



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 09:56 PM UTC

PDB ID : 8BR0 / pdb_00008br0
Title : ExoY Nucleotidyl Cyclase domain from *Vibrio nigripulchritudo* MARTX toxin (residue Q3455 to L3863) in complex with 3'deoxyCTP and two manganese cations bound to Latrunculin-B-ADP-Mn-actin
Authors : Texeira-Nuns, M.; Retailleau, P.; Renault, L.
Deposited on : 2022-11-22
Resolution : 2.22 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

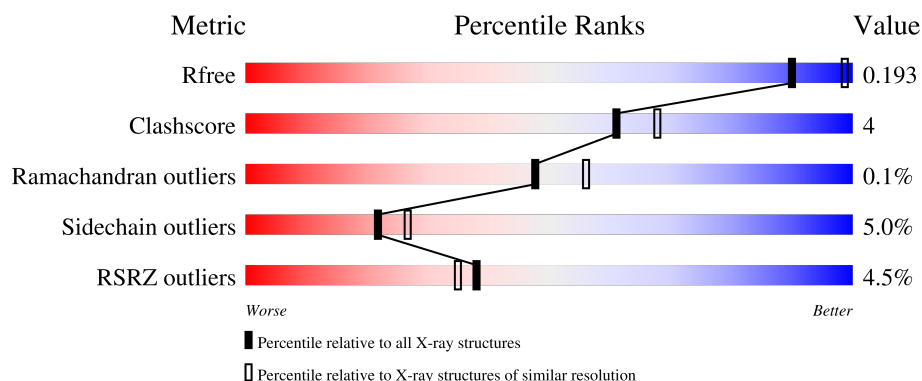
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.22 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	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

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	3% 84% 10% 6%
1	C	375	7% 88% 9% ..
2	B	591	3% 57% 10% 33%
2	D	591	3% 58% 9% 33%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12638 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	354	Total	C	N	O	S	0	1	0
			2768	1757	461	532	18			
1	C	365	Total	C	N	O	S	0	1	0
			2858	1811	481	547	19			

- Molecule 2 is a protein called Putative Adenylate cyclase, Profilin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	398	Total	C	N	O	S	0	0	0
			3144	1992	519	624	9			
2	D	398	Total	C	N	O	S	0	1	0
			3157	1998	524	626	9			

There are 20 discrepancies between the modelled and reference sequences:

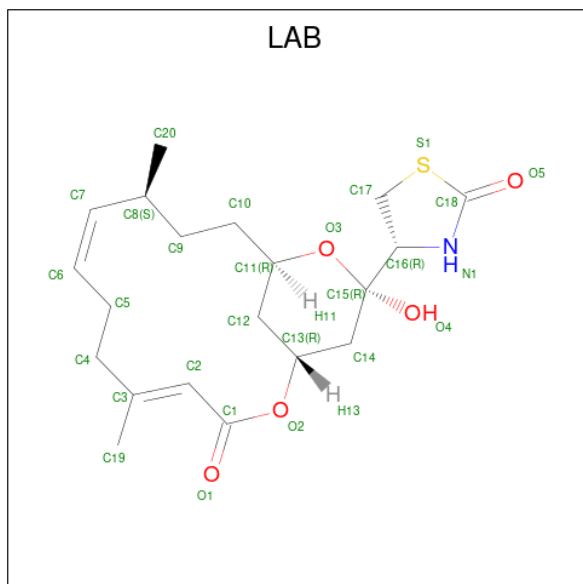
Chain	Residue	Modelled	Actual	Comment	Reference
B	451	GLY	-	expression tag	UNP A0A6N3LUE9
B	452	PRO	-	expression tag	UNP A0A6N3LUE9
B	453	GLY	-	expression tag	UNP A0A6N3LUE9
B	454	SER	-	expression tag	UNP A0A6N3LUE9
B	897	PRO	-	linker	UNP A0A6N3LUE9
B	898	PRO	-	linker	UNP A0A6N3LUE9
B	899	PRO	-	linker	UNP A0A6N3LUE9
B	900	PRO	-	linker	UNP A0A6N3LUE9
B	901	GLY	-	linker	UNP A0A6N3LUE9
B	902	GLY	-	linker	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
D	897	PRO	-	linker	UNP A0A6N3LUE9
D	898	PRO	-	linker	UNP A0A6N3LUE9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	899	PRO	-	linker	UNP A0A6N3LUE9
D	900	PRO	-	linker	UNP A0A6N3LUE9
D	901	GLY	-	linker	UNP A0A6N3LUE9
D	902	GLY	-	linker	UNP A0A6N3LUE9

- Molecule 3 is LATRUNCULIN B (CCD ID: LAB) (formula: $C_{20}H_{29}NO_5S$) (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'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

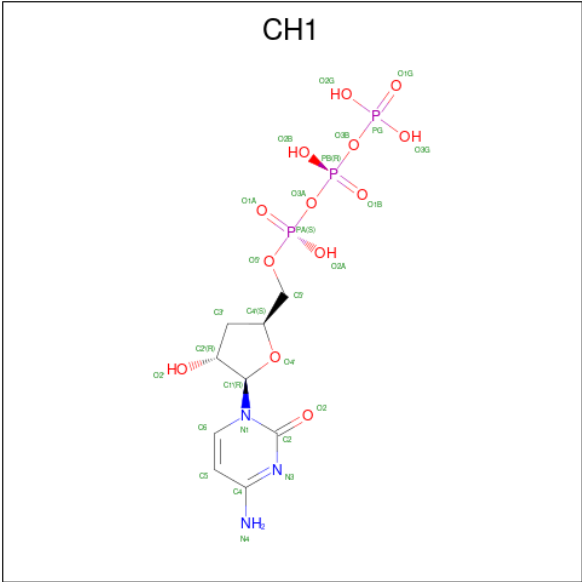


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
4	C	1	Total 27	C 10	N 5	O 10	P 2	0	0

- Molecule 5 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 6 is 3'-DEOXY-CYTIDINE-5'-TRIPHOSPHATE (CCD ID: CH1) (formula: $\text{C}_9\text{H}_{16}\text{N}_3\text{O}_{13}\text{P}_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	0	0
			28	9	3	13	3		
6	D	1	Total	C	N	O	P	0	0
			28	9	3	13	3		

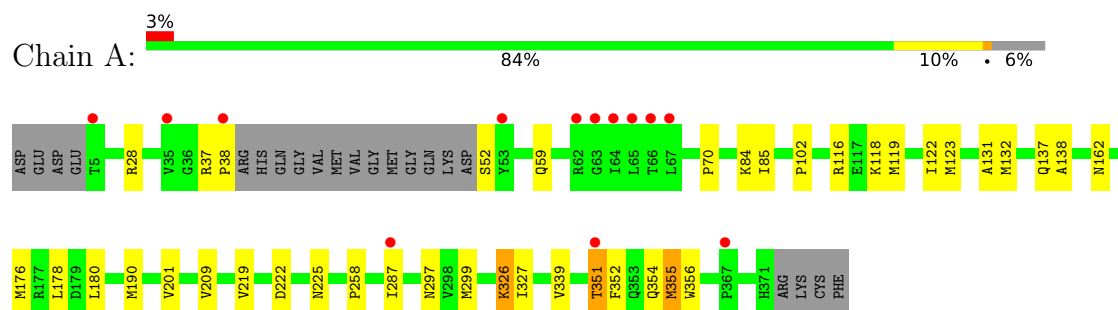
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	147	Total	O	0	0
			147	147		
7	B	132	Total	O	0	0
			132	132		
7	C	71	Total	O	0	0
			71	71		
7	D	191	Total	O	0	0
			191	191		

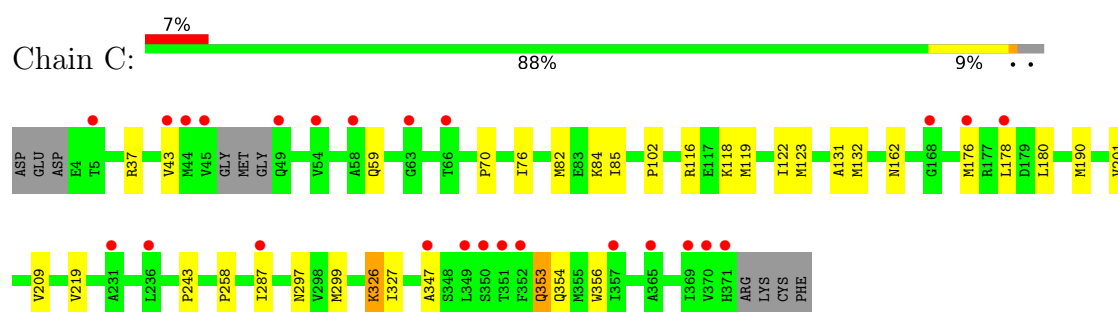
3 Residue-property plots

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.

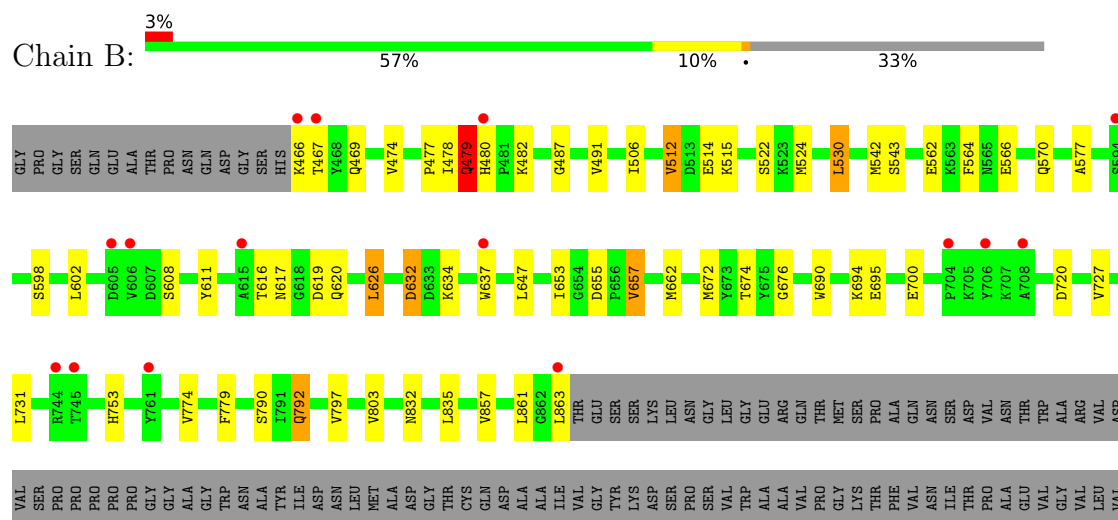
- Molecule 1: Actin, alpha skeletal muscle, intermediate form



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



- Molecule 2: Putative Adenylate cyclase, Profilin-1



GLY	LYS	ASP	GLY	SER	PHE	TYR	VAL	ASN	GLY	LEU	THR	LEU	GLY	GLN	LYS	CYS	SER	VAL	ILE	ARG	ASP	SER	LEU	GLN	ASP	GLY	GLU	PHE	SER	MET	ASP	LEU	ARG	THR	LYS	THR	GLY	GLY	ALA	PRO	THR	PHE	ASN	VAL	THR	VAL	THR	LYS	THR	LYS	ASP	LYS	THR	LEU	VAL	LEU
LEU	MET	GLY	LYS	GLY	VAL	HIS	GLY	GLY	ASN	LEU	ILE	ASP	ASN	LYS	CYS	TYR	GLY	ALA	SER	HIS	LEU	ARG	SER	LEU	GLN	ASP	GLY	PHE	SER	MET	ASP	LEU	ARG	THR	LYS	THR	GLY	GLY	ALA	PRO	THR	PHE	ASN	VAL	THR	VAL	THR	LYS	THR	LYS	ASP	LYS	THR	LEU	VAL	LEU

● Molecule 2: Putative Adenylate cyclase,Profilin-1



LEU	ARG	ARG	SER	GLN	TYR																					N832	S833	G834	L835	E590	S598	L602	E603	L604	D605	V606	D607	S608	G609	M610	Y611	L626	V631	M637	L647	I653	G654	D655	M662	T674	M690	E691	K694	E695	P704	K718	Q719	D720	L731	H753	V774	F779	S790	I791	Q792	V797	W803	A577
ARG	ASP	GLY	THR	GLN	ALA	ASP	GLY	ILE	VAL	GLY	TYR	LYS	ASP	SER	LEU	PRO	SER	THR	LYS	THR	PHE	ASN	VAL	THR	VAL	ILE	THR	PRO	ALA	ASP	GLY	VAL	VAL	GLY	LYS	ASP	ARG	SER	PRO	PRO	PHE	THR	ASN	THR	LEU	GLY	LYS	GLY	TYR	ILE	ASP	ASN	VAL	THR	ILE													
LEU	ARG	ARG	SER	GLN	TYR	ASP	GLN	GLY	GLY	PHE	SER	MET	ASP	LEU	ARG	THR	LYS	THR	THR	GLY	ALA	VAL	GLY	VAL	VAL	PRO	GLY	THR	LYS	THR	ASN	VAL	THR	THR	THR	VAL	VAL	GLY	LYS	ASP	ARG	SER	PRO	PRO	GLY	ASN	ALA	GLY	THR	TRP	ASN	ALA	TYR	ILE	ASP													

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.47Å 132.50Å 96.22Å 90.00° 110.40° 90.00°	Depositor
Resolution (Å)	48.05 – 2.22 48.05 – 2.22	Depositor EDS
% Data completeness (in resolution range)	71.8 (48.05-2.22) 71.7 (48.05-2.22)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.22Å)	Xtriage
Refinement program	BUSTER 2.10.4 (3-FEB-2022)	Depositor
R, R_{free}	0.208 , 0.243 0.197 , 0.193	Depositor DCC
R_{free} test set	3203 reflections (3.70%)	wwPDB-VP
Wilson B-factor (Å ²)	53.4	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.016 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12638	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LAB, ADP, CH1, MN

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	0.73	0/2831	1.03	1/3841 (0.0%)
1	C	0.70	1/2922 (0.0%)	1.02	0/3961
2	B	0.73	0/3212	1.06	2/4353 (0.0%)
2	D	0.75	0/3229	1.05	3/4375 (0.1%)
All	All	0.73	1/12194 (0.0%)	1.04	6/16530 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	37	ARG	CA-C	5.12	1.59	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	608	SER	N-CA-C	-6.13	104.53	112.68
1	A	352	PHE	N-CA-C	-6.11	106.16	113.97
2	D	720	ASP	CA-CB-CG	5.76	118.36	112.60
2	B	720	ASP	CA-CB-CG	5.24	117.83	112.60
2	D	525	TYR	N-CA-C	5.12	118.08	109.95
2	B	564	PHE	CA-CB-CG	-5.07	108.73	113.80

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	2768	0	2738	27	0
1	C	2858	0	2828	21	0
2	B	3144	0	3056	30	0
2	D	3157	0	3070	26	0
3	A	27	0	29	4	0
3	C	27	0	29	4	0
4	A	27	0	12	0	0
4	C	27	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	28	0	12	0	0
6	D	28	0	12	0	0
7	A	147	0	0	3	0
7	B	132	0	0	0	0
7	C	71	0	0	0	0
7	D	191	0	0	0	0
All	All	12638	0	11798	101	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 4.

All (101) 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)
2:B:479:GLN:HG2	2:B:480:HIS:H	1.44	0.81
2:B:479:GLN:H	2:B:479:GLN:CD	1.96	0.74
2:B:530:LEU:HD13	2:B:753:HIS:CD2	2.26	0.71
2:D:530:LEU:HD13	2:D:753:HIS:CD2	2.27	0.70
1:C:59:GLN:HG3	3:C:401:LAB:C7	2.24	0.67
1:C:59:GLN:HG3	3:C:401:LAB:H7	1.78	0.65
2:D:655:ASP:HA	2:D:662:MET:HE3	1.78	0.65
2:D:515:LYS:HE2	2:D:543[A]:SER:OG	1.96	0.65
1:A:59:GLN:HG3	3:A:401:LAB:C7	2.30	0.62
2:B:515:LYS:HE2	2:B:543:SER:OG	1.99	0.61
3:A:401:LAB:H11	3:A:401:LAB:H51	1.84	0.60
1:A:70:PRO:HG2	1:A:85:ILE:HD12	1.85	0.59
1:C:162:ASN:HB2	1:C:176:MET:HB2	1.84	0.59
2:B:655:ASP:HA	2:B:662:MET:HE3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:ASN:HB2	1:A:176:MET:HB2	1.84	0.58
1:C:70:PRO:HG2	1:C:85:ILE:HD12	1.85	0.57
1:A:131:ALA:HB1	1:A:356:TRP:HB3	1.87	0.57
1:C:116:ARG:HA	1:C:119:MET:HG2	1.85	0.57
1:A:116:ARG:HA	1:A:119:MET:HG2	1.87	0.56
1:A:351:THR:HB	2:B:863:LEU:HA	1.89	0.55
1:A:222:ASP:OD2	1:A:225[B]:ASN:ND2	2.37	0.55
2:B:469:GLN:HG2	2:B:474:VAL:HG22	1.89	0.55
2:D:469:GLN:HG2	2:D:474:VAL:HG22	1.89	0.54
1:A:326:LYS:NZ	1:A:327:ILE:H	2.06	0.54
2:B:797:VAL:HG22	2:B:803:VAL:HG22	1.90	0.53
1:C:326:LYS:NZ	1:C:327:ILE:H	2.07	0.53
2:B:602:LEU:HB3	2:B:611:TYR:HB3	1.91	0.53
1:A:219:VAL:HG22	1:A:258:PRO:HB2	1.90	0.52
1:C:131:ALA:HB1	1:C:356:TRP:HB3	1.89	0.52
1:C:326:LYS:HZ2	1:C:326:LYS:HA	1.75	0.52
1:C:219:VAL:HG22	1:C:258:PRO:HB2	1.92	0.52
2:D:797:VAL:HG22	2:D:803:VAL:HG22	1.91	0.51
2:B:466:LYS:HG2	2:B:477:PRO:HG2	1.90	0.51
1:A:190:MET:HG3	1:A:209:VAL:HG11	1.93	0.51
2:D:604:LEU:HG	2:D:611:TYR:CZ	2.45	0.50
1:C:190:MET:HG3	1:C:209:VAL:HG11	1.94	0.50
1:C:353:GLN:O	1:C:353:GLN:HG3	2.11	0.50
2:B:655:ASP:OD1	2:B:657:VAL:HG13	2.12	0.49
1:C:243:PRO:O	2:D:704:PRO:HD3	2.12	0.49
1:A:351:THR:HB	2:B:863:LEU:HB3	1.94	0.48
2:D:779:PHE:HA	2:D:792:GLN:OE1	2.12	0.48
2:D:604:LEU:HD22	2:D:608:SER:O	2.14	0.48
1:A:326:LYS:HZ1	1:A:327:ILE:H	1.62	0.48
2:B:617:ASN:HD21	2:B:620:GLN:HG3	1.79	0.48
2:D:506:ILE:HG12	2:D:774:VAL:HG12	1.96	0.47
2:B:779:PHE:HA	2:B:792:GLN:OE1	2.13	0.47
2:B:790:SER:HB2	2:B:792:GLN:OE1	2.15	0.47
2:B:832:ASN:HA	2:B:835:LEU:HD22	1.97	0.47
2:D:606:VAL:HB	2:D:609:GLY:HA3	1.97	0.47
2:D:790:SER:HB2	2:D:792:GLN:OE1	2.15	0.47
2:B:487:GLY:HA3	2:B:512:VAL:HG22	1.97	0.47
1:A:326:LYS:HZ2	1:A:326:LYS:HA	1.79	0.47
2:D:608:SER:O	2:D:609:GLY:C	2.58	0.47
2:B:626:LEU:HB3	2:B:637:TRP:HB3	1.96	0.46
2:D:577:ALA:HB1	2:D:653:ILE:HG23	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:626:LEU:HB3	2:D:637:TRP:HB3	1.97	0.46
1:A:28:ARG:HG2	7:A:546:HOH:O	2.15	0.46
2:D:487:GLY:HA2	2:D:514:GLU:HA	1.98	0.46
1:A:118:LYS:HE3	1:A:122:ILE:HD11	1.98	0.45
2:D:605:ASP:O	2:D:606:VAL:C	2.58	0.45
2:D:832:ASN:HA	2:D:835:LEU:HD22	1.97	0.45
1:C:70:PRO:HG2	1:C:85:ILE:CD1	2.46	0.45
2:B:479:GLN:HG2	2:B:480:HIS:N	2.23	0.45
1:A:123:MET:HG3	1:A:132:MET:HE3	1.99	0.45
1:A:138:ALA:HA	7:A:506:HOH:O	2.16	0.45
1:C:102:PRO:HB3	1:C:131:ALA:HB3	1.98	0.45
2:B:577:ALA:HB1	2:B:653:ILE:HG23	1.98	0.45
1:C:123:MET:HG3	1:C:132:MET:HE3	1.99	0.45
2:D:607:ASP:HB2	2:D:608:SER:H	1.62	0.44
2:B:506:ILE:HG12	2:B:774:VAL:HG12	1.98	0.44
1:A:59:GLN:HG3	3:A:401:LAB:H7	1.97	0.44
1:C:59:GLN:HB2	3:C:401:LAB:H7	2.00	0.44
2:B:487:GLY:HA2	2:B:514:GLU:HA	2.00	0.43
1:C:347:ALA:HA	1:C:353:GLN:NE2	2.33	0.43
1:A:70:PRO:HG2	1:A:85:ILE:CD1	2.47	0.43
1:A:102:PRO:HB3	1:A:131:ALA:HB3	1.99	0.43
1:C:178:LEU:HG	1:C:180:LEU:HB3	2.00	0.43
2:B:857:VAL:HG13	2:B:861:LEU:HD12	2.00	0.43
1:A:351:THR:HB	2:B:863:LEU:CB	2.49	0.42
2:D:487:GLY:HA3	2:D:512:VAL:HG22	2.01	0.42
1:A:178:LEU:HG	1:A:180:LEU:HB3	2.01	0.42
2:D:482:LYS:HG3	2:D:484:ILE:HD11	2.02	0.42
1:C:118:LYS:HE3	1:C:122:ILE:HD11	2.01	0.42
1:C:326:LYS:HZ1	1:C:327:ILE:H	1.68	0.41
2:D:690:TRP:CE2	2:D:694:LYS:HD2	2.55	0.41
1:C:76:ILE:HD13	1:C:82:MET:HG2	2.03	0.41
3:C:401:LAB:H52	3:C:401:LAB:H11	2.01	0.41
1:A:59:GLN:HB2	3:A:401:LAB:H7	2.03	0.41
1:A:38:PRO:HG3	1:A:52:SER:N	2.36	0.41
7:A:543:HOH:O	2:B:676:GLY:HA2	2.21	0.41
2:B:506:ILE:HB	2:B:672:MET:HB2	2.03	0.41
2:B:632:ASP:HB2	2:B:634:LYS:HE3	2.03	0.41
2:D:606:VAL:O	2:D:609:GLY:N	2.54	0.41
1:A:137:GLN:HG2	1:A:339:VAL:HG11	2.03	0.41
2:B:522:SER:HB2	2:B:524:MET:HE3	2.03	0.41
2:D:604:LEU:HG	2:D:611:TYR:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:THR:HB	2:B:863:LEU:CA	2.49	0.40
1:A:355:MET:HE3	1:A:355:MET:HB3	1.99	0.40
2:B:690:TRP:CE2	2:B:694:LYS:HD2	2.56	0.40
2:D:510:ARG:HB3	2:D:511:PRO:HD2	2.03	0.40
2:D:522:SER:HB2	2:D:524:MET:HE3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	351/375 (94%)	338 (96%)	13 (4%)	0	100	100
1	C	362/375 (96%)	348 (96%)	14 (4%)	0	100	100
2	B	396/591 (67%)	385 (97%)	10 (2%)	1 (0%)	36	41
2	D	397/591 (67%)	382 (96%)	14 (4%)	1 (0%)	36	41
All	All	1506/1932 (78%)	1453 (96%)	51 (3%)	2 (0%)	48	56

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	609	GLY
2	B	479	GLN

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	301/318 (95%)	291 (97%)	10 (3%)	33	44
1	C	310/318 (98%)	301 (97%)	9 (3%)	37	49
2	B	345/504 (68%)	320 (93%)	25 (7%)	13	14
2	D	348/504 (69%)	327 (94%)	21 (6%)	17	20
All	All	1304/1644 (79%)	1239 (95%)	65 (5%)	22	27

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ARG
1	A	84	LYS
1	A	201	VAL
1	A	287	ILE
1	A	297	ASN
1	A	299	MET
1	A	326	LYS
1	A	351	THR
1	A	354	GLN
1	A	355	MET
2	B	467	THR
2	B	478	ILE
2	B	479	GLN
2	B	482	LYS
2	B	491	VAL
2	B	512	VAL
2	B	530	LEU
2	B	542	MET
2	B	562	GLU
2	B	566	GLU
2	B	570	GLN
2	B	598	SER
2	B	608	SER
2	B	616	THR
2	B	619	ASP
2	B	626	LEU
2	B	632	ASP
2	B	647	LEU
2	B	657	VAL
2	B	674	THR
2	B	695	GLU

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Mol	Chain	Res	Type
2	B	700	GLU
2	B	727	VAL
2	B	731	LEU
2	B	792	GLN
1	C	43	VAL
1	C	84	LYS
1	C	201	VAL
1	C	287	ILE
1	C	297	ASN
1	C	299	MET
1	C	326	LYS
1	C	353	GLN
1	C	354	GLN
2	D	466	LYS
2	D	467	THR
2	D	479	GLN
2	D	491	VAL
2	D	512	VAL
2	D	530	LEU
2	D	542	MET
2	D	562	GLU
2	D	566	GLU
2	D	570	GLN
2	D	590	GLU
2	D	598	SER
2	D	603	GLU
2	D	607	ASP
2	D	626	LEU
2	D	647	LEU
2	D	674	THR
2	D	691	GLU
2	D	695	GLU
2	D	731	LEU
2	D	792	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	796	ASN
2	B	815	GLN
1	C	246	GLN
1	C	280	ASN

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Mol	Chain	Res	Type
1	C	353	GLN
2	D	640	HIS
2	D	712	ASN
2	D	719	GLN
2	D	796	ASN
2	D	800	GLN
2	D	815	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 6 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	$\# Z > 2$
3	LAB	A	401	-	28,29,29	0.87	1 (3%)	29,41,41	1.11	3 (10%)
3	LAB	C	401	-	28,29,29	0.85	1 (3%)	29,41,41	1.31	5 (17%)
6	CH1	D	1103	5	27,29,29	0.68	0	37,45,45	0.70	0
4	ADP	A	402	5	28,29,29	0.37	0	43,45,45	0.54	0
6	CH1	B	1103	5	27,29,29	0.68	1 (3%)	37,45,45	0.79	0
4	ADP	C	402	5	28,29,29	0.37	0	43,45,45	0.56	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LAB	A	401	-	-	4/21/49/49	0/2/3/3
3	LAB	C	401	-	-	6/21/49/49	0/2/3/3
6	CH1	D	1103	5	-	6/22/34/34	0/2/2/2
4	ADP	A	402	5	-	0/16/32/32	0/3/3/3
6	CH1	B	1103	5	-	7/22/34/34	0/2/2/2
4	ADP	C	402	5	-	0/16/32/32	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	4.38	1.62	1.54
3	C	401	LAB	C15-C16	4.25	1.62	1.54
6	B	1103	CH1	PG-O3G	-2.22	1.46	1.54

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	401	LAB	C3-C2-C1	3.25	135.12	127.36
3	C	401	LAB	C5-C6-C7	3.13	139.45	125.47
3	A	401	LAB	C3-C2-C1	2.79	134.03	127.36
3	A	401	LAB	C10-C9-C8	2.74	118.71	114.11
3	C	401	LAB	C10-C9-C8	2.65	118.57	114.11
3	C	401	LAB	O3-C15-C16	2.44	107.38	104.25
3	A	401	LAB	C14-C15-C16	-2.38	109.11	113.75
3	C	401	LAB	C14-C15-C16	-2.03	109.78	113.75

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	LAB	O3-C15-C16-C17
3	C	401	LAB	C5-C6-C7-C8
6	B	1103	CH1	PB-O3B-PG-O2G
6	B	1103	CH1	PB-O3B-PG-O3G
6	B	1103	CH1	C3'-C4'-C5'-O5'
6	D	1103	CH1	C3'-C4'-C5'-O5'
3	C	401	LAB	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
6	B	1103	CH1	C5'-O5'-PA-O1A
6	B	1103	CH1	O4'-C4'-C5'-O5'
6	B	1103	CH1	PA-O3A-PB-O2B
6	D	1103	CH1	PA-O3A-PB-O1B
6	D	1103	CH1	O4'-C4'-C5'-O5'
3	C	401	LAB	O2-C1-C2-C3
3	C	401	LAB	C19-C3-C4-C5
6	B	1103	CH1	C2'-C1'-N1-C6
6	D	1103	CH1	C2'-C1'-N1-C6
3	A	401	LAB	O2-C1-C2-C3
3	C	401	LAB	C11-C10-C9-C8
6	D	1103	CH1	PB-O3B-PG-O2G
3	C	401	LAB	O1-C1-C2-C3
3	A	401	LAB	C11-C10-C9-C8
3	A	401	LAB	C19-C3-C4-C5
6	D	1103	CH1	PA-O3A-PB-O2B

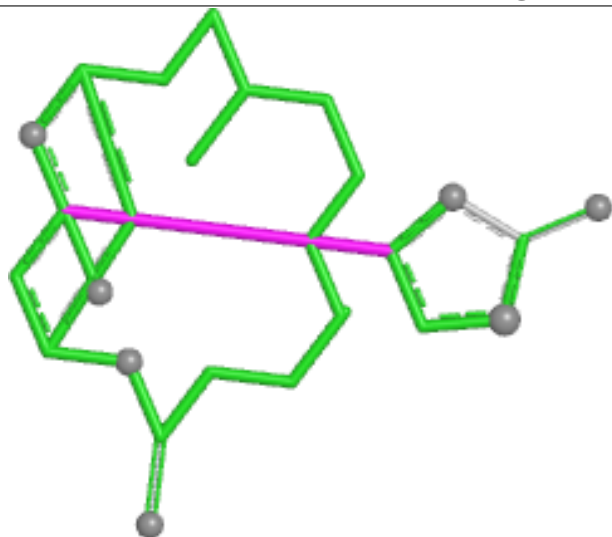
There are no ring outliers.

2 monomers are involved in 8 short contacts:

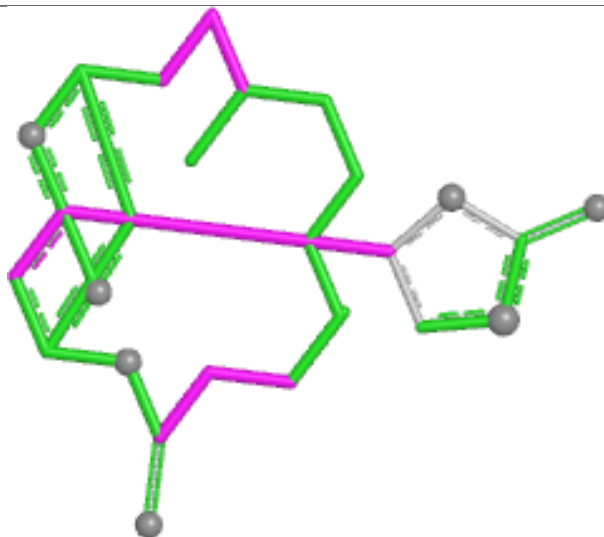
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	LAB	4	0
3	C	401	LAB	4	0

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.

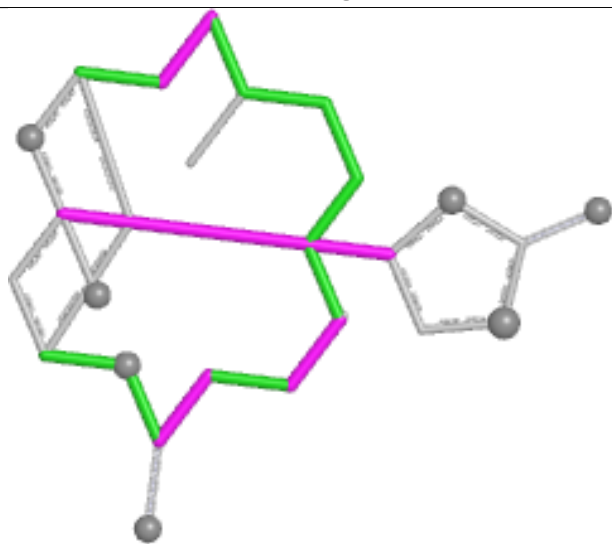
Ligand LAB A 401



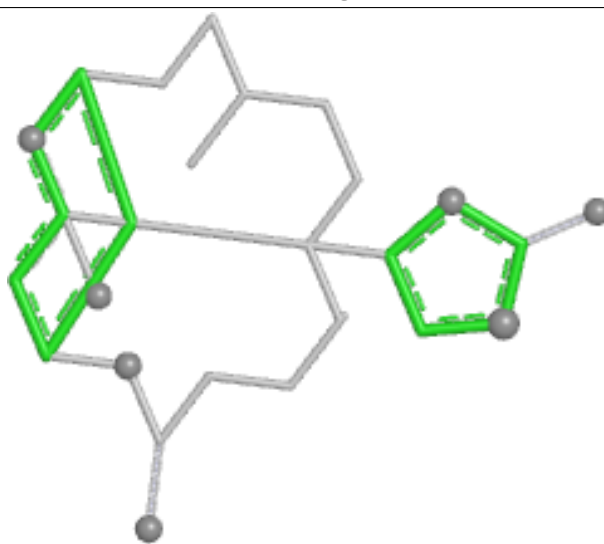
Bond lengths



Bond angles

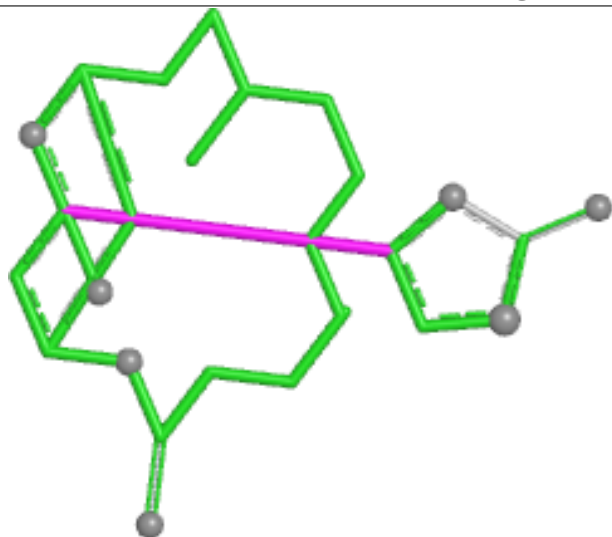


Torsions

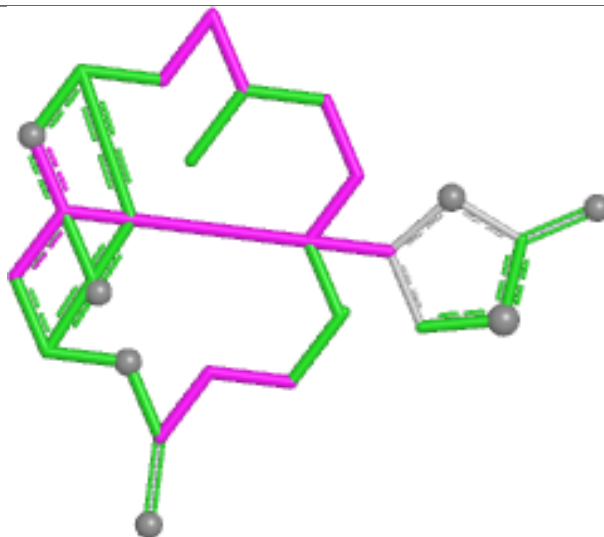


Rings

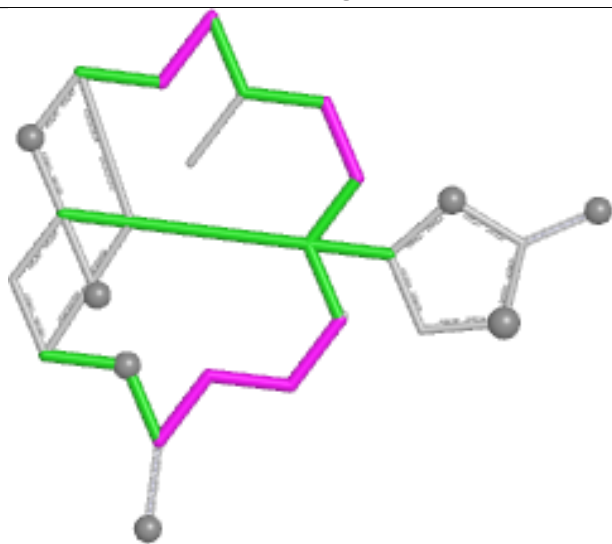
Ligand LAB C 401



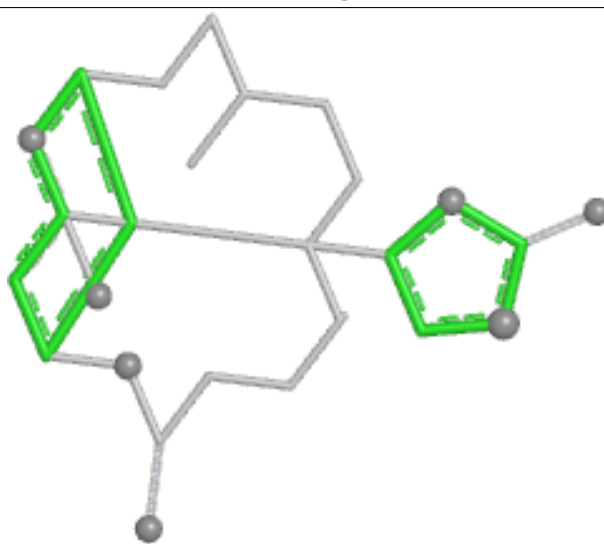
Bond lengths



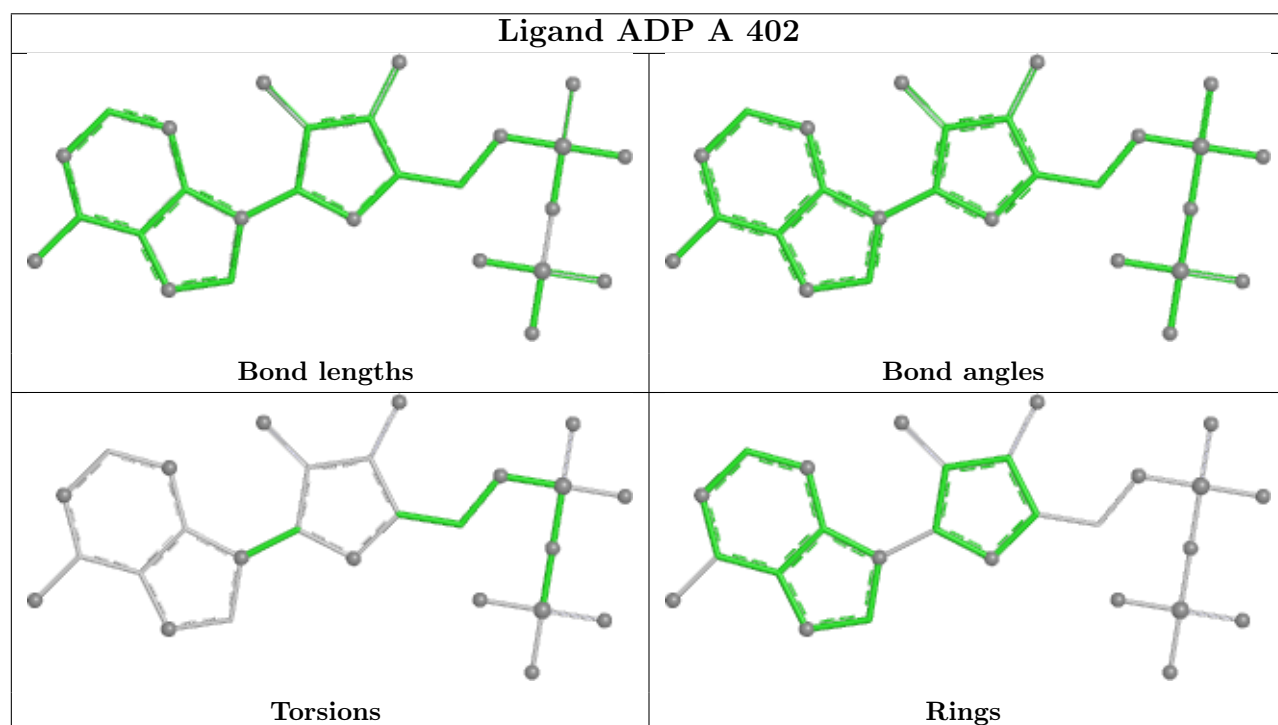
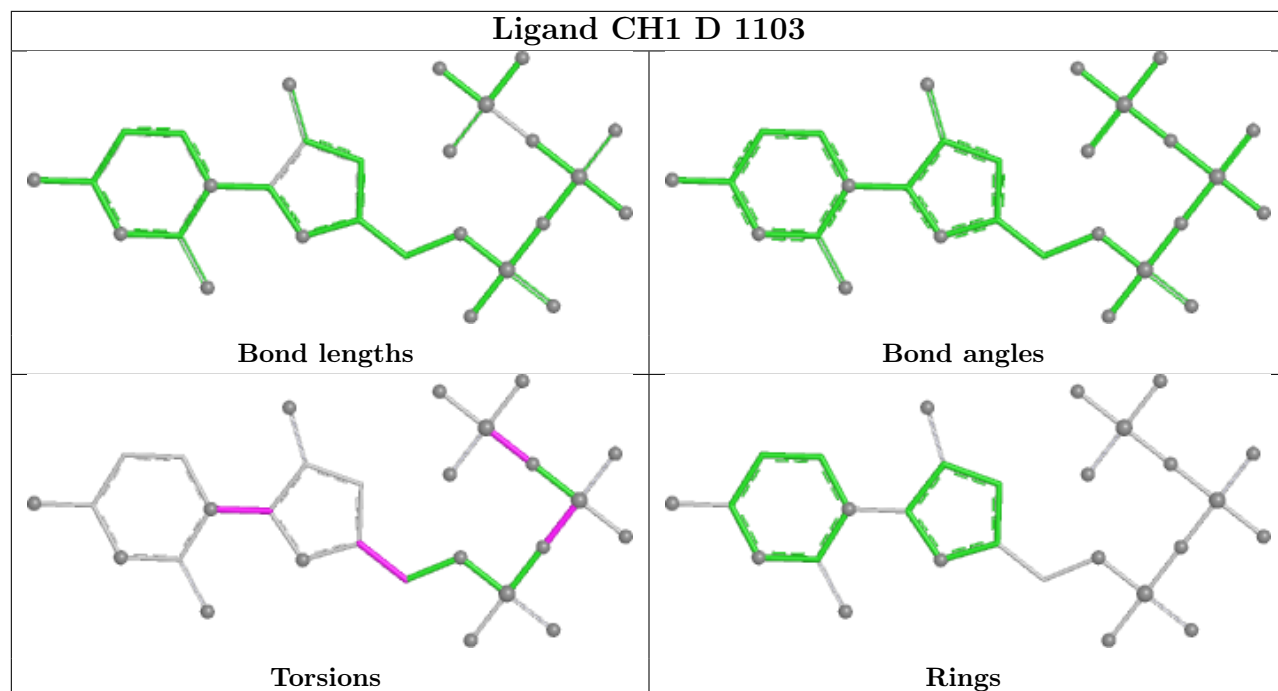
Bond angles

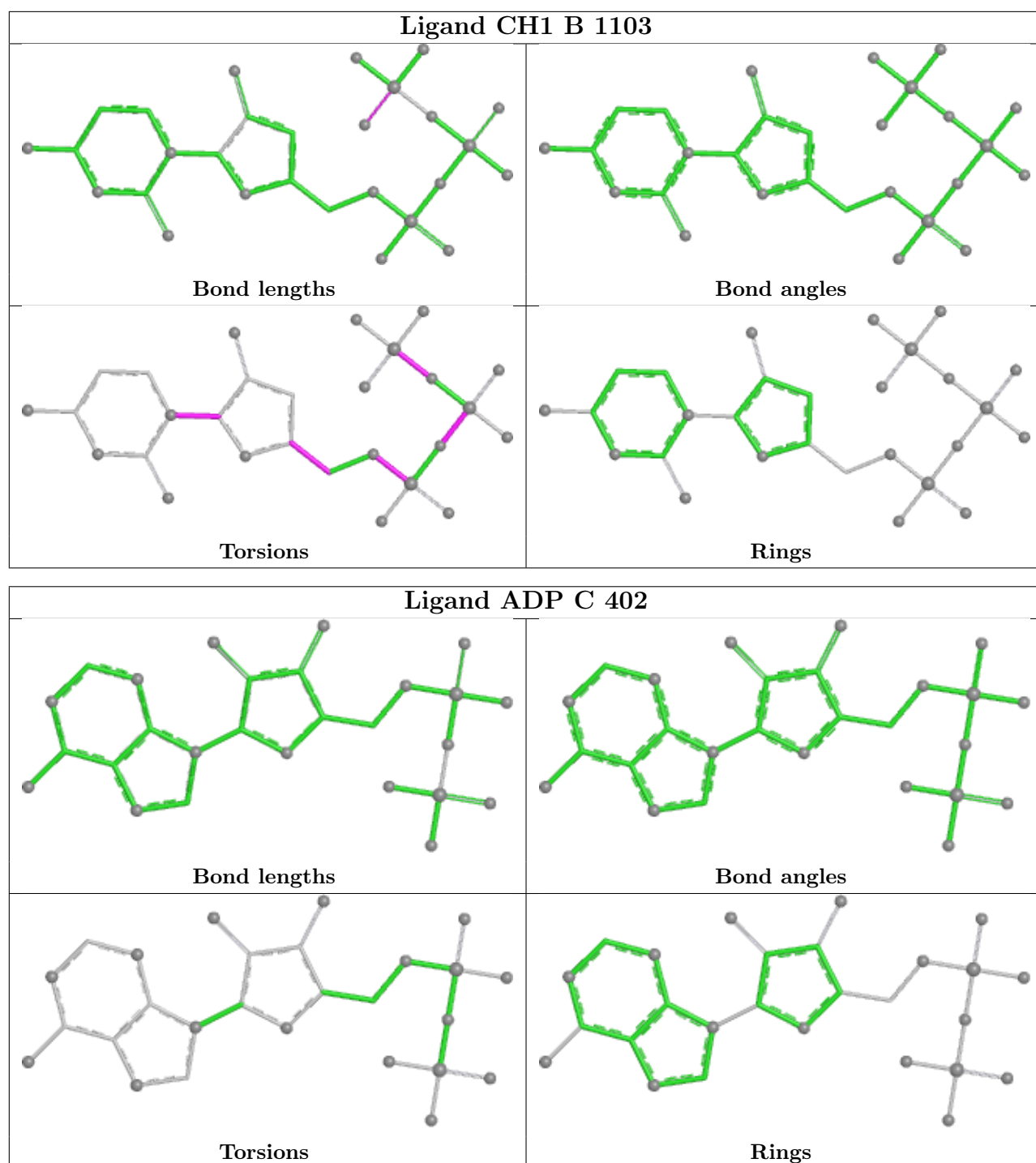


Torsions



Rings





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	354/375 (94%)	0.30	13 (3%)	45 42	31, 61, 104, 135	1 (0%)
1	C	365/375 (97%)	0.75	25 (6%)	23 20	46, 83, 137, 181	1 (0%)
2	B	398/591 (67%)	0.45	15 (3%)	44 41	38, 65, 120, 148	0
2	D	398/591 (67%)	0.31	15 (3%)	44 41	28, 59, 109, 130	1 (0%)
All	All	1515/1932 (78%)	0.45	68 (4%)	38 35	28, 67, 120, 181	3 (0%)

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	351	THR	4.9
1	A	64	ILE	4.6
2	D	606	VAL	4.4
1	C	45	VAL	4.3
2	B	606	VAL	4.2
1	C	352	PHE	3.9
1	C	43	VAL	3.9
2	D	609	GLY	3.9
2	D	464	SER	3.8
1	C	44	MET	3.7
2	B	708	ALA	3.7
1	C	350	SER	3.5
2	D	861	LEU	3.5
2	D	608	SER	3.3
1	C	347	ALA	3.3
1	A	38	PRO	3.2
1	C	5	THR	3.2
1	C	357	ILE	3.1
2	B	704	PRO	3.0
2	B	863	LEU	3.0
2	B	466	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	615	ALA	3.0
1	A	66	THR	3.0
2	B	706	TYR	3.0
1	C	49	GLN	2.9
1	C	231	ALA	2.9
1	C	236	LEU	2.9
2	D	479	GLN	2.9
1	A	62	ARG	2.8
1	A	5	THR	2.8
1	A	367	PRO	2.8
1	A	287	ILE	2.8
2	D	833	SER	2.7
1	A	67	LEU	2.7
2	B	745	THR	2.7
1	C	369	ILE	2.6
1	A	65	LEU	2.5
2	D	481	PRO	2.5
2	B	605	ASP	2.5
2	B	480	HIS	2.5
1	A	351	THR	2.4
1	C	287	ILE	2.4
1	C	63	GLY	2.3
1	C	365	ALA	2.3
1	C	370	VAL	2.3
2	B	637	TRP	2.3
2	B	467	THR	2.3
1	C	178	LEU	2.3
1	C	371	HIS	2.2
1	C	168	GLY	2.2
2	B	761	TYR	2.2
2	D	602	LEU	2.2
1	C	54	VAL	2.2
2	B	594	SER	2.2
1	C	66	THR	2.1
2	B	744	ARG	2.1
1	C	58	ALA	2.1
1	C	349	LEU	2.1
2	D	631	VAL	2.1
1	C	176	MET	2.1
2	D	480	HIS	2.1
1	A	63	GLY	2.1
2	D	478	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
2	D	484	ILE	2.0
1	A	53	TYR	2.0
1	A	35	VAL	2.0
2	D	718	LYS	2.0
2	D	637	TRP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

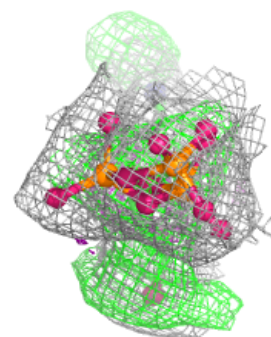
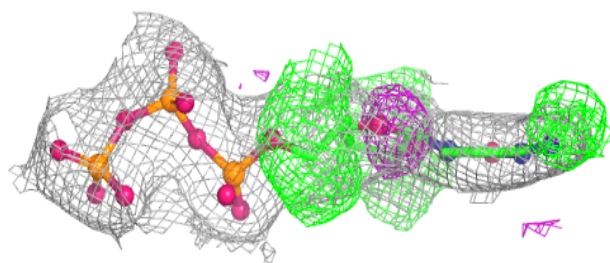
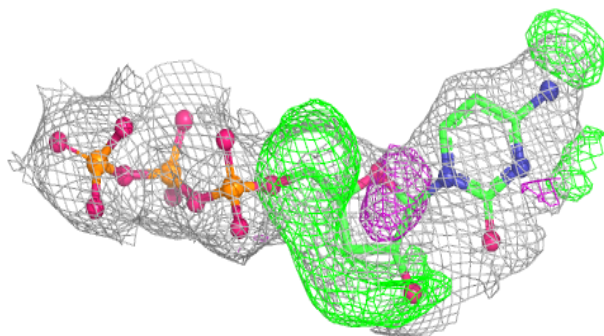
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	CH1	B	1103	28/28	0.87	0.13	53,56,65,65	0
6	CH1	D	1103	28/28	0.90	0.13	44,54,66,67	0
3	LAB	C	401	27/27	0.93	0.10	62,63,64,65	0
3	LAB	A	401	27/27	0.96	0.08	47,49,50,50	0
4	ADP	C	402	27/27	0.96	0.07	61,63,64,64	0
5	MN	D	1101	1/1	0.98	0.06	45,45,45,45	0
4	ADP	A	402	27/27	0.98	0.04	39,41,46,46	0
5	MN	C	403	1/1	0.98	0.05	90,90,90,90	0
5	MN	B	1101	1/1	0.99	0.03	54,54,54,54	0
5	MN	D	1102	1/1	0.99	0.02	45,45,45,45	0
5	MN	B	1102	1/1	0.99	0.07	54,54,54,54	0
5	MN	A	403	1/1	0.99	0.03	69,69,69,69	0

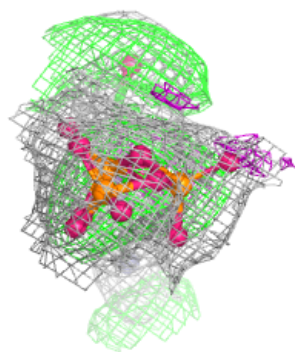
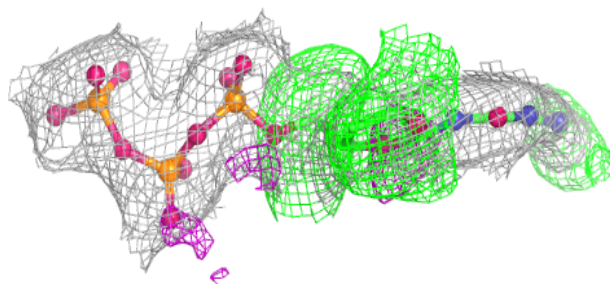
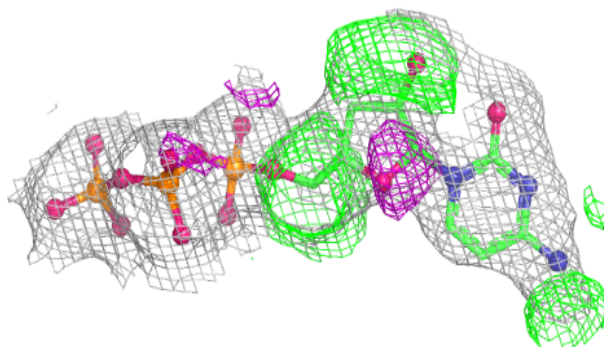
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around CH1 B 1103:

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

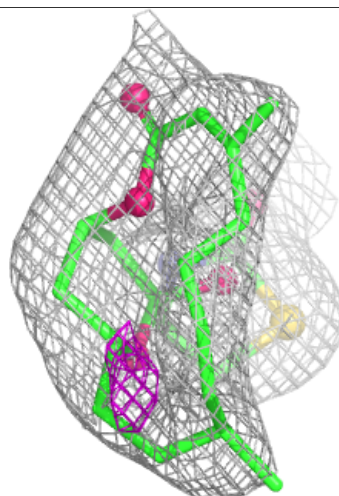
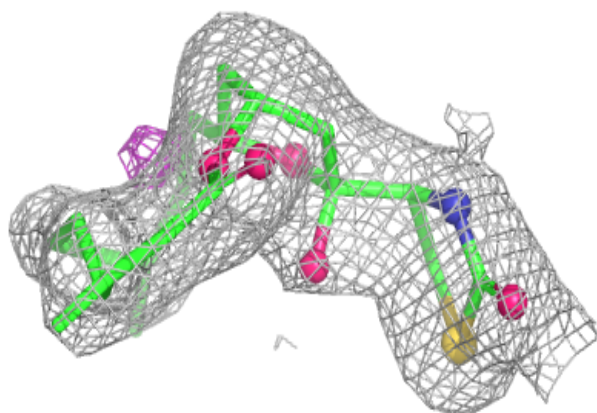
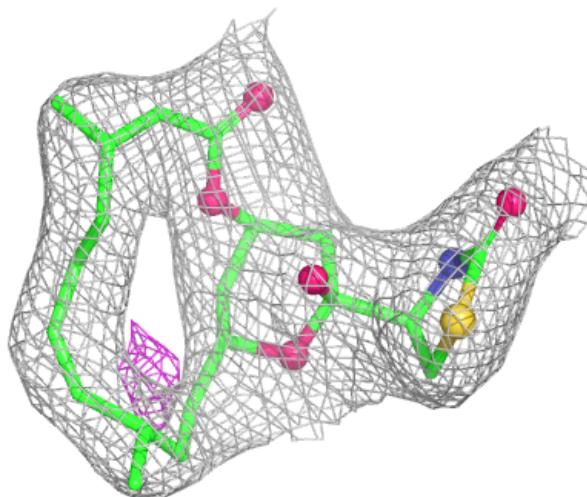
**Electron density around CH1 D 1103:**

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



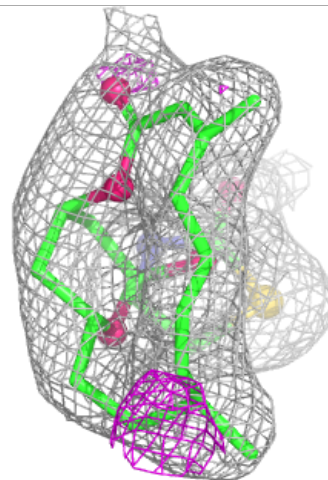
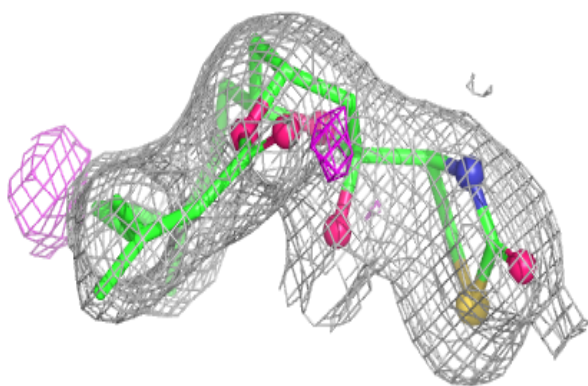
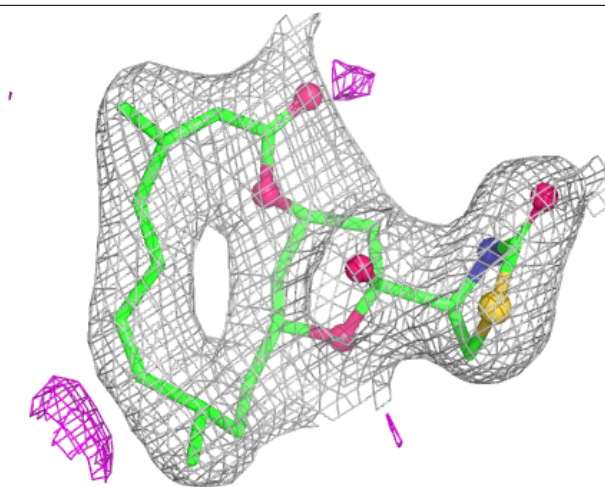
Electron density around LAB C 401:

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



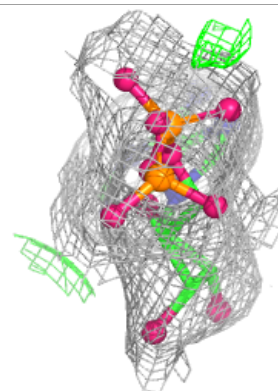
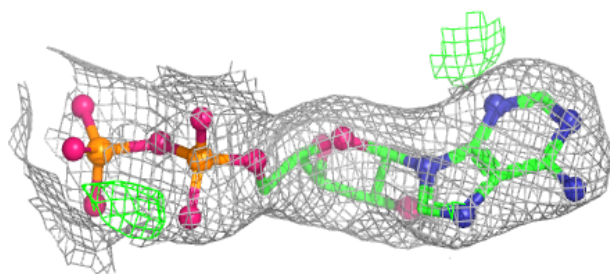
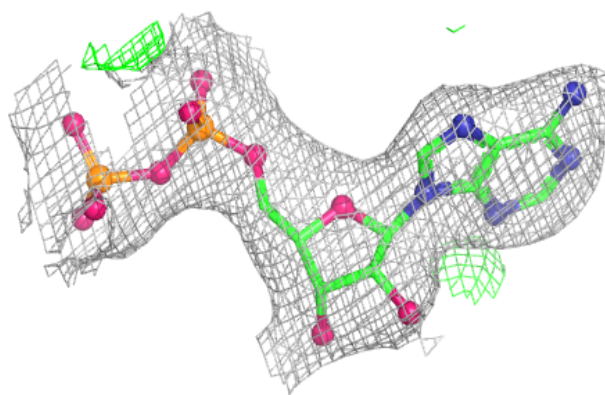
Electron density around LAB A 401:

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



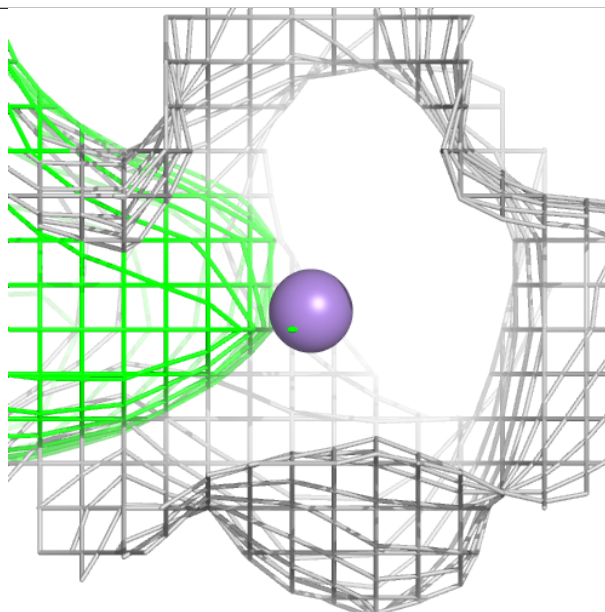
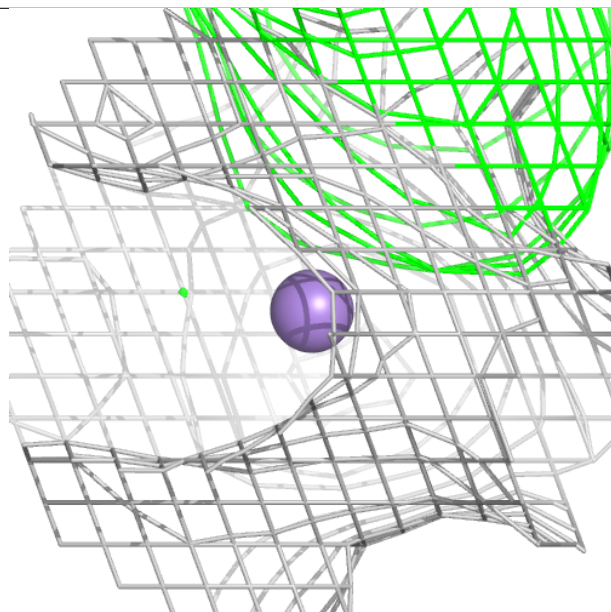
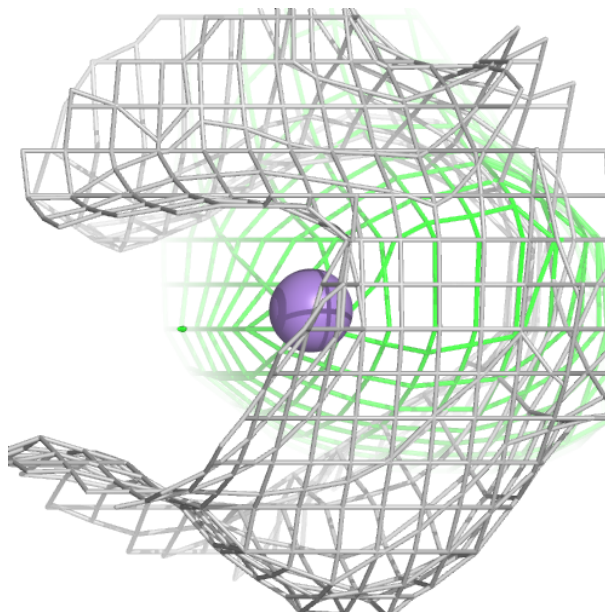
Electron density around ADP C 402:

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



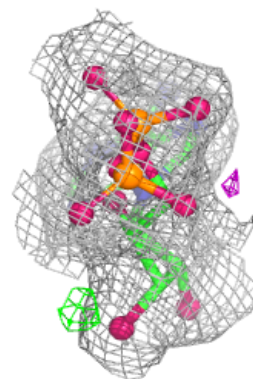
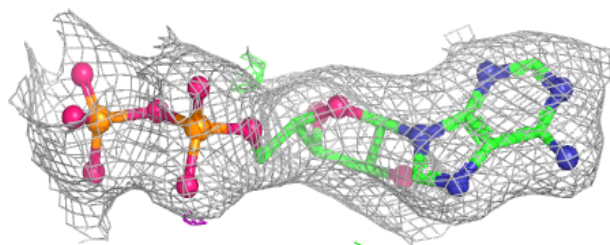
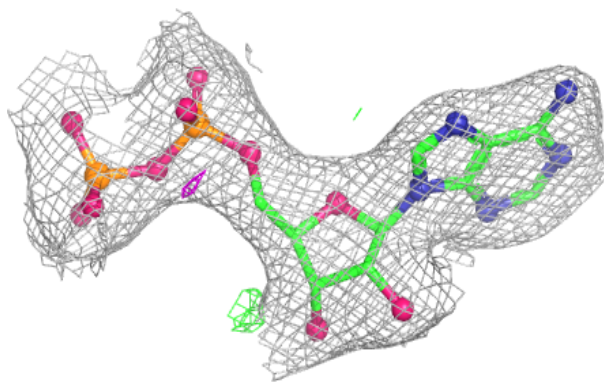
Electron density around MN D 1101:

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



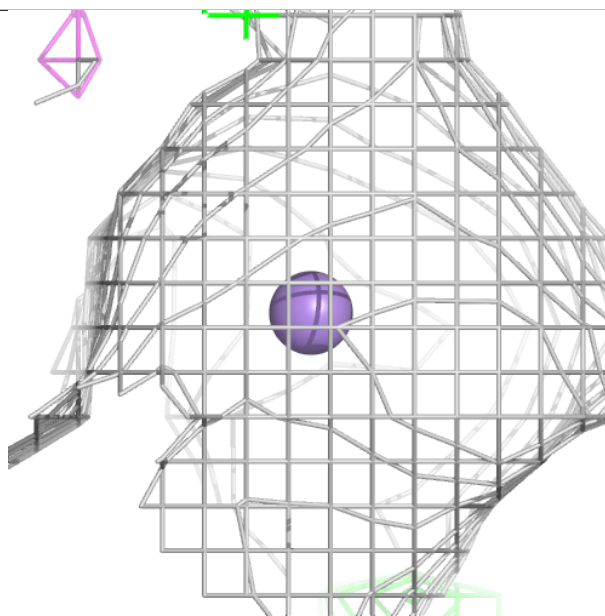
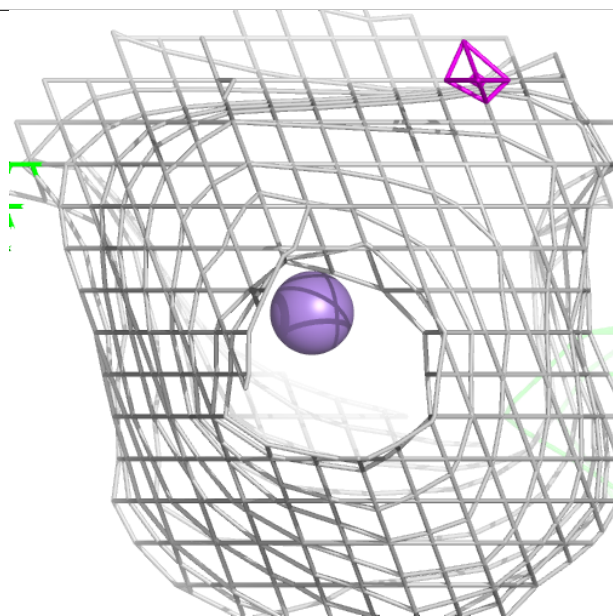
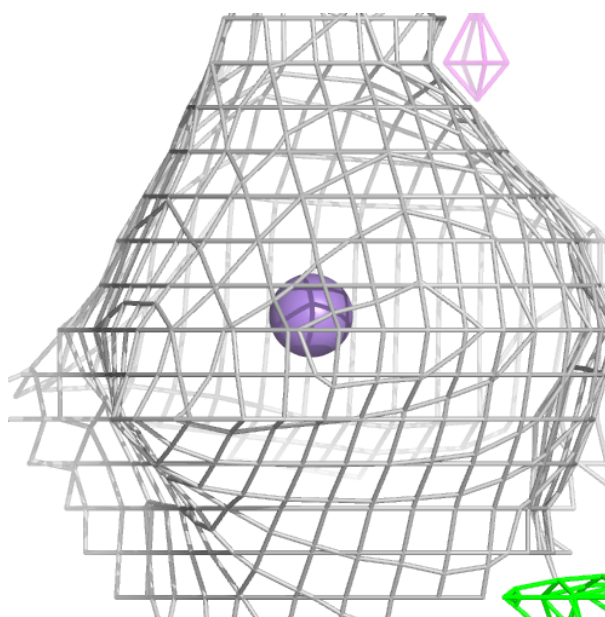
Electron density around ADP A 402:

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



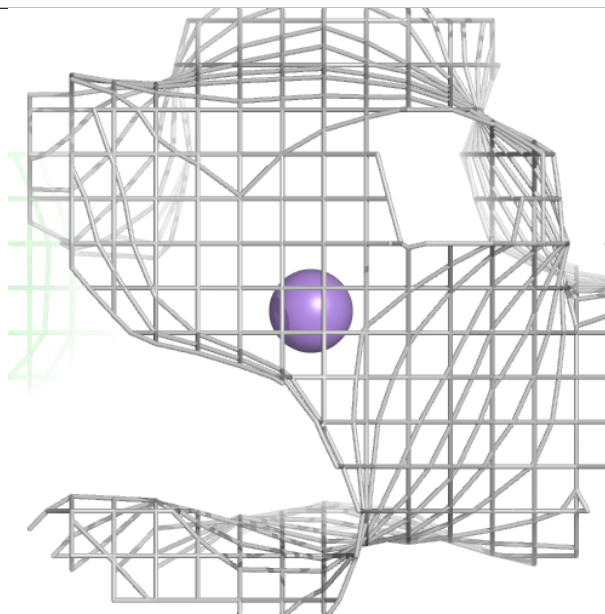
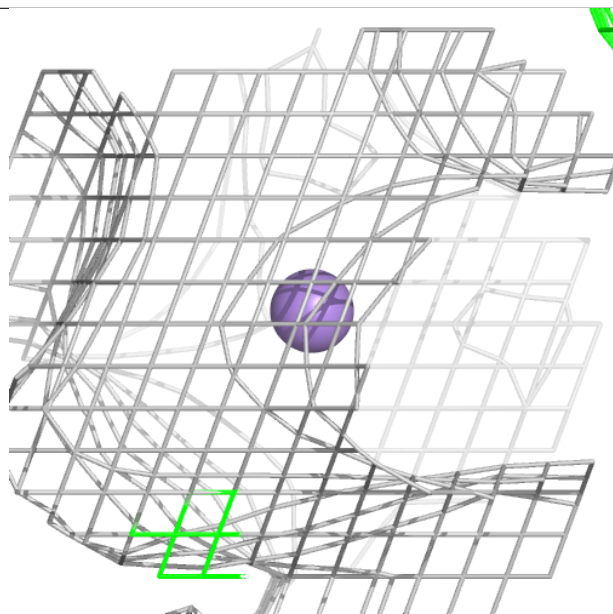
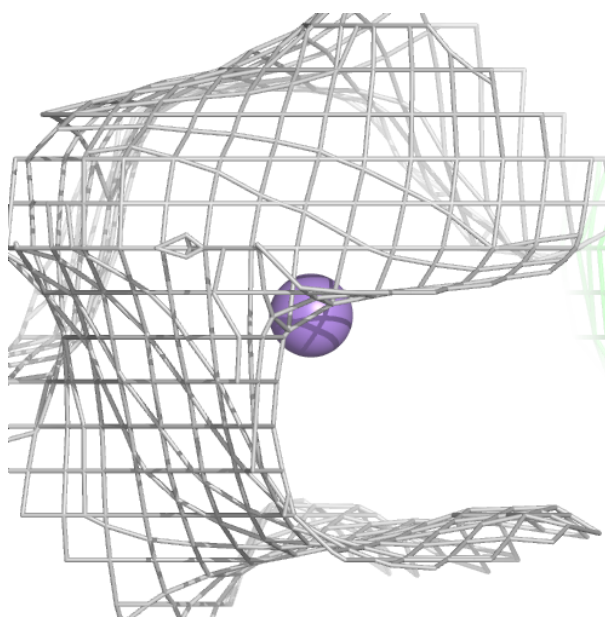
Electron density around MN C 403:

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



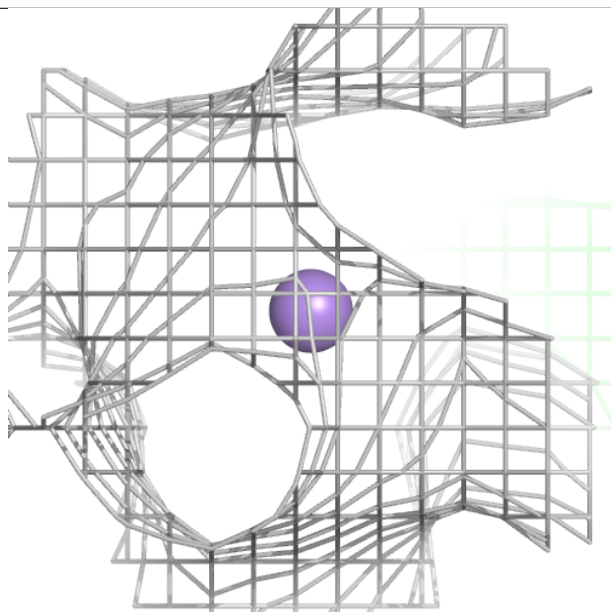
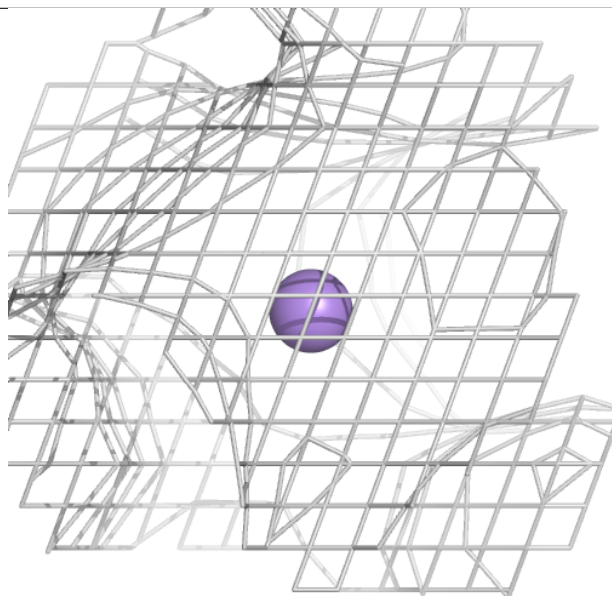
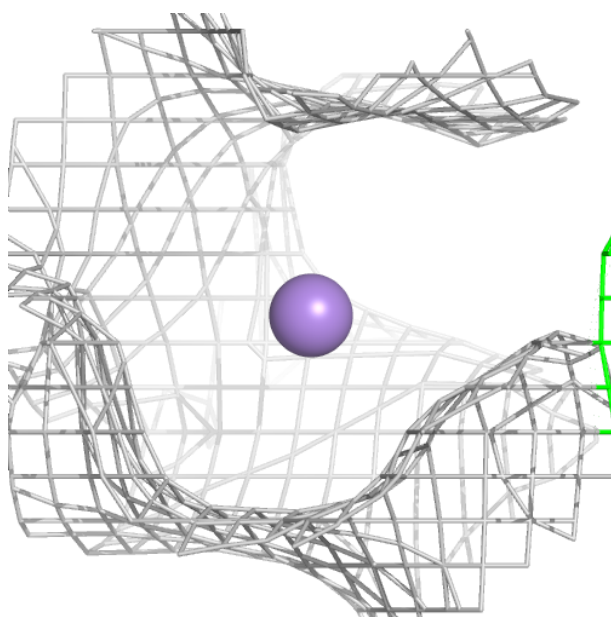
Electron density around MN B 1101:

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



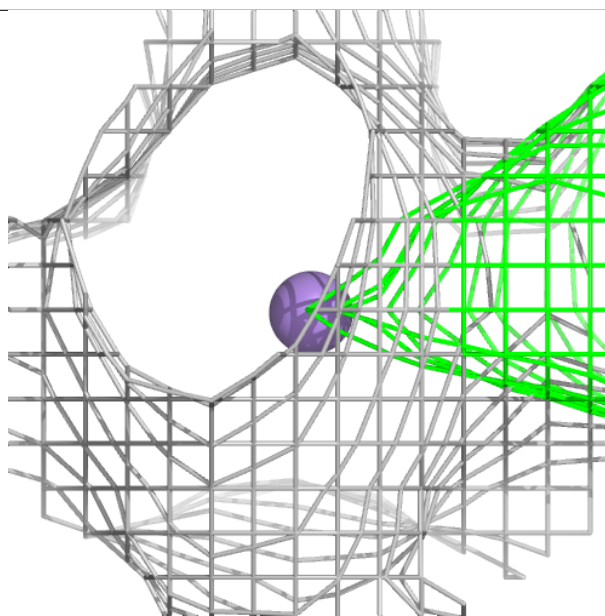
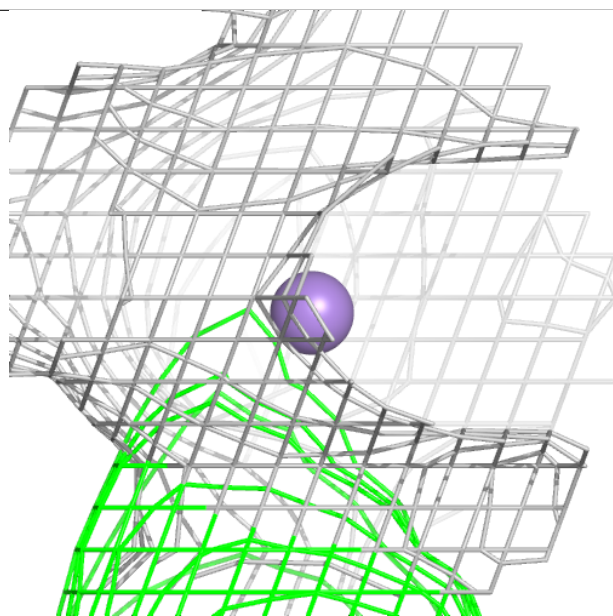
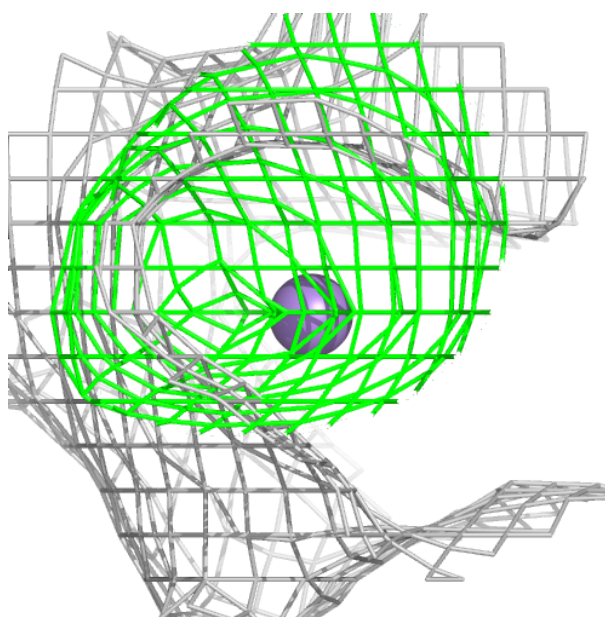
Electron density around MN D 1102:

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



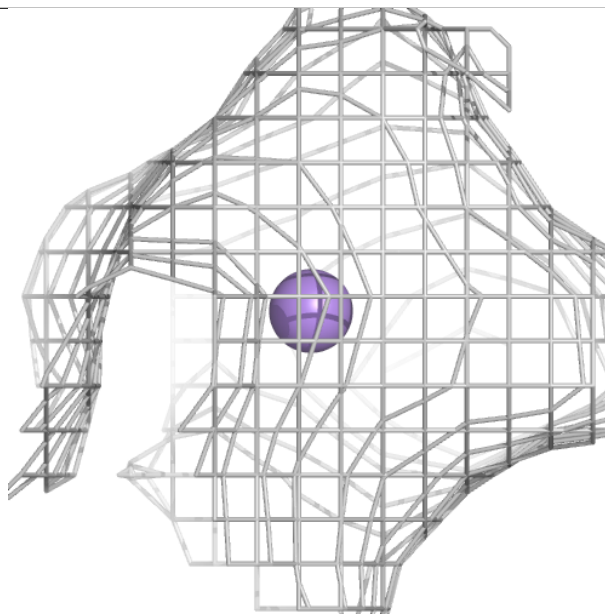
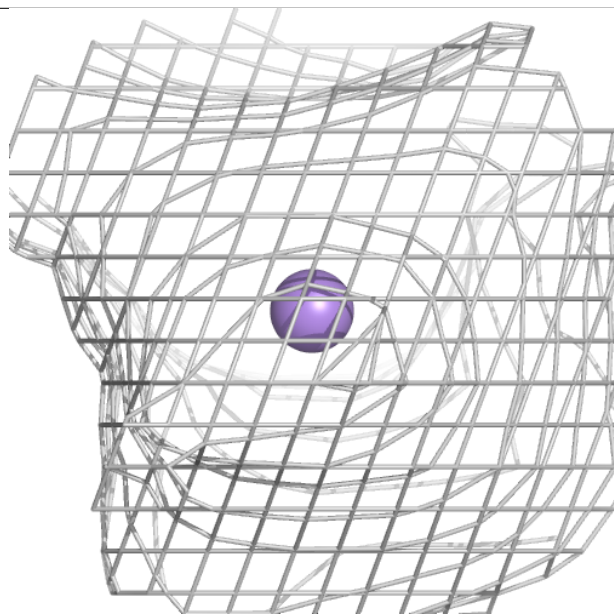
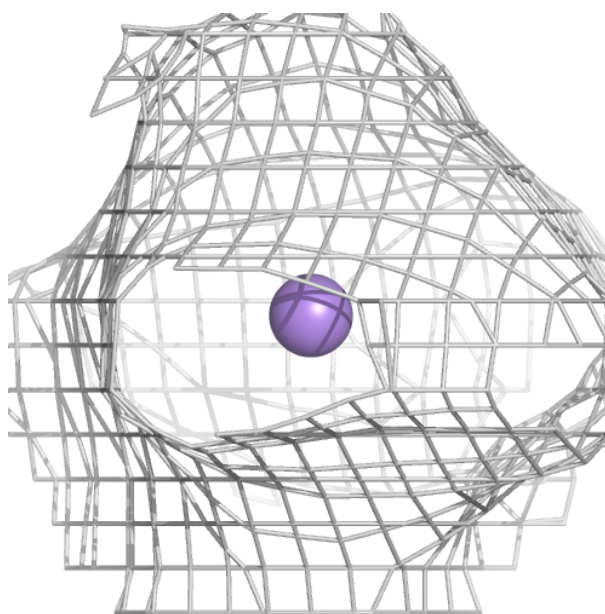
Electron density around MN B 1102:

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



Electron density around MN 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.