Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2024 – 10:25 am BST

PDB ID	:	8QJ0
Title	:	Room-temperature Serial Synchrotron Crystallography structure of Spinacia oleracea RuBisCO
Authors	:	Bjelcic, M.; Neutze, R.; Aurelius, O.; Nan, J.; Ursby, T.
Deposited on	:	2023-09-12
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 ⓘ 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:

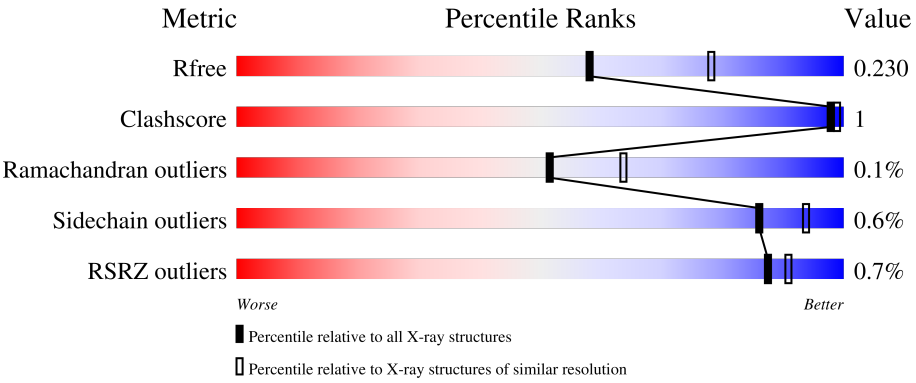
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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	S	123	97%
1	T	123	93% 7%
1	U	123	96%
1	V	123	2% 96%
2	L	475	% 87% 8%

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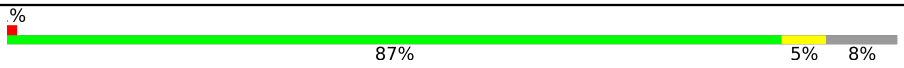
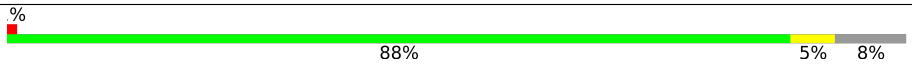
Mol	Chain	Length	Quality of chain
2	M	475	
2	N	475	
2	O	475	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 36264 atoms, of which 17380 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 Ribulose bisphosphate carboxylase small subunit, chloroplastic 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	S	123	Total	C	H	N	O	S	31	0	0
			2023	669	989	171	186	8			
1	T	123	Total	C	H	N	O	S	31	0	0
			2023	669	989	171	186	8			
1	U	123	Total	C	H	N	O	S	31	0	0
			2023	669	989	171	186	8			
1	V	123	Total	C	H	N	O	S	31	0	0
			2023	669	989	171	186	8			

- Molecule 2 is a protein called Ribulose bisphosphate carboxylase large chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	L	439	Total	C	H	N	O	S	109	0	0
			6786	2175	3351	606	637	17			
2	M	439	Total	C	H	N	O	S	109	0	0
			6786	2175	3351	606	637	17			
2	N	439	Total	C	H	N	O	S	107	0	0
			6799	2178	3360	607	637	17			
2	O	439	Total	C	H	N	O	S	107	0	0
			6802	2178	3362	608	637	17			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	1	Total	Mg	0	0
			1	1		
3	M	1	Total	Mg	0	0
			1	1		
3	N	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	O	1	Total Mg 1 1	0	0

- Molecule 4 is water.

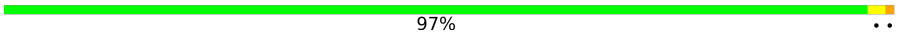
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	S	44	Total O 44 44	0	0
4	T	50	Total O 50 50	0	0
4	U	45	Total O 45 45	0	0
4	V	46	Total O 46 46	0	0
4	L	202	Total O 202 202	0	0
4	M	198	Total O 198 198	0	0
4	N	193	Total O 193 193	0	0
4	O	217	Total O 217 217	0	0

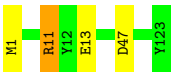
3 Residue-property plots (i)

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: Ribulose bisphosphate carboxylase small subunit, chloroplastic 2

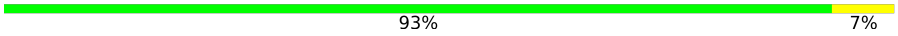
Chain S:

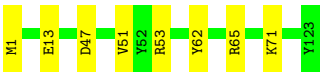




• Molecule 1: Ribulose bisphosphate carboxylase small subunit, chloroplastic 2

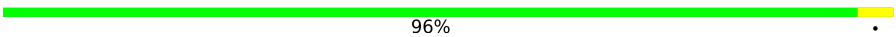
Chain T:

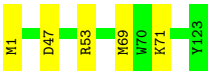




• Molecule 1: Ribulose bisphosphate carboxylase small subunit, chloroplastic 2

Chain U:



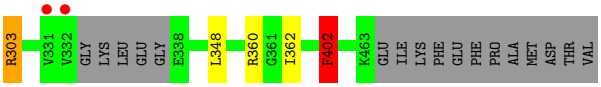


• Molecule 1: Ribulose bisphosphate carboxylase small subunit, chloroplastic 2

Chain V:

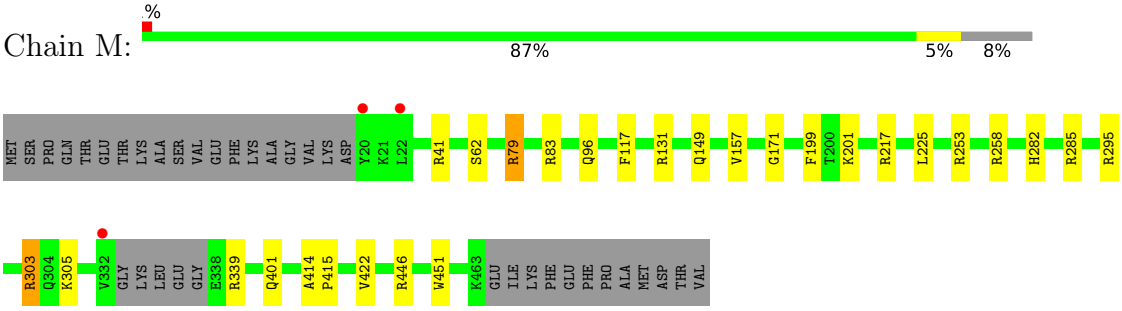
• Molecule 2: Ribulose bisphosphate carboxylase large chain

Chain L:



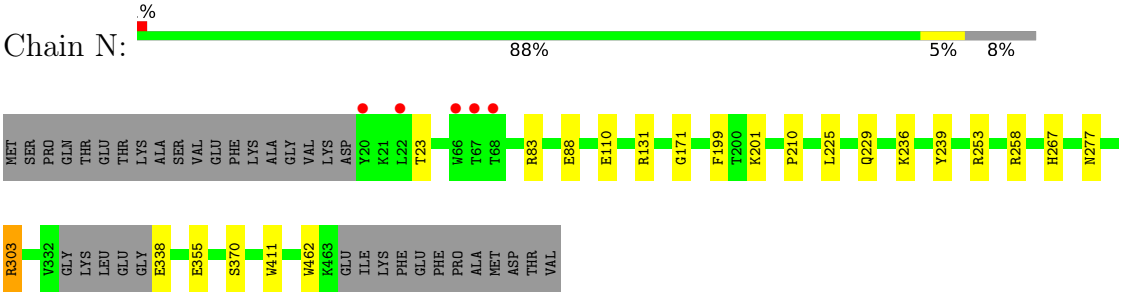
• Molecule 2: Ribulose bisphosphate carboxylase large chain

Chain M:



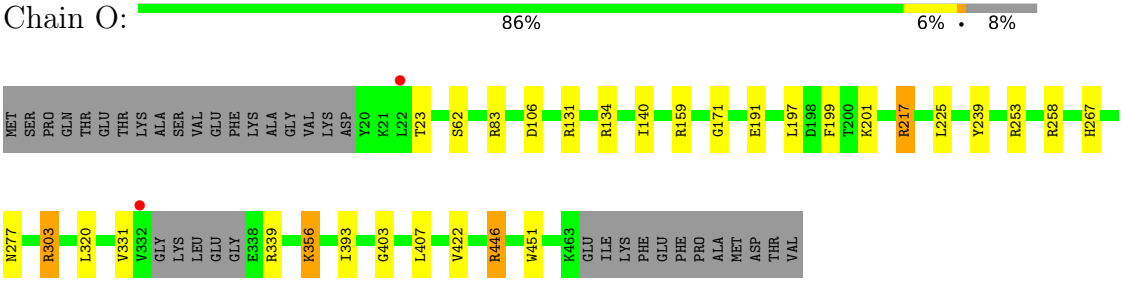
• Molecule 2: Ribulose bisphosphate carboxylase large chain

Chain N:



• Molecule 2: Ribulose bisphosphate carboxylase large chain

Chain O:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	158.60Å 157.12Å 202.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	97.78 – 2.30 97.78 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (97.78-2.30) 99.9 (97.78-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.74 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.181 , 0.227 0.190 , 0.230	Depositor DCC
R_{free} test set	5444 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å^2)	20.2	Xtriage
Anisotropy	0.278	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 42.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	36264	wwPDB-VP
Average B, all atoms (Å^2)	25.0	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 54.16 % 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 3.7999e-05. 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: KCX, MG

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	S	0.63	0/1069	1.07	4/1453 (0.3%)
1	T	0.61	0/1069	1.13	6/1453 (0.4%)
1	U	0.61	0/1069	1.08	3/1453 (0.2%)
1	V	0.64	0/1069	1.11	3/1453 (0.2%)
2	L	0.69	1/3507 (0.0%)	1.15	15/4763 (0.3%)
2	M	0.67	0/3507	1.09	11/4763 (0.2%)
2	N	0.70	1/3511 (0.0%)	1.13	10/4767 (0.2%)
2	O	0.69	0/3512	1.13	9/4767 (0.2%)
All	All	0.68	2/18313 (0.0%)	1.12	61/24872 (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	S	0	1
2	L	0	6
2	M	0	7
2	N	0	3
2	O	0	5
All	All	0	22

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	110	GLU	CD-OE2	5.46	1.31	1.25
2	L	223	GLU	CD-OE1	-5.31	1.19	1.25

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	360	ARG	NE-CZ-NH2	-12.85	113.88	120.30
2	N	253	ARG	NE-CZ-NH2	-10.33	115.13	120.30
2	L	266	MET	CG-SD-CE	9.64	115.63	100.20
2	O	134	ARG	NE-CZ-NH2	-9.36	115.62	120.30
2	L	360	ARG	NE-CZ-NH1	9.33	124.96	120.30
1	T	53	ARG	NE-CZ-NH2	-8.32	116.14	120.30
2	M	83	ARG	NE-CZ-NH2	-8.00	116.30	120.30
2	O	131	ARG	NE-CZ-NH2	7.97	124.28	120.30
1	T	65	ARG	NE-CZ-NH2	-7.92	116.34	120.30
2	N	303	ARG	NE-CZ-NH2	-7.90	116.35	120.30
2	N	83	ARG	NE-CZ-NH2	-7.77	116.41	120.30
2	M	303	ARG	NE-CZ-NH1	-7.53	116.54	120.30
2	N	303	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	S	47	ASP	CB-CA-C	6.83	124.05	110.40
1	V	65	ARG	NE-CZ-NH2	-6.76	116.92	120.30
2	L	131	ARG	NE-CZ-NH1	6.71	123.66	120.30
2	L	253	ARG	NE-CZ-NH2	-6.56	117.02	120.30
2	O	83	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	S	11	ARG	NE-CZ-NH2	-6.45	117.07	120.30
2	O	253	ARG	NE-CZ-NH2	-6.30	117.15	120.30
2	M	225	LEU	CB-CG-CD1	-6.22	100.42	111.00
2	L	258	ARG	NE-CZ-NH1	-6.21	117.19	120.30
1	V	47	ASP	CB-CA-C	6.21	122.82	110.40
2	L	303	ARG	NE-CZ-NH1	6.21	123.41	120.30
2	L	402	PHE	CB-CA-C	6.17	122.73	110.40
1	T	13	GLU	CB-CA-C	6.12	122.63	110.40
1	T	47	ASP	CB-CA-C	6.11	122.62	110.40
2	L	83	ARG	NE-CZ-NH2	-6.08	117.26	120.30
2	N	131	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	T	1	MET	CG-SD-CE	6.01	109.81	100.20
2	M	285	ARG	NE-CZ-NH2	5.97	123.28	120.30
1	U	53	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	S	1	MET	CG-SD-CE	5.90	109.64	100.20
1	V	13	GLU	CB-CA-C	5.74	121.89	110.40
2	L	303	ARG	NE-CZ-NH2	-5.74	117.43	120.30
2	O	239	TYR	CB-CG-CD2	-5.70	117.58	121.00
1	S	13	GLU	CB-CA-C	5.69	121.78	110.40
2	L	239	TYR	CB-CG-CD2	-5.65	117.61	121.00
2	O	303	ARG	CD-NE-CZ	5.64	131.50	123.60
1	T	71	LYS	CB-CA-C	5.60	121.59	110.40
2	N	239	TYR	CB-CG-CD1	5.52	124.31	121.00
2	L	239	TYR	CB-CG-CD1	5.47	124.28	121.00
1	U	71	LYS	CB-CA-C	5.45	121.31	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	N	253	ARG	NH1-CZ-NH2	5.42	125.36	119.40
2	M	225	LEU	CB-CG-CD2	5.41	120.20	111.00
2	O	217	ARG	NE-CZ-NH1	5.38	122.99	120.30
2	N	225	LEU	CB-CG-CD1	-5.37	101.86	111.00
2	L	225	LEU	CB-CG-CD1	-5.32	101.96	111.00
2	M	117	PHE	CB-CG-CD1	5.31	124.52	120.80
2	M	83	ARG	NE-CZ-NH1	5.29	122.94	120.30
2	O	356	LYS	CA-CB-CG	5.28	125.03	113.40
2	L	187	ARG	NE-CZ-NH1	5.28	122.94	120.30
2	N	88	GLU	N-CA-CB	5.27	120.08	110.60
2	M	131	ARG	CA-CB-CG	5.22	124.88	113.40
2	M	79	ARG	NE-CZ-NH1	-5.21	117.69	120.30
2	M	303	ARG	NE-CZ-NH2	5.20	122.90	120.30
1	U	47	ASP	CB-CA-C	5.18	120.76	110.40
2	N	225	LEU	CB-CG-CD2	5.17	119.78	111.00
2	L	258	ARG	CD-NE-CZ	5.14	130.80	123.60
2	O	339	ARG	CG-CD-NE	5.04	122.39	111.80
2	M	253	ARG	NE-CZ-NH2	-5.02	117.79	120.30

There are no chirality outliers.

All (22) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	L	187	ARG	Sidechain
2	L	217	ARG	Sidechain
2	L	258	ARG	Sidechain
2	L	303	ARG	Sidechain
2	L	402	PHE	Mainchain
2	L	79	ARG	Sidechain
2	M	217	ARG	Sidechain
2	M	258	ARG	Sidechain
2	M	295	ARG	Sidechain
2	M	303	ARG	Sidechain
2	M	339	ARG	Sidechain
2	M	446	ARG	Sidechain
2	M	79	ARG	Sidechain
2	N	258	ARG	Sidechain
2	N	303	ARG	Sidechain
2	N	462	TRP	Peptide
2	O	159	ARG	Sidechain
2	O	217	ARG	Sidechain
2	O	258	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	O	303	ARG	Sidechain
2	O	446	ARG	Sidechain
1	S	11	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	S	1034	989	986	0	0
1	T	1034	989	986	1	0
1	U	1034	989	986	2	0
1	V	1034	989	986	1	0
2	L	3435	3351	3330	4	0
2	M	3435	3351	3330	6	0
2	N	3439	3360	3341	4	1
2	O	3440	3362	3343	8	1
3	L	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
3	O	1	0	0	0	0
4	L	202	0	0	0	0
4	M	198	0	0	0	0
4	N	193	0	0	1	0
4	O	217	0	0	2	0
4	S	44	0	0	0	0
4	T	50	0	0	0	0
4	U	45	0	0	0	0
4	V	46	0	0	0	0
All	All	18884	17380	17288	24	1

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 1.

All (24) 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)
2:O:407:LEU:HD22	4:O:774:HOH:O	2.07	0.54
2:N:229:GLN:HE21	2:N:236:LYS:H	1.55	0.54
2:O:197:LEU:HD23	4:O:709:HOH:O	2.09	0.52
2:O:331:VAL:HG11	2:O:393:ILE:HD13	1.92	0.51
2:O:140:ILE:HD13	2:O:320:LEU:HD11	1.95	0.49
2:M:41:ARG:HH11	2:M:96:GLN:NE2	2.11	0.48
2:L:348:LEU:HD11	2:L:362:ILE:HD12	1.96	0.47
2:M:149:GLN:HE22	2:M:282:HIS:HA	1.79	0.47
2:L:172:CYS:HA	2:L:402:PHE:O	2.15	0.46
2:L:171:GLY:HA2	2:L:199:PHE:O	2.16	0.46
2:M:157:VAL:HG13	4:N:773:HOH:O	2.16	0.45
2:M:171:GLY:HA2	2:M:199:PHE:O	2.17	0.44
2:N:171:GLY:HA2	2:N:199:PHE:O	2.17	0.44
1:V:51:VAL:HG13	1:V:62:TYR:HB3	1.99	0.44
1:T:51:VAL:HG13	1:T:62:TYR:HB3	1.98	0.44
1:U:69:MET:HE3	2:O:191:GLU:HG3	2.01	0.43
1:U:1:MET:HE3	2:N:411:TRP:HA	2.00	0.42
2:L:267:HIS:HD2	2:L:277:ASN:OD1	2.02	0.42
2:O:171:GLY:HA2	2:O:199:PHE:O	2.19	0.41
2:N:267:HIS:HD2	2:N:277:ASN:OD1	2.04	0.41
2:M:414:ALA:HB3	2:M:415:PRO:HD3	2.03	0.40
2:M:422:VAL:HG13	2:M:451:TRP:CH2	2.56	0.40
2:O:267:HIS:HD2	2:O:277:ASN:OD1	2.04	0.40
2:O:422:VAL:HG13	2:O:451:TRP:CH2	2.57	0.40

All (1) 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)
2:N:370:SER:HG	2:O:106:ASP:OD2[4_555]	1.55	0.05

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	S	121/123 (98%)	114 (94%)	7 (6%)	0	100	100
1	T	121/123 (98%)	114 (94%)	7 (6%)	0	100	100
1	U	121/123 (98%)	115 (95%)	6 (5%)	0	100	100
1	V	121/123 (98%)	115 (95%)	6 (5%)	0	100	100
2	L	434/475 (91%)	423 (98%)	11 (2%)	0	100	100
2	M	434/475 (91%)	424 (98%)	9 (2%)	1 (0%)	47	58
2	N	434/475 (91%)	423 (98%)	11 (2%)	0	100	100
2	O	434/475 (91%)	424 (98%)	8 (2%)	2 (0%)	29	35
All	All	2220/2392 (93%)	2152 (97%)	65 (3%)	3 (0%)	51	64

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	62	SER
2	O	62	SER
2	O	403	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	S	112/112 (100%)	112 (100%)	0	100	100
1	T	112/112 (100%)	112 (100%)	0	100	100
1	U	112/112 (100%)	112 (100%)	0	100	100
1	V	112/112 (100%)	112 (100%)	0	100	100
2	L	354/386 (92%)	352 (99%)	2 (1%)	86	94
2	M	354/386 (92%)	352 (99%)	2 (1%)	86	94
2	N	355/386 (92%)	351 (99%)	4 (1%)	73	86
2	O	355/386 (92%)	351 (99%)	4 (1%)	73	86
All	All	1866/1992 (94%)	1854 (99%)	12 (1%)	86	94

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	23	THR
2	L	178	LEU
2	M	305	LYS
2	M	401	GLN
2	N	23	THR
2	N	210	PRO
2	N	338	GLU
2	N	355	GLU
2	O	23	THR
2	O	225	LEU
2	O	356	LYS
2	O	446	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	T	56	HIS
1	U	57	ASN
1	V	36	ASN
2	L	115	ASN
2	L	153	HIS
2	L	238	HIS
2	L	267	HIS
2	L	292	HIS
2	L	298	HIS
2	L	327	HIS
2	L	386	HIS
2	M	96	GLN
2	M	115	ASN
2	M	149	GLN
2	M	153	HIS
2	M	238	HIS
2	M	267	HIS
2	M	292	HIS
2	M	298	HIS
2	M	327	HIS
2	M	386	HIS
2	M	401	GLN
2	N	115	ASN
2	N	229	GLN
2	N	267	HIS

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Mol	Chain	Res	Type
2	N	292	HIS
2	N	298	HIS
2	N	327	HIS
2	N	386	HIS
2	O	115	ASN
2	O	238	HIS
2	O	267	HIS
2	O	292	HIS
2	O	298	HIS
2	O	304	GLN
2	O	327	HIS
2	O	386	HIS

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	$\#\|Z\| > 2$
2	KCX	M	201	2,3	9,11,12	1.71	1 (11%)	5,12,14	2.75	2 (40%)
2	KCX	N	201	2,3	9,11,12	1.74	1 (11%)	5,12,14	4.45	3 (60%)
2	KCX	L	201	2,3	9,11,12	1.53	1 (11%)	5,12,14	4.37	3 (60%)
2	KCX	O	201	2,3	9,11,12	1.63	1 (11%)	5,12,14	2.22	3 (60%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	KCX	M	201	2,3	-	0/9/10/12	-
2	KCX	N	201	2,3	-	0/9/10/12	-
2	KCX	L	201	2,3	-	0/9/10/12	-
2	KCX	O	201	2,3	-	0/9/10/12	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	201	KCX	CX-NZ	4.86	1.43	1.35
2	M	201	KCX	CX-NZ	4.58	1.43	1.35
2	O	201	KCX	CX-NZ	4.30	1.42	1.35
2	L	201	KCX	CX-NZ	3.98	1.42	1.35

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	N	201	KCX	OQ1-CX-NZ	8.18	137.63	124.96
2	L	201	KCX	OQ1-CX-NZ	7.94	137.27	124.96
2	N	201	KCX	CE-NZ-CX	-5.10	113.70	121.89
2	L	201	KCX	CE-NZ-CX	-5.01	113.85	121.89
2	M	201	KCX	OQ1-CX-NZ	4.82	132.43	124.96
2	O	201	KCX	CE-NZ-CX	-3.77	115.84	121.89
2	M	201	KCX	CE-NZ-CX	-3.05	116.99	121.89
2	L	201	KCX	CG-CD-CE	-2.32	102.58	113.56
2	O	201	KCX	OQ1-CX-NZ	2.13	128.26	124.96
2	N	201	KCX	CG-CD-CE	-2.08	103.69	113.56
2	O	201	KCX	CG-CD-CE	-2.05	103.86	113.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides 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, 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	S	123/123 (100%)	-0.32	0 100 100	13, 28, 53, 77	0
1	T	123/123 (100%)	-0.36	0 100 100	16, 27, 55, 80	0
1	U	123/123 (100%)	-0.18	0 100 100	14, 29, 53, 76	0
1	V	123/123 (100%)	-0.22	2 (1%) 72 77	12, 30, 58, 78	0
2	L	438/475 (92%)	-0.44	4 (0%) 84 88	9, 18, 51, 101	0
2	M	438/475 (92%)	-0.47	3 (0%) 87 91	9, 18, 49, 104	0
2	N	438/475 (92%)	-0.42	5 (1%) 80 85	9, 18, 49, 90	0
2	O	438/475 (92%)	-0.38	2 (0%) 91 94	10, 19, 50, 91	0
All	All	2244/2392 (93%)	-0.40	16 (0%) 87 91	9, 21, 53, 104	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	22	LEU	5.7
2	N	22	LEU	4.7
2	O	22	LEU	4.2
2	N	66	TRP	4.1
2	M	332	VAL	4.0
2	M	22	LEU	3.7
2	N	20	TYR	3.2
2	L	332	VAL	3.2
1	V	123	TYR	3.2
2	M	20	TYR	2.9
2	O	332	VAL	2.7
2	L	331	VAL	2.6
1	V	37	LYS	2.2
2	N	67	THR	2.1
2	N	68	THR	2.0
2	L	66	TRP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
2	KCX	L	201	12/13	0.95	0.11	11,19,19,23	0
2	KCX	N	201	12/13	0.96	0.13	12,18,20,21	0
2	KCX	O	201	12/13	0.96	0.11	12,16,20,21	0
2	KCX	M	201	12/13	0.97	0.11	12,16,19,19	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

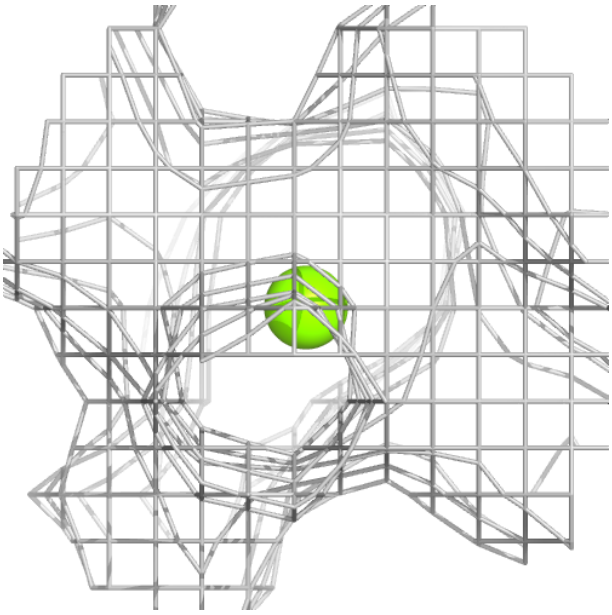
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

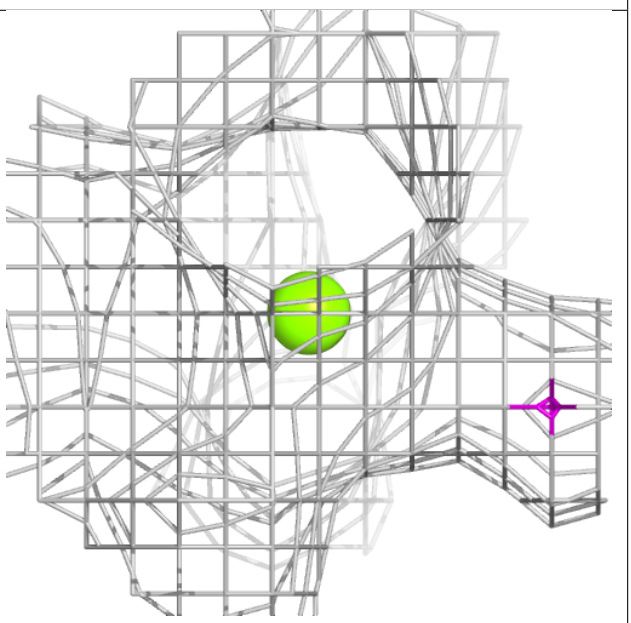
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	L	501	1/1	0.96	0.05	17,17,17,17	0
3	MG	M	501	1/1	0.97	0.04	18,18,18,18	0
3	MG	N	501	1/1	0.98	0.04	16,16,16,16	0
3	MG	O	501	1/1	0.98	0.06	20,20,20,20	0

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 MG L 501:

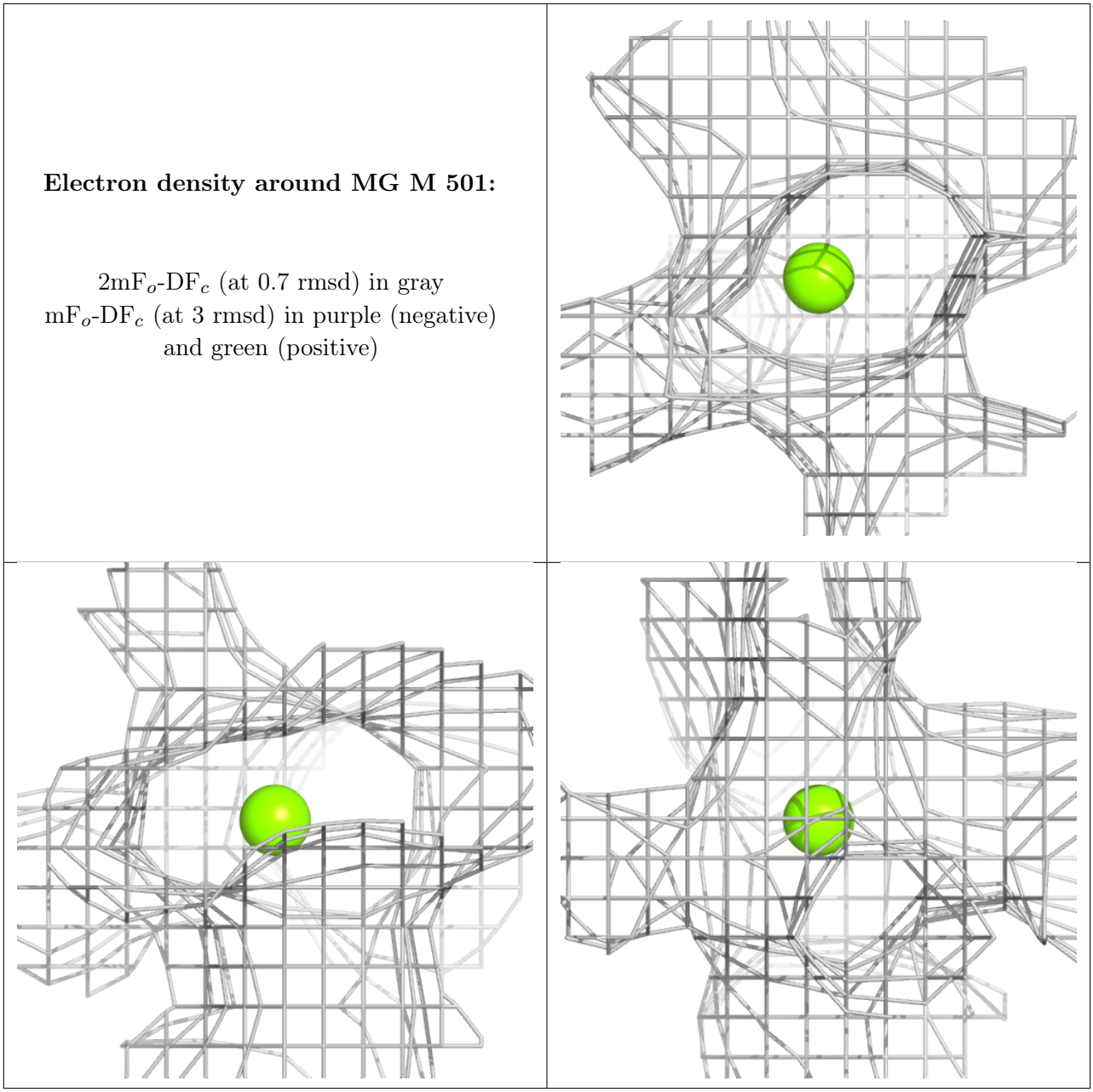
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





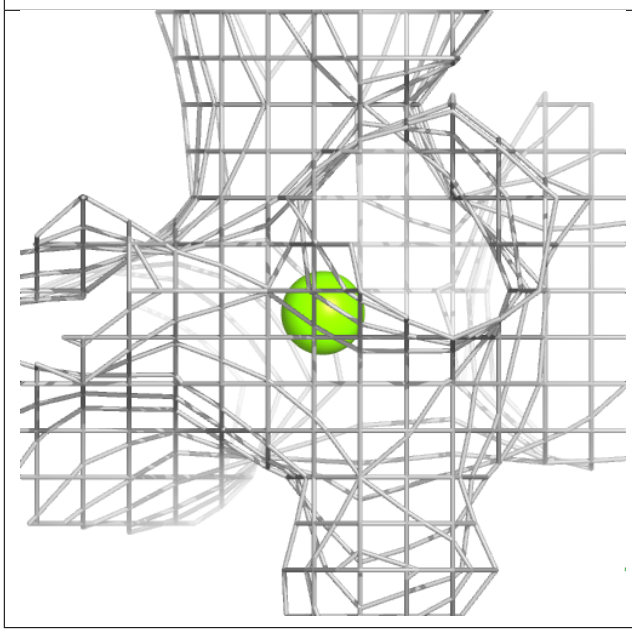
Electron density around MG M 501:

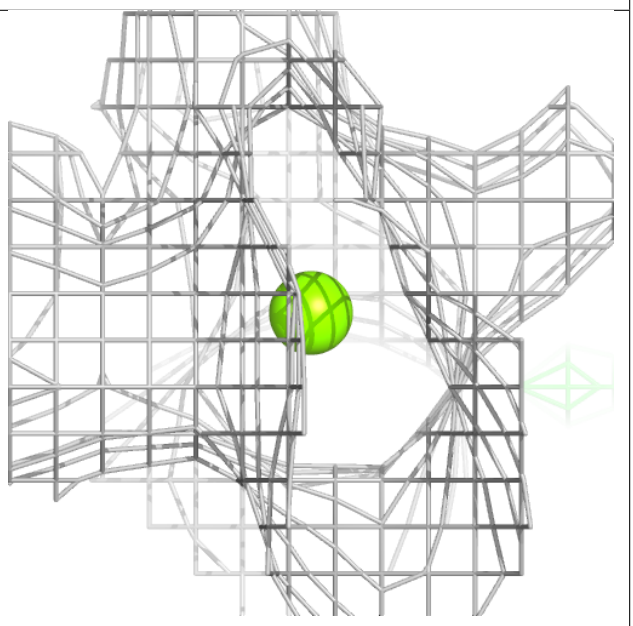
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around MG N 501:

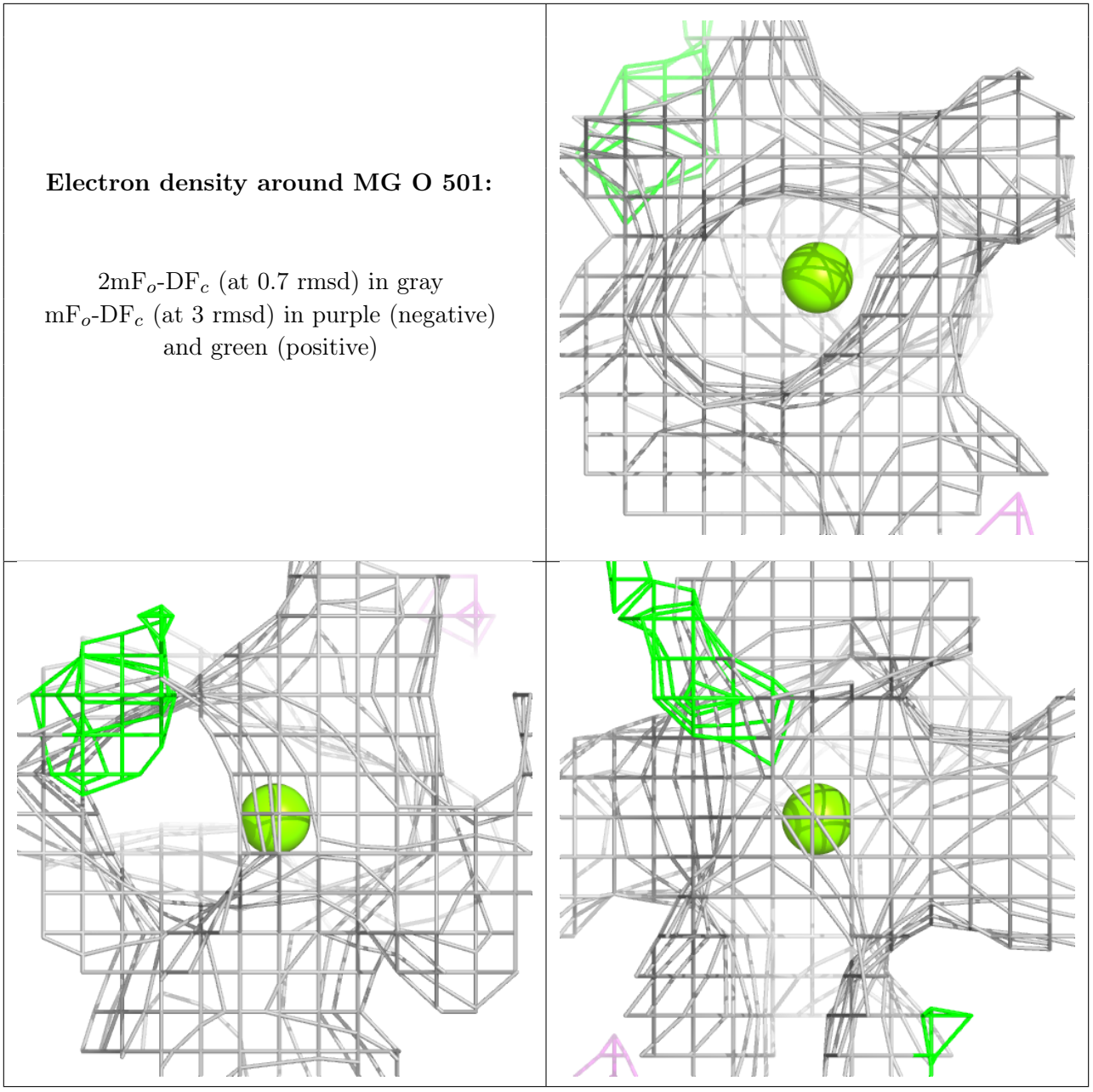
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





Electron density around MG O 501:

$2mF_o$-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.