wwPDB X-ray Structure Validation Summary Report (i)

Mar 3, 2025 – 03:08 pm GMT

PDB ID	:	8RMY
Title	:	Transglutaminase 3 in complex with inhibitor Z-don and DH patient-derived Fab DH63-A02
Authors	:	Heggelund, J.E.; Sollid, L.M.
Deposited on	:	2024-01-09
Resolution	:	2.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (1)) were used in the production of this report:

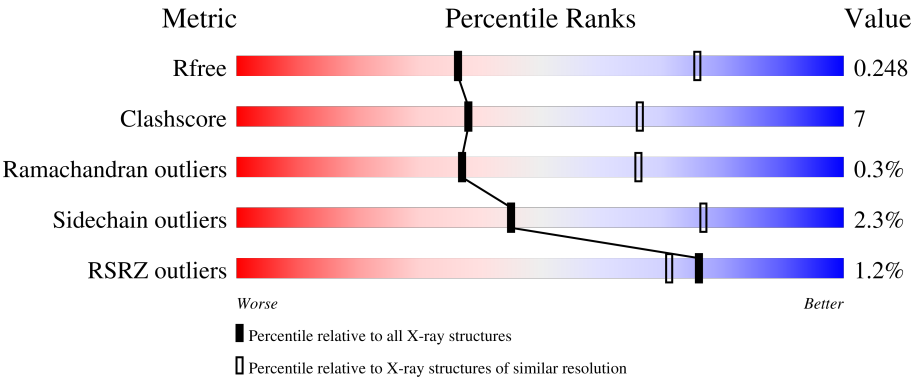
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41

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 2.90 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}	164625	2335 (2.90-2.90)
Clashscore	180529	2564 (2.90-2.90)
Ramachandran outliers	177936	2514 (2.90-2.90)
Sidechain outliers	177891	2516 (2.90-2.90)
RSRZ outliers	164620	2337 (2.90-2.90)

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	C	219	3% 71% 26%
1	F	219	76% 23%
2	A	464	90% 9%
2	D	464	% 91% 9%
3	B	221	3% 61% 26% 12%

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Mol	Chain	Length	Quality of chain
3	E	221	81% 16%
4	J	5	60% 20% 20%
4	K	5	60% 20% 20%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 13890 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 Antibody Fab fragment light chain IGKV4-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	F	219	Total	C	N	O	S	0	0	0
			1697	1063	283	345	6			
1	C	216	Total	C	N	O	S	0	0	0
			1674	1051	280	338	5			

- Molecule 2 is a protein called Protein-glutamine gamma-glutamyltransferase E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	462	Total	C	N	O	S	0	0	0
			3605	2269	636	687	13			
2	D	460	Total	C	N	O	S	0	0	0
			3589	2259	632	684	14			

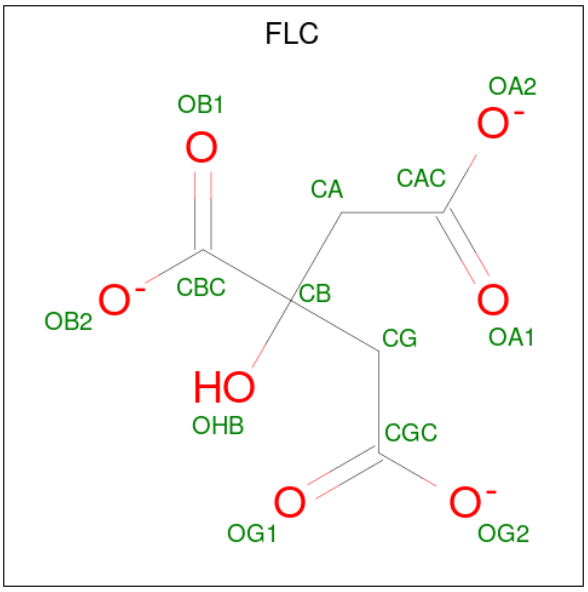
- Molecule 3 is a protein called Antibody Fab fragment heavy chain IGHV2-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	221	Total	C	N	O	S	0	0	0
			1660	1052	274	327	7			
3	B	195	Total	C	N	O	S	0	0	0
			1488	952	244	286	6			

- Molecule 4 is a protein called P6S-ONL-VAL-PRO-MLL.

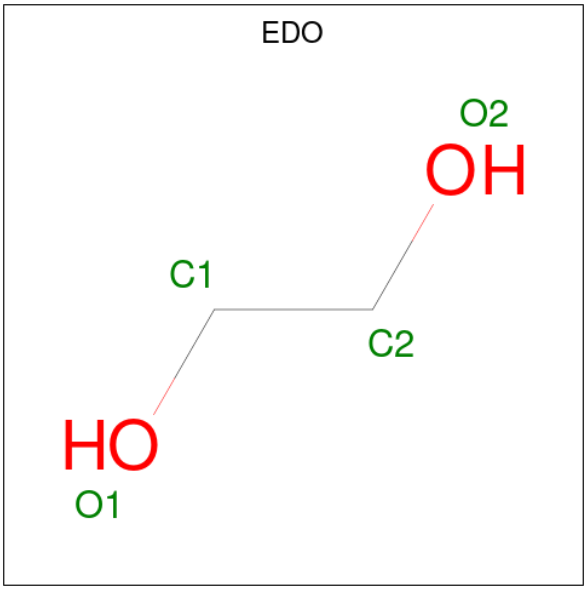
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	J	5	Total	C	N	O	0	0	0
			43	31	4	8			
4	K	5	Total	C	N	O	0	0	0
			43	31	4	8			

- Molecule 5 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 13 6 7	0	0
5	D	1	Total C O 13 6 7	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

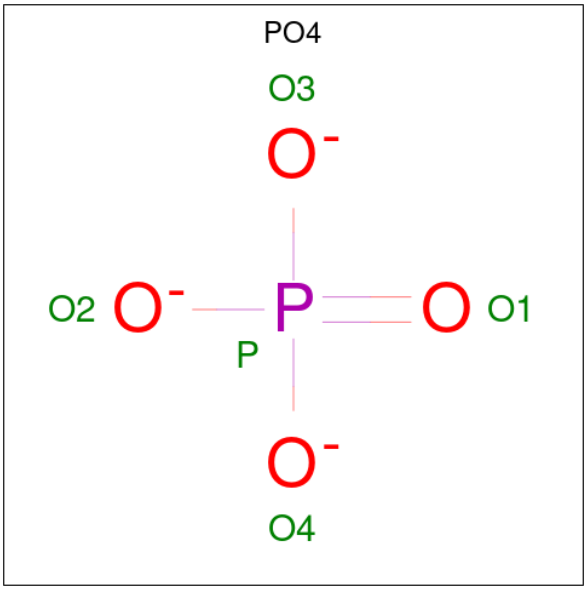


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 8 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total O P 5 4 1	0	0

- Molecule 9 is water.

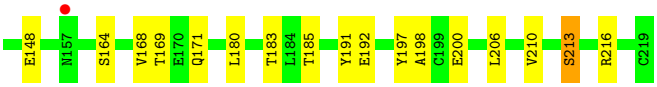
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	F	11	Total O 11 11	0	0
9	A	8	Total O 8 8	0	0
9	D	20	Total O 20 20	0	0
9	E	6	Total O 6 6	0	0
9	B	1	Total O 1 1	0	0

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.

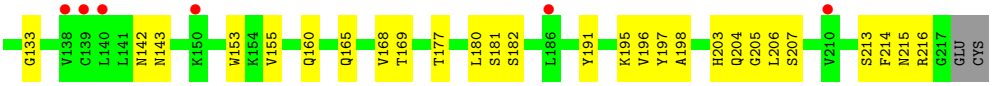
• Molecule 1: Antibody Fab fragment light chain IGKV4-1

Chain F:



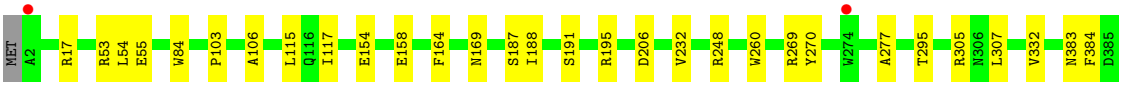
• Molecule 1: Antibody Fab fragment light chain IGKV4-1

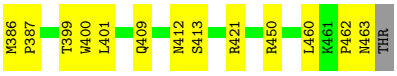
Chain C:



• Molecule 2: Protein-glutamine gamma-glutamyltransferase E

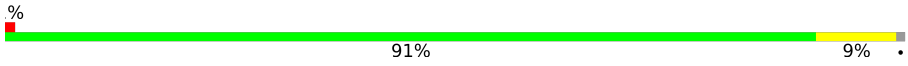
Chain A:

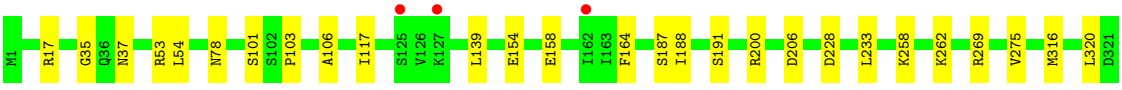


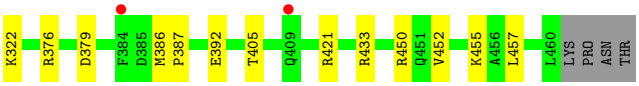


• Molecule 2: Protein-glutamine gamma-glutamyltransferase E

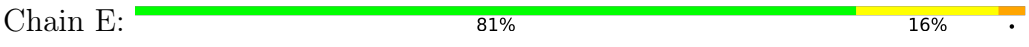
Chain D:

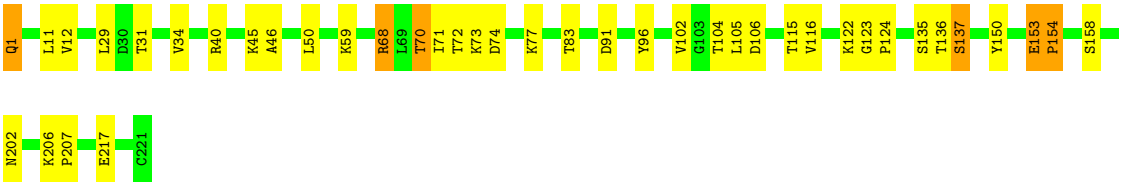




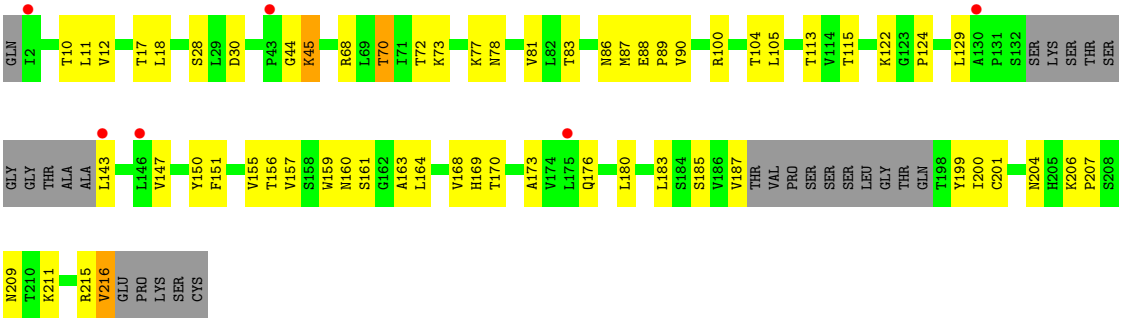


• Molecule 3: Antibody Fab fragment heavy chain IGHV2-5





• Molecule 3: Antibody Fab fragment heavy chain IGHV2-5



• Molecule 4: P6S-ONL-VAL-PRO-MLL

• Molecule 4: P6S-ONL-VAL-PRO-MLL

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	94.18Å 260.19Å 139.02Å 90.00° 95.10° 90.00°	Depositor
Resolution (Å)	69.20 – 2.90 69.20 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (69.20-2.90) 98.6 (69.20-2.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.18 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.88)	Depositor
R, R_{free}	0.195 , 0.242 0.203 , 0.248	Depositor DCC
R_{free} test set	3729 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	95.0	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 81.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13890	wwPDB-VP
Average B, all atoms (Å^2)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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: CA, MLL, ONL, EDO, FLC, PO4, P6S

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	C	0.47	0/1711	0.56	0/2325
1	F	0.59	1/1734 (0.1%)	0.63	0/2356
2	A	0.58	1/3692 (0.0%)	0.63	0/5010
2	D	0.55	1/3675 (0.0%)	0.61	1/4986 (0.0%)
3	B	0.48	0/1524	0.59	0/2083
3	E	0.56	0/1700	0.65	0/2325
4	J	0.68	0/14	0.71	0/19
4	K	0.41	0/14	0.81	0/19
All	All	0.55	3/14064 (0.0%)	0.62	1/19123 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	2
1	F	0	4
2	A	0	4
2	D	0	6
3	B	0	2
3	E	0	1
4	J	0	1
4	K	0	1
All	All	0	21

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	187	SER	CA-CB	-5.89	1.44	1.52
2	A	187	SER	CA-CB	-5.20	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	69	SER	CA-CB	-5.08	1.45	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	452	VAL	N-CA-CB	5.15	122.82	111.50

There are no chirality outliers.

5 of 21 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	133	GLY	Peptide
1	F	113	ARG	Sidechain
1	F	133	GLY	Peptide
1	F	18	ARG	Sidechain
1	F	200	GLU	Peptide

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	C	1674	0	1624	50	0
1	F	1697	0	1642	39	0
2	A	3605	0	3471	21	0
2	D	3589	0	3457	16	0
3	B	1488	0	1489	44	0
3	E	1660	0	1663	25	0
4	J	43	0	33	0	0
4	K	43	0	33	0	0
5	A	13	0	5	0	0
5	D	13	0	5	0	0
6	A	4	0	6	1	0
6	B	4	0	6	0	0
7	A	3	0	0	0	0
7	D	3	0	0	0	0
8	A	5	0	0	0	0
9	A	8	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	B	1	0	0	0	0
9	D	20	0	0	1	0
9	E	6	0	0	0	0
9	F	11	0	0	1	2
All	All	13890	0	13434	185	2

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.

The worst 5 of 185 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)
3:B:10:THR:HG21	3:B:207:PRO:HG3	1.25	1.17
2:D:379:ASP:OD1	2:D:455:LYS:NZ	2.05	0.89
1:C:3:VAL:H	1:C:26:SER:HB3	1.39	0.86
1:F:34:ASN:OD1	1:F:36:LYS:HB2	1.76	0.86
2:D:316:MET:HG3	3:E:102:VAL:HG11	1.59	0.85

All (2) 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)
9:F:304:HOH:O	9:F:304:HOH:O[2_655]	1.10	1.10
9:F:310:HOH:O	9:F:310:HOH:O[2_655]	2.03	0.17

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	C	214/219 (98%)	194 (91%)	19 (9%)	1 (0%)	25 56
1	F	217/219 (99%)	202 (93%)	14 (6%)	1 (0%)	25 56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	A	460/464 (99%)	440 (96%)	20 (4%)	0	100 100
2	D	458/464 (99%)	440 (96%)	17 (4%)	1 (0%)	44 73
3	B	189/221 (86%)	165 (87%)	24 (13%)	0	100 100
3	E	219/221 (99%)	207 (94%)	10 (5%)	2 (1%)	14 43
4	J	2/5 (40%)	2 (100%)	0	0	100 100
4	K	2/5 (40%)	2 (100%)	0	0	100 100
All	All	1761/1818 (97%)	1652 (94%)	104 (6%)	5 (0%)	37 66

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	100	LEU
3	E	154	PRO
1	C	143	ASN
2	D	228	ASP
3	E	137	SER

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	C	191/194 (98%)	184 (96%)	7 (4%)	29 64
1	F	194/194 (100%)	190 (98%)	4 (2%)	48 78
2	A	389/391 (100%)	387 (100%)	2 (0%)	86 96
2	D	387/391 (99%)	382 (99%)	5 (1%)	65 88
3	B	174/195 (89%)	165 (95%)	9 (5%)	19 50
3	E	195/195 (100%)	188 (96%)	7 (4%)	30 65
4	J	2/2 (100%)	2 (100%)	0	100 100
4	K	2/2 (100%)	1 (50%)	1 (50%)	0 0
All	All	1534/1564 (98%)	1499 (98%)	35 (2%)	45 77

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	113	THR
3	B	115	THR
3	B	201	CYS
2	A	450	ARG
2	A	206	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
4	MLL	K	5	4	9,9,9	0.35	0	11,11,11	0.60	0
4	MLL	J	5	4	9,9,9	0.44	0	11,11,11	0.73	1 (9%)
4	ONL	J	2	2,4	7,8,9	0.71	0	4,9,11	2.10	1 (25%)
4	ONL	K	2	2,4	7,8,9	0.62	0	4,9,11	1.88	1 (25%)

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
4	MLL	K	5	4	-	6/10/10/10	-
4	MLL	J	5	4	-	7/10/10/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ONL	J	2	2,4	-	5/6/7/9	-
4	ONL	K	2	2,4	-	2/6/7/9	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	J	2	ONL	CB-CG-CD	-3.76	110.70	114.57
4	K	2	ONL	CB-CG-CD	-3.72	110.75	114.57
4	J	5	MLL	C10-OXT-C	2.04	120.56	115.94

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	J	2	ONL	N-CA-CB-CG
4	J	2	ONL	C-CA-CB-CG
4	J	5	MLL	O-C-CA-N
4	J	5	MLL	O-C-OXT-C10
4	K	5	MLL	CA-C-OXT-C10

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 6 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	FLC	D	501	-	12,12,12	1.19	1 (8%)	17,17,17	1.30	2 (11%)
6	EDO	B	301	-	3,3,3	0.18	0	2,2,2	0.17	0
5	FLC	A	501	-	12,12,12	1.26	2 (16%)	17,17,17	1.20	2 (11%)
6	EDO	A	502	-	3,3,3	0.53	0	2,2,2	0.34	0
8	PO4	A	506	-	4,4,4	0.54	0	6,6,6	0.46	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	B	301	-	-	0/1/1/1	-
5	FLC	D	501	-	-	1/16/16/16	-
6	EDO	A	502	-	-	0/1/1/1	-
5	FLC	A	501	-	-	7/16/16/16	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	501	FLC	CB-CBC	2.32	1.55	1.53
5	A	501	FLC	OA2-CAC	-2.09	1.23	1.30
5	A	501	FLC	OG1-CGC	2.02	1.28	1.22

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	501	FLC	OB1-CBC-CB	-3.39	117.45	122.25
5	D	501	FLC	OB1-CBC-CB	-3.39	117.46	122.25
5	D	501	FLC	OB2-CBC-CB	2.36	117.15	113.05
5	A	501	FLC	OB2-CBC-CB	2.11	116.72	113.05

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	FLC	CA-CB-CBC-OB1
5	A	501	FLC	CA-CB-CBC-OB2
5	A	501	FLC	OHB-CB-CBC-OB1
5	A	501	FLC	OHB-CB-CBC-OB2
5	A	501	FLC	CG-CB-CBC-OB2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	502	EDO	1	0

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	C	216/219 (98%)	0.08	7 (3%) 50 44	89, 153, 218, 286	0
1	F	219/219 (100%)	-0.46	1 (0%) 87 84	66, 92, 126, 180	0
2	A	462/464 (99%)	-0.26	2 (0%) 89 86	69, 97, 134, 181	0
2	D	460/464 (99%)	-0.16	5 (1%) 77 72	73, 101, 144, 182	0
3	B	195/221 (88%)	0.16	6 (3%) 51 46	95, 152, 237, 283	0
3	E	221/221 (100%)	-0.39	0 100 100	73, 98, 121, 148	0
4	J	2/5 (40%)	-0.17	0 100 100	107, 107, 107, 108	0
4	K	2/5 (40%)	-0.05	0 100 100	105, 105, 105, 122	0
All	All	1777/1818 (97%)	-0.19	21 (1%) 76 71	66, 103, 190, 286	0

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	143	LEU	4.7
2	A	2	ALA	4.5
1	C	150	LYS	2.9
2	D	125	SER	2.8
1	C	186	LEU	2.7

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MLL	J	5	10/10	0.90	0.15	105,128,133,146	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ONL	J	2	9/10	0.94	0.10	87,89,104,162	0
4	MLL	K	5	10/10	0.94	0.13	89,113,139,149	0
4	ONL	K	2	9/10	0.96	0.09	83,103,122,124	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

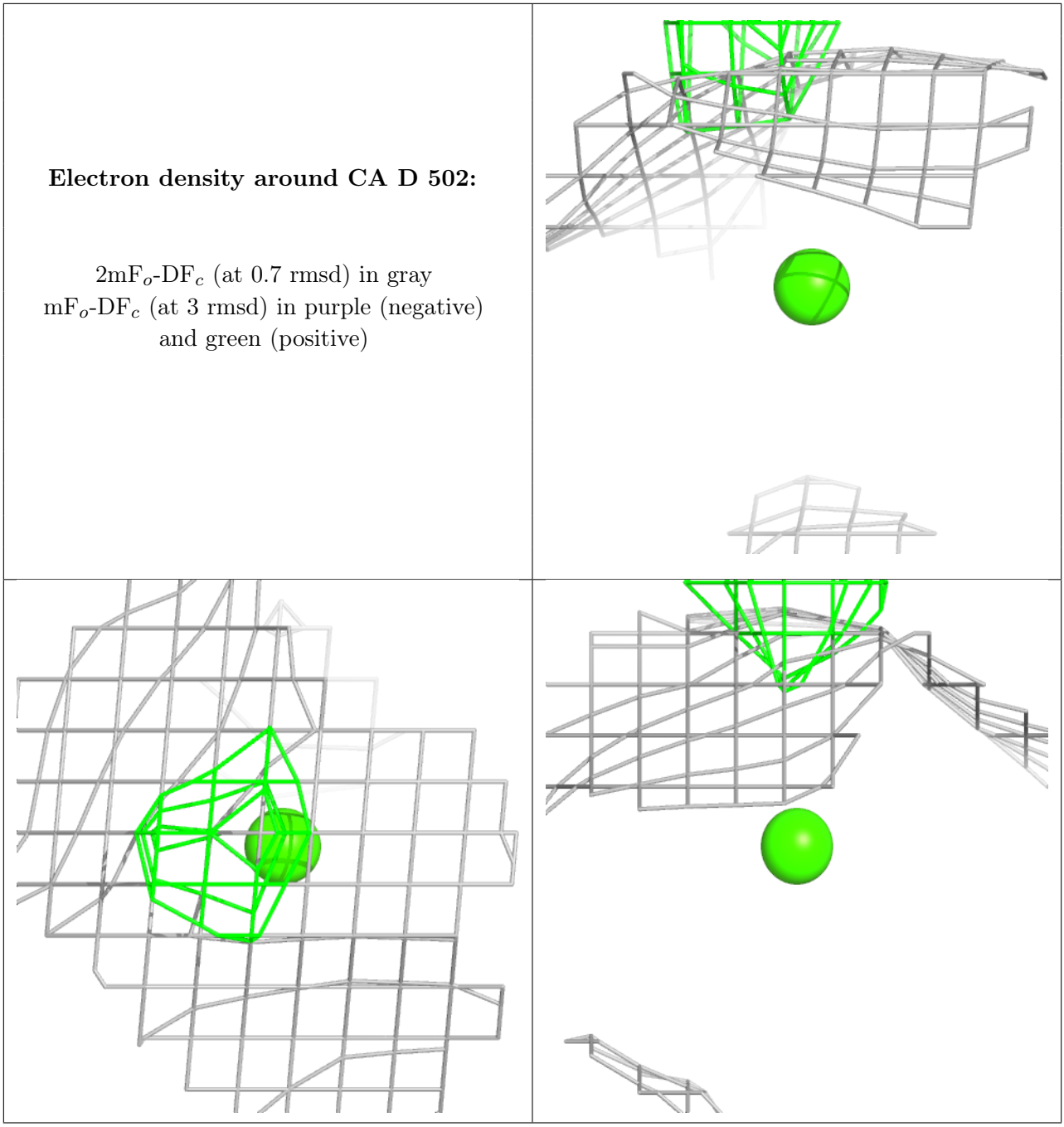
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	EDO	B	301	4/4	0.64	0.29	107,124,130,135	0
8	PO4	A	506	5/5	0.64	0.08	137,180,197,203	0
6	EDO	A	502	4/4	0.81	0.20	87,109,115,140	0
5	FLC	D	501	13/13	0.84	0.06	147,155,166,177	0
5	FLC	A	501	13/13	0.87	0.10	89,109,161,161	0
7	CA	D	502	1/1	0.98	0.06	96,96,96,96	0
7	CA	D	503	1/1	0.99	0.02	93,93,93,93	0
7	CA	A	504	1/1	0.99	0.04	76,76,76,76	0
7	CA	A	505	1/1	1.00	0.02	84,84,84,84	0
7	CA	D	504	1/1	1.00	0.02	84,84,84,84	0
7	CA	A	503	1/1	1.00	0.03	89,89,89,89	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.

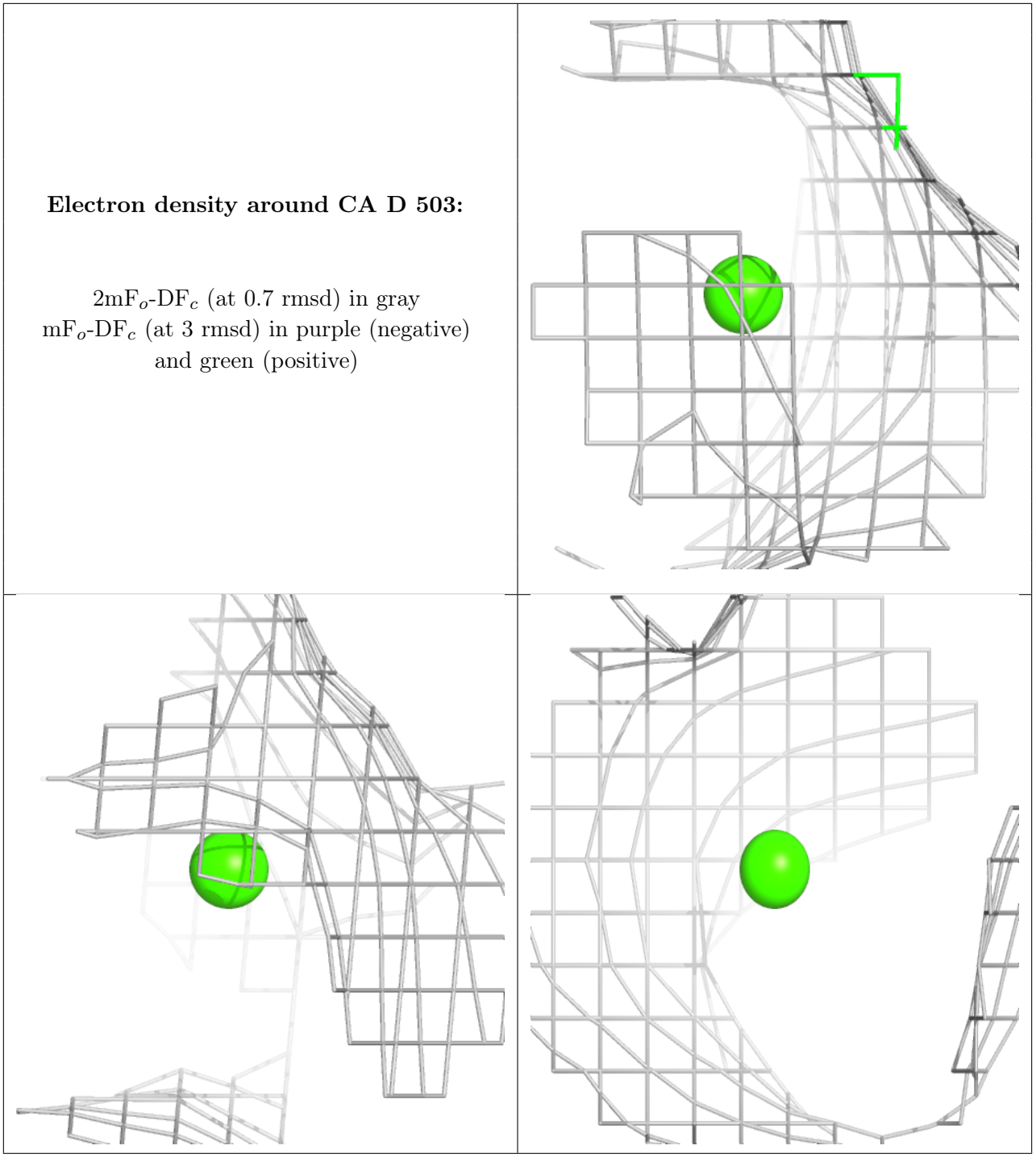
Electron density around CA D 502:

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



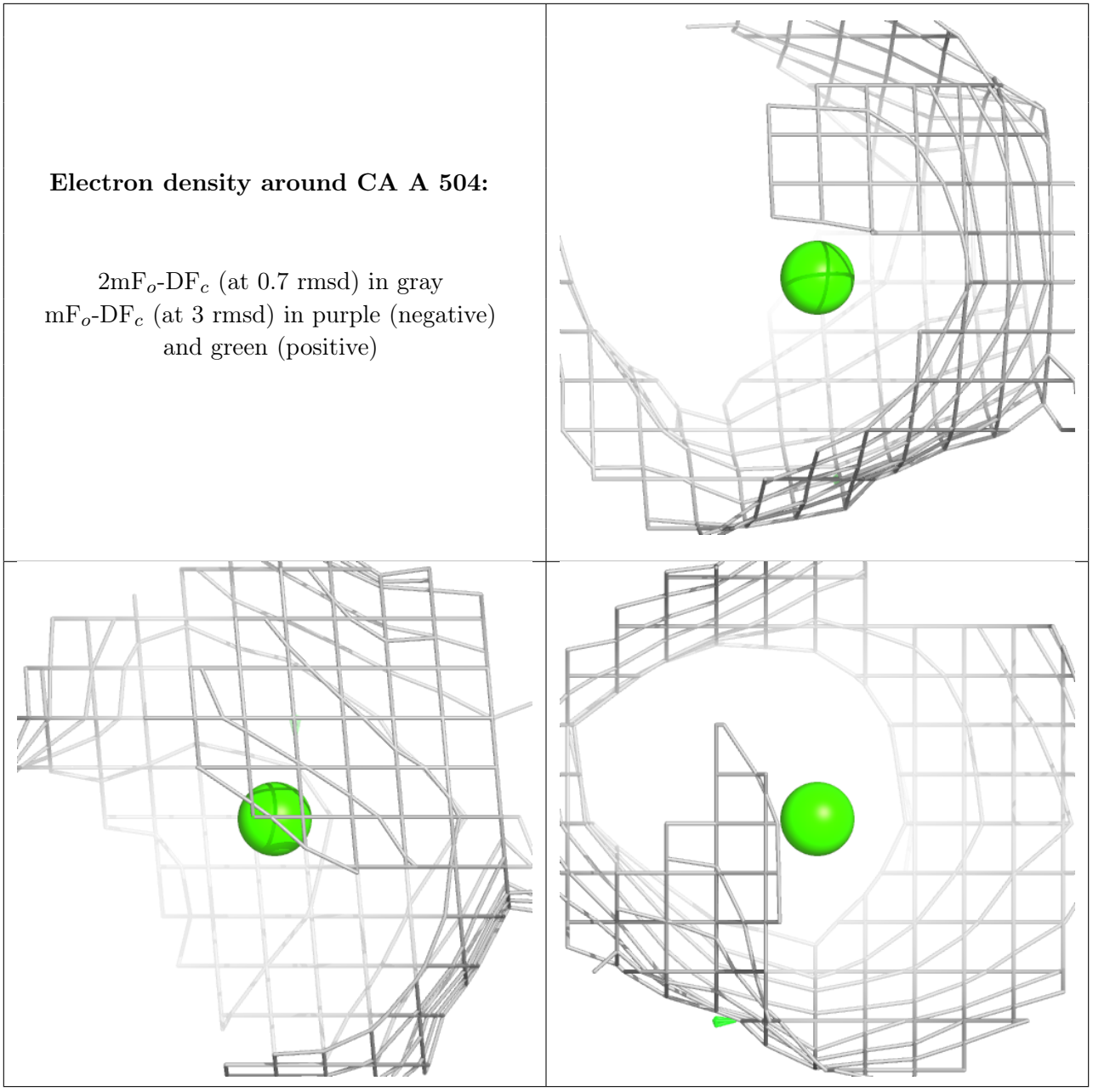
Electron density around CA D 503:

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



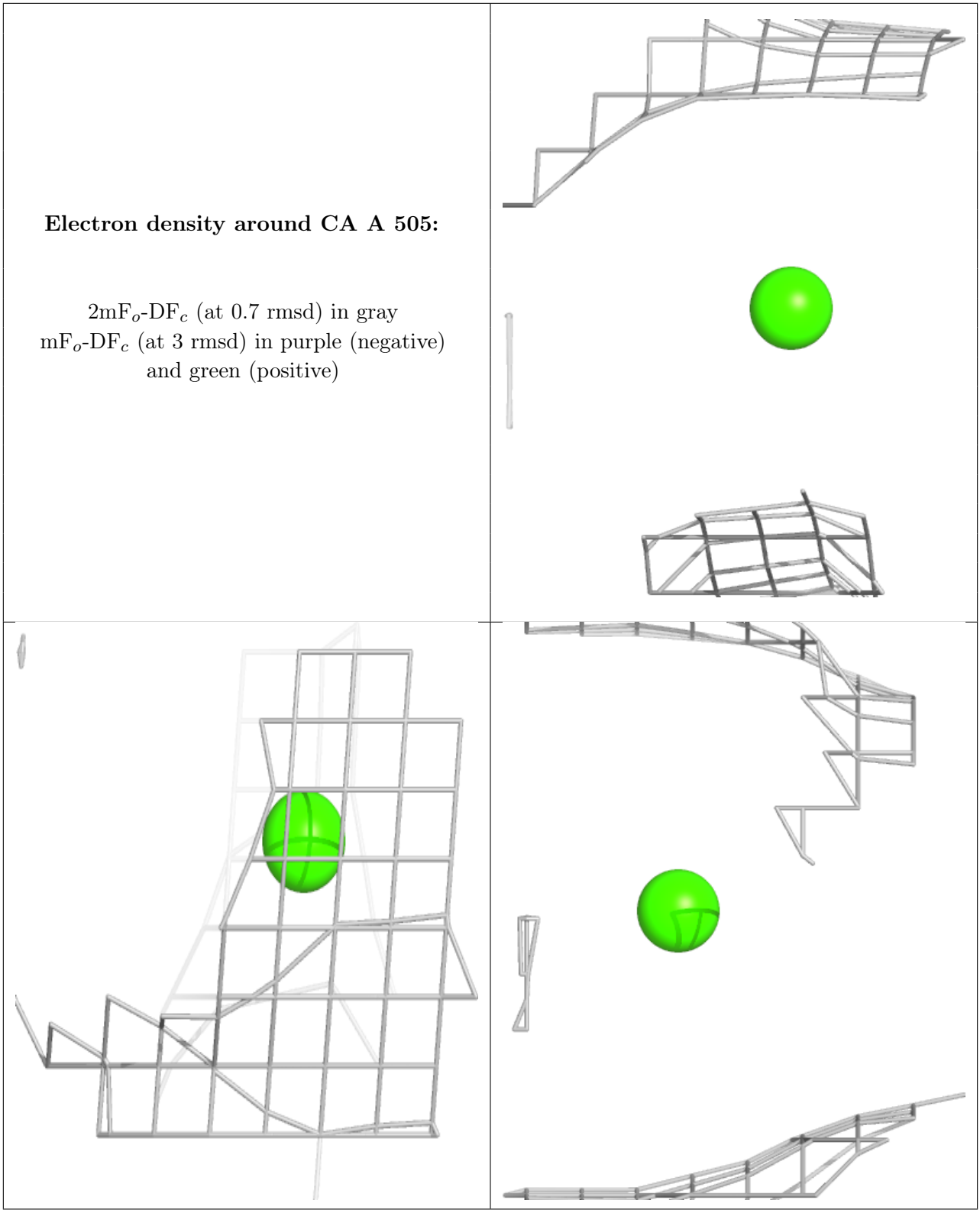
Electron density around CA A 504:

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



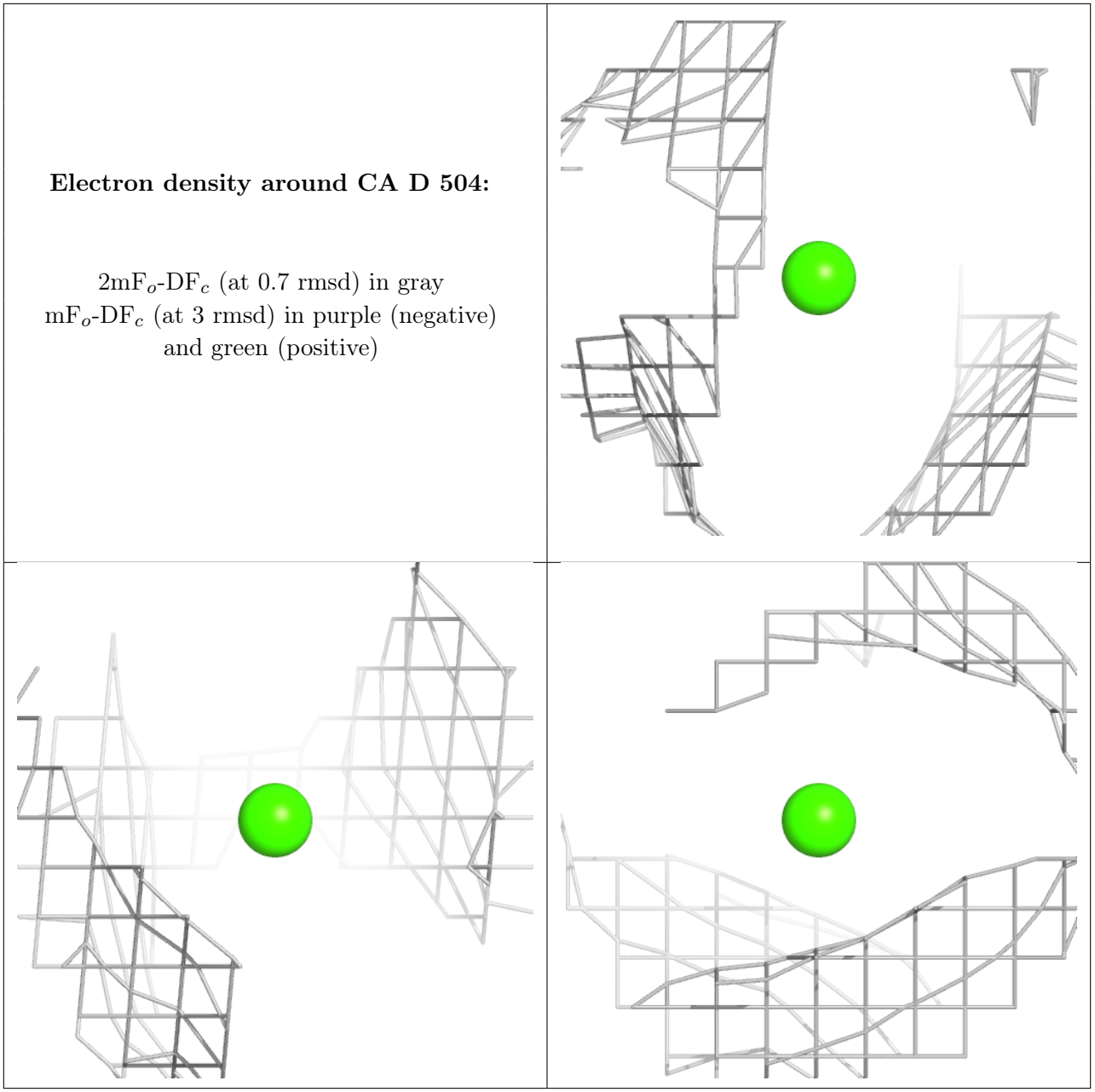
Electron density around CA A 505:

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



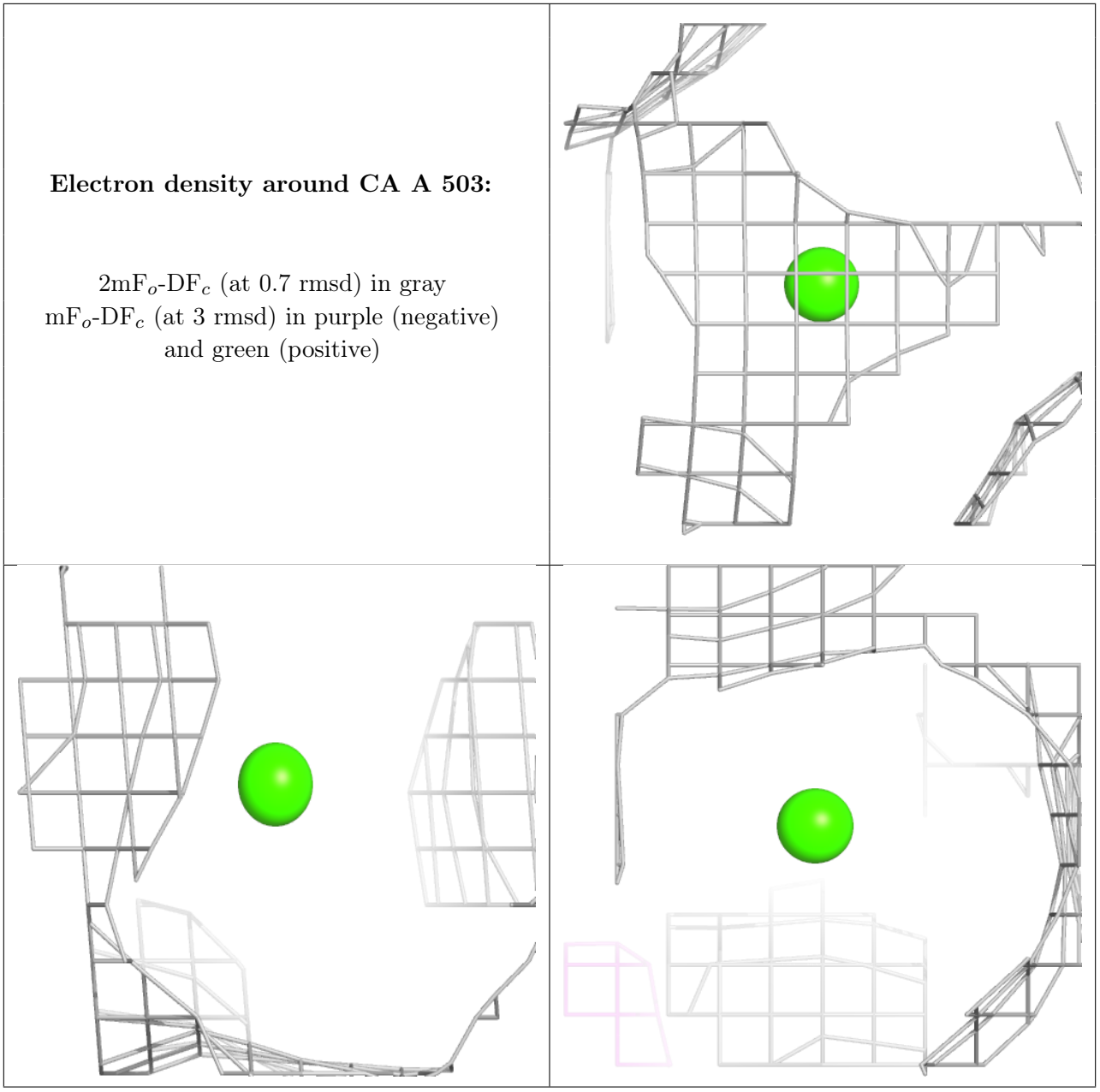
Electron density around CA D 504:

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



Electron density around 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)



6.5 Other polymers (i)

There are no such residues in this entry.