



# Full wwPDB X-ray Structure Validation Report ⓘ

May 4, 2026 – 10:28 PM JST

PDB ID : 9VR2 / pdb\_00009vr2  
Title : The crystal structure of MetRS-like protein from *Streptomyces candidus* in complex with L-Glu and L-N6-OH-lysine  
Authors : Zhang, Z.M.; Huang, H.S.  
Deposited on : 2025-07-05  
Resolution : 2.45 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](mailto: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>.

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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	:	1.8.5 (274361), CSD as541be (2020)
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

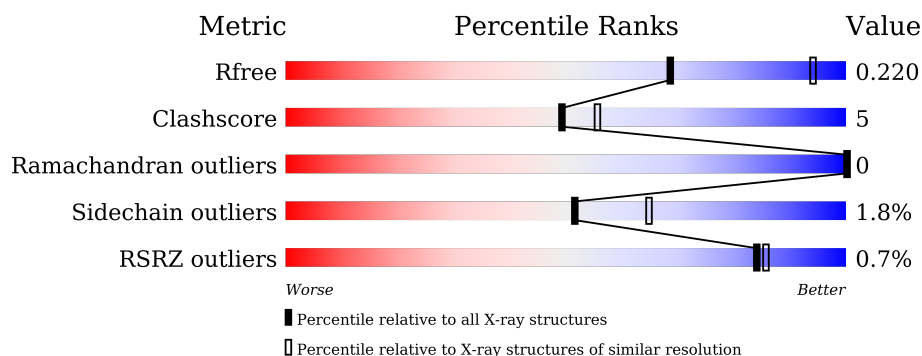
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.45 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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  $\geq 3$ , 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	A	560	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; bottom: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 100%; background: linear-gradient(to right, red 0%, red 1%, orange 1%, orange 83%, yellow 83%, yellow 94%, green 94%, green 100%);"></div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 100%; background: linear-gradient(to right, red 0%, red 1%, orange 1%, orange 83%, yellow 83%, yellow 94%, green 94%, green 100%);"></div> </div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> <span>%</span> <span>83%</span> <span>11%</span> <span>• 5%</span> </div> </div>
1	B	560	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; bottom: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 100%; background: linear-gradient(to right, red 0%, red 1%, orange 1%, orange 82%, yellow 82%, yellow 94%, green 94%, green 100%);"></div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 100%; background: linear-gradient(to right, red 0%, red 1%, orange 1%, orange 82%, yellow 82%, yellow 94%, green 94%, green 100%);"></div> </div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> <span>%</span> <span>82%</span> <span>12%</span> <span>• 5%</span> </div> </div>

## 2 Entry composition [i](#)

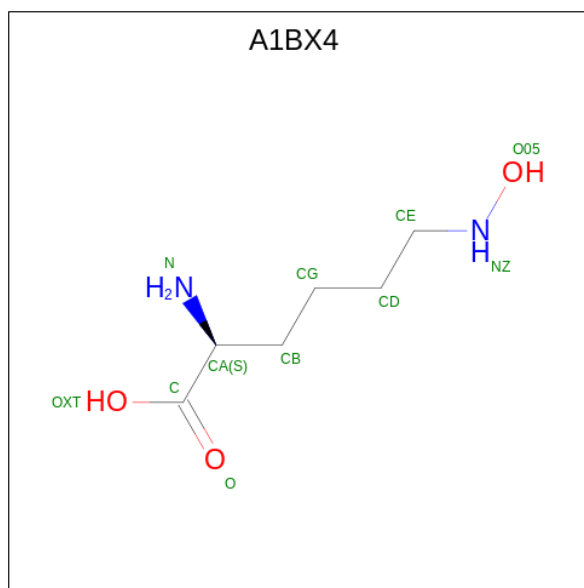
There are 6 unique types of molecules in this entry. The entry contains 8955 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Methionine-tRNA ligase.

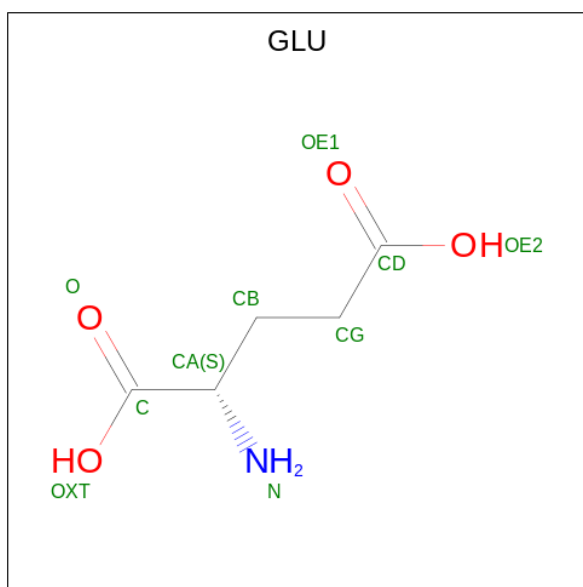
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	533	Total	C	N	O	S	0	1	0
			4111	2606	731	755	19			
1	B	531	Total	C	N	O	S	0	0	0
			4087	2589	728	751	19			

- Molecule 2 is N 6 -hydroxy-L-lysine (CCD ID: A1BX4) (formula:  $C_6H_{14}N_2O_3$ ) (labeled as "Ligand of Interest" by depositor).



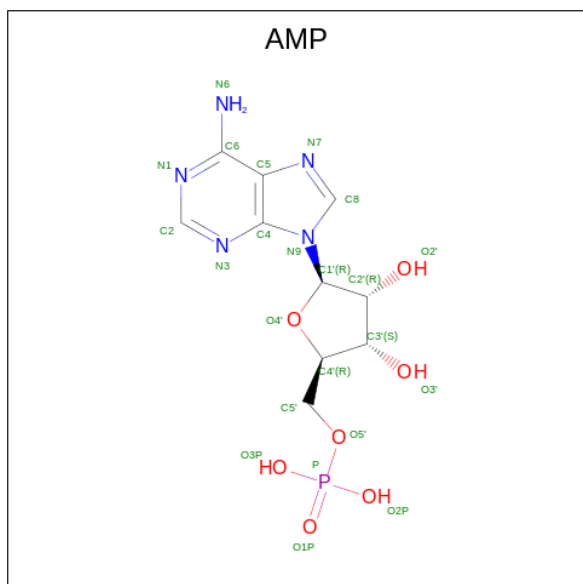
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			11	6	2	3		
2	B	1	Total	C	N	O	0	0
			11	6	2	3		

- Molecule 3 is GLUTAMIC ACID (CCD ID: GLU) (formula:  $C_5H_9NO_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			9	5	1	3		
3	B	1	Total	C	N	O	0	0
			9	5	1	3		

- Molecule 4 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula:  $C_{10}H_{14}N_5O_7P$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			22	10	5	6	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			22	10	5	6	1		

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	Zn	0	0
			3	3		
5	B	2	Total	Zn	0	0
			2	2		

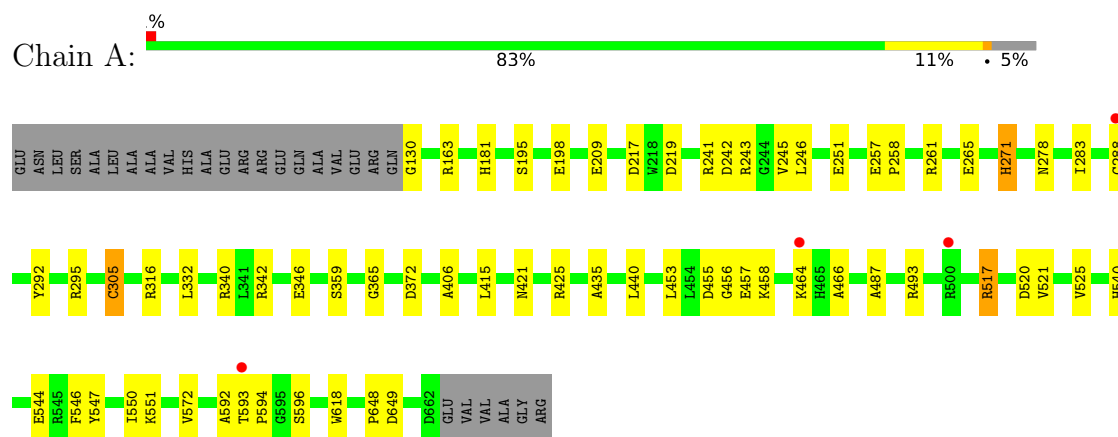
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	378	Total	O	0	0
			378	378		
6	B	290	Total	O	0	0
			290	290		

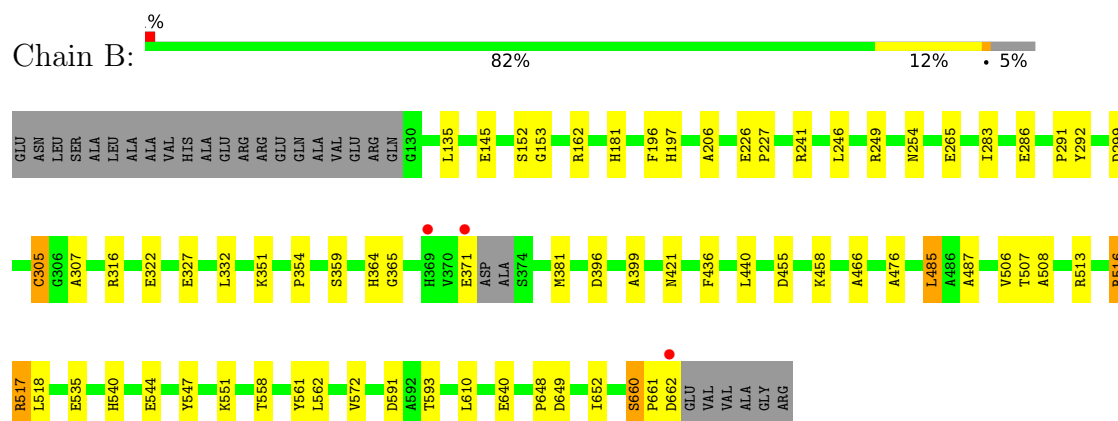
### 3 Residue-property plots [i](#)

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: Methionine-tRNA ligase



- Molecule 1: Methionine-tRNA ligase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.58Å 50.53Å 106.61Å 90.00° 89.82° 90.00°	Depositor
Resolution (Å)	41.67 – 2.45 41.67 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.6 (41.67-2.45) 99.5 (41.67-2.45)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.63 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.9_1692+SVN	Depositor
R, $R_{free}$	0.172 , 0.218 0.181 , 0.220	Depositor DCC
$R_{free}$ test set	2025 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.9	Xtriage
Anisotropy	0.576	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 40.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -l,k,h 0.015 for h,-k,-l 0.008 for -l,-k,-h	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8955	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: A1BX4, ZN, AMP

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	0.64	1/4224 (0.0%)	0.93	4/5756 (0.1%)
1	B	0.56	0/4194	0.89	15/5711 (0.3%)
All	All	0.60	1/8418 (0.0%)	0.91	19/11467 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	305	CYS	CB-SG	-5.55	1.62	1.81

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	265	GLU	CB-CA-C	-7.14	108.33	116.54
1	B	197	HIS	N-CA-C	6.36	118.29	111.36
1	B	305	CYS	N-CA-C	5.86	118.89	111.69
1	A	466	ALA	N-CA-C	5.84	117.13	108.60
1	B	466	ALA	N-CA-C	5.69	117.50	108.79
1	B	562	LEU	CA-C-N	5.37	125.01	119.05
1	B	562	LEU	C-N-CA	5.37	125.01	119.05
1	B	153	GLY	CA-C-N	5.29	125.10	119.28
1	B	153	GLY	C-N-CA	5.29	125.10	119.28
1	B	265	GLU	CB-CA-C	-5.28	110.47	116.54
1	A	251	GLU	N-CA-C	5.23	112.93	108.22
1	B	322	GLU	CA-C-N	-5.17	114.76	119.82
1	B	322	GLU	C-N-CA	-5.17	114.76	119.82
1	B	436	PHE	N-CA-C	5.16	116.99	111.36
1	B	640	GLU	CA-C-N	5.11	124.72	119.56
1	B	640	GLU	C-N-CA	5.11	124.72	119.56
1	B	652	ILE	N-CA-C	5.09	114.91	107.37
1	B	305	CYS	CB-CA-C	-5.01	101.54	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	271	HIS	N-CA-C	5.00	117.64	109.59

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	4111	0	3975	42	0
1	B	4087	0	3955	44	0
2	A	11	0	0	0	0
2	B	11	0	0	1	0
3	A	9	0	5	2	0
3	B	9	0	5	2	0
4	A	22	0	12	1	0
4	B	22	0	12	2	0
5	A	3	0	0	0	0
5	B	2	0	0	0	0
6	A	378	0	0	18	2
6	B	290	0	0	17	0
All	All	8955	0	7964	87	2

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 5.

All (87) 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:457:GLU:OE2	6:A:801:HOH:O	1.84	0.96
1:A:295:ARG:NH1	6:A:803:HOH:O	2.01	0.93
1:A:242:ASP:OD2	6:A:802:HOH:O	1.89	0.90
1:B:455:ASP:OD1	6:B:801:HOH:O	1.97	0.83
3:A:702:GLU:C	4:A:703:AMP:P	2.64	0.80
3:B:702:GLU:C	4:B:703:AMP:P	2.68	0.77
1:A:130:GLY:N	6:A:812:HOH:O	2.17	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:660:SER:OG	6:B:802:HOH:O	2.05	0.75
1:B:558:THR:O	6:B:803:HOH:O	2.06	0.74
1:B:381:MET:SD	6:B:1016:HOH:O	2.46	0.73
1:A:209:GLU:OE1	6:A:806:HOH:O	2.07	0.73
1:A:217:ASP:OD2	6:A:804:HOH:O	2.06	0.73
1:A:346:GLU:OE2	1:B:593:THR:OG1	2.06	0.72
1:A:455:ASP:OD1	6:A:805:HOH:O	2.06	0.72
1:B:249:ARG:NH2	6:B:811:HOH:O	2.23	0.71
1:B:299:ASP:O	6:B:804:HOH:O	2.07	0.71
1:B:544:GLU:HB2	6:B:848:HOH:O	1.92	0.69
1:B:476:ALA:O	6:B:802:HOH:O	2.10	0.68
1:B:396:ASP:OD2	6:B:805:HOH:O	2.10	0.68
1:A:219:ASP:OD2	6:A:809:HOH:O	2.12	0.67
1:A:592:ALA:O	6:A:808:HOH:O	2.12	0.67
1:A:547:TYR:CE2	1:A:551:LYS:HD2	2.32	0.65
1:A:517:ARG:NH1	1:A:520:ASP:OD2	2.30	0.65
1:A:457:GLU:OE1	6:A:811:HOH:O	2.15	0.65
1:A:209:GLU:OE2	6:A:810:HOH:O	2.14	0.65
1:B:516:ARG:NH1	6:B:818:HOH:O	2.30	0.63
1:B:399:ALA:O	6:B:807:HOH:O	2.17	0.60
1:B:551:LYS:NZ	6:B:825:HOH:O	2.35	0.59
1:A:340:ARG:NH1	6:A:813:HOH:O	2.18	0.58
1:B:291:PRO:HB2	1:B:354:PRO:HG2	1.86	0.58
1:B:535:GLU:OE1	6:B:808:HOH:O	2.17	0.57
1:B:327:GLU:OE1	6:B:809:HOH:O	2.17	0.57
1:A:406:ALA:HB1	1:A:440:LEU:HB3	1.87	0.57
1:A:295:ARG:NH2	6:A:807:HOH:O	2.09	0.56
1:A:457:GLU:CD	6:A:811:HOH:O	2.49	0.55
1:B:561:TYR:HB2	6:B:803:HOH:O	2.07	0.54
1:A:372:ASP:N	6:A:830:HOH:O	2.41	0.54
2:B:701:A1BX4:NZ	4:B:703:AMP:O2P	2.41	0.53
1:B:507:THR:OG1	1:B:662:ASP:OD2	2.27	0.53
1:B:547:TYR:CE2	1:B:551:LYS:HD2	2.44	0.53
1:A:456:GLY:O	6:A:814:HOH:O	2.19	0.53
1:A:195:SER:OG	1:A:198:GLU:HG3	2.09	0.52
1:A:283:ILE:HA	1:A:292:TYR:CE1	2.45	0.52
1:A:493:ARG:NH2	1:B:591:ASP:OD2	2.41	0.52
1:A:544:GLU:HG2	6:A:1063:HOH:O	2.10	0.52
1:A:271:HIS:CE1	1:A:278:ASN:HB3	2.46	0.51
1:A:163:ARG:HB3	1:A:618[B]:TRP:CZ3	2.46	0.51
1:B:286:GLU:OE2	1:B:458:LYS:NZ	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:LEU:HD12	1:B:162:ARG:HB2	1.94	0.50
1:A:546:PHE:O	1:A:550:ILE:HG13	2.12	0.49
1:B:421:ASN:OD1	3:B:702:GLU:HA	2.13	0.48
1:B:316:ARG:HD2	1:B:359:SER:O	2.13	0.48
1:A:243:ARG:NH2	1:A:435:ALA:O	2.46	0.48
1:A:593:THR:O	1:A:596:SER:OG	2.17	0.48
1:A:487:ALA:HB2	1:A:572:VAL:HG11	1.97	0.47
1:B:249:ARG:HD3	6:B:819:HOH:O	2.15	0.47
1:A:257:GLU:HB2	1:A:258:PRO:HD3	1.98	0.46
1:A:283:ILE:HD12	6:A:946:HOH:O	2.16	0.46
1:B:508:ALA:O	1:B:513:ARG:HG3	2.16	0.46
1:A:181:HIS:CG	1:A:365:GLY:HA2	2.51	0.45
1:B:254:ASN:ND2	6:B:834:HOH:O	2.45	0.45
1:B:518:LEU:HD23	1:B:610:LEU:HD13	1.98	0.45
1:A:648:PRO:O	1:A:649:ASP:HB2	2.15	0.45
1:A:316:ARG:HD2	1:A:359:SER:O	2.17	0.45
1:B:135:LEU:CD1	1:B:162:ARG:HB2	2.47	0.45
1:B:517:ARG:CZ	1:B:517:ARG:HA	2.48	0.44
1:A:241:ARG:HB2	1:A:246:LEU:HD12	1.99	0.44
1:B:648:PRO:O	1:B:649:ASP:HB2	2.17	0.44
1:B:661:PRO:HA	1:B:662:ASP:HA	1.64	0.44
1:A:421:ASN:OD1	3:A:702:GLU:HA	2.18	0.43
1:B:145:GLU:HG3	1:B:206:ALA:HB1	2.01	0.43
1:B:196:PHE:HB2	1:B:364:HIS:CD2	2.53	0.43
1:B:241:ARG:HB2	1:B:246:LEU:HD12	2.01	0.43
1:B:506:VAL:HB	1:B:662:ASP:OD1	2.19	0.43
1:A:415:LEU:HD13	1:A:425:ARG:HD2	2.01	0.43
1:B:152:SER:HB3	1:B:485:LEU:HD13	2.01	0.42
1:B:305:CYS:HB2	1:B:307:ALA:H	1.84	0.42
1:B:332:LEU:HD23	1:B:332:LEU:HA	1.94	0.42
1:B:283:ILE:HA	1:B:292:TYR:CE2	2.55	0.41
1:A:332:LEU:O	1:A:342:ARG:NH1	2.45	0.41
1:B:226:GLU:HA	1:B:227:PRO:HD2	1.83	0.41
1:A:453:LEU:HA	1:A:458:LYS:HA	2.03	0.41
1:A:593:THR:HA	1:A:594:PRO:HD3	1.91	0.41
1:B:181:HIS:CD2	1:B:365:GLY:HA2	2.56	0.41
1:B:487:ALA:HB2	1:B:572:VAL:HG11	2.02	0.41
1:A:521:VAL:O	1:A:525:VAL:HG23	2.21	0.40
1:B:181:HIS:CG	1:B:365:GLY:HA2	2.56	0.40

All (2) 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)
6:A:1021:HOH:O	6:A:1107:HOH:O[2_646]	2.09	0.11
6:A:912:HOH:O	6:A:960:HOH:O[1_565]	2.16	0.04

### 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	532/560 (95%)	520 (98%)	12 (2%)	0	100	100
1	B	527/560 (94%)	515 (98%)	12 (2%)	0	100	100
All	All	1059/1120 (95%)	1035 (98%)	24 (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	411/430 (96%)	404 (98%)	7 (2%)	53	67
1	B	409/430 (95%)	401 (98%)	8 (2%)	48	63
All	All	820/860 (95%)	805 (98%)	15 (2%)	51	65

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	245	VAL
1	A	261	ARG

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Mol	Chain	Res	Type
1	A	288	CYS
1	A	305	CYS
1	A	464	LYS
1	A	517	ARG
1	A	540	HIS
1	B	351	LYS
1	B	371	GLU
1	B	440	LEU
1	B	485	LEU
1	B	516	ARG
1	B	517	ARG
1	B	540	HIS
1	B	660	SER

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

Mol	Chain	Res	Type
1	A	449	ASN
1	B	379	GLN

### 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 [i](#)

Of 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 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	$\# Z  > 2$
2	A1BX4	B	701	-	8,10,10	0.96	0	9,11,11	1.12	1 (11%)
3	GLU	B	702	-	7,8,9	0.93	0	4,9,11	1.00	0
4	AMP	B	703	-	21,24,25	1.53	4 (19%)	31,35,38	2.08	9 (29%)
3	GLU	A	702	-	7,8,9	1.09	0	4,9,11	1.06	0
4	AMP	A	703	-	21,24,25	1.54	4 (19%)	31,35,38	2.12	11 (35%)
2	A1BX4	A	701	-	8,10,10	1.00	0	9,11,11	0.87	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
2	A1BX4	B	701	-	-	9/9/10/10	-
3	GLU	B	702	-	-	5/6/7/9	-
4	AMP	B	703	-	-	0/7/25/26	0/3/3/3
3	GLU	A	702	-	-	5/6/7/9	-
4	AMP	A	703	-	-	0/7/25/26	0/3/3/3
2	A1BX4	A	701	-	-	7/9/10/10	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	703	AMP	C5-C4	4.62	1.47	1.39
4	B	703	AMP	C5-C4	4.60	1.47	1.39
4	B	703	AMP	C5-N7	-2.80	1.33	1.39
4	A	703	AMP	C5-C6	2.65	1.48	1.41
4	A	703	AMP	C5-N7	-2.37	1.34	1.39
4	B	703	AMP	C5-C6	2.17	1.47	1.41
4	B	703	AMP	C4-N9	-2.07	1.33	1.37
4	A	703	AMP	C8-N7	2.07	1.35	1.31

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	703	AMP	C5-C4-N3	-5.98	118.94	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	703	AMP	C5-C4-N3	-5.95	118.98	126.75
4	B	703	AMP	N3-C4-N9	4.93	135.21	127.08
4	A	703	AMP	N3-C4-N9	4.60	134.67	127.08
4	A	703	AMP	C4-C5-N7	-3.81	105.98	110.62
4	A	703	AMP	C2-N3-C4	3.54	120.11	111.75
4	B	703	AMP	C2-N3-C4	3.34	119.65	111.75
4	B	703	AMP	C4-C5-N7	-3.15	106.78	110.62
4	A	703	AMP	C5-N7-C8	3.14	107.97	103.51
4	B	703	AMP	N3-C2-N1	-2.87	124.12	128.60
4	B	703	AMP	C5-N7-C8	2.84	107.54	103.51
4	A	703	AMP	N3-C2-N1	-2.82	124.19	128.60
4	B	703	AMP	C4-N9-C8	2.82	108.78	105.73
4	A	703	AMP	O4'-C1'-N9	2.77	113.51	108.06
4	A	703	AMP	C4-N9-C8	2.56	108.50	105.73
2	B	701	A1BX4	CB-CA-C	-2.21	105.05	110.30
4	A	703	AMP	C6-C5-N7	2.20	136.12	132.02
4	A	703	AMP	C2-N1-C6	2.10	122.38	118.77
4	B	703	AMP	N9-C8-N7	-2.06	111.09	113.91
4	B	703	AMP	C2-N1-C6	2.06	122.30	118.77
4	A	703	AMP	N9-C8-N7	-2.02	111.16	113.91

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	A1BX4	CG-CD-CE-NZ
2	A	701	A1BX4	O-C-CA-N
2	B	701	A1BX4	CG-CD-CE-NZ
2	B	701	A1BX4	C-CA-CB-CG
2	B	701	A1BX4	N-CA-CB-CG
2	B	701	A1BX4	O-C-CA-N
3	A	702	GLU	O-C-CA-CB
3	B	702	GLU	O-C-CA-CB
2	A	701	A1BX4	OXT-C-CA-N
2	B	701	A1BX4	OXT-C-CA-N
2	A	701	A1BX4	CE-CD-CG-CB
2	B	701	A1BX4	CA-CB-CG-CD
2	B	701	A1BX4	CE-CD-CG-CB
2	A	701	A1BX4	CA-CB-CG-CD
3	A	702	GLU	CA-CB-CG-CD
3	B	702	GLU	CA-CB-CG-CD
2	A	701	A1BX4	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
2	A	701	A1BX4	OXT-C-CA-CB
2	B	701	A1BX4	O-C-CA-CB
2	B	701	A1BX4	OXT-C-CA-CB
3	A	702	GLU	OE2-CD-CG-CB
3	B	702	GLU	OE2-CD-CG-CB
3	B	702	GLU	OE1-CD-CG-CB
3	A	702	GLU	OE1-CD-CG-CB
3	A	702	GLU	N-CA-CB-CG
3	B	702	GLU	N-CA-CB-CG

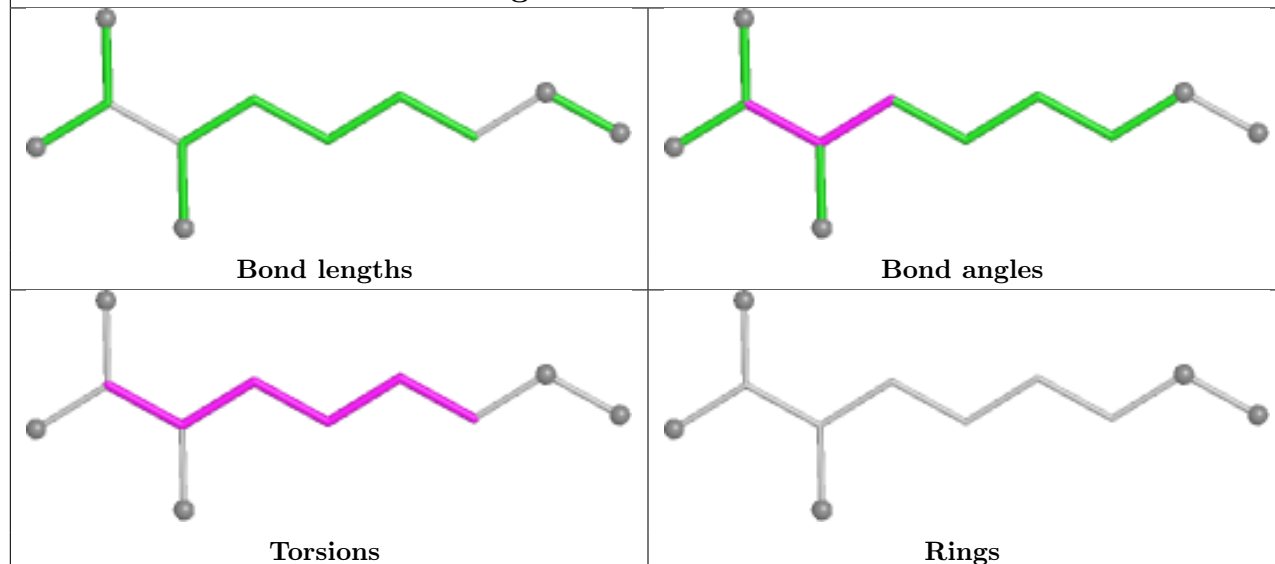
There are no ring outliers.

5 monomers are involved in 5 short contacts:

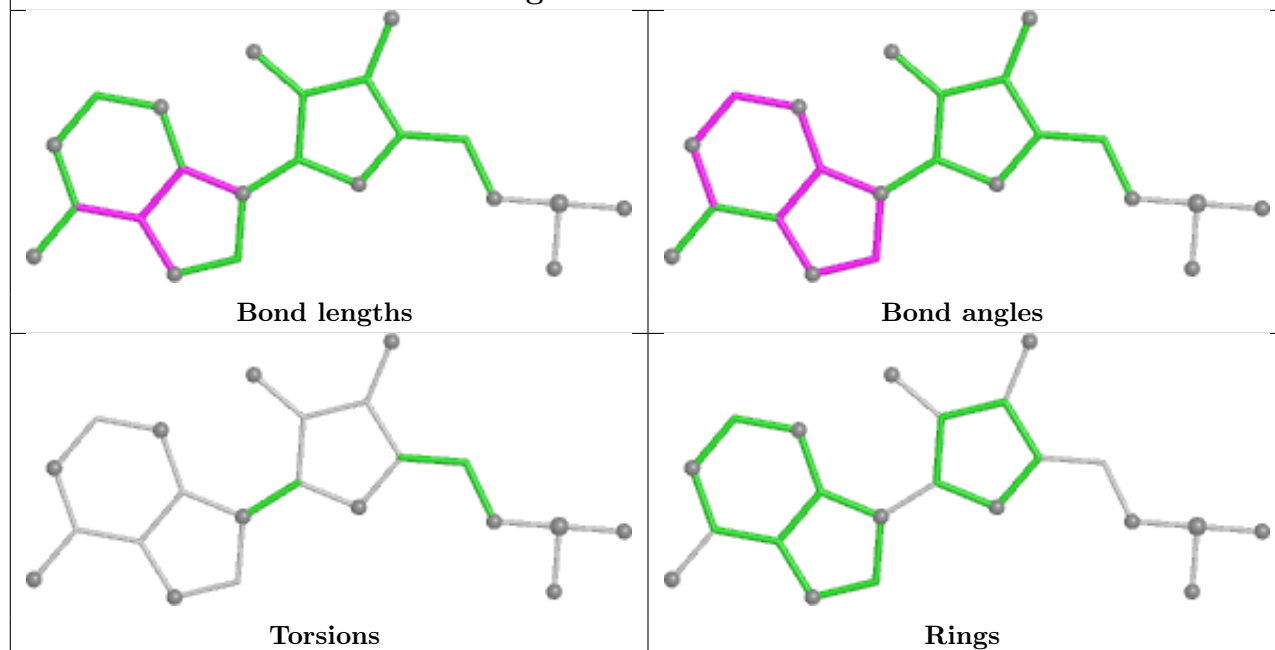
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	A1BX4	1	0
3	B	702	GLU	2	0
4	B	703	AMP	2	0
3	A	702	GLU	2	0
4	A	703	AMP	1	0

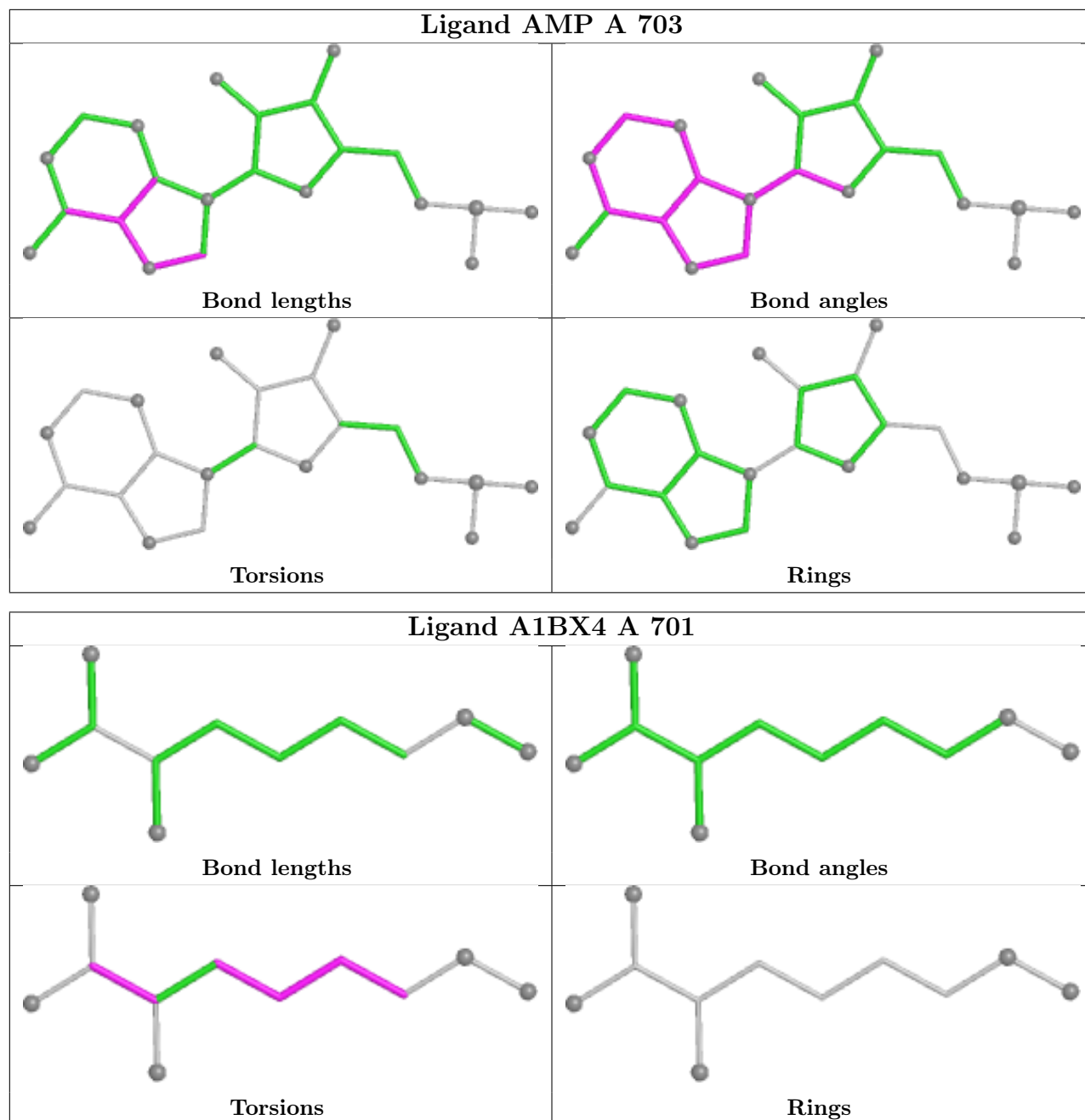
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 A1BX4 B 701



## Ligand AMP B 703





## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	533/560 (95%)	-0.48	4 (0%)	82 83	6, 14, 33, 53	1 (0%)
1	B	531/560 (94%)	-0.33	3 (0%)	85 87	12, 21, 39, 57	0
All	All	1064/1120 (95%)	-0.41	7 (0%)	84 86	6, 19, 37, 57	1 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	288	CYS	3.7
1	A	500	ARG	3.1
1	B	662	ASP	2.9
1	B	369	HIS	2.5
1	B	371	GLU	2.5
1	A	464	LYS	2.4
1	A	593	THR	2.2

### 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](#)

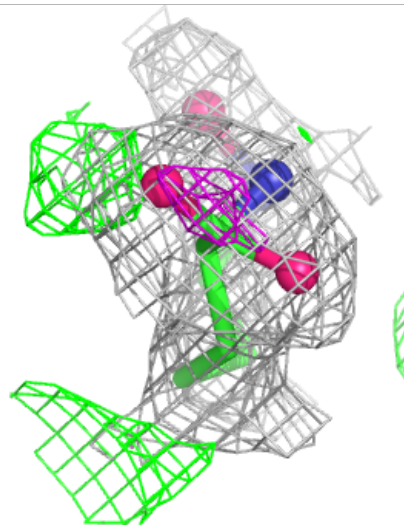
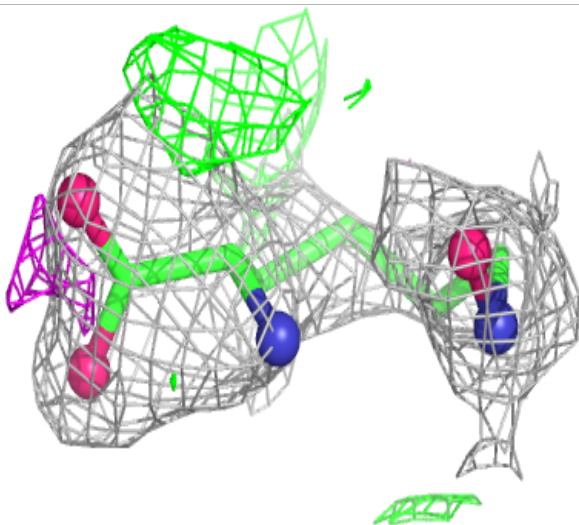
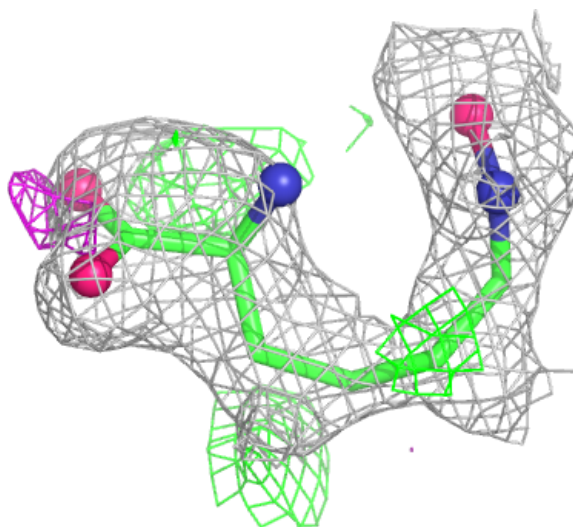
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	A1BX4	A	701	11/11	0.80	0.17	27,29,29,30	0
3	GLU	B	702	9/10	0.81	0.11	9,20,23,24	0
2	A1BX4	B	701	11/11	0.84	0.17	31,36,36,38	0
3	GLU	A	702	9/10	0.88	0.09	10,11,17,18	0
4	AMP	B	703	22/23	0.95	0.07	16,18,20,22	0
5	ZN	A	706	1/1	0.96	0.11	62,62,62,62	0
4	AMP	A	703	22/23	0.98	0.05	9,11,13,14	0
5	ZN	A	705	1/1	0.99	0.02	12,12,12,12	0
5	ZN	A	704	1/1	0.99	0.02	16,16,16,16	0
5	ZN	B	704	1/1	0.99	0.02	24,24,24,24	0
5	ZN	B	705	1/1	0.99	0.02	28,28,28,28	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.

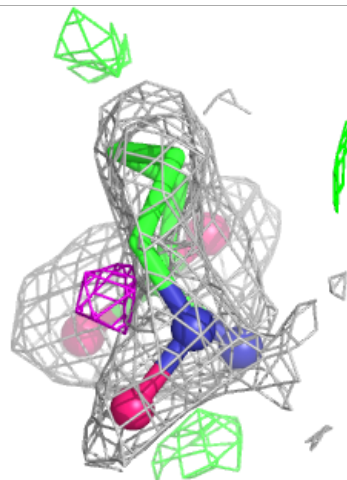
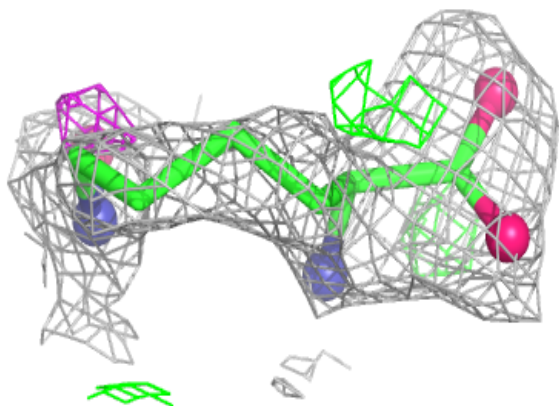
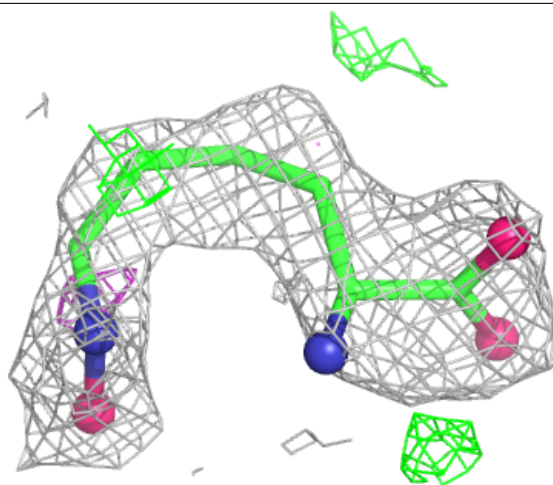
**Electron density around A1BX4 A 701:**

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



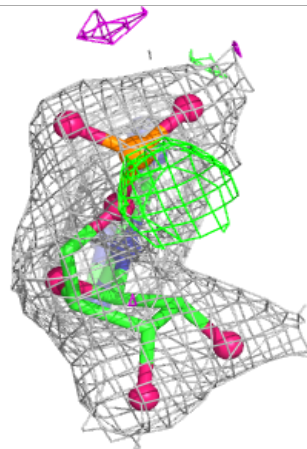
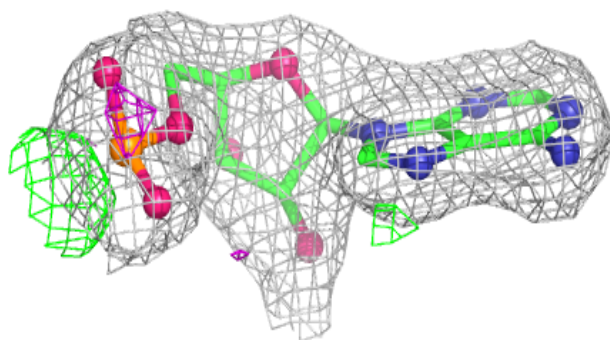
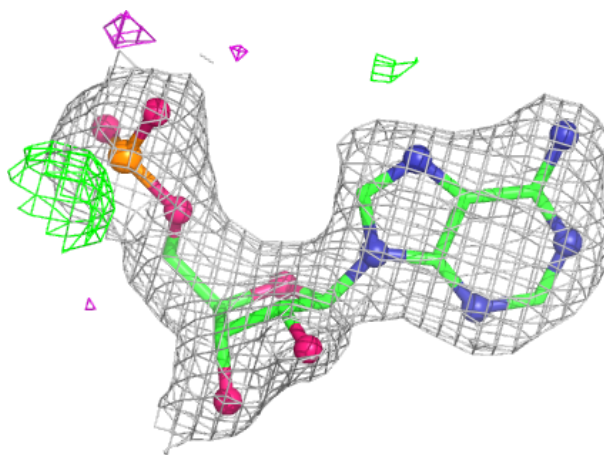
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and green (positive)



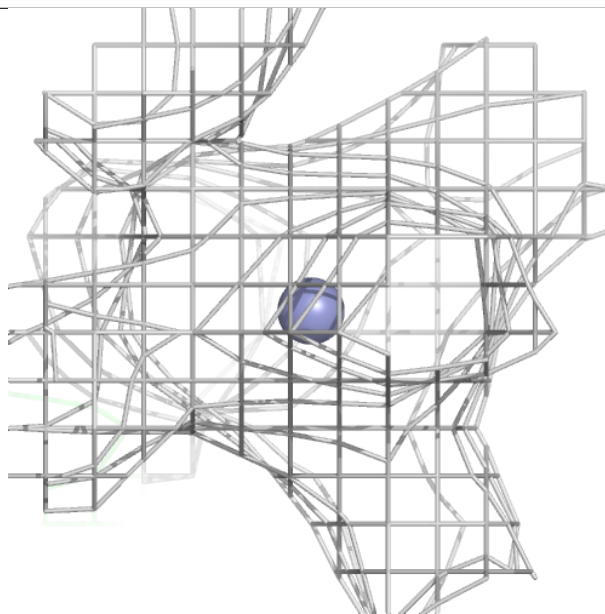
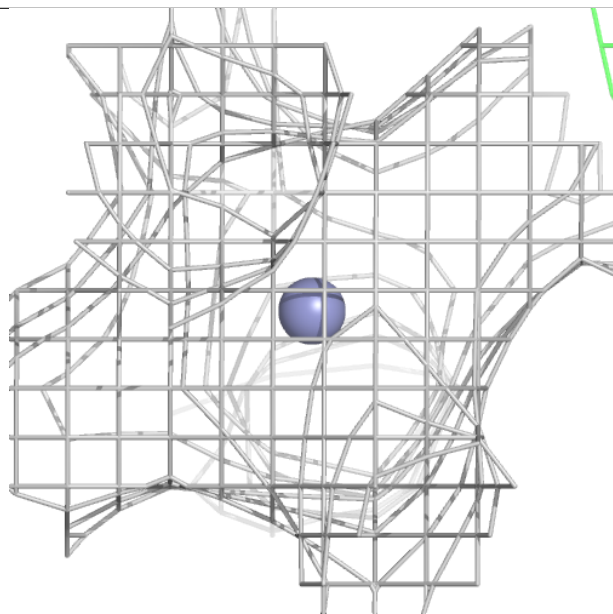
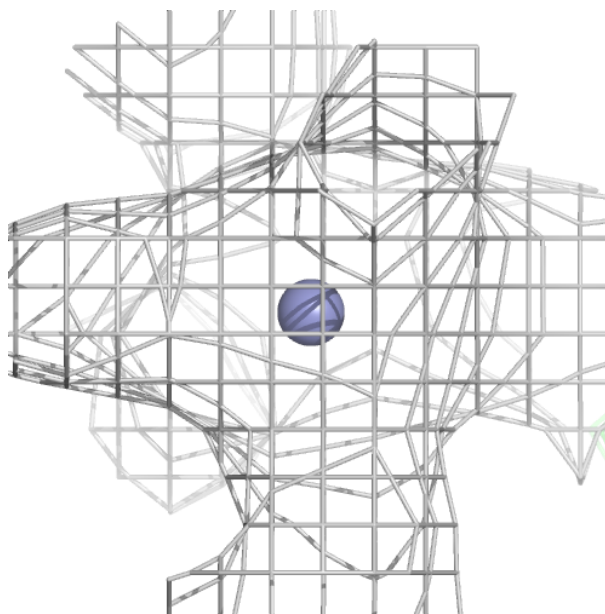
**Electron density around AMP B 703:**

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and green (positive)



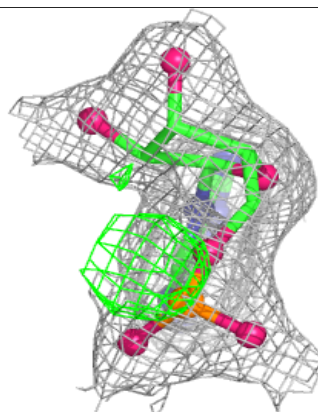
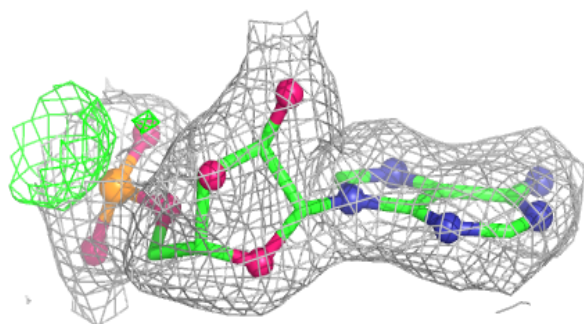
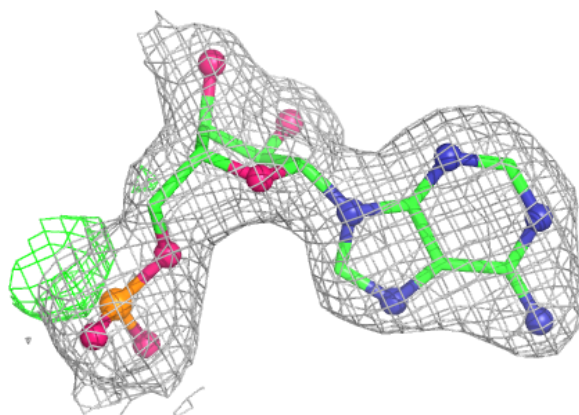
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and green (positive)



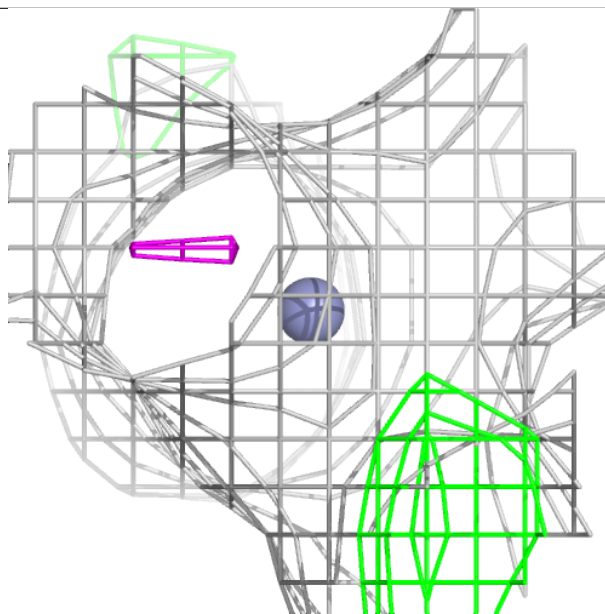
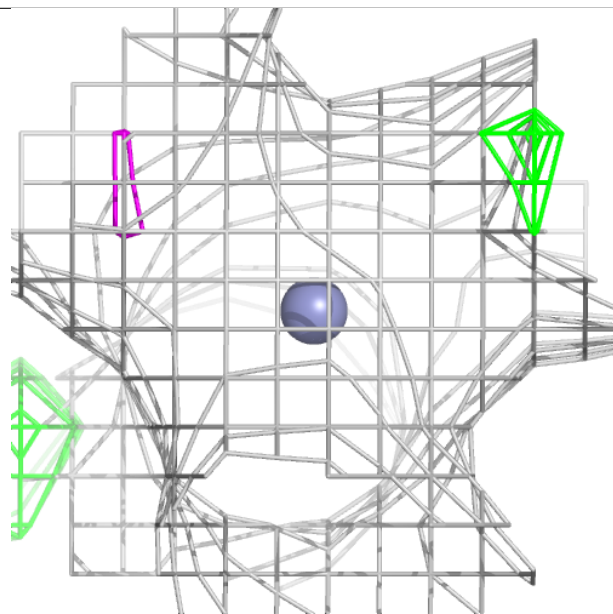
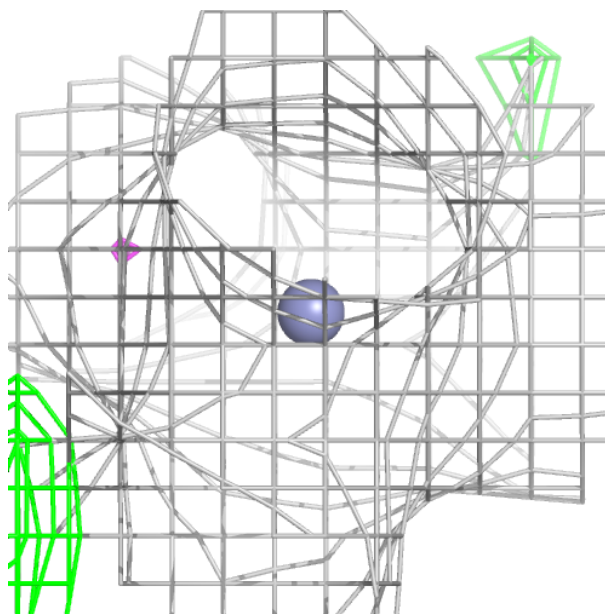
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and green (positive)



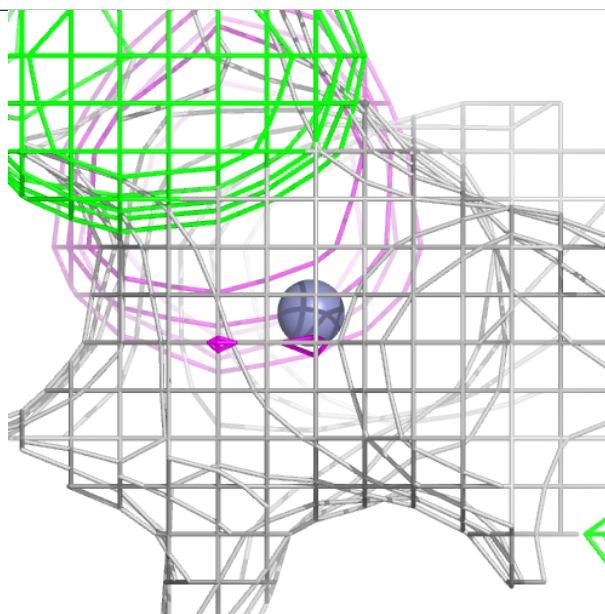
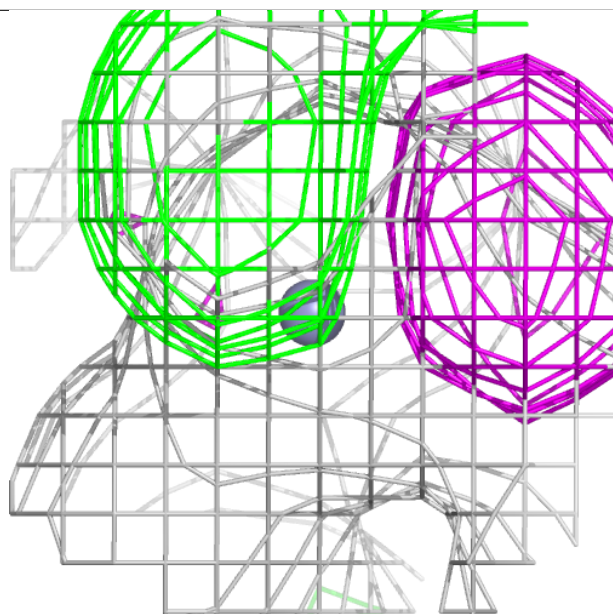
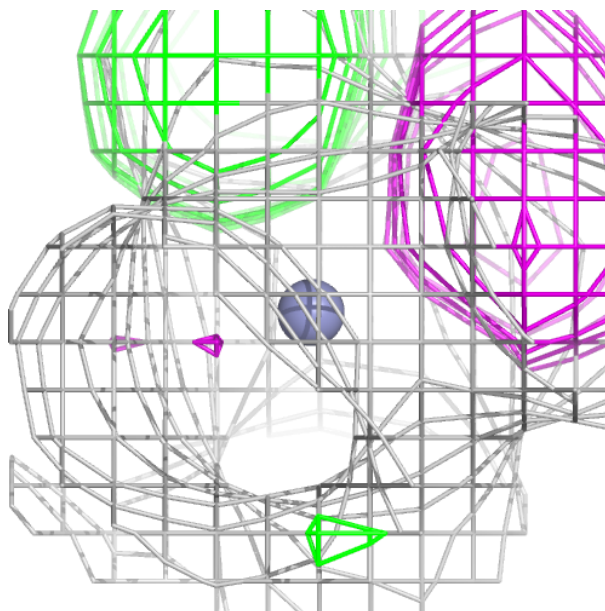
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



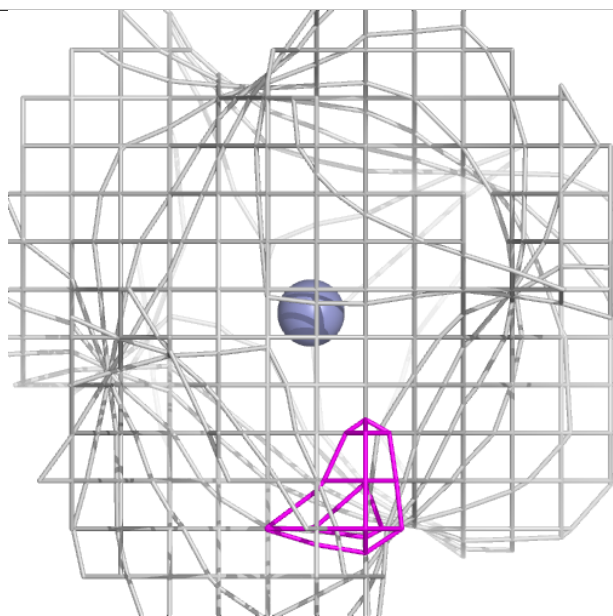
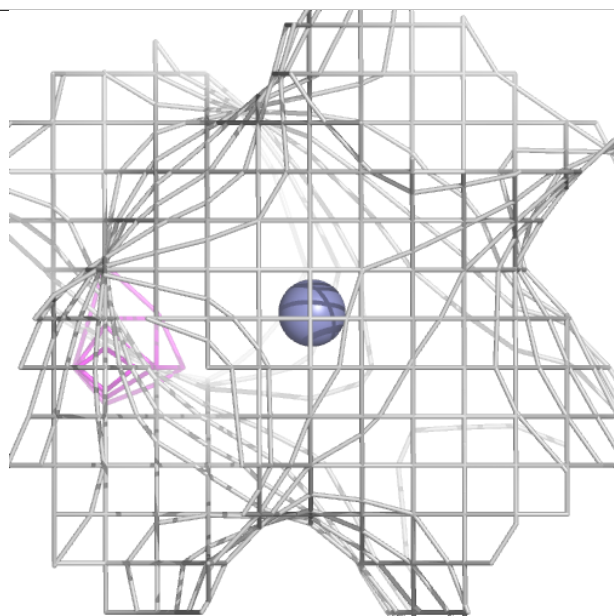
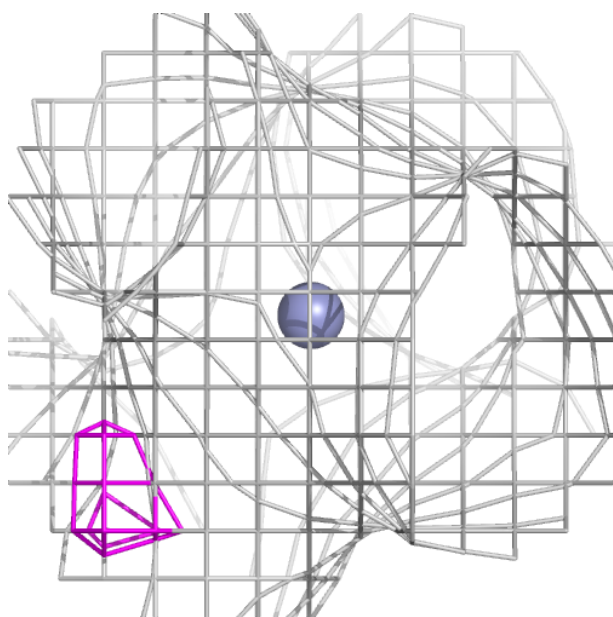
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and green (positive)



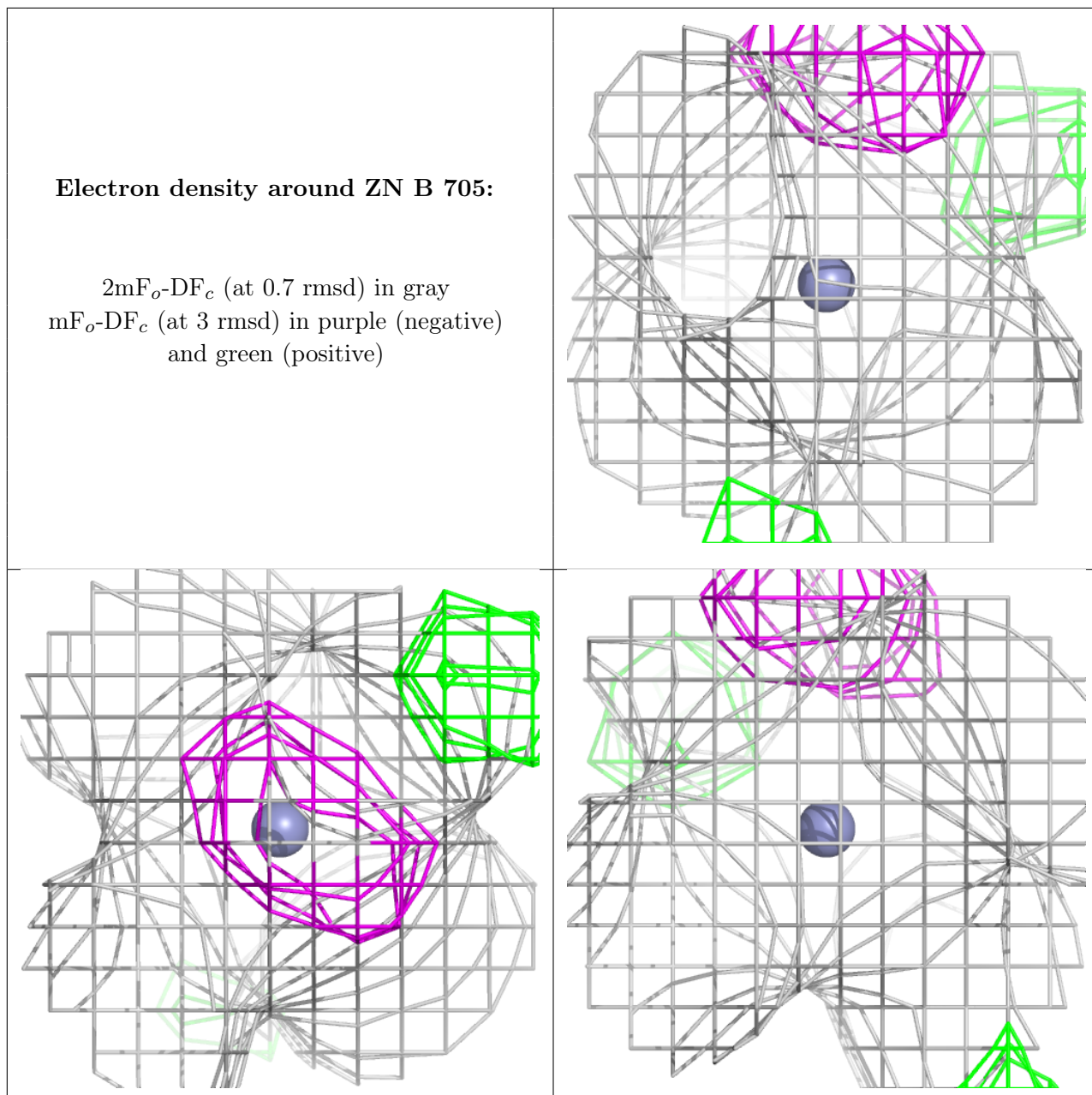
**Electron density around ZN B 704:**

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and green (positive)



**Electron density around ZN B 705:**

$2mF_o-DF_c$  (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.