



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:36 PM UTC

PDB ID : 7QNF / pdb_00007qnf
Title : CRYSTAL STRUCTURE OF E.coli ALCOHOL DEHYDROGENASE - FucO
MUTANT N151G, L259V COMPLEXED WITH FE, NAD⁺, AND ETHY-
LENE GLYCOL
Authors : Sridhar, S.; Kiema, T.R.; Wierenga, R.K.; Widersten, M.
Deposited on : 2021-12-20
Resolution : 2.14 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

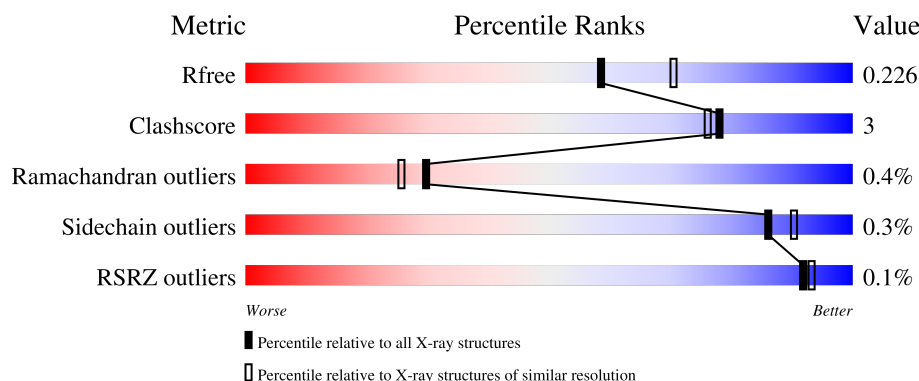
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

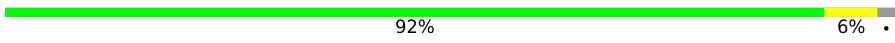
The reported resolution of this entry is 2.14 Å.

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	3689 (2.16-2.12)
Clashscore	190562	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)
RSRZ outliers	180081	3691 (2.16-2.12)

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	390	 92% 6% .
1	BBB	390	 89% 8% ..

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11873 atoms, of which 5798 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	C	H	N	O	S	65	2	0
			5723	1803	2864	497	544	15			
1	BBB	383	Total	C	H	N	O	S	65	0	0
			5688	1793	2846	493	541	15			

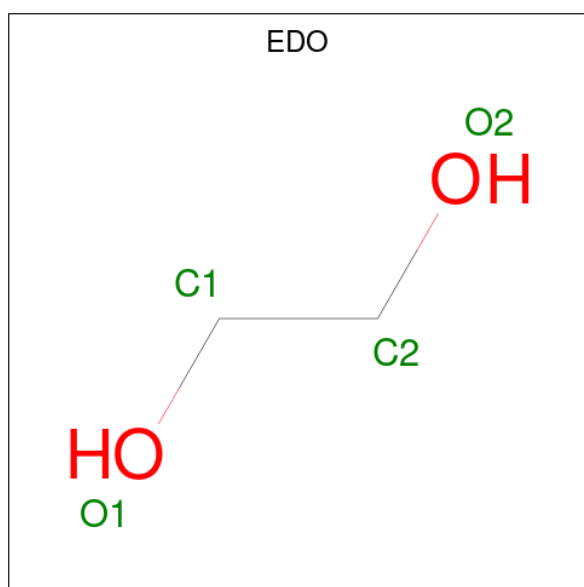
There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	1	MET	-	initiating methionine	UNP P0A9S2
AAA	151	GLY	ASN	engineered mutation	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	151	GLY	ASN	engineered mutation	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 FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

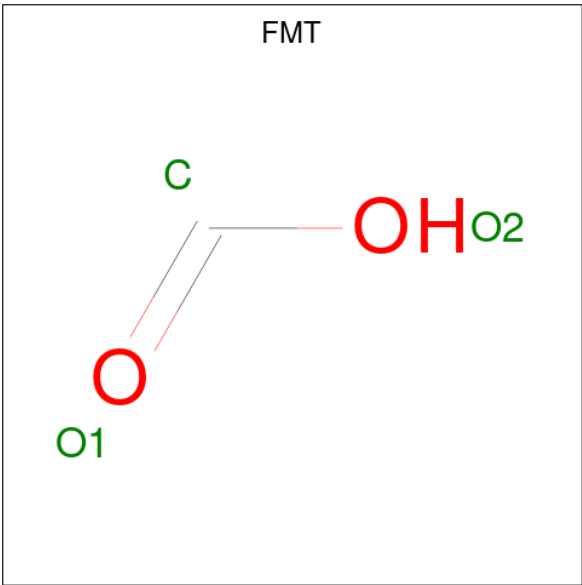
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AAA	1	Total Fe 1 1	0	0
2	BBB	1	Total Fe 1 1	0	0

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$) (labeled as "Ligand of Interest" by depositor).



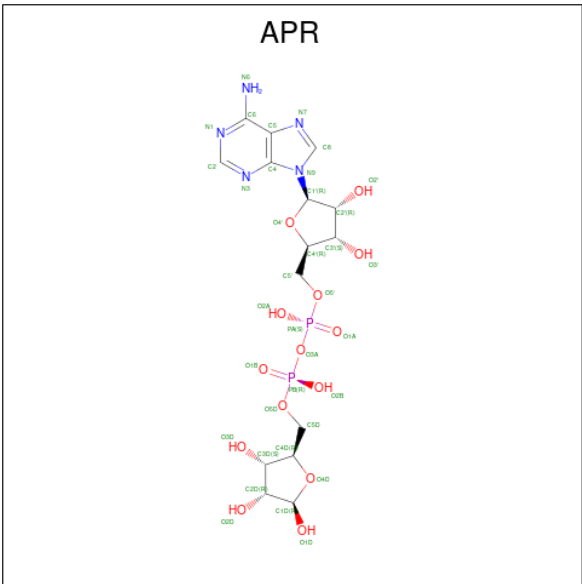
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total C H O 10 2 6 2	1	0
3	AAA	1	Total C H O 10 2 6 2	1	0
3	AAA	1	Total C H O 10 2 6 2	1	0
3	AAA	1	Total C H O 10 2 6 2	1	0
3	BBB	1	Total C H O 10 2 6 2	1	0
3	BBB	1	Total C H O 10 2 6 2	1	0
3	BBB	1	Total C H O 10 2 6 2	1	0

- Molecule 4 is FORMIC ACID (CCD ID: FMT) (formula: CH_2O_2) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	AAA	1	Total	C	H	O	1	0
			5	1	2	2		
4	AAA	1	Total	C	H	O	1	0
			5	1	2	2		

- Molecule 5 is ADENOSINE-5-DIPHOSPHORIBOSE (CCD ID: APR) (formula: $C_{15}H_{23}N_5O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	BBB	1	Total	C	H	N	O	P	5	0
			57	15	21	5	14	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	AAA	153	Total	O	0	0
			153	153		
6	BBB	113	Total	O	0	0
			113	113		

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.

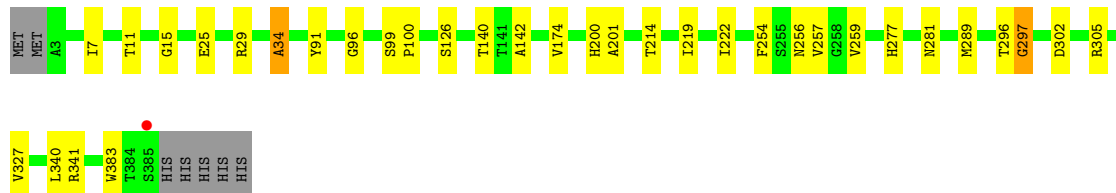
- Molecule 1: Lactaldehyde reductase

Chain AAA:  92% 6% .



- Molecule 1: Lactaldehyde reductase

Chain BBB:  89% 8% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	61.84Å 85.77Å 136.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.71 – 2.14 36.71 – 2.14	Depositor EDS
% Data completeness (in resolution range)	99.9 (36.71-2.14) 99.9 (36.71-2.14)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.179 , 0.226 0.179 , 0.226	Depositor DCC
R_{free} test set	2050 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	37.7	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 31.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	11873	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FE, APR, FMT, EDO

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	1.04	0/2916	1.46	2/3968 (0.1%)
1	BBB	1.04	0/2896	1.46	1/3942 (0.0%)
All	All	1.04	0/5812	1.46	3/7910 (0.0%)

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	2
All	All	0	3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	15	GLY	CA-C-O	-6.41	118.05	122.22
1	AAA	250	ALA	CA-C-N	5.77	126.51	119.99
1	AAA	250	ALA	C-N-CA	5.77	126.51	119.99

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AAA	142	ALA	Peptide
1	BBB	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	2859	2864	2854	13	0
1	BBB	2842	2846	2836	17	0
2	AAA	1	0	0	0	0
2	BBB	1	0	0	0	0
3	AAA	16	24	24	0	0
3	BBB	12	18	17	2	0
4	AAA	6	4	2	0	0
5	AAA	36	21	21	0	0
5	BBB	36	21	21	0	0
6	AAA	153	0	0	0	0
6	BBB	113	0	0	2	0
All	All	6075	5798	5775	32	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 3.

All (32) 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:ND2	1.92	0.67
1:BBB:7:ILE:H	1:BBB:256:ASN:HD21	1.44	0.64
1:AAA:7:ILE:H	1:AAA:256:ASN:HD21	1.46	0.64
1:AAA:34:ALA:HB2	1:AAA:91:TYR:CZ	2.35	0.62
1:BBB:340:LEU:HB2	1:BBB:383:TRP:HA	1.82	0.62
1:AAA:99:SER:HB2	1:AAA:100:PRO:HD3	1.83	0.59
1:BBB:7:ILE:H	1:BBB:256:ASN:ND2	2.03	0.56
1:AAA:35:LEU:HD22	1:AAA:84:PHE:HA	1.90	0.54
1:AAA:309:VAL:HG11	1:AAA:322:ALA:HB1	1.93	0.51
1:BBB:25:GLU:OE1	1:BBB:29:ARG:NH1	2.39	0.49
1:BBB:289:MET:SD	1:BBB:327:VAL:HG21	2.53	0.48
1:AAA:200:HIS:HB3	1:AAA:254:PHE:CD2	2.49	0.48
1:BBB:34:ALA:HB2	1:BBB:91:TYR:CZ	2.49	0.48
1:BBB:296:THR:O	1:BBB:297:GLY:C	2.57	0.47
1:BBB:99:SER:HB2	1:BBB:100:PRO:HD3	1.96	0.46
1:BBB:201:ALA:HB1	1:BBB:222:ILE:HG13	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:11:THR:O	1:BBB:174:VAL:HA	2.16	0.45
1:BBB:96:GLY:HA2	1:BBB:140:THR:OG1	2.17	0.44
1:AAA:25:GLU:OE1	1:AAA:29:ARG:NH1	2.45	0.43
1:BBB:277:HIS:CE1	1:BBB:281:ASN:HD21	2.36	0.43
1:BBB:214:THR:HG21	1:BBB:257:VAL:HG13	1.99	0.43
3:BBB:402:EDO:H21	6:BBB:511:HOH:O	2.18	0.43
1:AAA:302:ASP:OD1	1:AAA:305:ARG:NH2	2.52	0.42
1:AAA:80:GLY:HA3	1:AAA:107:ILE:HD11	2.01	0.42
1:AAA:49:ALA:HA	1:AAA:52:THR:OG1	2.20	0.42
3:BBB:402:EDO:C2	6:BBB:511:HOH:O	2.66	0.42
1:BBB:219:ILE:HD12	1:BBB:219:ILE:HA	1.88	0.42
1:BBB:200:HIS:HB3	1:BBB:254:PHE:CD2	2.55	0.42
1:BBB:214:THR:HG21	1:BBB:257:VAL:CG1	2.49	0.42
1:AAA:218:HIS:CE1	1:AAA:253:GLY:HA3	2.55	0.41
1:BBB:302:ASP:HA	1:BBB:305:ARG:NH1	2.34	0.41
1:AAA:218:HIS:HE1	1:AAA:254:PHE:N	2.20	0.40

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	383/390 (98%)	372 (97%)	10 (3%)	1 (0%)	36	33
1	BBB	381/390 (98%)	367 (96%)	12 (3%)	2 (0%)	24	19
All	All	764/780 (98%)	739 (97%)	22 (3%)	3 (0%)	30	26

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	259	VAL
1	BBB	297	GLY

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Mol	Chain	Res	Type
1	BBB	259	VAL

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	AAA	292/297 (98%)	292 (100%)	0	100	100
1	BBB	290/297 (98%)	288 (99%)	2 (1%)	76	81
All	All	582/594 (98%)	580 (100%)	2 (0%)	86	90

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BBB	126	SER
1	BBB	341	ARG

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

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 13 ligands modelled in this entry, 2 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	$\# Z > 2$
3	EDO	AAA	406	-	3,3,3	0.14	0	2,2,2	0.29	0
4	FMT	AAA	408	-	2,2,2	0.21	0	1,1,1	0.18	0
3	EDO	AAA	404	-	3,3,3	0.10	0	2,2,2	0.12	0
3	EDO	BBB	404	-	3,3,3	0.09	0	2,2,2	0.15	0
3	EDO	AAA	402	-	3,3,3	0.06	0	2,2,2	0.09	0
4	FMT	AAA	405	-	2,2,2	0.22	0	1,1,1	0.19	0
5	APR	BBB	405	-	39,39,39	0.45	0	56,60,60	0.45	0
3	EDO	AAA	403	-	3,3,3	0.11	0	2,2,2	0.08	0
5	APR	AAA	407	-	39,39,39	0.54	0	56,60,60	0.50	0
3	EDO	BBB	402	2	3,3,3	0.10	0	2,2,2	0.29	0
3	EDO	BBB	403	-	3,3,3	0.09	0	2,2,2	0.18	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	EDO	AAA	406	-	-	1/1/1/1	-
3	EDO	AAA	404	-	-	0/1/1/1	-
3	EDO	BBB	404	-	-	1/1/1/1	-
3	EDO	AAA	402	-	-	0/1/1/1	-
5	APR	BBB	405	-	-	1/22/54/54	0/4/4/4
3	EDO	AAA	403	-	-	1/1/1/1	-
5	APR	AAA	407	-	-	1/22/54/54	0/4/4/4
3	EDO	BBB	402	2	-	1/1/1/1	-
3	EDO	BBB	403	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

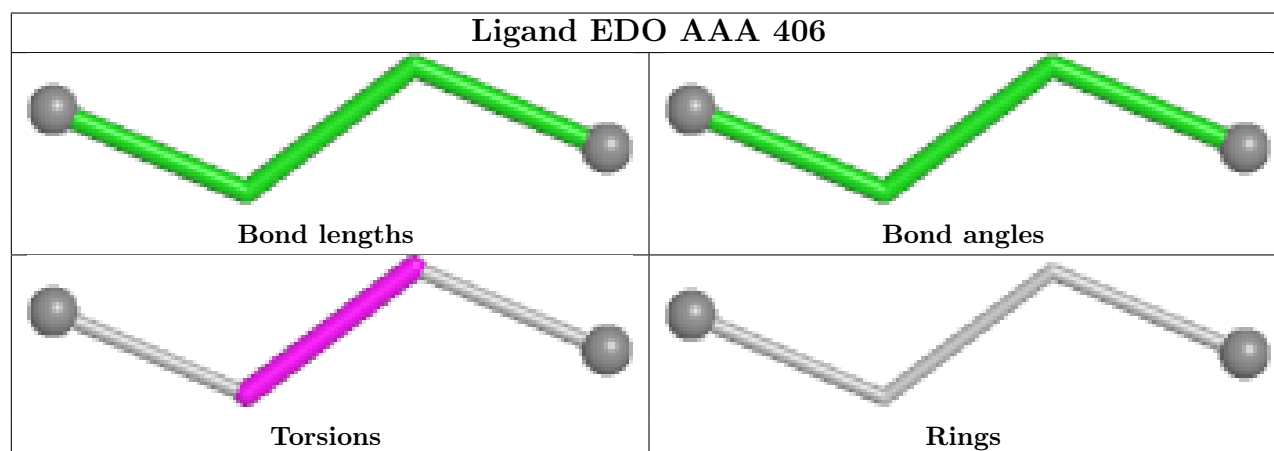
Mol	Chain	Res	Type	Atoms
3	AAA	406	EDO	O1-C1-C2-O2
3	BBB	402	EDO	O1-C1-C2-O2
5	AAA	407	APR	PA-O3A-PB-O5D
5	BBB	405	APR	PA-O3A-PB-O5D
3	BBB	404	EDO	O1-C1-C2-O2
3	AAA	403	EDO	O1-C1-C2-O2
3	BBB	403	EDO	O1-C1-C2-O2

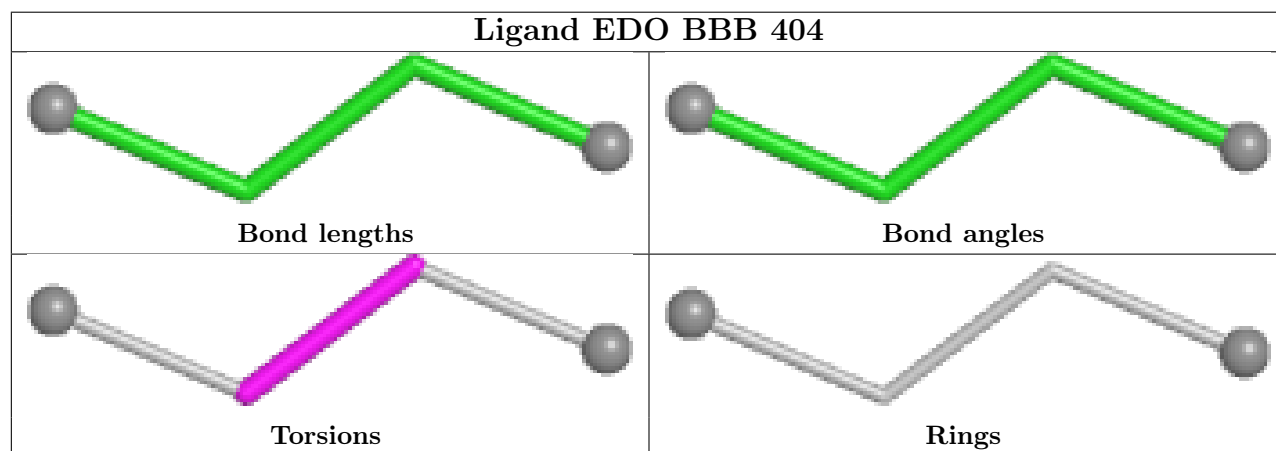
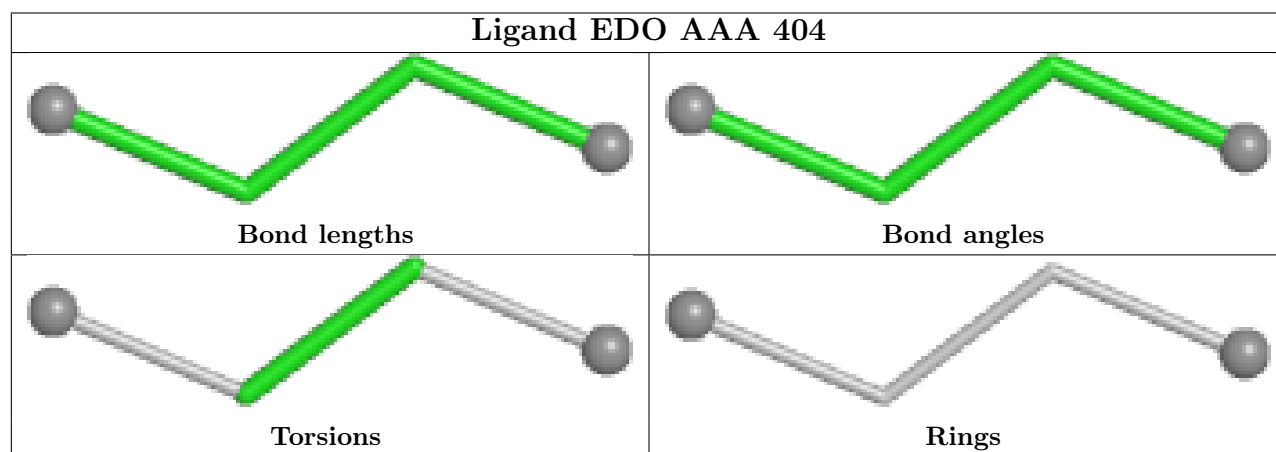
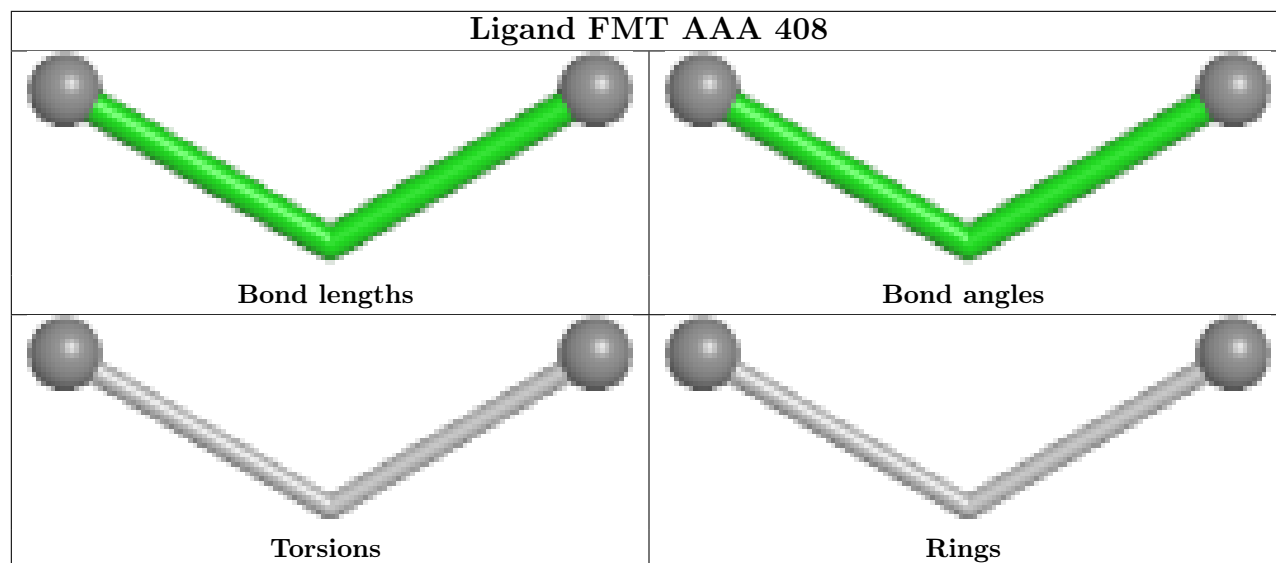
There are no ring outliers.

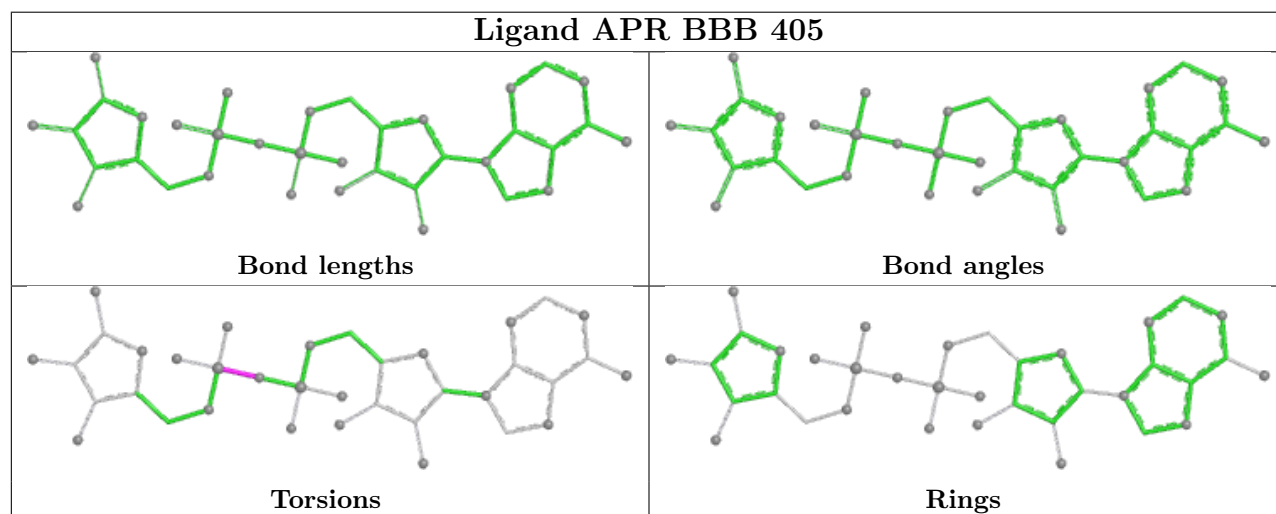
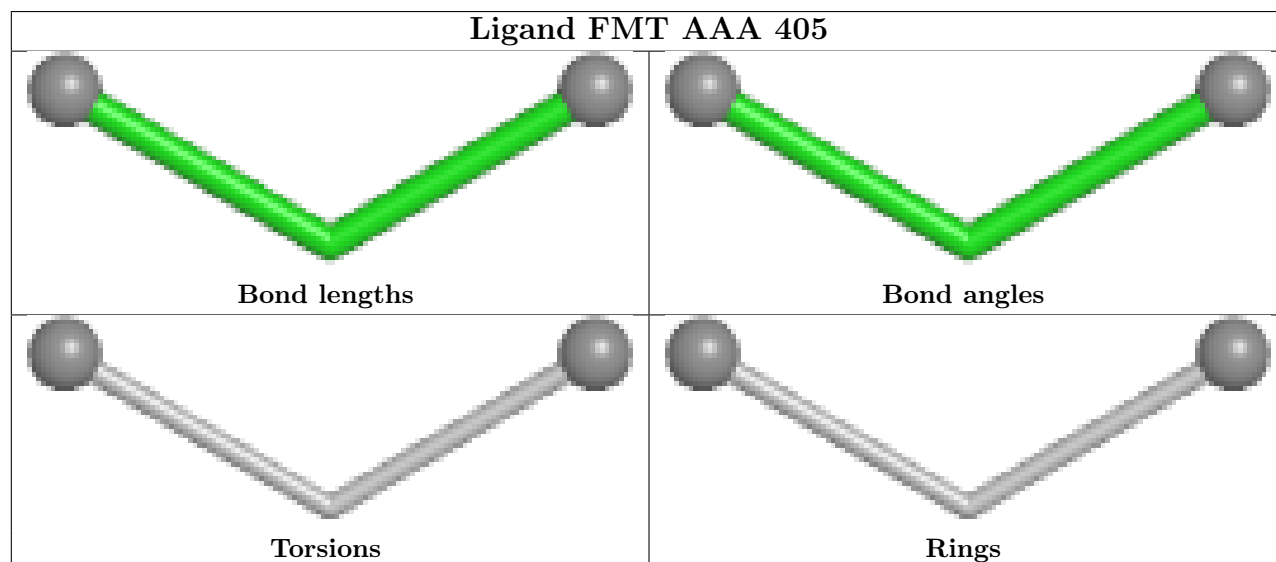
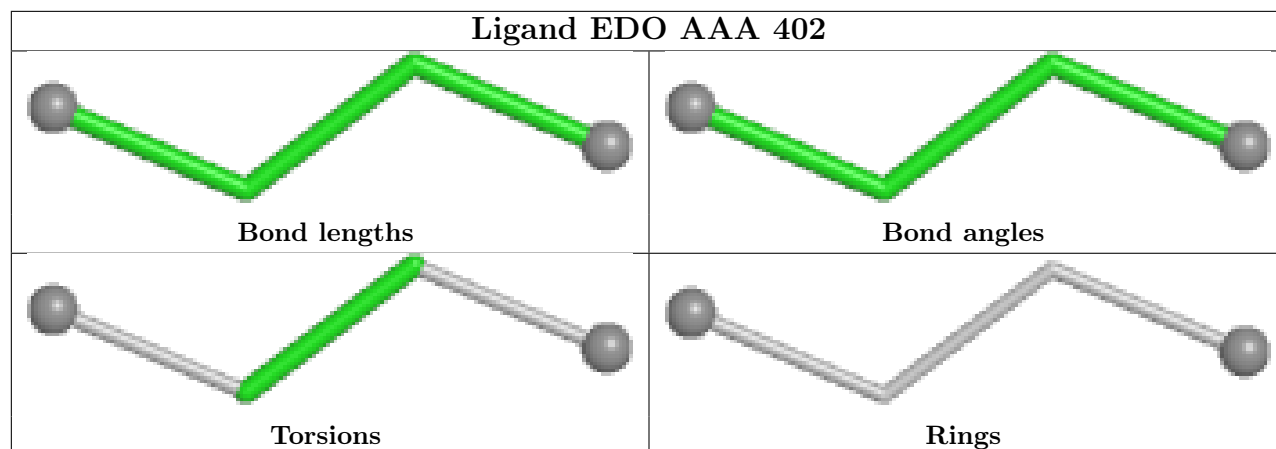
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	BBB	402	EDO	2	0

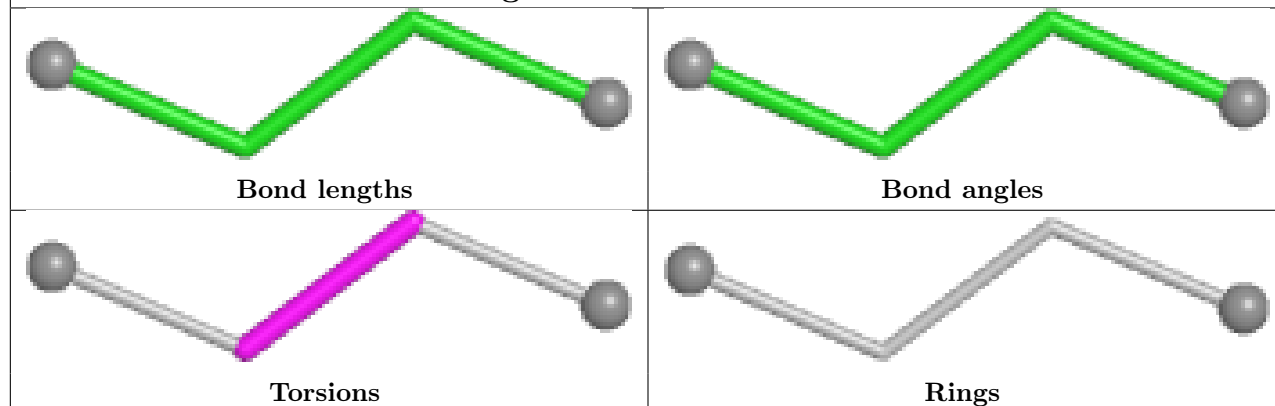
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.



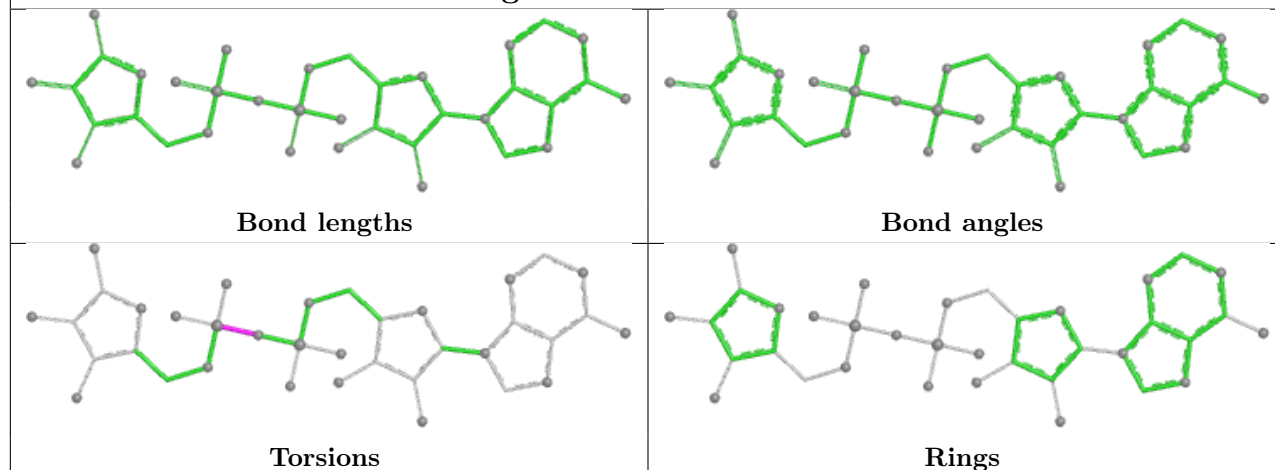




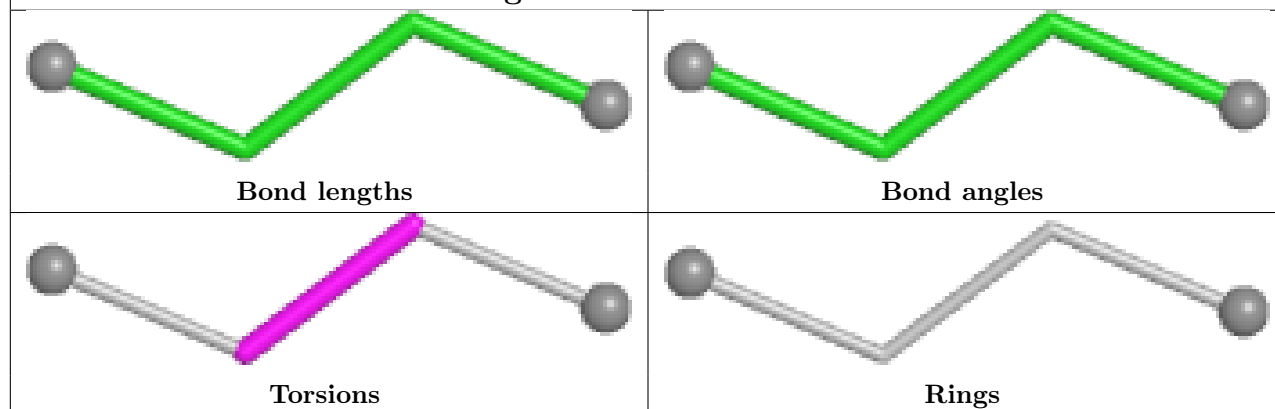
Ligand EDO AAA 403

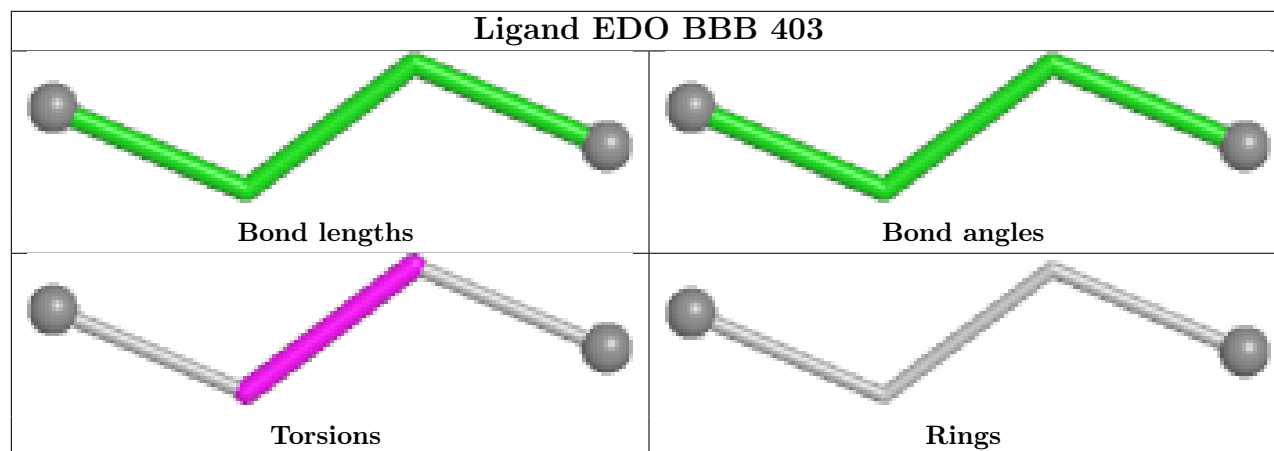


Ligand APR AAA 407



Ligand EDO BBB 402





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 [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	AAA	383/390 (98%)	-0.55	0	100 100	25, 40, 58, 75	2 (0%)
1	BBB	383/390 (98%)	-0.40	1 (0%)	90 92	27, 43, 73, 107	0
All	All	766/780 (98%)	-0.47	1 (0%)	92 93	25, 41, 66, 107	2 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	385	SER	3.7

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
4	FMT	AAA	405	3/3	0.74	0.19	68,68,70,72	1
3	EDO	BBB	404	4/4	0.78	0.15	63,70,74,74	1
3	EDO	AAA	406	4/4	0.86	0.17	61,63,63,63	1
4	FMT	AAA	408	3/3	0.87	0.14	63,63,63,65	1

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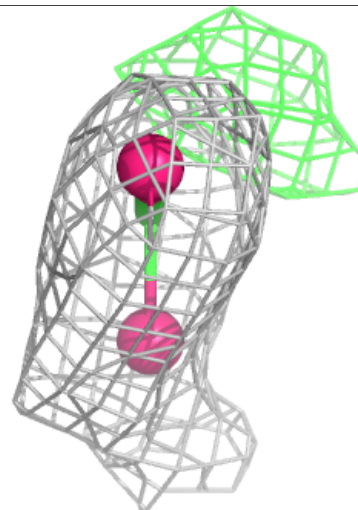
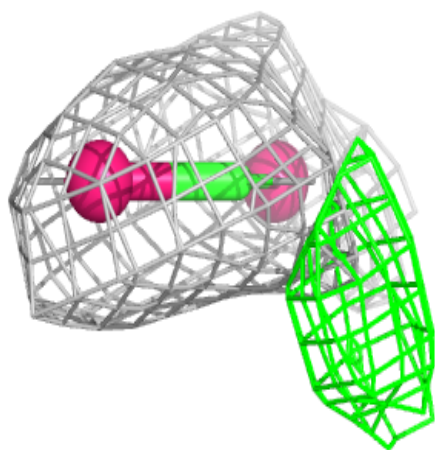
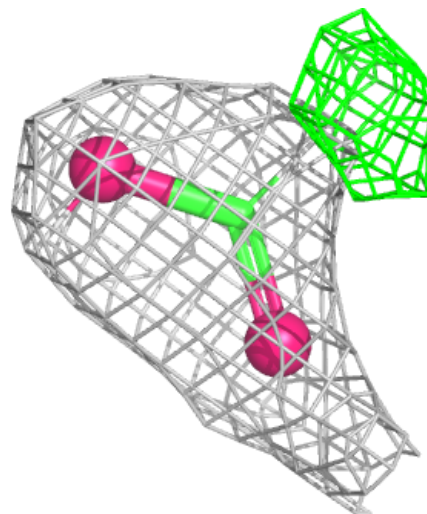
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	AAA	403	4/4	0.88	0.15	59,60,63,63	1
3	EDO	BBB	402	4/4	0.89	0.13	46,52,54,54	1
3	EDO	AAA	402	4/4	0.89	0.14	48,52,55,55	1
3	EDO	AAA	404	4/4	0.92	0.13	60,61,62,62	1
3	EDO	BBB	403	4/4	0.94	0.10	61,63,64,64	1
5	APR	AAA	407	36/36	0.98	0.05	32,36,41,42	5
5	APR	BBB	405	36/36	0.98	0.04	33,41,47,48	5
2	FE	BBB	401	1/1	1.00	0.01	33,33,33,33	0
2	FE	AAA	401	1/1	1.00	0.01	30,30,30,30	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.

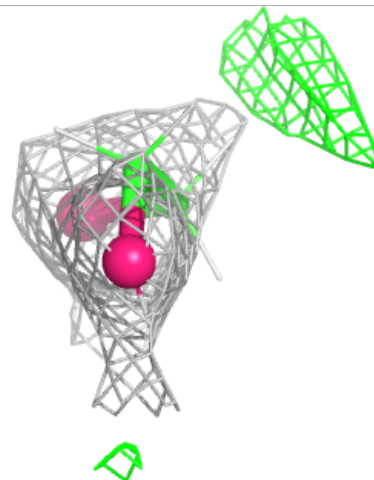
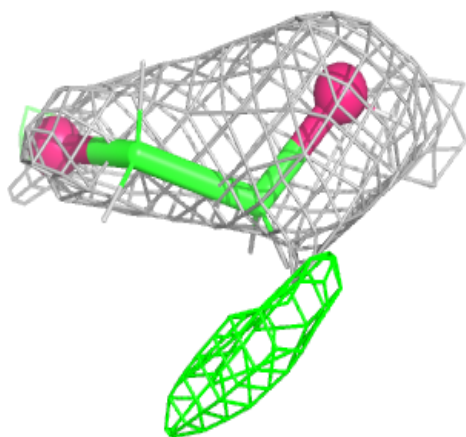
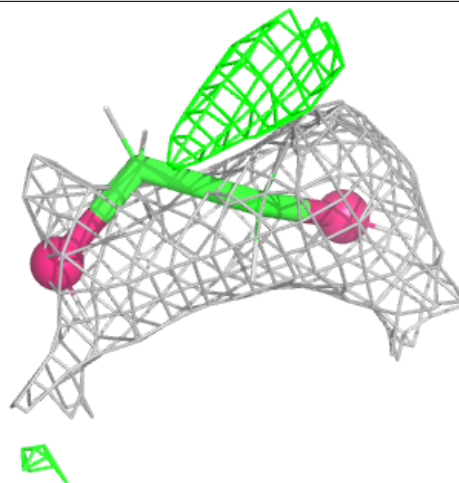
Electron density around FMT AAA 405:

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



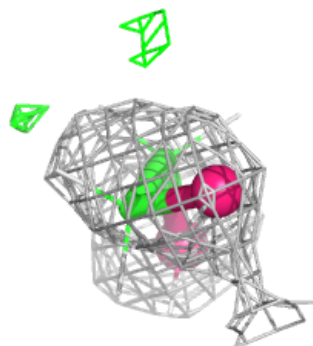
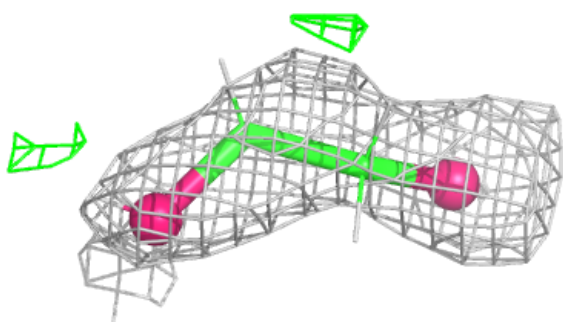
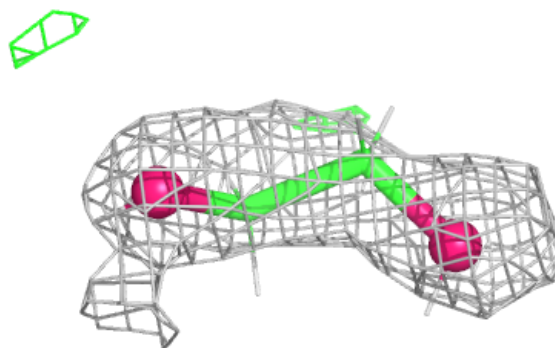
Electron density around EDO BBB 404:

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

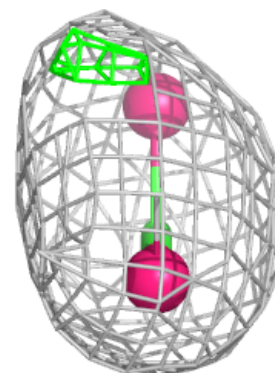
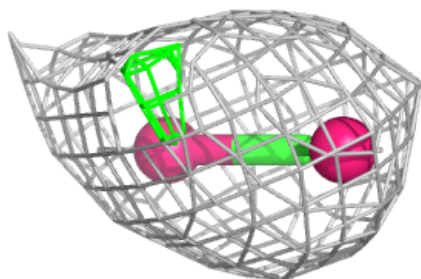
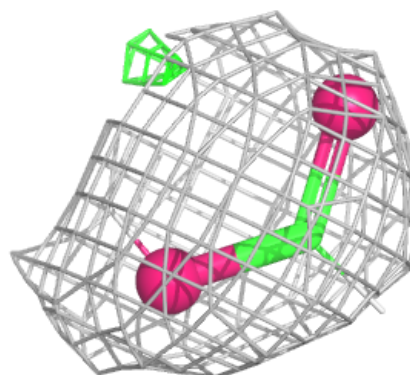


Electron density around EDO AAA 406:

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

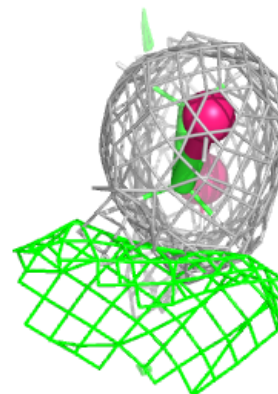
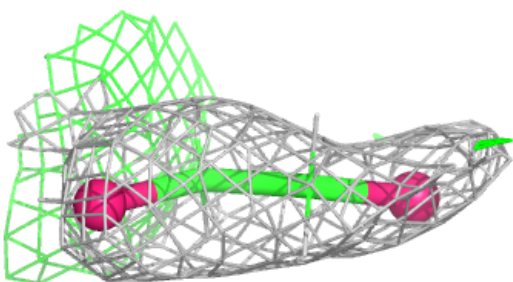
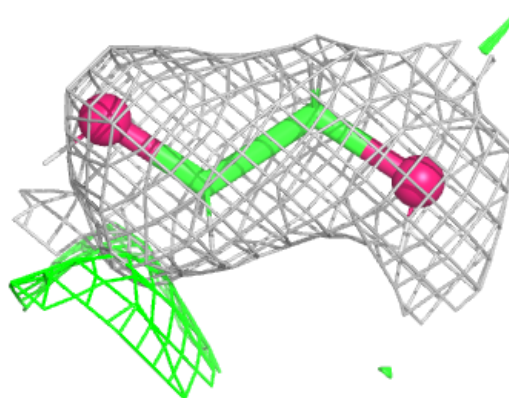
**Electron density around FMT AAA 408:**

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

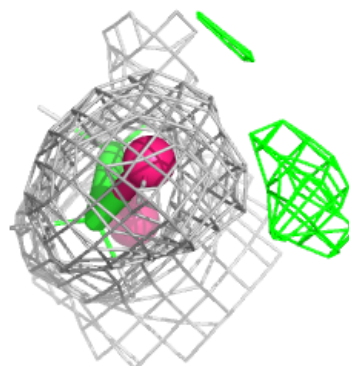
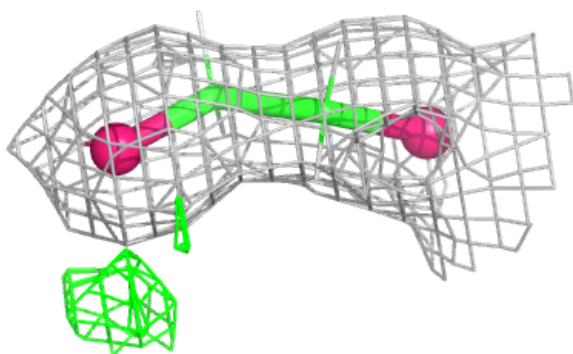
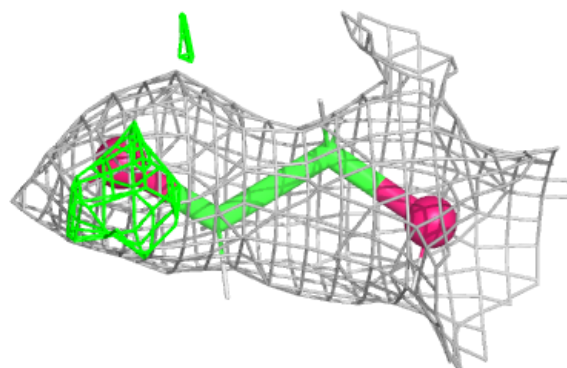


Electron density around EDO AAA 403:

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

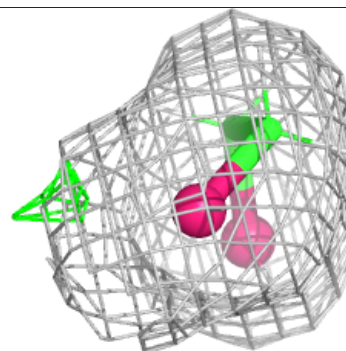
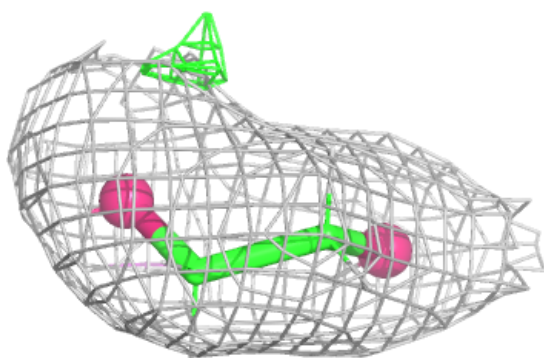
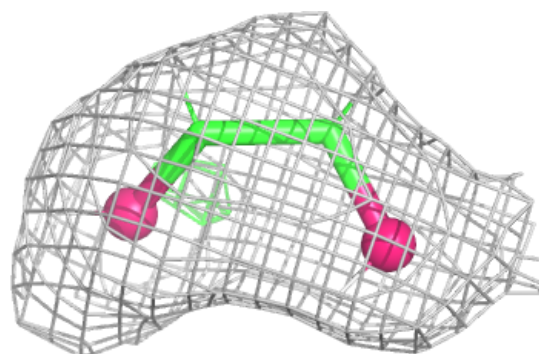
**Electron density around EDO BBB 402:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

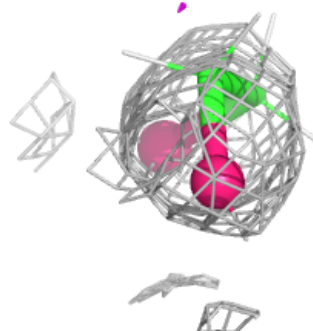
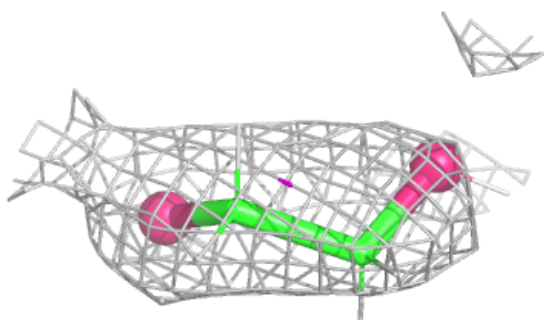
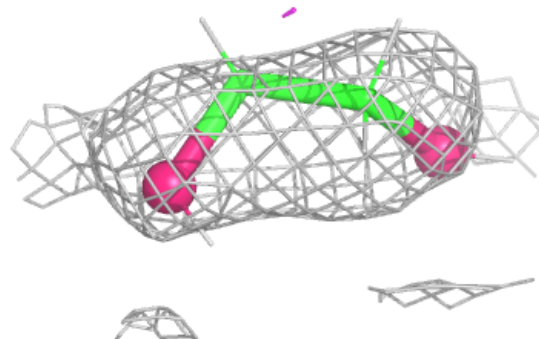


Electron density around EDO AAA 402:

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

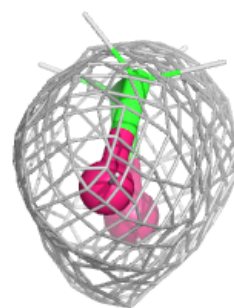
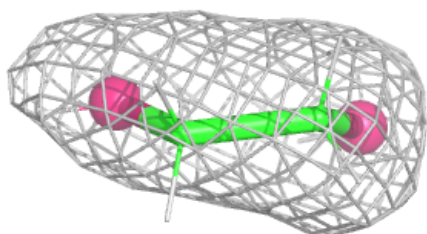
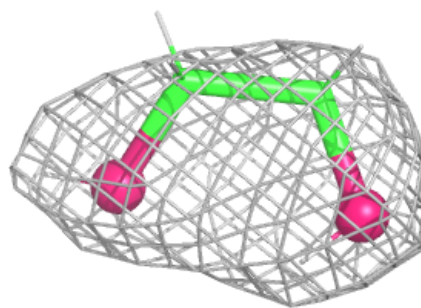
**Electron density around EDO AAA 404:**

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

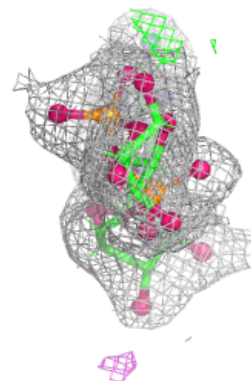
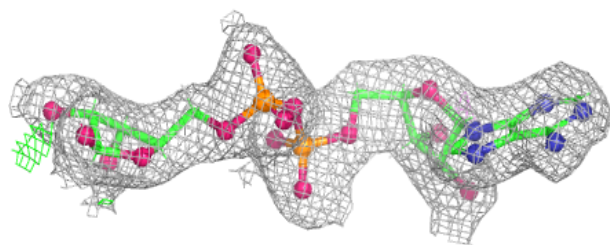
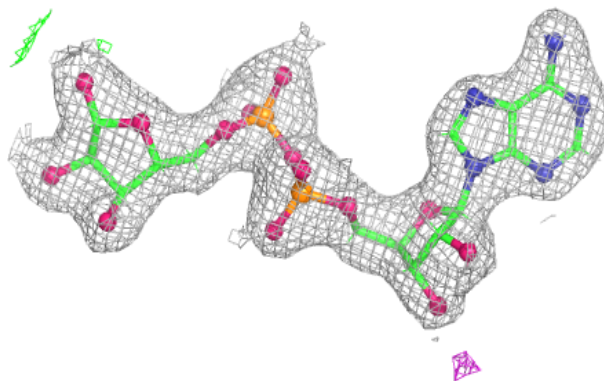


Electron density around EDO BBB 403:

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

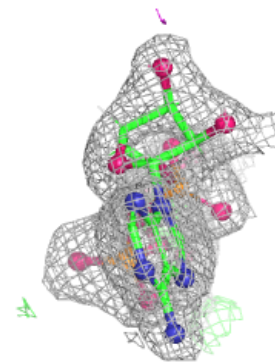
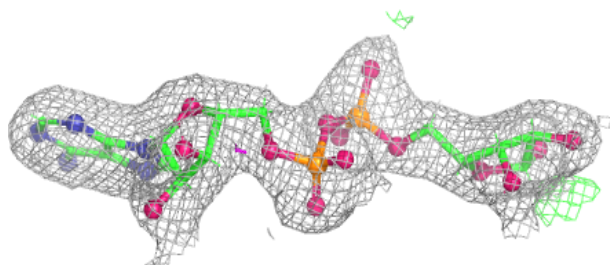
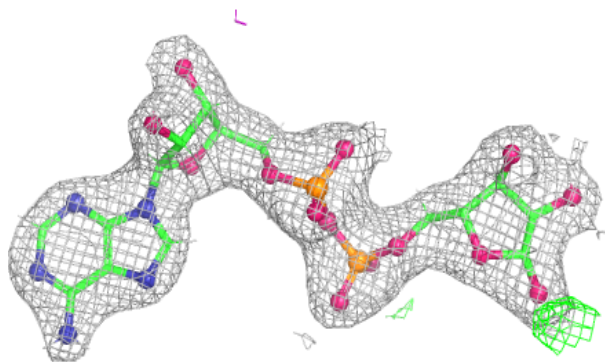
**Electron density around APR AAA 407:**

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



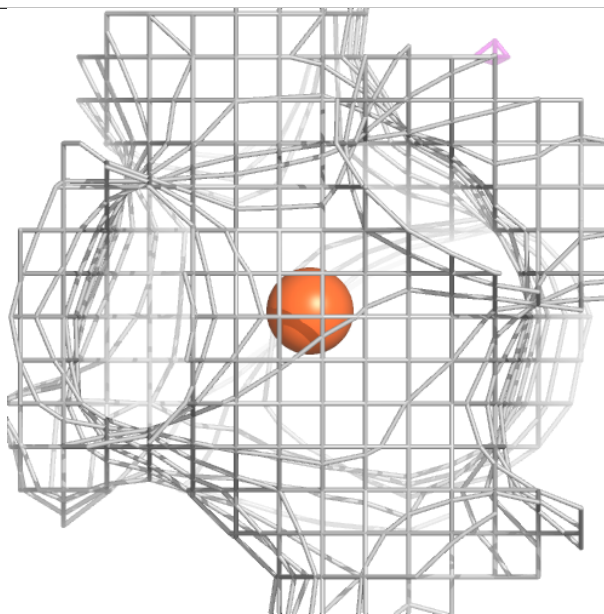
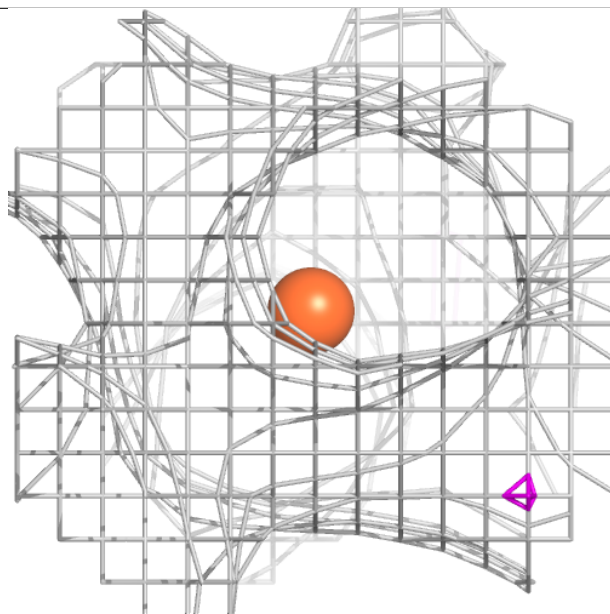
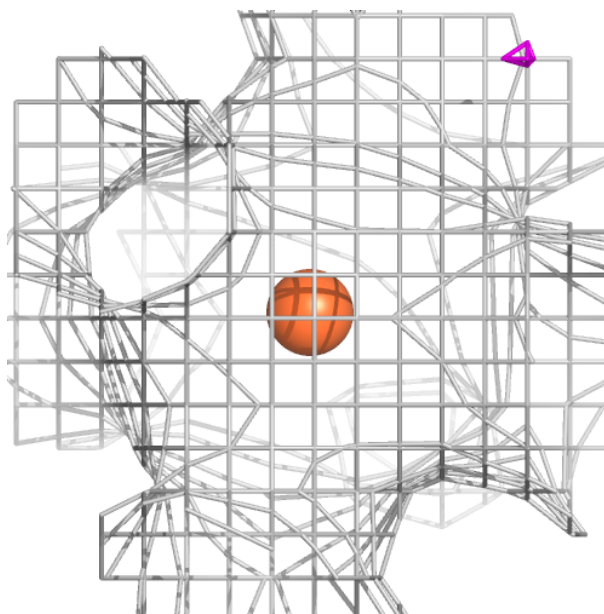
Electron density around APR BBB 405:

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and green (positive)



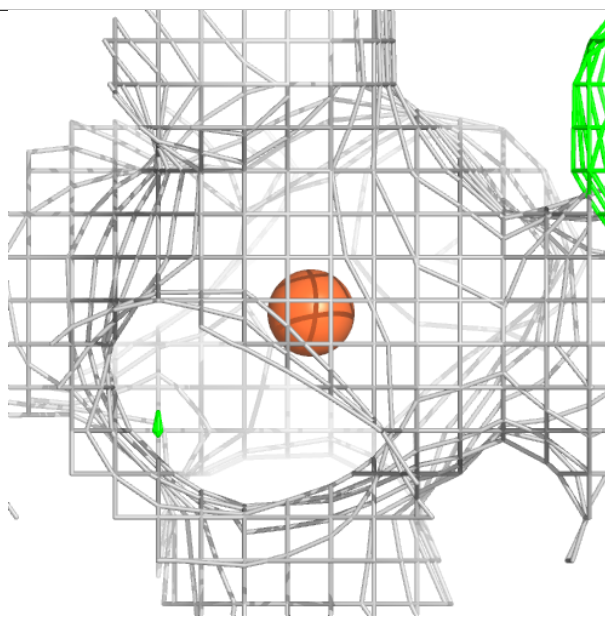
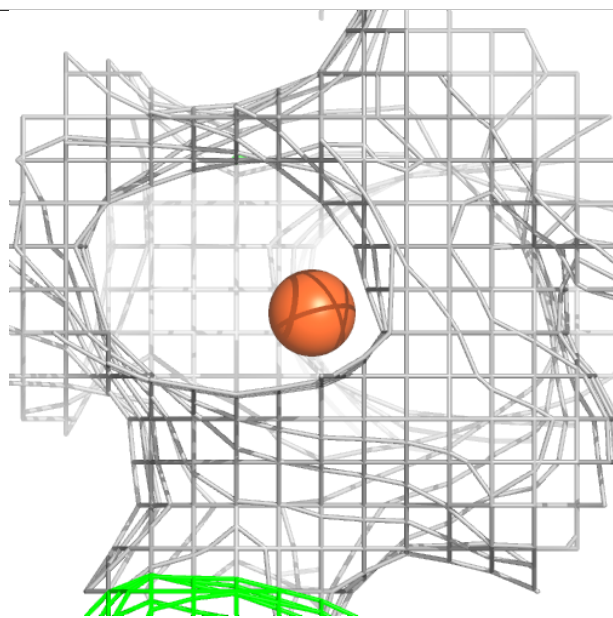
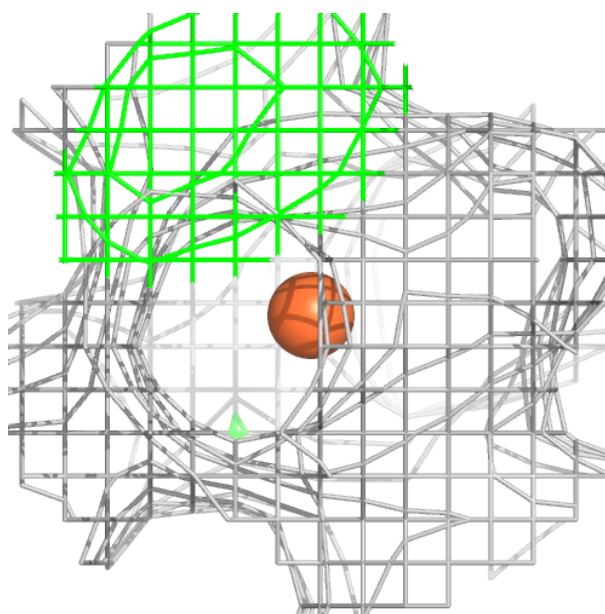
Electron density around FE BBB 401:

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



Electron density around FE 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.