Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 02:21 PM BST

PDB ID	:	6L7U
Title	:	Crystal structure of FKRP in complex with Ba ion, Ba-SAD data
Authors	:	Kuwabara, N.
Deposited on	:	2019-11-03
Resolution	:	2.24 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 following versions of software and data (see references ⓘ) were used in the production of this report:

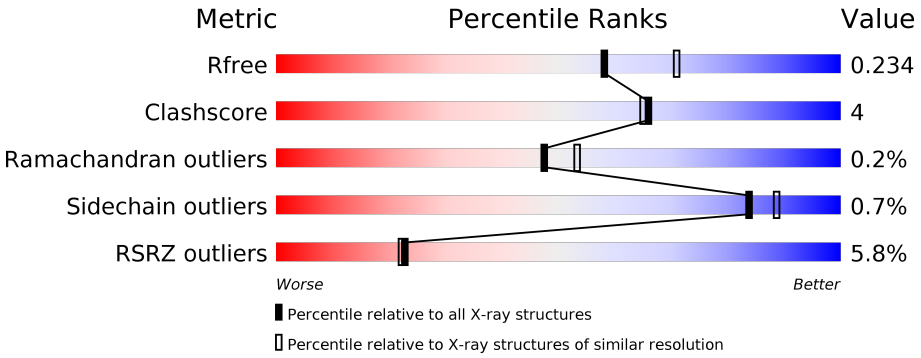
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance

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

The reported resolution of this entry is 2.24 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	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (2.26-2.22)

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 on 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	5% 87% 9%
1	B	455	8% 87% 10%
1	C	455	4% 87% 10%
1	D	455	5% 87% 7% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	D	502	-	-	-	X
3	NAG	D	503	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14108 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	442	Total	C	N	O	S	0	0	0
			3392	2174	600	609	9			
1	B	444	Total	C	N	O	S	0	0	0
			3420	2194	601	616	9			
1	C	441	Total	C	N	O	S	0	0	0
			3400	2184	598	609	9			
1	D	431	Total	C	N	O	S	0	0	0
			3319	2131	581	598	9			

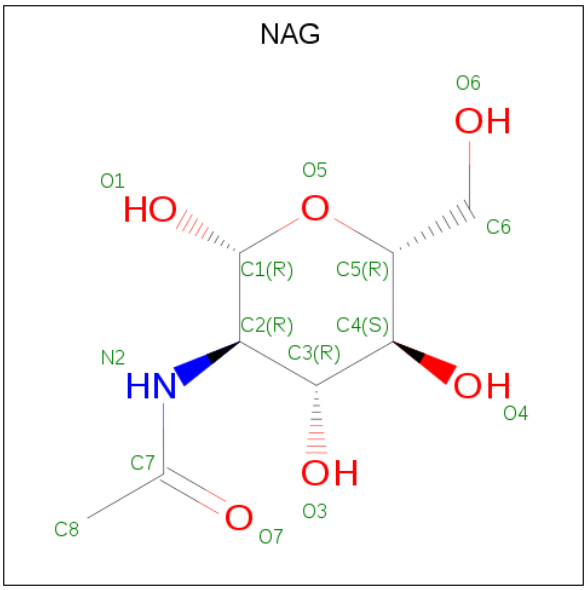
There are 16 discrepancies between the modelled and reference sequences:

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 author).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	C	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	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 BARIUM ION (three-letter code: BA) (formula: Ba) (labeled as "Ligand of Interest" by author).

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

- Molecule 5 is water.

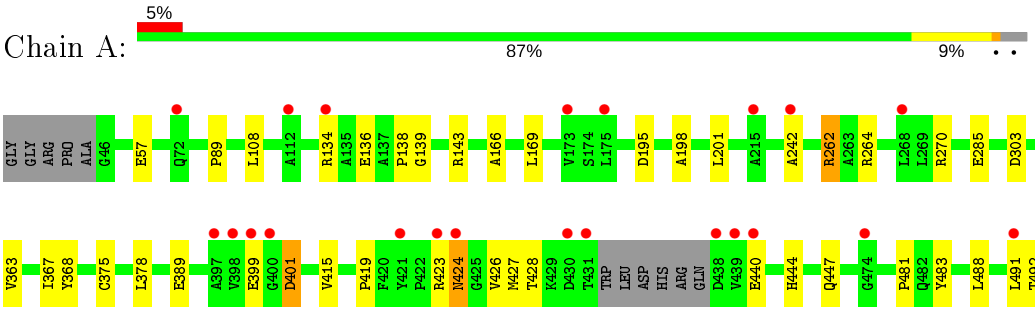
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	140	Total O 140 140	0	0
5	B	104	Total O 104 104	0	0
5	C	126	Total O 126 126	0	0
5	D	129	Total O 129 129	0	0

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.

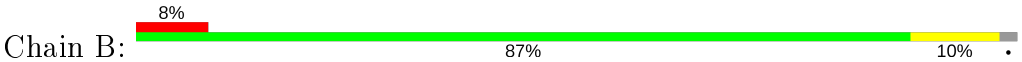
- Molecule 1: Fukutin-related protein

Chain A:



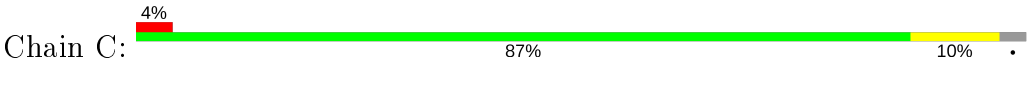
- Molecule 1: Fukutin-related protein

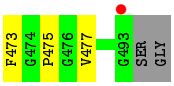
Chain B:



- Molecule 1: Fukutin-related protein

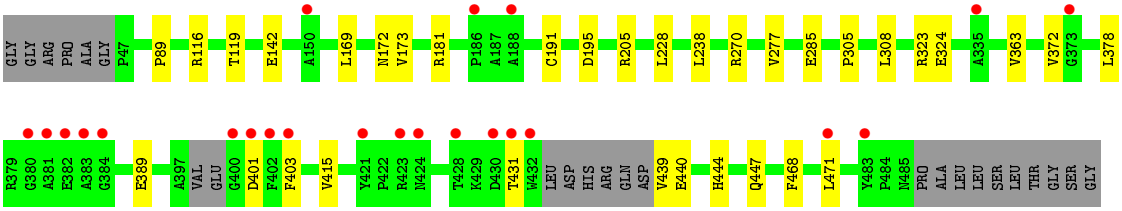
Chain C:





• Molecule 1: Fukutin-related protein

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	77.15Å 119.24Å 255.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.24 – 2.24 49.24 – 2.24	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.24-2.24) 99.9 (49.24-2.24)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.84 (at 2.24Å)	Xtriage
Refinement program	PHENIX 1.13_2998, PHENIX 1.13_2998	Depositor
R, R_{free}	0.200 , 0.234 0.200 , 0.234	Depositor DCC
R_{free} test set	5724 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	44.1	Xtriage
Anisotropy	0.630	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 36.9	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	14108	wwPDB-VP
Average B, all atoms (Å^2)	59.0	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 21.97 % 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 6.2721e-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, BA

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	0.27	0/3484	0.47	0/4775
1	B	0.27	0/3516	0.48	1/4820 (0.0%)
1	C	0.30	1/3494 (0.0%)	0.48	0/4787
1	D	0.27	0/3411	0.48	1/4675 (0.0%)
All	All	0.28	1/13905 (0.0%)	0.48	2/19057 (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
1	C	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	317	CYS	CB-SG	-8.20	1.68	1.82

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	181	ARG	NE-CZ-NH1	-5.67	117.47	120.30
1	B	149	ARG	NE-CZ-NH1	-5.33	117.63	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	422	PRO	Peptide

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	3392	0	3316	29	0
1	B	3420	0	3329	27	0
1	C	3400	0	3332	30	0
1	D	3319	0	3221	27	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
3	C	14	0	13	2	0
3	D	28	0	26	4	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	140	0	0	1	0
5	B	104	0	0	1	0
5	C	126	0	0	2	0
5	D	129	0	0	3	0
All	All	14108	0	13263	108	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 (108) 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:C:470:GLU:HG2	1:C:475:PRO:HA	1.45	0.93
1:D:378:LEU:HD23	1:D:378:LEU:O	1.75	0.86
1:A:339:ARG:HH11	1:A:339:ARG:HB2	1.44	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:302:GLY:HA3	1:C:304:THR:N	1.97	0.80
1:B:137:ALA:HB3	1:B:140:LEU:HD11	1.63	0.79
1:D:401:ASP:OD1	1:D:431:THR:HB	1.85	0.76
1:C:302:GLY:HA3	1:C:304:THR:H	1.51	0.74
1:A:134:ARG:NH2	1:A:242:ALA:O	2.26	0.69
1:D:378:LEU:HD23	1:D:378:LEU:C	2.14	0.67
1:C:443:GLU:OE2	1:C:447:GLN:NE2	2.28	0.67
1:D:172:ASN:HB2	3:D:502:NAG:N2	2.11	0.65
1:B:47:PRO:HG2	1:B:142:GLU:HG3	1.79	0.65
1:A:440:GLU:OE2	1:A:440:GLU:N	2.30	0.64
1:D:205:ARG:HA	3:D:503:NAG:H83	1.81	0.62
1:C:169:LEU:HD11	1:C:195:ASP:HB2	1.82	0.61
1:D:323:ARG:NH2	5:D:601:HOH:O	2.32	0.61
1:D:389:GLU:H	1:D:389:GLU:CD	2.03	0.61
1:D:169:LEU:HD11	1:D:195:ASP:HB2	1.83	0.61
1:C:373:GLY:O	1:C:379:ARG:NH1	2.34	0.61
1:C:389:GLU:CD	1:C:389:GLU:H	2.04	0.61
1:A:339:ARG:HB2	1:A:339:ARG:NH1	2.14	0.60
1:A:169:LEU:HD11	1:A:195:ASP:HB2	1.83	0.60
1:C:205:ARG:CZ	3:C:502:NAG:H82	2.32	0.60
1:D:270:ARG:NH2	5:D:602:HOH:O	2.35	0.60
1:A:270:ARG:NH1	5:A:602:HOH:O	2.34	0.59
1:C:259:ARG:HA	1:C:262:ARG:NH2	2.17	0.59
1:C:289:CYS:N	1:C:317:CYS:SG	2.65	0.58
1:A:488:LEU:O	1:A:492:THR:HG22	2.04	0.58
1:B:294:THR:HG22	1:B:295:ARG:O	2.03	0.57
1:A:389:GLU:H	1:A:389:GLU:CD	2.07	0.57
1:C:50:THR:HG21	1:C:121:VAL:HG22	1.86	0.56
1:B:256:LYS:O	1:B:260:GLU:HG3	2.06	0.56
1:C:73:GLN:NE2	1:C:136:GLU:O	2.39	0.56
1:A:426:VAL:HG12	1:A:428:THR:HG23	1.87	0.55
1:D:372:VAL:HG13	1:D:378:LEU:HD22	1.87	0.55
1:C:301:VAL:HG21	1:D:89:PRO:HB3	1.89	0.55
1:B:177:GLU:O	1:B:179:THR:HG23	2.08	0.53
1:D:116:ARG:O	1:D:119:THR:HG22	2.09	0.53
1:C:363:VAL:HB	1:C:415:VAL:HG22	1.90	0.53
1:D:468:PHE:O	1:D:471:LEU:HB3	2.09	0.53
1:D:378:LEU:HD21	1:D:403:PHE:CZ	2.44	0.52
1:B:134:ARG:HH22	1:B:136:GLU:HB2	1.75	0.51
1:A:368:TYR:CZ	1:A:427:MET:HE1	2.46	0.51
1:C:166:ALA:HB2	1:C:198:ALA:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:173:VAL:HB	1:D:228:LEU:HD13	1.93	0.51
1:C:110:ARG:NH1	5:C:608:HOH:O	2.43	0.51
1:A:375:CYS:HB3	1:A:378:LEU:HB2	1.94	0.50
1:A:108:LEU:HD21	1:B:272:LEU:HD13	1.94	0.50
1:B:98:ASN:OD1	1:D:119:THR:OG1	2.29	0.49
1:A:89:PRO:HB3	1:B:301:VAL:HG21	1.93	0.49
1:D:305:PRO:HD2	1:D:308:LEU:HD12	1.95	0.49
1:B:308:LEU:HD11	1:B:359:TRP:HB2	1.95	0.49
1:B:179:THR:HG22	1:B:276:LEU:HB3	1.95	0.49
3:D:502:NAG:O7	3:D:502:NAG:O3	2.28	0.48
1:D:172:ASN:HB2	3:D:502:NAG:HN2	1.77	0.48
1:C:470:GLU:CG	1:C:475:PRO:HA	2.32	0.48
1:D:378:LEU:C	1:D:378:LEU:CD2	2.80	0.48
1:B:289:CYS:SG	1:B:295:ARG:HA	2.54	0.48
1:C:473:PHE:HB2	1:C:477:VAL:HG11	1.96	0.48
1:B:149:ARG:HH12	1:B:203:ARG:HH22	1.60	0.48
1:B:202:LEU:HD11	1:B:207:LEU:HB2	1.95	0.48
1:B:97:PRO:HB2	1:D:119:THR:HG23	1.96	0.47
1:D:324:GLU:HG3	5:D:609:HOH:O	2.14	0.47
1:B:176:ARG:HD3	1:B:313:TRP:CD2	2.50	0.47
1:A:139:GLY:O	1:A:143:ARG:HG2	2.15	0.47
1:C:154:ARG:HD3	1:C:231:TRP:CD2	2.50	0.47
1:D:277:VAL:HB	1:D:285:GLU:HB2	1.96	0.47
1:B:369:LEU:O	1:B:372:VAL:HG13	2.14	0.46
1:A:444:HIS:HA	1:A:447:GLN:HG3	1.97	0.46
1:B:363:VAL:HB	1:B:415:VAL:HG22	1.97	0.46
1:B:323:ARG:NH2	5:B:608:HOH:O	2.49	0.46
1:D:439:VAL:HG22	1:D:440:GLU:H	1.81	0.45
1:A:363:VAL:HB	1:A:415:VAL:HG22	1.99	0.45
1:A:423:ARG:O	1:A:424:ASN:HB2	2.16	0.45
1:B:137:ALA:HB3	1:B:140:LEU:CD1	2.40	0.45
1:A:134:ARG:HE	1:A:134:ARG:HB3	1.50	0.44
1:A:339:ARG:HH11	1:A:339:ARG:CB	2.24	0.44
1:C:288:GLY:HA3	1:C:317:CYS:SG	2.57	0.44
1:B:159:PRO:HD3	1:B:235:LEU:HD11	1.99	0.44
1:D:363:VAL:HB	1:D:415:VAL:HG22	1.99	0.44
1:B:66:LEU:HD11	1:B:129:VAL:HG12	2.00	0.43
1:C:117:PRO:HB2	1:C:208:PHE:CE1	2.53	0.43
1:A:262:ARG:NH2	1:A:285:GLU:OE2	2.51	0.43
1:B:423:ARG:HD3	1:B:423:ARG:HA	1.88	0.43
1:B:79:VAL:HB	1:B:99:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:ALA:HB2	1:A:198:ALA:HB2	2.01	0.43
1:B:403:PHE:HB2	1:B:417:LEU:HB2	2.00	0.43
1:A:166:ALA:CB	1:A:198:ALA:HB2	2.49	0.42
1:C:377:GLN:HB3	1:C:394:TRP:CD2	2.54	0.42
1:A:57:GLU:OE2	1:A:264:ARG:NH2	2.51	0.42
1:C:403:PHE:HB2	1:C:417:LEU:HB2	2.02	0.42
1:C:79:VAL:HB	1:C:99:VAL:HG22	2.02	0.42
1:C:375:CYS:HB3	1:C:378:LEU:HD12	2.01	0.42
1:A:134:ARG:CZ	1:A:136:GLU:OE1	2.68	0.42
1:D:142:GLU:N	1:D:142:GLU:OE2	2.47	0.41
1:D:238:LEU:HD12	1:D:238:LEU:H	1.85	0.41
1:D:444:HIS:HA	1:D:447:GLN:CG	2.49	0.41
1:A:401:ASP:OD2	1:A:401:ASP:N	2.53	0.41
1:A:491:LEU:HD12	3:C:502:NAG:O6	2.20	0.41
1:A:483:TYR:CE1	1:C:313:TRP:HZ2	2.38	0.41
1:B:420:PHE:CZ	1:B:429:LYS:HD2	2.56	0.41
1:C:302:GLY:CA	1:C:304:THR:H	2.25	0.41
1:A:367:ILE:O	1:A:419:PRO:HA	2.21	0.41
1:C:67:VAL:HG21	1:C:93:LEU:HD22	2.03	0.41
1:C:134:ARG:HD3	1:C:136:GLU:OE1	2.21	0.40
1:B:447:GLN:HA	1:B:448:PRO:HA	1.91	0.40
1:C:259:ARG:HD2	5:C:624:HOH:O	2.21	0.40
1:A:352:ARG:CZ	1:A:481:PRO:HB3	2.52	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	438/455 (96%)	424 (97%)	11 (2%)	3 (1%)	22 20
1	B	442/455 (97%)	427 (97%)	15 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	437/455 (96%)	426 (98%)	11 (2%)	0	100 100
1	D	425/455 (93%)	416 (98%)	9 (2%)	0	100 100
All	All	1742/1820 (96%)	1693 (97%)	46 (3%)	3 (0%)	47 53

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	303	ASP
1	A	399	GLU
1	A	424	ASN

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	339/357 (95%)	335 (99%)	4 (1%)	71 78
1	B	342/357 (96%)	339 (99%)	3 (1%)	78 84
1	C	341/357 (96%)	339 (99%)	2 (1%)	86 90
1	D	331/357 (93%)	330 (100%)	1 (0%)	92 95
All	All	1353/1428 (95%)	1343 (99%)	10 (1%)	84 88

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	138	PRO
1	A	201	LEU
1	A	262	ARG
1	A	401	ASP
1	B	95	ARG
1	B	140	LEU
1	B	191	CYS
1	C	134	ARG
1	C	143	ARG

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Mol	Chain	Res	Type
1	D	191	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	435	HIS
1	C	424	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 13 ligands modelled in this entry, 8 are monoatomic - leaving 5 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	D	502	1	14,14,15	1.68	1 (7%)	17,19,21	1.41	2 (11%)
3	NAG	B	502	1	14,14,15	0.53	0	17,19,21	0.47	0
3	NAG	D	503	1	14,14,15	0.24	0	17,19,21	0.51	0
3	NAG	C	502	1	14,14,15	0.67	0	17,19,21	0.83	0
3	NAG	A	502	1	14,14,15	0.36	0	17,19,21	0.44	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	D	502	1	-	2/6/23/26	0/1/1/1
3	NAG	B	502	1	-	0/6/23/26	0/1/1/1
3	NAG	D	503	1	-	2/6/23/26	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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	502	NAG	C1-C2	5.95	1.61	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	502	NAG	C1-O5-C5	3.94	117.54	112.19
3	D	502	NAG	C3-C4-C5	-2.98	104.92	110.24

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	502	NAG	O5-C5-C6-O6
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	A	502	NAG	O5-C5-C6-O6
3	A	502	NAG	C4-C5-C6-O6
3	D	502	NAG	C1-C2-N2-C7
3	D	502	NAG	C3-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	502	NAG	3	0
3	D	503	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	502	NAG	2	0

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	442/455 (97%)	0.48	23 (5%)	27	26	32, 55, 94, 128	0
1	B	444/455 (97%)	0.50	37 (8%)	11	11	36, 56, 101, 130	0
1	C	441/455 (96%)	0.43	19 (4%)	35	34	33, 55, 86, 126	0
1	D	431/455 (94%)	0.40	23 (5%)	26	26	36, 55, 95, 143	0
All	All	1758/1820 (96%)	0.45	102 (5%)	23	22	32, 55, 95, 143	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	398	VAL	10.4
1	A	397	ALA	8.6
1	B	485	ASN	8.4
1	B	487	ALA	8.2
1	A	400	GLY	7.9
1	B	486	PRO	7.7
1	D	431	THR	7.2
1	A	399	GLU	6.5
1	B	488	LEU	6.5
1	A	439	VAL	6.2
1	D	400	GLY	6.2
1	D	432	TRP	5.9
1	B	399	GLU	5.9
1	A	493	GLY	5.8
1	B	150	ALA	4.8
1	C	139	GLY	4.7
1	D	430	ASP	4.4
1	B	489	LEU	4.4
1	C	137	ALA	4.3
1	B	401	ASP	4.3
1	A	438	ASP	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	439	VAL	4.2
1	B	432	TRP	4.1
1	B	484	PRO	4.0
1	A	431	THR	4.0
1	A	424	ASN	3.9
1	C	398	VAL	3.8
1	B	426	VAL	3.6
1	D	401	ASP	3.6
1	D	483	TYR	3.6
1	C	424	ASN	3.5
1	C	432	TRP	3.5
1	D	402	PHE	3.5
1	A	421	TYR	3.4
1	C	168	CYS	3.4
1	D	381	ALA	3.3
1	C	442	PRO	3.3
1	C	399	GLU	3.2
1	B	146	GLU	3.1
1	D	471	LEU	3.1
1	B	400	GLY	3.0
1	D	403	PHE	3.0
1	B	189	PRO	3.0
1	C	431	THR	3.0
1	B	289	CYS	2.9
1	C	302	GLY	2.9
1	A	268	LEU	2.9
1	B	438	ASP	2.9
1	B	436	ARG	2.9
1	B	255	TRP	2.8
1	B	425	GLY	2.8
1	A	423	ARG	2.8
1	D	421	TYR	2.8
1	B	435	HIS	2.7
1	D	373	GLY	2.7
1	D	383	ALA	2.7
1	A	134	ARG	2.6
1	B	433	LEU	2.6
1	B	482	GLN	2.6
1	C	426	VAL	2.6
1	A	474	GLY	2.6
1	B	108	LEU	2.6
1	D	186	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	424	ASN	2.5
1	B	431	THR	2.5
1	B	188	ALA	2.5
1	C	317	CYS	2.5
1	B	439	VAL	2.5
1	C	493	GLY	2.5
1	C	425	GLY	2.4
1	A	491	LEU	2.4
1	D	150	ALA	2.4
1	B	423	ARG	2.4
1	B	139	GLY	2.4
1	B	429	LYS	2.3
1	A	398	VAL	2.3
1	D	382	GLU	2.3
1	A	72	GLN	2.3
1	D	380	GLY	2.3
1	A	175	LEU	2.2
1	C	401	ASP	2.2
1	B	107	ALA	2.2
1	A	430	ASP	2.2
1	C	445	PHE	2.2
1	D	384	GLY	2.2
1	A	242	ALA	2.2
1	A	173	VAL	2.1
1	D	428	THR	2.1
1	D	423	ARG	2.1
1	C	73	GLN	2.1
1	C	173	VAL	2.1
1	D	188	ALA	2.1
1	A	440	GLU	2.1
1	A	215	ALA	2.1
1	B	280	GLU	2.0
1	A	112	ALA	2.0
1	B	138	PRO	2.0
1	B	384	GLY	2.0
1	B	249	ALA	2.0
1	B	253	ALA	2.0
1	B	383	ALA	2.0
1	D	335	ALA	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)

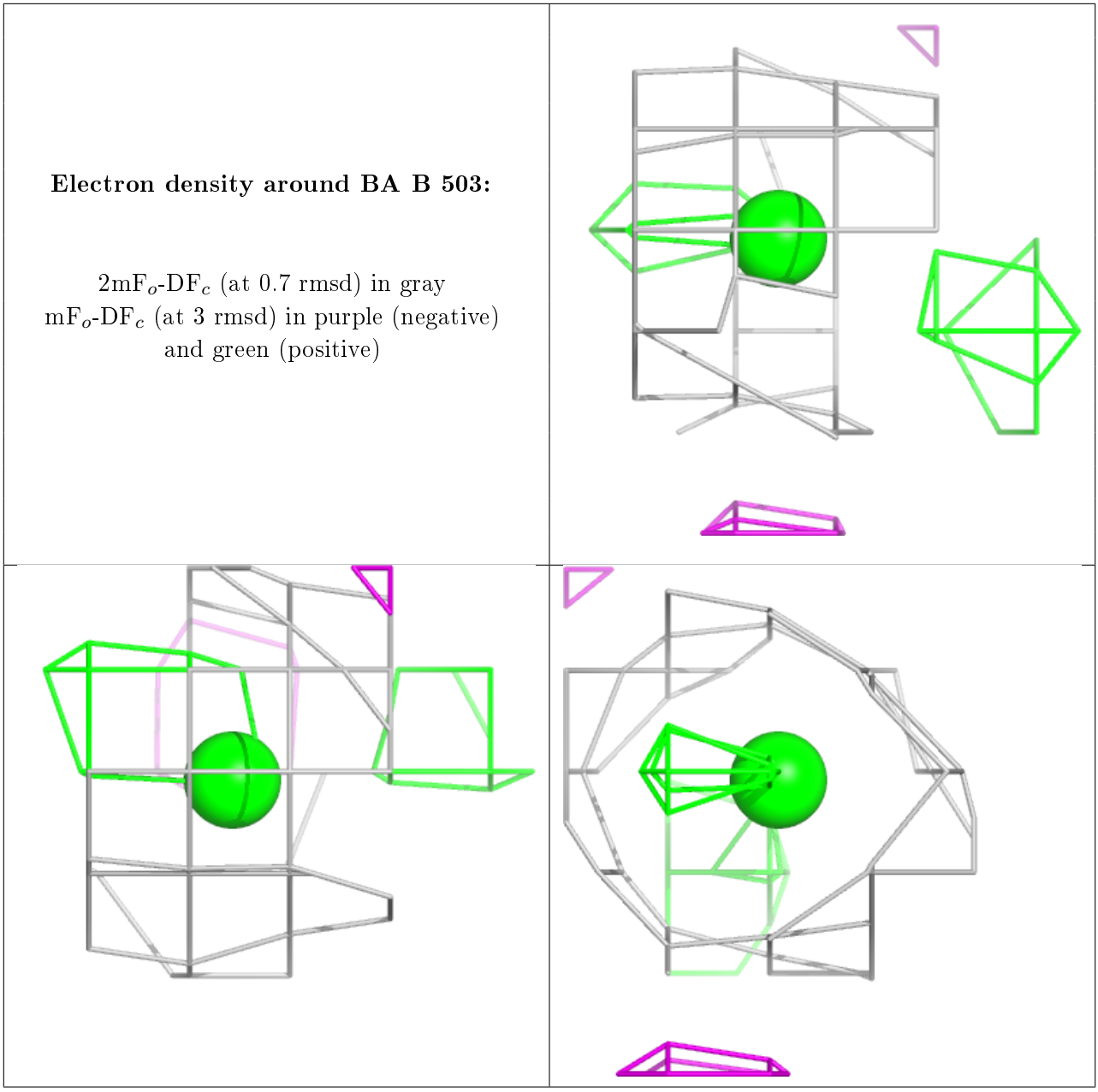
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
4	BA	B	503	1/1	0.22	0.17	248,248,248,248	0
4	BA	A	503	1/1	0.39	0.27	303,303,303,303	0
3	NAG	D	502	14/15	0.49	0.47	86,93,98,98	0
3	NAG	D	503	14/15	0.57	0.41	71,78,82,82	0
3	NAG	B	502	14/15	0.74	0.28	65,77,81,84	0
3	NAG	C	502	14/15	0.77	0.18	72,75,80,84	0
3	NAG	A	502	14/15	0.84	0.18	50,61,70,75	0
4	BA	C	503	1/1	0.84	0.33	278,278,278,278	0
4	BA	D	504	1/1	0.89	0.14	193,193,193,193	0
2	ZN	C	501	1/1	0.96	0.14	43,43,43,43	0
2	ZN	D	501	1/1	0.98	0.14	46,46,46,46	0
2	ZN	A	501	1/1	0.99	0.14	43,43,43,43	0
2	ZN	B	501	1/1	0.99	0.10	46,46,46,46	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.

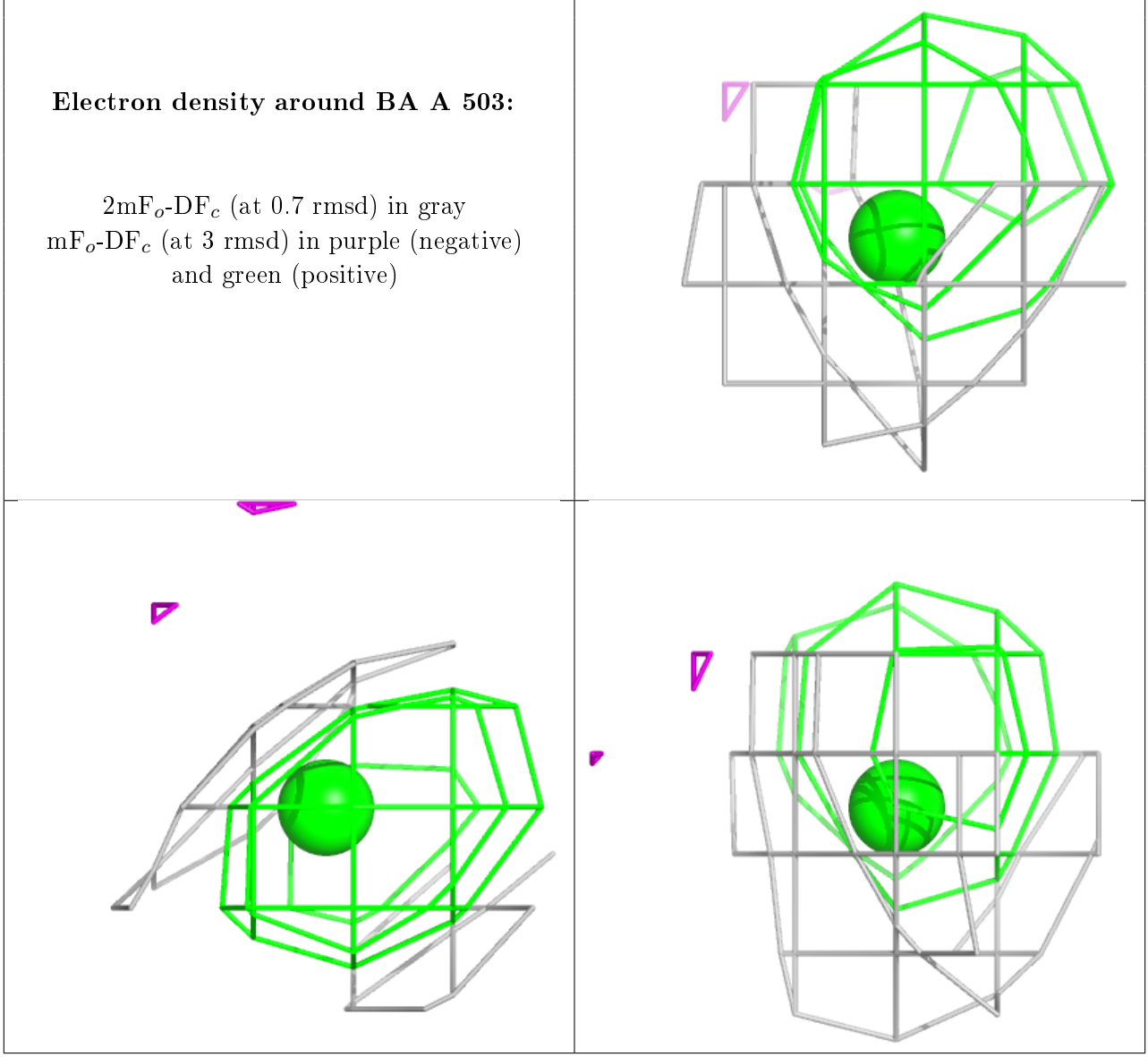
Electron density around BA B 503:

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



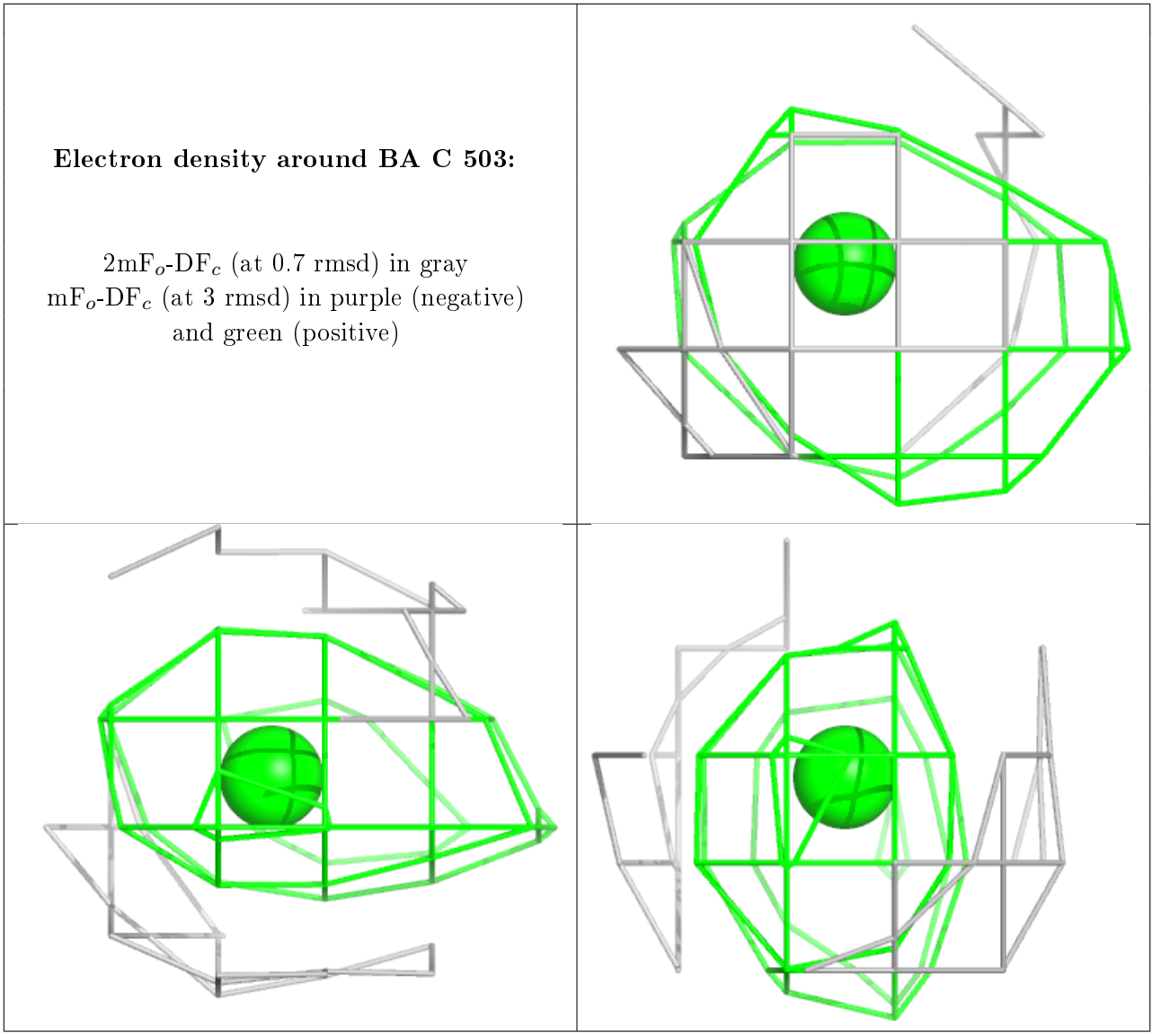
Electron density around BA A 503:

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



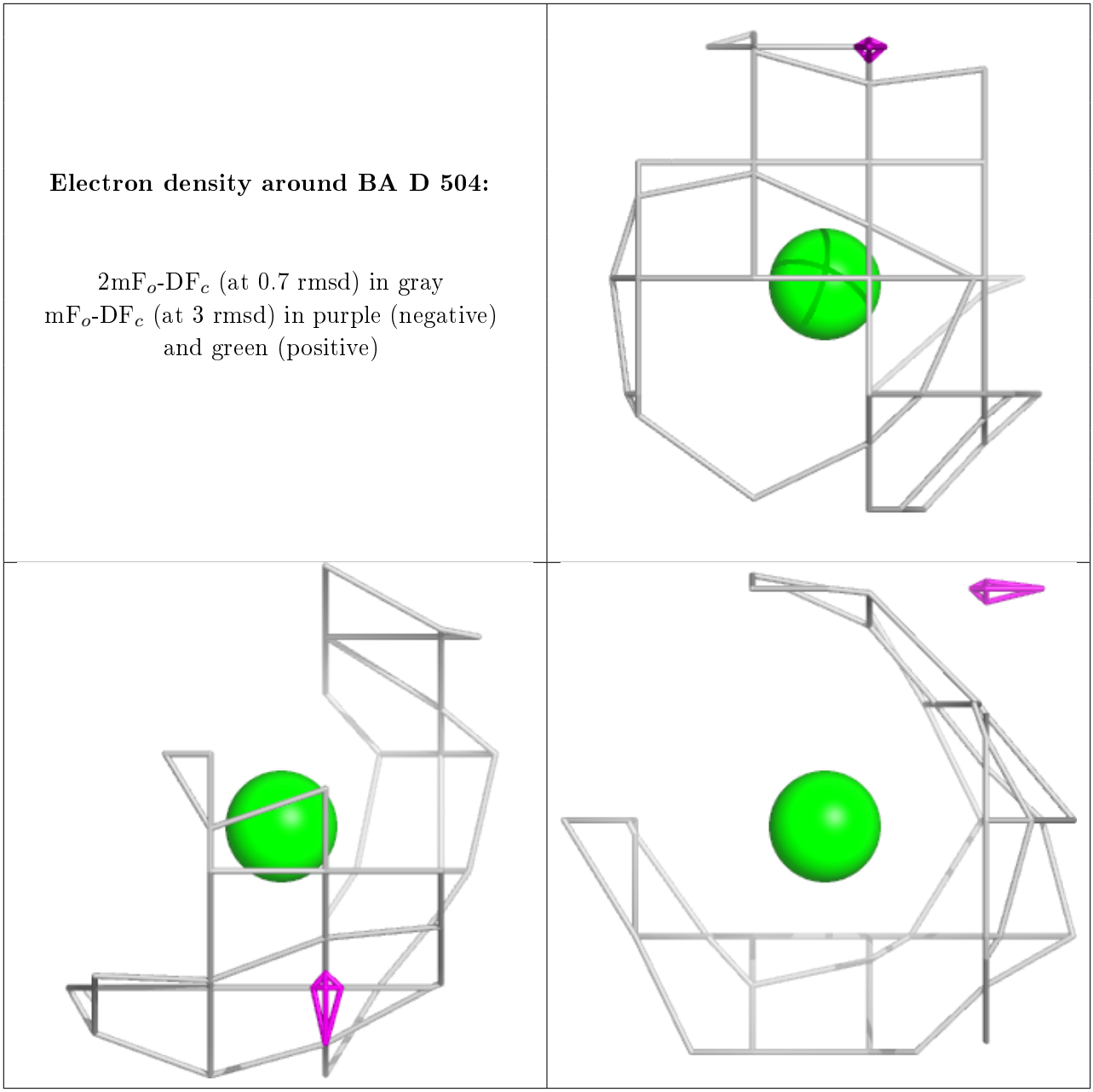
Electron density around BA C 503:

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



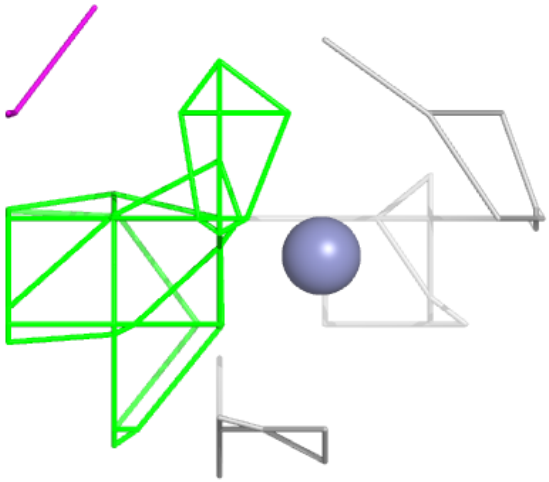
Electron density around BA D 504:

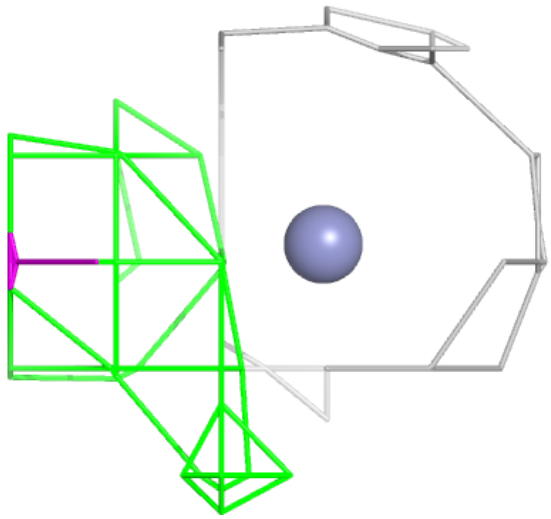
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

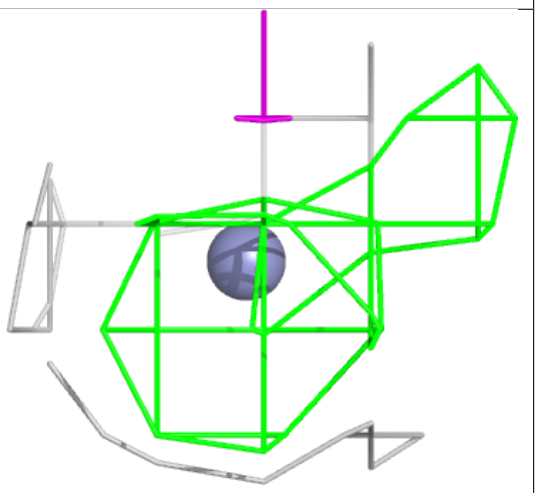


Electron density around ZN C 501:

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

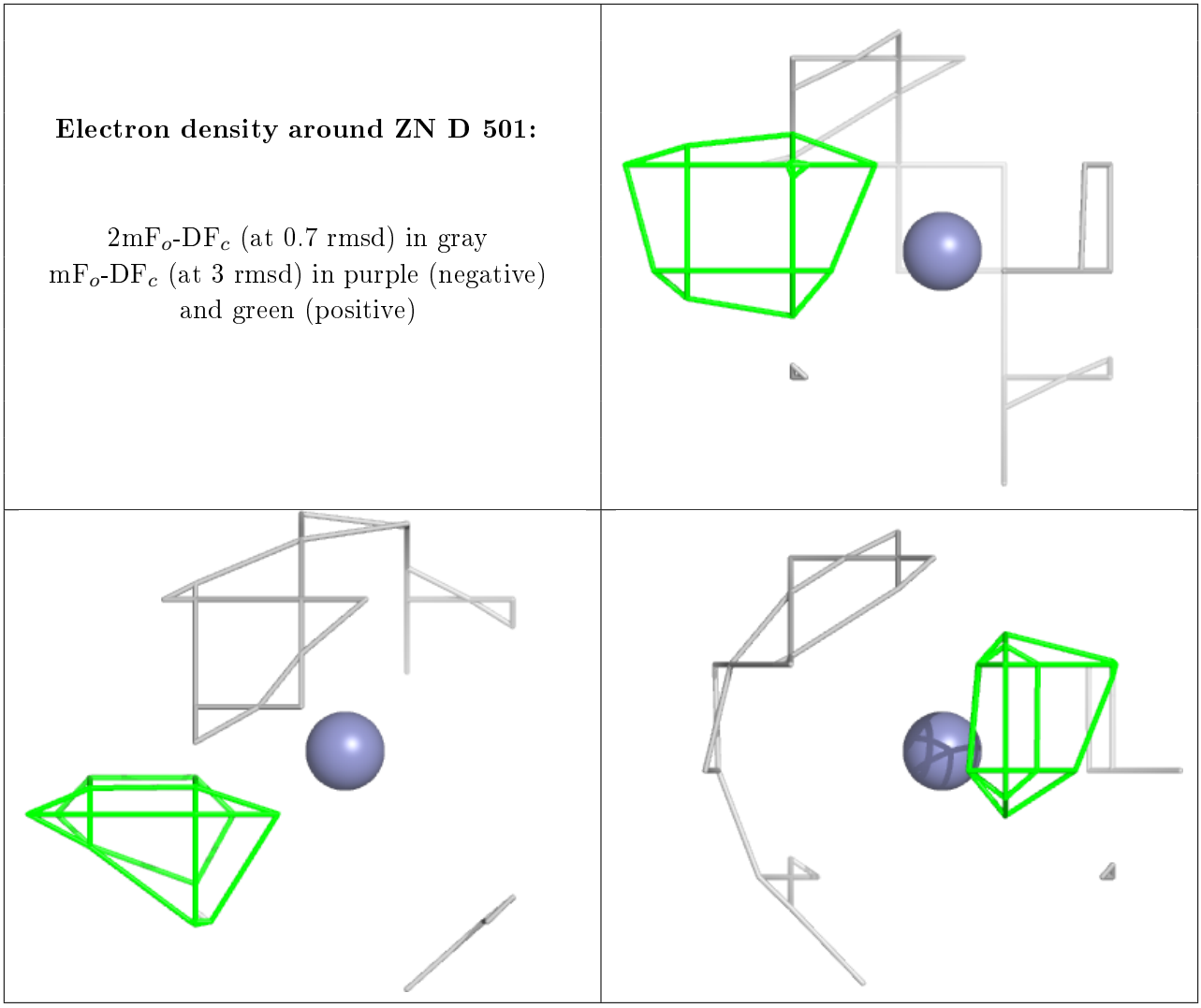






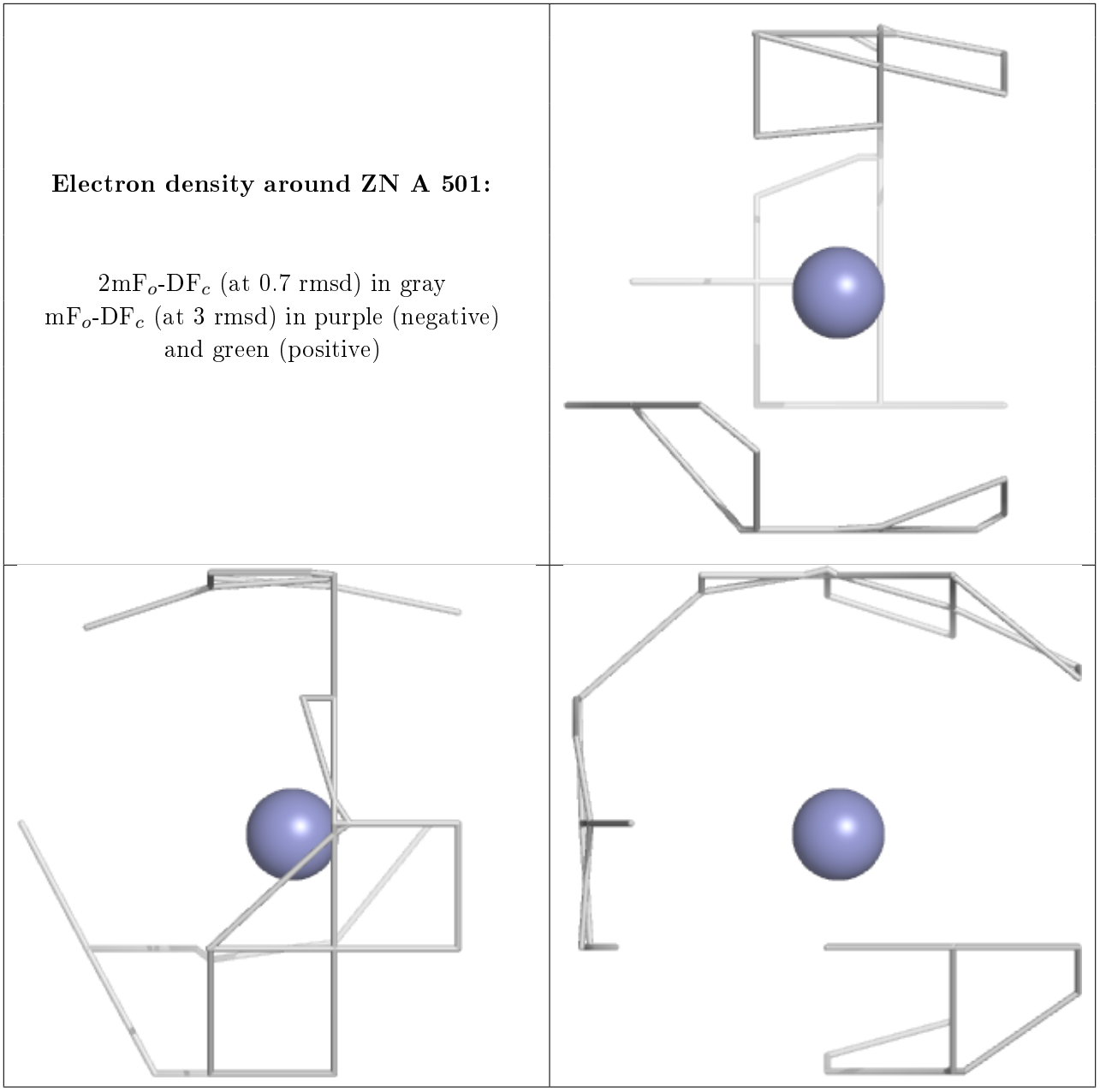
Electron density around ZN D 501:

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



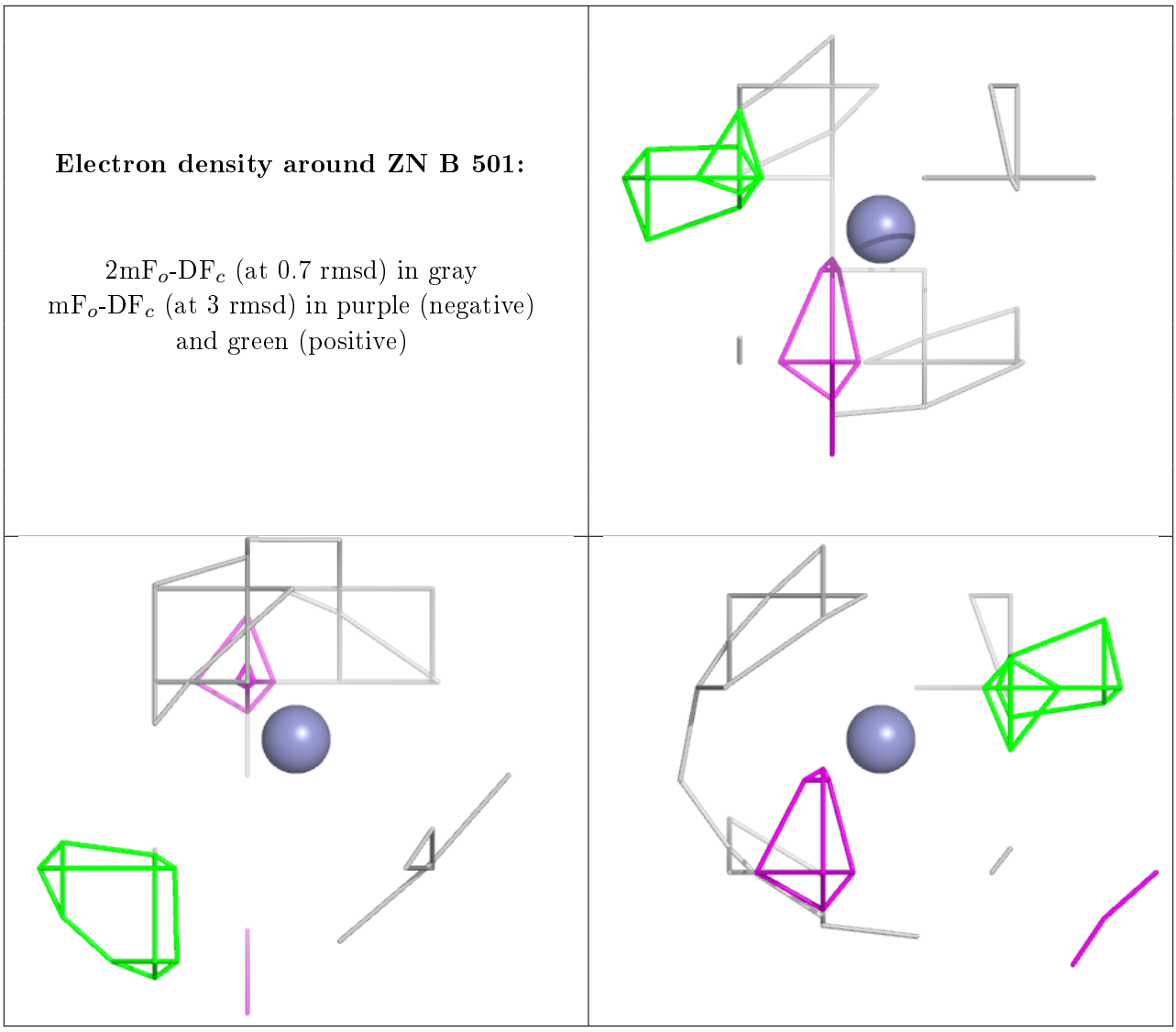
Electron density around ZN A 501:

$2mF_o$-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 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)



6.5 Other polymers

There are no such residues in this entry.