



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 14, 2024 – 07:47 am GMT

PDB ID : 6IAV
Title : CO-AZURIN FROM PSEUDOMONAS AERUGINOSA TREATED WITH HYDROSULFIDE
Authors : Palm, G.J.; Kohlhause, D.
Deposited on : 2018-11-27
Resolution : 2.00 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
Xtrriage (Phenix) : 1.13
EDS : 2.36
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

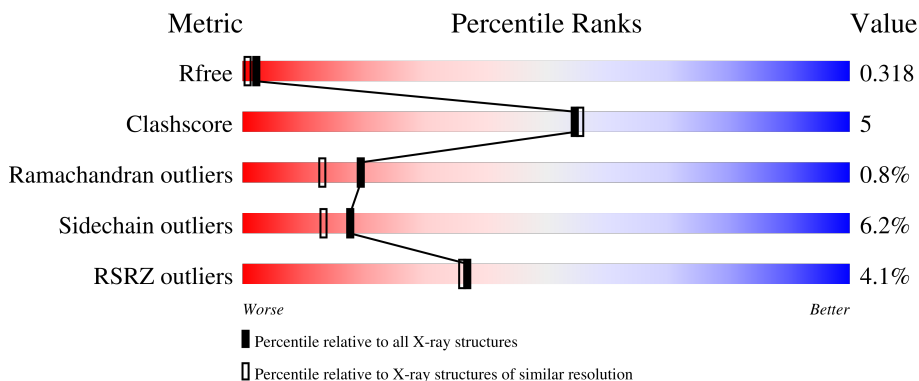
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	127	 83% 13% ..
1	B	127	 79% 17% ..
1	C	127	 88% 10% ..
1	D	127	 69% 27% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3918 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 Azurin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	127	977	613	163	191	10	0	3	0
1	B	127	967	605	162	190	10	0	1	0
1	C	127	966	604	162	190	10	0	1	0
1	D	127	972	608	163	191	10	0	2	0

- 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	A	1	Total 1	Co 1	0	0
2	B	1	Total 1	Co 1	0	0
2	C	1	Total 1	Co 1	0	0
2	D	1	Total 1	Co 1	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Ca 1	0	0
3	B	1	Total 1	Ca 1	0	0
3	C	1	Total 1	Ca 1	0	0

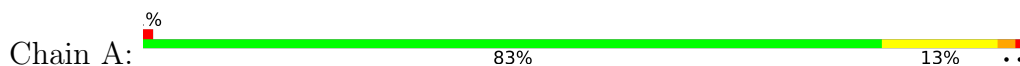
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	6	Total O 6 6	0	0
4	B	8	Total O 8 8	0	0
4	C	8	Total O 8 8	0	0
4	D	7	Total O 7 7	0	0

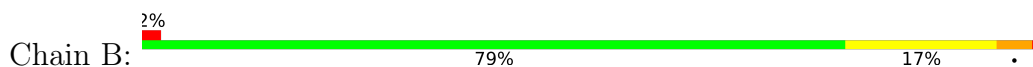
3 Residue-property plots [i](#)

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.

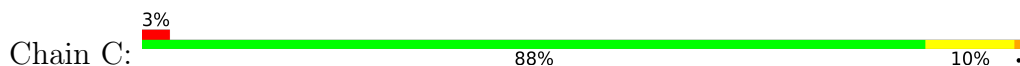
- Molecule 1: Azurin



- Molecule 1: Azurin



- Molecule 1: Azurin



- Molecule 1: Azurin



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	50.43Å 59.95Å 82.52Å 90.00° 90.43° 90.00°	Depositor
Resolution (Å)	50.48 – 2.00 50.43 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.2 (50.48-2.00) 96.2 (50.43-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.72 (at 2.00Å)	Xtrriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.250 , 0.310 0.255 , 0.318	Depositor DCC
R_{free} test set	1563 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	34.3	Xtrriage
Anisotropy	0.653	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 37.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.068 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3918	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.61 % 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 9.1418e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: CO, CA

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	1.32	3/1003 (0.3%)	1.47	7/1353 (0.5%)
1	B	1.30	6/987 (0.6%)	1.43	4/1331 (0.3%)
1	C	1.27	5/986 (0.5%)	1.31	2/1330 (0.2%)
1	D	1.38	10/995 (1.0%)	1.44	3/1342 (0.2%)
All	All	1.32	24/3971 (0.6%)	1.41	16/5356 (0.3%)

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	A	0	3
1	B	0	1
1	C	0	1
All	All	0	5

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	17	THR	C-O	8.06	1.38	1.23
1	B	51	SER	CB-OG	7.27	1.51	1.42
1	B	121	MET	C-O	-7.26	1.09	1.23
1	B	94	SER	CA-CB	-6.98	1.42	1.52
1	D	108	TYR	C-O	6.96	1.36	1.23
1	C	91	GLU	CD-OE1	-6.54	1.18	1.25
1	D	116	GLY	C-O	-6.16	1.13	1.23
1	C	33	LEU	C-O	6.14	1.35	1.23
1	D	8	GLN	C-O	6.09	1.34	1.23
1	D	107[A]	GLN	C-O	6.07	1.34	1.23
1	D	107[B]	GLN	C-O	6.07	1.34	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	15	PHE	C-O	-5.82	1.12	1.23
1	D	85	LYS	C-O	5.79	1.34	1.23
1	D	46	HIS	CE1-NE2	5.61	1.45	1.32
1	A	35	HIS	CE1-NE2	5.59	1.45	1.32
1	C	98	ASP	C-O	5.45	1.33	1.23
1	B	89	SER	CB-OG	5.35	1.49	1.42
1	C	94	SER	CA-CB	-5.31	1.45	1.52
1	C	105	GLY	C-O	5.31	1.32	1.23
1	D	30	THR	C-O	-5.17	1.13	1.23
1	D	5	VAL	C-O	5.14	1.33	1.23
1	B	3	CYS	C-O	5.10	1.33	1.23
1	A	77	ASP	C-O	5.09	1.33	1.23
1	B	46	HIS	CE1-NE2	5.03	1.44	1.32

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	128	LYS	CA-C-O	6.74	134.25	120.10
1	A	108	TYR	CB-CG-CD1	6.68	125.01	121.00
1	A	62	ASP	CB-CG-OD2	6.56	124.20	118.30
1	B	6	ASP	CB-CG-OD1	6.49	124.14	118.30
1	B	115	PRO	C-N-CA	6.43	135.81	122.30
1	D	110	PHE	CB-CA-C	5.93	122.26	110.40
1	A	108	TYR	CB-CG-CD2	-5.89	117.47	121.00
1	A	64	MET	CG-SD-CE	-5.79	90.94	100.20
1	B	94	SER	N-CA-CB	-5.59	102.11	110.50
1	C	79	ARG	NE-CZ-NH2	5.52	123.06	120.30
1	A	6	ASP	CB-CG-OD2	5.24	123.02	118.30
1	D	106	GLU	CB-CA-C	5.16	120.71	110.40
1	C	106	GLU	CB-CA-C	5.14	120.67	110.40
1	A	119	ALA	CB-CA-C	5.10	117.75	110.10
1	D	121	MET	CA-CB-CG	5.09	121.95	113.30
1	A	4	SER	N-CA-CB	5.04	118.06	110.50

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	37	GLY	Peptide
1	A	48	TRP	Mainchain
1	A	96	THR	Mainchain
1	B	37	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	C	37	GLY	Peptide

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	977	0	959	7	0
1	B	967	0	942	15	0
1	C	966	0	940	4	0
1	D	972	0	948	17	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	6	0	0	1	0
4	B	8	0	0	0	0
4	C	8	0	0	0	0
4	D	7	0	0	1	0
All	All	3918	0	3789	40	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 5.

All (40) 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:57:GLN:HE21	1:B:61:THR:HG23	1.32	0.93
1:B:57:GLN:NE2	1:B:61:THR:HG23	2.04	0.71
1:D:58:GLY:HA3	1:D:79:ARG:NH2	2.07	0.69
1:D:107[A]:GLN:HE22	1:D:124:THR:HG22	1.57	0.69
1:D:36:PRO:O	1:D:37:GLY:O	2.20	0.58
1:B:57:GLN:HE21	1:B:61:THR:CG2	2.09	0.57
1:C:36:PRO:O	1:C:37:GLY:O	2.22	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:MET:HE1	1:B:64:MET:SD	2.45	0.56
1:A:64:MET:HE1	1:B:115:PRO:HB3	1.88	0.55
1:D:7:ILE:HD11	1:D:20:ILE:HD11	1.90	0.54
1:A:36:PRO:O	1:A:37:GLY:O	2.26	0.53
1:B:36:PRO:O	1:B:37:GLY:O	2.26	0.52
1:A:64:MET:CE	1:B:64:MET:SD	2.98	0.52
1:D:58:GLY:HA3	1:D:79:ARG:HH22	1.74	0.50
1:A:57[A]:GLN:HG2	4:A:306:HOH:O	2.11	0.50
1:D:42:ASN:HA	1:D:68:LEU:HD13	1.93	0.50
1:D:29:PHE:O	1:D:96:THR:HA	2.13	0.48
1:B:13:MET:HB2	1:B:44[B]:MET:HE1	1.95	0.48
1:D:8:GLN:OE1	1:D:36:PRO:HG3	2.15	0.47
1:D:11:ASP:HA	1:D:44[A]:MET:HG2	1.97	0.47
1:B:11:ASP:HA	1:B:44[B]:MET:HG2	1.98	0.46
1:A:127:LEU:HD23	1:A:127:LEU:HA	1.78	0.46
1:D:26:CYS:O	4:D:301:HOH:O	2.21	0.46
1:C:120:LEU:N	1:C:120:LEU:HD23	2.32	0.45
1:D:74:LYS:HB3	1:D:77:ASP:HB2	1.98	0.45
1:B:11:ASP:HA	1:B:44[A]:MET:HG2	2.00	0.44
1:B:127:LEU:HD23	1:B:127:LEU:HA	1.52	0.44
1:C:7:ILE:HD11	1:C:20:ILE:HD11	2.00	0.43
1:C:127:LEU:HD23	1:C:127:LEU:HA	1.83	0.43
1:D:58:GLY:CA	1:D:79:ARG:HH22	2.31	0.43
1:D:49:VAL:O	1:D:110:PHE:HA	2.19	0.42
1:D:58:GLY:CA	1:D:79:ARG:NH2	2.78	0.42
1:A:10:ASN:O	1:A:46:HIS:NE2	2.42	0.42
1:B:103:LYS:HB3	1:B:103:LYS:HE2	1.87	0.42
1:B:13:MET:CA	1:B:44[B]:MET:CE	2.98	0.42
1:D:120:LEU:HD23	1:D:120:LEU:HA	1.85	0.41
1:B:46:HIS:CE1	1:B:121:MET:SD	3.13	0.41
1:D:127:LEU:HD23	1:D:127:LEU:HA	1.78	0.41
1:B:49:VAL:O	1:B:110:PHE:HA	2.20	0.41
1:D:11:ASP:HA	1:D:44[B]:MET:HG2	2.03	0.41

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	128/127 (101%)	119 (93%)	8 (6%)	1 (1%)	19	13
1	B	126/127 (99%)	119 (94%)	6 (5%)	1 (1%)	19	13
1	C	126/127 (99%)	121 (96%)	4 (3%)	1 (1%)	19	13
1	D	127/127 (100%)	122 (96%)	4 (3%)	1 (1%)	19	13
All	All	507/508 (100%)	481 (95%)	22 (4%)	4 (1%)	19	13

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	37	GLY
1	D	37	GLY
1	A	37	GLY
1	B	37	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	111/110 (101%)	105 (95%)	6 (5%)	22	18
1	B	109/110 (99%)	101 (93%)	8 (7%)	14	9
1	C	109/110 (99%)	106 (97%)	3 (3%)	43	44
1	D	110/110 (100%)	99 (90%)	11 (10%)	7	4
All	All	439/440 (100%)	411 (94%)	28 (6%)	18	13

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	SER
1	A	24	LYS
1	A	66	SER
1	A	120	LEU
1	A	122	LYS
1	A	127	LEU
1	B	24	LYS
1	B	66	SER
1	B	69	ASP
1	B	92	LYS
1	B	94	SER
1	B	122	LYS
1	B	126	THR
1	B	127	LEU
1	C	66	SER
1	C	122	LYS
1	C	127	LEU
1	D	24	LYS
1	D	27	LYS
1	D	57	GLN
1	D	70	LYS
1	D	92	LYS
1	D	104	GLU
1	D	107[A]	GLN
1	D	107[B]	GLN
1	D	115	PRO
1	D	122	LYS
1	D	127	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	57	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 7 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, 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	127/127 (100%)	0.10	1 (0%) 86 85	24, 45, 73, 84	0
1	B	127/127 (100%)	0.29	2 (1%) 72 70	34, 54, 84, 106	0
1	C	127/127 (100%)	0.34	4 (3%) 49 48	30, 56, 87, 100	0
1	D	127/127 (100%)	0.72	14 (11%) 5 5	22, 56, 96, 112	0
All	All	508/508 (100%)	0.36	21 (4%) 37 36	22, 54, 87, 112	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	25	SER	6.0
1	C	128	LYS	5.2
1	D	43	VAL	4.2
1	D	3	CYS	4.1
1	D	104	GLU	3.7
1	B	76	ASP	3.4
1	D	36	PRO	3.4
1	B	26	CYS	3.4
1	C	120	LEU	2.8
1	D	4	SER	2.8
1	D	103	LYS	2.8
1	D	12	GLN	2.6
1	D	26	CYS	2.6
1	D	39	LEU	2.5
1	D	33	LEU	2.5
1	D	2	GLU	2.4
1	A	88	GLY	2.3
1	D	37	GLY	2.2
1	D	128	LYS	2.1
1	C	43	VAL	2.1
1	C	87	ILE	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](#)

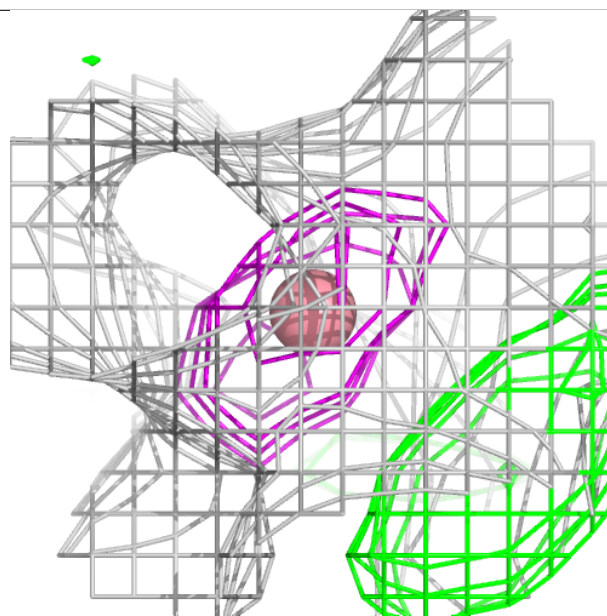
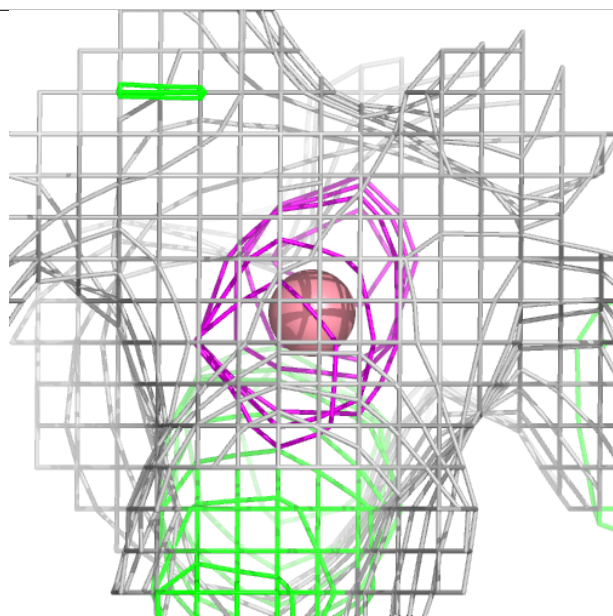
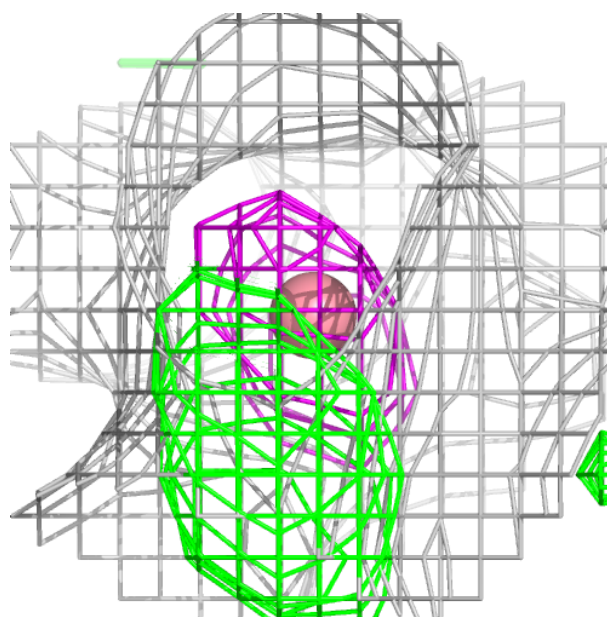
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	CA	C	202	1/1	0.83	0.07	91,91,91,91	0
3	CA	A	202	1/1	0.94	0.17	60,60,60,60	0
3	CA	B	202	1/1	0.95	0.07	71,71,71,71	0
2	CO	D	201	1/1	0.96	0.03	44,44,44,44	0
2	CO	B	201	1/1	0.97	0.04	47,47,47,47	0
2	CO	A	201	1/1	0.99	0.04	41,41,41,41	0
2	CO	C	201	1/1	0.99	0.04	54,54,54,54	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.

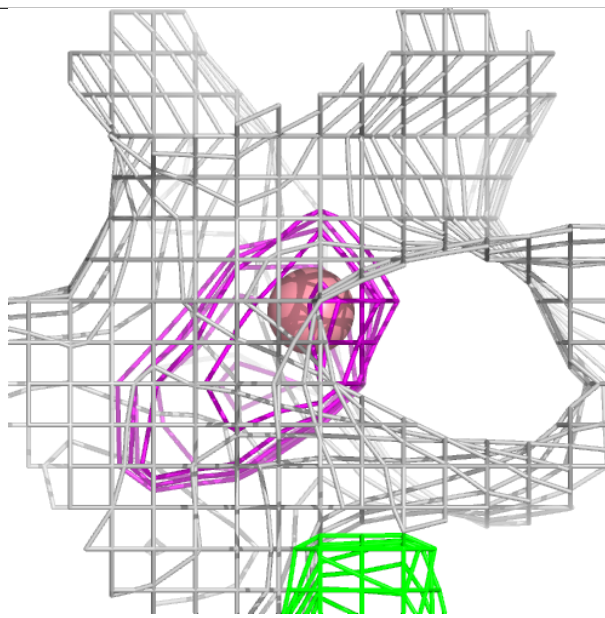
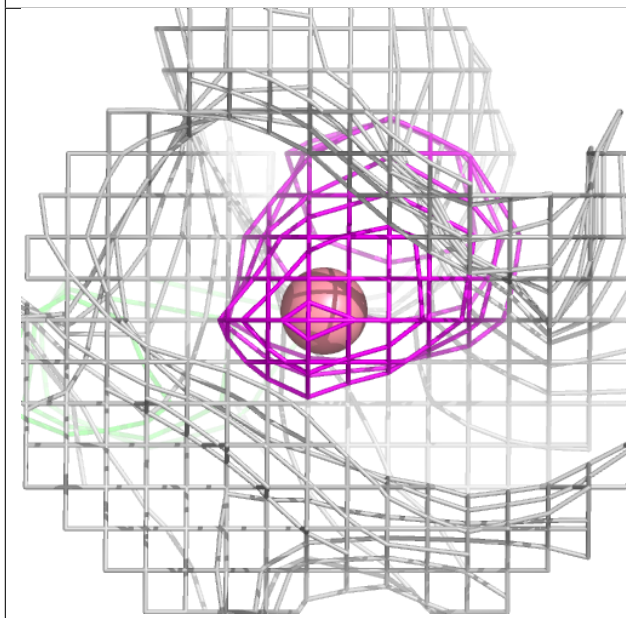
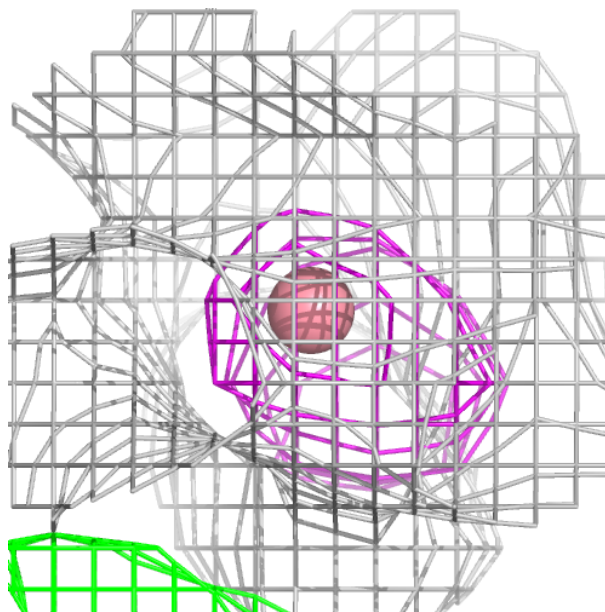
Electron density around CO D 201:

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



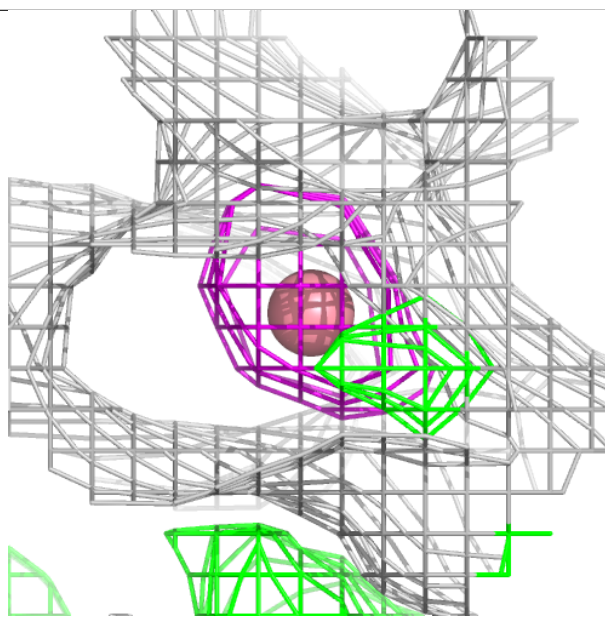
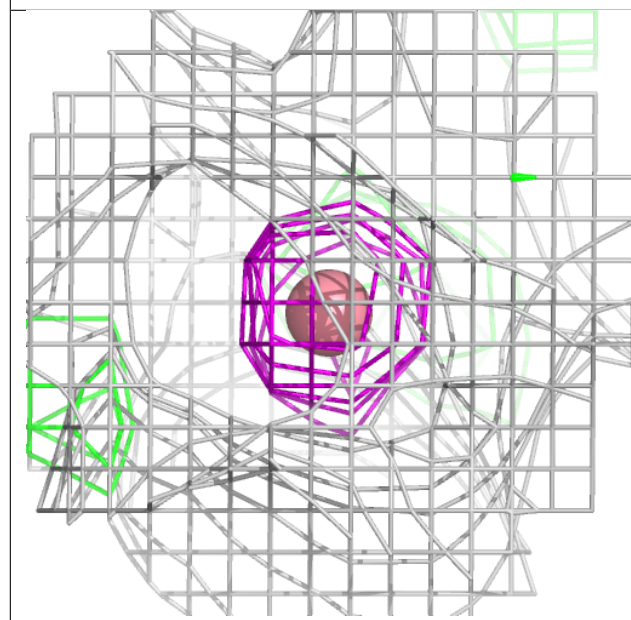
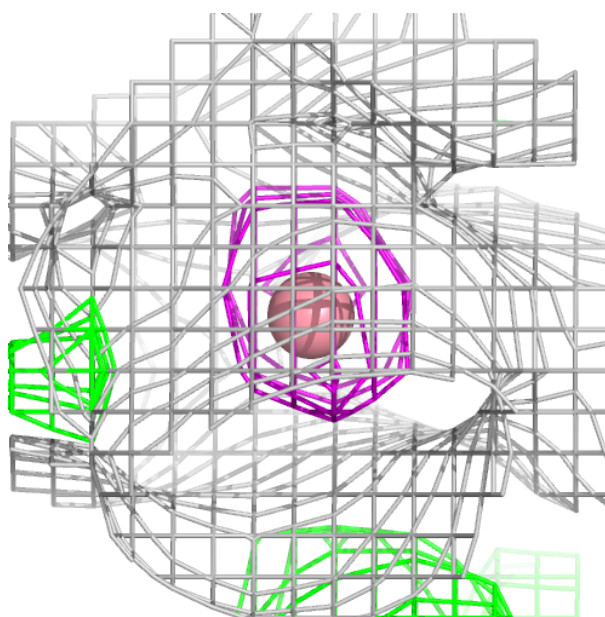
Electron density around CO B 201:

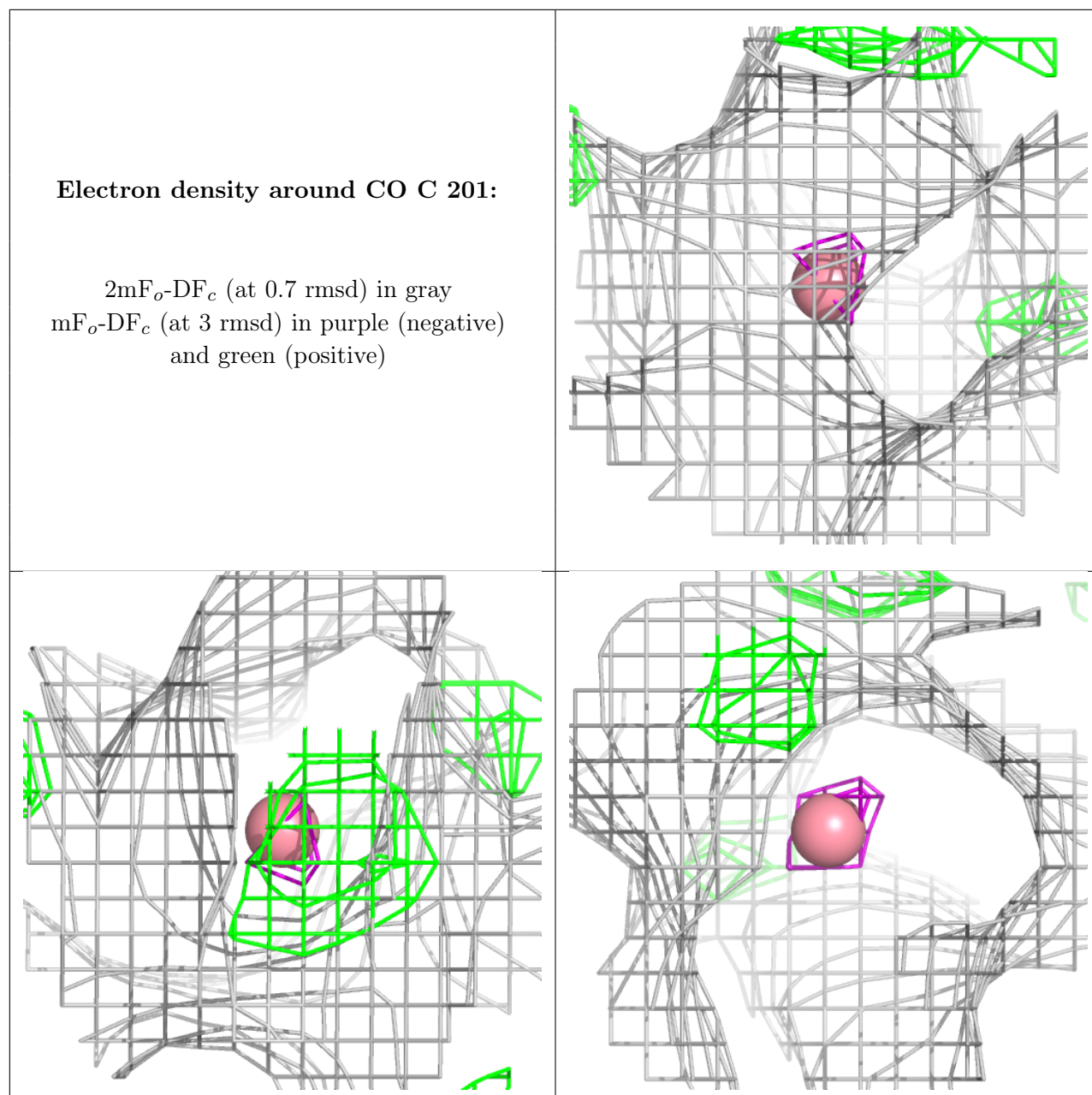
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CO 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.