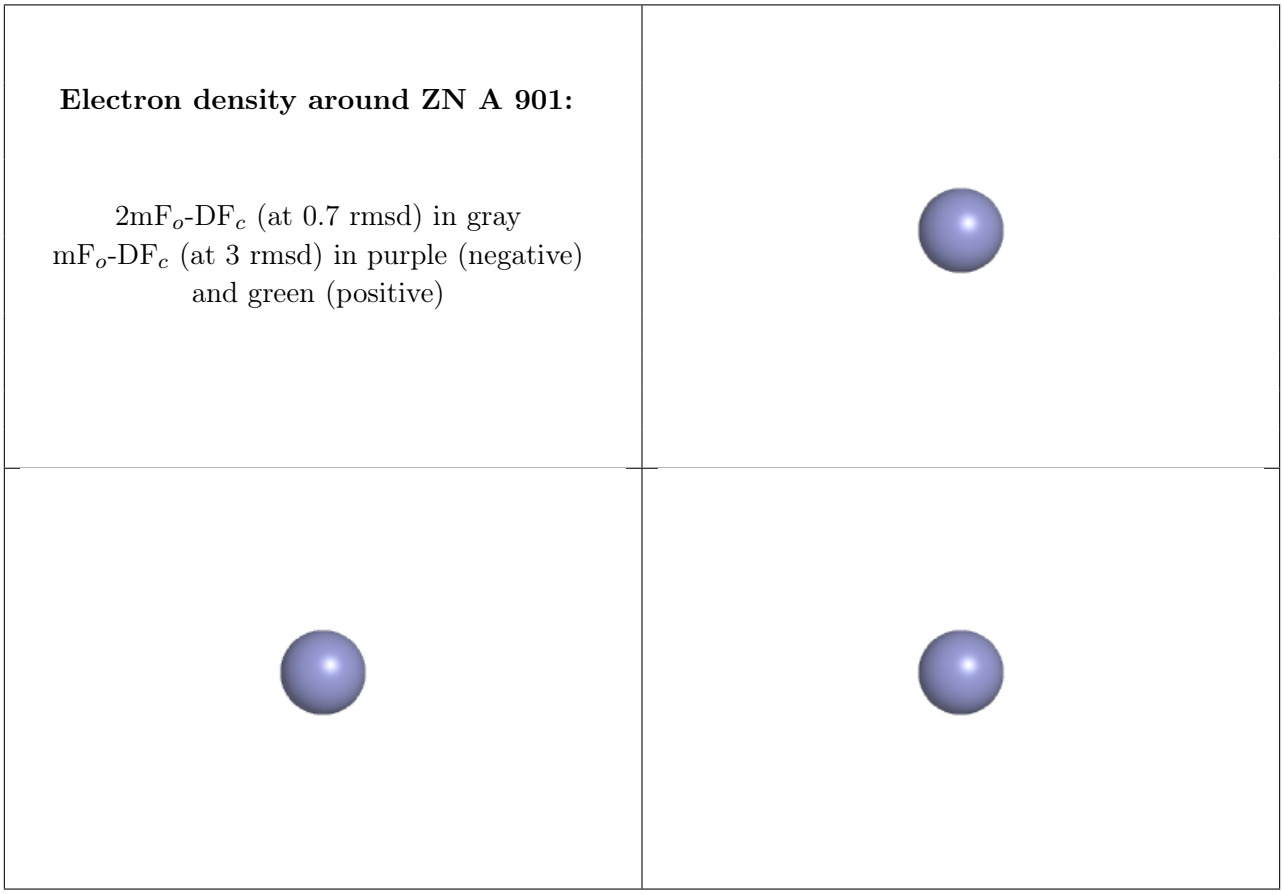
There are no monosaccharides in this entry.

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
4	ZN	A	901	1/1	0.98	0.06	256,256,256,256	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.



6.5 Other polymers (i)

There are no such residues in this entry.