



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:23 PM UTC

PDB ID : 8BR1 / pdb_00008br1
Title : ExoY Nucleotidyl Cyclase domain from *Vibrio nigripulchritudo* MARTX toxin, bound to Latrunculin-B-ATP-Mg-actin, and 3'-DEOXYADENOSINE-5'-TRI PHOSPHATE and 2 Mg ions
Authors : Teixeira-Nunes, M.; Renault, L.; Retailleau, P.
Deposited on : 2022-11-22
Resolution : 2.04 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

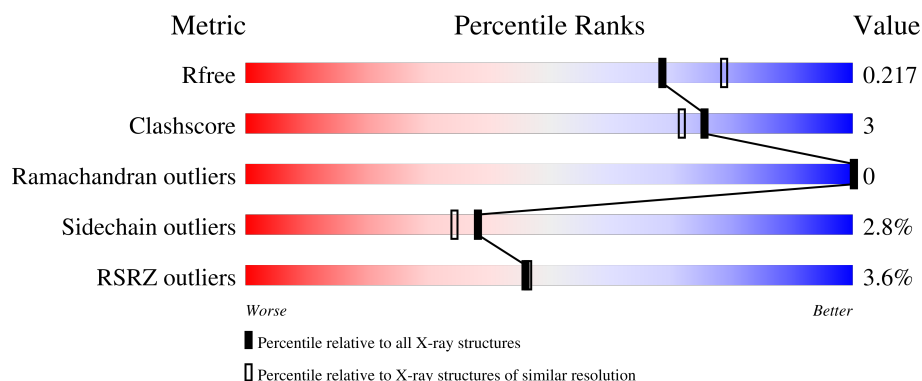
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



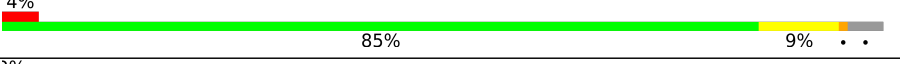

The reported resolution of this entry is 2.04 Å.

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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	375	
1	C	375	
2	B	413	
2	D	413	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 12811 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 Actin, alpha skeletal muscle, intermediate form.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	358	Total	C	N	O	S	0	0	0
			2801	1775	469	539	18			
1	C	365	Total	C	N	O	S	0	0	0
			2854	1808	479	548	19			

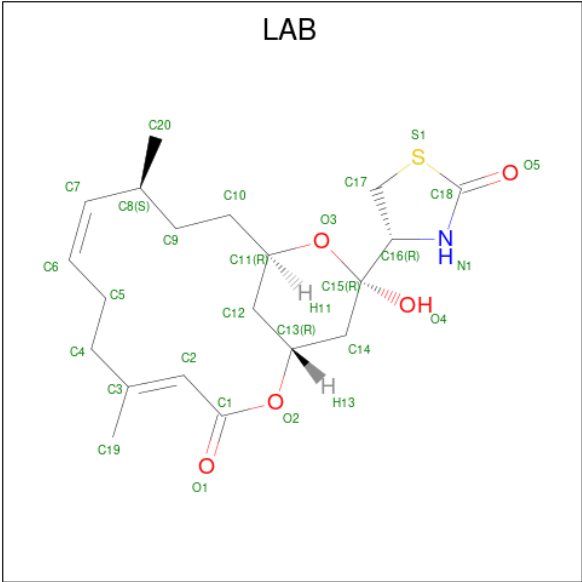
- Molecule 2 is a protein called Putative Adenylate cyclase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	398	Total	C	N	O	S	0	1	0
			3162	2002	526	625	9			
2	D	397	Total	C	N	O	S	0	0	0
			3146	1992	522	623	9			

There are 8 discrepancies between the modelled and reference sequences:

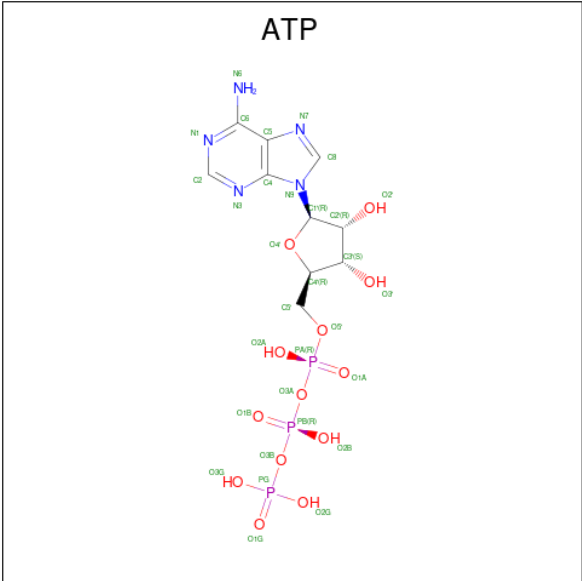
Chain	Residue	Modelled	Actual	Comment	Reference
B	451	GLY	-	expression tag	UNP A0A6N3LUE9
B	452	PRO	-	expression tag	UNP A0A6N3LUE9
B	453	GLY	-	expression tag	UNP A0A6N3LUE9
B	454	SER	-	expression tag	UNP A0A6N3LUE9
D	451	GLY	-	expression tag	UNP A0A6N3LUE9
D	452	PRO	-	expression tag	UNP A0A6N3LUE9
D	453	GLY	-	expression tag	UNP A0A6N3LUE9
D	454	SER	-	expression tag	UNP A0A6N3LUE9

- Molecule 3 is LATRUNCULIN B (CCD ID: LAB) (formula: C₂₀H₂₉NO₅S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			27	20	1	5	1		
3	C	1	Total	C	N	O	S	0	0
			27	20	1	5	1		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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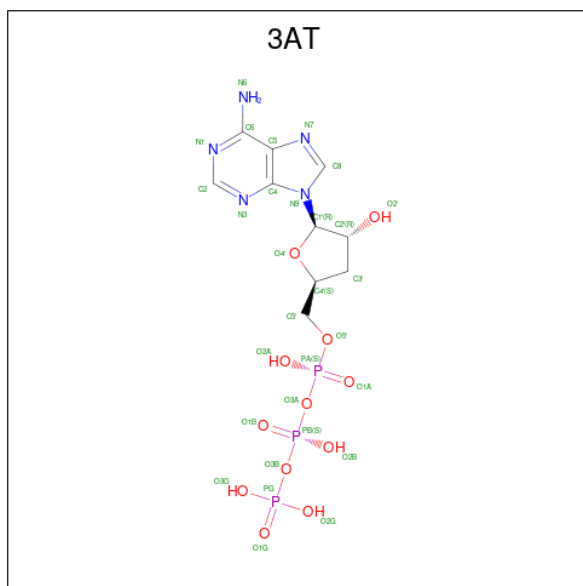
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		
5	B	2	Total	Mg	0	0
			2	2		
5	D	2	Total	Mg	0	0
			2	2		

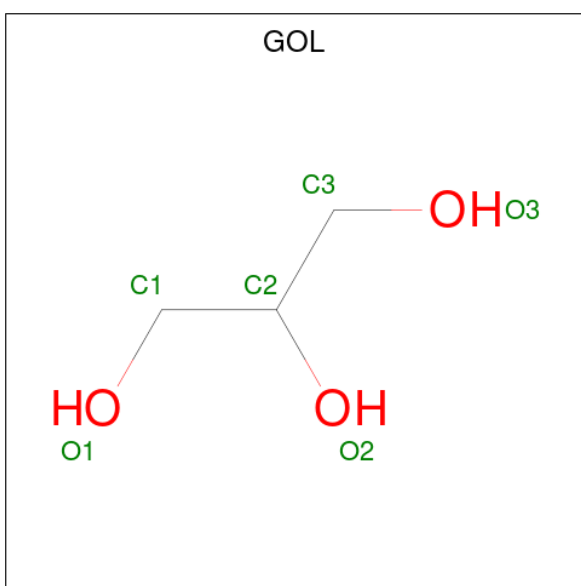
- Molecule 6 is 3'-DEOXYADENOSINE-5'-TRIPHOSPHATE (CCD ID: 3AT) (formula: C₁₀H₁₆N₅O₁₂P₃) (labeled as "Ligand of Interest" by depositor).





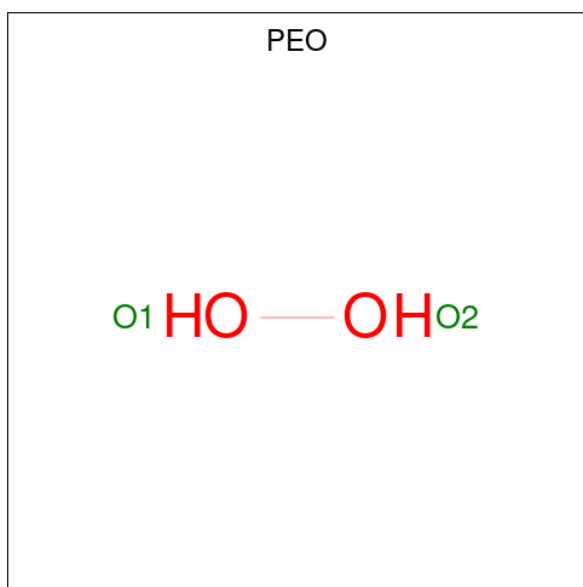
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	O	S	0	0
			5	4	1		
7	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is HYDROGEN PEROXIDE (CCD ID: PEO) (formula: H_2O_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total O 2 2	0	0

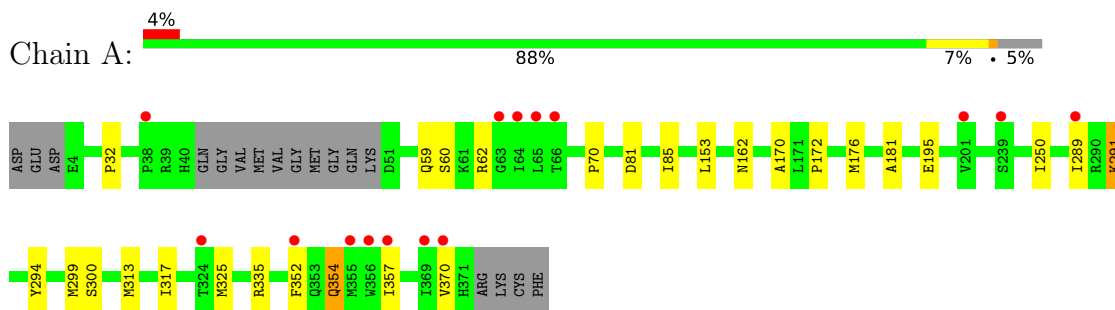
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	140	Total O 140 140	0	0
10	C	123	Total O 123 123	0	0
10	B	170	Total O 170 170	0	0
10	D	215	Total O 215 215	0	0

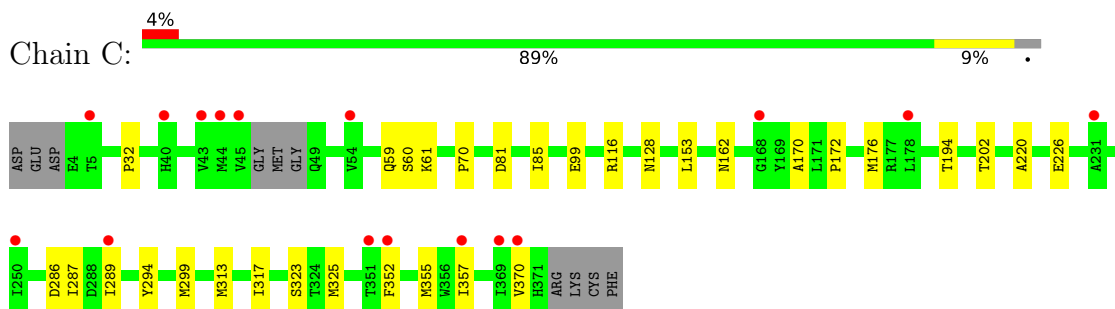
3 Residue-property plots

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.

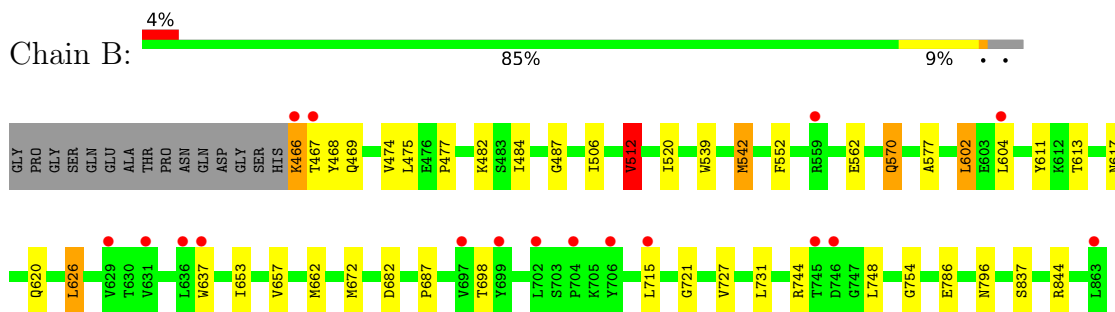
- Molecule 1: Actin, alpha skeletal muscle, intermediate form



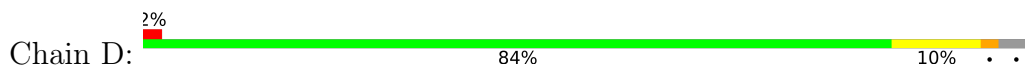
- Molecule 1: Actin, alpha skeletal muscle, intermediate form

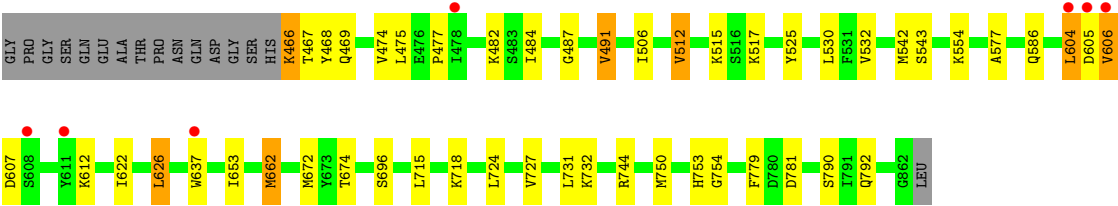


- Molecule 2: Putative Adenylate cyclase



- Molecule 2: Putative Adenylate cyclase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.12Å 132.44Å 96.40Å 90.00° 110.57° 90.00°	Depositor
Resolution (Å)	47.76 – 2.04 47.76 – 2.04	Depositor EDS
% Data completeness (in resolution range)	76.7 (47.76-2.04) 76.6 (47.76-2.04)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 2.05Å)	Xtriage
Refinement program	BUSTER 2.10.3 (20-MAY-2020)	Depositor
R, R_{free}	0.190 , 0.222 0.188 , 0.217	Depositor DCC
R_{free} test set	4302 reflections (3.81%)	wwPDB-VP
Wilson B-factor (Å ²)	51.1	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 49.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12811	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LAB, GOL, 3AT, SO4, MG, PEO, ATP

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	0.72	0/2862	1.02	3/3882 (0.1%)
1	C	0.71	0/2915	1.02	5/3952 (0.1%)
2	B	0.73	1/3234 (0.0%)	1.00	3/4378 (0.1%)
2	D	0.77	2/3214 (0.1%)	1.04	7/4353 (0.2%)
All	All	0.73	3/12225 (0.0%)	1.02	18/16565 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	662	MET	SD-CE	-7.73	1.60	1.79
2	D	662	MET	SD-CE	-6.57	1.63	1.79
2	D	525	TYR	CA-C	-5.21	1.46	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	289	ILE	N-CA-CB	-6.78	104.75	112.21
1	A	289	ILE	N-CA-CB	-6.46	105.10	112.21
1	C	352	PHE	CA-CB-CG	6.25	120.05	113.80
2	D	604	LEU	N-CA-C	5.89	117.65	110.41
2	D	606	VAL	N-CA-C	-5.71	106.90	111.81
2	B	698	THR	CB-CA-C	5.56	119.31	110.19
1	C	286	ASP	CA-CB-CG	5.39	117.99	112.60
2	D	525	TYR	N-CA-C	5.32	118.23	109.72
2	B	682	ASP	CA-CB-CG	-5.29	107.31	112.60
2	D	605	ASP	CA-C-N	-5.17	116.25	122.35
2	D	605	ASP	C-N-CA	-5.17	116.25	122.35
1	A	181	ALA	CA-C-N	5.09	125.75	119.99
1	A	181	ALA	C-N-CA	5.09	125.75	119.99
2	D	491	VAL	N-CA-CB	-5.09	102.94	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	202	THR	CA-C-N	5.08	127.09	120.28
1	C	202	THR	C-N-CA	5.08	127.09	120.28
2	D	622	ILE	N-CA-C	5.05	113.61	107.61
2	B	512	VAL	CB-CA-C	5.02	117.66	110.33

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	2801	0	2762	16	0
1	C	2854	0	2821	14	0
2	B	3162	0	3087	19	0
2	D	3146	0	3067	23	0
3	A	27	0	29	2	0
3	C	27	0	29	2	0
4	A	31	0	12	0	0
4	C	31	0	12	0	0
5	A	1	0	0	0	0
5	B	2	0	0	0	0
5	C	1	0	0	0	0
5	D	2	0	0	0	0
6	B	30	0	12	0	0
6	D	30	0	12	1	0
7	B	5	0	0	0	0
7	D	5	0	0	0	0
8	B	6	0	8	0	0
9	B	2	0	0	1	0
10	A	140	0	0	1	0
10	B	170	0	0	1	0
10	C	123	0	0	0	0
10	D	215	0	0	1	0
All	All	12811	0	11851	72	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 3.

All (72) 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)
9:B:1106:PEO:O1	9:B:1106:PEO:O2	1.52	1.24
2:D:530:LEU:HD22	6:D:1101:3AT:H2'1	1.64	0.79
2:D:606:VAL:HG11	2:D:612:LYS:HD2	1.69	0.74
1:A:170:ALA:O	1:A:172:PRO:HD3	2.04	0.57
2:D:530:LEU:HD23	2:D:753:HIS:CD2	2.39	0.57
1:C:170:ALA:O	1:C:172:PRO:HD3	2.04	0.57
2:B:487:GLY:HA3	2:B:512:VAL:HG22	1.89	0.54
1:C:153:LEU:HD22	1:C:313:MET:HE2	1.89	0.54
1:A:153:LEU:HD22	1:A:313:MET:HE2	1.89	0.54
2:D:790:SER:HB2	2:D:792:GLN:OE1	2.08	0.53
2:D:487:GLY:HA3	2:D:512:VAL:HG22	1.90	0.53
2:B:570:GLN:NE2	10:B:1305:HOH:O	2.41	0.53
1:A:291:LYS:HG3	1:A:325:MET:SD	2.49	0.53
2:B:482:LYS:HG3	2:B:484:ILE:HD11	1.92	0.52
2:D:482:LYS:HG3	2:D:484:ILE:HD11	1.91	0.52
1:A:162:ASN:HB2	1:A:176:MET:HB2	1.93	0.51
2:B:602:LEU:HD13	2:B:611:TYR:HB3	1.93	0.51
2:B:744:ARG:HD2	2:B:748:LEU:O	2.12	0.50
2:B:837:SER:OG	2:B:844[A]:ARG:NH2	2.44	0.50
1:A:294:TYR:CD2	1:A:325:MET:HG2	2.47	0.50
2:B:602:LEU:HD22	2:B:613:THR:HB	1.93	0.50
2:B:727:VAL:HG23	2:B:731:LEU:HD22	1.92	0.50
2:D:577:ALA:HB1	2:D:653:ILE:HG23	1.94	0.50
1:C:59:GLN:HG3	3:C:403:LAB:C7	2.43	0.49
1:C:162:ASN:HB2	1:C:176:MET:HB2	1.95	0.48
2:B:469:GLN:HG3	2:B:474:VAL:HG22	1.95	0.48
1:C:294:TYR:CD2	1:C:325:MET:HG2	2.48	0.48
2:D:469:GLN:HG3	2:D:474:VAL:HG22	1.96	0.47
2:B:577:ALA:HB1	2:B:653:ILE:HG23	1.96	0.47
1:A:195:GLU:HB2	10:A:501:HOH:O	2.13	0.47
2:D:727:VAL:HG23	2:D:731:LEU:HD22	1.96	0.47
2:D:517:LYS:NZ	10:D:1310:HOH:O	2.48	0.46
2:B:506:ILE:HB	2:B:672:MET:HB2	1.97	0.46
2:D:515:LYS:HE2	2:D:543:SER:OG	2.16	0.46
2:B:466:LYS:O	2:B:477:PRO:HG3	2.17	0.45
1:C:220:ALA:HB1	1:C:226:GLU:HG3	1.97	0.45
2:D:506:ILE:HB	2:D:672:MET:HB2	1.99	0.45
2:D:530:LEU:CD2	2:D:753:HIS:CD2	3.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:466:LYS:O	2:D:477:PRO:HG3	2.17	0.44
1:C:313:MET:O	1:C:317:ILE:HG12	2.17	0.44
2:D:779:PHE:HA	2:D:792:GLN:OE1	2.18	0.44
1:A:59:GLN:HG3	3:A:401:LAB:C7	2.47	0.44
2:B:626:LEU:HB3	2:B:637:TRP:CE3	2.53	0.44
2:D:731:LEU:HD22	2:D:754:GLY:HA2	2.00	0.44
1:C:61:LYS:NZ	2:D:696:SER:HA	2.33	0.43
2:D:626:LEU:HB3	2:D:637:TRP:CE3	2.54	0.43
2:D:532:VAL:HG21	2:D:662:MET:HE1	2.00	0.43
1:A:70:PRO:HG3	1:A:81:ASP:HB3	2.00	0.43
1:C:32:PRO:HG3	3:C:403:LAB:H6	2.01	0.43
1:A:313:MET:O	1:A:317:ILE:HG12	2.18	0.43
1:C:70:PRO:HG3	1:C:81:ASP:HB3	2.01	0.43
2:D:724:LEU:HD13	2:D:732:LYS:HG2	2.01	0.43
1:A:300:SER:HA	1:A:335:ARG:HB2	2.01	0.42
1:A:357:ILE:HD11	1:A:370:VAL:HA	2.01	0.42
2:D:718:LYS:HE3	2:D:718:LYS:HB2	1.82	0.42
1:A:70:PRO:HG2	1:A:85:ILE:HD12	2.02	0.42
1:A:352:PHE:C	1:A:354:GLN:H	2.27	0.42
1:C:357:ILE:HD11	1:C:370:VAL:HA	2.02	0.41
1:C:153:LEU:HD23	1:C:299:MET:HE3	2.02	0.41
2:B:520:ILE:O	2:B:744:ARG:NH2	2.53	0.41
2:B:731:LEU:HD22	2:B:754:GLY:HA2	2.00	0.41
1:A:32:PRO:HG3	3:A:401:LAB:H6	2.02	0.41
1:A:59:GLN:O	1:A:62:ARG:HB2	2.20	0.41
1:A:153:LEU:HD23	1:A:299:MET:HE3	2.03	0.41
2:B:539:TRP:CZ2	2:B:617:ASN:HB3	2.55	0.41
2:D:744:ARG:HD3	2:D:750:MET:HG2	2.01	0.41
1:C:99:GLU:HA	1:C:128:ASN:O	2.20	0.41
2:B:468:TYR:HB3	2:B:475:LEU:HB2	2.03	0.40
2:B:542:MET:HE3	2:B:552:PHE:HB3	2.04	0.40
1:C:70:PRO:HG2	1:C:85:ILE:HD12	2.02	0.40
2:B:687:PRO:HB3	2:B:721:GLY:C	2.47	0.40
2:D:468:TYR:HB3	2:D:475:LEU:HB2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	354/375 (94%)	347 (98%)	7 (2%)	0	100	100
1	C	361/375 (96%)	354 (98%)	7 (2%)	0	100	100
2	B	397/413 (96%)	386 (97%)	11 (3%)	0	100	100
2	D	395/413 (96%)	386 (98%)	9 (2%)	0	100	100
All	All	1507/1576 (96%)	1473 (98%)	34 (2%)	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	304/318 (96%)	300 (99%)	4 (1%)	61	63
1	C	310/318 (98%)	304 (98%)	6 (2%)	50	50
2	B	348/358 (97%)	334 (96%)	14 (4%)	28	22
2	D	346/358 (97%)	333 (96%)	13 (4%)	29	24
All	All	1308/1352 (97%)	1271 (97%)	37 (3%)	38	34

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	SER
1	A	250	ILE

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Mol	Chain	Res	Type
1	A	291	LYS
1	A	354	GLN
1	C	60	SER
1	C	116	ARG
1	C	194	THR
1	C	287	ILE
1	C	323	SER
1	C	355	MET
2	B	466	LYS
2	B	467	THR
2	B	512	VAL
2	B	542	MET
2	B	562	GLU
2	B	570	GLN
2	B	602	LEU
2	B	604	LEU
2	B	620	GLN
2	B	626	LEU
2	B	657	VAL
2	B	715	LEU
2	B	786	GLU
2	B	796	ASN
2	D	466	LYS
2	D	467	THR
2	D	491	VAL
2	D	512	VAL
2	D	542	MET
2	D	554	LYS
2	D	586	GLN
2	D	604	LEU
2	D	607	ASP
2	D	626	LEU
2	D	674	THR
2	D	715	LEU
2	D	781	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	ASN
1	A	121	GLN
1	A	128	ASN

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Mol	Chain	Res	Type
1	C	111	ASN
1	C	225	ASN
2	B	576	ASN
2	B	586	GLN
2	B	712	ASN
2	B	796	ASN
2	B	800	GLN
2	D	479	GLN
2	D	576	ASN
2	D	681	GLN
2	D	712	ASN
2	D	796	ASN
2	D	800	GLN
2	D	815	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 16 ligands modelled in this entry, 6 are monoatomic - leaving 10 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
7	SO4	D	1104	-	4,4,4	0.17	0	6,6,6	0.29	0
3	LAB	C	403	-	28,29,29	0.73	1 (3%)	29,41,41	0.89	1 (3%)
6	3AT	B	1101	5	30,32,32	0.48	0	42,50,50	0.60	0
8	GOL	B	1105	-	5,5,5	0.35	0	5,5,5	0.33	0
4	ATP	C	401	5	32,33,33	0.43	0	48,52,52	0.55	0
4	ATP	A	402	5	32,33,33	0.50	0	48,52,52	0.70	2 (4%)
7	SO4	B	1104	-	4,4,4	0.30	0	6,6,6	0.19	0
9	PEO	B	1106	-	1,1,1	0.71	0	-		
3	LAB	A	401	-	28,29,29	0.93	1 (3%)	29,41,41	0.90	2 (6%)
6	3AT	D	1101	5	30,32,32	0.61	1 (3%)	42,50,50	0.57	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LAB	C	403	-	-	2/21/49/49	0/2/3/3
6	3AT	B	1101	5	-	7/22/34/34	0/3/3/3
8	GOL	B	1105	-	-	0/4/4/4	-
4	ATP	C	401	5	-	3/22/38/38	0/3/3/3
4	ATP	A	402	5	-	3/22/38/38	0/3/3/3
3	LAB	A	401	-	-	2/21/49/49	0/2/3/3
6	3AT	D	1101	5	-	6/22/34/34	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	LAB	C15-C16	4.71	1.63	1.54
3	C	403	LAB	C15-C16	3.54	1.61	1.54
6	D	1101	3AT	PA-O5'	2.52	1.69	1.59

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	403	LAB	O3-C15-C16	2.86	107.92	104.25
4	A	402	ATP	O3'-C3'-C2'	-2.78	102.89	111.82
3	A	401	LAB	O3-C15-C16	2.24	107.12	104.25
3	A	401	LAB	C3-C2-C1	2.13	132.44	127.36
4	A	402	ATP	O2B-PB-O1B	2.11	122.28	112.44

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	1101	3AT	O4'-C4'-C5'-O5'
6	B	1101	3AT	C3'-C4'-C5'-O5'
6	D	1101	3AT	O4'-C4'-C5'-O5'
6	D	1101	3AT	C3'-C4'-C5'-O5'
4	C	401	ATP	PB-O3B-PG-O2G
6	B	1101	3AT	PB-O3B-PG-O3G
6	D	1101	3AT	PB-O3B-PG-O2G
4	C	401	ATP	PG-O3B-PB-O1B
6	D	1101	3AT	C4'-C5'-O5'-PA
4	A	402	ATP	C5'-O5'-PA-O1A
4	C	401	ATP	C5'-O5'-PA-O1A
6	B	1101	3AT	C5'-O5'-PA-O1A
6	B	1101	3AT	C4'-C5'-O5'-PA
3	A	401	LAB	O2-C1-C2-C3
6	D	1101	3AT	PA-O3A-PB-O2B
3	C	403	LAB	O2-C1-C2-C3
3	A	401	LAB	O1-C1-C2-C3
3	C	403	LAB	O1-C1-C2-C3
4	A	402	ATP	PG-O3B-PB-O1B
6	B	1101	3AT	PA-O3A-PB-O2B
4	A	402	ATP	PB-O3B-PG-O2G
6	B	1101	3AT	PA-O3A-PB-O1B
6	D	1101	3AT	PA-O3A-PB-O1B

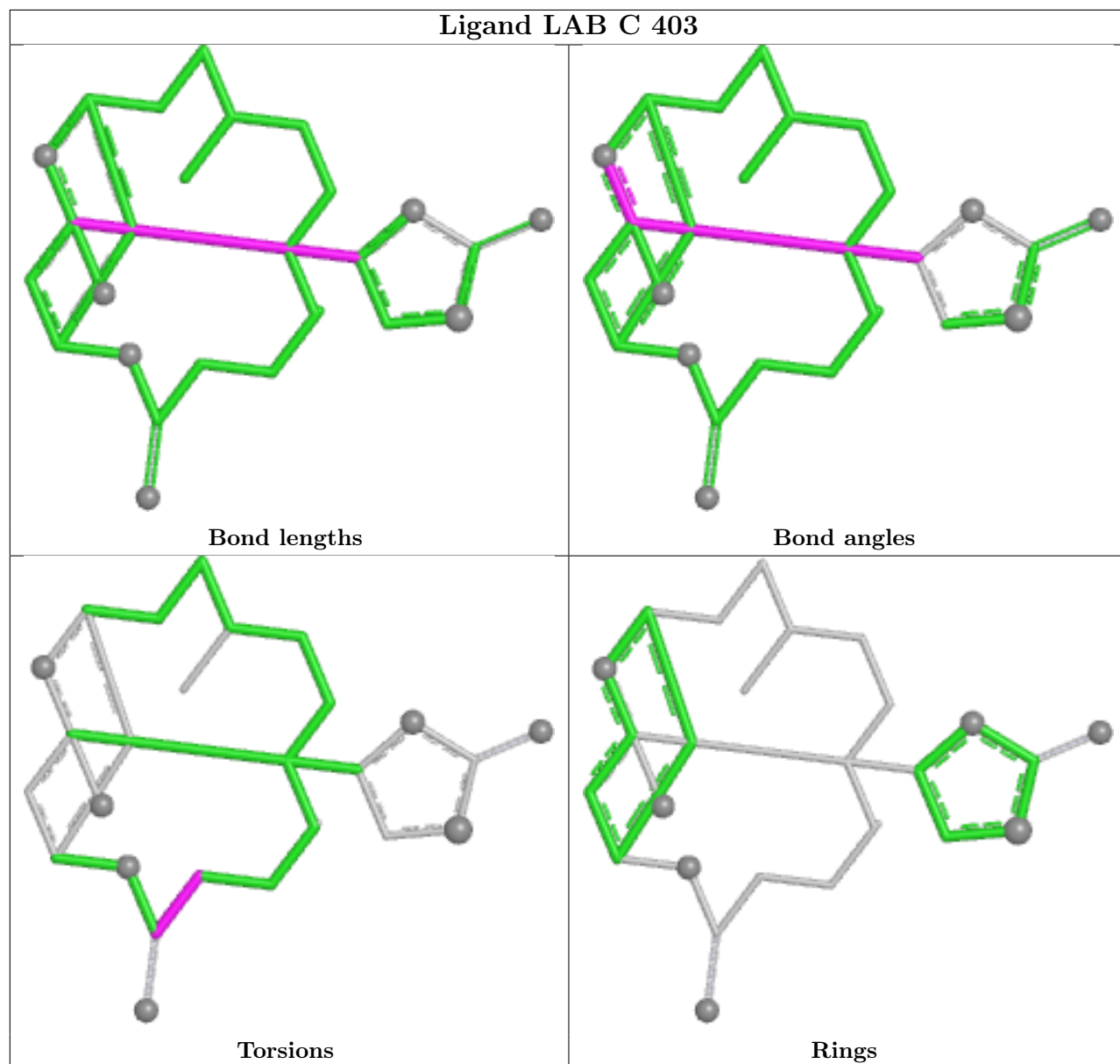
There are no ring outliers.

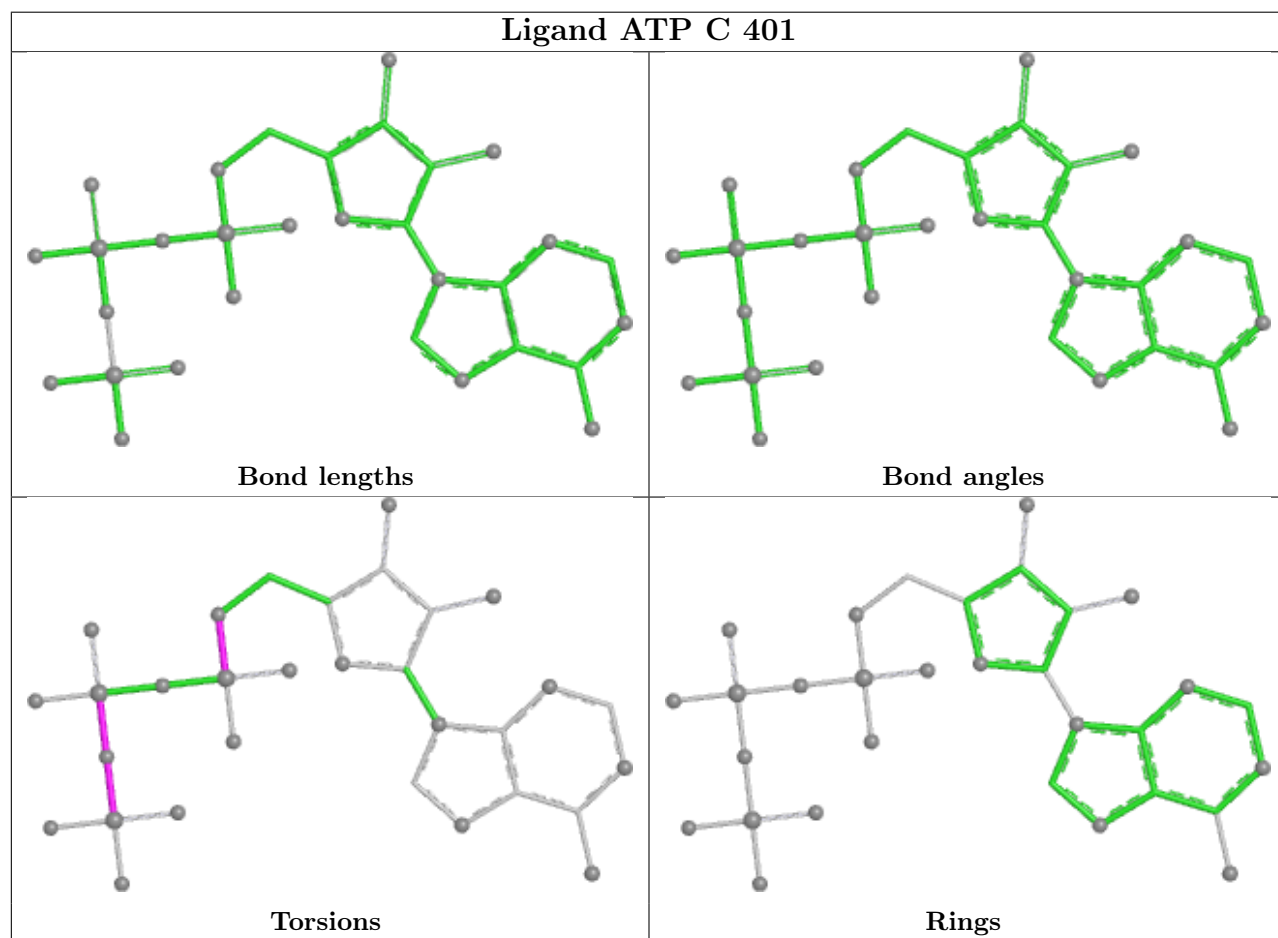
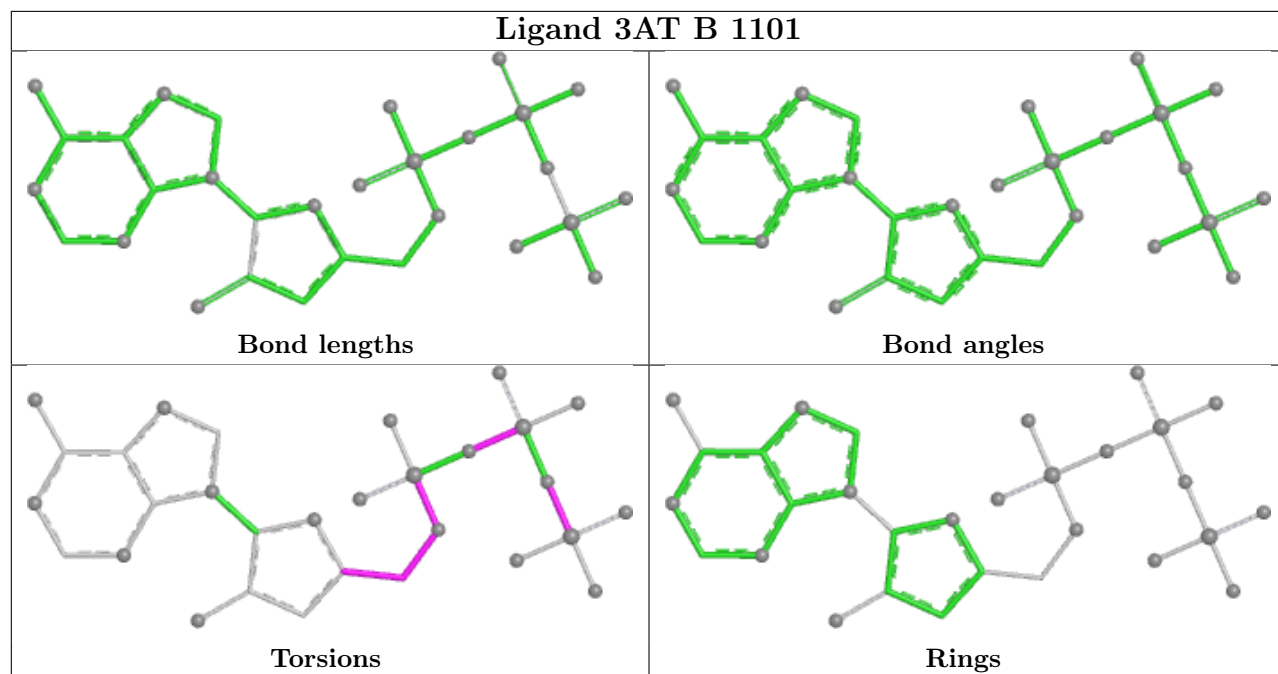
4 monomers are involved in 6 short contacts:

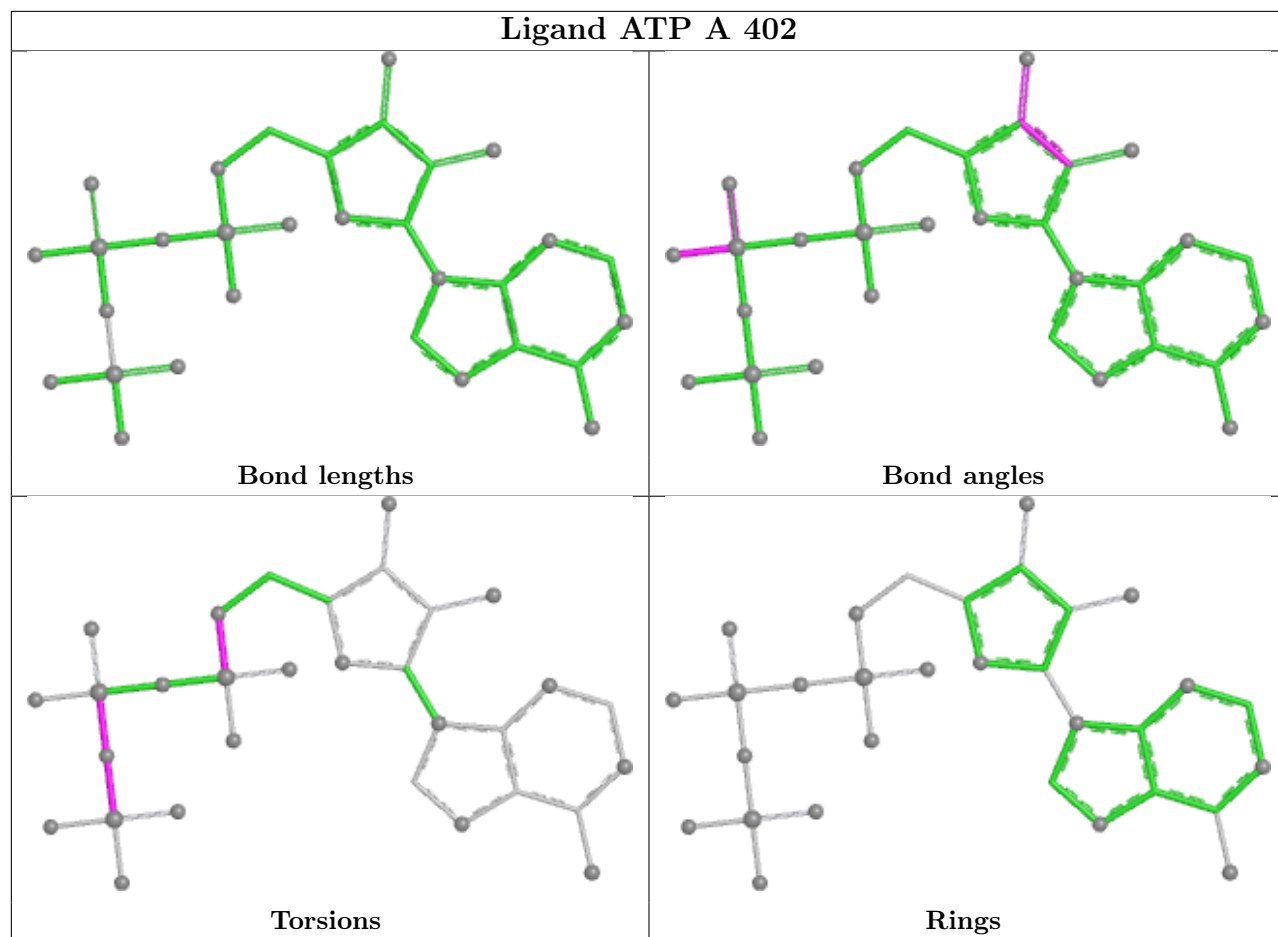
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	403	LAB	2	0
9	B	1106	PEO	1	0
3	A	401	LAB	2	0
6	D	1101	3AT	1	0

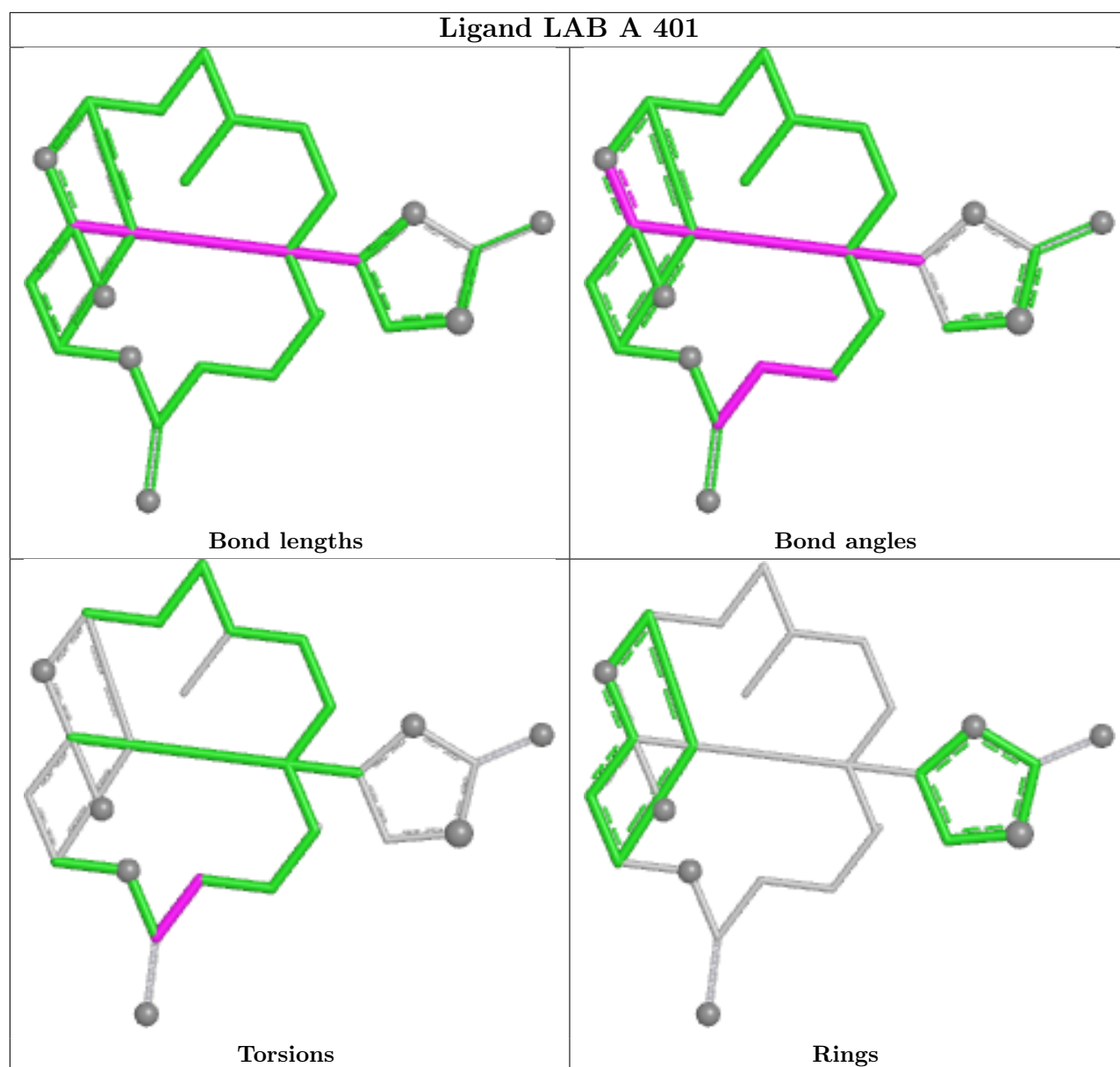
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

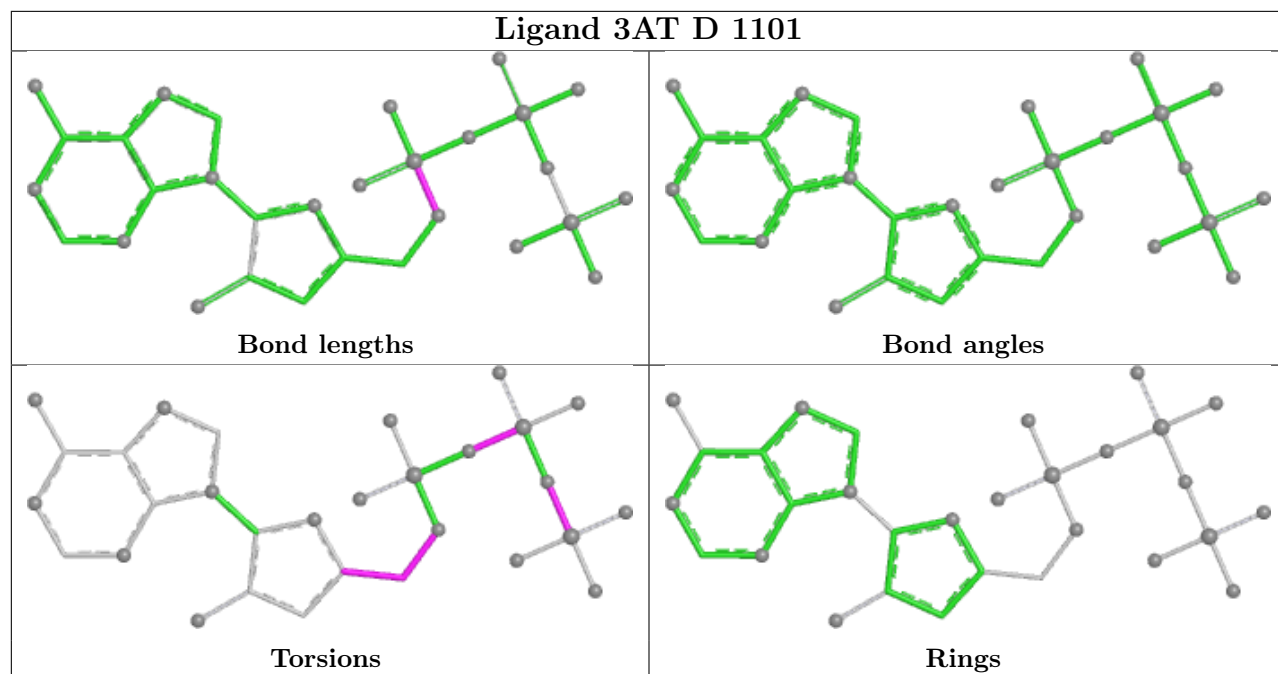
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











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 ⓘ

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	358/375 (95%)	0.36	15 (4%)	40 40	38, 56, 84, 103	0
1	C	365/375 (97%)	0.54	16 (4%)	39 39	45, 64, 105, 115	0
2	B	398/413 (96%)	0.49	17 (4%)	40 40	34, 57, 94, 107	1 (0%)
2	D	397/413 (96%)	0.23	7 (1%)	67 69	38, 52, 82, 95	0
All	All	1518/1576 (96%)	0.40	55 (3%)	46 46	34, 57, 90, 115	1 (0%)

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	45	VAL	3.9
1	A	324	THR	3.8
2	D	606	VAL	3.5
1	A	356	TRP	3.4
2	D	608	SER	3.4
2	D	604	LEU	3.0
1	C	43	VAL	3.0
1	C	231	ALA	3.0
1	A	355	MET	3.0
1	A	289	ILE	2.8
1	A	357	ILE	2.8
1	A	201	VAL	2.8
1	A	38	PRO	2.8
1	C	352	PHE	2.7
1	C	351	THR	2.7
2	B	466	LYS	2.7
1	A	64	ILE	2.6
2	B	697	VAL	2.6
1	C	5	THR	2.6
2	B	631	VAL	2.5
1	A	63	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	370	VAL	2.4
2	B	629	VAL	2.4
1	A	369	ILE	2.4
1	C	369	ILE	2.4
1	C	168	GLY	2.4
1	A	66	THR	2.4
1	C	289	ILE	2.3
2	B	702	LEU	2.3
2	B	706	TYR	2.3
2	D	611	TYR	2.3
1	C	357	ILE	2.3
1	C	250	ILE	2.2
2	D	478	ILE	2.2
2	D	605	ASP	2.2
2	B	604	LEU	2.2
2	B	863	LEU	2.2
2	B	559	ARG	2.2
2	B	467	THR	2.2
1	C	54	VAL	2.2
2	B	699	TYR	2.2
1	C	44	MET	2.2
2	B	704	PRO	2.1
2	B	745	THR	2.2
2	B	636	LEU	2.1
2	B	637	TRP	2.1
2	D	637	TRP	2.1
1	C	370	VAL	2.1
1	C	40	HIS	2.1
1	A	352	PHE	2.1
1	A	239	SER	2.1
1	A	65	LEU	2.0
2	B	746	ASP	2.0
1	C	178	LEU	2.0
2	B	715	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 oligosaccharides in this entry.

6.4 Ligands ⓘ

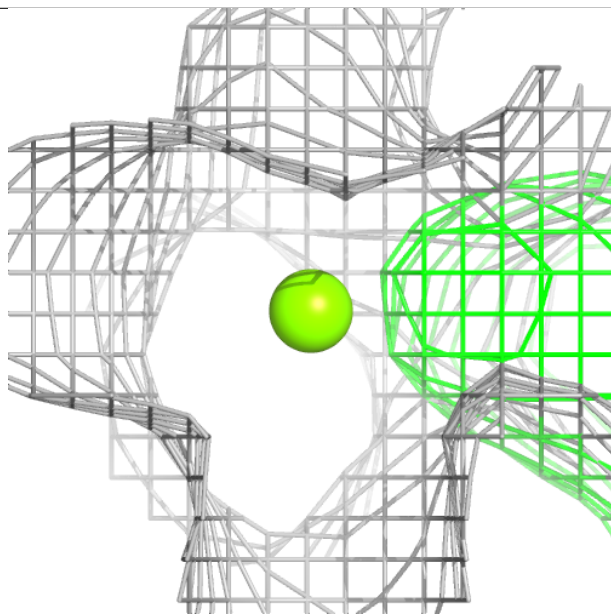
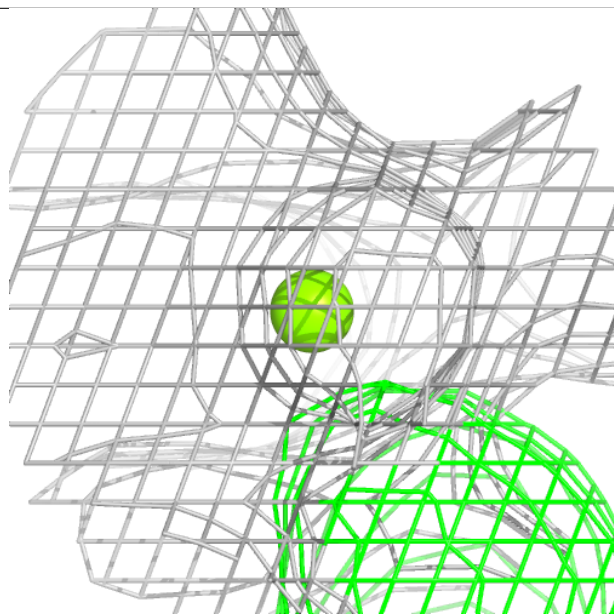
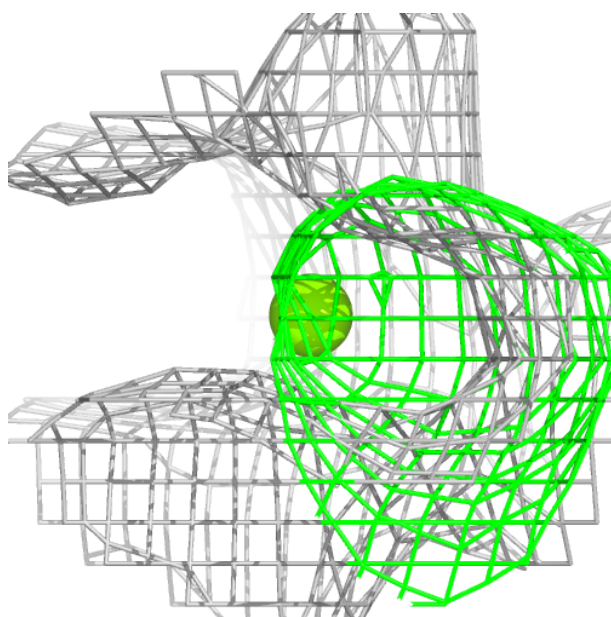
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	GOL	B	1105	6/6	0.77	0.21	64,65,66,66	0
9	PEO	B	1106	2/2	0.83	0.10	76,76,76,77	0
7	SO4	D	1104	5/5	0.89	0.23	64,64,64,65	5
5	MG	D	1102	1/1	0.89	0.08	51,51,51,51	0
7	SO4	B	1104	5/5	0.89	0.19	80,80,81,81	5
6	3AT	B	1101	30/30	0.92	0.11	45,56,60,61	0
6	3AT	D	1101	30/30	0.93	0.10	40,55,60,61	0
5	MG	B	1102	1/1	0.94	0.07	54,54,54,54	0
3	LAB	A	401	27/27	0.95	0.09	48,52,54,55	0
3	LAB	C	403	27/27	0.95	0.09	56,59,60,60	0
4	ATP	C	401	31/31	0.96	0.07	47,49,52,53	0
4	ATP	A	402	31/31	0.97	0.07	41,44,48,49	0
5	MG	A	403	1/1	0.99	0.05	44,44,44,44	0
5	MG	D	1103	1/1	0.99	0.05	41,41,41,41	0
5	MG	C	402	1/1	1.00	0.02	50,50,50,50	0
5	MG	B	1103	1/1	1.00	0.06	51,51,51,51	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.

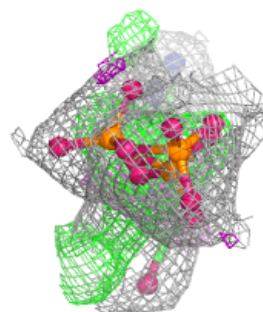
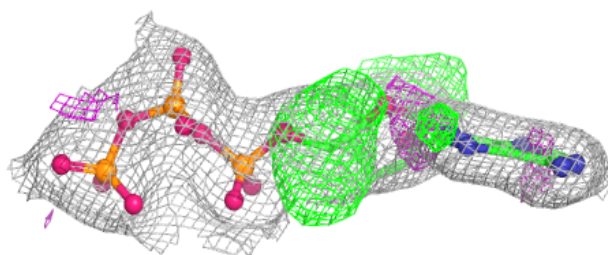
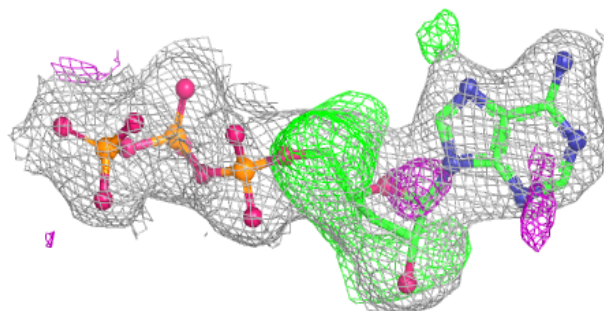
Electron density around MG D 1102:

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

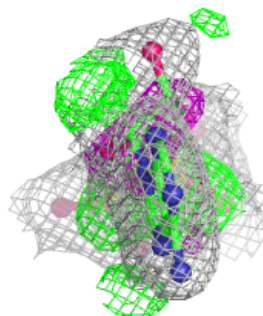
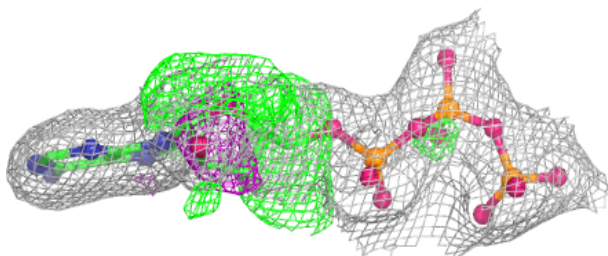
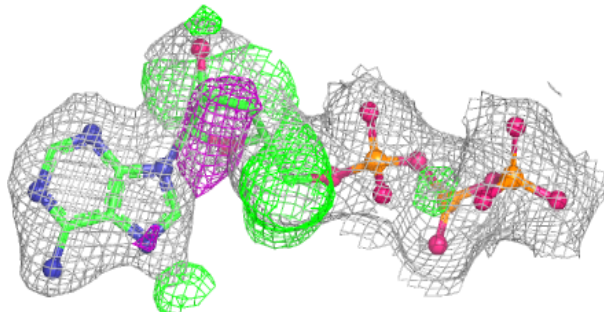


Electron density around 3AT B 1101:

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

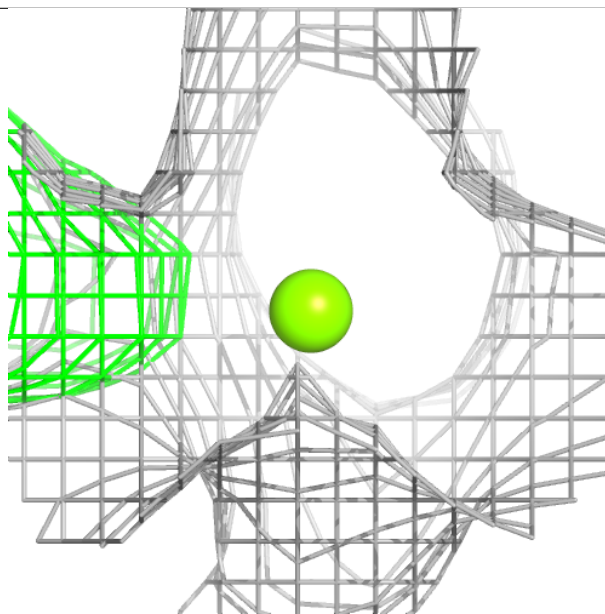
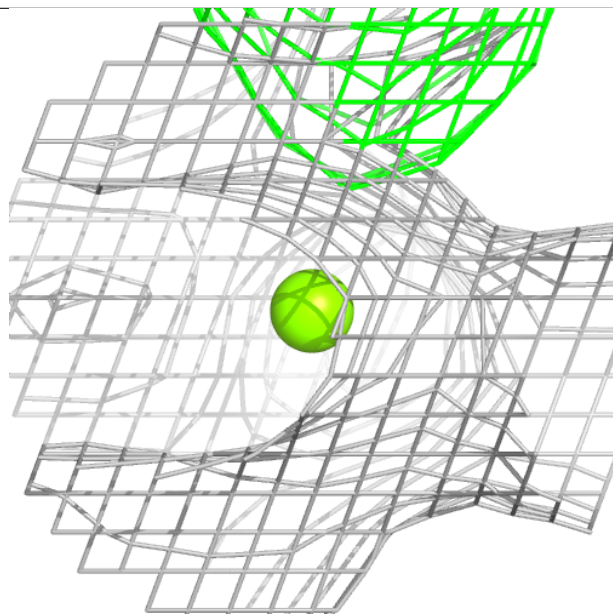
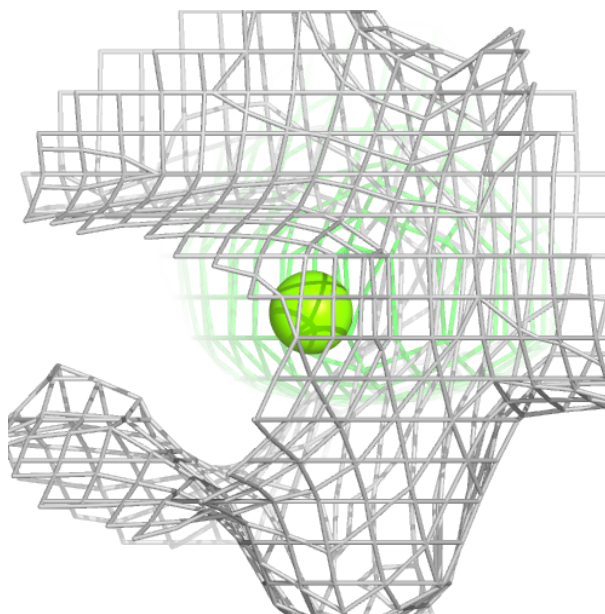
**Electron density around 3AT D 1101:**

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



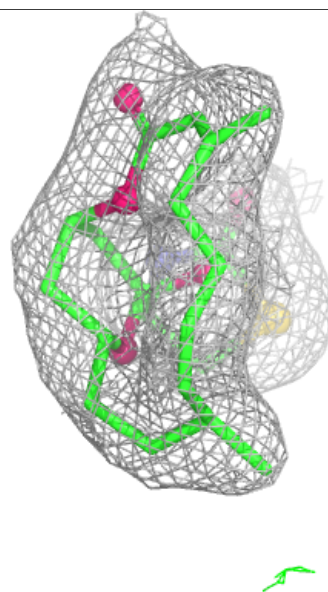
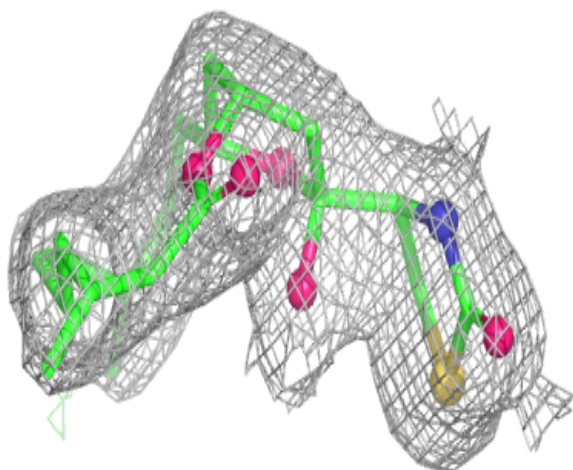
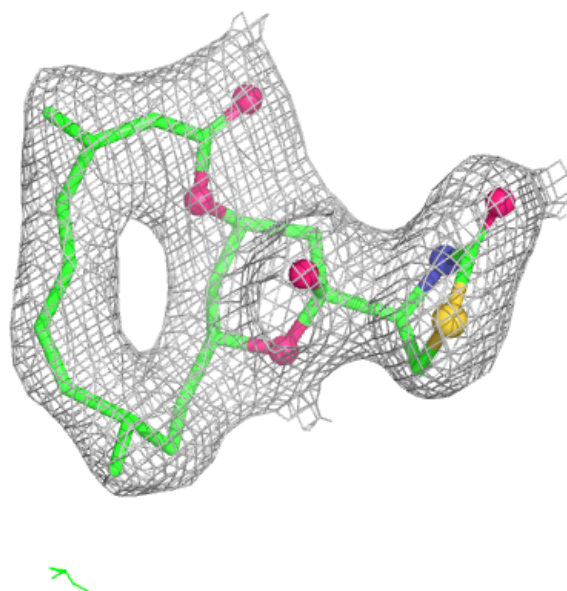
Electron density around MG B 1102:

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and green (positive)



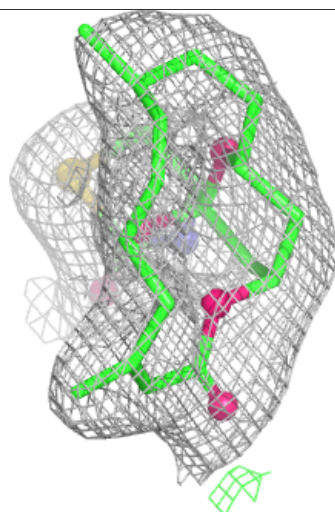
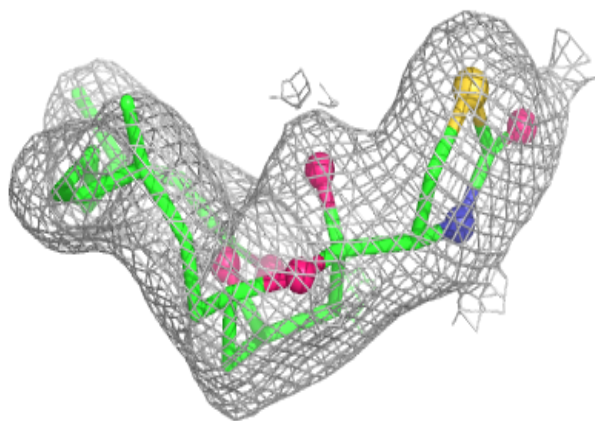
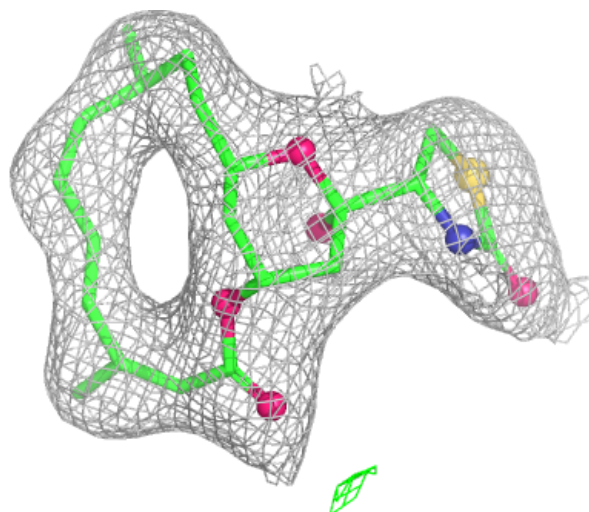
Electron density around LAB A 401:

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



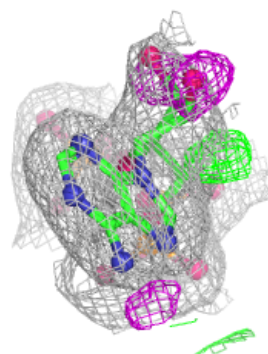
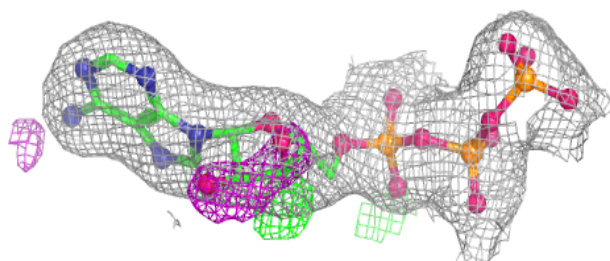
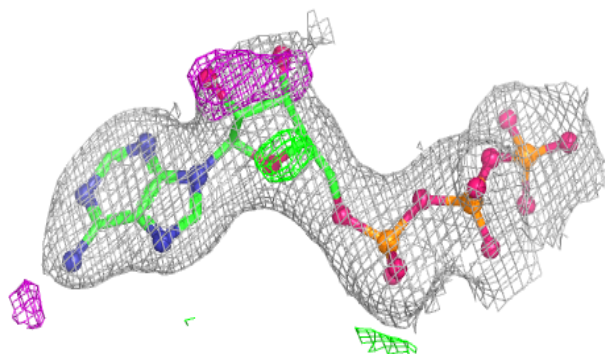
Electron density around LAB C 403:

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and green (positive)

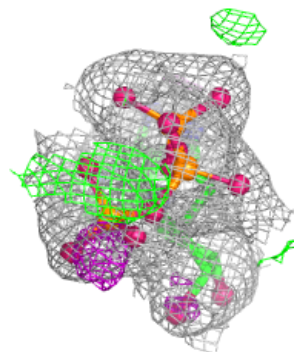
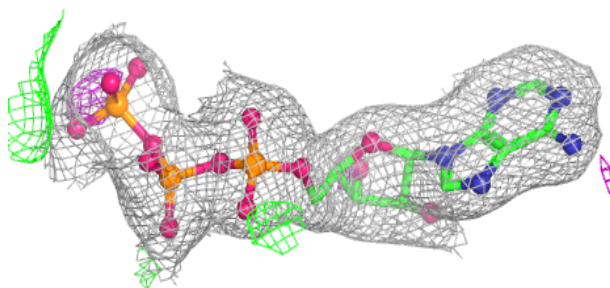
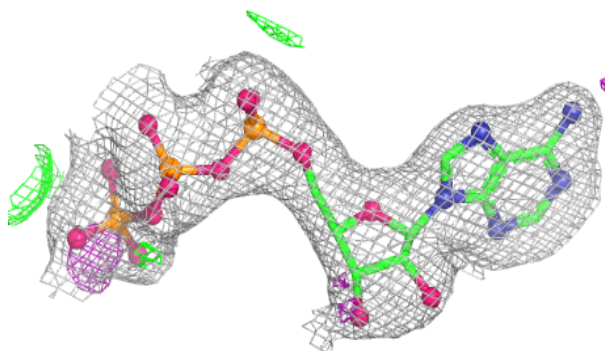


Electron density around ATP C 401:

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

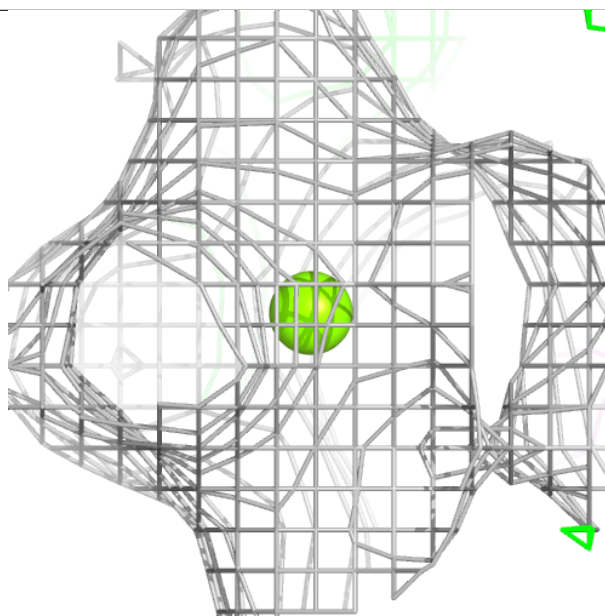
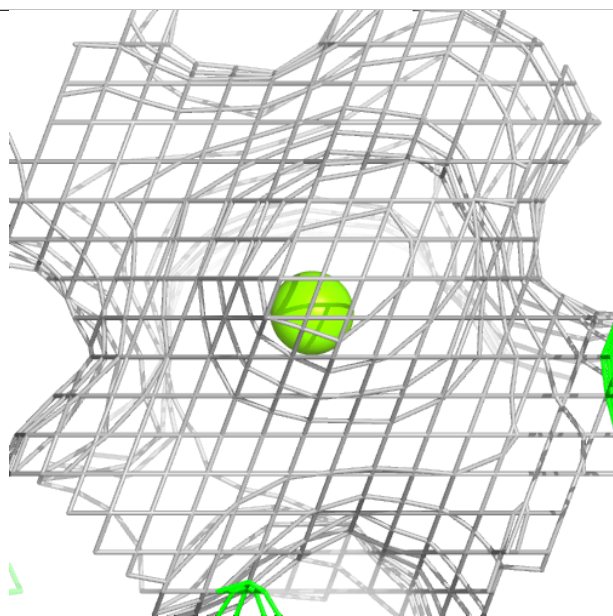
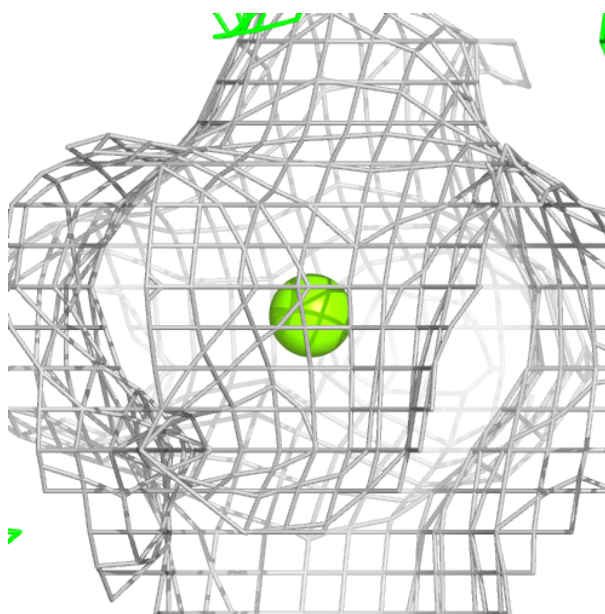
**Electron density around ATP A 402:**

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



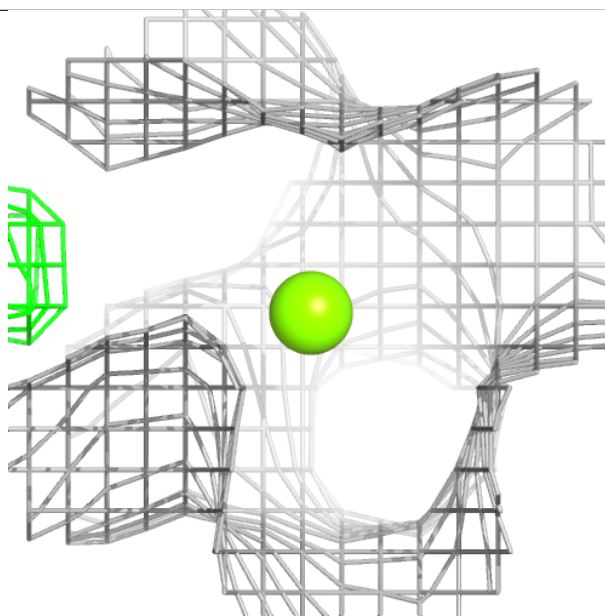
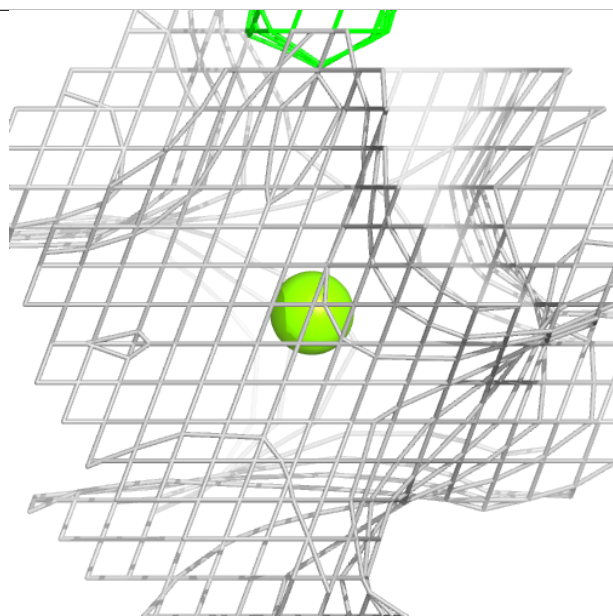
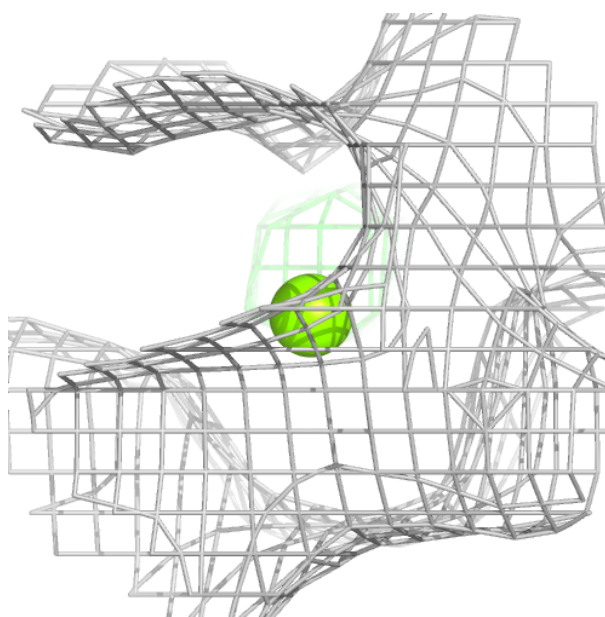
Electron density around MG A 403:

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



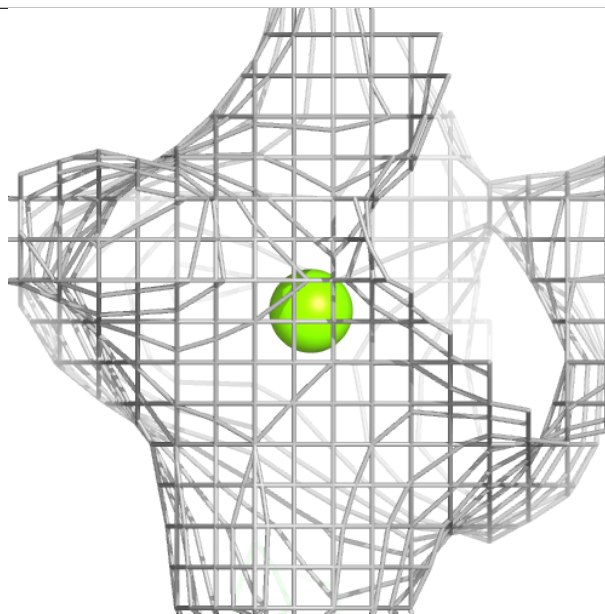
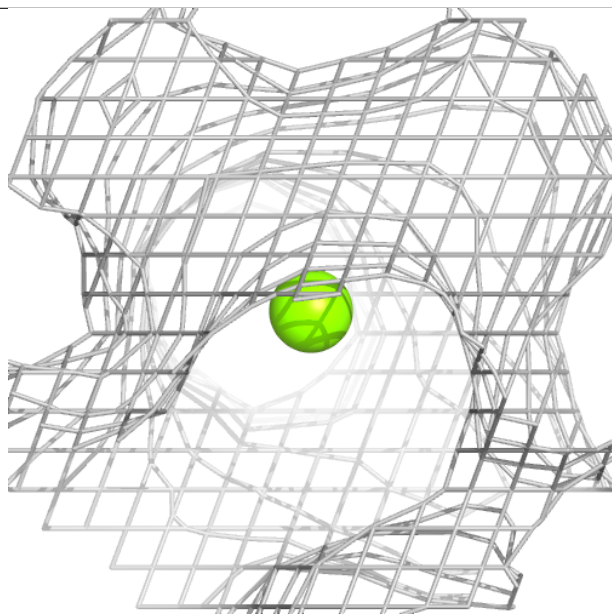
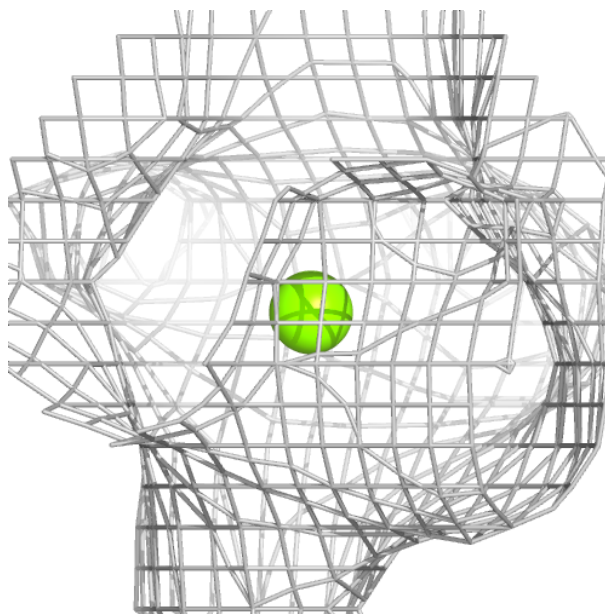
Electron density around MG D 1103:

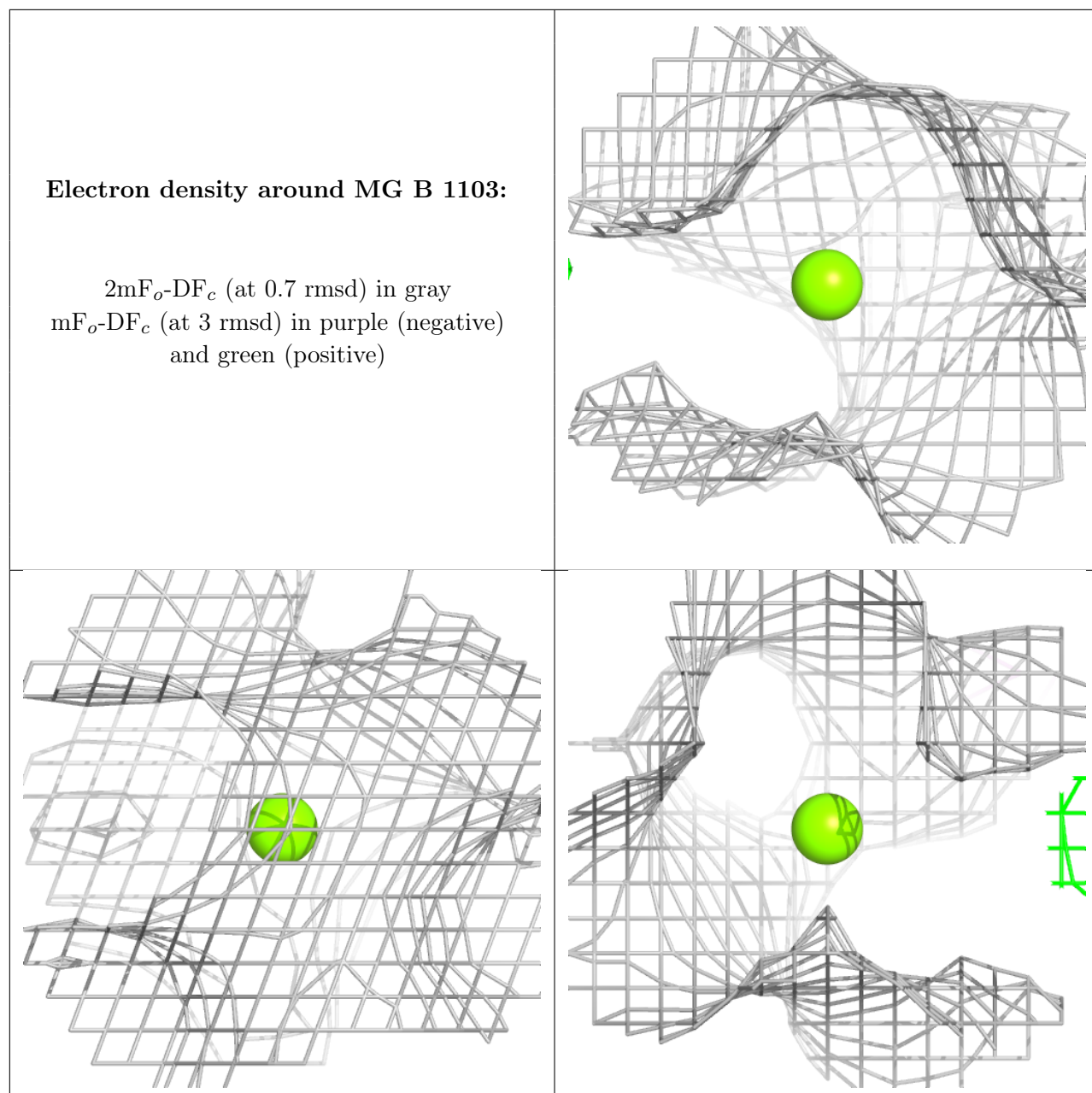
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MG C 402:

$2mF_o-DF_c$ (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.