



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2022 – 02:04 PM EDT

PDB ID : 7T7O
Title : Structure of SPAC806.04c protein from fission yeast covalently bound to BeF3
Authors : Jacewicz, A.; Sanchez, A.M.; Shuman, S.
Deposited on : 2021-12-15
Resolution : 2.16 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

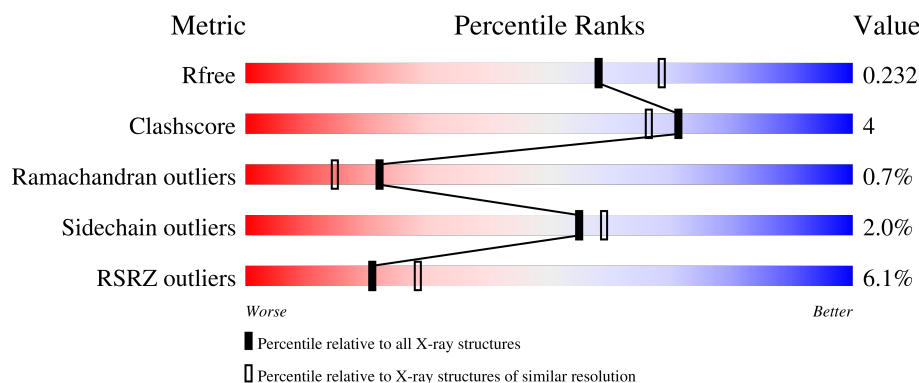
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.16 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	<div> <div>6%</div> <div>88%</div> <div>10%</div> </div>
1	B	439	<div> <div>6%</div> <div>90%</div> <div>8%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7265 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
1	B	438	Total	Be	C	F	N	O	S	0	0	0
			3528	1	2276	3	574	661	13			
1	A	433	Total	Be	C	F	N	O	S	0	1	0
			3497	1	2257	3	568	655	13			

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

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

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

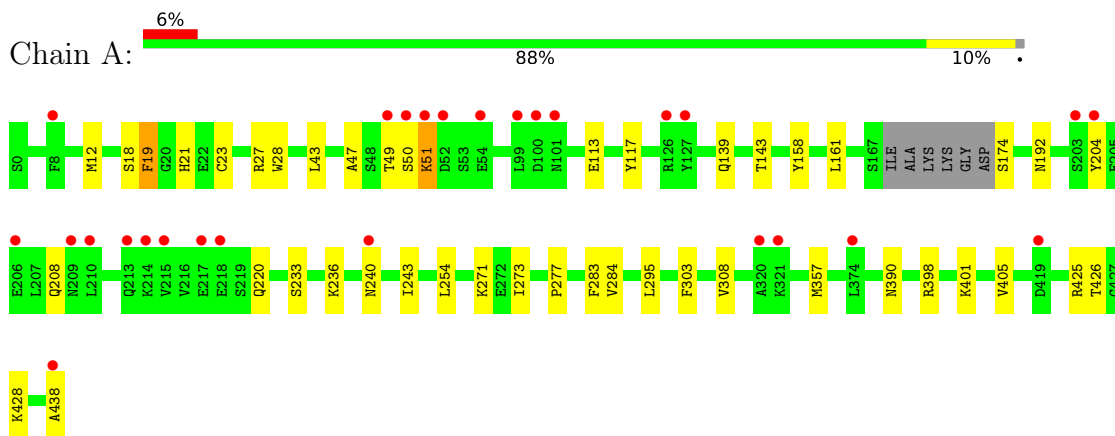


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	117	Total	O	0	0
			117	117		
4	A	116	Total	O	0	0
			116	116		

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



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	57.94Å 116.50Å 151.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.35 – 2.16 46.35 – 2.16	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.35-2.16) 99.9 (46.35-2.16)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 2.16Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.202 , 0.235 0.198 , 0.232	Depositor DCC
R_{free} test set	1390 reflections (2.49%)	wwPDB-VP
Wilson B-factor (Å ²)	27.6	Xtriage
Anisotropy	0.518	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 41.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7265	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.72% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, BFD, CO

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	0.43	0/3577	0.60	0/4852
1	B	0.40	0/3606	0.60	0/4892
All	All	0.42	0/7183	0.60	0/9744

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	3497	0	3436	27	0
1	B	3528	0	3468	22	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	5	0	0	0	0
4	A	116	0	0	0	0
4	B	117	0	0	1	0
All	All	7265	0	6904	49	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 4.

All (49) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:ASN:HD22	1:A:271:LYS:HD2	1.52	0.74
1:B:277:PRO:HG3	1:B:326:LEU:HD11	1.74	0.69
1:A:47:ALA:HB1	1:A:51:LYS:HD2	1.75	0.69
1:B:164:GLU:HG3	1:B:170:LYS:HD2	1.78	0.65
1:B:164:GLU:O	1:B:166:ASN:N	2.26	0.64
1:B:196:LEU:HB2	1:B:285:SER:HB3	1.82	0.61
1:A:23:CYS:HA	1:A:27:ARG:HB2	1.85	0.57
1:B:94:GLU:OE1	1:B:97:LYS:NZ	2.34	0.56
1:B:164:GLU:C	1:B:166:ASN:H	2.11	0.54
1:A:139:GLN:O	1:A:143:THR:HG23	2.10	0.52
1:B:164:GLU:HG2	1:B:165:LEU:N	2.25	0.52
1:A:398:ARG:HH12	1:A:405:VAL:HG22	1.74	0.51
1:B:188:SER:OG	1:B:257:ASP:OD1	2.28	0.51
1:A:303:PHE:HB2	1:A:308:VAL:HG11	1.92	0.51
1:A:18:SER:O	1:A:21:HIS:HB3	2.11	0.51
1:A:50:SER:O	1:A:51:LYS:HB2	2.10	0.51
1:A:426:THR:OG1	1:A:428:LYS:HG2	2.11	0.50
1:A:23:CYS:HB3	1:A:28:TRP:CE2	2.45	0.50
1:B:160:LEU:HA	1:B:163:GLU:HG3	1.93	0.49
1:B:72:ASP:HA	1:B:77:ARG:HH11	1.78	0.48
1:B:23:CYS:HA	1:B:27:ARG:HB2	1.95	0.48
1:B:202:LEU:HD22	1:B:206:GLU:HG2	1.94	0.48
1:B:243:ILE:O	1:B:273:ILE:HA	2.14	0.47
1:A:47:ALA:HB1	1:A:51:LYS:CD	2.44	0.47
1:A:143:THR:HG22	1:A:204:TYR:CE1	2.50	0.47
1:A:158:TYR:O	1:A:161:LEU:HB2	2.14	0.47
1:A:254:LEU:HD23	1:A:295:LEU:HD22	1.97	0.47
1:A:243:ILE:HB	1:A:273:ILE:HD13	1.98	0.46
1:A:192:ASN:OD1	1:A:401[A]:LYS:NZ	2.49	0.46
1:B:117:TYR:CZ	1:B:283:PHE:HA	2.51	0.45
1:A:113:GLU:HG2	1:A:283:PHE:CZ	2.52	0.45
1:B:2:LYS:HD3	1:B:2:LYS:HA	1.50	0.44
1:B:154:LEU:HD13	1:B:256:VAL:HG12	2.00	0.44
1:B:51:LYS:HE2	1:B:51:LYS:HB2	1.54	0.44
1:A:19:PHE:CD1	1:A:425:ARG:HD3	2.52	0.44
1:B:19:PHE:HB3	1:B:109:TRP:CH2	2.53	0.44
1:A:240:ASN:HD22	1:A:271:LYS:CD	2.26	0.43
1:A:47:ALA:HB1	1:A:51:LYS:NZ	2.33	0.43
1:A:117:TYR:CZ	1:A:283:PHE:HA	2.53	0.43
1:B:72:ASP:OD1	1:B:77:ARG:NH1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:ASN:CG	1:A:271:LYS:HB3	2.39	0.43
1:B:7:PRO:HD2	1:B:375:TRP:CZ2	2.54	0.42
1:A:12:MET:HE3	1:A:12:MET:HB3	1.94	0.42
1:A:233:SER:HA	1:A:236:LYS:HE3	2.01	0.42
1:B:26:ARG:NE	4:B:602:HOH:O	2.39	0.41
1:B:300:ASP:OD1	1:B:300:ASP:N	2.51	0.41
1:A:390:ASN:HB3	1:A:438:ALA:HB3	2.03	0.41
1:A:243:ILE:HD12	1:A:357:MET:HB3	2.03	0.40
1:A:43:LEU:O	1:A:47:ALA:HB2	2.20	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	429/439 (98%)	418 (97%)	7 (2%)	4 (1%)	17	11
1	B	435/439 (99%)	424 (98%)	9 (2%)	2 (0%)	29	22
All	All	864/878 (98%)	842 (98%)	16 (2%)	6 (1%)	22	15

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	49	THR
1	A	51	LYS
1	A	284	VAL
1	B	277	PRO
1	B	284	VAL
1	A	277	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	379/382 (99%)	375 (99%)	4 (1%)	73	78
1	B	381/382 (100%)	370 (97%)	11 (3%)	42	42
All	All	760/764 (100%)	745 (98%)	15 (2%)	55	59

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	2	LYS
1	B	19	PHE
1	B	139	GLN
1	B	148	ARG
1	B	160	LEU
1	B	162	GLU
1	B	163	GLU
1	B	233	SER
1	B	244	ASP
1	B	263	TYR
1	B	295	LEU
1	A	19	PHE
1	A	174	SER
1	A	208	GLN
1	A	220	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	98	GLN
1	B	240	ASN
1	A	166	ASN
1	A	240	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 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	$\# Z > 2$
1	BFD	A	248	1,2	8,11,12	0.86	0	3,15,17	0.80	0
1	BFD	B	248	1,2	8,11,12	0.81	0	3,15,17	0.91	0

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
1	BFD	A	248	1,2	-	1/5/11/13	-
1	BFD	B	248	1,2	-	1/5/11/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	248	BFD	O-C-CA-CB
1	A	248	BFD	O-C-CA-CB

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 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	502	-	4,4,4	0.78	0	6,6,6	0.45	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.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	432/439 (98%)	0.12	27 (6%) 20 27	18, 27, 54, 91	0
1	B	437/439 (99%)	0.29	26 (5%) 22 30	18, 27, 49, 86	1 (0%)
All	All	869/878 (98%)	0.21	53 (6%) 21 28	18, 27, 51, 91	1 (0%)

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	51	LYS	7.7
1	B	163	GLU	6.9
1	B	438	ALA	6.5
1	A	50	SER	6.5
1	A	100	ASP	5.0
1	A	210	LEU	4.9
1	B	85	GLU	4.8
1	A	49	THR	4.2
1	B	162	GLU	4.2
1	B	64	ASN	3.9
1	A	218	GLU	3.9
1	B	419	ASP	3.8
1	A	206	GLU	3.8
1	A	214	LYS	3.8
1	A	101	ASN	3.7
1	B	60	LYS	3.7
1	A	203	SER	3.6
1	B	214	LYS	3.5
1	B	239	HIS	3.3
1	B	127	TYR	3.2
1	B	126	ARG	3.2
1	A	209	ASN	3.2
1	A	204	TYR	3.2
1	B	215	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	87	GLN	3.1
1	A	374	LEU	3.1
1	B	418	LYS	3.1
1	B	86	GLY	3.1
1	B	237	ASP	3.0
1	B	160	LEU	3.0
1	B	218	GLU	2.9
1	B	54	GLU	2.9
1	A	52	ASP	2.8
1	A	438	ALA	2.8
1	B	83	GLU	2.8
1	A	419	ASP	2.7
1	B	166	ASN	2.7
1	A	215	VAL	2.6
1	A	8	PHE	2.5
1	A	127	TYR	2.5
1	A	217	GLU	2.4
1	A	126	ARG	2.4
1	B	165	LEU	2.3
1	B	1	MET	2.3
1	A	213	GLN	2.3
1	B	66	LEU	2.2
1	A	240	ASN	2.2
1	A	320	ALA	2.2
1	B	164	GLU	2.2
1	A	54	GLU	2.2
1	A	99	LEU	2.1
1	A	321	LYS	2.1
1	B	217	GLU	2.1

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

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(\AA^2)	Q<0.9
1	BFD	B	248	12/13	0.96	0.15	17,19,23,24	0
1	BFD	A	248	12/13	0.97	0.10	17,19,21,26	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

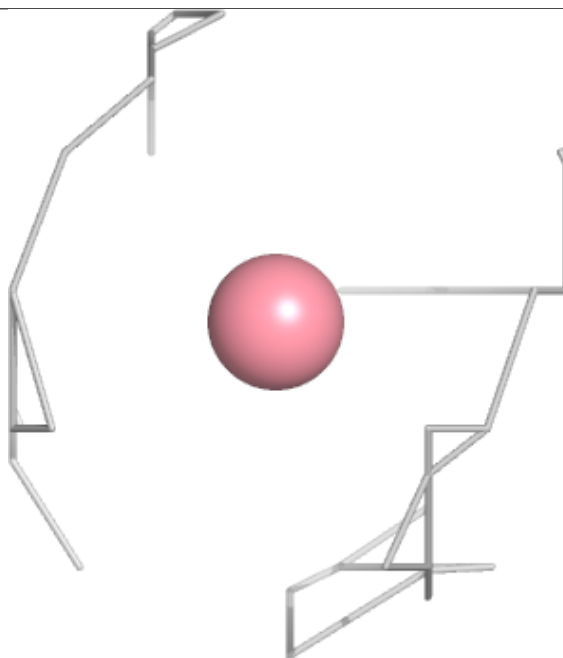
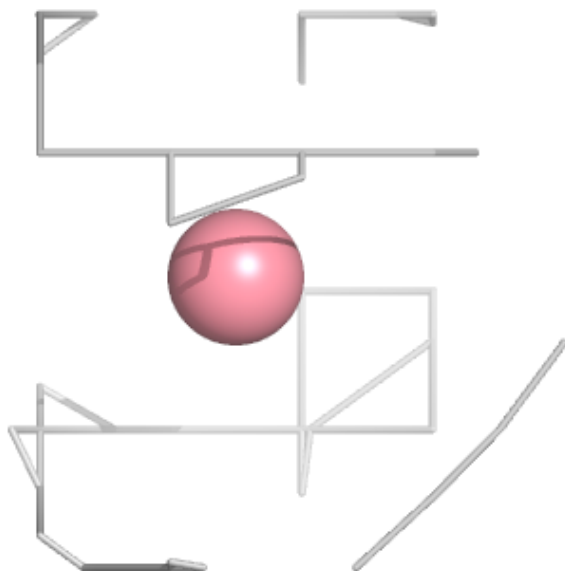
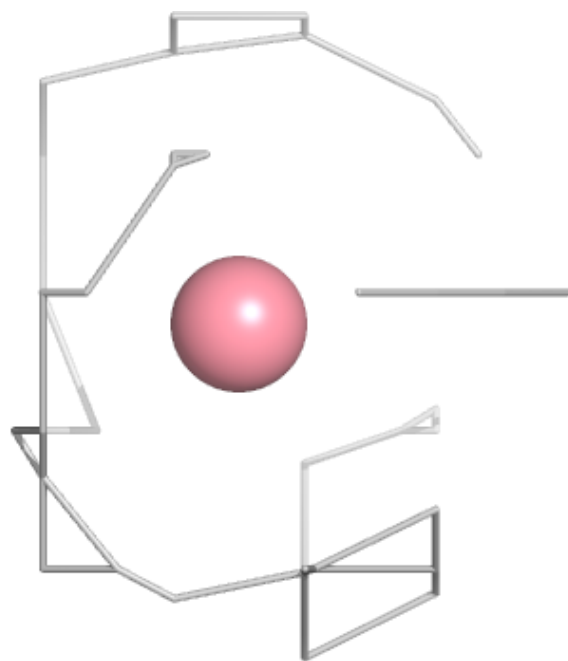
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

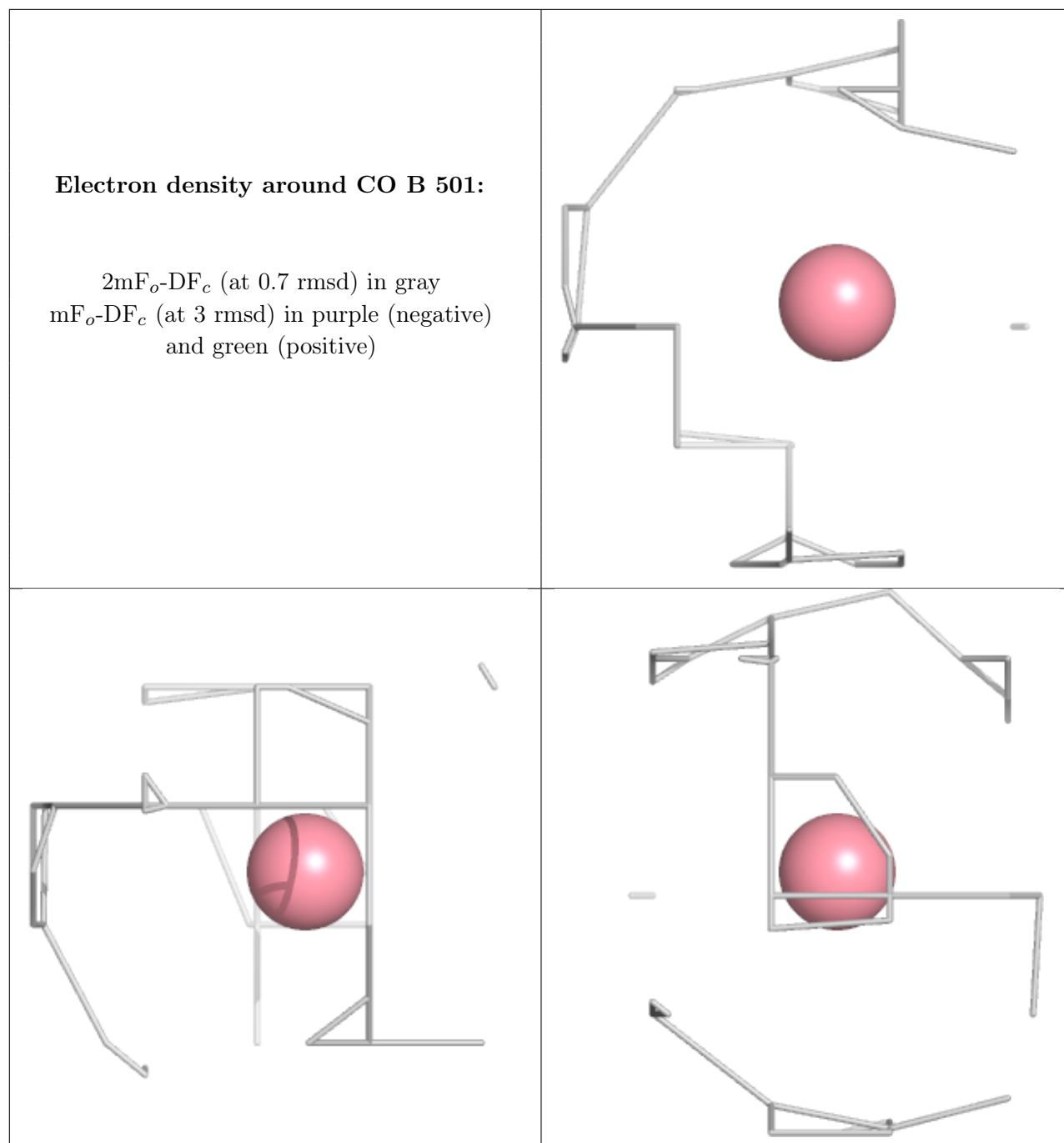
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	PO4	A	502	5/5	0.95	0.23	57,58,65,72	1
2	CO	A	501	1/1	0.98	0.10	26,26,26,26	1
2	CO	B	501	1/1	0.99	0.07	25,25,25,25	1

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 A 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.