



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 10, 2026 – 10:13 pm BST

PDB ID : 9TPY / pdb_00009tpy
Title : HomA ectodomain (EDC-HomA)
Authors : Rodriguez-Banqueri, A.; Goulas, T.; Eckhard, U.; Gomis-Ruth, F.X.
Deposited on : 2025-12-19
Resolution : 2.85 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 : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

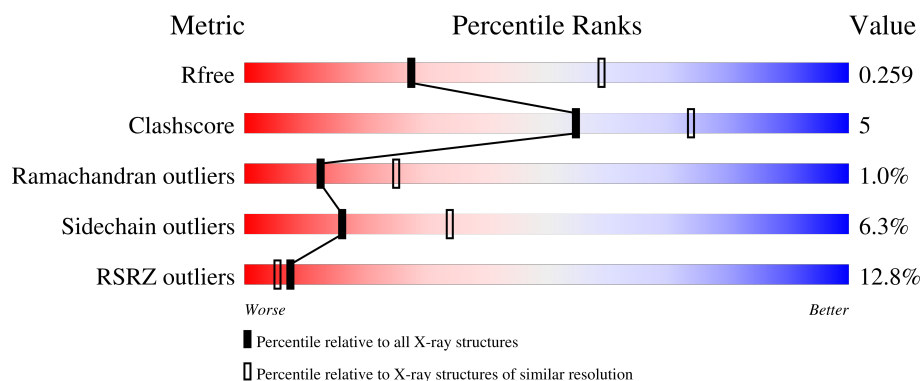
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	487	8% 70% 12% • 16%
1	B	487	15% 70% 11% • 17%
1	C	487	9% 70% 12% • 17%
1	D	487	10% 69% 12% • 17%
1	E	487	9% 69% 10% • 19%

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Mol	Chain	Length	Quality of chain
1	F	487	
1	G	487	
1	H	487	

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
4	IOD	C	507	-	-	X	-
6	PGE	D	503	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 24235 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 HomA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	409	Total	C	N	O	S	0	0	0
			3059	1923	519	608	9			
1	B	405	Total	C	N	O	S	0	0	0
			3064	1930	512	613	9			
1	C	405	Total	C	N	O	S	0	0	0
			3066	1929	517	611	9			
1	D	406	Total	C	N	O	S	0	0	0
			3086	1932	526	619	9			
1	E	395	Total	C	N	O	S	0	0	0
			2984	1880	500	595	9			
1	F	396	Total	C	N	O	S	0	0	0
			2990	1879	502	600	9			
1	G	393	Total	C	N	O	S	0	0	0
			2819	1760	480	570	9			
1	H	396	Total	C	N	O	S	0	0	0
			2911	1826	492	585	8			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	initiating methionine	UNP O25414
A	-1	HIS	-	expression tag	UNP O25414
A	0	HIS	-	expression tag	UNP O25414
A	1	HIS	-	expression tag	UNP O25414
A	2	HIS	-	expression tag	UNP O25414
A	3	HIS	-	expression tag	UNP O25414
A	4	HIS	-	expression tag	UNP O25414
A	5	SER	-	expression tag	UNP O25414
A	6	SER	-	expression tag	UNP O25414
A	7	GLY	-	expression tag	UNP O25414
A	8	GLU	-	expression tag	UNP O25414
A	9	VAL	-	expression tag	UNP O25414
A	10	LEU	-	expression tag	UNP O25414

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Chain	Residue	Modelled	Actual	Comment	Reference
A	11	PHE	-	expression tag	UNP O25414
A	12	GLN	-	expression tag	UNP O25414
A	13	GLY	-	expression tag	UNP O25414
A	14	MET	-	expression tag	UNP O25414
A	15	GLY	-	expression tag	UNP O25414
A	16	ASN	-	expression tag	UNP O25414
A	481	SER	-	insertion	UNP O25414
B	-2	MET	-	initiating methionine	UNP O25414
B	-1	HIS	-	expression tag	UNP O25414
B	0	HIS	-	expression tag	UNP O25414
B	1	HIS	-	expression tag	UNP O25414
B	2	HIS	-	expression tag	UNP O25414
B	3	HIS	-	expression tag	UNP O25414
B	4	HIS	-	expression tag	UNP O25414
B	5	SER	-	expression tag	UNP O25414
B	6	SER	-	expression tag	UNP O25414
B	7	GLY	-	expression tag	UNP O25414
B	8	GLU	-	expression tag	UNP O25414
B	9	VAL	-	expression tag	UNP O25414
B	10	LEU	-	expression tag	UNP O25414
B	11	PHE	-	expression tag	UNP O25414
B	12	GLN	-	expression tag	UNP O25414
B	13	GLY	-	expression tag	UNP O25414
B	14	MET	-	expression tag	UNP O25414
B	15	GLY	-	expression tag	UNP O25414
B	16	ASN	-	expression tag	UNP O25414
B	481	SER	-	insertion	UNP O25414
C	-2	MET	-	initiating methionine	UNP O25414
C	-1	HIS	-	expression tag	UNP O25414
C	0	HIS	-	expression tag	UNP O25414
C	1	HIS	-	expression tag	UNP O25414
C	2	HIS	-	expression tag	UNP O25414
C	3	HIS	-	expression tag	UNP O25414
C	4	HIS	-	expression tag	UNP O25414
C	5	SER	-	expression tag	UNP O25414
C	6	SER	-	expression tag	UNP O25414
C	7	GLY	-	expression tag	UNP O25414
C	8	GLU	-	expression tag	UNP O25414
C	9	VAL	-	expression tag	UNP O25414
C	10	LEU	-	expression tag	UNP O25414
C	11	PHE	-	expression tag	UNP O25414
C	12	GLN	-	expression tag	UNP O25414

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Chain	Residue	Modelled	Actual	Comment	Reference
C	13	GLY	-	expression tag	UNP O25414
C	14	MET	-	expression tag	UNP O25414
C	15	GLY	-	expression tag	UNP O25414
C	16	ASN	-	expression tag	UNP O25414
C	481	SER	-	insertion	UNP O25414
D	-2	MET	-	initiating methionine	UNP O25414
D	-1	HIS	-	expression tag	UNP O25414
D	0	HIS	-	expression tag	UNP O25414
D	1	HIS	-	expression tag	UNP O25414
D	2	HIS	-	expression tag	UNP O25414
D	3	HIS	-	expression tag	UNP O25414
D	4	HIS	-	expression tag	UNP O25414
D	5	SER	-	expression tag	UNP O25414
D	6	SER	-	expression tag	UNP O25414
D	7	GLY	-	expression tag	UNP O25414
D	8	GLU	-	expression tag	UNP O25414
D	9	VAL	-	expression tag	UNP O25414
D	10	LEU	-	expression tag	UNP O25414
D	11	PHE	-	expression tag	UNP O25414
D	12	GLN	-	expression tag	UNP O25414
D	13	GLY	-	expression tag	UNP O25414
D	14	MET	-	expression tag	UNP O25414
D	15	GLY	-	expression tag	UNP O25414
D	16	ASN	-	expression tag	UNP O25414
D	481	SER	-	insertion	UNP O25414
E	-2	MET	-	initiating methionine	UNP O25414
E	-1	HIS	-	expression tag	UNP O25414
E	0	HIS	-	expression tag	UNP O25414
E	1	HIS	-	expression tag	UNP O25414
E	2	HIS	-	expression tag	UNP O25414
E	3	HIS	-	expression tag	UNP O25414
E	4	HIS	-	expression tag	UNP O25414
E	5	SER	-	expression tag	UNP O25414
E	6	SER	-	expression tag	UNP O25414
E	7	GLY	-	expression tag	UNP O25414
E	8	GLU	-	expression tag	UNP O25414
E	9	VAL	-	expression tag	UNP O25414
E	10	LEU	-	expression tag	UNP O25414
E	11	PHE	-	expression tag	UNP O25414
E	12	GLN	-	expression tag	UNP O25414
E	13	GLY	-	expression tag	UNP O25414
E	14	MET	-	expression tag	UNP O25414

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Chain	Residue	Modelled	Actual	Comment	Reference
E	15	GLY	-	expression tag	UNP O25414
E	16	ASN	-	expression tag	UNP O25414
E	481	SER	-	insertion	UNP O25414
F	-2	MET	-	initiating methionine	UNP O25414
F	-1	HIS	-	expression tag	UNP O25414
F	0	HIS	-	expression tag	UNP O25414
F	1	HIS	-	expression tag	UNP O25414
F	2	HIS	-	expression tag	UNP O25414
F	3	HIS	-	expression tag	UNP O25414
F	4	HIS	-	expression tag	UNP O25414
F	5	SER	-	expression tag	UNP O25414
F	6	SER	-	expression tag	UNP O25414
F	7	GLY	-	expression tag	UNP O25414
F	8	GLU	-	expression tag	UNP O25414
F	9	VAL	-	expression tag	UNP O25414
F	10	LEU	-	expression tag	UNP O25414
F	11	PHE	-	expression tag	UNP O25414
F	12	GLN	-	expression tag	UNP O25414
F	13	GLY	-	expression tag	UNP O25414
F	14	MET	-	expression tag	UNP O25414
F	15	GLY	-	expression tag	UNP O25414
F	16	ASN	-	expression tag	UNP O25414
F	481	SER	-	insertion	UNP O25414
G	-2	MET	-	initiating methionine	UNP O25414
G	-1	HIS	-	expression tag	UNP O25414
G	0	HIS	-	expression tag	UNP O25414
G	1	HIS	-	expression tag	UNP O25414
G	2	HIS	-	expression tag	UNP O25414
G	3	HIS	-	expression tag	UNP O25414
G	4	HIS	-	expression tag	UNP O25414
G	5	SER	-	expression tag	UNP O25414
G	6	SER	-	expression tag	UNP O25414
G	7	GLY	-	expression tag	UNP O25414
G	8	GLU	-	expression tag	UNP O25414
G	9	VAL	-	expression tag	UNP O25414
G	10	LEU	-	expression tag	UNP O25414
G	11	PHE	-	expression tag	UNP O25414
G	12	GLN	-	expression tag	UNP O25414
G	13	GLY	-	expression tag	UNP O25414
G	14	MET	-	expression tag	UNP O25414
G	15	GLY	-	expression tag	UNP O25414
G	16	ASN	-	expression tag	UNP O25414

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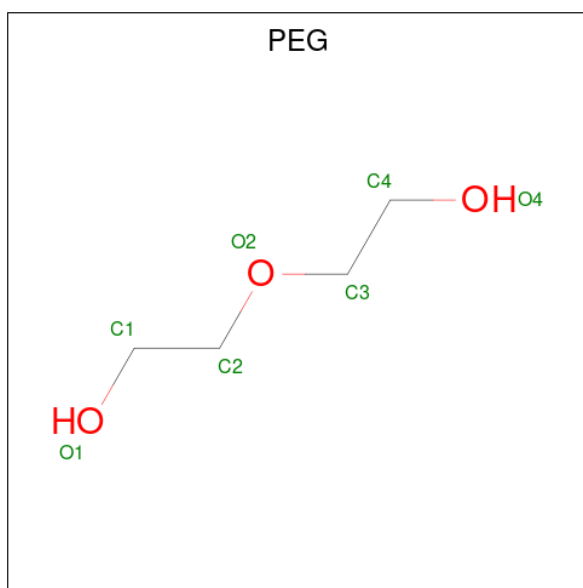
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Chain	Residue	Modelled	Actual	Comment	Reference
G	481	SER	-	insertion	UNP O25414
H	-2	MET	-	initiating methionine	UNP O25414
H	-1	HIS	-	expression tag	UNP O25414
H	0	HIS	-	expression tag	UNP O25414
H	1	HIS	-	expression tag	UNP O25414
H	2	HIS	-	expression tag	UNP O25414
H	3	HIS	-	expression tag	UNP O25414
H	4	HIS	-	expression tag	UNP O25414
H	5	SER	-	expression tag	UNP O25414
H	6	SER	-	expression tag	UNP O25414
H	7	GLY	-	expression tag	UNP O25414
H	8	GLU	-	expression tag	UNP O25414
H	9	VAL	-	expression tag	UNP O25414
H	10	LEU	-	expression tag	UNP O25414
H	11	PHE	-	expression tag	UNP O25414
H	12	GLN	-	expression tag	UNP O25414
H	13	GLY	-	expression tag	UNP O25414
H	14	MET	-	expression tag	UNP O25414
H	15	GLY	-	expression tag	UNP O25414
H	16	ASN	-	expression tag	UNP O25414
H	481	SER	-	insertion	UNP O25414

- 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 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	E	1	Total Zn 1 1	0	0
2	F	1	Total Zn 1 1	0	0
2	G	1	Total Zn 1 1	0	0
2	H	1	Total Zn 1 1	0	0

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).

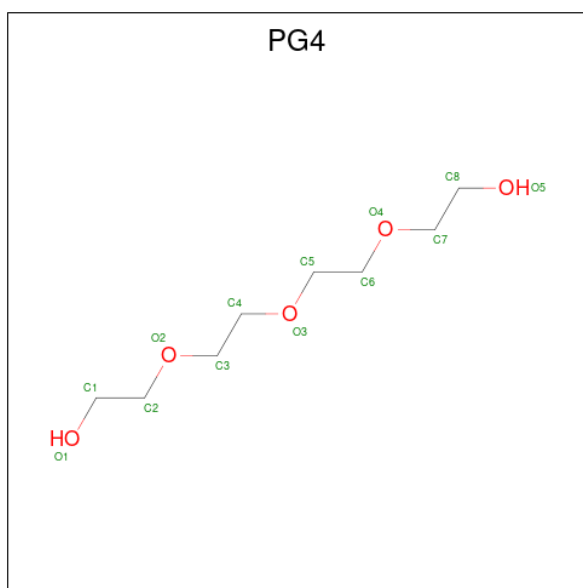


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	C	1	Total	C	O	0	0
			7	4	3		
3	E	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is IODIDE ION (CCD ID: IOD) (formula: I).

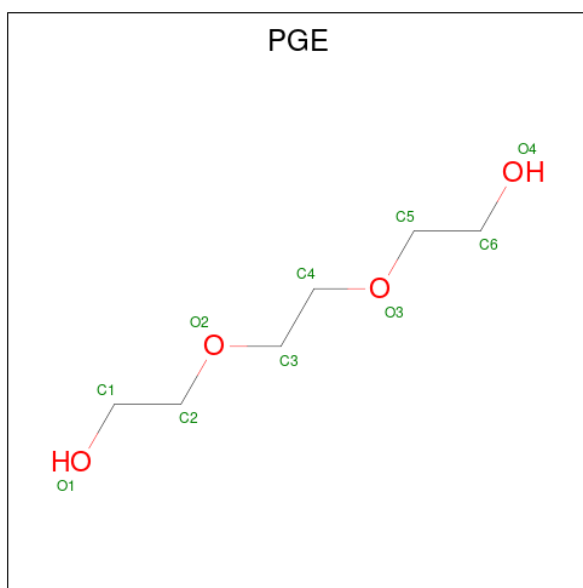
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	I	0	0
			5	5		
4	B	5	Total	I	0	0
			5	5		
4	C	5	Total	I	0	0
			5	5		
4	D	5	Total	I	0	0
			5	5		
4	E	4	Total	I	0	0
			4	4		
4	F	4	Total	I	0	0
			4	4		
4	G	4	Total	I	0	0
			4	4		
4	H	4	Total	I	0	0
			4	4		

- Molecule 5 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			13	8	5		

- Molecule 6 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



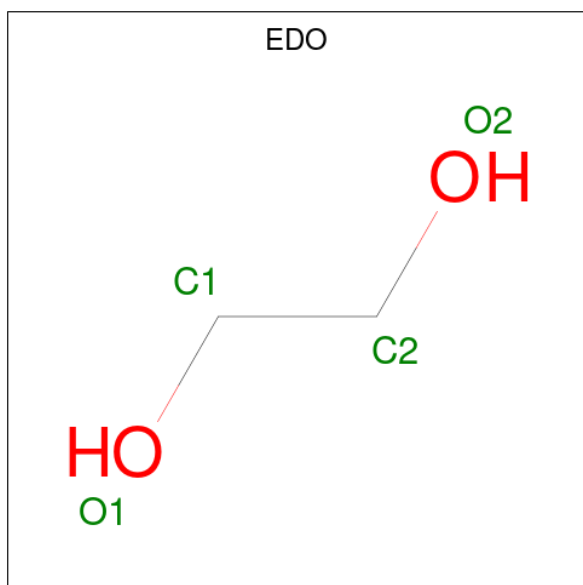
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	C	O	0	0
			10	6	4		
6	D	1	Total	C	O	0	0
			10	6	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	F	1	Total	C	O	0	0
			10	6	4		
6	H	1	Total	C	O	0	0
			10	6	4		

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	E	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	19	Total	O	0	0
			19	19		
8	B	23	Total	O	0	0
			23	23		
8	C	20	Total	O	0	0
			20	20		
8	D	20	Total	O	0	0
			20	20		
8	E	10	Total	O	0	0
			10	10		
8	F	16	Total	O	0	0
			16	16		

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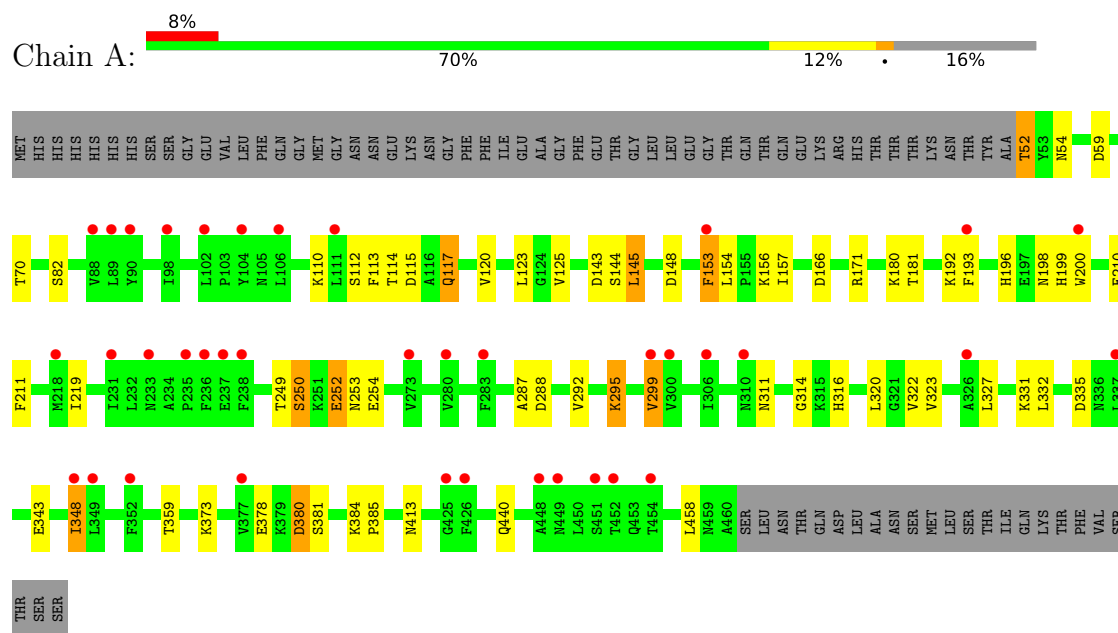
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	G	9	Total	O	0	0
			9	9		
8	H	17	Total	O	0	0
			17	17		

3 Residue-property plots [i](#)

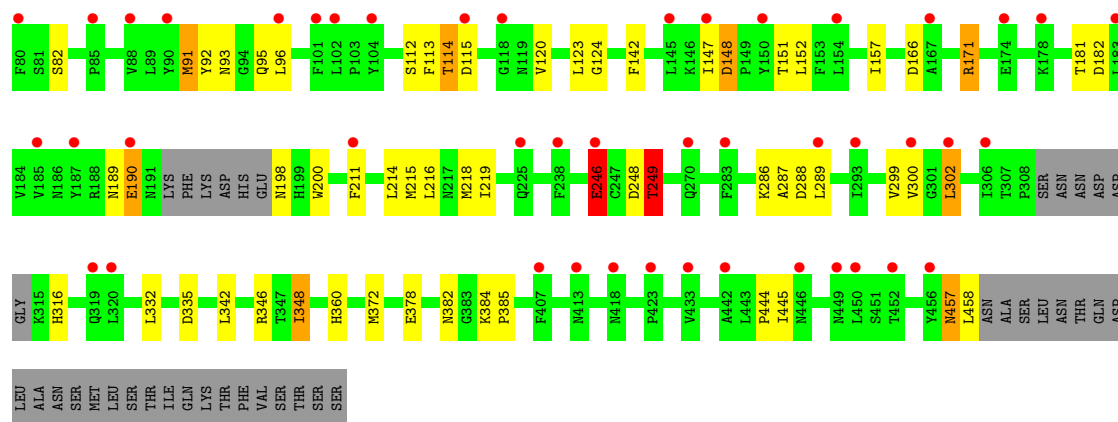
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

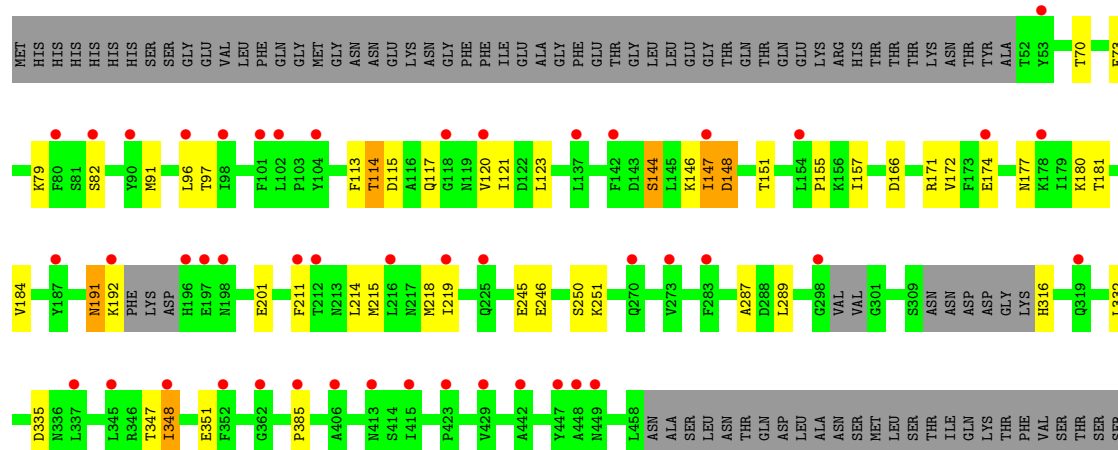


• Molecule 1: HomA

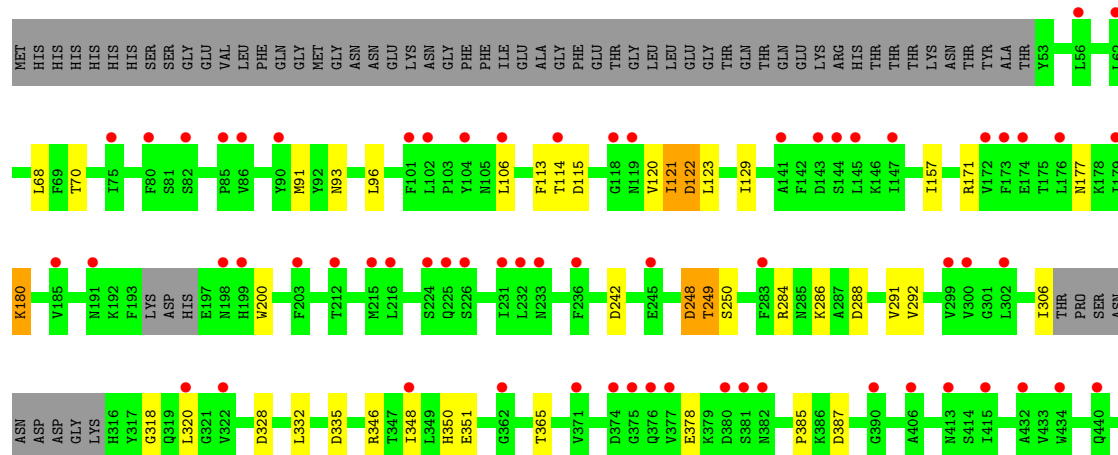


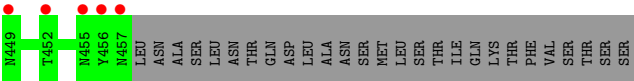


• Molecule 1: HomA

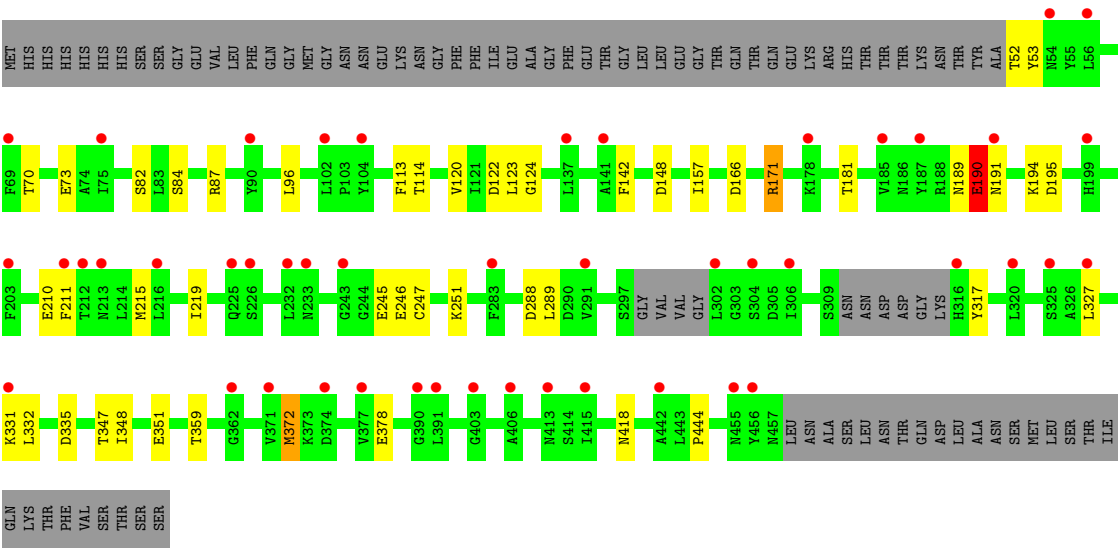


• Molecule 1: HomA





● Molecule 1: HomA



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	60.90Å 126.60Å 155.10Å 84.50° 84.40° 83.50°	Depositor
Resolution (Å)	93.31 – 2.85 93.31 – 2.85	Depositor EDS
% Data completeness (in resolution range)	98.1 (93.31-2.85) 98.1 (93.31-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 2.86Å)	Xtriage
Refinement program	BUSTER 2.10.4 (24-FEB-2021)	Depositor
R, R_{free}	0.241 , 0.266 0.241 , 0.259	Depositor DCC
R_{free} test set	949 reflections (0.89%)	wwPDB-VP
Wilson B-factor (Å ²)	105.4	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 105.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	24235	wwPDB-VP
Average B, all atoms (Å ²)	131.0	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 35.80 % 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 5.5154e-04. 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: PEG, PG4, ZN, PGE, EDO, IOD

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	0.76	1/3120 (0.0%)	1.07	10/4264 (0.2%)
1	B	0.75	1/3128 (0.0%)	1.03	3/4273 (0.1%)
1	C	0.77	1/3127 (0.0%)	1.06	10/4267 (0.2%)
1	D	0.80	1/3148 (0.0%)	1.08	13/4296 (0.3%)
1	E	0.73	1/3043 (0.0%)	1.05	10/4159 (0.2%)
1	F	0.73	1/3048 (0.0%)	1.01	2/4158 (0.0%)
1	G	0.72	1/2867 (0.0%)	0.99	2/3928 (0.1%)
1	H	0.76	1/2966 (0.0%)	1.04	8/4061 (0.2%)
All	All	0.75	8/24447 (0.0%)	1.04	58/33406 (0.2%)

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	70	THR	CA-C	11.99	1.58	1.52
1	D	70	THR	CA-C	9.68	1.58	1.52
1	G	70	THR	CA-C	8.96	1.57	1.52
1	F	70	THR	CA-C	8.92	1.57	1.52
1	H	70	THR	CA-C	8.49	1.57	1.52

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	153	PHE	CA-CB-CG	9.03	122.83	113.80
1	B	193	PHE	CA-CB-CG	8.60	122.40	113.80
1	A	199	HIS	CA-C-N	8.15	134.69	122.95
1	A	199	HIS	C-N-CA	8.15	134.69	122.95
1	E	91	MET	CA-C-N	8.01	132.07	120.38

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	3059	0	2876	30	0
1	B	3064	0	2873	33	0
1	C	3066	0	2911	28	0
1	D	3086	0	2914	35	0
1	E	2984	0	2820	30	0
1	F	2990	0	2806	33	0
1	G	2819	0	2557	18	0
1	H	2911	0	2667	22	0
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
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	7	0	10	2	0
3	C	7	0	10	2	0
3	E	7	0	10	2	0
4	A	5	0	0	1	0
4	B	5	0	0	1	0
4	C	5	0	0	3	0
4	D	5	0	0	1	0
4	E	4	0	0	0	0
4	F	4	0	0	0	0
4	G	4	0	0	2	0
4	H	4	0	0	0	0
5	B	13	0	18	0	0
6	D	20	0	28	7	0
6	F	10	0	14	1	0
6	H	10	0	14	5	0
7	E	4	0	6	0	0
8	A	19	0	0	0	0
8	B	23	0	0	0	0
8	C	20	0	0	0	0
8	D	20	0	0	0	0
8	E	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	F	16	0	0	0	0
8	G	9	0	0	1	0
8	H	17	0	0	0	0
All	All	24235	0	22534	222	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 5.

The worst 5 of 222 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:381:SER:HA	1:F:251:LYS:HB3	1.41	0.98
1:B:250:SER:HA	1:B:385:PRO:HD2	1.49	0.94
1:F:148:ASP:HB2	1:F:151:THR:HG23	1.52	0.90
1:D:246:GLU:HA	6:D:503:PGE:H6	1.60	0.81
1:B:373:LYS:HB2	1:B:379:LYS:NZ	1.96	0.81

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	407/487 (84%)	380 (93%)	21 (5%)	6 (2%)	8	18
1	B	403/487 (83%)	377 (94%)	22 (6%)	4 (1%)	12	25
1	C	403/487 (83%)	374 (93%)	23 (6%)	6 (2%)	8	18
1	D	404/487 (83%)	373 (92%)	28 (7%)	3 (1%)	18	35
1	E	389/487 (80%)	364 (94%)	23 (6%)	2 (0%)	24	42
1	F	388/487 (80%)	365 (94%)	19 (5%)	4 (1%)	12	25
1	G	387/487 (80%)	365 (94%)	21 (5%)	1 (0%)	36	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	390/487 (80%)	362 (93%)	23 (6%)	5 (1%)	9	21
All	All	3171/3896 (81%)	2960 (93%)	180 (6%)	31 (1%)	12	25

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	299	VAL
1	C	196	HIS
1	C	251	LYS
1	C	312	ASP
1	F	146	LYS

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	326/427 (76%)	301 (92%)	25 (8%)	12	25
1	B	329/427 (77%)	301 (92%)	28 (8%)	10	22
1	C	332/427 (78%)	313 (94%)	19 (6%)	18	39
1	D	336/427 (79%)	310 (92%)	26 (8%)	12	25
1	E	324/427 (76%)	302 (93%)	22 (7%)	14	30
1	F	322/427 (75%)	308 (96%)	14 (4%)	26	50
1	G	284/427 (66%)	267 (94%)	17 (6%)	17	36
1	H	302/427 (71%)	291 (96%)	11 (4%)	31	56
All	All	2555/3416 (75%)	2393 (94%)	162 (6%)	16	34

5 of 162 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	332	LEU
1	G	249	THR
1	E	458	LEU
1	F	219	ILE

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Mol	Chain	Res	Type
1	G	387	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	95	GLN
1	G	108	ASN
1	G	418	ASN
1	C	54	ASN
1	B	455	ASN

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 53 ligands modelled in this entry, 44 are monoatomic - leaving 9 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	$\# Z > 2$
3	PEG	C	502	-	6,6,6	0.47	0	5,5,5	0.20	0
6	PGE	D	502	-	9,9,9	0.30	0	8,8,8	0.23	0
7	EDO	E	503	-	3,3,3	0.70	0	2,2,2	0.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PEG	E	502	-	6,6,6	0.19	0	5,5,5	0.17	0
6	PGE	H	502	-	9,9,9	0.27	0	8,8,8	0.24	0
6	PGE	D	503	-	9,9,9	0.37	0	8,8,8	0.22	0
3	PEG	A	502	-	6,6,6	0.55	0	5,5,5	0.35	0
6	PGE	F	502	-	9,9,9	0.26	0	8,8,8	0.36	0
5	PG4	B	502	-	12,12,12	0.15	0	11,11,11	0.09	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	PEG	C	502	-	-	2/4/4/4	-
6	PGE	D	502	-	-	3/7/7/7	-
7	EDO	E	503	-	-	0/1/1/1	-
3	PEG	E	502	-	-	1/4/4/4	-
6	PGE	H	502	-	-	3/7/7/7	-
6	PGE	D	503	-	-	3/7/7/7	-
3	PEG	A	502	-	-	1/4/4/4	-
6	PGE	F	502	-	-	1/7/7/7	-
5	PG4	B	502	-	-	5/10/10/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	503	PGE	O2-C3-C4-O3
3	A	502	PEG	O1-C1-C2-O2
3	C	502	PEG	O2-C3-C4-O4
6	H	502	PGE	C1-C2-O2-C3
6	D	503	PGE	C1-C2-O2-C3

There are no ring outliers.

7 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	502	PEG	2	0
6	D	502	PGE	1	0
3	E	502	PEG	2	0
6	H	502	PGE	5	0
6	D	503	PGE	6	0
3	A	502	PEG	2	0
6	F	502	PGE	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	A	409/487 (83%)	0.66	38 (9%) 14 11	83, 124, 183, 201	0
1	B	405/487 (83%)	1.00	72 (17%) 4 3	90, 144, 197, 212	0
1	C	405/487 (83%)	0.66	42 (10%) 11 9	84, 116, 176, 188	0
1	D	406/487 (83%)	0.71	49 (12%) 8 6	83, 116, 175, 191	0
1	E	395/487 (81%)	0.71	46 (11%) 9 7	86, 128, 175, 199	0
1	F	396/487 (81%)	0.73	47 (11%) 9 7	82, 124, 178, 193	0
1	G	393/487 (80%)	0.98	69 (17%) 4 3	92, 151, 191, 217	0
1	H	396/487 (81%)	0.72	47 (11%) 9 7	85, 128, 176, 205	0
All	All	3205/3896 (82%)	0.77	410 (12%) 7 5	82, 129, 184, 217	0

The worst 5 of 410 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	376	GLN	7.0
1	A	452	THR	6.8
1	G	390	GLY	6.0
1	G	226	SER	5.9
1	G	102	LEU	5.9

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 ⓘ

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
3	PEG	E	502	7/7	0.70	0.15	132,132,134,134	0
3	PEG	A	502	7/7	0.73	0.19	103,105,107,107	0
6	PGE	F	502	10/10	0.75	0.14	99,101,102,102	0
6	PGE	H	502	10/10	0.80	0.14	109,113,114,114	0
7	EDO	E	503	4/4	0.81	0.14	115,115,115,115	0
6	PGE	D	503	10/10	0.86	0.13	90,98,100,101	0
5	PG4	B	502	13/13	0.87	0.15	147,147,148,148	0
6	PGE	D	502	10/10	0.88	0.10	97,101,104,104	0
3	PEG	C	502	7/7	0.90	0.12	99,100,101,102	0
4	IOD	G	505	1/1	0.91	0.10	106,106,106,106	1
4	IOD	B	505	1/1	0.93	0.09	134,134,134,134	1
4	IOD	B	503	1/1	0.95	0.11	136,136,136,136	1
4	IOD	H	506	1/1	0.95	0.08	118,118,118,118	1
2	ZN	B	501	1/1	0.95	0.13	175,175,175,175	0
4	IOD	G	504	1/1	0.95	0.07	140,140,140,140	1
4	IOD	H	504	1/1	0.96	0.06	99,99,99,99	1
4	IOD	B	506	1/1	0.96	0.06	121,121,121,121	1
4	IOD	E	506	1/1	0.97	0.06	88,88,88,88	1
4	IOD	F	504	1/1	0.97	0.06	99,99,99,99	1
4	IOD	G	503	1/1	0.97	0.06	130,130,130,130	1
4	IOD	A	503	1/1	0.97	0.07	108,108,108,108	1
4	IOD	A	505	1/1	0.97	0.05	97,97,97,97	1
4	IOD	H	503	1/1	0.97	0.05	101,101,101,101	1
4	IOD	A	506	1/1	0.97	0.05	116,116,116,116	1
2	ZN	F	501	1/1	0.97	0.13	126,126,126,126	0
2	ZN	G	501	1/1	0.97	0.11	171,171,171,171	0
2	ZN	H	501	1/1	0.97	0.13	143,143,143,143	0
4	IOD	B	507	1/1	0.97	0.05	87,87,87,87	1
4	IOD	C	503	1/1	0.97	0.06	109,109,109,109	1
4	IOD	C	507	1/1	0.97	0.06	84,84,84,84	1
4	IOD	E	504	1/1	0.97	0.05	117,117,117,117	1
4	IOD	G	502	1/1	0.98	0.05	111,111,111,111	1
4	IOD	C	505	1/1	0.98	0.04	104,104,104,104	1
2	ZN	D	501	1/1	0.98	0.14	116,116,116,116	0
4	IOD	D	504	1/1	0.98	0.05	107,107,107,107	1
4	IOD	D	507	1/1	0.98	0.04	102,102,102,102	1
4	IOD	D	508	1/1	0.98	0.05	84,84,84,84	1

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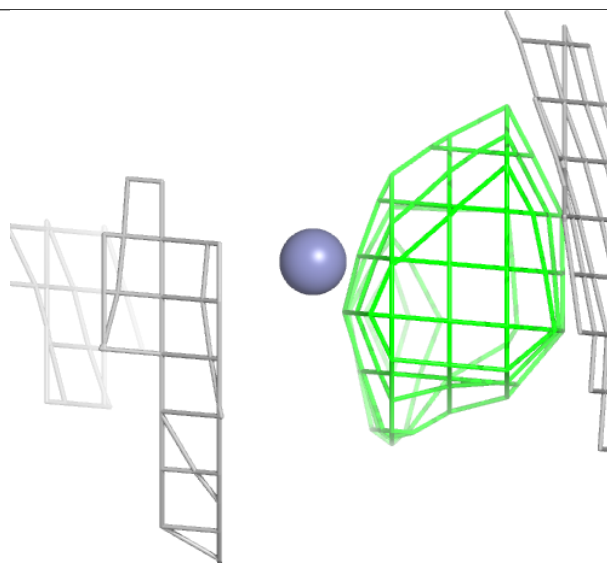
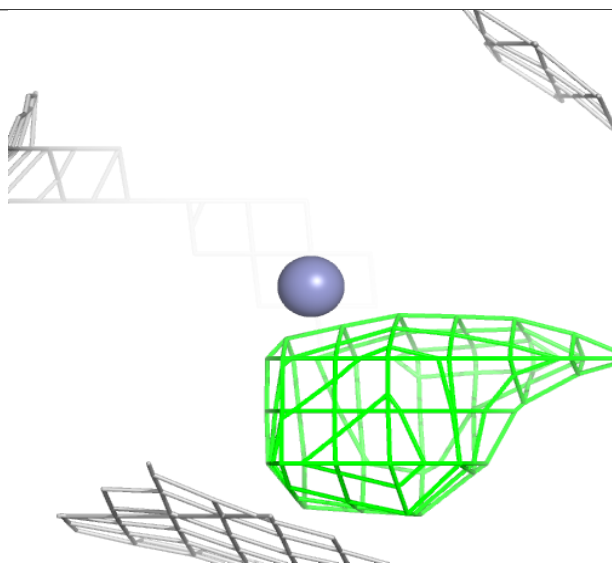
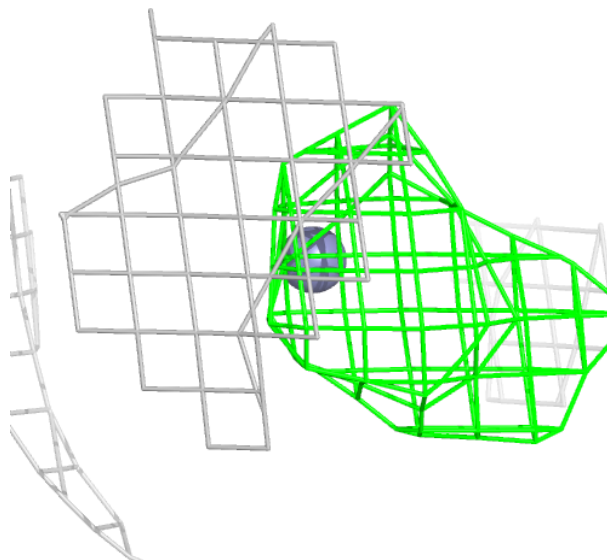
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	IOD	H	505	1/1	0.98	0.04	102,102,102,102	1
2	ZN	A	501	1/1	0.98	0.12	133,133,133,133	0
4	IOD	E	505	1/1	0.98	0.04	105,105,105,105	1
4	IOD	A	504	1/1	0.98	0.06	115,115,115,115	1
4	IOD	F	503	1/1	0.98	0.05	109,109,109,109	1
4	IOD	B	504	1/1	0.98	0.05	94,94,94,94	1
4	IOD	F	505	1/1	0.98	0.04	114,114,114,114	1
4	IOD	F	506	1/1	0.98	0.05	90,90,90,90	1
4	IOD	A	507	1/1	0.99	0.03	88,88,88,88	1
4	IOD	D	505	1/1	0.99	0.05	105,105,105,105	1
4	IOD	E	507	1/1	0.99	0.03	90,90,90,90	1
4	IOD	D	506	1/1	0.99	0.03	96,96,96,96	1
2	ZN	C	501	1/1	0.99	0.11	114,114,114,114	0
4	IOD	C	506	1/1	0.99	0.03	86,86,86,86	1
2	ZN	E	501	1/1	0.99	0.13	141,141,141,141	0
4	IOD	C	504	1/1	1.00	0.09	101,101,101,101	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.

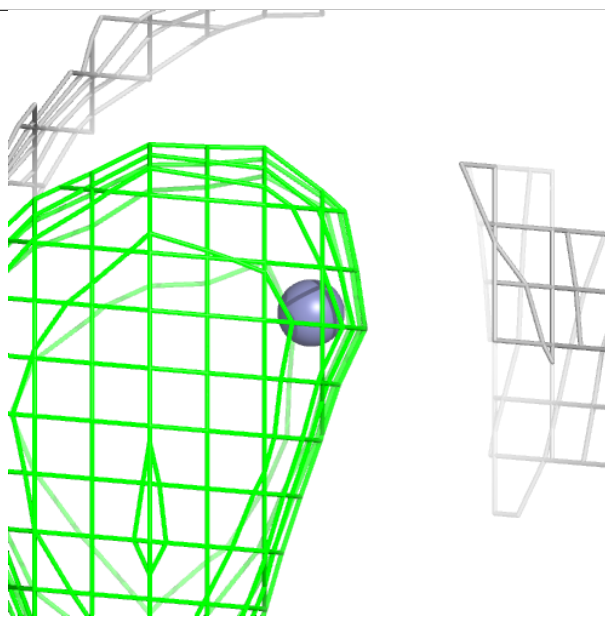
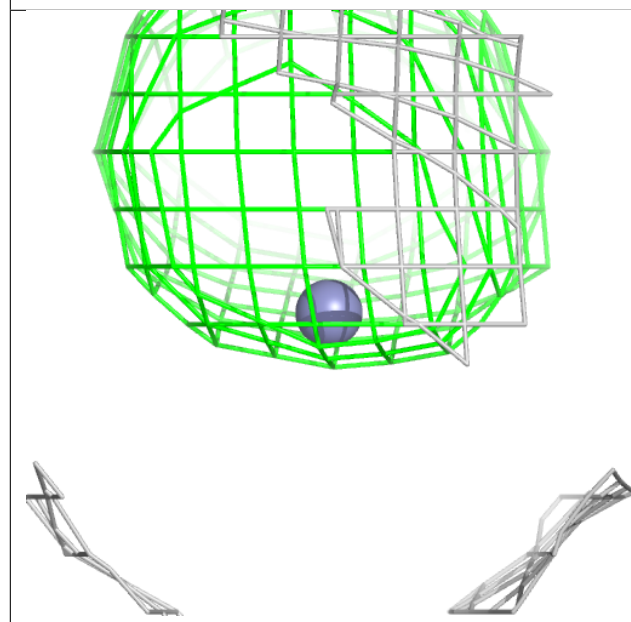
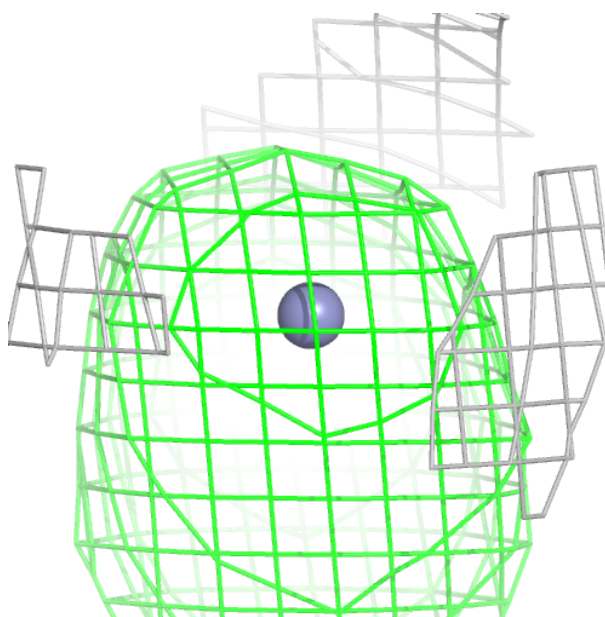
Electron density around ZN B 501:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



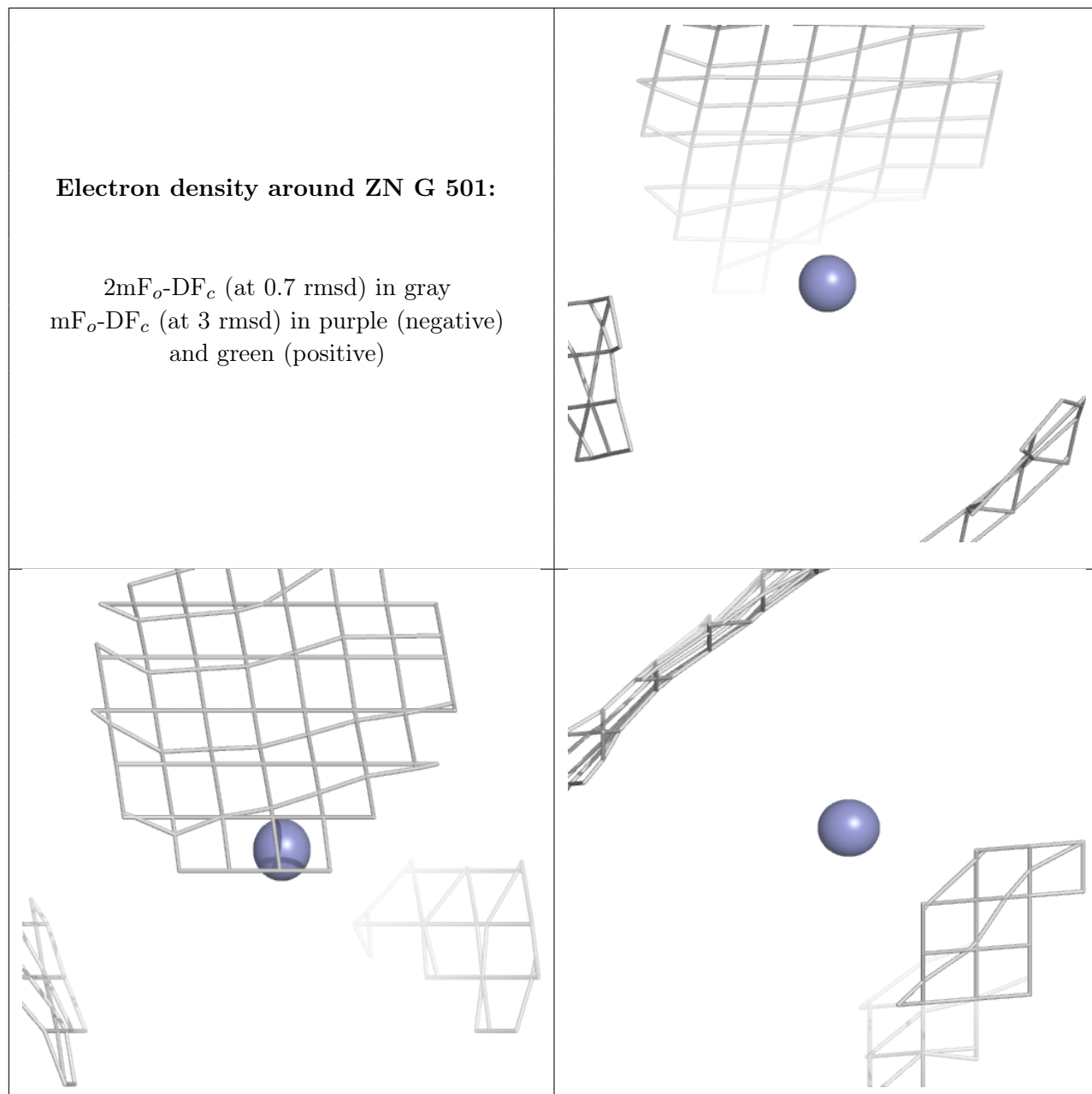
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and green (positive)



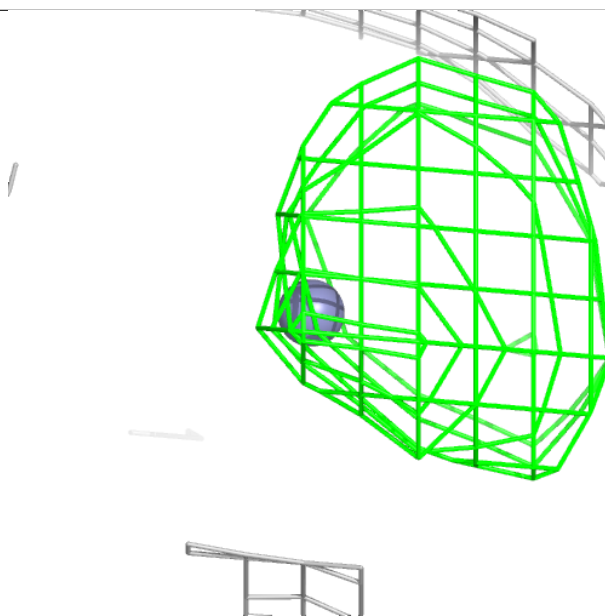
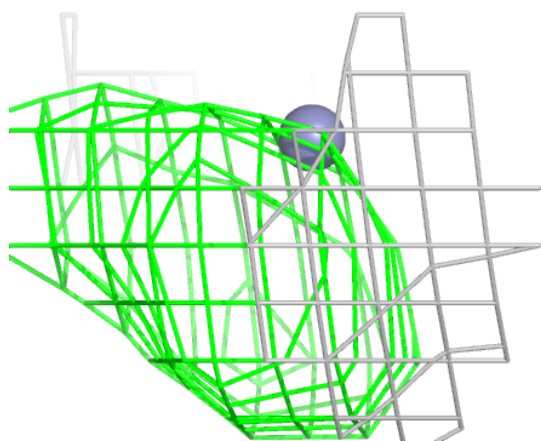
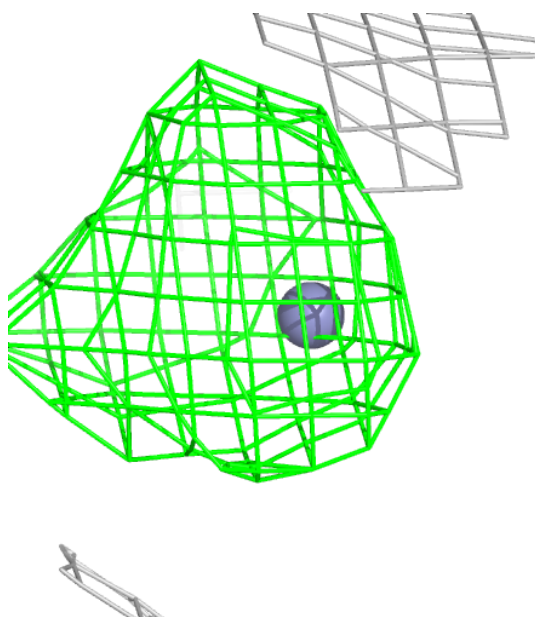
Electron density around ZN G 501:

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and green (positive)



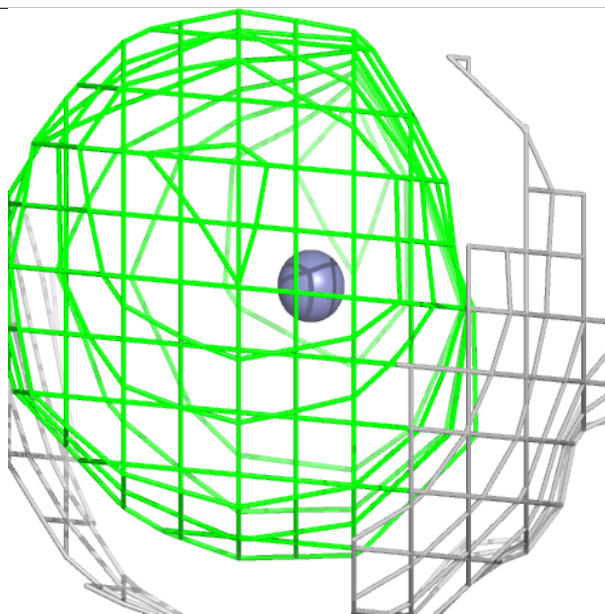
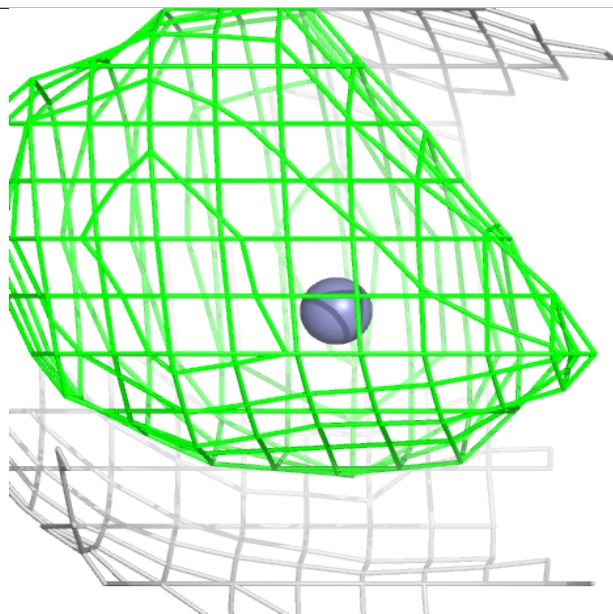
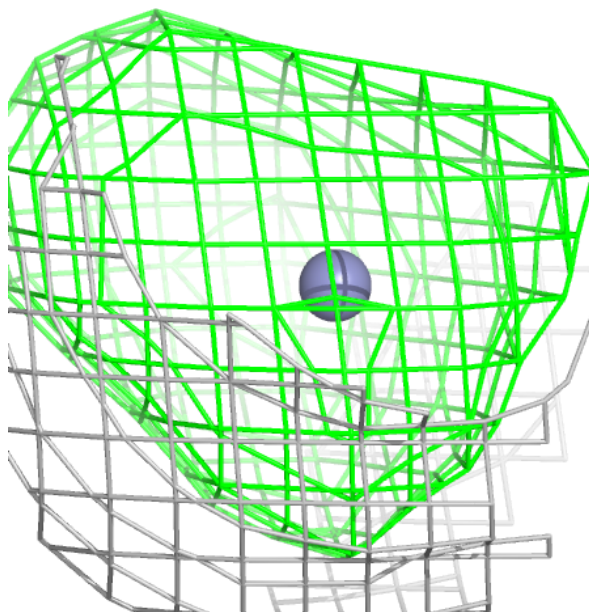
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and green (positive)



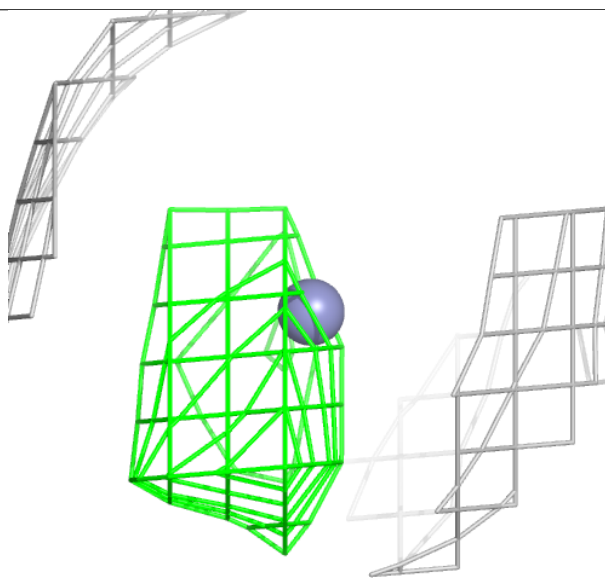
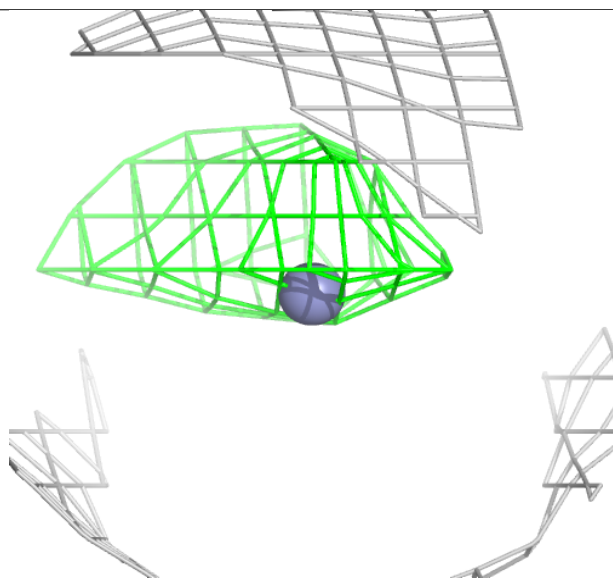
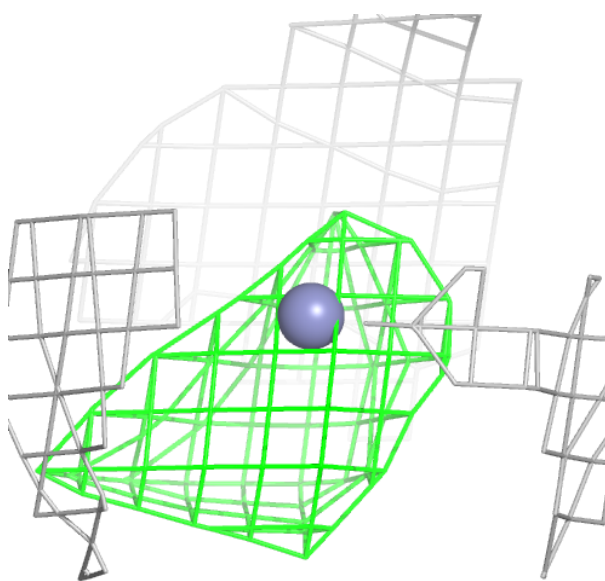
Electron density around ZN D 501:

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



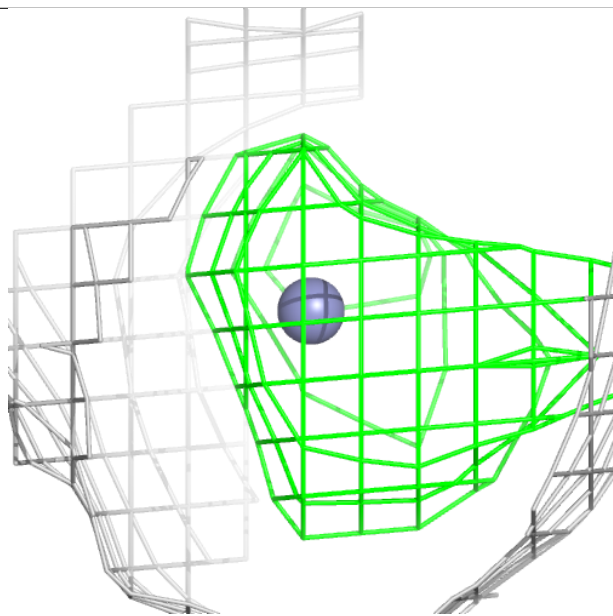
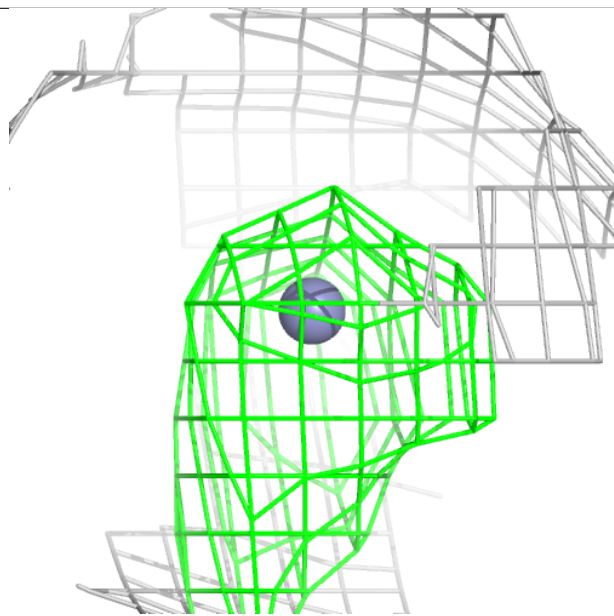
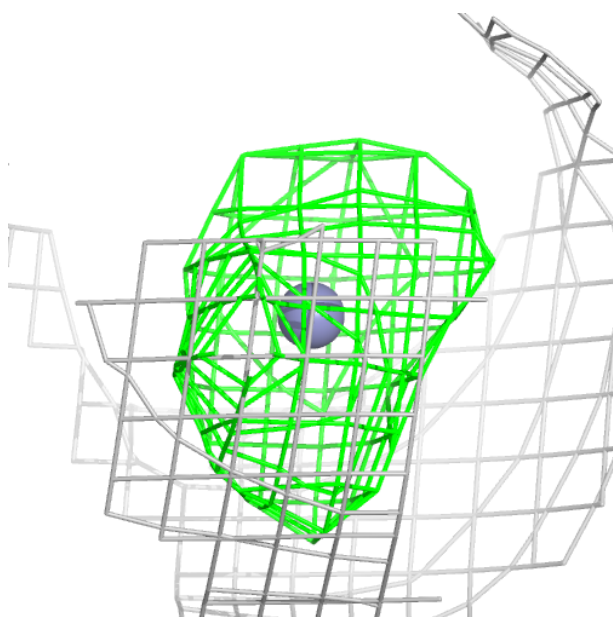
Electron density around ZN A 501:

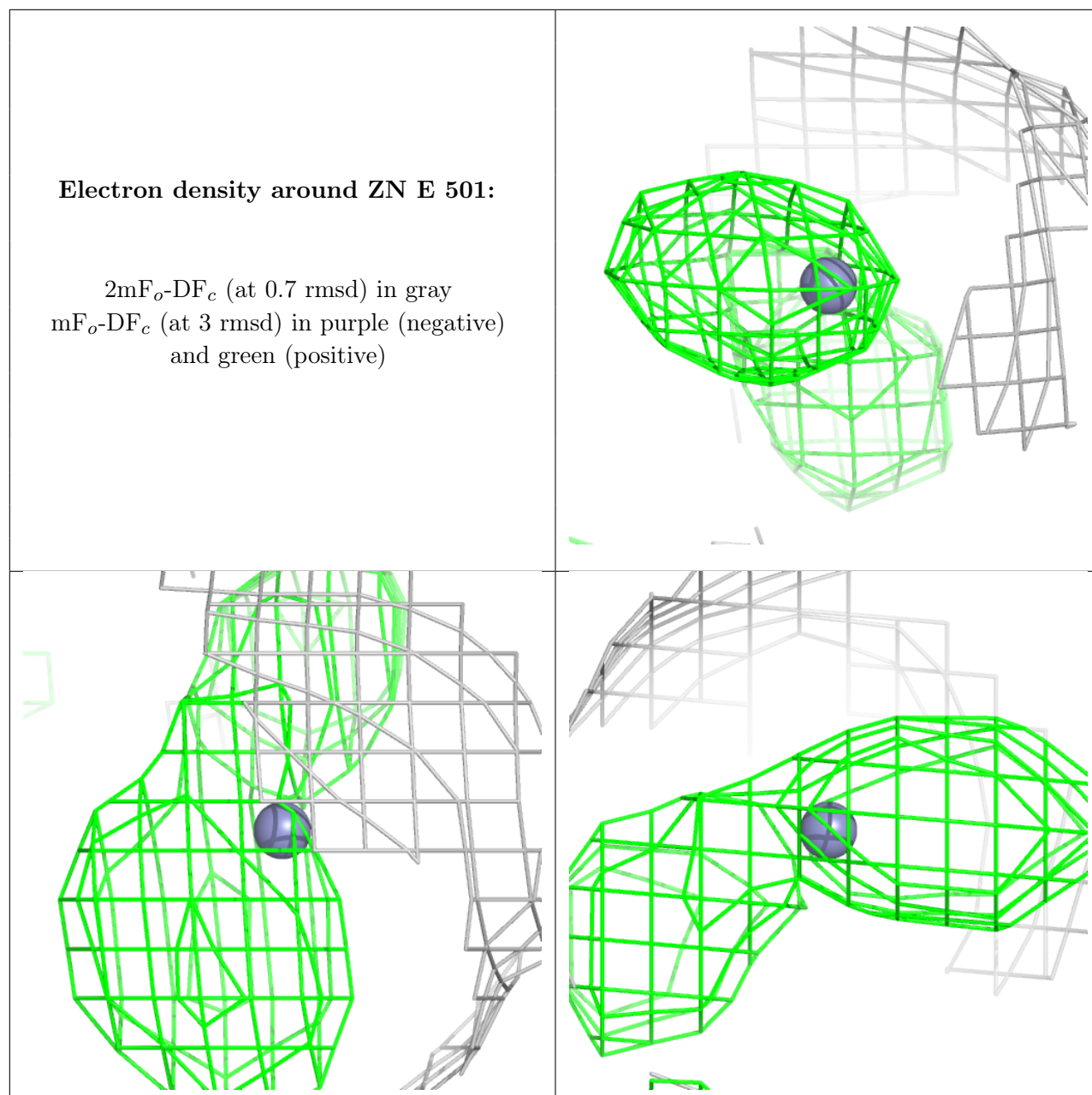
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers ⓘ

There are no such residues in this entry.