



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:59 PM UTC

PDB ID : 8D40 / pdb_00008d40
Title : Crystal structure of human CELSR1 EC1-4
Authors : Tamilselvan, E.; Sotomayor, M.
Deposited on : 2022-06-01
Resolution : 3.55 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

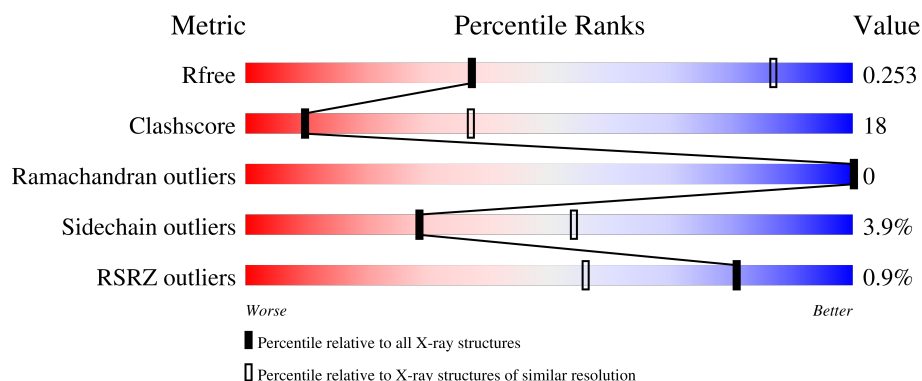
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.55 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1410 (3.62-3.50)
Clashscore	190562	1480 (3.62-3.50)
Ramachandran outliers	187476	1440 (3.62-3.50)
Sidechain outliers	187428	1441 (3.62-3.50)
RSRZ outliers	180081	1409 (3.62-3.50)

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

Mol	Chain	Length	Quality of chain
1	A	457	
1	B	457	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6673 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 Cadherin EGF LAG seven-pass G-type receptor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	422	Total	C	N	O	S	0	0	0
			3307	2066	565	672	4			
1	B	427	Total	C	N	O	S	0	0	0
			3340	2085	571	680	4			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q9NYQ6
A	449	LEU	-	expression tag	UNP Q9NYQ6
A	450	GLU	-	expression tag	UNP Q9NYQ6
A	451	HIS	-	expression tag	UNP Q9NYQ6
A	452	HIS	-	expression tag	UNP Q9NYQ6
A	453	HIS	-	expression tag	UNP Q9NYQ6
A	454	HIS	-	expression tag	UNP Q9NYQ6
A	455	HIS	-	expression tag	UNP Q9NYQ6
A	456	HIS	-	expression tag	UNP Q9NYQ6
B	0	MET	-	initiating methionine	UNP Q9NYQ6
B	449	LEU	-	expression tag	UNP Q9NYQ6
B	450	GLU	-	expression tag	UNP Q9NYQ6
B	451	HIS	-	expression tag	UNP Q9NYQ6
B	452	HIS	-	expression tag	UNP Q9NYQ6
B	453	HIS	-	expression tag	UNP Q9NYQ6
B	454	HIS	-	expression tag	UNP Q9NYQ6
B	455	HIS	-	expression tag	UNP Q9NYQ6
B	456	HIS	-	expression tag	UNP Q9NYQ6

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Na 1 1	0	0
2	B	2	Total Na 2 2	0	0

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	8	Total Ca 8 8	0	0
3	B	7	Total Ca 7 7	0	0

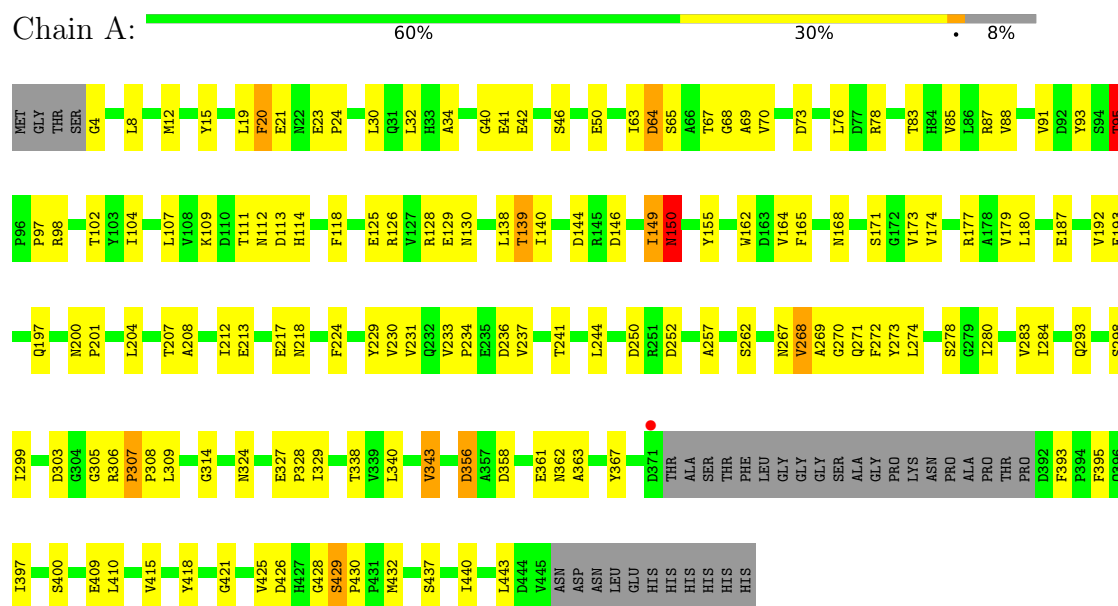
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	4	Total O 4 4	0	0
4	B	4	Total O 4 4	0	0

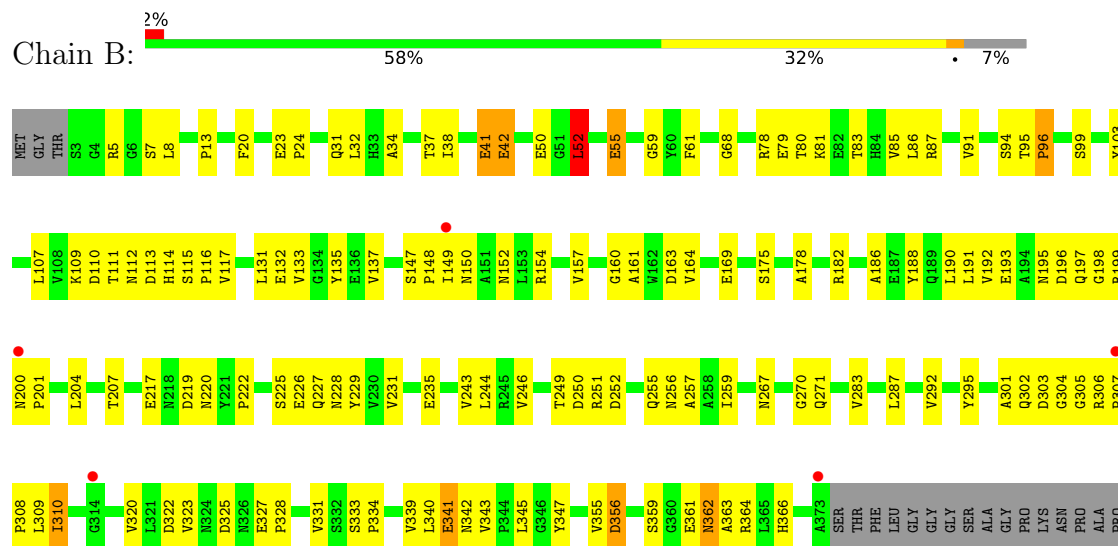
3 Residue-property plots

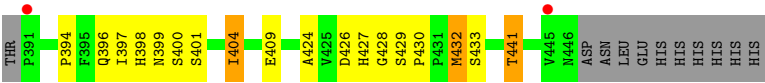
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Cadherin EGF LAG seven-pass G-type receptor 1



• Molecule 1: Cadherin EGF LAG seven-pass G-type receptor 1





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	305.65Å 90.36Å 94.95Å 90.00° 96.17° 90.00°	Depositor
Resolution (Å)	47.24 – 3.55 47.24 – 3.55	Depositor EDS
% Data completeness (in resolution range)	98.2 (47.24-3.55) 98.2 (47.24-3.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 3.57Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.216 , 0.252 0.217 , 0.253	Depositor DCC
R_{free} test set	1483 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å ²)	102.7	Xtriage
Anisotropy	0.690	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 95.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6673	wwPDB-VP
Average B, all atoms (Å ²)	133.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	1.10	0/3375	1.53	23/4603 (0.5%)
1	B	1.10	2/3409 (0.1%)	1.58	25/4650 (0.5%)
All	All	1.10	2/6784 (0.0%)	1.55	48/9253 (0.5%)

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	A	0	1
1	B	0	2
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	328	PRO	C-O	-5.45	1.17	1.23
1	B	331	VAL	C-O	-5.20	1.18	1.24

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	96	PRO	N-CA-C	-13.49	94.24	110.70
1	A	73	ASP	CA-CB-CG	8.28	120.88	112.60
1	A	95	THR	CA-CB-OG1	-7.79	97.91	109.60
1	B	325	ASP	CA-CB-CG	7.50	120.10	112.60
1	B	55	GLU	CB-CA-C	-7.26	100.71	112.03
1	B	113	ASP	CB-CA-C	-7.13	96.23	110.42
1	B	428	GLY	CA-C-O	-6.88	114.20	121.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	114	HIS	CB-CA-C	6.70	120.78	109.80
1	A	361	GLU	N-CA-C	-6.59	105.27	113.38
1	A	65	SER	CA-C-N	6.54	129.28	120.65
1	A	65	SER	C-N-CA	6.54	129.28	120.65
1	A	307	PRO	CB-CA-C	6.49	118.84	110.92
1	A	162	TRP	N-CA-C	-6.48	104.56	113.18
1	B	52	LEU	CA-C-N	6.43	129.14	120.65
1	B	52	LEU	C-N-CA	6.43	129.14	120.65
1	A	293	GLN	CB-CA-C	-6.30	97.62	109.72
1	B	356	ASP	CA-CB-CG	6.28	118.88	112.60
1	B	96	PRO	CB-CA-C	6.22	118.51	110.92
1	B	80	THR	CB-CA-C	6.18	122.00	110.70
1	A	362	ASN	N-CA-C	-6.15	105.74	113.18
1	B	131	LEU	CA-C-N	6.14	130.02	120.75
1	B	131	LEU	C-N-CA	6.14	130.02	120.75
1	B	394	PRO	N-CA-C	6.10	125.04	112.47
1	A	428	GLY	CA-C-N	5.99	128.23	120.44
1	A	428	GLY	C-N-CA	5.99	128.23	120.44
1	B	441	THR	CA-CB-OG1	-5.88	100.78	109.60
1	B	31	GLN	CB-CA-C	5.83	121.42	111.68
1	B	81	LYS	CB-CA-C	-5.83	101.73	110.24
1	B	362	ASN	N-CA-C	-5.68	102.99	110.43
1	B	341	GLU	CA-C-O	-5.59	115.63	121.55
1	B	113	ASP	CA-CB-CG	5.57	118.17	112.60
1	A	20	PHE	CA-C-O	-5.54	114.57	121.50
1	A	64	ASP	CA-CB-CG	5.43	118.03	112.60
1	A	343	VAL	N-CA-CB	5.37	116.94	110.33
1	B	409	GLU	CB-CG-CD	5.31	121.63	112.60
1	A	268	VAL	N-CA-C	-5.27	104.31	110.05
1	B	13	PRO	CB-CA-C	-5.25	104.68	112.55
1	A	284	ILE	N-CA-C	-5.24	108.02	113.10
1	B	219	ASP	CA-CB-CG	5.20	117.80	112.60
1	A	102	THR	CA-CB-OG1	-5.17	101.84	109.60
1	A	197	GLN	N-CA-C	-5.11	104.84	111.74
1	A	356	ASP	CA-C-N	5.10	127.37	120.38
1	A	356	ASP	C-N-CA	5.10	127.37	120.38
1	A	20	PHE	CA-C-N	5.04	129.05	120.88
1	A	20	PHE	C-N-CA	5.04	129.05	120.88
1	A	150	ASN	CB-CA-C	5.04	119.14	111.02
1	B	219	ASP	N-CA-C	-5.03	105.19	113.50
1	B	249	THR	CA-CB-OG1	-5.02	102.07	109.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	429	SER	Peptide
1	B	137	VAL	Peptide
1	B	59	GLY	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	3307	0	3152	114	0
1	B	3340	0	3183	115	0
2	A	1	0	0	0	0
2	B	2	0	0	0	0
3	A	8	0	0	2	0
3	B	7	0	0	0	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
All	All	6673	0	6335	229	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 18.

All (229) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:SER:OG	1:B:334:PRO:HD3	1.41	1.17
1:A:19:LEU:HD12	1:A:20:PHE:O	1.48	1.11
1:A:306:ARG:HB2	1:A:307:PRO:HD3	1.21	1.09
1:A:274:LEU:CD2	1:A:299:ILE:HD11	1.81	1.09
1:A:306:ARG:HB2	1:A:307:PRO:CD	1.84	1.05
1:A:267:ASN:ND2	1:A:270:GLY:O	1.90	1.04
1:B:250:ASP:OD2	1:B:257:ALA:HA	1.60	0.99
1:B:95:THR:HB	1:B:96:PRO:HD3	1.48	0.94
1:A:299:ILE:HG22	1:A:314:GLY:HA3	1.49	0.94
1:A:218:ASN:HD22	1:A:305:GLY:HA3	1.33	0.93
1:B:5:ARG:CZ	1:B:7:SER:HB3	2.03	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:GLU:O	1:B:342:ASN:CG	2.17	0.87
1:B:333:SER:OG	1:B:334:PRO:CD	2.23	0.87
1:A:144:ASP:OD2	1:A:146:ASP:HB2	1.75	0.86
1:A:4:GLY:HA2	1:A:40:GLY:HA2	1.58	0.85
1:A:338:THR:HB	1:A:443:LEU:HD11	1.58	0.85
1:A:19:LEU:CD1	1:A:20:PHE:O	2.26	0.84
1:A:299:ILE:CG2	1:A:314:GLY:HA3	2.08	0.83
1:A:274:LEU:HD21	1:A:299:ILE:HD11	1.61	0.81
1:B:95:THR:HB	1:B:96:PRO:CD	2.11	0.79
1:A:274:LEU:HD23	1:A:299:ILE:HD11	1.65	0.78
1:B:306:ARG:HG2	1:B:307:PRO:HD2	1.66	0.78
1:A:299:ILE:HG22	1:A:314:GLY:CA	2.14	0.76
1:A:237:VAL:CG2	1:A:241:THR:HG21	2.16	0.76
1:B:340:LEU:O	1:B:343:VAL:HG23	1.86	0.75
1:B:397:ILE:HG22	1:B:404:ILE:HG12	1.71	0.73
1:B:306:ARG:HG2	1:B:308:PRO:HD2	1.71	0.72
1:A:328:PRO:O	1:A:329:ILE:HG13	1.88	0.72
1:A:139:THR:HG22	1:A:173:VAL:HG23	1.69	0.72
1:B:50:GLU:HG2	1:B:55:GLU:OE2	1.89	0.72
1:A:274:LEU:CD2	1:A:299:ILE:CD1	2.63	0.71
1:B:308:PRO:O	1:B:309:LEU:C	2.33	0.71
1:B:259:ILE:HD11	1:B:301:ALA:HB1	1.71	0.71
1:B:398:HIS:HB3	1:B:401:SER:HB2	1.72	0.70
1:B:306:ARG:CG	1:B:307:PRO:HD2	2.21	0.70
1:A:218:ASN:ND2	1:A:305:GLY:HA3	2.07	0.69
1:B:306:ARG:HG2	1:B:307:PRO:CD	2.24	0.68
1:A:4:GLY:HA2	1:A:40:GLY:CA	2.23	0.68
1:B:157:VAL:HG23	1:B:190:LEU:HD21	1.76	0.68
1:A:140:ILE:HD11	1:A:192:VAL:HG11	1.76	0.67
1:B:83:THR:HG22	1:B:107:LEU:HD13	1.78	0.66
1:A:356:ASP:HB3	1:A:363:ALA:HA	1.79	0.65
1:A:429:SER:HB2	1:A:430:PRO:CD	2.28	0.64
1:A:112:ASN:HB2	1:A:150:ASN:OD1	1.98	0.64
1:B:5:ARG:CZ	1:B:7:SER:CB	2.76	0.63
1:B:52:LEU:HD21	1:B:85:VAL:HG12	1.80	0.63
1:B:306:ARG:HD2	1:B:308:PRO:HG2	1.78	0.63
1:B:163:ASP:OD1	1:B:164:VAL:HG23	1.99	0.63
1:B:306:ARG:CG	1:B:308:PRO:HD2	2.28	0.63
1:B:342:ASN:OD1	1:B:342:ASN:C	2.42	0.62
1:A:83:THR:HG22	1:A:107:LEU:HD12	1.81	0.62
1:B:217:GLU:HA	1:B:306:ARG:NH1	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:SER:HG	1:B:334:PRO:HD3	1.57	0.61
1:A:237:VAL:HG22	1:A:241:THR:HG21	1.82	0.61
1:B:256:ASN:HA	1:B:305:GLY:HA3	1.83	0.61
1:B:152:ASN:O	1:B:197:GLN:HB2	2.01	0.61
1:A:41:GLU:HG2	1:A:42:GLU:HG2	1.83	0.60
1:A:112:ASN:OD1	3:A:503:CA:CA	1.78	0.60
1:A:19:LEU:HD11	1:A:76:LEU:HD12	1.83	0.60
1:A:250:ASP:HB3	1:A:257:ALA:HA	1.84	0.59
1:B:302:GLN:CD	1:B:309:LEU:HD21	2.28	0.58
1:A:234:PRO:HB2	1:A:236:ASP:OD1	2.02	0.58
1:B:5:ARG:HB2	1:B:38:ILE:HB	1.84	0.58
1:A:64:ASP:O	1:A:67:THR:O	2.20	0.58
1:A:8:LEU:HD11	1:A:34:ALA:HB1	1.84	0.58
1:A:303:ASP:OD2	3:A:506:CA:CA	1.79	0.58
1:A:421:GLY:HA2	1:A:437:SER:HA	1.85	0.58
1:A:63:ILE:HG22	1:A:70:VAL:HG22	1.85	0.58
1:A:367:TYR:HB3	1:A:397:ILE:HD11	1.87	0.57
1:A:140:ILE:CD1	1:A:192:VAL:HG11	2.34	0.57
1:A:63:ILE:HA	1:A:69:ALA:O	2.06	0.56
1:A:327:GLU:HB2	1:A:432:MET:HE3	1.87	0.56
1:B:222:PRO:HB2	1:B:259:ILE:HD12	1.86	0.56
1:A:299:ILE:HG22	1:A:314:GLY:C	2.30	0.55
1:A:234:PRO:CB	1:A:236:ASP:OD1	2.54	0.55
1:B:222:PRO:CB	1:B:259:ILE:HD12	2.36	0.55
1:B:222:PRO:HB2	1:B:259:ILE:CD1	2.37	0.55
1:B:96:PRO:CD	1:B:96:PRO:O	2.54	0.54
1:A:4:GLY:CA	1:A:40:GLY:CA	2.85	0.54
1:B:78:ARG:NH2	1:B:79:GLU:OE2	2.41	0.54
1:A:168:ASN:HB3	1:A:171:SER:HB3	1.90	0.54
1:A:410:LEU:CD1	1:A:418:TYR:OH	2.56	0.54
1:B:327:GLU:HB3	1:B:432:MET:HB3	1.91	0.54
1:B:110:ASP:OD2	1:B:147:SER:HB2	2.09	0.53
1:A:128:ARG:HH12	1:A:217:GLU:CD	2.18	0.52
1:B:304:GLY:HA2	1:B:309:LEU:HG	1.91	0.52
1:A:95:THR:O	1:A:97:PRO:HD3	2.10	0.52
1:A:150:ASN:N	1:A:150:ASN:HD22	2.07	0.52
1:B:364:ARG:NH1	1:B:427:HIS:CE1	2.78	0.52
1:A:409:GLU:O	1:A:410:LEU:HG	2.10	0.52
1:B:270:GLY:O	1:B:271:GLN:HB2	2.09	0.52
1:B:303:ASP:OD1	1:B:303:ASP:O	2.28	0.52
1:B:267:ASN:ND2	1:B:270:GLY:O	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:ASN:CG	1:B:251:ARG:HB2	2.35	0.52
1:A:358:ASP:O	1:A:363:ALA:HB2	2.11	0.52
1:B:228:ASN:OD1	1:B:229:TYR:O	2.27	0.52
1:B:235:GLU:HG2	1:B:323:VAL:HG23	1.92	0.51
1:B:154:ARG:HB3	1:B:195:ASN:HD21	1.75	0.51
1:A:19:LEU:HD12	1:A:20:PHE:N	2.25	0.51
1:B:426:ASP:OD1	1:B:432:MET:N	2.43	0.51
1:B:133:VAL:HG22	1:B:178:ALA:HA	1.91	0.51
1:A:241:THR:HG22	1:A:283:VAL:CG2	2.40	0.51
1:B:147:SER:HB3	1:B:149:ILE:HD12	1.91	0.51
1:B:341:GLU:O	1:B:342:ASN:OD1	2.28	0.51
1:B:148:PRO:C	1:B:150:ASN:O	2.54	0.51
1:B:149:ILE:CG2	1:B:199:ARG:NH2	2.74	0.51
1:A:340:LEU:HB2	1:A:343:VAL:HG13	1.93	0.50
1:B:250:ASP:HB3	1:B:257:ALA:HB1	1.92	0.50
1:A:224:PHE:CZ	1:A:299:ILE:HG23	2.47	0.50
1:B:429:SER:CB	1:B:430:PRO:CD	2.90	0.50
1:A:298:SER:HA	1:A:314:GLY:O	2.11	0.50
1:A:64:ASP:HB3	1:A:69:ALA:HB3	1.94	0.50
1:B:182:ARG:NH2	1:B:252:ASP:HA	2.27	0.49
1:A:46:SER:HG	1:A:93:TYR:HH	1.56	0.49
1:A:118:PHE:CD2	1:A:208:ALA:HB2	2.47	0.49
1:A:299:ILE:HG23	1:A:314:GLY:HA3	1.94	0.49
1:A:410:LEU:HD12	1:A:418:TYR:OH	2.12	0.49
1:B:322:ASP:CB	1:B:359:SER:HB3	2.41	0.49
1:B:339:VAL:O	1:B:339:VAL:HG13	2.13	0.49
1:A:125:GLU:C	1:A:126:ARG:HG2	2.38	0.48
1:A:429:SER:HB2	1:A:430:PRO:HD3	1.94	0.48
1:B:191:LEU:HD12	1:B:192:VAL:N	2.27	0.48
1:B:150:ASN:HB3	1:B:196:ASP:OD2	2.13	0.48
1:A:4:GLY:CA	1:A:40:GLY:HA3	2.43	0.48
1:B:199:ARG:O	1:B:200:ASN:C	2.56	0.48
1:A:19:LEU:HD12	1:A:19:LEU:C	2.39	0.48
1:A:125:GLU:HG3	1:A:138:LEU:HD22	1.94	0.48
1:A:268:VAL:HG12	1:A:269:ALA:N	2.29	0.48
1:A:271:GLN:O	1:A:272:PHE:CD2	2.67	0.47
1:A:303:ASP:HB2	1:A:309:LEU:H	1.79	0.47
1:A:21:GLU:CG	1:A:78:ARG:H	2.26	0.47
1:A:324:ASN:ND2	1:A:426:ASP:OD2	2.46	0.47
1:A:155:TYR:HA	1:A:193:GLU:O	2.14	0.47
1:A:165:PHE:CE2	1:A:212:ILE:HD13	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:ASN:N	1:A:150:ASN:ND2	2.61	0.47
1:B:196:ASP:HB2	1:B:204:LEU:O	2.14	0.47
1:A:4:GLY:CA	1:A:40:GLY:HA2	2.37	0.47
1:A:250:ASP:OD2	1:A:252:ASP:HB2	2.15	0.47
1:A:271:GLN:O	1:A:272:PHE:CG	2.68	0.47
1:B:41:GLU:HG2	1:B:42:GLU:H	1.80	0.47
1:B:112:ASN:HD21	1:B:204:LEU:HB2	1.78	0.47
1:B:430:PRO:O	1:B:432:MET:HE3	2.15	0.47
1:B:196:ASP:C	1:B:198:GLY:N	2.69	0.47
1:B:309:LEU:HD23	1:B:309:LEU:O	2.14	0.47
1:B:340:LEU:HB2	1:B:343:VAL:HG23	1.96	0.47
1:A:237:VAL:CG2	1:A:241:THR:CG2	2.91	0.46
1:B:356:ASP:HB3	1:B:363:ALA:HA	1.96	0.46
1:B:231:VAL:HG11	1:B:244:LEU:HB2	1.98	0.46
1:A:262:SER:O	1:A:299:ILE:HD12	2.15	0.46
1:B:200:ASN:HB3	1:B:201:PRO:HD3	1.97	0.46
1:B:361:GLU:HA	1:B:361:GLU:OE1	2.16	0.46
1:A:50:GLU:OE2	1:A:87:ARG:NH2	2.49	0.45
1:A:113:ASP:OD1	1:A:114:HIS:N	2.50	0.45
1:A:278:SER:HB3	1:A:280:ILE:HG13	1.98	0.45
1:B:424:ALA:O	1:B:433:SER:HA	2.16	0.45
1:B:87:ARG:HG3	1:B:103:TYR:CE2	2.51	0.45
1:B:441:THR:O	1:B:441:THR:OG1	2.34	0.45
1:B:287:LEU:HD23	1:B:320:VAL:HG22	1.99	0.45
1:A:138:LEU:HD23	1:A:174:VAL:HG21	1.98	0.45
1:A:130:ASN:HA	1:A:179:VAL:HG22	1.99	0.45
1:B:182:ARG:HG2	1:B:186:ALA:HB2	1.98	0.44
1:B:225:SER:HB2	1:B:229:TYR:OH	2.18	0.44
1:B:359:SER:O	1:B:362:ASN:O	2.35	0.44
1:A:23:GLU:O	1:A:24:PRO:C	2.59	0.44
1:B:303:ASP:OD1	1:B:310:ILE:N	2.50	0.44
1:A:21:GLU:HG3	1:A:78:ARG:H	1.82	0.44
1:B:5:ARG:NE	1:B:7:SER:HB3	2.32	0.44
1:A:30:LEU:HD22	1:A:104:ILE:HD12	1.99	0.44
1:B:112:ASN:ND2	1:B:204:LEU:HD13	2.32	0.44
1:B:160:GLY:O	1:B:161:ALA:HB3	2.18	0.43
1:B:292:VAL:HG11	1:B:295:TYR:CE1	2.53	0.43
1:A:63:ILE:CG2	1:A:70:VAL:HG22	2.48	0.43
1:B:8:LEU:HD11	1:B:34:ALA:HB1	1.99	0.43
1:B:154:ARG:HG2	1:B:169:GLU:HB3	2.00	0.43
1:B:235:GLU:OE1	1:B:323:VAL:N	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:361:GLU:C	1:B:362:ASN:O	2.53	0.43
1:B:429:SER:HB3	1:B:430:PRO:HD3	2.00	0.43
1:A:149:ILE:HD13	1:A:149:ILE:HA	1.77	0.43
1:A:32:LEU:HD13	1:A:88:VAL:HG11	2.01	0.43
1:B:227:GLN:CD	1:B:227:GLN:H	2.26	0.43
1:A:273:TYR:CD1	1:A:273:TYR:C	2.97	0.43
1:A:340:LEU:HB2	1:A:343:VAL:CG1	2.49	0.43
1:B:147:SER:O	1:B:150:ASN:O	2.36	0.42
1:A:19:LEU:O	1:A:109:LYS:HG3	2.20	0.42
1:A:129:GLU:HA	1:A:180:LEU:HB2	2.00	0.42
1:A:32:LEU:O	1:A:68:GLY:HA3	2.19	0.42
1:A:112:ASN:HD21	1:A:204:LEU:HB2	1.83	0.42
1:B:61:PHE:CD1	1:B:86:LEU:HD11	2.54	0.42
1:A:12:MET:HB2	1:A:15:TYR:CZ	2.55	0.42
1:B:91:VAL:HG22	1:B:99:SER:HB2	2.02	0.42
1:B:135:TYR:O	1:B:175:SER:HA	2.19	0.42
1:A:4:GLY:C	1:A:98:ARG:HH22	2.28	0.41
1:A:111:THR:O	1:A:201:PRO:HD3	2.20	0.41
1:B:20:PHE:CD1	1:B:109:LYS:HB2	2.55	0.41
1:B:343:VAL:HG11	1:B:347:TYR:CD1	2.55	0.41
1:B:343:VAL:CG1	1:B:347:TYR:CG	3.03	0.41
1:A:20:PHE:CZ	1:A:109:LYS:HD2	2.55	0.41
1:A:278:SER:HB3	1:A:280:ILE:CG1	2.51	0.41
1:B:115:SER:O	1:B:116:PRO:C	2.62	0.41
1:B:366:HIS:ND1	1:B:399:ASN:HB3	2.35	0.41
1:B:5:ARG:NE	1:B:37:THR:OG1	2.52	0.41
1:A:164:VAL:O	1:A:177:ARG:HB2	2.20	0.41
1:A:340:LEU:CB	1:A:343:VAL:HG13	2.50	0.41
1:B:193:GLU:HB2	1:B:207:THR:HG22	2.02	0.41
1:B:426:ASP:OD1	1:B:432:MET:O	2.39	0.41
1:B:164:VAL:HG11	1:B:188:TYR:CE2	2.56	0.41
1:B:345:LEU:HD13	1:B:345:LEU:HA	1.91	0.41
1:B:96:PRO:O	1:B:96:PRO:HD2	2.21	0.41
1:A:111:THR:HA	1:A:200:ASN:HB3	2.02	0.41
1:A:241:THR:HG22	1:A:283:VAL:HG22	2.02	0.41
1:B:340:LEU:HB2	1:B:343:VAL:CG2	2.51	0.41
1:A:229:TYR:HD2	1:A:244:LEU:HD21	1.86	0.41
1:B:112:ASN:HB3	1:B:201:PRO:HD2	2.03	0.41
1:B:252:ASP:HB3	1:B:256:ASN:HB3	2.01	0.41
1:B:255:GLN:C	1:B:257:ALA:H	2.27	0.41
1:A:20:PHE:CE1	1:A:109:LYS:HD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:PHE:CE2	1:A:440:ILE:HD12	2.56	0.40
1:B:94:SER:OG	1:B:96:PRO:HD2	2.20	0.40
1:B:23:GLU:HA	1:B:24:PRO:HD3	1.85	0.40
1:A:64:ASP:CB	1:A:69:ALA:HB3	2.52	0.40
1:A:112:ASN:ND2	1:A:204:LEU:HB2	2.36	0.40
1:A:234:PRO:HB3	1:A:236:ASP:OD1	2.21	0.40
1:A:393:PHE:CE2	1:A:395:PHE:HB2	2.56	0.40
1:B:32:LEU:HD23	1:B:32:LEU:HA	1.95	0.40
1:A:192:VAL:O	1:A:207:THR:HB	2.21	0.40
1:B:343:VAL:HG12	1:B:347:TYR:HB3	2.02	0.40
1:A:307:PRO:HA	1:A:308:PRO:HD2	1.90	0.40
1:B:32:LEU:O	1:B:68:GLY:HA3	2.22	0.40
1:B:111:THR:HA	1:B:200:ASN:CB	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	418/457 (92%)	363 (87%)	55 (13%)	0	100	100
1	B	423/457 (93%)	351 (83%)	72 (17%)	0	100	100
All	All	841/914 (92%)	714 (85%)	127 (15%)	0	100	100

There are no Ramachandran outliers to report.

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	368/395 (93%)	354 (96%)	14 (4%)	29	55
1	B	372/395 (94%)	357 (96%)	15 (4%)	28	53
All	All	740/790 (94%)	711 (96%)	29 (4%)	28	54

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	VAL
1	A	91	VAL
1	A	95	THR
1	A	139	THR
1	A	149	ILE
1	A	150	ASN
1	A	187	GLU
1	A	213	GLU
1	A	230	VAL
1	A	231	VAL
1	A	233	VAL
1	A	400	SER
1	A	415	VAL
1	A	425	VAL
1	B	41	GLU
1	B	42	GLU
1	B	52	LEU
1	B	117	VAL
1	B	132	GLU
1	B	226	GLU
1	B	243	VAL
1	B	246	VAL
1	B	283	VAL
1	B	310	ILE
1	B	355	VAL
1	B	396	GLN
1	B	400	SER
1	B	404	ILE
1	B	432	MET

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

Mol	Chain	Res	Type
1	A	16	GLN
1	A	267	ASN
1	A	302	GLN
1	A	336	GLN
1	B	31	GLN
1	B	152	ASN
1	B	195	ASN
1	B	197	GLN
1	B	253	GLN
1	B	255	GLN
1	B	267	ASN
1	B	399	ASN
1	B	446	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 18 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	422/457 (92%)	-0.28	1 (0%) 91 80	94, 133, 171, 213	0
1	B	427/457 (93%)	-0.29	7 (1%) 70 42	78, 130, 172, 219	0
All	All	849/914 (92%)	-0.28	8 (0%) 81 56	78, 131, 172, 219	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	445	VAL	3.9
1	B	391	PRO	3.2
1	B	314	GLY	3.0
1	B	149	ILE	2.4
1	B	200	ASN	2.2
1	B	373	ALA	2.2
1	B	307	PRO	2.2
1	A	371	ASP	2.2

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

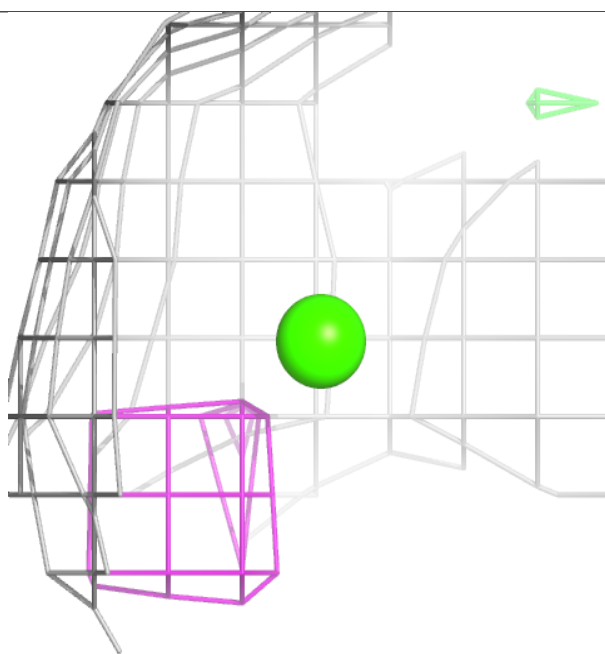
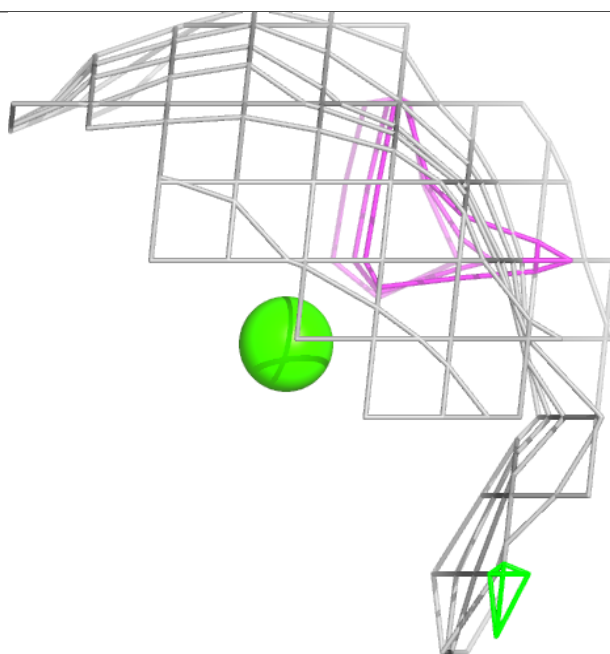
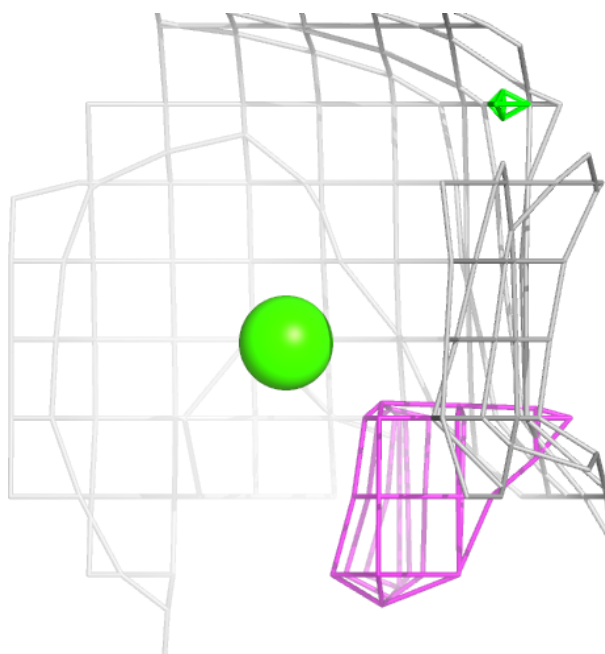
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CA	B	507	1/1	0.92	0.07	151,151,151,151	0
3	CA	A	507	1/1	0.95	0.07	175,175,175,175	0
2	NA	A	501	1/1	0.97	0.04	111,111,111,111	0
3	CA	B	503	1/1	0.97	0.05	125,125,125,125	0
2	NA	B	502	1/1	0.97	0.04	103,103,103,103	0
2	NA	B	504	1/1	0.98	0.05	95,95,95,95	0
3	CA	A	502	1/1	0.98	0.04	125,125,125,125	0
3	CA	A	504	1/1	0.98	0.04	135,135,135,135	0
3	CA	A	503	1/1	0.99	0.04	121,121,121,121	0
3	CA	B	506	1/1	0.99	0.03	122,122,122,122	0
3	CA	A	509	1/1	0.99	0.02	110,110,110,110	0
3	CA	B	509	1/1	0.99	0.03	93,93,93,93	0
3	CA	A	505	1/1	1.00	0.02	121,121,121,121	0
3	CA	B	505	1/1	1.00	0.02	142,142,142,142	0
3	CA	A	508	1/1	1.00	0.04	109,109,109,109	0
3	CA	A	506	1/1	1.00	0.02	122,122,122,122	0
3	CA	B	508	1/1	1.00	0.02	86,86,86,86	0
3	CA	B	501	1/1	1.00	0.02	108,108,108,108	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.

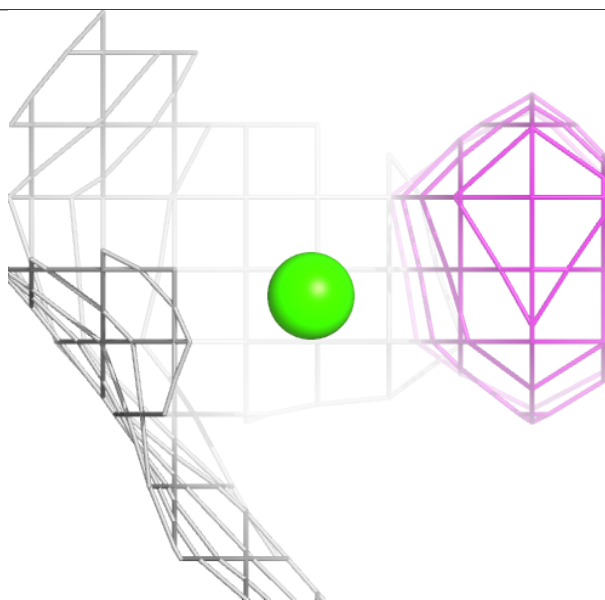
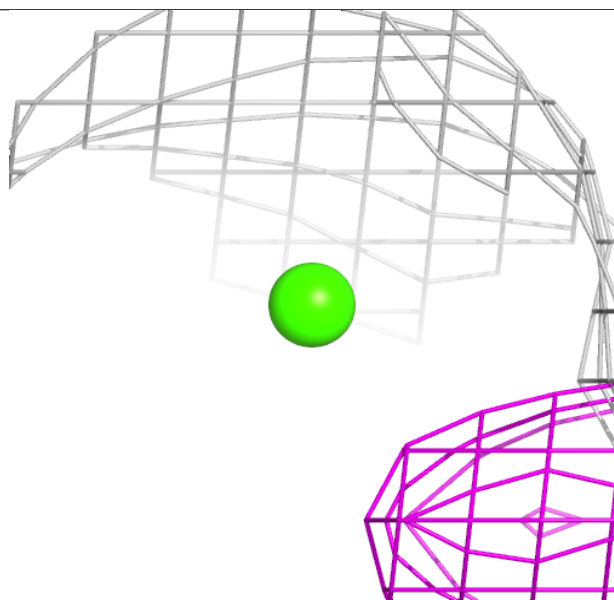
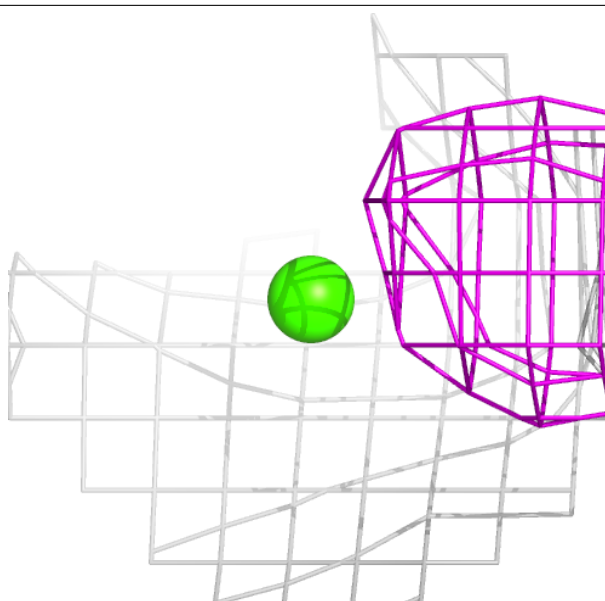
Electron density around CA B 507:

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



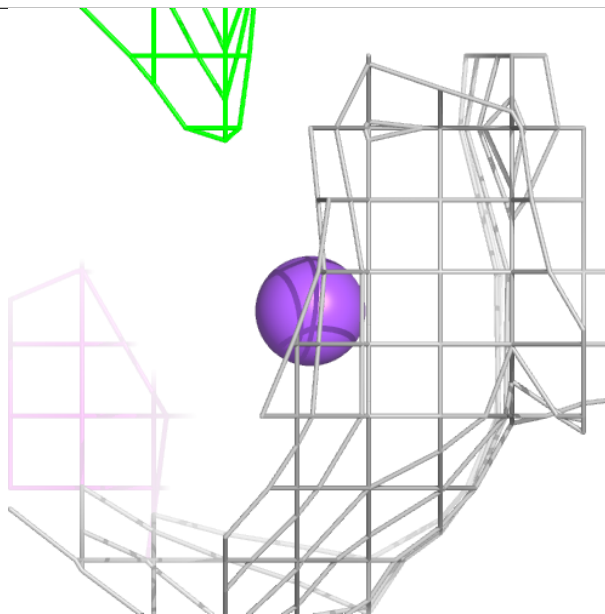
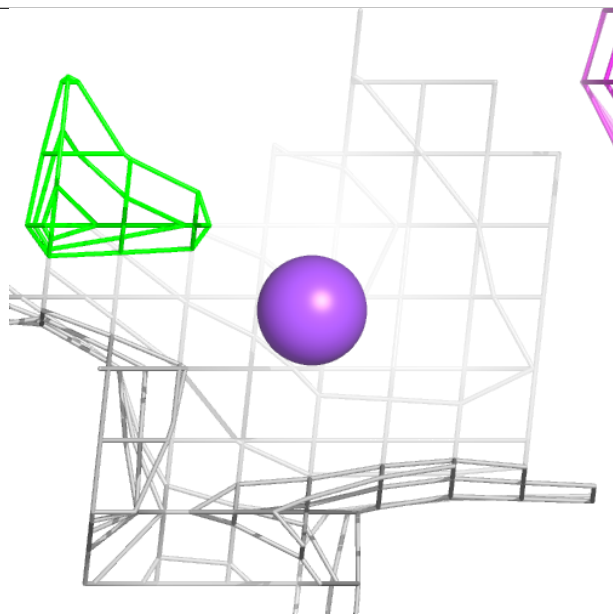
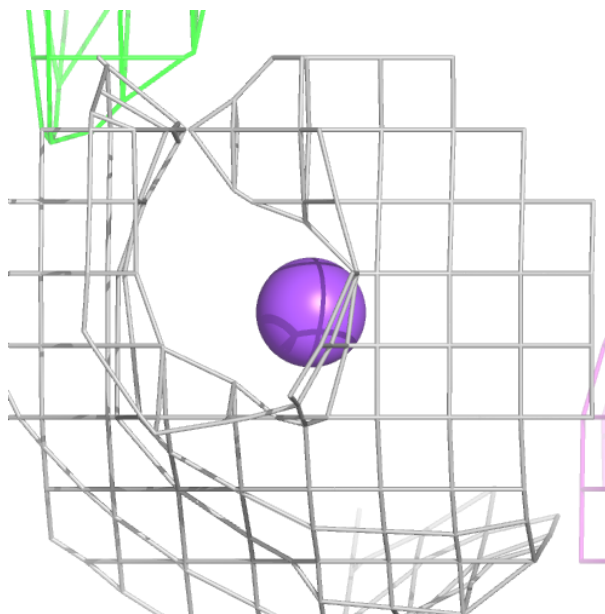
Electron density around CA A 507:

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



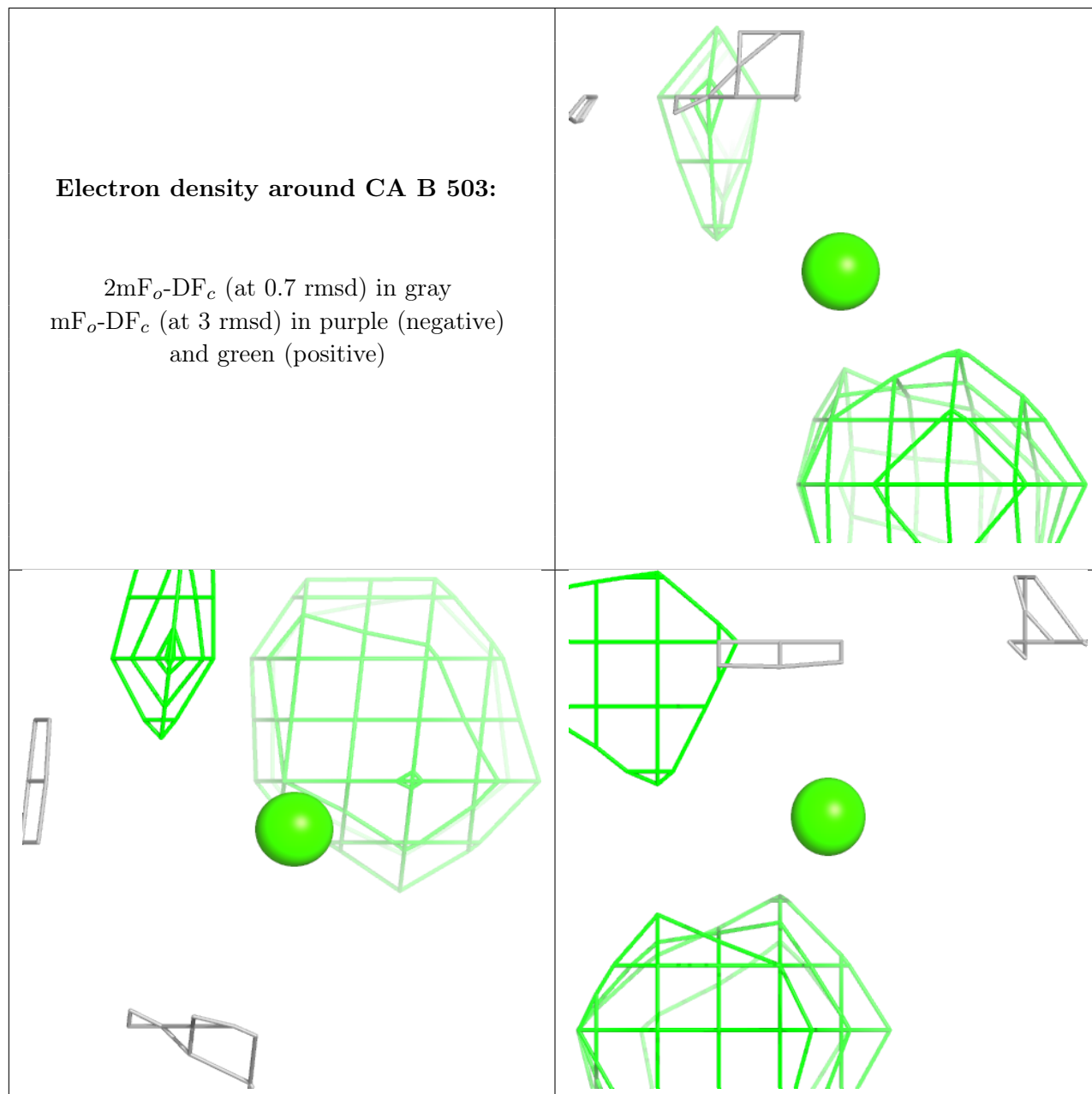
Electron density around NA A 501:

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



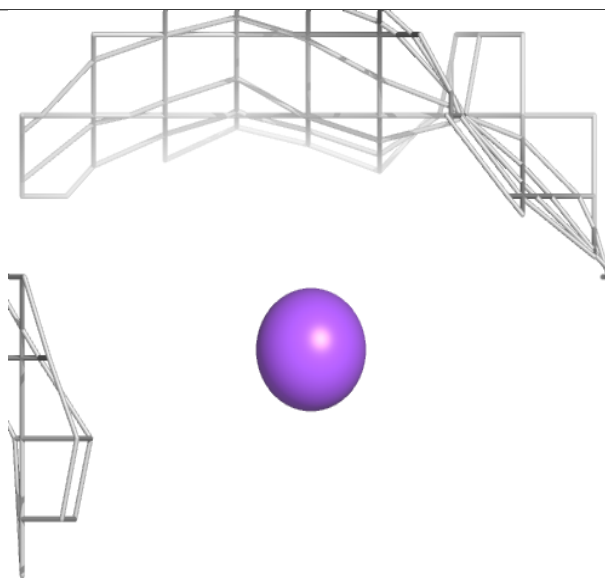
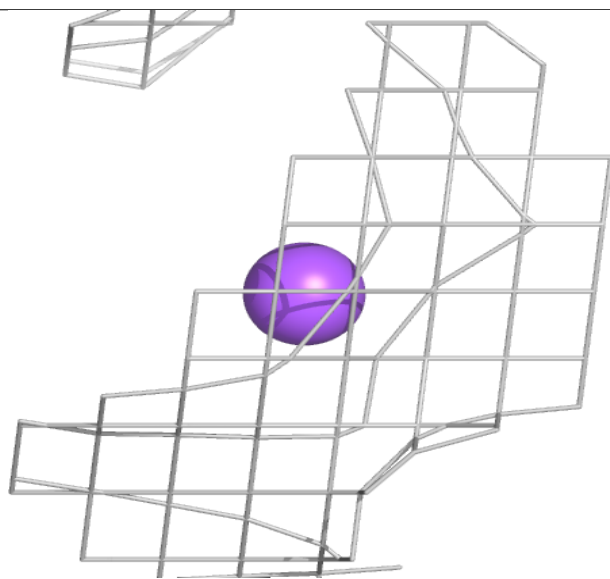
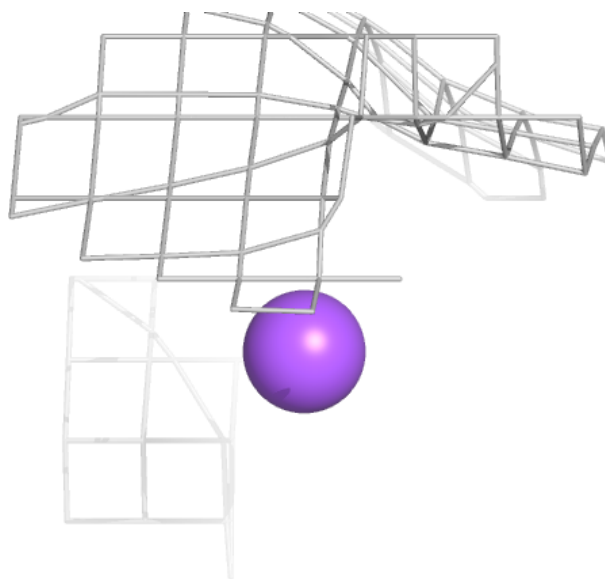
Electron density around CA B 503:

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



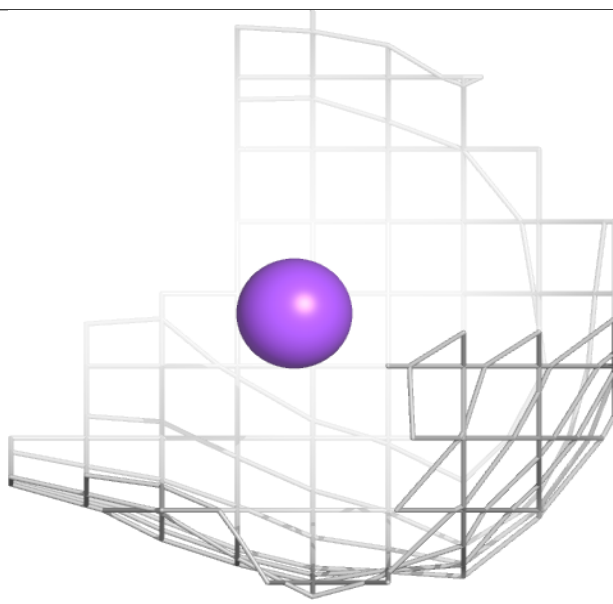
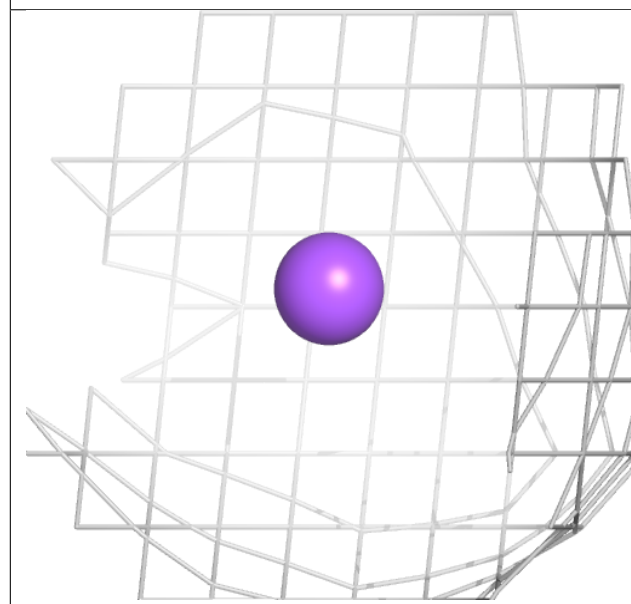
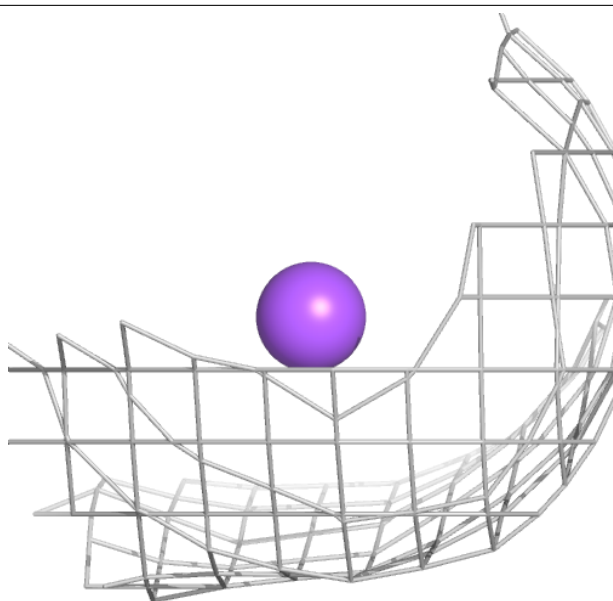
Electron density around NA B 502:

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



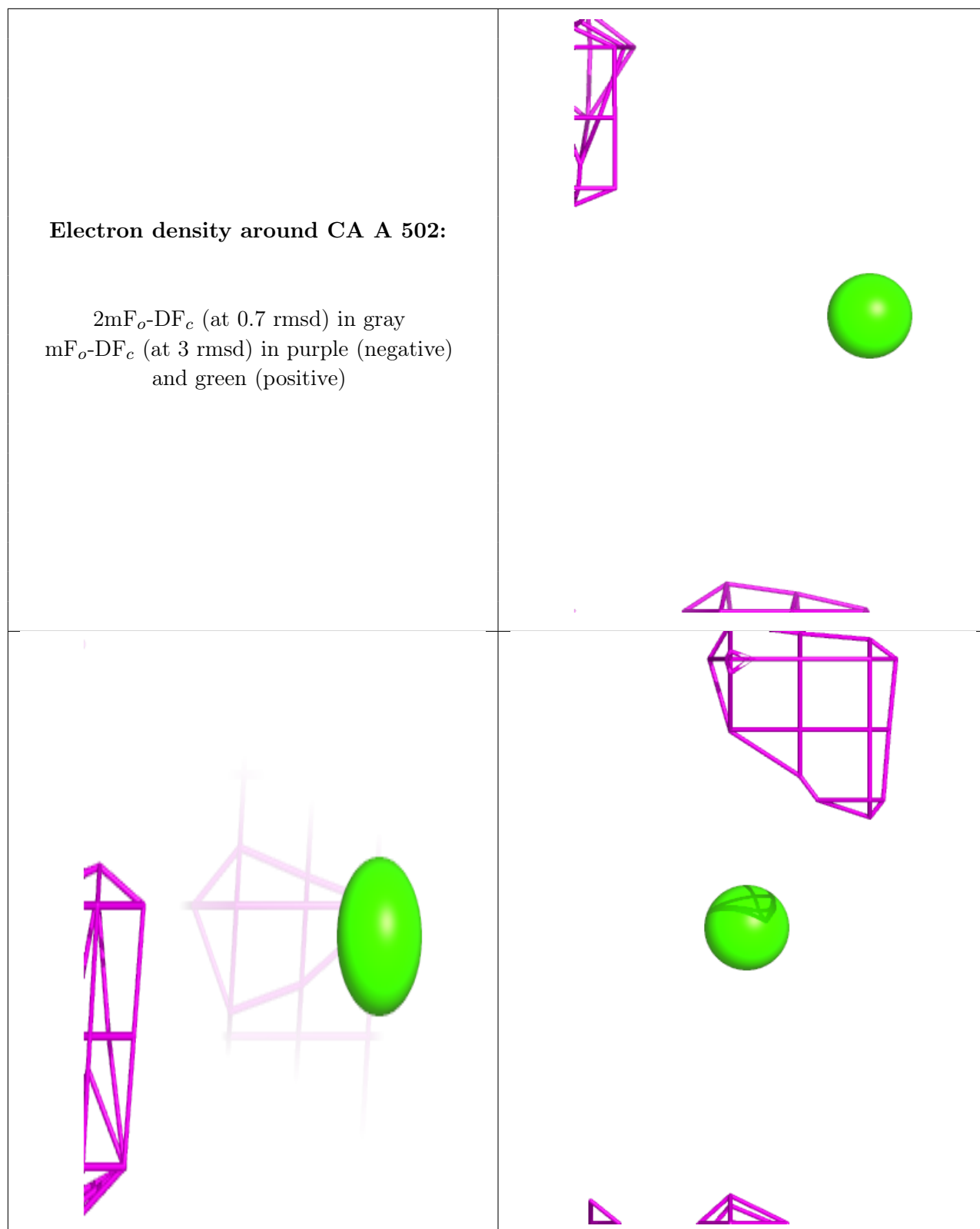
Electron density around NA B 504:

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



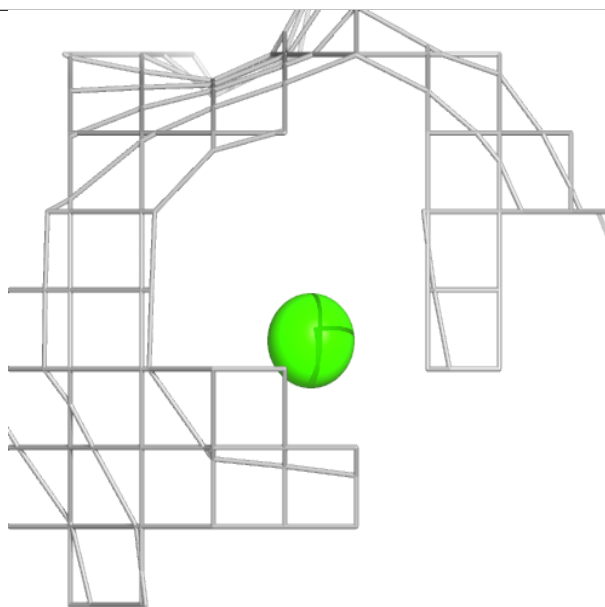
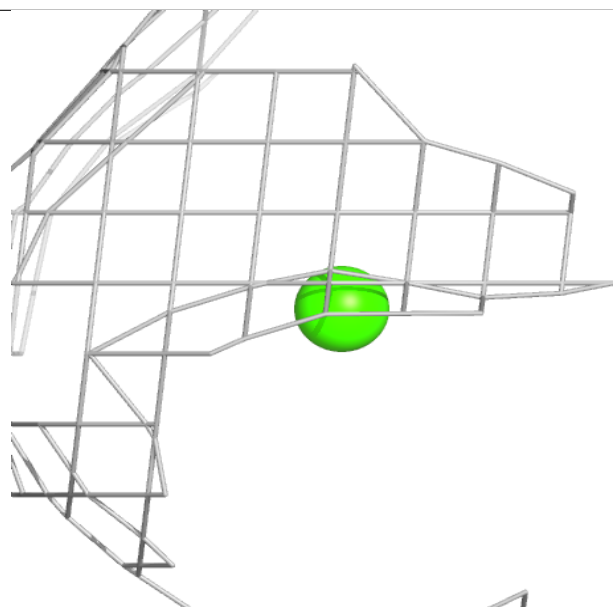
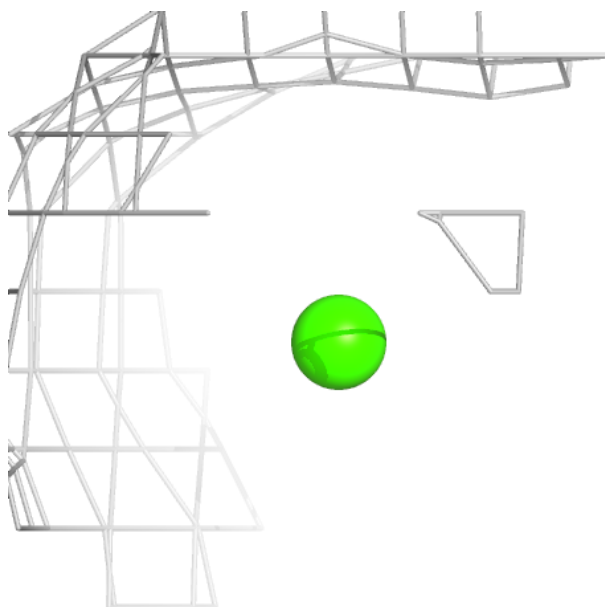
Electron density around CA A 502:

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



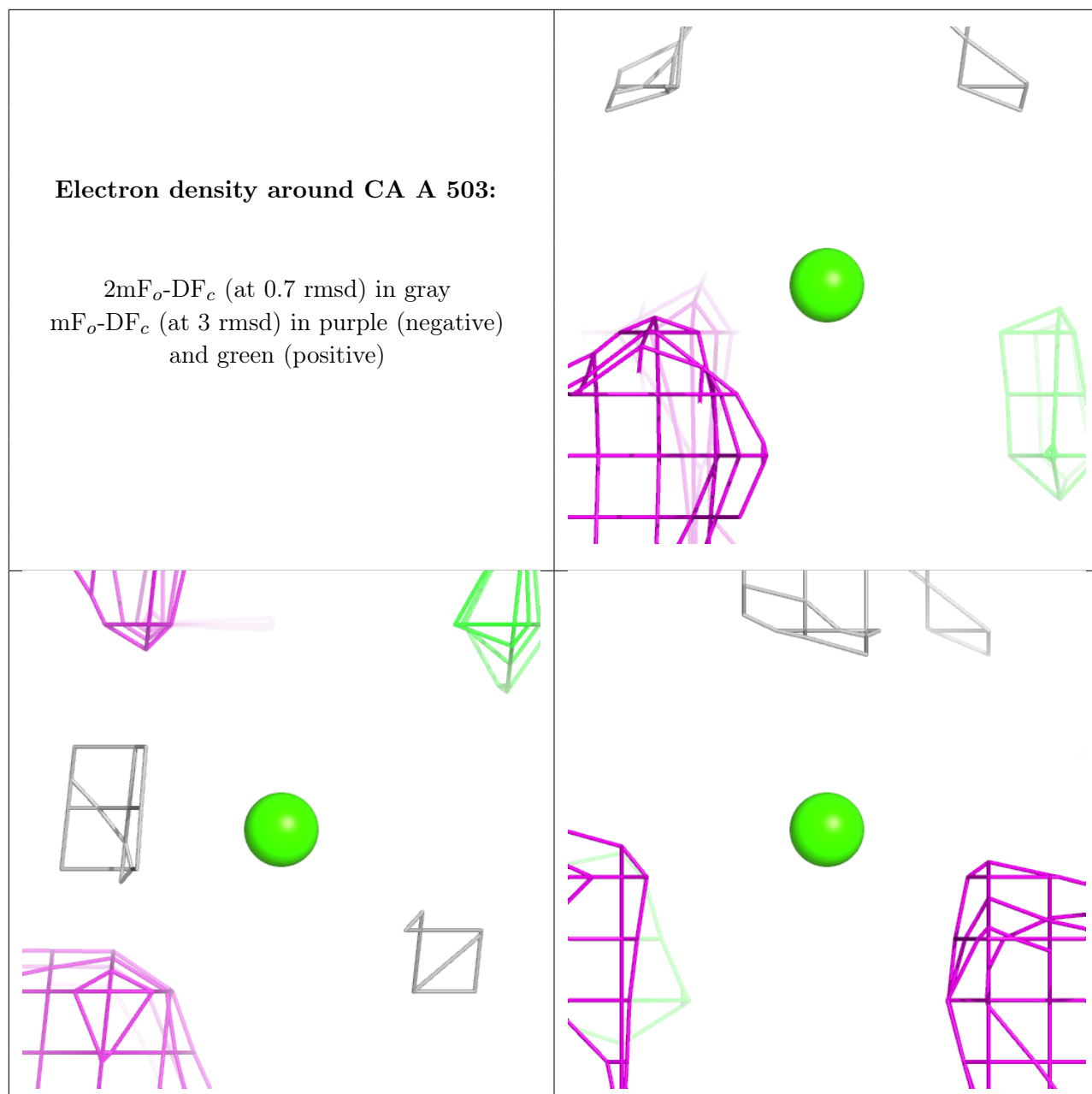
Electron density around CA A 504:

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



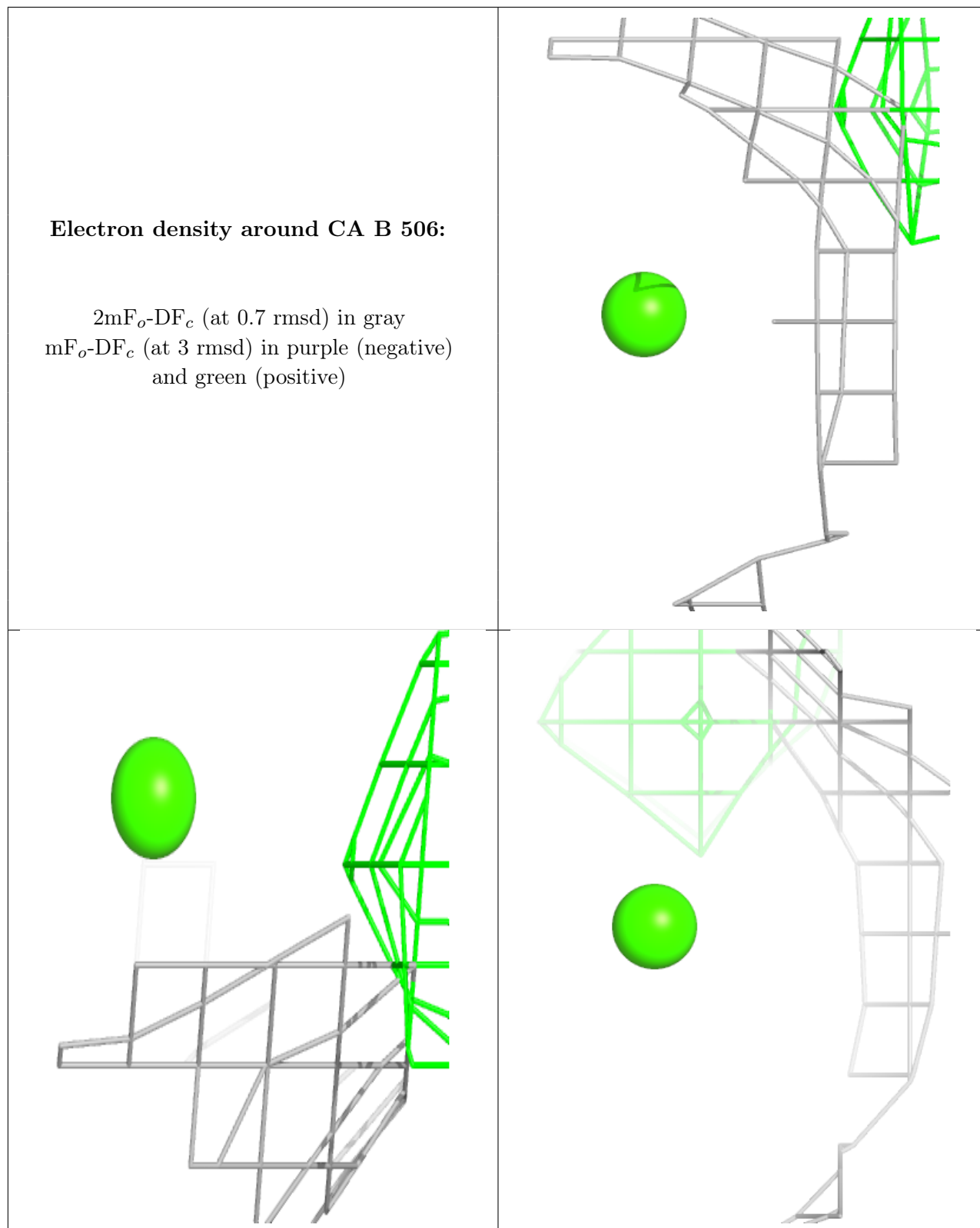
Electron density around CA A 503:

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



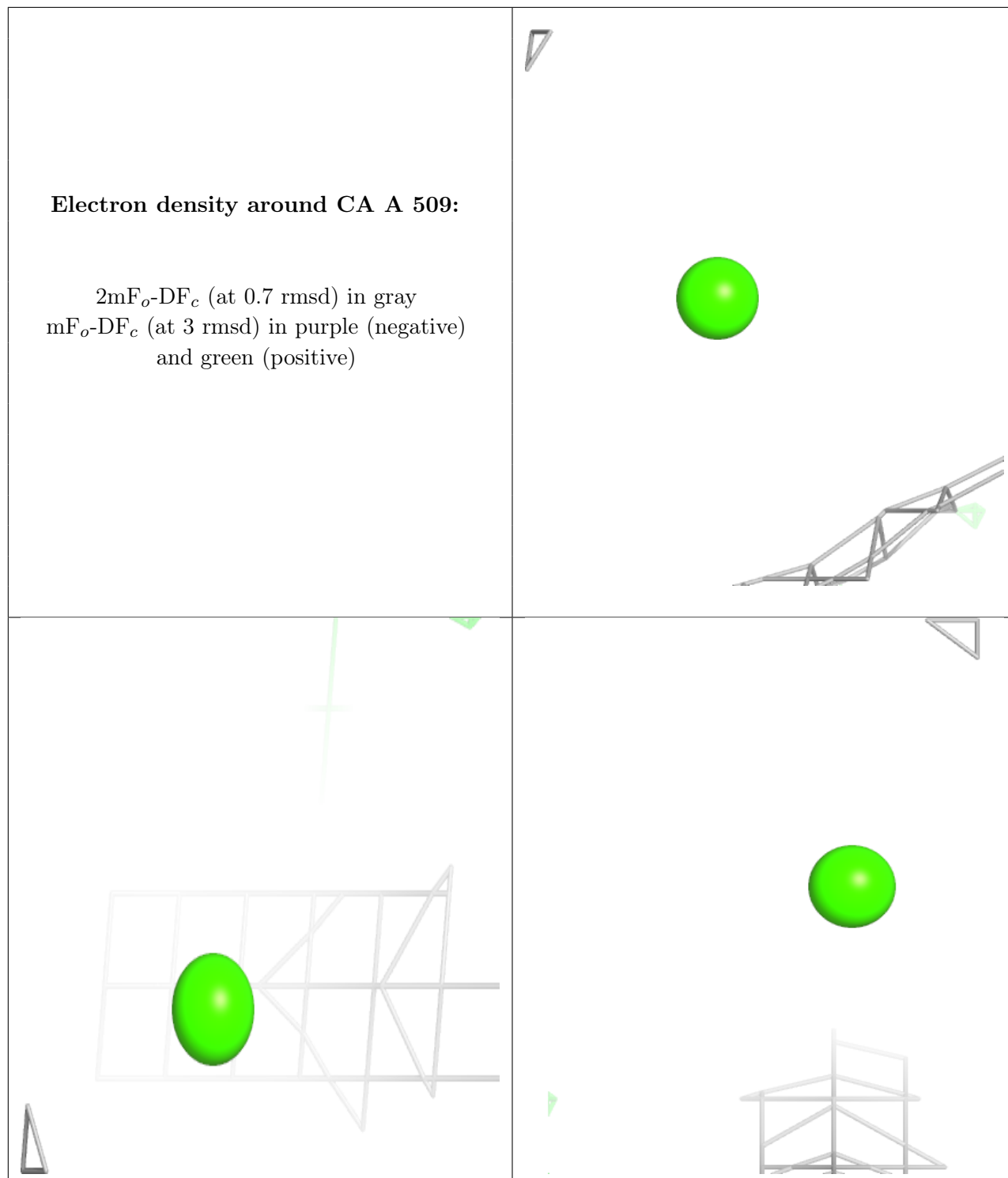
Electron density around CA B 506:

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



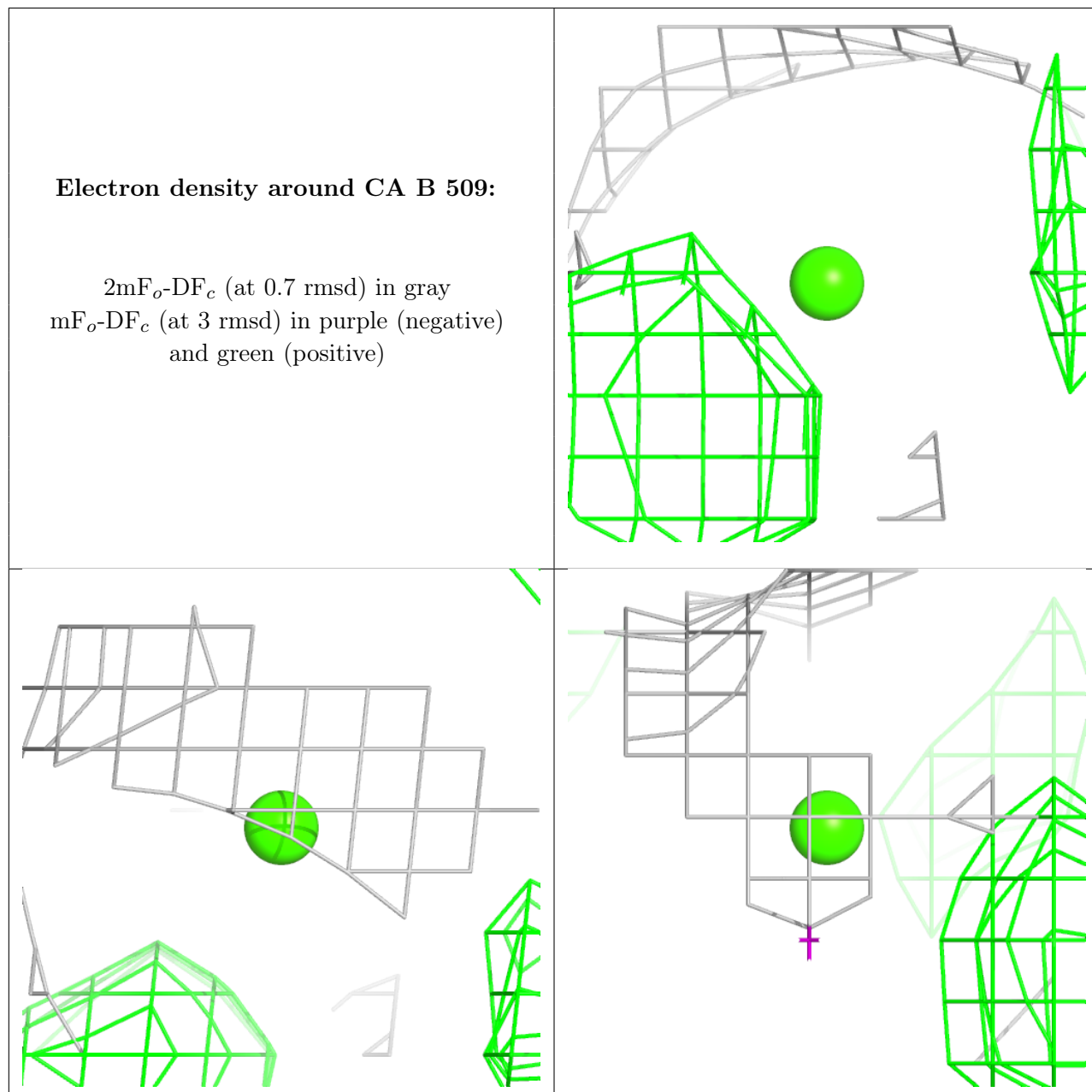
Electron density around CA A 509:

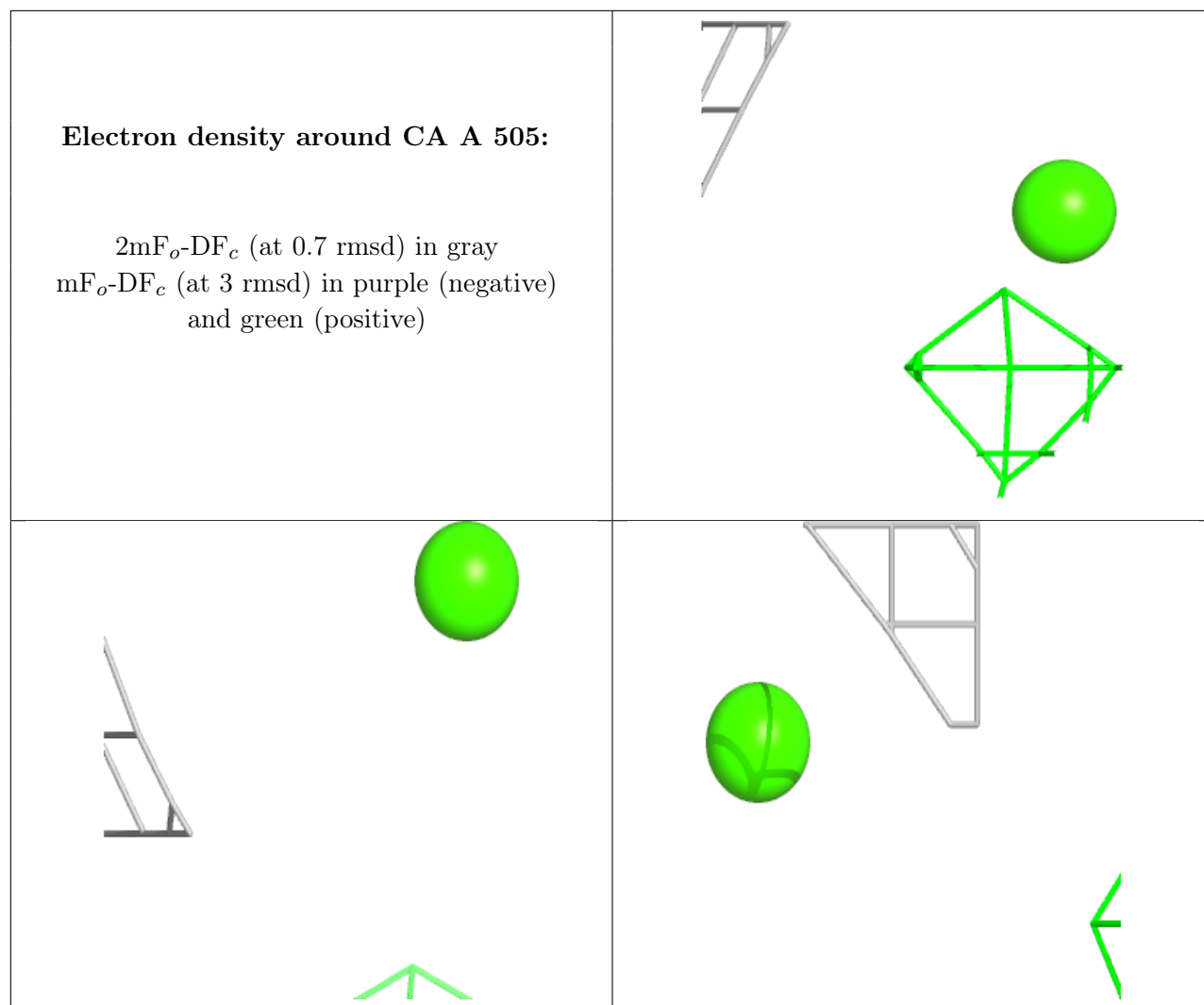
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CA B 509:

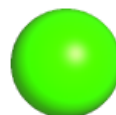
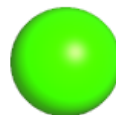
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





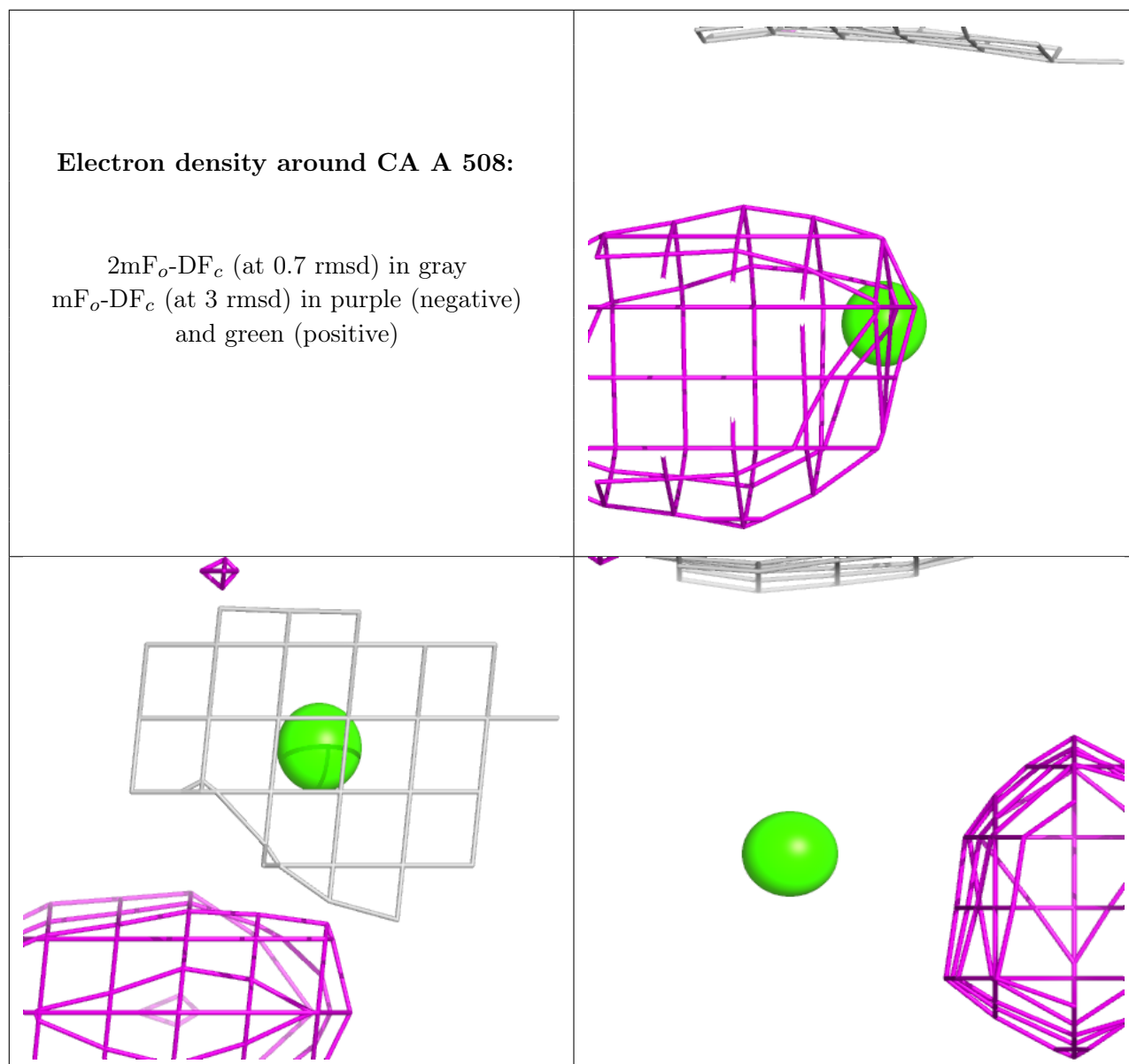
Electron density around CA B 505:

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



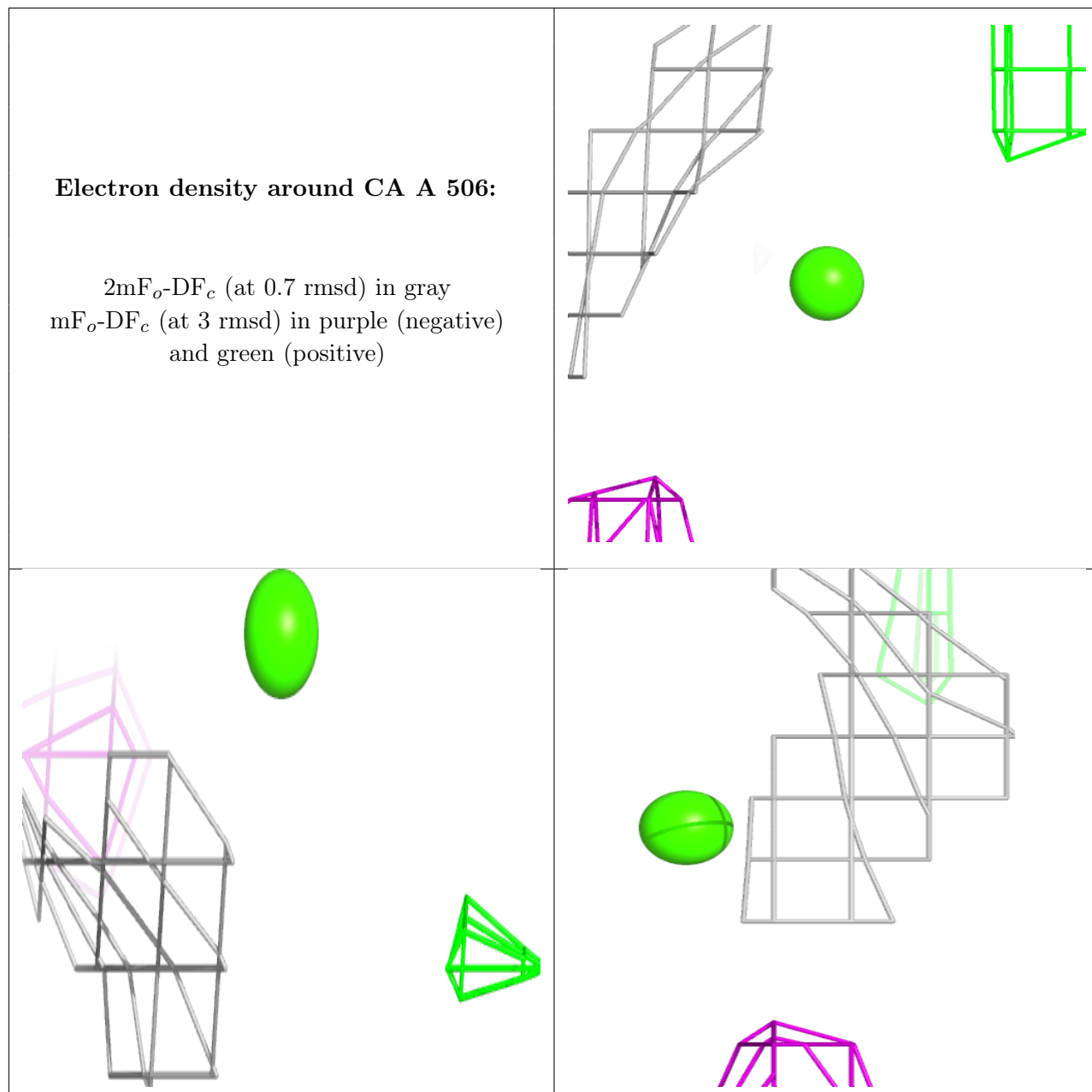
Electron density around CA A 508:

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



Electron density around CA A 506:

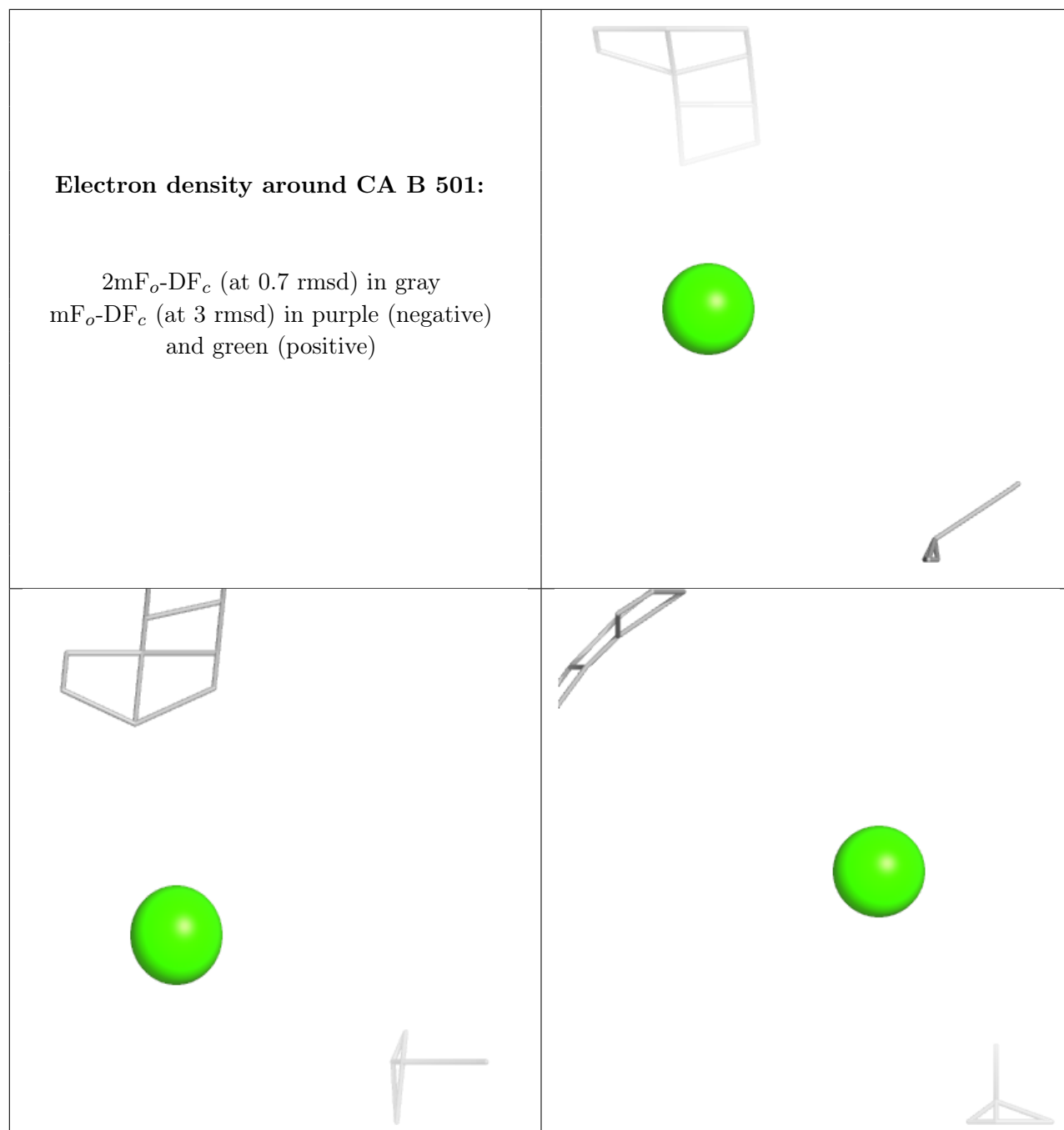
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CA B 508:

$2mF_o-DF_c$ (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.