Full wwPDB X-ray Structure Validation Report (i)

May 17, 2023 – 07:24 pm BST

PDB ID	:	8OSI
Title	:	Genetically encoded green ratiometric calcium indicator FNCaMP in calcium-bound state
Authors	:	Varfolomeeva, L.A.; Boyko, K.M.; Nikolaeva, A.Y.; Subach, O.M.; Subach, F.V.
Deposited on	:	2023-04-19
Resolution	:	2.42 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

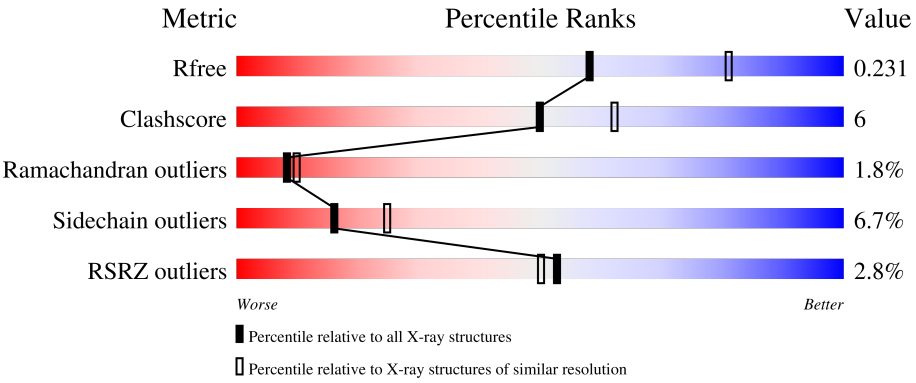
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.42 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4647 (2.44-2.40)
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)
RSRZ outliers	127900	4543 (2.44-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	463	2% 70% 12% 14%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3251 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 mNeonGreen,Calmodulin,Protein kinase domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	400	3179	1990	529	636	24	0	0	0

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-41	MET	-	initiating methionine	UNP A0A1S4NYF2
A	-40	GLY	-	expression tag	UNP A0A1S4NYF2
A	-39	GLY	-	expression tag	UNP A0A1S4NYF2
A	-38	SER	-	expression tag	UNP A0A1S4NYF2
A	-37	HIS	-	expression tag	UNP A0A1S4NYF2
A	-36	HIS	-	expression tag	UNP A0A1S4NYF2
A	-35	HIS	-	expression tag	UNP A0A1S4NYF2
A	-34	HIS	-	expression tag	UNP A0A1S4NYF2
A	-33	HIS	-	expression tag	UNP A0A1S4NYF2
A	-32	HIS	-	expression tag	UNP A0A1S4NYF2
A	-31	GLY	-	expression tag	UNP A0A1S4NYF2
A	-10	GLU	-	linker	UNP A0A1S4NYF2
A	-9	ASN	-	linker	UNP A0A1S4NYF2
A	-8	LEU	-	linker	UNP A0A1S4NYF2
A	-7	TYR	-	linker	UNP A0A1S4NYF2
A	-6	PHE	-	linker	UNP A0A1S4NYF2
A	-5	GLN	-	linker	UNP A0A1S4NYF2
A	-4	GLY	-	linker	UNP A0A1S4NYF2
A	-3	HIS	-	linker	UNP A0A1S4NYF2
A	-2	MET	-	linker	UNP A0A1S4NYF2
A	-1	ARG	-	linker	UNP A0A1S4NYF2
A	0	SER	-	linker	UNP A0A1S4NYF2
A	8	GLU	ASP	engineered mutation	UNP A0A1S4NYF2
A	28	ILE	VAL	engineered mutation	UNP A0A1S4NYF2
A	53	MET	LYS	engineered mutation	UNP A0A1S4NYF2
A	107	THR	SER	engineered mutation	UNP A0A1S4NYF2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	128	GLU	LYS	engineered mutation	UNP A0A1S4NYF2
A	146	GLU	-	linker	UNP A0A1S4NYF2
A	147	ALA	-	linker	UNP A0A1S4NYF2
A	148	GLN	-	linker	UNP A0A1S4NYF2
A	164	LEU	ALA	engineered mutation	UNP A0A100IBH9
A	170	LEU	LYS	engineered mutation	UNP A0A100IBH9
A	189	ASP	GLY	engineered mutation	UNP A0A100IBH9
A	190	LEU	GLN	engineered mutation	UNP A0A100IBH9
A	207	GLY	ASP	engineered mutation	UNP A0A100IBH9
A	208	GLY	ASN	engineered mutation	UNP A0A100IBH9
A	209	ASP	ASN	engineered mutation	UNP A0A100IBH9
A	222	THR	ALA	engineered mutation	UNP A0A100IBH9
A	224	GLU	LYS	engineered mutation	UNP A0A100IBH9
A	227	TYR	ASP	engineered mutation	UNP A0A100IBH9
A	228	ARG	THR	engineered mutation	UNP A0A100IBH9
A	230	THR	SER	engineered mutation	UNP A0A100IBH9
A	237	LEU	ALA	engineered mutation	UNP A0A100IBH9
A	238	CYS	PHE	engineered mutation	UNP A0A100IBH9
A	246	ASP	ASN	engineered mutation	UNP A0A100IBH9
A	250	VAL	SER	engineered mutation	UNP A0A100IBH9
A	257	ALA	VAL	engineered mutation	UNP A0A100IBH9
A	264	GLU	LYS	engineered mutation	UNP A0A100IBH9
A	294	LYS	MET	engineered mutation	UNP A0A100IBH9
A	298	GLY	-	linker	UNP A0A100IBH9
A	299	GLY	-	linker	UNP A0A100IBH9
A	300	GLY	-	linker	UNP A0A100IBH9
A	301	GLY	-	linker	UNP A0A100IBH9
A	302	SER	-	linker	UNP A0A100IBH9
A	303	GLY	-	linker	UNP A0A100IBH9
A	304	GLY	-	linker	UNP A0A100IBH9
A	305	SER	-	linker	UNP A0A100IBH9
A	306	GLY	-	linker	UNP A0A100IBH9
A	307	MET	-	linker	UNP A0A100IBH9
A	310	LEU	THR	engineered mutation	UNP A0A254U4M1
A	312	LYS	HIS	engineered mutation	UNP A0A254U4M1
A	323	ARG	LYS	engineered mutation	UNP A0A254U4M1
A	328	MET	-	linker	UNP A0A254U4M1
A	329	TYR	-	linker	UNP A0A254U4M1
A	330	PHE	-	linker	UNP A0A254U4M1
A	335	VAL	ARG	engineered mutation	UNP A0A1S4NYF2
A	340	CYS	TYR	engineered mutation	UNP A0A1S4NYF2
A	342	ASP	ASN	engineered mutation	UNP A0A1S4NYF2

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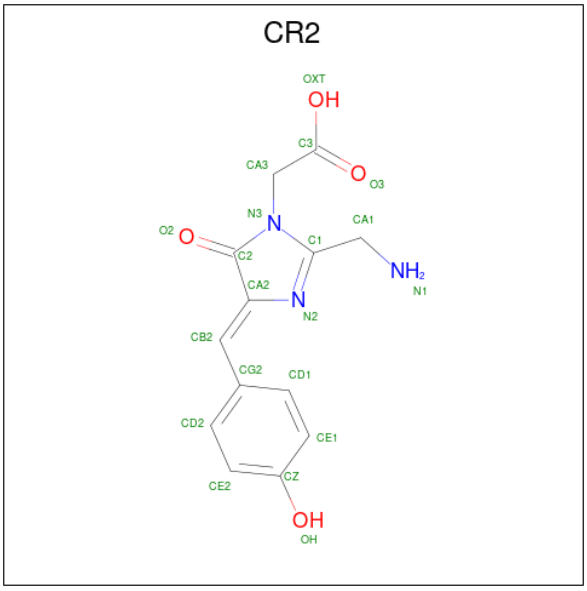
Chain	Residue	Modelled	Actual	Comment	Reference
A	347	VAL	ILE	engineered mutation	UNP A0A1S4NYF2
A	350	LEU	PHE	engineered mutation	UNP A0A1S4NYF2
A	353	ALA	SER	engineered mutation	UNP A0A1S4NYF2
A	354	PHE	TYR	engineered mutation	UNP A0A1S4NYF2
A	355	ILE	THR	engineered mutation	UNP A0A1S4NYF2
A	357	ASP	GLY	engineered mutation	UNP A0A1S4NYF2
A	395	ILE	LYS	engineered mutation	UNP A0A1S4NYF2
A	413	GLY	VAL	engineered mutation	UNP A0A1S4NYF2

- Molecule 2 is {(4Z)-2-(aminomethyl)-4-[(4-hydroxyphenyl)methylidene]-5-oxo-4,5-dihydro-1H-imidazol-1-yl}acetic acid (three-letter code: CR2) (formula: $C_{13}H_{13}N_3O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 19 13 3 3	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	4	Total Ca 4 4	0	0

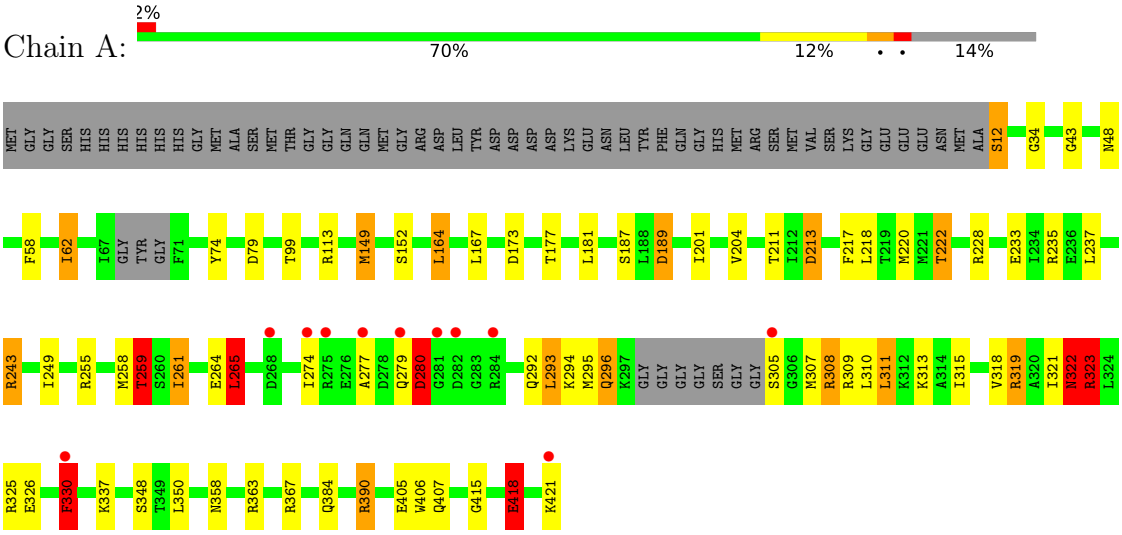
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	49	Total O 49 49	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: mNeonGreen,Calmodulin,Protein kinase domain-containing protein



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	151.40Å 151.40Å 61.97Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.95 – 2.42 47.95 – 2.42	Depositor EDS
% Data completeness (in resolution range)	99.4 (47.95-2.42) 99.4 (47.95-2.42)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.21 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.8.0405	Depositor
R, R_{free}	0.196 , 0.231 0.196 , 0.231	Depositor DCC
R_{free} test set	1539 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	63.6	Xtriage
Anisotropy	0.376	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 39.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.033 for -h,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	3251	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.44% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CR2, 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	0.72	1/3241 (0.0%)	1.36	32/4371 (0.7%)

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	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	213	ASP	CG-OD1	5.75	1.38	1.25

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	322	ASN	N-CA-CB	8.79	126.43	110.60
1	A	384	GLN	CB-CA-C	-8.49	93.42	110.40
1	A	177	THR	N-CA-CB	7.59	124.73	110.30
1	A	319	ARG	NE-CZ-NH2	-7.45	116.57	120.30
1	A	177	THR	CB-CA-C	-7.27	91.96	111.60
1	A	325	ARG	CG-CD-NE	-6.98	97.14	111.80
1	A	243	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	A	323	ARG	NE-CZ-NH2	-6.61	117.00	120.30
1	A	213	ASP	CB-CG-OD2	-6.61	112.36	118.30
1	A	243	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	A	113	ARG	NE-CZ-NH1	6.59	123.60	120.30
1	A	99	THR	OG1-CB-CG2	-6.54	94.96	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	62	ILE	N-CA-CB	6.43	125.59	110.80
1	A	390	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	A	264	GLU	CB-CA-C	6.33	123.05	110.40
1	A	259	THR	CA-CB-CG2	6.06	120.89	112.40
1	A	235	ARG	CB-CA-C	6.03	122.45	110.40
1	A	322	ASN	CB-CA-C	-5.93	98.53	110.40
1	A	319	ARG	CB-CG-CD	-5.85	96.39	111.60
1	A	367	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	A	79	ASP	CB-CG-OD1	5.84	123.56	118.30
1	A	418	GLU	CB-CG-CD	5.79	129.82	114.20
1	A	243	ARG	CD-NE-CZ	5.61	131.46	123.60
1	A	330	PHE	CB-CA-C	5.59	121.58	110.40
1	A	228	ARG	CB-CA-C	-5.57	99.25	110.40
1	A	177	THR	CA-CB-CG2	5.51	120.12	112.40
1	A	189	ASP	CB-CA-C	5.40	121.20	110.40
1	A	330	PHE	CA-CB-CG	5.15	126.27	113.90
1	A	367	ARG	CG-CD-NE	-5.12	101.04	111.80
1	A	358	ASN	CB-CA-C	5.11	120.62	110.40
1	A	280	ASP	CB-CG-OD1	5.06	122.86	118.30
1	A	12	SER	CB-CA-C	5.00	119.61	110.10

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	243	ARG	Sidechain
1	A	305	SER	Peptide
1	A	308	ARG	Sidechain
1	A	309	ARG	Sidechain
1	A	319	ARG	Sidechain
1	A	323	ARG	Sidechain

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	3179	0	3029	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	19	0	11	3	0
3	A	4	0	0	0	0
4	A	49	0	0	0	0
All	All	3251	0	3040	36	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 6.

All (36) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:ILE:O	1:A:322:ASN:HB2	1.77	0.84
1:A:415:GLY:HA2	1:A:418:GLU:HG3	1.61	0.82
1:A:296:GLN:HG3	1:A:308:ARG:HH21	1.47	0.79
1:A:321:ILE:O	1:A:322:ASN:CB	2.36	0.70
1:A:58:PHE:CD1	1:A:62:ILE:HD11	2.26	0.70
1:A:318:VAL:O	1:A:321:ILE:O	2.10	0.69
1:A:261:ILE:O	1:A:261:ILE:HG12	1.95	0.66
1:A:296:GLN:HG3	1:A:308:ARG:NH2	2.12	0.65
1:A:218:LEU:O	1:A:222:THR:HB	1.96	0.65
1:A:415:GLY:HA2	1:A:418:GLU:CG	2.28	0.63
1:A:58:PHE:CE1	1:A:62:ILE:HD11	2.35	0.60
1:A:350:LEU:CD2	2:A:501:CR2:HE1	2.41	0.51
1:A:233:GLU:OE2	1:A:323:ARG:HD2	2.11	0.51
1:A:237:LEU:HD22	1:A:318:VAL:HG12	1.91	0.51
1:A:255:ARG:O	1:A:259:THR:HG23	2.09	0.51
1:A:265:LEU:CD2	1:A:307:MET:HE1	2.42	0.50
1:A:277:ALA:HB2	1:A:293:LEU:HD13	1.94	0.49
1:A:164:LEU:HD13	1:A:217:PHE:HZ	1.77	0.49
1:A:265:LEU:HD21	1:A:307:MET:HE1	1.95	0.49
1:A:363:ARG:HH11	1:A:363:ARG:HG2	1.79	0.48
1:A:405:GLU:OE1	2:A:501:CR2:N2	2.47	0.48
1:A:337:LYS:O	1:A:348:SER:HA	2.13	0.47
1:A:294:LYS:HG3	1:A:315:ILE:HG21	1.97	0.47
1:A:167:LEU:HD12	1:A:313:LYS:HE2	1.96	0.46
1:A:390:ARG:HG2	1:A:407:GLN:HG2	1.97	0.46
1:A:390:ARG:HA	1:A:406:TRP:O	2.16	0.46
1:A:310:LEU:HD23	1:A:310:LEU:HA	1.78	0.45
1:A:292:GLN:O	1:A:296:GLN:HG2	2.17	0.45
1:A:34:GLY:HA3	1:A:48:ASN:O	2.17	0.44
1:A:258:MET:HE2	1:A:310:LEU:HD13	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:GLY:HA2	1:A:74:TYR:O	2.18	0.44
1:A:293:LEU:HD22	1:A:311:LEU:HD13	2.01	0.43
1:A:405:GLU:OE1	2:A:501:CR2:HD2	2.18	0.42
1:A:204:VAL:HG21	1:A:220:MET:HG3	2.01	0.42
1:A:164:LEU:HD13	1:A:217:PHE:CZ	2.55	0.41
1:A:279:GLN:O	1:A:280:ASP:HB3	2.21	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	394/463 (85%)	373 (95%)	14 (4%)	7 (2%)	8 10

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	280	ASP
1	A	296	GLN
1	A	322	ASN
1	A	330	PHE
1	A	149	MET
1	A	265	LEU
1	A	326	GLU

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	344/391 (88%)	321 (93%)	23 (7%)	16 25

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	SER
1	A	149	MET
1	A	152	SER
1	A	164	LEU
1	A	173	ASP
1	A	181	LEU
1	A	187	SER
1	A	189	ASP
1	A	201	ILE
1	A	211	THR
1	A	213	ASP
1	A	222	THR
1	A	249	ILE
1	A	259	THR
1	A	261	ILE
1	A	265	LEU
1	A	274	ILE
1	A	293	LEU
1	A	295	MET
1	A	311	LEU
1	A	330	PHE
1	A	418	GLU
1	A	421	LYS

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

Mol	Chain	Res	Type
1	A	35	GLN
1	A	175	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
2	CR2	A	501	1	20,20,21	0.99	1 (5%)	25,27,29	2.56	10 (40%)

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
2	CR2	A	501	1	-	0/6/25/26	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	CR2	C1-N3	2.35	1.40	1.37

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	CR2	O2-C2-CA2	-5.58	127.83	130.96
2	A	501	CR2	C1-CA1-N1	-5.15	101.45	112.85
2	A	501	CR2	CA2-C2-N3	4.62	105.56	103.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	CR2	CA1-C1-N2	-4.04	118.86	124.28
2	A	501	CR2	CG2-CB2-CA2	3.48	134.20	129.94
2	A	501	CR2	O3-C3-CA3	-3.44	115.99	126.39
2	A	501	CR2	CA1-C1-N3	2.90	126.40	122.52
2	A	501	CR2	CB2-CA2-N2	2.89	132.83	128.83
2	A	501	CR2	C2-N3-C1	-2.80	106.62	107.99
2	A	501	CR2	CB2-CA2-C2	-2.40	119.41	122.28

There are no chirality outliers.

There are no torsion outliers.

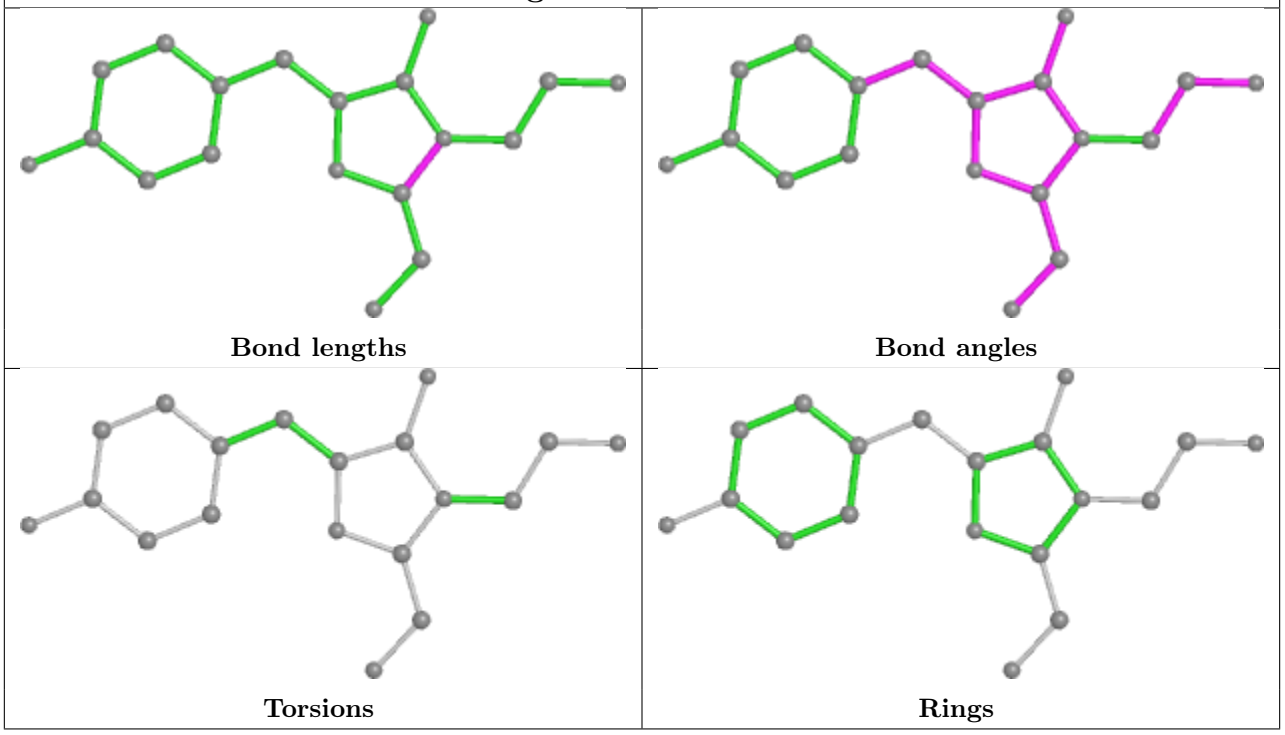
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	CR2	3	0

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

Ligand CR2 A 501



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	400/463 (86%)	-0.02	11 (2%) 53 50	41, 63, 110, 138	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	281	GLY	4.3
1	A	305	SER	3.3
1	A	277	ALA	3.3
1	A	284	ARG	3.2
1	A	275	ARG	2.9
1	A	274	ILE	2.9
1	A	279	GLN	2.3
1	A	421	LYS	2.3
1	A	268	ASP	2.1
1	A	282	ASP	2.1
1	A	330	PHE	2.1

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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

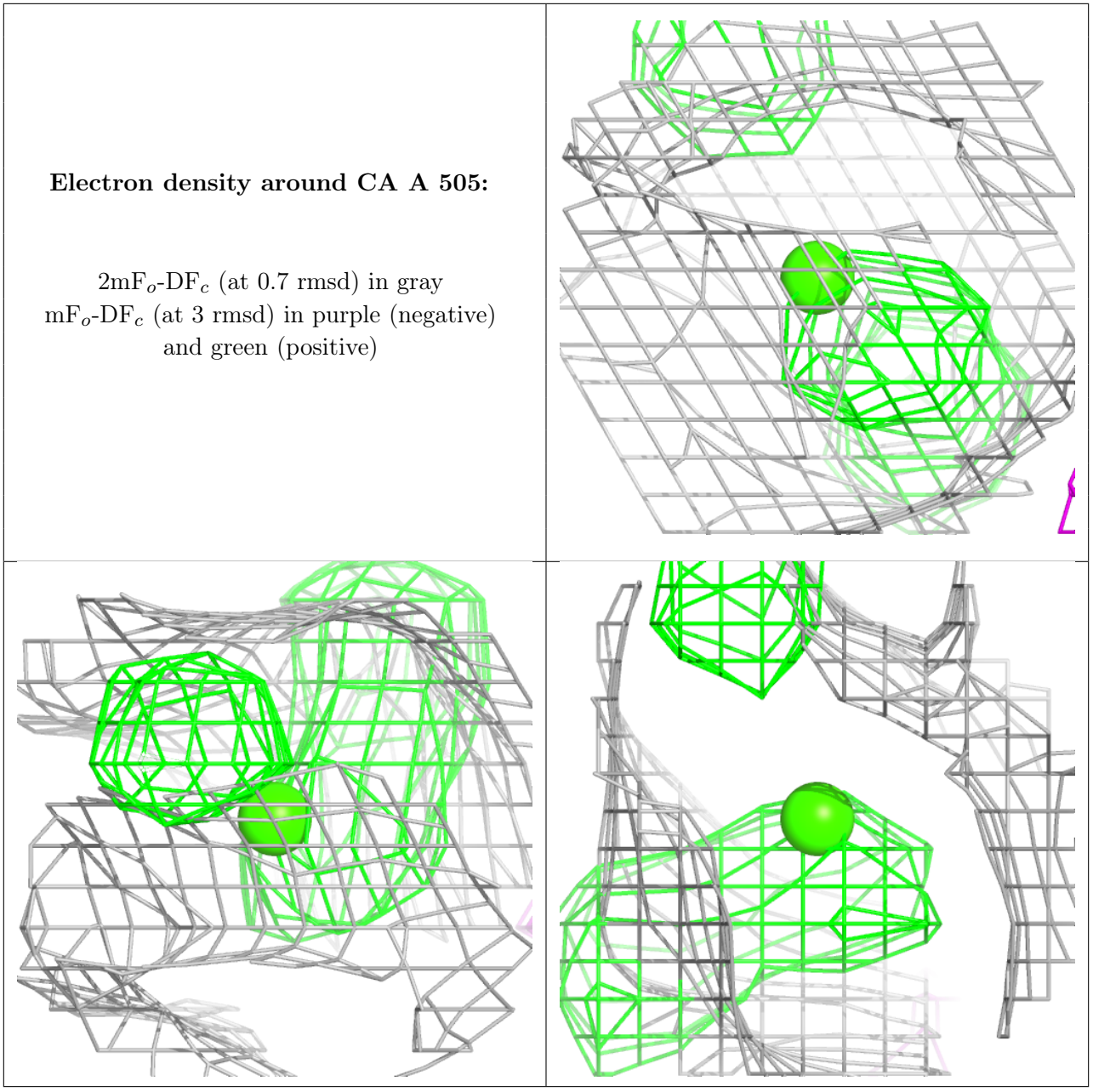
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CA	A	505	1/1	0.93	0.16	74,74,74,74	0
3	CA	A	503	1/1	0.95	0.04	98,98,98,98	0
3	CA	A	502	1/1	0.97	0.15	69,69,69,69	0
2	CR2	A	501	19/20	0.98	0.14	37,52,62,65	0
3	CA	A	504	1/1	0.99	0.06	70,70,70,70	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.

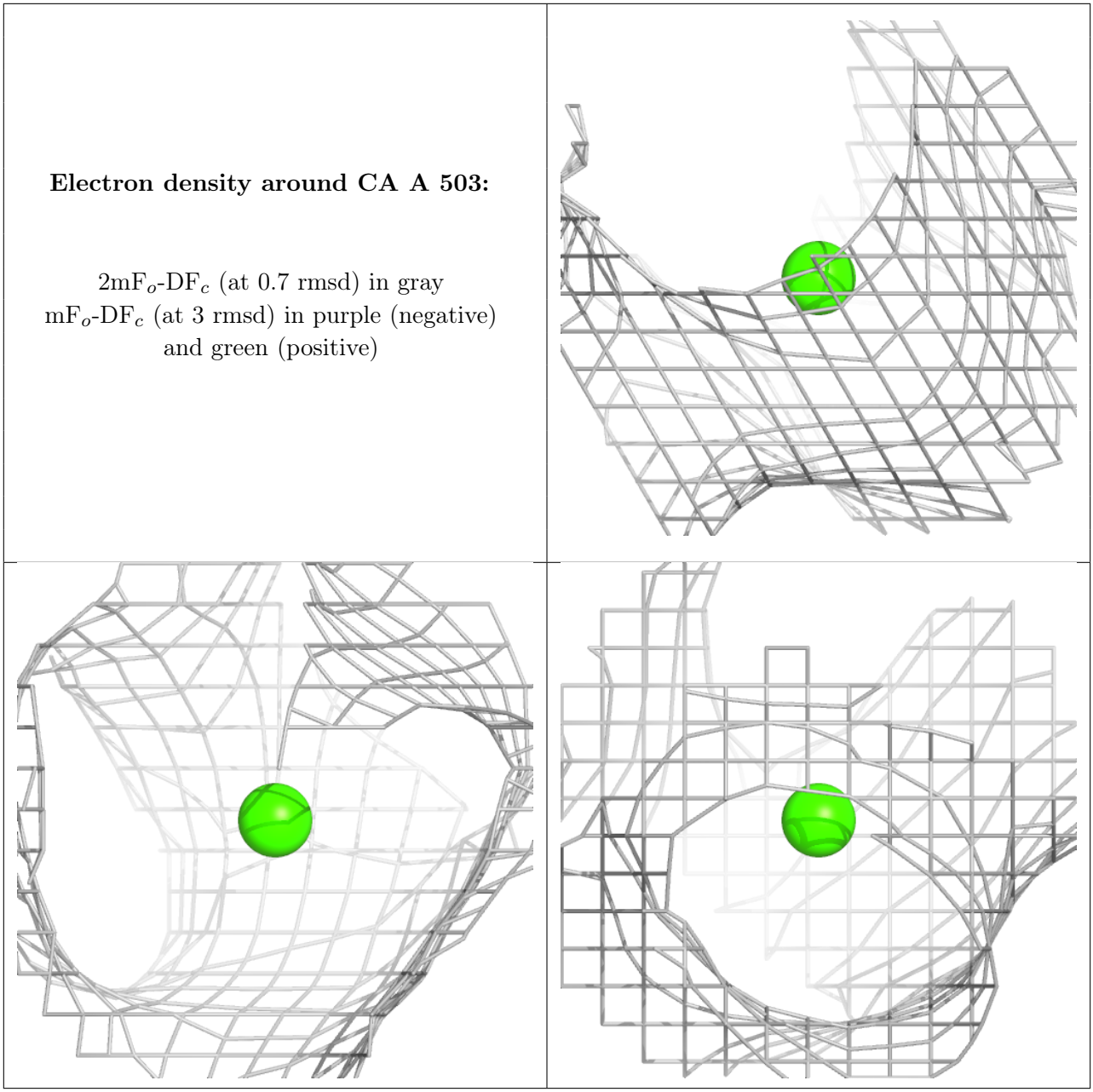
Electron density around CA A 505:

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



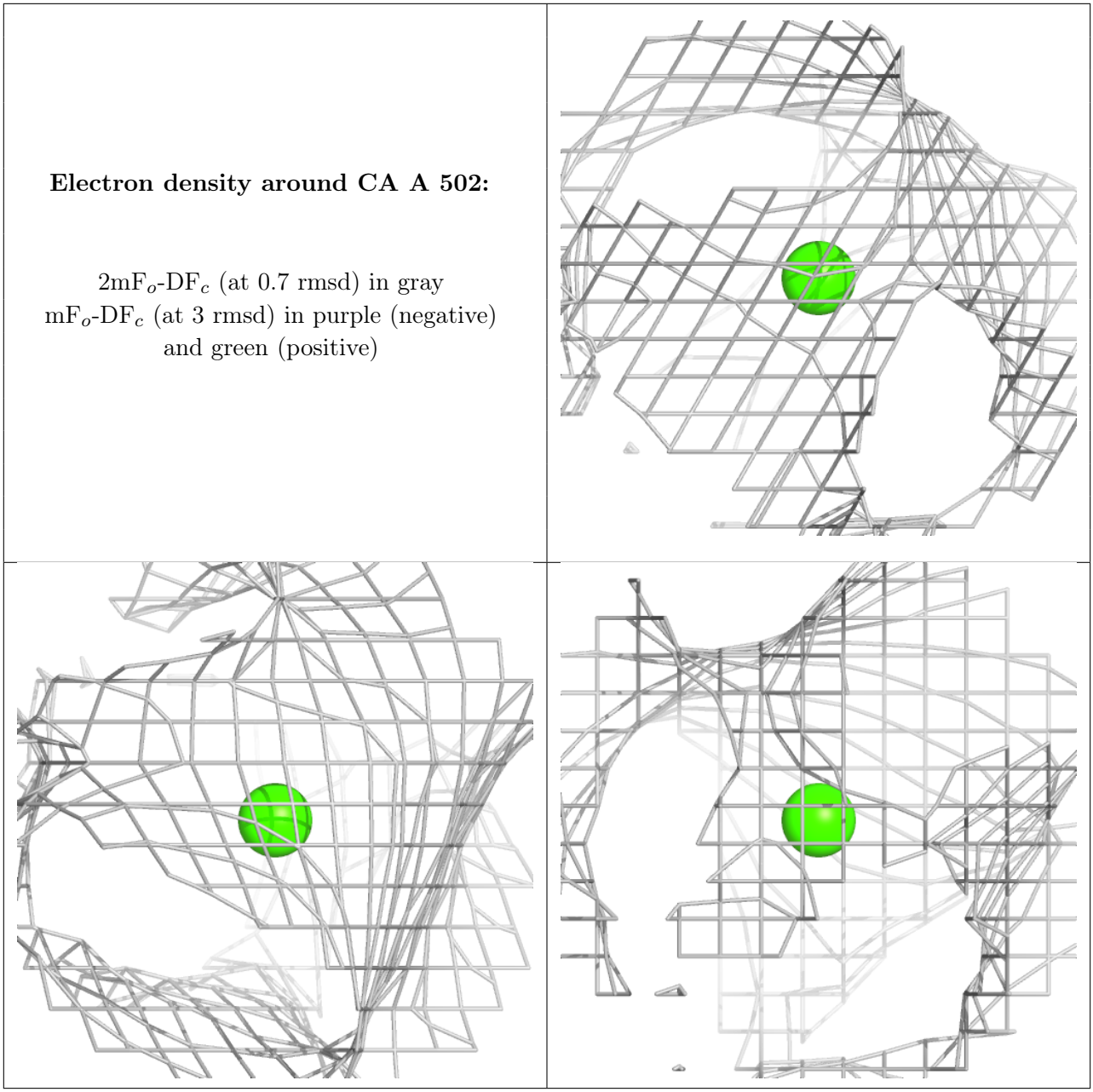
Electron density around CA A 503:

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



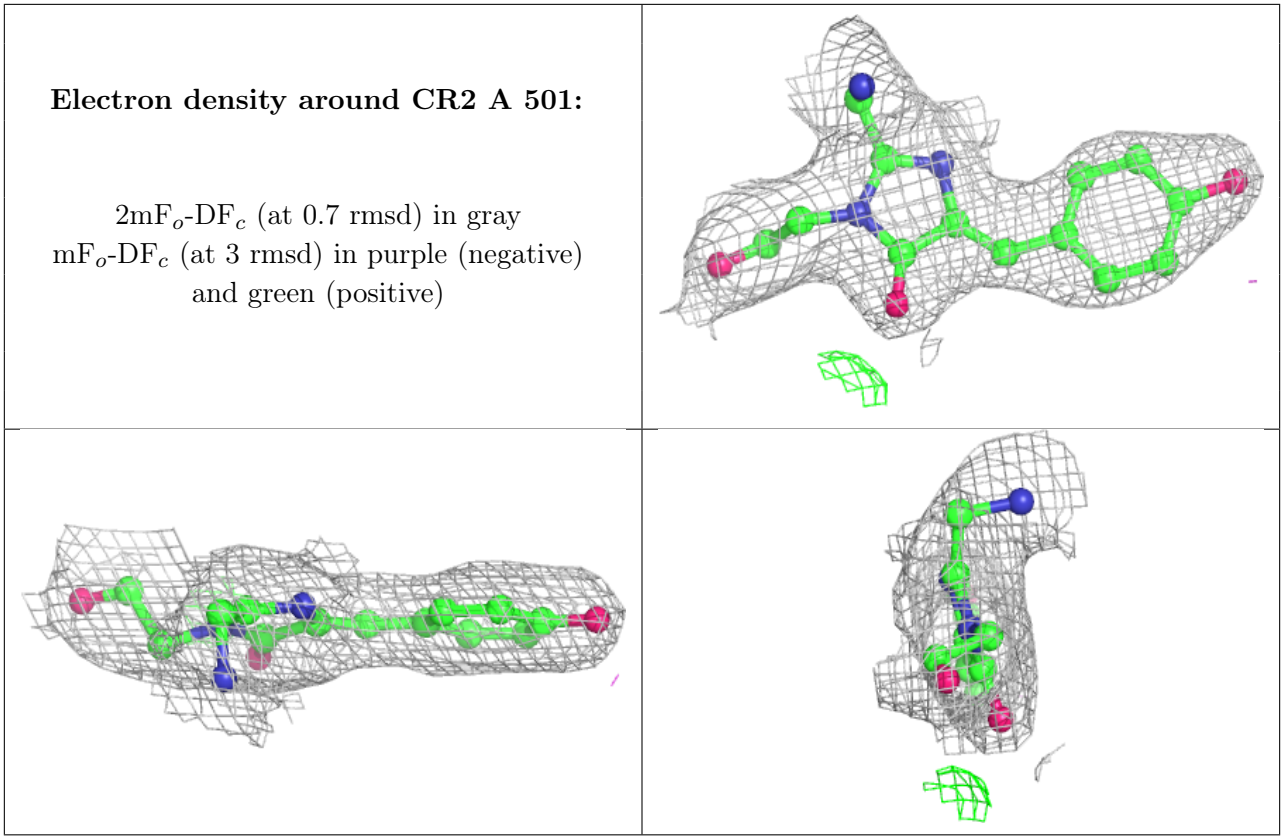
Electron density around CA A 502:

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



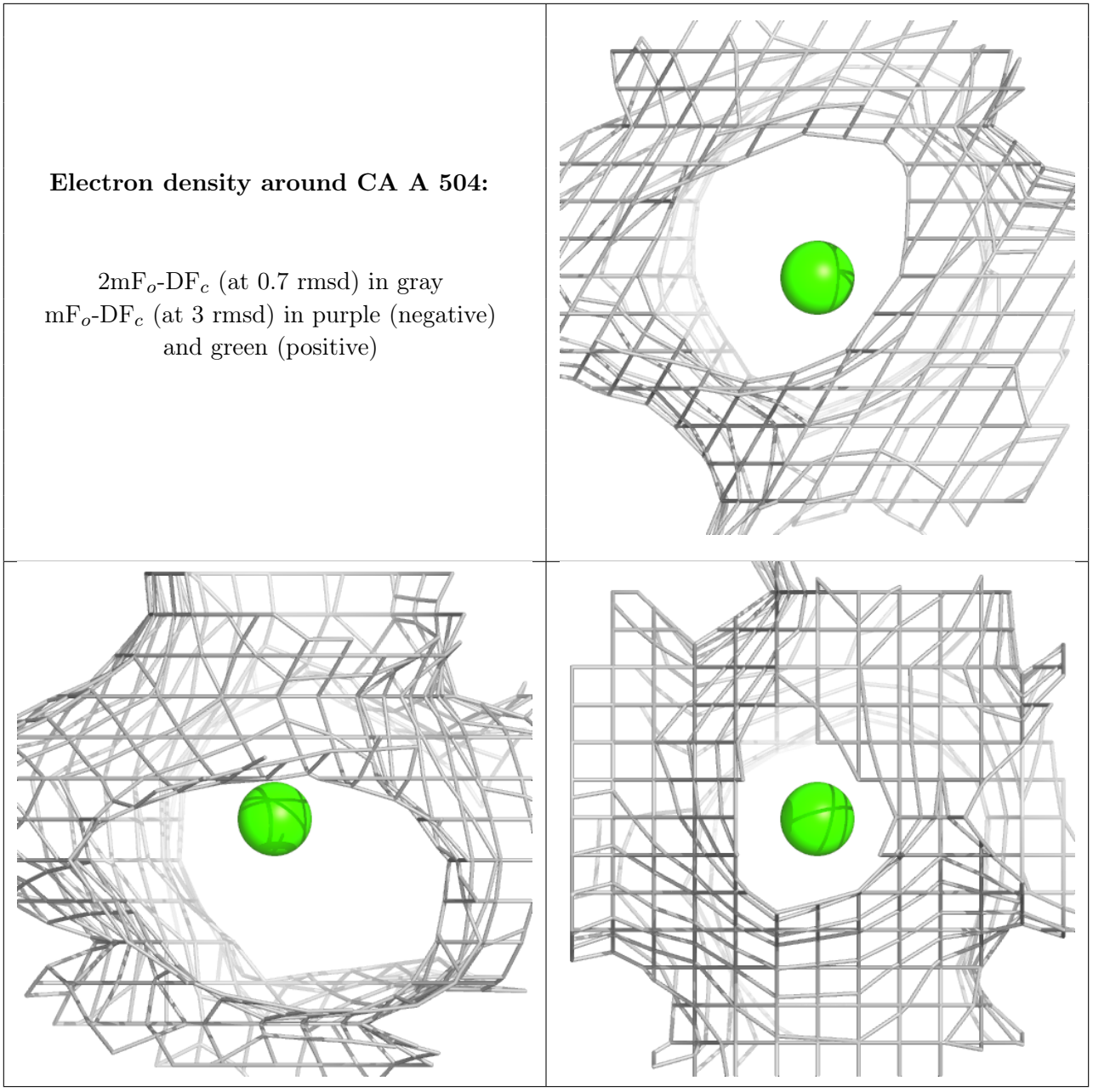
Electron density around CR2 A 501:

$2mF_o$-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 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)



6.5 Other polymers

There are no such residues in this entry.