Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 01:02 AM EDT

PDB ID	:	7TD5
Title	:	Structure of human PRC2-EZH1 containing phosphorylated SUZ12
Authors	:	Gong, L.; Jiao, L.; Liu, X.
Deposited on	:	2021-12-30
Resolution	:	2.99 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:

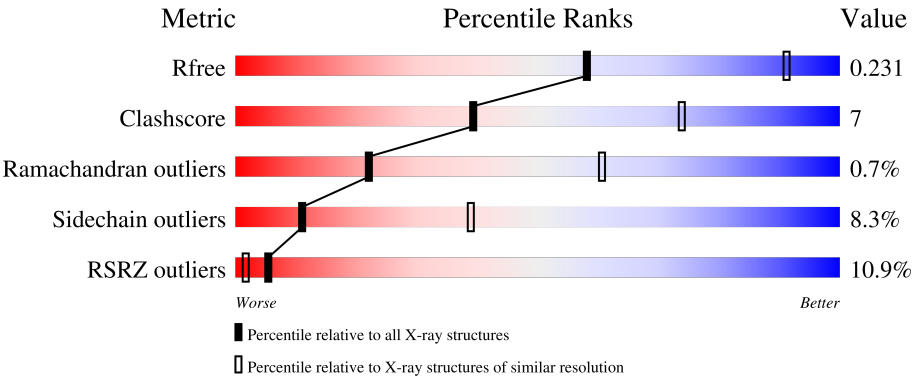
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.99 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	747	3% 53% 13% 33%
1	F	747	17% 48% 11% 40%
2	B	373	% 76% 23%
2	G	373	4% 76% 22%
3	C	179	% 49% 24% 26%

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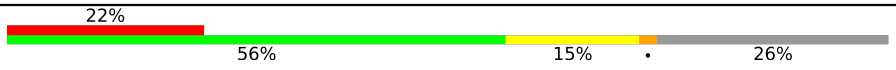
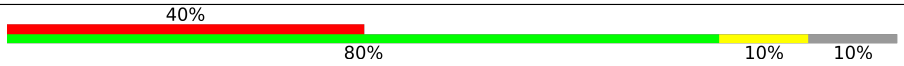
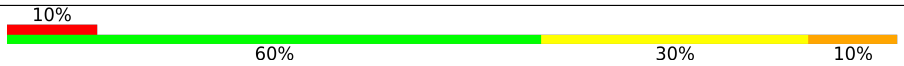
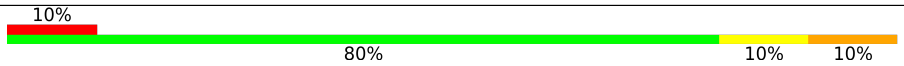
Mol	Chain	Length	Quality of chain
3	H	179	
4	D	10	
4	I	10	
5	E	10	
5	J	10	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 16191 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 Histone-lysine N-methyltransferase EZH1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	497	Total	C	N	O	S	0	0	0
			3999	2524	692	740	43			
1	F	447	Total	C	N	O	S	0	0	0
			3597	2262	625	669	41			

- Molecule 2 is a protein called Polycomb protein EED.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	373	Total	C	N	O	S	0	0	0
			3031	1920	533	556	22			
2	G	372	Total	C	N	O	S	0	0	0
			3020	1914	529	555	22			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	69	SER	-	expression tag	UNP O75530
B	70	TRP	-	expression tag	UNP O75530
B	71	SER	-	expression tag	UNP O75530
B	72	HIS	-	expression tag	UNP O75530
B	73	PRO	-	expression tag	UNP O75530
B	74	GLN	-	expression tag	UNP O75530
B	75	PHE	-	expression tag	UNP O75530
B	76	GLU	-	expression tag	UNP O75530
G	69	SER	-	expression tag	UNP O75530
G	70	TRP	-	expression tag	UNP O75530
G	71	SER	-	expression tag	UNP O75530
G	72	HIS	-	expression tag	UNP O75530
G	73	PRO	-	expression tag	UNP O75530
G	74	GLN	-	expression tag	UNP O75530
G	75	PHE	-	expression tag	UNP O75530
G	76	GLU	-	expression tag	UNP O75530

- Molecule 3 is a protein called Polycomb protein SUZ12.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	132	Total	C	N	O	P	S	0	0	0
			1099	689	188	209	1	12			
3	H	132	Total	C	N	O	P	S	0	0	0
			1099	689	188	209	1	12			

- Molecule 4 is a protein called THR-LYS-ALA-ALA-ARG-MET-SER-ALA-PRO-SER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	10	Total	C	N	O	S	0	0	0
			69	41	14	13	1			
4	I	9	Total	C	N	O	S	0	0	0
			63	38	13	11	1			

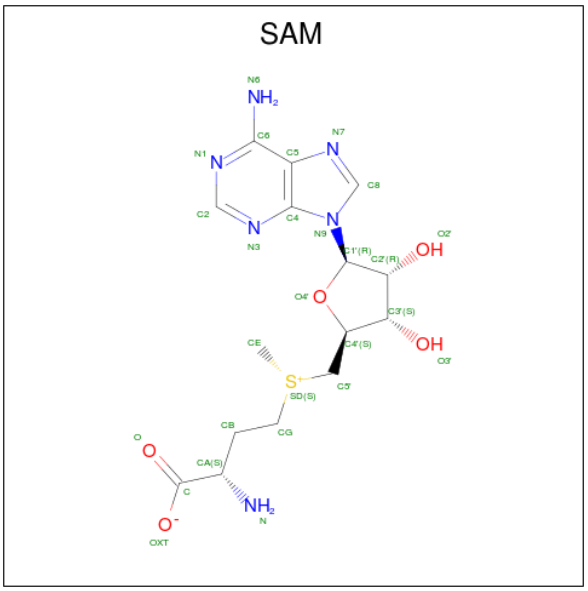
- Molecule 5 is a protein called THR-LYS-ALA-ALA-ARG-M3L-SER-ALA-PRO-ALA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	10	Total	C	N	O	0	0	0
			72	45	15	12			
5	J	10	Total	C	N	O	0	0	0
			72	45	15	12			

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	8	Total	Zn	0	0
			8	8		
6	F	8	Total	Zn	0	0
			8	8		

- Molecule 7 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: $C_{15}H_{22}N_6O_5S$) (labeled as "Ligand of Interest" by depositor).



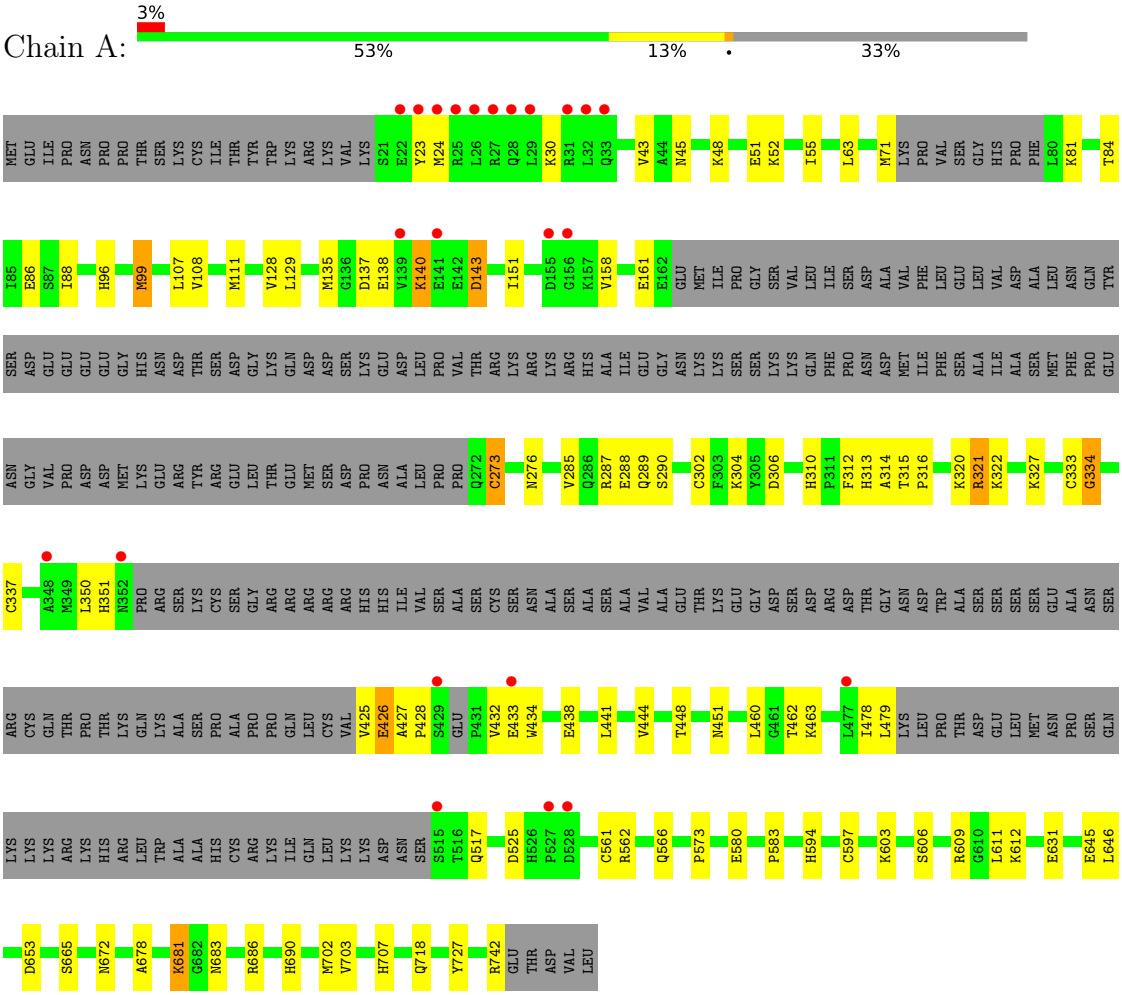
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
7	F	1	Total	C	N	O	S	0	0
			27	15	6	5	1		

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.

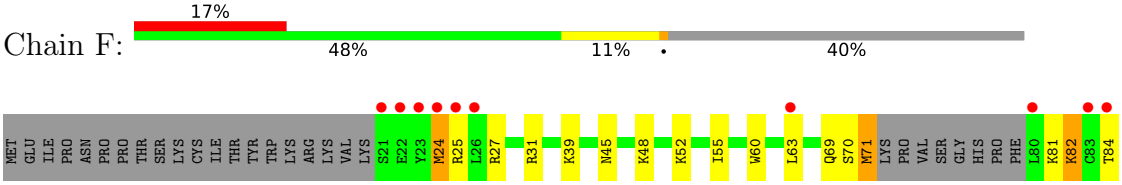
• Molecule 1: Histone-lysine N-methyltransferase EZH1

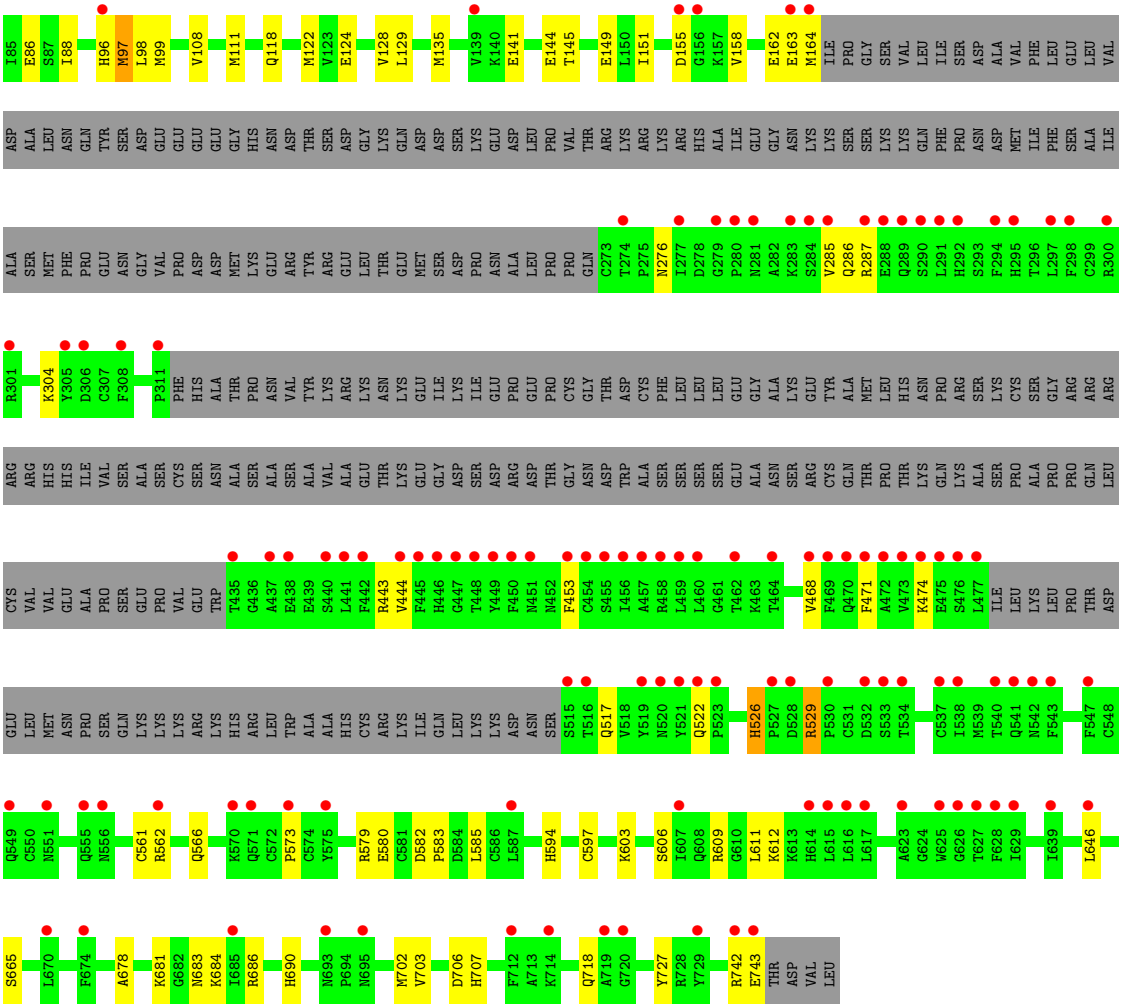
Chain A:



• Molecule 1: Histone-lysine N-methyltransferase EZH1

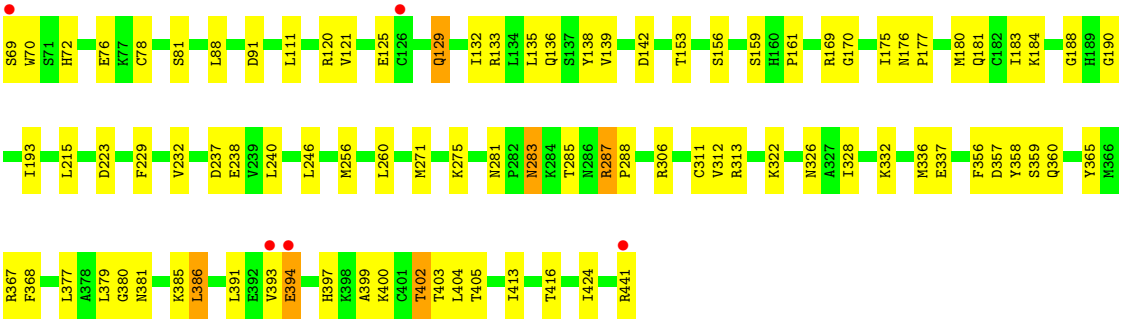
Chain F:





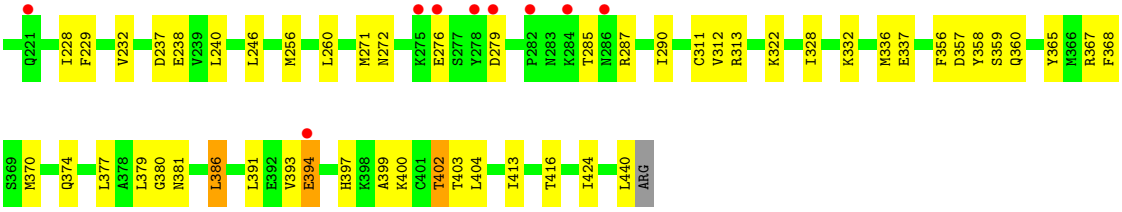
• Molecule 2: Polycomb protein EED

Chain B:

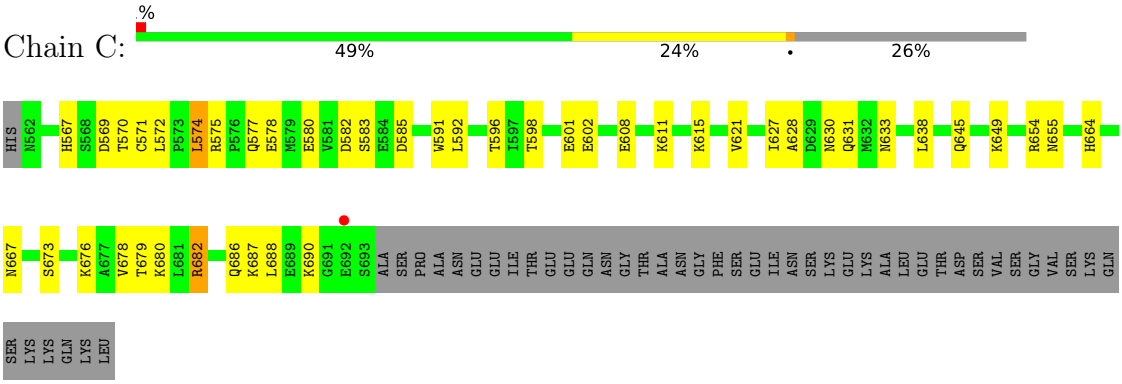


• Molecule 2: Polycomb protein EED

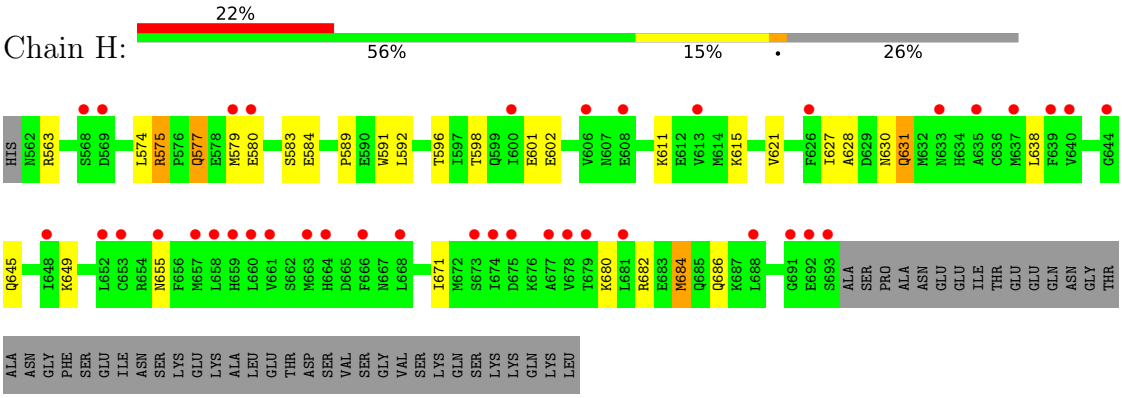
Chain G:



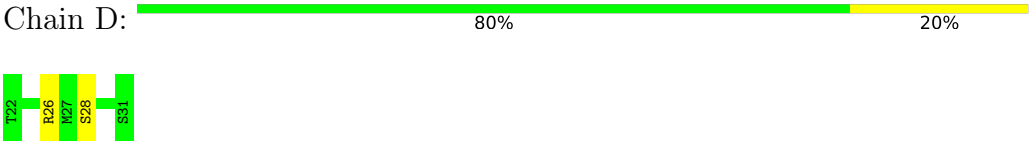
• Molecule 3: Polycomb protein SUZ12



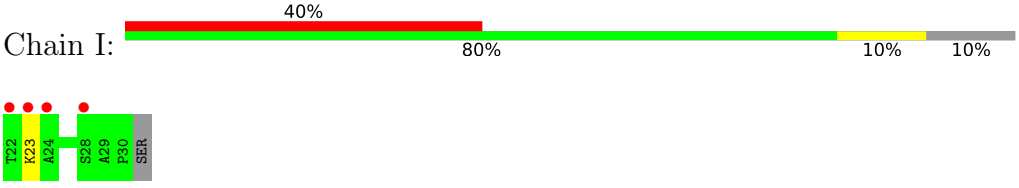
• Molecule 3: Polycomb protein SUZ12



• Molecule 4: THR-LYS-ALA-ALA-ARG-MET-SER-ALA-PRO-SER



• Molecule 4: THR-LYS-ALA-ALA-ARG-MET-SER-ALA-PRO-SER

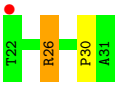


• Molecule 5: THR-LYS-ALA-ALA-ARG-M3L-SER-ALA-PRO-ALA

Chain E:

• Molecule 5: THR-LYS-ALA-ALA-ARG-M3L-SER-ALA-PRO-ALA

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	231.87Å 64.43Å 254.50Å 90.00° 109.89° 90.00°	Depositor
Resolution (Å)	42.52 – 2.99 49.62 – 2.99	Depositor EDS
% Data completeness (in resolution range)	85.7 (42.52-2.99) 85.7 (49.62-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.32 (at 3.01Å)	Xtriage
Refinement program	BUSTER 2.10.4 (16-JUL-2021)	Depositor
R, R_{free}	0.196 , 0.230 0.199 , 0.231	Depositor DCC
R_{free} test set	2988 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å^2)	51.3	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 65.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	16191	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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: SEP, ZN, SAM, M3L

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	0.47	0/4087	0.63	0/5508
1	F	0.33	0/3673	0.56	0/4946
2	B	0.47	0/3111	0.66	0/4213
2	G	0.38	0/3100	0.63	0/4199
3	C	0.54	0/1108	0.63	0/1483
3	H	0.32	0/1108	0.54	0/1483
4	D	0.53	0/69	0.57	0/91
4	I	0.37	0/63	0.56	0/83
5	E	0.65	0/60	0.71	0/80
5	J	0.47	0/60	0.58	0/80
All	All	0.42	0/16439	0.61	0/22166

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

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	3999	0	3869	64	0
1	F	3597	0	3468	50	0
2	B	3031	0	2938	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	3020	0	2925	51	0
3	C	1099	0	1078	39	0
3	H	1099	0	1078	20	0
4	D	69	0	73	1	0
4	I	63	0	68	0	0
5	E	72	0	83	2	0
5	J	72	0	83	1	0
6	A	8	0	0	0	0
6	F	8	0	0	0	0
7	A	27	0	22	0	0
7	F	27	0	22	0	0
All	All	16191	0	15707	235	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 7.

All (235) 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:321:ARG:NH1	3:C:664:HIS:CE1	2.14	1.16
1:A:321:ARG:HH11	3:C:664:HIS:CE1	1.73	1.07
1:F:84:THR:HG22	1:F:96:HIS:HD2	1.21	1.06
1:A:84:THR:HG22	1:A:96:HIS:HD2	1.20	1.00
2:G:70:TRP:HB3	2:G:357:ASP:OD2	1.73	0.88
1:A:84:THR:HG22	1:A:96:HIS:CD2	2.09	0.88
1:A:322:LYS:H	3:C:667:ASN:HD21	1.23	0.87
1:F:84:THR:HG22	1:F:96:HIS:CD2	2.11	0.85
1:F:27:ARG:HH11	1:F:31:ARG:HH11	1.20	0.84
1:A:690:HIS:HD2	1:A:727:TYR:H	1.26	0.83
1:F:690:HIS:HD2	1:F:727:TYR:H	1.26	0.83
3:C:628:ALA:H	3:C:631:GLN:HE21	1.28	0.82
5:J:26:ARG:HH22	5:J:30:PRO:HB3	1.43	0.82
2:B:70:TRP:NE1	2:B:397:HIS:O	2.17	0.77
1:A:276:ASN:HD21	3:C:655:ASN:HD21	1.31	0.76
1:A:321:ARG:HH12	3:C:664:HIS:CD2	2.03	0.76
1:A:276:ASN:ND2	3:C:655:ASN:HD21	1.83	0.75
1:F:27:ARG:HH11	1:F:31:ARG:NH1	1.83	0.75
1:F:27:ARG:NH1	1:F:31:ARG:HH11	1.84	0.75
3:C:601:GLU:HG2	3:C:615:LYS:NZ	2.02	0.73
3:H:601:GLU:HG2	3:H:615:LYS:NZ	2.03	0.72
1:A:321:ARG:NH1	3:C:664:HIS:NE2	2.37	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:232:VAL:HG21	3:C:591:TRP:CE3	2.26	0.71
2:G:74:GLN:NE2	2:G:400:LYS:NZ	2.38	0.71
1:A:321:ARG:NH1	3:C:664:HIS:ND1	2.39	0.71
1:A:140:LYS:HB2	1:A:143:ASP:HB2	1.73	0.69
1:F:276:ASN:ND2	3:H:655:ASN:HD21	1.91	0.68
1:A:517:GLN:HB2	1:A:672:ASN:OD1	1.93	0.67
3:C:627:ILE:H	3:C:631:GLN:HE22	1.41	0.67
1:A:287:ARG:HG3	1:A:444:VAL:HA	1.77	0.66
1:F:52:LYS:HB2	2:G:246:LEU:HD13	1.76	0.66
3:C:627:ILE:H	3:C:631:GLN:NE2	1.93	0.66
1:A:690:HIS:CD2	1:A:727:TYR:H	2.13	0.65
1:A:52:LYS:HB2	2:B:246:LEU:HD13	1.78	0.65
2:G:215:LEU:HB2	2:G:229:PHE:HB2	1.79	0.65
2:B:161:PRO:O	2:B:177:PRO:HD2	1.96	0.64
2:G:370:MET:HE1	2:G:374:GLN:HB3	1.78	0.64
2:G:161:PRO:O	2:G:177:PRO:HD2	1.97	0.64
1:F:70:SER:HB3	2:G:135:LEU:HD23	1.80	0.64
1:F:287:ARG:HG3	1:F:444:VAL:HA	1.78	0.64
1:F:276:ASN:HD21	3:H:655:ASN:HD21	1.46	0.64
1:F:684:LYS:HE3	3:H:584:GLU:HG3	1.81	0.63
1:A:151:ILE:HG12	1:A:158:VAL:HG21	1.81	0.62
1:F:27:ARG:NH1	1:F:31:ARG:NH1	2.43	0.62
2:B:215:LEU:HB2	2:B:229:PHE:HB2	1.82	0.61
3:C:628:ALA:H	3:C:631:GLN:NE2	1.96	0.61
5:E:26:ARG:HH22	5:E:30:PRO:HD3	1.65	0.61
3:C:575:ARG:HD3	3:C:578:GLU:OE2	2.02	0.60
1:F:690:HIS:CD2	1:F:727:TYR:H	2.13	0.60
2:B:69:SER:HA	2:G:359:SER:HB2	1.83	0.60
3:H:627:ILE:H	3:H:631:GLN:HE22	1.48	0.60
1:A:566:GLN:HB3	1:A:603:LYS:HG2	1.84	0.59
2:B:183:ILE:HG13	2:B:184:LYS:H	1.67	0.59
2:G:183:ILE:HG13	2:G:184:LYS:H	1.66	0.59
1:F:151:ILE:HG12	1:F:158:VAL:HG21	1.84	0.59
2:G:76:GLU:HB3	2:G:400:LYS:NZ	2.18	0.59
2:B:142:ASP:OD2	2:B:169:ARG:HD2	2.02	0.59
1:A:321:ARG:NH1	3:C:664:HIS:CG	2.71	0.58
1:F:678:ALA:O	1:F:686:ARG:NH2	2.36	0.58
1:F:566:GLN:HB3	1:F:603:LYS:HG2	1.84	0.58
3:C:601:GLU:HG2	3:C:615:LYS:HZ1	1.69	0.57
1:A:678:ALA:O	1:A:686:ARG:NH2	2.35	0.57
1:A:334:GLY:HA2	1:A:337:CYS:HB2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:GLU:HB2	1:A:140:LYS:HE3	1.86	0.56
1:A:322:LYS:N	3:C:667:ASN:HD21	2.00	0.56
1:A:321:ARG:HH12	3:C:664:HIS:CG	2.22	0.56
1:F:471:PHE:HA	1:F:474:LYS:CE	2.35	0.56
2:G:360:GLN:O	2:G:381:ASN:HB2	2.06	0.56
1:A:45:ASN:HA	1:A:48:LYS:HD3	1.88	0.56
3:H:601:GLU:HG2	3:H:615:LYS:HZ1	1.68	0.55
2:G:78:CYS:HB3	2:G:402:THR:HB	1.88	0.55
2:B:70:TRP:HB3	2:B:357:ASP:OD2	2.05	0.55
2:G:189:HIS:HD2	2:G:212:ASP:OD2	1.90	0.55
3:H:575:ARG:HE	3:H:577:GLN:HE21	1.54	0.55
2:B:386:LEU:HD21	2:B:416:THR:HG21	1.88	0.55
3:C:598:THR:O	3:C:602:GLU:HG2	2.05	0.55
2:G:216:ARG:HG2	2:G:228:ILE:HG12	1.89	0.55
2:G:232:VAL:HG21	3:H:591:TRP:CE3	2.42	0.55
1:F:45:ASN:HA	1:F:48:LYS:HD3	1.88	0.54
1:F:24:MET:SD	1:F:25:ARG:N	2.80	0.54
2:G:386:LEU:HD21	2:G:416:THR:HG21	1.89	0.54
3:H:601:GLU:HA	3:H:611:LYS:HE3	1.90	0.54
1:A:441:LEU:HD11	3:C:654:ARG:HG2	1.89	0.54
1:F:526:HIS:HB2	1:F:529:ARG:HG3	1.90	0.54
1:A:71:MET:HG3	2:B:136:GLN:HA	1.89	0.54
3:C:582:ASP:HB3	3:C:585:ASP:HB2	1.89	0.54
1:F:453:PHE:HD1	1:F:468:VAL:HG12	1.73	0.54
2:B:70:TRP:HD1	2:B:72:HIS:H	1.57	0.53
2:B:78:CYS:HB3	2:B:402:THR:HB	1.89	0.53
3:H:628:ALA:H	3:H:631:GLN:HE21	1.57	0.53
2:G:76:GLU:HB3	2:G:400:LYS:HZ2	1.74	0.53
2:B:175:ILE:O	2:B:177:PRO:HD3	2.09	0.53
1:A:321:ARG:NH1	3:C:664:HIS:CD2	2.71	0.52
1:F:286:GLN:HA	1:F:443:ARG:HD3	1.91	0.52
3:C:678:VAL:O	3:C:682:ARG:HG2	2.10	0.52
2:G:74:GLN:NE2	2:G:400:LYS:HZ2	2.06	0.52
1:A:322:LYS:H	3:C:667:ASN:ND2	2.01	0.52
2:G:175:ILE:O	2:G:177:PRO:HD3	2.09	0.52
2:B:281:ASN:O	2:B:285:THR:HG22	2.08	0.52
2:G:74:GLN:NE2	2:G:400:LYS:HZ3	2.07	0.52
3:C:679:THR:HG22	3:C:680:LYS:HE3	1.92	0.51
1:F:609:ARG:HB2	1:F:611:LEU:HG	1.92	0.51
1:A:517:GLN:HE21	1:A:672:ASN:HD21	1.59	0.51
2:B:76:GLU:HB3	2:B:400:LYS:HE3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:601:GLU:HG2	3:C:615:LYS:HZ3	1.75	0.51
2:B:359:SER:HB2	2:G:69:SER:HA	1.92	0.50
3:C:645:GLN:HG3	3:C:688:LEU:HD11	1.92	0.50
2:G:70:TRP:NE1	2:G:397:HIS:O	2.43	0.50
2:B:360:GLN:O	2:B:381:ASN:HB2	2.10	0.50
1:A:609:ARG:HB2	1:A:611:LEU:HG	1.93	0.50
1:F:471:PHE:HA	1:F:474:LYS:HE2	1.93	0.50
1:A:351:HIS:HB2	1:A:451:ASN:HD21	1.77	0.50
2:B:70:TRP:HE3	2:B:357:ASP:H	1.60	0.50
2:G:370:MET:HE2	2:G:391:LEU:CD1	2.41	0.50
1:A:107:LEU:HD21	2:B:169:ARG:HD3	1.94	0.49
2:B:136:GLN:NE2	2:B:138:TYR:OH	2.45	0.49
3:H:601:GLU:HA	3:H:611:LYS:CE	2.42	0.49
1:F:129:LEU:HB3	1:F:158:VAL:HG22	1.95	0.49
1:A:111:MET:O	2:B:190:GLY:HA3	2.13	0.49
1:F:71:MET:SD	2:G:136:GLN:HG3	2.53	0.49
1:F:594:HIS:HB3	1:F:597:CYS:HB2	1.95	0.49
2:G:370:MET:HE1	2:G:374:GLN:CB	2.43	0.49
3:H:628:ALA:H	3:H:631:GLN:NE2	2.11	0.48
1:A:316:PRO:HB2	1:A:320:LYS:NZ	2.29	0.48
2:B:91:ASP:OD1	2:B:120:ARG:NH1	2.38	0.48
2:B:328:ILE:HB	2:B:356:PHE:HB2	1.96	0.48
3:H:601:GLU:HG2	3:H:615:LYS:HZ3	1.76	0.48
2:G:170:GLY:HA2	2:G:193:ILE:HG13	1.96	0.47
3:C:567:HIS:CE1	3:C:574:LEU:HD12	2.48	0.47
2:G:111:LEU:HD12	2:G:424:ILE:HD12	1.95	0.47
1:F:145:THR:O	1:F:149:GLU:HG2	2.14	0.47
1:F:122:MET:HA	1:F:646:LEU:HB2	1.96	0.47
3:H:682:ARG:O	3:H:686:GLN:OE1	2.32	0.47
1:A:129:LEU:HB3	1:A:158:VAL:HG22	1.95	0.47
2:B:111:LEU:HD12	2:B:424:ILE:HD12	1.95	0.47
1:A:583:PRO:HB2	3:C:628:ALA:HB2	1.96	0.47
2:B:368:PHE:HB3	2:B:379:LEU:HD13	1.97	0.47
1:F:583:PRO:HB2	3:H:628:ALA:HB2	1.96	0.47
3:H:598:THR:O	3:H:602:GLU:HG2	2.15	0.47
2:G:386:LEU:HD13	2:G:404:LEU:HD12	1.97	0.46
2:B:386:LEU:HD13	2:B:404:LEU:HD12	1.98	0.46
1:F:471:PHE:HA	1:F:474:LYS:HE3	1.97	0.46
2:G:70:TRP:HE1	2:G:397:HIS:CA	2.28	0.46
3:H:680:LYS:O	3:H:684:MET:HG2	2.15	0.46
1:A:478:ILE:HG22	1:A:479:LEU:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:580:GLU:HG3	1:A:703:VAL:HG22	1.96	0.46
1:F:118:GLN:OE1	3:H:584:GLU:OE1	2.33	0.46
2:B:311:CYS:HB3	2:B:322:LYS:HG2	1.98	0.46
2:G:272:ASN:O	2:G:276:GLU:OE1	2.34	0.46
2:G:88:LEU:HD11	2:G:132:ILE:HB	1.97	0.46
2:G:368:PHE:HB3	2:G:379:LEU:HD13	1.97	0.46
3:C:567:HIS:CE1	3:C:574:LEU:CD1	2.98	0.46
1:F:60:TRP:HA	1:F:63:LEU:HD12	1.97	0.46
1:F:70:SER:HB3	2:G:135:LEU:CD2	2.45	0.46
1:A:52:LYS:HA	1:A:55:ILE:HD12	1.97	0.46
1:A:99:MET:HG2	2:B:139:VAL:HB	1.98	0.46
1:A:702:MET:HE2	1:A:707:HIS:CE1	2.51	0.46
1:F:81:LYS:HG3	1:F:82:LYS:H	1.80	0.46
1:F:39:LYS:HE3	2:G:394:GLU:HG2	1.97	0.45
1:A:594:HIS:HB3	1:A:597:CYS:HB2	1.98	0.45
2:B:240:LEU:O	2:B:367:ARG:NH2	2.49	0.45
1:F:52:LYS:HA	1:F:55:ILE:HD12	1.98	0.45
3:C:633:ASN:ND2	3:C:673:SER:OG	2.39	0.45
1:F:580:GLU:HG3	1:F:703:VAL:HG22	1.99	0.45
1:A:425:VAL:HG23	1:A:426:GLU:OE1	2.16	0.45
1:A:137:ASP:HA	5:E:26:ARG:HD2	1.98	0.45
1:A:702:MET:CE	1:A:707:HIS:CE1	2.99	0.45
2:B:88:LEU:HD11	2:B:132:ILE:HB	1.98	0.45
1:F:82:LYS:HB2	1:F:98:LEU:HD12	1.97	0.45
2:B:380:GLY:HA3	2:B:413:ILE:HB	1.99	0.45
3:C:601:GLU:HA	3:C:611:LYS:HE2	1.98	0.45
1:F:702:MET:CE	1:F:707:HIS:CE1	3.00	0.45
2:G:380:GLY:HA3	2:G:413:ILE:HB	1.99	0.45
3:H:589:PRO:HD2	3:H:592:LEU:HD12	1.99	0.45
1:A:683:ASN:O	1:A:686:ARG:HG2	2.17	0.45
3:C:676:LYS:O	3:C:680:LYS:HG2	2.17	0.45
2:B:125:GLU:HB2	2:B:135:LEU:HG	1.99	0.44
1:A:285:VAL:HG13	1:A:289:GLN:HB3	1.99	0.44
2:B:385:LYS:HG3	2:B:405:THR:HG22	1.98	0.44
2:B:170:GLY:HA2	2:B:193:ILE:HG13	2.00	0.44
2:B:238:GLU:HB2	2:B:256:MET:HG3	2.00	0.44
1:A:81:LYS:O	1:A:99:MET:HB2	2.18	0.44
1:A:302:CYS:SG	1:A:310:HIS:CE1	3.11	0.44
2:G:240:LEU:O	2:G:367:ARG:NH2	2.50	0.44
3:C:649:LYS:HE2	3:C:688:LEU:HD13	1.99	0.44
2:G:311:CYS:HB3	2:G:322:LYS:HG2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:312:VAL:O	2:B:313:ARG:NH1	2.51	0.44
2:G:238:GLU:HB2	2:G:256:MET:HG3	1.98	0.43
2:G:70:TRP:HE1	2:G:397:HIS:HA	1.83	0.43
1:F:582:ASP:HB3	1:F:585:LEU:HB2	2.00	0.43
1:F:561:CYS:HB3	1:F:573:PRO:HG2	2.00	0.43
2:B:129:GLN:O	2:B:129:GLN:HG3	2.18	0.43
3:C:570:THR:OG1	3:C:572:LEU:HD13	2.19	0.43
2:G:393:VAL:HG11	2:G:399:ALA:HA	2.01	0.43
1:F:683:ASN:O	1:F:686:ARG:HG2	2.19	0.43
1:A:653:ASP:OD1	4:D:26:ARG:NH2	2.52	0.43
2:G:125:GLU:HB2	2:G:135:LEU:HG	1.99	0.43
2:B:283:ASN:ND2	2:B:283:ASN:H	2.17	0.43
1:A:333:CYS:N	1:A:334:GLY:CA	2.82	0.42
1:A:561:CYS:HB3	1:A:573:PRO:HG2	2.00	0.42
2:B:328:ILE:HG13	2:B:358:TYR:HE2	1.84	0.42
2:B:287:ARG:H	2:B:287:ARG:HG2	1.58	0.42
1:F:99:MET:HG3	2:G:137:SER:OG	2.18	0.42
1:A:315:THR:HB	1:A:525:ASP:OD2	2.19	0.42
2:G:237:ASP:HB3	2:G:256:MET:HB2	2.01	0.42
2:G:370:MET:CE	2:G:391:LEU:CD1	2.97	0.42
1:A:645:GLU:HG3	1:A:681:LYS:HG3	2.02	0.42
1:F:97:MET:HB3	1:F:97:MET:HE2	1.78	0.42
2:G:312:VAL:O	2:G:313:ARG:NH1	2.52	0.42
1:A:478:ILE:HG22	1:A:479:LEU:HG	2.01	0.42
1:A:580:GLU:HB2	1:A:703:VAL:HG13	2.01	0.42
1:F:81:LYS:HG3	1:F:82:LYS:N	2.35	0.42
2:G:337:GLU:H	2:G:337:GLU:CD	2.22	0.42
2:B:393:VAL:HG11	2:B:399:ALA:HA	2.01	0.42
2:G:377:LEU:HB2	2:G:391:LEU:HD11	2.02	0.42
1:A:460:LEU:C	1:A:462:THR:H	2.24	0.41
2:B:326:ASN:HA	2:B:358:TYR:CE1	2.56	0.41
2:G:328:ILE:HB	2:G:356:PHE:HB2	2.01	0.41
1:A:276:ASN:HD21	3:C:655:ASN:ND2	2.07	0.41
2:B:237:ASP:HB3	2:B:256:MET:HB2	2.02	0.41
1:F:111:MET:O	2:G:190:GLY:HA3	2.21	0.41
2:G:183:ILE:HG13	2:G:184:LYS:N	2.34	0.41
1:A:315:THR:HA	1:A:316:PRO:HD3	1.85	0.41
1:A:434:TRP:CZ2	1:A:463:LYS:HG2	2.56	0.41
1:A:43:VAL:HG21	2:B:394:GLU:HG3	2.03	0.41
2:B:337:GLU:H	2:B:337:GLU:CD	2.22	0.41
1:F:81:LYS:HE3	1:F:82:LYS:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:579:ARG:HG2	1:F:702:MET:HB3	2.03	0.41
2:B:377:LEU:HB2	2:B:391:LEU:HD11	2.03	0.41
1:A:306:ASP:HA	1:A:312:PHE:HZ	1.87	0.40
1:A:438:GLU:OE2	1:A:463:LYS:HD3	2.21	0.40
2:B:288:PRO:HD3	3:C:578:GLU:HG2	2.02	0.40
2:G:328:ILE:HG13	2:G:358:TYR:HE1	1.86	0.40
3:C:678:VAL:O	3:C:682:ARG:CG	2.69	0.40
3:H:575:ARG:NE	3:H:577:GLN:HE21	2.19	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	485/747 (65%)	453 (93%)	25 (5%)	7 (1%)	11 43
1	F	437/747 (58%)	411 (94%)	25 (6%)	1 (0%)	47 82
2	B	371/373 (100%)	351 (95%)	18 (5%)	2 (0%)	29 68
2	G	370/373 (99%)	355 (96%)	12 (3%)	3 (1%)	19 57
3	C	129/179 (72%)	124 (96%)	5 (4%)	0	100 100
3	H	129/179 (72%)	125 (97%)	4 (3%)	0	100 100
4	D	8/10 (80%)	6 (75%)	2 (25%)	0	100 100
4	I	7/10 (70%)	6 (86%)	1 (14%)	0	100 100
5	E	7/10 (70%)	6 (86%)	0	1 (14%)	0 1
5	J	7/10 (70%)	6 (86%)	1 (14%)	0	100 100
All	All	1950/2638 (74%)	1843 (94%)	93 (5%)	14 (1%)	22 60

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	273	CYS
1	A	313	HIS
1	F	742	ARG
1	A	314	ALA
1	A	426	GLU
1	A	427	ALA
2	B	365	TYR
2	G	71	SER
2	G	365	TYR
5	E	30	PRO
1	A	428	PRO
2	B	188	GLY
2	G	188	GLY
1	A	334	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	446/670 (67%)	413 (93%)	33 (7%)	13 44
1	F	402/670 (60%)	371 (92%)	31 (8%)	13 42
2	B	336/336 (100%)	312 (93%)	24 (7%)	14 46
2	G	335/336 (100%)	310 (92%)	25 (8%)	13 43
3	C	124/164 (76%)	109 (88%)	15 (12%)	5 21
3	H	124/164 (76%)	109 (88%)	15 (12%)	5 21
4	D	7/7 (100%)	6 (86%)	1 (14%)	3 15
4	I	6/7 (86%)	5 (83%)	1 (17%)	2 11
5	E	5/5 (100%)	3 (60%)	2 (40%)	0 0
5	J	5/5 (100%)	4 (80%)	1 (20%)	1 7
All	All	1790/2364 (76%)	1642 (92%)	148 (8%)	11 39

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	TYR
1	A	24	MET
1	A	30	LYS
1	A	51	GLU
1	A	63	LEU
1	A	86	GLU
1	A	88	ILE
1	A	99	MET
1	A	108	VAL
1	A	128	VAL
1	A	135	MET
1	A	140	LYS
1	A	143	ASP
1	A	161	GLU
1	A	273	CYS
1	A	288	GLU
1	A	290	SER
1	A	304	LYS
1	A	321	ARG
1	A	327	LYS
1	A	350	LEU
1	A	432	VAL
1	A	433	GLU
1	A	448	THR
1	A	562	ARG
1	A	606	SER
1	A	612	LYS
1	A	631	GLU
1	A	646	LEU
1	A	665	SER
1	A	681	LYS
1	A	718	GLN
1	A	742	ARG
2	B	81	SER
2	B	121	VAL
2	B	129	GLN
2	B	133	ARG
2	B	153	THR
2	B	156	SER
2	B	159	SER
2	B	176	ASN
2	B	180	MET
2	B	181	GLN

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Mol	Chain	Res	Type
2	B	223	ASP
2	B	260	LEU
2	B	271	MET
2	B	275	LYS
2	B	283	ASN
2	B	287	ARG
2	B	306	ARG
2	B	332	LYS
2	B	336	MET
2	B	386	LEU
2	B	394	GLU
2	B	402	THR
2	B	403	THR
2	B	441	ARG
3	C	569	ASP
3	C	571	CYS
3	C	574	LEU
3	C	577	GLN
3	C	580	GLU
3	C	592	LEU
3	C	596	THR
3	C	608	GLU
3	C	621	VAL
3	C	630	ASN
3	C	638	LEU
3	C	682	ARG
3	C	686	GLN
3	C	687	LYS
3	C	690	LYS
4	D	28	SER
5	E	22	THR
5	E	23	LYS
1	F	24	MET
1	F	69	GLN
1	F	71	MET
1	F	82	LYS
1	F	86	GLU
1	F	88	ILE
1	F	97	MET
1	F	108	VAL
1	F	124	GLU
1	F	128	VAL

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Mol	Chain	Res	Type
1	F	135	MET
1	F	141	GLU
1	F	144	GLU
1	F	155	ASP
1	F	162	GLU
1	F	163	GLU
1	F	164	MET
1	F	285	VAL
1	F	304	LYS
1	F	517	GLN
1	F	522	GLN
1	F	526	HIS
1	F	529	ARG
1	F	562	ARG
1	F	606	SER
1	F	612	LYS
1	F	665	SER
1	F	681	LYS
1	F	706	ASP
1	F	718	GLN
1	F	743	GLU
2	G	81	SER
2	G	107	GLU
2	G	120	ARG
2	G	121	VAL
2	G	122	THR
2	G	136	GLN
2	G	153	THR
2	G	159	SER
2	G	176	ASN
2	G	180	MET
2	G	185	HIS
2	G	189	HIS
2	G	260	LEU
2	G	271	MET
2	G	279	ASP
2	G	285	THR
2	G	287	ARG
2	G	290	ILE
2	G	332	LYS
2	G	336	MET
2	G	386	LEU

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Mol	Chain	Res	Type
2	G	394	GLU
2	G	402	THR
2	G	403	THR
2	G	440	LEU
3	H	563	ARG
3	H	574	LEU
3	H	575	ARG
3	H	577	GLN
3	H	579	MET
3	H	580	GLU
3	H	596	THR
3	H	621	VAL
3	H	630	ASN
3	H	631	GLN
3	H	638	LEU
3	H	645	GLN
3	H	649	LYS
3	H	671	ILE
3	H	684	MET
4	I	23	LYS
5	J	26	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	GLN
1	A	96	HIS
1	A	118	GLN
1	A	276	ASN
1	A	451	ASN
1	A	517	GLN
1	A	556	ASN
1	A	636	ASN
1	A	690	HIS
1	A	707	HIS
2	B	72	HIS
2	B	136	GLN
2	B	160	HIS
2	B	176	ASN
2	B	213	HIS
2	B	272	ASN
2	B	283	ASN

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Mol	Chain	Res	Type
3	C	562	ASN
3	C	631	GLN
3	C	633	ASN
3	C	642	ASN
3	C	667	ASN
1	F	96	HIS
1	F	118	GLN
1	F	276	ASN
1	F	295	HIS
1	F	556	ASN
1	F	571	GLN
1	F	608	GLN
1	F	636	ASN
1	F	690	HIS
1	F	704	ASN
1	F	707	HIS
2	G	72	HIS
2	G	74	GLN
2	G	160	HIS
2	G	176	ASN
2	G	181	GLN
2	G	189	HIS
2	G	213	HIS
2	G	374	GLN
3	H	577	GLN
3	H	624	HIS
3	H	631	GLN
3	H	642	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)

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
5	M3L	J	27	5	10,11,12	0.44	0	9,14,16	0.26	0
3	SEP	H	583	3	8,9,10	1.15	1 (12%)	8,12,14	2.30	3 (37%)
5	M3L	E	27	5	10,11,12	0.45	0	9,14,16	0.27	0
3	SEP	C	583	3	8,9,10	1.22	1 (12%)	8,12,14	4.68	4 (50%)

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
5	M3L	J	27	5	-	0/9/10/12	-
3	SEP	H	583	3	-	1/5/8/10	-
5	M3L	E	27	5	-	0/9/10/12	-
3	SEP	C	583	3	-	1/5/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	583	SEP	P-OG	-2.69	1.51	1.60
3	H	583	SEP	P-OG	-2.42	1.52	1.60

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	583	SEP	OG-CB-CA	10.17	118.04	108.14
3	C	583	SEP	O3P-P-OG	-6.26	90.07	106.73
3	H	583	SEP	OG-CB-CA	5.10	113.11	108.14
3	C	583	SEP	OG-P-O1P	4.47	119.02	106.47
3	H	583	SEP	P-OG-CB	-2.57	111.22	118.30
3	H	583	SEP	O3P-P-OG	2.53	113.48	106.73
3	C	583	SEP	O3P-P-O2P	2.22	116.13	107.64

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	583	SEP	CA-CB-OG-P

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Mol	Chain	Res	Type	Atoms
3	H	583	SEP	CA-CB-OG-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 16 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	$\#\|Z\| > 2$
7	SAM	F	1009	-	24,29,29	0.72	0	23,42,42	0.92	2 (8%)
7	SAM	A	1009	-	24,29,29	0.72	0	23,42,42	1.01	2 (8%)

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
7	SAM	F	1009	-	-	2/12/33/33	0/3/3/3
7	SAM	A	1009	-	-	2/12/33/33	0/3/3/3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	1009	SAM	C5-C6-N6	2.49	124.14	120.35
7	F	1009	SAM	C5-C6-N6	2.37	123.95	120.35
7	A	1009	SAM	O-C-CA	-2.18	114.45	122.14
7	F	1009	SAM	O-C-CA	-2.04	114.95	122.14

There are no chirality outliers.

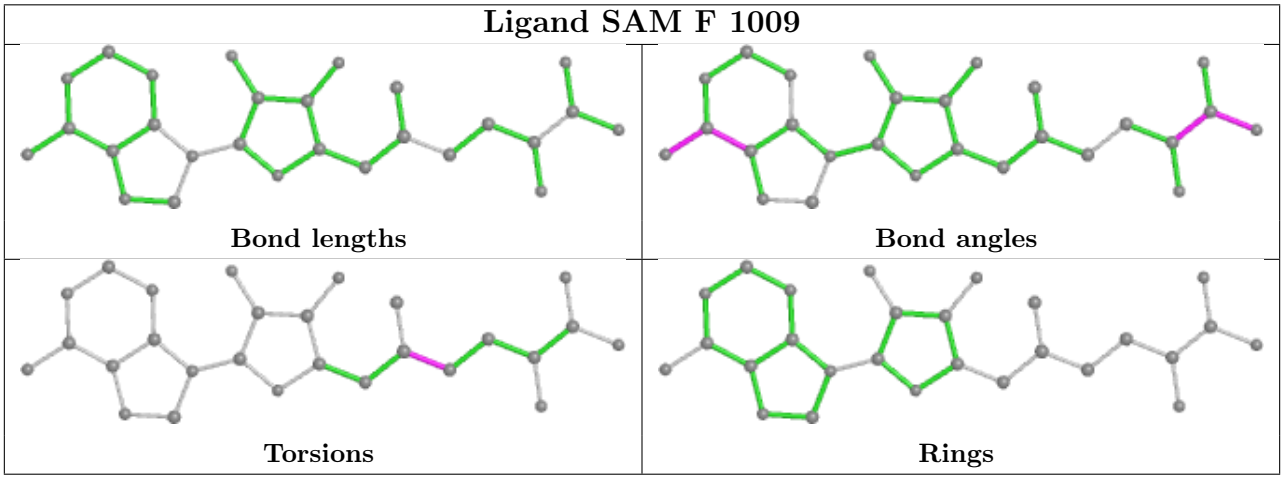
All (4) torsion outliers are listed below:

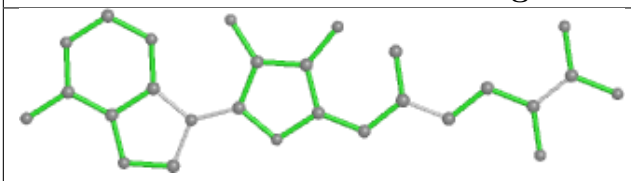
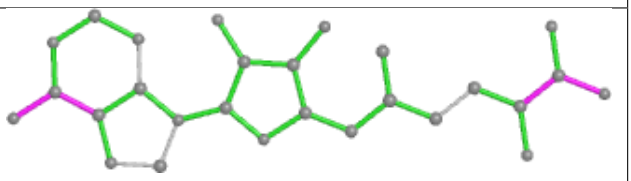
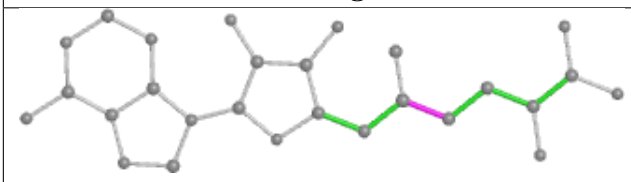
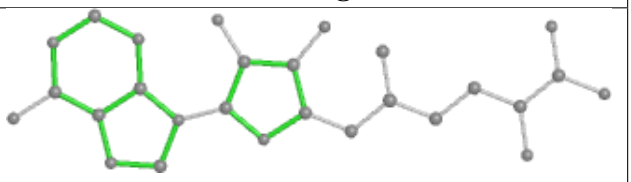
Mol	Chain	Res	Type	Atoms
7	A	1009	SAM	CB-CG-SD-CE
7	A	1009	SAM	CB-CG-SD-C5'
7	F	1009	SAM	CB-CG-SD-CE
7	F	1009	SAM	CB-CG-SD-C5'

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



Ligand SAM A 1009	
 Bond lengths	 Bond angles
 Torsions	 Rings

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	497/747 (66%)	0.17	23 (4%) 32 12	16, 53, 96, 130	0
1	F	447/747 (59%)	1.31	129 (28%) 0 0	71, 115, 193, 201	0
2	B	373/373 (100%)	0.04	5 (1%) 77 51	17, 50, 83, 97	0
2	G	372/373 (99%)	0.28	14 (3%) 40 16	38, 78, 115, 146	0
3	C	131/179 (73%)	-0.14	1 (0%) 86 65	18, 35, 73, 88	0
3	H	131/179 (73%)	1.38	39 (29%) 0 0	84, 122, 151, 157	0
4	D	10/10 (100%)	0.16	0 100 100	49, 59, 69, 72	0
4	I	9/10 (90%)	1.77	4 (44%) 0 0	108, 111, 114, 114	0
5	E	9/10 (90%)	0.60	1 (11%) 5 1	55, 63, 78, 79	0
5	J	9/10 (90%)	1.10	1 (11%) 5 1	70, 76, 84, 86	0
All	All	1988/2638 (75%)	0.50	217 (10%) 5 2	16, 72, 152, 201	0

All (217) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	515	SER	7.4
1	F	521	TYR	7.2
1	F	23	TYR	7.0
1	F	538	ILE	6.6
1	A	26	LEU	6.5
1	F	446	HIS	6.3
1	F	540	THR	6.2
5	J	22	THR	6.0
3	H	681	LEU	5.5
1	F	437	ALA	5.4
1	F	516	THR	5.3
3	H	688	LEU	5.2
1	F	291	LEU	5.0

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Mol	Chain	Res	Type	RSRZ
3	H	666	PHE	5.0
1	F	450	PHE	5.0
1	F	542	ASN	5.0
1	A	155	ASP	5.0
3	H	692	GLU	4.9
1	F	295	HIS	4.9
1	A	139	VAL	4.8
1	F	22	GLU	4.8
1	F	442	PHE	4.7
1	F	462	THR	4.7
1	A	24	MET	4.7
1	F	454	CYS	4.7
1	F	26	LEU	4.6
1	F	556	ASN	4.5
1	F	459	LEU	4.5
1	F	473	VAL	4.5
1	F	522	GLN	4.5
1	F	470	GLN	4.5
1	F	156	GLY	4.4
1	F	155	ASP	4.4
1	F	471	PHE	4.4
1	F	571	GLN	4.3
1	F	300	ARG	4.3
1	F	458	ARG	4.3
1	A	25	ARG	4.3
3	H	657	MET	4.3
1	F	294	PHE	4.3
3	H	674	ILE	4.3
1	F	139	VAL	4.2
1	F	607	ILE	4.2
1	F	695	ASN	4.2
1	F	283	LYS	4.2
1	F	616	LEU	4.1
3	H	675	ASP	4.0
1	F	448	THR	4.0
1	F	457	ALA	4.0
1	F	685	ILE	4.0
1	F	24	MET	3.9
1	F	533	SER	3.9
1	F	555	GLN	3.8
1	F	551	ASN	3.8
1	F	469	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
3	H	653	CYS	3.8
1	A	352	ASN	3.7
1	A	527	PRO	3.6
5	E	22	THR	3.6
1	F	292	HIS	3.6
1	F	562	ARG	3.6
1	F	639	ILE	3.6
1	F	280	PRO	3.6
2	B	394	GLU	3.6
3	H	659	HIS	3.6
3	H	691	GLY	3.5
1	A	23	TYR	3.5
3	H	661	VAL	3.5
1	F	537	CYS	3.5
3	H	677	ALA	3.4
1	F	445	PHE	3.4
1	F	440	SER	3.4
1	F	277	ILE	3.3
2	G	69	SER	3.3
3	H	663	MET	3.3
3	H	655	ASN	3.3
1	F	543	PHE	3.3
1	F	438	GLU	3.3
1	F	468	VAL	3.3
1	F	573	PRO	3.2
1	F	281	ASN	3.2
1	F	617	LEU	3.2
3	H	658	LEU	3.2
3	H	660	LEU	3.2
1	F	441	LEU	3.2
4	I	22	THR	3.2
1	F	456	ILE	3.2
1	F	449	TYR	3.2
1	A	27	ARG	3.2
1	F	306	ASP	3.2
1	F	284	SER	3.2
1	F	301	ARG	3.2
1	F	587	LEU	3.2
1	F	444	VAL	3.1
1	F	541	GLN	3.1
1	F	475	GLU	3.1
1	A	28	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	477	LEU	3.1
1	F	464	THR	3.1
3	H	652	LEU	3.0
2	G	160	HIS	3.0
3	H	635	ALA	3.0
1	F	519	TYR	3.0
1	A	477	LEU	3.0
1	F	288	GLU	3.0
1	F	164	MET	3.0
2	G	284	LYS	3.0
1	A	348	ALA	3.0
3	C	692	GLU	3.0
1	F	305	TYR	2.9
1	F	289	GLN	2.9
1	F	549	GLN	2.9
1	F	298	PHE	2.9
1	F	455	SER	2.9
1	F	534	THR	2.9
2	G	159	SER	2.9
1	A	29	LEU	2.9
1	F	453	PHE	2.8
3	H	606	VAL	2.8
1	F	84	THR	2.8
1	F	523	PRO	2.8
1	F	629	ILE	2.8
3	H	648	ILE	2.8
3	H	639	PHE	2.8
3	H	608	GLU	2.8
3	H	644	GLY	2.8
3	H	600	ILE	2.8
3	H	579	MET	2.7
1	F	547	PHE	2.7
3	H	626	PHE	2.7
1	F	274	THR	2.7
1	F	460	LEU	2.7
2	B	126	CYS	2.7
1	F	615	LEU	2.7
2	G	282	PRO	2.7
3	H	633	ASN	2.6
1	A	31	ARG	2.6
1	F	474	LYS	2.6
3	H	613	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	515	SER	2.6
1	F	570	LYS	2.6
1	F	674	PHE	2.5
1	A	32	LEU	2.5
1	F	96	HIS	2.5
1	F	476	SER	2.5
1	F	714	LYS	2.5
2	G	275	LYS	2.5
1	F	614	HIS	2.5
3	H	673	SER	2.5
1	F	297	LEU	2.5
3	H	668	LEU	2.5
1	F	625	TRP	2.5
3	H	678	VAL	2.5
1	F	472	ALA	2.5
4	I	28	SER	2.5
1	F	742	ARG	2.5
1	F	626	GLY	2.5
3	H	693	SER	2.4
1	A	22	GLU	2.4
1	F	520	ASN	2.4
4	I	23	LYS	2.4
3	H	664	HIS	2.4
1	F	80	LEU	2.4
1	F	163	GLU	2.4
1	F	532	ASP	2.4
2	B	441	ARG	2.4
1	F	287	ARG	2.4
3	H	569	ASP	2.4
1	A	141	GLU	2.3
1	F	451	ASN	2.3
4	I	24	ALA	2.3
1	F	729	TYR	2.3
3	H	580	GLU	2.3
1	A	156	GLY	2.3
2	G	133	ARG	2.3
1	A	429	SER	2.3
1	F	712	PHE	2.3
1	F	693	ASN	2.3
1	F	21	SER	2.3
2	B	69	SER	2.2
1	F	528	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	63	LEU	2.2
2	G	286	ASN	2.2
1	F	311	PRO	2.2
1	F	527	PRO	2.2
2	G	221	GLN	2.2
1	F	447	GLY	2.2
1	F	719	ALA	2.2
3	H	637	MET	2.2
1	A	433	GLU	2.2
1	F	290	SER	2.2
1	F	575	TYR	2.2
2	G	276	GLU	2.2
1	F	435	THR	2.2
1	F	646	LEU	2.2
1	F	720	GLY	2.1
1	F	670	LEU	2.1
1	F	627	THR	2.1
1	F	83	CYS	2.1
2	B	393	VAL	2.1
3	H	679	THR	2.1
1	F	628	PHE	2.1
1	F	285	VAL	2.1
2	G	162	LEU	2.1
1	F	530	PRO	2.1
2	G	394	GLU	2.1
1	F	308	PHE	2.1
2	G	279	ASP	2.0
3	H	568	SER	2.0
1	F	743	GLU	2.0
3	H	640	VAL	2.0
1	F	25	ARG	2.0
1	F	623	ALA	2.0
2	G	278	TYR	2.0
1	F	279	GLY	2.0
1	A	33	GLN	2.0
1	A	528	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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	SEP	H	583	10/11	0.97	0.21	109,111,117,120	0
5	M3L	E	27	12/13	0.97	0.22	27,32,47,47	0
5	M3L	J	27	12/13	0.98	0.23	56,59,65,65	0
3	SEP	C	583	10/11	0.99	0.15	27,40,42,45	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

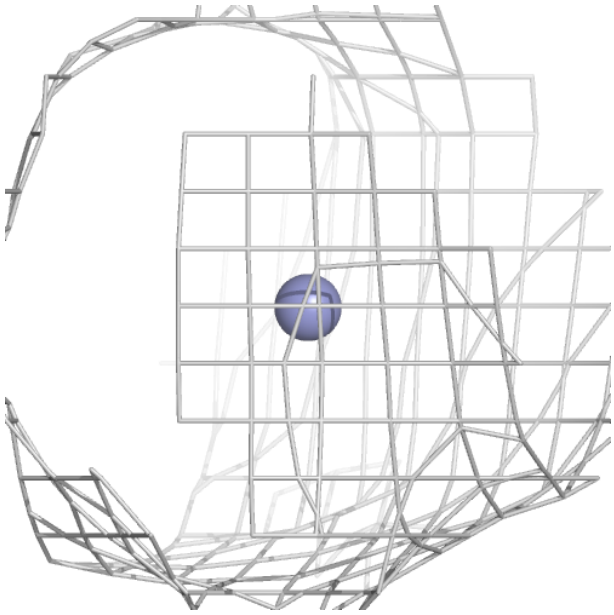
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

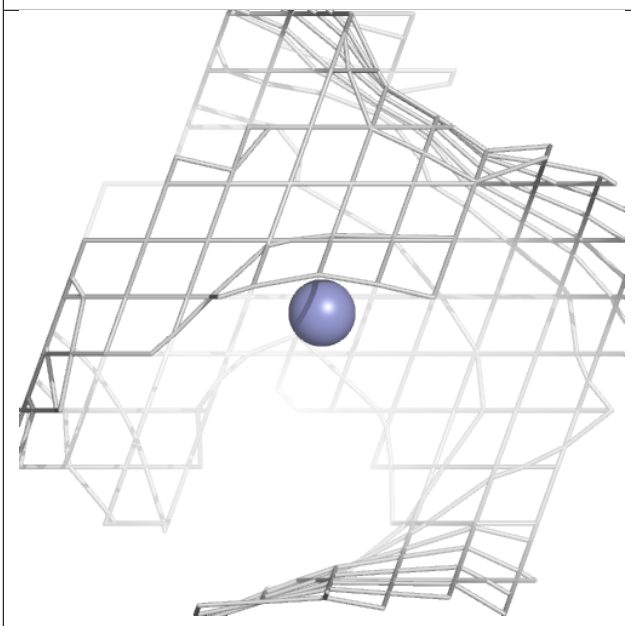
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	ZN	F	1002	1/1	0.41	0.16	189,189,189,189	0
7	SAM	F	1009	27/27	0.94	0.19	105,106,106,107	0
6	ZN	F	1005	1/1	0.95	0.06	188,188,188,188	0
6	ZN	F	1004	1/1	0.95	0.05	167,167,167,167	0
6	ZN	F	1003	1/1	0.97	0.04	159,159,159,159	0
7	SAM	A	1009	27/27	0.97	0.20	45,47,49,50	0
6	ZN	F	1001	1/1	0.97	0.08	137,137,137,137	0
6	ZN	F	1006	1/1	0.98	0.09	137,137,137,137	0
6	ZN	F	1008	1/1	0.98	0.09	130,130,130,130	0
6	ZN	A	1001	1/1	0.99	0.14	33,33,33,33	0
6	ZN	A	1004	1/1	0.99	0.11	66,66,66,66	0
6	ZN	F	1007	1/1	0.99	0.05	132,132,132,132	0
6	ZN	A	1007	1/1	1.00	0.13	41,41,41,41	0
6	ZN	A	1008	1/1	1.00	0.14	37,37,37,37	0
6	ZN	A	1003	1/1	1.00	0.12	47,47,47,47	0
6	ZN	A	1002	1/1	1.00	0.10	48,48,48,48	0
6	ZN	A	1005	1/1	1.00	0.11	55,55,55,55	0
6	ZN	A	1006	1/1	1.00	0.14	37,37,37,37	0

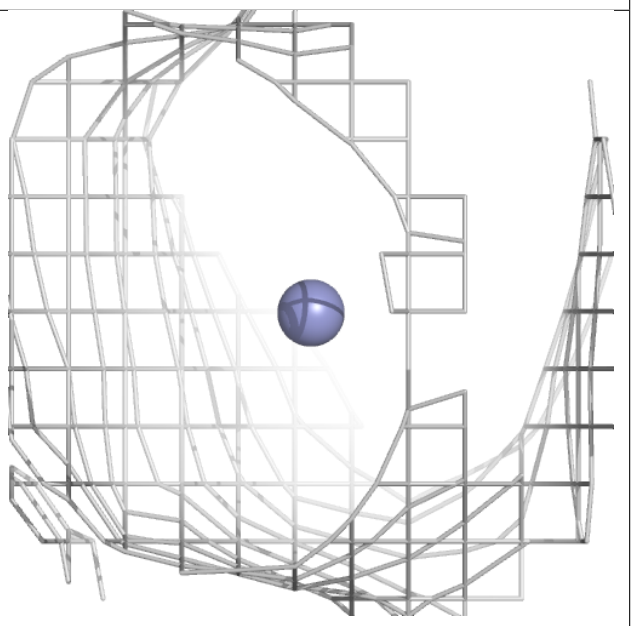
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ZN F 1002:

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

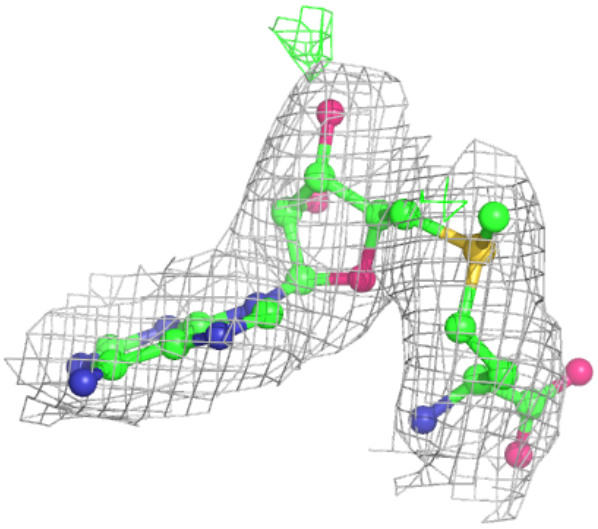


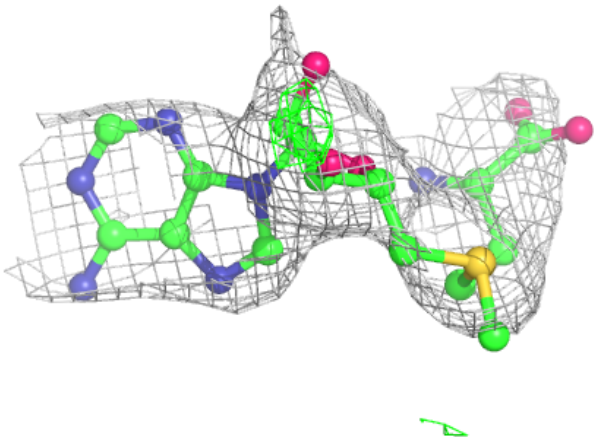


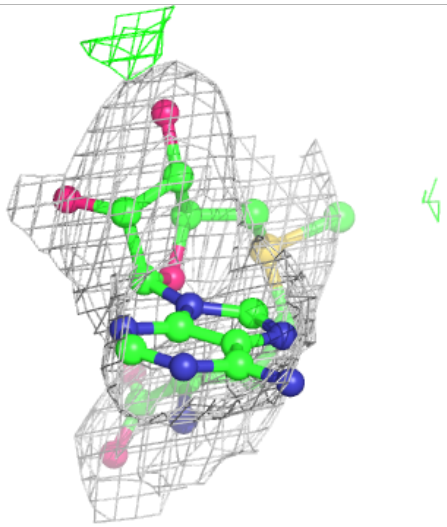


Electron density around SAM F 1009:

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

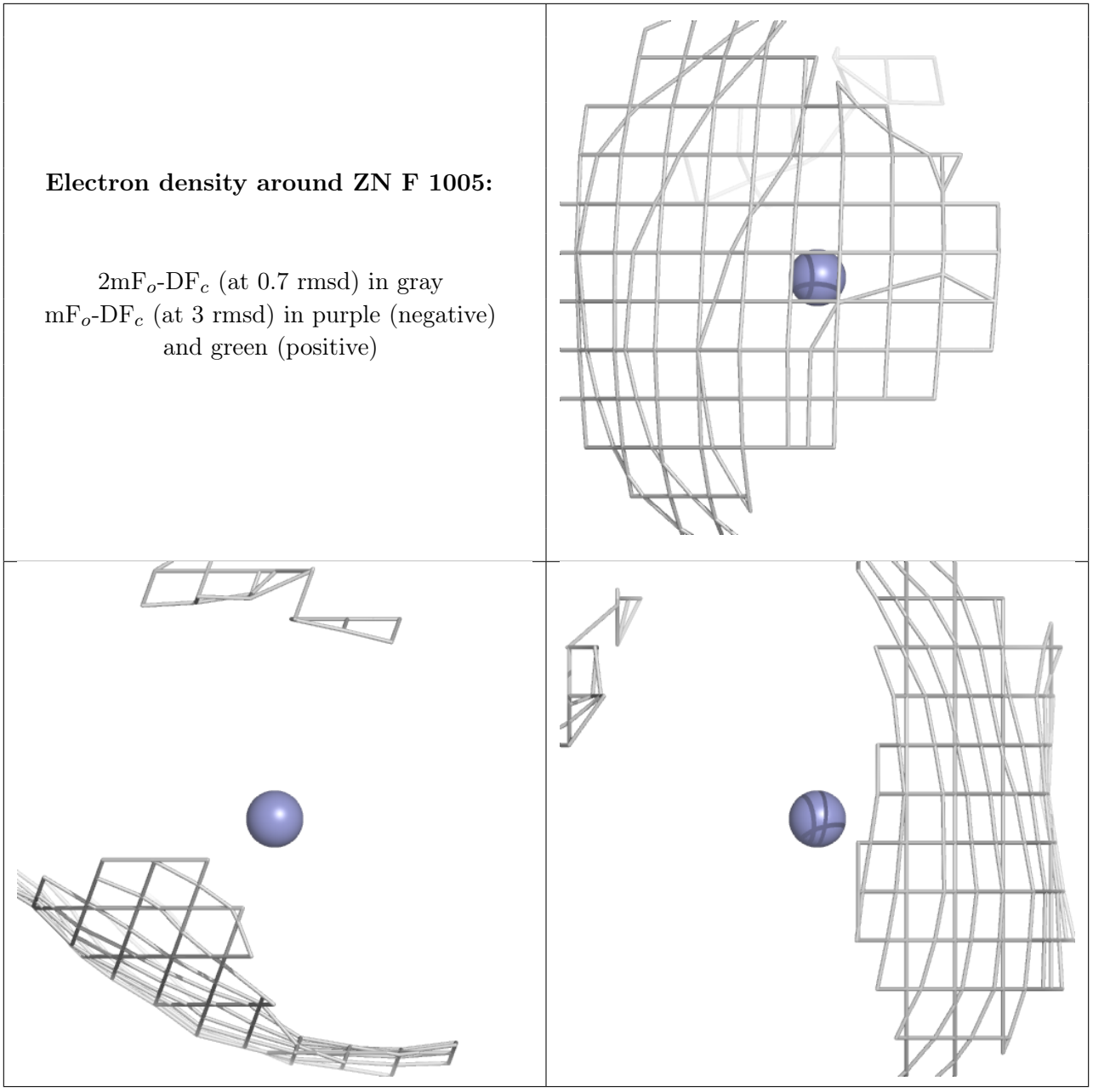






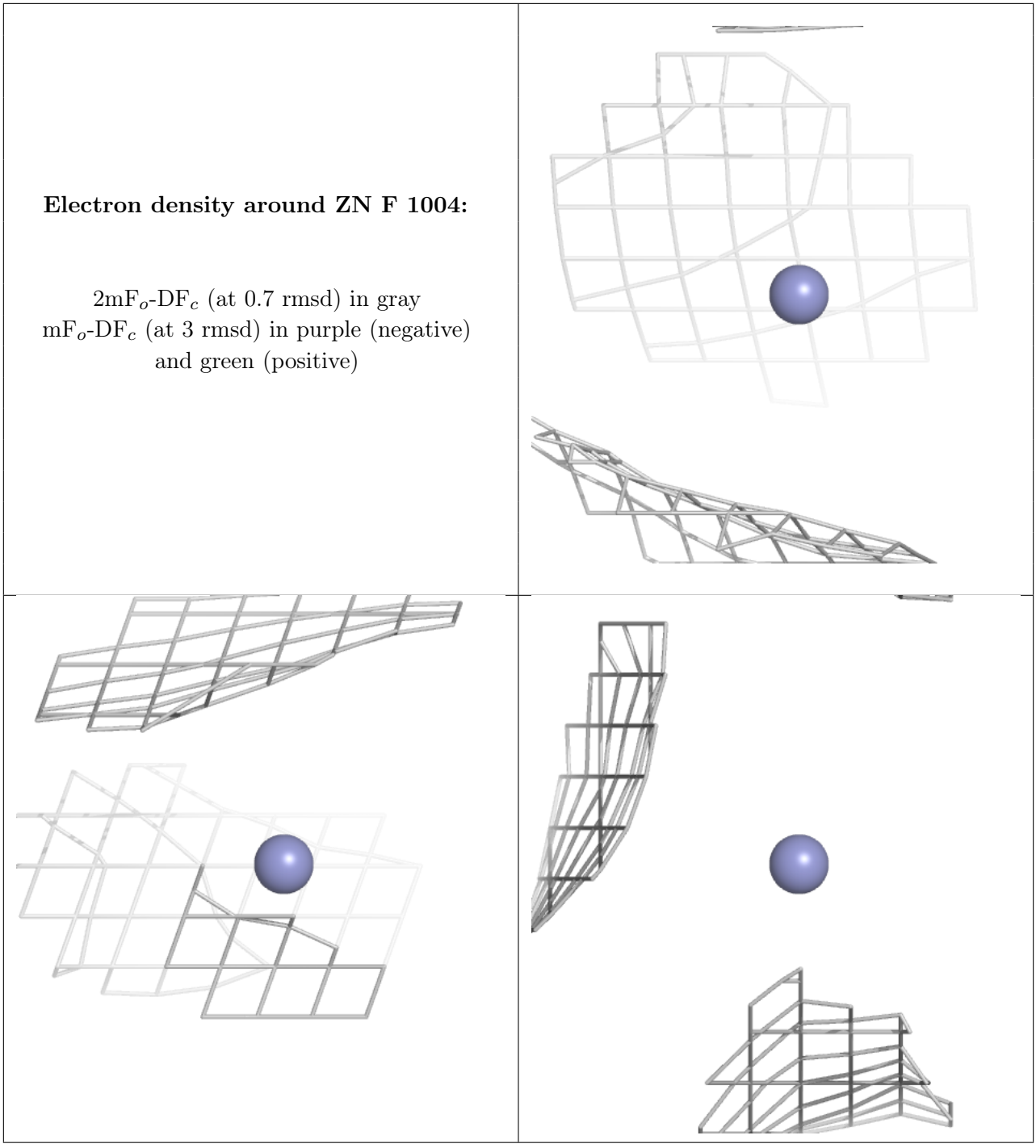
Electron density around ZN F 1005:

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



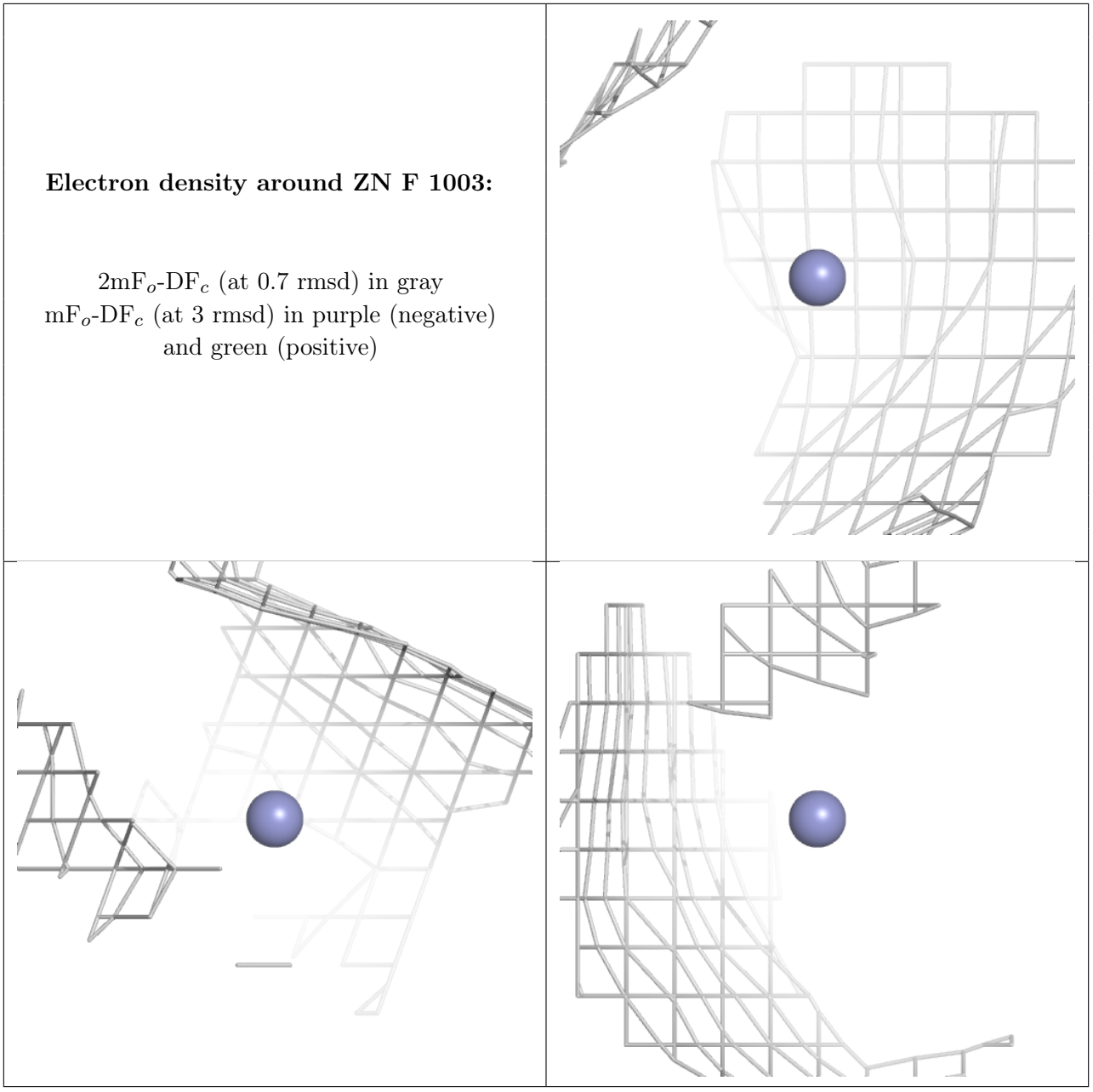
Electron density around ZN F 1004:

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



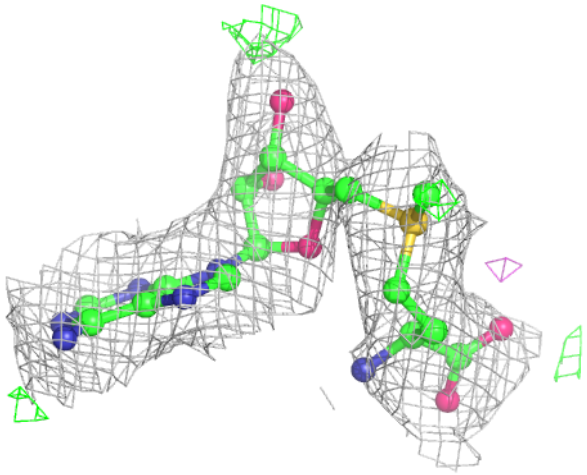
Electron density around ZN F 1003:

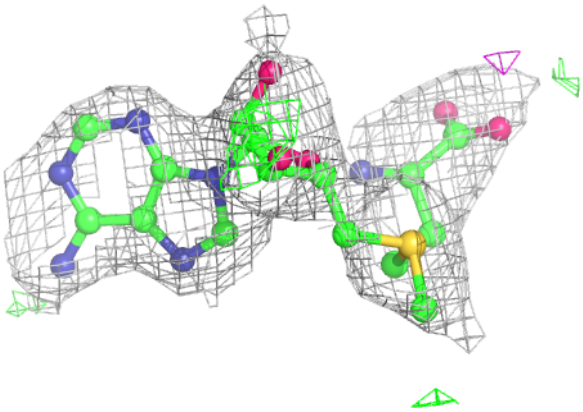
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

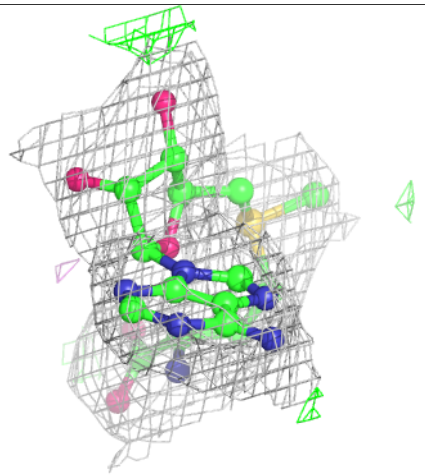


Electron density around SAM A 1009:

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

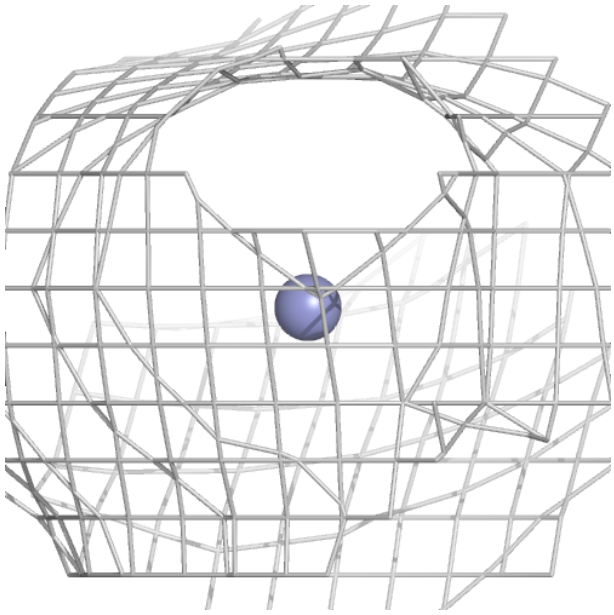


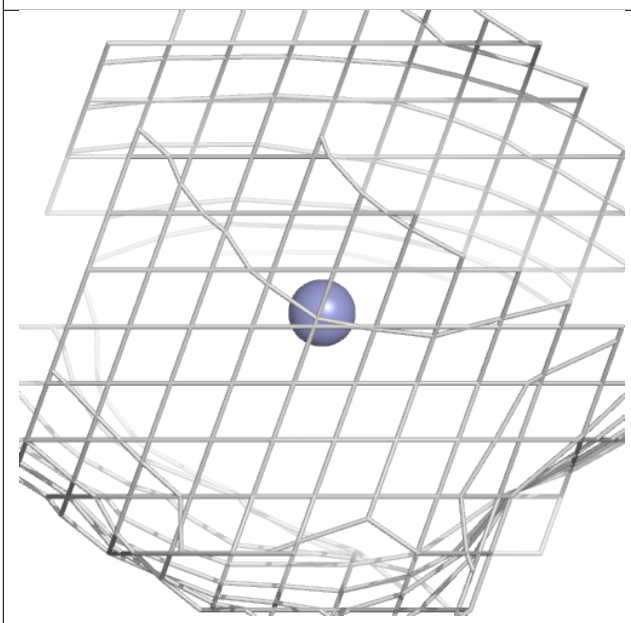


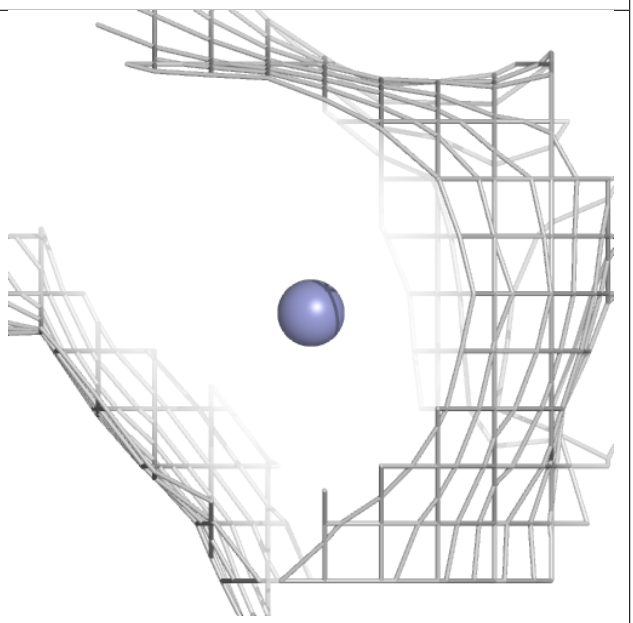


Electron density around ZN F 1001:

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

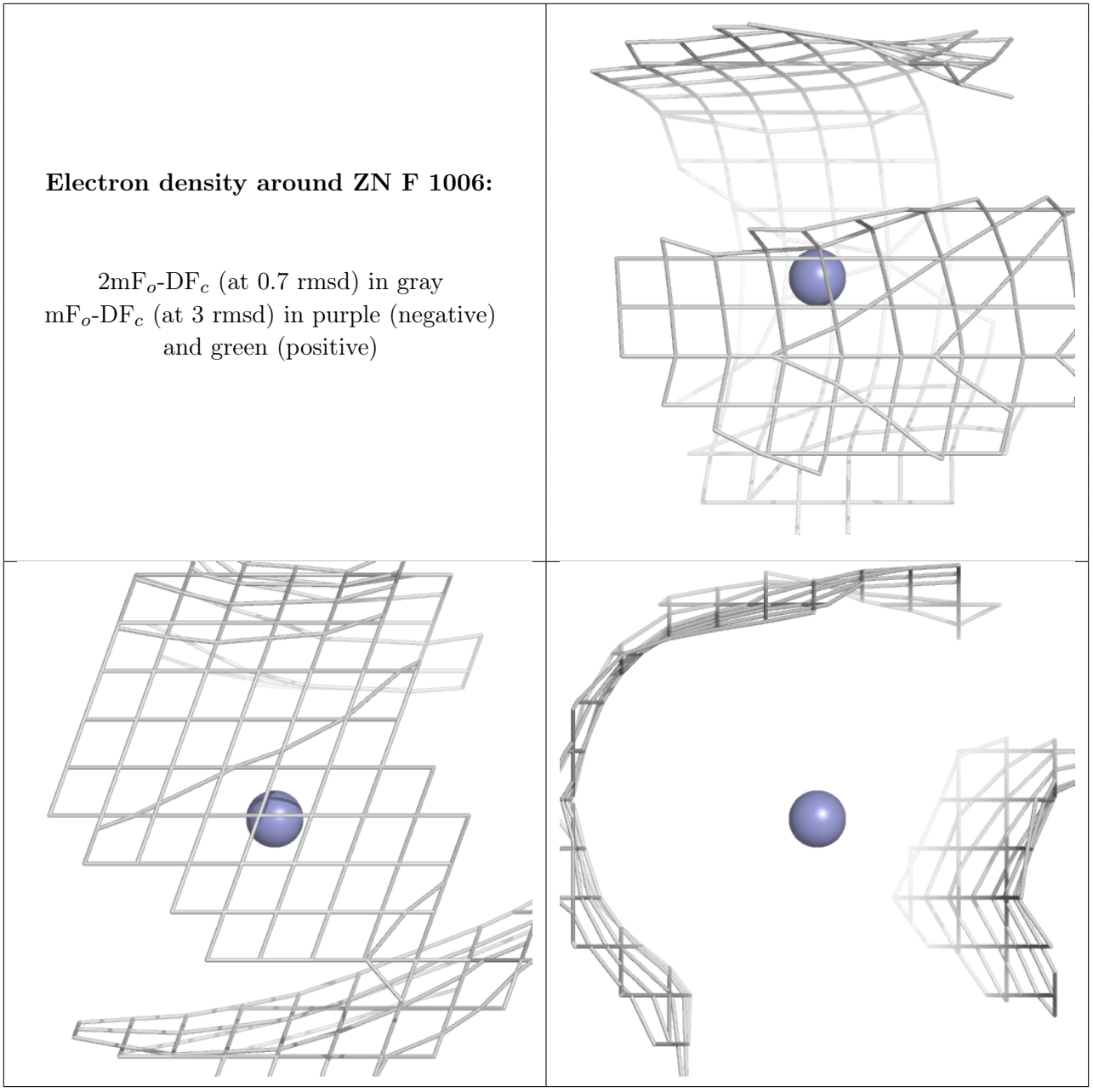






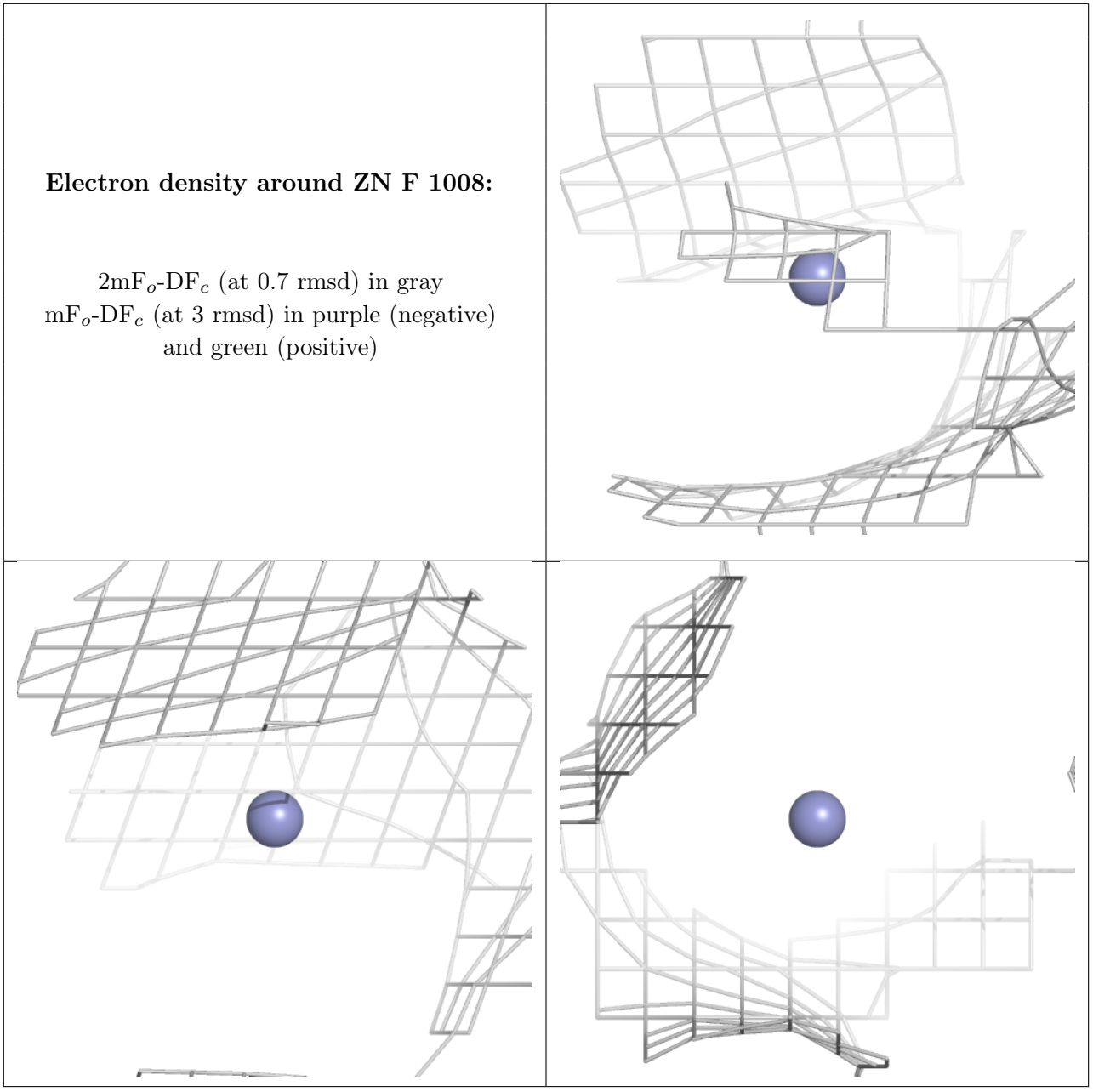
Electron density around ZN F 1006:

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



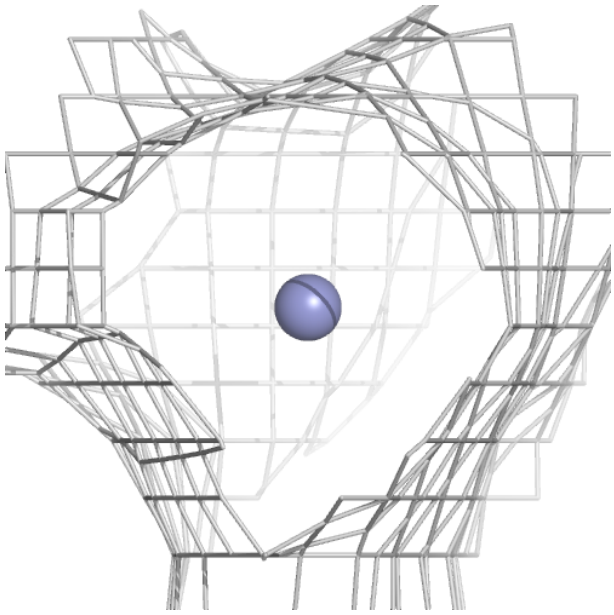
Electron density around ZN F 1008:

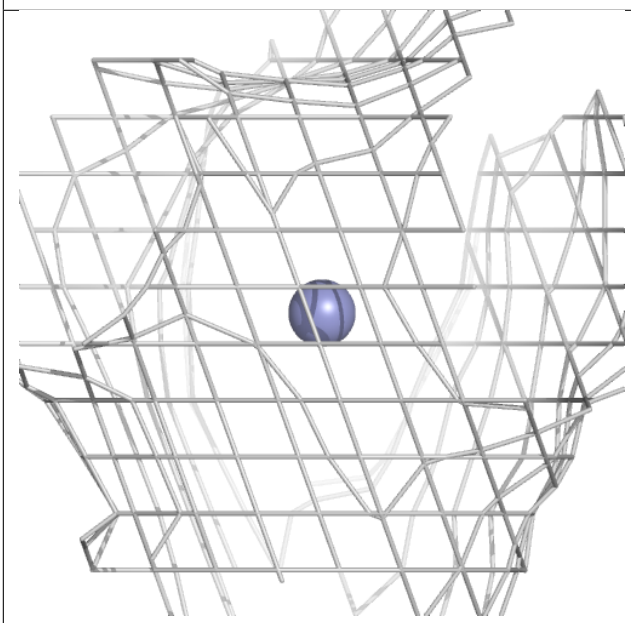
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

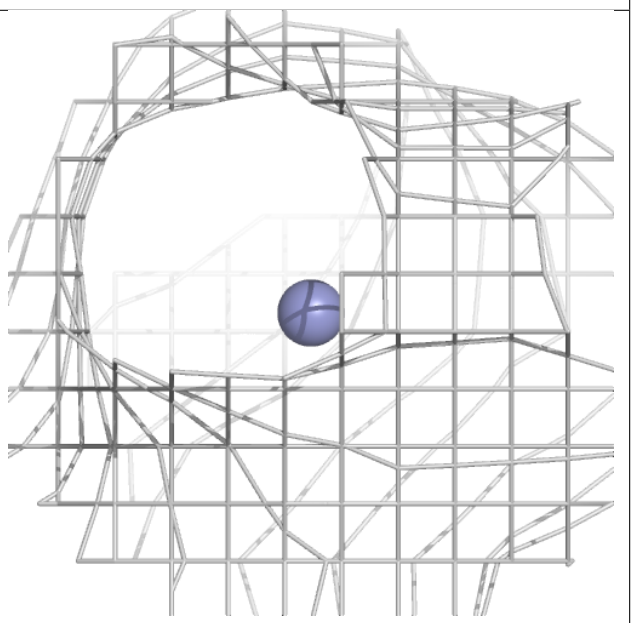


Electron density around ZN A 1001:

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

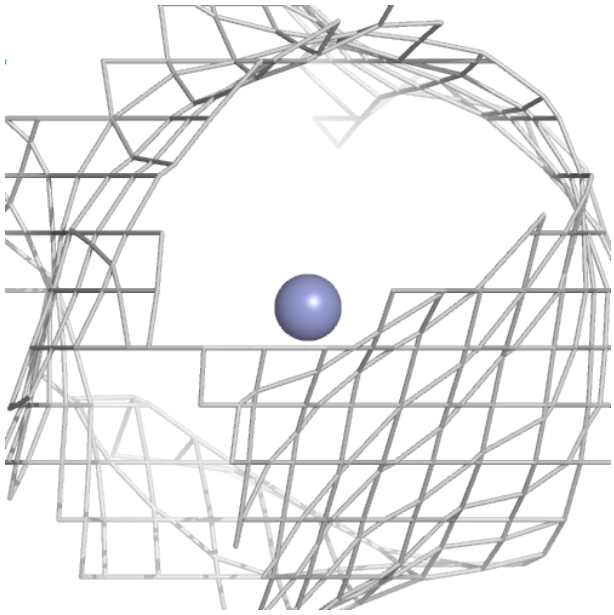


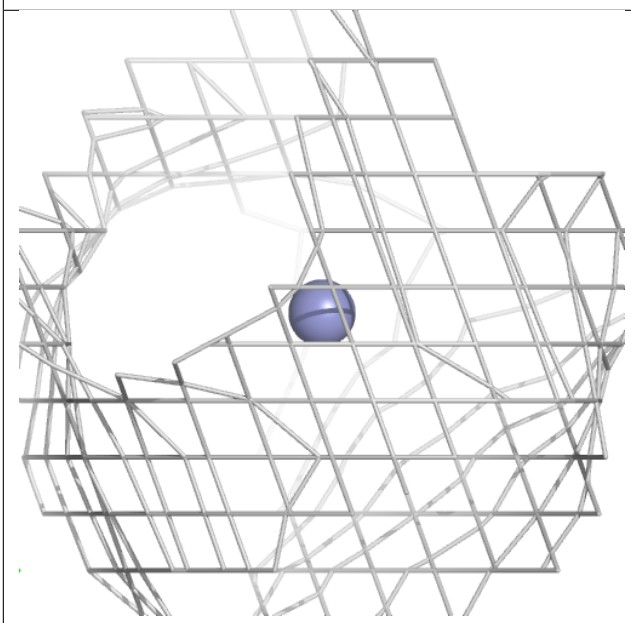


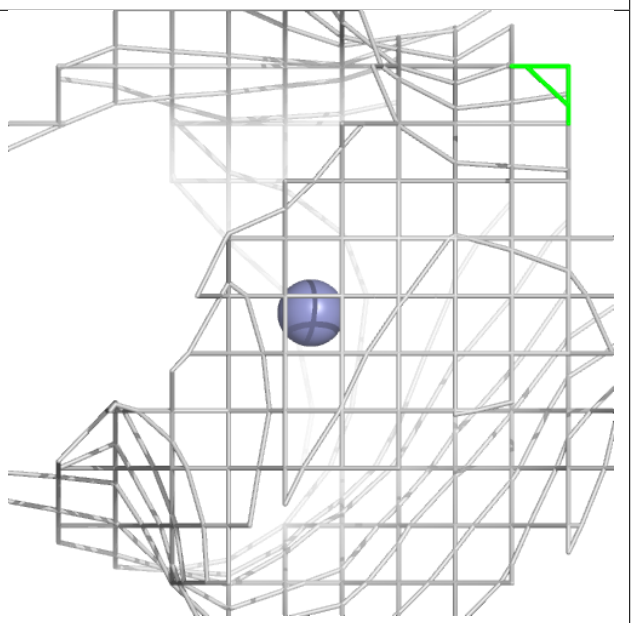


Electron density around ZN A 1004:

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

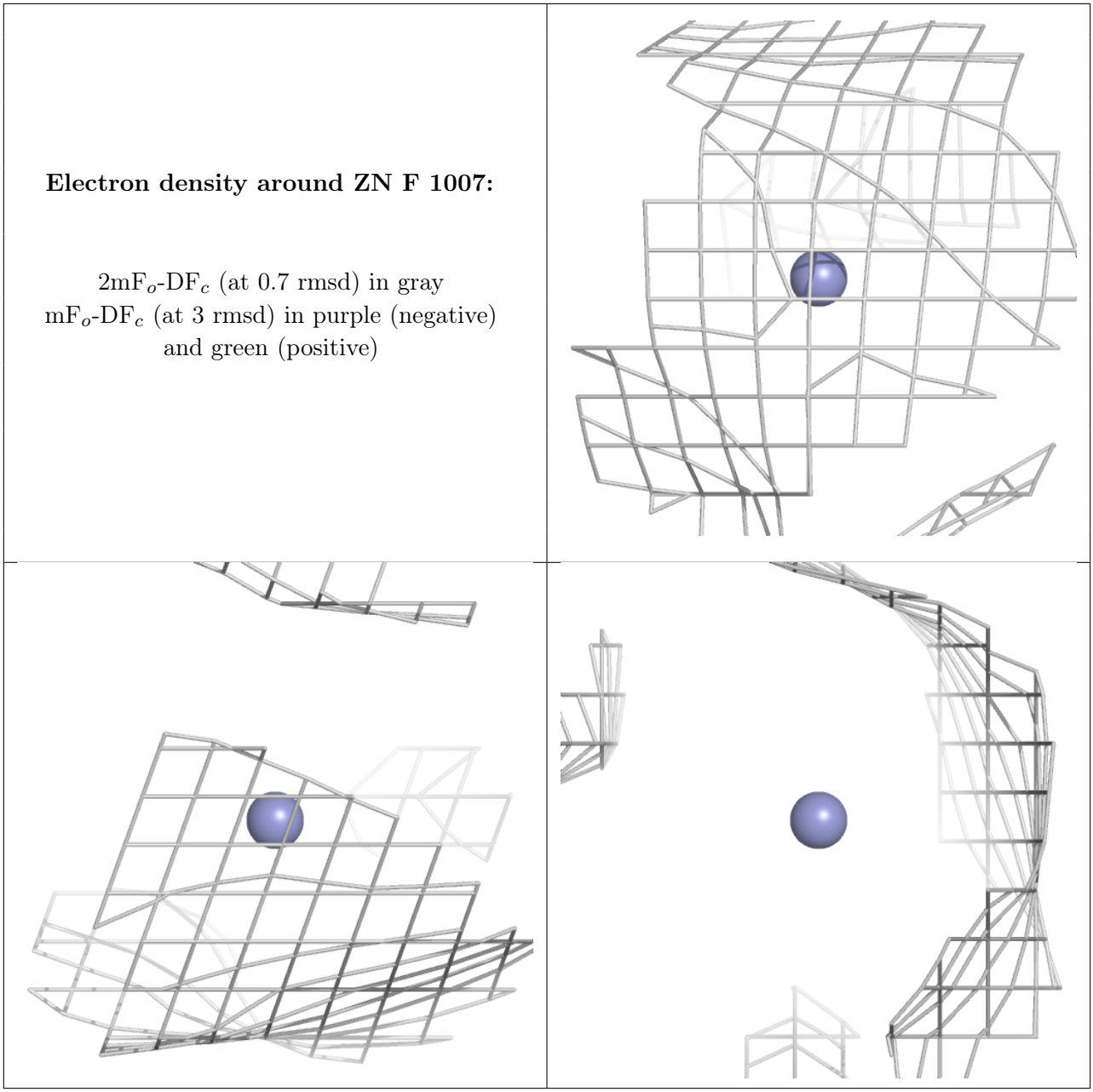






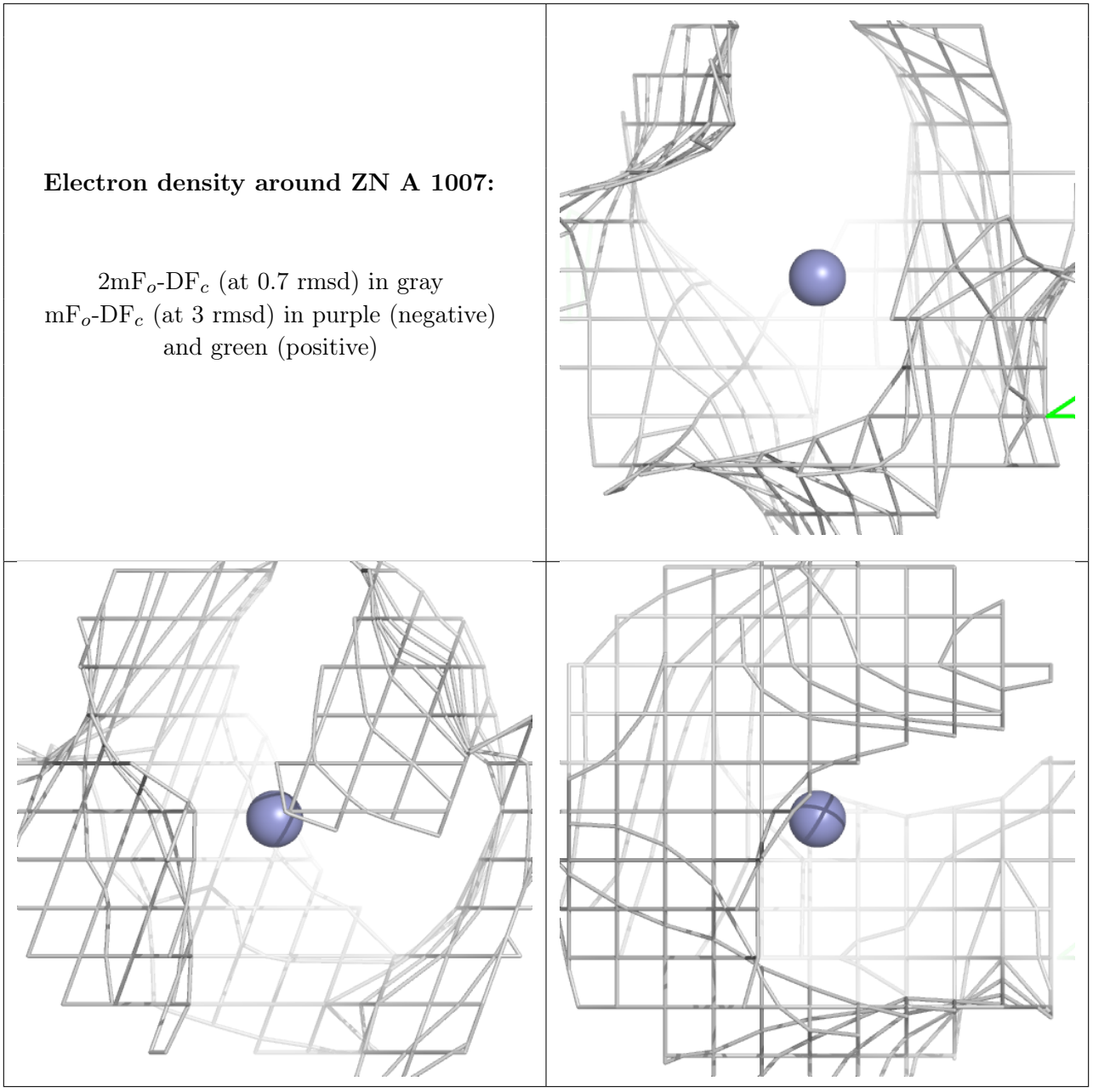
Electron density around ZN F 1007:

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



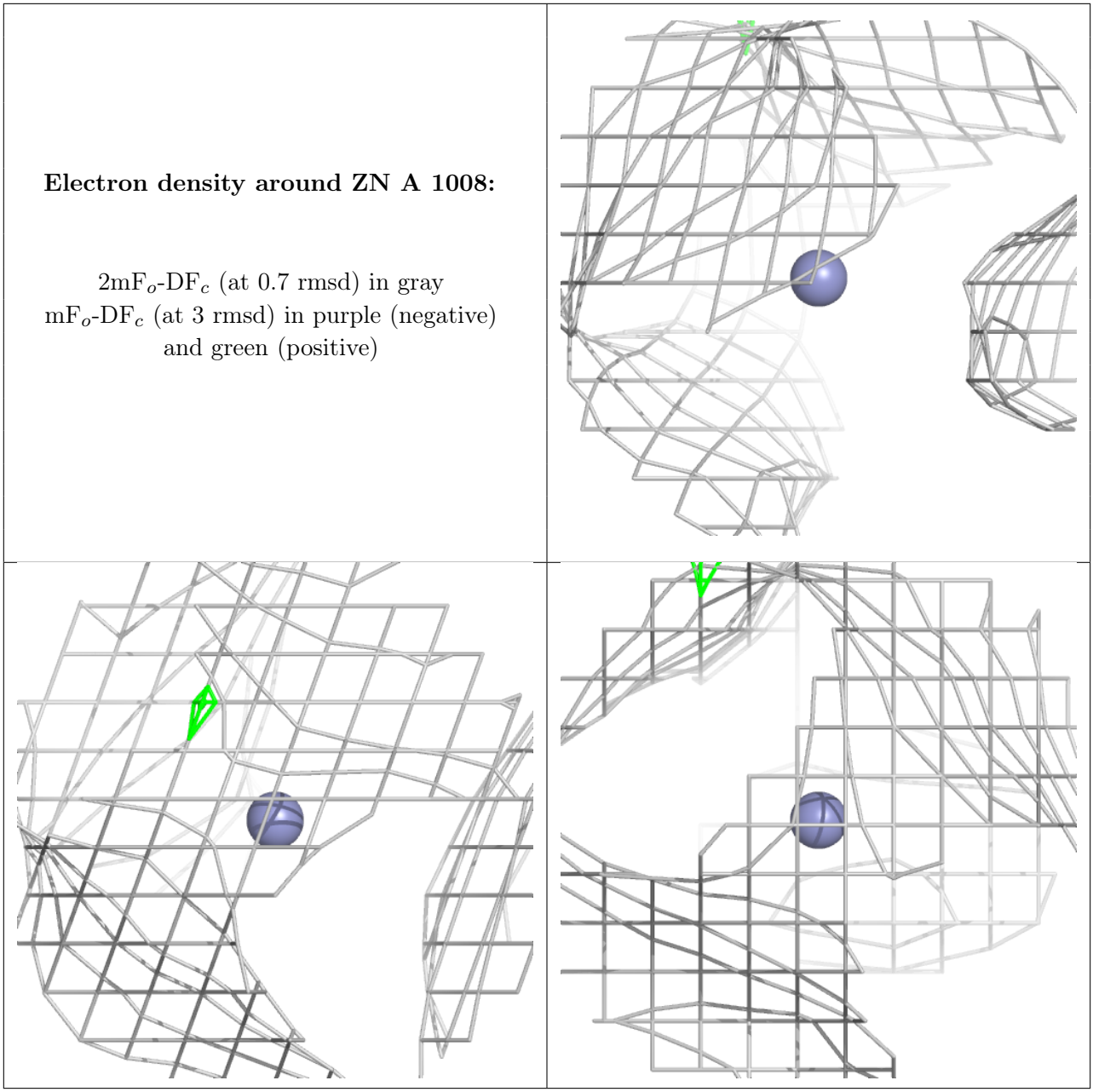
Electron density around ZN A 1007:

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



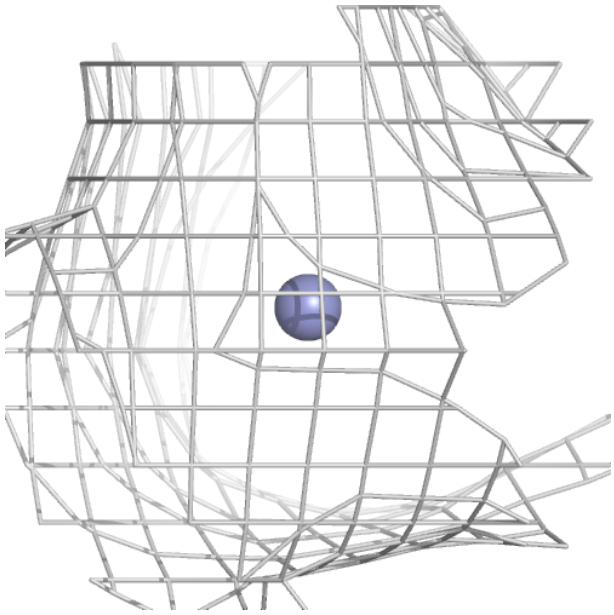
Electron density around ZN A 1008:

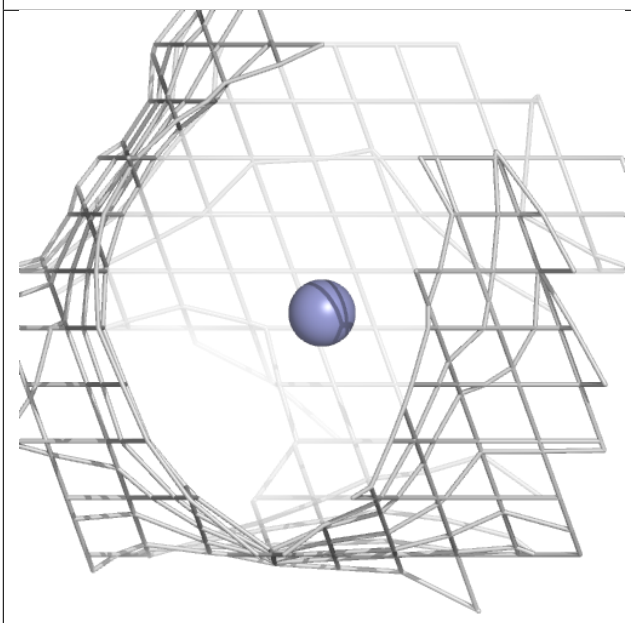
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

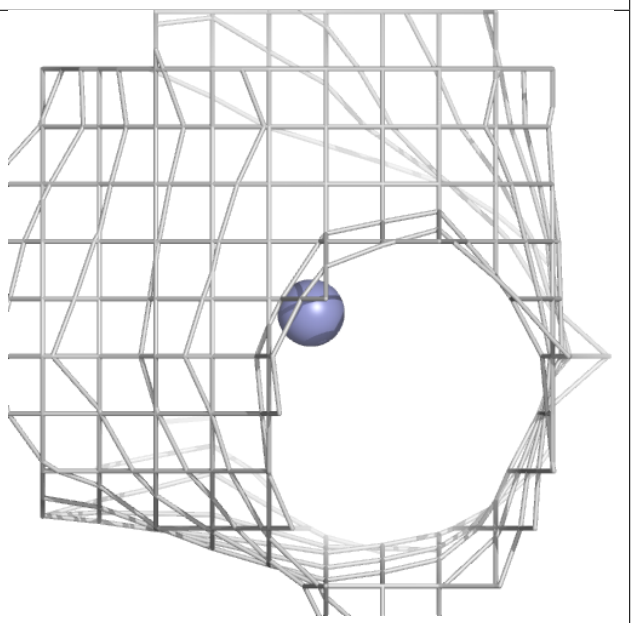


Electron density around ZN A 1003:

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

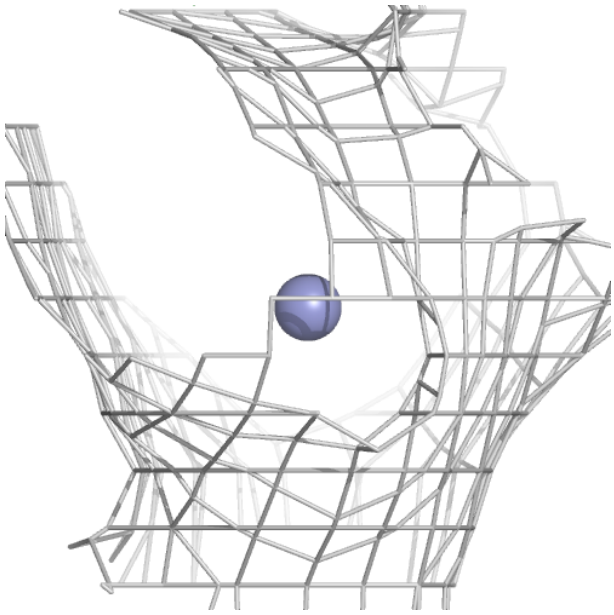


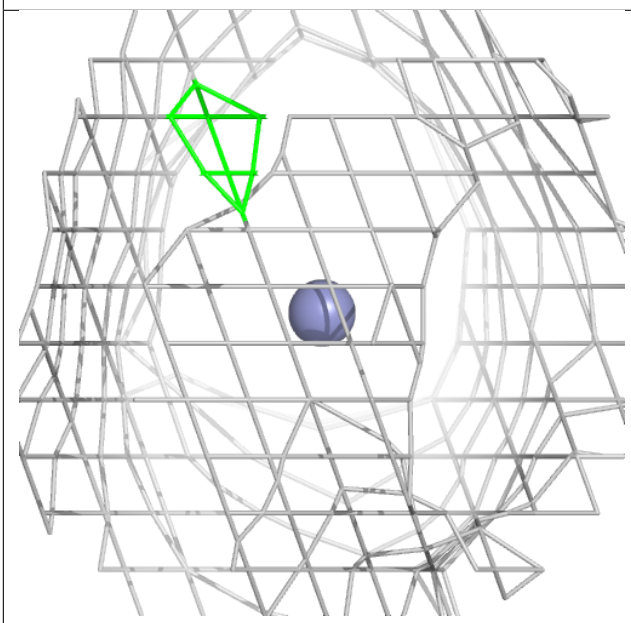


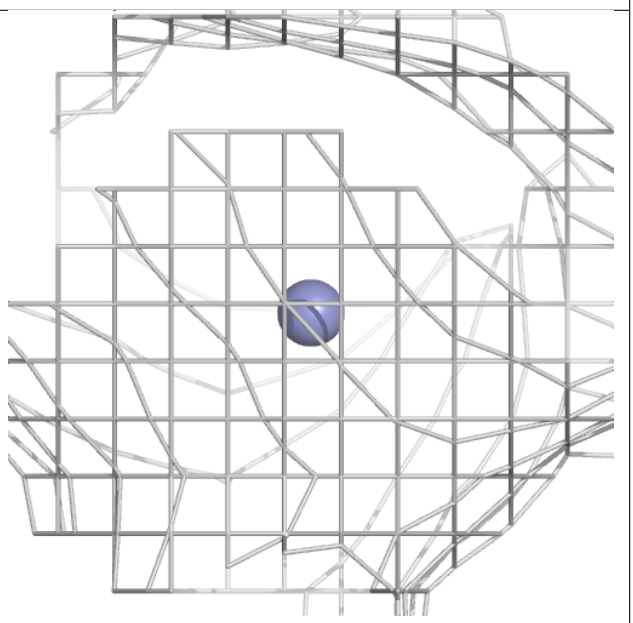


Electron density around ZN A 1002:

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

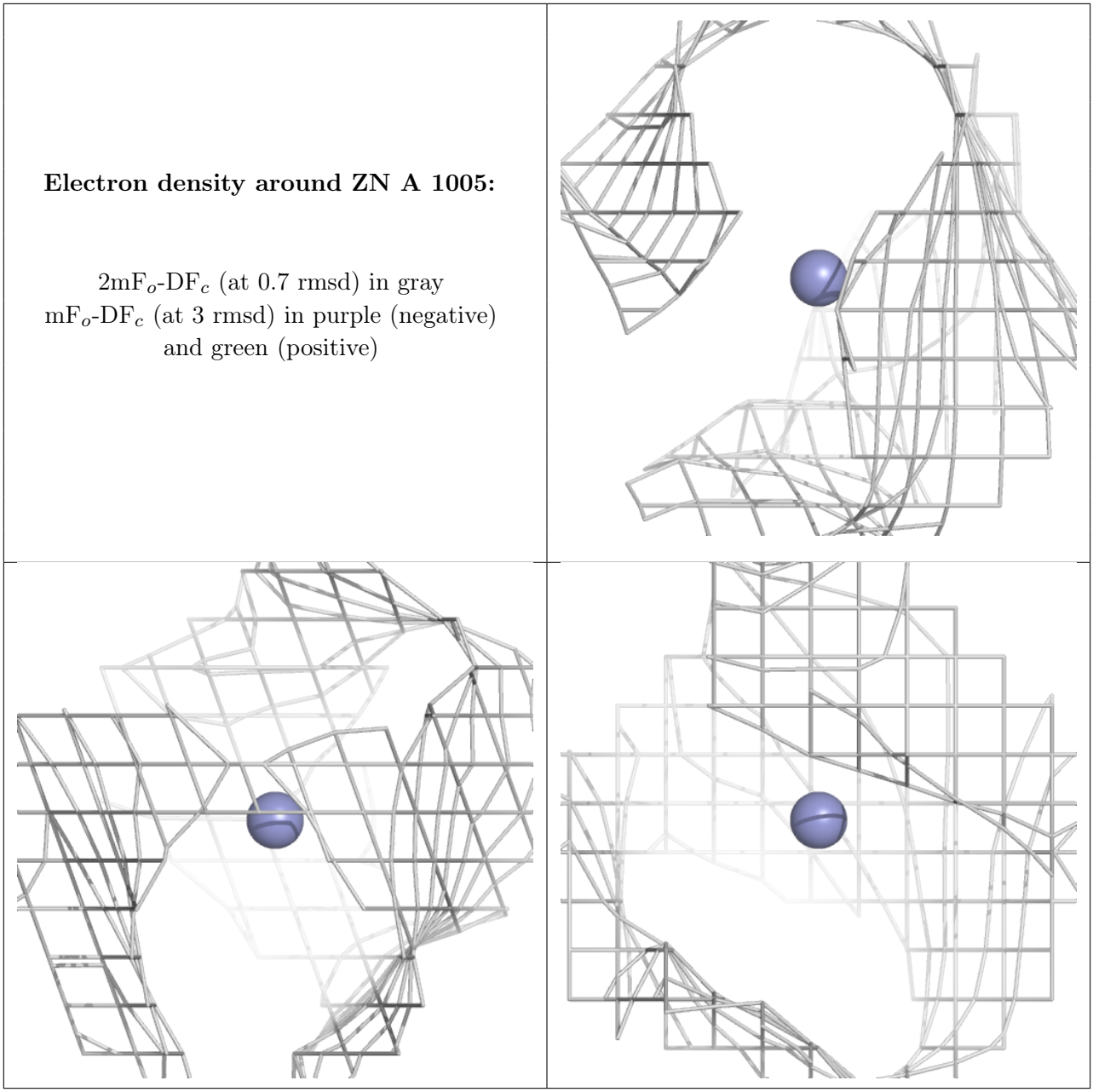






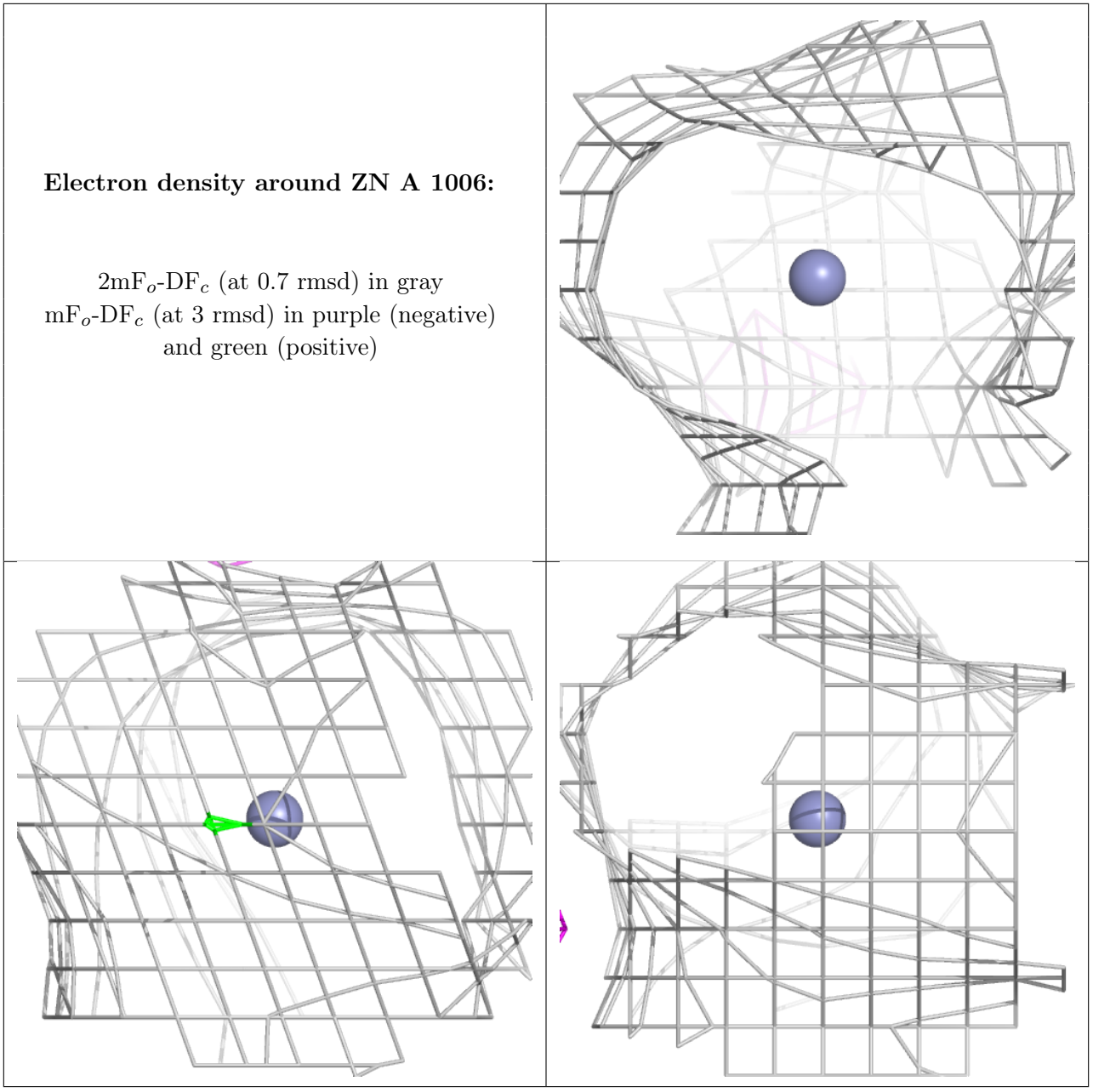
Electron density around ZN A 1005:

$2mF_o$-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 1006:

$2mF_o$-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.