



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:46 AM UTC

PDB ID : 10UI / pdb_000010ui
Title : Crystal structure of Formyl-coenzyme A transferase from Brucella melitensis in complex with Zinc
Authors : Seattle Structural Genomics Center for Infectious Disease; Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2026-02-09
Resolution : 2.34 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

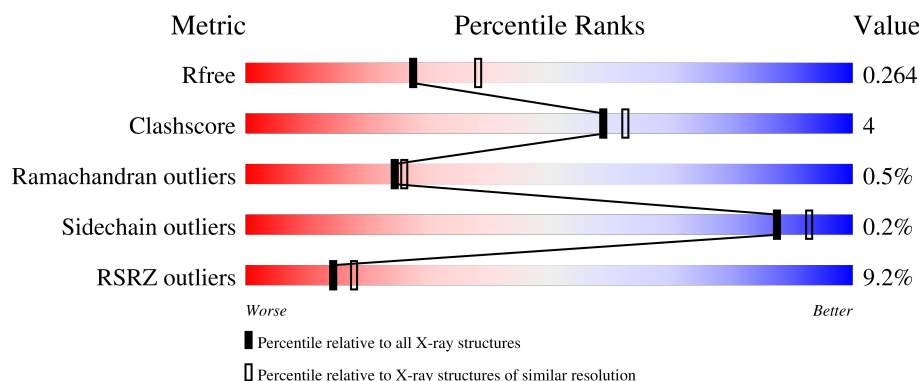
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.34 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	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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	409	
1	B	409	
1	C	409	
1	D	409	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12288 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 Formyl-coenzyme a transferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	403	Total	C	N	O	S	0	2	0
			3054	1928	538	573	15			
1	B	403	Total	C	N	O	S	0	1	0
			3047	1923	536	573	15			
1	C	402	Total	C	N	O	S	0	0	0
			3025	1909	529	572	15			
1	D	400	Total	C	N	O	S	0	1	0
			3012	1904	525	568	15			

There are 32 discrepancies between the modelled and reference sequences:

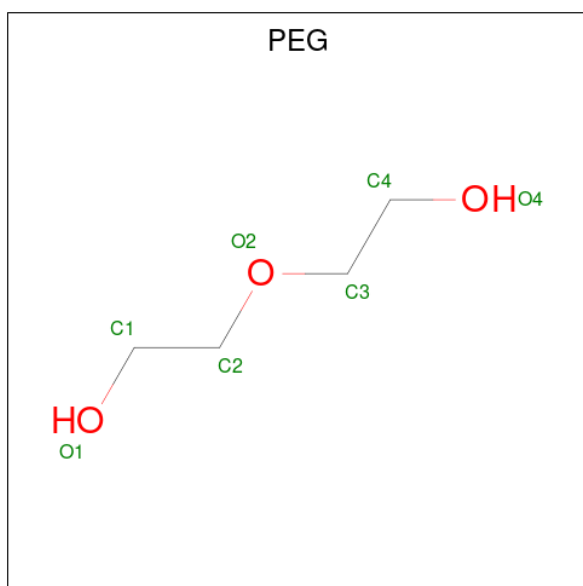
Chain	Residue	Modelled	Actual	Comment	Reference
A	42	MET	-	expression tag	UNP Q8YDF2
A	43	ALA	-	expression tag	UNP Q8YDF2
A	44	HIS	-	expression tag	UNP Q8YDF2
A	45	HIS	-	expression tag	UNP Q8YDF2
A	46	HIS	-	expression tag	UNP Q8YDF2
A	47	HIS	-	expression tag	UNP Q8YDF2
A	48	HIS	-	expression tag	UNP Q8YDF2
A	49	HIS	-	expression tag	UNP Q8YDF2
B	42	MET	-	expression tag	UNP Q8YDF2
B	43	ALA	-	expression tag	UNP Q8YDF2
B	44	HIS	-	expression tag	UNP Q8YDF2
B	45	HIS	-	expression tag	UNP Q8YDF2
B	46	HIS	-	expression tag	UNP Q8YDF2
B	47	HIS	-	expression tag	UNP Q8YDF2
B	48	HIS	-	expression tag	UNP Q8YDF2
B	49	HIS	-	expression tag	UNP Q8YDF2
C	42	MET	-	expression tag	UNP Q8YDF2
C	43	ALA	-	expression tag	UNP Q8YDF2
C	44	HIS	-	expression tag	UNP Q8YDF2
C	45	HIS	-	expression tag	UNP Q8YDF2
C	46	HIS	-	expression tag	UNP Q8YDF2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	47	HIS	-	expression tag	UNP Q8YDF2
C	48	HIS	-	expression tag	UNP Q8YDF2
C	49	HIS	-	expression tag	UNP Q8YDF2
D	42	MET	-	expression tag	UNP Q8YDF2
D	43	ALA	-	expression tag	UNP Q8YDF2
D	44	HIS	-	expression tag	UNP Q8YDF2
D	45	HIS	-	expression tag	UNP Q8YDF2
D	46	HIS	-	expression tag	UNP Q8YDF2
D	47	HIS	-	expression tag	UNP Q8YDF2
D	48	HIS	-	expression tag	UNP Q8YDF2
D	49	HIS	-	expression tag	UNP Q8YDF2

- Molecule 2 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

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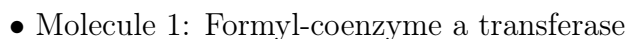
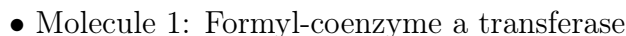
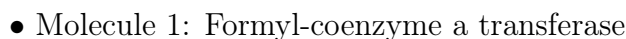
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Zn 1	0	0
3	C	1	Total 1	Zn 1	0	0
3	D	1	Total 1	Zn 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	38	Total 38	O 38	0	0
4	B	56	Total 56	O 56	0	0
4	C	17	Total 17	O 17	0	0
4	D	21	Total 21	O 21	0	0

- Molecule 1: Formyl-coenzyme a transferase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	54.27Å 127.95Å 224.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.85 – 2.34 48.85 – 2.34	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.85-2.34) 100.0 (48.85-2.34)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 2.34Å)	Xtriage
Refinement program	PHENIX (2.0_5936: ???)	Depositor
R, R_{free}	0.217 , 0.263 0.220 , 0.264	Depositor DCC
R_{free} test set	3418 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	37.2	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12288	wwPDB-VP
Average B, all atoms (Å ²)	56.0	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 27.35 % 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 2.2348e-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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.18	0/3119	0.34	0/4232
1	B	0.21	0/3108	0.36	0/4217
1	C	0.17	0/3082	0.35	0/4184
1	D	0.17	0/3071	0.36	0/4167
All	All	0.19	0/12380	0.35	0/16800

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 [i](#)

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	3054	0	3070	25	0
1	B	3047	0	3063	29	0
1	C	3025	0	3032	25	0
1	D	3012	0	3027	48	0
2	A	7	0	10	0	0
2	B	7	0	10	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	1	0	0	0	0
4	A	38	0	0	1	0
4	B	56	0	0	0	0
4	C	17	0	0	0	0
4	D	21	0	0	0	0
All	All	12288	0	12212	107	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 4.

All (107) 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:357:LYS:HG2	1:B:358:MET:HE2	1.62	0.81
1:D:218:ILE:HG22	1:D:222:MET:HE3	1.62	0.79
1:A:376:ASN:HB2	1:B:181:GLU:OE1	1.90	0.71
1:D:77:MET:HE1	1:D:229:LEU:HD11	1.74	0.68
1:D:59:LEU:HB3	1:D:141:VAL:HG22	1.77	0.65
1:B:357:LYS:NZ	1:B:358:MET:HE3	2.12	0.65
1:C:101:TYR:CE2	1:C:102:LYS:HD2	2.32	0.64
1:A:222:MET:HE1	1:B:219:VAL:HG13	1.79	0.64
1:D:131:ILE:HG21	1:D:155:ILE:CG2	2.28	0.64
1:D:131:ILE:HG21	1:D:155:ILE:HG21	1.79	0.64
1:C:230:ALA:HB2	1:D:77:MET:HE3	1.81	0.63
1:C:324:THR:HG23	1:C:327:GLY:H	1.62	0.63
1:D:130:ILE:HD13	1:D:425:LEU:HD11	1.81	0.62
1:D:218:ILE:HG22	1:D:222:MET:CE	2.28	0.62
1:B:357:LYS:HG2	1:B:358:MET:CE	2.30	0.60
1:D:133:GLU:OE1	1:D:136:LYS:HE3	2.02	0.59
1:C:209:THR:HG21	1:D:202:GLY:HA2	1.85	0.58
1:D:425:LEU:HD12	1:D:431:LEU:HD12	1.83	0.58
1:A:423:SER:O	1:A:427:ASP:OD2	2.21	0.58
1:B:315:GLU:OE2	1:B:315:GLU:N	2.28	0.58
1:C:59:LEU:HB3	1:C:141:VAL:HG22	1.86	0.57
1:C:128:LEU:HD22	1:C:132:HIS:HE1	1.70	0.56
1:C:128:LEU:CD2	1:C:132:HIS:HE1	2.19	0.56
1:D:421:SER:O	1:D:425:LEU:HD23	2.08	0.54
1:B:141:VAL:HG23	1:B:167:ILE:HD11	1.89	0.53
1:B:122:LEU:O	1:B:128:LEU:HD21	2.08	0.53
1:A:226:GLN:HB3	1:B:77:MET:HE1	1.91	0.53
1:B:191:VAL:HG21	1:B:248:LEU:HD23	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:311:ILE:HD12	1:C:313:LEU:HB2	1.90	0.52
1:D:425:LEU:HD13	1:D:429:LEU:HD12	1.92	0.52
1:A:209:THR:HG21	1:B:202:GLY:HA2	1.92	0.51
1:D:118:LEU:CD2	1:D:425:LEU:HD21	2.41	0.51
1:D:358:MET:HA	1:D:358:MET:HE2	1.92	0.51
1:C:270:PRO:HG2	1:D:368:VAL:HB	1.93	0.51
1:B:290:ASP:HB2	1:C:290:ASP:HB2	1.92	0.50
1:D:122:LEU:HB3	1:D:153:LEU:HD13	1.93	0.50
1:A:61:LEU:HD23	1:A:84:ILE:HB	1.94	0.49
1:D:122:LEU:HD13	1:D:153:LEU:HD13	1.94	0.49
1:A:301:ARG:HG2	1:A:301:ARG:HH11	1.76	0.49
1:B:357:LYS:HZ2	1:B:358:MET:HE3	1.77	0.49
1:C:230:ALA:CB	1:D:77:MET:HE3	2.43	0.48
1:D:71:THR:HG22	1:D:142:VAL:HG21	1.95	0.48
1:B:337:PRO:HB2	1:B:338:PRO:HD3	1.94	0.48
1:D:391:LEU:HG	1:D:416:MET:HE2	1.95	0.48
1:D:148:GLY:C	1:D:151:GLU:OE1	2.56	0.48
1:D:102:LYS:HB2	1:D:391:LEU:HD22	1.95	0.48
1:C:260:GLY:O	1:C:264:LEU:HG	2.14	0.48
1:D:118:LEU:HD22	1:D:425:LEU:CD2	2.44	0.48
1:A:368:VAL:HB	1:B:270:PRO:HG2	1.96	0.47
1:A:236:LYS:HE2	1:B:233:TYR:CE1	2.50	0.47
1:A:312:ASP:O	1:A:313:LEU:HD12	2.14	0.47
1:B:315:GLU:H	1:B:315:GLU:CD	2.13	0.46
1:C:123:LYS:NZ	1:C:153:LEU:HD21	2.31	0.46
1:C:100:ASN:OD1	1:C:100:ASN:C	2.59	0.46
1:B:283:TYR:CE1	1:B:296:ALA:HB1	2.50	0.46
1:C:138:ALA:O	1:C:167:ILE:HD11	2.16	0.46
1:C:436:LEU:HD12	1:C:436:LEU:N	2.31	0.46
1:D:244:ILE:HG22	1:D:246:VAL:HG23	1.97	0.46
1:D:136:LYS:HB2	1:D:137:GLN:OE1	2.17	0.45
1:B:357:LYS:HZ3	1:B:358:MET:HE3	1.82	0.45
1:B:344:ARG:NH1	1:C:370:GLU:OE2	2.49	0.45
1:A:222:MET:HE1	1:B:219:VAL:CG1	2.46	0.45
1:D:305:ILE:HG21	1:D:358:MET:HB3	1.99	0.44
1:A:301:ARG:HD3	1:A:301:ARG:H	1.83	0.44
1:D:120:LEU:HD12	1:D:445:ILE:HG22	1.99	0.44
1:A:141:VAL:HG23	1:A:167:ILE:HD11	1.99	0.44
1:C:230:ALA:HB2	1:D:77:MET:CE	2.46	0.44
1:C:431:LEU:HB2	1:C:436:LEU:HD11	1.99	0.44
1:D:120:LEU:HD11	1:D:127:GLY:HA2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:148:GLY:CA	1:D:151:GLU:OE1	2.66	0.43
1:D:120:LEU:HD21	1:D:127:GLY:O	2.19	0.43
1:A:376:ASN:CB	1:B:181:GLU:OE1	2.64	0.43
1:A:256:LEU:O	1:A:257:ILE:C	2.62	0.43
1:C:256:LEU:O	1:C:257:ILE:C	2.62	0.43
1:D:390:HIS:HB2	1:D:416:MET:HE3	2.00	0.43
1:A:219:VAL:HG13	1:B:222:MET:HE1	1.99	0.43
1:D:256:LEU:O	1:D:257:ILE:C	2.61	0.43
1:B:120:LEU:CD2	1:B:122:LEU:HD23	2.49	0.43
1:B:202:GLY:O	1:B:274:GLY:HA2	2.18	0.43
1:C:128:LEU:HD13	1:C:132:HIS:CE1	2.53	0.42
1:C:98:VAL:O	1:D:279:THR:HG23	2.19	0.42
1:D:382:VAL:O	1:D:398:ARG:HG2	2.18	0.42
1:D:277:HIS:CG	1:D:278:PRO:HD2	2.54	0.42
1:D:64:VAL:O	1:D:68:PRO:HG2	2.20	0.42
1:D:371:ALA:O	1:D:377:VAL:HG21	2.19	0.42
1:B:277:HIS:HB2	1:B:283:TYR:HD2	1.84	0.42
1:C:432:ASP:O	1:C:436:LEU:HD13	2.19	0.42
1:D:135:ALA:CB	1:D:160:LEU:HD22	2.50	0.42
1:C:439:LEU:HB3	1:C:444:VAL:HG13	2.01	0.42
1:A:301:ARG:HD3	1:A:301:ARG:N	2.35	0.41
1:A:62:SER:HB2	1:A:67:GLY:HA3	2.02	0.41
1:A:123:LYS:NZ	1:A:152:ARG:HH21	2.18	0.41
1:D:404:LYS:O	1:D:407:GLU:HG3	2.20	0.41
1:D:118:LEU:HD21	1:D:425:LEU:HD21	2.03	0.41
1:A:275:ASN:HA	1:B:210[A]:ARG:HG2	2.03	0.41
1:A:348:ARG:HG2	4:A:616:HOH:O	2.19	0.41
1:A:277:HIS:CG	1:A:278:PRO:HD2	2.56	0.41
1:A:336:ILE:HB	1:A:337:PRO:HD3	2.03	0.41
1:C:395:SER:HB2	1:D:264:LEU:HB3	2.03	0.41
1:D:128:LEU:HG	1:D:132:HIS:NE2	2.36	0.41
1:D:60:ASP:CG	1:D:71:THR:HG21	2.46	0.41
1:A:290:ASP:HB2	1:D:290:ASP:HB2	2.03	0.40
1:A:64:VAL:HG12	1:A:65:LEU:N	2.36	0.40
1:B:426:GLY:O	1:B:430:GLY:HA2	2.22	0.40
1:D:120:LEU:CD1	1:D:445:ILE:HG22	2.52	0.40
1:D:440:ILE:HD13	1:D:445:ILE:O	2.20	0.40
1:B:277:HIS:CG	1:B:278:PRO:HD2	2.56	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	403/409 (98%)	399 (99%)	2 (0%)	2 (0%)	24	26
1	B	402/409 (98%)	397 (99%)	3 (1%)	2 (0%)	24	26
1	C	400/409 (98%)	395 (99%)	3 (1%)	2 (0%)	24	26
1	D	397/409 (97%)	391 (98%)	4 (1%)	2 (0%)	24	26
All	All	1602/1636 (98%)	1582 (99%)	12 (1%)	8 (0%)	24	26

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	64	VAL
1	A	257	ILE
1	B	64	VAL
1	B	257	ILE
1	C	64	VAL
1	C	257	ILE
1	D	257	ILE
1	D	64	VAL

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	318/322 (99%)	318 (100%)	0	100	100
1	B	317/322 (98%)	317 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	314/322 (98%)	313 (100%)	1 (0%)	86	91
1	D	313/322 (97%)	312 (100%)	1 (0%)	86	91
All	All	1262/1288 (98%)	1260 (100%)	2 (0%)	87	93

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	188	ASP
1	D	97	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	GLN
1	A	177	GLN
1	A	350	HIS
1	A	376	ASN
1	B	302	GLN
1	B	364	GLN
1	C	86	ASN
1	C	132	HIS
1	C	177	GLN
1	C	390	HIS
1	D	177	GLN
1	D	349	GLN
1	D	390	HIS

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 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	$\# Z > 2$
2	PEG	B	501	-	6,6,6	0.26	0	5,5,5	0.32	0
2	PEG	A	501	-	6,6,6	0.25	0	5,5,5	0.33	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
2	PEG	B	501	-	-	1/4/4/4	-
2	PEG	A	501	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	PEG	O2-C3-C4-O4
2	A	501	PEG	O1-C1-C2-O2
2	B	501	PEG	O2-C3-C4-O4
2	A	501	PEG	C4-C3-O2-C2

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	403/409 (98%)	0.18	8 (1%) 65 70	19, 45, 82, 116	2 (0%)
1	B	403/409 (98%)	-0.03	4 (0%) 79 82	17, 39, 61, 76	1 (0%)
1	C	402/409 (98%)	0.89	41 (10%) 12 14	35, 65, 96, 124	0
1	D	400/409 (97%)	1.26	95 (23%) 2 1	23, 69, 110, 164	1 (0%)
All	All	1608/1636 (98%)	0.58	148 (9%) 14 18	17, 52, 96, 164	4 (0%)

All (148) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	155	ILE	6.1
1	D	122	LEU	5.8
1	D	150	VAL	5.4
1	D	431	LEU	5.2
1	B	48	HIS	4.5
1	D	160	LEU	4.5
1	D	50	ALA	4.3
1	D	131	ILE	4.3
1	C	49	HIS	4.3
1	D	134	LEU	4.0
1	D	153	LEU	4.0
1	D	185	PRO	3.9
1	D	442	ALA	3.9
1	D	135	ALA	3.8
1	D	125	ARG	3.8
1	D	163	LEU	3.7
1	D	425	LEU	3.7
1	D	429	LEU	3.6
1	D	180	PRO	3.5
1	D	127	GLY	3.5
1	D	450	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	59	LEU	3.4
1	D	377	VAL	3.4
1	D	391	LEU	3.3
1	D	443	GLY	3.3
1	C	238	THR	3.3
1	C	377	VAL	3.3
1	D	389	ALA	3.3
1	D	149	THR	3.3
1	C	182	ALA	3.2
1	C	450	PRO	3.2
1	A	48	HIS	3.2
1	D	440	ILE	3.2
1	D	424	VAL	3.2
1	D	448	TYR	3.2
1	D	229	LEU	3.2
1	D	436	LEU	3.2
1	D	178	THR	3.2
1	D	101	TYR	3.1
1	D	439	LEU	3.1
1	D	130	ILE	3.1
1	D	128	LEU	3.1
1	C	383	VAL	3.1
1	D	159	SER	3.0
1	C	375	PRO	3.0
1	D	379	ALA	2.9
1	D	157	TYR	2.9
1	D	428	VAL	2.9
1	D	87	ILE	2.9
1	C	379	ALA	2.9
1	D	154	LYS	2.8
1	A	436	LEU	2.8
1	D	119	ALA	2.8
1	C	424	VAL	2.8
1	D	151	GLU	2.8
1	C	231	ALA	2.8
1	D	409	ALA	2.8
1	D	441	ALA	2.8
1	D	156	ASP	2.8
1	D	146	ARG	2.8
1	D	238	THR	2.7
1	B	376	ASN	2.7
1	D	120	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	50	ALA	2.7
1	C	162	ALA	2.7
1	D	162	ALA	2.7
1	D	411	TYR	2.7
1	D	121	ASP	2.7
1	D	444	VAL	2.7
1	D	433	GLY	2.6
1	D	434	ASN	2.6
1	C	101	TYR	2.6
1	B	49	HIS	2.5
1	D	169	TYR	2.5
1	D	51	LEU	2.5
1	C	237	THR	2.5
1	C	157	TYR	2.5
1	C	439	LEU	2.5
1	C	151	GLU	2.5
1	C	372	PHE	2.5
1	A	49	HIS	2.5
1	D	148	GLY	2.5
1	C	147	SER	2.4
1	D	388	SER	2.4
1	D	53	LEU	2.4
1	D	446	TYR	2.4
1	C	442	ALA	2.4
1	C	391	LEU	2.4
1	D	61	LEU	2.4
1	D	386	LEU	2.4
1	B	205	ASP	2.4
1	C	185	PRO	2.4
1	D	410	ALA	2.4
1	C	382	VAL	2.4
1	C	389	ALA	2.4
1	D	124	SER	2.4
1	C	440	ILE	2.4
1	D	84	ILE	2.4
1	D	132	HIS	2.4
1	D	233	TYR	2.3
1	C	443	GLY	2.3
1	D	103	GLY	2.3
1	D	182	ALA	2.3
1	A	431	LEU	2.3
1	D	123	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	375	PRO	2.3
1	D	421	SER	2.3
1	C	122	LEU	2.3
1	D	118	LEU	2.3
1	C	376	ASN	2.3
1	C	163	LEU	2.3
1	D	417	LEU	2.3
1	D	376	ASN	2.3
1	D	187	TYR	2.3
1	D	88	GLN	2.3
1	D	58	VAL	2.3
1	D	181	GLU	2.2
1	C	155	ILE	2.2
1	D	152	ARG	2.2
1	C	433	GLY	2.2
1	D	137	GLN	2.2
1	D	138	ALA	2.2
1	C	240	LEU	2.2
1	C	373	GLU	2.2
1	D	126	GLU	2.2
1	C	378	LYS	2.2
1	C	187	TYR	2.2
1	C	408	ASN	2.2
1	D	78	GLY	2.2
1	D	298	GLY	2.2
1	C	178	THR	2.2
1	D	422	ALA	2.2
1	C	358	MET	2.1
1	A	150	VAL	2.1
1	A	450	PRO	2.1
1	C	449	GLN	2.1
1	A	147	SER	2.1
1	C	180	PRO	2.1
1	D	140	VAL	2.1
1	D	165	PRO	2.1
1	D	426	GLY	2.1
1	A	181	GLU	2.1
1	D	183	GLN	2.1
1	D	383	VAL	2.1
1	C	181	GLU	2.0
1	D	382	VAL	2.0
1	D	416	MET	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	299	ASN	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](#)

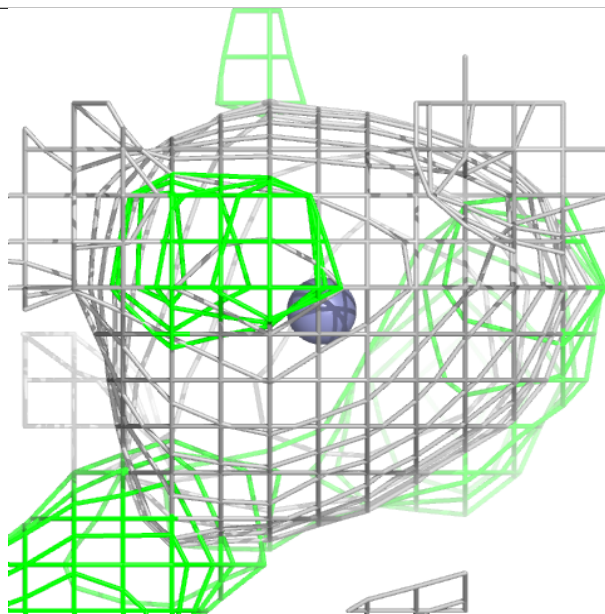
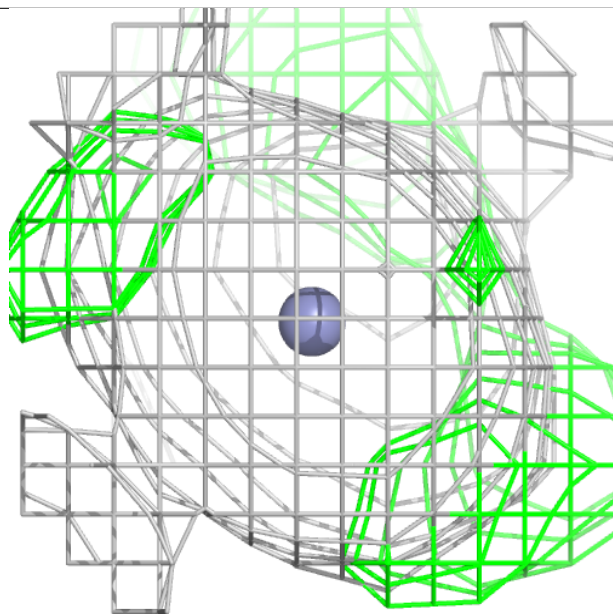
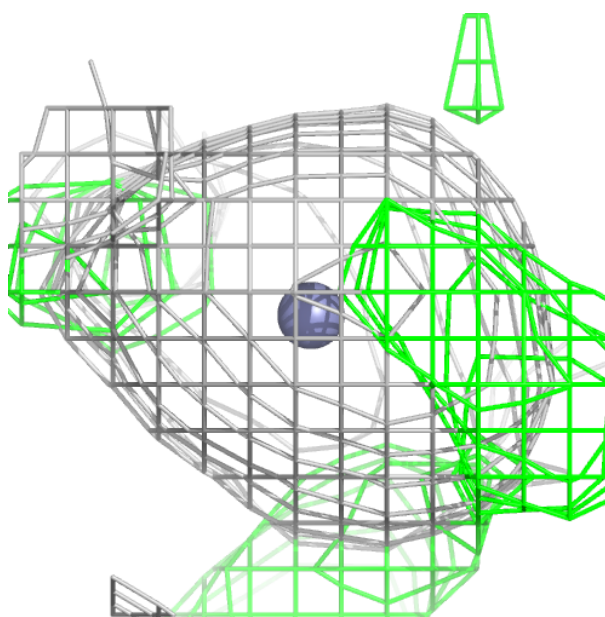
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	PEG	B	501	7/7	0.84	0.13	46,48,50,53	0
2	PEG	A	501	7/7	0.87	0.13	52,59,69,71	0
3	ZN	A	502	1/1	0.94	0.08	62,62,62,62	0
3	ZN	C	501	1/1	0.96	0.07	55,55,55,55	0
3	ZN	D	501	1/1	0.97	0.07	54,54,54,54	0
3	ZN	B	502	1/1	0.98	0.09	40,40,40,40	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.

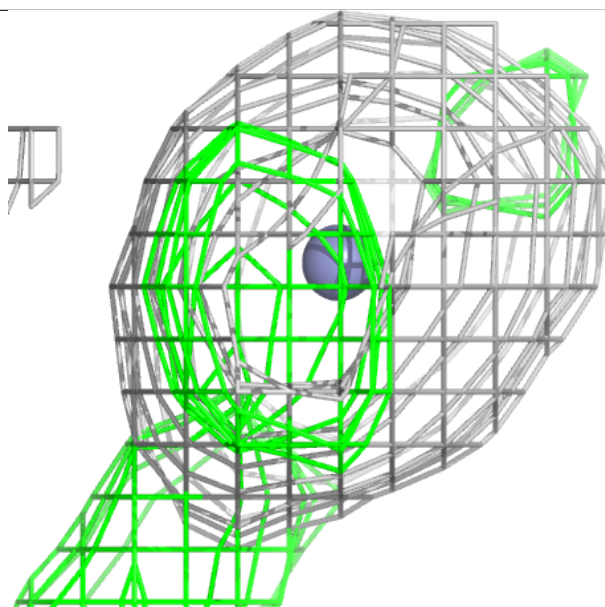
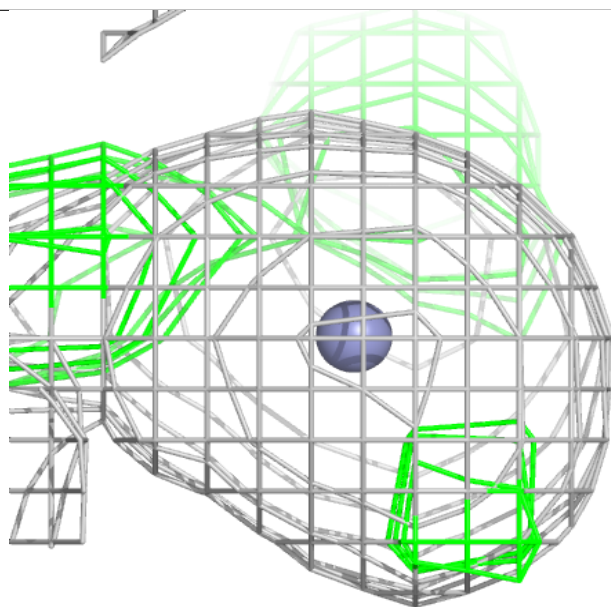
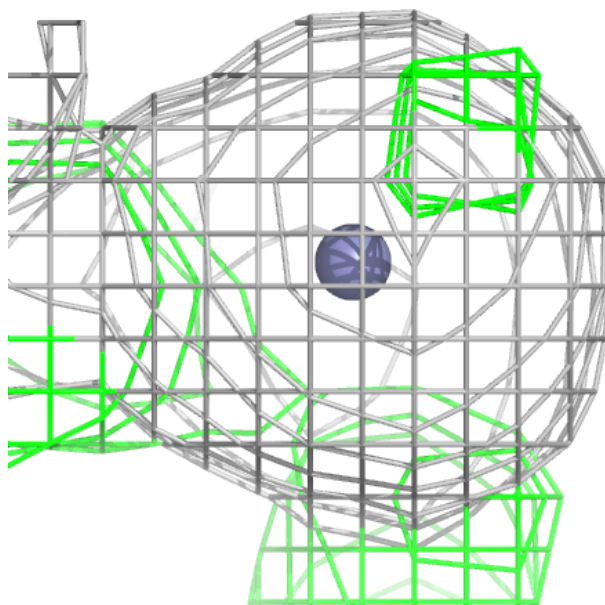
Electron density around ZN A 502:

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



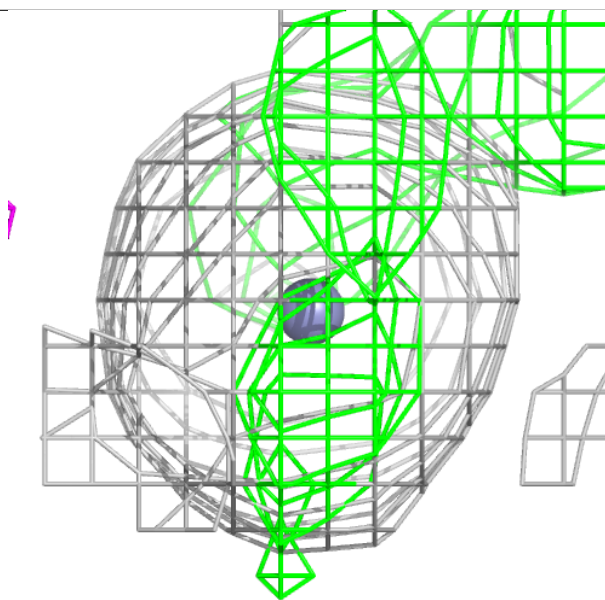
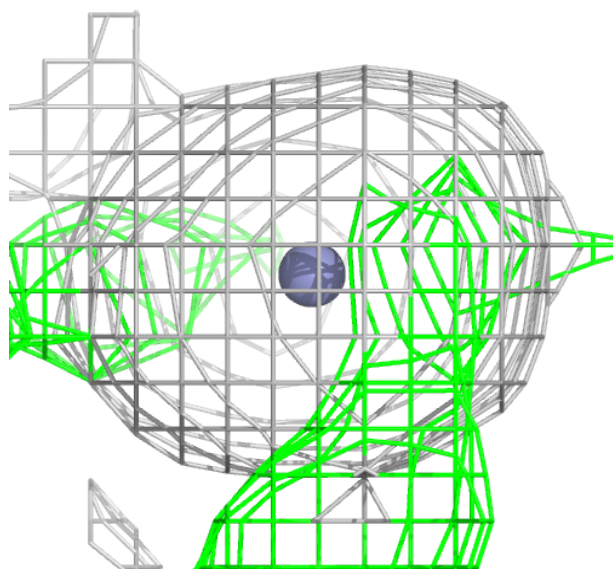
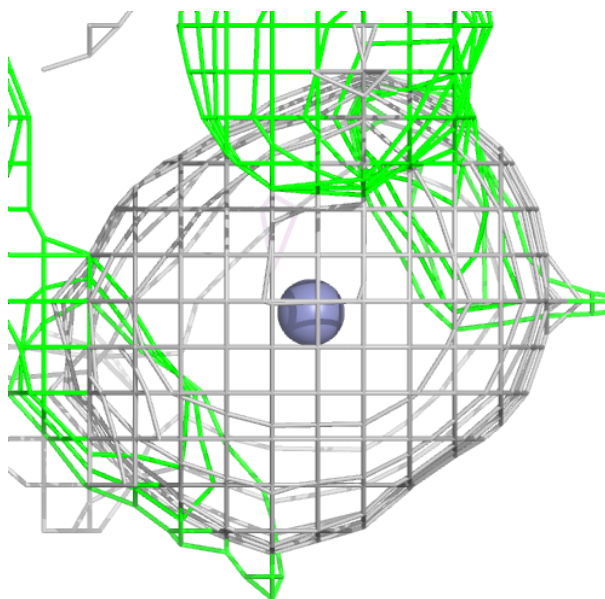
Electron density around ZN C 501:

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



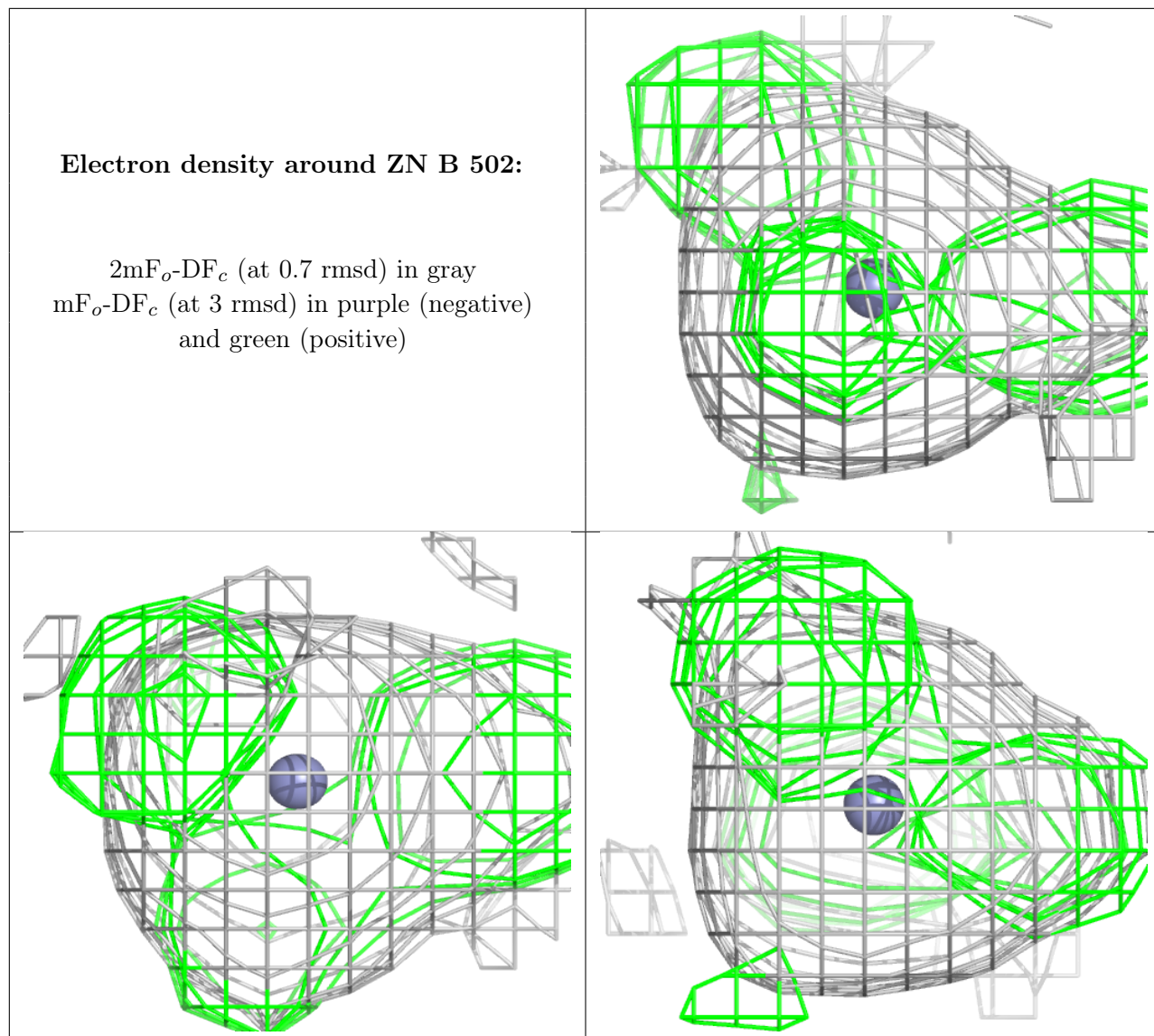
Electron density around ZN D 501:

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



Electron density around ZN B 502:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.