



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2020 – 06:00 PM BST

PDB ID : 6OLY
Title : Full-length MthK channel at 3.1 angstrom resolution
Authors : Rothberg, B.S.
Deposited on : 2019-04-17
Resolution : 3.11 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
Xtriage (Phenix)	:	1.13
EDS	:	2.13
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

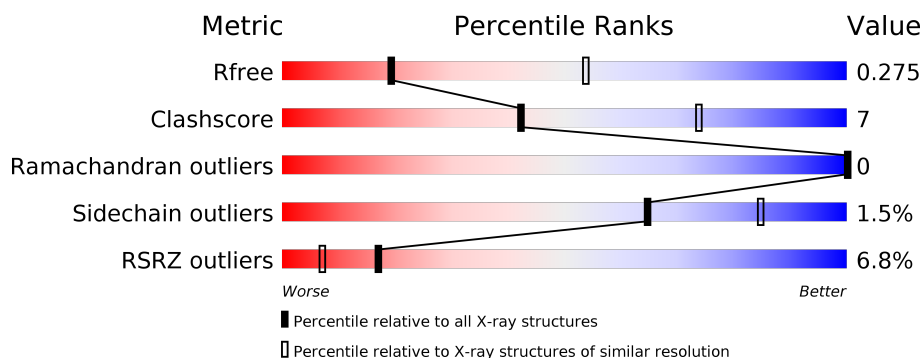
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.11 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	1292 (3.14-3.10)
Clashscore	141614	1389 (3.14-3.10)
Ramachandran outliers	138981	1337 (3.14-3.10)
Sidechain outliers	138945	1337 (3.14-3.10)
RSRZ outliers	127900	1260 (3.14-3.10)

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 $\leq 5\%$. 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	348	<div> <div>6%</div> <div> <div></div> <div>74%</div> <div>15%</div> <div>10%</div> </div> </div>
1	B	348	<div> <div>7%</div> <div> <div></div> <div>73%</div> <div>17%</div> <div>10%</div> </div> </div>
1	C	348	<div> <div>6%</div> <div> <div></div> <div>78%</div> <div>13%</div> <div>9%</div> </div> </div>
1	D	348	<div> <div>5%</div> <div> <div></div> <div>79%</div> <div>10%</div> <div>10%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8775 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 Calcium-gated potassium channel MthK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	313	Total	C	N	O	S	0	0	0
			2201	1370	390	433	8			
1	B	314	Total	C	N	O	S	0	0	0
			2193	1361	390	435	7			
1	C	318	Total	C	N	O	S	0	0	0
			2198	1362	393	436	7			
1	D	312	Total	C	N	O	S	0	0	0
			2153	1334	386	426	7			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	107	ILE	MET	engineered mutation	UNP O27564
A	337	LEU	-	expression tag	UNP O27564
A	338	VAL	-	expression tag	UNP O27564
A	339	PRO	-	expression tag	UNP O27564
A	340	ARG	-	expression tag	UNP O27564
A	341	GLY	-	expression tag	UNP O27564
A	342	SER	-	expression tag	UNP O27564
A	343	HIS	-	expression tag	UNP O27564
A	344	HIS	-	expression tag	UNP O27564
A	345	HIS	-	expression tag	UNP O27564
A	346	HIS	-	expression tag	UNP O27564
A	347	HIS	-	expression tag	UNP O27564
A	348	HIS	-	expression tag	UNP O27564
B	107	ILE	MET	engineered mutation	UNP O27564
B	337	LEU	-	expression tag	UNP O27564
B	338	VAL	-	expression tag	UNP O27564
B	339	PRO	-	expression tag	UNP O27564
B	340	ARG	-	expression tag	UNP O27564
B	341	GLY	-	expression tag	UNP O27564
B	342	SER	-	expression tag	UNP O27564
B	343	HIS	-	expression tag	UNP O27564

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Chain	Residue	Modelled	Actual	Comment	Reference
B	344	HIS	-	expression tag	UNP O27564
B	345	HIS	-	expression tag	UNP O27564
B	346	HIS	-	expression tag	UNP O27564
B	347	HIS	-	expression tag	UNP O27564
B	348	HIS	-	expression tag	UNP O27564
C	107	ILE	MET	engineered mutation	UNP O27564
C	337	LEU	-	expression tag	UNP O27564
C	338	VAL	-	expression tag	UNP O27564
C	339	PRO	-	expression tag	UNP O27564
C	340	ARG	-	expression tag	UNP O27564
C	341	GLY	-	expression tag	UNP O27564
C	342	SER	-	expression tag	UNP O27564
C	343	HIS	-	expression tag	UNP O27564
C	344	HIS	-	expression tag	UNP O27564
C	345	HIS	-	expression tag	UNP O27564
C	346	HIS	-	expression tag	UNP O27564
C	347	HIS	-	expression tag	UNP O27564
C	348	HIS	-	expression tag	UNP O27564
D	107	ILE	MET	engineered mutation	UNP O27564
D	337	LEU	-	expression tag	UNP O27564
D	338	VAL	-	expression tag	UNP O27564
D	339	PRO	-	expression tag	UNP O27564
D	340	ARG	-	expression tag	UNP O27564
D	341	GLY	-	expression tag	UNP O27564
D	342	SER	-	expression tag	UNP O27564
D	343	HIS	-	expression tag	UNP O27564
D	344	HIS	-	expression tag	UNP O27564
D	345	HIS	-	expression tag	UNP O27564
D	346	HIS	-	expression tag	UNP O27564
D	347	HIS	-	expression tag	UNP O27564
D	348	HIS	-	expression tag	UNP O27564

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by author).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	3	Total Ca 3 3	0	0
2	A	3	Total Ca 3 3	0	0
2	D	3	Total Ca 3 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	3	Total 3	Ca 3	0	0

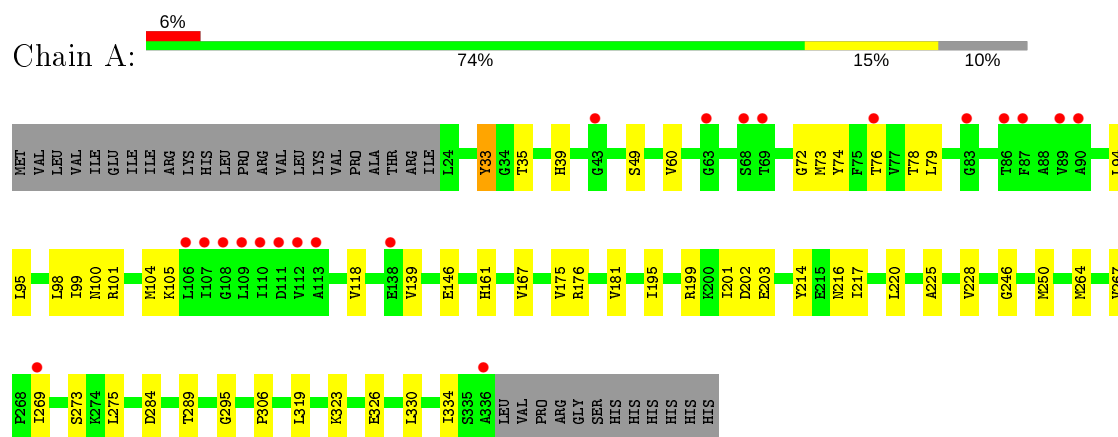
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	5	Total 5	O 5	0	0
3	B	2	Total 2	O 2	0	0
3	C	5	Total 5	O 5	0	0
3	D	6	Total 6	O 6	0	0

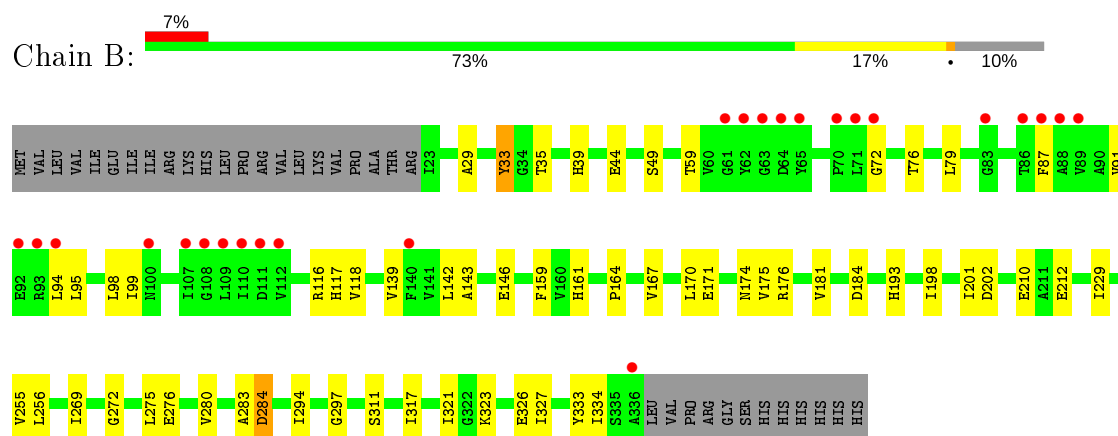
3 Residue-property plots [i](#)

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.

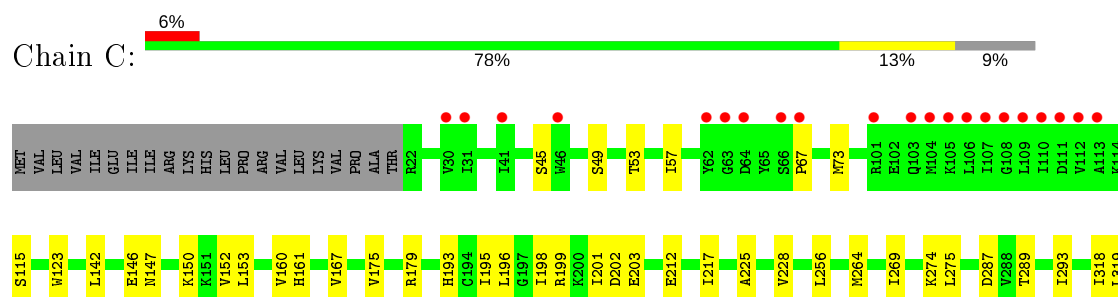
- Molecule 1: Calcium-gated potassium channel MthK

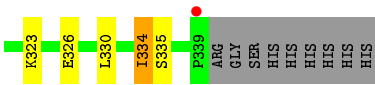


- Molecule 1: Calcium-gated potassium channel MthK

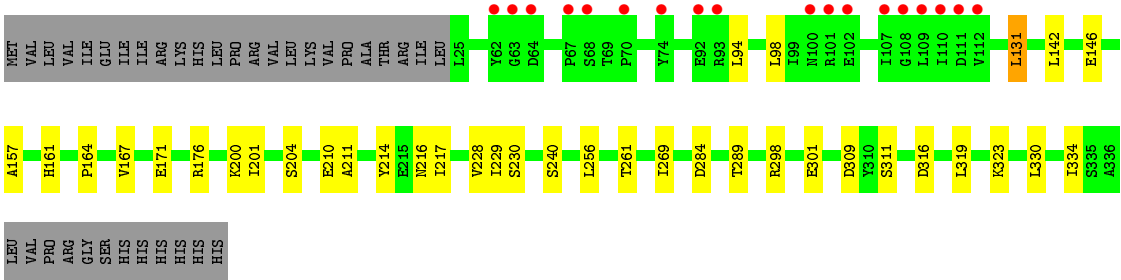
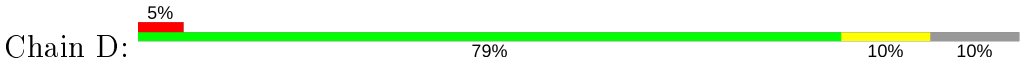


- Molecule 1: Calcium-gated potassium channel MthK





● Molecule 1: Calcium-gated potassium channel MthK



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	137.46 Å 137.46 Å 373.03 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.70 – 3.11 39.70 – 3.11	Depositor EDS
% Data completeness (in resolution range)	98.3 (39.70-3.11) 91.5 (39.70-3.11)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 3.12 Å)	Xtriage
Refinement program	PHENIX (dev_3374: ???)	Depositor
R, R_{free}	0.236 , 0.275 0.236 , 0.275	Depositor DCC
R_{free} test set	1899 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	83.3	Xtriage
Anisotropy	0.425	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 69.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8775	wwPDB-VP
Average B, all atoms (Å ²)	135.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.29% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.37	0/2230	0.55	0/3036
1	B	0.35	0/2219	0.54	0/3020
1	C	0.37	0/2224	0.58	1/3030 (0.0%)
1	D	0.40	0/2178	0.59	1/2964 (0.0%)
All	All	0.37	0/8851	0.57	2/12050 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	334	ILE	CG1-CB-CG2	-6.78	96.49	111.40
1	D	131	LEU	CB-CG-CD2	-5.53	101.60	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2201	0	2002	33	0
1	B	2193	0	1993	36	0
1	C	2198	0	1971	31	0
1	D	2153	0	1928	19	1
2	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
3	A	5	0	0	0	0
3	B	2	0	0	2	0
3	C	5	0	0	3	0
3	D	6	0	0	1	0
All	All	8775	0	7894	115	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (115) 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:275:LEU:HD12	1:C:334:ILE:HD12	1.67	0.76
1:D:269:ILE:HG12	1:D:334:ILE:HD11	1.67	0.75
1:D:261:THR:HG22	1:D:323:LYS:HG2	1.72	0.72
1:B:184:ASP:OD2	3:B:501:HOH:O	2.09	0.71
1:A:269:ILE:HG12	1:A:334:ILE:HD11	1.71	0.71
1:A:264:MET:HE3	1:A:319:LEU:HD21	1.74	0.70
1:C:212:GLU:OE2	3:C:501:HOH:O	2.09	0.69
1:B:269:ILE:HG12	1:B:334:ILE:HD11	1.74	0.69
1:B:72:GLY:O	1:B:76:THR:N	2.23	0.68
1:D:298:ARG:NH1	1:D:316:ASP:OD1	2.26	0.67
1:C:287:ASP:OD2	3:C:502:HOH:O	2.13	0.66
1:D:301:GLU:OE2	3:D:501:HOH:O	2.12	0.66
1:A:72:GLY:O	1:A:76:THR:N	2.28	0.66
1:A:101:ARG:O	1:A:105:LYS:N	2.28	0.64
1:B:212:GLU:OE2	3:B:501:HOH:O	2.15	0.63
1:A:167:VAL:HG13	1:A:201:ILE:HD11	1.81	0.63
1:C:269:ILE:HG12	1:C:334:ILE:HD11	1.79	0.63
1:C:147:ASN:O	1:C:150:LYS:HG2	1.99	0.63
1:A:246:GLY:O	1:A:250:MET:HG3	2.00	0.62
1:B:297:GLY:N	1:B:317:ILE:O	2.31	0.61
1:A:216:ASN:ND2	1:C:193:HIS:CE1	2.68	0.61
1:C:275:LEU:HD12	1:C:334:ILE:CD1	2.31	0.60
1:A:175:VAL:HG13	1:A:181:VAL:HG21	1.83	0.60
1:A:146:GLU:HG2	1:A:161:HIS:ND1	2.16	0.60
1:B:171:GLU:OE2	1:B:176:ARG:NH2	2.35	0.59
1:D:167:VAL:HG13	1:D:201:ILE:HD11	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:202:ASP:OD2	3:C:503:HOH:O	2.17	0.56
1:D:167:VAL:HG21	1:D:200:LYS:HE2	1.88	0.56
1:C:323:LYS:HB2	1:C:326:GLU:HG2	1.88	0.55
1:D:211:ALA:HB3	1:D:230:SER:HB3	1.87	0.54
1:B:94:LEU:O	1:B:98:LEU:HG	2.08	0.54
1:C:45:SER:O	1:C:49:SER:OG	2.23	0.54
1:A:176:ARG:HA	1:A:202:ASP:HB2	1.89	0.53
1:A:323:LYS:HB2	1:A:326:GLU:HG2	1.90	0.53
1:B:33:TYR:HE2	1:B:79:LEU:HA	1.72	0.53
1:B:294:ILE:HD13	1:B:321:ILE:HD11	1.91	0.53
1:A:275:LEU:HD12	1:A:334:ILE:HG13	1.90	0.52
1:B:272:GLY:N	1:B:276:GLU:OE1	2.43	0.52
1:B:175:VAL:HG11	1:B:198:ILE:HG23	1.91	0.52
1:A:100:ASN:O	1:A:104:MET:N	2.41	0.52
1:C:175:VAL:HG11	1:C:198:ILE:HG23	1.91	0.52
1:D:171:GLU:OE2	1:D:176:ARG:NH2	2.43	0.52
1:C:289:THR:HG21	1:C:330:LEU:HA	1.91	0.51
1:B:176:ARG:HA	1:B:202:ASP:HB2	1.92	0.51
1:D:94:LEU:O	1:D:98:LEU:N	2.43	0.51
1:C:264:MET:HE3	1:C:319:LEU:HD21	1.92	0.50
1:B:323:LYS:O	1:B:327:ILE:HG12	2.10	0.50
1:A:33:TYR:CE2	1:A:79:LEU:HD13	2.47	0.49
1:A:216:ASN:ND2	1:C:193:HIS:HE1	2.09	0.49
1:A:176:ARG:HB2	1:A:201:ILE:HG22	1.95	0.49
1:B:116:ARG:HG3	1:B:117:HIS:H	1.77	0.49
1:B:280:VAL:HA	1:B:283:ALA:HB3	1.94	0.49
1:C:146:GLU:HG2	1:C:161:HIS:ND1	2.28	0.48
1:D:289:THR:HG21	1:D:330:LEU:HA	1.96	0.47
1:D:214:TYR:O	1:D:217:ILE:HG12	2.14	0.47
1:B:146:GLU:HG2	1:B:161:HIS:ND1	2.29	0.47
1:B:35:THR:HA	1:B:49:SER:HB3	1.96	0.47
1:B:39:HIS:HA	1:B:44:GLU:O	2.15	0.47
1:B:275:LEU:HD21	1:B:333:TYR:CZ	2.50	0.46
1:C:274:LYS:HG3	1:C:335:SER:O	2.15	0.46
1:C:142:LEU:HD13	1:C:160:VAL:HG12	1.97	0.46
1:A:199:ARG:HD3	1:A:203:GLU:HA	1.98	0.46
1:B:87:PHE:O	1:B:91:VAL:HG13	2.16	0.46
1:B:175:VAL:HG13	1:B:181:VAL:HG21	1.98	0.46
1:A:216:ASN:HD21	1:C:193:HIS:HE1	1.63	0.46
1:D:210:GLU:HA	1:D:229:ILE:O	2.17	0.45
1:D:146:GLU:HG2	1:D:161:HIS:ND1	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:VAL:HG21	1:A:330:LEU:HD23	1.99	0.45
1:B:95:LEU:HA	1:B:98:LEU:HD12	1.98	0.45
1:B:280:VAL:O	1:B:284:ASP:N	2.47	0.45
1:D:256:LEU:HD23	1:D:256:LEU:HA	1.78	0.45
1:A:217:ILE:HG23	1:A:228:VAL:HG11	1.98	0.45
1:D:142:LEU:HG	1:D:164:PRO:HG3	1.99	0.45
1:B:29:ALA:O	1:B:33:TYR:HB3	2.17	0.45
1:C:293:ILE:HD12	1:C:318:ILE:HG23	1.99	0.45
1:A:35:THR:O	1:A:39:HIS:HB2	2.18	0.44
1:A:273:SER:OG	1:A:334:ILE:O	2.18	0.44
1:A:35:THR:HG23	1:A:49:SER:HB2	1.98	0.44
1:A:94:LEU:O	1:A:98:LEU:N	2.49	0.44
1:B:256:LEU:HA	1:B:256:LEU:HD23	1.67	0.44
1:A:74:TYR:CZ	1:A:78:THR:HG21	2.53	0.44
1:B:116:ARG:HG3	1:B:117:HIS:N	2.32	0.44
1:B:323:LYS:HB2	1:B:326:GLU:HG2	2.00	0.44
1:C:196:LEU:HD23	1:C:196:LEU:HA	1.77	0.44
1:A:95:LEU:O	1:A:99:ILE:N	2.50	0.43
1:D:217:ILE:HG23	1:D:228:VAL:HG11	2.00	0.43
1:D:319:LEU:HD12	1:D:319:LEU:HA	1.79	0.43
1:B:142:LEU:HG	1:B:164:PRO:HG3	1.99	0.43
1:B:95:LEU:O	1:B:99:ILE:HG13	2.17	0.43
1:C:115:SER:HB3	1:C:179:ARG:HH11	1.81	0.43
1:C:123:TRP:CZ3	1:C:152:VAL:HG22	2.53	0.43
1:A:289:THR:O	1:A:326:GLU:HB2	2.19	0.43
1:B:143:ALA:HB3	1:B:159:PHE:HE1	1.84	0.43
1:A:216:ASN:O	1:A:220:LEU:HD13	2.19	0.43
1:C:256:LEU:HD23	1:C:256:LEU:HA	1.63	0.43
1:C:67:PRO:HB3	1:C:73:MET:N	2.34	0.43
1:A:295:GLY:HA2	1:A:306:PRO:HD3	2.01	0.42
1:C:195:ILE:HD13	1:C:225:ALA:HB2	2.00	0.42
1:D:131:LEU:HD21	1:D:157:ALA:HB2	2.02	0.42
1:A:60:VAL:HG22	1:B:59:THR:HA	2.02	0.41
1:B:118:VAL:HB	1:B:139:VAL:HG22	2.01	0.41
1:B:167:VAL:HG13	1:B:201:ILE:HD11	2.02	0.41
1:C:53:THR:O	1:C:57:ILE:HG12	2.21	0.41
1:C:167:VAL:HG13	1:C:201:ILE:HD11	2.02	0.41
1:C:289:THR:O	1:C:326:GLU:HB2	2.21	0.41
1:B:255:VAL:HG23	1:B:256:LEU:HG	2.03	0.41
1:B:210:GLU:HA	1:B:229:ILE:O	2.20	0.40
1:C:199:ARG:HD3	1:C:203:GLU:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:VAL:HB	1:A:139:VAL:HG22	2.03	0.40
1:A:214:TYR:O	1:A:217:ILE:HG12	2.21	0.40
1:A:195:ILE:HD13	1:A:225:ALA:HB2	2.03	0.40
1:C:153:LEU:HD13	1:C:153:LEU:HA	1.83	0.40
1:C:217:ILE:HG23	1:C:228:VAL:HG11	2.03	0.40
1:D:261:THR:CG2	1:D:323:LYS:HG2	2.47	0.40
1:B:170:LEU:HD23	1:B:170:LEU:HA	1.90	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:204:SER:OG	1:D:309:ASP:O[12_555]	2.07	0.13

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	311/348 (89%)	301 (97%)	10 (3%)	0	100	100
1	B	312/348 (90%)	302 (97%)	10 (3%)	0	100	100
1	C	316/348 (91%)	308 (98%)	8 (2%)	0	100	100
1	D	310/348 (89%)	300 (97%)	10 (3%)	0	100	100
All	All	1249/1392 (90%)	1211 (97%)	38 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	202/299 (68%)	199 (98%)	3 (2%)	65	85
1	B	201/299 (67%)	196 (98%)	5 (2%)	47	75
1	C	196/299 (66%)	196 (100%)	0	100	100
1	D	191/299 (64%)	187 (98%)	4 (2%)	53	78
All	All	790/1196 (66%)	778 (98%)	12 (2%)	65	85

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	TYR
1	A	73	MET
1	A	284	ASP
1	B	33	TYR
1	B	174	ASN
1	B	193	HIS
1	B	284	ASP
1	B	311	SER
1	D	216	ASN
1	D	240	SER
1	D	284	ASP
1	D	311	SER

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

Mol	Chain	Res	Type
1	A	216	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 [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 12 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

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, 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	313/348 (89%)	0.26	21 (6%) 17 7	58, 125, 266, 375	0
1	B	314/348 (90%)	0.13	25 (7%) 12 5	61, 130, 259, 415	0
1	C	318/348 (91%)	0.15	22 (6%) 16 7	63, 117, 272, 355	0
1	D	312/348 (89%)	0.12	18 (5%) 23 10	53, 100, 275, 324	0
All	All	1257/1392 (90%)	0.17	86 (6%) 17 7	53, 117, 269, 415	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	107	ILE	12.5
1	A	108	GLY	9.0
1	C	109	LEU	7.5
1	C	107	ILE	7.5
1	A	76	THR	7.3
1	A	69	THR	7.1
1	B	111	ASP	6.2
1	C	108	GLY	6.2
1	A	110	ILE	5.9
1	C	63	GLY	5.9
1	A	86	THR	5.9
1	B	62	TYR	5.5
1	C	62	TYR	5.5
1	C	106	LEU	5.4
1	A	109	LEU	5.3
1	C	104	MET	4.9
1	C	105	LYS	4.9
1	A	111	ASP	4.8
1	D	102	GLU	4.8
1	C	110	ILE	4.7
1	B	109	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	65	TYR	4.6
1	B	88	ALA	4.5
1	D	100	ASN	4.4
1	A	106	LEU	4.4
1	A	87	PHE	4.1
1	B	63	GLY	4.1
1	B	108	GLY	4.1
1	B	89	VAL	4.1
1	D	107	ILE	4.0
1	B	64	ASP	4.0
1	B	61	GLY	4.0
1	B	107	ILE	4.0
1	C	113	ALA	3.9
1	D	63	GLY	3.9
1	A	336	ALA	3.9
1	A	112	VAL	3.9
1	D	67	PRO	3.7
1	D	92	GLU	3.6
1	C	67	PRO	3.5
1	C	66	SER	3.5
1	B	112	VAL	3.5
1	A	83	GLY	3.5
1	B	110	ILE	3.4
1	A	68	SER	3.3
1	D	101	ARG	3.3
1	D	93	ARG	3.1
1	B	92	GLU	3.1
1	D	112	VAL	3.0
1	C	64	ASP	3.0
1	C	112	VAL	3.0
1	A	43	GLY	3.0
1	A	138	GLU	3.0
1	B	86	THR	2.9
1	D	108	GLY	2.9
1	D	68	SER	2.9
1	A	63	GLY	2.8
1	B	93	ARG	2.8
1	D	111	ASP	2.8
1	B	72	GLY	2.7
1	C	339	PRO	2.7
1	B	100	ASN	2.7
1	C	46	TRP	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	70	PRO	2.7
1	B	336	ALA	2.7
1	C	111	ASP	2.6
1	B	87	PHE	2.6
1	B	94	LEU	2.6
1	C	101	ARG	2.6
1	A	90	ALA	2.5
1	C	103	GLN	2.4
1	A	113	ALA	2.4
1	C	30	VAL	2.4
1	D	70	PRO	2.4
1	D	110	ILE	2.4
1	B	140	PHE	2.4
1	B	83	GLY	2.3
1	A	89	VAL	2.3
1	C	31	ILE	2.3
1	C	41	ILE	2.3
1	B	71	LEU	2.1
1	D	64	ASP	2.1
1	D	62	TYR	2.1
1	A	269	ILE	2.0
1	D	109	LEU	2.0
1	D	74	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, 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.

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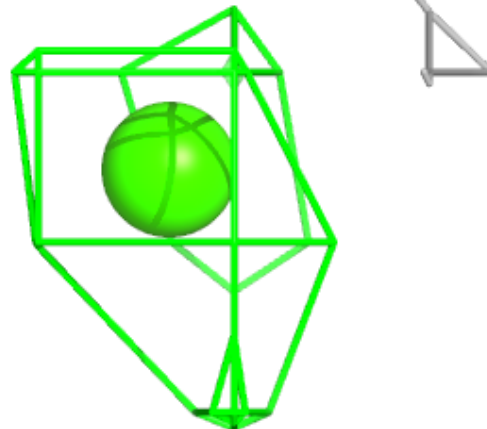
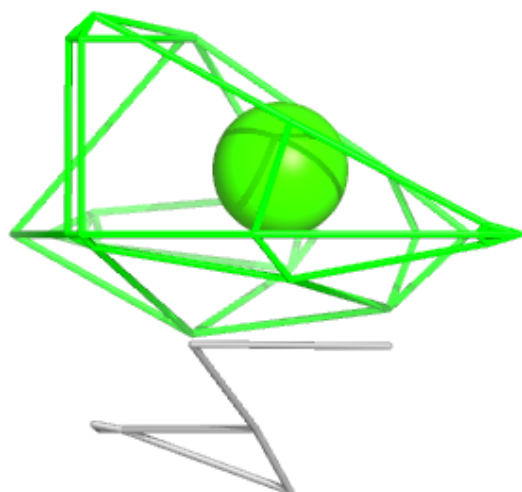
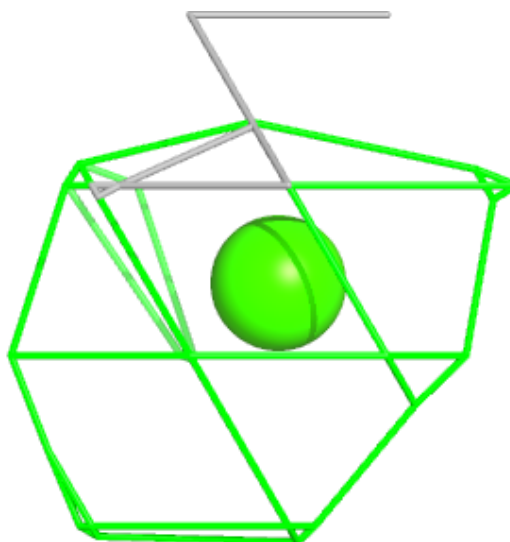
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	CA	A	403	1/1	0.90	0.23	137,137,137,137	0
2	CA	B	402	1/1	0.97	0.28	87,87,87,87	0
2	CA	D	402	1/1	0.97	0.38	112,112,112,112	0
2	CA	B	403	1/1	0.97	0.09	83,83,83,83	0
2	CA	B	401	1/1	0.98	0.33	98,98,98,98	0
2	CA	A	401	1/1	0.98	0.27	79,79,79,79	0
2	CA	C	403	1/1	0.98	0.18	104,104,104,104	0
2	CA	A	402	1/1	0.99	0.39	123,123,123,123	0
2	CA	D	401	1/1	0.99	0.21	82,82,82,82	0
2	CA	D	403	1/1	0.99	0.12	89,89,89,89	0
2	CA	C	402	1/1	0.99	0.37	72,72,72,72	0
2	CA	C	401	1/1	1.00	0.22	84,84,84,84	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.

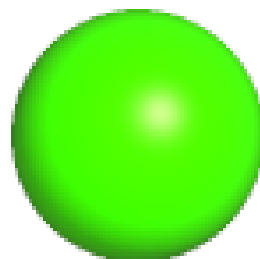
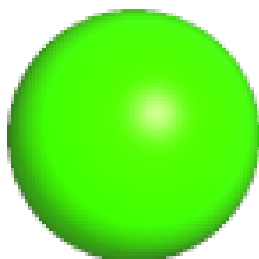
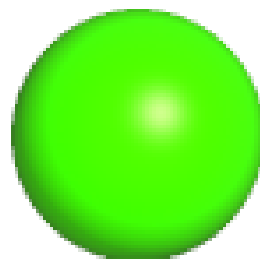
Electron density around CA A 403:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



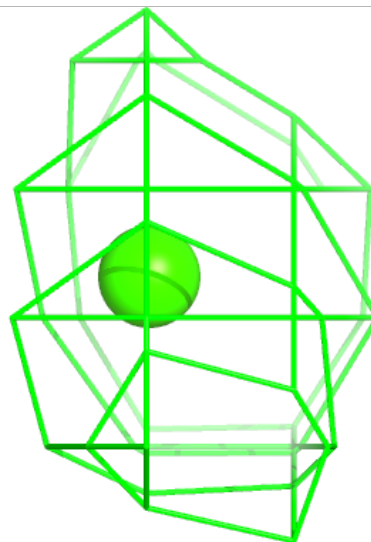
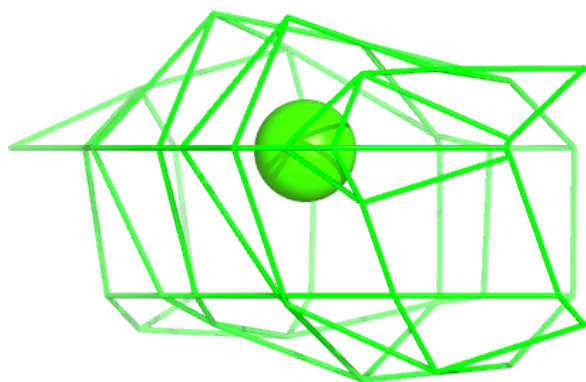
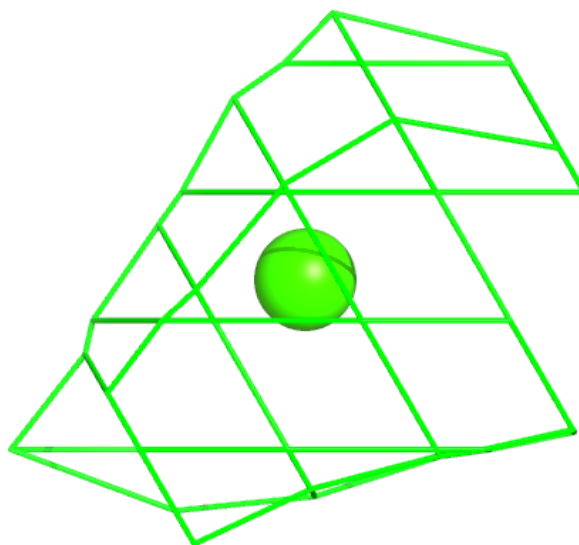
Electron density around CA B 402:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



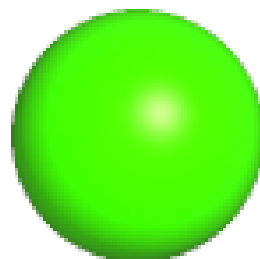
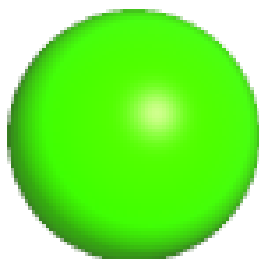
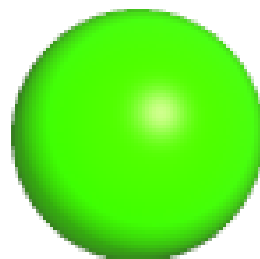
Electron density around CA D 402:

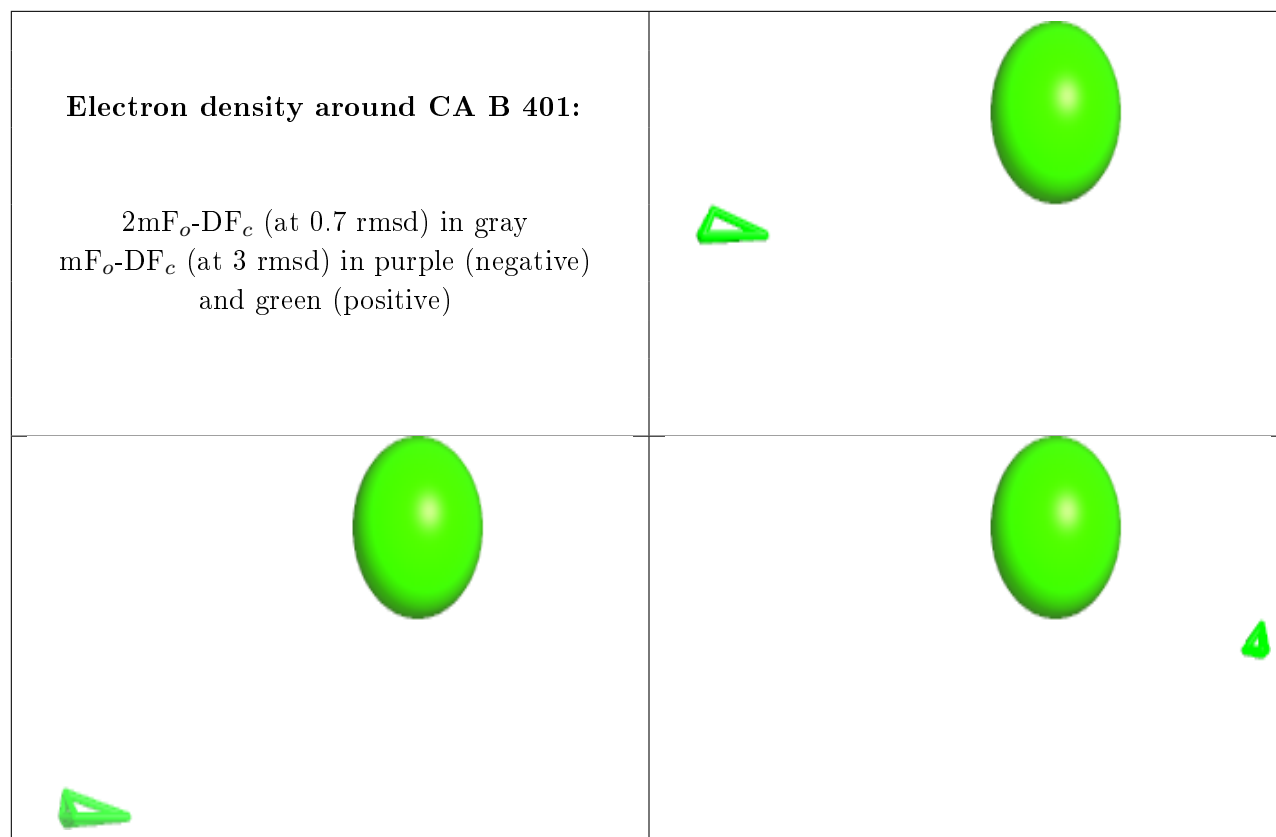
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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

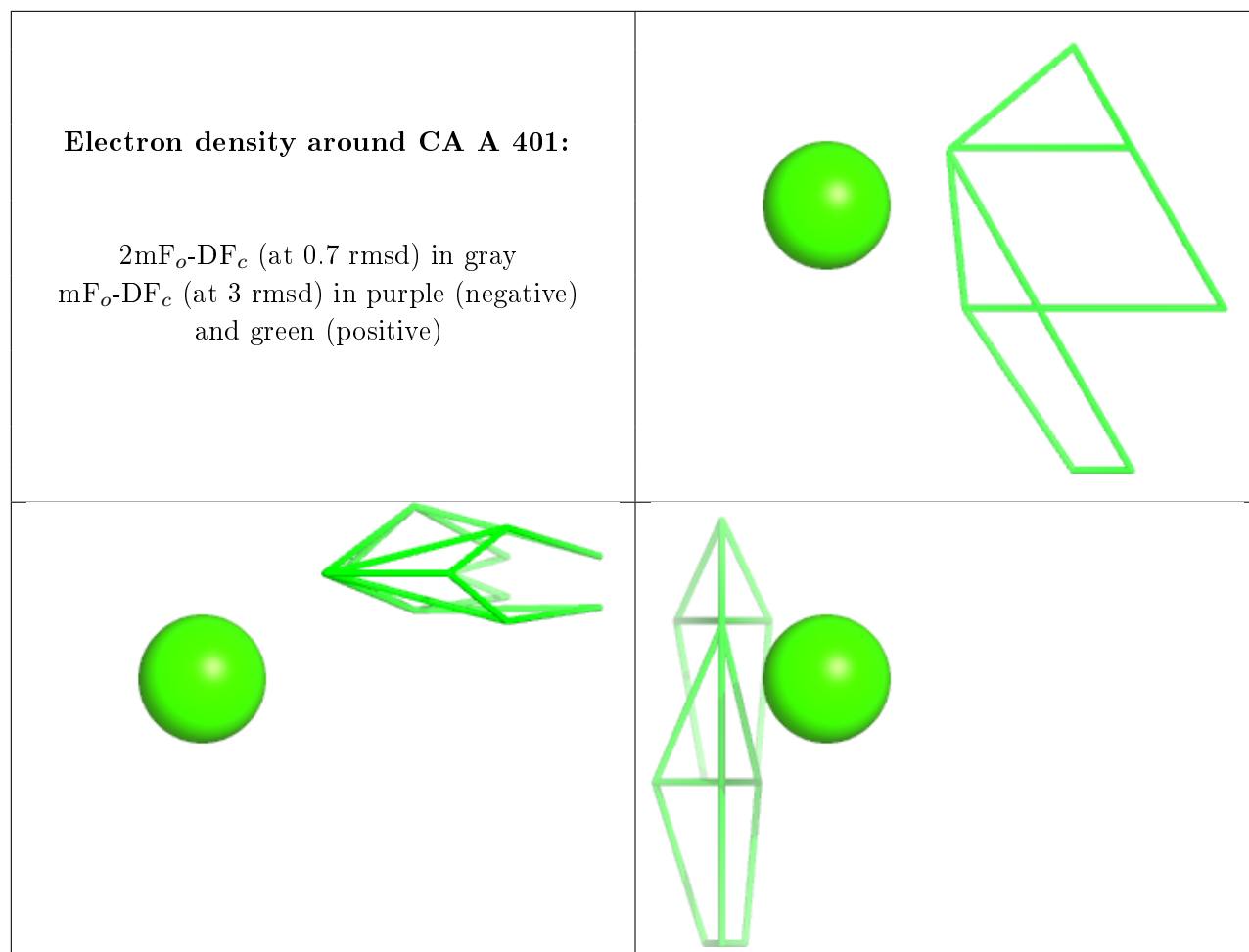


Electron density around CA B 403:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

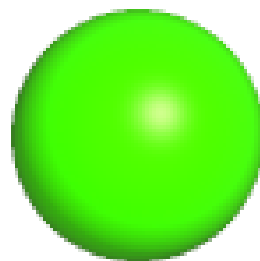
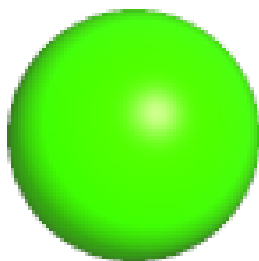
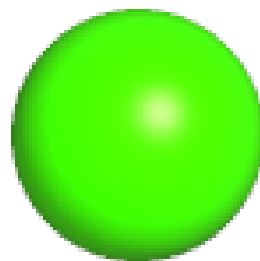






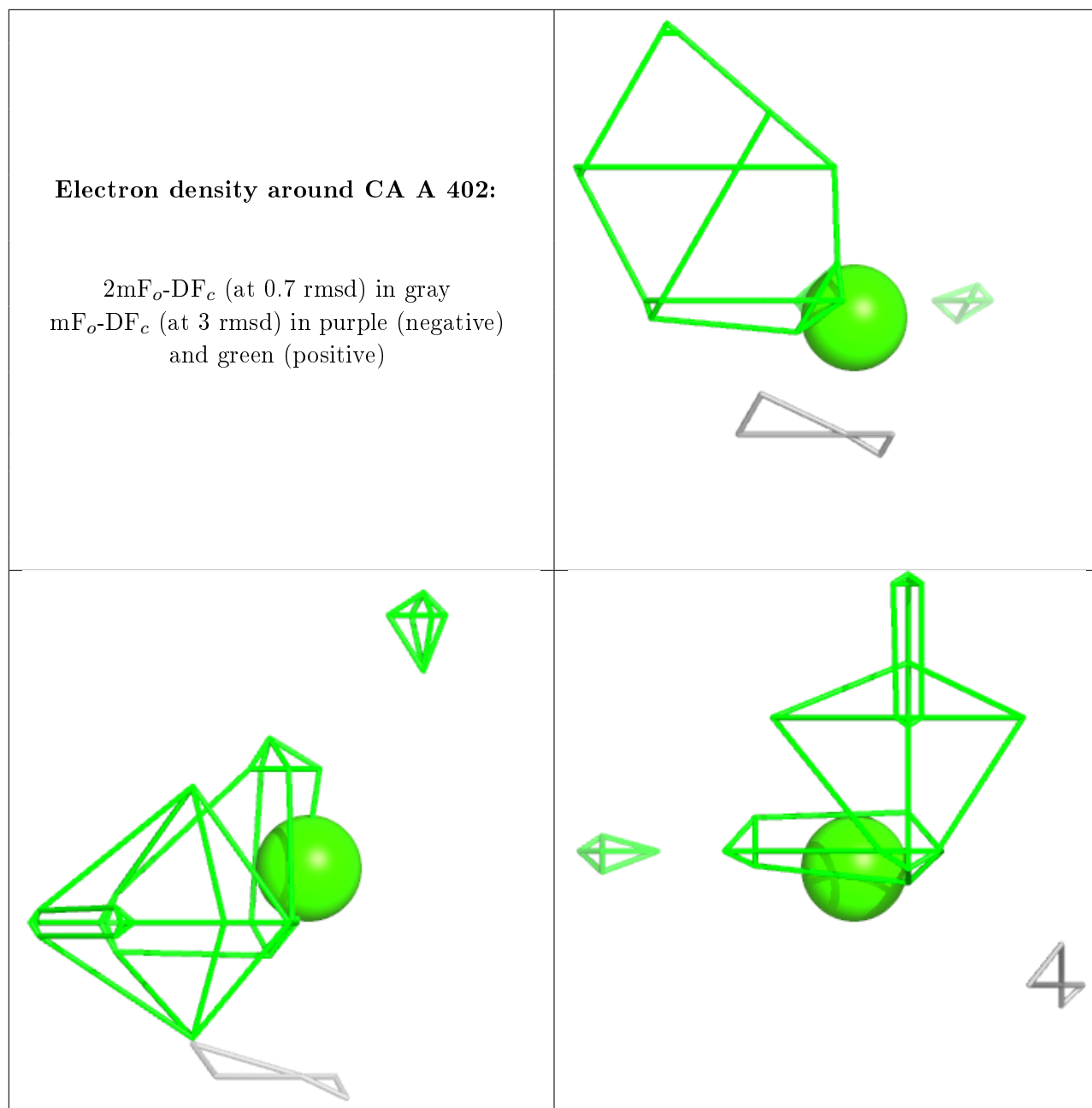
Electron density around CA C 403:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



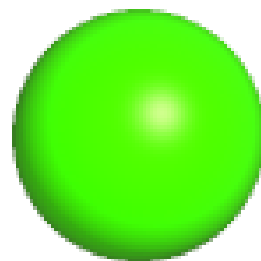
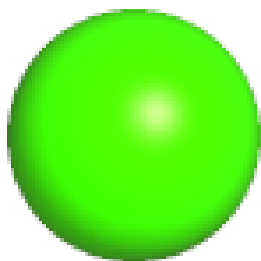
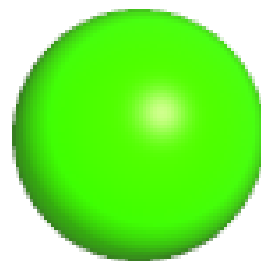
Electron density around CA A 402:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



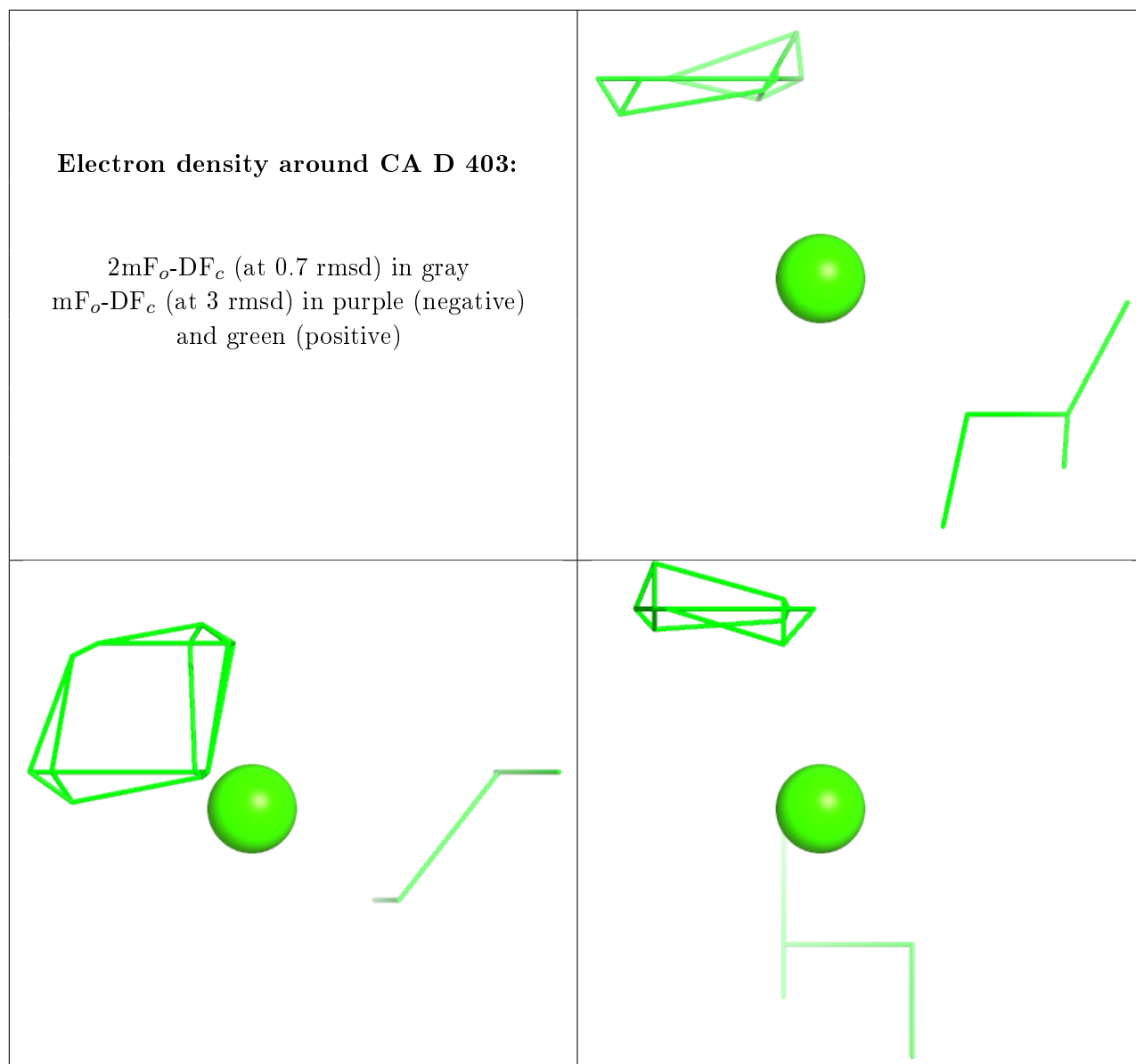
Electron density around CA D 401:

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and green (positive)



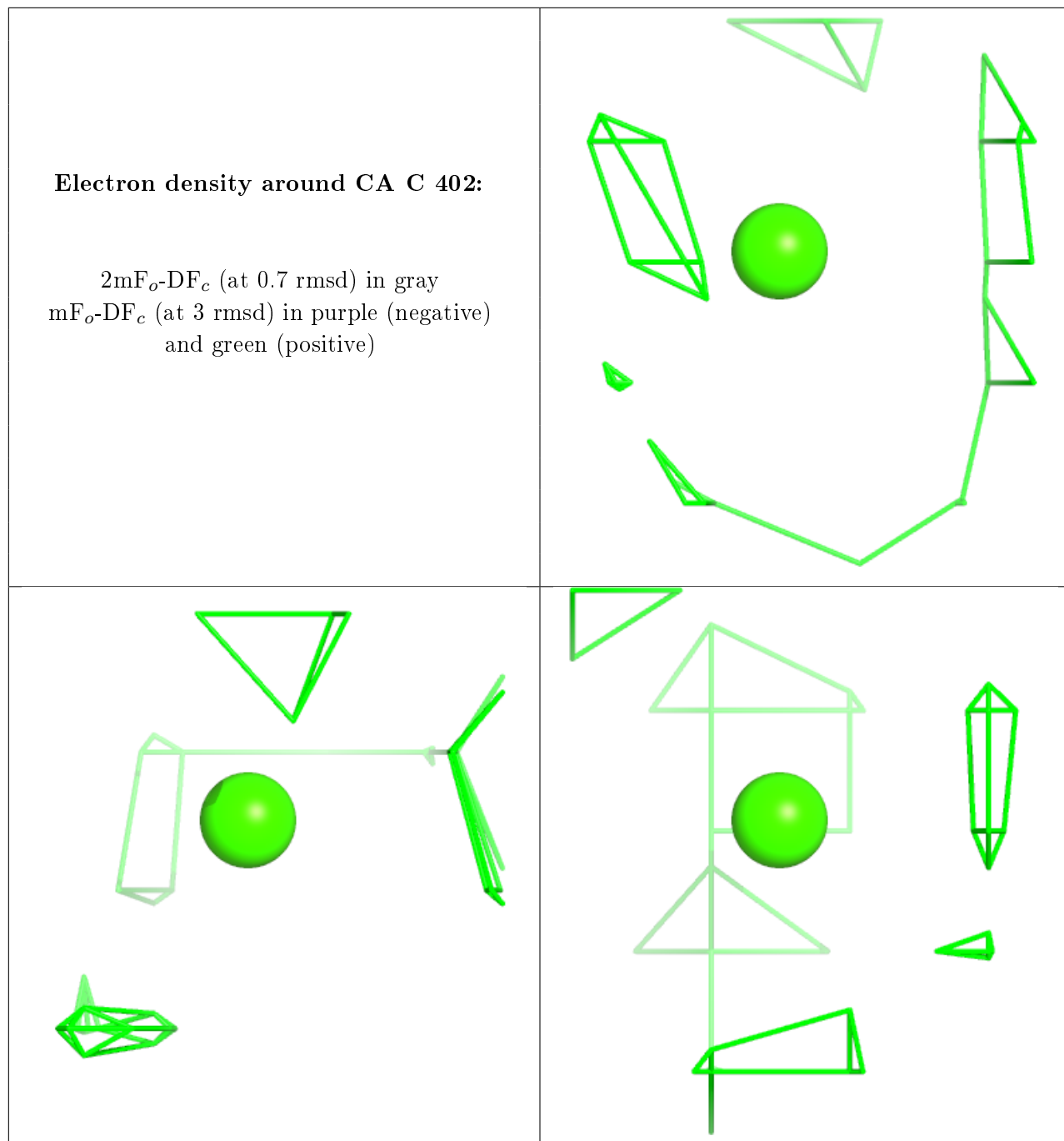
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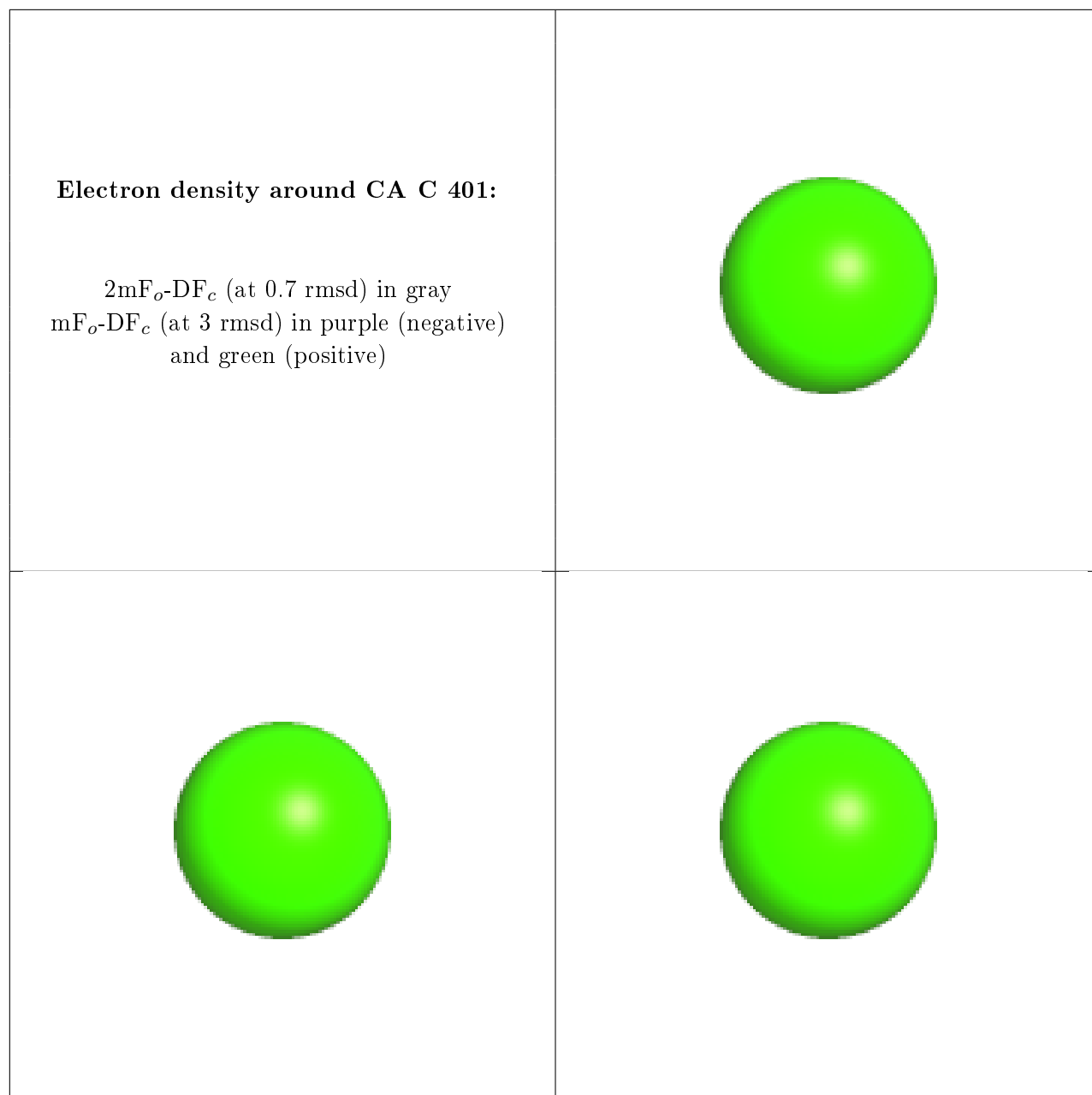
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CA C 402:

$2mF_o-DF_c$ (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.