Full wwPDB X-ray Structure Validation Report (i)

Nov 16, 2023 – 07:31 AM JST

PDB ID	:	6L7T
Title	:	Crystal structure of FKRP in complex with Mg ion, Zinc low remote data
Authors	:	Kuwabara, N.
Deposited on	:	2019-11-03
Resolution	:	2.41 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

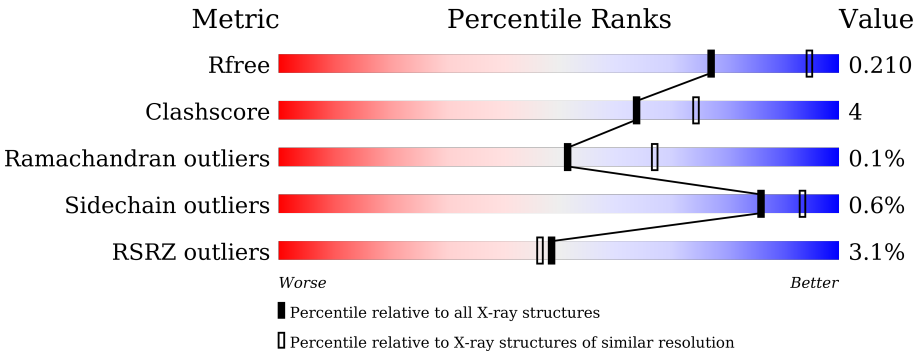
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.41 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	4647 (2.44-2.40)
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)
RSRZ outliers	127900	4543 (2.44-2.40)

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	455	2% 86% 11% ·
1	B	455	5% 89% 8% ·
1	C	455	2% 87% 10% ·
1	D	455	2% 85% 9% 5%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 14642 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 Fukutin-related protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	0	0	0
			3410	2188	603	610	9			
1	B	445	Total	C	N	O	S	0	0	0
			3424	2196	602	617	9			
1	C	441	Total	C	N	O	S	0	0	0
			3410	2190	602	609	9			
1	D	430	Total	C	N	O	S	0	1	0
			3318	2128	584	597	9			

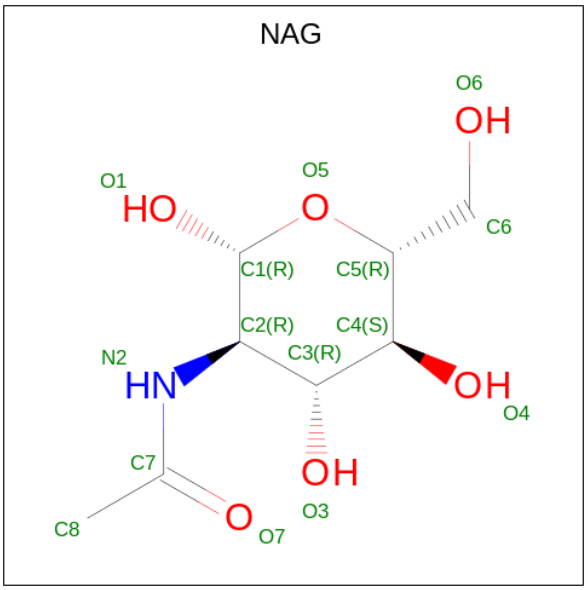
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	41	GLY	-	expression tag	UNP Q9H9S5
A	42	GLY	-	expression tag	UNP Q9H9S5
A	43	ARG	-	expression tag	UNP Q9H9S5
A	44	PRO	-	expression tag	UNP Q9H9S5
B	41	GLY	-	expression tag	UNP Q9H9S5
B	42	GLY	-	expression tag	UNP Q9H9S5
B	43	ARG	-	expression tag	UNP Q9H9S5
B	44	PRO	-	expression tag	UNP Q9H9S5
C	41	GLY	-	expression tag	UNP Q9H9S5
C	42	GLY	-	expression tag	UNP Q9H9S5
C	43	ARG	-	expression tag	UNP Q9H9S5
C	44	PRO	-	expression tag	UNP Q9H9S5
D	41	GLY	-	expression tag	UNP Q9H9S5
D	42	GLY	-	expression tag	UNP Q9H9S5
D	43	ARG	-	expression tag	UNP Q9H9S5
D	44	PRO	-	expression tag	UNP Q9H9S5

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	C	1	Total C N O 14 8 1 5	0	0
3	D	1	Total C N O 14 8 1 5	0	0
3	D	1	Total C N O 14 8 1 5	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	B	2	Total Mg 2 2	0	0
4	C	1	Total Mg 1 1	0	0
4	D	2	Total Mg 2 2	0	0

- Molecule 5 is water.

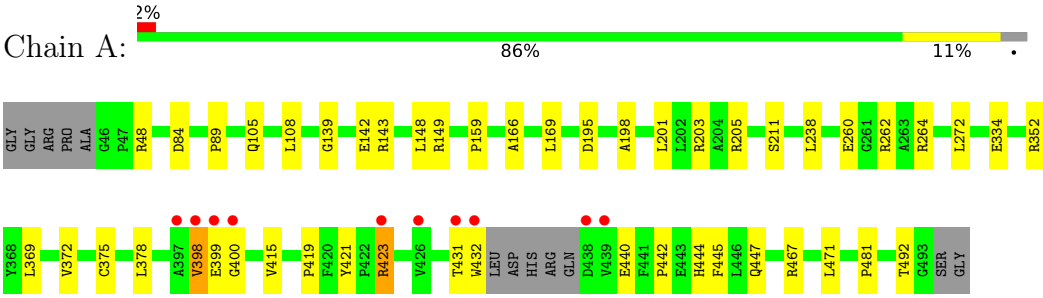
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	273	Total O 273 273	0	0
5	B	202	Total O 202 202	0	0
5	C	266	Total O 266 266	0	0
5	D	231	Total O 231 231	0	0

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.

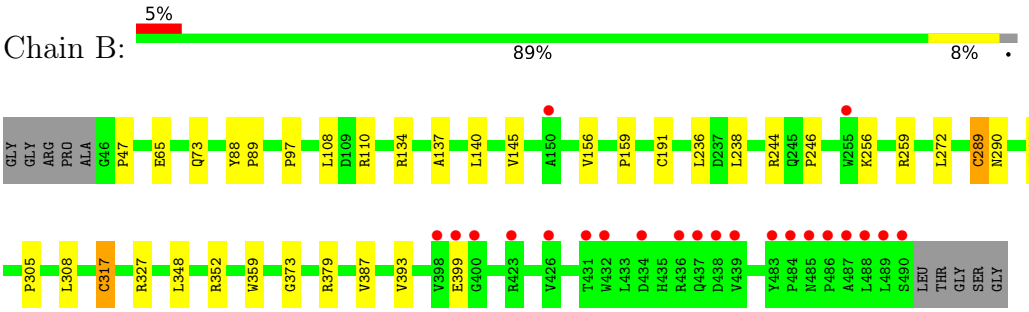
• Molecule 1: Fukutin-related protein

Chain A:



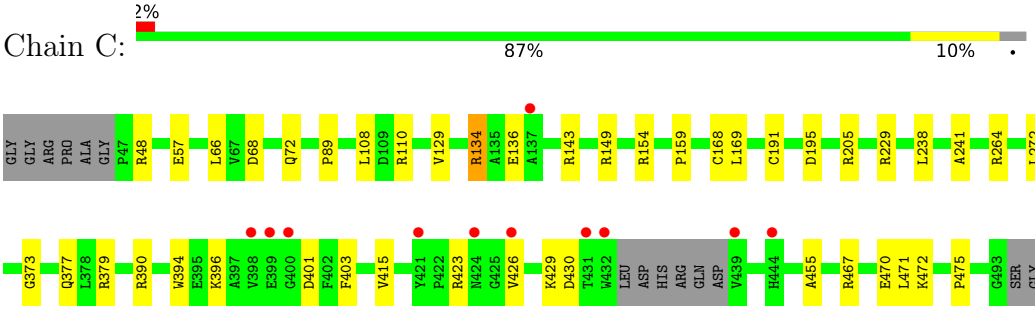
• Molecule 1: Fukutin-related protein

Chain B:



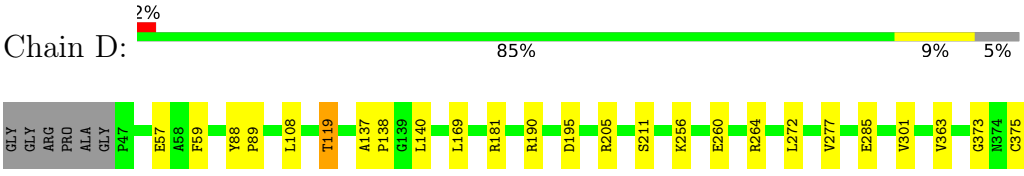
• Molecule 1: Fukutin-related protein

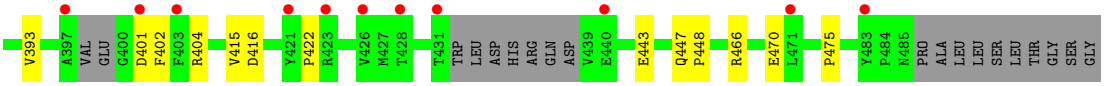
Chain C:



• Molecule 1: Fukutin-related protein

Chain D:




V393
A397
VAL
GLU
G400
D401
F402
F403
R404
V415
D416
Y421
P422
R423
V426
M427
T428
T431
TRP
LEU
ASP
HIS
ARG
GLN
ASP
V439
E440
E443
Q447
P448
R466
E470
L471
P475
Y483
P484
N485
PRO
ALA
LEU
LEU
SER
LEU
THR
GLY
SER
GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	77.00Å 119.48Å 257.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.05 – 2.41 49.05 – 2.41	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.05-2.41) 99.6 (49.05-2.41)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.35 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.178 , 0.210 0.178 , 0.210	Depositor DCC
R_{free} test set	4583 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	40.7	Xtriage
Anisotropy	0.561	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 48.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14642	wwPDB-VP
Average B, all atoms (Å^2)	49.0	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 22.26 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.9057e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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, NAG, MG

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	0.31	0/3504	0.52	0/4802
1	B	0.33	2/3520 (0.1%)	0.51	0/4826
1	C	0.30	0/3504	0.50	0/4798
1	D	0.30	0/3412	0.51	0/4674
All	All	0.31	2/13940 (0.0%)	0.51	0/19100

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	317	CYS	CB-SG	-5.86	1.72	1.81
1	B	289	CYS	CB-SG	-5.25	1.73	1.81

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	3410	0	3336	35	0
1	B	3424	0	3330	28	0
1	C	3410	0	3355	30	0
1	D	3318	0	3230	29	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	28	0	26	0	0
3	B	28	0	26	0	0
3	C	14	0	13	0	0
3	D	28	0	26	1	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
4	D	2	0	0	0	0
5	A	273	0	0	2	0
5	B	202	0	0	2	0
5	C	266	0	0	2	0
5	D	231	0	0	3	0
All	All	14642	0	13342	112	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 (112) 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:48:ARG:HH22	1:A:149:ARG:HH12	1.28	0.79
1:A:142:GLU:OE2	1:A:142:GLU:N	2.17	0.76
1:C:429:LYS:HG3	1:C:430:ASP:H	1.54	0.71
1:B:65:GLU:OE2	1:B:134:ARG:NH2	2.24	0.70
1:D:401:ASP:OD1	1:D:402:PHE:HD1	1.75	0.69
1:A:398:VAL:HG23	1:A:399:GLU:H	1.59	0.66
1:D:401:ASP:OD1	1:D:402:PHE:CD1	2.51	0.63
1:B:97:PRO:HB2	1:D:119:THR:HG23	1.84	0.60
1:C:136:GLU:HG3	1:C:241:ALA:HB3	1.84	0.59
1:C:373:GLY:O	1:C:379:ARG:NH1	2.34	0.59
1:A:432:TRP:HH2	1:A:440:GLU:HB3	1.68	0.58
1:C:134:ARG:HD3	1:C:136:GLU:OE2	2.04	0.57
1:D:375:CYS:HB3	1:D:378:LEU:HD13	1.87	0.57
1:D:363:VAL:HB	1:D:415:VAL:HG22	1.86	0.57
1:C:390:ARG:NH2	5:C:604:HOH:O	2.38	0.56
1:D:470:GLU:OE2	1:D:475:PRO:HA	2.06	0.56
1:A:48:ARG:NH2	1:A:149:ARG:HH12	2.02	0.55
1:A:139:GLY:O	1:A:143:ARG:HG2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:429:LYS:HG3	1:C:430:ASP:N	2.22	0.55
1:C:467:ARG:O	1:C:471:LEU:HG	2.07	0.54
1:B:137:ALA:HB3	1:B:140:LEU:HD11	1.89	0.54
1:C:89:PRO:HB3	1:D:301:VAL:HG21	1.90	0.54
1:A:262:ARG:NH2	5:A:604:HOH:O	2.34	0.54
1:A:169:LEU:HD11	1:A:195:ASP:HB2	1.89	0.53
1:C:363:VAL:HB	1:C:415:VAL:HG22	1.92	0.52
1:D:181:ARG:NH1	5:D:605:HOH:O	2.35	0.52
1:A:108:LEU:HD21	1:B:272:LEU:HD13	1.92	0.52
1:B:294:THR:HG22	1:B:295:ARG:O	2.09	0.52
1:B:387:VAL:HG22	1:B:393:VAL:HG22	1.92	0.52
1:C:169:LEU:HD11	1:C:195:ASP:HB2	1.92	0.52
1:D:205:ARG:HA	3:D:503:NAG:H83	1.92	0.51
1:B:289:CYS:HB2	1:B:317:CYS:HB2	1.91	0.51
1:D:401:ASP:OD1	1:D:401:ASP:N	2.41	0.51
1:C:108:LEU:HD21	1:D:272:LEU:HD13	1.92	0.50
1:A:159:PRO:HD2	1:A:238:LEU:O	2.11	0.50
1:A:375:CYS:HB3	1:A:378:LEU:HB2	1.93	0.50
1:C:57:GLU:OE2	1:C:264:ARG:NH2	2.45	0.50
1:C:159:PRO:HD2	1:C:238:LEU:O	2.12	0.50
1:A:421:TYR:HE2	1:A:423:ARG:HD2	1.77	0.50
1:D:256:LYS:O	1:D:260:GLU:HG2	2.12	0.49
1:D:169:LEU:HD11	1:D:195:ASP:HB2	1.95	0.49
1:C:136:GLU:HG3	1:C:241:ALA:CB	2.43	0.49
1:C:396:LYS:HD3	1:C:403:PHE:CE2	2.47	0.48
1:D:57:GLU:OE2	1:D:264:ARG:NH2	2.46	0.48
1:B:327:ARG:NH2	5:B:603:HOH:O	2.34	0.48
1:B:256:LYS:HZ2	1:B:259:ARG:HD3	1.77	0.48
1:A:442:PRO:HB2	1:A:444:HIS:NE2	2.29	0.48
1:B:305:PRO:HD2	1:B:308:LEU:HD12	1.95	0.48
1:A:352:ARG:CZ	1:A:481:PRO:HB3	2.44	0.48
1:A:363:VAL:HB	1:A:415:VAL:HG22	1.95	0.48
1:B:47:PRO:HB3	1:B:145:VAL:HG11	1.95	0.48
1:A:442:PRO:HB2	1:A:444:HIS:CD2	2.48	0.48
1:B:290:ASN:OD1	1:B:293:THR:HG23	2.14	0.48
1:A:369:LEU:O	1:A:372:VAL:HG13	2.14	0.47
1:C:66:LEU:HD11	1:C:129:VAL:HG12	1.96	0.47
1:C:470:GLU:HG2	1:C:475:PRO:HA	1.95	0.47
1:A:272:LEU:HD13	1:B:108:LEU:HD21	1.97	0.47
1:C:68:ASP:O	1:C:72:GLN:HG3	2.14	0.47
1:A:432:TRP:CH2	1:A:440:GLU:HB3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:LYS:CE	1:B:259:ARG:HD3	2.44	0.47
1:D:137:ALA:HB3	1:D:140:LEU:HD11	1.97	0.47
1:C:377:GLN:HB3	1:C:394:TRP:CD2	2.50	0.46
1:B:134:ARG:NH2	1:B:244:ARG:HD2	2.30	0.46
1:A:444:HIS:HA	1:A:447:GLN:HG3	1.96	0.46
1:C:48:ARG:NH1	1:C:149:ARG:HH21	2.14	0.46
1:C:110:ARG:O	1:D:211:SER:HB2	2.15	0.46
1:C:401:ASP:O	1:C:429:LYS:NZ	2.29	0.46
1:A:89:PRO:HB3	1:B:301:VAL:HG21	1.97	0.45
1:B:244:ARG:O	1:B:246:PRO:HD3	2.16	0.45
1:D:466:ARG:O	1:D:470:GLU:HG3	2.17	0.45
1:A:334:GLU:OE2	5:A:601:HOH:O	2.21	0.45
1:D:190:ARG:NH2	5:D:608:HOH:O	2.43	0.44
1:D:404:ARG:HH21	1:D:416:ASP:CG	2.20	0.44
1:A:203:ARG:HD3	1:A:205:ARG:NH2	2.32	0.44
1:B:73:GLN:NE2	5:B:601:HOH:O	2.25	0.44
1:A:84:ASP:O	1:A:105:GLN:HB3	2.18	0.44
1:A:166:ALA:CB	1:A:198:ALA:HB2	2.48	0.44
1:B:373:GLY:O	1:B:379:ARG:HD3	2.17	0.43
1:B:159:PRO:HD2	1:B:238:LEU:O	2.18	0.43
1:A:211:SER:HB2	1:B:110:ARG:O	2.18	0.43
1:C:205:ARG:HA	1:C:205:ARG:HD2	1.64	0.43
1:B:88:TYR:HA	1:B:89:PRO:C	2.39	0.43
1:C:264:ARG:HD3	5:C:772:HOH:O	2.18	0.43
1:C:423:ARG:O	1:C:426:VAL:HG12	2.19	0.43
1:A:492:THR:HG22	1:C:229:ARG:HA	2.01	0.42
1:C:143:ARG:CZ	1:C:238:LEU:HD21	2.48	0.42
1:D:59:PHE:CE2	1:D:256:LYS:HD2	2.54	0.42
1:D:447:GLN:HA	1:D:448:PRO:HA	1.82	0.42
1:D:466:ARG:NH1	5:D:602:HOH:O	2.27	0.42
1:B:289:CYS:SG	1:B:295:ARG:HA	2.59	0.42
1:D:422:PRO:HB3	1:D:443:GLU:OE1	2.19	0.42
1:B:308:LEU:HD21	1:B:359:TRP:HB2	2.01	0.42
1:B:256:LYS:NZ	1:B:259:ARG:HD3	2.34	0.42
1:D:88:TYR:HA	1:D:89:PRO:C	2.39	0.42
1:A:148:LEU:HD22	1:A:201:LEU:HD23	2.01	0.42
1:D:373:GLY:O	1:D:379:ARG:HD3	2.20	0.42
1:B:156:VAL:HB	1:B:236:LEU:HD11	2.02	0.42
1:C:154:ARG:HA	1:C:154:ARG:HD2	1.85	0.42
1:D:387:VAL:HG22	1:D:393:VAL:HG22	2.01	0.41
1:B:256:LYS:HE3	1:B:259:ARG:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:256:LYS:HB2	1:D:256:LYS:HE3	1.77	0.41
1:D:277:VAL:HB	1:D:285:GLU:HB2	2.01	0.41
1:C:323:ARG:HG2	1:C:455:ALA:HB1	2.02	0.41
1:A:166:ALA:HA	1:A:195:ASP:O	2.21	0.41
1:A:352:ARG:NH1	1:A:481:PRO:HB3	2.36	0.41
1:A:400:GLY:HA2	1:A:431:THR:HG21	2.03	0.41
1:B:348:LEU:HD21	1:B:352:ARG:NH2	2.36	0.40
1:A:367:ILE:O	1:A:419:PRO:HA	2.21	0.40
1:A:442:PRO:HG2	1:A:445:PHE:CE2	2.55	0.40
1:A:467:ARG:O	1:A:471:LEU:HD22	2.21	0.40
1:A:260:GLU:O	1:A:264:ARG:HG3	2.22	0.40
1:C:272:LEU:HD13	1:D:108:LEU:HD21	2.03	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	439/455 (96%)	425 (97%)	13 (3%)	1 (0%)	47	61
1	B	443/455 (97%)	432 (98%)	10 (2%)	1 (0%)	47	61
1	C	437/455 (96%)	429 (98%)	8 (2%)	0	100	100
1	D	425/455 (93%)	419 (99%)	6 (1%)	0	100	100
All	All	1744/1820 (96%)	1705 (98%)	37 (2%)	2 (0%)	51	67

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	399	GLU
1	A	398	VAL

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	341/357 (96%)	340 (100%)	1 (0%)	92 97
1	B	342/357 (96%)	341 (100%)	1 (0%)	92 97
1	C	343/357 (96%)	339 (99%)	4 (1%)	71 84
1	D	332/357 (93%)	330 (99%)	2 (1%)	86 93
All	All	1358/1428 (95%)	1350 (99%)	8 (1%)	86 93

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	423	ARG
1	B	191	CYS
1	C	134	ARG
1	C	168	CYS
1	C	191	CYS
1	C	472	LYS
1	D	119	THR
1	D	138	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	424	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 17 ligands modelled in this entry, 10 are monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	A	503	1	14,14,15	0.22	0	17,19,21	0.81	1 (5%)
3	NAG	D	502	1	14,14,15	1.34	1 (7%)	17,19,21	1.52	3 (17%)
3	NAG	D	503	1	14,14,15	0.30	0	17,19,21	0.53	0
3	NAG	B	503	1	14,14,15	0.45	0	17,19,21	0.61	0
3	NAG	C	502	1	14,14,15	0.22	0	17,19,21	0.76	1 (5%)
3	NAG	A	502	1	14,14,15	0.37	0	17,19,21	0.44	0
3	NAG	B	502	1	14,14,15	0.54	0	17,19,21	0.45	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	503	1	-	2/6/23/26	0/1/1/1
3	NAG	D	502	1	-	0/6/23/26	0/1/1/1
3	NAG	D	503	1	-	3/6/23/26	0/1/1/1
3	NAG	B	503	1	-	1/6/23/26	0/1/1/1
3	NAG	C	502	1	-	2/6/23/26	0/1/1/1
3	NAG	A	502	1	-	2/6/23/26	0/1/1/1
3	NAG	B	502	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	502	NAG	O5-C1	4.88	1.51	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	502	NAG	C1-O5-C5	4.43	118.19	112.19
3	D	502	NAG	C2-N2-C7	2.79	126.88	122.90
3	A	503	NAG	C1-O5-C5	2.64	115.77	112.19
3	C	502	NAG	C1-O5-C5	2.47	115.54	112.19
3	D	502	NAG	O3-C3-C2	2.06	113.73	109.47

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	502	NAG	C4-C5-C6-O6
3	D	503	NAG	C8-C7-N2-C2
3	D	503	NAG	O7-C7-N2-C2
3	C	502	NAG	O5-C5-C6-O6
3	A	502	NAG	O5-C5-C6-O6
3	A	502	NAG	C4-C5-C6-O6
3	A	503	NAG	C4-C5-C6-O6
3	B	502	NAG	C4-C5-C6-O6
3	B	502	NAG	O5-C5-C6-O6
3	B	503	NAG	O5-C5-C6-O6
3	A	503	NAG	O5-C5-C6-O6
3	D	503	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	503	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	443/455 (97%)	-0.18	10 (2%)	60	57	25, 43, 78, 105	0
1	B	445/455 (97%)	0.02	22 (4%)	29	27	27, 49, 89, 115	0
1	C	441/455 (96%)	-0.22	11 (2%)	57	54	25, 44, 76, 106	0
1	D	430/455 (94%)	-0.08	11 (2%)	56	53	27, 47, 85, 112	0
All	All	1759/1820 (96%)	-0.12	54 (3%)	49	46	25, 46, 83, 115	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	486	PRO	7.6
1	A	398	VAL	7.3
1	B	487	ALA	7.1
1	B	485	ASN	7.0
1	B	488	LEU	6.6
1	B	398	VAL	6.6
1	B	489	LEU	5.0
1	C	432	TRP	4.8
1	A	431	THR	4.6
1	B	484	PRO	4.5
1	A	438	ASP	4.5
1	B	432	TRP	4.1
1	A	399	GLU	4.0
1	B	426	VAL	3.7
1	C	424	ASN	3.6
1	B	483	TYR	3.5
1	A	432	TRP	3.3
1	C	399	GLU	3.1
1	B	150	ALA	3.0
1	D	423	ARG	3.0
1	D	431	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	490	SER	3.0
1	D	471	LEU	3.0
1	B	434	ASP	2.9
1	B	399	GLU	2.9
1	B	255	TRP	2.9
1	D	403	PHE	2.9
1	D	428	THR	2.9
1	C	431	THR	2.8
1	B	431	THR	2.7
1	C	421	TYR	2.7
1	C	439	VAL	2.7
1	B	439	VAL	2.6
1	A	400	GLY	2.6
1	B	423	ARG	2.6
1	C	426	VAL	2.6
1	A	397	ALA	2.5
1	B	436	ARG	2.5
1	C	400	GLY	2.4
1	B	437	GLN	2.4
1	D	397	ALA	2.4
1	C	137	ALA	2.3
1	B	438	ASP	2.2
1	A	423	ARG	2.2
1	D	421	TYR	2.2
1	D	440	GLU	2.2
1	D	426	VAL	2.1
1	C	444	HIS	2.1
1	D	401	ASP	2.1
1	A	439	VAL	2.1
1	C	398	VAL	2.1
1	A	426	VAL	2.0
1	B	400	GLY	2.0
1	D	483	TYR	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)

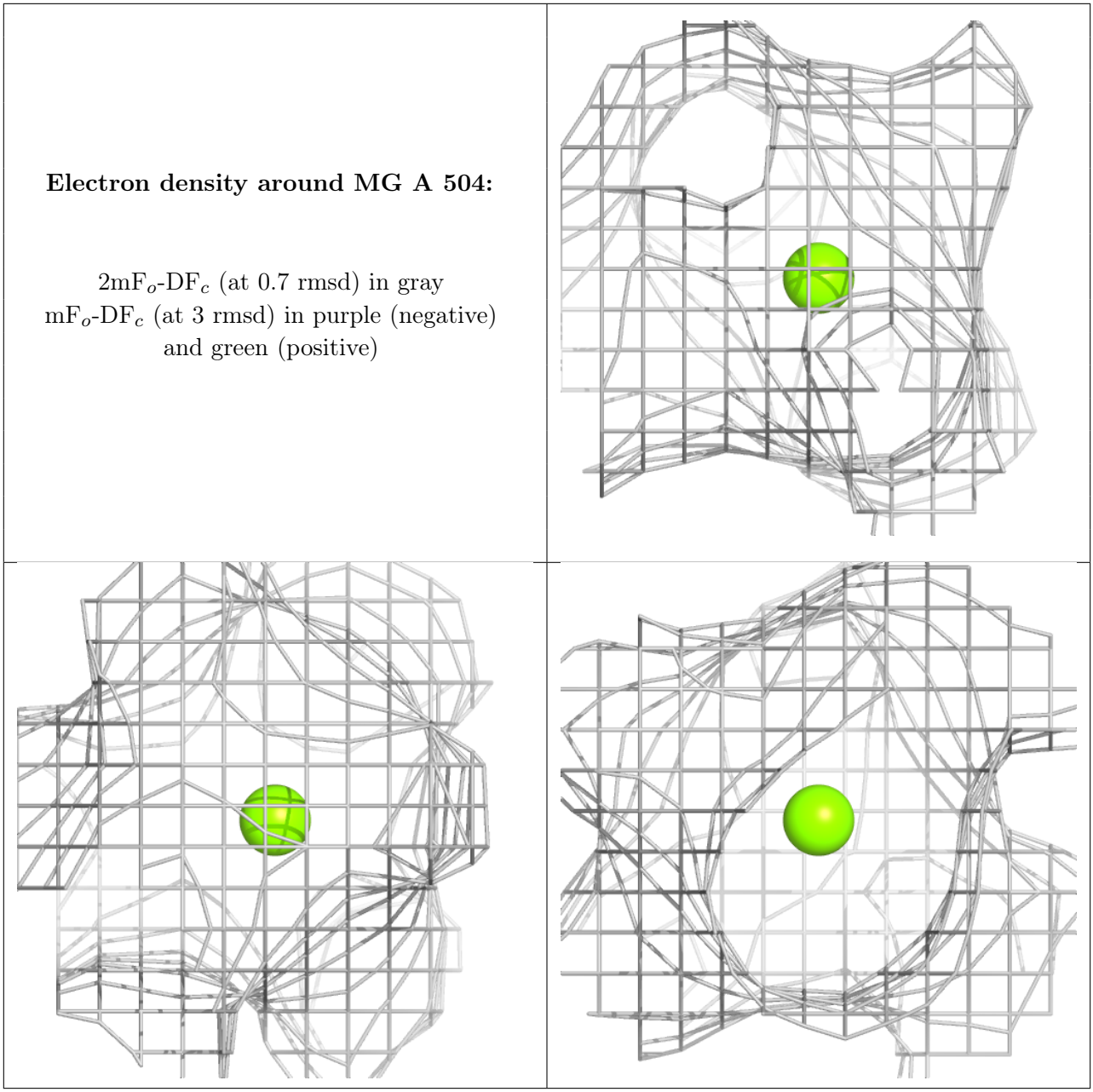
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	NAG	D	502	14/15	0.72	0.29	74,80,87,89	0
3	NAG	B	503	14/15	0.73	0.27	68,78,83,86	0
3	NAG	D	503	14/15	0.80	0.19	64,68,74,78	0
3	NAG	A	503	14/15	0.85	0.19	51,55,57,61	0
3	NAG	B	502	14/15	0.88	0.22	59,66,76,78	0
4	MG	A	504	1/1	0.92	0.07	71,71,71,71	0
3	NAG	C	502	14/15	0.93	0.13	50,55,59,60	0
4	MG	C	503	1/1	0.93	0.04	58,58,58,58	0
4	MG	B	504	1/1	0.94	0.09	65,65,65,65	0
4	MG	B	505	1/1	0.94	0.09	57,57,57,57	0
2	ZN	B	501	1/1	0.94	0.11	47,47,47,47	0
4	MG	D	505	1/1	0.94	0.26	102,102,102,102	0
3	NAG	A	502	14/15	0.95	0.14	47,53,62,64	0
4	MG	D	504	1/1	0.96	0.10	80,80,80,80	0
2	ZN	D	501	1/1	0.99	0.06	40,40,40,40	0
2	ZN	A	501	1/1	0.99	0.03	35,35,35,35	0
2	ZN	C	501	1/1	1.00	0.06	36,36,36,36	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.

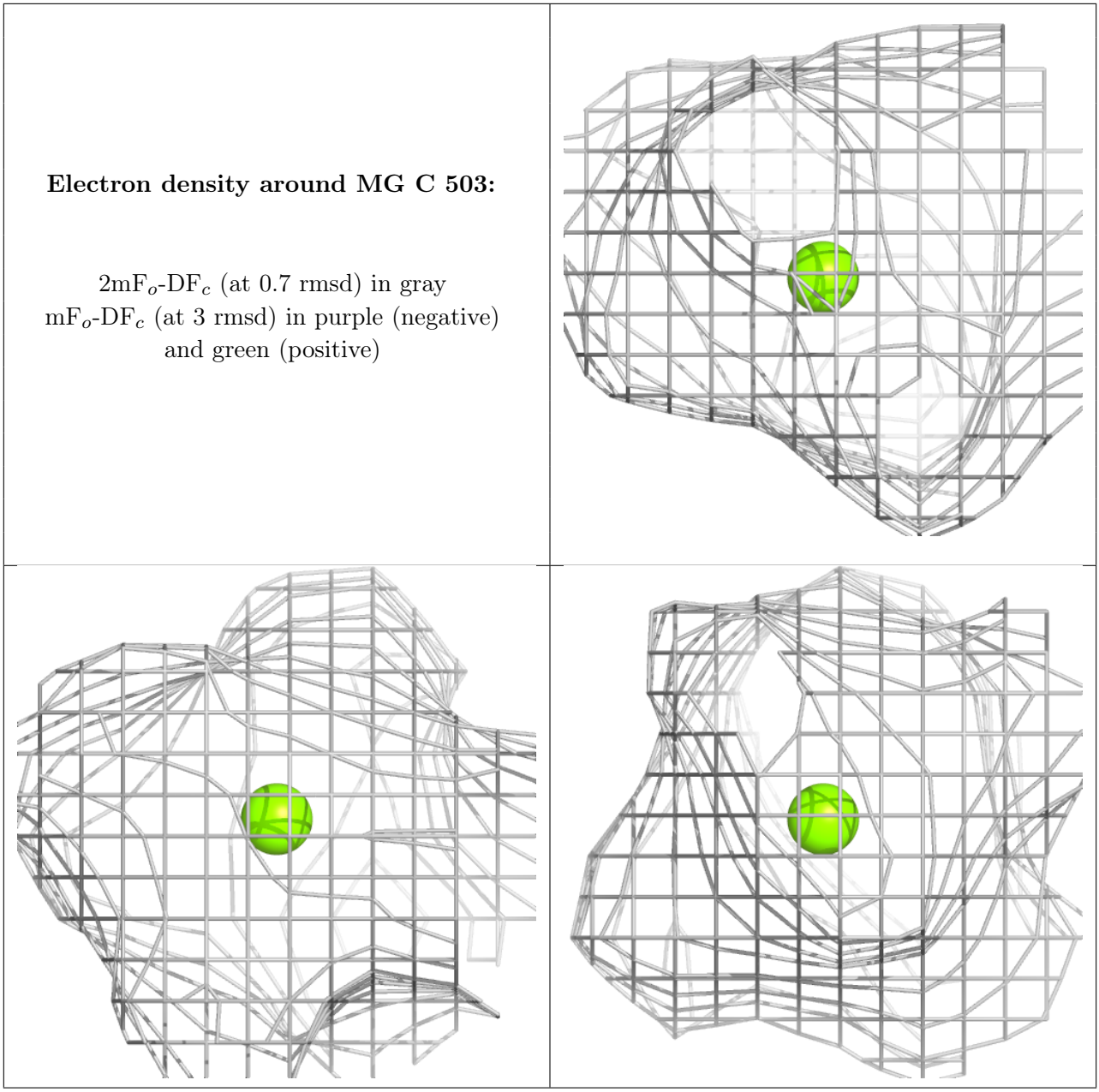
Electron density around MG A 504:

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



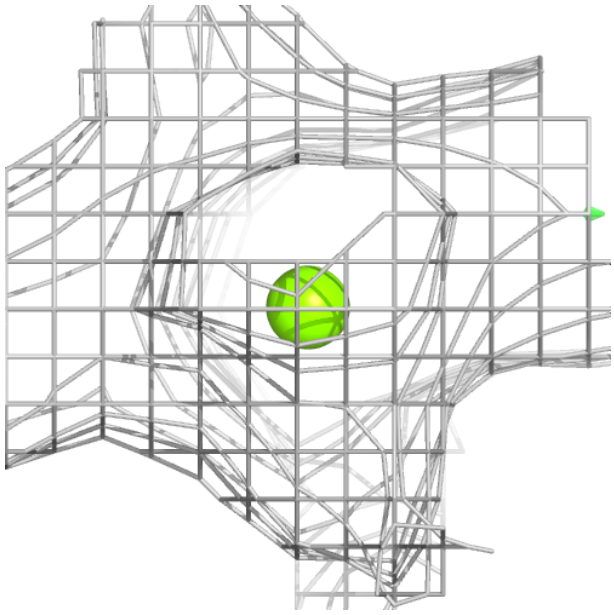
Electron density around MG C 503:

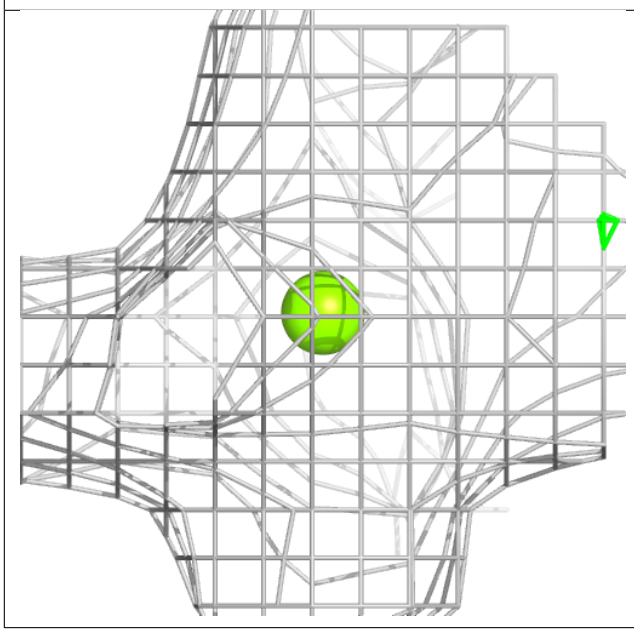
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

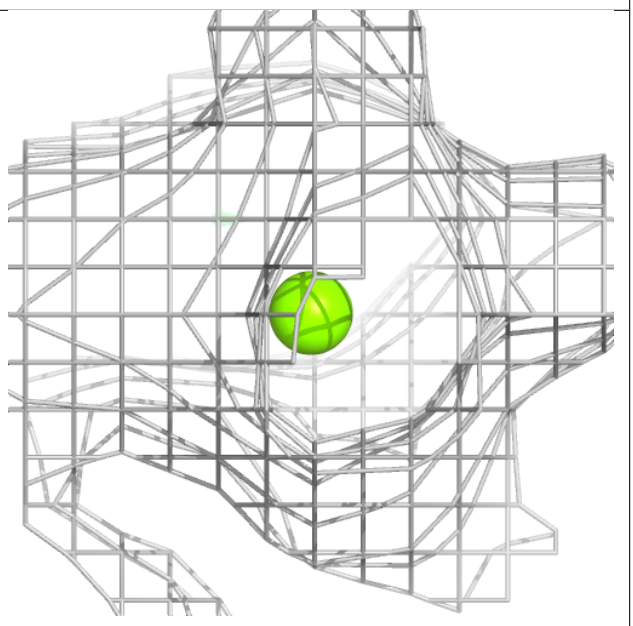


Electron density around MG B 504:

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

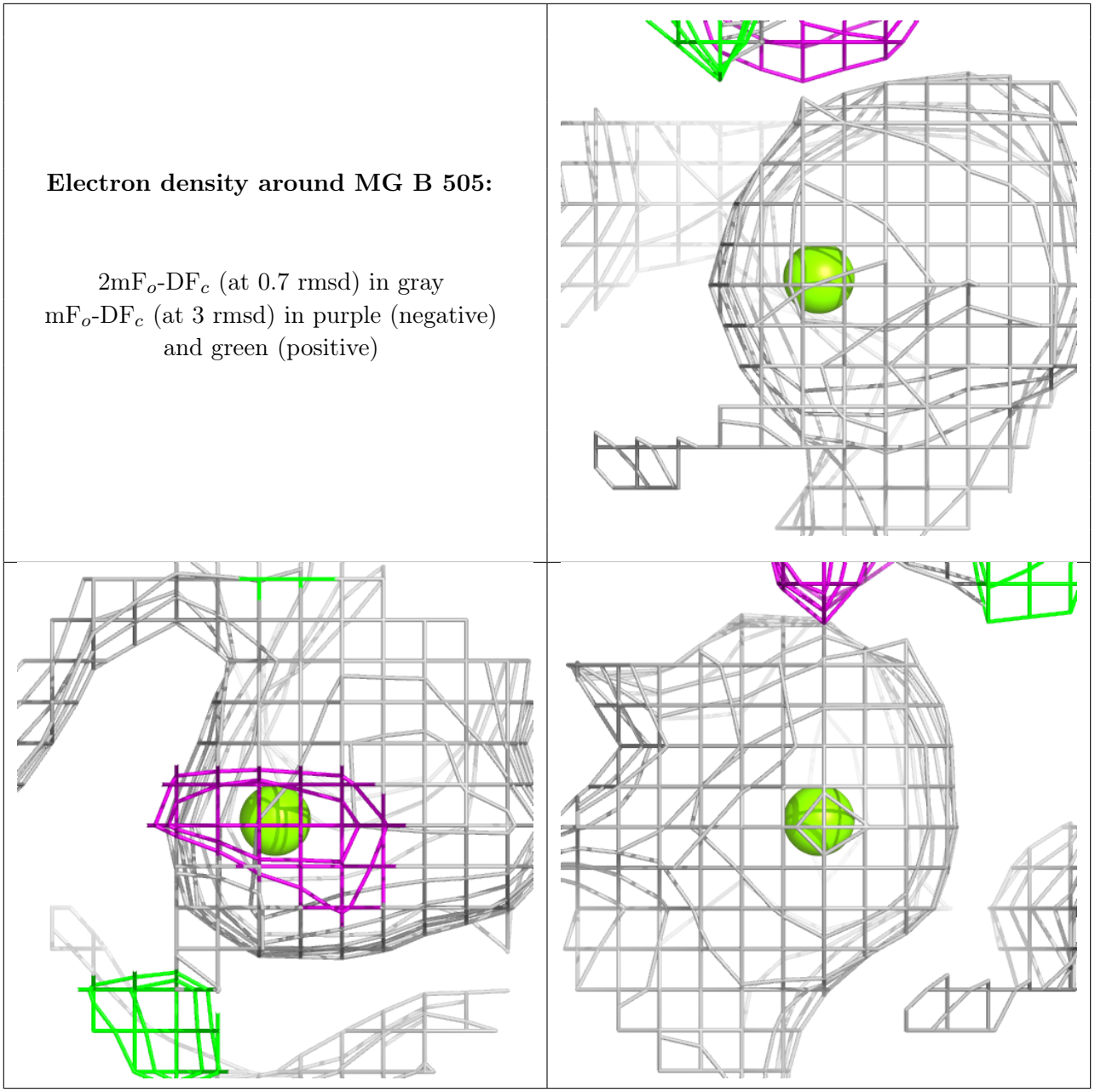






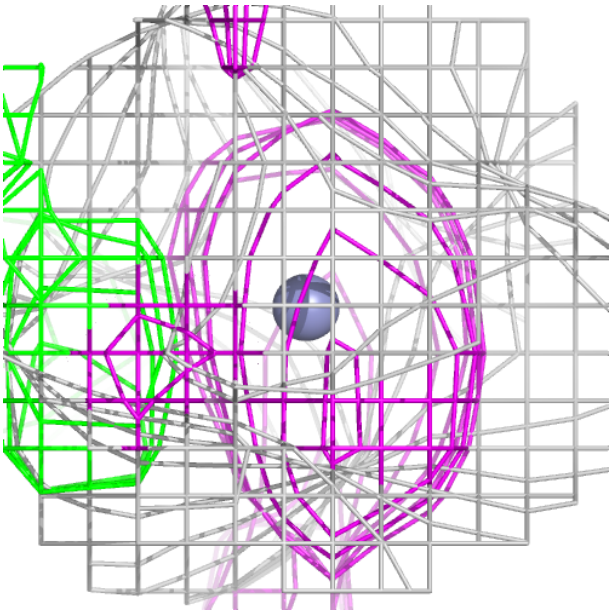
Electron density around MG B 505:

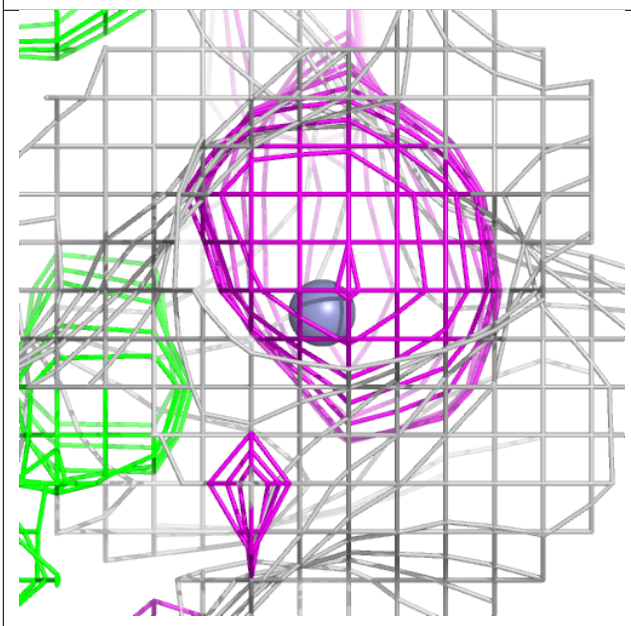
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

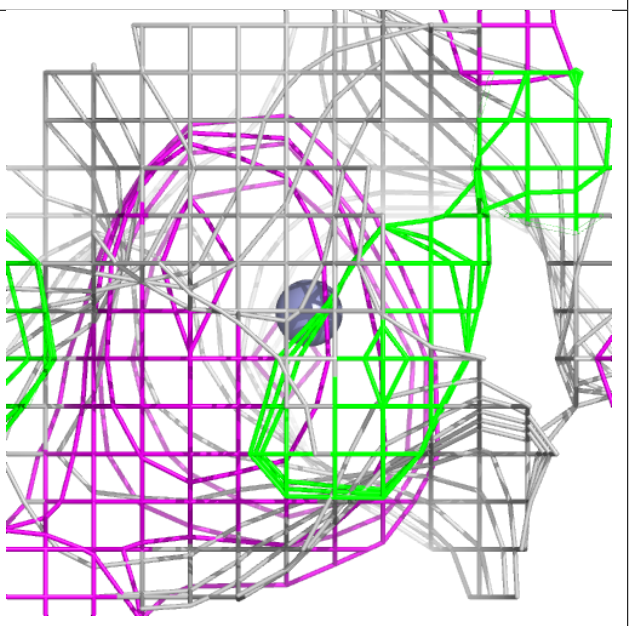


Electron density around ZN B 501:

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

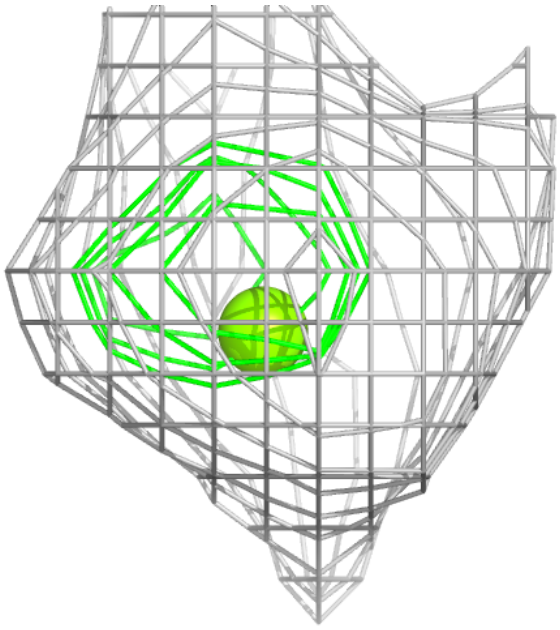


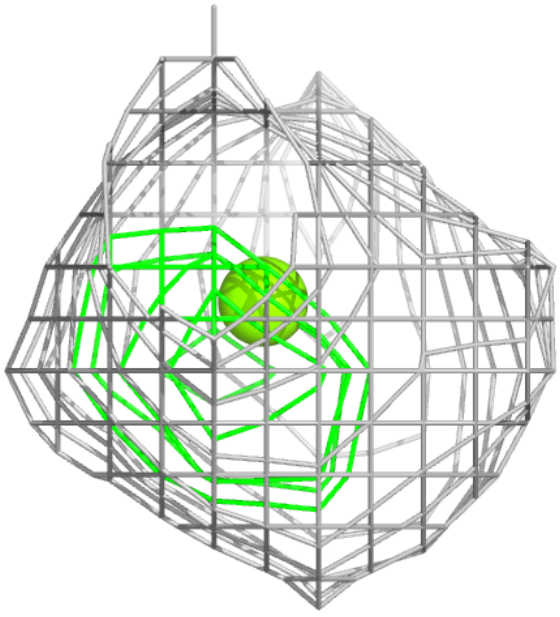


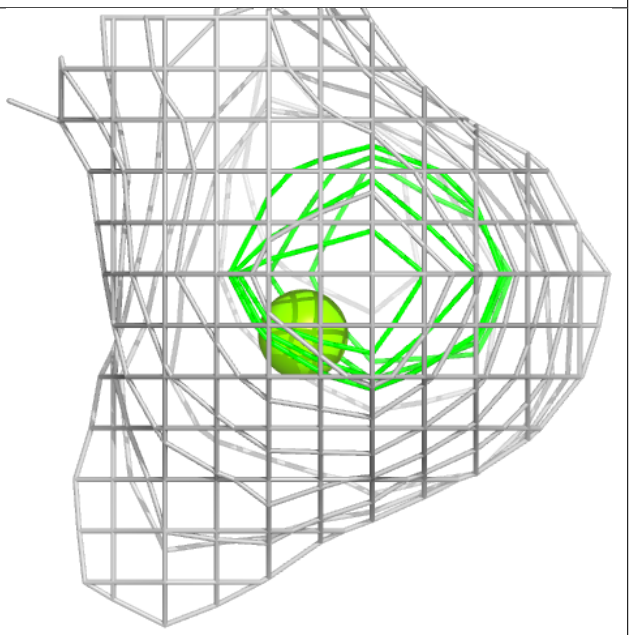


Electron density around MG D 505:

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

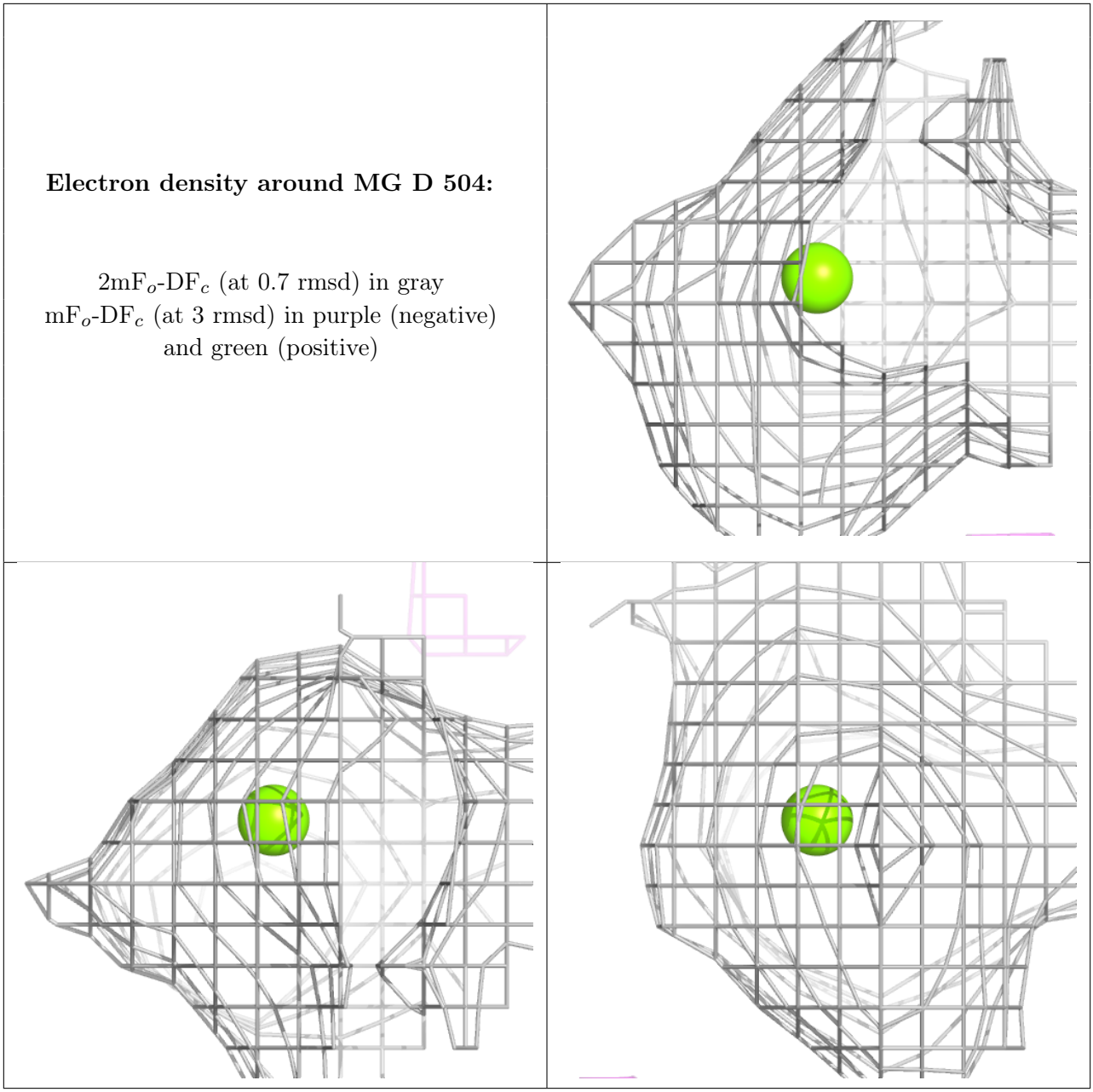






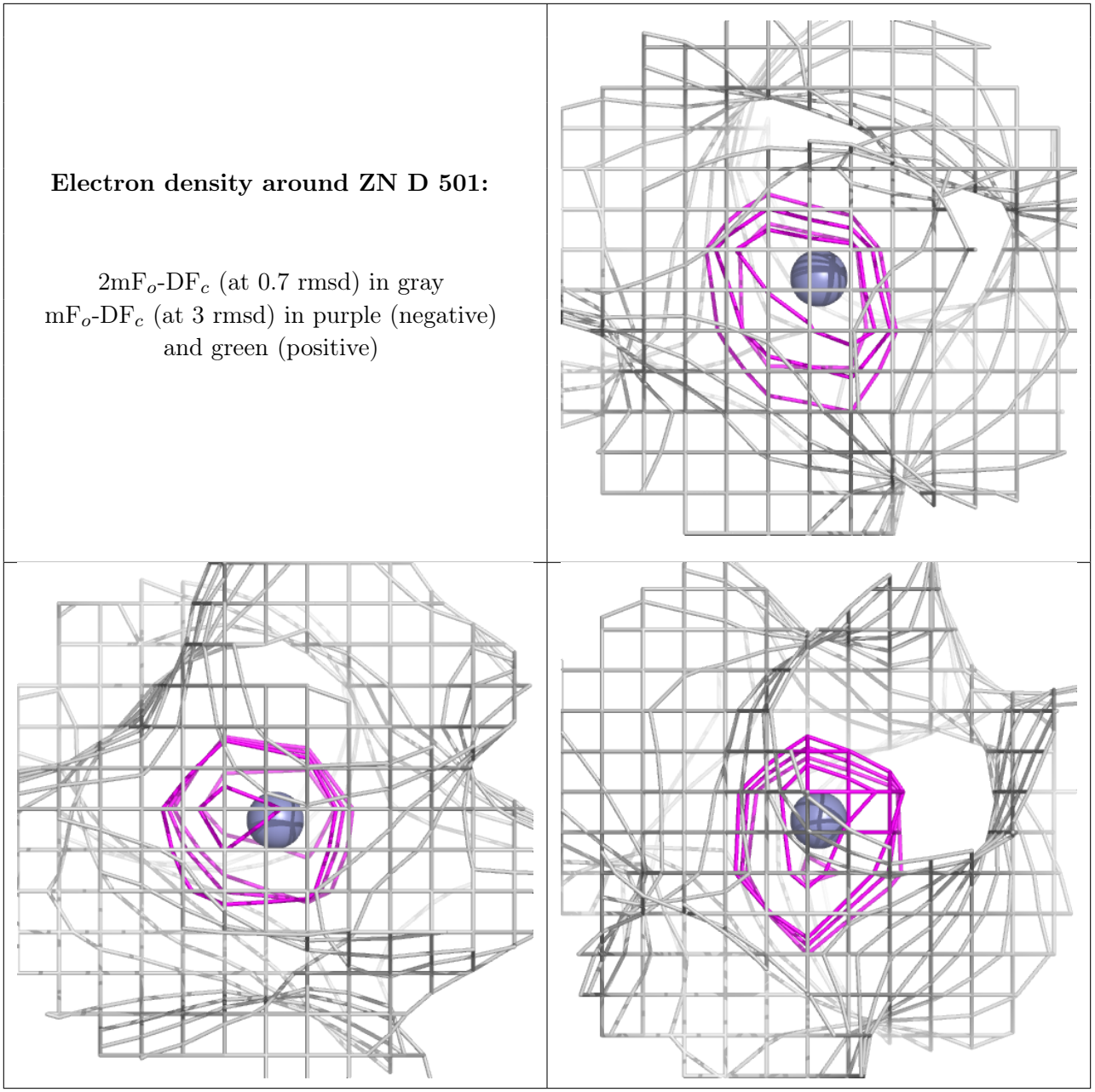
Electron density around MG D 504:

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



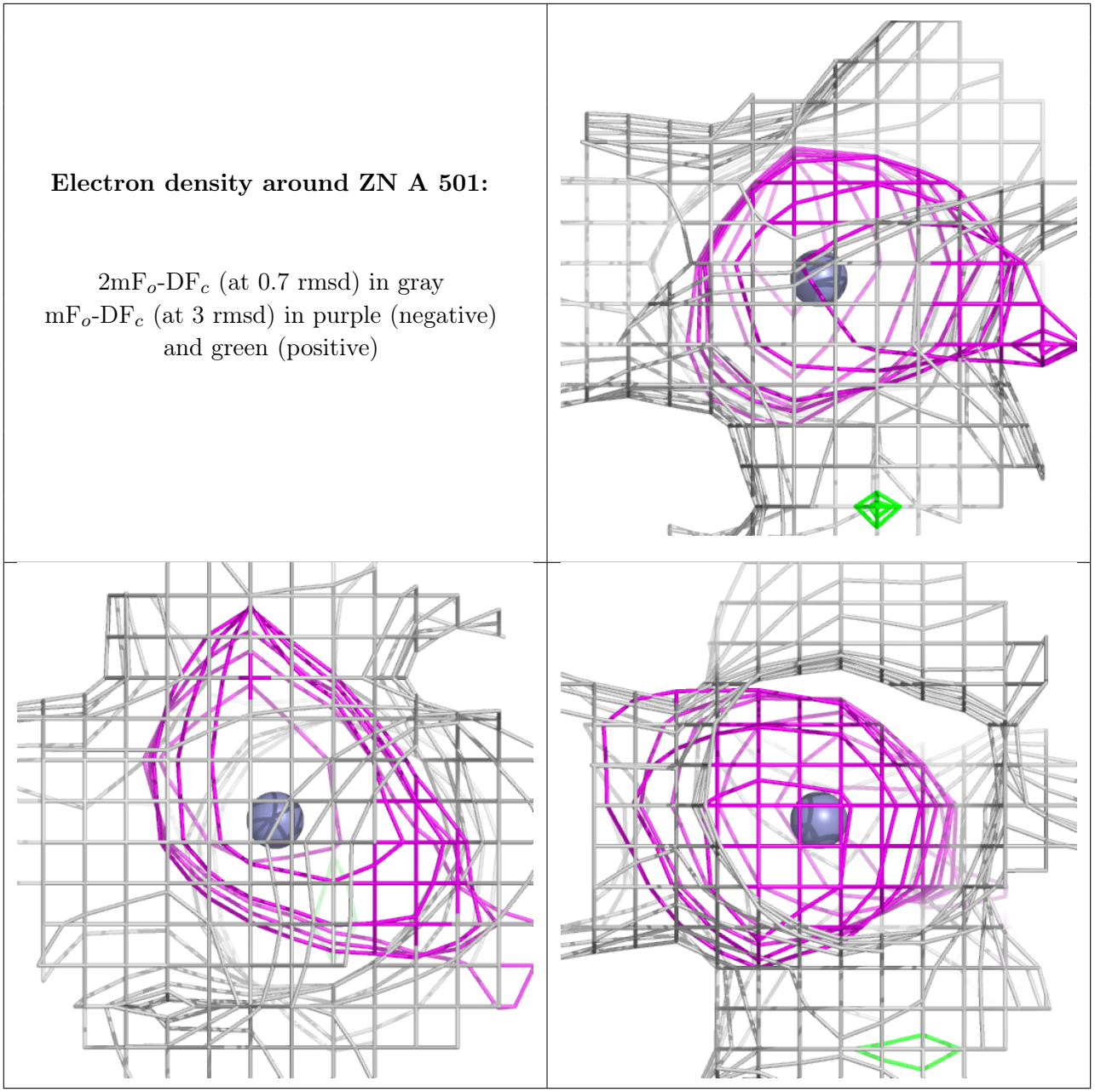
Electron density around ZN D 501:

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



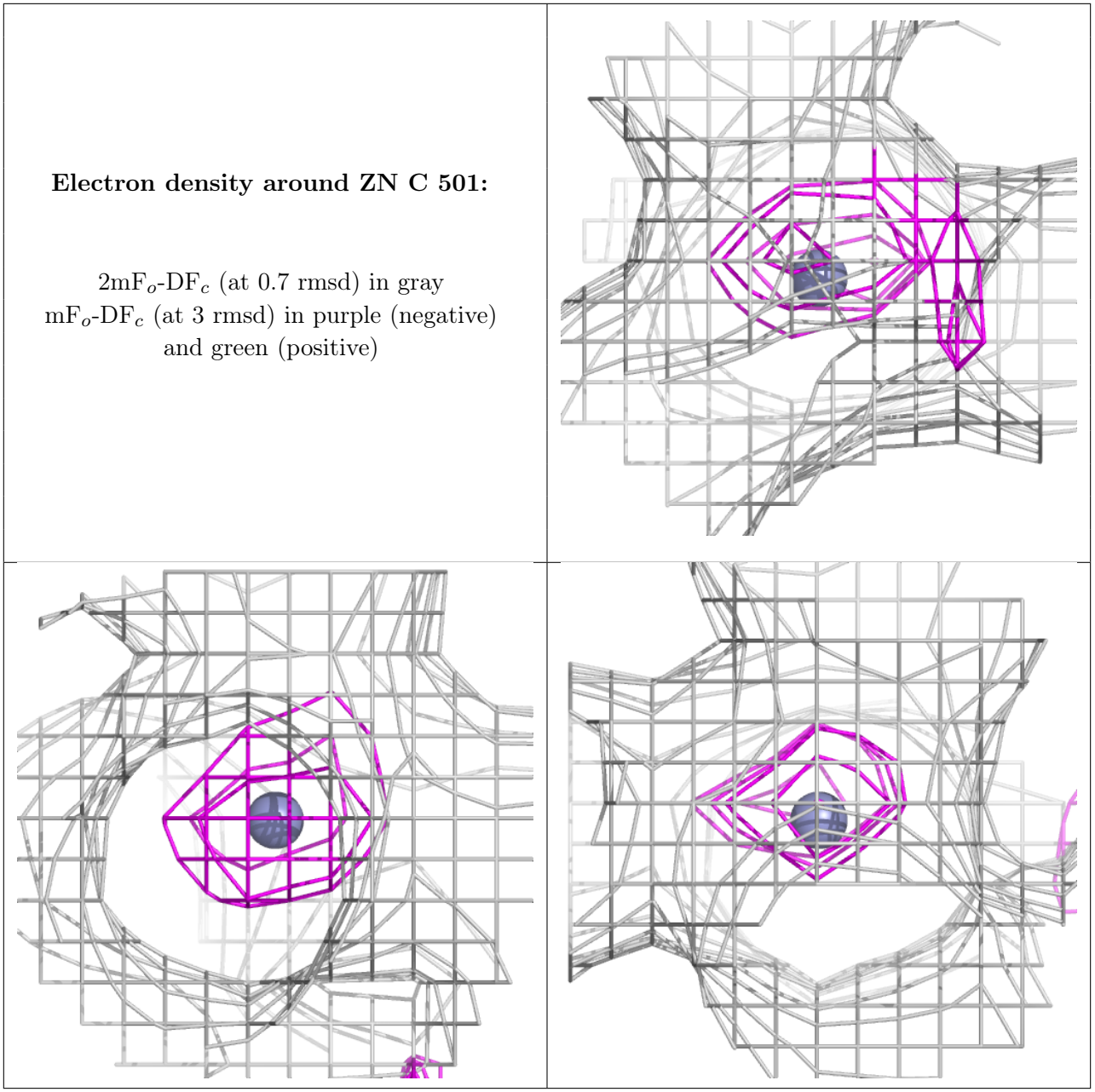
Electron density around ZN A 501:

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



Electron density around ZN C 501:

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



6.5 Other polymers (i)

There are no such residues in this entry.