



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 02:12 AM UTC

PDB ID : 9ON4 / pdb_00009on4
Title : Crystal structure of Zn²⁺ bound Calprotectin variant I73K
Authors : Garcia, V.; Chazin, W.C.
Deposited on : 2025-05-14
Resolution : 1.66 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
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

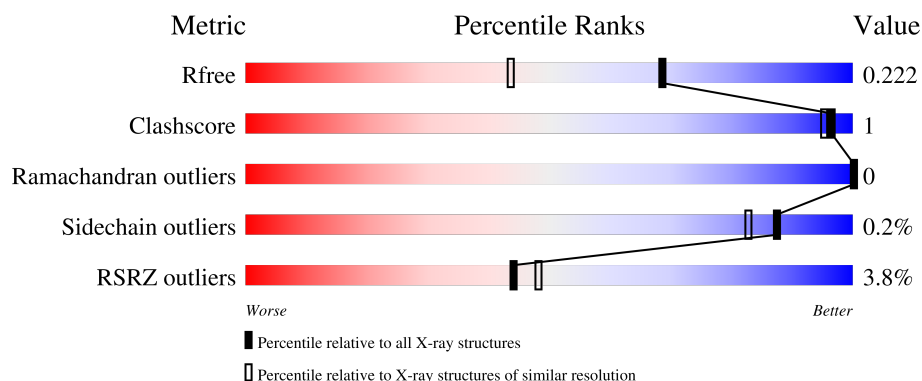
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.66 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	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (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	A	93	 3% 91% 5%
1	C	93	 2% 87% 5% 8%
1	E	93	 3% 94% 5%
1	G	93	 2% 90% 5% 8%
1	IA	93	 3% 88% 6% 5%

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Mol	Chain	Length	Quality of chain
1	KA	93	
1	MA	93	
1	PA	93	
2	B	114	
2	D	114	
2	F	114	
2	H	114	
2	JA	114	
2	LA	114	
2	NA	114	
2	OA	114	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13773 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 Protein S100-A8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	88	Total	C	N	O	S	0	0	0
			702	457	116	127	2			
1	C	86	Total	C	N	O	S	0	1	0
			688	447	114	126	1			
1	E	88	Total	C	N	O	S	0	1	0
			718	465	118	133	2			
1	G	86	Total	C	N	O	S	0	0	0
			695	452	115	126	2			
1	IA	88	Total	C	N	O	S	0	3	0
			721	470	116	133	2			
1	KA	88	Total	C	N	O	S	0	0	0
			708	459	117	130	2			
1	MA	88	Total	C	N	O	S	0	0	0
			710	461	116	131	2			
1	PA	90	Total	C	N	O	S	0	0	0
			698	451	114	131	2			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	42	SER	CYS	engineered mutation	UNP P05109
A	73	LYS	ILE	engineered mutation	UNP P05109
C	42	SER	CYS	engineered mutation	UNP P05109
C	73	LYS	ILE	engineered mutation	UNP P05109
E	42	SER	CYS	engineered mutation	UNP P05109
E	73	LYS	ILE	engineered mutation	UNP P05109
G	42	SER	CYS	engineered mutation	UNP P05109
G	73	LYS	ILE	engineered mutation	UNP P05109
IA	42	SER	CYS	engineered mutation	UNP P05109
IA	73	LYS	ILE	engineered mutation	UNP P05109
KA	42	SER	CYS	engineered mutation	UNP P05109
KA	73	LYS	ILE	engineered mutation	UNP P05109
MA	42	SER	CYS	engineered mutation	UNP P05109

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Chain	Residue	Modelled	Actual	Comment	Reference
MA	73	LYS	ILE	engineered mutation	UNP P05109
PA	42	SER	CYS	engineered mutation	UNP P05109
PA	73	LYS	ILE	engineered mutation	UNP P05109

- Molecule 2 is a protein called Protein S100-A9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	108	Total	C	N	O	S	0	0	0
			871	548	152	166	5			
2	D	108	Total	C	N	O	S	0	0	1
			851	536	145	165	5			
2	F	109	Total	C	N	O	S	0	0	0
			885	554	157	169	5			
2	H	108	Total	C	N	O	S	0	1	0
			857	539	147	166	5			
2	JA	108	Total	C	N	O	S	0	0	0
			870	544	153	168	5			
2	LA	108	Total	C	N	O	S	0	1	0
			882	553	156	168	5			
2	NA	108	Total	C	N	O	S	0	1	0
			885	556	156	168	5			
2	OA	108	Total	C	N	O	S	0	0	0
			855	537	149	164	5			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	3	SER	CYS	engineered mutation	UNP P06702
D	3	SER	CYS	engineered mutation	UNP P06702
F	3	SER	CYS	engineered mutation	UNP P06702
H	3	SER	CYS	engineered mutation	UNP P06702
JA	3	SER	CYS	engineered mutation	UNP P06702
LA	3	SER	CYS	engineered mutation	UNP P06702
NA	3	SER	CYS	engineered mutation	UNP P06702
OA	3	SER	CYS	engineered mutation	UNP P06702

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total 2	Ca 2	0	0
3	C	1	Total 1	Ca 1	0	0
3	D	2	Total 2	Ca 2	0	0
3	E	2	Total 2	Ca 2	0	0
3	F	2	Total 2	Ca 2	0	0
3	G	1	Total 1	Ca 1	0	0
3	H	1	Total 1	Ca 1	0	0
3	IA	2	Total 2	Ca 2	0	0
3	JA	2	Total 2	Ca 2	0	0
3	KA	1	Total 1	Ca 1	0	0
3	LA	2	Total 2	Ca 2	0	0
3	MA	1	Total 1	Ca 1	0	0
3	NA	2	Total 2	Ca 2	0	0
3	PA	1	Total 1	Ca 1	0	0
3	OA	2	Total 2	Ca 2	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Zn 1	0	0
4	D	1	Total 1	Zn 1	0	0
4	F	1	Total 1	Zn 1	0	0
4	H	1	Total 1	Zn 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	JA	1	Total 1	Zn 1	0	0
4	LA	1	Total 1	Zn 1	0	0
4	NA	1	Total 1	Zn 1	0	0
4	OA	1	Total 1	Zn 1	0	0

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	1	Total 1	Cl 1	0	0
5	H	1	Total 1	Cl 1	0	0

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	1	Total 1	Mg 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	55	Total 55	O 55	0	0
7	B	92	Total 92	O 92	0	0
7	C	69	Total 69	O 69	0	0
7	D	62	Total 62	O 62	0	0
7	E	69	Total 69	O 69	0	0
7	F	119	Total 119	O 119	0	0
7	G	63	Total 63	O 63	0	0
7	H	76	Total 76	O 76	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	IA	62	Total 62	O 62	0	0
7	JA	81	Total 81	O 81	0	0
7	KA	77	Total 77	O 77	0	0
7	LA	99	Total 99	O 99	0	0
7	MA	63	Total 63	O 63	0	0
7	NA	72	Total 72	O 72	0	0
7	PA	35	Total 35	O 35	0	0
7	OA	47	Total 47	O 47	0	0

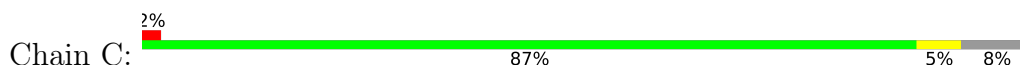
3 Residue-property plots [i](#)

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.

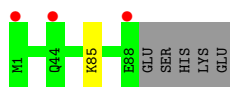
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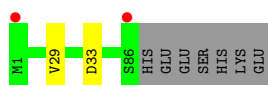
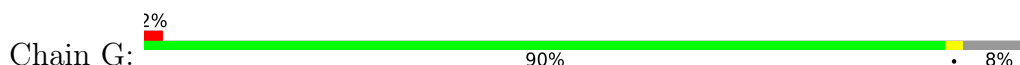
- Molecule 1: Protein S100-A8



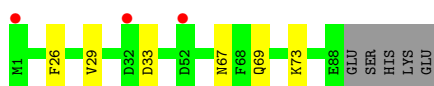
- Molecule 1: Protein S100-A8



- Molecule 1: Protein S100-A8



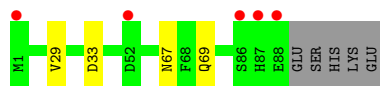
- Molecule 1: Protein S100-A8



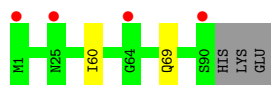
- Molecule 1: Protein S100-A8



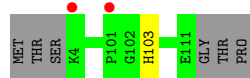
- Molecule 1: Protein S100-A8



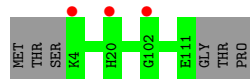
- Molecule 1: Protein S100-A8



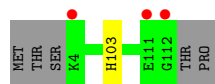
- Molecule 2: Protein S100-A9



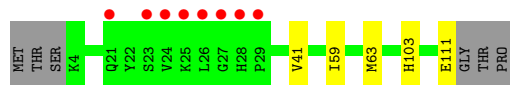
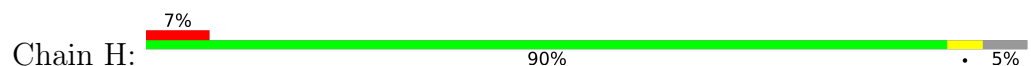
- Molecule 2: Protein S100-A9



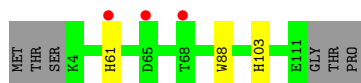
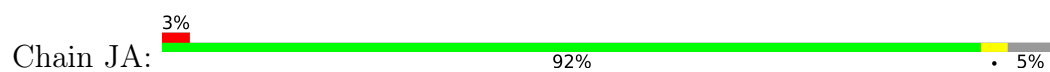
- Molecule 2: Protein S100-A9



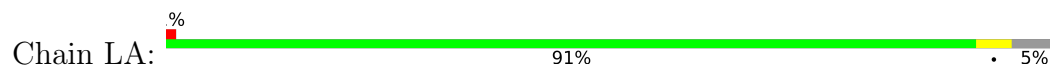
- Molecule 2: Protein S100-A9



- Molecule 2: Protein S100-A9



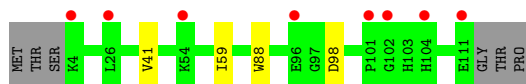
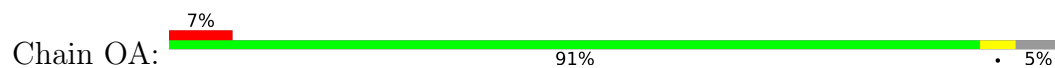
• Molecule 2: Protein S100-A9



• Molecule 2: Protein S100-A9



• Molecule 2: Protein S100-A9



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	106.48Å 83.58Å 109.69Å 90.00° 97.74° 90.00°	Depositor
Resolution (Å)	36.23 – 1.66 36.23 – 1.66	Depositor EDS
% Data completeness (in resolution range)	93.5 (36.23-1.66) 93.5 (36.23-1.66)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 1.66Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.183 , 0.221 0.184 , 0.222	Depositor DCC
R_{free} test set	1832 reflections (0.82%)	wwPDB-VP
Wilson B-factor (Å ²)	25.0	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 39.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13773	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.46% 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: CL, ZN, MG, CA

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	0.23	0/716	0.46	0/965
1	C	0.28	0/701	0.53	2/943 (0.2%)
1	E	0.26	0/735	0.46	0/989
1	G	0.25	0/708	0.45	0/951
1	IA	0.29	0/748	0.45	0/1006
1	KA	0.29	0/722	0.48	0/972
1	MA	0.27	0/724	0.45	0/973
1	PA	0.22	0/711	0.40	0/960
2	B	0.25	0/889	0.47	0/1194
2	D	0.23	0/868	0.45	0/1166
2	F	0.27	0/903	0.48	0/1210
2	H	0.26	0/880	0.46	0/1183
2	JA	0.27	0/888	0.47	0/1192
2	LA	0.26	0/904	0.47	0/1213
2	NA	0.23	0/907	0.41	0/1217
2	OA	0.20	0/873	0.41	0/1176
All	All	0.25	0/12877	0.46	2/17310 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	41	GLU	CA-C-N	-5.13	113.41	123.56
1	C	41	GLU	C-N-CA	-5.13	113.41	123.56

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	702	0	693	2	0
1	C	688	0	691	3	0
1	E	718	0	717	1	0
1	G	695	0	710	1	0
1	IA	721	0	727	5	0
1	KA	708	0	705	1	0
1	MA	710	0	714	2	0
1	PA	698	0	675	2	0
2	B	871	0	821	1	0
2	D	851	0	788	0	0
2	F	885	0	852	1	0
2	H	857	0	799	2	0
2	JA	870	0	820	4	0
2	LA	882	0	839	2	0
2	NA	885	0	844	1	0
2	OA	855	0	785	3	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	IA	2	0	0	0	0
3	JA	2	0	0	0	0
3	KA	1	0	0	0	0
3	LA	2	0	0	0	0
3	MA	1	0	0	0	0
3	NA	2	0	0	0	0
3	OA	2	0	0	0	0
3	PA	1	0	0	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
4	H	1	0	0	0	0
4	JA	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	LA	1	0	0	0	0
4	NA	1	0	0	0	0
4	OA	1	0	0	0	0
5	F	1	0	0	0	0
5	H	1	0	0	0	0
6	H	1	0	0	0	0
7	A	55	0	0	0	0
7	B	92	0	0	1	0
7	C	69	0	0	0	0
7	D	62	0	0	0	0
7	E	69	0	0	1	0
7	F	119	0	0	1	0
7	G	63	0	0	0	0
7	H	76	0	0	1	0
7	IA	62	0	0	0	0
7	JA	81	0	0	1	0
7	KA	77	0	0	0	0
7	LA	99	0	0	0	0
7	MA	63	0	0	0	0
7	NA	72	0	0	0	0
7	OA	47	0	0	0	0
7	PA	35	0	0	0	0
All	All	13773	0	12180	25	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.

All (25) 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)
2:NA:41:VAL:HG11	2:NA:59:ILE:HD12	1.94	0.50
2:LA:90:SER:O	2:LA:94:MET:HG3	2.11	0.50
1:A:73:LYS:HE3	1:C:60:ILE:HD12	1.94	0.50
1:MA:67:ASN:OD1	1:MA:69:GLN:HG2	2.12	0.49
2:JA:103:HIS:HA	7:JA:311:HOH:O	2.13	0.48
1:C:57:GLU:HG2	1:C:73:LYS:HE2	1.97	0.46
1:IA:73:LYS:HE3	1:PA:60:ILE:HD12	1.98	0.45
1:KA:81:ALA:O	1:KA:85:LYS:HG2	2.15	0.45
1:A:49:LYS:HD2	1:A:54:TRP:CE2	2.52	0.45
2:B:103:HIS:HA	7:B:301:HOH:O	2.16	0.45
1:IA:69:GLN:HB3	2:JA:88:TRP:CZ3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:29:VAL:HG13	1:G:33:ASP:HB2	2.00	0.44
1:IA:67:ASN:OD1	1:IA:69:GLN:HG2	2.17	0.44
2:LA:41:VAL:HG11	2:LA:59:ILE:HD12	2.00	0.44
2:JA:61:HIS:CD2	2:OA:98:ASP:HB3	2.52	0.44
1:IA:29:VAL:HG13	1:IA:33:ASP:HB2	1.99	0.43
1:MA:29:VAL:HG13	1:MA:33:ASP:HB2	1.99	0.43
1:PA:69:GLN:HB2	2:OA:88:TRP:CZ3	2.52	0.43
2:OA:41:VAL:HG11	2:OA:59:ILE:HD12	2.02	0.42
2:F:103:HIS:HA	7:F:301:HOH:O	2.19	0.42
1:C:33:ASP:CB	1:C:33:ASP:OD2	2.67	0.42
1:IA:26:PHE:CG	2:JA:103:HIS:HB2	2.55	0.41
2:H:103:HIS:HA	7:H:302:HOH:O	2.20	0.41
2:H:41:VAL:HG11	2:H:59:ILE:HD12	2.03	0.41
1:E:85:LYS:HG3	7:E:239:HOH:O	2.22	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	86/93 (92%)	85 (99%)	1 (1%)	0	100	100
1	C	85/93 (91%)	84 (99%)	1 (1%)	0	100	100
1	E	87/93 (94%)	86 (99%)	1 (1%)	0	100	100
1	G	84/93 (90%)	83 (99%)	1 (1%)	0	100	100
1	IA	89/93 (96%)	88 (99%)	1 (1%)	0	100	100
1	KA	86/93 (92%)	86 (100%)	0	0	100	100
1	MA	86/93 (92%)	84 (98%)	2 (2%)	0	100	100
1	PA	88/93 (95%)	88 (100%)	0	0	100	100
2	B	106/114 (93%)	106 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	106/114 (93%)	105 (99%)	1 (1%)	0	100	100
2	F	107/114 (94%)	107 (100%)	0	0	100	100
2	H	107/114 (94%)	106 (99%)	1 (1%)	0	100	100
2	JA	106/114 (93%)	105 (99%)	1 (1%)	0	100	100
2	LA	107/114 (94%)	107 (100%)	0	0	100	100
2	NA	107/114 (94%)	107 (100%)	0	0	100	100
2	OA	106/114 (93%)	106 (100%)	0	0	100	100
All	All	1543/1656 (93%)	1533 (99%)	10 (1%)	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	71/83 (86%)	71 (100%)	0	100	100
1	C	71/83 (86%)	71 (100%)	0	100	100
1	E	76/83 (92%)	76 (100%)	0	100	100
1	G	74/83 (89%)	74 (100%)	0	100	100
1	IA	77/83 (93%)	77 (100%)	0	100	100
1	KA	74/83 (89%)	74 (100%)	0	100	100
1	MA	76/83 (92%)	76 (100%)	0	100	100
1	PA	70/83 (84%)	70 (100%)	0	100	100
2	B	91/103 (88%)	91 (100%)	0	100	100
2	D	88/103 (85%)	88 (100%)	0	100	100
2	F	96/103 (93%)	96 (100%)	0	100	100
2	H	90/103 (87%)	87 (97%)	3 (3%)	33	11
2	JA	93/103 (90%)	93 (100%)	0	100	100
2	LA	95/103 (92%)	95 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	NA	95/103 (92%)	95 (100%)	0	100	100
2	OA	87/103 (84%)	87 (100%)	0	100	100
All	All	1324/1488 (89%)	1321 (100%)	3 (0%)	87	83

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	63[A]	MET
2	H	63[B]	MET
2	H	111	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	69	GLN
2	D	21	GLN
2	F	11	ASN
2	F	34	GLN
1	G	69	GLN
2	H	73	GLN
2	H	104	HIS
1	PA	87	HIS
2	OA	11	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 36 ligands modelled in this entry, 36 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	88/93 (94%)	0.25	3 (3%)	48	52	20, 26, 34, 45	0
1	C	86/93 (92%)	0.13	2 (2%)	61	66	16, 24, 37, 43	1 (1%)
1	E	88/93 (94%)	0.15	3 (3%)	48	52	15, 23, 36, 44	4 (4%)
1	G	86/93 (92%)	0.35	2 (2%)	61	66	19, 27, 41, 46	0
1	IA	88/93 (94%)	0.14	3 (3%)	48	52	16, 24, 39, 45	4 (4%)
1	KA	88/93 (94%)	0.01	3 (3%)	48	52	19, 24, 31, 46	0
1	MA	88/93 (94%)	0.30	5 (5%)	29	33	21, 26, 41, 61	2 (2%)
1	PA	90/93 (96%)	0.67	4 (4%)	39	42	23, 32, 40, 54	1 (1%)
2	B	108/114 (94%)	0.31	2 (1%)	66	71	20, 26, 42, 54	0
2	D	108/114 (94%)	0.46	3 (2%)	55	60	21, 29, 38, 44	1 (0%)
2	F	109/114 (95%)	0.12	3 (2%)	55	60	20, 25, 34, 56	2 (1%)
2	H	108/114 (94%)	0.58	8 (7%)	20	23	20, 29, 43, 52	2 (1%)
2	JA	108/114 (94%)	0.38	3 (2%)	55	60	20, 28, 39, 42	1 (0%)
2	LA	108/114 (94%)	0.22	1 (0%)	81	86	18, 26, 36, 48	1 (0%)
2	NA	108/114 (94%)	0.60	7 (6%)	25	28	19, 31, 41, 58	1 (0%)
2	OA	108/114 (94%)	0.74	8 (7%)	20	23	23, 34, 49, 59	0
All	All	1567/1656 (94%)	0.35	60 (3%)	44	48	15, 27, 41, 61	20 (1%)

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	4	LYS	7.2
2	F	112	GLY	4.4
2	H	21	GLN	3.5
1	IA	1	MET	3.5
2	F	4	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	MA	86	SER	3.3
2	OA	102	GLY	3.3
1	PA	1	MET	3.3
2	NA	26	LEU	3.2
2	JA	68	THR	3.1
2	OA	101	PRO	3.0
2	H	24	VAL	2.9
2	H	27	GLY	2.9
2	NA	101	PRO	2.9
2	H	29	PRO	2.8
1	KA	26	PHE	2.8
2	NA	4	LYS	2.8
1	MA	52	ASP	2.8
1	G	86	SER	2.8
2	H	26	LEU	2.7
2	D	102	GLY	2.7
2	NA	24	VAL	2.6
2	LA	4	LYS	2.6
2	B	4	LYS	2.6
1	E	88	GLU	2.6
2	JA	65	ASP	2.5
2	OA	111	GLU	2.5
2	OA	96	GLU	2.5
1	MA	1	MET	2.5
1	PA	90	SER	2.5
2	F	111	GLU	2.5
2	OA	104	HIS	2.4
1	C	86	SER	2.4
1	IA	32[A]	ASP	2.4
2	B	101	PRO	2.4
1	G	1	MET	2.4
2	JA	61	HIS	2.4
2	OA	54	LYS	2.3
1	E	44	GLN	2.3
2	OA	4	LYS	2.3
1	KA	69	GLN	2.3
1	MA	87	HIS	2.2
2	H	28	HIS	2.2
1	A	1	MET	2.2
2	NA	88	TRP	2.1
2	OA	26	LEU	2.1
2	H	25	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	1	MET	2.1
1	A	26	PHE	2.1
1	C	1	MET	2.1
1	A	44	GLN	2.1
1	IA	52	ASP	2.1
2	H	23	SER	2.1
2	D	20	HIS	2.1
1	KA	1	MET	2.1
2	NA	104	HIS	2.1
1	MA	88	GLU	2.0
1	PA	25	ASN	2.0
1	PA	64	GLY	2.0
2	NA	30	ASP	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 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(\AA^2)	Q<0.9
6	MG	H	203	1/1	0.88	0.10	28,28,28,28	0
3	CA	NA	202	1/1	0.96	0.09	31,31,31,31	0
3	CA	JA	201	1/1	0.97	0.05	26,26,26,26	0
3	CA	F	201	1/1	0.98	0.04	22,22,22,22	0
3	CA	OA	202	1/1	0.98	0.07	30,30,30,30	0
4	ZN	F	204	1/1	0.98	0.03	18,18,18,18	1
4	ZN	LA	203	1/1	0.98	0.05	23,23,23,23	1
4	ZN	NA	203	1/1	0.98	0.03	24,24,24,24	1
5	CL	F	203	1/1	0.98	0.05	30,30,30,30	0
5	CL	H	201	1/1	0.98	0.09	30,30,30,30	0

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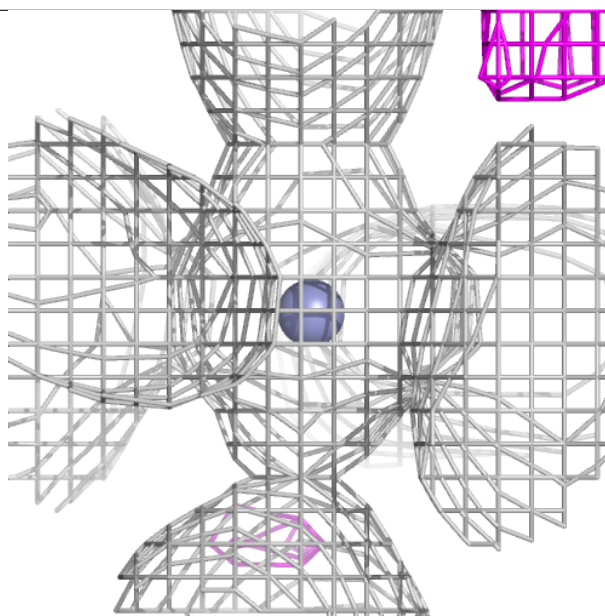
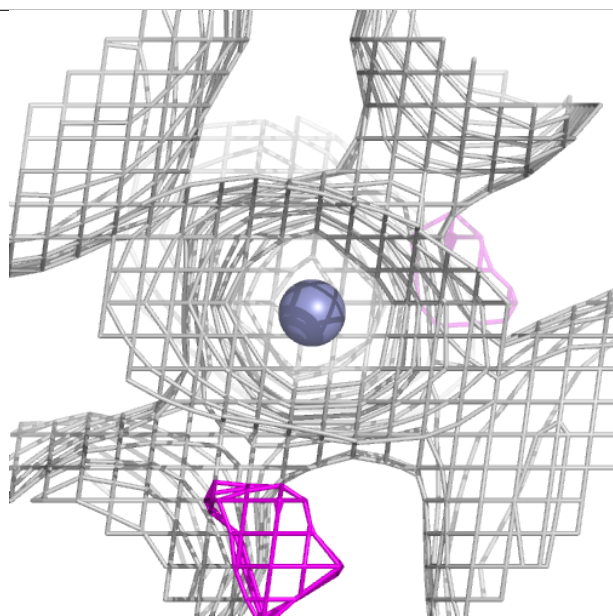
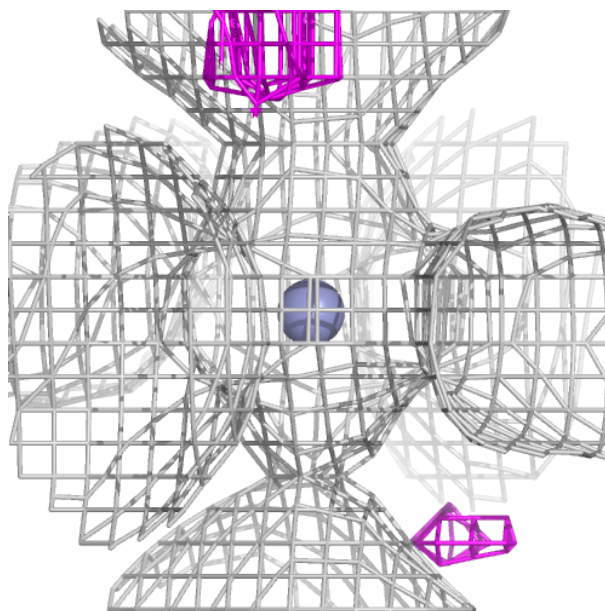
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	CA	D	202	1/1	0.98	0.04	25,25,25,25	0
3	CA	B	202	1/1	0.99	0.04	21,21,21,21	0
3	CA	JA	202	1/1	0.99	0.03	25,25,25,25	0
3	CA	LA	201	1/1	0.99	0.04	22,22,22,22	0
3	CA	LA	202	1/1	0.99	0.05	21,21,21,21	0
3	CA	MA	200	1/1	0.99	0.03	20,20,20,20	0
3	CA	NA	201	1/1	0.99	0.03	23,23,23,23	0
3	CA	D	201	1/1	0.99	0.03	25,25,25,25	0
3	CA	PA	200	1/1	0.99	0.04	24,24,24,24	0
3	CA	OA	201	1/1	0.99	0.03	22,22,22,22	0
3	CA	A	200	1/1	0.99	0.02	22,22,22,22	0
4	ZN	B	203	1/1	0.99	0.03	28,28,28,28	1
3	CA	E	101	1/1	0.99	0.03	19,19,19,19	0
4	ZN	H	204	1/1	0.99	0.04	22,22,22,22	1
3	CA	E	102	1/1	0.99	0.21	28,28,28,28	0
3	CA	B	201	1/1	0.99	0.04	22,22,22,22	0
4	ZN	OA	203	1/1	0.99	0.04	39,39,39,39	1
3	CA	F	202	1/1	0.99	0.03	22,22,22,22	0
3	CA	H	202	1/1	0.99	0.03	23,23,23,23	0
3	CA	IA	102	1/1	0.99	0.23	30,30,30,30	0
3	CA	KA	200	1/1	1.00	0.02	20,20,20,20	0
3	CA	G	200	1/1	1.00	0.03	21,21,21,21	0
4	ZN	D	203	1/1	1.00	0.02	23,23,23,23	1
3	CA	C	200	1/1	1.00	0.04	19,19,19,19	0
3	CA	IA	101	1/1	1.00	0.02	20,20,20,20	0
4	ZN	JA	203	1/1	1.00	0.01	21,21,21,21	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.

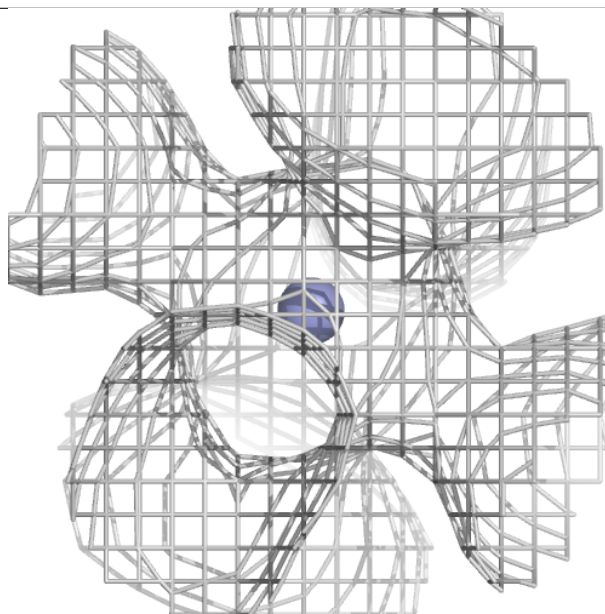
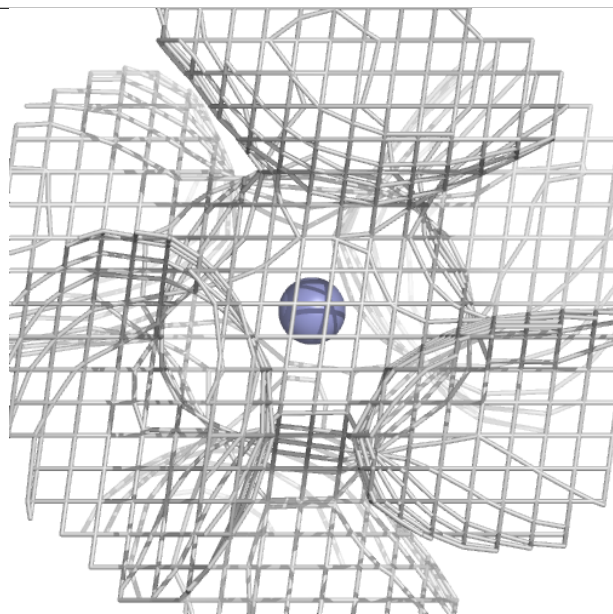
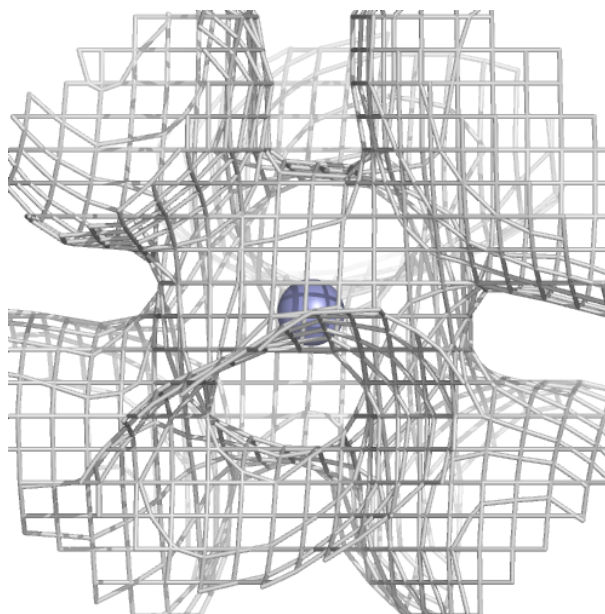
Electron density around ZN F 204:

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



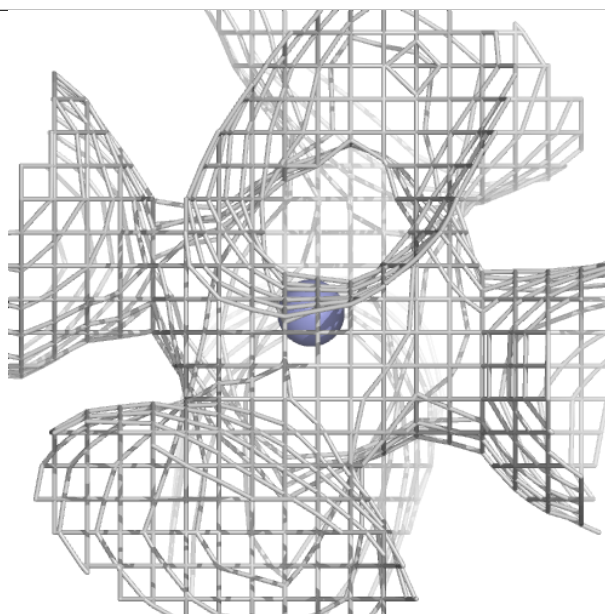
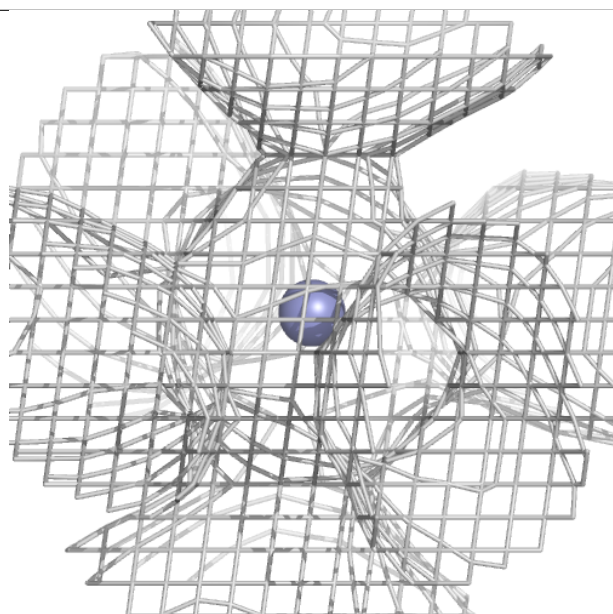
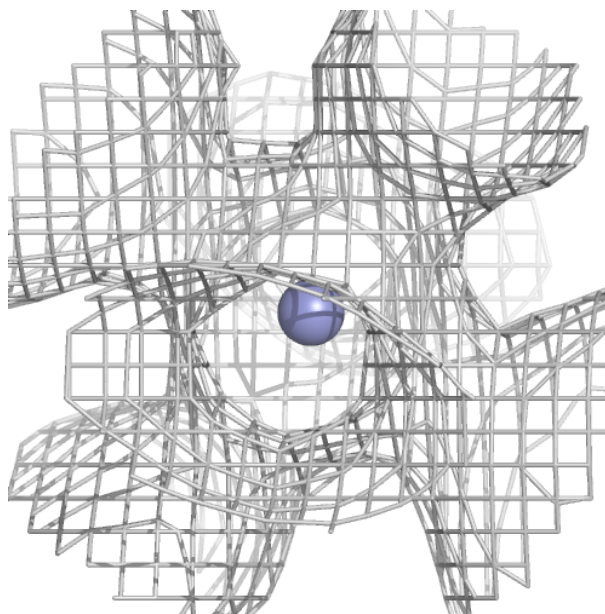
Electron density around ZN LA 203:

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



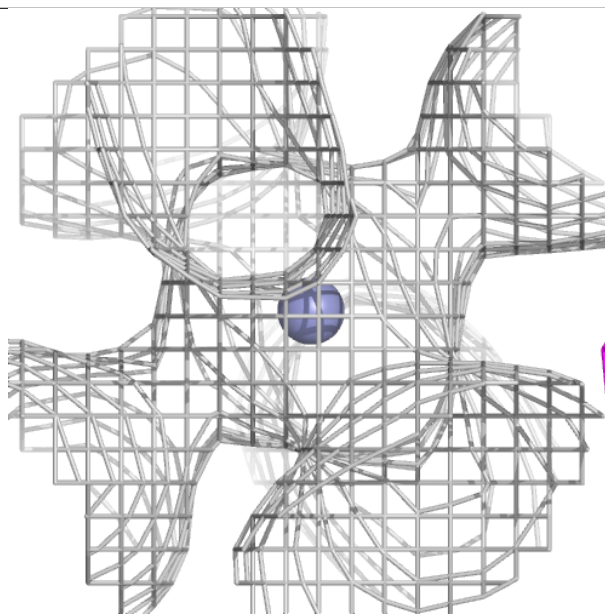
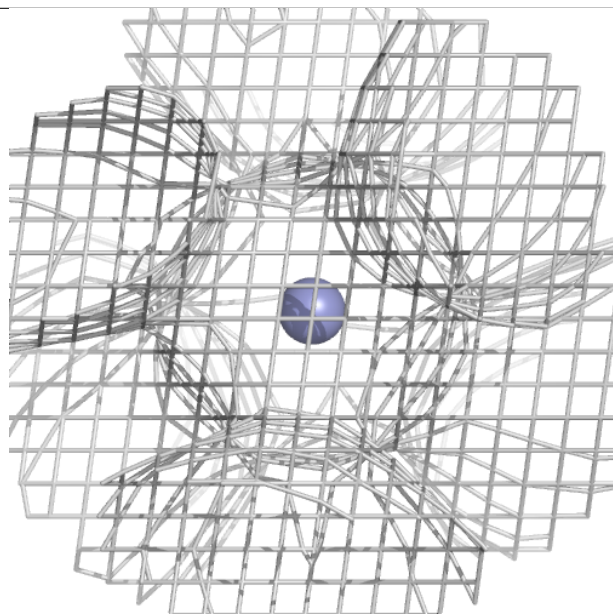
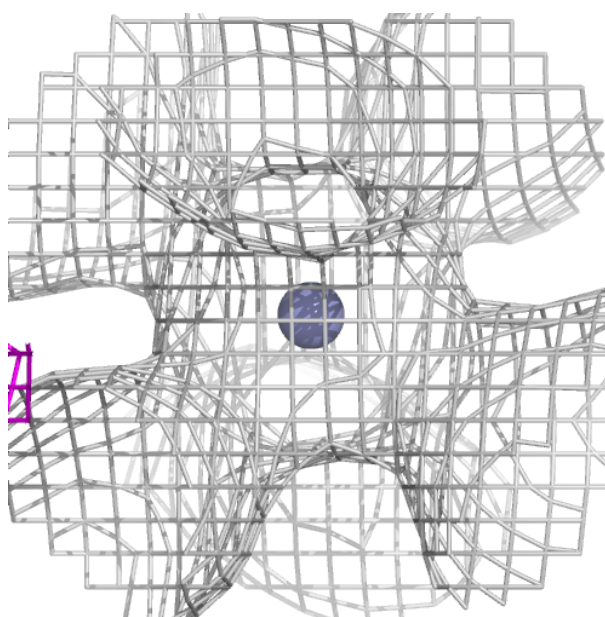
Electron density around ZN NA 203:

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



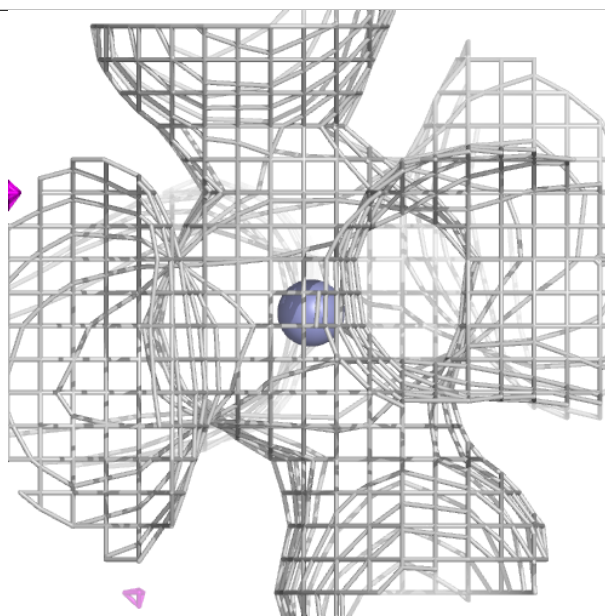
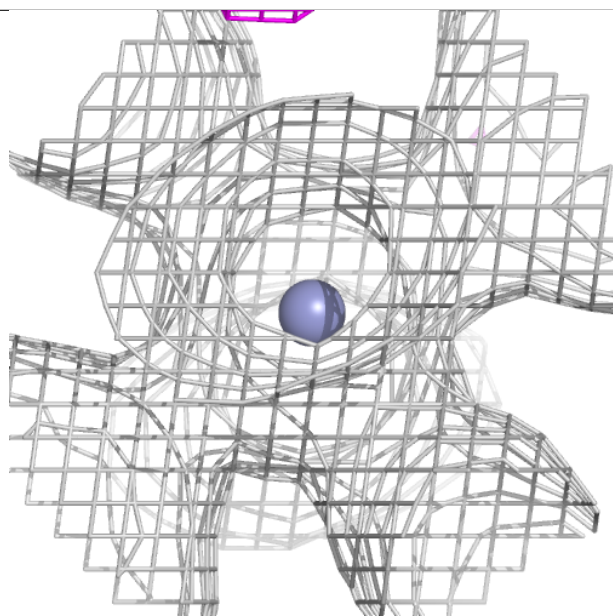
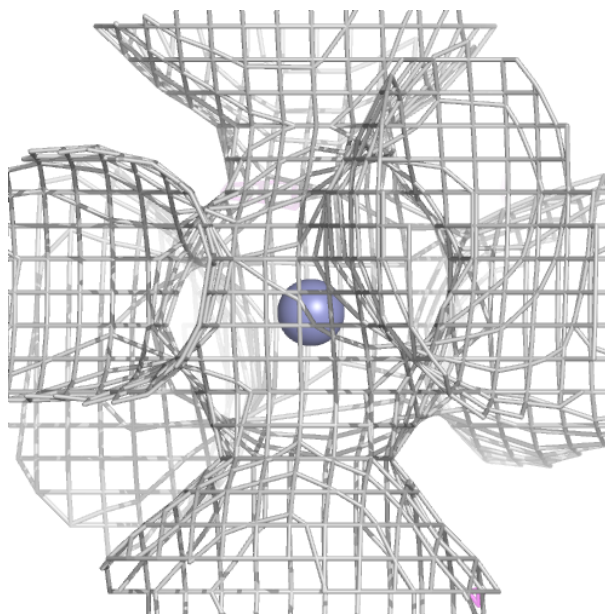
Electron density around ZN B 203:

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



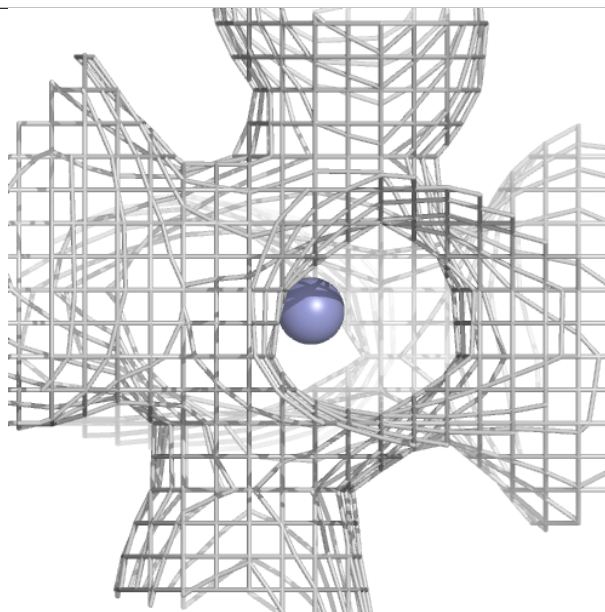
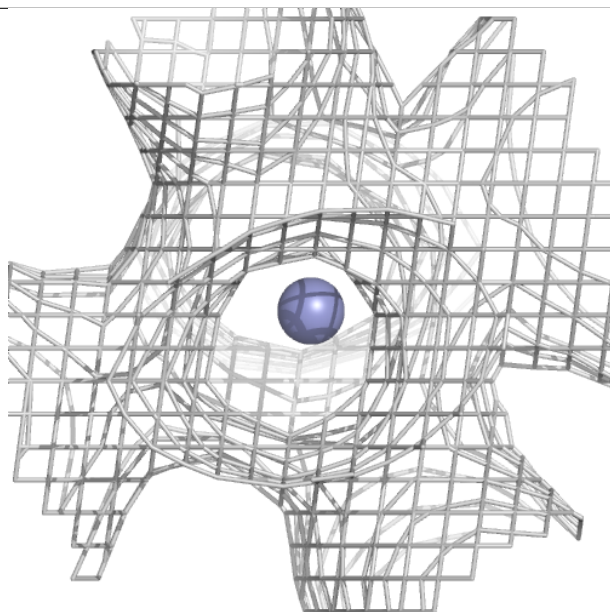
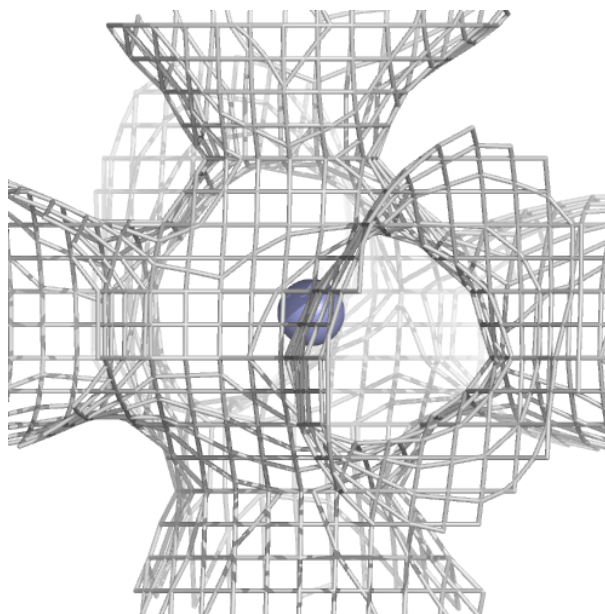
Electron density around ZN H 204:

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



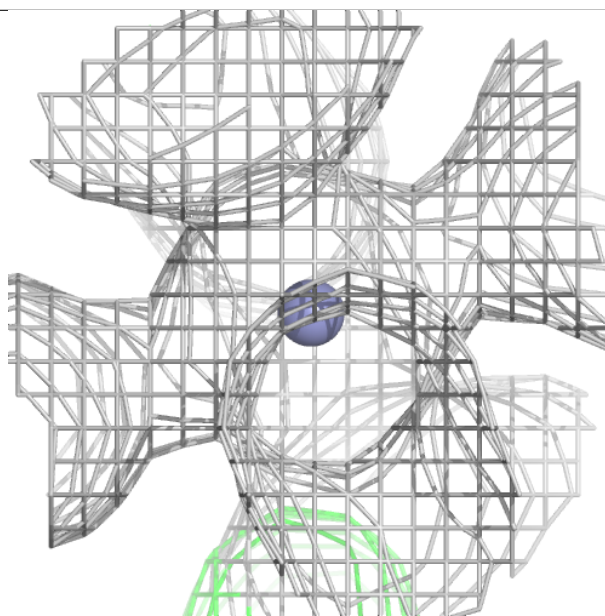
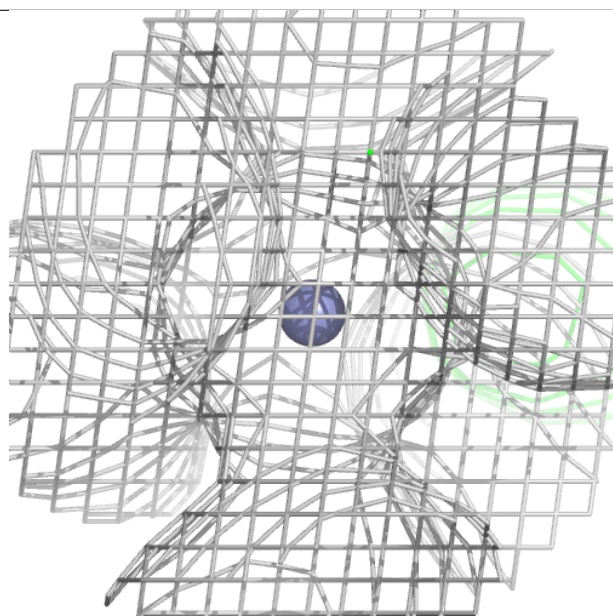
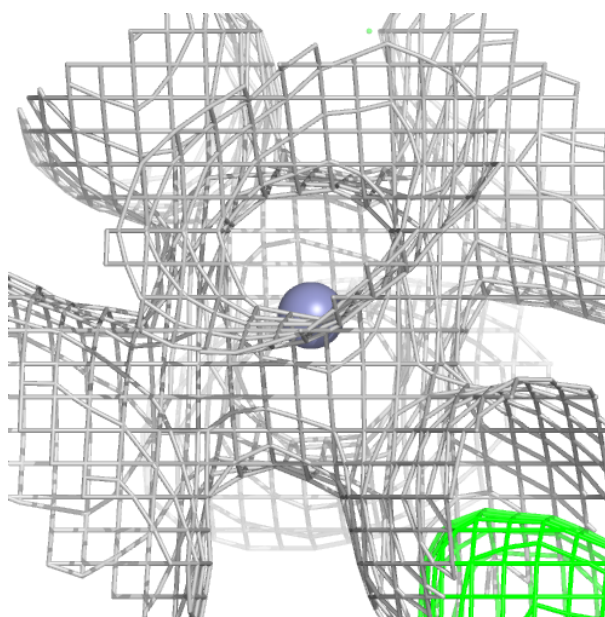
Electron density around ZN OA 203:

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



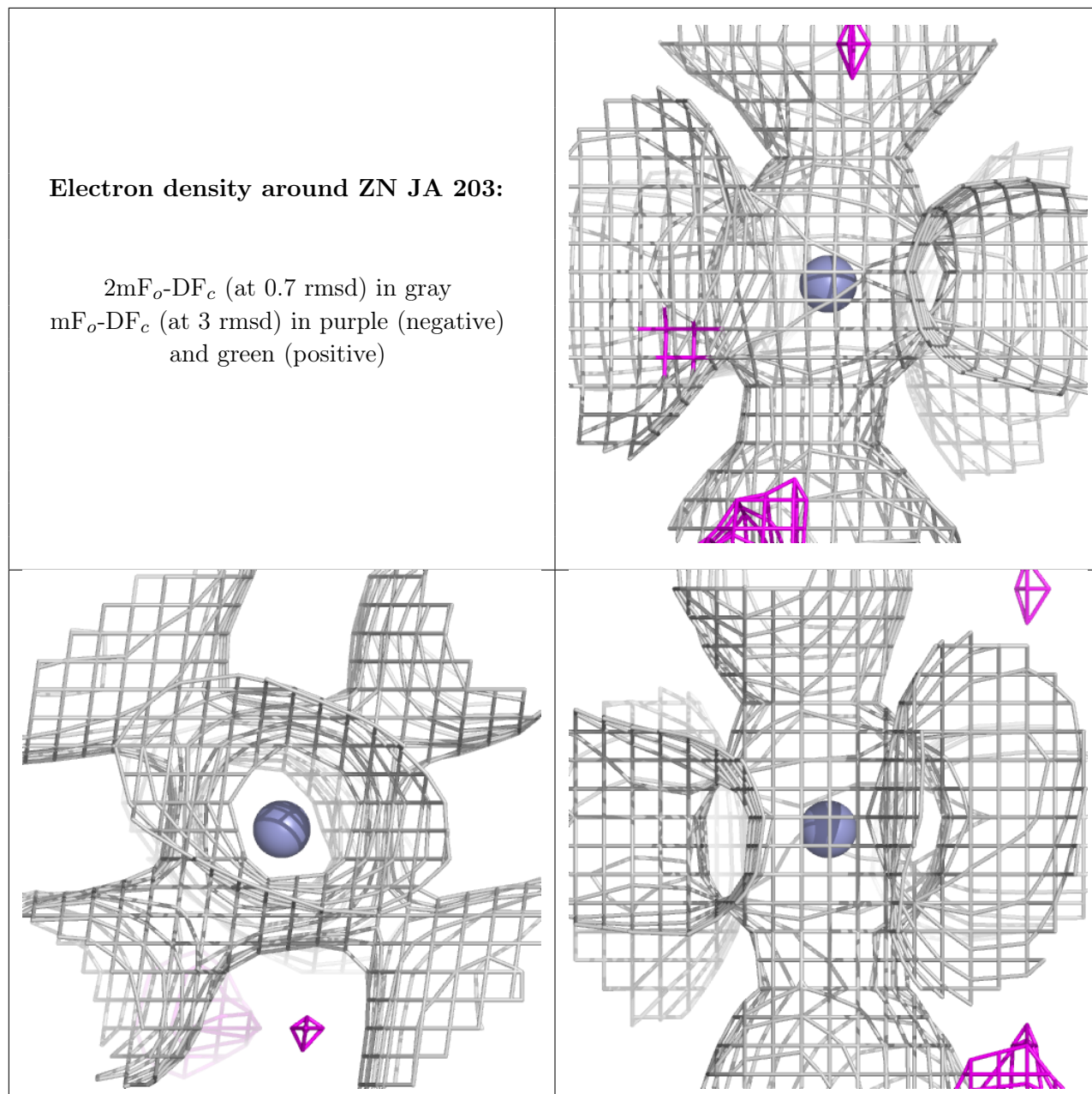
Electron density around ZN D 203:

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



Electron density around ZN JA 203:

$2mF_o-DF_c$ (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.