Full wwPDB X-ray Structure Validation Report (i)

Jan 20, 2024 – 09:59 pm GMT

PDB ID	:	7R2G
Title	:	USP15 D1D2 in catalytically-competent state bound to mitoxantrone stack (isoform 2)
Authors	:	Priyanka, A.; Sixma, T.K.
Deposited on	:	2022-02-04
Resolution	:	1.98 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 (i) 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 (i)) were used in the production of this report:

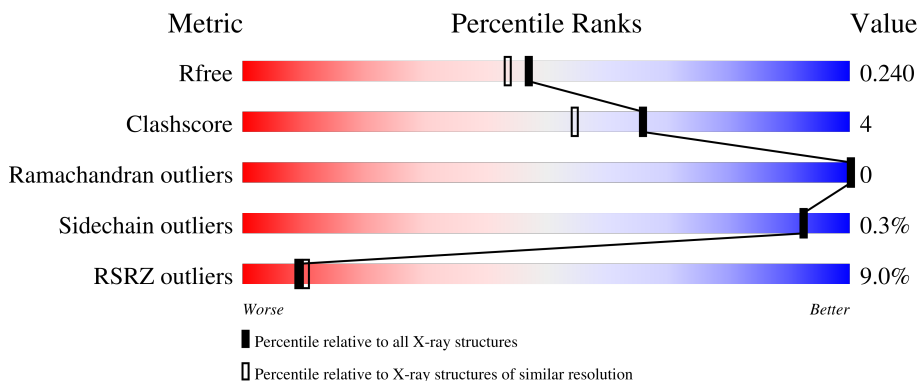|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.98 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		0.240
Clashscore		4
Ramachandran outliers		0
Sidechain outliers		0.3%
RSRZ outliers		9.0%

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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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	A	362	10% / 88% / 8% •
1	B	362	7% / 89% / 8% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

WORLDWIDE wwPDB PROTEIN DATA BANK

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MIX	B	1014	-	-	-	X

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 6126 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 Ubiquitin carboxyl-terminal hydrolase 15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	346	Total	C	N	O	S	0	0	0
			2780	1781	462	521	16			
1	B	351	Total	C	N	O	S	0	0	0
			2822	1806	471	529	16			

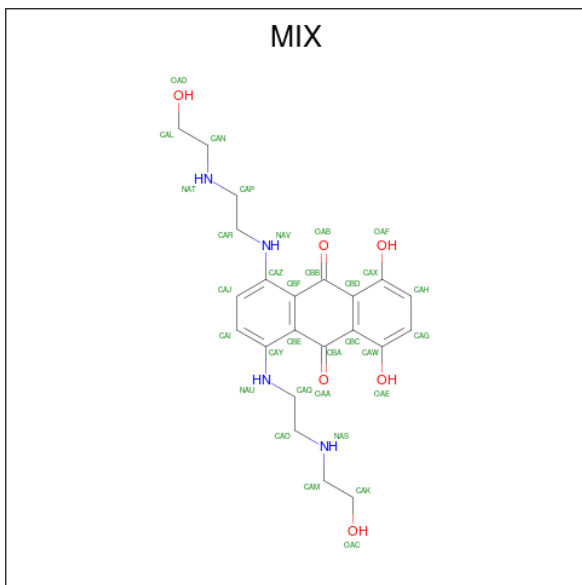- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
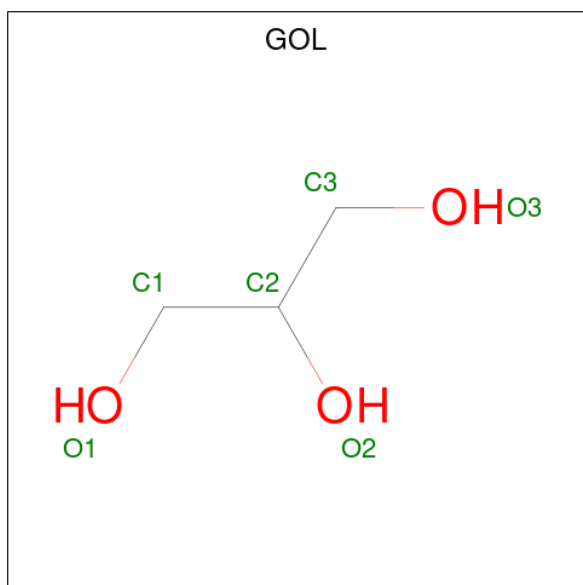
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total C O 6 3 3			0	0

- Molecule 4 is 1,4-DIHYDROXY-5,8-BIS({2-[(2-HYDROXYETHYL)AMINO]ETHYL}AMI NO)-9,10-ANTHRACENEDIONE (three-letter code: MIX) (formula: $C_{22}H_{28}N_4O_6$) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total 32	C 22	N 4	O 6	0	0
4	B	1	Total 32	C 22	N 4	O 6	0	0
4	B	1	Total 32	C 22	N 4	O 6	0	0
4	B	1	Total 32	C 22	N 4	O 6	0	0
4	B	1	Total 32	C 22	N 4	O 6	0	0
4	B	1	Total 32	C 22	N 4	O 6	0	0
4	B	1	Total 32	C 22	N 4	O 6	0	0
4	B	1	Total 32	C 22	N 4	O 6	0	0
4	B	1	Total 32	C 22	N 4	O 6	0	0
4	B	1	Total 32	C 22	N 4	O 6	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total 32	C 22	N 4	O 6	0	0
4	B	1	Total 32	C 22	N 4	O 6	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	52	Total 52	O 52	0	0
5	B	80	Total 80	O 80	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: Ubiquitin carboxyl-terminal hydrolase 15

Chain A:

• Molecule 1: Ubiquitin carboxyl-terminal hydrolase 15

Chain B:
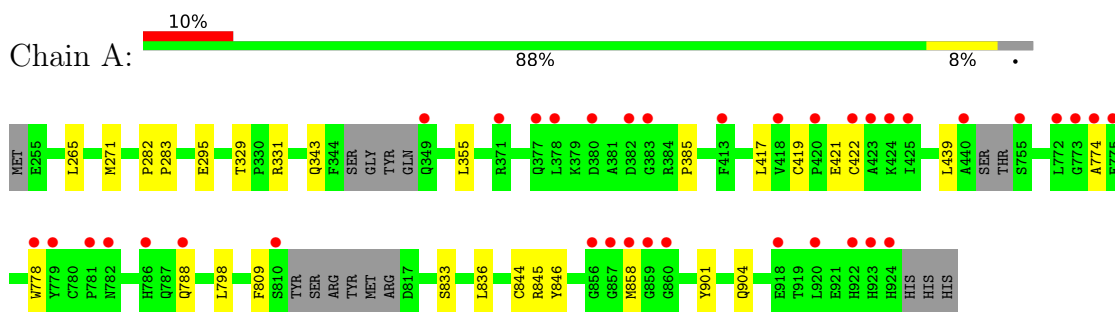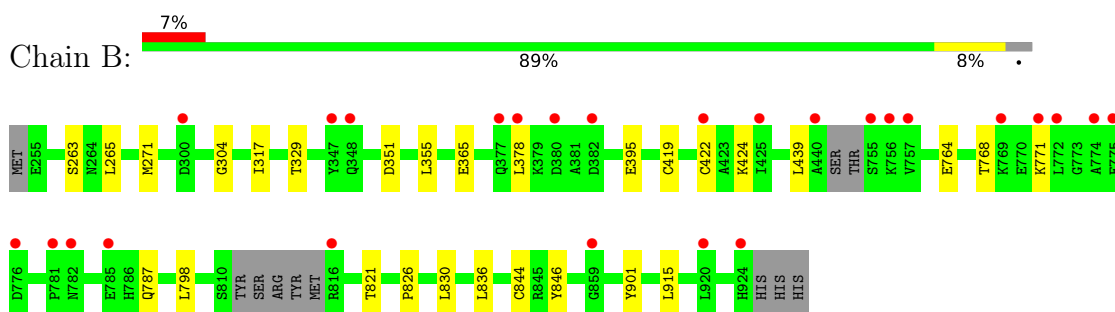
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	63.88Å 97.40Å 62.99Å 90.00° 90.01° 90.00°	Depositor
Resolution (Å)	44.89 – 1.98 44.85 – 1.98	Depositor EDS
% Data completeness (in resolution range)	96.7 (44.89-1.98) 96.7 (44.85-1.98)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.62 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.204 , 0.238 0.212 , 0.240	Depositor DCC
R_{free} test set	2444 reflections (4.71%)	wwPDB-VP
Wilson B-factor (Å^2)	32.5	Xtriage
Anisotropy	0.765	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 35.4	EDS
L-test for twinning[2]	$< |L| > = 0.46, < L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.026 for -l,k,h 0.316 for -h,-k,l 0.035 for l,-k,h	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	6126	wwPDB-VP
Average B, all atoms (Å^2)	54.0	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.*

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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: MIX, GOL, ZN

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	0.81	1/2851 (0.0%)	0.80	0/3858
1	B	0.79	1/2895 (0.0%)	0.80	0/3918
All	All	0.80	2/5746 (0.0%)	0.80	0/7776

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	295	GLU	CD-OE1	8.42	1.34	1.25
1	B	821	THR	C-O	5.90	1.34	1.23

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2780	0	2691	18	1
1	B	2822	0	2730	19	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	B	6	0	8	1	0
4	B	384	0	312	11	1
5	A	52	0	0	0	0

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PROTEIN DATA BANK

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	80	0	0	2	0
All	All	6126	0	5741	47	1

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 (47) 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:419:CYS:SG	1:A:421:GLU:O	2.36	0.83
1:B:764:GLU:O	1:B:768:THR:HG23	1.79	0.82
1:A:417:LEU:HD13	1:A:778:TRP:CD1	2.29	0.67
1:B:798:LEU:HD12	1:B:844:CYS:SG	2.36	0.66
1:A:798:LEU:HG	1:A:836:LEU:HD21	1.83	0.60
1:B:798:LEU:HG	1:B:836:LEU:HD21	1.87	0.55
1:A:271:MET:HA	1:A:355:LEU:CD2	2.38	0.53
1:A:385:PRO:HB3	1:B:304:GLY:O	2.08	0.53
1:B:422:CYS:SG	1:B:424:LYS:HB2	2.48	0.52
1:A:265:LEU:HD21	1:A:329:THR:HG23	1.91	0.51
1:B:844:CYS:HG	1:B:846:TYR:HE1	1.60	0.50
1:A:417:LEU:HD13	1:A:778:TRP:NE1	2.28	0.49
1:A:421:GLU:O	1:A:422:CYS:SG	2.71	0.48
4:B:1011:MIX:HAT	4:B:1012:MIX:HAS	1.61	0.48
1:B:263:SER:OG	1:B:329:THR:HA	2.13	0.48
1:A:282:PRO:N	1:A:283:PRO:HD2	2.30	0.47
1:B:439:LEU:HD12	1:B:439:LEU:N	2.31	0.46
4:B:1004:MIX:NAV	4:B:1004:MIX:OAB	2.48	0.46
1:B:419:CYS:SG	1:B:787:GLN:HG3	2.56	0.46
1:A:774:ALA:N	1:A:788:GLN:HE21	2.13	0.46
4:B:1005:MIX:OAB	4:B:1005:MIX:NAV	2.50	0.45
4:B:1007:MIX:OAB	4:B:1007:MIX:NAV	2.49	0.45
1:A:265:LEU:HD22	1:A:331:ARG:NH2	2.32	0.45
1:B:271:MET:HA	1:B:355:LEU:CD2	2.48	0.44
1:B:365:GLU:HA	1:B:365:GLU:OE1	2.19	0.43
1:A:833:SER:HA	1:A:844:CYS:SG	2.58	0.43
1:B:826:PRO:HG2	1:B:830:LEU:HB2	2.01	0.43
4:B:1008:MIX:OAB	4:B:1008:MIX:NAV	2.52	0.43
4:B:1011:MIX:HAR2	4:B:1012:MIX:CAI	2.49	0.42
1:A:439:LEU:HD12	1:A:439:LEU:N	2.34	0.42
1:B:317:ILE:HD13	1:B:317:ILE:HA	1.90	0.42
1:A:809:PHE:CE1	1:A:858:MET:HA	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:LEU:HD21	1:B:329:THR:HG23	2.01	0.42
1:A:833:SER:CA	1:A:844:CYS:SG	3.08	0.41
1:B:846:TYR:HB3	1:B:901:TYR:HB3	2.02	0.41
4:B:1004:MIX:HAR1	4:B:1005:MIX:OAA	2.20	0.41
1:B:395:GLU:HG3	5:B:1123:HOH:O	2.20	0.41
1:B:351:ASP:HB2	3:B:1002:GOL:H32	2.02	0.41
1:A:846:TYR:HB3	1:A:901:TYR:HB3	2.02	0.41
1:B:304:GLY:HA3	5:B:1121:HOH:O	2.19	0.41
4:B:1006:MIX:OAB	4:B:1006:MIX:NAV	2.53	0.41
4:B:1009:MIX:OAA	4:B:1009:MIX:NAU	2.53	0.41
4:B:1006:MIX:OAA	4:B:1006:MIX:NAU	2.53	0.40
1:A:282:PRO:N	1:A:283:PRO:CD	2.84	0.40
1:B:915:LEU:HD13	1:B:915:LEU:C	2.41	0.40
4:B:1008:MIX:OAA	4:B:1008:MIX:NAU	2.53	0.40
1:A:845:ARG:HD2	1:A:904:GLN:OE1	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:GLN:NE2	4:B:1014:MIX:OAE[2_654]	2.12	0.08

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	338/362 (93%)	329 (97%)	9 (3%)	0	100	100
1	B	345/362 (95%)	336 (97%)	9 (3%)	0	100	100
All	All	683/724 (94%)	665 (97%)	18 (3%)	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	306/321 (95%)	306 (100%)	0	100	100
1	B	310/321 (97%)	308 (99%)	2 (1%)	86	85
All	All	616/642 (96%)	614 (100%)	2 (0%)	92	92

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

Mol	Chain	Res	Type
1	B	378	LEU
1	B	771	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	267	ASN
1	A	788	GLN
1	B	256	GLN
1	B	267	ASN
1	B	924	HIS

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 15 ligands modelled in this entry, 2 are monoatomic - leaving 13 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	$\#|Z| > 2$
4	MIX	B	1004	-	34,34,34	0.43	0	44,46,46	0.64	0
4	MIX	B	1012	-	34,34,34	0.46	0	44,46,46	0.54	0
4	MIX	B	1003	-	34,34,34	0.49	0	44,46,46	0.57	0
4	MIX	B	1010	-	34,34,34	0.45	0	44,46,46	0.55	0
4	MIX	B	1014	-	34,34,34	0.49	0	44,46,46	0.61	0
4	MIX	B	1005	-	34,34,34	0.43	0	44,46,46	0.56	0
3	GOL	B	1002	-	5,5,5	0.13	0	5,5,5	0.29	0
4	MIX	B	1007	-	34,34,34	0.39	0	44,46,46	0.60	0
4	MIX	B	1008	-	34,34,34	0.44	0	44,46,46	0.55	0
4	MIX	B	1013	-	34,34,34	0.42	0	44,46,46	0.56	0
4	MIX	B	1011	-	34,34,34	0.43	0	44,46,46	0.56	0
4	MIX	B	1009	-	34,34,34	0.48	0	44,46,46	0.62	0
4	MIX	B	1006	-	34,34,34	0.41	0	44,46,46	0.56	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	MIX	B	1004	-	-	5/14/30/30	0/3/3/3
4	MIX	B	1012	-	-	6/14/30/30	0/3/3/3
4	MIX	B	1003	-	-	10/14/30/30	0/3/3/3
4	MIX	B	1010	-	-	9/14/30/30	0/3/3/3
4	MIX	B	1014	-	-	9/14/30/30	0/3/3/3
4	MIX	B	1005	-	-	4/14/30/30	0/3/3/3
3	GOL	B	1002	-	-	3/4/4/4	-
4	MIX	B	1007	-	-	6/14/30/30	0/3/3/3
4	MIX	B	1008	-	-	1/14/30/30	0/3/3/3
4	MIX	B	1013	-	-	9/14/30/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MIX	B	1011	-	-	7/14/30/30	0/3/3/3
4	MIX	B	1009	-	-	4/14/30/30	0/3/3/3
4	MIX	B	1006	-	-	8/14/30/30	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (81) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1006	MIX	OAD-CAL-CAN-NAT
4	B	1008	MIX	OAC-CAK-CAM-NAS
4	B	1010	MIX	OAD-CAL-CAN-NAT
4	B	1011	MIX	OAD-CAL-CAN-NAT
4	B	1004	MIX	NAS-CAO-CAQ-NAU
4	B	1005	MIX	NAT-CAP-CAR-NAV
4	B	1010	MIX	NAT-CAP-CAR-NAV
4	B	1014	MIX	CAJ-CAZ-NAV-CAR
4	B	1003	MIX	NAS-CAO-CAQ-NAU
4	B	1003	MIX	NAT-CAP-CAR-NAV
4	B	1003	MIX	CAI-CAY-NAU-CAQ
4	B	1004	MIX	CAJ-CAZ-NAV-CAR
4	B	1006	MIX	CAI-CAY-NAU-CAQ
4	B	1010	MIX	CAI-CAY-NAU-CAQ
4	B	1011	MIX	CAI-CAY-NAU-CAQ
4	B	1014	MIX	CBF-CAZ-NAV-CAR
4	B	1004	MIX	OAD-CAL-CAN-NAT
4	B	1013	MIX	OAC-CAK-CAM-NAS
4	B	1014	MIX	NAT-CAP-CAR-NAV
4	B	1010	MIX	NAS-CAO-CAQ-NAU
4	B	1014	MIX	CAK-CAM-NAS-CAO
4	B	1014	MIX	NAS-CAO-CAQ-NAU
4	B	1007	MIX	CAI-CAY-NAU-CAQ
4	B	1003	MIX	CBE-CAY-NAU-CAQ
4	B	1003	MIX	CBF-CAZ-NAV-CAR
4	B	1004	MIX	CBF-CAZ-NAV-CAR
4	B	1006	MIX	CBE-CAY-NAU-CAQ
4	B	1007	MIX	CBE-CAY-NAU-CAQ
4	B	1007	MIX	CBF-CAZ-NAV-CAR
4	B	1010	MIX	CBE-CAY-NAU-CAQ

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Mol	Chain	Res	Type	Atoms
4	B	1011	MIX	CBE-CAY-NAU-CAQ
4	B	1013	MIX	CBF-CAZ-NAV-CAR
4	B	1007	MIX	CAJ-CAZ-NAV-CAR
4	B	1013	MIX	CAJ-CAZ-NAV-CAR
4	B	1003	MIX	OAC-CAK-CAM-NAS
4	B	1003	MIX	OAD-CAL-CAN-NAT
4	B	1005	MIX	OAD-CAL-CAN-NAT
4	B	1012	MIX	OAC-CAK-CAM-NAS
3	B	1002	GOL	O1-C1-C2-C3
4	B	1013	MIX	CBE-CAY-NAU-CAQ
4	B	1003	MIX	CAJ-CAZ-NAV-CAR
4	B	1013	MIX	NAT-CAP-CAR-NAV
4	B	1013	MIX	CAI-CAY-NAU-CAQ
4	B	1010	MIX	CAR-CAP-NAT-CAN
4	B	1005	MIX	NAS-CAO-CAQ-NAU
4	B	1011	MIX	CAR-CAP-NAT-CAN
4	B	1013	MIX	CAP-CAR-NAV-CAZ
4	B	1004	MIX	OAC-CAK-CAM-NAS
4	B	1005	MIX	OAC-CAK-CAM-NAS
4	B	1009	MIX	OAC-CAK-CAM-NAS
4	B	1010	MIX	OAC-CAK-CAM-NAS
4	B	1003	MIX	CAR-CAP-NAT-CAN
4	B	1013	MIX	CAQ-CAO-NAS-CAM
4	B	1006	MIX	NAT-CAP-CAR-NAV
4	B	1009	MIX	CAL-CAN-NAT-CAP
4	B	1014	MIX	CBE-CAY-NAU-CAQ
4	B	1010	MIX	CAO-CAQ-NAU-CAY
3	B	1002	GOL	O2-C2-C3-O3
4	B	1006	MIX	CAR-CAP-NAT-CAN
4	B	1010	MIX	CAP-CAR-NAV-CAZ
4	B	1006	MIX	CAP-CAR-NAV-CAZ
4	B	1011	MIX	CAL-CAN-NAT-CAP
4	B	1014	MIX	CAI-CAY-NAU-CAQ
4	B	1011	MIX	CAJ-CAZ-NAV-CAR
4	B	1014	MIX	OAC-CAK-CAM-NAS
4	B	1006	MIX	CBF-CAZ-NAV-CAR
4	B	1011	MIX	CBF-CAZ-NAV-CAR
4	B	1013	MIX	OAD-CAL-CAN-NAT
4	B	1003	MIX	CAQ-CAO-NAS-CAM
4	B	1012	MIX	CBE-CAY-NAU-CAQ
4	B	1006	MIX	CAJ-CAZ-NAV-CAR
4	B	1007	MIX	OAC-CAK-CAM-NAS

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Mol	Chain	Res	Type	Atoms
3	B	1002	GOL	C1-C2-C3-O3
4	B	1012	MIX	CAR-CAP-NAT-CAN
4	B	1007	MIX	NAS-CAO-CAQ-NAU
4	B	1014	MIX	CAL-CAN-NAT-CAP
4	B	1012	MIX	NAS-CAO-CAQ-NAU
4	B	1012	MIX	NAT-CAP-CAR-NAV
4	B	1012	MIX	CAI-CAY-NAU-CAQ
4	B	1009	MIX	CAK-CAM-NAS-CAO
4	B	1009	MIX	CBE-CAY-NAU-CAQ

There are no ring outliers.

10 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1004	MIX	2	0
4	B	1012	MIX	2	0
4	B	1014	MIX	0	1
4	B	1005	MIX	2	0
3	B	1002	GOL	1	0
4	B	1007	MIX	1	0
4	B	1008	MIX	2	0
4	B	1011	MIX	2	0
4	B	1009	MIX	1	0
4	B	1006	MIX	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 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 MIX B 1004

Bond lengths

Bond angles

Torsions

Rings

Ligand MIX B 1012

Bond lengths

Bond angles

Torsions

Rings

Ligand MIX B 1003

Bond lengths

Bond angles

Torsions

Rings

Ligand MIX B 1010

Bond lengths

Bond angles

Torsions

Rings

Ligand MIX B 1014

Bond lengths

Bond angles

Torsions

Rings

Ligand MIX B 1005

Bond lengths

Bond angles

Torsions

Rings

Ligand MIX B 1007

Bond lengths

Bond angles

Torsions

Rings

Ligand MIX B 1008

Bond lengths

Bond angles

Torsions

Rings

Ligand MIX B 1013

Bond lengths

Bond angles

Torsions

Rings

Ligand MIX B 1011

Bond lengths

Bond angles

Torsions

Rings

Ligand MIX B 1009

Bond lengths

Bond angles

Torsions

Rings

Ligand MIX B 1006

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(Å²)	Q<0.9
1	A	346/362 (95%)	0.62	37 (10%)	6	6	27, 45, 99, 125	0
1	B	351/362 (96%)	0.44	26 (7%)	14	16	27, 45, 90, 109	0
All	All	697/724 (96%)	0.53	63 (9%)	9	10	27, 45, 95, 125	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	810	SER	10.7
1	A	857	GLY	10.2
1	A	859	GLY	9.3
1	A	858	MET	8.0
1	A	349	GLN	5.9
1	A	378	LEU	5.5
1	B	378	LEU	5.4
1	A	440	ALA	5.3
1	A	775	GLU	5.0
1	A	774	ALA	4.8
1	A	423	ALA	4.8
1	B	348	GLN	4.8
1	A	425	ILE	4.6
1	A	856	GLY	4.4
1	A	922	HIS	4.4
1	B	347	TYR	4.2
1	B	756	LYS	4.0
1	B	772	LEU	3.9
1	B	422	CYS	3.9
1	B	755	SER	3.9
1	A	924	HIS	3.8
1	A	778	TRP	3.7
1	A	422	CYS	3.7
1	A	380	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	424	LYS	3.6
1	B	377	GLN	3.6
1	A	377	GLN	3.6
1	A	779	TYR	3.5
1	A	772	LEU	3.4
1	B	440	ALA	3.4
1	A	773	GLY	3.3
1	A	786	HIS	3.3
1	B	775	GLU	3.1
1	A	383	GLY	3.1
1	B	771	LYS	3.0
1	A	788	GLN	3.0
1	A	420	PRO	2.9
1	B	816	ARG	2.8
1	A	418	VAL	2.8
1	B	859	GLY	2.7
1	A	918	GLU	2.7
1	A	413	PHE	2.5
1	A	382	ASP	2.5
1	B	785	GLU	2.5
1	B	300	ASP	2.5
1	B	382	ASP	2.5
1	A	782	ASN	2.4
1	A	860	GLY	2.4
1	B	924	HIS	2.4
1	B	380	ASP	2.3
1	B	774	ALA	2.3
1	A	371	ARG	2.3
1	B	920	LEU	2.2
1	A	923	HIS	2.2
1	B	776	ASP	2.2
1	A	755	SER	2.2
1	B	757	VAL	2.2
1	B	425	ILE	2.2
1	A	781	PRO	2.2
1	B	781	PRO	2.1
1	B	769	LYS	2.1
1	B	782	ASN	2.1
1	A	920	LEU	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 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
4	MIX	B	1014	32/32	0.65	0.42	115,133,143,144	0
4	MIX	B	1012	32/32	0.76	0.32	106,122,134,135	0
3	GOL	B	1002	6/6	0.76	0.15	46,54,54,62	0
4	MIX	B	1009	32/32	0.79	0.25	102,109,116,118	0
4	MIX	B	1010	32/32	0.79	0.26	108,116,131,131	0
2	ZN	A	1001	1/1	0.81	0.06	101,101,101,101	0
4	MIX	B	1011	32/32	0.81	0.29	108,127,132,136	0
4	MIX	B	1008	32/32	0.85	0.27	99,107,125,128	0
4	MIX	B	1013	32/32	0.85	0.26	112,127,136,137	0
4	MIX	B	1006	32/32	0.85	0.25	94,105,128,128	0
2	ZN	B	1001	1/1	0.86	0.30	71,71,71,71	1
4	MIX	B	1005	32/32	0.87	0.23	98,103,135,136	0
4	MIX	B	1007	32/32	0.89	0.26	87,106,130,131	0
4	MIX	B	1003	32/32	0.90	0.18	82,90,105,107	0
4	MIX	B	1004	32/32	0.90	0.24	85,92,116,118	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.
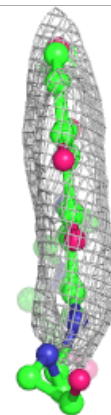
Electron density around MIX B 1014:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
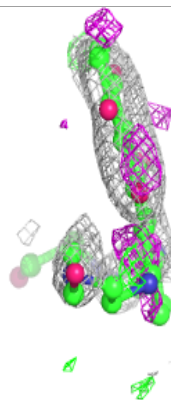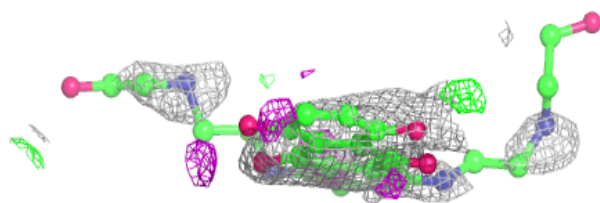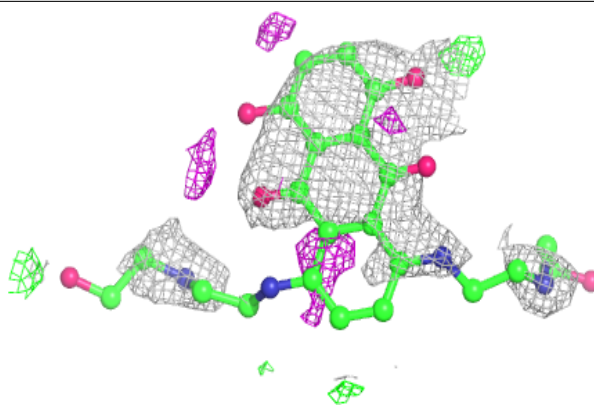
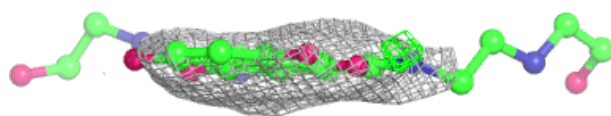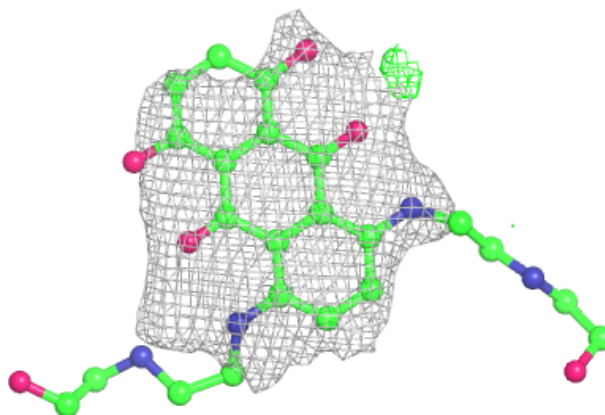
Electron density around MIX B 1012:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
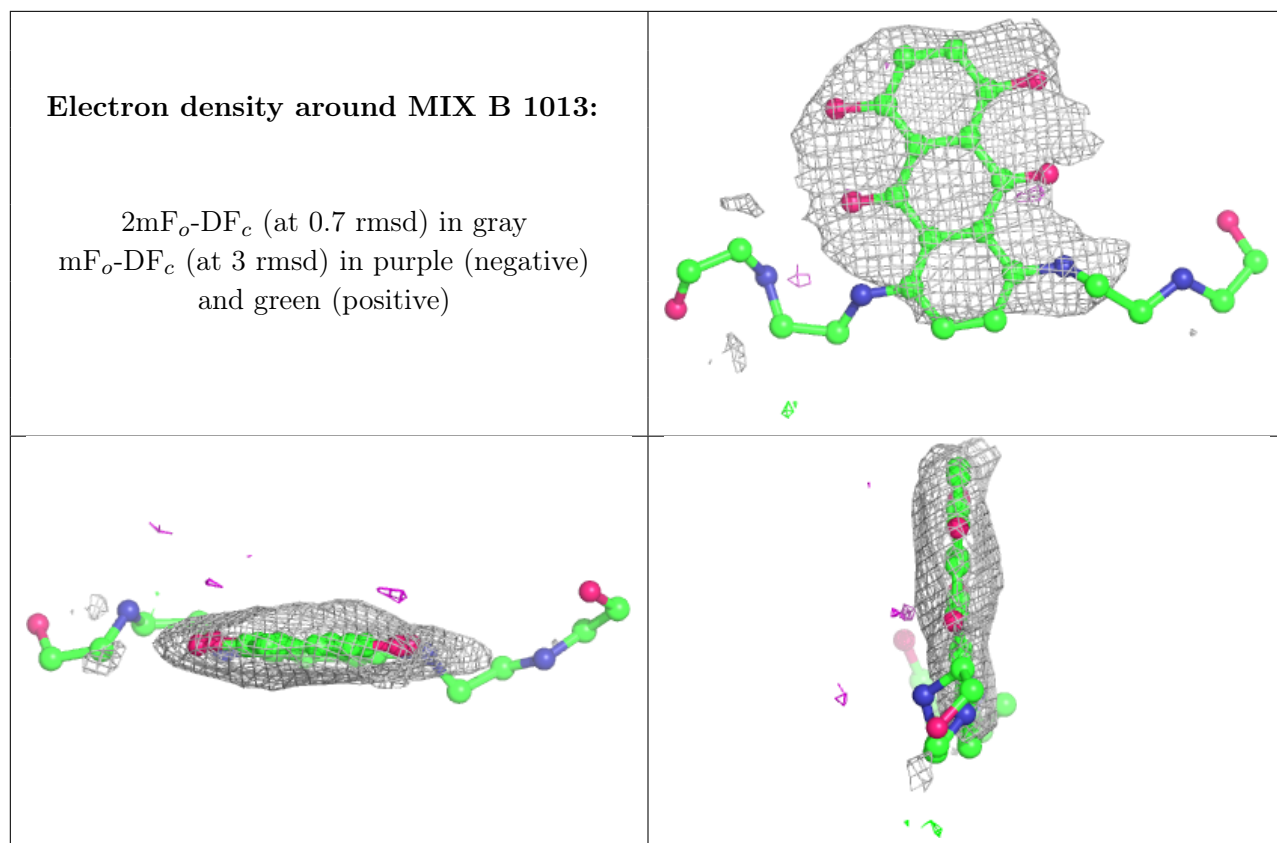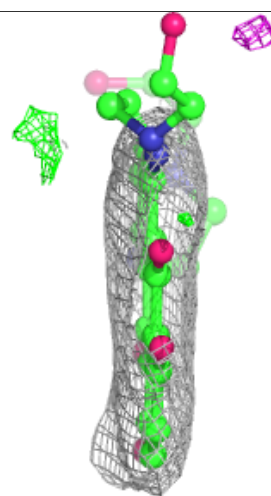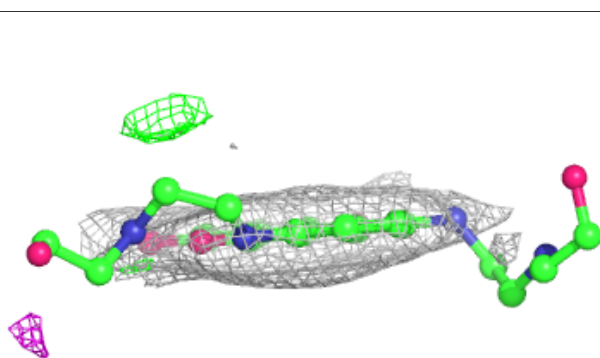mF_o-DF_c (at 3 rmsd) in purple (negative)
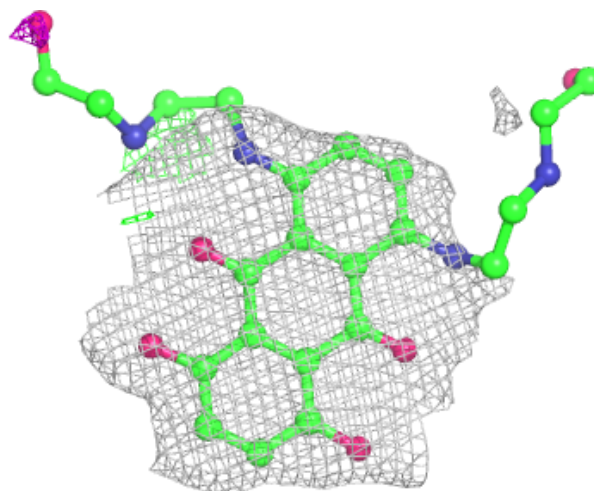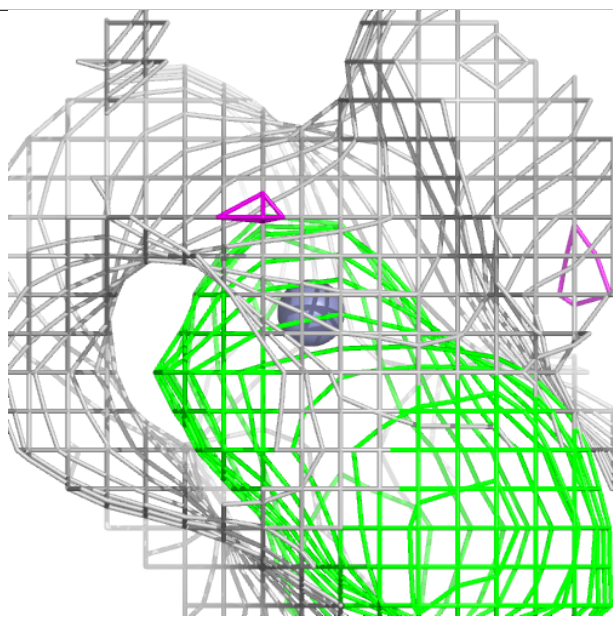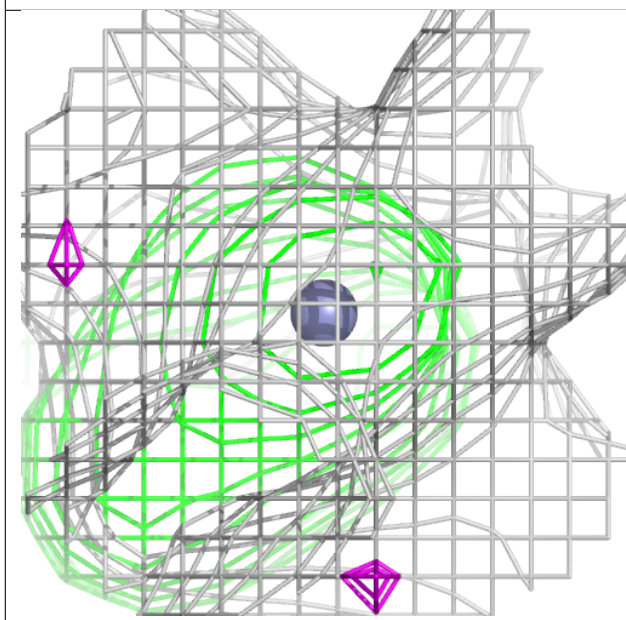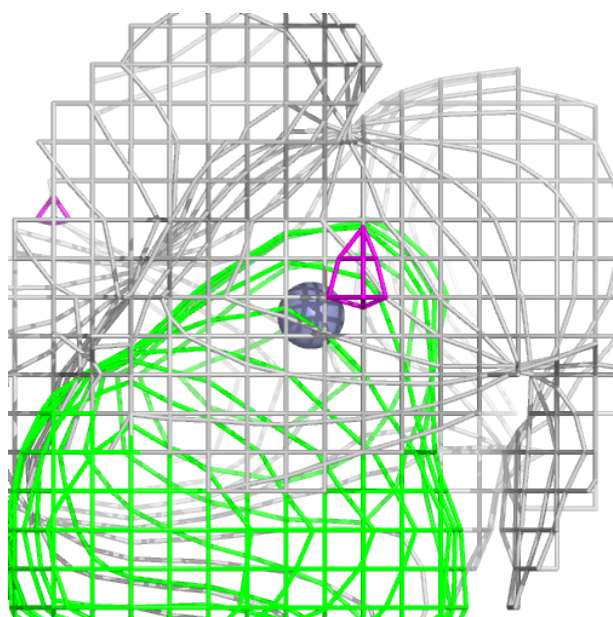and green (positive)
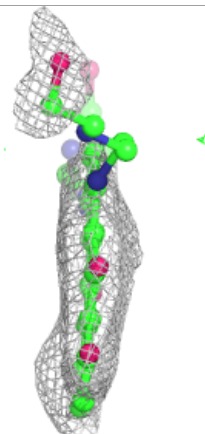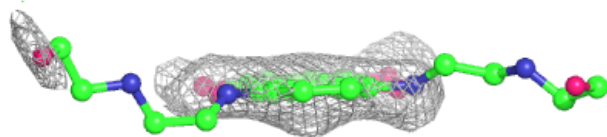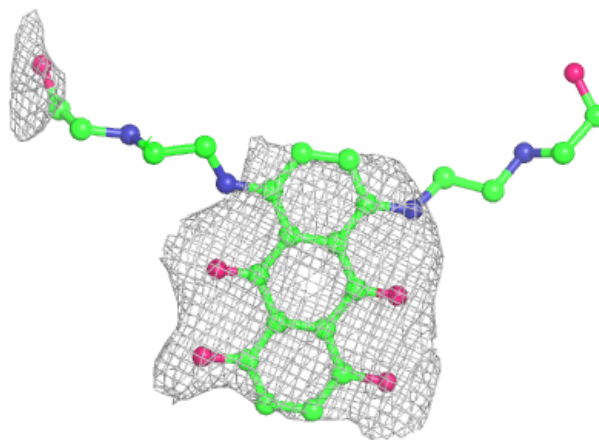
Electron density around MIX B 1009:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
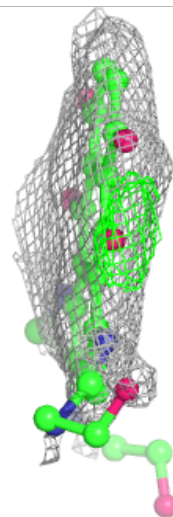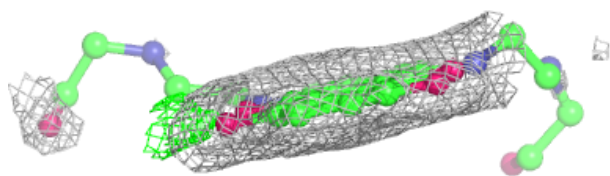mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
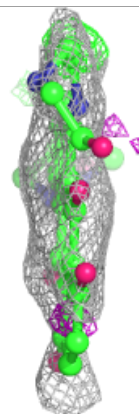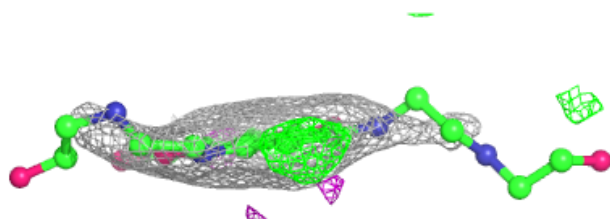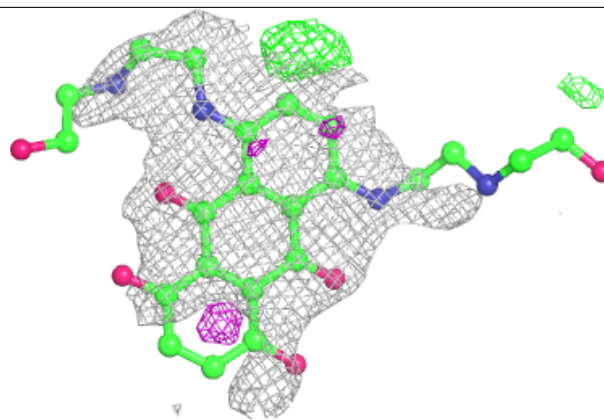
Electron density around MIX B 1010:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
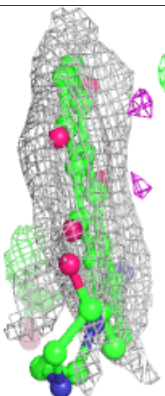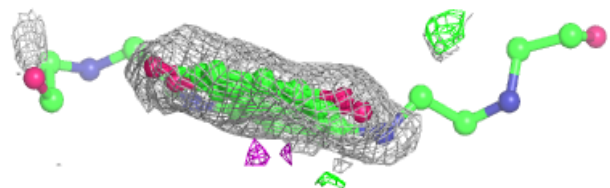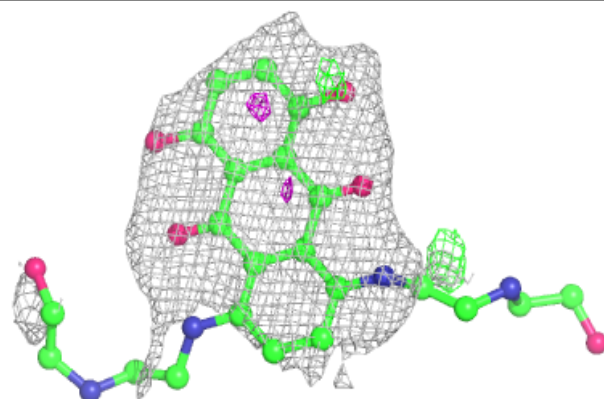
Electron density around ZN A 1001:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
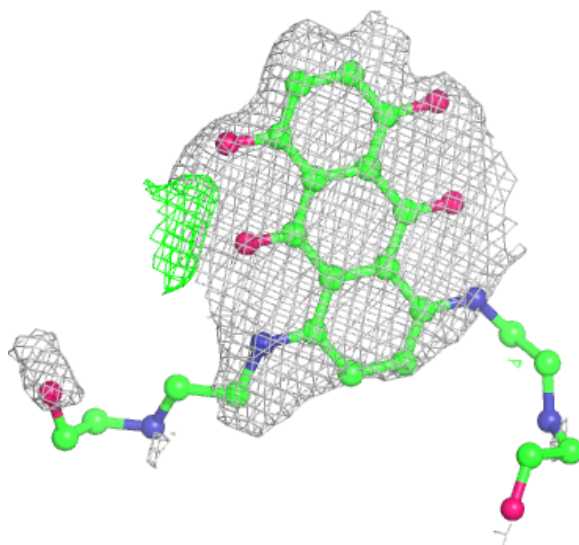and green (positive)
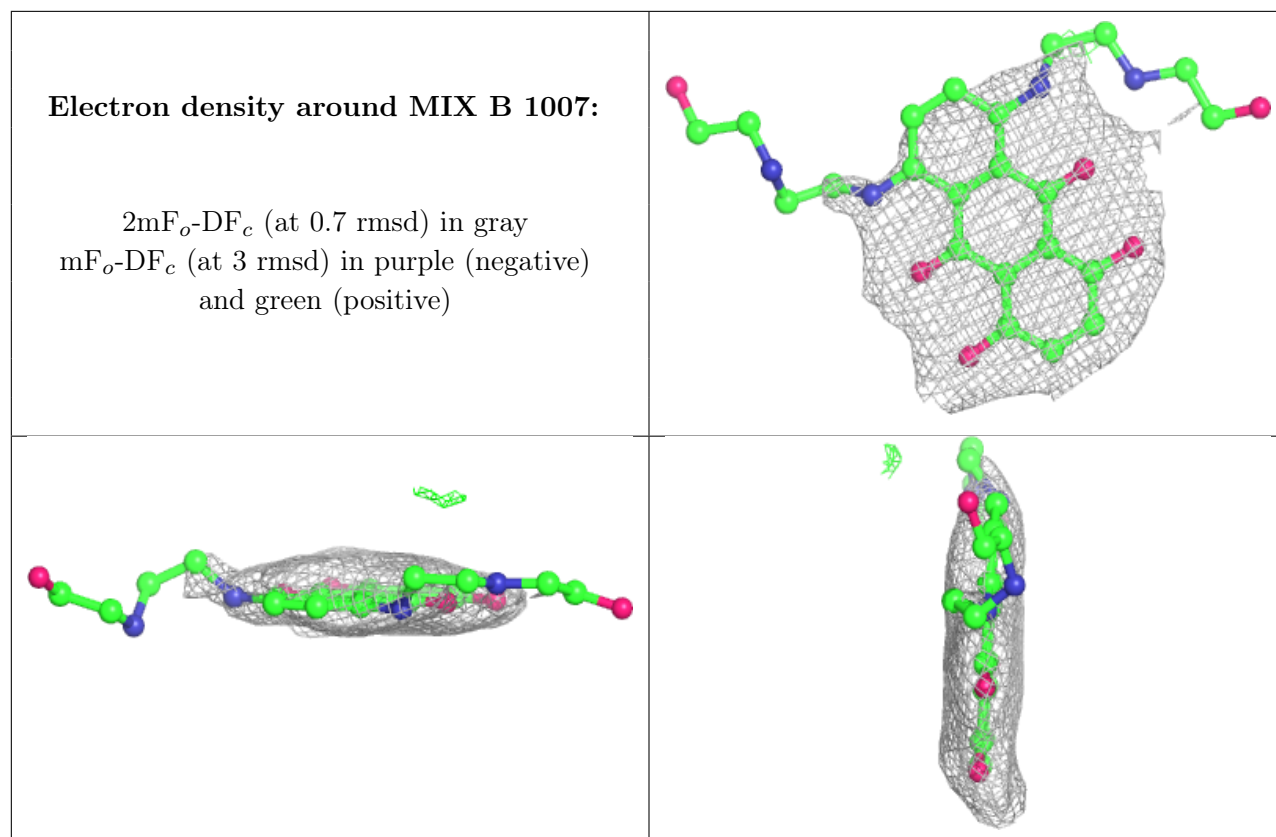
Electron density around MIX B 1011:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
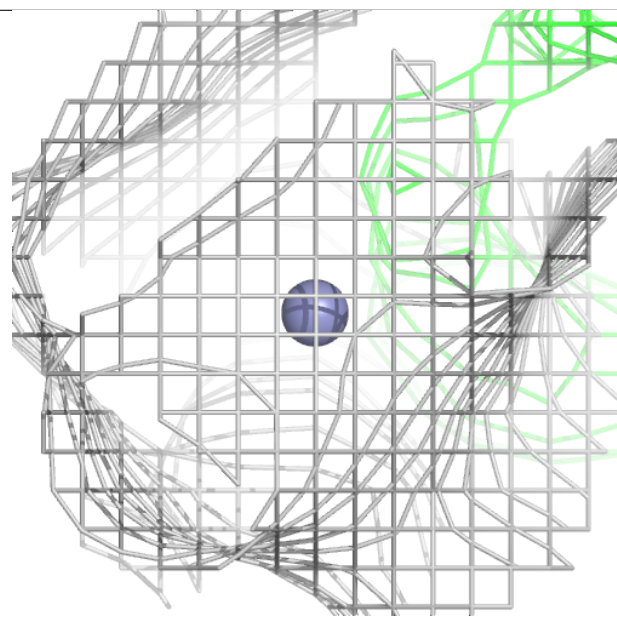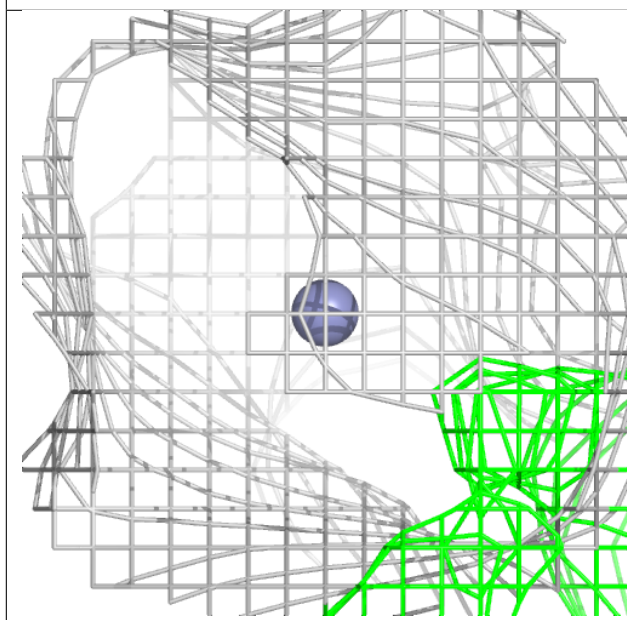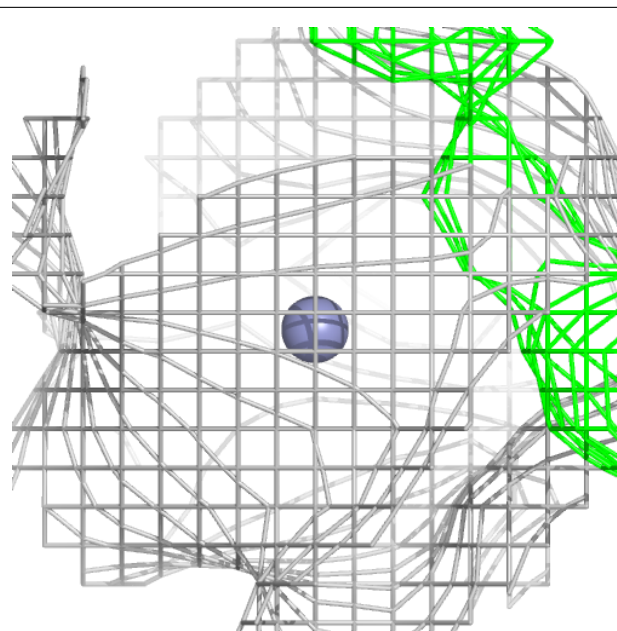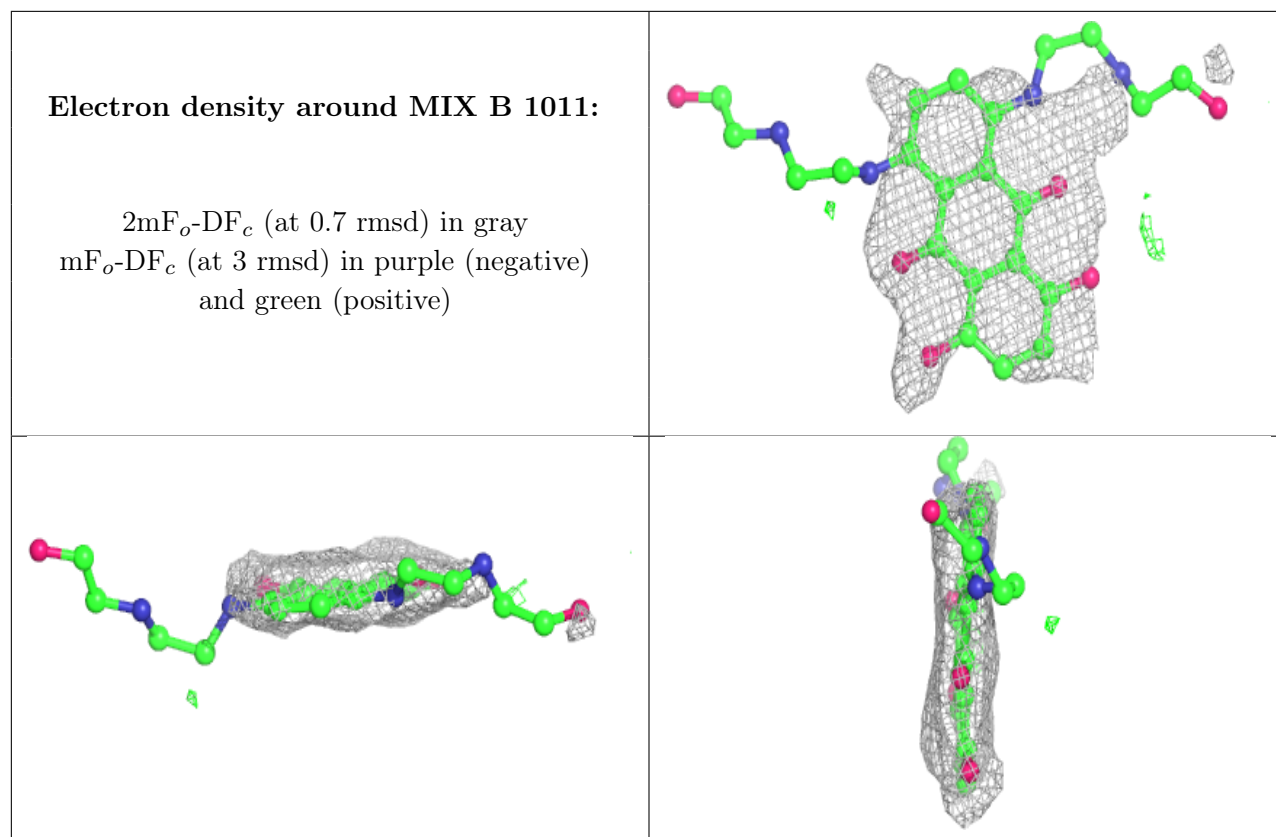
Electron density around MIX B 1008:

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

Electron density around MIX B 1013:

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

Electron density around MIX B 1006:

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

Electron density around ZN B 1001:

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

**Electron density around MIX B 1005:**

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

Electron density around MIX B 1007:

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

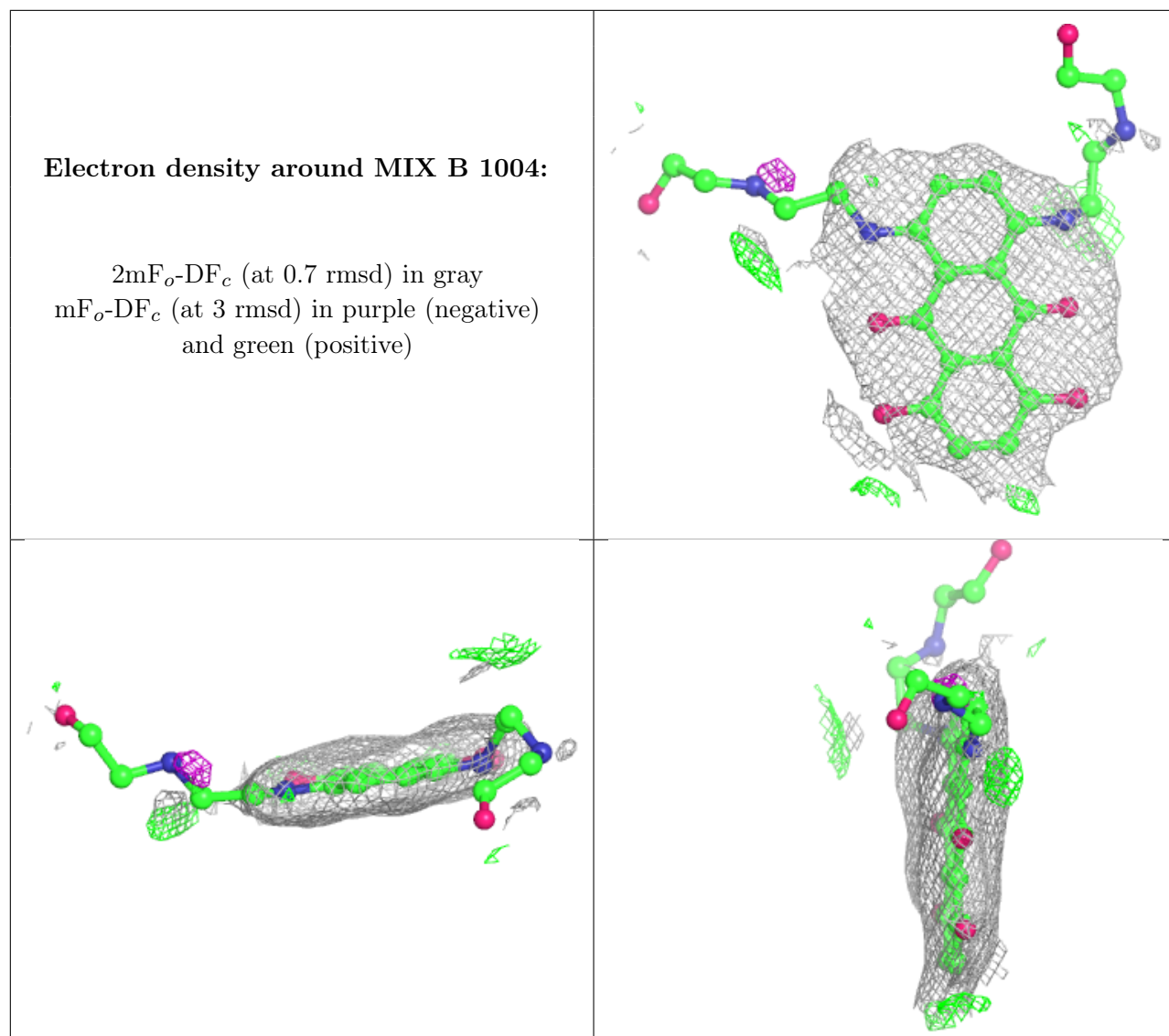**Electron density around MIX B 1003:**

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

Electron density around MIX B 1004:

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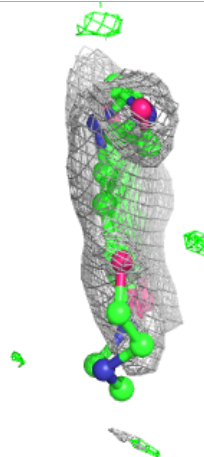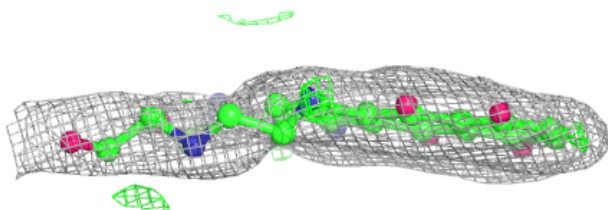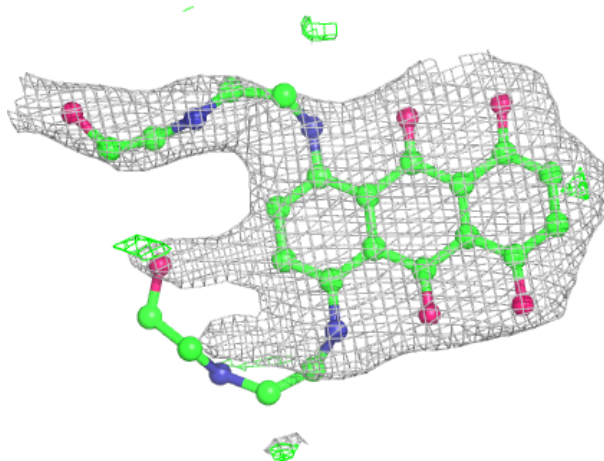
6.5 Other polymers (i)

There are no such residues in this entry.