Full wwPDB X-ray Structure Validation Report (i)

Apr 22, 2025 – 10:16 AM JST

PDB ID	:	8Y0M / pdb_00008y0m
Title	:	beta-glucosidase mutant M279V_T308S_K361R_D433N_N514C
Authors	:	Matsuzaki, C.; Katayama, T.
Deposited on	:	2024-01-22
Resolution	:	2.30 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:

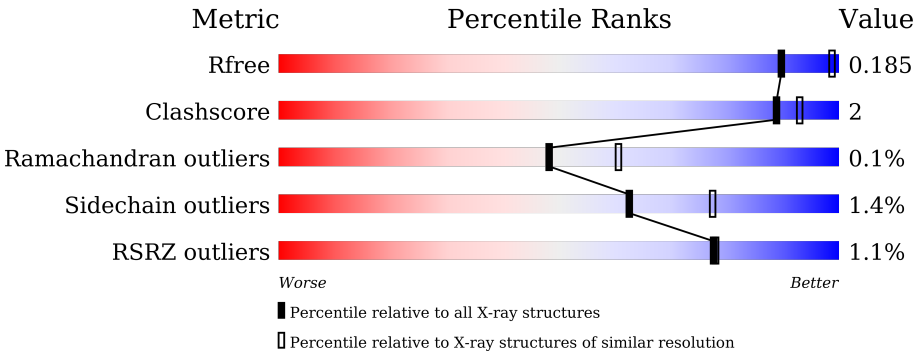
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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 2.30 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	5963 (2.30-2.30)
Clashscore	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (2.30-2.30)
RSRZ outliers	164620	5963 (2.30-2.30)

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	861	86% · 9%
1	B	861	86% · 9%
1	C	861	86% 5% 9%
1	D	861	86% 5% 9%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 26960 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 beta-glucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	781	Total	C	N	O	S	0	0	0
			5976	3783	1017	1152	24			
1	B	781	Total	C	N	O	S	0	0	0
			5976	3783	1017	1152	24			
1	C	781	Total	C	N	O	S	0	0	0
			5976	3783	1017	1152	24			
1	D	781	Total	C	N	O	S	0	0	0
			5976	3783	1017	1152	24			

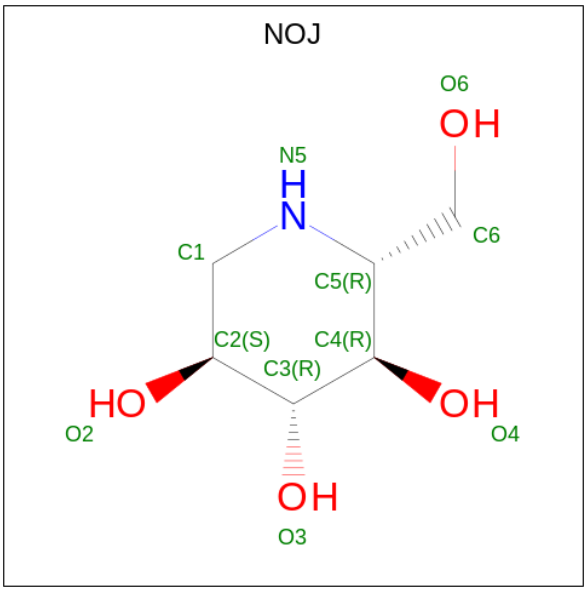
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	VAL	MET	engineered mutation	UNP Q0ZUL0
A	308	SER	THR	engineered mutation	UNP Q0ZUL0
A	361	ARG	LYS	engineered mutation	UNP Q0ZUL0
A	433	ASN	ASP	engineered mutation	UNP Q0ZUL0
A	514	CYS	ASN	engineered mutation	UNP Q0ZUL0
B	279	VAL	MET	engineered mutation	UNP Q0ZUL0
B	308	SER	THR	engineered mutation	UNP Q0ZUL0
B	361	ARG	LYS	engineered mutation	UNP Q0ZUL0
B	433	ASN	ASP	engineered mutation	UNP Q0ZUL0
B	514	CYS	ASN	engineered mutation	UNP Q0ZUL0
C	279	VAL	MET	engineered mutation	UNP Q0ZUL0
C	308	SER	THR	engineered mutation	UNP Q0ZUL0
C	361	ARG	LYS	engineered mutation	UNP Q0ZUL0
C	433	ASN	ASP	engineered mutation	UNP Q0ZUL0
C	514	CYS	ASN	engineered mutation	UNP Q0ZUL0
D	279	VAL	MET	engineered mutation	UNP Q0ZUL0
D	308	SER	THR	engineered mutation	UNP Q0ZUL0
D	361	ARG	LYS	engineered mutation	UNP Q0ZUL0
D	433	ASN	ASP	engineered mutation	UNP Q0ZUL0
D	514	CYS	ASN	engineered mutation	UNP Q0ZUL0

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 3 is 1-DEOXYNOJIRIMYCIN (CCD ID: NOJ) (formula: $C_6H_{13}NO_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 11 6 1 4	0	0
3	B	1	Total C N O 11 6 1 4	0	0
3	C	1	Total C N O 11 6 1 4	0	0
3	D	1	Total C N O 11 6 1 4	0	0

- Molecule 4 is water.

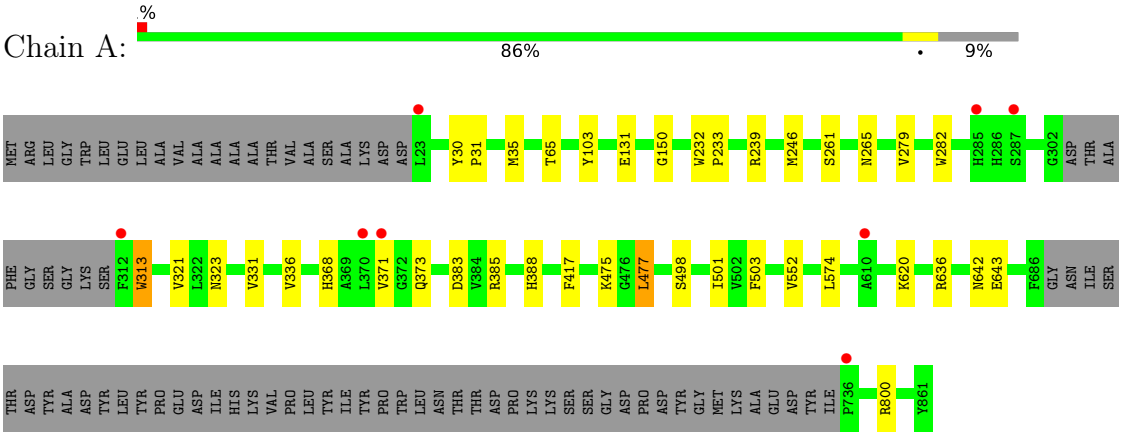
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	773	Total O 773 773	0	0
4	B	801	Total O 801 801	0	0
4	C	715	Total O 715 715	0	0
4	D	713	Total O 713 713	0	0

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.

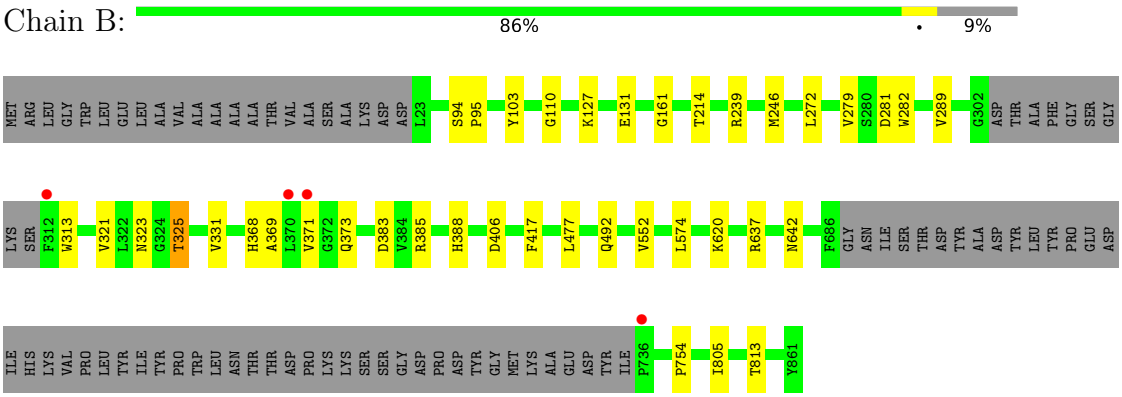
• Molecule 1: beta-glucosidase

Chain A:



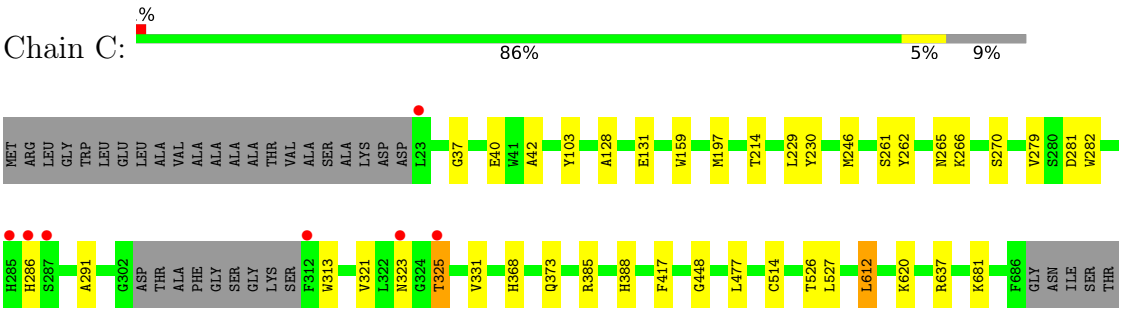
• Molecule 1: beta-glucosidase

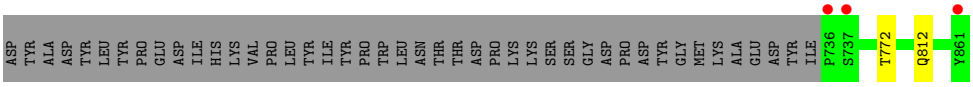
Chain B:



• Molecule 1: beta-glucosidase

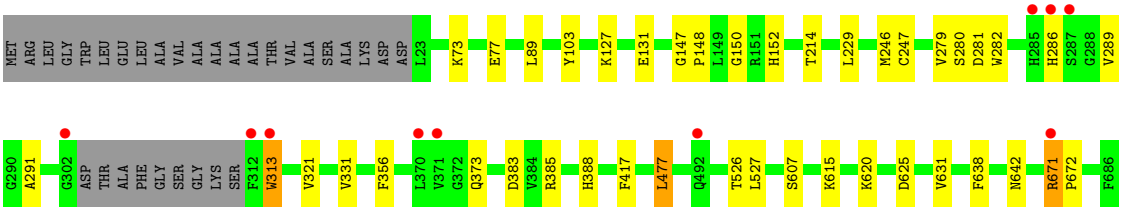
Chain C:





• Molecule 1: beta-glucosidase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	138.19Å 150.16Å 174.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.20 – 2.30 40.20 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.20-2.30) 99.9 (40.20-2.30)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.18 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.162 , 0.180 0.168 , 0.185	Depositor DCC
R_{free} test set	8013 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	21.7	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 46.7	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	0.96	EDS
Total number of atoms	26960	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.83 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.4744e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: MG, NOJ

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	0.30	0/6133	0.59	0/8357
1	B	0.30	0/6133	0.59	0/8357
1	C	0.30	0/6133	0.59	0/8357
1	D	0.30	0/6133	0.59	0/8357
All	All	0.30	0/24532	0.59	0/33428

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	5976	0	5718	22	0
1	B	5976	0	5718	24	0
1	C	5976	0	5718	27	0
1	D	5976	0	5718	25	0
2	A	2	0	0	0	0
2	B	3	0	0	0	0
2	C	2	0	0	0	0
2	D	3	0	0	1	0
3	A	11	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	11	0	13	1	0
3	C	11	0	13	1	0
3	D	11	0	13	1	0
4	A	773	0	0	1	0
4	B	801	0	0	1	0
4	C	715	0	0	1	0
4	D	713	0	0	3	0
All	All	26960	0	22924	85	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 (85) 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:B:323:ASN:OD1	1:B:325:THR:HG23	1.79	0.82
2:D:903:MG:MG	4:D:1001:HOH:O	1.24	0.80
1:A:620:LYS:H	1:D:373:GLN:HE22	1.37	0.70
1:D:625:ASP:OD2	4:D:1001:HOH:O	2.10	0.69
1:D:152:HIS:NE2	4:D:1001:HOH:O	2.27	0.67
1:B:131:GLU:OE1	1:B:388:HIS:NE2	2.29	0.65
1:A:131:GLU:OE1	1:A:388:HIS:NE2	2.28	0.65
1:C:323:ASN:HB2	1:C:325:THR:HG23	1.80	0.64
1:B:383:ASP:OD1	1:B:385:ARG:HD3	1.99	0.64
1:D:131:GLU:OE1	1:D:388:HIS:NE2	2.27	0.63
1:D:671:ARG:HD2	1:D:672:PRO:O	1.98	0.63
1:C:131:GLU:OE1	1:C:388:HIS:NE2	2.28	0.61
1:D:281:ASP:OD1	3:D:904:NOJ:H11	2.04	0.58
1:A:383:ASP:OD1	1:A:385:ARG:HD3	2.04	0.57
1:B:323:ASN:OD1	1:B:325:THR:CG2	2.54	0.55
1:D:286:HIS:HB2	1:D:291:ALA:HB2	1.88	0.55
1:B:321:VAL:HG21	1:B:331:VAL:HG21	1.89	0.55
1:B:620:LYS:H	1:C:373:GLN:HE22	1.55	0.55
1:D:321:VAL:HG21	1:D:331:VAL:HG21	1.89	0.55
1:A:321:VAL:HG21	1:A:331:VAL:HG21	1.89	0.54
1:D:526:THR:HG22	1:D:527:LEU:O	2.09	0.53
1:C:197:MET:SD	1:C:612:LEU:CD2	2.98	0.52
1:B:103:TYR:CE1	1:D:477:LEU:HD22	2.45	0.52
1:B:281:ASP:OD1	3:B:904:NOJ:H11	2.09	0.52
1:B:373:GLN:HE22	1:C:620:LYS:H	1.57	0.52
1:A:321:VAL:CG2	1:A:331:VAL:HG21	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:ALA:HA	1:C:131:GLU:HG3	1.93	0.51
1:A:475:LYS:O	1:C:385:ARG:NH2	2.42	0.49
1:C:321:VAL:HG21	1:C:331:VAL:HG21	1.95	0.49
1:B:477:LEU:HD22	1:D:103:TYR:CE1	2.48	0.48
1:A:239:ARG:NH2	4:A:1003:HOH:O	2.44	0.48
1:A:103:TYR:CE1	1:C:477:LEU:HD22	2.49	0.48
1:B:552:VAL:HG12	1:B:574:LEU:HD11	1.95	0.48
1:A:477:LEU:HD22	1:C:103:TYR:CE1	2.49	0.47
1:B:127:LYS:O	1:B:131:GLU:HG3	2.13	0.47
1:B:369:ALA:HB3	1:B:371:VAL:O	2.15	0.47
1:B:368:HIS:HE1	1:C:214:THR:OG1	1.98	0.47
1:A:620:LYS:H	1:D:373:GLN:NE2	2.09	0.47
1:C:514:CYS:SG	4:C:1561:HOH:O	2.61	0.46
1:C:262:TYR:CZ	1:C:266:LYS:HD3	2.50	0.46
1:D:77:GLU:HA	1:D:89:LEU:O	2.16	0.46
1:A:65:THR:HG1	1:A:313:TRP:HD1	1.62	0.45
1:B:321:VAL:CG2	1:B:331:VAL:HG21	2.47	0.45
1:C:229:LEU:HD23	1:C:230:TYR:CE2	2.52	0.44
1:C:281:ASP:OD1	3:C:903:NOJ:H11	2.17	0.44
1:C:526:THR:HG22	1:C:527:LEU:O	2.17	0.44
1:B:246:MET:HA	1:B:279:VAL:O	2.17	0.44
1:D:246:MET:HA	1:D:279:VAL:O	2.18	0.44
1:A:373:GLN:HE22	1:D:620:LYS:H	1.66	0.44
1:B:94:SER:HB2	1:B:95:PRO:CD	2.48	0.43
1:B:620:LYS:H	1:C:373:GLN:NE2	2.16	0.43
1:C:261:SER:O	1:C:265:ASN:HB2	2.19	0.43
1:C:772:THR:OG1	1:C:812:GLN:HG2	2.18	0.43
1:D:127:LYS:O	1:D:131:GLU:HG3	2.17	0.43
1:D:147:GLY:HA2	1:D:148:PRO:C	2.39	0.43
1:A:552:VAL:HG12	1:A:574:LEU:HD11	2.00	0.43
1:C:37:GLY:O	1:C:42:ALA:HA	2.19	0.43
1:C:321:VAL:CG2	1:C:331:VAL:HG21	2.48	0.42
1:D:247:CYS:SG	1:D:280:SER:HA	2.59	0.42
1:A:35:MET:SD	1:A:336:VAL:HG13	2.59	0.42
1:A:501:ILE:HG22	1:A:503:PHE:CE1	2.55	0.42
1:A:323:ASN:OD1	1:A:323:ASN:C	2.58	0.42
1:A:368:HIS:HE1	1:D:214:THR:OG1	2.03	0.42
1:D:73:LYS:HE3	1:D:356:PHE:O	2.19	0.42
1:C:159:TRP:CZ2	1:C:448:GLY:HA3	2.55	0.42
1:C:286:HIS:HB2	1:C:291:ALA:HB2	2.02	0.42
1:C:266:LYS:O	1:C:270:SER:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:805:ILE:HG21	1:B:813:THR:HG21	2.01	0.42
1:C:246:MET:HA	1:C:279:VAL:O	2.19	0.42
1:D:383:ASP:OD1	1:D:385:ARG:HD3	2.20	0.42
1:B:272:LEU:O	1:B:754:PRO:HA	2.20	0.41
1:D:313:TRP:CD1	1:D:313:TRP:C	2.94	0.41
1:A:261:SER:O	1:A:265:ASN:HB2	2.21	0.41
1:D:229:LEU:HD22	1:D:631:VAL:HA	2.02	0.41
1:A:30:TYR:HB3	1:A:31:PRO:HA	2.02	0.41
1:A:800:ARG:HD3	1:A:800:ARG:HA	1.94	0.41
1:D:607:SER:HB3	1:D:638:PHE:CE2	2.55	0.41
1:A:246:MET:HA	1:A:279:VAL:O	2.21	0.41
1:B:214:THR:OG1	1:C:368:HIS:HE1	2.04	0.41
1:C:323:ASN:HB2	1:C:325:THR:CG2	2.49	0.41
1:D:321:VAL:CG2	1:D:331:VAL:HG21	2.50	0.41
1:B:110:GLY:HA3	1:B:161:GLY:O	2.21	0.40
1:B:239:ARG:NH2	4:B:1009:HOH:O	2.52	0.40
1:B:323:ASN:OD1	1:B:323:ASN:C	2.59	0.40
1:A:232:TRP:HB3	1:A:233:PRO:CD	2.52	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	775/861 (90%)	749 (97%)	25 (3%)	1 (0%)	48	60
1	B	775/861 (90%)	750 (97%)	25 (3%)	0	100	100
1	C	775/861 (90%)	748 (96%)	27 (4%)	0	100	100
1	D	775/861 (90%)	747 (96%)	27 (4%)	1 (0%)	48	60
All	All	3100/3444 (90%)	2994 (97%)	104 (3%)	2 (0%)	48	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	150	GLY
1	A	150	GLY

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	631/695 (91%)	622 (99%)	9 (1%)	62	77
1	B	631/695 (91%)	622 (99%)	9 (1%)	62	77
1	C	631/695 (91%)	623 (99%)	8 (1%)	65	79
1	D	631/695 (91%)	622 (99%)	9 (1%)	62	77
All	All	2524/2780 (91%)	2489 (99%)	35 (1%)	62	77

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	282	TRP
1	A	313	TRP
1	A	371	VAL
1	A	417	PHE
1	A	477	LEU
1	A	498	SER
1	A	636	ARG
1	A	642	ASN
1	A	643	GLU
1	B	282	TRP
1	B	289	VAL
1	B	313	TRP
1	B	325	THR
1	B	406	ASP
1	B	417	PHE
1	B	492	GLN
1	B	637	ARG
1	B	642	ASN
1	C	40	GLU
1	C	282	TRP

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Mol	Chain	Res	Type
1	C	313	TRP
1	C	325	THR
1	C	417	PHE
1	C	612	LEU
1	C	637	ARG
1	C	681	LYS
1	D	282	TRP
1	D	289	VAL
1	D	313	TRP
1	D	417	PHE
1	D	477	LEU
1	D	615	LYS
1	D	642	ASN
1	D	671	ARG
1	D	801	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	368	HIS
1	A	373	GLN
1	A	468	ASN
1	B	368	HIS
1	B	373	GLN
1	B	468	ASN
1	B	642	ASN
1	C	368	HIS
1	C	373	GLN
1	C	468	ASN
1	C	642	ASN
1	C	808	HIS
1	D	368	HIS
1	D	373	GLN
1	D	468	ASN
1	D	642	ASN
1	D	808	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 10 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
3	NOJ	B	904	-	11,11,11	0.26	0	13,15,15	0.95	1 (7%)
3	NOJ	A	903	-	11,11,11	0.31	0	13,15,15	1.14	2 (15%)
3	NOJ	D	904	-	11,11,11	0.26	0	13,15,15	0.90	1 (7%)
3	NOJ	C	903	-	11,11,11	0.26	0	13,15,15	1.04	2 (15%)

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
3	NOJ	B	904	-	-	0/2/19/19	0/1/1/1
3	NOJ	A	903	-	-	0/2/19/19	0/1/1/1
3	NOJ	D	904	-	-	0/2/19/19	0/1/1/1
3	NOJ	C	903	-	-	0/2/19/19	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	903	NOJ	C1-N5-C5	2.96	116.00	109.61
3	C	903	NOJ	C1-C2-C3	2.59	113.37	110.33
3	A	903	NOJ	C1-C2-C3	2.47	113.23	110.33
3	B	904	NOJ	C1-N5-C5	2.46	114.92	109.61
3	D	904	NOJ	C1-N5-C5	2.30	114.59	109.61
3	C	903	NOJ	C1-N5-C5	2.14	114.25	109.61

There are no chirality outliers.

There are no torsion outliers.

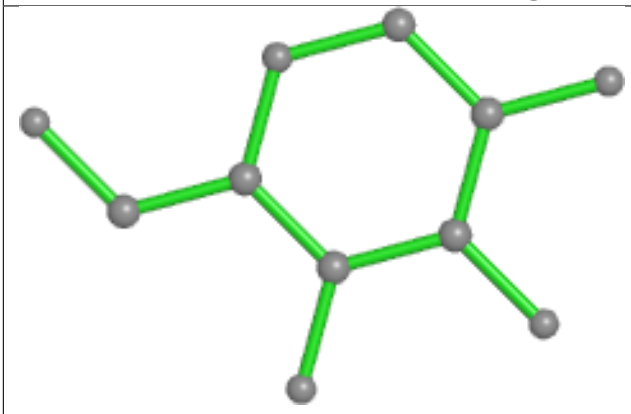
There are no ring outliers.

3 monomers are involved in 3 short contacts:

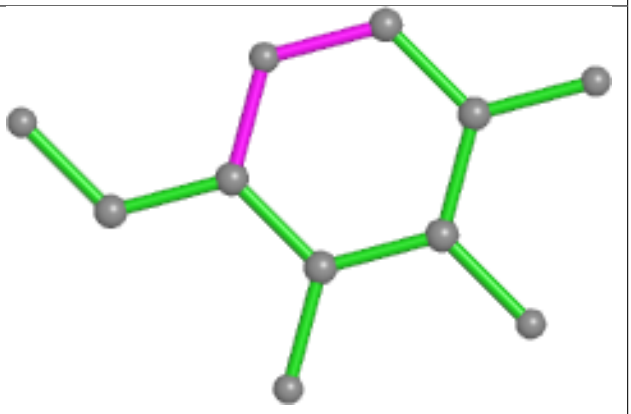
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	904	NOJ	1	0
3	D	904	NOJ	1	0
3	C	903	NOJ	1	0

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.

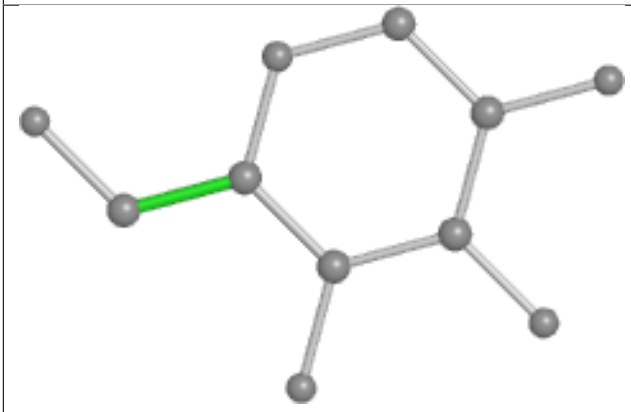
Ligand NOJ B 904



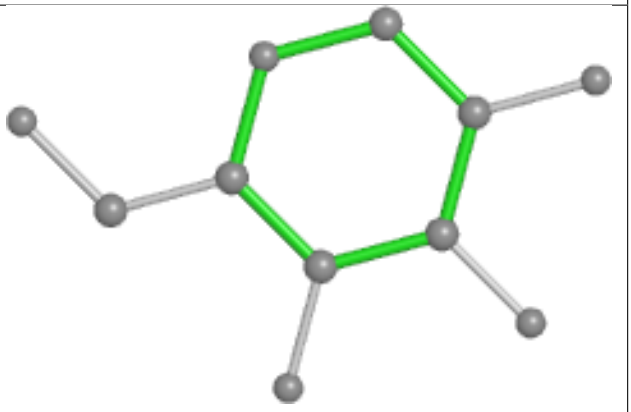
Bond lengths



Bond angles

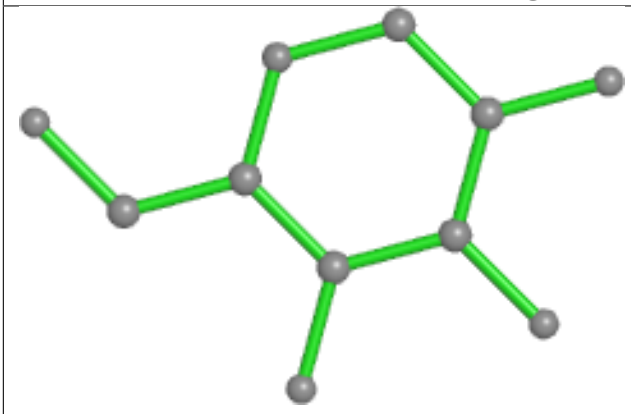


Torsions

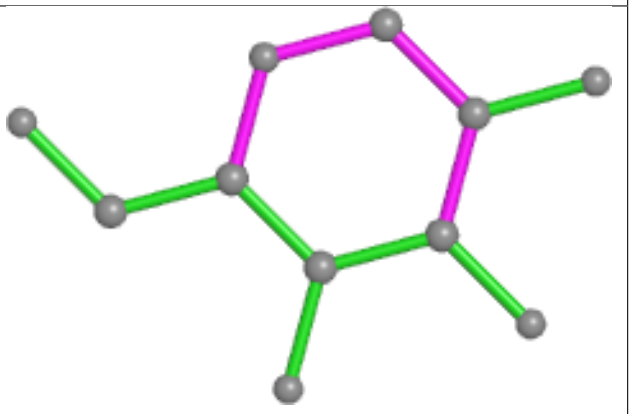


Rings

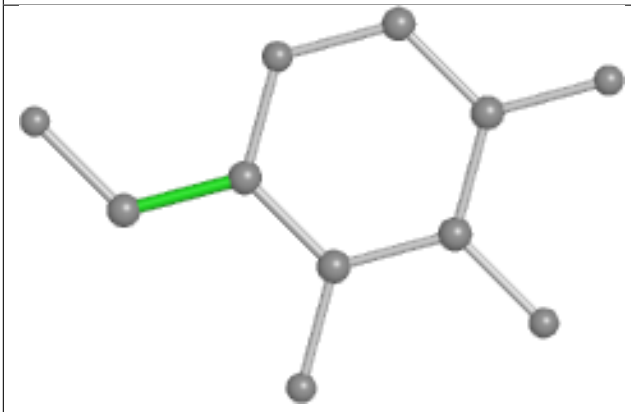
Ligand NOJ A 903



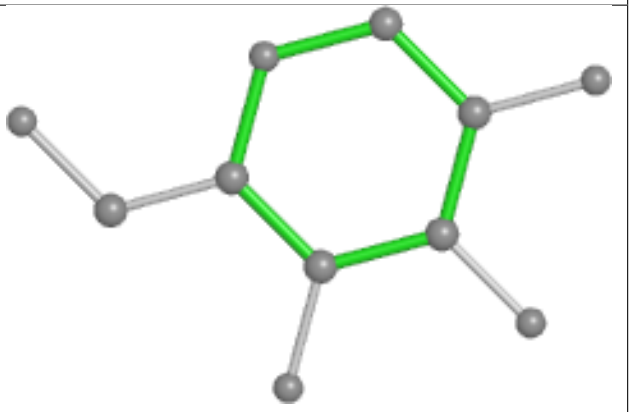
Bond lengths



Bond angles

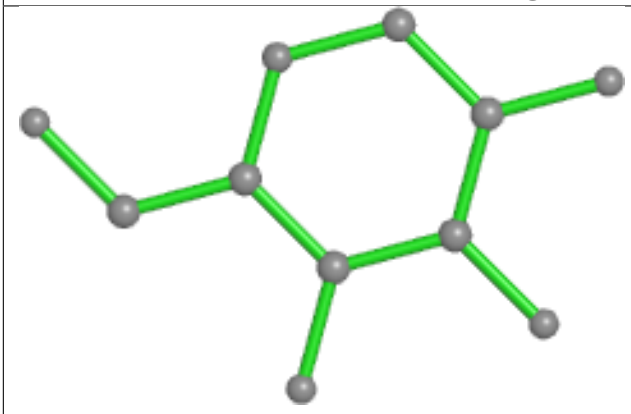


Torsions

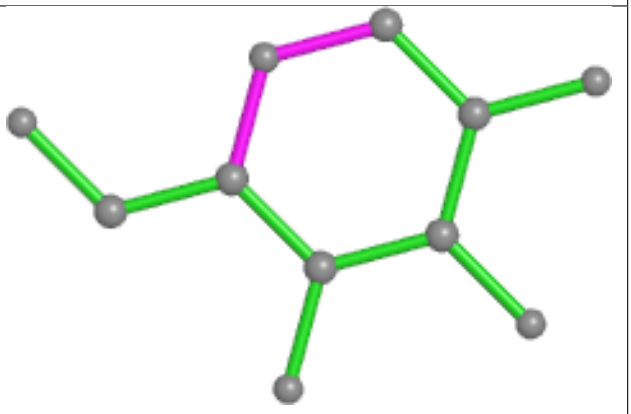


Rings

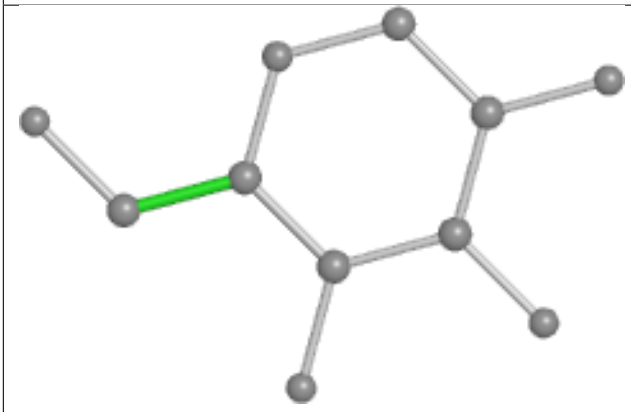
Ligand NOJ D 904



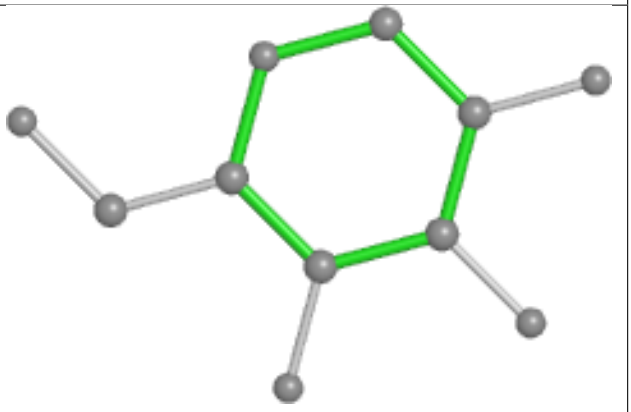
Bond lengths



Bond angles

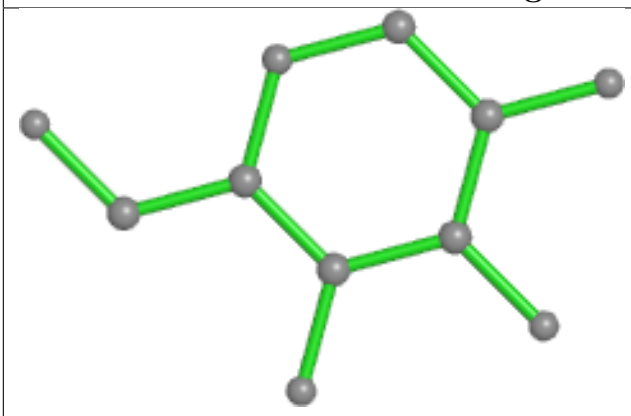


Torsions

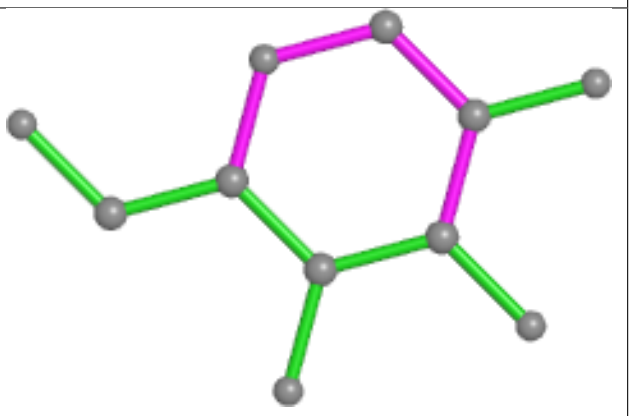


Rings

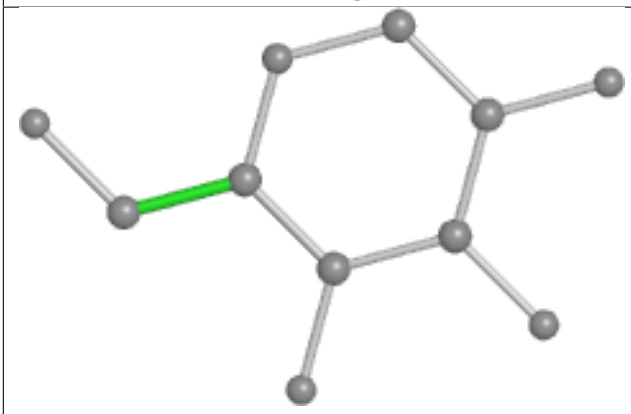
Ligand NOJ C 903



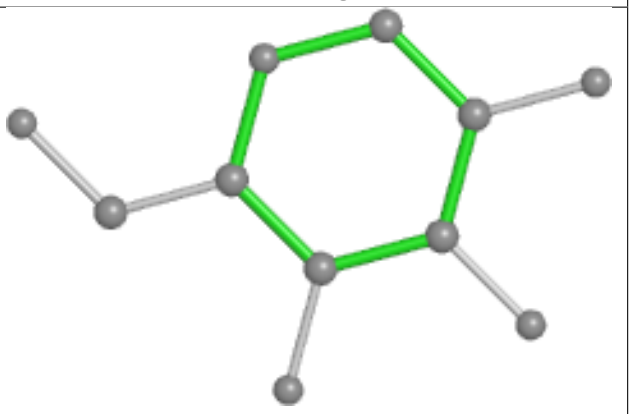
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	781/861 (90%)	-0.51	8 (1%)	79	79	14, 20, 33, 62	0
1	B	781/861 (90%)	-0.52	4 (0%)	87	88	14, 20, 32, 65	0
1	C	781/861 (90%)	-0.47	10 (1%)	74	75	15, 20, 38, 66	0
1	D	781/861 (90%)	-0.45	12 (1%)	71	72	14, 21, 39, 70	0
All	All	3124/3444 (90%)	-0.49	34 (1%)	77	78	14, 20, 36, 70	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	312	PHE	5.1
1	B	312	PHE	5.0
1	A	287	SER	3.9
1	A	312	PHE	3.8
1	D	671	ARG	3.6
1	D	736	PRO	3.4
1	D	737	SER	3.2
1	A	370	LEU	3.2
1	D	370	LEU	3.2
1	A	736	PRO	3.1
1	C	737	SER	3.0
1	D	302	GLY	2.9
1	D	285	HIS	2.9
1	C	286	HIS	2.9
1	C	312	PHE	2.8
1	B	371	VAL	2.8
1	C	285	HIS	2.7
1	D	371	VAL	2.6
1	D	287	SER	2.5
1	C	861	TYR	2.5
1	B	736	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	492	GLN	2.4
1	B	370	LEU	2.3
1	C	325	THR	2.3
1	C	287	SER	2.3
1	A	285	HIS	2.2
1	D	313	TRP	2.2
1	A	23	LEU	2.2
1	C	323	ASN	2.2
1	A	371	VAL	2.2
1	D	286	HIS	2.2
1	C	736	PRO	2.1
1	C	23	LEU	2.1
1	A	610	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	NOJ	C	903	11/11	0.96	0.07	15,16,16,16	0
3	NOJ	A	903	11/11	0.97	0.05	14,15,15,15	0
3	NOJ	B	904	11/11	0.97	0.06	16,16,17,17	0
2	MG	B	903	1/1	0.97	0.14	5,5,5,5	0
2	MG	D	903	1/1	0.98	0.10	9,9,9,9	0
2	MG	D	901	1/1	0.98	0.03	25,25,25,25	0
3	NOJ	D	904	11/11	0.98	0.05	17,17,17,17	0
2	MG	D	902	1/1	0.99	0.01	28,28,28,28	0
2	MG	B	902	1/1	0.99	0.02	20,20,20,20	0
2	MG	A	902	1/1	0.99	0.03	23,23,23,23	0

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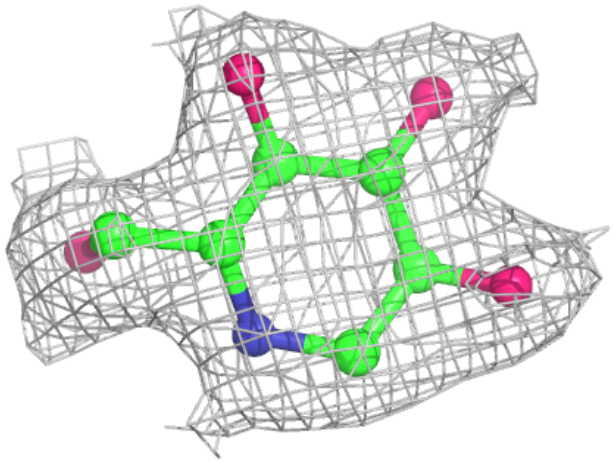
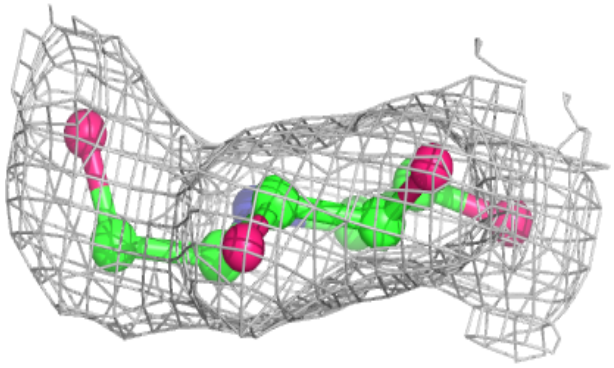
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MG	C	901	1/1	0.99	0.02	25,25,25,25	0
2	MG	C	902	1/1	0.99	0.03	26,26,26,26	0
2	MG	B	901	1/1	0.99	0.02	20,20,20,20	0
2	MG	A	901	1/1	1.00	0.01	18,18,18,18	0

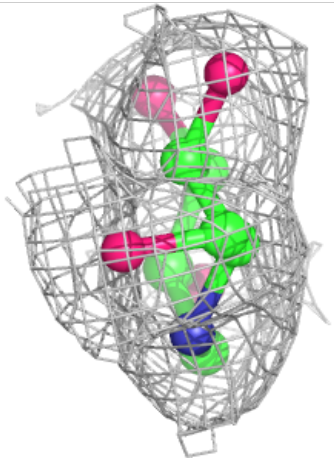
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NOJ C 903:

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

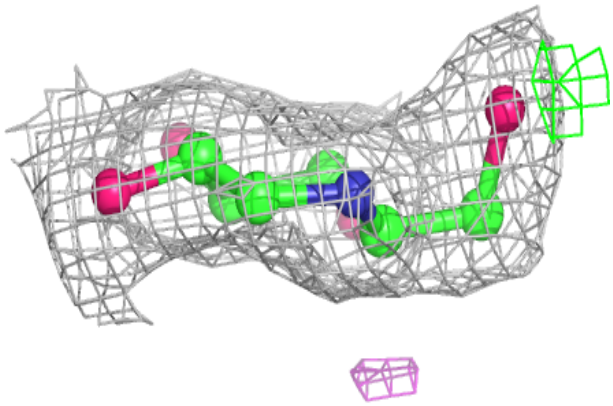


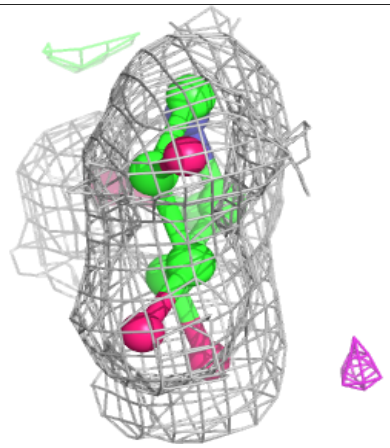




Electron density around NOJ A 903:

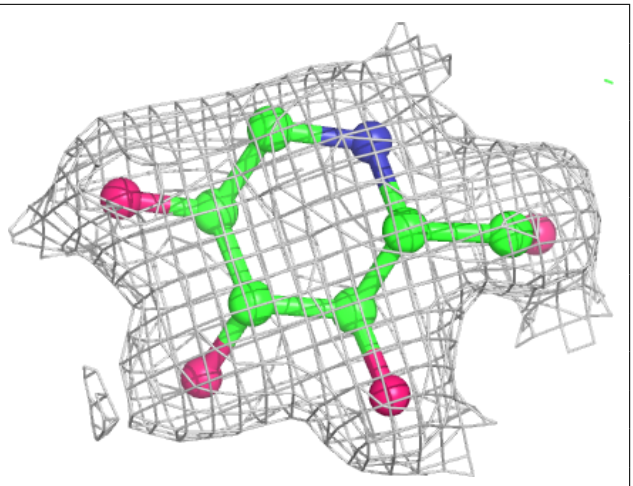
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

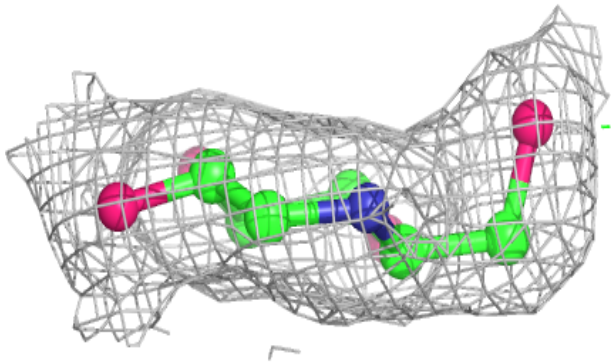


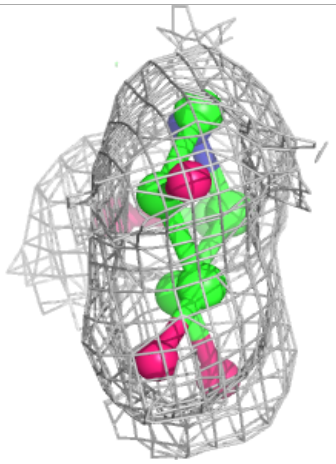


Electron density around NOJ B 904:

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

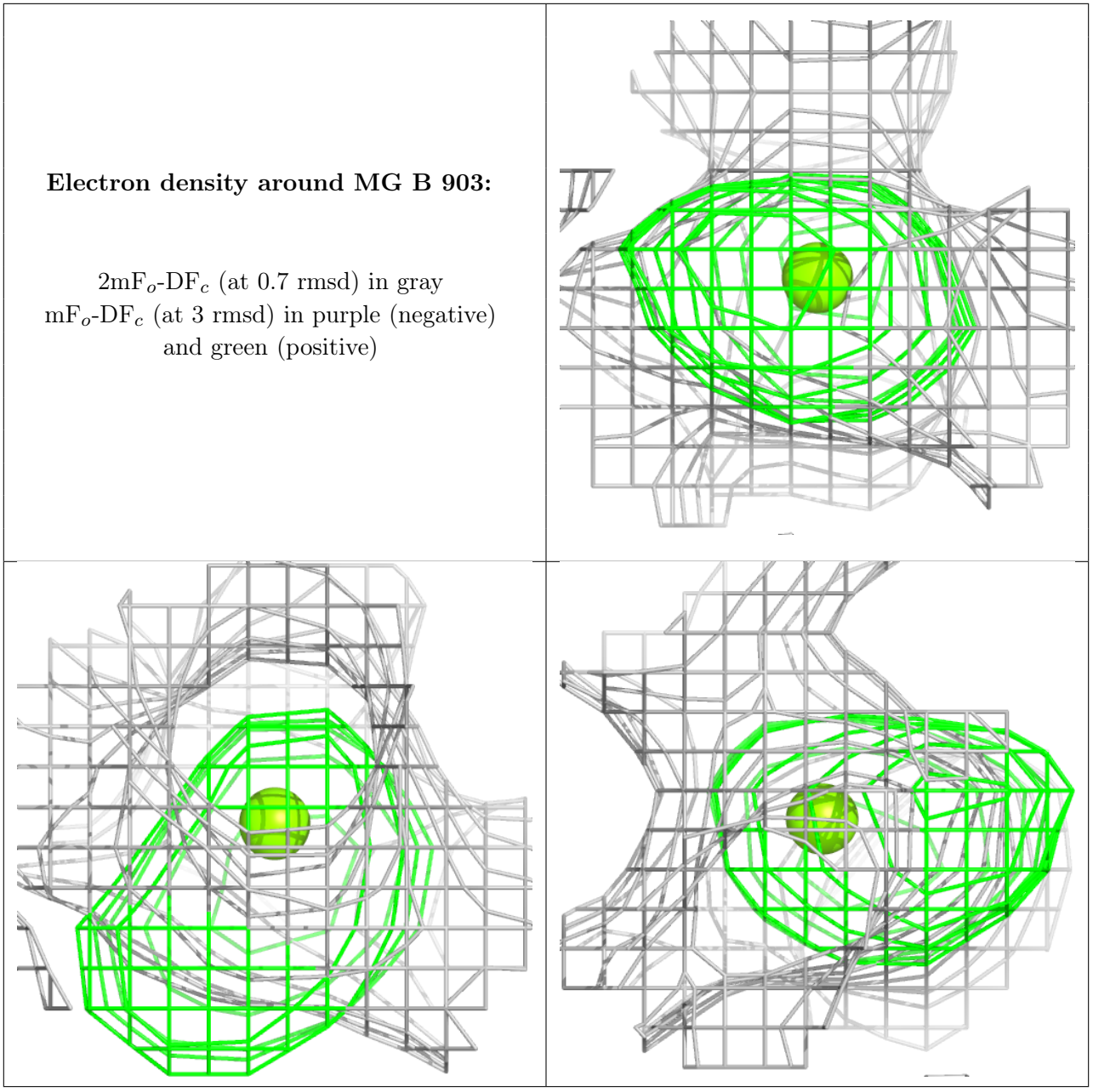






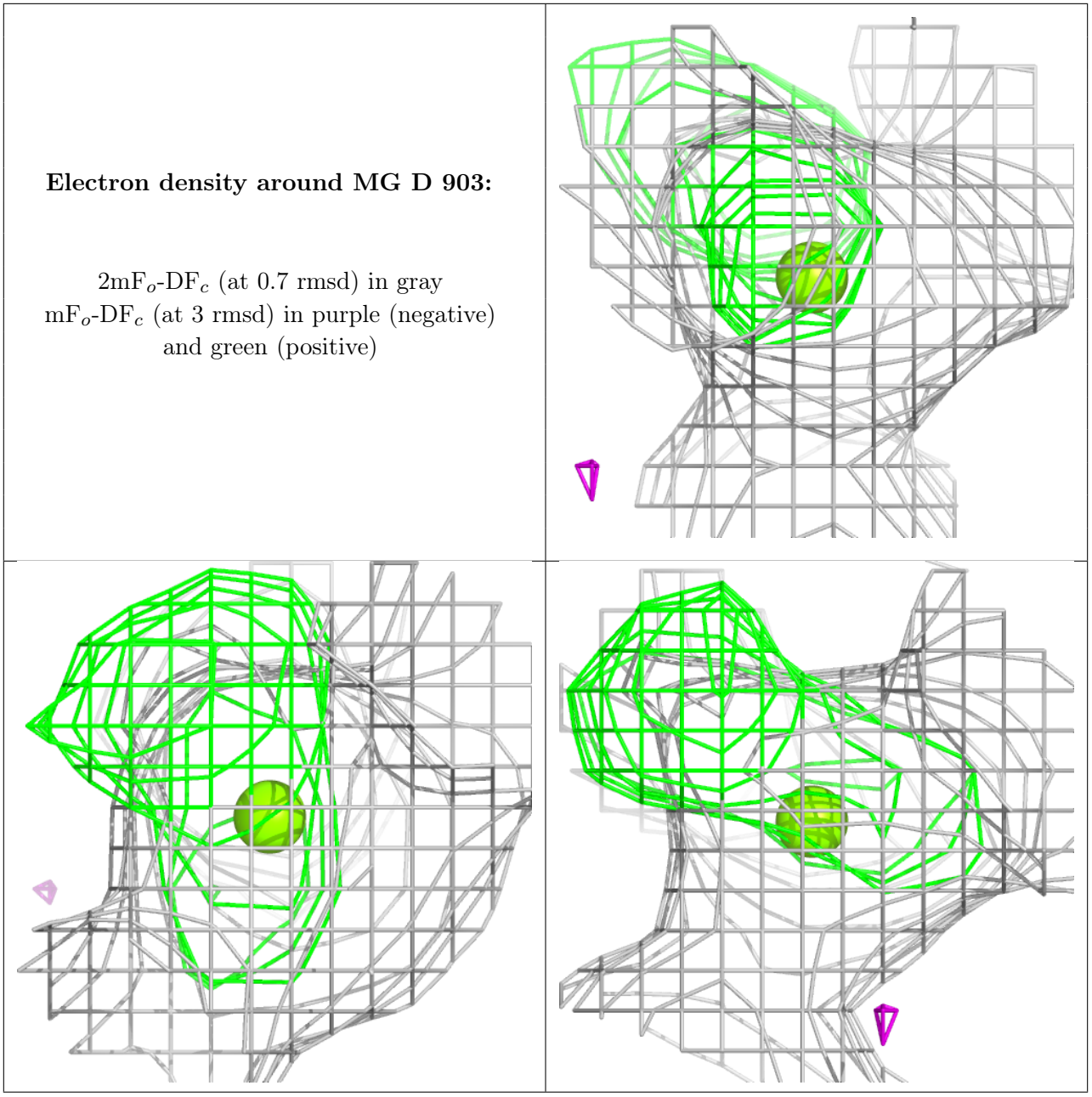
Electron density around MG B 903:

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



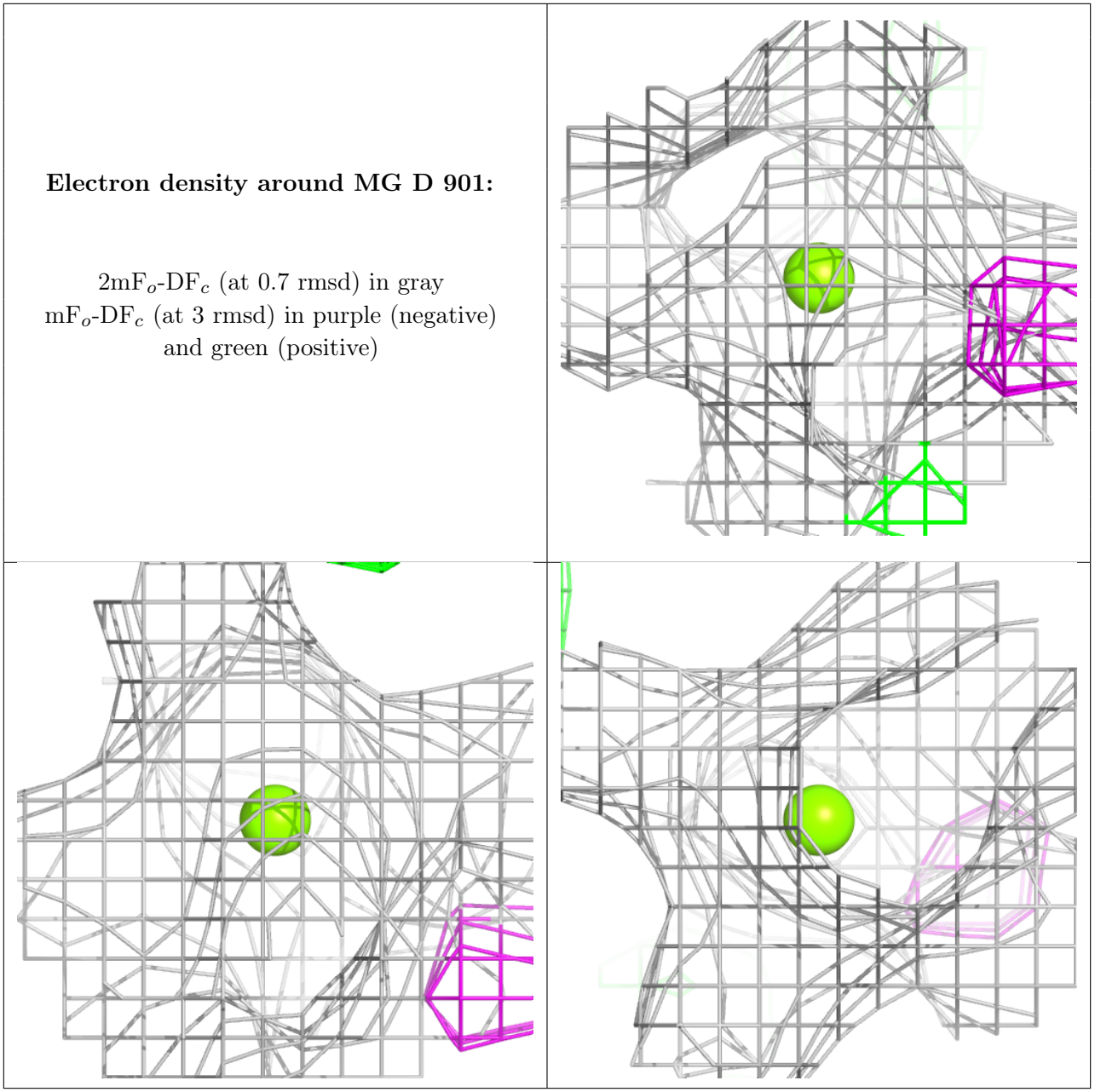
Electron density around MG D 903:

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



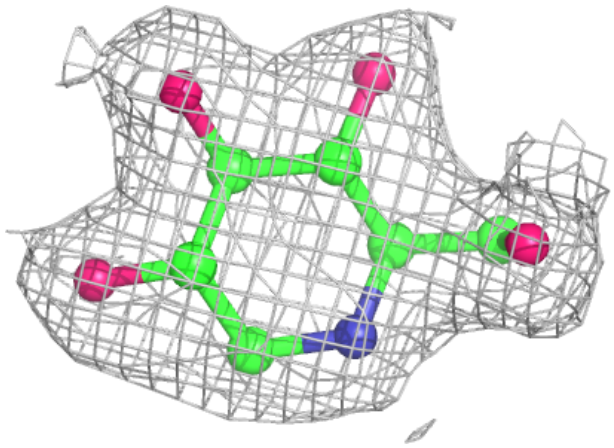
Electron density around MG D 901:

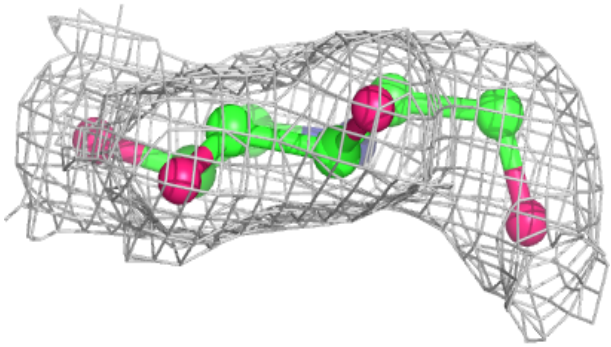
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

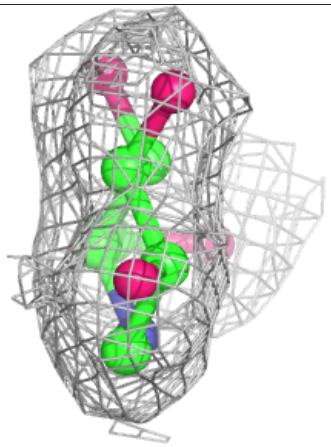


Electron density around NOJ D 904:

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

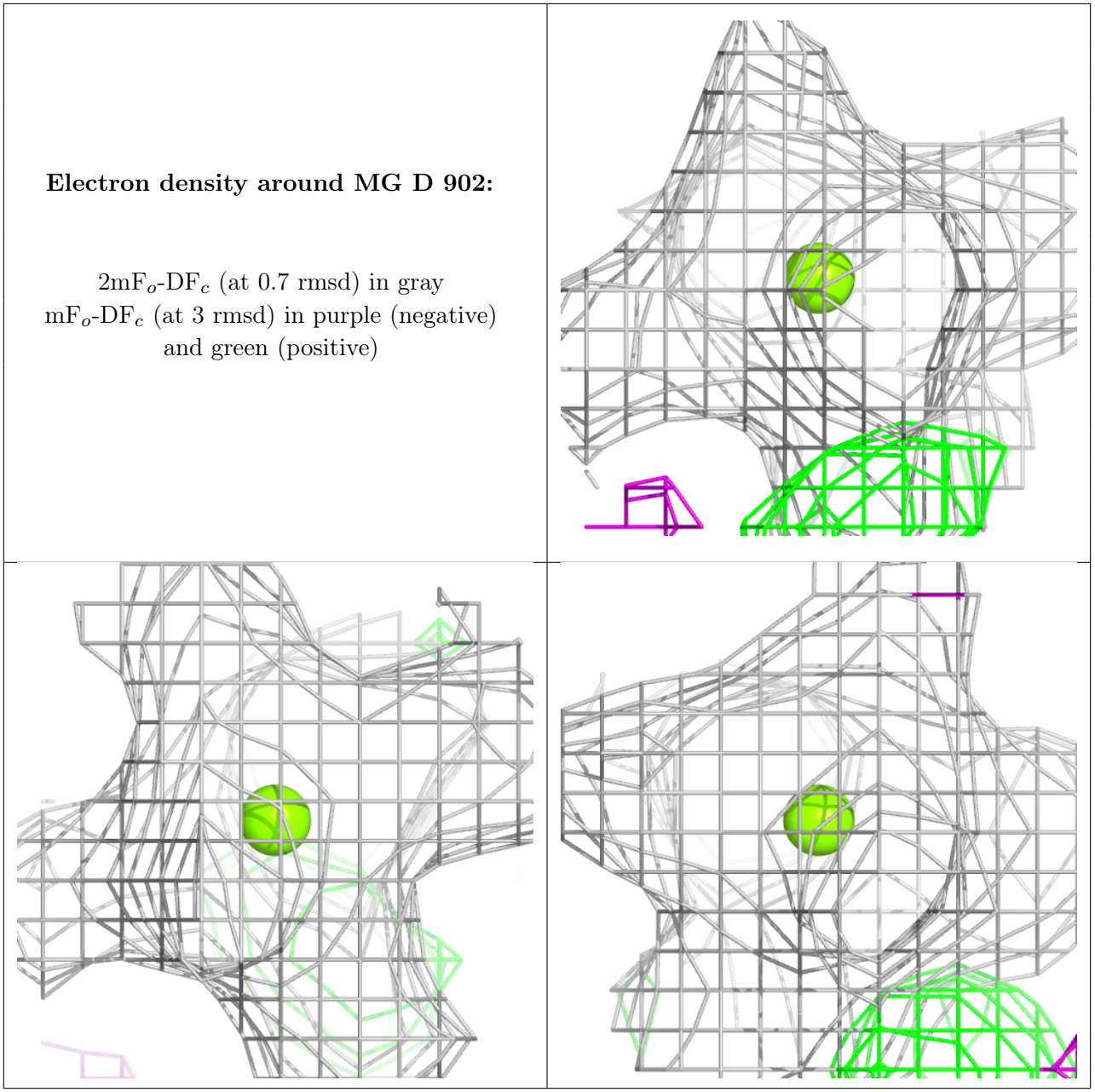






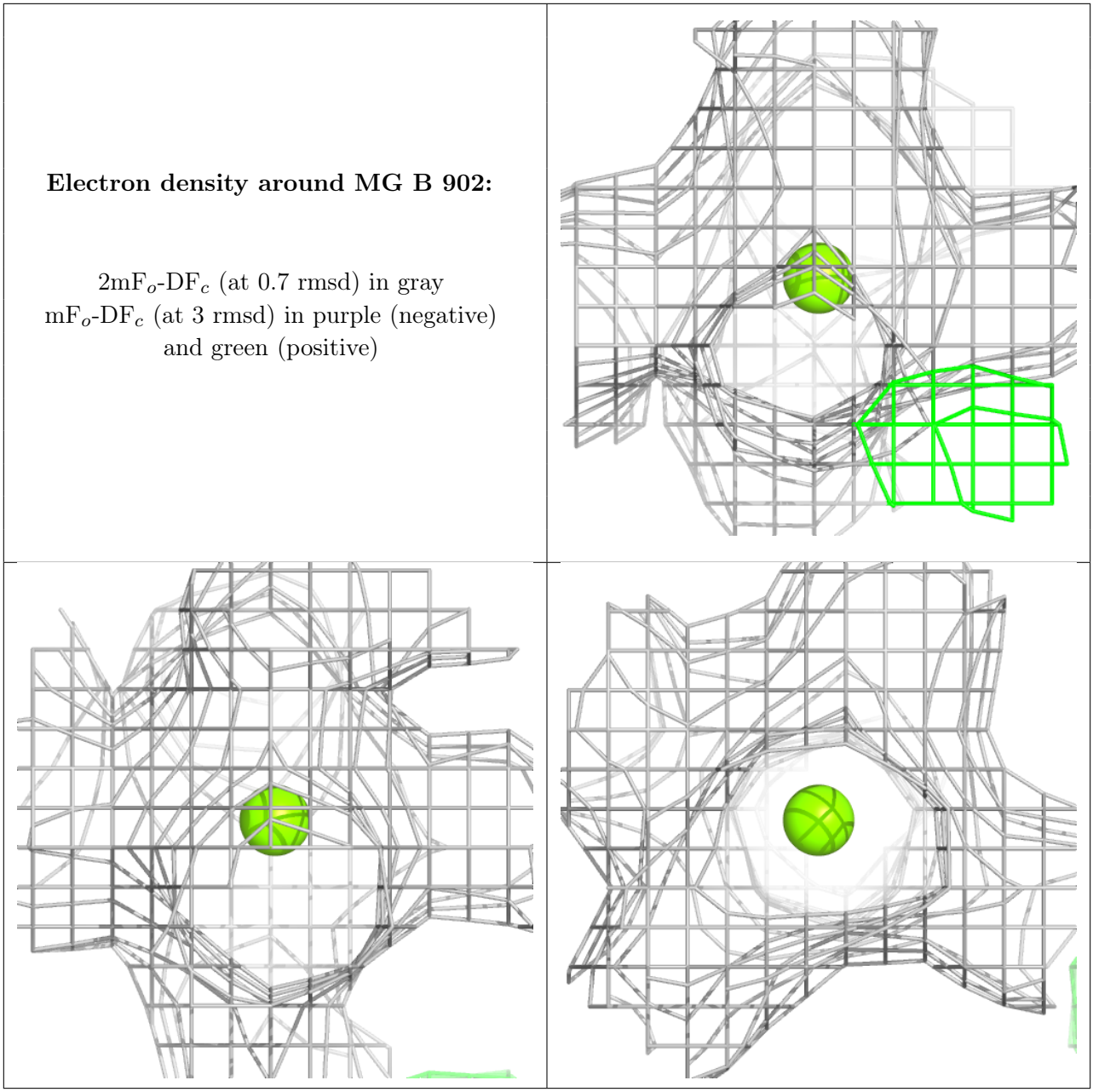
Electron density around MG D 902:

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



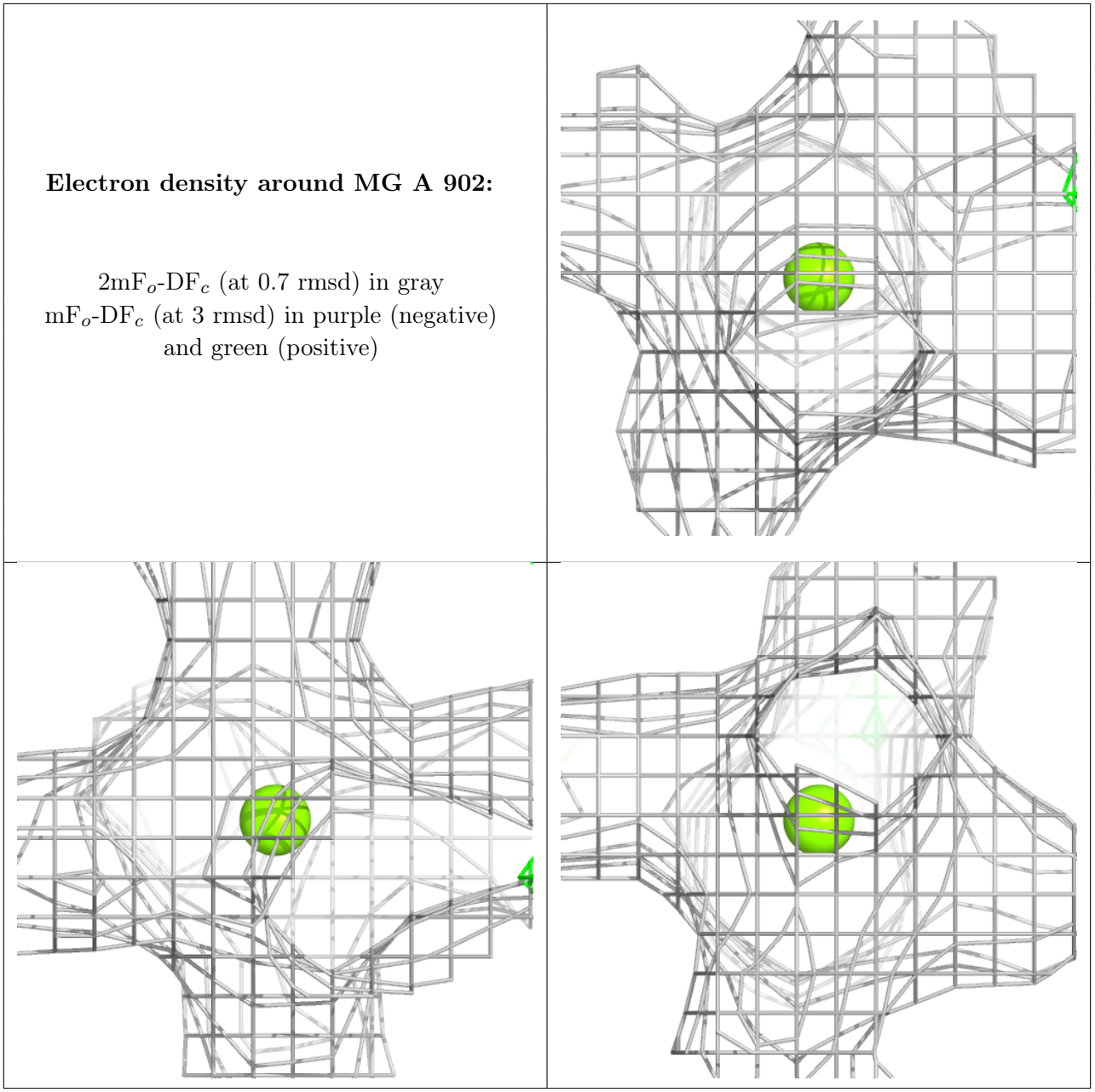
Electron density around MG B 902:

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



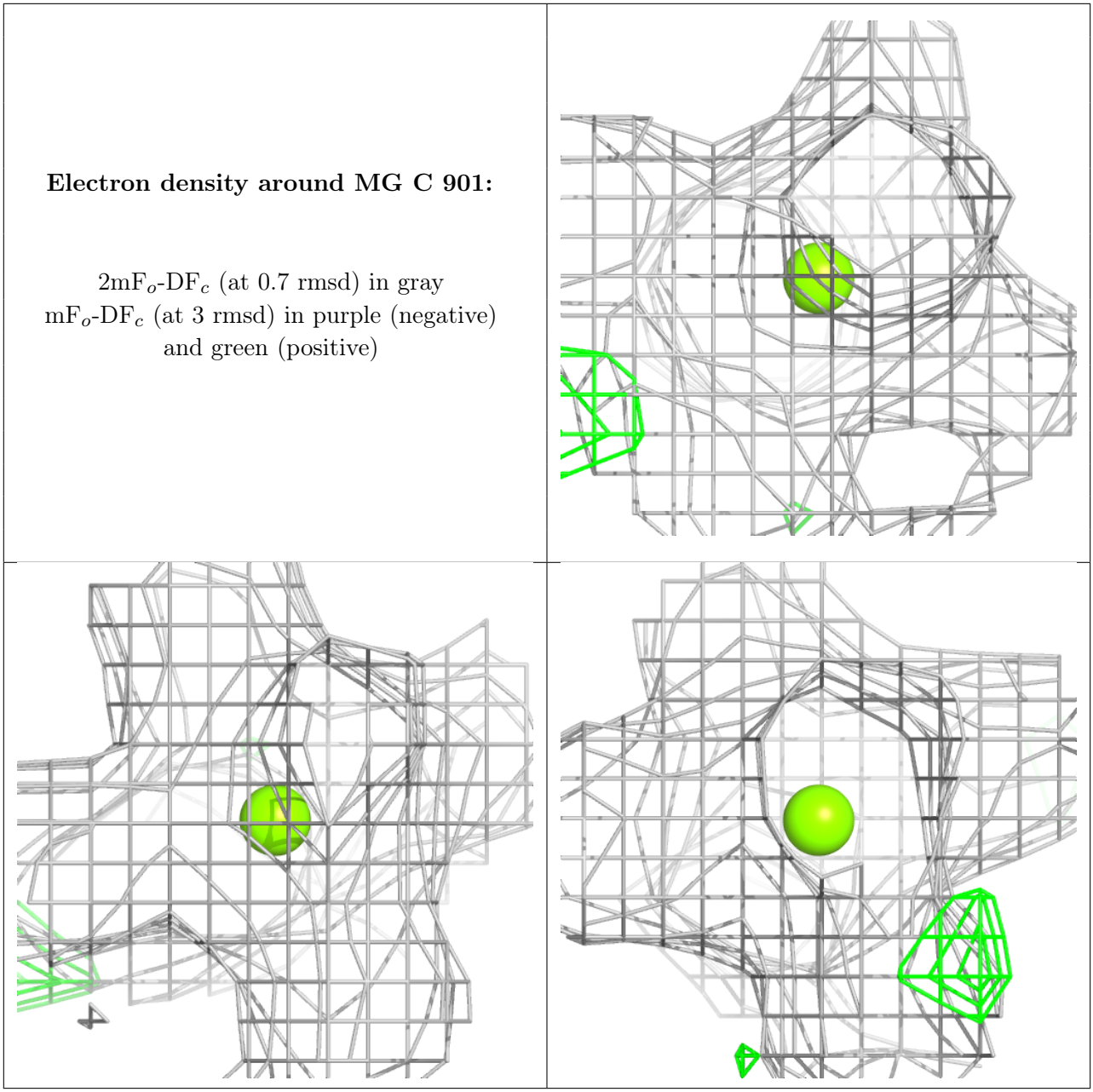
Electron density around MG A 902:

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



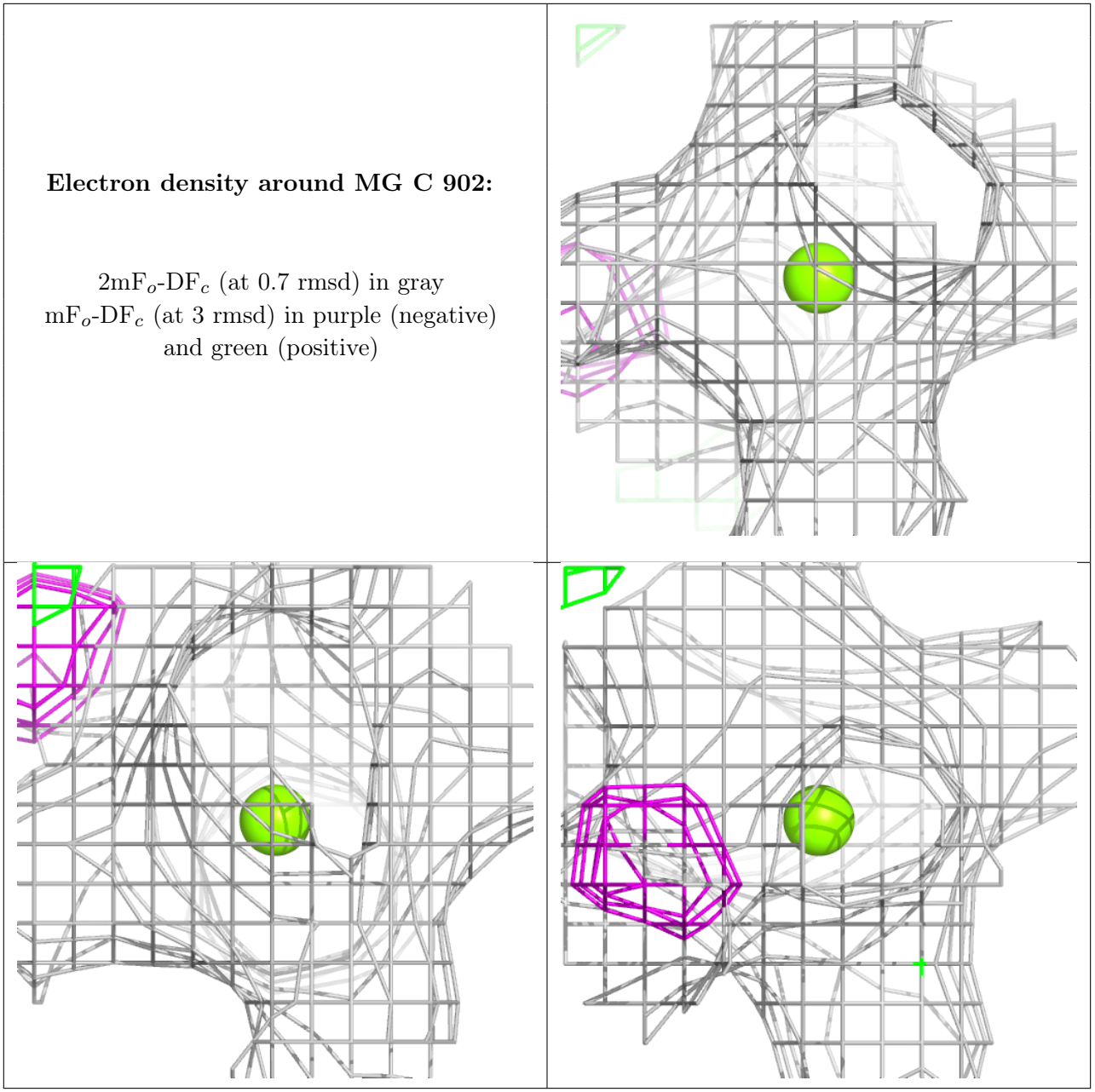
Electron density around MG C 901:

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



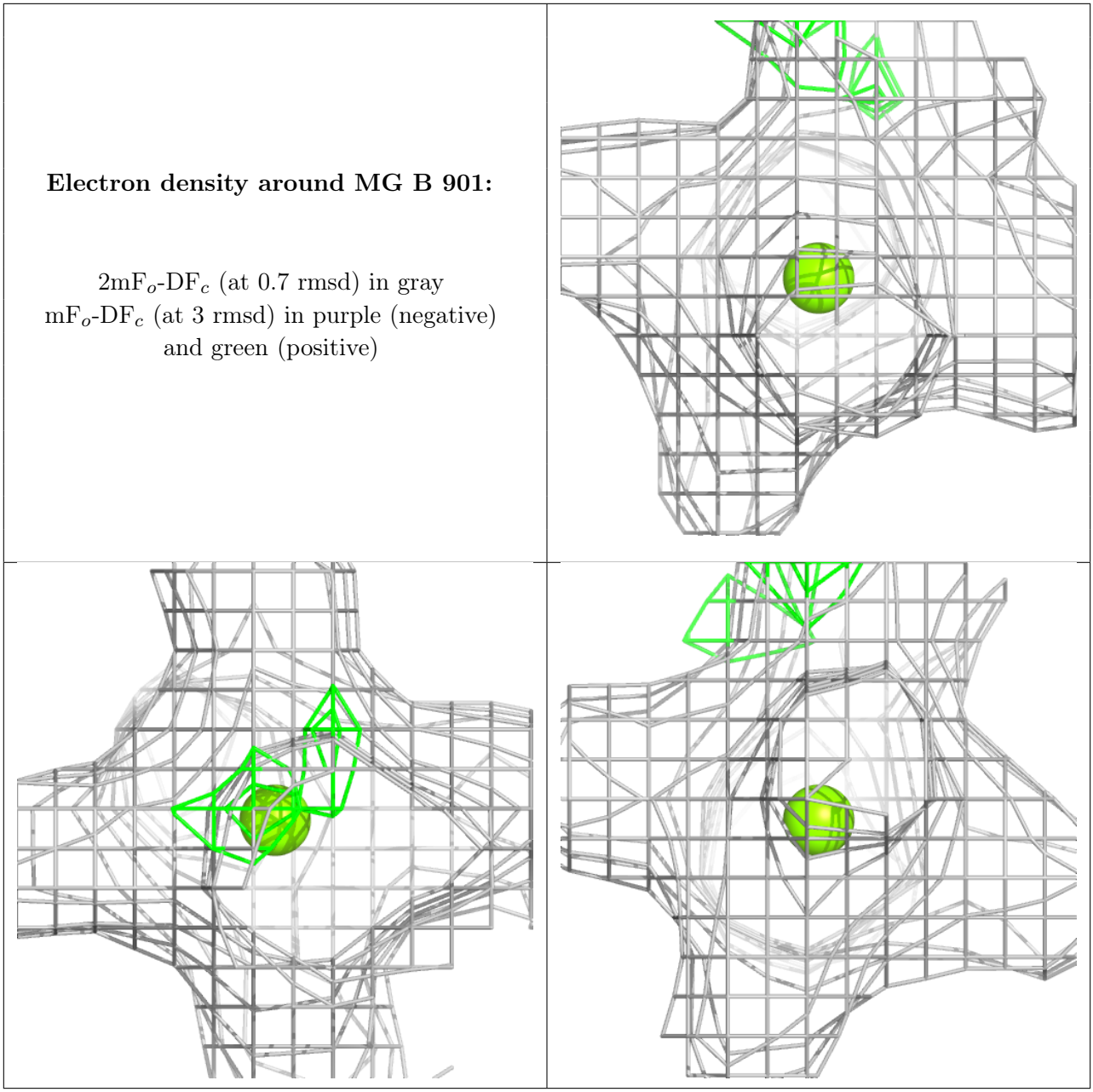
Electron density around MG C 902:

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



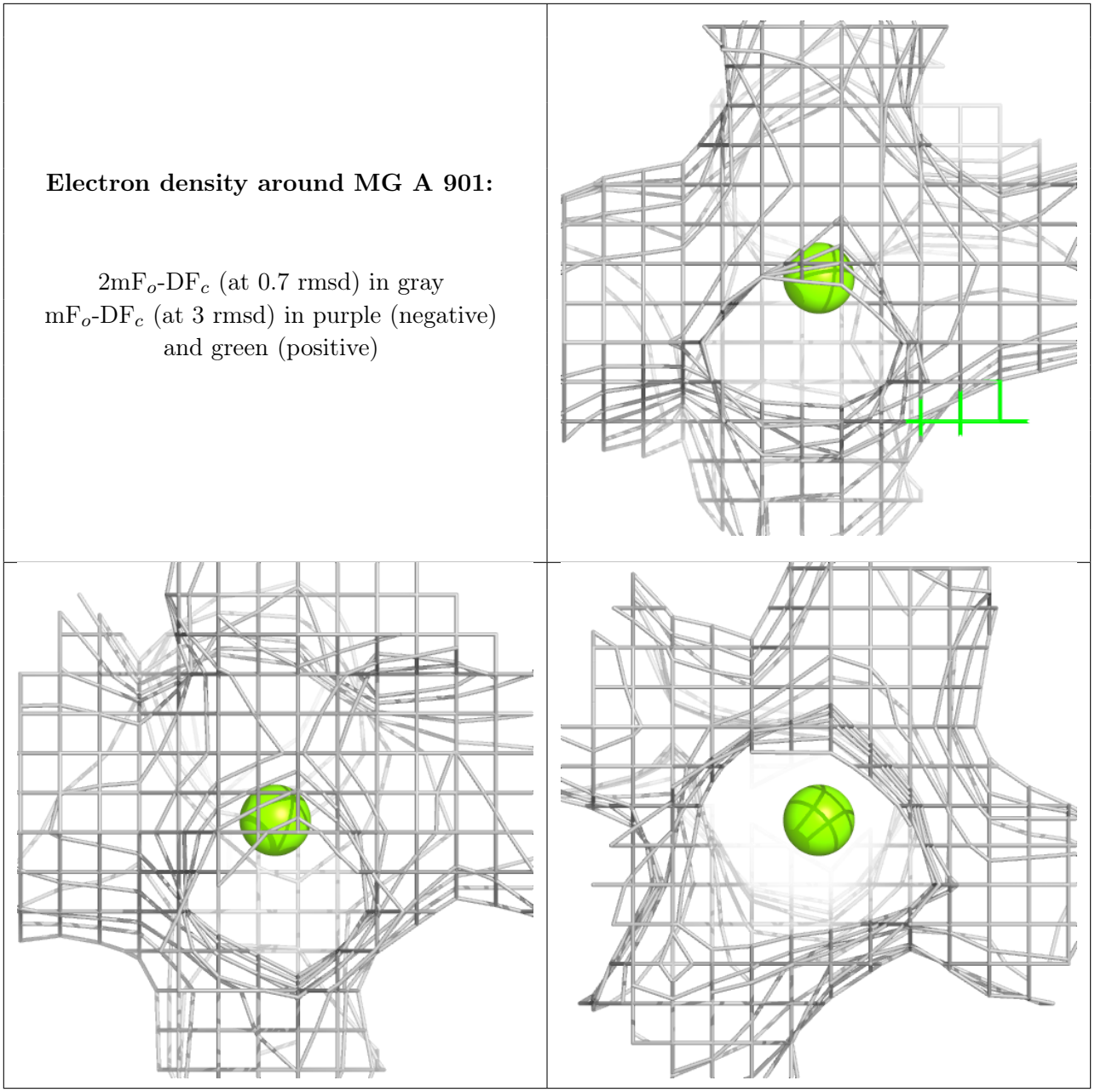
Electron density around MG B 901:

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



Electron density around MG A 901:

$2mF_o$-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.