W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Dec 20, 2022 – 03:30 pm GMT

PDB ID	:	7QLG
Title	:	CRYSTAL STRUCTURE OF E.coli ALCOHOL DEHYDROGENASE - FucO MUTANT L259V COMPLEXED WITH FE, NADH, AND GLYCEROL
Authors	:	Sridhar, S.; Kiema, T.R.; Widertsen, M.; Wierenga, R.K.
Deposited on	:	2021-12-20
Resolution	:	2.00 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

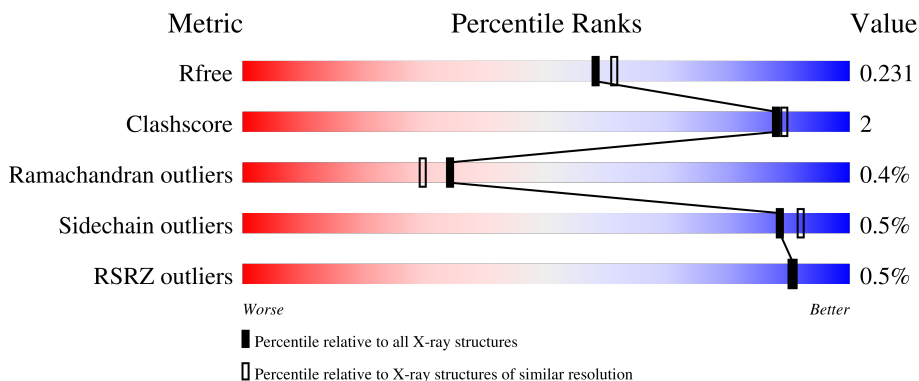|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.3
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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	Percentile Ranks	Value
Rfree		0.231
Clashscore		2
Ramachandran outliers		0.4%
Sidechain outliers		0.5%
RSRZ outliers		0.5%

Worse ⟶ *Better*

▊ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

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 <=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	390	92% 6% ·
1	BBB	390	92% 6% ·

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 11829 atoms, of which 5784 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 Lactaldehyde reductase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	383	Total 5695	C 1795	H 2849	N 494	O 542	S 15	65	0	0
1	BBB	383	Total 5707	C 1799	H 2857	N 494	O 542	S 15	65	1	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	1	MET	-	initiating methionine	UNP P0A9S2
AAA	259	VAL	LEU	engineered mutation	UNP P0A9S2
AAA	315	GLY	SER	engineered mutation	UNP P0A9S2
AAA	384	THR	-	expression tag	UNP P0A9S2
AAA	385	SER	-	expression tag	UNP P0A9S2
AAA	386	HIS	-	expression tag	UNP P0A9S2
AAA	387	HIS	-	expression tag	UNP P0A9S2
AAA	388	HIS	-	expression tag	UNP P0A9S2
AAA	389	HIS	-	expression tag	UNP P0A9S2
AAA	390	HIS	-	expression tag	UNP P0A9S2
BBB	1	MET	-	initiating methionine	UNP P0A9S2
BBB	259	VAL	LEU	engineered mutation	UNP P0A9S2
BBB	315	GLY	SER	engineered mutation	UNP P0A9S2
BBB	384	THR	-	expression tag	UNP P0A9S2
BBB	385	SER	-	expression tag	UNP P0A9S2
BBB	386	HIS	-	expression tag	UNP P0A9S2
BBB	387	HIS	-	expression tag	UNP P0A9S2
BBB	388	HIS	-	expression tag	UNP P0A9S2
BBB	389	HIS	-	expression tag	UNP P0A9S2
BBB	390	HIS	-	expression tag	UNP P0A9S2

- Molecule 2 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).

WORLDWIDE
wwPDB
PROTEIN DATA BANK

NAI
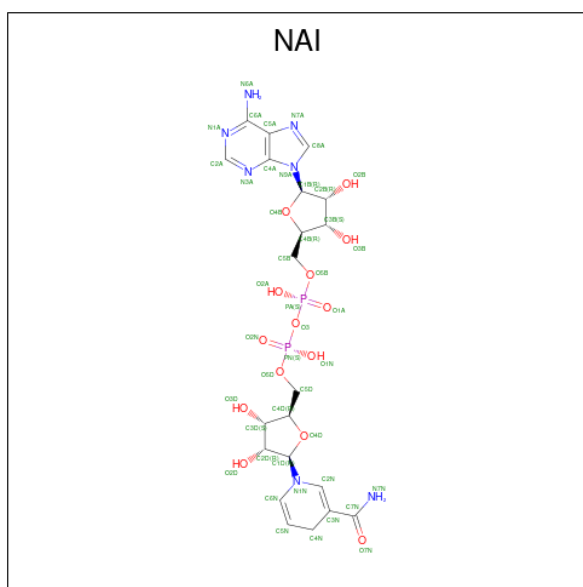
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	AAA	1	Total	C	H	N	O	P	6	0
			71	21	27	7	14	2		
2	BBB	1	Total	C	H	N	O	P	6	0
			71	21	27	7	14	2		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).

GOL
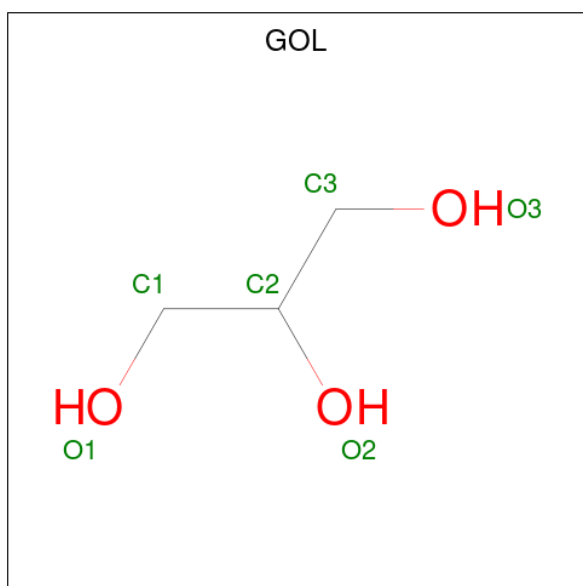
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	AAA	1	Total	C	H	O	2	0
			14	3	8	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	AAA	1	Total 14	C 3	H 8	O 3	2	0
3	BBB	1	Total 14	C 3	H 8	O 3	2	0

- Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	1	Total 1	Fe 1	0	0
4	BBB	1	Total 1	Fe 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	127	Total 127	O 127	0	0
5	BBB	114	Total 114	O 114	0	0

3 Residue-property plots ⓘ

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: Lactaldehyde reductase

Chain AAA:
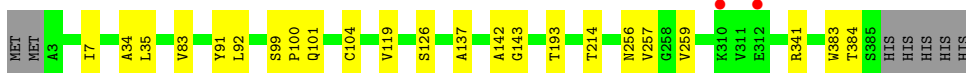
• Molecule 1: Lactaldehyde reductase

Chain BBB:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	69.78Å 55.36Å 107.69Å 90.00° 103.67° 90.00°	Depositor
Resolution (Å)	51.66 – 2.00 51.61 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.8 (51.66-2.00) 98.8 (51.61-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.61 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.186 , 0.227 0.194 , 0.231	Depositor DCC
R_{free} test set	2602 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å^2)	20.3	Xtriage
Anisotropy	0.673	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.45 , 40.4	EDS
L-test for twinning [2]	$<|L|> = 0.49, <L^2> = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11829	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.35% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ 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: NAI, GOL, FE

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	0.68	0/2900	0.76	0/3948
1	BBB	0.67	0/2907	0.73	0/3958
All	All	0.68	0/5807	0.75	0/7906

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	AAA	0	1
1	BBB	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AAA	142	ALA	Peptide
1	BBB	34	ALA	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	AAA	2846	2849	2839	11	0
1	BBB	2850	2857	2848	12	0
2	AAA	44	27	27	0	0
2	BBB	44	27	27	0	0
3	AAA	12	16	16	0	0
3	BBB	6	8	8	0	0
4	AAA	1	0	0	0	0
4	BBB	1	0	0	0	0
5	AAA	127	0	0	0	0
5	BBB	114	0	0	1	0
All	All	6045	5784	5765	23	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 2.

The worst 5 of 23 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:AAA:7:ILE:H	1:AAA:256:ASN:HD21	1.49	0.58
1:BBB:7:ILE:H	1:BBB:256:ASN:HD21	1.52	0.57
1:BBB:7:ILE:H	1:BBB:256:ASN:ND2	2.04	0.55
1:AAA:34:ALA:HB2	1:AAA:91:TYR:CZ	2.42	0.55
1:BBB:99:SER:HB2	1:BBB:100:PRO:HD3	1.87	0.54

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	AAA	381/390 (98%)	373 (98%)	6 (2%)	2 (0%)	29	23
1	BBB	382/390 (98%)	374 (98%)	7 (2%)	1 (0%)	41	37
All	All	763/780 (98%)	747 (98%)	13 (2%)	3 (0%)	34	30

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	259	VAL
1	BBB	259	VAL
1	AAA	119	VAL

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	291/298 (98%)	289 (99%)	2 (1%)	84	88
1	BBB	292/298 (98%)	291 (100%)	1 (0%)	92	95
All	All	583/596 (98%)	580 (100%)	3 (0%)	88	92

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	126	SER
1	AAA	384	THR
1	BBB	33	LYS

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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	GOL	AAA	402	-	5,5,5	0.11	0	5,5,5	0.28	0
3	GOL	BBB	403	-	5,5,5	0.12	0	5,5,5	0.41	0
2	NAI	BBB	402	-	42,48,48	0.58	0	47,73,73	0.78	1 (2%)
2	NAI	AAA	401	-	42,48,48	0.65	0	47,73,73	0.72	1 (2%)
3	GOL	AAA	404	-	5,5,5	0.18	0	5,5,5	0.40	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
3	GOL	AAA	402	-	-	3/4/4/4	-
3	GOL	BBB	403	-	-	3/4/4/4	-
2	NAI	BBB	402	-	-	6/25/72/72	0/5/5/5
2	NAI	AAA	401	-	-	3/25/72/72	0/5/5/5
3	GOL	AAA	404	-	-	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(^{o})	Ideal(^{o})
2	BBB	402	NAI	C5A-C6A-N6A	2.68	124.43	120.35
2	AAA	401	NAI	C5A-C6A-N6A	2.41	124.01	120.35

There are no chirality outliers.

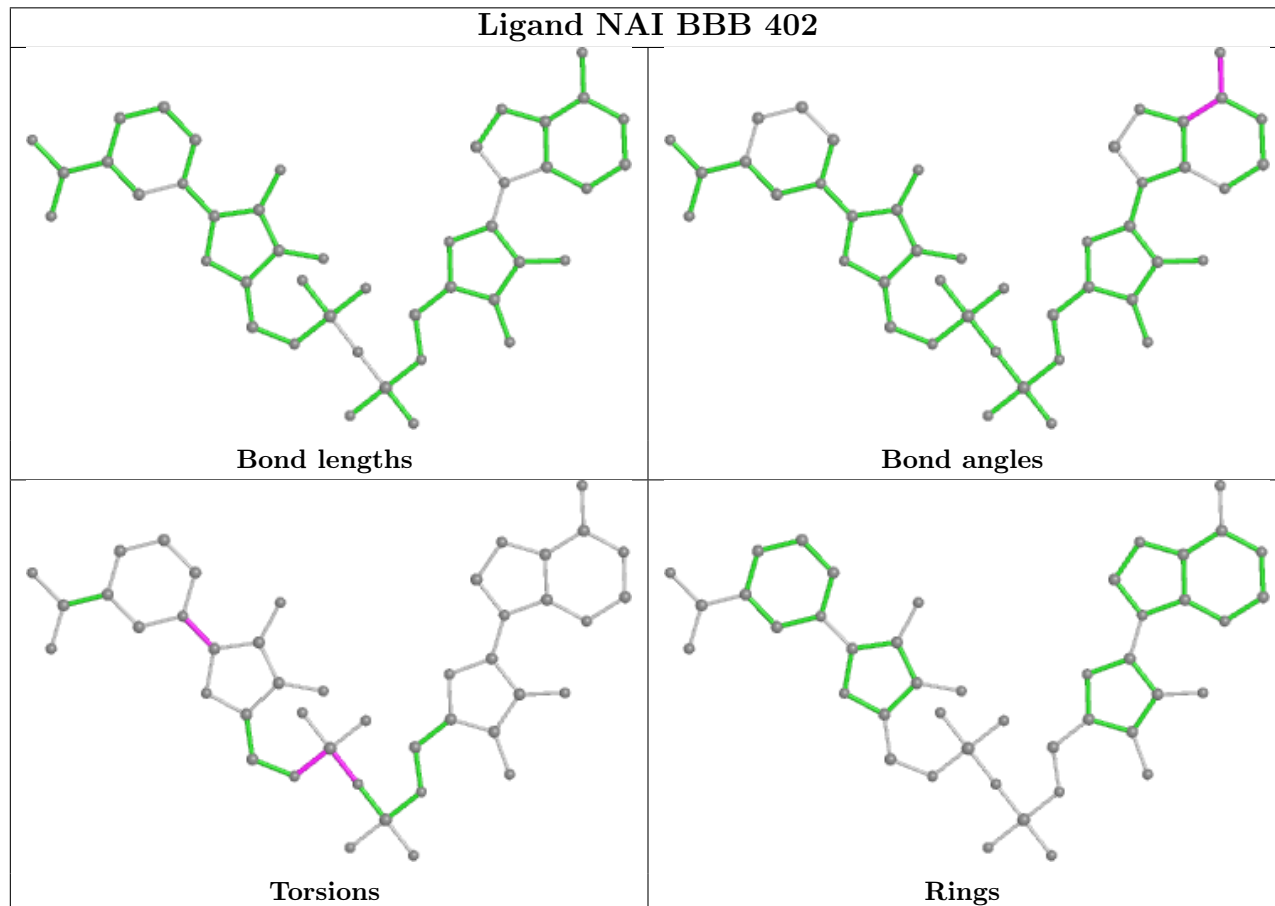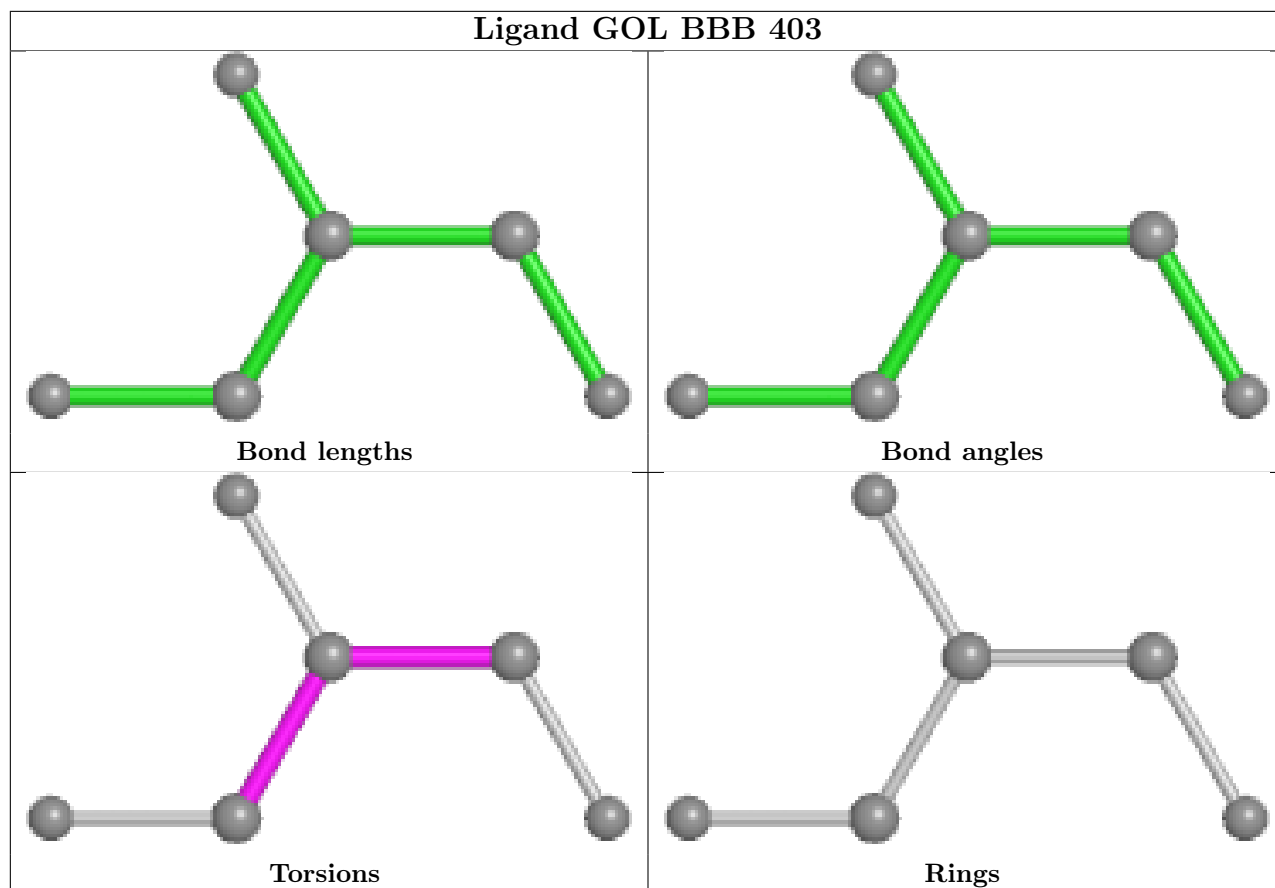5 of 17 torsion outliers are listed below:

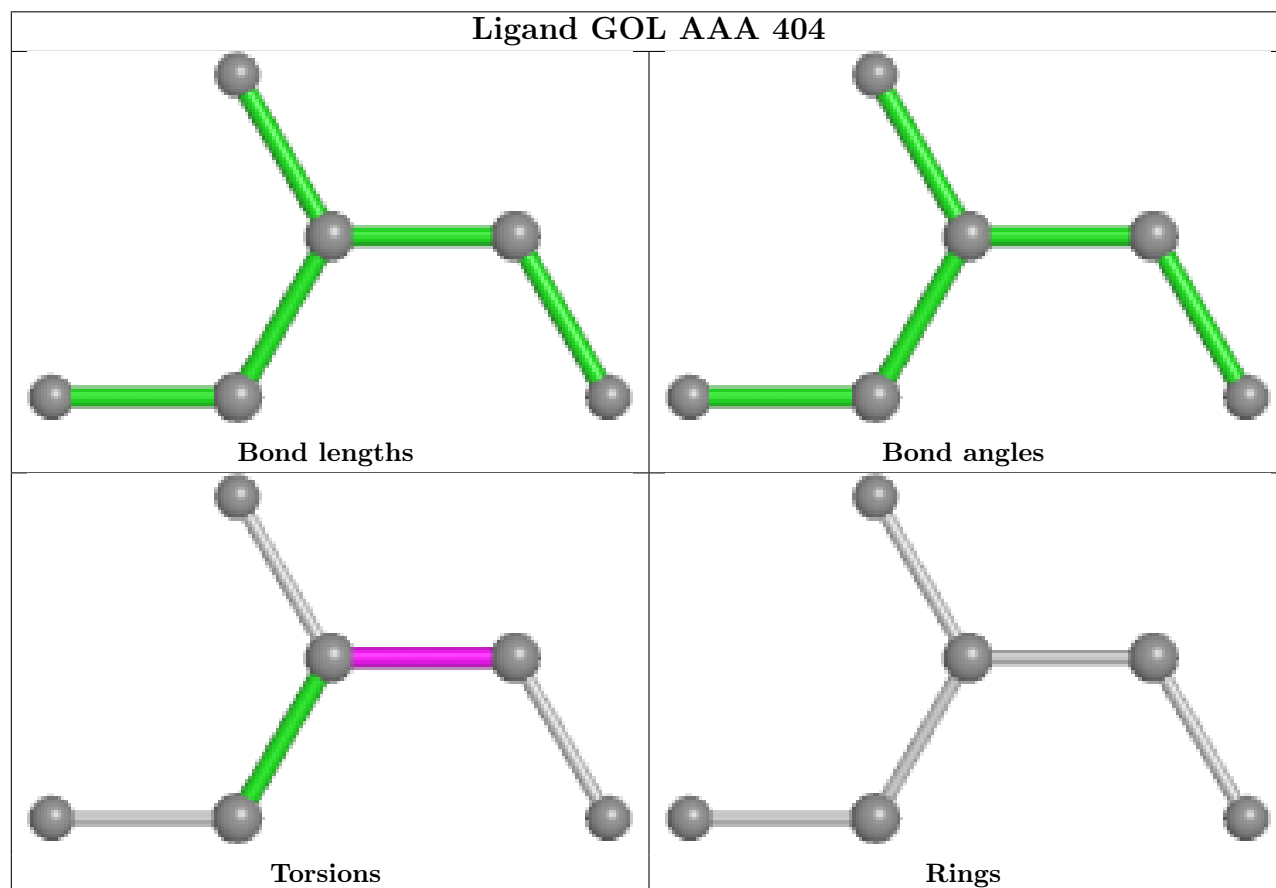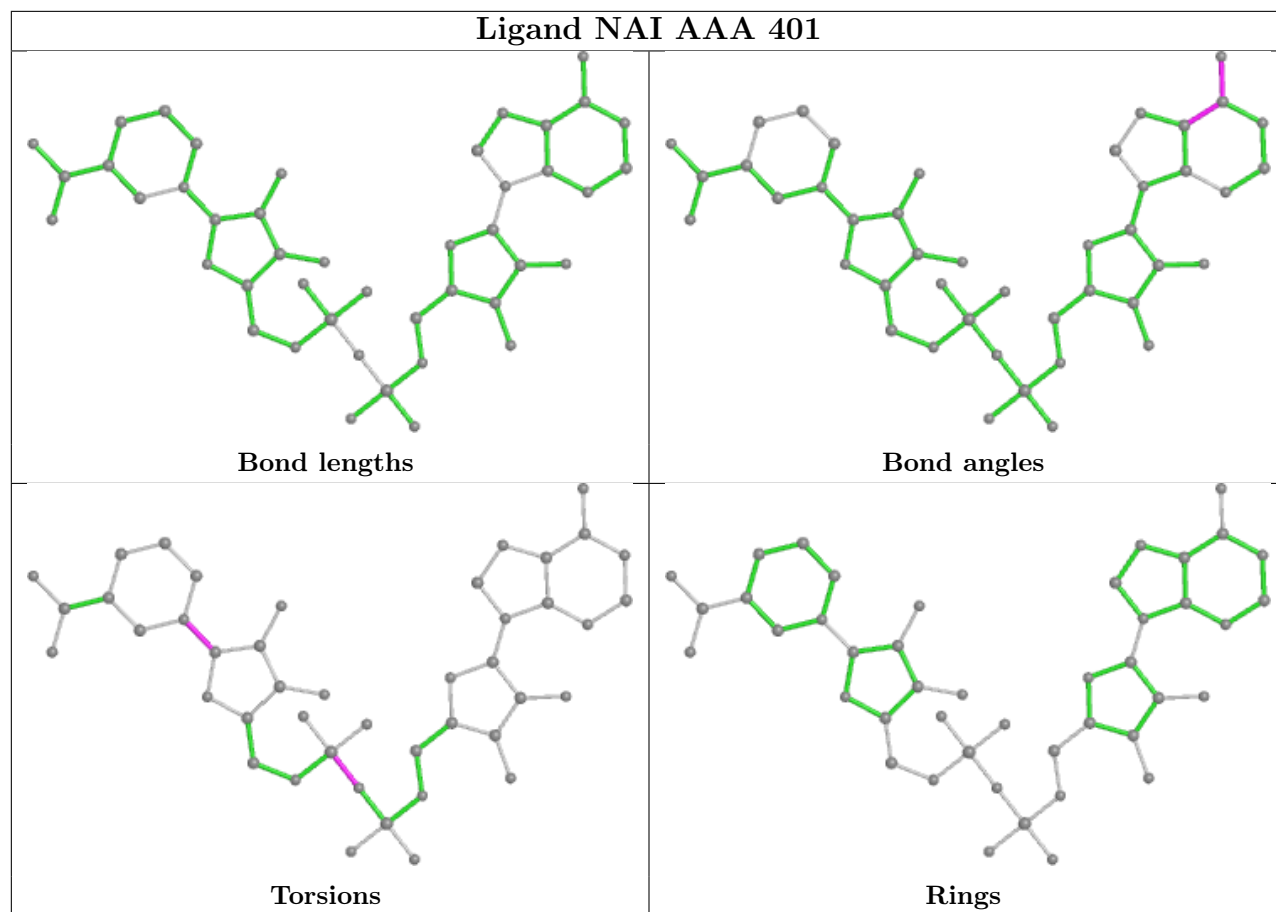| Mol	Chain	Res	Type	Atoms
3	AAA	402	GOL	O1-C1-C2-C3
3	AAA	404	GOL	O1-C1-C2-C3
3	BBB	403	GOL	O1-C1-C2-C3
3	BBB	403	GOL	O1-C1-C2-O2
3	BBB	403	GOL	C1-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand GOL AAA 402

Bond lengths   Bond angles

Torsions   Rings

Ligand GOL BBB 403

Bond lengths

Bond angles

Torsions

Rings

Ligand NAI BBB 402

Bond lengths

Bond angles

Torsions

Rings

Ligand NAI AAA 401

Bond lengths

Bond angles

Torsions

Rings

Ligand GOL AAA 404

Bond lengths

Bond angles

Torsions

Rings
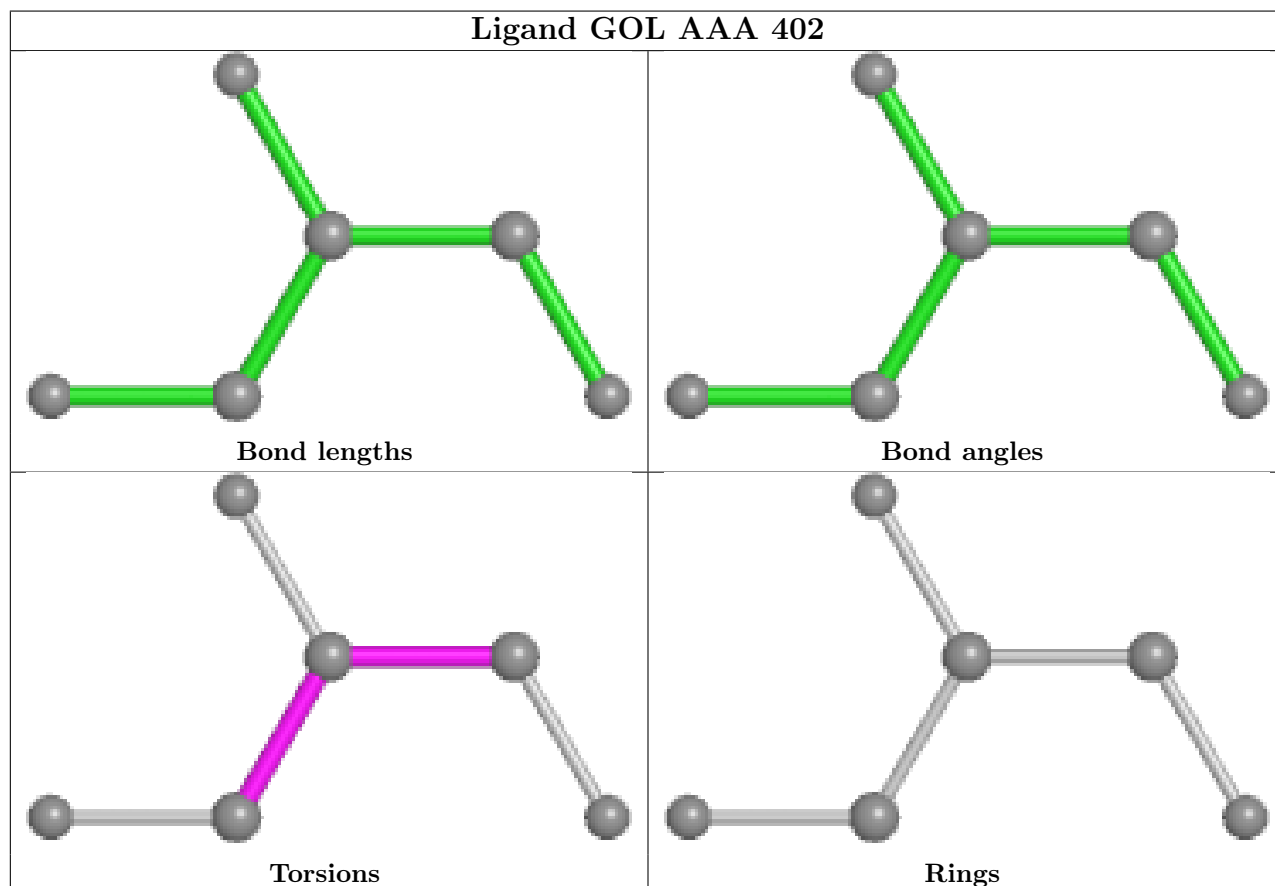
5.7 Other polymers ⓘ

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 ⓘ

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	383/390 (98%)	-0.35	2 (0%)	91	90	12, 20, 33, 59	0
1	BBB	383/390 (98%)	-0.35	2 (0%)	91	90	13, 20, 34, 57	0
All	All	766/780 (98%)	-0.35	4 (0%)	91	90	12, 20, 34, 59	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	312	GLU	2.8
1	AAA	310	LYS	2.3
1	AAA	312	GLU	2.2
1	BBB	158	GLU	2.1

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 monosaccharides 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	GOL	BBB	403	6/6	0.71	0.19	40,41,43,43	2

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	AAA	404	6/6	0.81	0.23	37,38,40,41	2
3	GOL	AAA	402	6/6	0.85	0.18	41,46,48,49	2
2	NAI	BBB	402	44/44	0.96	0.11	14,20,31,36	6
4	FE	AAA	403	1/1	0.96	0.07	41,41,41,41	0
2	NAI	AAA	401	44/44	0.97	0.11	17,21,44,49	6
4	FE	BBB	401	1/1	0.98	0.07	41,41,41,41	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.
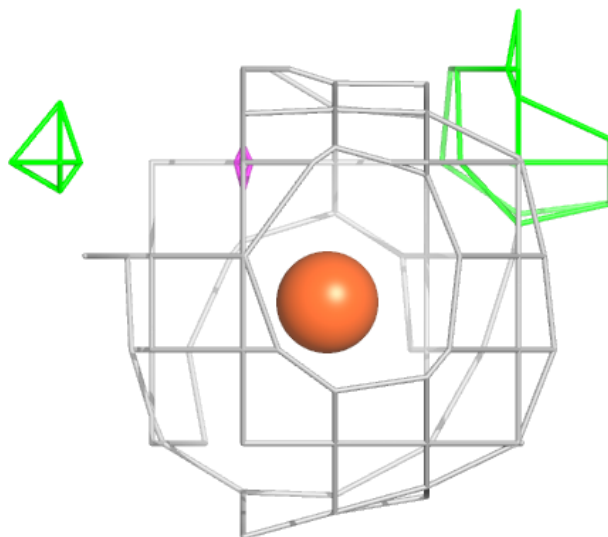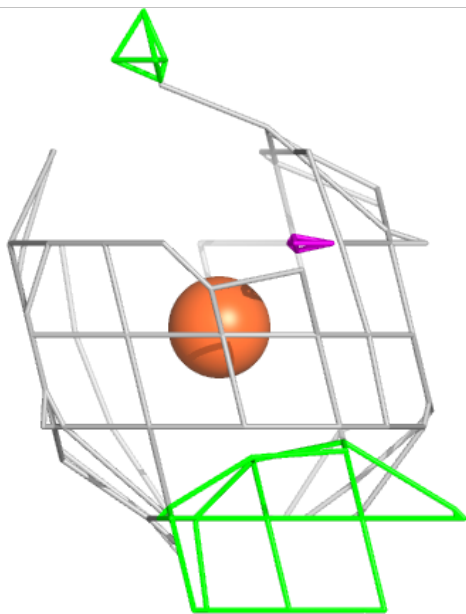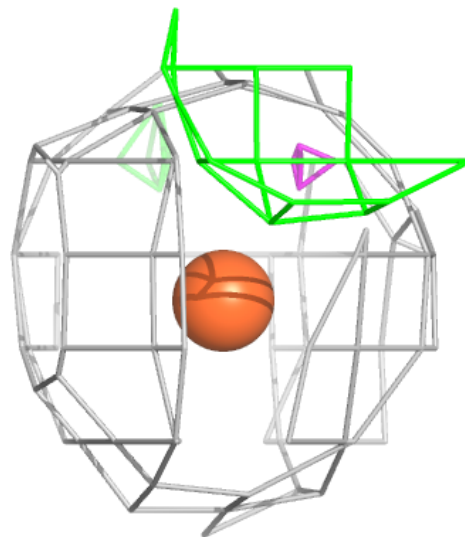

Electron density around GOL BBB 403:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
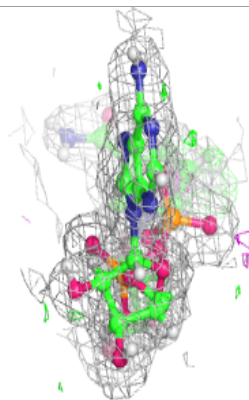mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
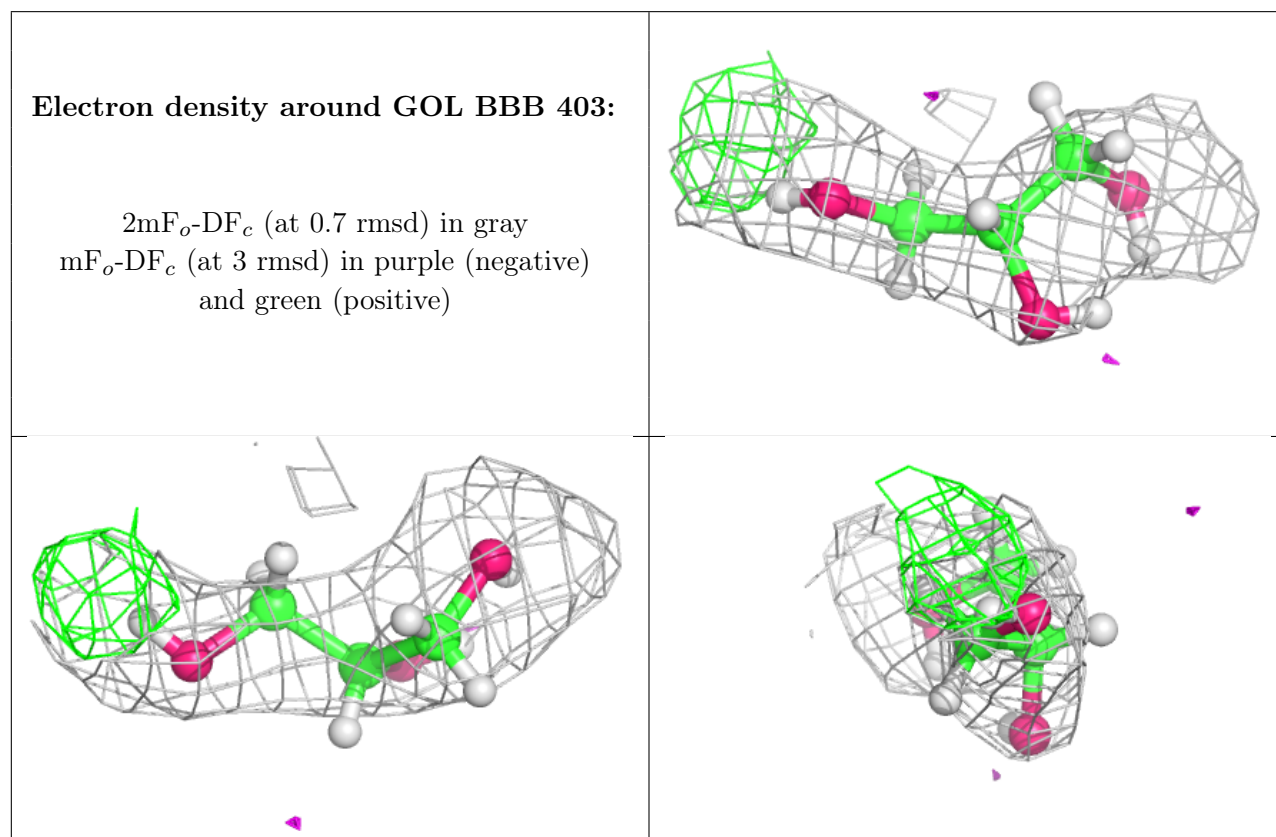
Electron density around GOL AAA 404:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
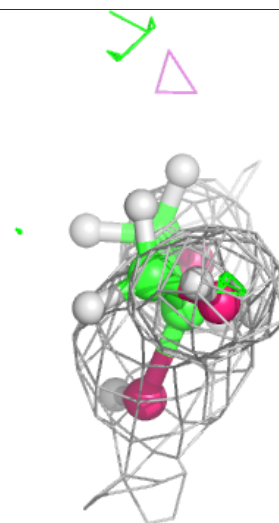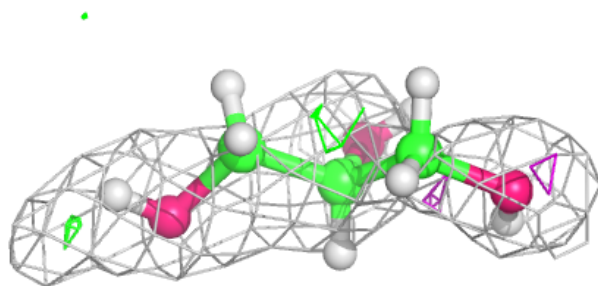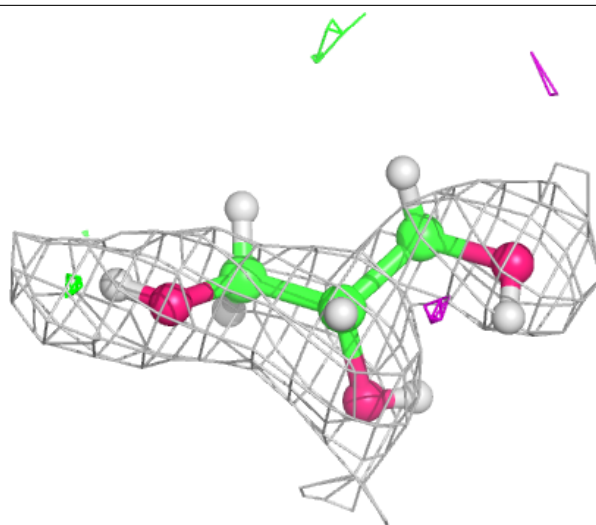
Electron density around GOL AAA 402:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
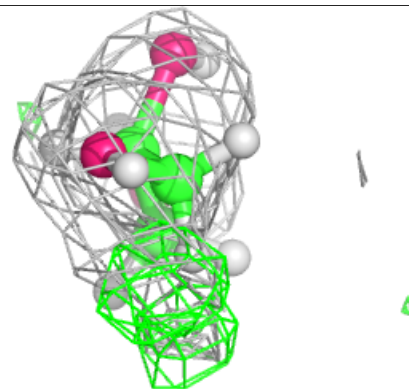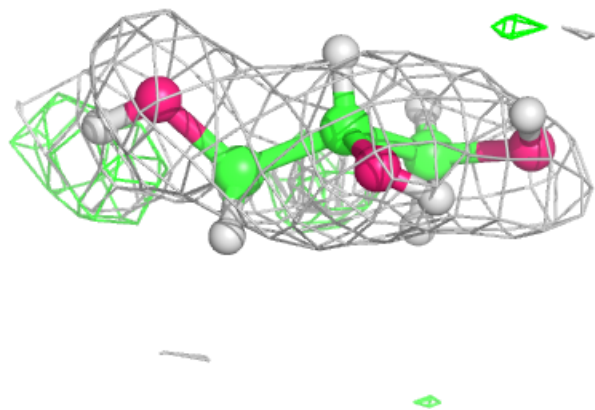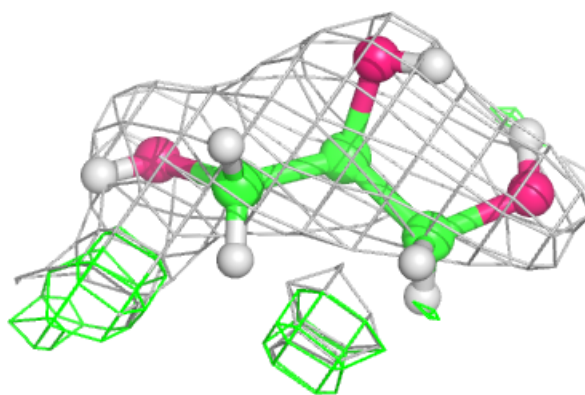
Electron density around NAI BBB 402:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
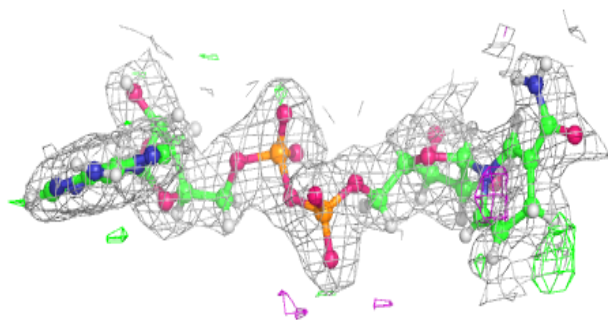$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
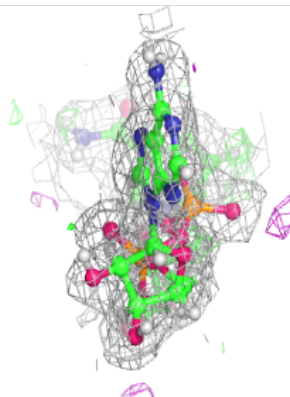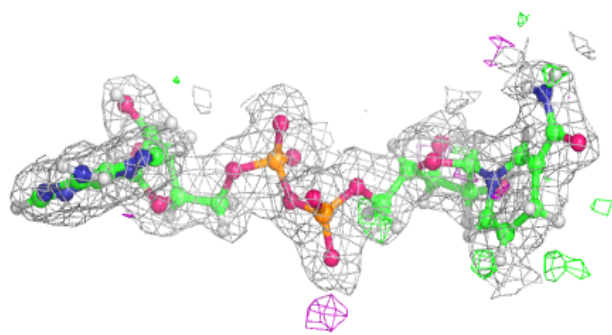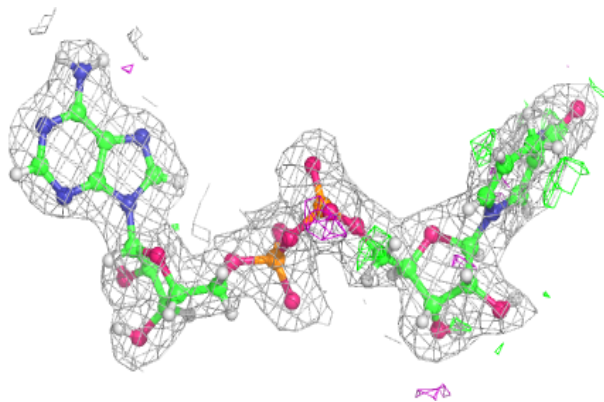
Electron density around FE AAA 403:

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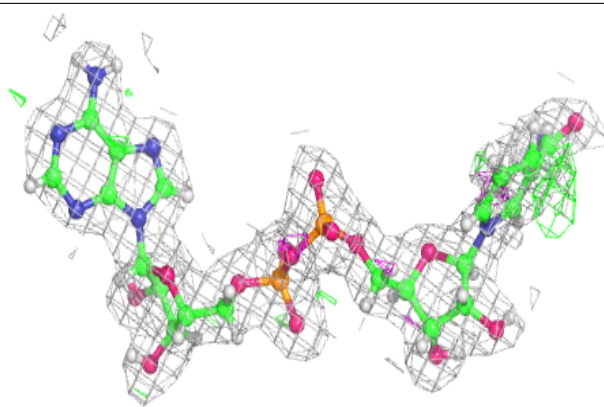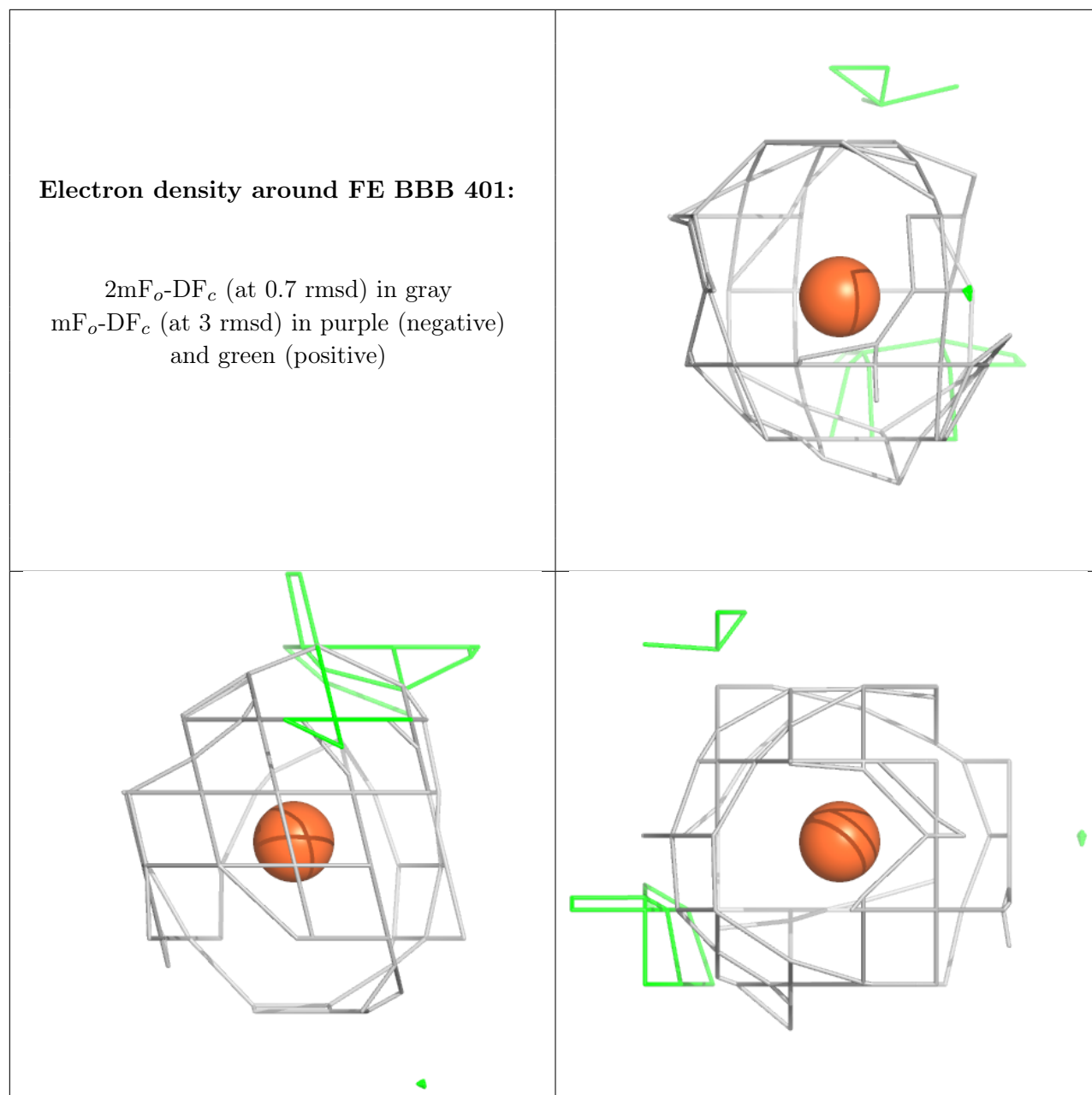and green (positive)

Electron density around NAI AAA 401:

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

Electron density around FE BBB 401:

$2mF_o$-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.