



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:08 AM UTC

PDB ID : 6PSD / pdb_00006psd
Title : Complex of CRACR2a with a Dynein Light Intermediate Chain Peptide
Authors : Dominguez, R.; Lee, I.G.
Deposited on : 2019-07-12
Resolution : 2.66 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
Xtrriage (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

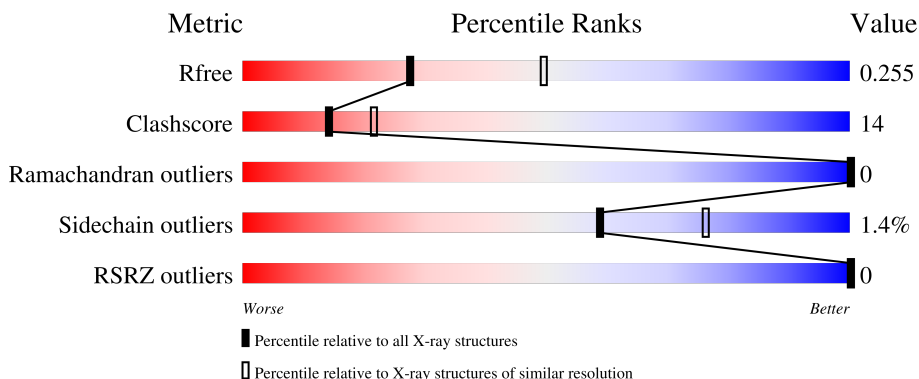
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.66 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.






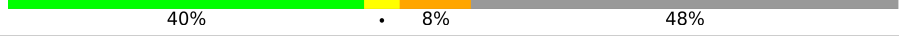



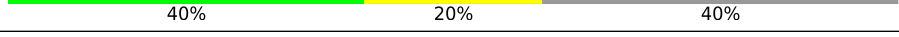

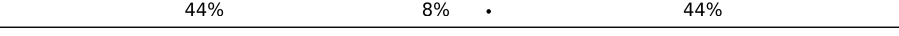
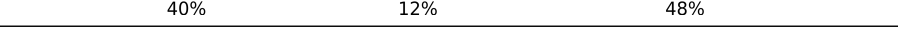
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	76	71% 22% . .
1	C	76	59% 34% . 5%
1	E	76	66% 29% . .
1	G	76	61% 33% 7%
1	I	76	74% 20% . . .

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Mol	Chain	Length	Quality of chain
1	K	76	 64% 28% • •
1	M	76	 83% 11% • 5%
1	O	76	 54% 37% • 5%
2	B	25	 40% • 8% 48%
2	D	25	 48% 12% 40%
2	F	25	 52% 48%
2	H	25	 52% • 44%
2	J	25	 40% 20% 40%
2	L	25	 48% 12% 40%
2	N	25	 44% 8% • 44%
2	P	25	 40% 12% 48%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5599 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 EF-hand calcium-binding domain-containing protein 4B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	E	73	Total 589	C 377	N 96	O 113	S 3	0	0	0
1	C	72	Total 585	C 375	N 95	O 112	S 3	0	0	0
1	A	73	Total 589	C 377	N 96	O 113	S 3	0	0	0
1	G	71	Total 579	C 372	N 94	O 110	S 3	0	0	0
1	I	73	Total 594	C 380	N 97	O 114	S 3	0	0	0
1	K	73	Total 589	C 377	N 96	O 113	S 3	0	0	0
1	M	72	Total 585	C 375	N 95	O 112	S 3	0	0	0
1	O	72	Total 583	C 374	N 95	O 111	S 3	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	46	GLY	-	expression tag	UNP Q9BSW2
C	46	GLY	-	expression tag	UNP Q9BSW2
A	46	GLY	-	expression tag	UNP Q9BSW2
G	46	GLY	-	expression tag	UNP Q9BSW2
I	46	GLY	-	expression tag	UNP Q9BSW2
K	46	GLY	-	expression tag	UNP Q9BSW2
M	46	GLY	-	expression tag	UNP Q9BSW2
O	46	GLY	-	expression tag	UNP Q9BSW2

- Molecule 2 is a protein called cDNA FLJ10219 fis, clone HEMBA1007018, highly similar to Cytoplasmic dynein 1 light intermediate chain 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	F	13	Total	C	N	O	0	0	0
			99	65	15	19			
2	D	15	Total	C	N	O	0	0	0
			114	74	18	22			
2	B	13	Total	C	N	O	0	0	0
			99	66	16	17			
2	H	14	Total	C	N	O	0	0	0
			105	68	16	21			
2	J	15	Total	C	N	O	0	0	0
			112	72	17	23			
2	L	15	Total	C	N	O	0	0	0
			114	74	18	22			
2	N	14	Total	C	N	O	0	0	0
			108	71	17	20			
2	P	13	Total	C	N	O	0	0	0
			99	65	15	19			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		
3	A	1	Total	Ca	0	0
			1	1		
3	G	1	Total	Ca	0	0
			1	1		
3	I	1	Total	Ca	0	0
			1	1		
3	K	1	Total	Ca	0	0
			1	1		
3	M	1	Total	Ca	0	0
			1	1		
3	O	1	Total	Ca	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	4	Total	O	0	0
			4	4		

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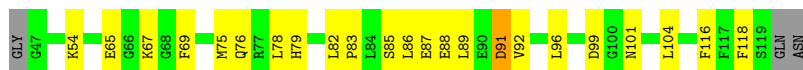
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	5	Total O 5 5	0	0
4	A	6	Total O 6 6	0	0
4	I	6	Total O 6 6	0	0
4	K	8	Total O 8 8	0	0
4	M	3	Total O 3 3	0	0
4	O	2	Total O 2 2	0	0
4	F	3	Total O 3 3	0	0
4	D	4	Total O 4 4	0	0
4	B	2	Total O 2 2	0	0
4	H	1	Total O 1 1	0	0
4	J	2	Total O 2 2	0	0
4	P	2	Total O 2 2	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.

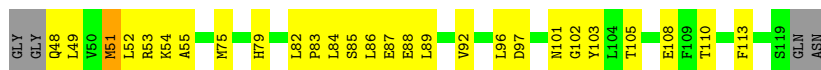
- Molecule 1: EF-hand calcium-binding domain-containing protein 4B

Chain E: 66% 29% . .



- Molecule 1: EF-hand calcium-binding domain-containing protein 4B

Chain C: 59% 34% . 5%



- Molecule 1: EF-hand calcium-binding domain-containing protein 4B

Chain A: 71% 22% . .



- Molecule 1: EF-hand calcium-binding domain-containing protein 4B

Chain G: 61% 33% 7%



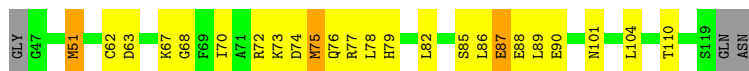
- Molecule 1: EF-hand calcium-binding domain-containing protein 4B

Chain I: 74% 20% . .



- Molecule 1: EF-hand calcium-binding domain-containing protein 4B

Chain K: 64% 28% . .



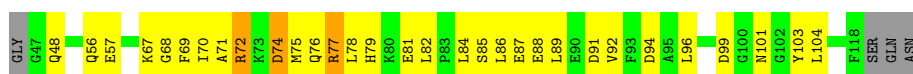
- Molecule 1: EF-hand calcium-binding domain-containing protein 4B

Chain M: 83% 11% 5%



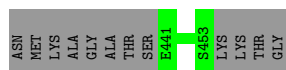
- Molecule 1: EF-hand calcium-binding domain-containing protein 4B

Chain O: 54% 37% 5%



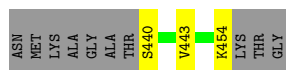
- Molecule 2: cDNA FLJ10219 fis, clone HEMBA1007018, highly similar to Cytoplasmic dynein 1 light intermediate chain 1

Chain F: 52% 48%



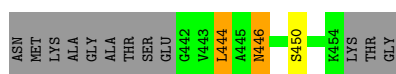
- Molecule 2: cDNA FLJ10219 fis, clone HEMBA1007018, highly similar to Cytoplasmic dynein 1 light intermediate chain 1

Chain D: 48% 12% 40%



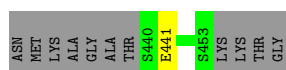
- Molecule 2: cDNA FLJ10219 fis, clone HEMBA1007018, highly similar to Cytoplasmic dynein 1 light intermediate chain 1

Chain B: 40% 8% 48%



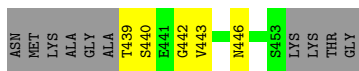
- Molecule 2: cDNA FLJ10219 fis, clone HEMBA1007018, highly similar to Cytoplasmic dynein 1 light intermediate chain 1

Chain H: 52% 44%



- Molecule 2: cDNA FLJ10219 fis, clone HEMBA1007018, highly similar to Cytoplasmic dynein 1 light intermediate chain 1

Chain J: 



- Molecule 2: cDNA FLJ10219 fis, clone HEMBA1007018, highly similar to Cytoplasmic dynein 1 light intermediate chain 1

Chain L: 



- Molecule 2: cDNA FLJ10219 fis, clone HEMBA1007018, highly similar to Cytoplasmic dynein 1 light intermediate chain 1

Chain N: 



- Molecule 2: cDNA FLJ10219 fis, clone HEMBA1007018, highly similar to Cytoplasmic dynein 1 light intermediate chain 1

Chain P: 



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.29Å 161.99Å 56.90Å 90.00° 104.01° 90.00°	Depositor
Resolution (Å)	43.35 – 2.66 43.35 – 2.66	Depositor EDS
% Data completeness (in resolution range)	92.6 (43.35-2.66) 92.0 (43.35-2.66)	Depositor EDS
R_{merge}	0.36	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.197 , 0.232 (Not available) , 0.255	Depositor DCC
R_{free} test set	3009 reflections (8.61%)	wwPDB-VP
Wilson B-factor (Å ²)	30.7	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 30.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	0.287 for l,-k,h	Xtriage
Reported twinning fraction	0.338 for H, K, L 0.662 for L, -K, H	Depositor
Outliers	0 of 29543 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5599	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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	1.13	2/602 (0.3%)	1.03	4/807 (0.5%)
1	C	1.21	3/598 (0.5%)	0.99	0/802
1	E	1.32	5/602 (0.8%)	0.92	1/807 (0.1%)
1	G	0.87	0/592	0.78	0/794
1	I	1.15	0/607	0.90	2/814 (0.2%)
1	K	1.26	3/602 (0.5%)	0.91	0/807
1	M	1.05	2/598 (0.3%)	0.77	0/802
1	O	0.99	0/596	0.89	2/799 (0.3%)
2	B	1.34	1/100 (1.0%)	1.03	1/133 (0.8%)
2	D	1.09	0/115	0.81	0/153
2	F	0.89	0/100	0.73	0/134
2	H	1.02	0/106	0.95	1/142 (0.7%)
2	J	0.97	0/113	0.72	0/152
2	L	1.39	0/115	1.62	2/153 (1.3%)
2	N	1.15	0/109	1.16	1/145 (0.7%)
2	P	1.01	0/100	0.79	0/134
All	All	1.13	16/5655 (0.3%)	0.92	14/7578 (0.2%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	51	MET	SD-CE	-7.22	1.61	1.79
1	K	51	MET	SD-CE	-6.93	1.62	1.79
1	A	51	MET	SD-CE	-6.82	1.62	1.79
1	E	91	ASP	C-N	-6.48	1.25	1.33
1	E	83	PRO	N-CD	-6.30	1.39	1.47
1	K	75	MET	SD-CE	-6.15	1.64	1.79
1	E	92	VAL	C-N	-5.91	1.26	1.33
2	B	446	ASN	N-CA	-5.83	1.39	1.46
1	C	52	LEU	C-O	-5.74	1.16	1.24
1	C	53	ARG	N-CA	-5.64	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	47	GLY	N-CA	5.54	1.54	1.45
1	E	54	LYS	CA-C	-5.39	1.45	1.52
1	C	54	LYS	C-O	-5.33	1.17	1.24
1	K	87	GLU	C-O	-5.13	1.18	1.24
1	E	83	PRO	CA-CB	-5.09	1.48	1.53
1	M	56	GLN	C-O	-5.03	1.18	1.24

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	445	ALA	CA-C-N	11.50	135.39	120.44
2	L	445	ALA	C-N-CA	11.50	135.39	120.44
2	N	443	VAL	N-CA-C	-9.44	101.58	111.58
1	I	119	SER	N-CA-C	-8.49	100.92	111.11
1	A	67	LYS	N-CA-C	6.77	118.66	111.28
1	O	74	ASP	N-CA-C	-6.49	104.13	111.14
1	O	77	ARG	N-CA-C	-6.39	104.18	112.23
1	A	65	GLU	CB-CA-C	-6.29	98.22	110.11
1	A	65	GLU	N-CA-CB	5.97	119.15	110.26
2	B	444	LEU	N-CA-C	-5.93	104.73	111.14
1	I	118	PHE	N-CA-C	5.61	119.81	112.92
2	H	441	GLU	N-CA-C	-5.37	105.99	112.54
1	A	68	GLY	CA-C-O	5.21	123.66	118.77
1	E	92	VAL	O-C-N	5.21	127.31	121.90

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	589	0	557	12	0
1	C	585	0	554	21	0
1	E	589	0	557	14	0
1	G	579	0	549	18	0
1	I	594	0	562	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	589	0	557	28	0
1	M	585	0	554	6	0
1	O	583	0	552	40	0
2	B	99	0	102	3	0
2	D	114	0	113	2	0
2	F	99	0	95	0	0
2	H	105	0	100	0	0
2	J	112	0	107	2	0
2	L	114	0	113	1	0
2	N	108	0	108	2	0
2	P	99	0	95	4	0
3	A	1	0	0	0	0
3	C	1	0	0	1	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
3	K	1	0	0	0	0
3	M	1	0	0	0	0
3	O	1	0	0	0	0
4	A	6	0	0	0	0
4	B	2	0	0	0	0
4	C	5	0	0	0	0
4	D	4	0	0	0	0
4	E	4	0	0	0	0
4	F	3	0	0	0	0
4	H	1	0	0	0	0
4	I	6	0	0	0	0
4	J	2	0	0	0	0
4	K	8	0	0	0	0
4	M	3	0	0	0	0
4	O	2	0	0	0	0
4	P	2	0	0	0	0
All	All	5599	0	5275	154	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 14.

All (154) 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:O:75:MET:O	1:O:78:LEU:N	1.78	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:70:ILE:HB	1:K:104:LEU:HD23	1.25	1.13
1:K:70:ILE:CB	1:K:104:LEU:HD23	1.87	1.04
1:E:75:MET:O	1:E:89:LEU:HD13	1.66	0.96
1:O:72:ARG:NH1	1:O:94:ASP:OD1	2.04	0.91
1:A:92:VAL:HG23	2:B:444:LEU:HD23	1.57	0.86
1:E:91:ASP:OD1	1:A:80:LYS:NZ	2.08	0.85
1:O:92:VAL:HG23	2:P:444:LEU:HD23	1.59	0.83
1:O:75:MET:HE1	1:O:92:VAL:HG13	1.60	0.82
1:K:70:ILE:HB	1:K:104:LEU:CD2	2.08	0.80
1:G:62:CYS:O	1:G:77:ARG:NH1	2.15	0.80
1:C:51:MET:HE1	1:C:110:THR:HG23	1.64	0.79
1:K:70:ILE:HD12	1:K:104:LEU:CD2	2.12	0.78
1:O:79:HIS:ND1	1:O:86:LEU:HD23	1.99	0.78
1:G:79:HIS:ND1	1:G:79:HIS:O	2.18	0.77
1:G:67:LYS:NZ	1:G:74:ASP:OD2	2.17	0.77
1:O:48:GLN:N	1:O:48:GLN:OE1	2.18	0.77
1:M:52:LEU:O	1:M:56:GLN:HG3	1.85	0.76
1:O:92:VAL:CG2	2:P:444:LEU:HD23	2.16	0.76
1:A:89:LEU:O	1:A:92:VAL:HG12	1.87	0.75
2:J:442:GLY:O	2:J:446:ASN:ND2	2.20	0.74
1:O:85:SER:O	1:O:88:GLU:N	2.21	0.74
1:K:70:ILE:CD1	1:K:104:LEU:HD23	2.19	0.71
1:O:78:LEU:O	1:O:82:LEU:HB2	1.91	0.69
1:K:67:LYS:NZ	1:K:74:ASP:OD2	2.26	0.68
1:O:96:LEU:HB3	1:O:104:LEU:HD21	1.75	0.68
1:C:79:HIS:ND1	1:C:84:LEU:O	2.26	0.68
1:C:51:MET:HE2	1:C:55:ALA:HB2	1.76	0.67
1:C:101:ASN:O	1:C:103:TYR:N	2.28	0.66
2:D:454:LYS:O	2:D:454:LYS:HG2	1.93	0.66
1:G:57:GLU:O	1:G:61:THR:OG1	2.13	0.66
1:E:65:GLU:O	1:E:65:GLU:HG2	1.95	0.66
1:K:78:LEU:HB3	1:K:82:LEU:HD23	1.77	0.65
1:O:71:ALA:N	1:O:74:ASP:OD2	2.19	0.65
1:K:70:ILE:HD12	1:K:104:LEU:HD23	1.76	0.65
1:C:51:MET:HE3	1:C:113:PHE:HD2	1.60	0.65
1:K:86:LEU:O	1:K:90:GLU:HG3	1.97	0.64
2:J:440:SER:O	2:J:443:VAL:HG12	1.97	0.64
1:C:101:ASN:C	1:C:103:TYR:H	2.06	0.63
2:N:441:GLU:HB3	2:N:443:VAL:HG23	1.79	0.63
1:E:65:GLU:OE2	1:E:67:LYS:NZ	2.31	0.63
1:A:87:GLU:O	1:A:91:ASP:OD1	2.16	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:VAL:CG2	2:B:444:LEU:HD23	2.29	0.62
1:A:73:LYS:O	1:A:76:GLN:HG3	2.01	0.61
1:I:101:ASN:O	1:K:72:ARG:HD2	2.00	0.61
1:O:99:ASP:CG	1:O:101:ASN:HB2	2.26	0.61
1:C:85:SER:O	1:C:88:GLU:HG3	2.00	0.60
1:O:75:MET:C	1:O:78:LEU:H	2.03	0.60
1:O:75:MET:O	1:O:76:GLN:C	2.43	0.60
1:K:72:ARG:O	1:K:76:GLN:HG2	2.02	0.60
1:O:75:MET:O	1:O:77:ARG:N	2.34	0.60
1:K:70:ILE:CD1	1:K:104:LEU:CD2	2.79	0.60
1:A:96:LEU:HB3	1:A:104:LEU:HD21	1.82	0.59
1:K:76:GLN:OE1	1:K:86:LEU:HD22	2.04	0.58
1:I:118:PHE:O	1:I:119:SER:C	2.48	0.57
1:E:96:LEU:HB3	1:E:104:LEU:HD21	1.87	0.56
1:E:85:SER:N	1:E:88:GLU:OE1	2.36	0.56
2:D:440:SER:O	2:D:443:VAL:HG12	2.05	0.56
1:K:85:SER:O	1:K:88:GLU:N	2.38	0.56
1:O:79:HIS:ND1	1:O:86:LEU:CD2	2.69	0.56
1:A:73:LYS:HA	1:A:76:GLN:HG2	1.89	0.55
1:K:70:ILE:HD12	1:K:104:LEU:HD21	1.89	0.54
1:O:75:MET:C	1:O:77:ARG:N	2.61	0.54
1:I:89:LEU:HA	1:I:92:VAL:CG1	2.37	0.54
1:C:101:ASN:C	1:C:103:TYR:N	2.64	0.54
1:O:81:GLU:O	1:O:82:LEU:HD12	2.08	0.54
1:I:54:LYS:HD2	1:I:57:GLU:OE1	2.07	0.54
1:K:62:CYS:SG	1:K:75:MET:HE1	2.48	0.53
1:E:67:LYS:HD2	1:E:69:PHE:CZ	2.44	0.53
1:C:51:MET:CE	1:C:55:ALA:HB2	2.38	0.53
1:K:70:ILE:CG1	1:K:104:LEU:HD23	2.38	0.53
1:O:89:LEU:O	1:O:92:VAL:HG12	2.09	0.53
1:I:89:LEU:HA	1:I:92:VAL:HG12	1.91	0.52
1:G:111:THR:O	1:G:115:HIS:ND1	2.41	0.52
1:G:78:LEU:C	1:G:80:LYS:H	2.17	0.52
1:E:79:HIS:HB2	1:E:86:LEU:HD23	1.91	0.51
1:G:48:GLN:HG2	1:G:49:LEU:HD23	1.91	0.51
1:K:75:MET:O	1:K:89:LEU:HD22	2.10	0.51
1:K:70:ILE:CG2	1:K:104:LEU:HD23	2.40	0.51
1:O:101:ASN:OD1	1:O:103:TYR:HB2	2.11	0.51
2:P:444:LEU:O	2:P:447:PHE:N	2.42	0.51
1:O:96:LEU:CB	1:O:104:LEU:HD21	2.41	0.51
1:M:76:GLN:HG2	1:M:86:LEU:HD21	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:LEU:O	1:C:92:VAL:HG22	2.11	0.50
1:C:85:SER:O	1:C:88:GLU:CG	2.60	0.50
1:G:74:ASP:O	1:G:78:LEU:HD23	2.10	0.50
1:A:86:LEU:HA	1:A:89:LEU:HB2	1.94	0.50
1:I:87:GLU:O	1:I:91:ASP:OD1	2.29	0.50
1:C:48:GLN:OE1	1:C:49:LEU:CD1	2.60	0.50
1:E:78:LEU:HB3	1:E:82:LEU:HD12	1.94	0.49
1:M:79:HIS:CD2	1:M:86:LEU:HG	2.47	0.49
1:O:75:MET:CE	1:O:92:VAL:HG13	2.37	0.49
1:G:56:GLN:O	1:G:57:GLU:C	2.54	0.49
1:C:51:MET:CE	1:C:113:PHE:HD2	2.25	0.49
2:B:446:ASN:O	2:B:450:SER:OG	2.27	0.49
1:O:67:LYS:HB3	1:O:69:PHE:CE1	2.47	0.48
1:C:97:ASP:OD2	1:C:102:GLY:N	2.47	0.48
1:K:63:ASP:OD1	1:K:67:LYS:HG3	2.13	0.48
1:G:50:VAL:N	1:O:56:GLN:OE1	2.46	0.48
2:P:447:PHE:CE2	2:P:451:LEU:HD11	2.48	0.48
1:A:67:LYS:HB3	1:A:69:PHE:CE1	2.49	0.47
1:O:70:ILE:HB	1:O:104:LEU:HB2	1.96	0.47
1:E:99:ASP:OD2	1:E:101:ASN:OD1	2.32	0.47
1:O:75:MET:O	1:O:78:LEU:CA	2.61	0.47
1:K:70:ILE:HB	1:K:104:LEU:HB3	1.95	0.47
1:G:78:LEU:C	1:G:80:LYS:N	2.71	0.47
1:K:75:MET:HA	1:K:75:MET:HE2	1.96	0.47
1:K:68:GLY:HA2	1:M:49:LEU:CD1	2.45	0.46
1:O:99:ASP:OD1	1:O:101:ASN:HB2	2.15	0.46
1:E:65:GLU:HG3	1:K:101:ASN:O	2.16	0.46
1:O:85:SER:O	1:O:86:LEU:C	2.58	0.46
1:I:92:VAL:HG13	1:I:93:PHE:N	2.31	0.46
1:G:94:ASP:HA	1:G:97:ASP:HB3	1.98	0.45
1:G:79:HIS:CD2	1:G:86:LEU:HG	2.52	0.45
1:G:89:LEU:O	1:G:92:VAL:HB	2.16	0.45
1:O:75:MET:O	1:O:78:LEU:HB2	2.16	0.45
1:C:92:VAL:O	1:C:96:LEU:HG	2.16	0.45
1:O:75:MET:HA	1:O:78:LEU:HD12	1.99	0.45
1:O:101:ASN:OD1	1:O:103:TYR:HD2	2.00	0.44
1:G:70:ILE:HG21	1:G:75:MET:HE3	1.99	0.44
1:I:70:ILE:HB	1:I:104:LEU:HB2	1.99	0.44
1:K:51:MET:HE1	1:K:110:THR:HG23	1.98	0.44
1:O:85:SER:H	1:O:88:GLU:HB2	1.83	0.44
1:C:48:GLN:OE1	1:C:49:LEU:HD13	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:87:GLU:O	1:O:91:ASP:OD1	2.36	0.44
1:A:101:ASN:HB2	1:A:103:TYR:H	1.83	0.43
1:E:101:ASN:ND2	1:I:65:GLU:CD	2.76	0.43
1:C:82:LEU:HA	1:C:83:PRO:HD2	1.75	0.43
1:C:75:MET:O	1:C:89:LEU:HD13	2.18	0.43
1:O:87:GLU:O	1:O:91:ASP:CG	2.61	0.43
1:G:54:LYS:O	1:G:55:ALA:C	2.61	0.43
1:O:79:HIS:CE1	1:O:84:LEU:O	2.72	0.43
1:E:76:GLN:O	1:E:76:GLN:HG2	2.16	0.43
1:O:79:HIS:C	1:O:81:GLU:H	2.27	0.43
2:L:440:SER:O	2:L:443:VAL:HG12	2.19	0.43
1:C:105:THR:OG1	1:C:108:GLU:HB2	2.19	0.42
1:A:51:MET:HE2	1:A:52:LEU:HG	2.00	0.42
1:I:73:LYS:O	1:I:76:GLN:HB2	2.19	0.42
1:G:73:LYS:O	1:G:77:ARG:HG2	2.20	0.42
1:O:71:ALA:HB3	1:O:74:ASP:CG	2.45	0.42
1:K:86:LEU:HA	1:K:89:LEU:HD12	2.01	0.42
1:G:49:LEU:HD13	1:O:68:GLY:HA2	2.01	0.41
1:E:116:PHE:O	1:E:118:PHE:N	2.53	0.41
1:I:78:LEU:N	1:I:78:LEU:HD23	2.35	0.41
1:I:89:LEU:C	1:I:92:VAL:HG12	2.46	0.41
1:M:69:PHE:CD1	1:M:69:PHE:C	2.98	0.41
1:C:86:LEU:O	1:C:87:GLU:C	2.61	0.41
1:C:101:ASN:HB3	3:C:201:CA:CA	1.80	0.41
1:O:56:GLN:O	1:O:57:GLU:C	2.64	0.41
1:I:92:VAL:HG13	1:I:93:PHE:H	1.85	0.41
1:K:79:HIS:HB2	1:K:86:LEU:CD2	2.51	0.41
1:M:92:VAL:HG11	2:N:447:PHE:CD2	2.56	0.40
1:O:79:HIS:O	1:O:79:HIS:HD2	2.03	0.40
1:K:73:LYS:O	1:K:77:ARG:HG3	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	71/76 (93%)	70 (99%)	1 (1%)	0	100	100
1	C	70/76 (92%)	68 (97%)	2 (3%)	0	100	100
1	E	71/76 (93%)	69 (97%)	2 (3%)	0	100	100
1	G	69/76 (91%)	64 (93%)	5 (7%)	0	100	100
1	I	71/76 (93%)	69 (97%)	2 (3%)	0	100	100
1	K	71/76 (93%)	69 (97%)	2 (3%)	0	100	100
1	M	70/76 (92%)	66 (94%)	4 (6%)	0	100	100
1	O	70/76 (92%)	68 (97%)	2 (3%)	0	100	100
2	B	11/25 (44%)	10 (91%)	1 (9%)	0	100	100
2	D	13/25 (52%)	13 (100%)	0	0	100	100
2	F	11/25 (44%)	10 (91%)	1 (9%)	0	100	100
2	H	12/25 (48%)	11 (92%)	1 (8%)	0	100	100
2	J	13/25 (52%)	13 (100%)	0	0	100	100
2	L	13/25 (52%)	10 (77%)	3 (23%)	0	100	100
2	N	12/25 (48%)	11 (92%)	1 (8%)	0	100	100
2	P	11/25 (44%)	9 (82%)	2 (18%)	0	100	100
All	All	659/808 (82%)	630 (96%)	29 (4%)	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	62/64 (97%)	62 (100%)	0	100	100
1	C	62/64 (97%)	61 (98%)	1 (2%)	55	74
1	E	62/64 (97%)	61 (98%)	1 (2%)	55	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	61/64 (95%)	61 (100%)	0	100	100
1	I	63/64 (98%)	61 (97%)	2 (3%)	34	55
1	K	62/64 (97%)	61 (98%)	1 (2%)	55	74
1	M	62/64 (97%)	62 (100%)	0	100	100
1	O	61/64 (95%)	60 (98%)	1 (2%)	55	74
2	B	11/19 (58%)	11 (100%)	0	100	100
2	D	13/19 (68%)	13 (100%)	0	100	100
2	F	11/19 (58%)	11 (100%)	0	100	100
2	H	12/19 (63%)	12 (100%)	0	100	100
2	J	13/19 (68%)	12 (92%)	1 (8%)	12	20
2	L	13/19 (68%)	13 (100%)	0	100	100
2	N	12/19 (63%)	11 (92%)	1 (8%)	10	18
2	P	11/19 (58%)	11 (100%)	0	100	100
All	All	591/664 (89%)	583 (99%)	8 (1%)	59	76

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

Mol	Chain	Res	Type
1	E	87	GLU
1	C	51	MET
1	I	48	GLN
1	I	119	SER
1	K	87	GLU
1	O	72	ARG
2	J	439	THR
2	N	443	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	60	GLN
1	E	76	GLN
1	E	101	ASN
1	K	101	ASN
1	K	107	GLN
1	M	76	GLN

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Mol	Chain	Res	Type
1	M	79	HIS
1	M	115	HIS
1	O	79	HIS
1	O	115	HIS
2	L	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 8 ligands modelled in this entry, 8 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	73/76 (96%)	-1.40	0 100 100	32, 57, 95, 115	0
1	C	72/76 (94%)	-1.33	0 100 100	30, 71, 118, 139	0
1	E	73/76 (96%)	-1.46	0 100 100	24, 52, 90, 100	0
1	G	71/76 (93%)	-1.13	0 100 100	51, 78, 120, 139	0
1	I	73/76 (96%)	-1.46	0 100 100	32, 57, 89, 107	0
1	K	73/76 (96%)	-1.61	0 100 100	30, 42, 69, 83	0
1	M	72/76 (94%)	-1.40	0 100 100	30, 64, 89, 108	0
1	O	72/76 (94%)	-1.18	0 100 100	41, 78, 133, 135	0
2	B	13/25 (52%)	-1.48	0 100 100	28, 38, 68, 102	0
2	D	15/25 (60%)	-1.33	0 100 100	36, 61, 100, 106	0
2	F	13/25 (52%)	-1.49	0 100 100	35, 43, 68, 82	0
2	H	14/25 (56%)	-1.17	0 100 100	47, 61, 89, 97	0
2	J	15/25 (60%)	-1.51	0 100 100	23, 43, 61, 77	0
2	L	15/25 (60%)	-1.39	0 100 100	31, 47, 98, 100	0
2	N	14/25 (56%)	-1.27	0 100 100	46, 69, 102, 115	0
2	P	13/25 (52%)	-1.27	0 100 100	45, 55, 86, 122	0
All	All	691/808 (85%)	-1.37	0 100 100	23, 60, 106, 139	0

There are no RSRZ outliers to report.

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

There are no oligosaccharides in this entry.

6.4 Ligands

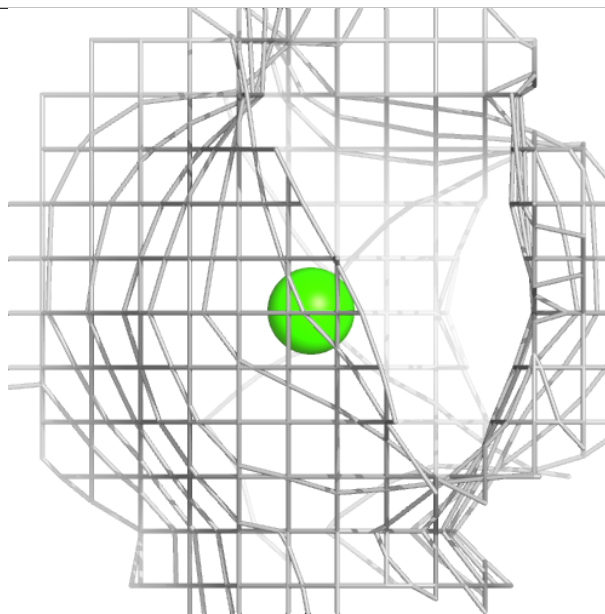
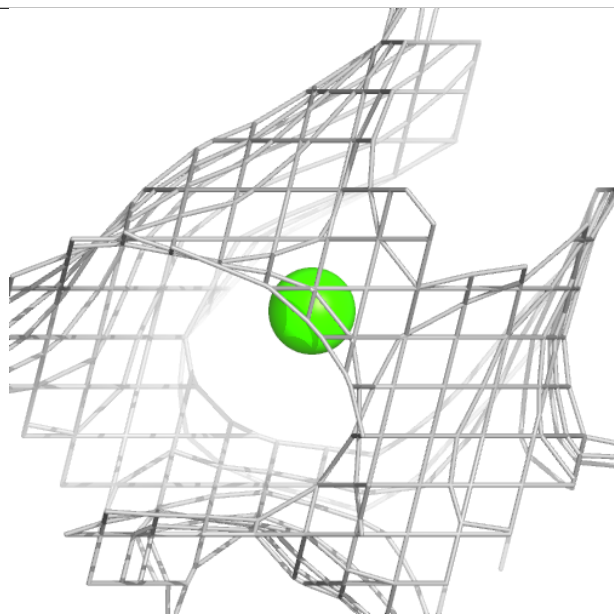
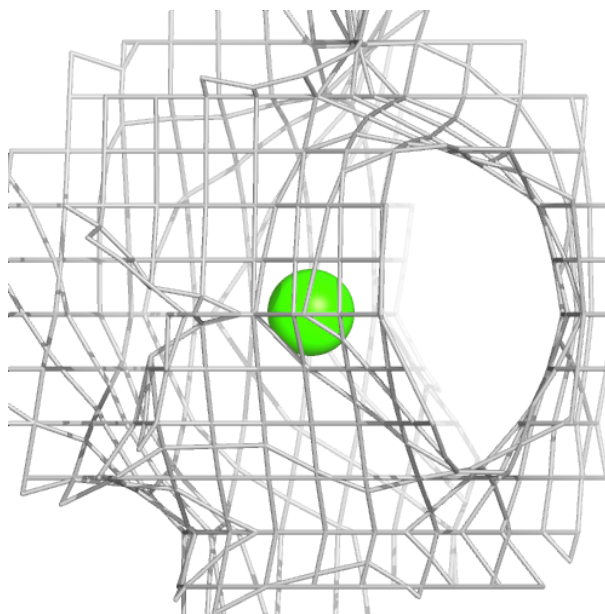
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	E	201	1/1	1.00	0.01	36,36,36,36	0
3	CA	C	201	1/1	1.00	0.01	64,64,64,64	0
3	CA	A	201	1/1	1.00	0.01	41,41,41,41	0
3	CA	G	201	1/1	1.00	0.02	54,54,54,54	0
3	CA	I	201	1/1	1.00	0.01	51,51,51,51	0
3	CA	K	201	1/1	1.00	0.02	30,30,30,30	0
3	CA	M	201	1/1	1.00	0.02	47,47,47,47	0
3	CA	O	201	1/1	1.00	0.01	69,69,69,69	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.

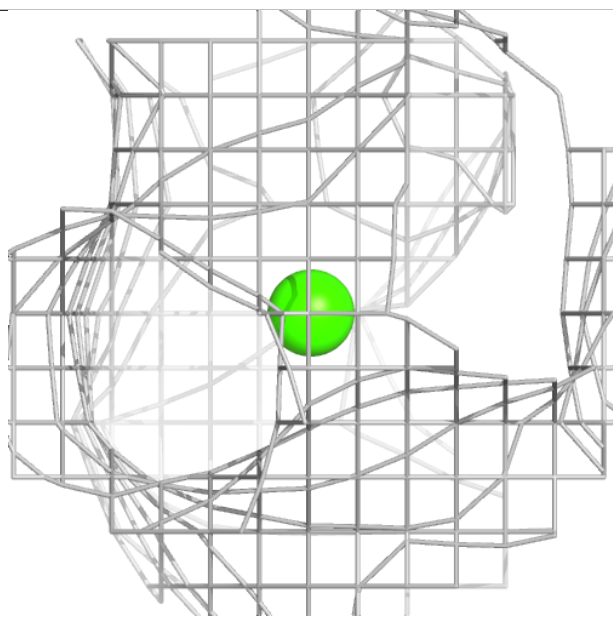
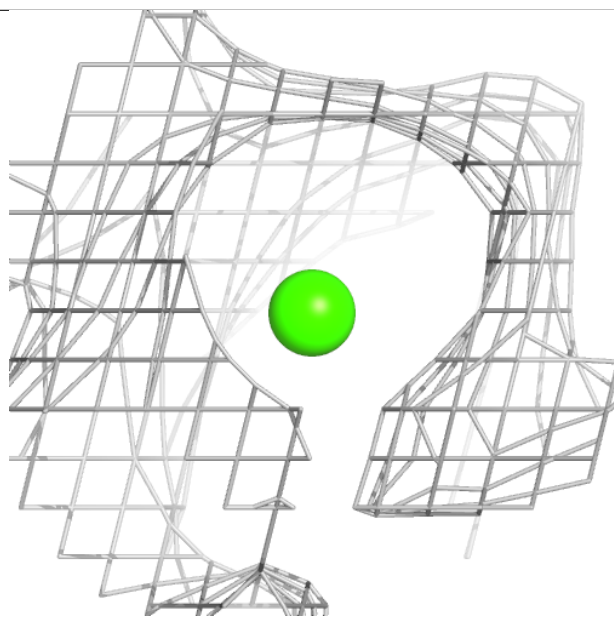
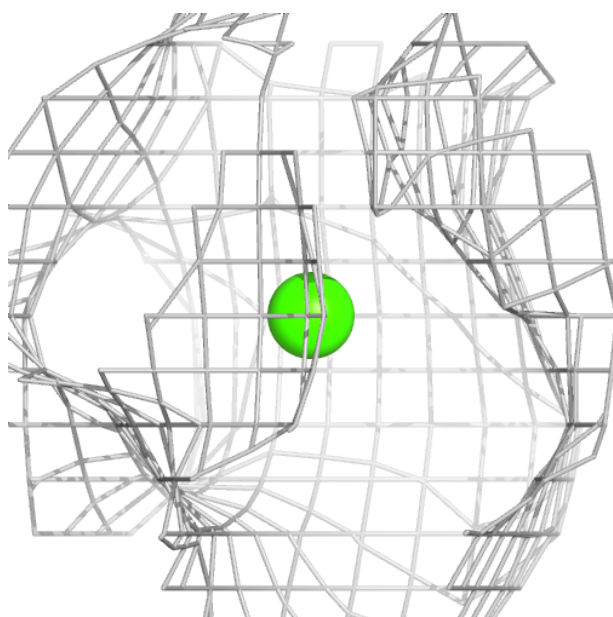
Electron density around CA E 201:

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



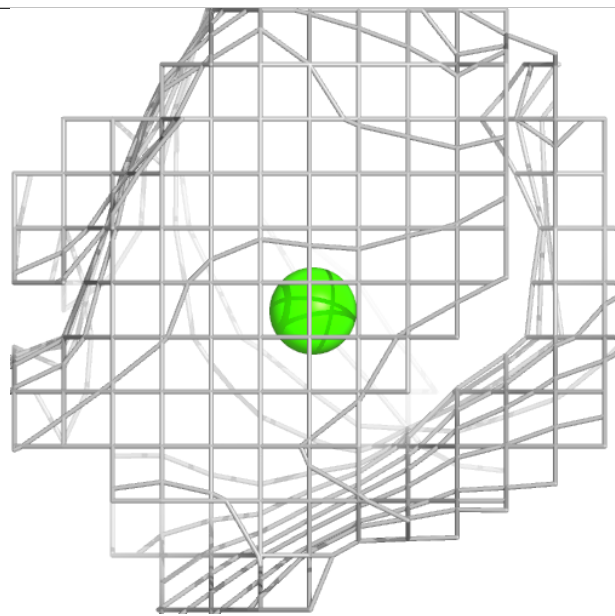
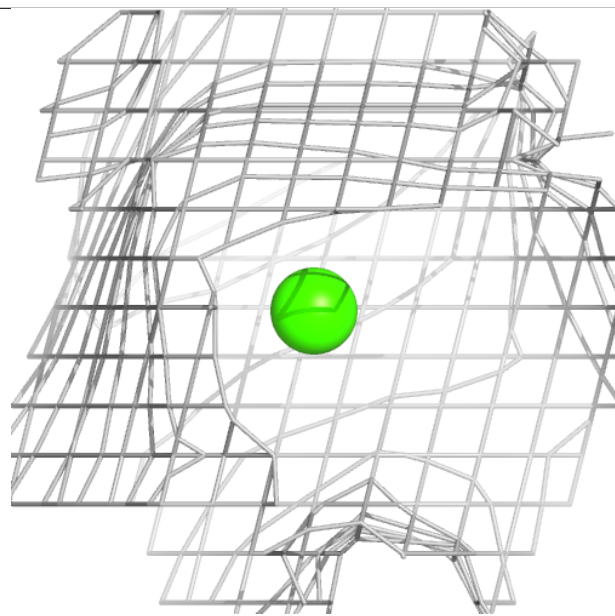
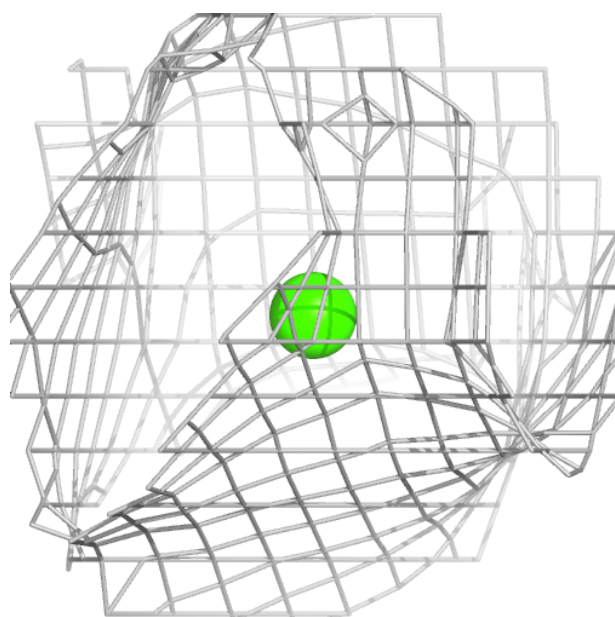
Electron density around CA C 201:

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



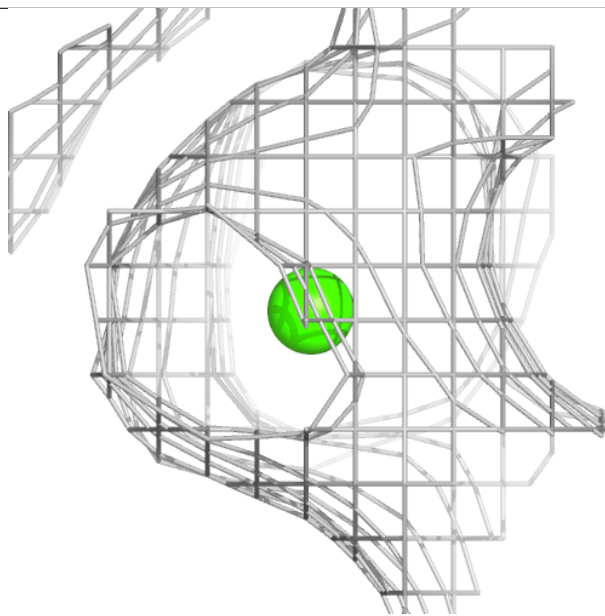
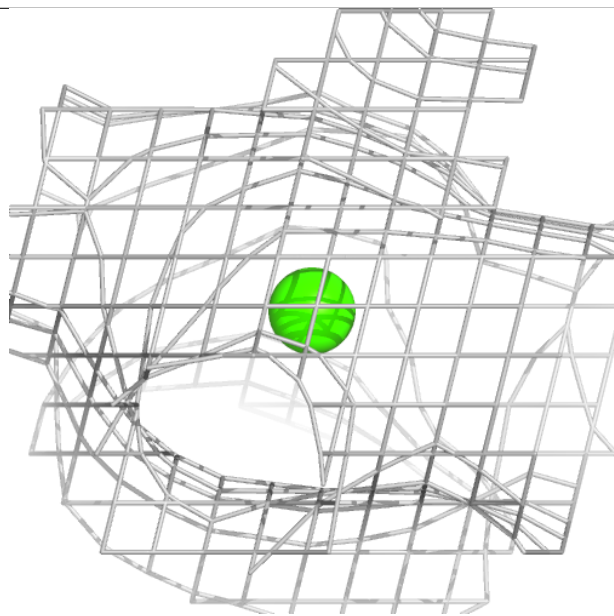
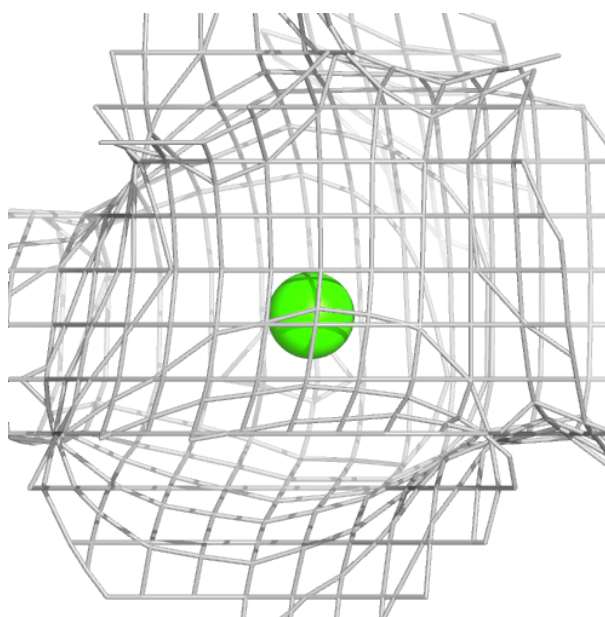
Electron density around CA A 201:

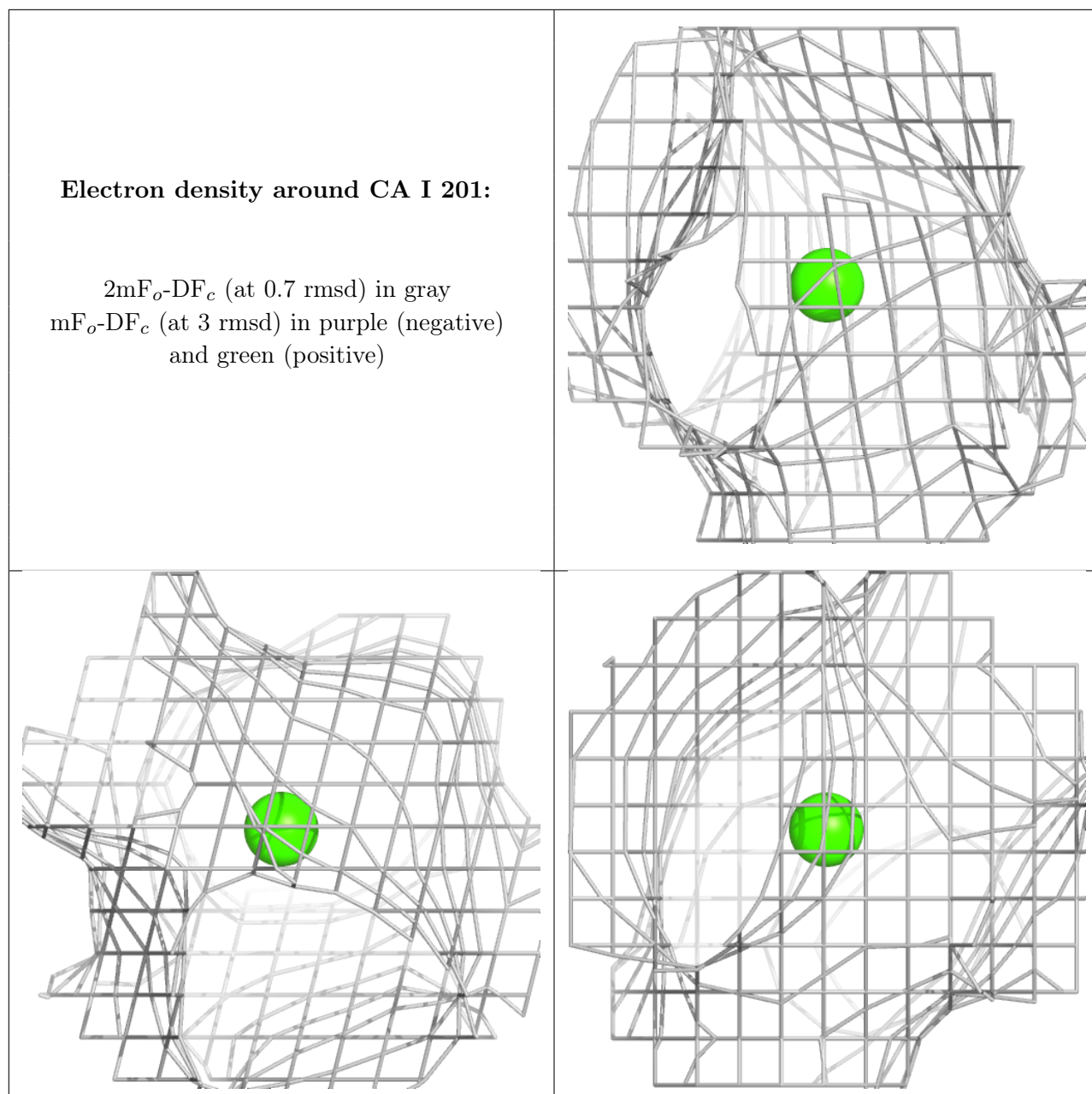
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CA G 201:

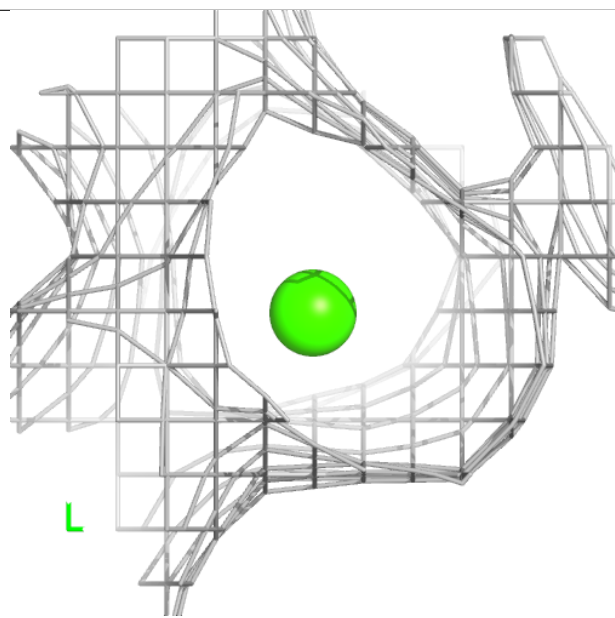
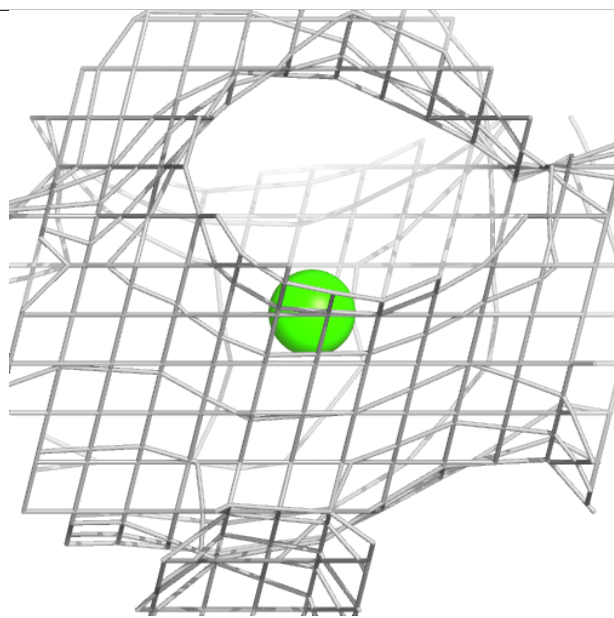
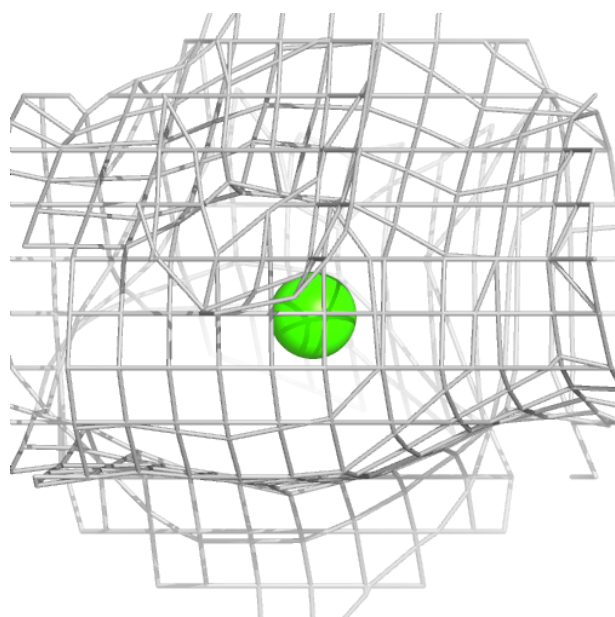
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





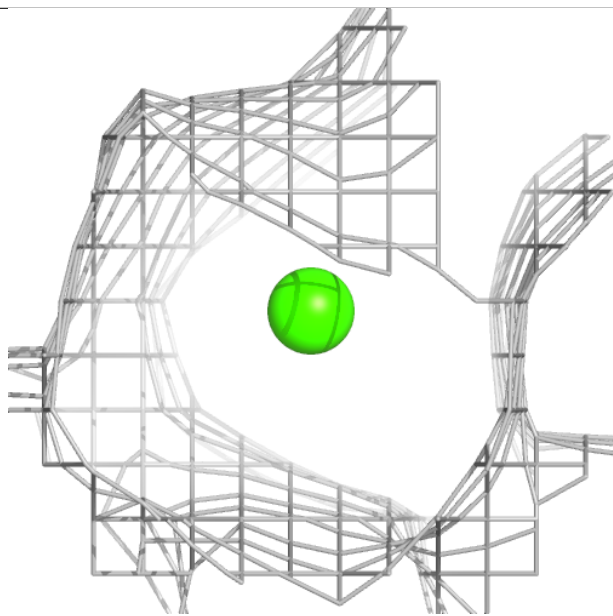
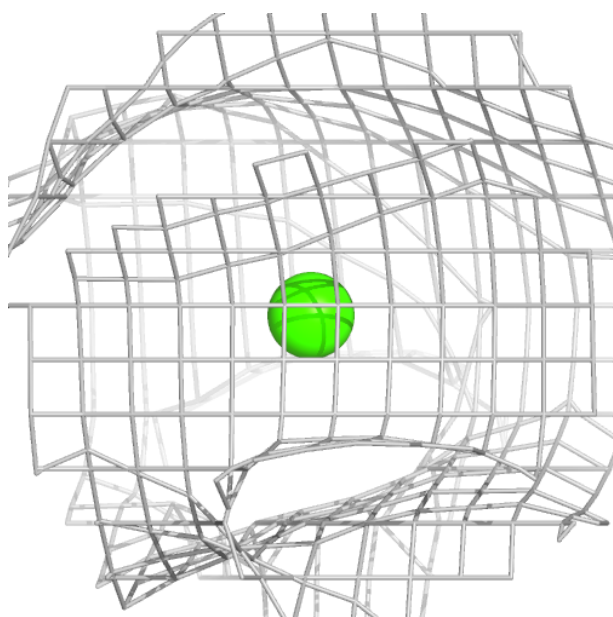
Electron density around CA K 201:

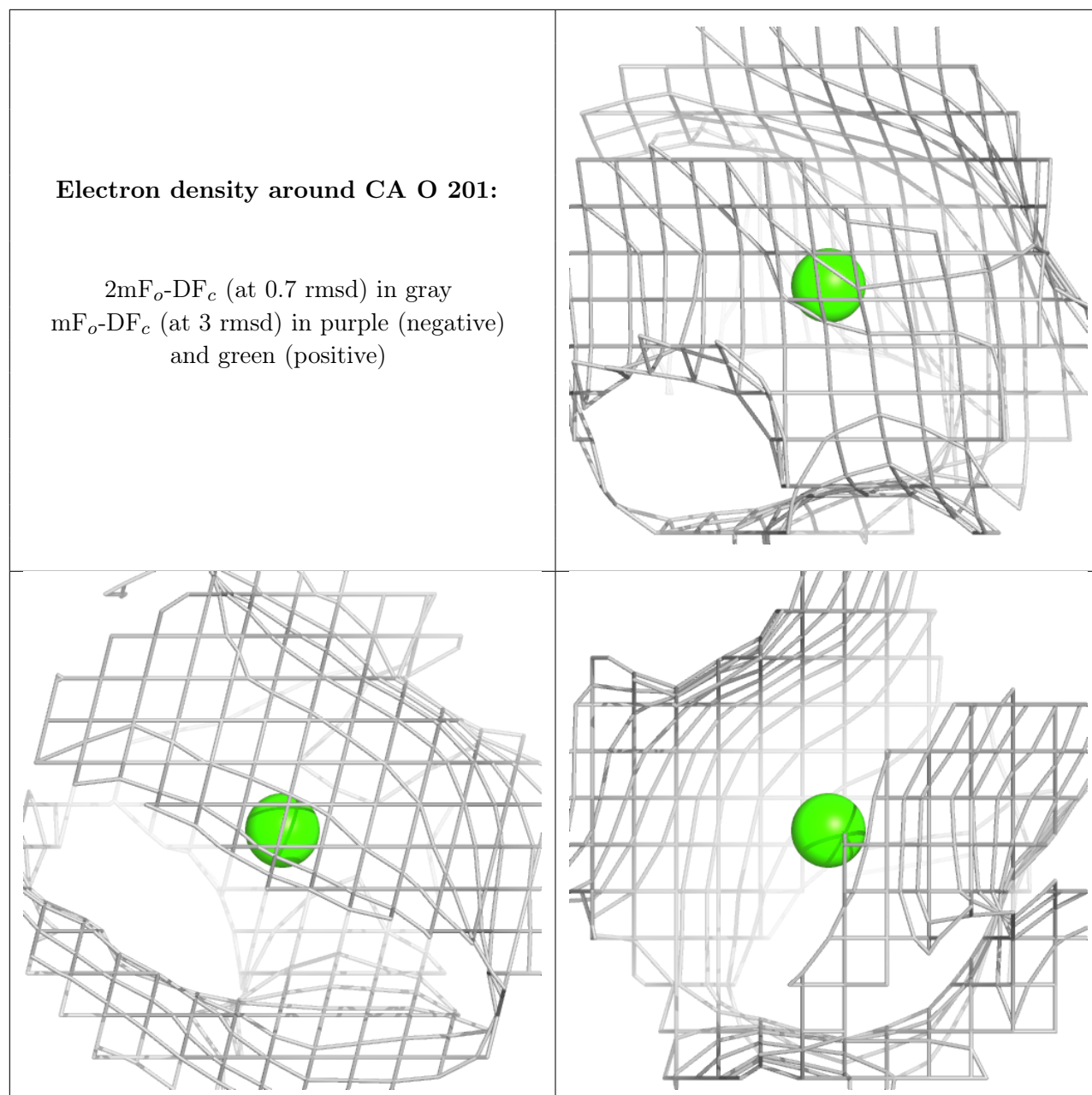
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CA M 201:

$2mF_o-DF_c$ (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.