



Full wwPDB X-ray Structure Validation Report ⓘ

May 31, 2022 – 06:11 pm BST

PDB ID : 7Z5H
Title : human Zn MATCAP
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Deposited on : 2022-03-09
Resolution : 2.50 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 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 : 2.28.1
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) : 2.28.1

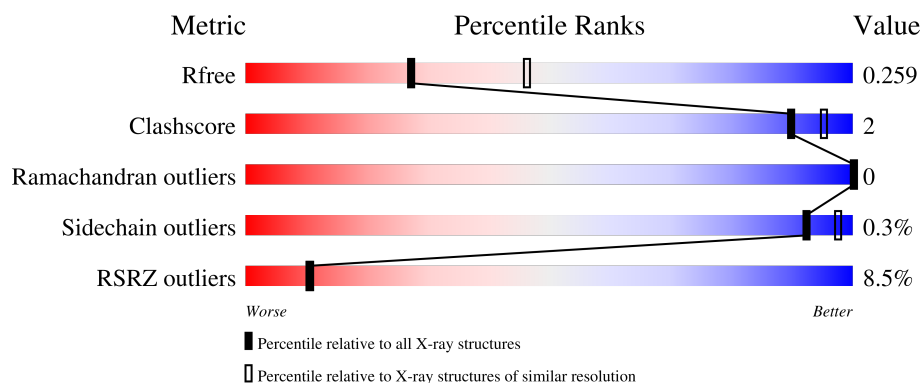
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	335	<div> <div>4%</div> <div>94%</div> <div>5%</div> </div>
1	B	335	<div> <div>21%</div> <div>92%</div> <div>6%</div> </div>
1	C	335	<div> <div>7%</div> <div>95%</div> <div>.</div> </div>
1	D	335	<div> <div>%</div> <div>94%</div> <div>5%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21714 atoms, of which 10703 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 Uncharacterized protein KIAA0895-like.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	332	Total	C	H	N	O	S	77	0	0
			5408	1722	2686	495	491	14			
1	B	330	Total	C	H	N	O	S	77	0	0
			5376	1712	2671	493	486	14			
1	C	330	Total	C	H	N	O	S	77	0	0
			5376	1712	2671	493	486	14			
1	D	331	Total	C	H	N	O	S	77	0	0
			5389	1716	2675	494	490	14			

- 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	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		

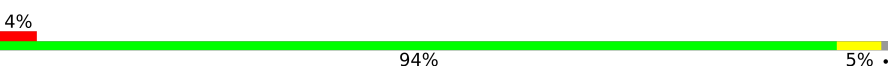
- Molecule 3 is water.

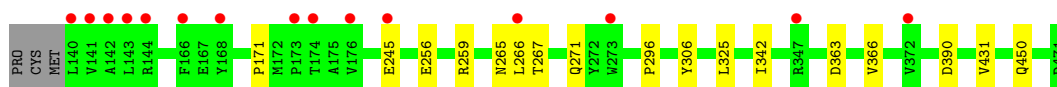
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	66	Total	O	0	0
			66	66		
3	B	12	Total	O	0	0
			12	12		
3	C	24	Total	O	0	0
			24	24		
3	D	59	Total	O	0	0
			59	59		

3 Residue-property plots

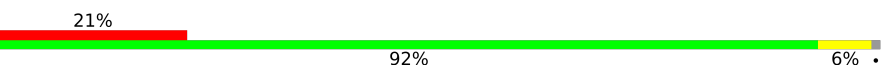
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

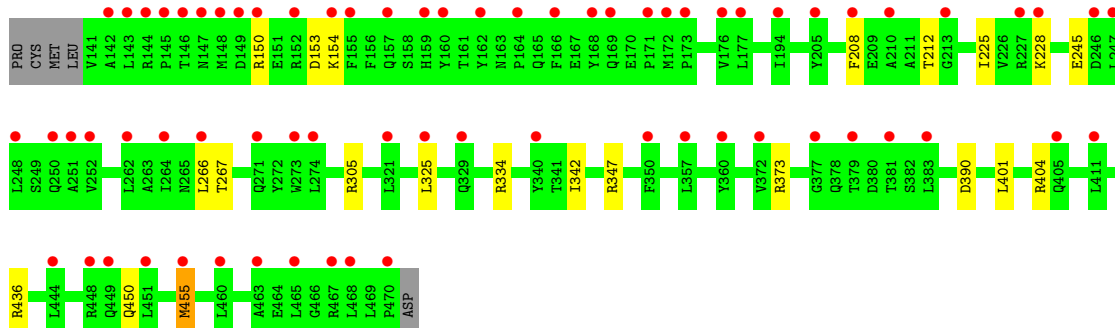
- Molecule 1: Uncharacterized protein KIAA0895-like

Chain A: 



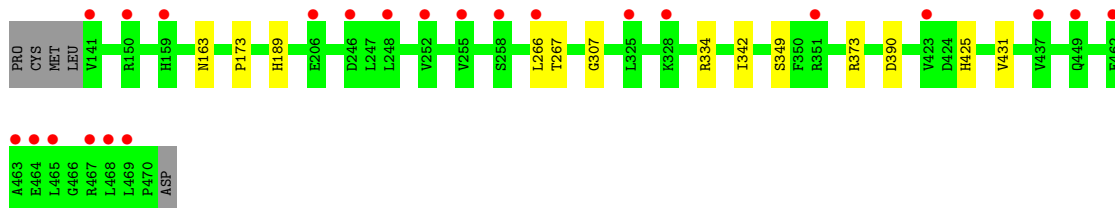
- Molecule 1: Uncharacterized protein KIAA0895-like

Chain B: 



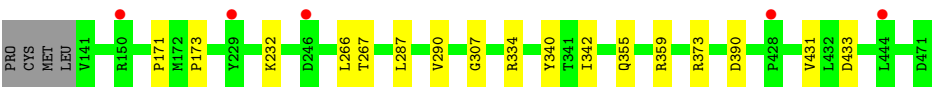
- Molecule 1: Uncharacterized protein KIAA0895-like

Chain C: 



- Molecule 1: Uncharacterized protein KIAA0895-like

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	55.65Å 88.07Å 165.58Å 90.00° 90.77° 90.00°	Depositor
Resolution (Å)	47.08 – 2.50 47.04 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.08-2.50) 100.0 (47.04-2.50)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0267, REFMAC 5.8.0267	Depositor
R, R_{free}	0.232 , 0.255 0.237 , 0.259	Depositor DCC
R_{free} test set	2762 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	39.5	Xtriage
Anisotropy	0.436	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.011 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	21714	wwPDB-VP
Average B, all atoms (Å ²)	60.0	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 22.18 % 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 6.0116e-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

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	0.35	0/2787	0.58	1/3771 (0.0%)
1	B	0.32	0/2770	0.59	2/3749 (0.1%)
1	C	0.32	0/2770	0.57	0/3749
1	D	0.34	0/2779	0.57	0/3760
All	All	0.33	0/11106	0.58	3/15029 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	455	MET	CA-CB-CG	6.58	124.48	113.30
1	A	271	GLN	CA-CB-CG	5.14	124.71	113.40
1	B	436	ARG	NE-CZ-NH2	-5.07	117.76	120.30

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	2722	2686	2672	10	0
1	B	2705	2671	2657	15	0
1	C	2705	2671	2657	9	0
1	D	2714	2675	2661	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	66	0	0	0	0
3	B	12	0	0	0	0
3	C	24	0	0	0	0
3	D	59	0	0	0	0
All	All	11011	10703	10647	38	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 (38) 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:B:208:PHE:O	1:B:212:THR:HG22	1.69	0.91
1:B:150:ARG:O	1:B:153:ASP:OD1	1.89	0.90
1:B:401:LEU:HD22	1:B:455:MET:HE3	1.79	0.65
1:B:401:LEU:HD22	1:B:455:MET:CE	2.26	0.65
1:C:163:ASN:ND2	1:C:349:SER:OG	2.34	0.61
1:A:171:PRO:O	1:B:305:ARG:NH1	2.36	0.59
1:A:296:PRO:HB2	1:A:306:TYR:CE2	2.39	0.57
1:A:363:ASP:OD2	1:A:366:VAL:HG23	2.04	0.57
1:B:325:LEU:O	1:B:450:GLN:OE1	2.27	0.52
1:D:340:TYR:OH	1:D:359:ARG:NH2	2.44	0.50
1:B:153:ASP:OD1	1:B:154:LYS:N	2.44	0.50
1:A:342:ILE:HD11	1:A:390:ASP:HB2	1.94	0.49
1:C:342:ILE:HD11	1:C:390:ASP:HB2	1.93	0.49
1:B:342:ILE:HD11	1:B:390:ASP:HB2	1.94	0.49
1:D:342:ILE:HD11	1:D:390:ASP:HB2	1.93	0.49
1:A:325:LEU:O	1:A:450:GLN:NE2	2.30	0.47
1:B:347:ARG:HB3	1:C:189:HIS:CE1	2.50	0.47
1:B:245:GLU:HG2	1:B:266:LEU:HD11	1.98	0.46
1:D:287:LEU:HA	1:D:290:VAL:HG22	1.97	0.46
1:A:245:GLU:HG2	1:A:266:LEU:HD11	1.98	0.45
1:C:307:GLY:HA3	1:D:173:PRO:HA	1.98	0.45
1:B:334:ARG:NH2	1:B:373:ARG:HH11	2.15	0.45
1:A:266:LEU:HD12	1:A:267:THR:N	2.32	0.45
1:B:266:LEU:HD12	1:B:267:THR:N	2.34	0.43
1:B:455:MET:HE2	1:B:455:MET:HB3	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:334:ARG:NH2	1:D:373:ARG:HH11	2.16	0.43
1:C:266:LEU:HD12	1:C:267:THR:N	2.34	0.42
1:D:266:LEU:HD12	1:D:267:THR:N	2.34	0.42
1:C:173:PRO:HA	1:D:307:GLY:HA3	2.02	0.42
1:C:334:ARG:NH2	1:C:373:ARG:HH11	2.17	0.42
1:A:256:GLU:O	1:A:259:ARG:HG2	2.20	0.42
1:A:296:PRO:CB	1:A:306:TYR:CE2	3.03	0.42
1:D:431:VAL:HG23	1:D:431:VAL:O	2.21	0.41
1:C:425:HIS:CE1	1:D:171:PRO:HB2	2.56	0.41
1:B:225:ILE:O	1:B:228:LYS:HG2	2.21	0.40
1:A:431:VAL:O	1:A:431:VAL:HG23	2.22	0.40
1:B:404:ARG:HD3	1:B:455:MET:HE1	2.03	0.40
1:C:431:VAL:HG23	1:C:431:VAL:O	2.21	0.40

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	A	330/335 (98%)	321 (97%)	9 (3%)	0	100	100
1	B	328/335 (98%)	319 (97%)	9 (3%)	0	100	100
1	C	328/335 (98%)	318 (97%)	10 (3%)	0	100	100
1	D	329/335 (98%)	321 (98%)	8 (2%)	0	100	100
All	All	1315/1340 (98%)	1279 (97%)	36 (3%)	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	288/291 (99%)	287 (100%)	1 (0%)	92	97
1	B	286/291 (98%)	286 (100%)	0	100	100
1	C	286/291 (98%)	286 (100%)	0	100	100
1	D	287/291 (99%)	284 (99%)	3 (1%)	76	90
All	All	1147/1164 (98%)	1143 (100%)	4 (0%)	92	97

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	265	ASN
1	D	232	LYS
1	D	355	GLN
1	D	433	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	242	GLN
1	A	265	ASN
1	B	189	HIS
1	B	242	GLN
1	B	329	GLN
1	B	450	GLN
1	C	157	GLN
1	C	163	ASN
1	C	189	HIS
1	C	292	ASN
1	C	298	HIS
1	D	157	GLN
1	D	189	HIS
1	D	292	ASN
1	D	298	HIS

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Mol	Chain	Res	Type
1	D	355	GLN

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 4 ligands modelled in this entry, 4 are 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, 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	332/335 (99%)	0.72	15 (4%) 33 36	32, 51, 78, 108	0
1	B	330/335 (98%)	1.37	69 (20%) 1 0	50, 74, 110, 131	0
1	C	330/335 (98%)	0.87	23 (6%) 16 16	44, 59, 92, 125	0
1	D	331/335 (98%)	0.68	5 (1%) 73 75	28, 48, 71, 106	0
All	All	1323/1340 (98%)	0.91	112 (8%) 10 10	28, 58, 98, 131	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	168	TYR	7.4
1	B	252	VAL	6.6
1	B	247	LEU	6.2
1	B	176	VAL	6.1
1	B	173	PRO	5.4
1	B	162	TYR	5.2
1	B	172	MET	5.0
1	B	164	PRO	4.8
1	B	383	LEU	4.8
1	B	372	VAL	4.6
1	C	467	ARG	4.6
1	B	166	PHE	4.6
1	B	149	ASP	4.5
1	D	246	ASP	4.5
1	C	246	ASP	4.3
1	B	148	MET	4.2
1	C	463	ALA	4.2
1	B	169	GLN	4.1
1	B	449	GLN	4.0
1	C	255	VAL	3.9
1	C	465	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	381	THR	3.8
1	B	143	LEU	3.8
1	B	154	LYS	3.8
1	A	173	PRO	3.6
1	B	470	PRO	3.6
1	B	321	LEU	3.5
1	D	444	LEU	3.3
1	A	140	LEU	3.2
1	B	377	GLY	3.2
1	B	451	LEU	3.2
1	B	194	ILE	3.2
1	B	246	ASP	3.2
1	B	144	ARG	3.1
1	B	150	ARG	3.1
1	B	444	LEU	3.1
1	A	176	VAL	3.1
1	B	205	TYR	3.0
1	B	251	ALA	3.0
1	B	146	THR	3.0
1	B	142	ALA	2.9
1	C	462	GLU	2.9
1	C	468	LEU	2.9
1	C	248	LEU	2.9
1	B	463	ALA	2.8
1	B	460	LEU	2.8
1	D	428	PRO	2.8
1	C	449	GLN	2.8
1	A	141	VAL	2.7
1	B	177	LEU	2.7
1	A	168	TYR	2.7
1	B	160	TYR	2.6
1	C	159	HIS	2.6
1	C	258	SER	2.6
1	B	468	LEU	2.6
1	C	150	ARG	2.6
1	B	329	GLN	2.6
1	B	266	LEU	2.6
1	B	357	LEU	2.6
1	C	351	ARG	2.6
1	B	274	LEU	2.6
1	C	469	LEU	2.6
1	B	379	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	144	ARG	2.5
1	B	155	PHE	2.5
1	B	157	GLN	2.5
1	B	405	GLN	2.5
1	B	152	ARG	2.4
1	A	174	THR	2.4
1	B	350	PHE	2.4
1	B	467	ARG	2.4
1	B	340	TYR	2.4
1	C	141	VAL	2.4
1	C	423	VAL	2.4
1	A	372	VAL	2.4
1	C	206	GLU	2.4
1	B	227	ARG	2.3
1	D	150	ARG	2.3
1	B	250	GLN	2.3
1	B	159	HIS	2.3
1	B	411	LEU	2.3
1	C	325	LEU	2.3
1	C	266	LEU	2.3
1	B	171	PRO	2.3
1	C	328	LYS	2.3
1	A	266	LEU	2.3
1	B	248	LEU	2.3
1	B	325	LEU	2.3
1	C	252	VAL	2.3
1	B	210	ALA	2.3
1	D	229	TYR	2.3
1	B	465	LEU	2.2
1	B	360	TYR	2.2
1	A	245	GLU	2.2
1	B	228	LYS	2.2
1	A	347	ARG	2.2
1	B	448	ARG	2.2
1	B	271	GLN	2.2
1	B	147	ASN	2.2
1	C	437	VAL	2.2
1	B	208	PHE	2.2
1	B	455	MET	2.1
1	B	273	TRP	2.1
1	B	213	GLY	2.1
1	B	264	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	166	PHE	2.1
1	B	262	LEU	2.1
1	C	464	GLU	2.1
1	A	142	ALA	2.0
1	A	273	TRP	2.0
1	A	143	LEU	2.0
1	B	145	PRO	2.0

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 monosaccharides in this entry.

6.4 Ligands [i](#)

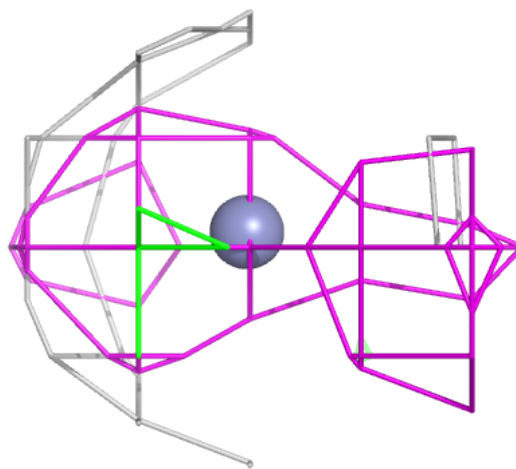
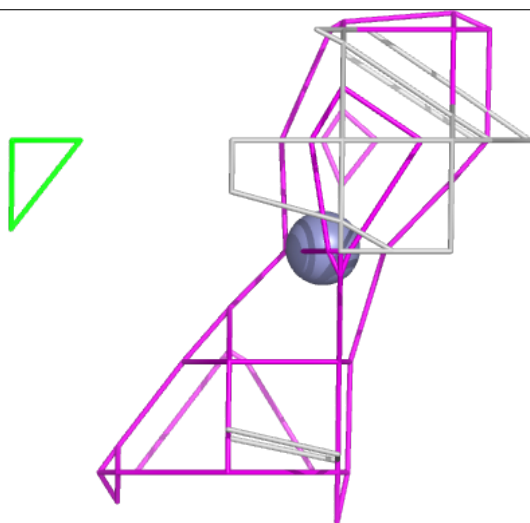
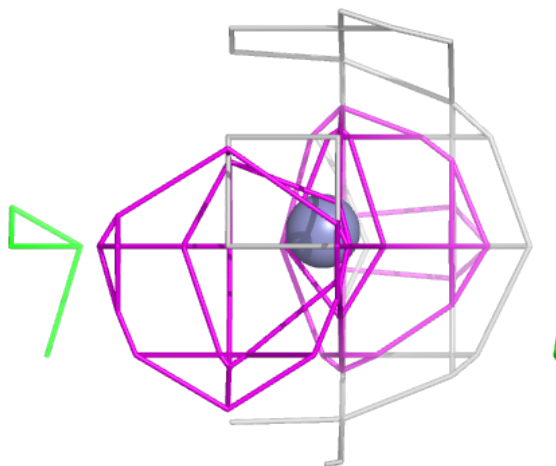
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ZN	C	501	1/1	0.90	0.06	57,57,57,57	0
2	ZN	B	501	1/1	0.92	0.08	55,55,55,55	0
2	ZN	A	501	1/1	0.93	0.07	46,46,46,46	0
2	ZN	D	501	1/1	0.97	0.08	44,44,44,44	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.

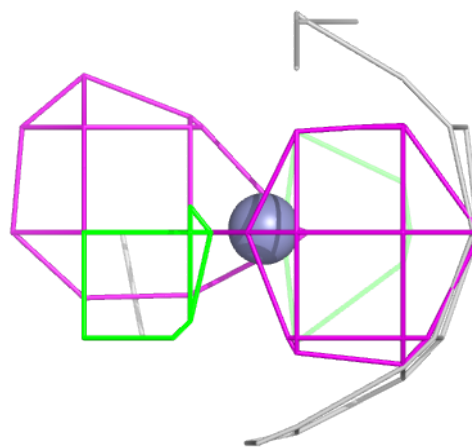
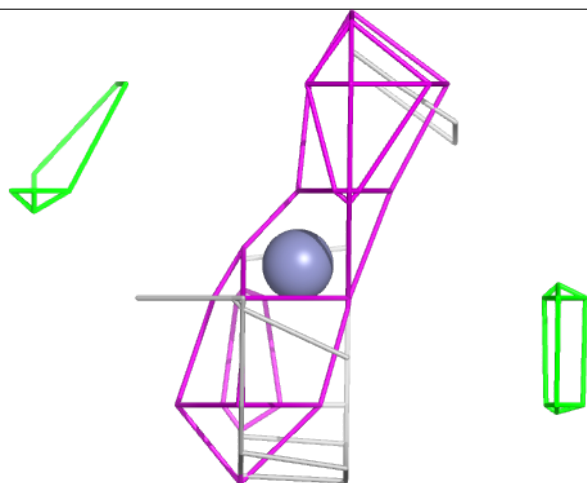
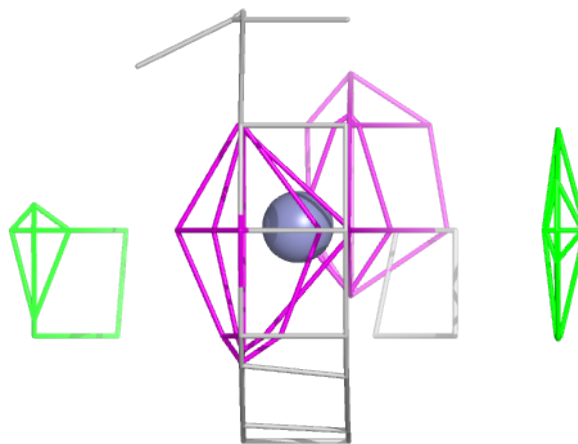
Electron density around ZN C 501:

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



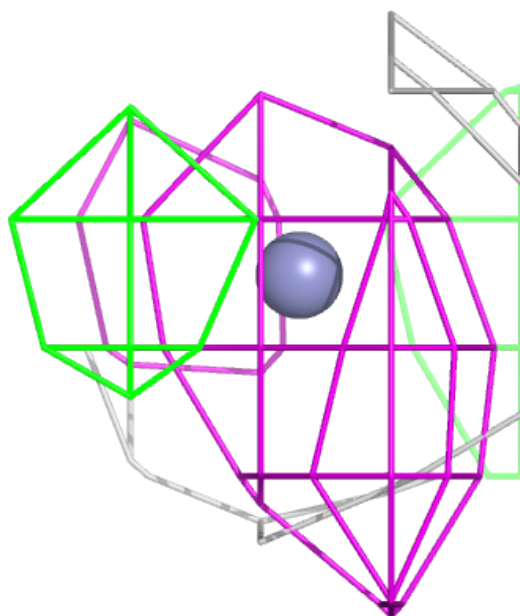
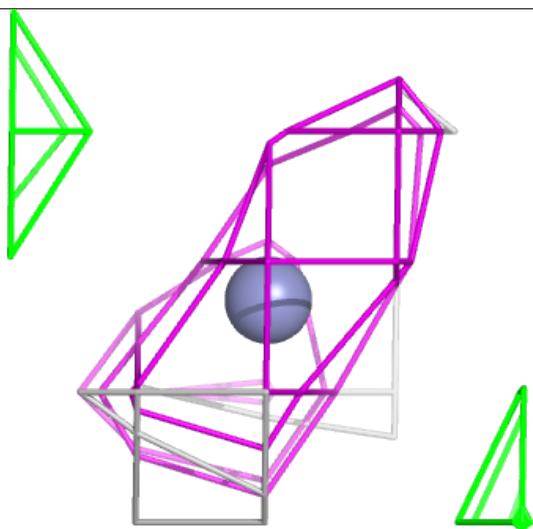
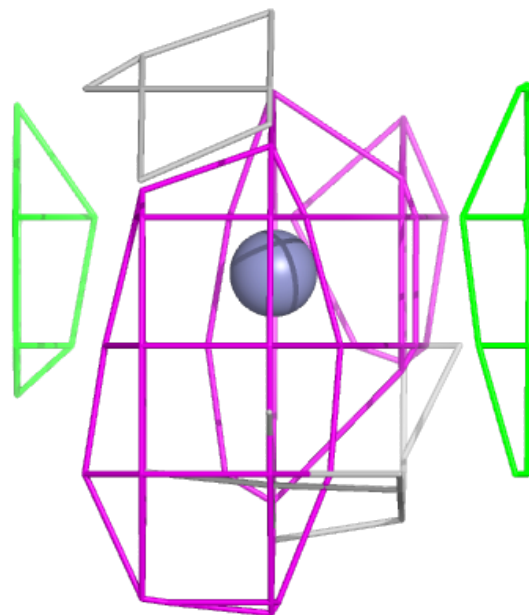
Electron density around ZN B 501:

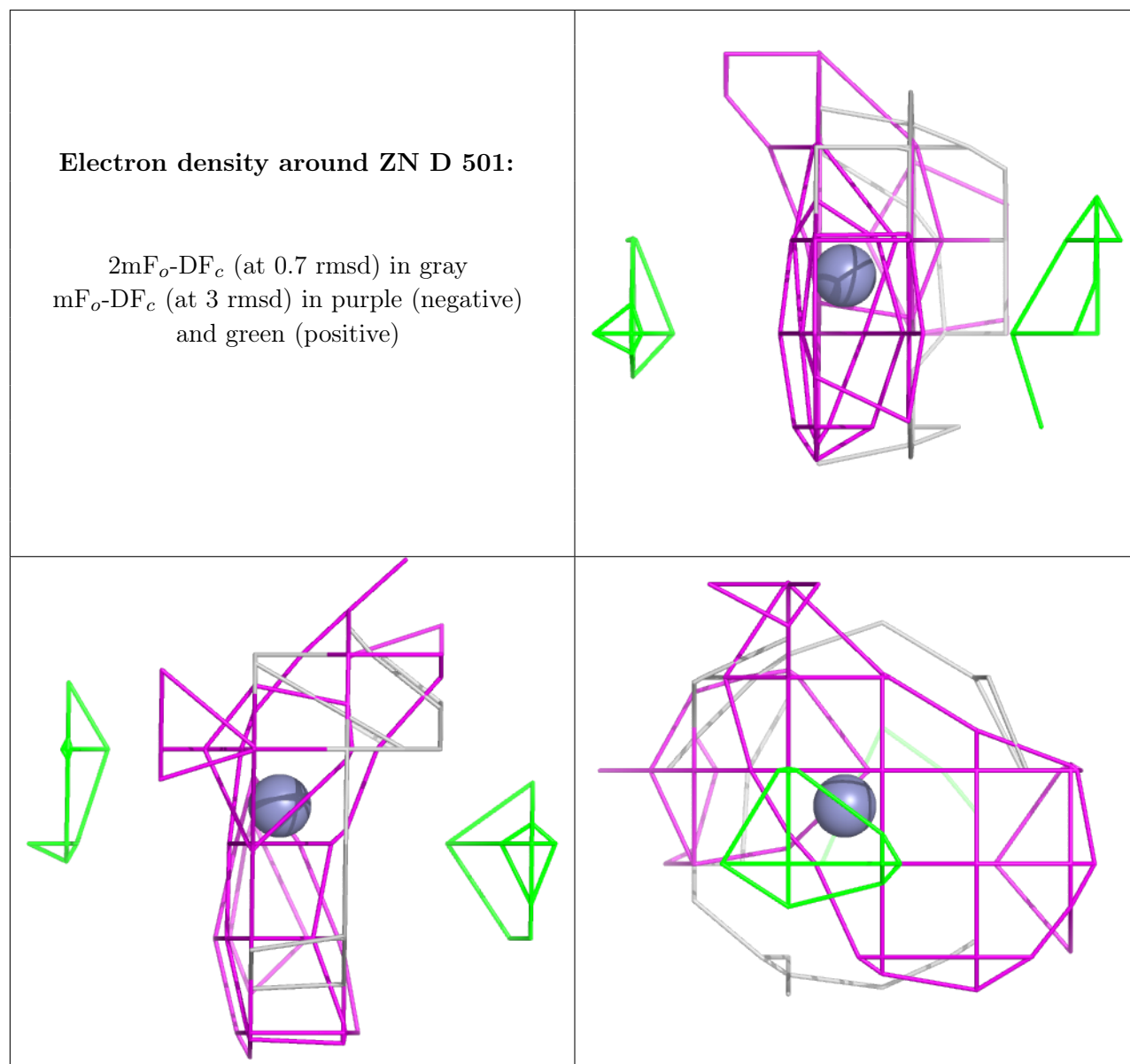
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZN A 501:

$2mF_o-DF_c$ (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.