



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:08 PM UTC

PDB ID : 8BHU / pdb_00008bhu
Title : Crystal Structure of SilF (Ag(I) form)
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Deposited on : 2022-11-01
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

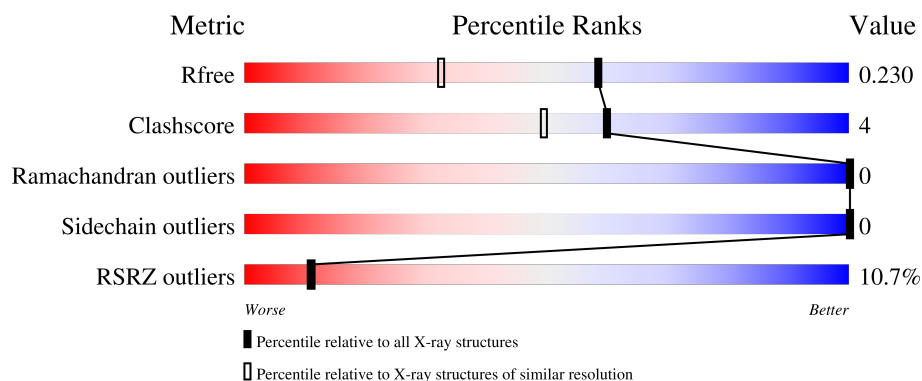
1 Overall quality at a glance

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	AAA	120	
1	BBB	120	
1	CCC	120	
1	DDD	120	
1	EEE	120	

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Mol	Chain	Length	Quality of chain
1	FFF	120	5% 58% 8% 35%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7457 atoms, of which 3667 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 SilF.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	77	Total	C	H	N	O	S	14	0	0
			1183	371	599	102	108	3			
1	BBB	80	Total	C	H	N	O	S	15	0	0
			1231	385	622	107	114	3			
1	CCC	78	Total	C	H	N	O	S	14	0	0
			1200	376	607	104	110	3			
1	DDD	79	Total	C	H	N	O	S	15	0	0
			1214	380	614	105	112	3			
1	EEE	77	Total	C	H	N	O	S	14	0	0
			1183	371	599	102	108	3			
1	FFF	78	Total	C	H	N	O	S	14	0	0
			1200	376	607	104	110	3			

- Molecule 2 is SILVER ION (CCD ID: AG) (formula: Ag) (labeled as "Ligand of Interest" by depositor).

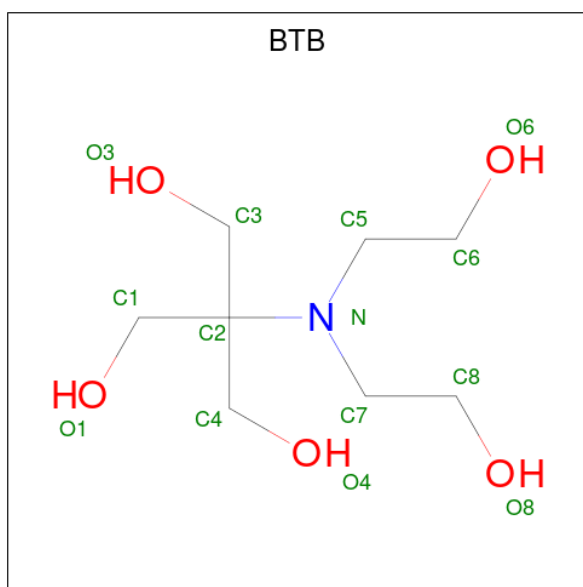
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	AAA	1	Total	Ag	0	0
			1	1		
2	BBB	1	Total	Ag	0	0
			1	1		
2	CCC	1	Total	Ag	0	0
			1	1		
2	DDD	1	Total	Ag	0	0
			1	1		
2	EEE	1	Total	Ag	0	0
			1	1		
2	FFF	1	Total	Ag	0	0
			1	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	AAA	1	Total	O	S	0	0
			5	4	1		
3	BBB	1	Total	O	S	0	0
			5	4	1		
3	CCC	1	Total	O	S	0	0
			5	4	1		
3	DDD	1	Total	O	S	0	0
			5	4	1		
3	DDD	1	Total	O	S	0	0
			5	4	1		
3	EEE	1	Total	O	S	0	0
			5	4	1		
3	FFF	1	Total	O	S	0	0
			5	4	1		
3	FFF	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (CCD ID: BTB) (formula: C₈H₁₉NO₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	BBB	1	Total	C	H	N	O	4	0
			33	8	19	1	5		

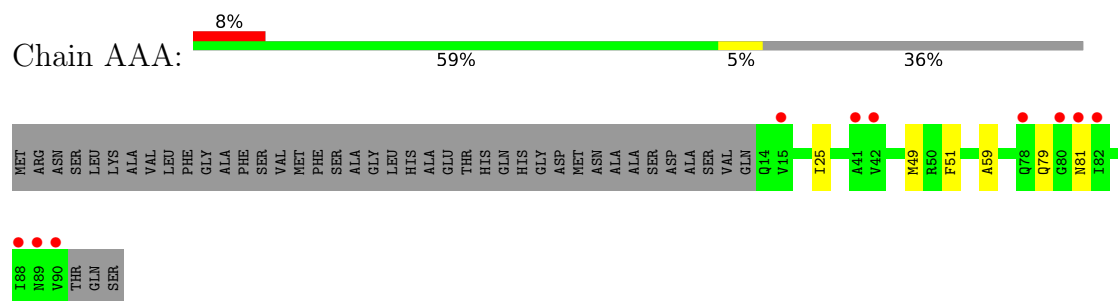
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	30	Total	O	0	0
			30	30		
5	BBB	30	Total	O	0	0
			30	30		
5	CCC	22	Total	O	0	0
			22	22		
5	DDD	30	Total	O	0	0
			30	30		
5	EEE	27	Total	O	0	0
			27	27		
5	FFF	28	Total	O	0	0
			28	28		

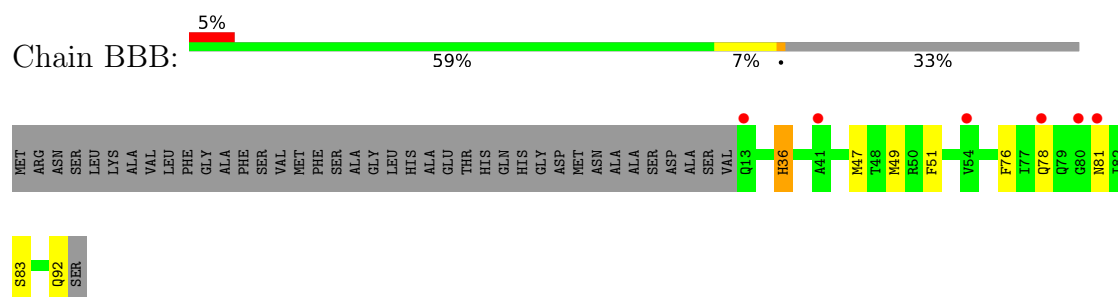
3 Residue-property plots [i](#)

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.

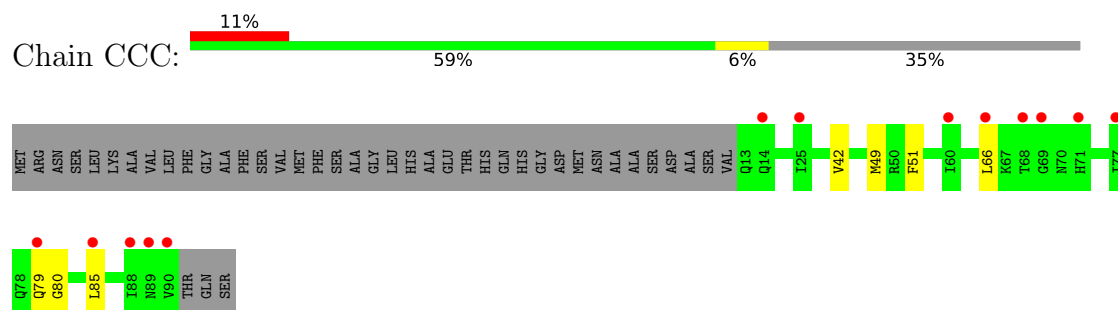
- Molecule 1: SilF



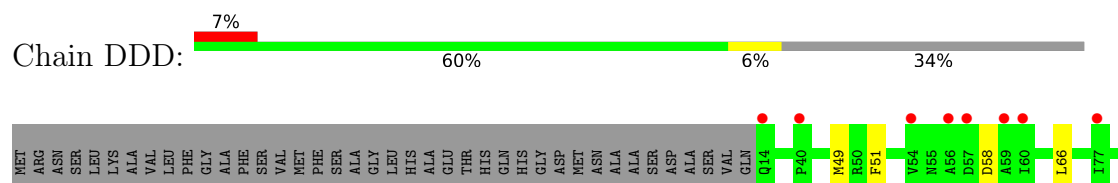
- Molecule 1: SilF



- Molecule 1: SilF

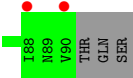


- Molecule 1: SilF

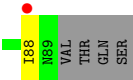
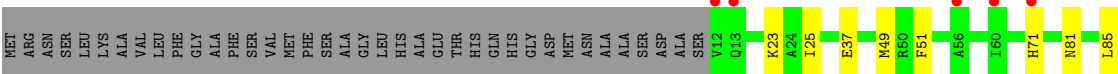




● Molecule 1: SilF



● Molecule 1: SilF



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	60.94Å 81.59Å 95.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	62.11 – 1.70 62.11 – 1.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (62.11-1.70) 100.0 (62.11-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.199 , 0.230 0.199 , 0.230	Depositor DCC
R_{free} test set	2620 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	26.6	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 25.3	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	0.96	EDS
Total number of atoms	7457	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.12% 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: AG, BTB, SO4

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	AAA	1.11	0/593	1.20	0/802
1	BBB	1.12	1/618 (0.2%)	1.21	1/836 (0.1%)
1	CCC	1.04	0/602	1.22	0/814
1	DDD	1.05	1/609 (0.2%)	1.26	0/824
1	EEE	1.07	0/593	1.23	1/802 (0.1%)
1	FFF	1.02	0/602	1.30	0/814
All	All	1.07	2/3617 (0.1%)	1.24	2/4892 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BBB	36	HIS	CE1-NE2	5.32	1.37	1.32
1	DDD	58	ASP	C-O	5.25	1.30	1.24

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	92	GLN	CA-C-O	-5.54	111.38	120.80
1	EEE	54	VAL	N-CA-C	-5.22	107.50	111.62

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	AAA	584	599	596	6	0
1	BBB	609	622	619	8	0
1	CCC	593	607	604	9	0
1	DDD	600	614	611	6	0
1	EEE	584	599	596	7	0
1	FFF	593	607	604	7	0
2	AAA	1	0	0	0	0
2	BBB	1	0	0	0	0
2	CCC	1	0	0	0	0
2	DDD	1	0	0	0	0
2	EEE	1	0	0	0	0
2	FFF	1	0	0	0	0
3	AAA	5	0	0	0	0
3	BBB	5	0	0	0	0
3	CCC	5	0	0	0	0
3	DDD	10	0	0	0	0
3	EEE	5	0	0	1	0
3	FFF	10	0	0	1	0
4	BBB	14	19	19	0	0
5	AAA	30	0	0	1	0
5	BBB	30	0	0	0	0
5	CCC	22	0	0	0	0
5	DDD	30	0	0	0	0
5	EEE	27	0	0	0	0
5	FFF	28	0	0	0	0
All	All	3790	3667	3649	31	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 (31) 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:CCC:79:GLN:HG2	1:EEE:42:VAL:O	1.67	0.93
1:BBB:76:PHE:HE2	1:BBB:78:GLN:HE21	1.19	0.87
1:BBB:78:GLN:NE2	1:BBB:83:SER:OG	2.25	0.68
1:FFF:23:LYS:HE3	3:FFF:103:SO4:O2	2.00	0.62
1:CCC:79:GLN:NE2	1:EEE:78:GLN:HE22	2.05	0.55
1:BBB:81:ASN:O	1:DDD:81:ASN:HB3	2.06	0.54
1:CCC:66:LEU:HD21	1:FFF:25:ILE:CG2	2.38	0.54
1:FFF:85:LEU:HD21	1:FFF:88:ILE:HD11	1.93	0.51
1:EEE:19:SER:HB2	1:EEE:71:HIS:CE1	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AAA:226:HOH:O	1:EEE:81:ASN:HB2	2.11	0.50
1:AAA:25:ILE:HD11	1:AAA:59:ALA:HB1	1.95	0.49
1:BBB:47:MET:HE1	1:DDD:82:ILE:HD12	1.95	0.48
1:CCC:66:LEU:HD21	1:FFF:25:ILE:HG23	1.96	0.48
1:AAA:81:ASN:HB3	1:CCC:80:GLY:O	2.14	0.48
1:CCC:49:MET:HE2	1:CCC:51:PHE:CZ	2.49	0.47
1:BBB:36:HIS:CE1	1:BBB:47:MET:HG2	2.50	0.46
1:BBB:81:ASN:HB3	1:FFF:81:ASN:O	2.14	0.46
1:DDD:51:PHE:HB3	1:DDD:85:LEU:HG	1.99	0.45
1:AAA:25:ILE:HG23	1:DDD:66:LEU:HD21	1.99	0.45
1:BBB:76:PHE:HE2	1:BBB:78:GLN:NE2	2.00	0.42
1:BBB:49:MET:HE2	1:BBB:51:PHE:CZ	2.55	0.42
1:CCC:51:PHE:HB3	1:CCC:85:LEU:HG	2.01	0.42
1:EEE:82:ILE:CD1	1:EEE:84:LEU:HD21	2.49	0.42
1:FFF:49:MET:HE2	1:FFF:51:PHE:CZ	2.55	0.42
1:EEE:50:ARG:NH2	3:EEE:102:SO4:O2	2.52	0.42
1:AAA:49:MET:HE2	1:AAA:51:PHE:CZ	2.54	0.42
1:DDD:49:MET:HE2	1:DDD:51:PHE:CZ	2.55	0.42
1:FFF:37:GLU:OE2	1:FFF:71:HIS:CE1	2.73	0.41
1:CCC:79:GLN:CG	1:EEE:42:VAL:O	2.54	0.41
1:AAA:79:GLN:HG3	1:CCC:42:VAL:O	2.21	0.41
1:AAA:25:ILE:CG2	1:DDD:66:LEU:HD21	2.51	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	AAA	75/120 (62%)	75 (100%)	0	0	100	100
1	BBB	78/120 (65%)	77 (99%)	1 (1%)	0	100	100
1	CCC	76/120 (63%)	76 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	DDD	77/120 (64%)	77 (100%)	0	0	100	100
1	EEE	75/120 (62%)	75 (100%)	0	0	100	100
1	FFF	76/120 (63%)	76 (100%)	0	0	100	100
All	All	457/720 (64%)	456 (100%)	1 (0%)	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	AAA	64/97 (66%)	64 (100%)	0	100	100
1	BBB	67/97 (69%)	67 (100%)	0	100	100
1	CCC	65/97 (67%)	65 (100%)	0	100	100
1	DDD	66/97 (68%)	66 (100%)	0	100	100
1	EEE	64/97 (66%)	64 (100%)	0	100	100
1	FFF	65/97 (67%)	65 (100%)	0	100	100
All	All	391/582 (67%)	391 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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, 6 are monoatomic - leaving 9 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	SO4	CCC	102	-	4,4,4	0.50	0	6,6,6	0.13	0
3	SO4	BBB	103	-	4,4,4	0.53	0	6,6,6	0.15	0
3	SO4	DDD	103	-	4,4,4	0.35	0	6,6,6	0.18	0
4	BTB	BBB	101	-	13,13,13	1.55	3 (23%)	7,16,16	0.61	0
3	SO4	EEE	102	-	4,4,4	0.45	0	6,6,6	0.09	0
3	SO4	FFF	102	-	4,4,4	0.51	0	6,6,6	0.13	0
3	SO4	AAA	102	-	4,4,4	0.54	0	6,6,6	0.20	0
3	SO4	DDD	102	-	4,4,4	0.46	0	6,6,6	0.11	0
3	SO4	FFF	103	-	4,4,4	0.35	0	6,6,6	0.19	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
4	BTB	BBB	101	-	-	2/21/21/21	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	BBB	101	BTB	C2-N	3.44	1.55	1.48
4	BBB	101	BTB	C5-N	3.33	1.52	1.48
4	BBB	101	BTB	C7-N	2.27	1.51	1.48

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	BBB	101	BTB	N-C5-C6-O6
4	BBB	101	BTB	N-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	EEE	102	SO4	1	0
3	FFF	103	SO4	1	0

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	AAA	77/120 (64%)	0.72	10 (12%) 7 7	18, 30, 62, 82	0
1	BBB	80/120 (66%)	0.38	6 (7%) 20 22	20, 28, 45, 68	0
1	CCC	78/120 (65%)	0.93	13 (16%) 4 4	21, 34, 58, 70	0
1	DDD	79/120 (65%)	0.60	8 (10%) 12 13	20, 29, 48, 59	0
1	EEE	77/120 (64%)	0.65	7 (9%) 15 15	20, 31, 50, 61	0
1	FFF	78/120 (65%)	0.47	6 (7%) 19 21	21, 30, 47, 54	0
All	All	469/720 (65%)	0.62	50 (10%) 11 11	18, 30, 52, 82	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	90	VAL	6.9
1	CCC	90	VAL	5.7
1	EEE	90	VAL	4.7
1	AAA	81	ASN	4.3
1	AAA	80	GLY	4.3
1	AAA	88	ILE	4.3
1	EEE	71	HIS	3.9
1	EEE	81	ASN	3.6
1	CCC	79	GLN	3.4
1	DDD	77	ILE	3.4
1	BBB	81	ASN	3.3
1	EEE	82	ILE	3.1
1	CCC	25	ILE	3.1
1	DDD	59	ALA	3.1
1	DDD	56	ALA	3.0
1	DDD	54	VAL	3.0
1	AAA	41	ALA	3.0
1	FFF	56	ALA	2.9
1	CCC	66	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	DDD	60	ILE	2.9
1	FFF	88	ILE	2.9
1	CCC	14	GLN	2.6
1	BBB	80	GLY	2.6
1	EEE	14	GLN	2.6
1	BBB	78	GLN	2.6
1	CCC	85	LEU	2.6
1	CCC	88	ILE	2.6
1	AAA	89	ASN	2.6
1	CCC	89	ASN	2.6
1	DDD	14	GLN	2.5
1	DDD	57	ASP	2.4
1	BBB	41	ALA	2.4
1	DDD	40	PRO	2.4
1	FFF	13	GLN	2.4
1	FFF	60	ILE	2.4
1	CCC	68	THR	2.3
1	CCC	60	ILE	2.3
1	CCC	77	ILE	2.3
1	BBB	54	VAL	2.3
1	EEE	88	ILE	2.2
1	AAA	78	GLN	2.2
1	BBB	13	GLN	2.1
1	AAA	15	VAL	2.1
1	FFF	12	VAL	2.1
1	AAA	42	VAL	2.1
1	EEE	56	ALA	2.0
1	CCC	71	HIS	2.0
1	FFF	71	HIS	2.0
1	CCC	69	GLY	2.0
1	AAA	82	ILE	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands

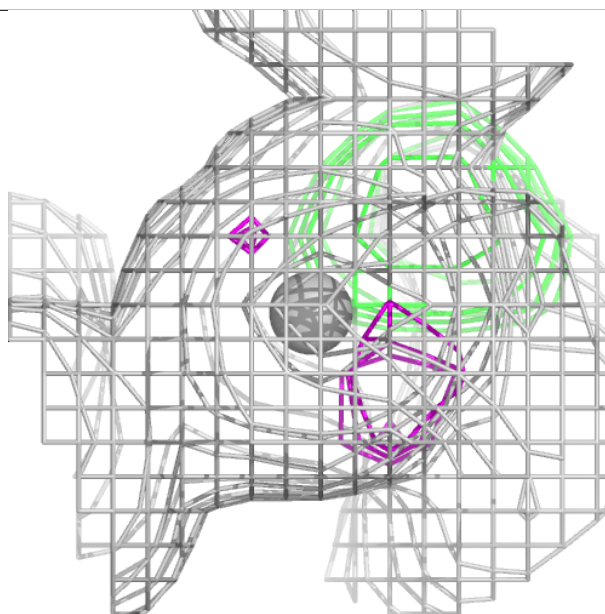
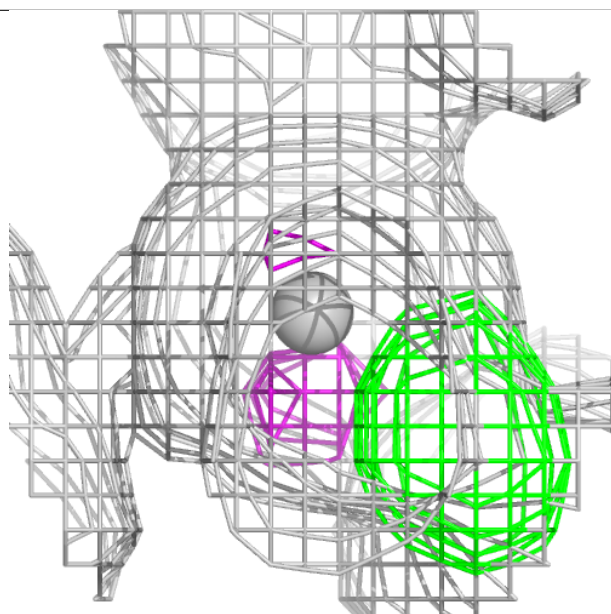
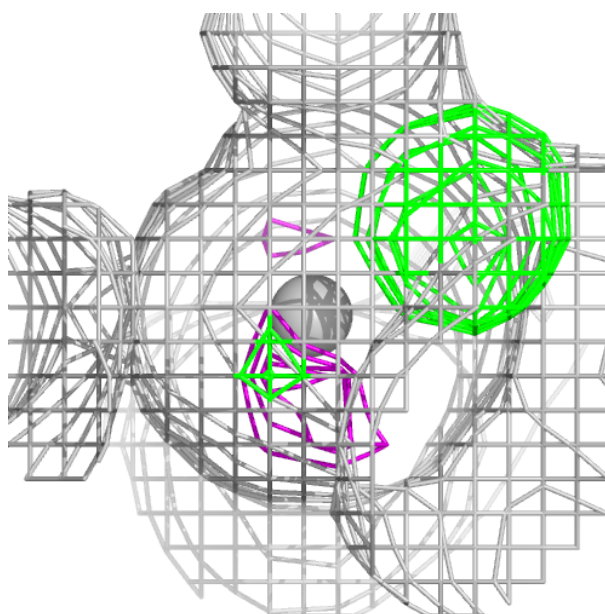
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	SO4	FFF	103	5/5	0.80	0.12	63,64,71,78	0
3	SO4	DDD	103	5/5	0.85	0.10	60,61,67,73	0
4	BTB	BBB	101	14/14	0.87	0.11	34,40,49,49	4
3	SO4	EEE	102	5/5	0.94	0.10	48,50,56,57	0
3	SO4	FFF	102	5/5	0.94	0.10	42,44,48,57	0
3	SO4	CCC	102	5/5	0.94	0.09	47,49,55,56	0
3	SO4	BBB	103	5/5	0.94	0.11	49,53,57,58	0
3	SO4	AAA	102	5/5	0.96	0.08	44,48,48,51	0
3	SO4	DDD	102	5/5	0.97	0.07	42,45,47,51	0
2	AG	DDD	101	1/1	0.99	0.03	26,26,26,26	0
2	AG	BBB	102	1/1	0.99	0.03	27,27,27,27	0
2	AG	AAA	101	1/1	1.00	0.02	23,23,23,23	0
2	AG	EEE	101	1/1	1.00	0.02	26,26,26,26	0
2	AG	FFF	101	1/1	1.00	0.02	25,25,25,25	0
2	AG	CCC	101	1/1	1.00	0.02	26,26,26,26	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.

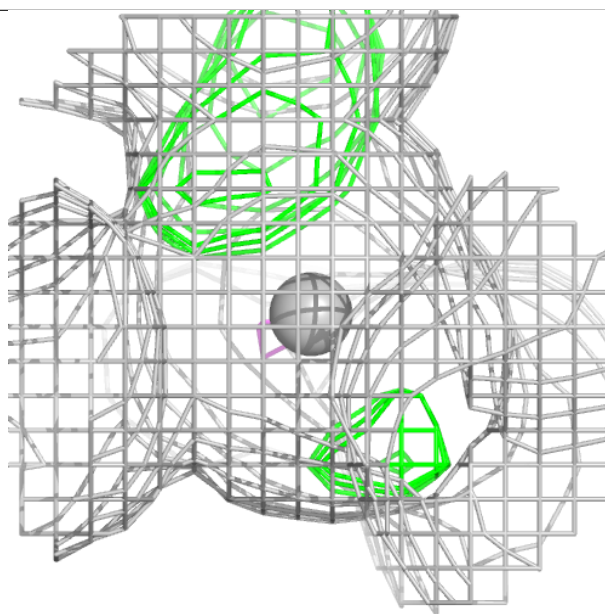
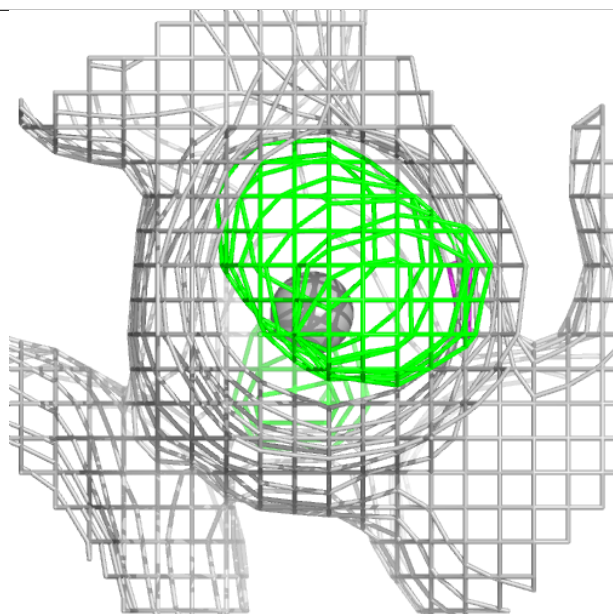
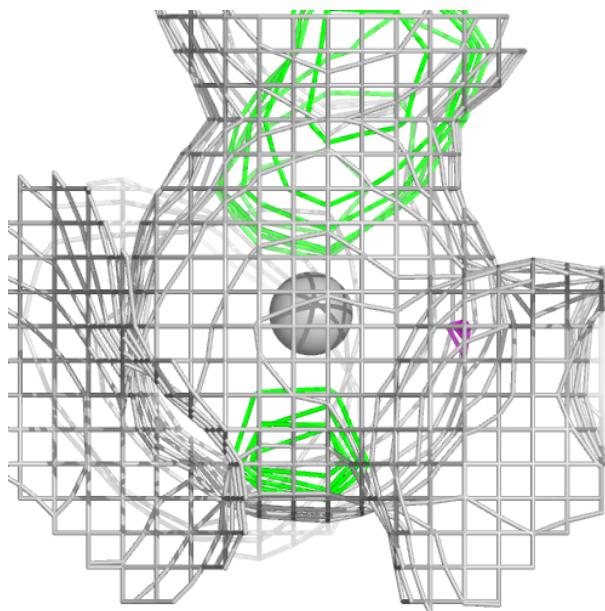
Electron density around AG DDD 101:

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



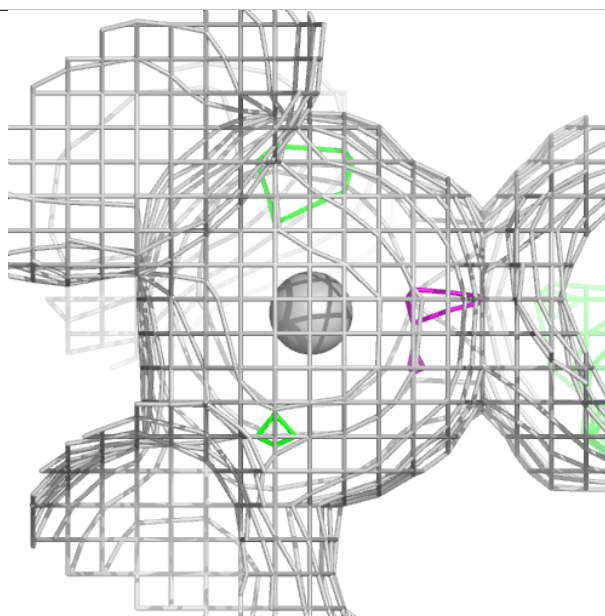
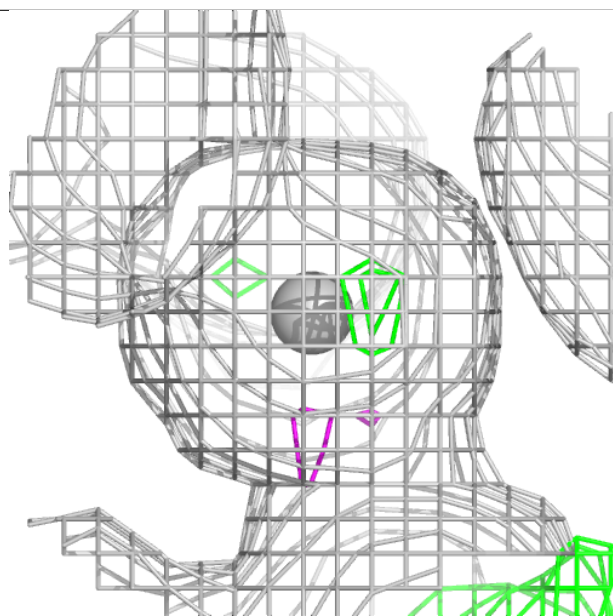
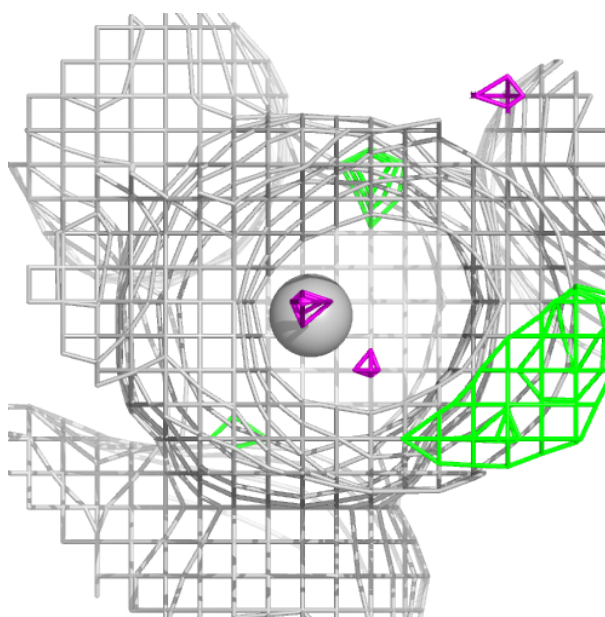
Electron density around AG BBB 102:

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



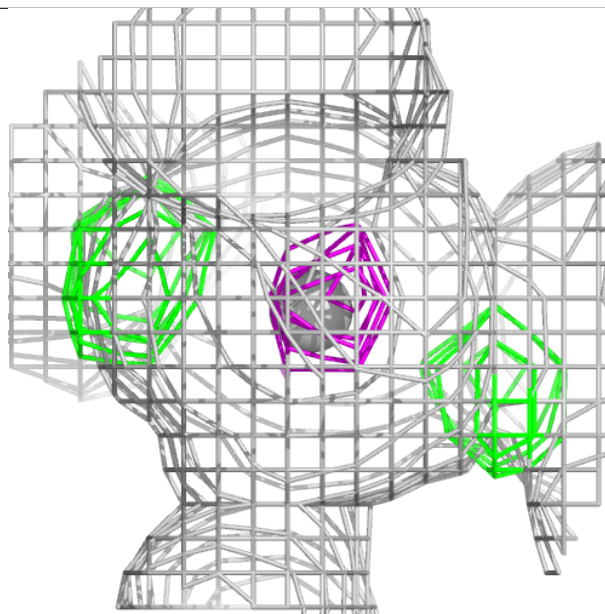
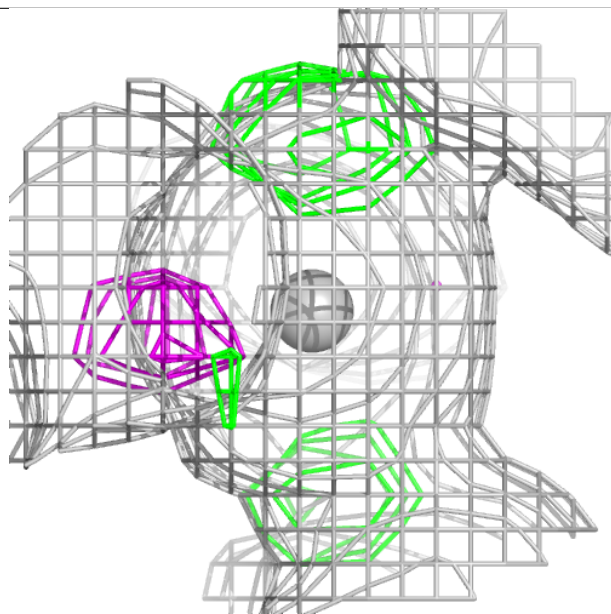
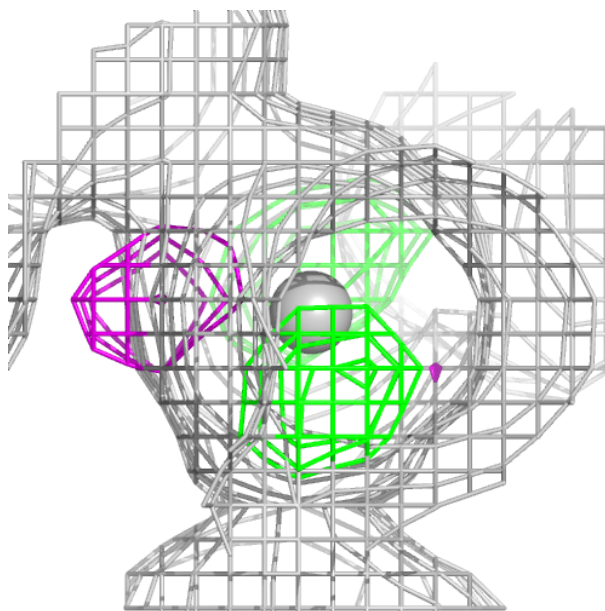
Electron density around AG AAA 101:

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



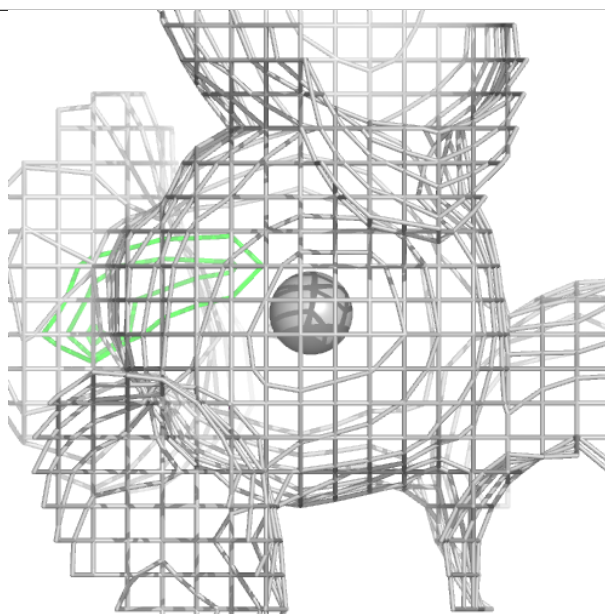
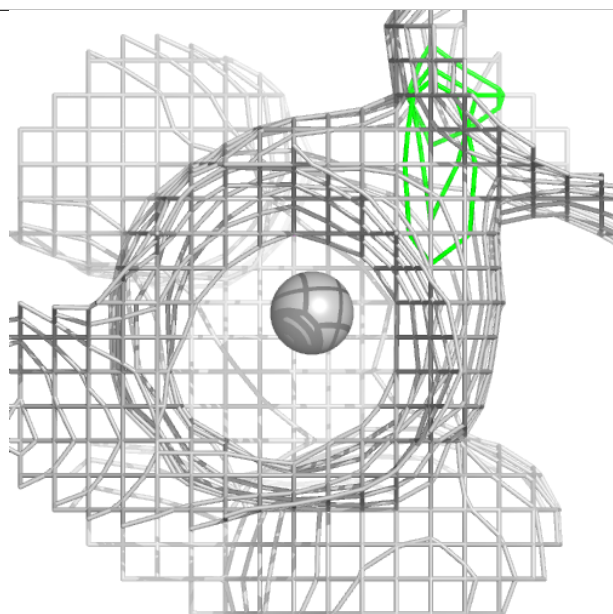
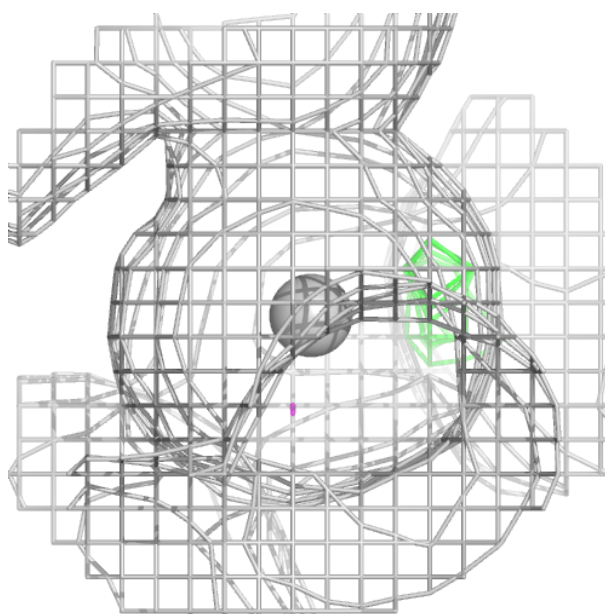
Electron density around AG EEE 101:

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



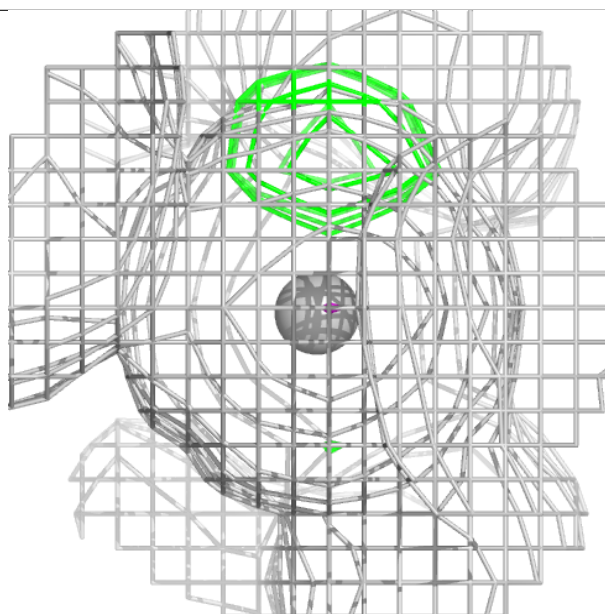
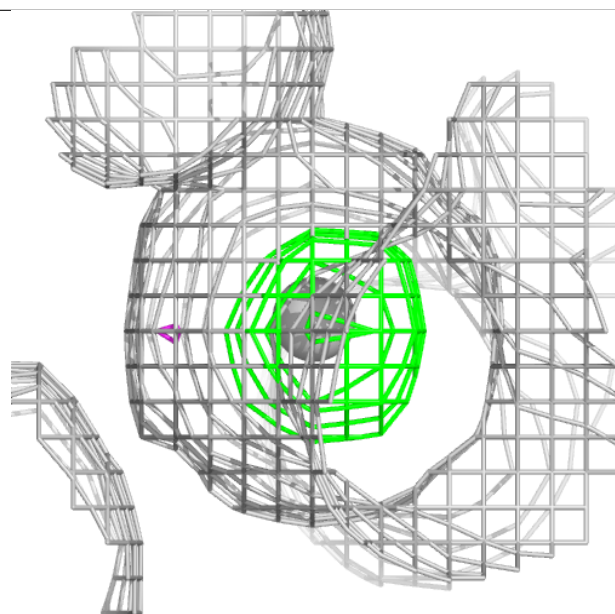
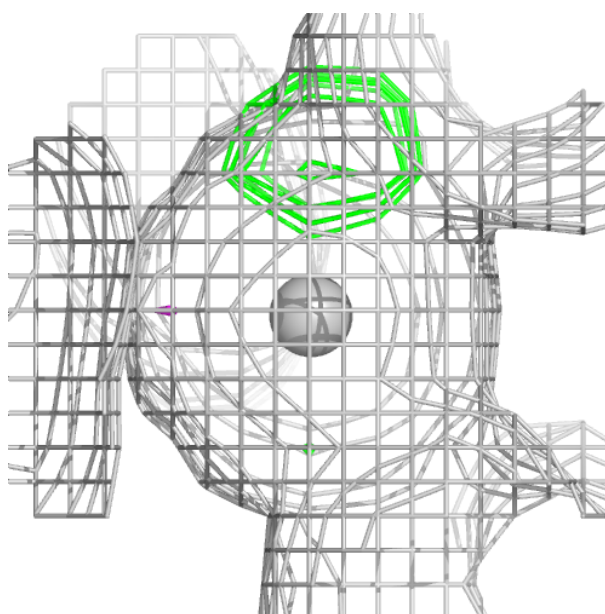
Electron density around AG FFF 101:

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



Electron density around AG CCC 101:

$2mF_o-DF_c$ (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.