



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:03 AM UTC

PDB ID : 6ZA2 / pdb_00006za2
Title : Crystal structure of dimeric latent PorU from Porphyromonas gingivalis
Authors : Gomis-Ruth, F.X.; Goulas, T.; Guevara, T.; Rodriguez-Banqueri, A.; Potempa, J.; Sola, M.
Deposited on : 2020-06-04
Resolution : 3.35 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

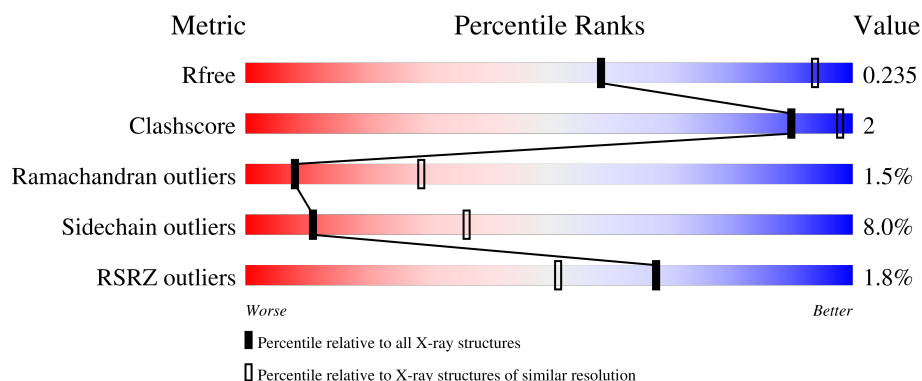
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

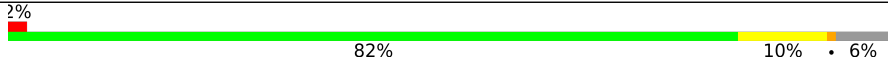
The reported resolution of this entry is 3.35 Å.

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	1099 (3.40-3.32)
Clashscore	190562	1116 (3.40-3.32)
Ramachandran outliers	187476	1101 (3.40-3.32)
Sidechain outliers	187428	1101 (3.40-3.32)
RSRZ outliers	180081	1099 (3.40-3.32)

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	1156	 2% 81% 11% • 6%
1	B	1156	 2% 82% 10% • 6%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 31870 atoms, of which 15484 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 Por secretion system protein porU.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1081	Total	C	H	N	O	S	7821	0	0
			16048	5189	7821	1406	1598	34			
1	B	1083	Total	C	H	N	O	S	7663	0	0
			15814	5128	7663	1395	1595	33			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	GLY	-	expression tag	UNP B2RGP6
A	4	SER	-	expression tag	UNP B2RGP6
A	5	SER	-	expression tag	UNP B2RGP6
A	6	HIS	-	expression tag	UNP B2RGP6
A	7	HIS	-	expression tag	UNP B2RGP6
A	8	HIS	-	expression tag	UNP B2RGP6
A	9	HIS	-	expression tag	UNP B2RGP6
A	10	HIS	-	expression tag	UNP B2RGP6
A	11	HIS	-	expression tag	UNP B2RGP6
A	12	SER	-	expression tag	UNP B2RGP6
A	13	GLN	-	expression tag	UNP B2RGP6
A	14	ASP	-	expression tag	UNP B2RGP6
A	15	PRO	-	expression tag	UNP B2RGP6
A	16	ASN	-	expression tag	UNP B2RGP6
A	17	SER	-	expression tag	UNP B2RGP6
A	18	SER	-	expression tag	UNP B2RGP6
A	19	SER	-	expression tag	UNP B2RGP6
A	20	ALA	-	expression tag	UNP B2RGP6
A	21	ARG	-	expression tag	UNP B2RGP6
A	22	LEU	-	expression tag	UNP B2RGP6
A	23	GLN	-	expression tag	UNP B2RGP6
B	-21	GLY	-	expression tag	UNP B2RGP6
B	-20	SER	-	expression tag	UNP B2RGP6
B	-19	SER	-	expression tag	UNP B2RGP6
B	-18	HIS	-	expression tag	UNP B2RGP6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	HIS	-	expression tag	UNP B2RGP6
B	-16	HIS	-	expression tag	UNP B2RGP6
B	-15	HIS	-	expression tag	UNP B2RGP6
B	-14	HIS	-	expression tag	UNP B2RGP6
B	-13	HIS	-	expression tag	UNP B2RGP6
B	-12	SER	-	expression tag	UNP B2RGP6
B	-11	GLN	-	expression tag	UNP B2RGP6
B	-10	ASP	-	expression tag	UNP B2RGP6
B	-9	PRO	-	expression tag	UNP B2RGP6
B	-8	ASN	-	expression tag	UNP B2RGP6
B	-7	SER	-	expression tag	UNP B2RGP6
B	-6	SER	-	expression tag	UNP B2RGP6
B	-5	SER	-	expression tag	UNP B2RGP6
B	-4	ALA	-	expression tag	UNP B2RGP6
B	-3	ARG	-	expression tag	UNP B2RGP6
B	-2	LEU	-	expression tag	UNP B2RGP6
B	-1	GLN	-	expression tag	UNP B2RGP6

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

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

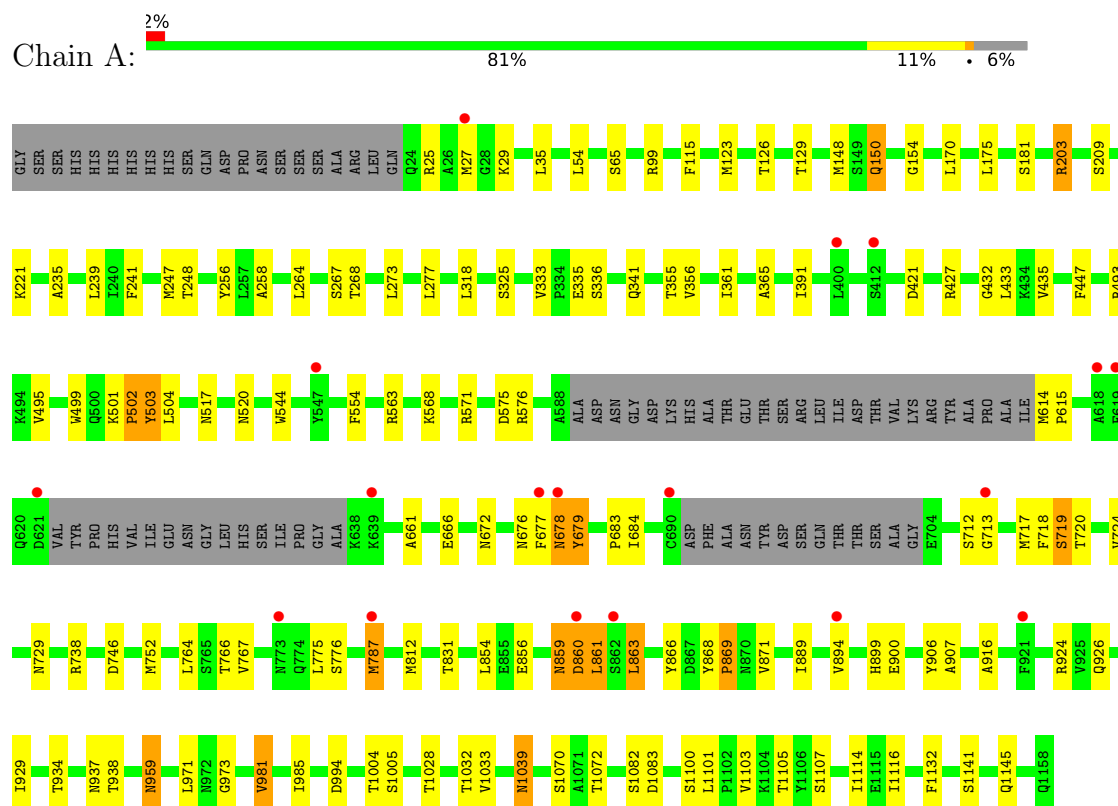
- Molecule 3 is water.

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

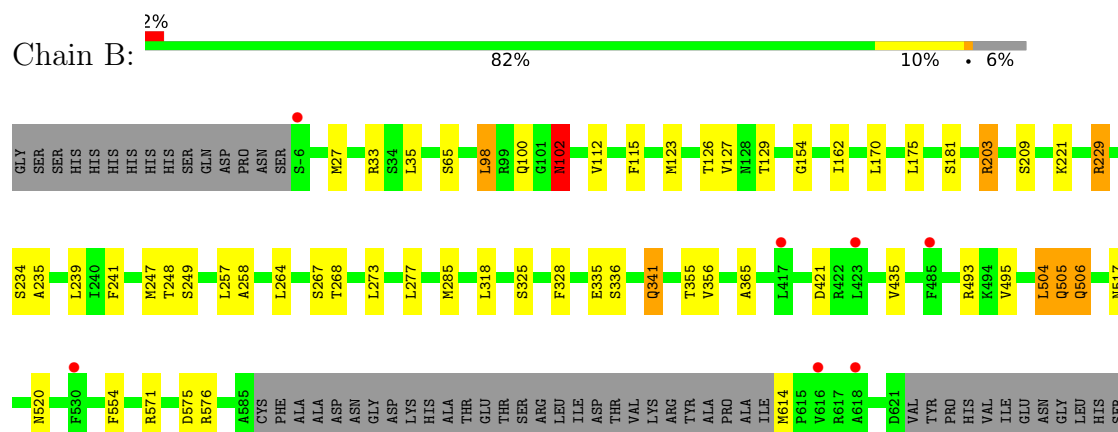
3 Residue-property plots

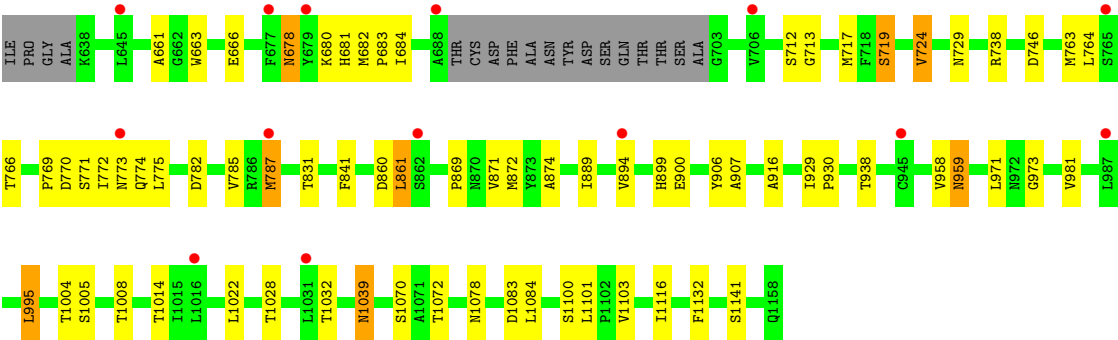
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Por secretion system protein porU



- Molecule 1: Por secretion system protein porU





4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	171.70Å 171.70Å 440.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	88.48 – 3.35 88.48 – 3.35	Depositor EDS
% Data completeness (in resolution range)	100.0 (88.48-3.35) 100.0 (88.48-3.35)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 3.33Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.202 , 0.243 0.206 , 0.235	Depositor DCC
R_{free} test set	836 reflections (1.49%)	wwPDB-VP
Wilson B-factor (Å ²)	125.7	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 126.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	31870	wwPDB-VP
Average B, all atoms (Å ²)	140.0	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.*

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	0.89	2/8404 (0.0%)	1.12	21/11434 (0.2%)
1	B	0.89	0/8323	1.14	30/11338 (0.3%)
All	All	0.89	2/16727 (0.0%)	1.13	51/22772 (0.2%)

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	2
1	B	0	2
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	148	MET	SD-CE	-5.12	1.66	1.79
1	A	568	LYS	CA-C	5.08	1.59	1.52

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	571	ARG	CD-NE-CZ	11.36	140.31	124.40
1	B	554	PHE	CA-CB-CG	9.52	123.32	113.80
1	B	100	GLN	N-CA-C	-9.10	101.31	108.78
1	A	336	SER	N-CA-C	-8.30	102.47	112.59
1	A	554	PHE	CA-CB-CG	8.07	121.87	113.80
1	A	937	ASN	CA-CB-CG	8.05	120.65	112.60
1	B	959	ASN	CA-CB-CG	7.94	120.54	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1039	ASN	CA-CB-CG	7.73	120.33	112.60
1	B	1039	ASN	CA-CB-CG	6.92	119.52	112.60
1	B	336	SER	N-CA-C	-6.82	104.27	112.59
1	A	1132	PHE	CA-CB-CG	6.74	120.54	113.80
1	A	959	ASN	CA-CB-CG	6.59	119.19	112.60
1	B	1132	PHE	CA-CB-CG	6.48	120.28	113.80
1	A	869	PRO	N-CA-C	-6.47	99.14	112.47
1	B	102	ASN	CA-CB-CG	6.39	118.99	112.60
1	B	869	PRO	N-CA-C	-6.21	99.67	112.47
1	A	676	ASN	CA-C-N	6.13	133.24	121.54
1	A	676	ASN	C-N-CA	6.13	133.24	121.54
1	B	770	ASP	CA-CB-CG	6.08	118.68	112.60
1	B	517	ASN	CA-CB-CG	6.07	118.67	112.60
1	A	517	ASN	CA-CB-CG	5.99	118.58	112.60
1	B	365	ALA	N-CA-C	5.79	113.43	108.22
1	A	432	GLY	CA-C-N	-5.79	112.74	122.29
1	A	432	GLY	C-N-CA	-5.79	112.74	122.29
1	A	571	ARG	CD-NE-CZ	5.79	132.50	124.40
1	A	860	ASP	CA-CB-CG	5.75	118.35	112.60
1	B	341	GLN	N-CA-C	-5.75	99.16	108.41
1	B	899	HIS	CA-C-N	5.74	132.51	121.54
1	B	899	HIS	C-N-CA	5.74	132.51	121.54
1	B	678	ASN	N-CA-C	-5.71	100.84	109.85
1	B	1083	ASP	CA-CB-CG	5.41	118.01	112.60
1	A	447	PHE	CA-CB-CG	-5.39	108.41	113.80
1	B	98	LEU	N-CA-CB	5.36	119.32	110.69
1	B	506	GLN	CA-C-N	5.34	131.91	122.67
1	B	506	GLN	C-N-CA	5.34	131.91	122.67
1	A	365	ALA	N-CA-C	5.31	113.00	108.22
1	B	27	MET	CA-C-N	5.28	125.73	120.98
1	B	27	MET	C-N-CA	5.28	125.73	120.98
1	B	505	GLN	CA-C-N	5.28	131.62	121.54
1	B	505	GLN	C-N-CA	5.28	131.62	121.54
1	B	681	HIS	N-CA-C	5.25	117.95	110.24
1	B	746	ASP	CA-CB-CG	5.24	117.84	112.60
1	B	678	ASN	CA-CB-CG	5.22	117.82	112.60
1	A	973	GLY	N-CA-C	5.18	118.10	112.29
1	B	680	LYS	CA-C-N	5.18	128.46	121.05
1	B	680	LYS	C-N-CA	5.18	128.46	121.05
1	A	859	ASN	CA-CB-CG	5.15	117.75	112.60
1	B	973	GLY	N-CA-C	5.13	118.04	112.29
1	A	863	LEU	N-CA-C	5.08	117.52	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	746	ASP	CA-CB-CG	5.07	117.67	112.60
1	A	503	TYR	N-CA-CB	5.00	117.21	109.91

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	614	MET	Mainchain
1	A	929	ILE	Mainchain
1	B	614	MET	Mainchain
1	B	929	ILE	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8227	7821	7821	33	0
1	B	8151	7663	7665	30	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
All	All	16386	15484	15486	58	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 2.

All (58) 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:684:ILE:HD13	1:A:787:MET:HE1	1.68	0.74
1:B:684:ILE:HD13	1:B:787:MET:HE1	1.72	0.72
1:A:861:LEU:HD11	1:B:738:ARG:HG2	1.73	0.69
1:A:985:ILE:HG23	1:A:1033:VAL:HG12	1.77	0.65
1:A:738:ARG:HG2	1:B:861:LEU:HD11	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:504:LEU:C	1:B:504:LEU:HD22	2.24	0.62
1:A:333:VAL:HG21	1:A:361:ILE:HG12	1.87	0.57
1:A:427:ARG:HB3	1:A:433:LEU:HD21	1.87	0.56
1:B:717:MET:HE3	1:B:719:SER:HB2	1.87	0.56
1:A:717:MET:HE3	1:A:719:SER:HB2	1.88	0.54
1:A:563:ARG:HD2	1:B:663:TRP:CE2	2.43	0.54
1:B:874:ALA:HB3	1:B:1008:THR:OG1	2.09	0.53
1:B:229:ARG:NH2	1:B:285:MET:HE2	2.24	0.52
1:B:241:PHE:CE1	1:B:264:LEU:HD22	2.45	0.52
1:A:860:ASP:C	1:A:861:LEU:HG	2.35	0.51
1:A:241:PHE:CE1	1:A:264:LEU:HD22	2.45	0.51
1:A:499:TRP:CE3	1:A:504:LEU:HB3	2.47	0.50
1:A:235:ALA:HB1	1:A:277:LEU:HD11	1.94	0.50
1:A:1103:VAL:HB	1:A:1116:ILE:HD11	1.94	0.49
1:A:563:ARG:HD2	1:B:663:TRP:CZ2	2.47	0.49
1:B:235:ALA:HB1	1:B:277:LEU:HD11	1.95	0.49
1:B:1103:VAL:HB	1:B:1116:ILE:HD11	1.94	0.49
1:B:860:ASP:C	1:B:861:LEU:HG	2.37	0.49
1:B:995:LEU:HD13	1:B:995:LEU:N	2.28	0.49
1:B:684:ILE:CD1	1:B:787:MET:HE1	2.43	0.47
1:A:907:ALA:HB3	1:A:916:ALA:HB3	1.97	0.47
1:B:907:ALA:HB3	1:B:916:ALA:HB3	1.97	0.46
1:B:782:ASP:HB3	1:B:785:VAL:HG23	1.98	0.45
1:A:812:MET:HE3	1:A:926:GLN:HB3	1.97	0.45
1:B:763:MET:HE1	1:B:775:LEU:HD11	1.99	0.45
1:A:718:PHE:HZ	1:A:752:MET:HE2	1.82	0.45
1:B:769:PRO:HA	1:B:773:ASN:HB2	2.00	0.44
1:A:150:GLN:H	1:A:150:GLN:CD	2.26	0.44
1:A:766:THR:O	1:A:766:THR:HG23	2.18	0.44
1:A:1114:ILE:HG23	1:B:249:SER:OG	2.18	0.44
1:A:544:TRP:CZ3	1:A:767:VAL:HG11	2.53	0.43
1:A:678:ASN:O	1:A:679:TYR:C	2.61	0.43
1:B:264:LEU:HD12	1:B:264:LEU:N	2.33	0.43
1:A:866:TYR:C	1:A:868:TYR:H	2.28	0.42
1:A:868:TYR:N	1:A:869:PRO:HD3	2.35	0.42
1:B:162:ILE:HD11	1:B:328:PHE:CE1	2.55	0.42
1:A:264:LEU:N	1:A:264:LEU:HD12	2.34	0.42
1:A:854:LEU:HD23	1:A:854:LEU:HA	1.96	0.42
1:A:720:THR:HG23	1:A:776:SER:O	2.20	0.41
1:B:115:PHE:C	1:B:123:MET:HE3	2.45	0.41
1:A:221:LYS:HG3	1:A:247:MET:HE1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:LYS:HG3	1:B:247:MET:HE1	2.03	0.41
1:B:724:VAL:HG21	1:B:775:LEU:HB3	2.01	0.41
1:A:493:ARG:CB	1:A:495:VAL:HG13	2.51	0.41
1:A:672:ASN:OD1	1:A:677:PHE:HB3	2.21	0.41
1:A:724:VAL:HG21	1:A:775:LEU:HB3	2.02	0.41
1:B:112:VAL:HG22	1:B:127:VAL:HG12	2.03	0.41
1:B:841:PHE:CD2	1:B:841:PHE:N	2.88	0.41
1:B:493:ARG:CB	1:B:495:VAL:HG13	2.51	0.41
1:B:766:THR:HB	1:B:769:PRO:HD2	2.02	0.41
1:A:115:PHE:C	1:A:123:MET:HE3	2.47	0.40
1:B:493:ARG:HB3	1:B:495:VAL:HG13	2.02	0.40
1:A:493:ARG:HB3	1:A:495:VAL:HG13	2.03	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	1073/1156 (93%)	993 (92%)	64 (6%)	16 (2%)	8	29
1	B	1075/1156 (93%)	1004 (93%)	55 (5%)	16 (2%)	8	29
All	All	2148/2312 (93%)	1997 (93%)	119 (6%)	32 (2%)	8	29

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	712	SER
1	A	894	VAL
1	A	981	VAL
1	B	258	ALA
1	B	712	SER
1	B	894	VAL

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Mol	Chain	Res	Type
1	B	900	GLU
1	B	981	VAL
1	A	25	ARG
1	A	203	ARG
1	A	258	ALA
1	A	678	ASN
1	B	203	ARG
1	B	506	GLN
1	B	729	ASN
1	B	930	PRO
1	A	615	PRO
1	A	661	ALA
1	A	679	TYR
1	B	102	ASN
1	B	661	ALA
1	A	683	PRO
1	A	729	ASN
1	B	771	SER
1	B	181	SER
1	B	683	PRO
1	A	181	SER
1	A	713	GLY
1	B	713	GLY
1	A	502	PRO
1	B	154	GLY
1	A	154	GLY

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	859/978 (88%)	789 (92%)	70 (8%)	11	36
1	B	839/978 (86%)	773 (92%)	66 (8%)	11	37
All	All	1698/1956 (87%)	1562 (92%)	136 (8%)	11	36

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	MET
1	A	29	LYS
1	A	35	LEU
1	A	54	LEU
1	A	65	SER
1	A	99	ARG
1	A	126	THR
1	A	129	THR
1	A	150	GLN
1	A	170	LEU
1	A	175	LEU
1	A	203	ARG
1	A	209	SER
1	A	239	LEU
1	A	248	THR
1	A	256	TYR
1	A	267	SER
1	A	268	THR
1	A	273	LEU
1	A	318	LEU
1	A	325	SER
1	A	335	GLU
1	A	341	GLN
1	A	355	THR
1	A	356	VAL
1	A	391	ILE
1	A	421	ASP
1	A	435	VAL
1	A	501	LYS
1	A	502	PRO
1	A	503	TYR
1	A	520	ASN
1	A	575	ASP
1	A	576	ARG
1	A	666	GLU
1	A	719	SER
1	A	764	LEU
1	A	787	MET
1	A	831	THR
1	A	856	GLU
1	A	859	ASN
1	A	861	LEU
1	A	863	LEU

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Mol	Chain	Res	Type
1	A	871	VAL
1	A	889	ILE
1	A	899	HIS
1	A	900	GLU
1	A	906	TYR
1	A	924	ARG
1	A	934	THR
1	A	938	THR
1	A	959	ASN
1	A	971	LEU
1	A	981	VAL
1	A	994	ASP
1	A	1004	THR
1	A	1005	SER
1	A	1028	THR
1	A	1032	THR
1	A	1039	ASN
1	A	1070	SER
1	A	1072	THR
1	A	1082	SER
1	A	1083	ASP
1	A	1100	SER
1	A	1101	LEU
1	A	1105	THR
1	A	1107	SER
1	A	1141	SER
1	A	1145	GLN
1	B	33	ARG
1	B	35	LEU
1	B	65	SER
1	B	98	LEU
1	B	102	ASN
1	B	126	THR
1	B	129	THR
1	B	170	LEU
1	B	175	LEU
1	B	203	ARG
1	B	209	SER
1	B	229	ARG
1	B	234	SER
1	B	239	LEU
1	B	248	THR

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Mol	Chain	Res	Type
1	B	257	LEU
1	B	267	SER
1	B	268	THR
1	B	273	LEU
1	B	318	LEU
1	B	325	SER
1	B	335	GLU
1	B	341	GLN
1	B	355	THR
1	B	356	VAL
1	B	421	ASP
1	B	435	VAL
1	B	504	LEU
1	B	505	GLN
1	B	520	ASN
1	B	575	ASP
1	B	576	ARG
1	B	666	GLU
1	B	678	ASN
1	B	682	MET
1	B	719	SER
1	B	724	VAL
1	B	764	LEU
1	B	772	ILE
1	B	774	GLN
1	B	787	MET
1	B	831	THR
1	B	861	LEU
1	B	871	VAL
1	B	872	MET
1	B	889	ILE
1	B	906	TYR
1	B	938	THR
1	B	958	VAL
1	B	959	ASN
1	B	971	LEU
1	B	995	LEU
1	B	1004	THR
1	B	1005	SER
1	B	1014	THR
1	B	1022	LEU
1	B	1028	THR

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Mol	Chain	Res	Type
1	B	1032	THR
1	B	1039	ASN
1	B	1070	SER
1	B	1072	THR
1	B	1078	ASN
1	B	1084	LEU
1	B	1100	SER
1	B	1101	LEU
1	B	1141	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	385	GLN
1	A	414	GLN
1	A	522	ASN
1	A	733	ASN
1	A	788	ASN
1	A	1038	ASN
1	A	1043	HIS
1	A	1085	ASN
1	B	150	GLN
1	B	385	GLN
1	B	414	GLN
1	B	646	GLN
1	B	733	ASN
1	B	788	ASN
1	B	975	ASN
1	B	1038	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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	1081/1156 (93%)	-0.23	18 (1%)	69 53	37, 66, 128, 234	0
1	B	1083/1156 (93%)	-0.04	21 (1%)	66 49	36, 71, 152, 241	0
All	All	2164/2312 (93%)	-0.14	39 (1%)	67 51	36, 68, 144, 241	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	862	SER	4.4
1	B	618	ALA	3.5
1	A	860	ASP	3.4
1	B	-6	SER	3.3
1	A	621	ASP	3.1
1	A	690	CYS	3.1
1	A	678	ASN	3.1
1	B	706	VAL	3.0
1	B	423	LEU	2.9
1	A	773	ASN	2.9
1	B	530	PHE	2.8
1	B	765	SER	2.8
1	A	412	SER	2.7
1	B	485	PHE	2.7
1	B	688	ALA	2.7
1	A	677	PHE	2.7
1	A	618	ALA	2.6
1	B	894	VAL	2.5
1	A	787	MET	2.5
1	A	27	MET	2.5
1	B	677	PHE	2.5
1	B	679	TYR	2.5
1	B	987	LEU	2.4
1	B	787	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	713	GLY	2.4
1	A	894	VAL	2.3
1	A	862	SER	2.3
1	B	417	LEU	2.3
1	A	639	LYS	2.2
1	A	547	TYR	2.2
1	B	945	CYS	2.2
1	B	645	LEU	2.1
1	A	921	PHE	2.1
1	B	773	ASN	2.1
1	A	400	LEU	2.1
1	B	1031	LEU	2.1
1	B	616	VAL	2.1
1	B	1016	LEU	2.1
1	A	619	PHE	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

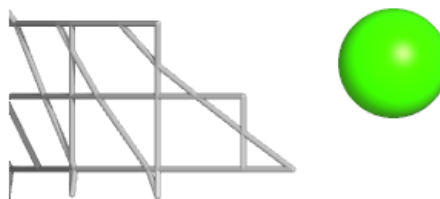
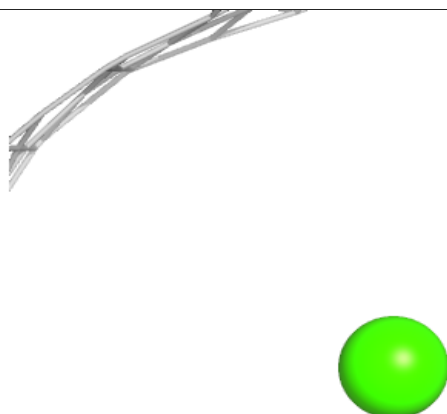
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	B	2002	1/1	0.96	0.05	213,213,213,213	0
2	CA	A	2002	1/1	0.97	0.04	169,169,169,169	0
2	CA	A	2001	1/1	0.99	0.07	106,106,106,106	0
2	CA	B	2001	1/1	1.00	0.06	103,103,103,103	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

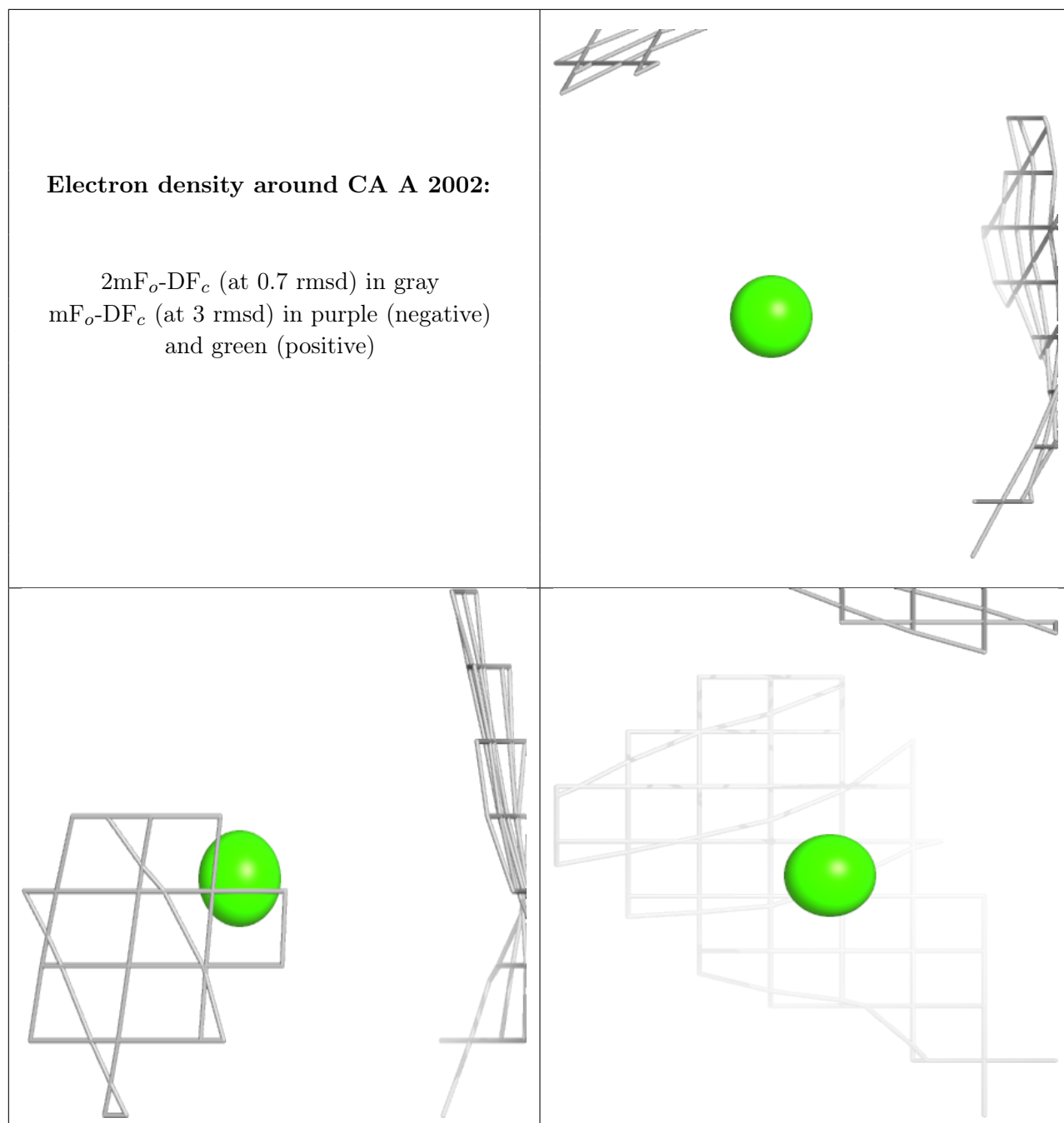
Electron density around CA B 2002:

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



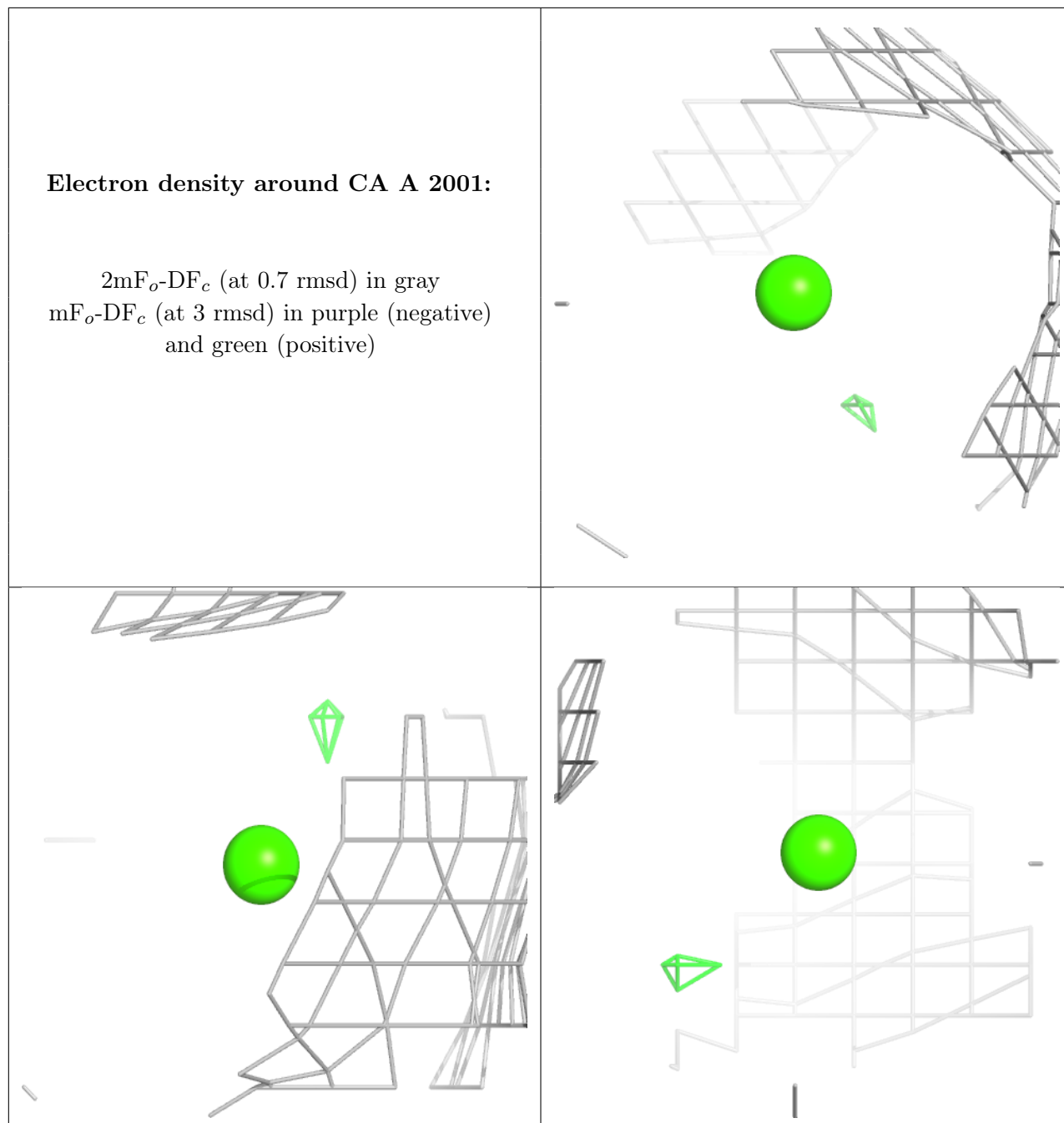
Electron density around CA A 2002:

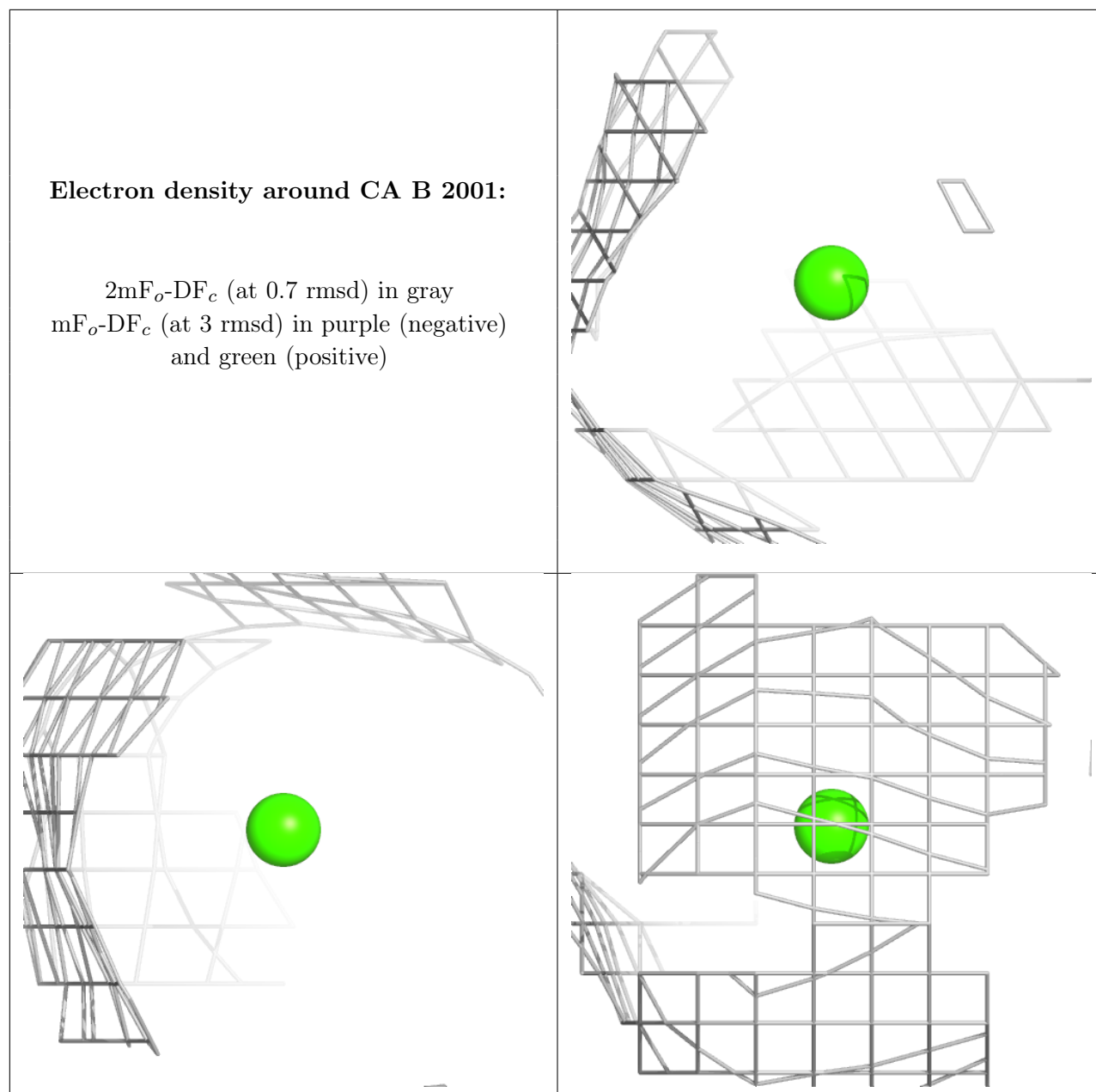
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CA A 2001:

$2mF_o-DF_c$ (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.