



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:35 AM UTC

PDB ID : 6GRR / pdb_00006grr
Title : Crystal structure of Escherichia coli amine oxidase mutant I342F/E573Q
Authors : Gaule, T.G.; Smith, M.A.; Tych, K.M.; Pirrat, P.; Trinh, C.H.; Pearson, A.R.; Knowles, P.F.; McPherson, M.J.
Deposited on : 2018-06-12
Resolution : 1.70 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
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

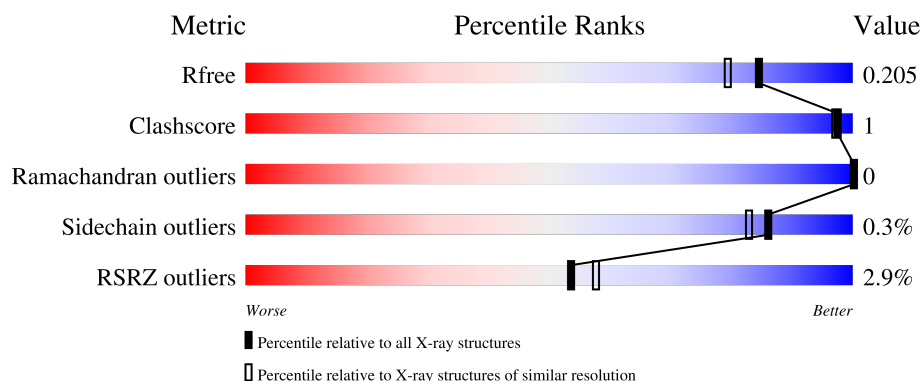
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	718	% 97% .
2	B	720	4% 98% .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12661 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 Amine oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	718	Total	C	N	O	S	0	1	0
			5673	3610	966	1074	23			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	342	PHE	ILE	engineered mutation	UNP A0A2K0PX72
A	573	GLN	GLU	engineered mutation	UNP A0A2K0PX72

- Molecule 2 is a protein called Amine oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	720	Total	C	N	O	S	0	3	0
			5712	3633	976	1080	23			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	342	PHE	ILE	engineered mutation	UNP A0A2K0PX72
B	573	GLN	GLU	engineered mutation	UNP A0A2K0PX72

- Molecule 3 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

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

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	654	Total	O	0	1
			655	655		
6	B	551	Total	O	0	0
			551	551		

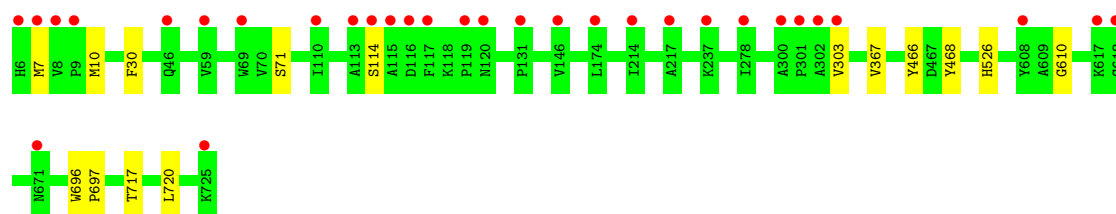
3 Residue-property plots [i](#)

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: Amine oxidase



- Molecule 2: Amine oxidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	135.15Å 166.84Å 79.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	105.05 – 1.70 105.02 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.2 (105.05-1.70) 99.2 (105.02-1.70)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.166 , 0.193 0.178 , 0.205	Depositor DCC
R_{free} test set	6714 reflections (3.39%)	wwPDB-VP
Wilson B-factor (Å ²)	27.0	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 33.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12661	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% 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: GOL, CU, 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	0.69	0/5819	0.83	3/7922 (0.0%)
2	B	0.68	0/5859	0.80	0/7975
All	All	0.68	0/11678	0.81	3/15897 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	148	GLN	N-CA-CB	-11.22	96.46	110.03
1	A	148	GLN	N-CA-C	8.69	122.28	110.29
1	A	147	ASP	CB-CA-C	6.89	123.65	109.95

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	5673	0	5549	10	0
2	B	5712	0	5587	10	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	36	0	48	0	0
5	B	30	0	40	0	0
6	A	655	0	0	0	0
6	B	551	0	0	1	0
All	All	12661	0	11224	18	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 1.

All (18) 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:7:MET:HE1	1:A:59:VAL:HG11	1.73	0.71
2:B:303:VAL:O	6:B:901:HOH:O	2.10	0.68
1:A:129:LEU:HD12	1:A:130:PRO:HD2	1.84	0.60
2:B:10:MET:HE1	2:B:30:PHE:CE1	2.46	0.51
2:B:10:MET:HE1	2:B:30:PHE:CD1	2.49	0.47
1:A:516:ASP:HB3	1:A:519:ILE:HB	1.97	0.46
1:A:90:GLU:OE2	1:A:322[A]:MET:HE2	2.18	0.44
2:B:466:TYR:CE2	2:B:526:HIS:HE1	2.34	0.44
1:A:326:ARG:NH2	2:B:303:VAL:HG23	2.32	0.44
1:A:610:GLY:HA3	2:B:610:GLY:HA3	2.00	0.44
1:A:13:THR:HG22	1:A:75:ILE:CD1	2.47	0.43
2:B:717:THR:HB	2:B:720:LEU:HG	2.01	0.43
2:B:7:MET:HG2	2:B:71:SER:HA	1.99	0.43
2:B:367:VAL:HG21	2:B:468:TYR:OH	2.20	0.42
1:A:642:ARG:CD	1:A:672:GLU:HG2	2.51	0.41
2:B:696:TRP:CD2	2:B:697:PRO:HA	2.56	0.40
1:A:15:LYS:HA	1:A:15:LYS:HE2	2.03	0.40
1:A:117:PHE:CZ	1:A:121:THR:HB	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	717/718 (100%)	708 (99%)	9 (1%)	0	100	100
2	B	721/720 (100%)	709 (98%)	12 (2%)	0	100	100
All	All	1438/1438 (100%)	1417 (98%)	21 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	611/610 (100%)	608 (100%)	3 (0%)	81	76
2	B	615/612 (100%)	614 (100%)	1 (0%)	87	84
All	All	1226/1222 (100%)	1222 (100%)	4 (0%)	86	83

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ASP
1	A	67	LYS
1	A	147	ASP
2	B	114	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	143	ASN
1	A	201	ASN
1	A	307	GLN
1	A	324	HIS
1	A	327	ASN
1	A	350	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	529	ASN
1	A	567	GLN
1	A	599	ASN
1	A	660	HIS
2	B	201	ASN
2	B	263	ASN
2	B	327	ASN
2	B	350	ASN
2	B	567	GLN
2	B	573	GLN
2	B	574	GLN
2	B	599	ASN

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 [i](#)

Of 15 ligands modelled in this entry, 4 are monoatomic - leaving 11 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	$\# Z > 2$
5	GOL	A	807	-	5,5,5	0.59	0	5,5,5	0.74	0
5	GOL	A	803	-	5,5,5	0.37	0	5,5,5	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	B	804	-	5,5,5	0.48	0	5,5,5	1.35	1 (20%)
5	GOL	B	806	-	5,5,5	0.32	0	5,5,5	0.87	0
5	GOL	A	805	-	5,5,5	0.44	0	5,5,5	1.01	0
5	GOL	A	804	-	5,5,5	0.55	0	5,5,5	0.32	0
5	GOL	B	803	-	5,5,5	0.39	0	5,5,5	0.52	0
5	GOL	B	805	-	5,5,5	0.33	0	5,5,5	0.42	0
5	GOL	B	807	-	5,5,5	0.15	0	5,5,5	0.52	0
5	GOL	A	806	-	5,5,5	0.39	0	5,5,5	0.60	0
5	GOL	A	808	-	5,5,5	0.61	0	5,5,5	1.35	1 (20%)

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
5	GOL	A	807	-	-	4/4/4/4	-
5	GOL	A	803	-	-	0/4/4/4	-
5	GOL	B	804	-	-	2/4/4/4	-
5	GOL	B	806	-	-	2/4/4/4	-
5	GOL	A	805	-	-	3/4/4/4	-
5	GOL	A	804	-	-	0/4/4/4	-
5	GOL	B	803	-	-	0/4/4/4	-
5	GOL	B	805	-	-	2/4/4/4	-
5	GOL	B	807	-	-	0/4/4/4	-
5	GOL	A	806	-	-	3/4/4/4	-
5	GOL	A	808	-	-	2/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	804	GOL	C3-C2-C1	2.28	120.14	111.80
5	A	808	GOL	C3-C2-C1	2.10	119.48	111.80

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	806	GOL	O1-C1-C2-C3
5	A	807	GOL	O1-C1-C2-C3
5	A	807	GOL	C1-C2-C3-O3
5	A	807	GOL	O2-C2-C3-O3
5	A	808	GOL	C1-C2-C3-O3
5	A	808	GOL	O2-C2-C3-O3
5	B	804	GOL	C1-C2-C3-O3
5	B	804	GOL	O2-C2-C3-O3
5	B	805	GOL	C1-C2-C3-O3
5	A	805	GOL	O1-C1-C2-C3
5	A	805	GOL	C1-C2-C3-O3
5	B	806	GOL	O1-C1-C2-C3
5	A	806	GOL	O1-C1-C2-O2
5	A	807	GOL	O1-C1-C2-O2
5	B	805	GOL	O2-C2-C3-O3
5	B	806	GOL	O1-C1-C2-O2
5	A	806	GOL	O2-C2-C3-O3
5	A	805	GOL	O1-C1-C2-O2

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	718/718 (100%)	0.07	10 (1%) 73 77	12, 29, 49, 70	1 (0%)
2	B	720/720 (100%)	0.33	31 (4%) 40 44	14, 33, 60, 87	3 (0%)
All	All	1438/1438 (100%)	0.20	41 (2%) 53 58	12, 31, 54, 87	4 (0%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	301	PRO	4.7
2	B	725	LYS	4.0
2	B	302	ALA	4.0
2	B	6	HIS	3.7
2	B	303	VAL	3.5
2	B	117	PHE	3.4
2	B	119	PRO	3.4
1	A	130	PRO	3.4
2	B	115	ALA	3.3
2	B	120	ASN	3.1
2	B	46	GLN	3.1
1	A	148	GLN	3.0
2	B	59	VAL	2.8
1	A	608	TYR	2.8
2	B	7	MET	2.6
2	B	671	ASN	2.6
2	B	278	ILE	2.5
2	B	9	PRO	2.5
2	B	300	ALA	2.5
1	A	147	ASP	2.4
2	B	8	VAL	2.4
2	B	214	ILE	2.4
2	B	69	TRP	2.4
2	B	617	LYS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	7	MET	2.2
2	B	174	LEU	2.2
2	B	131	PRO	2.2
2	B	113	ALA	2.1
1	A	617	LYS	2.1
1	A	149	PRO	2.1
2	B	110	ILE	2.1
1	A	670	ASP	2.1
2	B	116	ASP	2.1
2	B	237	LYS	2.1
2	B	618	GLY	2.1
1	A	303	VAL	2.1
1	A	671	ASN	2.1
2	B	146	VAL	2.0
2	B	608	TYR	2.0
2	B	217	ALA	2.0
2	B	114	SER	2.0

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(Å ²)	Q<0.9
5	GOL	B	806	6/6	0.83	0.17	42,54,56,59	0
5	GOL	A	807	6/6	0.87	0.15	50,55,57,57	0
5	GOL	A	808	6/6	0.88	0.12	30,39,40,44	0
5	GOL	B	804	6/6	0.88	0.13	32,42,44,46	0
5	GOL	A	805	6/6	0.88	0.15	42,51,53,58	0
5	GOL	A	803	6/6	0.89	0.11	44,45,46,47	0

Continued on next page...

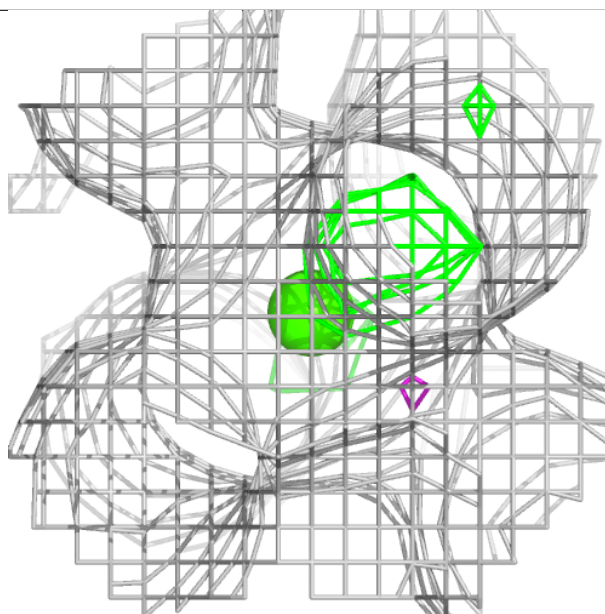
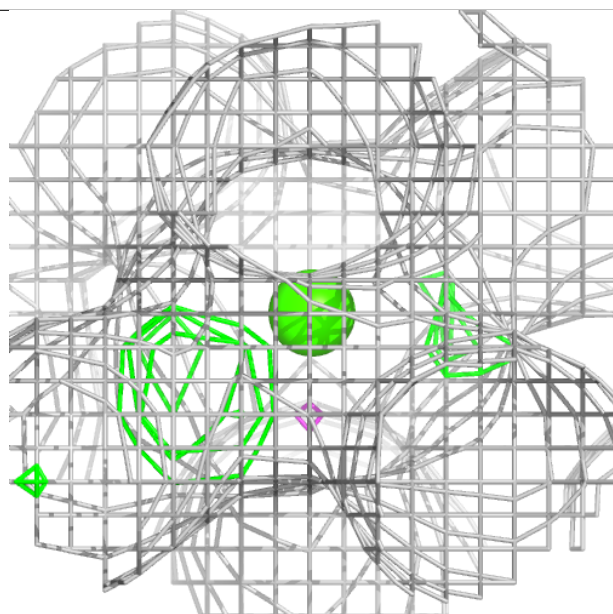
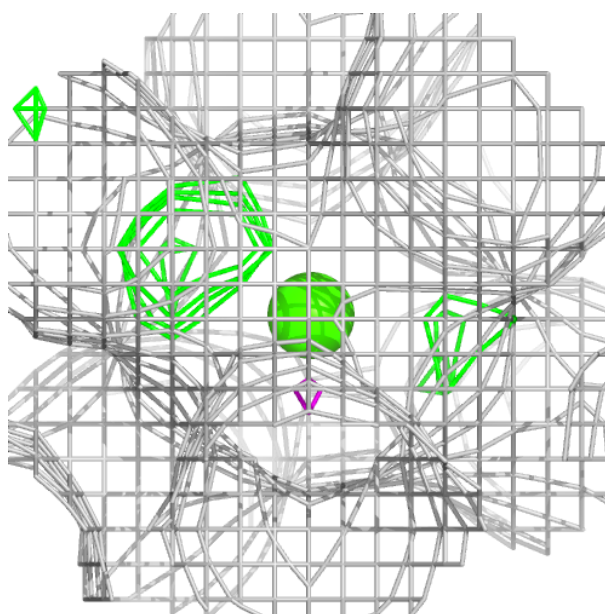
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GOL	B	805	6/6	0.90	0.13	68,68,69,69	0
5	GOL	A	806	6/6	0.91	0.12	34,45,47,50	0
5	GOL	A	804	6/6	0.91	0.10	34,38,40,41	0
5	GOL	B	807	6/6	0.91	0.11	31,43,45,53	0
5	GOL	B	803	6/6	0.96	0.08	28,31,33,36	0
4	CA	B	802	1/1	0.98	0.04	28,28,28,28	0
3	CU	A	801	1/1	0.99	0.02	26,26,26,26	0
3	CU	B	801	1/1	0.99	0.02	26,26,26,26	0
4	CA	A	802	1/1	0.99	0.03	23,23,23,23	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.

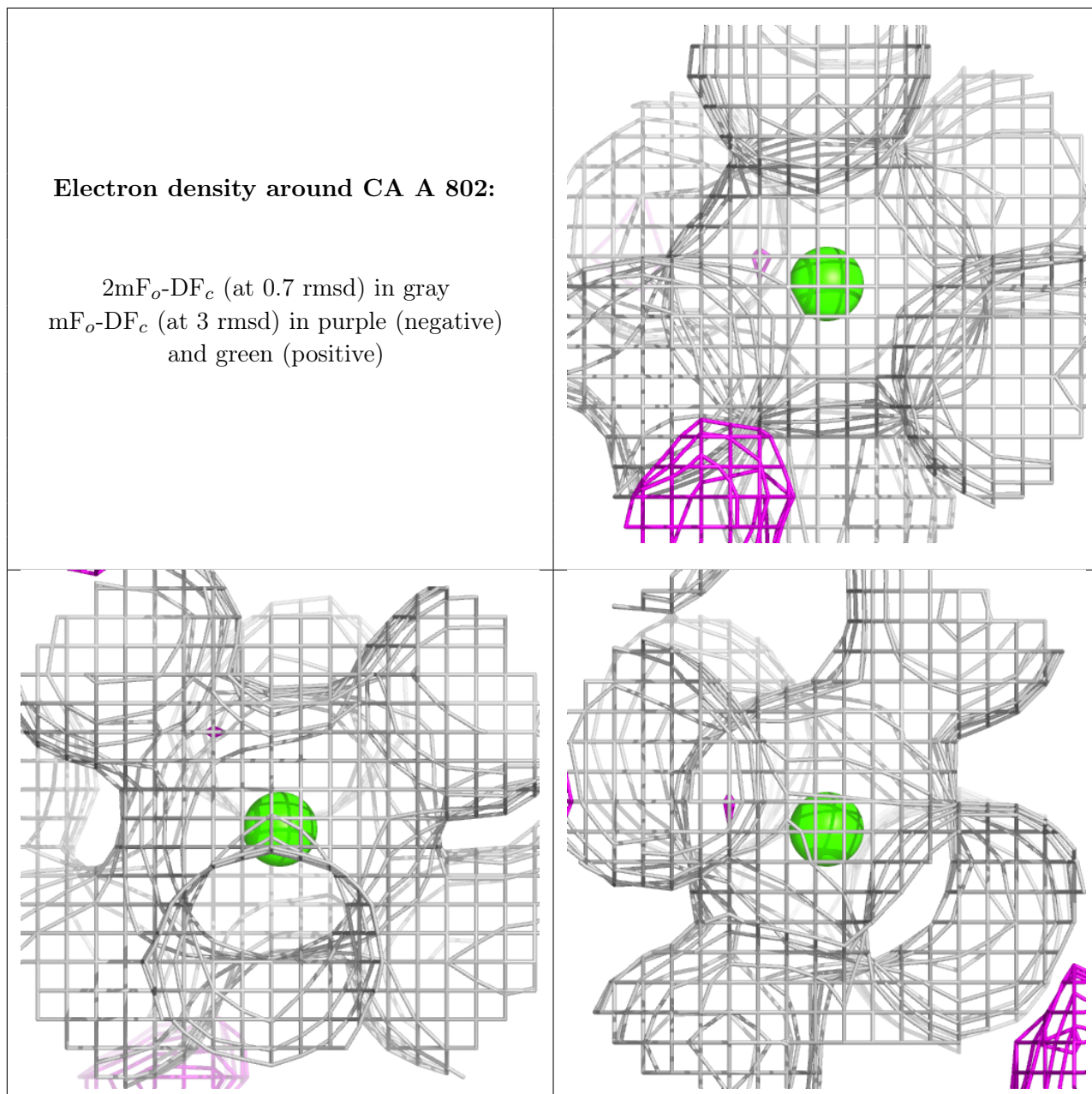
Electron density around CA B 802:

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



Electron density around CA A 802:

$2mF_o-DF_c$ (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.