WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Oct 15, 2023 – 10:35 AM EDT

PDB ID	:	8DZK
Title	:	Dbr1 in complex with 5-mer cleavage product
Authors	:	Clark, N.E.; Taylor, A.B.
Deposited on	:	2022-08-08
Resolution	:	2.10 Å(reported)

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

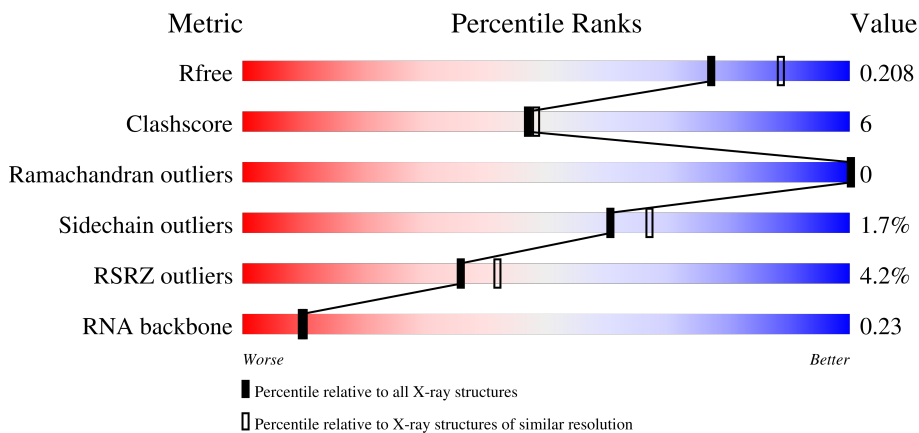|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.10 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		0.208
Clashscore		6
Ramachandran outliers		0
Sidechain outliers		1.7%
RSRZ outliers		4.2%
RNA backbone		0.23

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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)
RNA backbone	3102	1000 (2.54-1.66)

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	356	3% / 88% / 10% ·
1	B	356	2% / 79% / 18% ··
1	C	356	2% / 85% / 12% ··
1	D	356	5% / 85% / 12% ··

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Mol	Chain	Length	Quality of chain
1	E	356	8% 85% 12%
2	F	5	60% 20% 20%
2	G	5	60% 20% 20%
2	N	5	60% 20% 20%
2	O	5	20% 20% 20% 40% 20%
2	P	5	20% 20% 20% 40% 20%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 15212 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 RNA lariat debranching enzyme, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	349	Total 2857	C 1857	N 465	O 520	S 15	0	0	0
1	B	349	Total 2879	C 1869	N 470	O 524	S 16	0	3	0
1	C	349	Total 2857	C 1857	N 465	O 520	S 15	0	0	0
1	D	349	Total 2857	C 1857	N 465	O 520	S 15	0	0	0
1	E	349	Total 2857	C 1857	N 465	O 520	S 15	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP C4M1P9
A	0	ALA	-	expression tag	UNP C4M1P9
B	-1	GLY	-	expression tag	UNP C4M1P9
B	0	ALA	-	expression tag	UNP C4M1P9
C	-1	GLY	-	expression tag	UNP C4M1P9
C	0	ALA	-	expression tag	UNP C4M1P9
D	-1	GLY	-	expression tag	UNP C4M1P9
D	0	ALA	-	expression tag	UNP C4M1P9
E	-1	GLY	-	expression tag	UNP C4M1P9
E	0	ALA	-	expression tag	UNP C4M1P9

- Molecule 2 is a RNA chain called RNA (5'-R(P*(G46)P*UP*GP*UP*U)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	F	5	Total 90	C 38	N 14	O 32	P 5	S 1	0	0	0
2	G	4	Total 71	C 29	N 12	O 25	P 4	S 1	0	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	N	5	Total	C	N	O	P	S	0	0	0
			90	38	14	32	5	1			
2	O	4	Total	C	N	O	P	S	0	0	0
			49	19	2	23	4	1			
2	P	4	Total	C	N	O	P	S	0	0	0
			49	19	2	23	4	1			

- Molecule 3 is FE (II) ION (three-letter code: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Fe	0	0
			1	1		
3	B	1	Total	Fe	0	0
			1	1		
3	C	1	Total	Fe	0	0
			1	1		
3	D	1	Total	Fe	0	0
			1	1		
3	E	1	Total	Fe	0	0
			1	1		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		
4	B	1	Total	Zn	0	0
			1	1		
4	C	1	Total	Zn	0	0
			1	1		
4	D	1	Total	Zn	0	0
			1	1		
4	E	1	Total	Zn	0	0
			1	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

SO4

O1

O

O3 O⁻ —— S —— O⁻ O4

S

O

O2

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 5	O 4	S 1	0	0
5	A	1	Total 5	O 4	S 1	0	0
5	B	1	Total 5	O 4	S 1	0	0
5	B	1	Total 5	O 4	S 1	0	0
5	C	1	Total 5	O 4	S 1	0	0
5	D	1	Total 5	O 4	S 1	0	0
5	E	1	Total 5	O 4	S 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	103	Total 103	O 103	0	0
6	B	107	Total 107	O 107	0	0
6	C	99	Total 99	O 99	0	0
6	D	115	Total 115	O 115	0	0
6	E	80	Total 80	O 80	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total 1	O 1	0	0
6	G	3	Total 3	O 3	0	0
6	N	1	Total 1	O 1	0	0
6	P	2	Total 2	O 2	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: RNA lariat debranching enzyme, putative
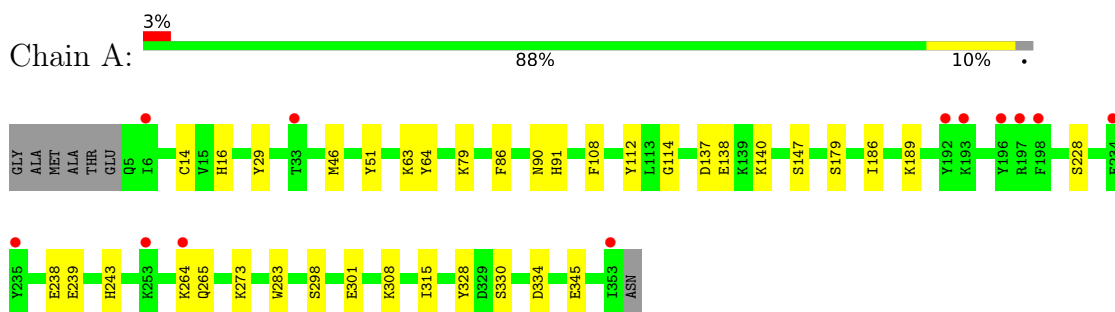
Chain A:

• Molecule 1: RNA lariat debranching enzyme, putative

Chain B:

• Molecule 1: RNA lariat debranching enzyme, putative

Chain C:

• Molecule 1: RNA lariat debranching enzyme, putative

Chain D:

• Molecule 1: RNA lariat debranching enzyme, putative
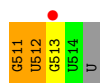
Chain E:

• Molecule 2: RNA (5'-R(P*(G46)P*UP*GP*UP*U)-3')

Chain F:

• Molecule 2: RNA (5'-R(P*(G46)P*UP*GP*UP*U)-3')

Chain G:

• Molecule 2: RNA (5'-R(P*(G46)P*UP*GP*UP*U)-3')

Chain N:

• Molecule 2: RNA (5'-R(P*(G46)P*UP*GP*UP*U)-3')

Chain O:

• Molecule 2: RNA (5'-R(P*(G46)P*UP*GP*UP*U)-3')

Chain P:

20%

20%　　　　20%　　　　40%　　　　20%

G511 U512 G513 U514 U
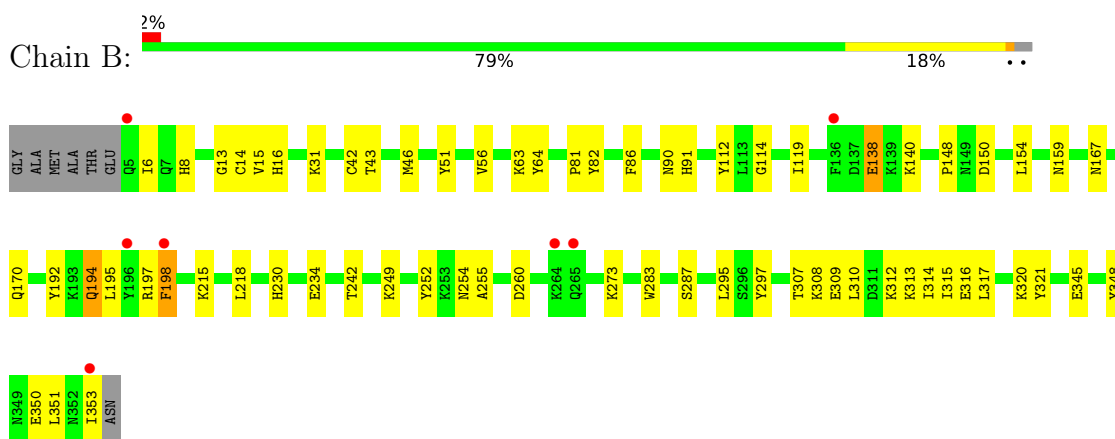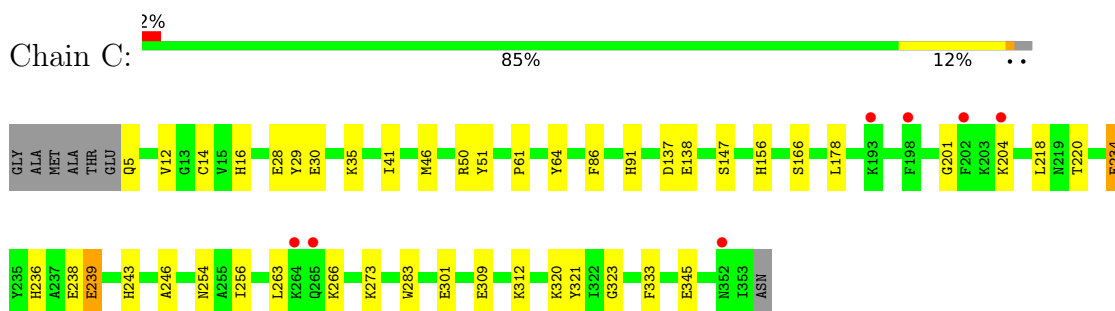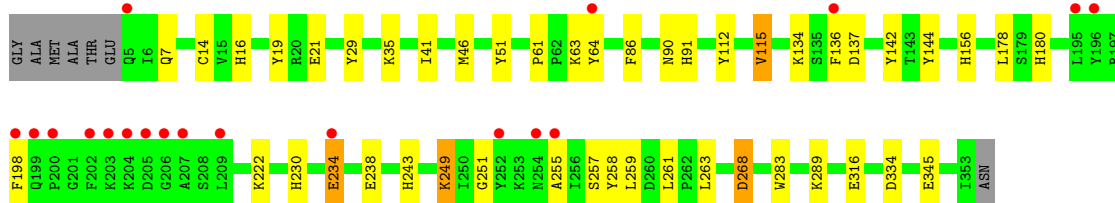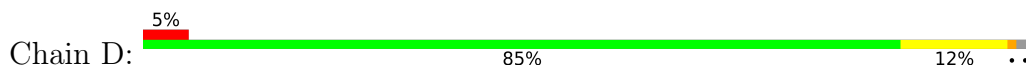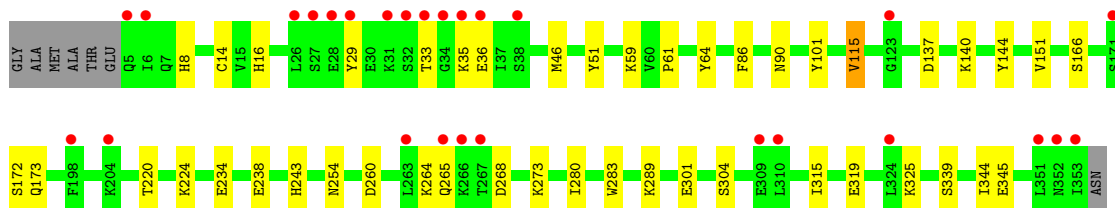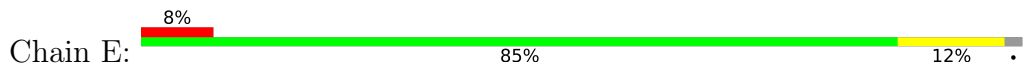
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	73.27Å 143.34Å 214.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.12 – 2.10 50.12 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.9 (50.12-2.10) 96.0 (50.12-2.10)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.92 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.20_4459	Depositor
R, R_{free}	0.178 , 0.209 0.177 , 0.208	Depositor DCC
R_{free} test set	6317 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	48.4	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 48.4	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15212	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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: G46, SO4, FE2, 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	0.43	0/2935	0.61	0/3967
1	B	0.44	0/2958	0.65	0/3998
1	C	0.42	0/2935	0.60	0/3967
1	D	0.44	0/2935	0.59	0/3967
1	E	0.39	0/2935	0.59	0/3967
2	F	1.25	1/72 (1.4%)	1.13	1/109 (0.9%)
2	G	0.36	0/51	0.93	0/78
2	N	1.26	1/72 (1.4%)	1.22	1/109 (0.9%)
2	O	0.33	0/38	0.90	0/57
2	P	0.44	0/38	1.22	0/57
All	All	0.44	2/14969 (0.0%)	0.62	2/20276 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	515	U	P-O5'	-10.34	1.49	1.59
2	F	515	U	P-O5'	-10.31	1.49	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	N	515	U	O5'-P-OP2	8.54	120.95	110.70
2	F	515	U	O5'-P-OP2	8.12	120.44	110.70

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	2857	0	2831	22	0
1	B	2879	0	2845	50	0
1	C	2857	0	2831	28	0
1	D	2857	0	2831	44	0
1	E	2857	0	2831	35	0
2	F	90	0	43	4	0
2	G	71	0	33	3	0
2	N	90	0	43	2	0
2	O	49	0	23	2	0
2	P	49	0	23	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
5	A	10	0	0	0	0
5	B	10	0	0	0	0
5	C	5	0	0	0	0
5	D	5	0	0	0	0
5	E	5	0	0	1	0
6	A	103	0	0	0	0
6	B	107	0	0	0	0
6	C	99	0	0	3	0
6	D	115	0	0	3	0
6	E	80	0	0	1	0
6	F	1	0	0	0	0
6	G	3	0	0	0	0
6	N	1	0	0	0	0
6	P	2	0	0	0	0
All	All	15212	0	14334	179	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 6.

The worst 5 of 179 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:D:136:PHE:CE1	1:D:137:ASP:OD2	1.99	1.14
1:D:136:PHE:HE1	1:D:137:ASP:OD2	1.31	1.05
1:A:273:LYS:HG3	1:A:315:ILE:HG13	1.44	0.98
1:E:234:GLU:HG3	1:E:254:ASN:HB2	1.52	0.91
1:D:134:LYS:HD2	1:D:136:PHE:HE2	1.39	0.85

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	A	347/356 (98%)	340 (98%)	7 (2%)	0	100	100
1	B	350/356 (98%)	342 (98%)	8 (2%)	0	100	100
1	C	347/356 (98%)	338 (97%)	9 (3%)	0	100	100
1	D	347/356 (98%)	339 (98%)	8 (2%)	0	100	100
1	E	347/356 (98%)	341 (98%)	6 (2%)	0	100	100
All	All	1738/1780 (98%)	1700 (98%)	38 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	A	316/320 (99%)	310 (98%)	6 (2%)	57	63
1	B	319/320 (100%)	313 (98%)	6 (2%)	57	63
1	C	316/320 (99%)	310 (98%)	6 (2%)	57	63
1	D	316/320 (99%)	311 (98%)	5 (2%)	62	69
1	E	316/320 (99%)	312 (99%)	4 (1%)	69	75
All	All	1583/1600 (99%)	1556 (98%)	27 (2%)	60	67

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	138	GLU
1	C	239	GLU
1	E	115	VAL
1	C	234	GLU
1	D	51	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	194	GLN
1	D	91	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	F	2/5 (40%)	0	0
2	G	2/5 (40%)	0	0
2	N	3/5 (60%)	0	0
2	O	2/5 (40%)	2 (100%)	0
2	P	2/5 (40%)	2 (100%)	0
All	All	11/25 (44%)	4 (36%)	0

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	O	512	U
2	O	513	G

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Mol	Chain	Res	Type
2	P	512	U
2	P	513	G

There are no RNA pucker outliers to report.

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

5 non-standard protein/DNA/RNA residues are modelled in this entry.

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	#$|Z| > 2$
2	G46	N	511	3,4,2	20,26,26	1.35	3 (15%)	22,40,40	1.29	2 (9%)
2	G46	G	511	3,4,2	20,26,26	1.30	2 (10%)	22,40,40	1.37	5 (22%)
2	G46	O	511	3,4,2	11,13,26	0.88	0	13,19,40	1.62	2 (15%)
2	G46	P	511	3,4,2	11,13,26	1.29	1 (9%)	13,19,40	1.73	4 (30%)
2	G46	F	511	3,4,2	20,26,26	1.10	1 (5%)	22,40,40	1.09	2 (9%)

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
2	G46	N	511	3,4,2	-	4/5/26/26	0/3/3/3
2	G46	G	511	3,4,2	-	0/5/26/26	0/3/3/3
2	G46	O	511	3,4,2	-	0/5/19/26	0/1/1/3
2	G46	P	511	3,4,2	-	3/5/19/26	0/1/1/3
2	G46	F	511	3,4,2	-	2/5/26/26	0/3/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	511	G46	P-O1P	-3.61	1.47	1.56
2	G	511	G46	P-O1P	-3.34	1.48	1.56
2	N	511	G46	P-O1P	-3.34	1.48	1.56
2	N	511	G46	C6-N1	-2.55	1.34	1.37
2	N	511	G46	P-O5'	2.15	1.61	1.57

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	511	G46	O4'-C4'-C3'	3.86	108.12	104.70
2	O	511	G46	O4'-C4'-C3'	3.75	108.02	104.70
2	N	511	G46	O5'-P-O3P	-3.13	102.88	114.42
2	O	511	G46	C1'-C2'-C3'	2.95	106.13	101.63
2	P	511	G46	O5'-P-O3P	-2.72	104.41	114.42

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	N	511	G46	C5'-O5'-P-O1P
2	N	511	G46	C5'-O5'-P-O3P
2	N	511	G46	O4'-C4'-C5'-O5'
2	P	511	G46	C3'-C4'-C5'-O5'
2	F	511	G46	O4'-C4'-C5'-O5'

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	N	511	G46	2	0
2	G	511	G46	3	0
2	O	511	G46	1	0
2	P	511	G46	2	0
2	F	511	G46	4	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6　Ligand geometry　ⓘ

Of 17 ligands modelled in this entry, 10 are monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
5	SO4	A	403	-	4,4,4	0.25	0	6,6,6	0.07	0
5	SO4	B	404	-	4,4,4	0.13	0	6,6,6	0.12	0
5	SO4	E	403	-	4,4,4	0.13	0	6,6,6	0.20	0
5	SO4	B	403	-	4,4,4	0.15	0	6,6,6	0.24	0
5	SO4	D	403	-	4,4,4	0.18	0	6,6,6	0.28	0
5	SO4	C	403	-	4,4,4	0.10	0	6,6,6	0.28	0
5	SO4	A	404	-	4,4,4	0.13	0	6,6,6	0.39	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	403	SO4	1	0

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	A	349/356 (98%)	0.25	12 (3%)	45	51	37, 52, 80, 103	0
1	B	349/356 (98%)	0.22	7 (2%)	65	69	36, 52, 78, 107	0
1	C	349/356 (98%)	0.36	7 (2%)	65	69	40, 54, 75, 94	0
1	D	349/356 (98%)	0.48	19 (5%)	25	31	36, 55, 95, 122	0
1	E	349/356 (98%)	0.55	27 (7%)	13	17	38, 57, 92, 121	0
2	F	4/5 (80%)	0.17	0	100	100	64, 64, 75, 82	4 (100%)
2	G	3/5 (60%)	-0.19	0	100	100	72, 72, 86, 92	3 (100%)
2	N	4/5 (80%)	-0.22	0	100	100	75, 75, 87, 98	4 (100%)
2	O	3/5 (60%)	1.48	1 (33%)	0	0	89, 89, 119, 120	3 (100%)
2	P	3/5 (60%)	1.24	1 (33%)	0	0	87, 87, 102, 126	2 (66%)
All	All	1762/1805 (97%)	0.37	74 (4%)	36	42	36, 54, 87, 126	16 (0%)

The worst 5 of 74 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	136	PHE	6.5
1	B	198	PHE	6.0
1	E	353	ILE	6.0
1	D	202	PHE	5.9
1	D	198	PHE	5.0

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

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
2	G46	P	511	13/24	0.89	0.25	54,80,88,92	13
2	G46	G	511	24/24	0.91	0.23	51,77,81,86	24
2	G46	O	511	13/24	0.92	0.24	66,94,101,111	13
2	G46	N	511	24/24	0.94	0.19	53,71,74,79	24
2	G46	F	511	24/24	0.95	0.13	48,62,65,68	24

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	SO4	A	403	5/5	0.86	0.19	88,91,97,162	0
5	SO4	A	404	5/5	0.94	0.15	59,66,70,78	0
5	SO4	B	404	5/5	0.94	0.24	76,76,78,89	0
5	SO4	C	403	5/5	0.95	0.10	67,69,73,77	0
5	SO4	B	403	5/5	0.96	0.14	63,64,69,78	0
4	ZN	A	402	1/1	0.97	0.11	63,63,63,63	0
4	ZN	B	402	1/1	0.98	0.17	63,63,63,63	0
5	SO4	D	403	5/5	0.98	0.12	54,56,59,61	0
5	SO4	E	403	5/5	0.98	0.10	56,59,62,68	0
4	ZN	C	402	1/1	0.99	0.13	70,70,70,70	0
4	ZN	D	402	1/1	0.99	0.11	77,77,77,77	0
4	ZN	E	402	1/1	0.99	0.12	55,55,55,55	0
3	FE2	A	401	1/1	0.99	0.15	39,39,39,39	0
3	FE2	C	401	1/1	0.99	0.19	45,45,45,45	0
3	FE2	B	401	1/1	1.00	0.16	41,41,41,41	0
3	FE2	D	401	1/1	1.00	0.14	54,54,54,54	0
3	FE2	E	401	1/1	1.00	0.21	45,45,45,45	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.
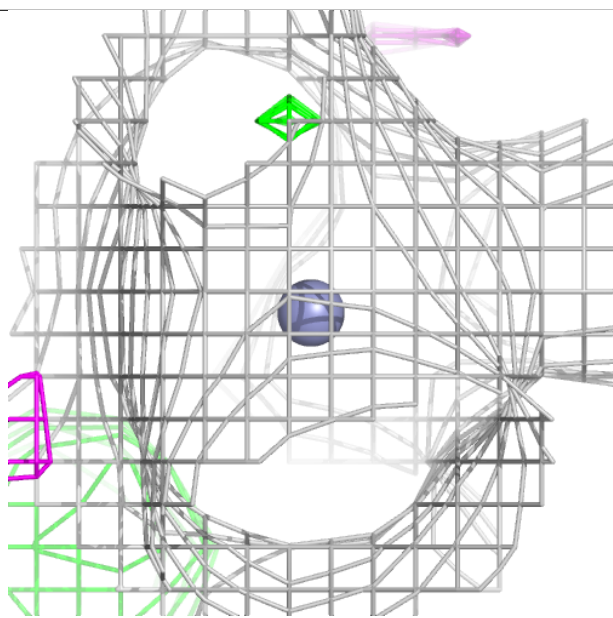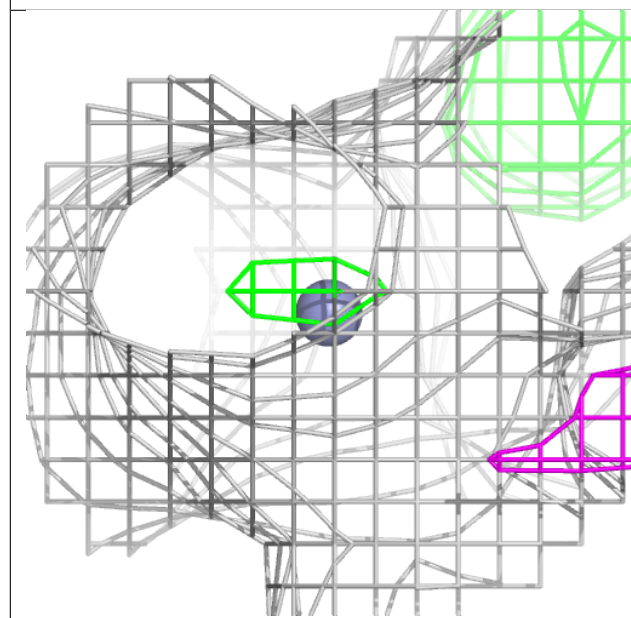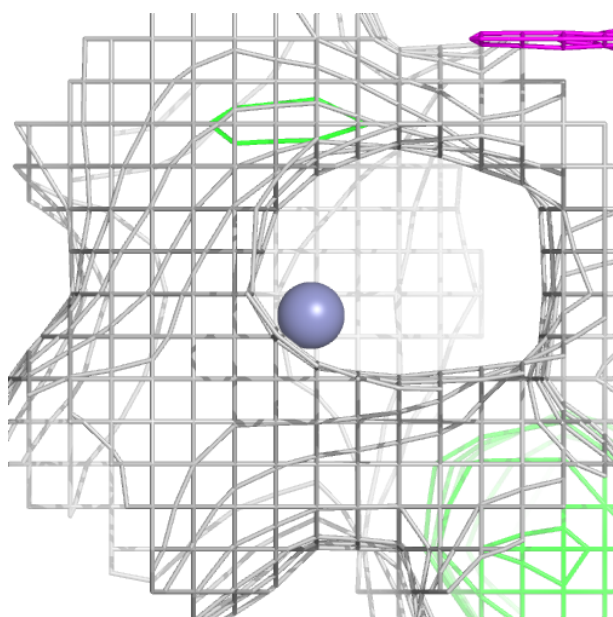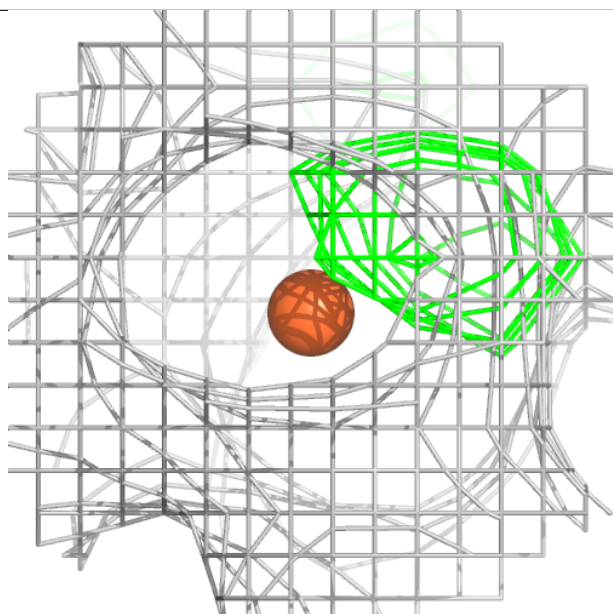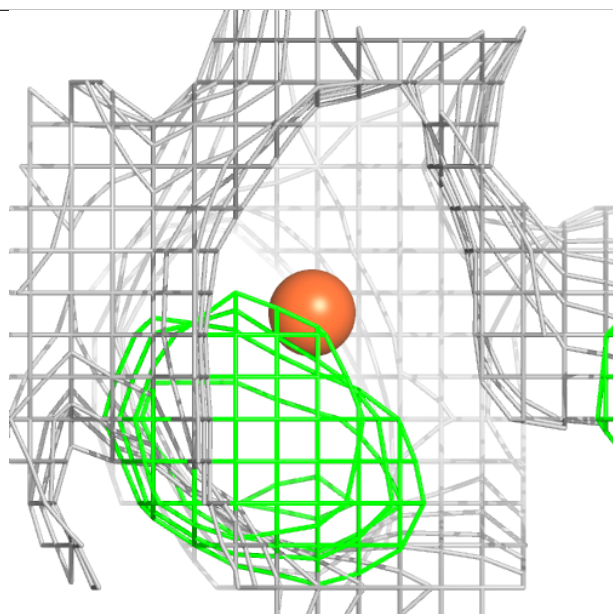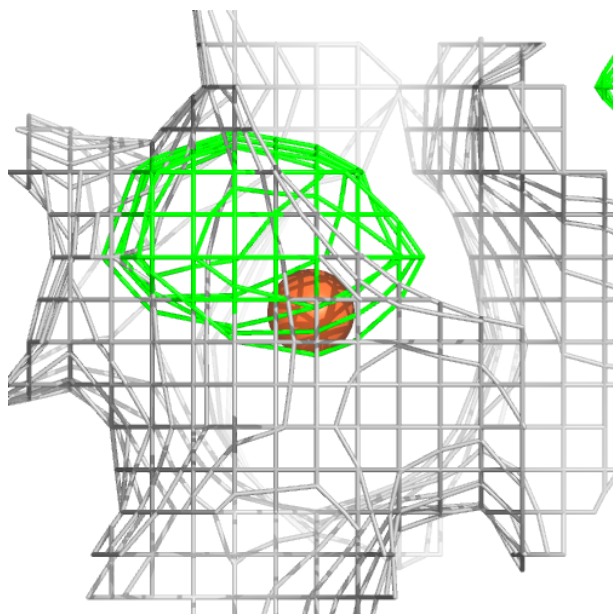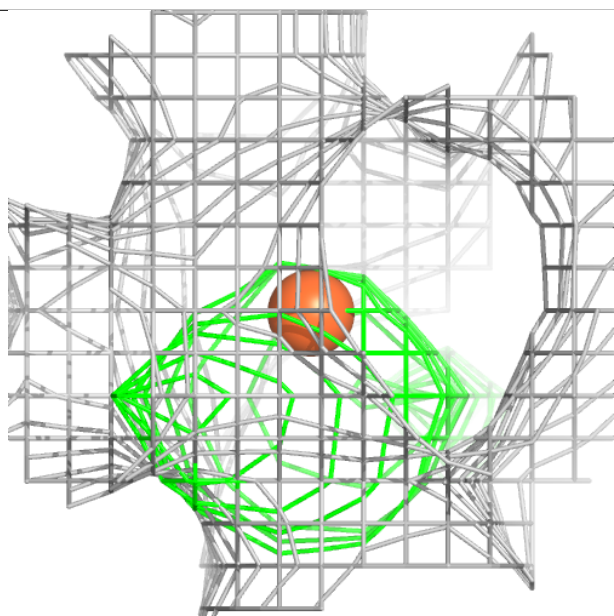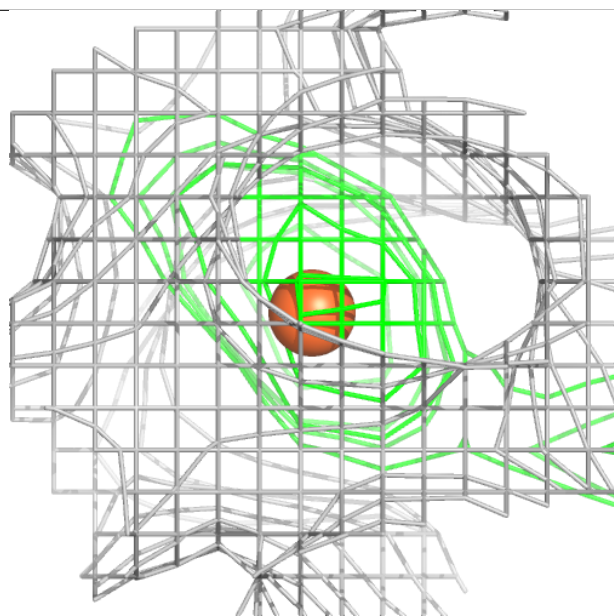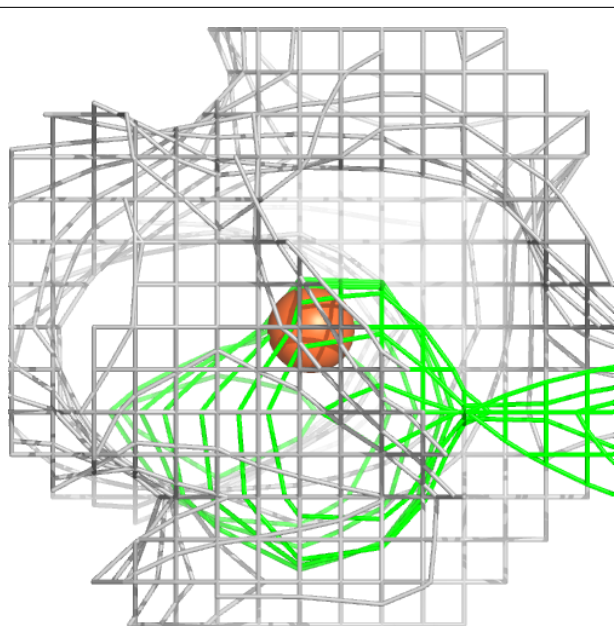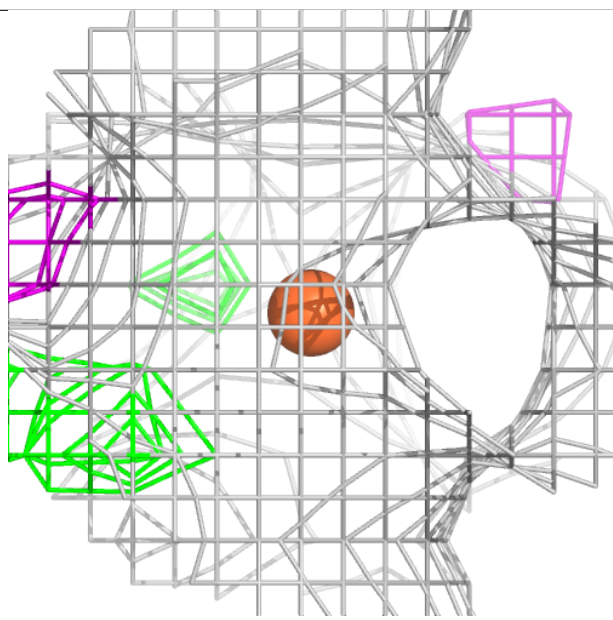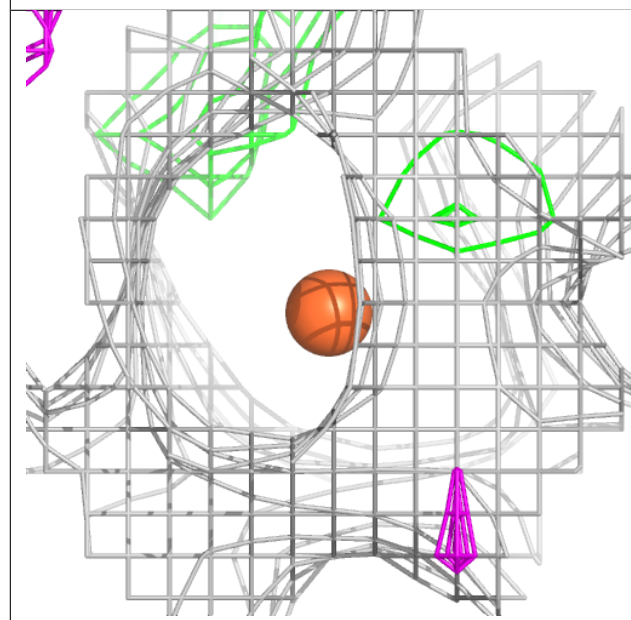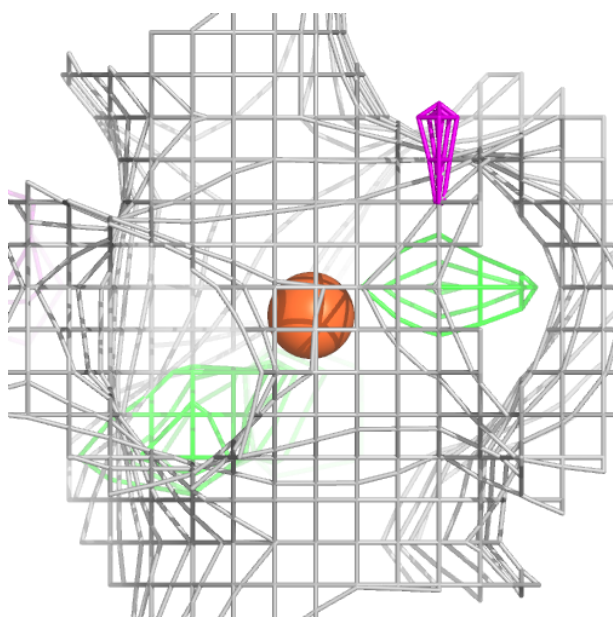
Electron density around ZN A 402:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
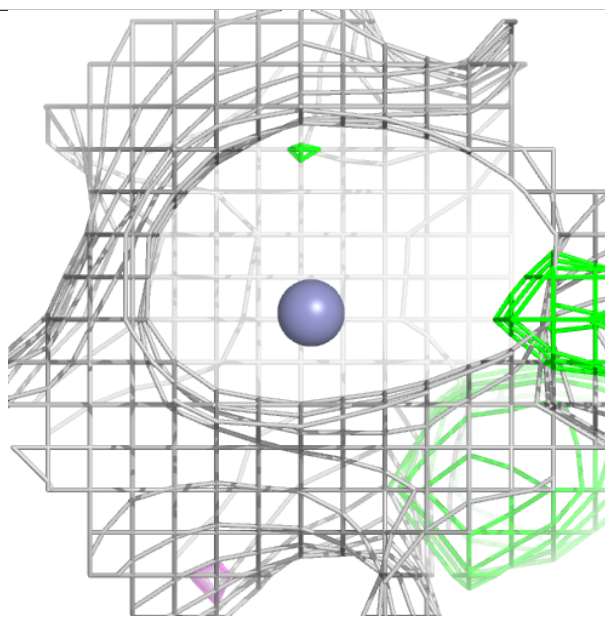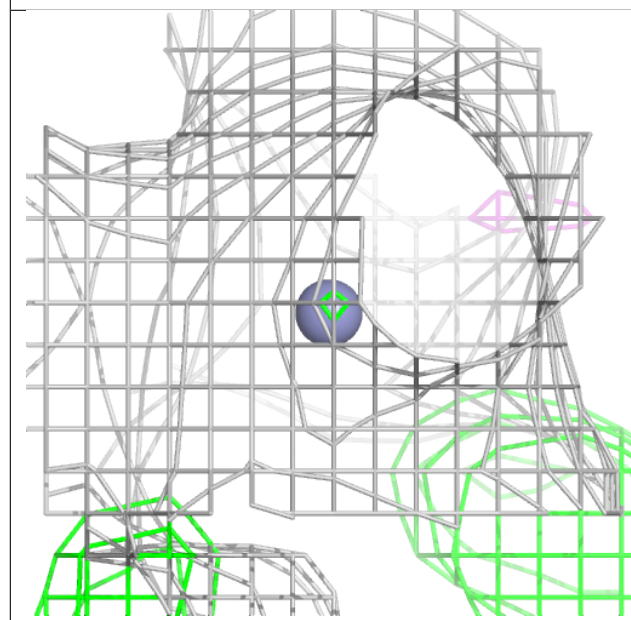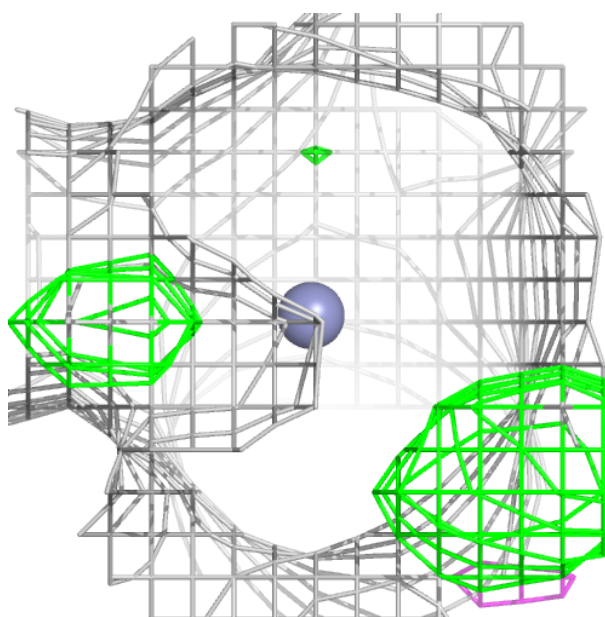
Electron density around ZN B 402:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray

$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
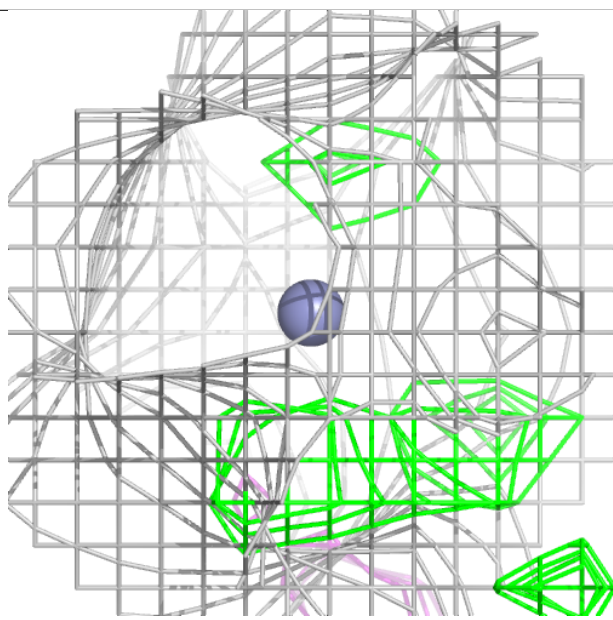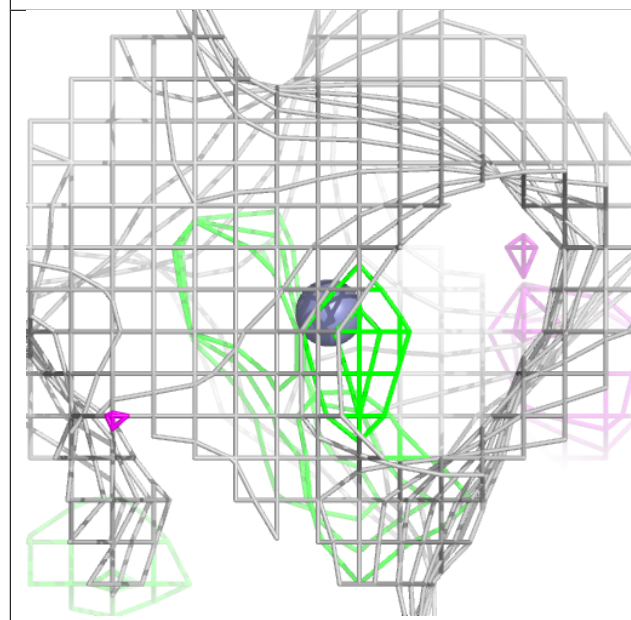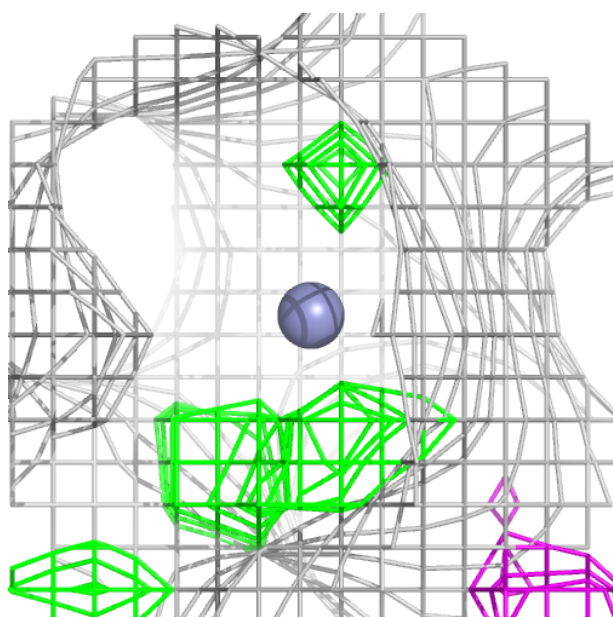
Electron density around ZN C 402:

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$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
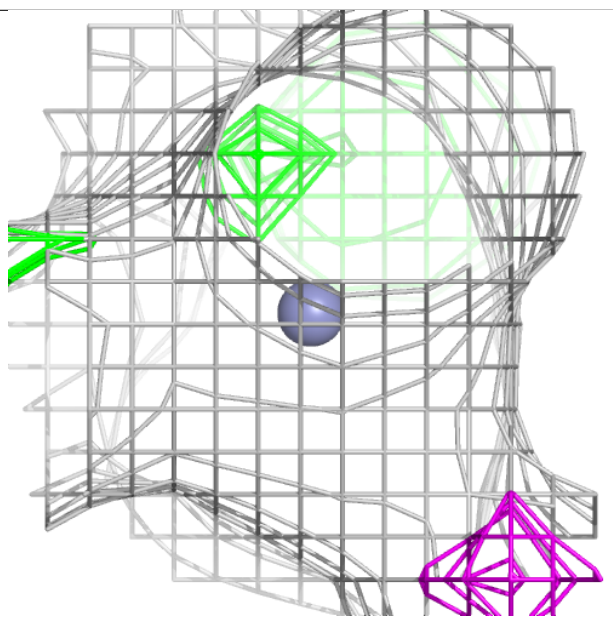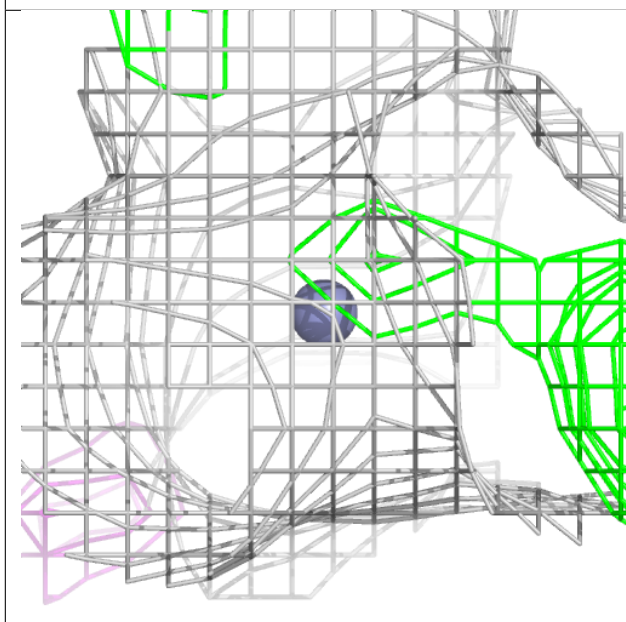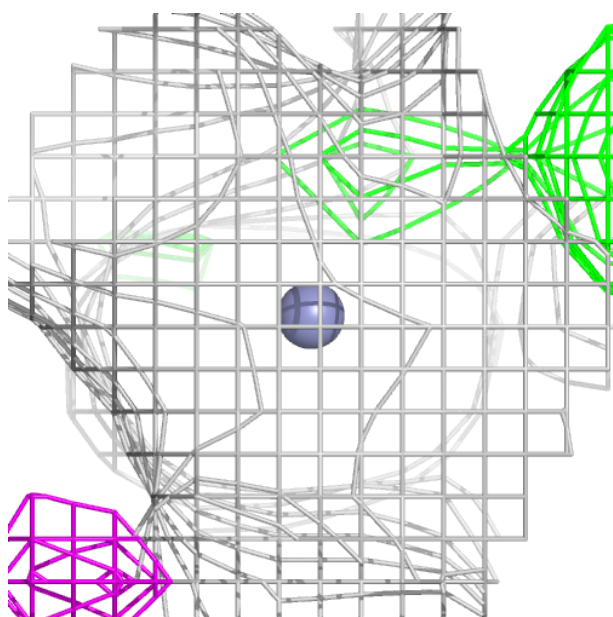
Electron density around ZN D 402:

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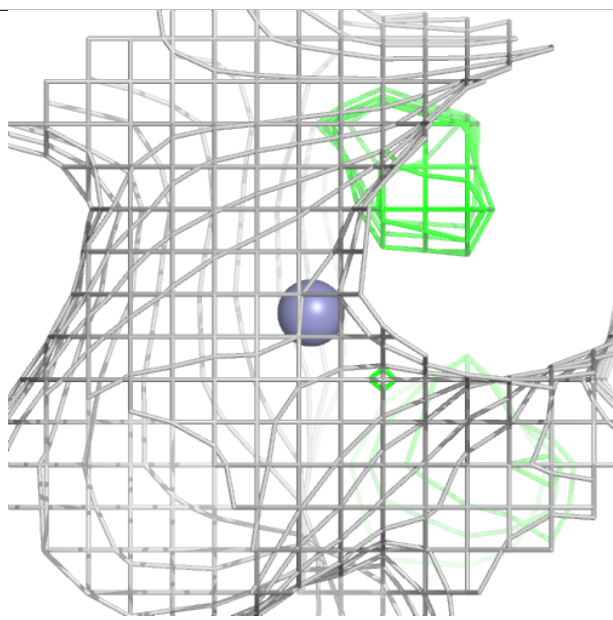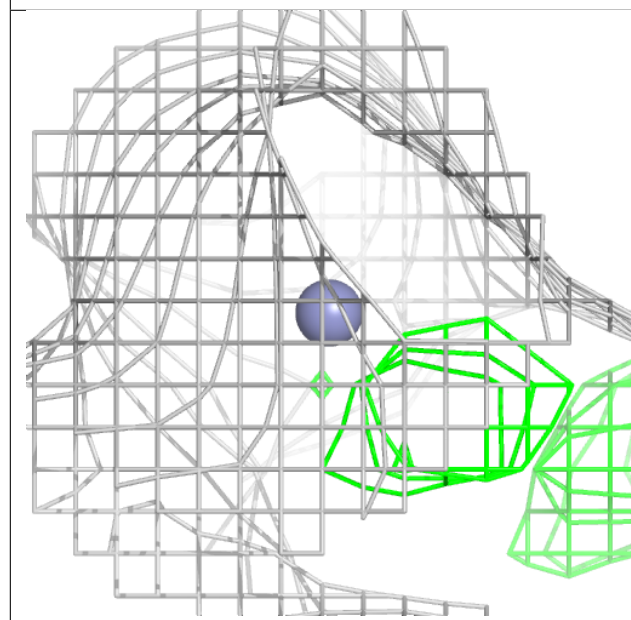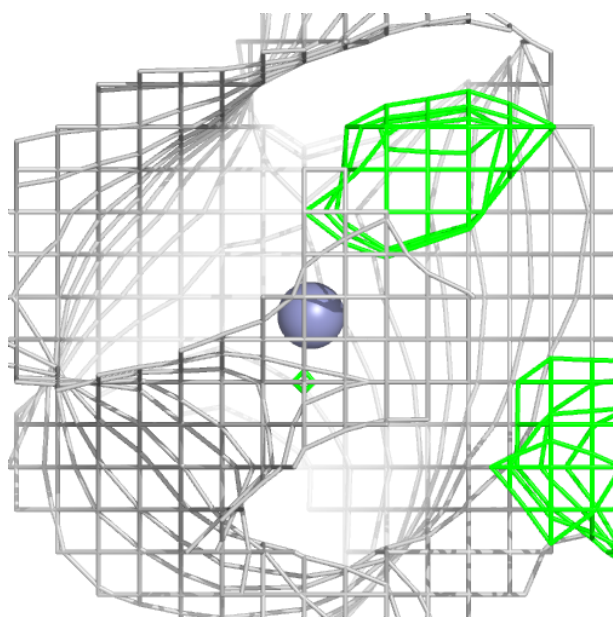
Electron density around ZN E 402:

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

Electron density around FE2 A 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 FE2 C 401:

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

Electron density around FE2 B 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 FE2 D 401:
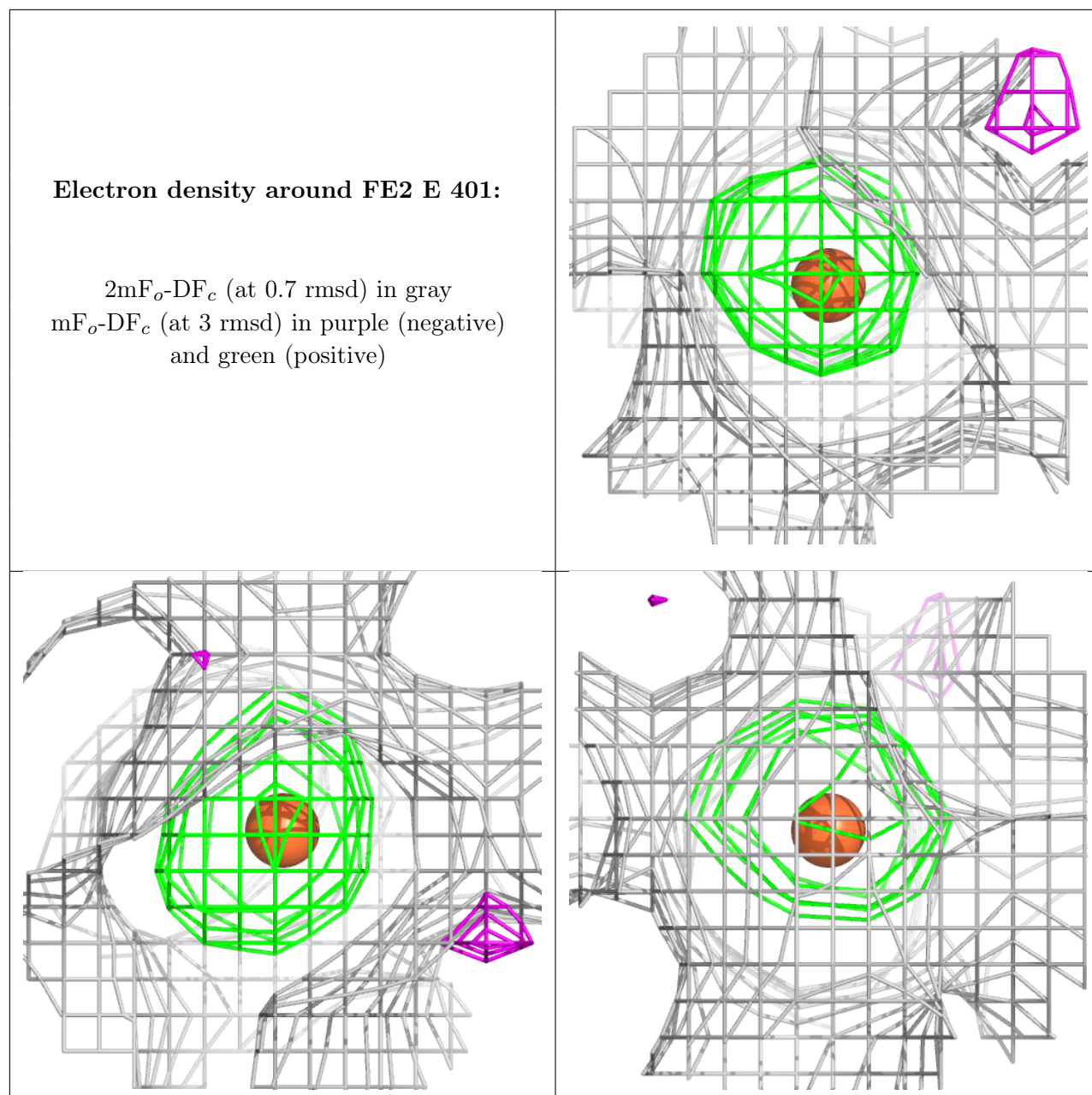
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around FE2 E 401:

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mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
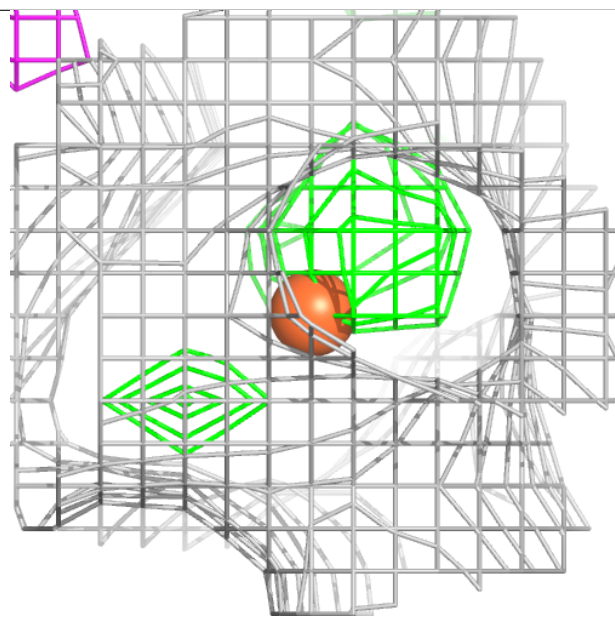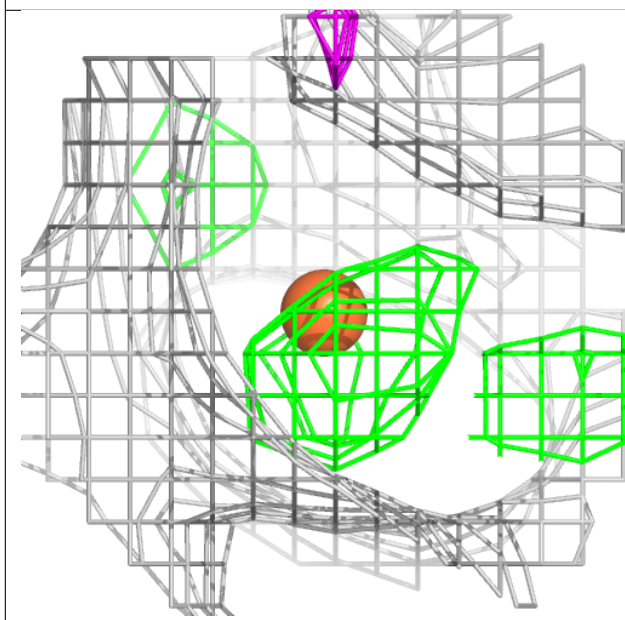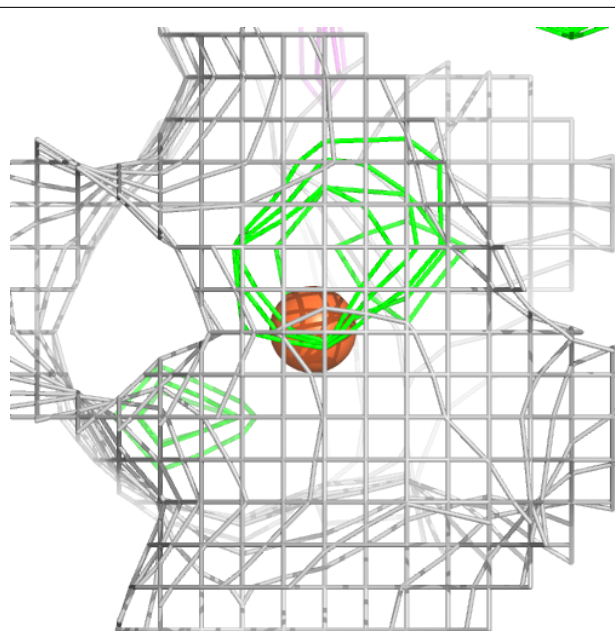
6.5 Other polymers (i)

There are no such residues in this entry.