



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2022 – 02:07 PM EDT

PDB ID : 7T7K
Title : Structure of SPAC806.04c protein from fission yeast bound to Co2+
Authors : Jacewicz, A.; Sanchez, A.M.; Shuman, S.
Deposited on : 2021-12-15
Resolution : 1.90 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 following versions of software and data (see [references ⓘ](#)) 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 : 2.28.1
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) : 2.28.1

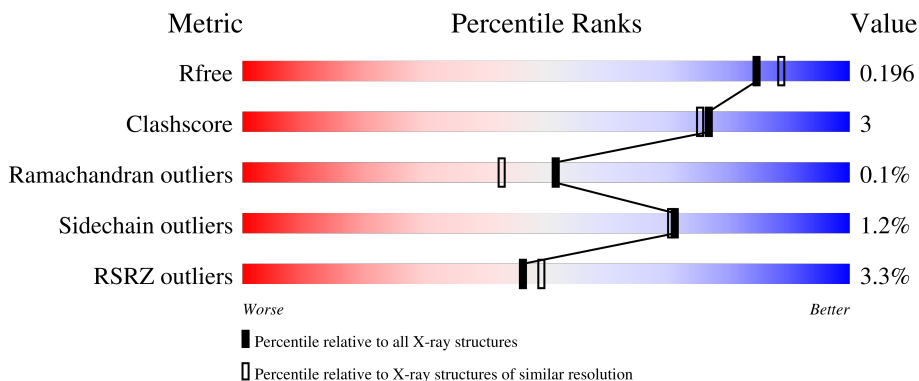
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

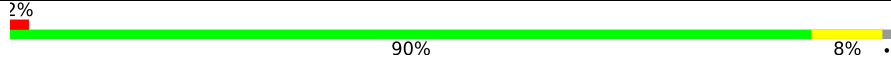
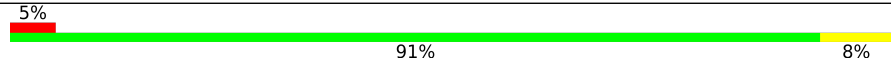
The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	439	 2% 90% 8%
1	B	439	 5% 91% 8%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7822 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 Damage-control phosphatase SPAC806.04c.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	438	3520	2273	573	661	13	1	0	0
1	A	433	3490	2254	567	656	13	0	1	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	SER	-	expression tag	UNP Q9UT55
A	0	SER	-	expression tag	UNP Q9UT55

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	K	0	0
			1	1		
2	A	3	Total	K	0	0
			3	3		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

- Molecule 4 is COBALT (II) ION (three-letter code: CO) (formula: Co) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	2	Total Co 2 2	0	0
4	A	2	Total Co 2 2	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 1 1	0	0

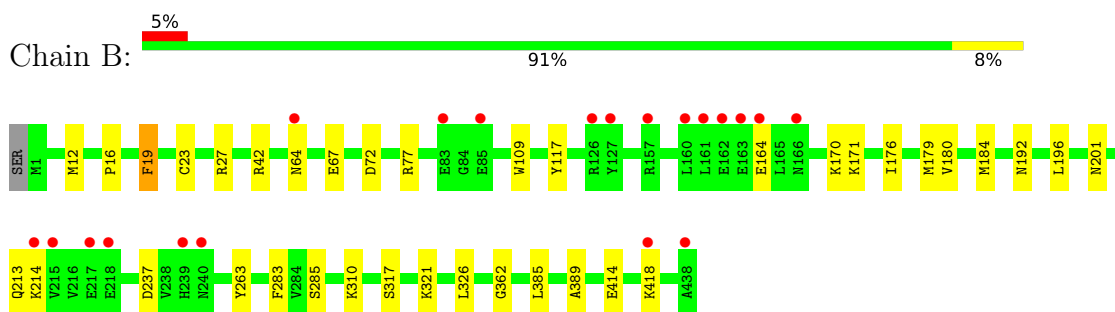
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	353	Total O 353 353	0	0
6	A	409	Total O 410 410	0	1

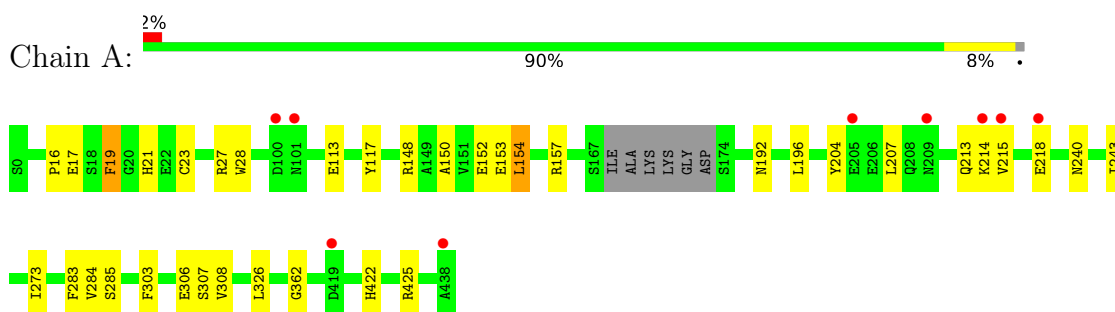
3 Residue-property plots [i](#)

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: Damage-control phosphatase SPAC806.04c



- Molecule 1: Damage-control phosphatase SPAC806.04c



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.65Å 116.31Å 151.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.42 – 1.90 46.42 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.42-1.90) 99.9 (46.42-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 1.90Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.164 , 0.196 0.166 , 0.196	Depositor DCC
R_{free} test set	2074 reflections (2.51%)	wwPDB-VP
Wilson B-factor (Å ²)	24.5	Xtrriage
Anisotropy	0.305	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 53.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7822	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.77% 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: K, PO4, CO, CL

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	0.41	0/3583	0.60	2/4863 (0.0%)
1	B	0.38	0/3611	0.60	2/4902 (0.0%)
All	All	0.39	0/7194	0.60	4/9765 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	326	LEU	CA-CB-CG	5.95	128.98	115.30
1	A	326	LEU	CA-CB-CG	5.54	128.03	115.30
1	A	154	LEU	CB-CG-CD2	5.12	119.71	111.00
1	B	12	MET	CA-CB-CG	5.04	121.87	113.30

There are no chirality outliers.

There are no planarity outliers.

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	A	3490	0	3429	19	0
1	B	3520	0	3457	20	0
2	A	3	0	0	0	0
2	B	1	0	0	0	0
3	A	25	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	15	0	0	2	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	1	0	0	1	0
6	A	410	0	0	3	0
6	B	353	0	0	8	0
All	All	7822	0	6886	42	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 3.

All (42) 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)
5:A:511:CL:CL	6:A:837:HOH:O	2.35	0.81
3:B:503:PO4:O1	6:B:601:HOH:O	2.12	0.67
1:A:150:ALA:O	1:A:154:LEU:HD23	1.95	0.65
1:A:422:HIS:ND1	6:A:603:HOH:O	2.30	0.65
1:B:23:CYS:HA	1:B:27:ARG:HB2	1.81	0.62
1:B:164:GLU:HG3	1:B:170:LYS:HD2	1.83	0.60
1:B:67:GLU:OE1	6:B:602:HOH:O	2.16	0.59
1:B:213:GLN:OE1	6:B:603:HOH:O	2.17	0.58
1:B:418:LYS:N	1:B:418:LYS:HD3	2.18	0.57
1:B:196:LEU:HB2	1:B:285:SER:HB3	1.87	0.57
1:A:23:CYS:HA	1:A:27:ARG:HB2	1.86	0.56
1:A:243:ILE:HB	1:A:273:ILE:HD13	1.89	0.54
1:A:153:GLU:HG2	1:A:213:GLN:NE2	2.23	0.54
1:A:215:VAL:HG13	6:A:889:HOH:O	2.08	0.54
1:A:214:LYS:O	1:A:218:GLU:HG3	2.09	0.51
1:B:310:LYS:NZ	6:B:614:HOH:O	2.42	0.50
1:A:153:GLU:HG2	1:A:213:GLN:HE21	1.76	0.50
1:B:117:TYR:CZ	1:B:283:PHE:HA	2.47	0.49
1:A:23:CYS:HB3	1:A:28:TRP:CE2	2.47	0.49
1:B:176:ILE:HD12	1:B:179:MET:HB2	1.95	0.49
1:B:237:ASP:OD1	1:B:237:ASP:N	2.39	0.48
1:B:42:ARG:NH1	6:B:613:HOH:O	2.40	0.48
1:A:148:ARG:O	1:A:152:GLU:HG3	2.12	0.48
1:B:72:ASP:OD1	1:B:77:ARG:NH1	2.47	0.47
1:A:204:TYR:CD1	1:A:207:LEU:HD23	2.48	0.47
1:A:192:ASN:OD1	1:A:362:GLY:HA2	2.16	0.46
1:B:385:LEU:HB2	1:B:389:ALA:HB2	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:414:GLU:O	1:B:418:LYS:HE2	2.16	0.45
3:B:504:PO4:O4	6:B:604:HOH:O	2.21	0.45
1:B:214:LYS:HG3	6:B:740:HOH:O	2.16	0.44
1:B:19:PHE:HB3	1:B:109:TRP:CH2	2.53	0.43
1:A:303:PHE:HB2	1:A:308:VAL:HG11	2.00	0.43
1:A:117:TYR:CZ	1:A:283:PHE:HA	2.53	0.43
1:A:113:GLU:HG2	1:A:283:PHE:CZ	2.54	0.42
1:A:16:PRO:HA	1:A:21:HIS:CD2	2.54	0.42
1:B:180:VAL:O	1:B:184:MET:HG2	2.20	0.42
1:A:306:GLU:HG3	1:A:307:SER:N	2.34	0.42
1:B:64:ASN:ND2	6:B:602:HOH:O	2.54	0.41
1:A:19:PHE:CD1	1:A:425:ARG:HD3	2.56	0.41
1:B:192:ASN:OD1	1:B:362:GLY:HA2	2.21	0.41
1:B:317:SER:O	1:B:321:LYS:HG3	2.21	0.41
1:A:196:LEU:HB2	1:A:285:SER:HB3	2.02	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	430/439 (98%)	423 (98%)	6 (1%)	1 (0%)	47	38
1	B	436/439 (99%)	427 (98%)	9 (2%)	0	100	100
All	All	866/878 (99%)	850 (98%)	15 (2%)	1 (0%)	51	42

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	284	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	380/383 (99%)	376 (99%)	4 (1%)	73	73
1	B	381/383 (100%)	376 (99%)	5 (1%)	69	68
All	All	761/766 (99%)	752 (99%)	9 (1%)	71	70

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	16	PRO
1	B	19	PHE
1	B	171	LYS
1	B	201	ASN
1	B	263	TYR
1	A	17	GLU
1	A	19	PHE
1	A	157	ARG
1	A	240	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	64	ASN
1	A	213	GLN

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 17 ligands modelled in this entry, 9 are monoatomic - leaving 8 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	PO4	A	506	-	4,4,4	0.75	0	6,6,6	0.53	0
3	PO4	A	508	-	4,4,4	0.92	0	6,6,6	0.70	0
3	PO4	A	507	-	4,4,4	1.02	0	6,6,6	0.50	0
3	PO4	B	504	-	4,4,4	0.88	0	6,6,6	0.33	0
3	PO4	B	503	-	4,4,4	0.88	0	6,6,6	0.52	0
3	PO4	A	505	-	4,4,4	0.69	0	6,6,6	0.81	0
3	PO4	A	504	-	4,4,4	0.90	0	6,6,6	0.46	0
3	PO4	B	502	-	4,4,4	0.89	0	6,6,6	0.42	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 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	504	PO4	1	0
3	B	503	PO4	1	0

5.7 Other polymers [i](#)

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, 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	433/439 (98%)	-0.17	9 (2%) 63 66	17, 25, 46, 65	4 (0%)
1	B	438/439 (99%)	0.12	20 (4%) 32 35	18, 25, 45, 90	2 (0%)
All	All	871/878 (99%)	-0.02	29 (3%) 46 49	17, 25, 46, 90	6 (0%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	163	GLU	6.4
1	B	85	GLU	6.2
1	B	166	ASN	4.5
1	B	214	LYS	4.5
1	B	162	GLU	4.4
1	B	438	ALA	4.4
1	A	215	VAL	4.1
1	B	160	LEU	3.5
1	A	100	ASP	3.2
1	B	164	GLU	3.1
1	B	418	LYS	3.0
1	B	240	ASN	3.0
1	A	214	LYS	3.0
1	A	205	GLU	2.8
1	B	217	GLU	2.8
1	B	239	HIS	2.8
1	B	83	GLU	2.8
1	B	215	VAL	2.8
1	B	218	GLU	2.7
1	B	64	ASN	2.7
1	A	101	ASN	2.7
1	A	419	ASP	2.6
1	A	218	GLU	2.5
1	B	126	ARG	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	161	LEU	2.3
1	A	438	ALA	2.2
1	B	157	ARG	2.1
1	A	209	ASN	2.1
1	B	127	TYR	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 monosaccharides in this entry.

6.4 Ligands [i](#)

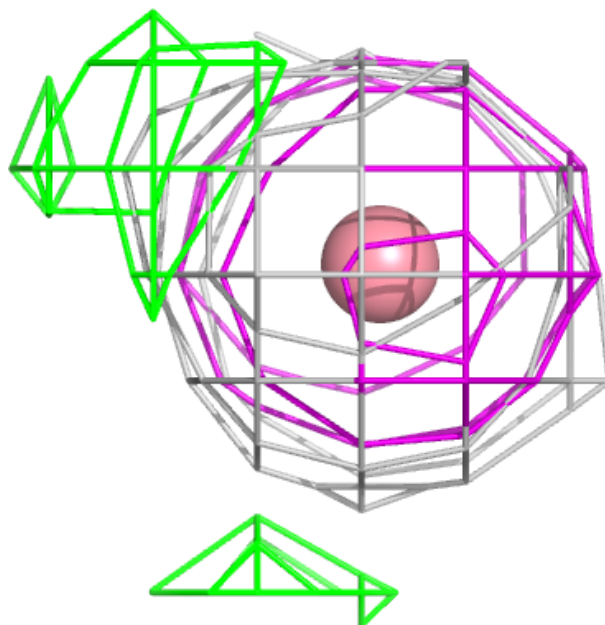
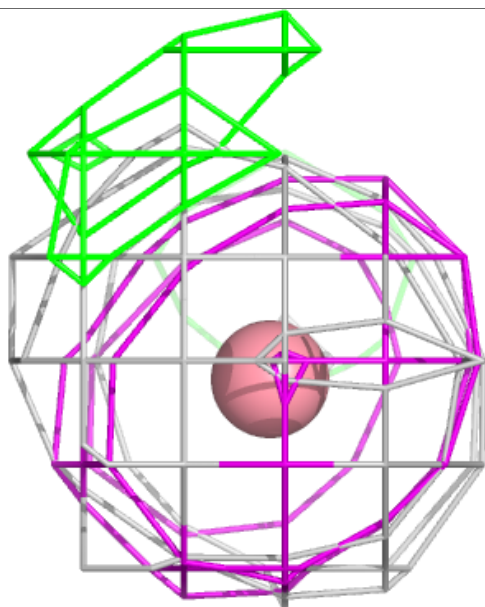
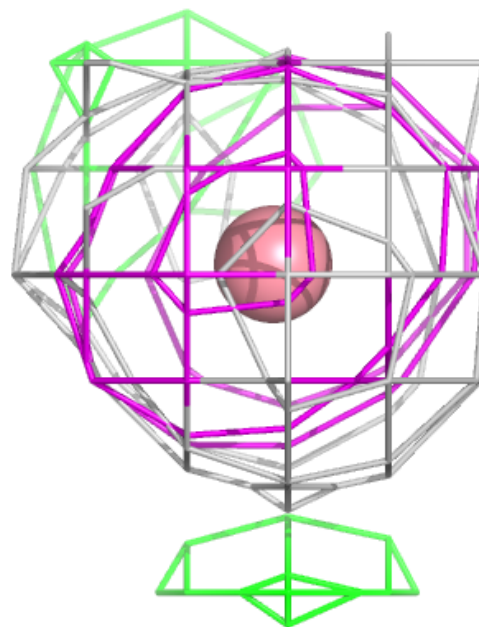
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PO4	B	504	5/5	0.80	0.32	34,38,53,59	5
3	PO4	B	503	5/5	0.86	0.16	41,42,56,59	5
3	PO4	B	502	5/5	0.88	0.20	57,59,79,88	5
2	K	A	503	1/1	0.89	0.51	46,46,46,46	1
3	PO4	A	505	5/5	0.90	0.11	27,34,46,47	5
2	K	A	501	1/1	0.91	0.10	61,61,61,61	1
3	PO4	A	506	5/5	0.91	0.18	56,61,67,83	0
3	PO4	A	507	5/5	0.92	0.19	36,41,48,49	5
2	K	A	502	1/1	0.93	0.17	48,48,48,48	1
3	PO4	A	504	5/5	0.96	0.18	55,61,62,67	5
3	PO4	A	508	5/5	0.97	0.08	29,30,38,42	5
4	CO	B	505	1/1	0.97	0.15	19,19,19,19	1
5	CL	A	511	1/1	0.97	0.07	38,38,38,38	1
2	K	B	501	1/1	0.98	0.06	23,23,23,23	1
4	CO	A	509	1/1	0.99	0.23	21,21,21,21	0
4	CO	A	510	1/1	0.99	0.39	21,21,21,21	1
4	CO	B	506	1/1	0.99	0.21	19,19,19,19	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.

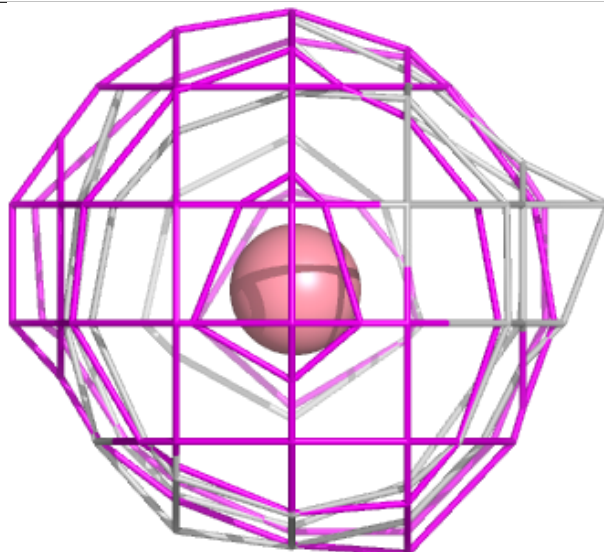
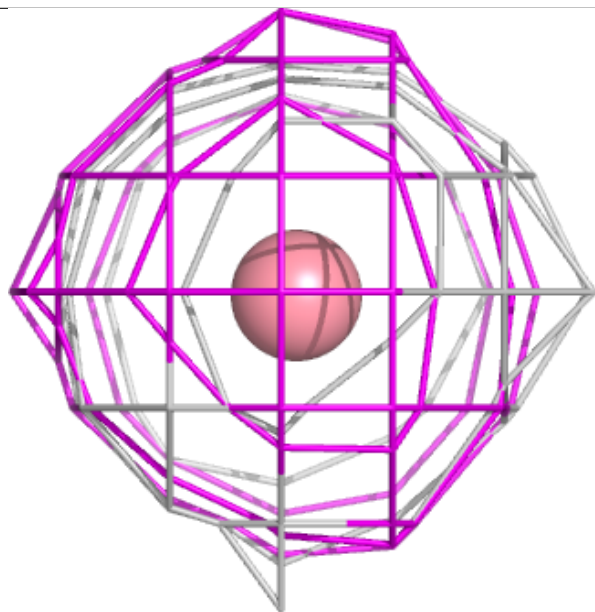
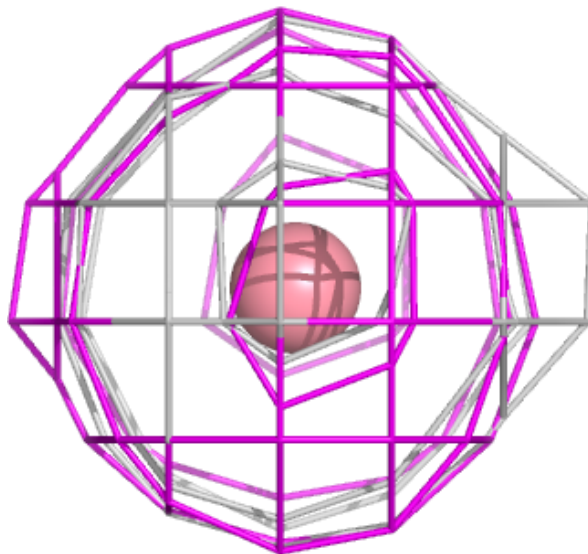
Electron density around CO B 505:

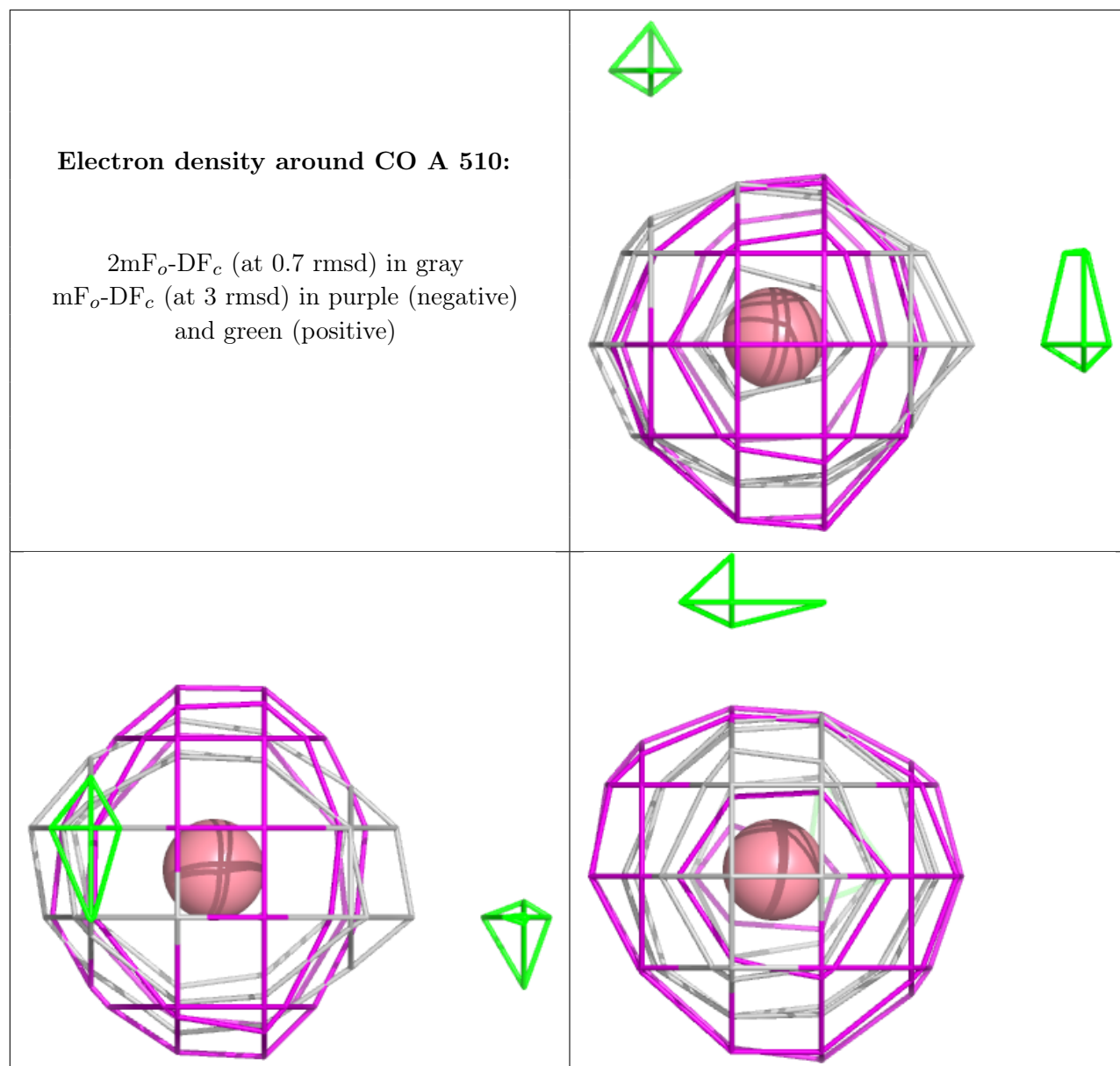
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

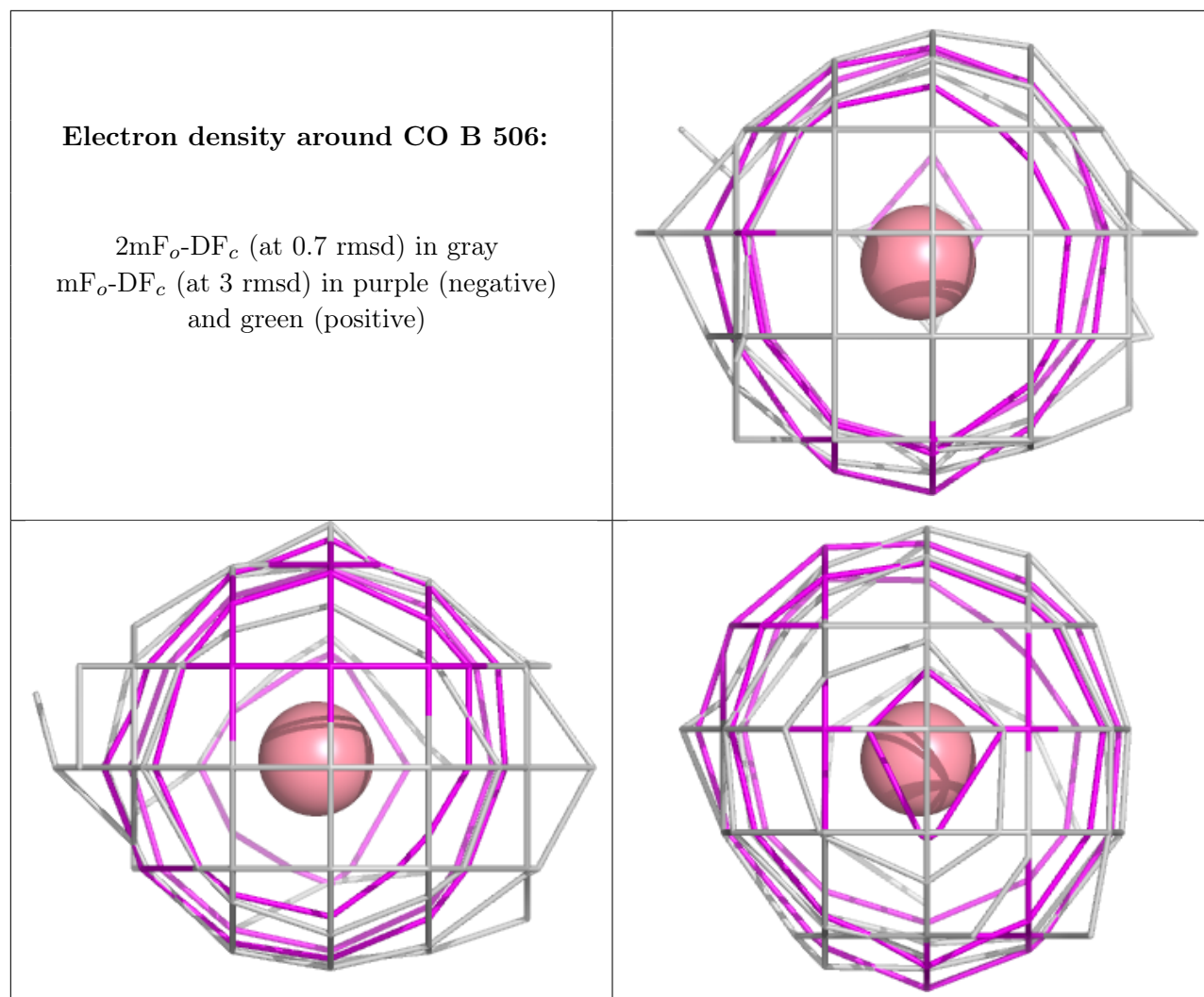


Electron density around CO A 509:

$2mF_o-DF_c$ (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.