wwPDB X-ray Structure Validation Summary Report (i)

Feb 15, 2021 – 03:13 PM GMT

PDB ID	:	6Y1R
Title	:	Nb22-LBT
Authors	:	Pompidor, G.; Zimmermann, S.; Loew, C.; Schneider, T.
Deposited on	:	2020-02-13
Resolution	:	1.85 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 following versions of software and data (see references (1)) were used in the production of this report:

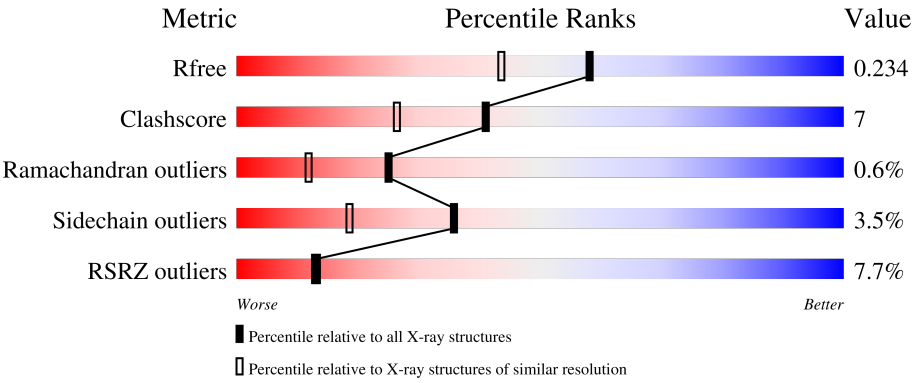
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.17
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.17

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 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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	147	3% 88% 7%
1	B	147	6% 70% 16% 12%
1	C	147	10% 84% 10%
1	D	147	5% 86% 9% 5%
1	E	147	12% 73% 16% 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	C	204	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10521 atoms, of which 4933 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.

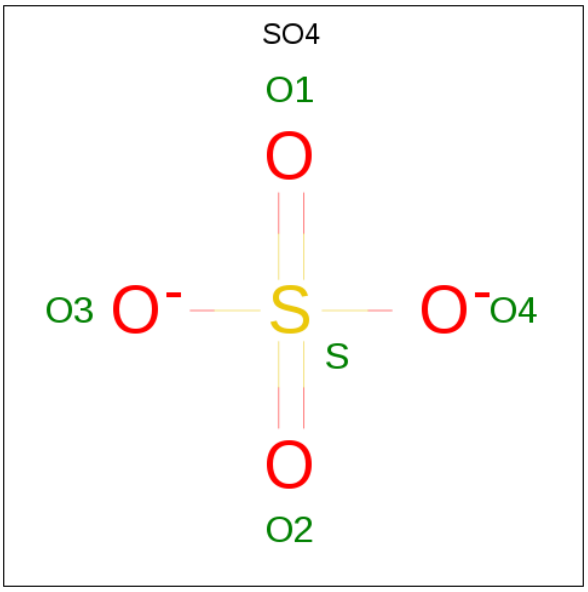
- Molecule 1 is a protein called Nb22-LBT.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	141	Total	C	H	N	O	S	0	2	0
			2103	668	1023	191	215	6			
1	B	129	Total	C	H	N	O	S	0	2	0
			1922	612	932	173	199	6			
1	C	141	Total	C	H	N	O	S	0	3	0
			2121	672	1035	193	215	6			
1	D	139	Total	C	H	N	O	S	0	1	0
			2052	652	995	189	211	5			
1	E	135	Total	C	H	N	O	S	0	2	0
			1968	628	948	176	210	6			

- Molecule 2 is TERBIUM(III) ION (three-letter code: TB) (formula: Tb) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Tb	0	0
			2	2		
2	B	1	Total	Tb	0	0
			1	1		
2	C	3	Total	Tb	0	0
			3	3		
2	D	1	Total	Tb	0	0
			1	1		
2	E	2	Total	Tb	0	0
			2	2		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0

- Molecule 4 is water.

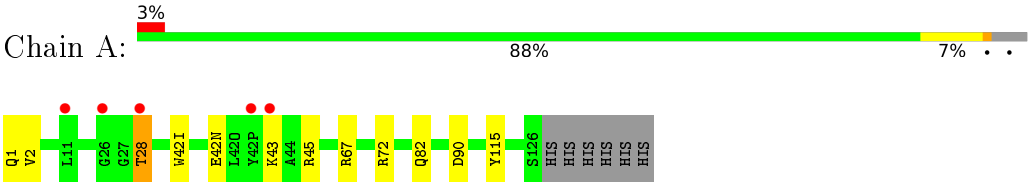
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	74	Total O 74 74	0	0
4	B	53	Total O 53 53	0	0
4	C	62	Total O 62 62	0	0
4	D	63	Total O 63 63	0	0
4	E	64	Total O 64 64	0	0

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.

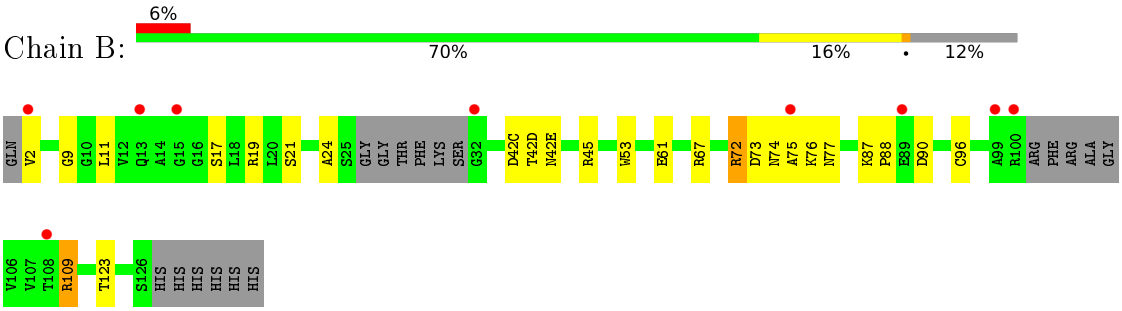
- Molecule 1: Nb22-LBT

Chain A:



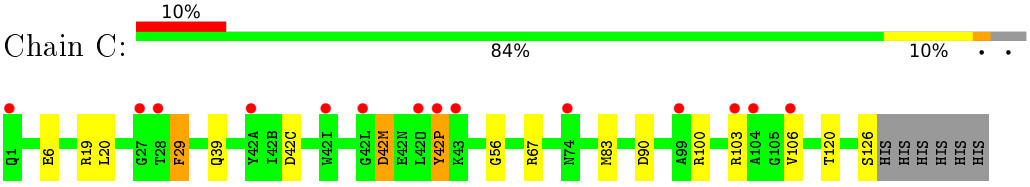
- Molecule 1: Nb22-LBT

Chain B:



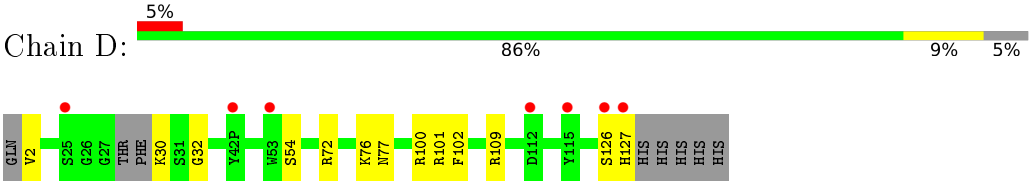
- Molecule 1: Nb22-LBT

Chain C:



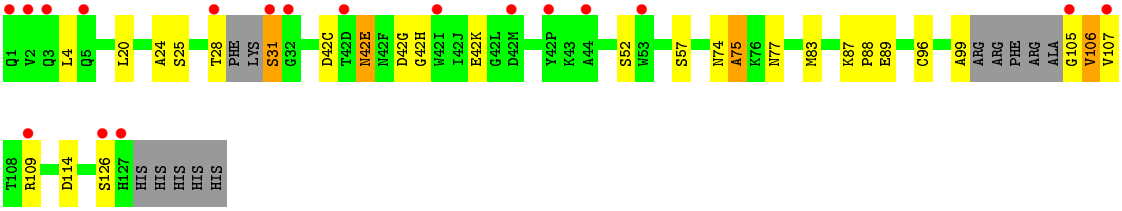
- Molecule 1: Nb22-LBT

Chain D:



- Molecule 1: Nb22-LBT

Chain E:


Q1
V2
Q3
L4
Q5
L20
A24
S25
T28
PHE
LYS
S31
G32
D42C
T42D
N42E
N42F
D42G
G42H
W42I
I42J
E42K
G42L
D42M
Y42P
K43
A44
S52
W53
S57
N74
A75
K76
N77
M83
K87
P88
E89
C96
A99
ARG
ARG
PHE
ARG
ALA
G105
V106
V107
T108
R109
D114
S126
H127
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	45.47Å 49.42Å 81.35Å 91.71° 99.18° 102.61°	Depositor
Resolution (Å)	80.13 – 1.85 80.13 – 1.73	Depositor EDS
% Data completeness (in resolution range)	93.2 (80.13-1.85) 90.0 (80.13-1.73)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.00 (at 1.73Å)	Xtriage
Refinement program	PHENIX 1.16-3549	Depositor
R, R_{free}	0.204 , 0.234 0.204 , 0.234	Depositor DCC
R_{free} test set	3235 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	26.3	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 50.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10521	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.97% 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: SO4, TB

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	0.44	1/1106 (0.1%)	0.66	0/1491
1	B	0.35	0/1012	0.56	0/1364
1	C	0.39	0/1115	0.62	0/1503
1	D	0.44	0/1079	0.63	0/1453
1	E	0.49	0/1043	0.67	0/1407
All	All	0.43	1/5355 (0.0%)	0.63	0/7218

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	28	THR	C-O	-5.24	1.13	1.23

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	1080	1023	1023	8	0
1	B	990	932	932	20	0
1	C	1086	1035	1035	13	0
1	D	1057	995	994	10	0
1	E	1020	948	948	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	2	0	0	0	0
2	B	1	0	0	0	0
2	C	3	0	0	0	0
2	D	1	0	0	0	0
2	E	2	0	0	0	0
3	B	5	0	0	0	0
3	C	10	0	0	2	0
3	D	10	0	0	1	0
3	E	5	0	0	0	0
4	A	74	0	0	4	1
4	B	53	0	0	8	0
4	C	62	0	0	3	0
4	D	63	0	0	2	0
4	E	64	0	0	8	1
All	All	5588	4933	4932	72	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 7.

The worst 5 of 72 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:E:109:ARG:NH1	4:E:301:HOH:O	1.91	1.02
1:B:76:LYS:NZ	4:B:302:HOH:O	2.04	0.89
1:A:82[B]:GLN:OE1	4:A:301:HOH:O	1.91	0.88
1:E:114:ASP:OD1	4:E:302:HOH:O	1.96	0.83
1:D:54:SER:OG	3:D:203:SO4:O1	1.95	0.83

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)
4:A:360:HOH:O	4:E:352:HOH:O[1_666]	2.18	0.02

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	141/147 (96%)	135 (96%)	6 (4%)	0	100 100
1	B	125/147 (85%)	121 (97%)	4 (3%)	0	100 100
1	C	142/147 (97%)	137 (96%)	5 (4%)	0	100 100
1	D	136/147 (92%)	133 (98%)	3 (2%)	0	100 100
1	E	131/147 (89%)	120 (92%)	7 (5%)	4 (3%)	4 0
All	All	675/735 (92%)	646 (96%)	25 (4%)	4 (1%)	25 12

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	25	SER
1	E	42(E)	ASN
1	E	75	ALA
1	E	106	VAL

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	109/113 (96%)	106 (97%)	3 (3%)	43 27
1	B	101/113 (89%)	93 (92%)	8 (8%)	12 2
1	C	110/113 (97%)	104 (94%)	6 (6%)	21 7
1	D	106/113 (94%)	104 (98%)	2 (2%)	57 43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	104/113 (92%)	103 (99%)	1 (1%)	76 69
All	All	530/565 (94%)	510 (96%)	20 (4%)	36 16

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	42(M)	ASP
1	D	100	ARG
1	E	31	SER
1	D	109	ARG
1	B	72	ARG

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)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 9 are monoatomic - leaving 6 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	SO4	C	204	-	4,4,4	0.14	0	6,6,6	0.14	0
3	SO4	C	203	-	4,4,4	0.14	0	6,6,6	0.22	0
3	SO4	B	202	-	4,4,4	0.16	0	6,6,6	0.22	0
3	SO4	E	203	-	4,4,4	0.17	0	6,6,6	0.18	0
3	SO4	D	202	-	4,4,4	0.16	0	6,6,6	0.18	0
3	SO4	D	203	-	4,4,4	0.16	0	6,6,6	0.07	0

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.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	204	SO4	2	0
3	D	203	SO4	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	A	141/147 (95%)	0.09	5 (3%) 44 41	16, 29, 48, 75	0
1	B	129/147 (87%)	0.32	9 (6%) 16 15	22, 39, 61, 79	0
1	C	141/147 (95%)	0.46	14 (9%) 7 7	16, 30, 63, 78	0
1	D	139/147 (94%)	0.19	7 (5%) 28 27	20, 32, 62, 85	0
1	E	135/147 (91%)	0.65	18 (13%) 3 3	19, 37, 66, 78	0
All	All	685/735 (93%)	0.34	53 (7%) 13 13	16, 33, 64, 85	0

The worst 5 of 53 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	42(P)	TYR	8.1
1	E	31	SER	6.9
1	E	127	HIS	5.8
1	A	42(P)	TYR	5.2
1	E	42(D)	THR	5.1

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

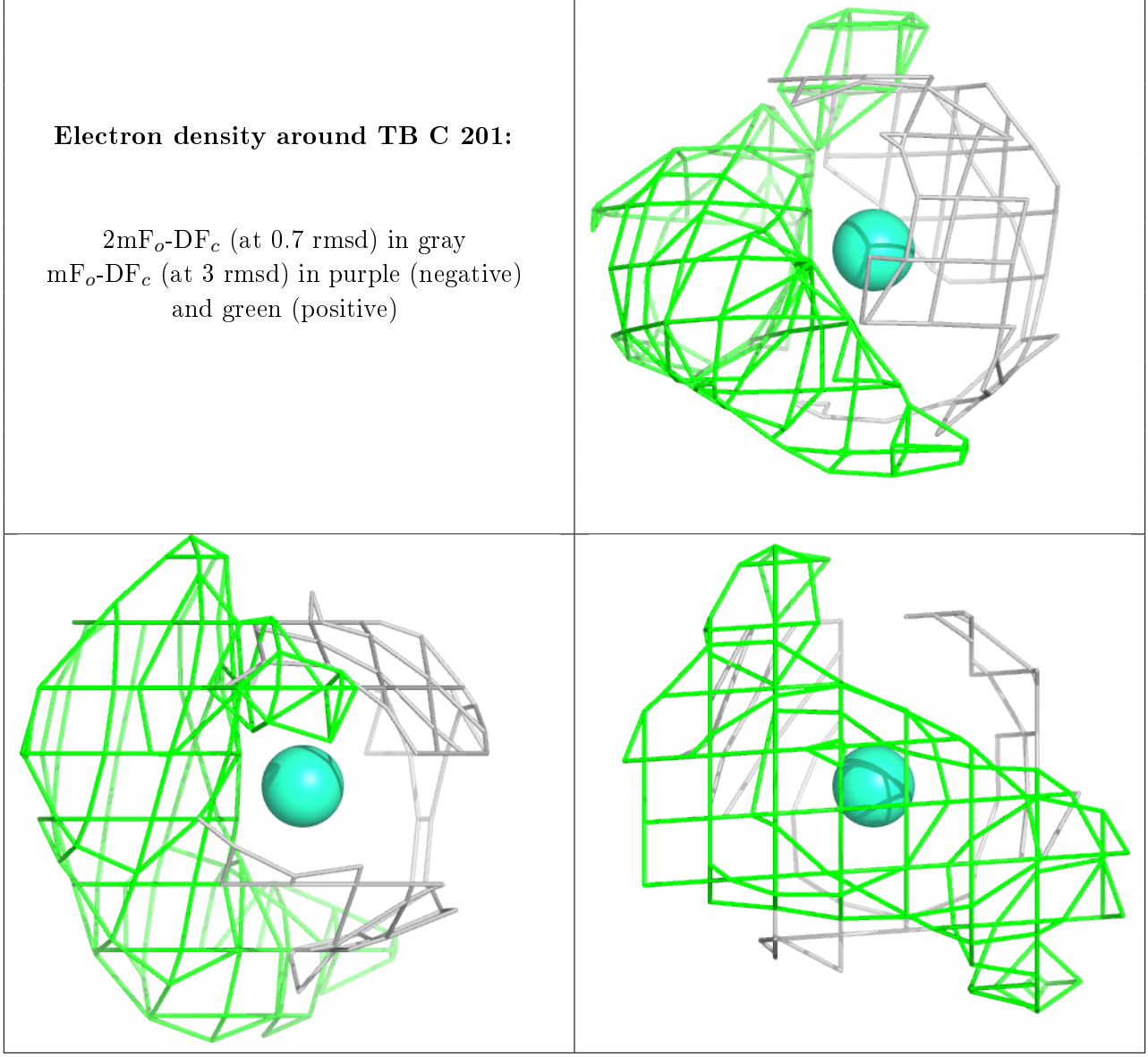
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	C	204	5/5	0.91	0.12	42,46,47,50	5
3	SO4	C	203	5/5	0.93	0.13	42,43,47,49	0
3	SO4	D	203	5/5	0.93	0.10	47,48,49,50	5
3	SO4	E	203	5/5	0.94	0.13	43,43,45,45	5
3	SO4	B	202	5/5	0.97	0.10	36,38,39,43	5
3	SO4	D	202	5/5	0.97	0.11	37,41,42,45	5
2	TB	C	201	1/1	0.99	0.15	40,40,40,40	1
2	TB	C	202	1/1	0.99	0.10	40,40,40,40	1
2	TB	E	201	1/1	0.99	0.11	36,36,36,36	1
2	TB	E	202	1/1	0.99	0.09	34,34,34,34	1
2	TB	B	201	1/1	0.99	0.15	40,40,40,40	1
2	TB	A	202	1/1	1.00	0.14	28,28,28,28	1
2	TB	A	201	1/1	1.00	0.16	28,28,28,28	1
2	TB	C	205	1/1	1.00	0.14	33,33,33,33	1
2	TB	D	201	1/1	1.00	0.13	32,32,32,32	1

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.

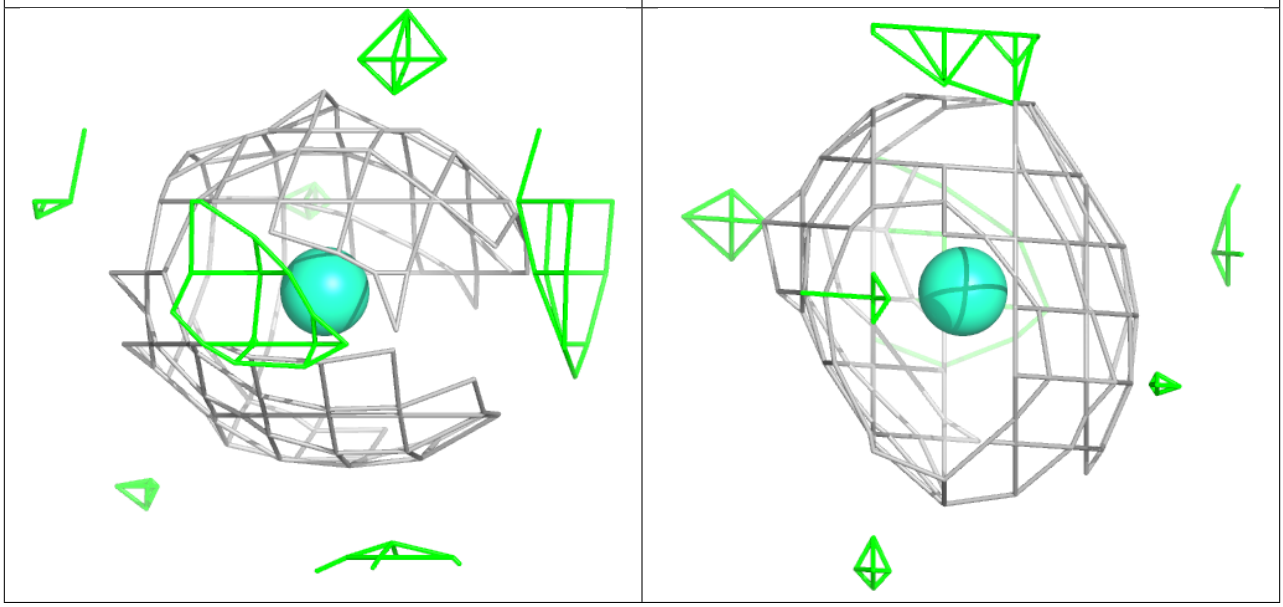
Electron density around TB C 201:

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



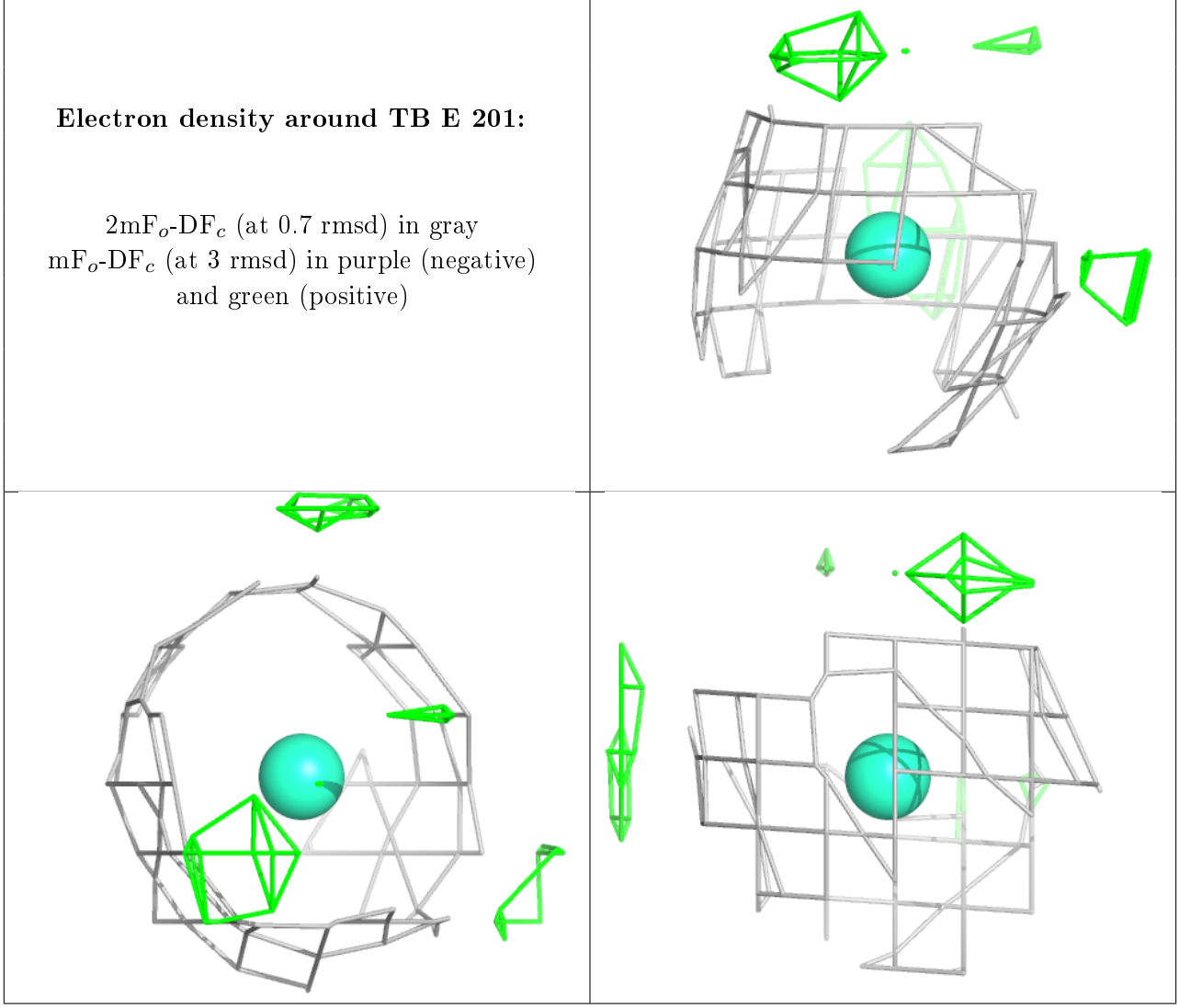
Electron density around TB C 202:

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



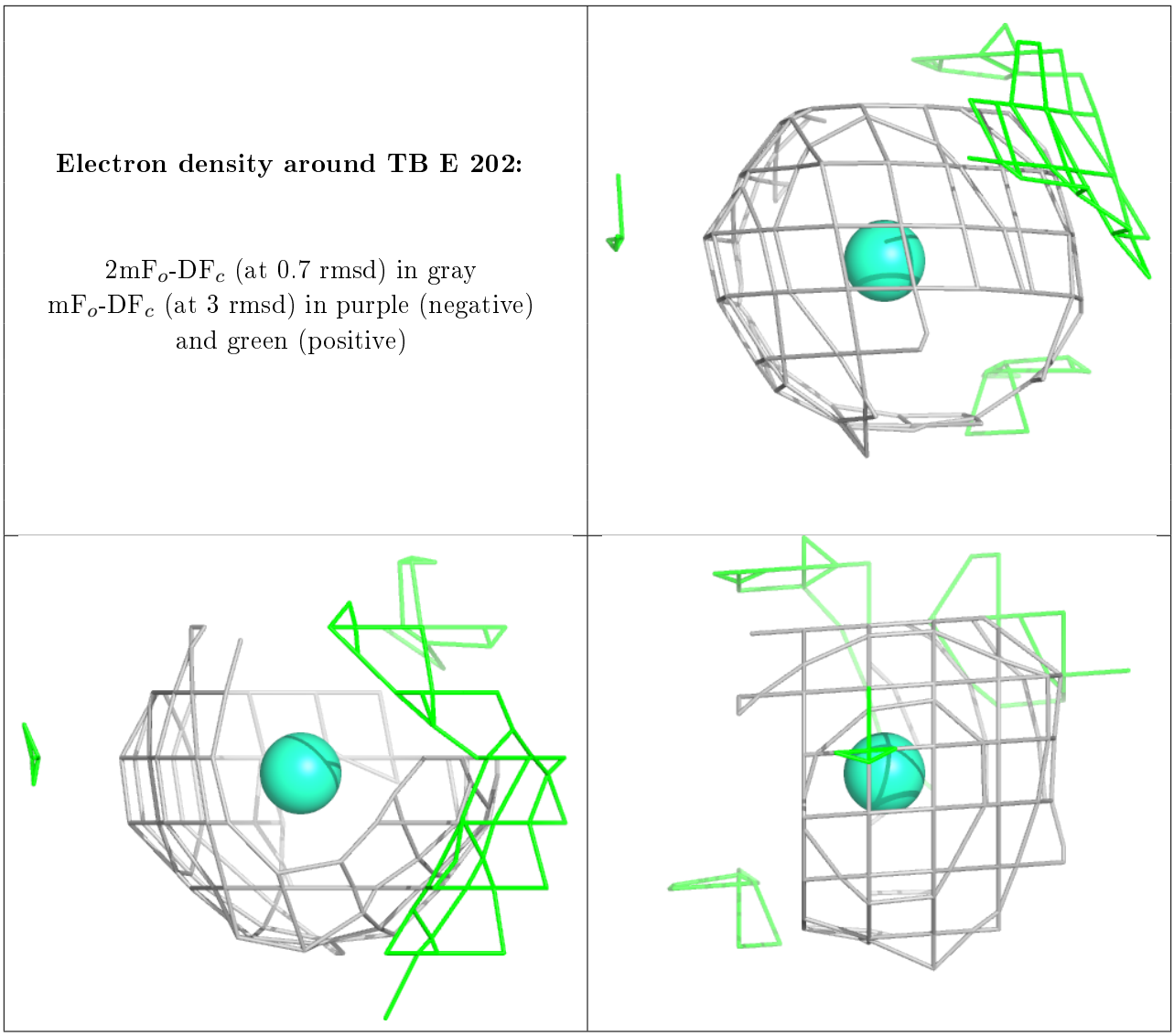
Electron density around TB E 201:

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



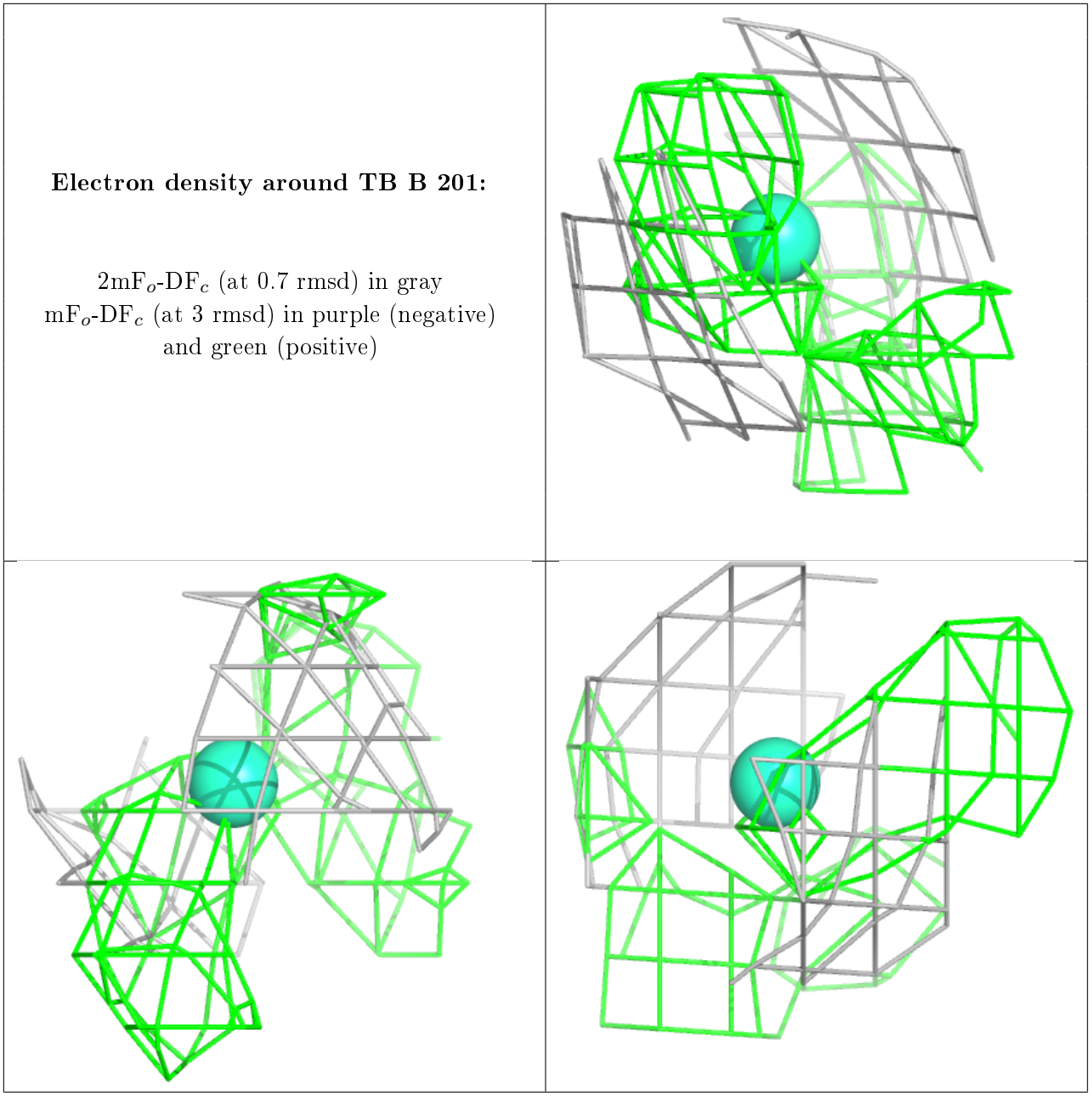
Electron density around TB E 202:

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



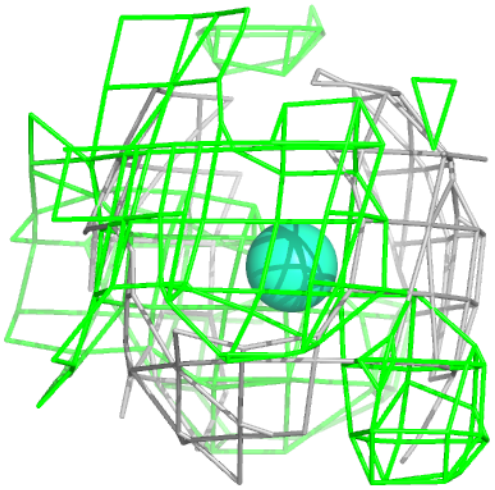
Electron density around TB B 201:

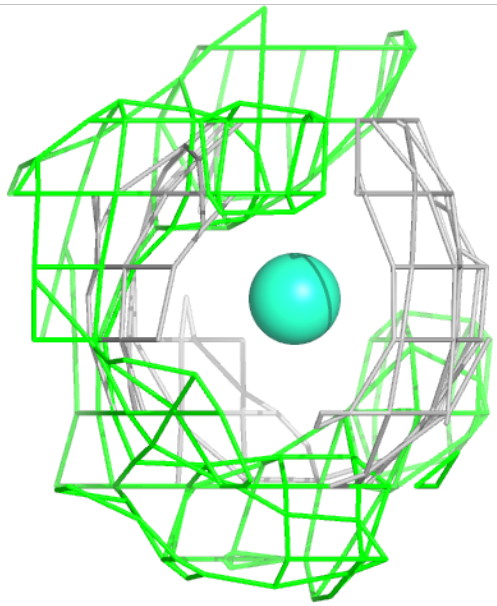
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

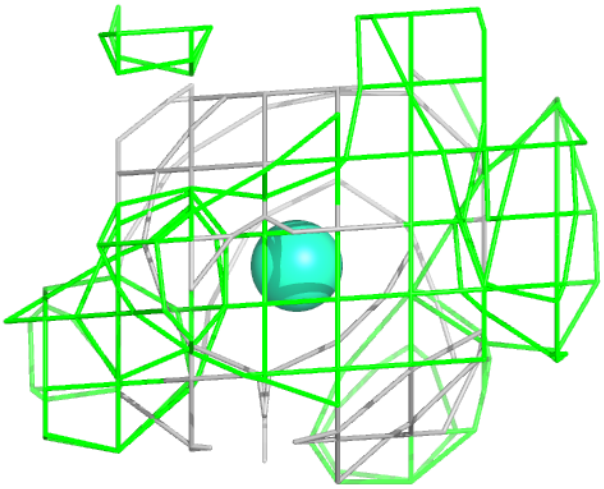


Electron density around TB A 202:

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

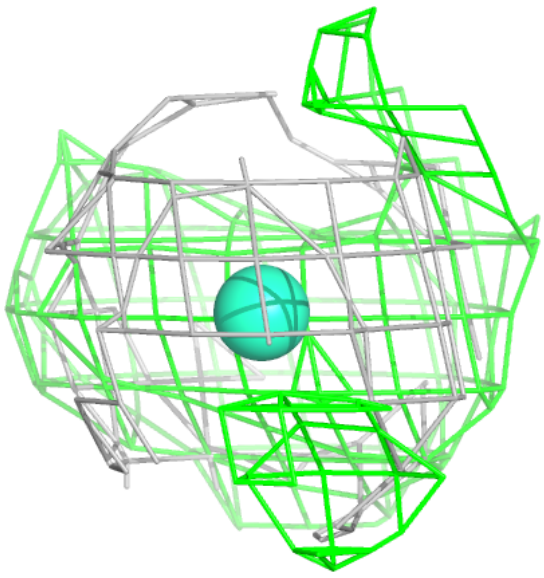


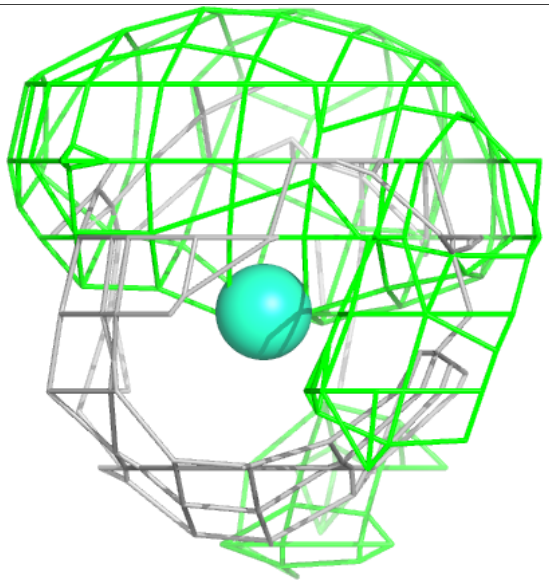


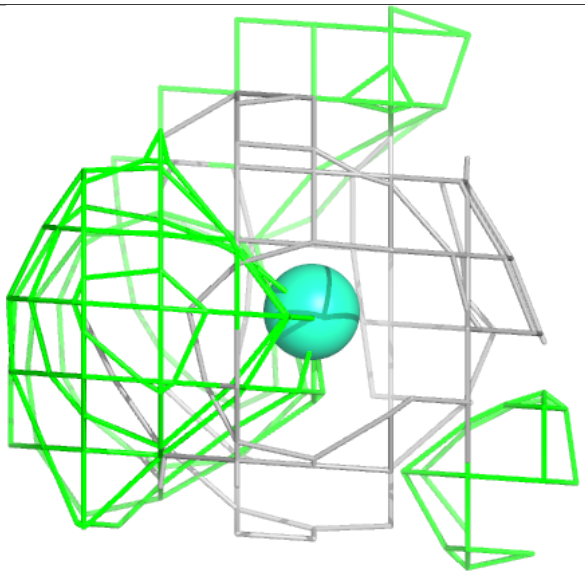


Electron density around TB A 201:

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

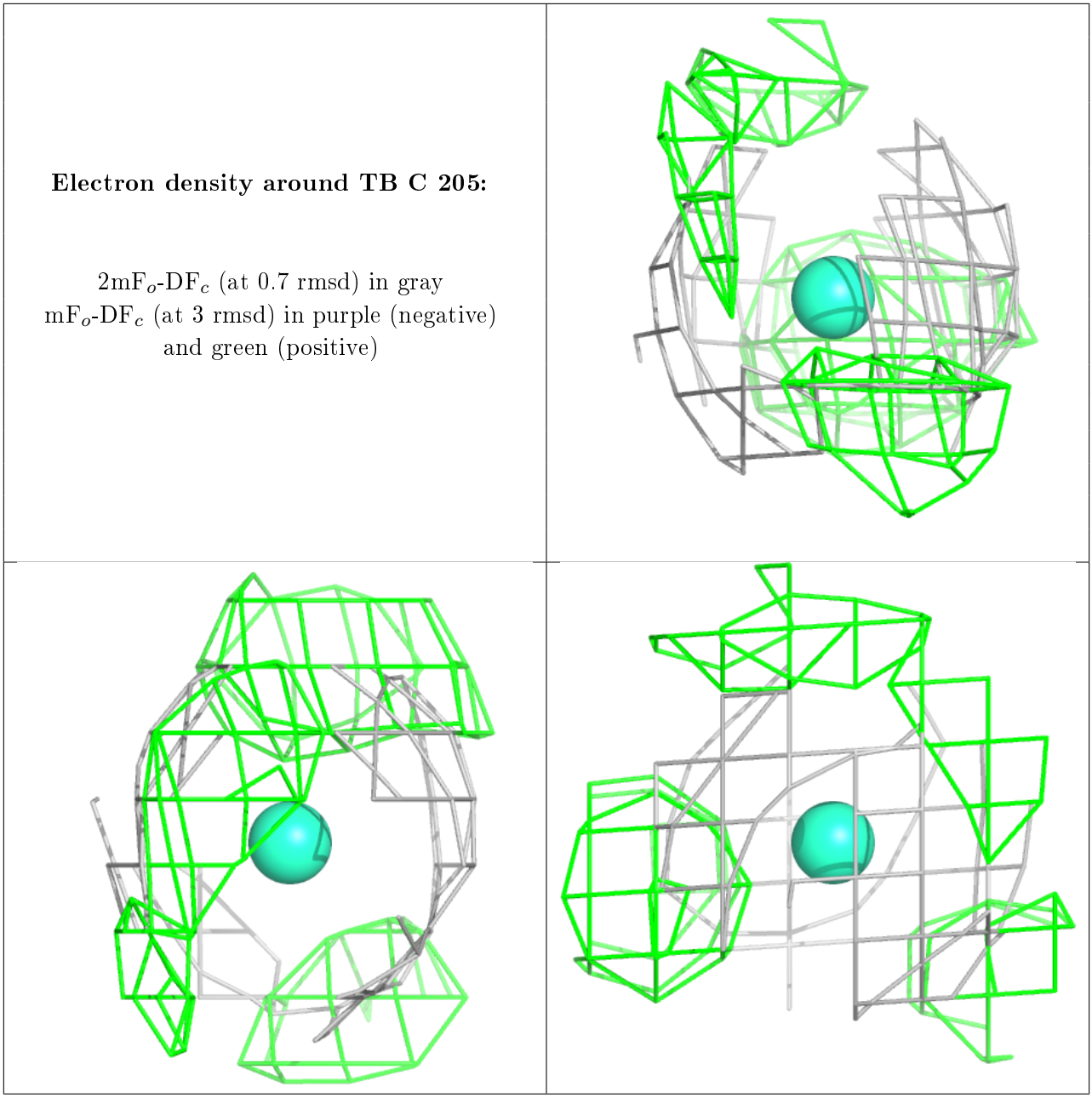






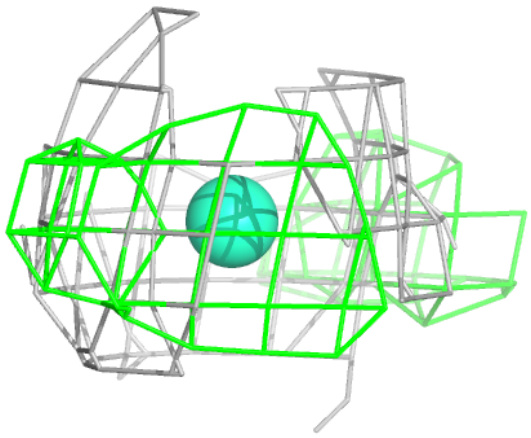
Electron density around TB C 205:

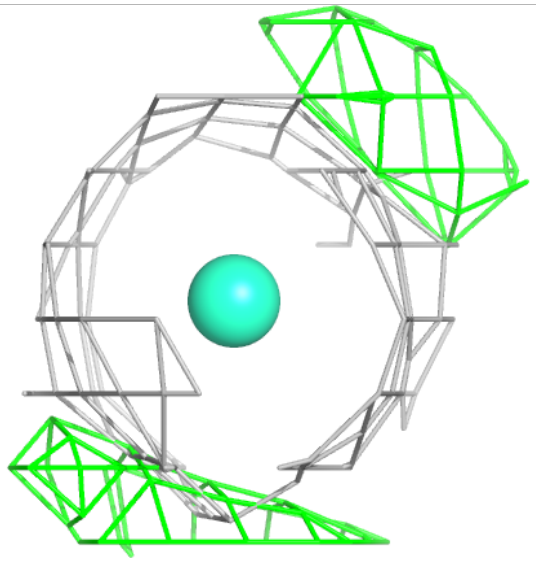
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

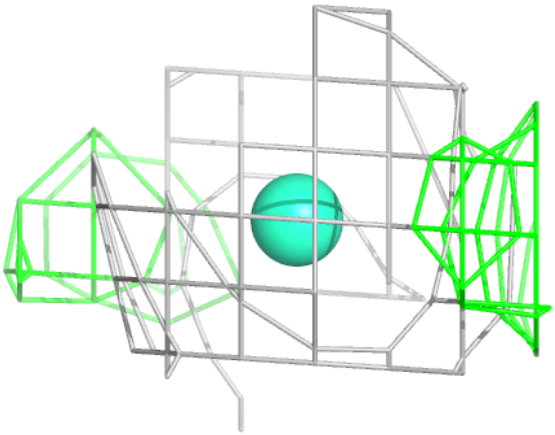


Electron density around TB D 201:

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







6.5 Other polymers

There are no such residues in this entry.