



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 07:43 AM UTC

PDB ID : 6IAV / pdb_00006iav
Title : CO-AZURIN FROM PSEUDOMONAS AERUGINOSA TREATED WITH
HYDROSULFIDE
Authors : Palm, G.J.; Kohlhaase, D.
Deposited on : 2018-11-27
Resolution : 2.00 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 ⓘ 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

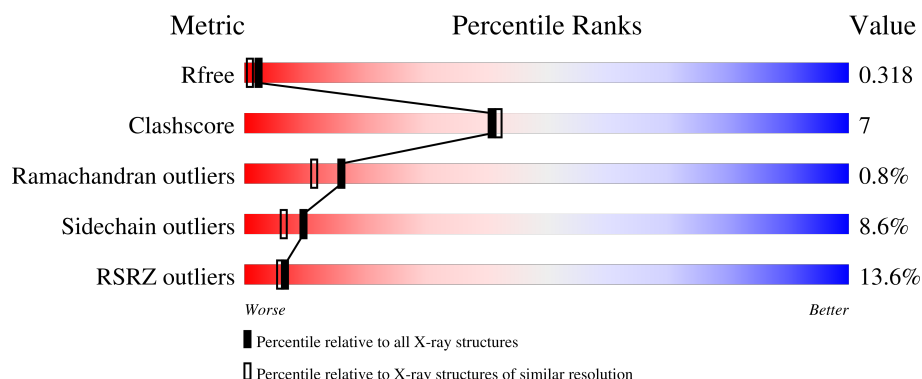
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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	5% 66% 29% ..
1	B	127	10% 62% 29% 7% .
1	C	127	11% 65% 31% ..
1	D	127	28% 49% 40% 10% .

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
1	A	127	Total	C	N	O	S	0	3	0
			977	613	163	191	10			
1	B	127	Total	C	N	O	S	0	1	0
			967	605	162	190	10			
1	C	127	Total	C	N	O	S	0	1	0
			966	604	162	190	10			
1	D	127	Total	C	N	O	S	0	2	0
			972	608	163	191	10			

- Molecule 2 is COBALT (II) ION (CCD ID: CO) (formula: Co) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

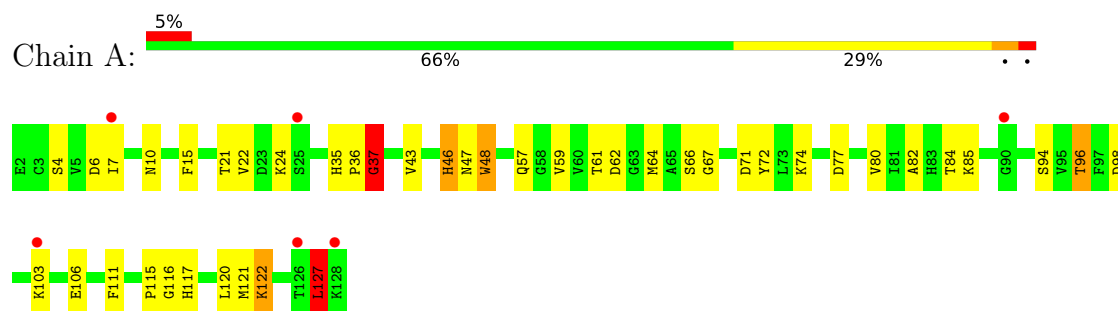
- Molecule 4 is water.

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

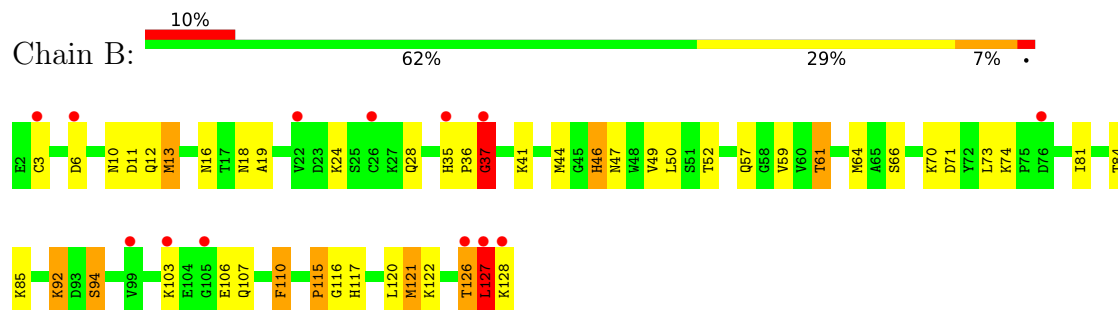
3 Residue-property plots [i](#)

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.

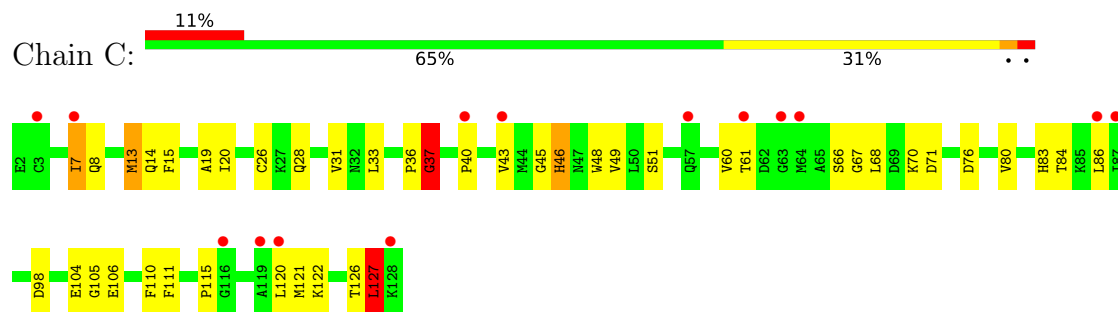
• Molecule 1: Azurin



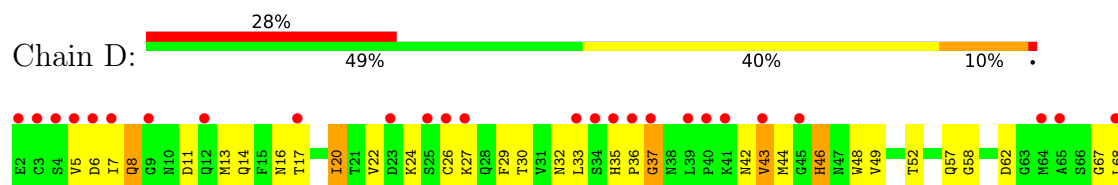
• Molecule 1: Azurin

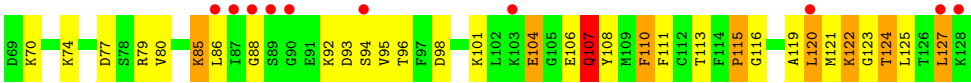


• Molecule 1: Azurin



• Molecule 1: Azurin





4 Data and refinement statistics

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 50.48 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.2 (50.48-2.00) 96.2 (50.48-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.72 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.250 , 0.310 0.255 , 0.318	Depositor DCC
R_{free} test set	1565 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å ²)	34.3	Xtriage
Anisotropy	0.653	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 51.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.068 for h,-k,-l	Xtriage
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

Xtriage'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	1.93	23/1003 (2.3%)	1.96	26/1353 (1.9%)
1	B	1.81	18/987 (1.8%)	1.96	24/1331 (1.8%)
1	C	1.78	19/986 (1.9%)	1.81	21/1330 (1.6%)
1	D	2.03	32/995 (3.2%)	1.98	27/1342 (2.0%)
All	All	1.89	92/3971 (2.3%)	1.93	98/5356 (1.8%)

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

The worst 5 of 92 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	46	HIS	CE1-NE2	13.01	1.45	1.32
1	A	35	HIS	CE1-NE2	12.96	1.45	1.32
1	D	17	THR	C-O	12.42	1.38	1.23
1	B	46	HIS	CE1-NE2	11.67	1.44	1.32
1	A	46	HIS	CE1-NE2	11.12	1.43	1.32

The worst 5 of 98 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	74	LYS	CA-C-O	-9.23	112.36	119.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	115	PRO	CA-C-N	8.96	135.81	122.10
1	B	115	PRO	C-N-CA	8.96	135.81	122.10
1	B	128	LYS	CA-C-O	7.91	134.25	120.80
1	C	76	ASP	CA-CB-CG	-7.89	104.71	112.60

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
1	C	37	GLY	Peptide

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	977	0	959	8	0
1	B	967	0	942	21	0
1	C	966	0	940	6	0
1	D	972	0	948	18	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	50	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 7.

The worst 5 of 50 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:A:64:MET:HE3	1:B:64:MET:SD	2.17	0.83
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

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%)	16	11
1	B	126/127 (99%)	119 (94%)	6 (5%)	1 (1%)	16	11
1	C	126/127 (99%)	121 (96%)	4 (3%)	1 (1%)	16	11
1	D	127/127 (100%)	122 (96%)	4 (3%)	1 (1%)	16	11
All	All	507/508 (100%)	481 (95%)	22 (4%)	4 (1%)	16	11

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%)	103 (93%)	8 (7%)	13	10
1	B	109/110 (99%)	98 (90%)	11 (10%)	7	4
1	C	109/110 (99%)	103 (94%)	6 (6%)	19	17
1	D	110/110 (100%)	97 (88%)	13 (12%)	5	3
All	All	439/440 (100%)	401 (91%)	38 (9%)	10	6

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	57	GLN
1	D	115	PRO
1	D	70	LYS
1	D	104	GLU
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 [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 oligosaccharides in this entry.

5.6 Ligand geometry

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

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	0.48	6 (4%) 36 35	24, 45, 73, 84	3 (2%)
1	B	127/127 (100%)	0.84	13 (10%) 12 11	34, 54, 84, 106	1 (0%)
1	C	127/127 (100%)	0.99	14 (11%) 10 9	30, 55, 86, 100	1 (0%)
1	D	127/127 (100%)	1.49	36 (28%) 1 1	22, 56, 96, 112	2 (1%)
All	All	508/508 (100%)	0.95	69 (13%) 7 6	22, 53, 87, 112	7 (1%)

The worst 5 of 69 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	43	VAL	4.7
1	D	68	LEU	4.7
1	D	128	LYS	4.6
1	D	36	PRO	4.3
1	D	39	LEU	4.1

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

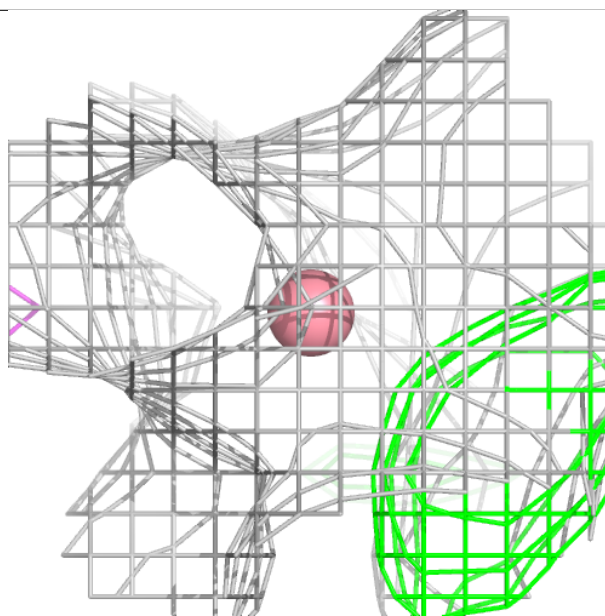
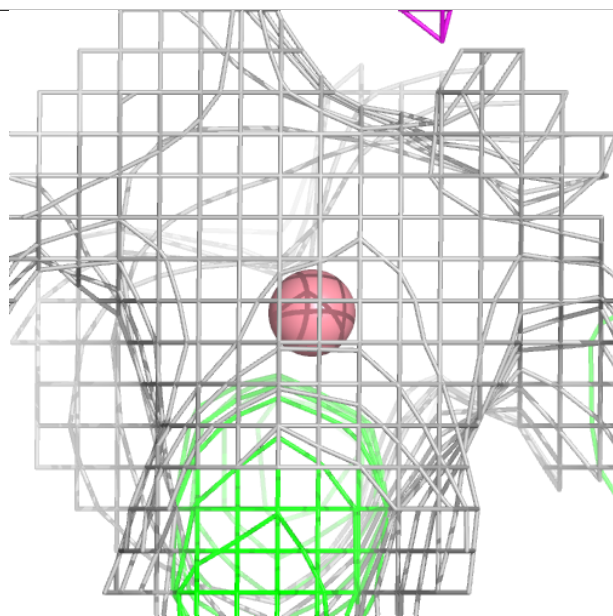
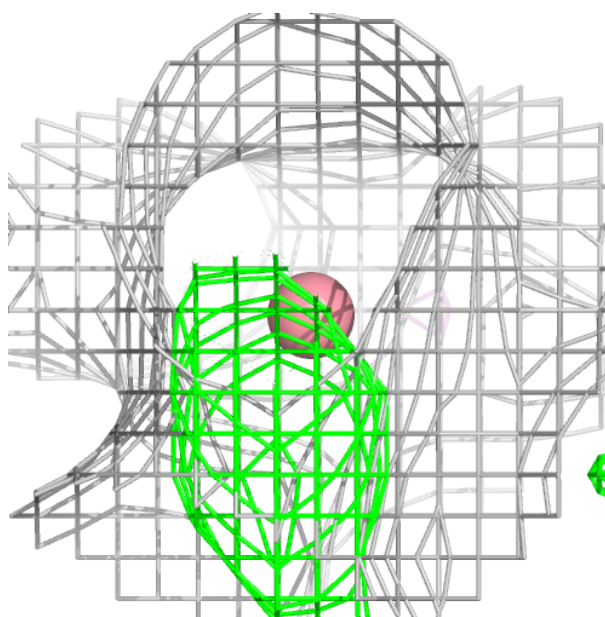
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CA	B	202	1/1	0.86	0.11	71,71,71,71	0
3	CA	C	202	1/1	0.86	0.12	91,91,91,91	0
3	CA	A	202	1/1	0.94	0.12	60,60,60,60	0
2	CO	D	201	1/1	0.95	0.05	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	0.98	0.04	41,41,41,41	0
2	CO	C	201	1/1	0.98	0.06	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.

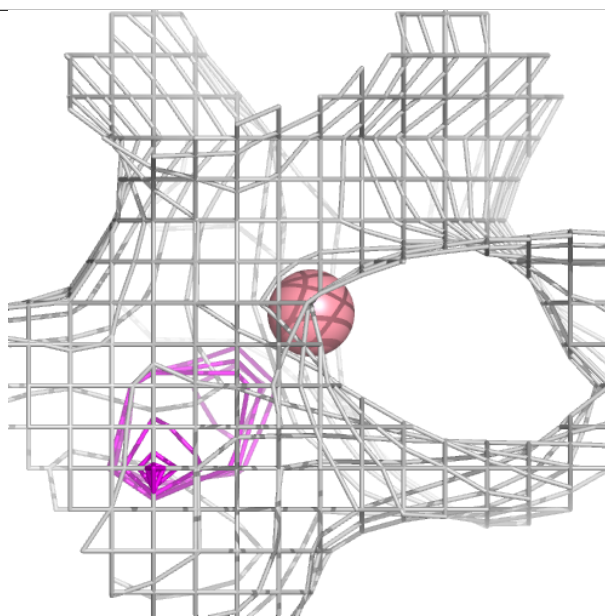
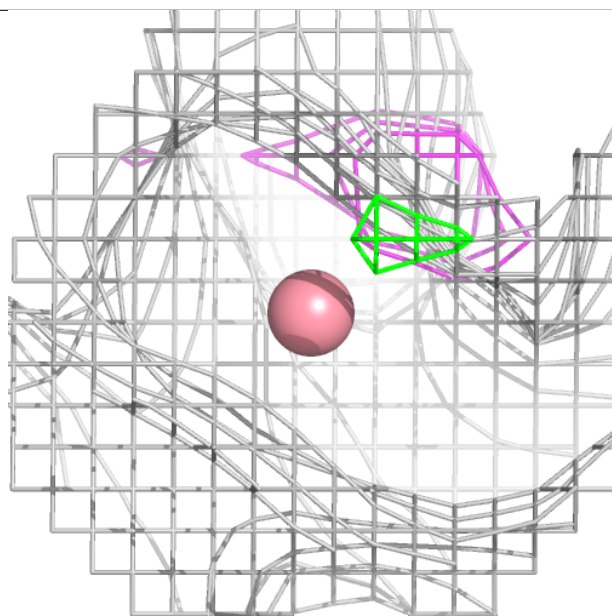
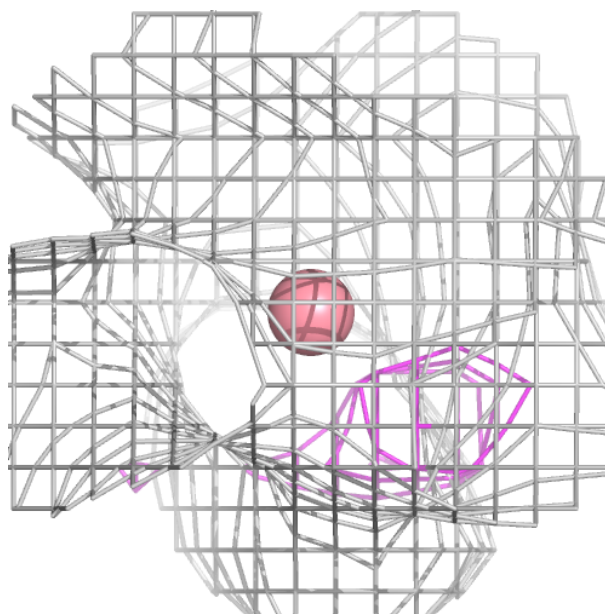
Electron density around CO D 201:

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



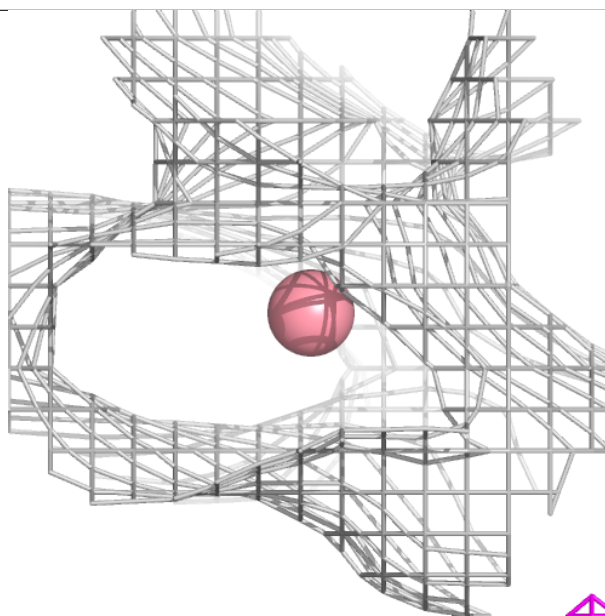
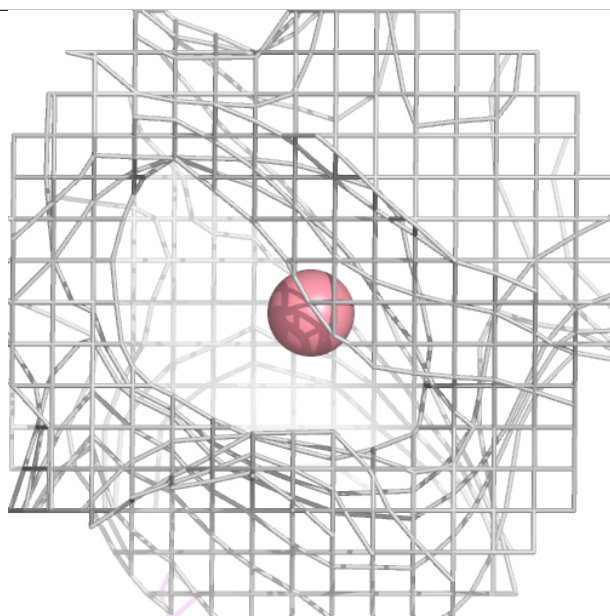
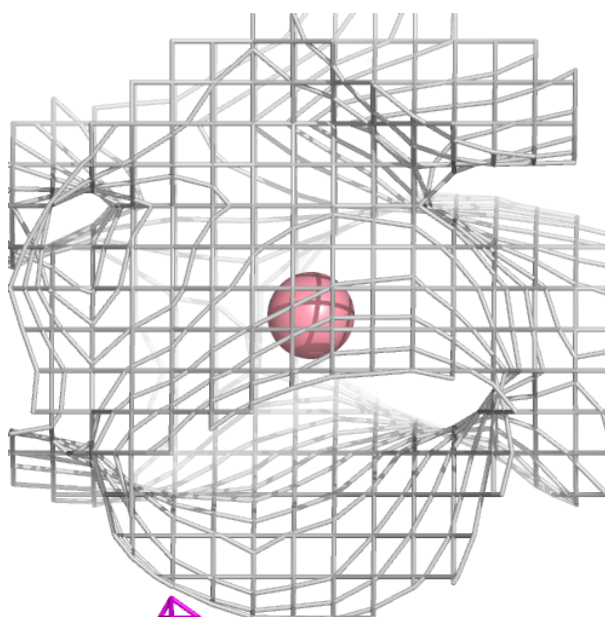
Electron density around CO B 201:

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



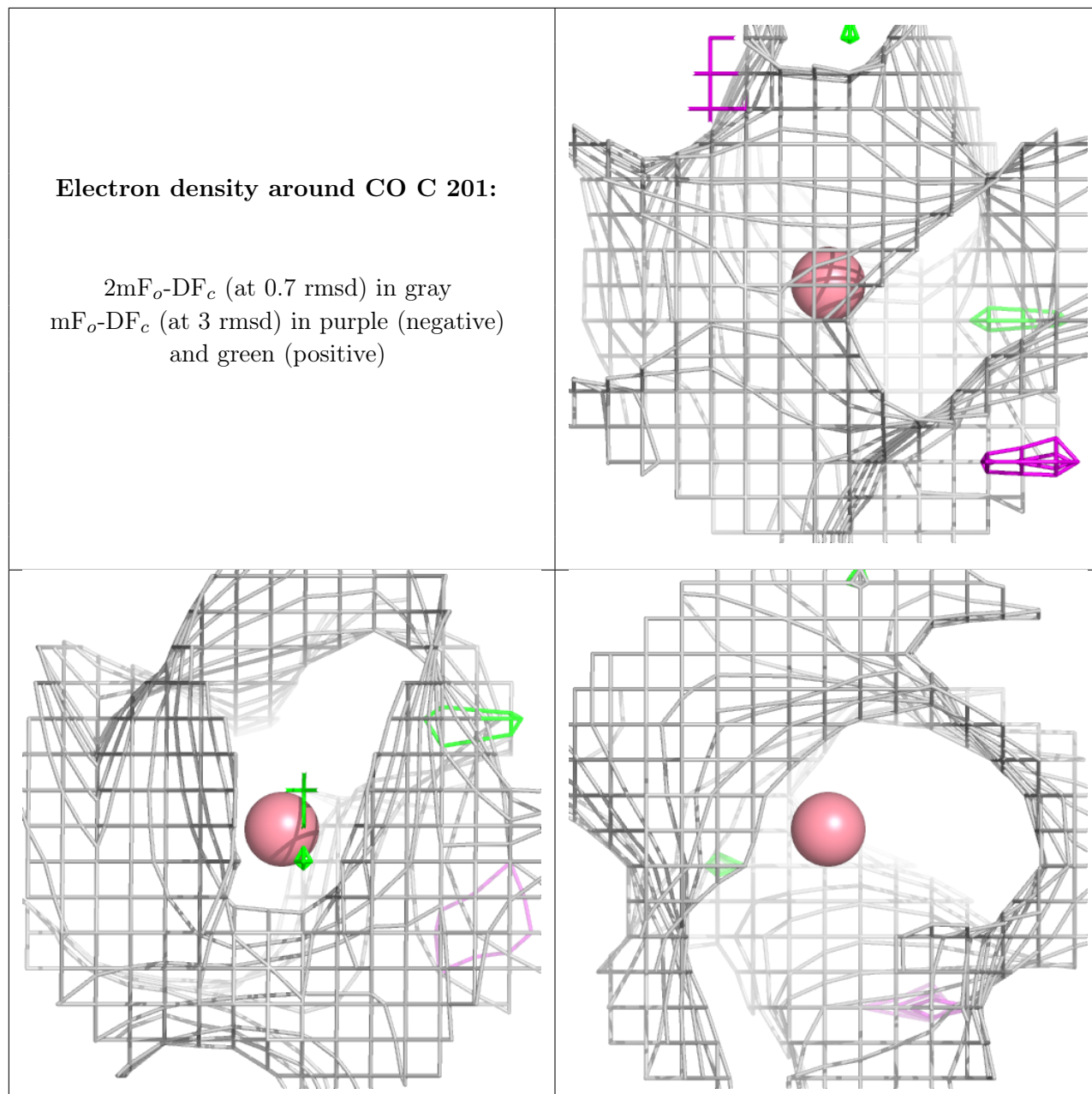
Electron density around CO A 201:

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



Electron density around CO 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)

**6.5 Other polymers** ⓘ

There are no such residues in this entry.