Full wwPDB X-ray Structure Validation Report (i)

Mar 28, 2022 – 07:12 pm BST

PDB ID	:	7PXP
Title	:	Benzoylsuccinyl-CoA thiolase
Authors	:	Ermler, U.; Heider, H.; Weidenweber, S.; Demmer, U.
Deposited on	:	2021-10-08
Resolution	:	2.00 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

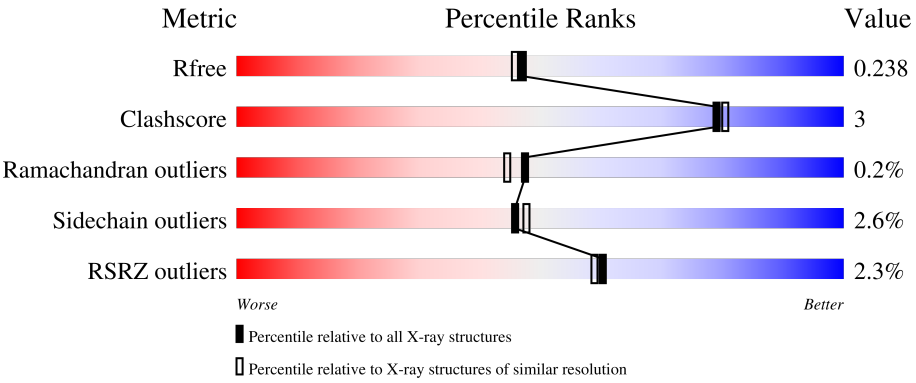
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.27
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	146	5% 83% 7% • 10%
1	B	146	3% 84% 5% 10%
1	E	146	3% 85% 6% 9%
1	F	146	% 83% 6% • 10%
2	C	392	3% 89% 9% •

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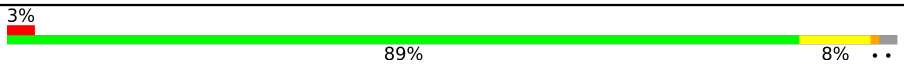
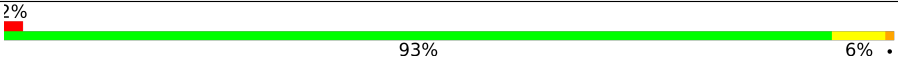
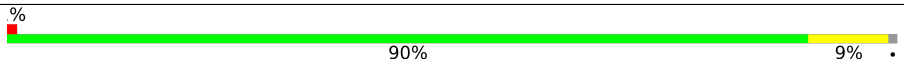
Mol	Chain	Length	Quality of chain
2	D	392	
2	G	392	
2	H	392	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 16076 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 Benzoylsuccinyl-CoA thiolase subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	132	Total	C	N	O	S	0	0	0
			1073	692	171	202	8			
1	B	131	Total	C	N	O	S	0	0	0
			1064	687	170	199	8			
1	E	133	Total	C	N	O	S	0	0	0
			1082	698	173	203	8			
1	F	131	Total	C	N	O	S	0	0	0
			1064	687	170	199	8			

- Molecule 2 is a protein called Benzoylsuccinyl-CoA thiolase subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	384	Total	C	N	O	S	0	0	0
			2841	1767	501	542	31			
2	D	385	Total	C	N	O	S	0	0	0
			2855	1775	506	543	31			
2	G	391	Total	C	N	O	S	0	0	0
			2892	1798	512	551	31			
2	H	387	Total	C	N	O	S	0	0	0
			2868	1785	507	545	31			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	391	GLY	-	expression tag	UNP Q39VG1
C	392	SER	-	expression tag	UNP Q39VG1
D	391	GLY	-	expression tag	UNP Q39VG1
D	392	SER	-	expression tag	UNP Q39VG1
G	391	GLY	-	expression tag	UNP Q39VG1
G	392	SER	-	expression tag	UNP Q39VG1
H	391	GLY	-	expression tag	UNP Q39VG1
H	392	SER	-	expression tag	UNP Q39VG1

- Molecule 3 is ZINC ION (three-letter code: 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
3	B	1	Total Zn 1 1	0	0
3	E	1	Total Zn 1 1	0	0
3	F	1	Total Zn 1 1	0	0

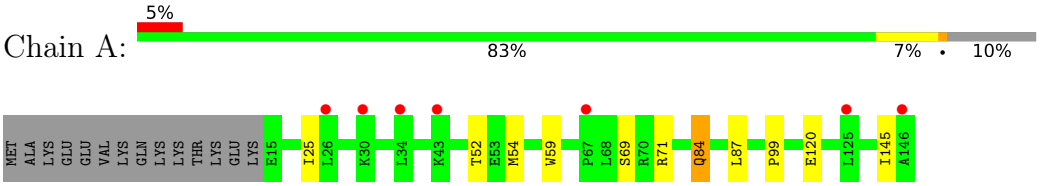
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	10	Total O 10 10	0	0
4	B	16	Total O 16 16	0	0
4	C	55	Total O 55 55	0	0
4	D	36	Total O 36 36	0	0
4	E	17	Total O 17 17	0	0
4	F	17	Total O 18 18	0	1
4	G	90	Total O 91 91	0	1
4	H	90	Total O 90 90	0	0

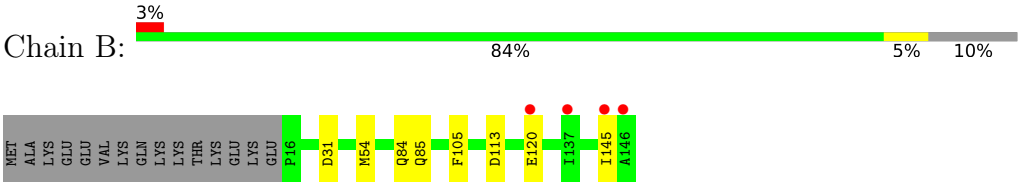
3 Residue-property plots (i)

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.

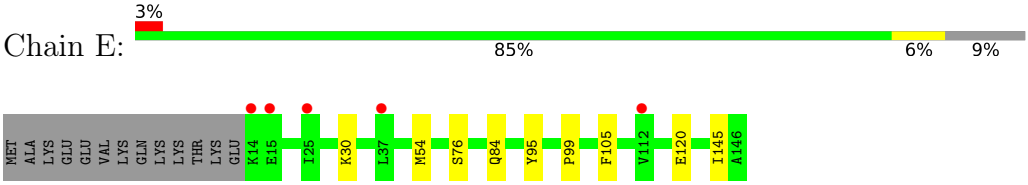
• Molecule 1: Benzoylsuccinyl-CoA thiolase subunit



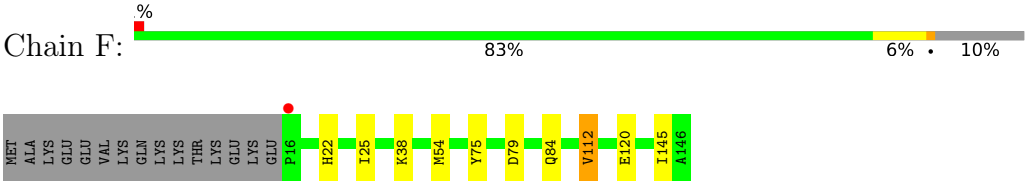
• Molecule 1: Benzoylsuccinyl-CoA thiolase subunit



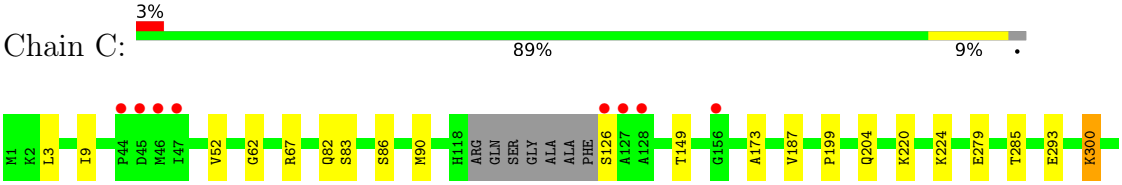
• Molecule 1: Benzoylsuccinyl-CoA thiolase subunit

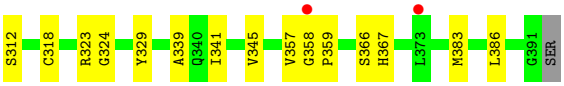


• Molecule 1: Benzoylsuccinyl-CoA thiolase subunit

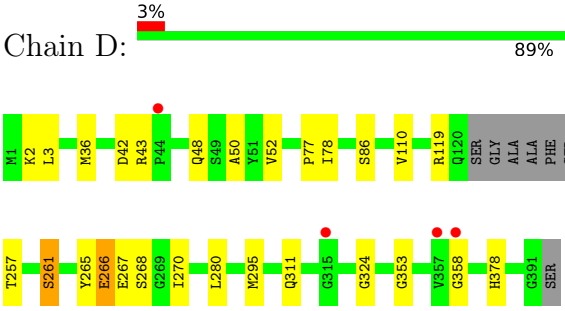


• Molecule 2: Benzoylsuccinyl-CoA thiolase subunit

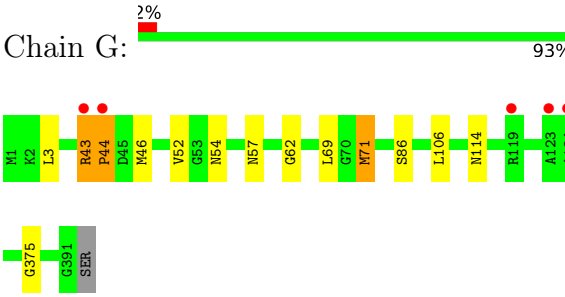




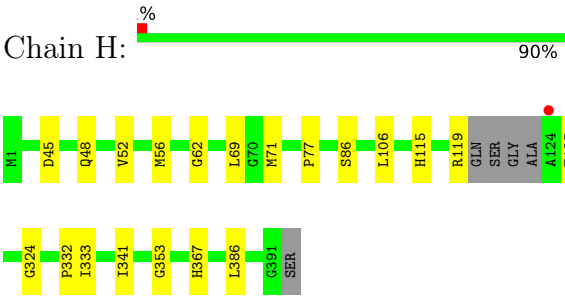
• Molecule 2: Benzoylsuccinyl-CoA thiolase subunit



• Molecule 2: Benzoylsuccinyl-CoA thiolase subunit



• Molecule 2: Benzoylsuccinyl-CoA thiolase subunit



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	80.79Å 105.51Å 142.54Å 90.00° 92.27° 90.00°	Depositor
Resolution (Å)	48.41 – 2.00 48.41 – 2.00	Depositor EDS
% Data completeness (in resolution range)	93.3 (48.41-2.00) 83.6 (48.41-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.98 (at 2.00Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.211 , 0.233 0.217 , 0.238	Depositor DCC
R_{free} test set	7666 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	31.6	Xtriage
Anisotropy	0.513	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.078 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	16076	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.46	0/1100	0.67	0/1488
1	B	0.45	0/1091	0.67	0/1475
1	E	0.47	0/1109	0.67	0/1499
1	F	0.46	0/1091	0.66	0/1475
2	C	0.50	0/2889	0.69	2/3898 (0.1%)
2	D	0.48	0/2903	0.69	0/3916
2	G	0.57	1/2942 (0.0%)	0.70	2/3970 (0.1%)
2	H	0.56	1/2917 (0.0%)	0.66	0/3935
All	All	0.51	2/16042 (0.0%)	0.68	4/21656 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	71	MET	SD-CE	-6.61	1.40	1.77
2	H	223	MET	SD-CE	-5.34	1.48	1.77

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	44	PRO	C-N-CA	5.32	134.99	121.70
2	C	357	VAL	C-N-CA	5.22	133.26	122.30
2	G	268	SER	N-CA-C	-5.08	97.28	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	300	LYS	CA-C-N	5.06	126.33	116.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	82	GLN	Peptide

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	1073	0	1044	5	0
1	B	1064	0	1039	2	0
1	E	1082	0	1057	5	0
1	F	1064	0	1039	5	0
2	C	2841	0	2824	16	0
2	D	2855	0	2840	18	0
2	G	2892	0	2873	18	0
2	H	2868	0	2851	25	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	10	0	0	1	0
4	B	16	0	0	0	0
4	C	55	0	0	1	0
4	D	36	0	0	0	0
4	E	17	0	0	0	0
4	F	18	0	0	0	0
4	G	91	0	0	0	0
4	H	90	0	0	0	0
All	All	16076	0	15567	87	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (87) 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:H:200:MET:HE3	2:H:284:PHE:HB3	1.41	0.97
2:H:200:MET:CE	2:H:284:PHE:HB3	2.07	0.85
2:H:115:HIS:CE1	2:H:332:PRO:HA	2.15	0.82
2:H:115:HIS:HE1	2:H:332:PRO:HA	1.46	0.77
2:G:54:ASN:HD21	2:G:57:ASN:HD22	1.34	0.76
2:D:280:LEU:HD21	2:D:295:MET:CE	2.17	0.75
2:G:265:TYR:O	2:G:268:SER:O	2.03	0.75
1:F:79:ASP:HB3	1:F:112:VAL:HG22	1.70	0.73
2:G:57:ASN:HD21	2:G:114:ASN:H	1.37	0.73
1:A:69:SER:OG	1:A:99:PRO:HD2	1.88	0.72
2:H:69:LEU:HB3	2:H:71:MET:HE3	1.72	0.69
2:G:44:PRO:HB3	2:G:71:MET:HG2	1.74	0.69
2:C:293:GLU:OE2	2:C:300:LYS:O	2.11	0.69
2:D:265:TYR:O	2:D:268:SER:O	2.11	0.69
2:G:69:LEU:HB3	2:G:71:MET:HE3	1.75	0.68
2:H:223:MET:HE3	2:H:231:PRO:HB3	1.79	0.64
2:H:223:MET:CE	2:H:231:PRO:HB3	2.30	0.62
2:H:200:MET:HE1	2:H:286:ILE:HG22	1.82	0.61
2:G:43:ARG:HH11	2:G:46:MET:HG2	1.66	0.60
2:C:149:THR:HG23	2:C:199:PRO:HD3	1.84	0.60
2:G:43:ARG:HE	2:G:46:MET:HB2	1.66	0.59
2:G:46:MET:HG3	2:G:106:LEU:CD2	2.34	0.58
2:H:56:MET:CE	2:H:115:HIS:HD2	2.17	0.58
2:H:200:MET:CE	2:H:286:ILE:HG22	2.34	0.57
2:H:69:LEU:CB	2:H:71:MET:HE3	2.34	0.56
2:D:280:LEU:HD21	2:D:295:MET:HE3	1.86	0.56
2:G:69:LEU:CB	2:G:71:MET:HE3	2.36	0.56
2:H:106:LEU:HD22	2:H:222:MET:HE2	1.88	0.56
2:G:249:ARG:NH2	2:G:375:GLY:O	2.35	0.56
2:D:280:LEU:CD2	2:D:295:MET:HE1	2.36	0.55
2:H:281:HIS:H	2:H:367:HIS:HD2	1.56	0.54
2:D:280:LEU:CD2	2:D:295:MET:CE	2.85	0.53
2:D:266:GLU:HG3	2:D:267:GLU:N	2.23	0.53
2:H:106:LEU:HD22	2:H:222:MET:CE	2.40	0.52
2:G:69:LEU:HB3	2:G:71:MET:CE	2.41	0.51
2:H:69:LEU:HB3	2:H:71:MET:CE	2.40	0.51
2:G:46:MET:HG3	2:G:106:LEU:HD23	1.93	0.50
2:H:56:MET:CE	2:H:115:HIS:CD2	2.95	0.49
1:F:79:ASP:CB	1:F:112:VAL:HG22	2.40	0.49
2:C:293:GLU:CD	2:C:300:LYS:O	2.50	0.49
2:C:83:SER:HB2	2:C:90:MET:SD	2.54	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:173:ALA:HB2	2:H:324:GLY:HA3	1.94	0.48
1:E:76:SER:C	2:H:146:MET:HE3	2.34	0.48
1:E:120:GLU:HB3	1:E:145:ILE:HD12	1.96	0.47
2:D:173:ALA:HB2	2:D:324:GLY:HA3	1.96	0.47
2:G:173:ALA:HB2	2:G:324:GLY:HA3	1.97	0.46
1:A:52:THR:HG22	4:A:304:HOH:O	2.15	0.46
1:F:22:HIS:HB3	1:F:25:ILE:HG22	1.98	0.46
2:C:359:PRO:HA	1:E:99:PRO:O	2.16	0.46
2:H:52:VAL:HG21	2:H:62:GLY:HA2	1.98	0.45
2:D:50:ALA:HB3	2:D:78:ILE:HG12	1.98	0.45
2:G:106:LEU:HB2	2:G:222:MET:HG2	1.98	0.45
2:C:279:GLU:O	2:C:366:SER:HA	2.17	0.45
2:C:173:ALA:HB2	2:C:324:GLY:HA3	1.99	0.45
1:E:95:TYR:N	2:H:146:MET:HE1	2.32	0.44
2:C:52:VAL:HG21	2:C:62:GLY:HA2	1.99	0.44
2:H:312:SER:HA	2:H:318:CYS:O	2.18	0.44
1:A:120:GLU:HB3	1:A:145:ILE:HD12	1.99	0.44
2:C:220:LYS:O	2:C:224:LYS:HG2	2.17	0.44
2:G:52:VAL:HG21	2:G:62:GLY:HA2	1.98	0.44
1:F:120:GLU:HB3	1:F:145:ILE:HD12	1.98	0.44
1:A:59:TRP:HH2	2:D:36:MET:HE2	1.82	0.44
1:B:120:GLU:HB3	1:B:145:ILE:HD12	2.00	0.44
2:H:115:HIS:CE1	2:H:333:ILE:H	2.36	0.43
2:C:312:SER:HA	2:C:318:CYS:O	2.18	0.43
2:C:367:HIS:HB2	2:C:383:MET:HG2	2.01	0.43
2:D:268:SER:C	2:D:270:ILE:H	2.22	0.43
2:H:48:GLN:O	2:H:77:PRO:HD2	2.18	0.43
2:D:186:THR:HG23	2:D:189:GLU:H	1.83	0.43
2:C:9:ILE:HG21	2:C:345:VAL:HG21	2.00	0.42
2:C:323:ARG:HG3	2:C:329:TYR:CE1	2.54	0.42
2:C:341:ILE:HG23	2:C:386:LEU:HD11	2.02	0.42
2:D:256:ILE:HG21	2:D:378:HIS:HB2	2.00	0.42
2:H:341:ILE:HG23	2:H:386:LEU:HD11	2.02	0.42
2:G:279:GLU:O	2:G:366:SER:HA	2.19	0.42
2:C:339:ALA:HB1	4:C:429:HOH:O	2.20	0.41
2:D:280:LEU:HD21	2:D:295:MET:HE1	1.93	0.41
2:C:204:GLN:HG2	2:C:285:THR:HG21	2.02	0.41
2:D:48:GLN:O	2:D:77:PRO:HD2	2.20	0.41
1:F:75:TYR:HE2	2:G:251:ILE:HG12	1.84	0.41
2:D:52:VAL:HA	2:D:110:VAL:O	2.19	0.41
2:D:280:LEU:HD23	2:D:295:MET:HE1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:185:ILE:HG13	2:G:189:GLU:HG3	2.01	0.41
2:D:257:THR:O	2:D:261:SER:HB2	2.21	0.41
1:A:84:GLN:HB3	1:A:87:LEU:HD13	2.02	0.41
1:E:105:PHE:CG	2:H:133:GLU:HG2	2.56	0.40
1:B:105:PHE:CG	2:D:133:GLU:HG2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	130/146 (89%)	128 (98%)	2 (2%)	0	100	100
1	B	129/146 (88%)	126 (98%)	3 (2%)	0	100	100
1	E	131/146 (90%)	129 (98%)	2 (2%)	0	100	100
1	F	129/146 (88%)	128 (99%)	1 (1%)	0	100	100
2	C	380/392 (97%)	368 (97%)	11 (3%)	1 (0%)	41	37
2	D	381/392 (97%)	364 (96%)	15 (4%)	2 (0%)	29	23
2	G	389/392 (99%)	373 (96%)	15 (4%)	1 (0%)	41	37
2	H	383/392 (98%)	370 (97%)	12 (3%)	1 (0%)	41	37
All	All	2052/2152 (95%)	1986 (97%)	61 (3%)	5 (0%)	47	44

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	358	GLY
2	D	358	GLY
2	H	353	GLY
2	D	353	GLY
2	G	353	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	119/132 (90%)	115 (97%)	4 (3%)	37	36
1	B	118/132 (89%)	113 (96%)	5 (4%)	30	27
1	E	120/132 (91%)	117 (98%)	3 (2%)	47	49
1	F	118/132 (89%)	114 (97%)	4 (3%)	37	36
2	C	297/302 (98%)	292 (98%)	5 (2%)	60	65
2	D	298/302 (99%)	286 (96%)	12 (4%)	31	29
2	G	301/302 (100%)	297 (99%)	4 (1%)	69	74
2	H	299/302 (99%)	292 (98%)	7 (2%)	50	53
All	All	1670/1736 (96%)	1626 (97%)	44 (3%)	46	48

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ILE
1	A	54	MET
1	A	71	ARG
1	A	84	GLN
1	B	31	ASP
1	B	54	MET
1	B	84	GLN
1	B	85	GLN
1	B	113	ASP
2	C	3	LEU
2	C	67	ARG
2	C	86	SER
2	C	126	SER
2	C	187	VAL
2	D	2	LYS
2	D	3	LEU
2	D	42	ASP
2	D	43	ARG
2	D	86	SER

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Mol	Chain	Res	Type
2	D	119	ARG
2	D	170	ARG
2	D	220	LYS
2	D	249	ARG
2	D	261	SER
2	D	266	GLU
2	D	311	GLN
1	E	30	LYS
1	E	54	MET
1	E	84	GLN
1	F	38	LYS
1	F	54	MET
1	F	84	GLN
1	F	112	VAL
2	G	3	LEU
2	G	43	ARG
2	G	86	SER
2	G	125	PHE
2	H	45	ASP
2	H	86	SER
2	H	119	ARG
2	H	125	PHE
2	H	164	MET
2	H	224	LYS
2	H	262	GLU

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

Mol	Chain	Res	Type
2	D	311	GLN
1	E	57	ASN
2	G	57	ASN
2	H	115	HIS
2	H	367	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	132/146 (90%)	0.46	7 (5%)	26	25	36, 52, 76, 102	0
1	B	131/146 (89%)	0.32	4 (3%)	49	48	30, 45, 65, 95	0
1	E	133/146 (91%)	0.34	5 (3%)	40	39	31, 43, 67, 98	0
1	F	131/146 (89%)	0.22	1 (0%)	86	85	28, 42, 64, 81	0
2	C	384/392 (97%)	0.18	10 (2%)	56	54	27, 38, 54, 74	0
2	D	385/392 (98%)	0.35	10 (2%)	56	54	30, 46, 65, 93	0
2	G	391/392 (99%)	0.02	9 (2%)	60	59	20, 30, 48, 82	0
2	H	387/392 (98%)	-0.03	2 (0%)	91	90	22, 33, 46, 87	0
All	All	2074/2152 (96%)	0.18	48 (2%)	60	59	20, 38, 63, 102	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	14	LYS	5.7
2	G	124	ALA	5.3
1	B	146	ALA	5.1
2	H	124	ALA	4.0
1	A	146	ALA	3.9
2	G	127	ALA	3.8
2	G	125	PHE	3.8
2	G	43	ARG	3.7
2	D	358	GLY	3.6
2	C	128	ALA	3.6
2	C	126	SER	3.6
2	G	126	SER	3.6
1	E	15	GLU	3.4
2	G	44	PRO	3.3
2	D	180	TRP	3.3
2	C	45	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
2	C	127	ALA	3.1
1	A	125	LEU	3.1
2	C	46	MET	3.1
1	A	34	LEU	3.0
2	G	119	ARG	3.0
2	D	229	ALA	2.9
1	F	16	PRO	2.8
1	E	25	ILE	2.8
1	E	112	VAL	2.8
2	D	191	VAL	2.7
2	C	156	GLY	2.6
2	C	44	PRO	2.6
2	D	156	GLY	2.6
1	A	30	LYS	2.5
2	G	123	ALA	2.5
2	C	358	GLY	2.5
2	D	44	PRO	2.5
2	D	315	GLY	2.5
2	D	177	PRO	2.4
2	H	126	SER	2.4
2	D	357	VAL	2.4
2	C	47	ILE	2.4
1	E	37	LEU	2.3
2	D	194	ARG	2.3
1	A	43	LYS	2.3
1	B	137	ILE	2.3
1	B	145	ILE	2.2
1	A	26	LEU	2.2
2	C	373	LEU	2.1
2	G	341	ILE	2.1
1	A	67	PRO	2.1
1	B	120	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

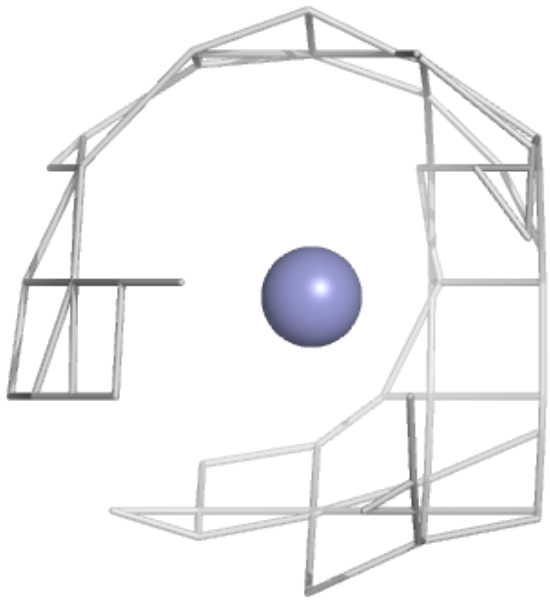
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

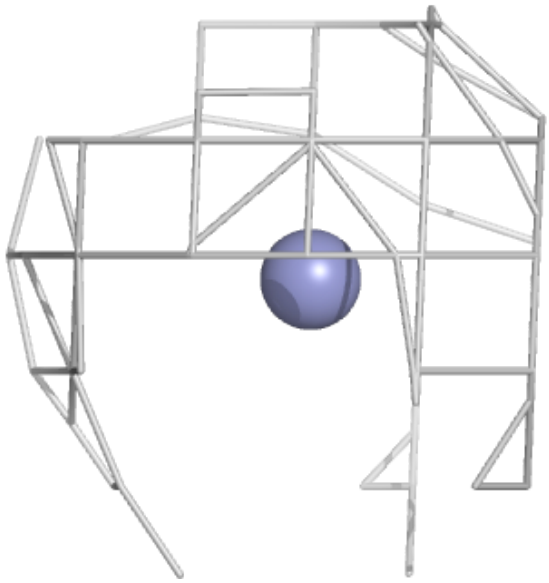
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ZN	B	201	1/1	0.99	0.08	31,31,31,31	0
3	ZN	A	201	1/1	1.00	0.12	56,56,56,56	0
3	ZN	E	201	1/1	1.00	0.11	36,36,36,36	0
3	ZN	F	201	1/1	1.00	0.11	49,49,49,49	0

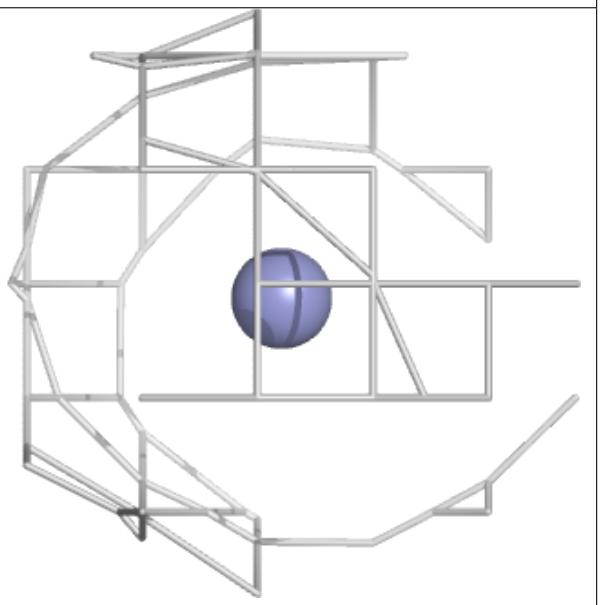
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ZN B 201:

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

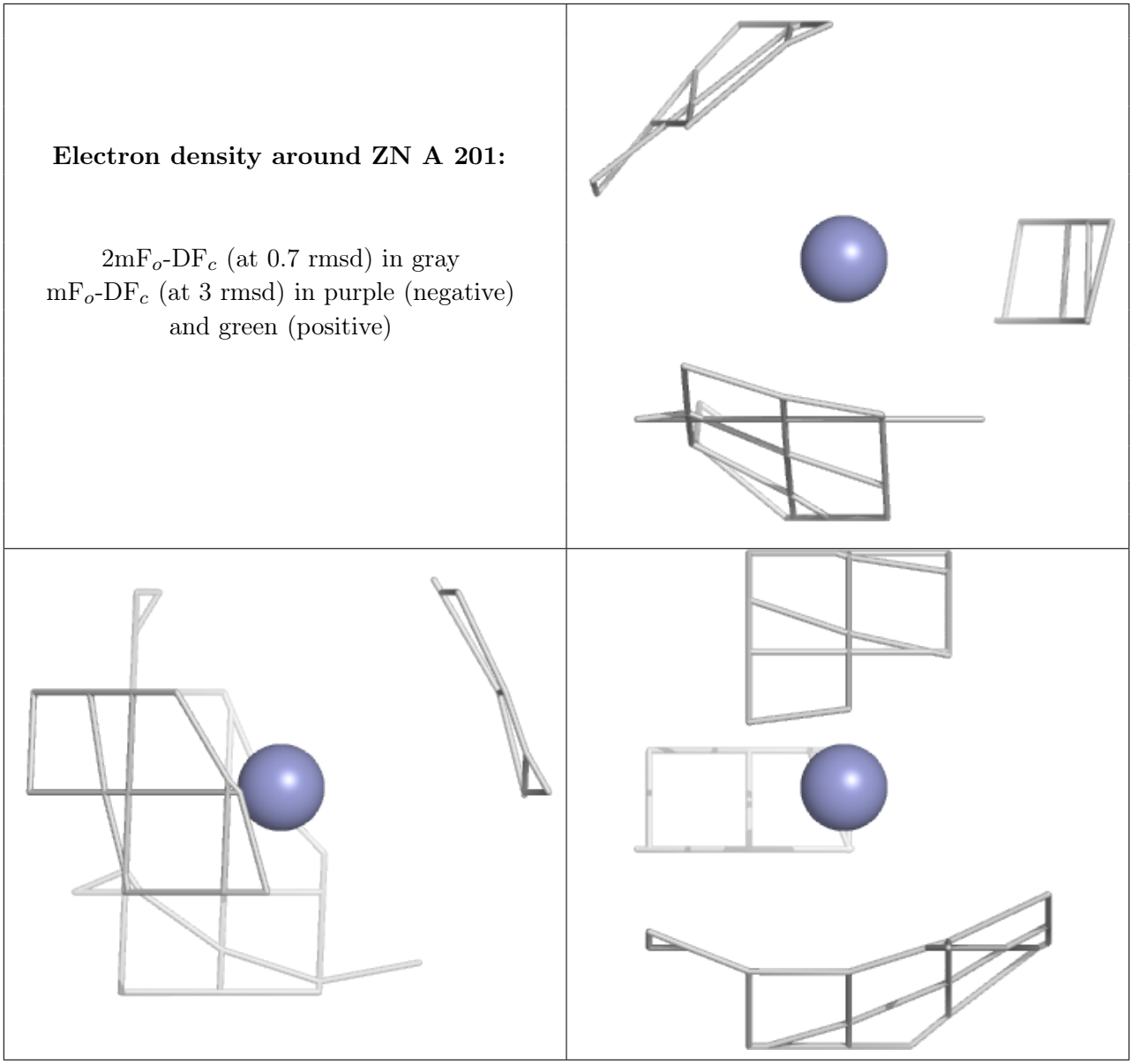






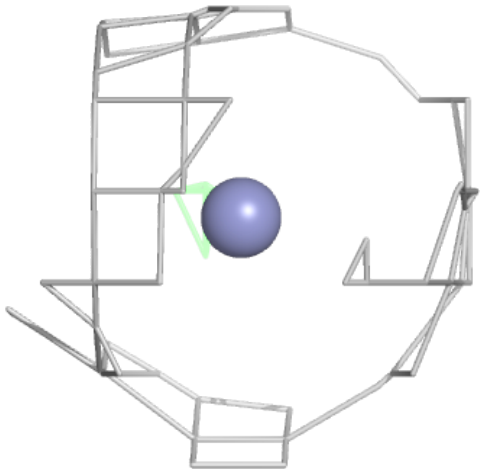
Electron density around ZN A 201:

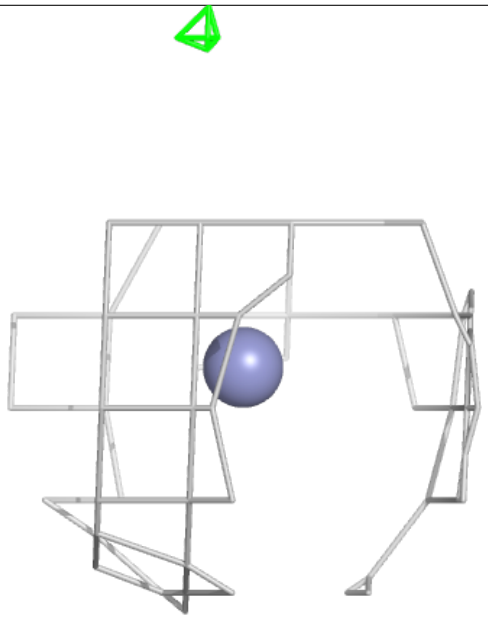
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

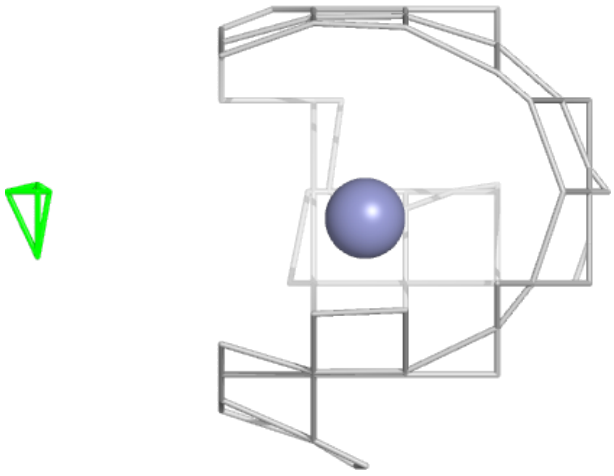


Electron density around ZN E 201:

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

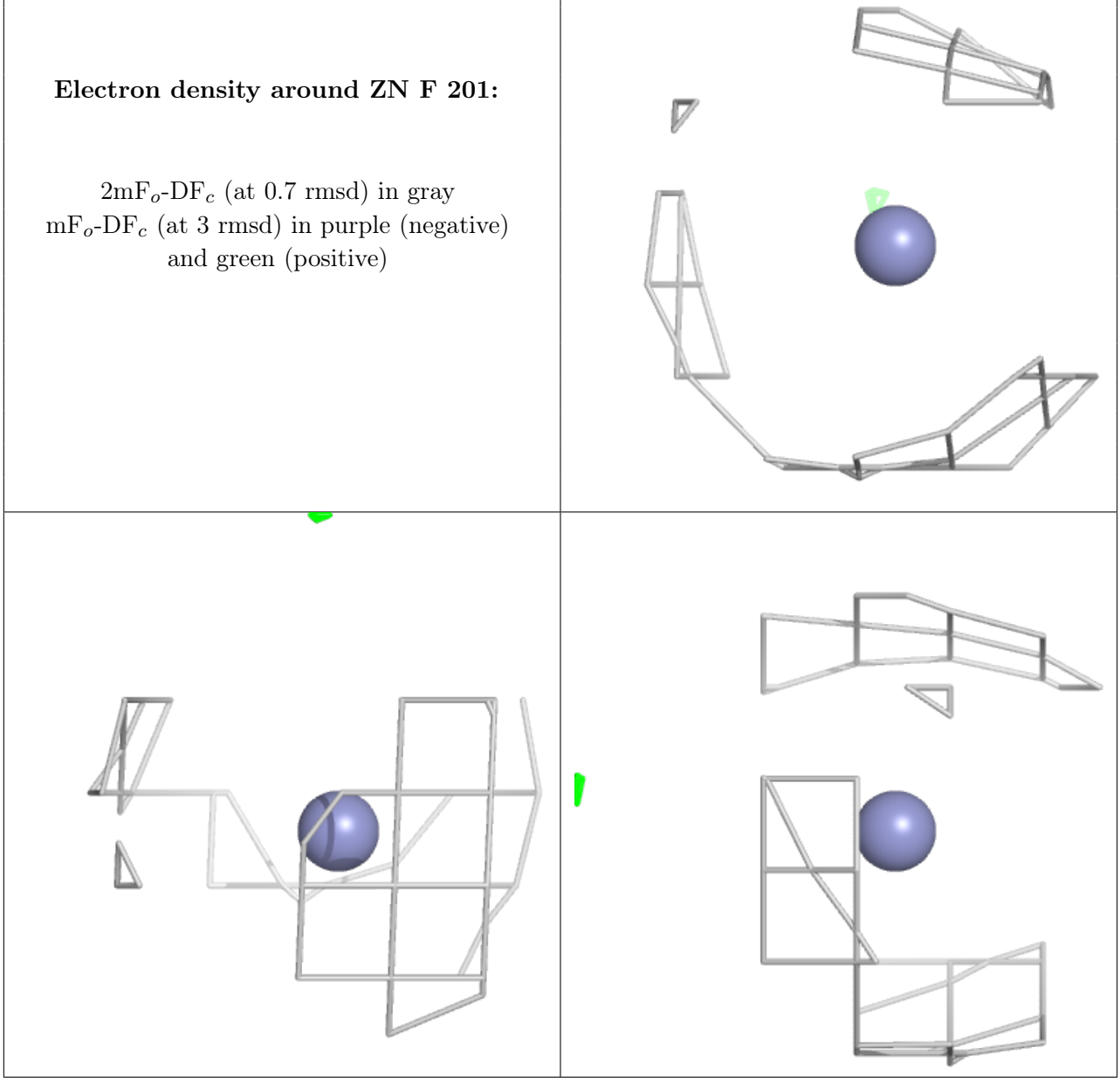






Electron density around ZN F 201:

$2mF_o$-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.