



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 7SH1 / pdb_00007sh1
Title : Class II UvrA protein - Ecm16
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Deposited on : 2021-10-07
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

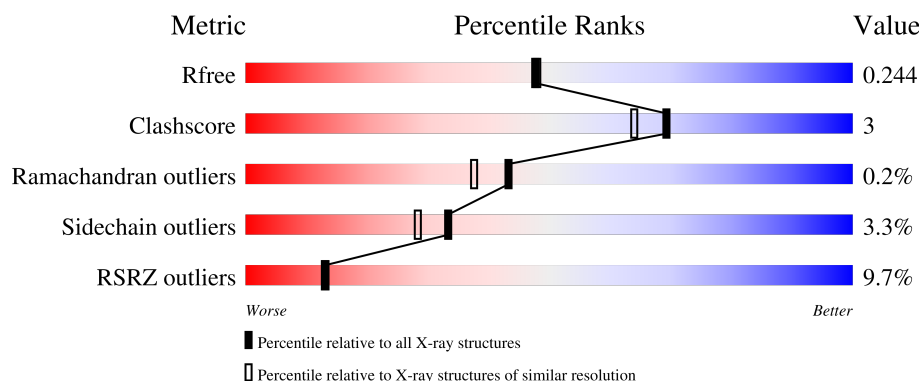
1 Overall quality at a glance

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	812	9% 67% 9% 23%
1	B	812	6% 67% 9% 23%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10007 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 Excinuclease ABC subunit UvrA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	626	Total	C	N	O	S	0	1	0
			4650	2892	842	896	20			
1	B	626	Total	C	N	O	S	0	0	0
			4626	2870	837	899	20			

There are 40 discrepancies between the modelled and reference sequences:

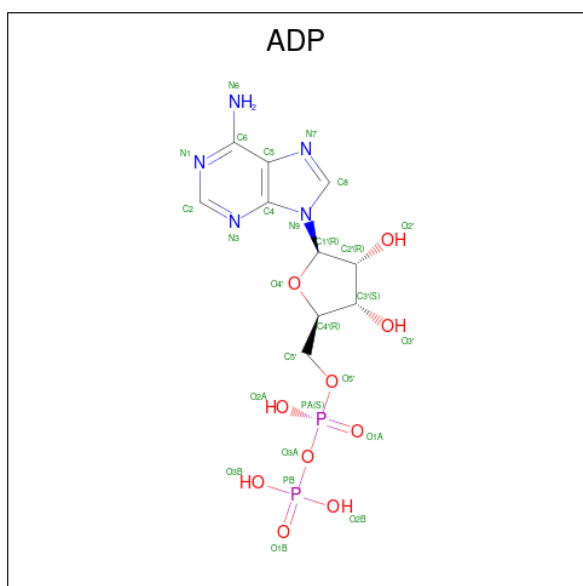
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q0X0A9
A	-18	GLY	-	expression tag	UNP Q0X0A9
A	-17	SER	-	expression tag	UNP Q0X0A9
A	-16	SER	-	expression tag	UNP Q0X0A9
A	-15	HIS	-	expression tag	UNP Q0X0A9
A	-14	HIS	-	expression tag	UNP Q0X0A9
A	-13	HIS	-	expression tag	UNP Q0X0A9
A	-12	HIS	-	expression tag	UNP Q0X0A9
A	-11	HIS	-	expression tag	UNP Q0X0A9
A	-10	HIS	-	expression tag	UNP Q0X0A9
A	-9	SER	-	expression tag	UNP Q0X0A9
A	-8	SER	-	expression tag	UNP Q0X0A9
A	-7	GLY	-	expression tag	UNP Q0X0A9
A	-6	LEU	-	expression tag	UNP Q0X0A9
A	-5	VAL	-	expression tag	UNP Q0X0A9
A	-4	PRO	-	expression tag	UNP Q0X0A9
A	-3	ARG	-	expression tag	UNP Q0X0A9
A	-2	GLY	-	expression tag	UNP Q0X0A9
A	-1	SER	-	expression tag	UNP Q0X0A9
A	0	HIS	-	expression tag	UNP Q0X0A9
B	-19	MET	-	initiating methionine	UNP Q0X0A9
B	-18	GLY	-	expression tag	UNP Q0X0A9
B	-17	SER	-	expression tag	UNP Q0X0A9
B	-16	SER	-	expression tag	UNP Q0X0A9
B	-15	HIS	-	expression tag	UNP Q0X0A9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP Q0X0A9
B	-13	HIS	-	expression tag	UNP Q0X0A9
B	-12	HIS	-	expression tag	UNP Q0X0A9
B	-11	HIS	-	expression tag	UNP Q0X0A9
B	-10	HIS	-	expression tag	UNP Q0X0A9
B	-9	SER	-	expression tag	UNP Q0X0A9
B	-8	SER	-	expression tag	UNP Q0X0A9
B	-7	GLY	-	expression tag	UNP Q0X0A9
B	-6	LEU	-	expression tag	UNP Q0X0A9
B	-5	VAL	-	expression tag	UNP Q0X0A9
B	-4	PRO	-	expression tag	UNP Q0X0A9
B	-3	ARG	-	expression tag	UNP Q0X0A9
B	-2	GLY	-	expression tag	UNP Q0X0A9
B	-1	SER	-	expression tag	UNP Q0X0A9
B	0	HIS	-	expression tag	UNP Q0X0A9

- Molecule 2 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
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Cl	0	0
			3	3		
4	B	2	Total	Cl	0	0
			2	2		

- 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	B	1	Total	Mg	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	309	Total	O	0	0
			309	309		
6	B	303	Total	O	0	0
			303	303		

SER	GLY	T351	L580	A716
ASP	ASP	F355	E586	V744
ILE	PRO	I358	F590	R764
ASP	VAL	G359	T591	F767
PRO	LYS	L360	C592	L774
ALA	VAL	S368	K593	L774
GLN	LYS	R379	A595	A777
LEU	GLY	L390	G596	A781
PHE	ASN	M412	V597	L781
ASP	THR	L415	ILE	G791
ALA	THR	K432	TYR	A792
GLY	THR	F433	THR	
ASP	TYR	E434	ASP	
GLY	GLU	T435	LEU	
LEU	GLY	I438	ALA	
ALA	LEU	V442	ILE	
ILE	LEU	L445	NET	
THR	ALA	T451	ALA	
THR	ARG	F458	GLY	
VAL	VAL	T470	V608	
VAL	ARG	V471	A609	
GLN	LYS	T472	T610	
THR	THR	D478	T611	
GLY	GLU	R479	D614	
PHE	THR	V492	G617	
PRO	THR	I530	K618	
HIS	ILE	D538	R619	
LYS	ARG	G539	V624	
ALA	ALA	K549	M640	
VAL	THR	R553	A645	
ARG	THR	M562	A654	
TYR	SER	I566	R655	
THR	ALA	F570	L663	
GLU	GLU	A571	L671	
GLU	GLU	K572	Q678	
ARG	ARG	A579	E687	
HIS	THR		G688	
GLY	THR		G699	
PHE	GLN		A700	
LEU	GLU		G701	
HIS	ARG		D707	
	HIS		E708	
	GLY		H714	
	PHE		L715	
	LEU			
	HIS			

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	141.13Å 141.13Å 173.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	122.22 – 2.04 122.22 – 2.04	Depositor EDS
% Data completeness (in resolution range)	100.0 (122.22-2.04) 100.0 (122.22-2.04)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.03Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.198 , 0.239 0.205 , 0.244	Depositor DCC
R_{free} test set	6157 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	38.5	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10007	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.24% 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: ZN, ADP, MG, CL

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	1.37	16/4715 (0.3%)	1.16	6/6385 (0.1%)
1	B	1.35	21/4691 (0.4%)	1.18	10/6355 (0.2%)
All	All	1.36	37/9406 (0.4%)	1.17	16/12740 (0.1%)

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	51	VAL	CA-CB	8.02	1.62	1.54
1	A	424	ASN	C-O	-6.86	1.15	1.23
1	B	708	GLU	CA-C	6.86	1.58	1.53
1	A	593	LYS	N-CA	6.61	1.54	1.46
1	B	63	THR	CA-C	6.54	1.57	1.52
1	B	432	LYS	CA-C	-6.38	1.46	1.52
1	A	564	GLU	N-CA	6.22	1.52	1.46
1	B	687	GLU	CA-C	-5.88	1.45	1.52
1	B	390	LEU	CA-C	-5.87	1.45	1.52
1	B	32	ASN	CA-C	-5.86	1.44	1.52
1	B	470	THR	CA-C	-5.80	1.45	1.53
1	A	419	LEU	N-CA	-5.72	1.39	1.46
1	B	434	GLU	CA-C	5.72	1.60	1.52
1	A	321	ALA	CA-C	5.70	1.60	1.52
1	B	593	LYS	N-CA	5.60	1.53	1.46
1	B	412	MET	N-CA	5.54	1.52	1.46
1	B	566	ILE	CA-CB	5.52	1.60	1.54
1	B	313	ILE	C-O	5.52	1.30	1.24
1	B	70	ARG	CA-C	5.45	1.59	1.52
1	B	570	PHE	CA-C	5.45	1.59	1.52
1	B	458	PHE	N-CA	-5.44	1.39	1.45
1	A	760	HIS	C-O	-5.42	1.17	1.24
1	A	742	GLN	CA-C	5.38	1.60	1.52
1	A	593	LYS	CA-C	5.33	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	472	THR	CA-CB	5.29	1.61	1.53
1	B	442	VAL	CA-C	-5.25	1.46	1.52
1	A	496	ARG	C-O	-5.24	1.17	1.23
1	A	417	LEU	CA-C	5.22	1.59	1.52
1	A	33	LEU	C-O	-5.19	1.17	1.23
1	B	26	HIS	CA-C	-5.18	1.46	1.52
1	B	716	ALA	N-CA	5.16	1.52	1.46
1	A	101	ALA	C-O	-5.14	1.17	1.24
1	A	766	VAL	C-O	-5.12	1.18	1.24
1	A	643	ALA	C-O	-5.11	1.18	1.24
1	A	327	SER	CA-C	5.10	1.59	1.52
1	B	744	VAL	N-CA	-5.02	1.40	1.46
1	A	55	GLY	CA-C	5.02	1.58	1.51

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	678	GLN	CA-C-N	-7.11	112.44	119.76
1	B	678	GLN	C-N-CA	-7.11	112.44	119.76
1	B	596	GLY	N-CA-C	-6.83	100.79	110.96
1	A	463	GLU	CA-C-N	6.46	127.15	119.98
1	A	463	GLU	C-N-CA	6.46	127.15	119.98
1	B	110	GLY	N-CA-C	-6.09	101.59	110.90
1	B	777	ALA	N-CA-C	5.97	117.46	111.07
1	B	351	THR	CB-CA-C	-5.72	101.86	110.90
1	A	668	GLU	N-CA-C	5.67	118.40	111.82
1	B	714	HIS	N-CA-CB	-5.31	102.77	110.36
1	A	723	ARG	N-CA-C	-5.28	105.61	111.36
1	A	618	LYS	N-CA-C	5.26	117.92	111.82
1	B	351	THR	N-CA-CB	5.21	117.63	110.07
1	B	596	GLY	CA-C-O	-5.14	116.14	121.63
1	A	536	GLY	N-CA-C	5.09	120.04	113.27
1	B	671	LEU	N-CA-C	5.02	118.29	112.97

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	4650	0	4683	34	0
1	B	4626	0	4651	32	0
2	A	54	0	24	1	0
2	B	54	0	24	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	3	0	0	0	0
4	B	2	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	309	0	0	5	0
6	B	303	0	0	5	1
All	All	10007	0	9382	65	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (65) 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:B:22:MET:HE2	1:B:39:GLU:HB3	1.65	0.77
1:A:488:GLN:O	6:A:901:HOH:O	2.09	0.71
1:A:325:GLN:HE22	1:A:760:HIS:H	1.39	0.71
1:A:699:GLY:O	6:A:902:HOH:O	2.09	0.70
1:A:723:ARG:NH2	1:B:478:ASP:OD1	2.25	0.70
1:A:139:ILE:O	6:A:903:HOH:O	2.13	0.67
1:A:26:HIS:HB2	1:A:94:VAL:HG13	1.75	0.67
1:A:357:GLN:O	1:A:411:ARG:HD2	1.95	0.66
1:B:358:ILE:HD11	1:B:360:LEU:HD12	1.84	0.60
1:A:70:ARG:NH1	1:A:74:GLU:OE2	2.35	0.59
1:B:640:MET:HE3	1:B:645:ALA:HB2	1.84	0.59
1:A:592:CYS:SG	1:A:593:LYS:N	2.75	0.58
1:B:595:ALA:HB2	1:B:619:ARG:CG	2.33	0.58
1:B:595:ALA:HB2	1:B:619:ARG:HG2	1.86	0.57
1:B:595:ALA:HB1	1:B:617:GLY:HA2	1.87	0.56
1:B:591:THR:HG21	1:B:614:ASP:OD2	2.06	0.55
1:A:338:ASP:OD1	1:A:340:SER:HB3	2.07	0.54
1:A:595:ALA:HB2	1:A:619:ARG:CG	2.38	0.54
1:B:767:PHE:CD2	1:B:774:LEU:HD13	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:HIS:HB2	1:B:94:VAL:HB	1.92	0.52
1:B:562:MET:HE1	1:B:663:LEU:HD23	1.92	0.52
1:A:592:CYS:O	1:A:593:LYS:NZ	2.39	0.52
1:A:583:PRO:HB3	1:A:593:LYS:HD2	1.92	0.51
1:A:121:THR:HG21	1:A:355:PHE:HZ	1.76	0.50
1:A:595:ALA:HB2	1:A:619:ARG:HG3	1.93	0.50
1:A:435:THR:O	1:A:438:ILE:HG12	2.11	0.50
1:B:451:THR:HG21	6:B:918:HOH:O	2.11	0.50
1:B:608:VAL:HG23	1:B:609:ALA:H	1.77	0.49
1:B:24:ARG:NH1	6:B:905:HOH:O	2.29	0.49
1:A:682:THR:HG21	2:A:801:ADP:N6	2.28	0.49
1:B:654:ALA:O	1:B:655:ARG:C	2.56	0.48
1:A:562:MET:HE2	1:A:662:VAL:CG1	2.42	0.48
1:A:42:LYS:HE3	1:A:97:GLY:O	2.12	0.48
1:B:358:ILE:HD12	1:B:379:ARG:HB3	1.96	0.48
1:A:640:MET:HE1	1:A:648:PHE:HB3	1.97	0.47
1:B:592:CYS:SG	1:B:593:LYS:N	2.88	0.47
1:B:26:HIS:HB3	6:B:940:HOH:O	2.15	0.46
1:B:435:THR:O	1:B:438:ILE:HG12	2.17	0.45
1:B:595:ALA:HB2	1:B:619:ARG:HG3	1.97	0.45
1:A:668:GLU:OE2	1:A:727:ARG:NH2	2.40	0.45
1:A:303:ARG:HD2	6:A:1006:HOH:O	2.16	0.45
1:A:442:VAL:HG11	1:A:465:LEU:HD22	1.99	0.44
1:A:592:CYS:O	1:A:593:LYS:CE	2.65	0.44
1:B:358:ILE:HG22	1:B:415:LEU:HD13	2.00	0.44
1:A:80:ILE:O	1:A:81:GLN:HB2	2.18	0.44
1:A:640:MET:HE1	1:A:648:PHE:CB	2.47	0.44
1:B:89:ARG:N	6:B:929:HOH:O	2.50	0.44
1:A:45:LEU:HD23	1:A:45:LEU:C	2.43	0.44
1:A:562:MET:HE1	1:A:663:LEU:CD2	2.48	0.44
1:B:70:ARG:NH1	1:B:74:GLU:OE2	2.51	0.43
1:A:131:PHE:HB3	1:A:145:PHE:CE2	2.53	0.43
1:A:595:ALA:HB2	1:A:619:ARG:HG2	1.99	0.43
1:B:593:LYS:N	1:B:593:LYS:HD3	2.33	0.43
1:B:358:ILE:HG22	1:B:415:LEU:CD1	2.49	0.43
1:B:358:ILE:HD11	1:B:360:LEU:CD1	2.48	0.42
1:A:20:HIS:HD2	6:A:1177:HOH:O	2.02	0.42
1:B:562:MET:HE1	1:B:663:LEU:CD2	2.50	0.42
1:A:102:ILE:HD12	1:A:393:VAL:HG11	2.02	0.42
1:A:519:THR:C	1:A:526:LYS:HD3	2.45	0.41
1:B:67:GLU:CD	1:B:89:ARG:HH11	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:LEU:HD22	1:B:98:LEU:HD21	2.03	0.41
1:A:471:VAL:O	1:A:475:HIS:HD2	2.03	0.41
1:B:121:THR:HG21	1:B:355:PHE:HZ	1.86	0.41
1:B:89:ARG:N	6:B:933:HOH:O	2.53	0.40
1:B:781:LEU:HD23	1:B:781:LEU:HA	1.98	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:1103:HOH:O	6:B:1123:HOH:O[6_765]	1.81	0.39

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	615/812 (76%)	597 (97%)	17 (3%)	1 (0%)	43	37
1	B	616/812 (76%)	596 (97%)	19 (3%)	1 (0%)	43	37
All	All	1231/1624 (76%)	1193 (97%)	36 (3%)	2 (0%)	43	37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	700	ALA
1	A	593	LYS

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	498/650 (77%)	481 (97%)	17 (3%)	32	27
1	B	497/650 (76%)	481 (97%)	16 (3%)	34	29
All	All	995/1300 (76%)	962 (97%)	33 (3%)	33	28

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	VAL
1	A	81	GLN
1	A	87	LEU
1	A	94	VAL
1	A	95	LEU
1	A	172	VAL
1	A	182	ILE
1	A	343	THR
1	A	353	GLU
1	A	406	PRO
1	A	432	LYS
1	A	492	VAL
1	A	572	LYS
1	A	598	ILE
1	A	608	VAL
1	A	621	GLN
1	A	635	SER
1	B	15	CYS
1	B	96	ASP
1	B	109	MET
1	B	111	THR
1	B	115	SER
1	B	149	VAL
1	B	351	THR
1	B	368	SER
1	B	445	LEU
1	B	479	ARG
1	B	492	VAL
1	B	538	ASP
1	B	549	LYS
1	B	562	MET
1	B	586	GLU
1	B	611	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	69	GLN
1	A	81	GLN
1	A	148	ASN
1	A	325	GLN
1	A	574	ASN
1	A	621	GLN
1	B	488	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 15 ligands modelled in this entry, 11 are monoatomic - leaving 4 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	ADP	A	802	-	28,29,29	1.51	6 (21%)	43,45,45	1.61	9 (20%)
2	ADP	B	802	-	28,29,29	1.43	4 (14%)	43,45,45	1.74	7 (16%)
2	ADP	B	801	5	28,29,29	1.99	7 (25%)	43,45,45	2.10	12 (27%)
2	ADP	A	801	5	28,29,29	1.62	8 (28%)	43,45,45	1.88	11 (25%)

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	ADP	A	802	-	-	0/16/32/32	0/3/3/3
2	ADP	B	802	-	-	1/16/32/32	0/3/3/3
2	ADP	B	801	5	-	1/16/32/32	0/3/3/3
2	ADP	A	801	5	-	3/16/32/32	0/3/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	ADP	C5-C4	5.59	1.49	1.39
2	A	802	ADP	C5-C4	4.24	1.46	1.39
2	A	801	ADP	C5-C4	3.99	1.46	1.39
2	B	802	ADP	C5-C4	3.90	1.46	1.39
2	B	801	ADP	PA-O3A	3.80	1.63	1.59
2	B	801	ADP	C5-N7	-3.75	1.32	1.39
2	A	801	ADP	C4-N9	-3.34	1.30	1.37
2	A	801	ADP	C5-C6	2.93	1.49	1.41
2	B	802	ADP	C5-N7	-2.84	1.33	1.39
2	B	802	ADP	C4-N9	-2.69	1.32	1.37
2	A	801	ADP	C5-N7	-2.62	1.34	1.39
2	B	802	ADP	C5-C6	2.56	1.48	1.41
2	B	801	ADP	C5-C6	2.54	1.48	1.41
2	A	802	ADP	O4'-C4'	-2.46	1.39	1.45
2	A	802	ADP	PB-O3B	-2.40	1.45	1.54
2	B	801	ADP	C2-N3	2.35	1.38	1.33
2	A	801	ADP	C8-N7	2.32	1.36	1.31
2	A	801	ADP	O4'-C4'	-2.30	1.39	1.45
2	B	801	ADP	C4-N9	-2.27	1.33	1.37
2	A	802	ADP	C4-N9	-2.22	1.33	1.37
2	A	801	ADP	PA-O3A	2.14	1.61	1.59
2	A	801	ADP	C2'-C1'	-2.09	1.46	1.53
2	A	802	ADP	C8-N7	2.08	1.35	1.31
2	A	802	ADP	C5-N7	-2.08	1.35	1.39
2	B	801	ADP	C2'-C3'	-2.01	1.47	1.53

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	ADP	C5-C4-N3	-5.89	118.61	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	ADP	C5-C4-N3	-5.48	119.17	126.72
2	B	801	ADP	N3-C4-N9	5.17	135.96	127.17
2	B	802	ADP	C5-C4-N3	-5.10	119.70	126.72
2	B	801	ADP	N3-C2-N1	-4.77	121.37	128.58
2	A	802	ADP	C5-C4-N3	-4.58	120.41	126.72
2	A	801	ADP	N3-C4-N9	4.55	134.91	127.17
2	B	802	ADP	N3-C2-N1	-4.39	121.93	128.58
2	B	802	ADP	N3-C4-N9	4.13	134.20	127.17
2	A	801	ADP	N3-C2-N1	-3.96	122.58	128.58
2	A	801	ADP	C2-N3-C4	3.92	121.41	111.83
2	A	802	ADP	N3-C4-N9	3.90	133.79	127.17
2	B	801	ADP	O2A-PA-O1A	3.60	129.21	112.44
2	B	801	ADP	C2-N3-C4	3.60	120.62	111.83
2	B	801	ADP	C2-N1-C6	3.57	124.59	118.73
2	B	801	ADP	O3B-PB-O2B	3.54	121.07	107.80
2	B	802	ADP	C2-N3-C4	3.47	120.31	111.83
2	B	802	ADP	C2-N1-C6	3.37	124.27	118.73
2	A	801	ADP	C4-N9-C8	3.12	109.02	105.74
2	A	802	ADP	C2-N3-C4	2.87	118.83	111.83
2	B	801	ADP	N6-C6-N1	2.73	124.46	118.38
2	A	801	ADP	O4'-C1'-N9	-2.66	102.97	108.09
2	A	802	ADP	O2'-C2'-C1'	2.59	119.01	110.10
2	A	802	ADP	N3-C2-N1	-2.48	124.83	128.58
2	B	801	ADP	O2A-PA-O3A	2.41	113.78	107.27
2	B	802	ADP	C4-N9-C8	2.38	108.24	105.74
2	B	802	ADP	C4-C5-N7	-2.36	107.88	110.58
2	A	801	ADP	O3B-PB-O2B	2.30	116.43	107.80
2	A	801	ADP	N6-C6-N1	2.22	123.33	118.38
2	B	801	ADP	C5-N7-C8	2.12	106.78	103.45
2	A	802	ADP	O3B-PB-O2B	2.09	115.64	107.80
2	A	802	ADP	O4'-C4'-C3'	2.08	109.29	105.15
2	A	801	ADP	O2A-PA-O1A	2.08	122.14	112.44
2	B	801	ADP	O3A-PA-O1A	-2.06	104.50	110.70
2	A	802	ADP	C5-C6-N6	-2.06	118.19	123.29
2	A	801	ADP	C4-C5-N7	-2.04	108.25	110.58
2	A	801	ADP	C5-C6-N6	-2.04	118.23	123.29
2	A	802	ADP	O3B-PB-O1B	2.04	118.77	110.83
2	B	801	ADP	C4-C5-N7	-2.01	108.29	110.58

There are no chirality outliers.

All (5) torsion outliers are listed below:

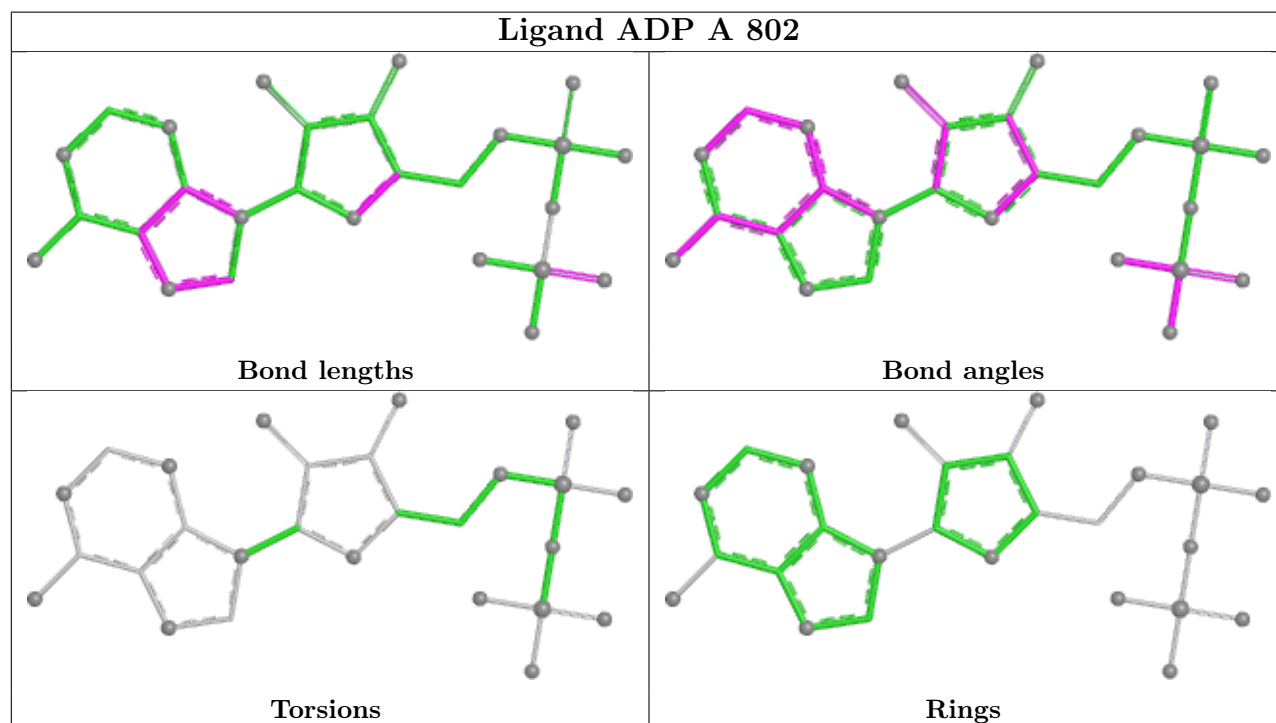
Mol	Chain	Res	Type	Atoms
2	A	801	ADP	PA-O3A-PB-O3B
2	A	801	ADP	C5'-O5'-PA-O1A
2	B	802	ADP	PA-O3A-PB-O3B
2	B	801	ADP	PA-O3A-PB-O3B
2	A	801	ADP	PA-O3A-PB-O1B

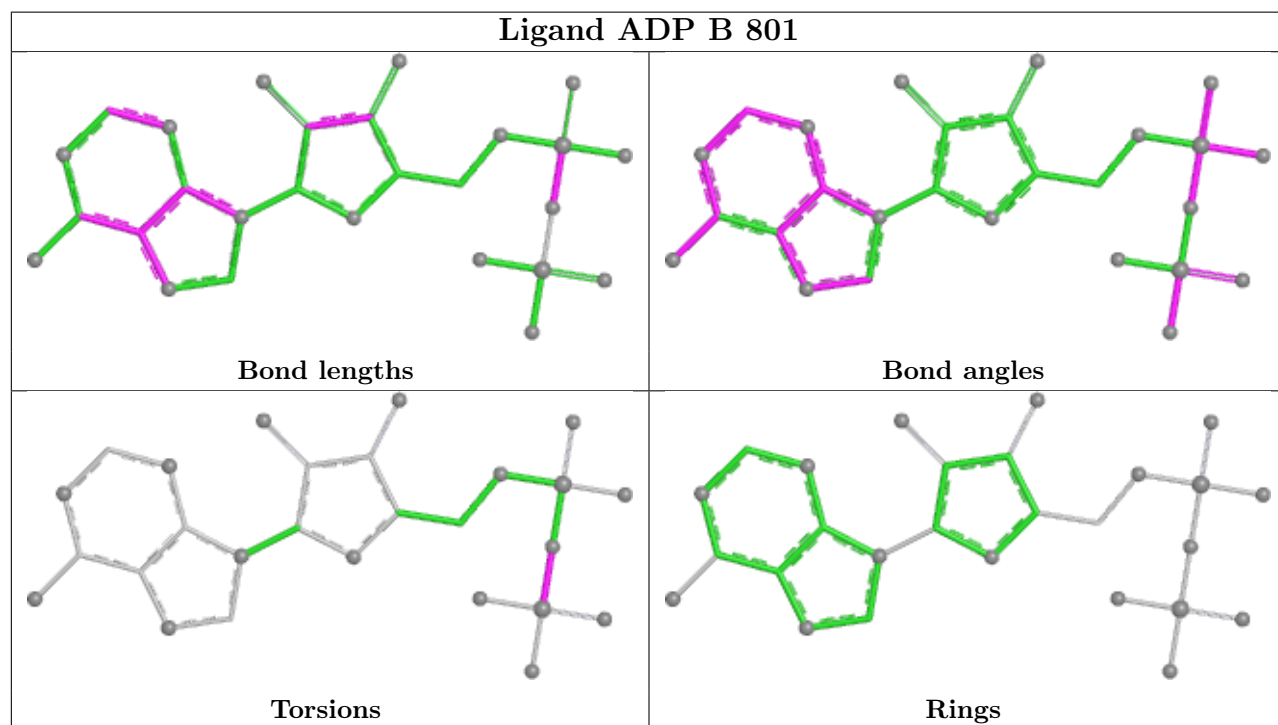
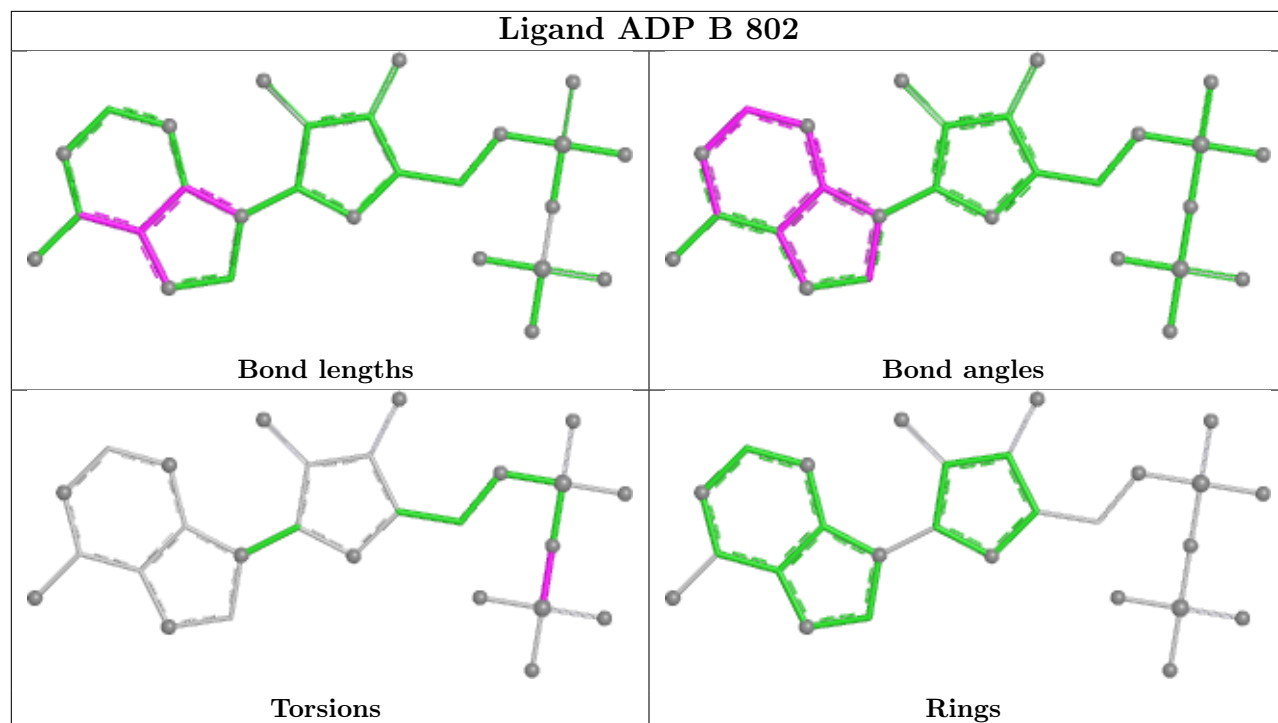
There are no ring outliers.

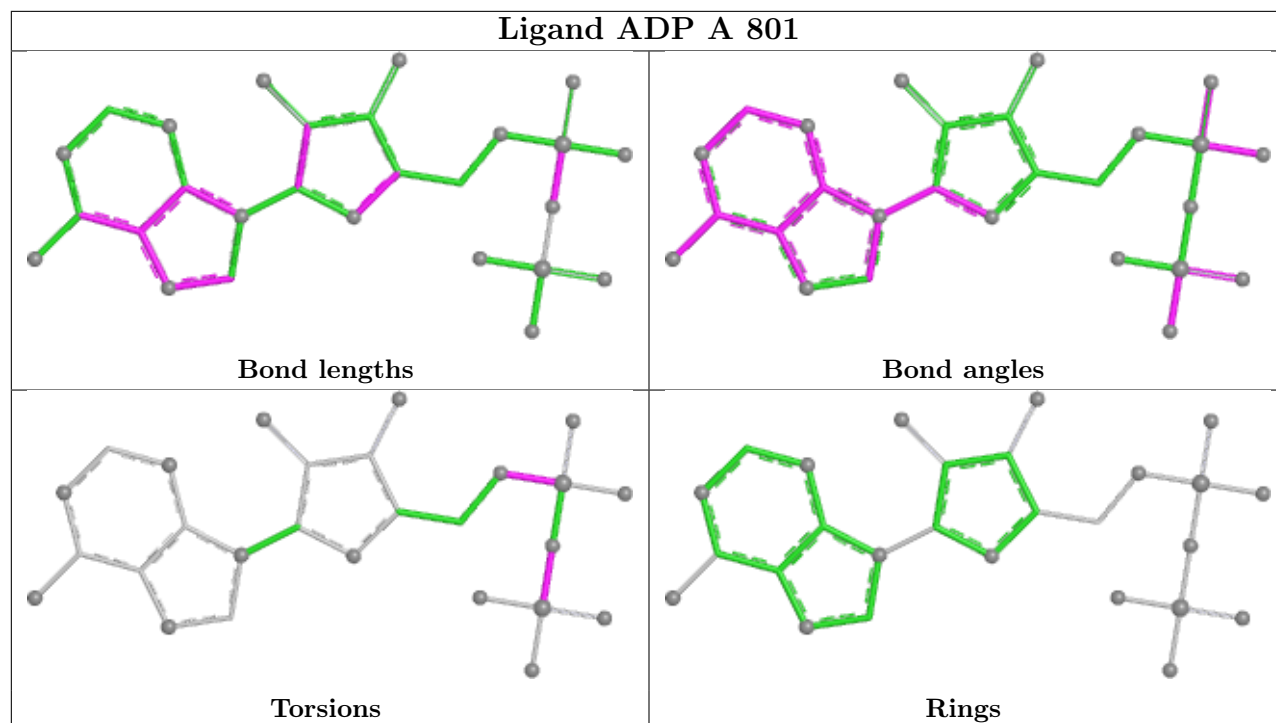
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	ADP	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	626/812 (77%)	0.65	77 (12%) 8 7	21, 44, 81, 105	1 (0%)
1	B	626/812 (77%)	0.57	45 (7%) 21 21	26, 43, 71, 101	0
All	All	1252/1624 (77%)	0.61	122 (9%) 13 13	21, 43, 78, 105	1 (0%)

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	110	GLY	7.9
1	B	78	ALA	7.7
1	A	113	LEU	7.0
1	A	598	ILE	6.9
1	A	608	VAL	6.1
1	B	608	VAL	6.0
1	A	182	ILE	5.9
1	B	149	VAL	5.5
1	A	80	ILE	4.9
1	B	609	ALA	4.7
1	B	108	PRO	4.6
1	A	172	VAL	4.6
1	A	580	LEU	4.4
1	A	581	PHE	4.2
1	A	616	GLY	4.2
1	B	792	ALA	4.2
1	A	79	PHE	4.0
1	A	87	LEU	3.9
1	A	573	ALA	3.8
1	A	173	GLY	3.7
1	A	593	LYS	3.7
1	A	148	ASN	3.6
1	A	792	ALA	3.5
1	A	583	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	571	ALA	3.4
1	A	575	GLY	3.4
1	A	700	ALA	3.3
1	A	613	GLU	3.3
1	A	342	THR	3.2
1	B	111	THR	3.2
1	B	700	ALA	3.2
1	A	339	PRO	3.2
1	B	572	LYS	3.2
1	A	597	VAL	3.2
1	B	593	LYS	3.2
1	B	716	ALA	3.1
1	A	296	CYS	3.1
1	A	576	VAL	3.1
1	A	337	THR	3.1
1	A	648	PHE	3.1
1	A	609	ALA	3.1
1	A	594	GLY	3.1
1	B	150	ALA	3.1
1	B	597	VAL	3.1
1	B	177	LEU	3.0
1	A	570	PHE	3.0
1	B	553	ARG	3.0
1	A	88	ALA	2.9
1	A	660	CYS	2.9
1	B	698	GLY	2.9
1	A	791	GLY	2.9
1	B	715	LEU	2.9
1	B	707	ASP	2.9
1	A	612	CYS	2.8
1	B	595	ALA	2.8
1	A	586	GLU	2.8
1	B	94	VAL	2.8
1	B	594	GLY	2.8
1	A	625	LEU	2.8
1	A	654	ALA	2.7
1	A	658	ALA	2.7
1	A	624	VAL	2.7
1	B	184	SER	2.7
1	B	337	THR	2.7
1	A	566	ILE	2.7
1	A	343	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	109	MET	2.6
1	B	151	SER	2.6
1	A	595	ALA	2.6
1	A	578	PRO	2.6
1	A	587	GLY	2.6
1	A	565	PRO	2.5
1	A	695	GLY	2.5
1	B	791	GLY	2.5
1	A	661	THR	2.5
1	B	591	THR	2.5
1	A	300	HIS	2.5
1	B	701	GLY	2.5
1	A	341	VAL	2.5
1	A	637	VAL	2.5
1	A	629	VAL	2.4
1	A	564	GLU	2.4
1	B	76	TYR	2.4
1	B	539	GLY	2.4
1	B	579	ALA	2.4
1	B	345	LEU	2.4
1	A	579	ALA	2.4
1	A	95	LEU	2.3
1	A	563	LEU	2.3
1	A	574	ASN	2.3
1	B	77	SER	2.3
1	A	611	THR	2.3
1	A	651	THR	2.3
1	B	89	ARG	2.3
1	A	577	LYS	2.3
1	B	530	ILE	2.3
1	B	624	VAL	2.3
1	A	299	CYS	2.3
1	B	764	ARG	2.2
1	B	341	VAL	2.2
1	B	142	GLN	2.2
1	A	649	PHE	2.1
1	A	78	ALA	2.1
1	A	733	LYS	2.1
1	A	622	PRO	2.1
1	A	657	PRO	2.1
1	B	610	THR	2.1
1	B	596	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	345	LEU	2.1
1	B	580	LEU	2.1
1	A	627	TYR	2.1
1	A	617	GLY	2.1
1	B	110	GLY	2.1
1	B	133	ARG	2.1
1	B	590	PRO	2.1
1	A	663	LEU	2.0
1	A	639	ALA	2.0
1	A	655	ARG	2.0
1	A	15	CYS	2.0
1	A	346	THR	2.0
1	A	610	THR	2.0
1	A	539	GLY	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
4	CL	A	807	1/1	0.86	0.15	88,88,88,88	0
4	CL	A	806	1/1	0.93	0.24	63,63,63,63	0
4	CL	B	805	1/1	0.94	0.11	58,58,58,58	0
4	CL	A	805	1/1	0.95	0.12	49,49,49,49	0
5	MG	B	807	1/1	0.96	0.08	49,49,49,49	0
4	CL	B	806	1/1	0.97	0.17	58,58,58,58	0
2	ADP	B	802	27/27	0.98	0.06	29,38,45,47	0
5	MG	A	808	1/1	0.98	0.05	59,59,59,59	0
3	ZN	A	804	1/1	0.98	0.06	67,67,67,67	0

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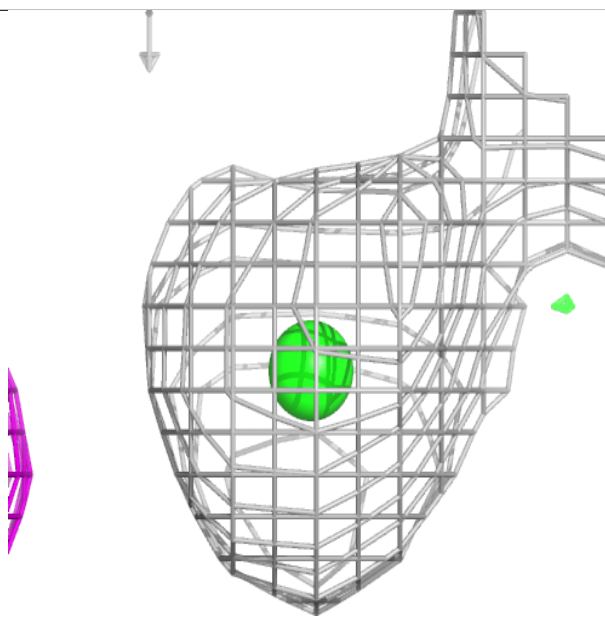
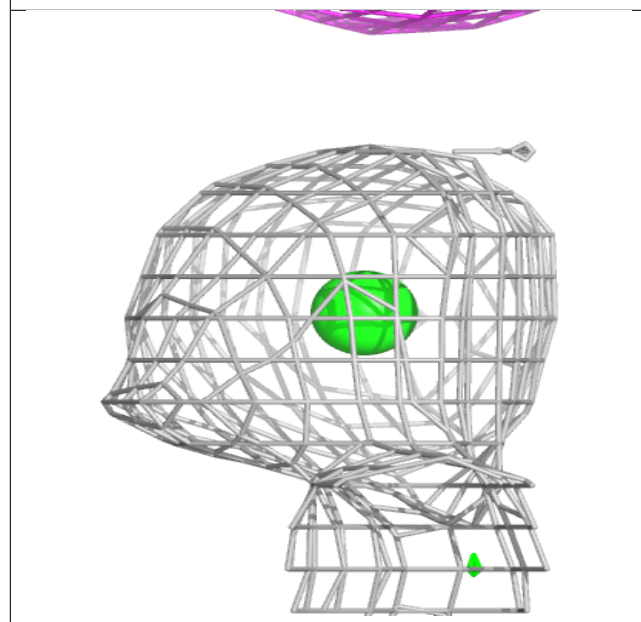
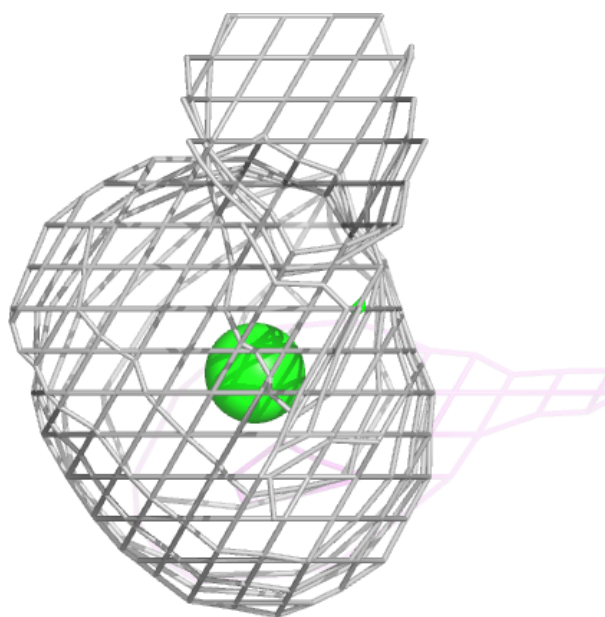
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ADP	A	801	27/27	0.99	0.06	24,36,49,53	0
3	ZN	A	803	1/1	0.99	0.09	65,65,65,65	0
2	ADP	A	802	27/27	0.99	0.04	24,33,39,40	0
3	ZN	B	803	1/1	0.99	0.03	48,48,48,48	0
3	ZN	B	804	1/1	0.99	0.03	65,65,65,65	0
2	ADP	B	801	27/27	0.99	0.05	24,30,43,48	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.

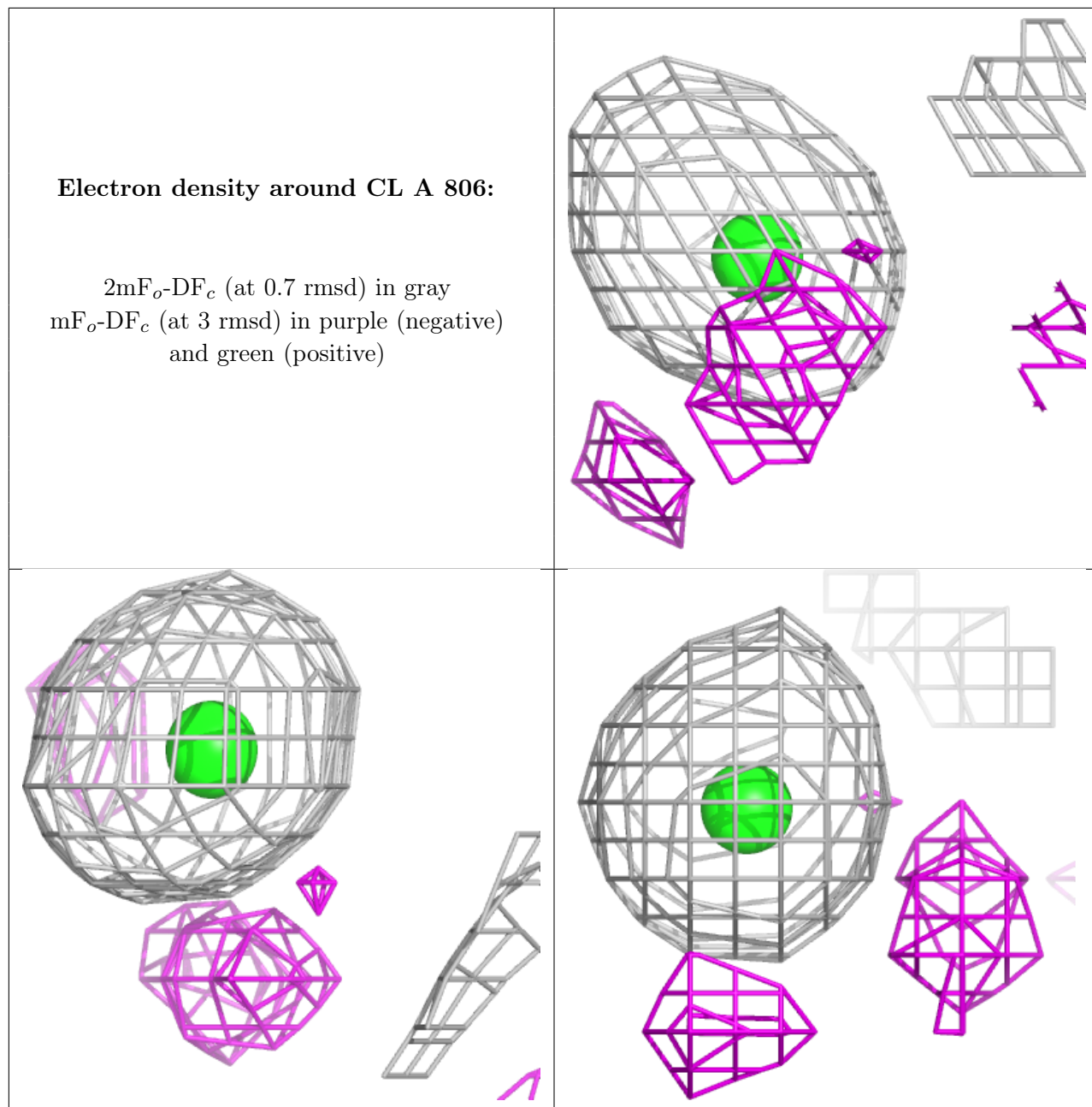
Electron density around CL A 807:

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



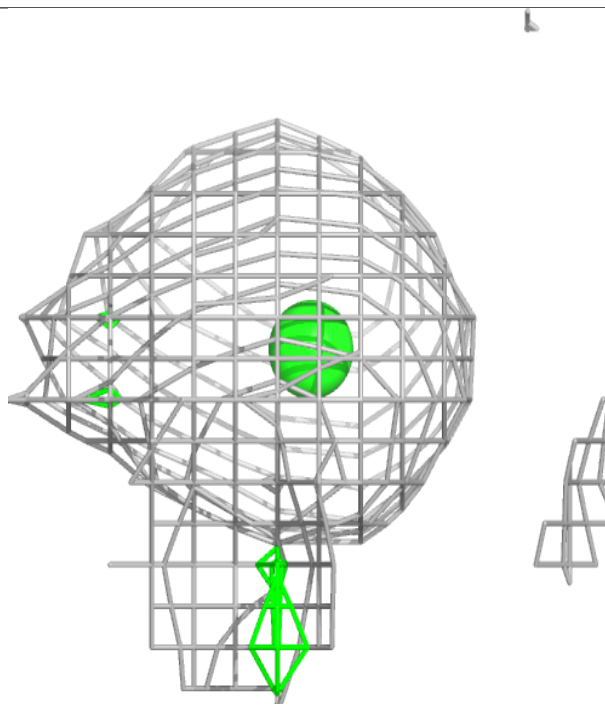
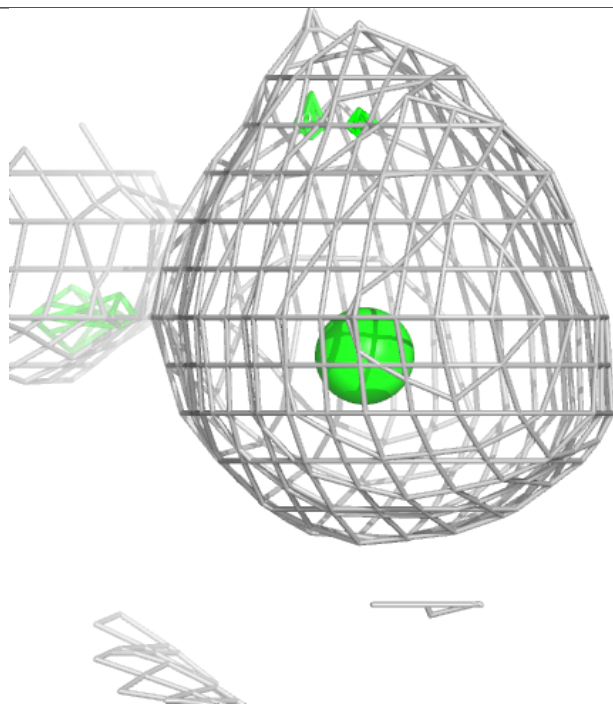
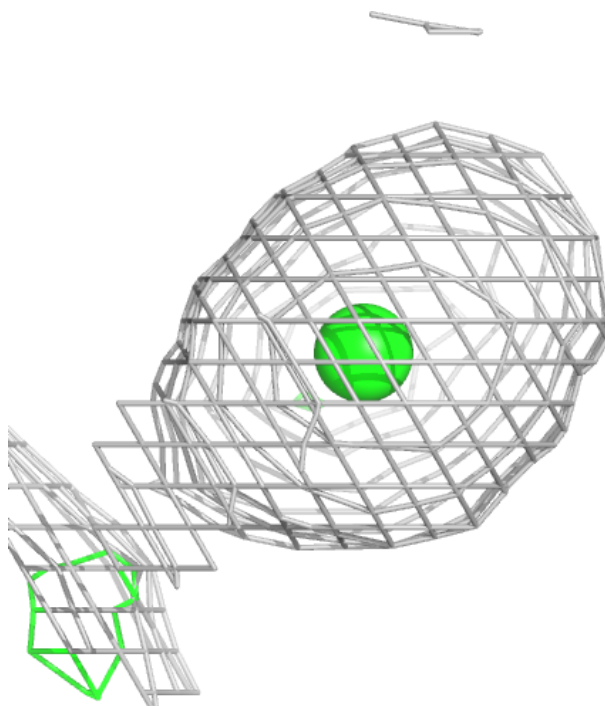
Electron density around CL A 806:

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



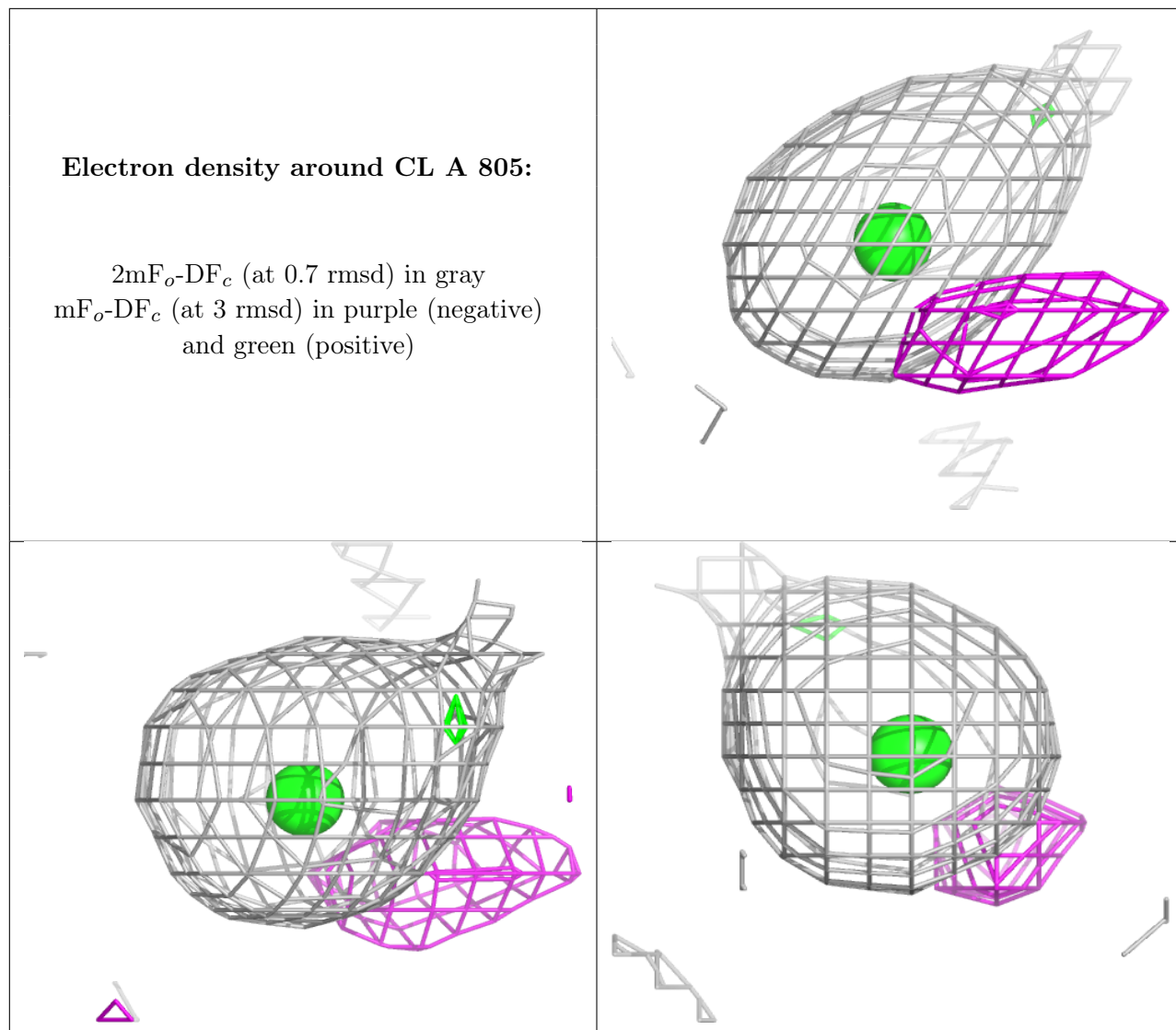
Electron density around CL B 805:

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



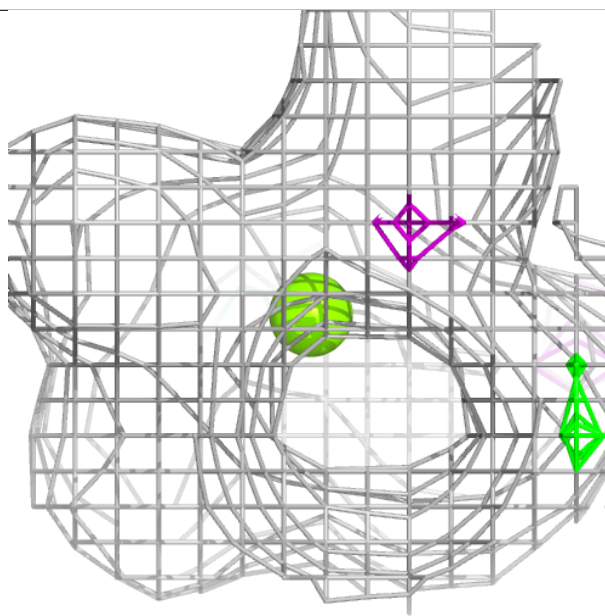
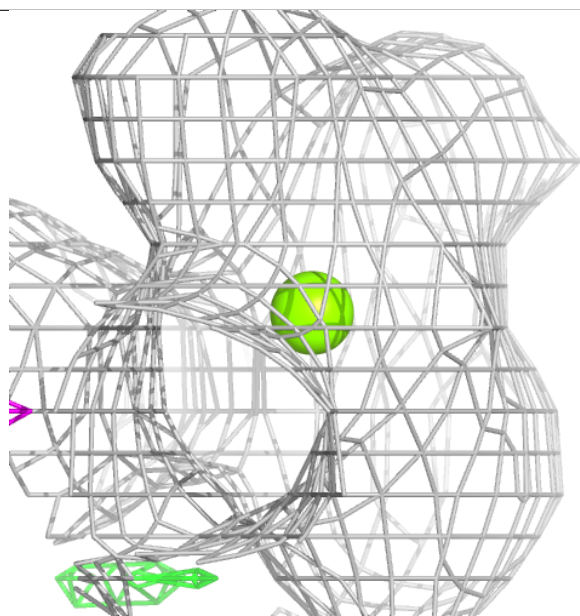
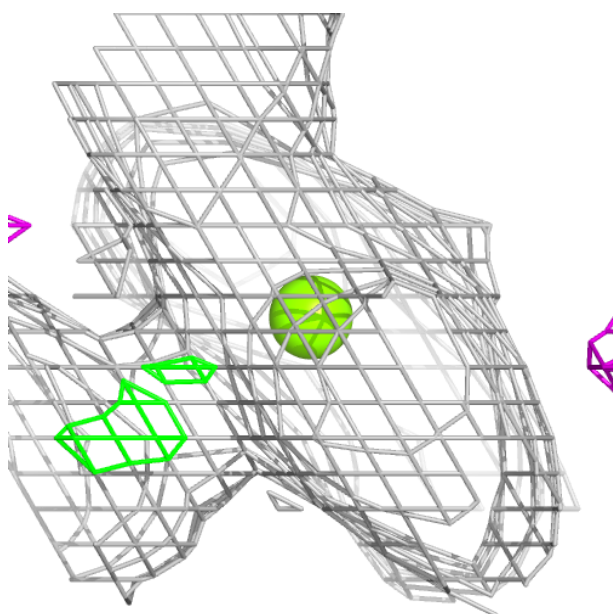
Electron density around CL A 805:

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



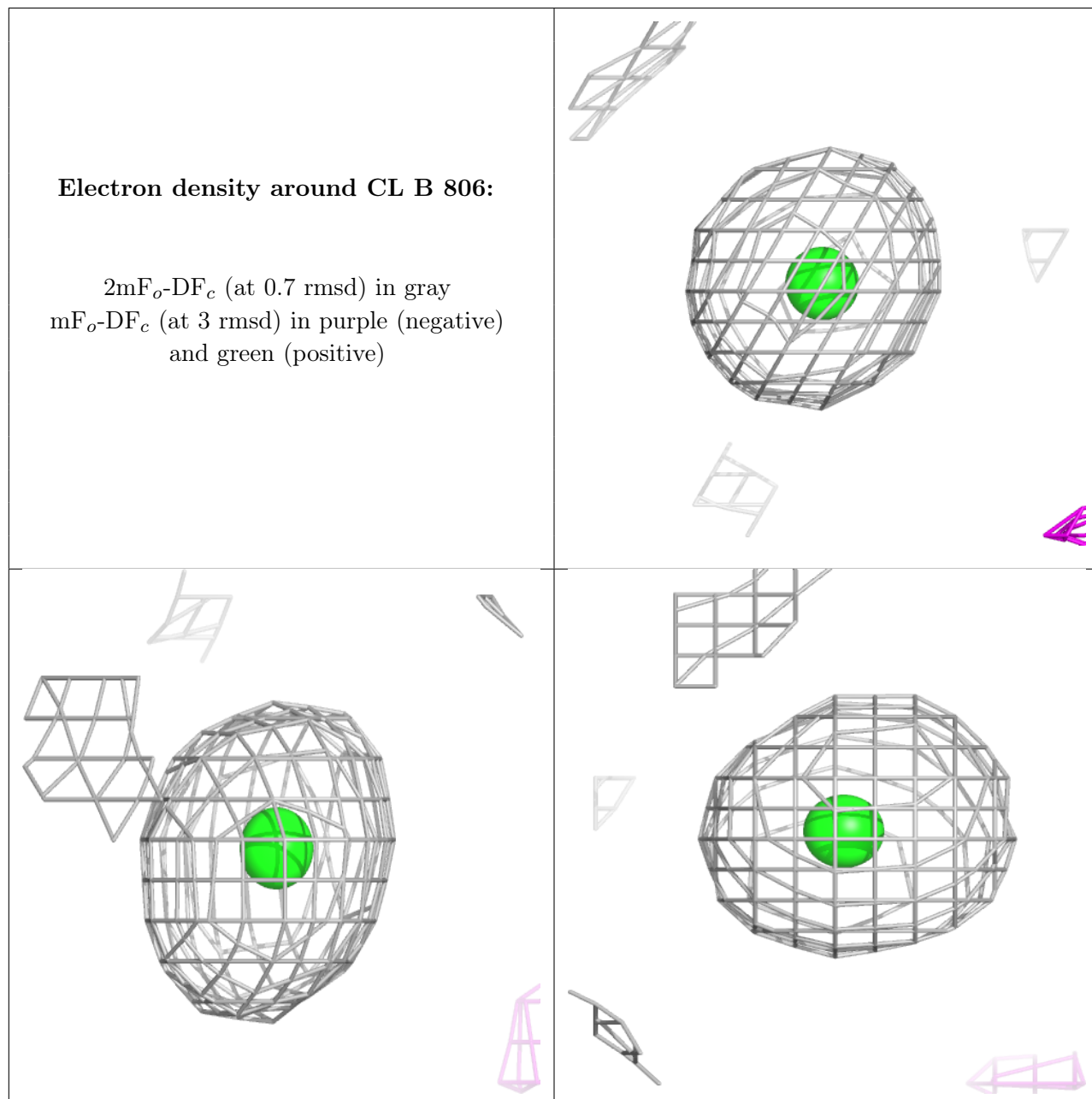
Electron density around MG B 807:

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



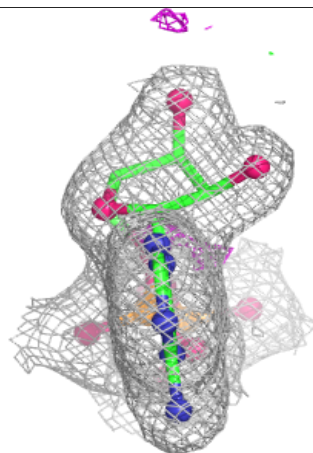
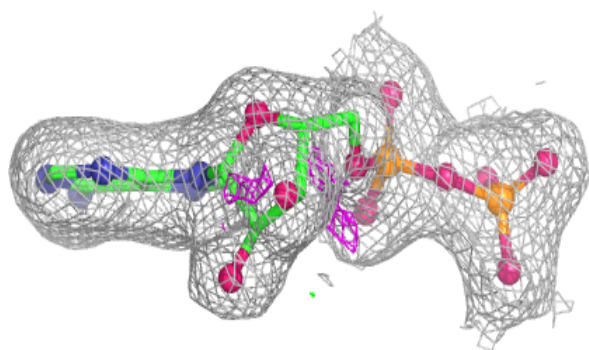
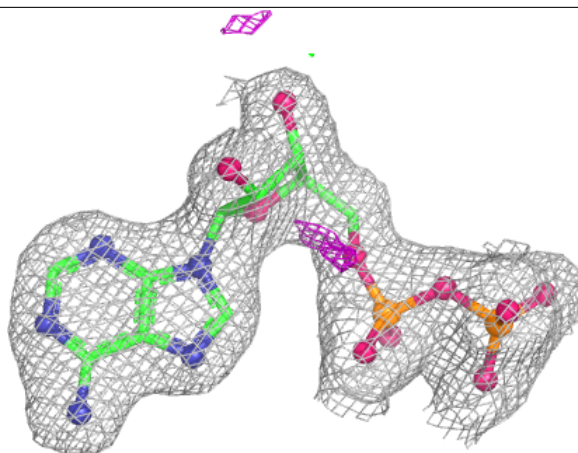
Electron density around CL B 806:

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



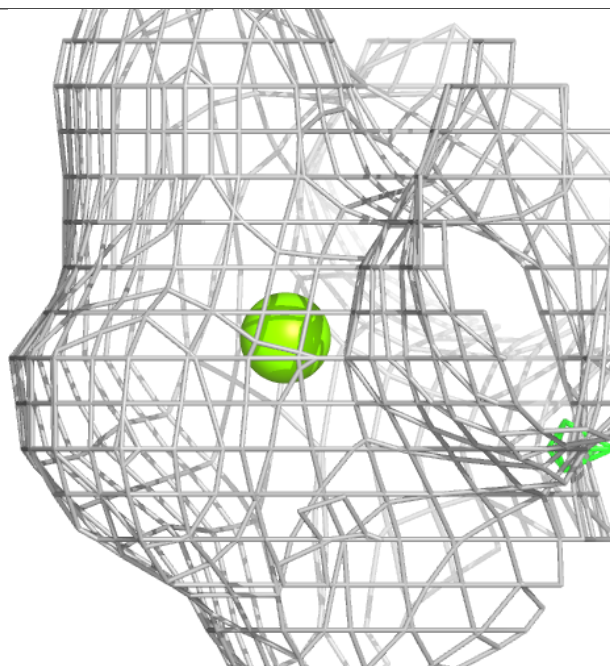
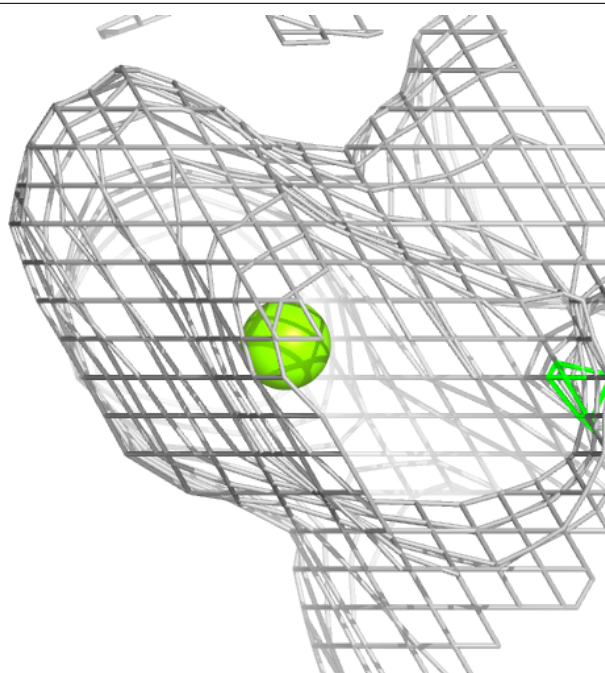
Electron density around ADP B 802:

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



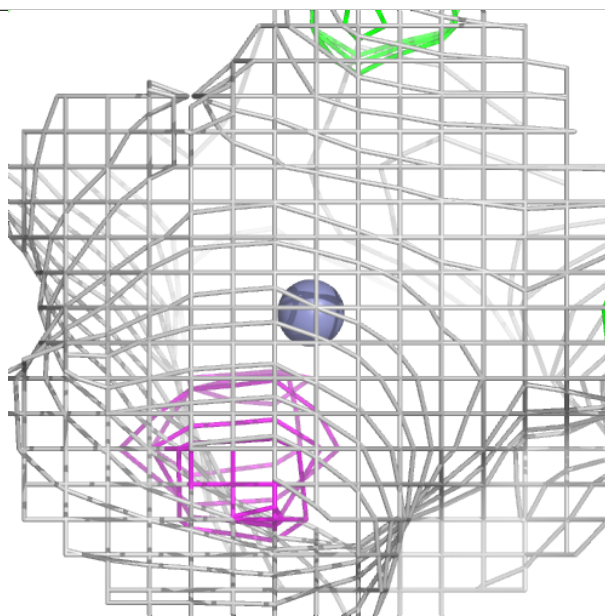
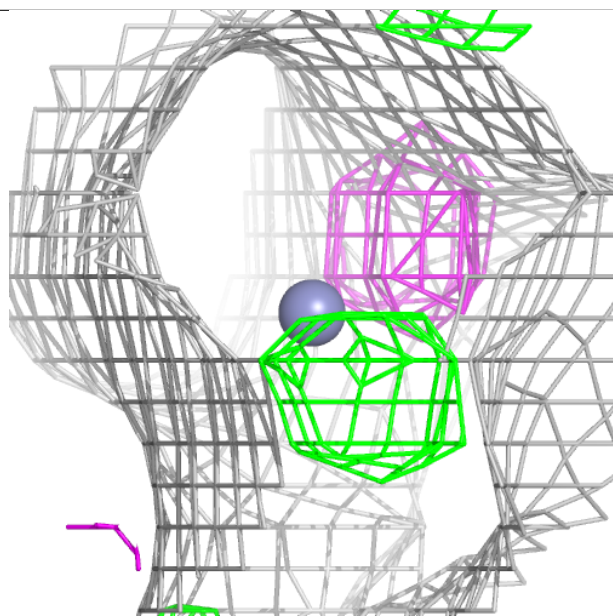
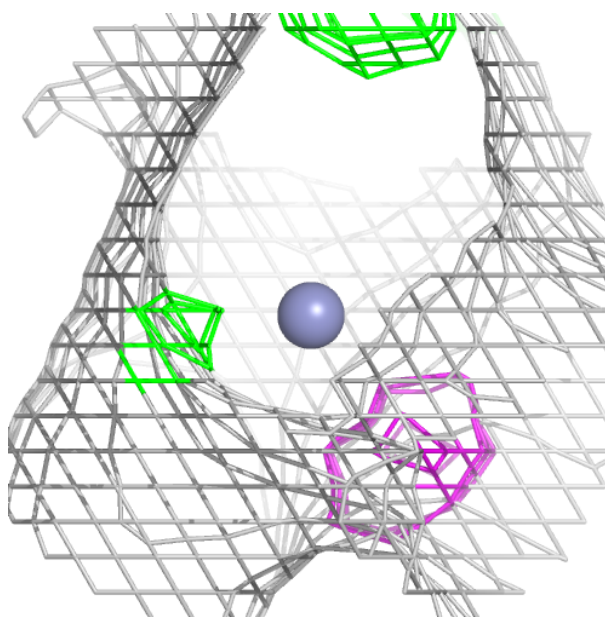
Electron density around MG A 808:

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



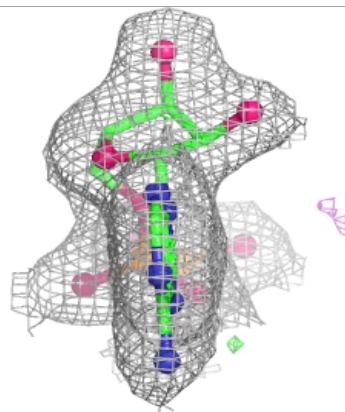
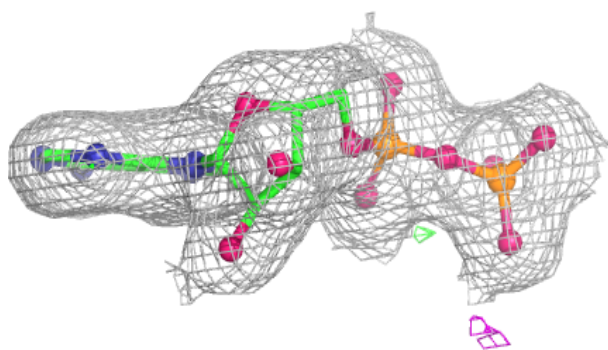
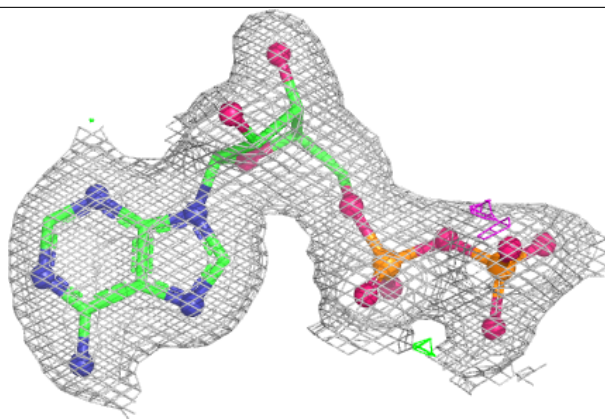
Electron density around ZN A 804:

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



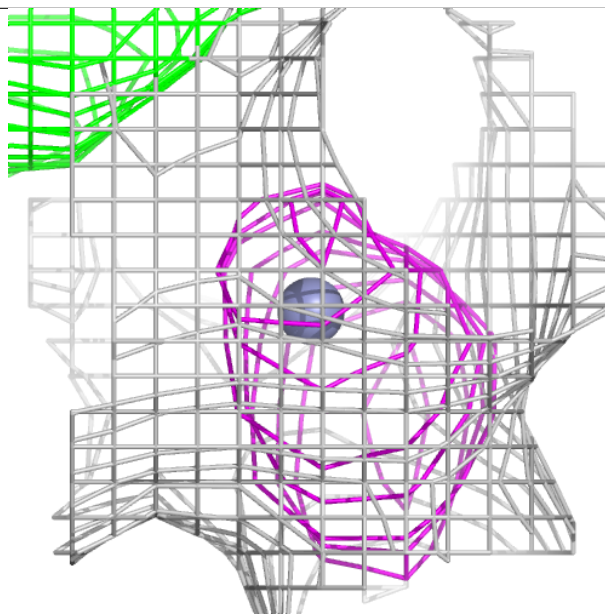
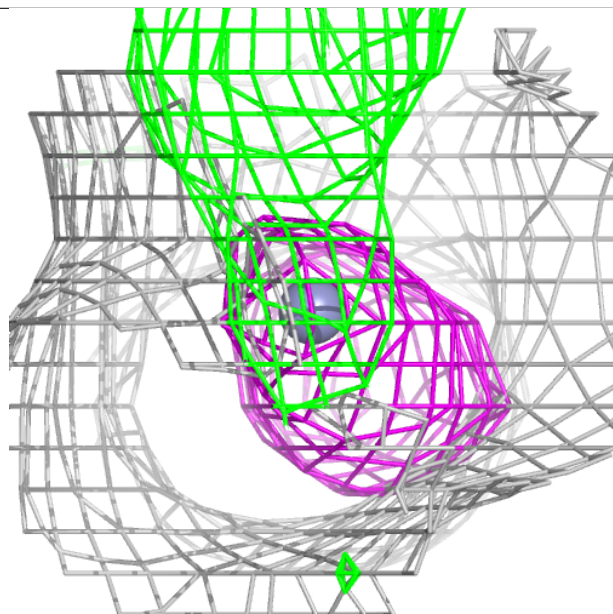
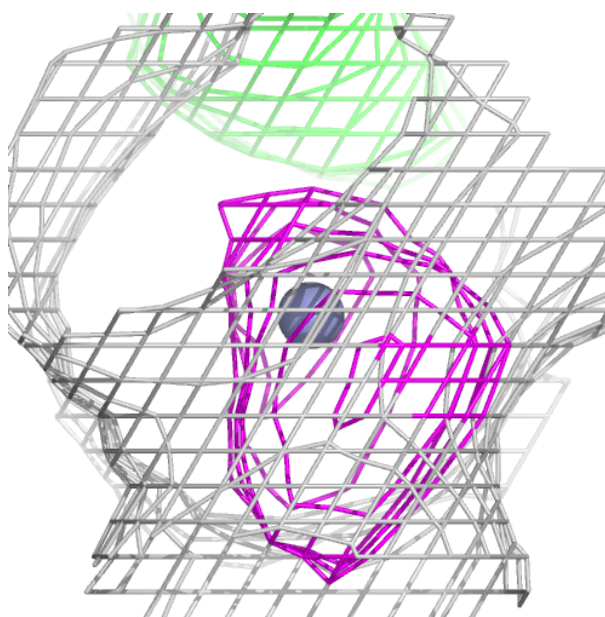
Electron density around ADP A 801:

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



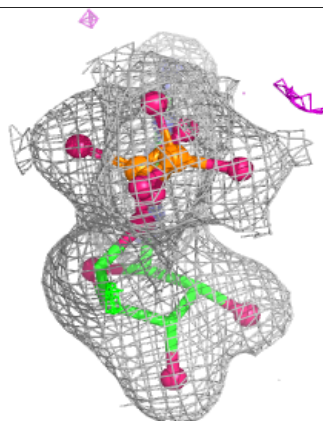
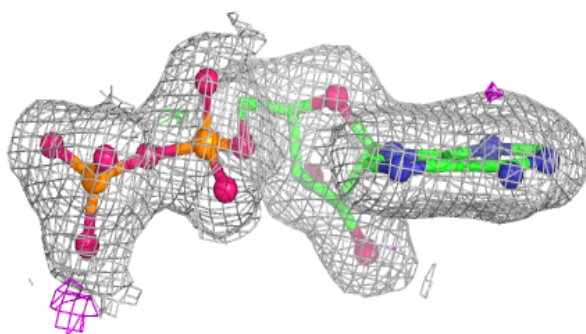
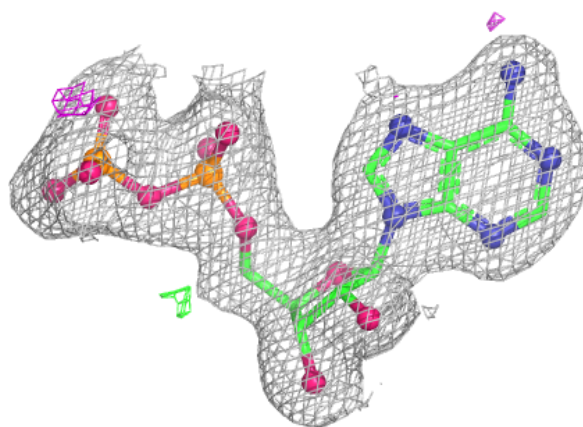
Electron density around ZN A 803:

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



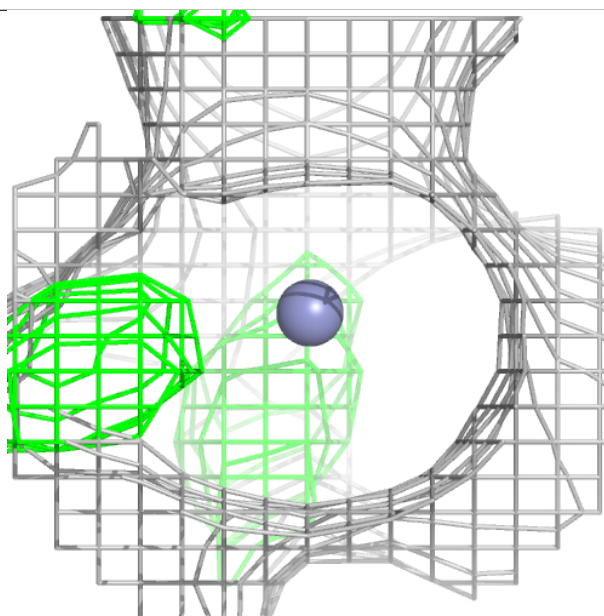
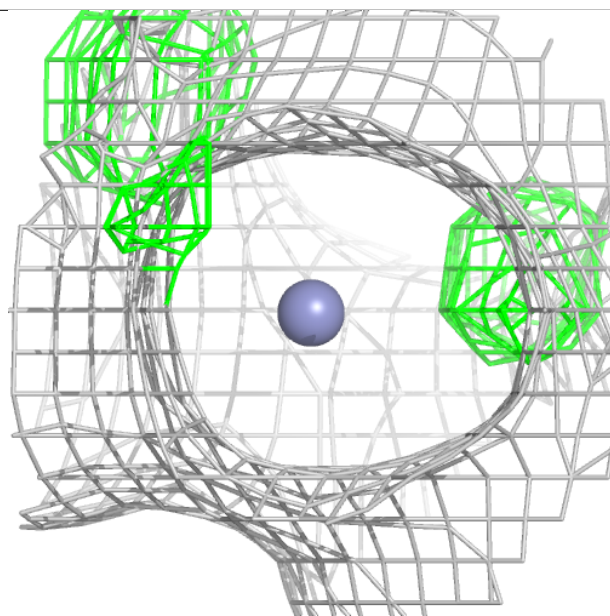
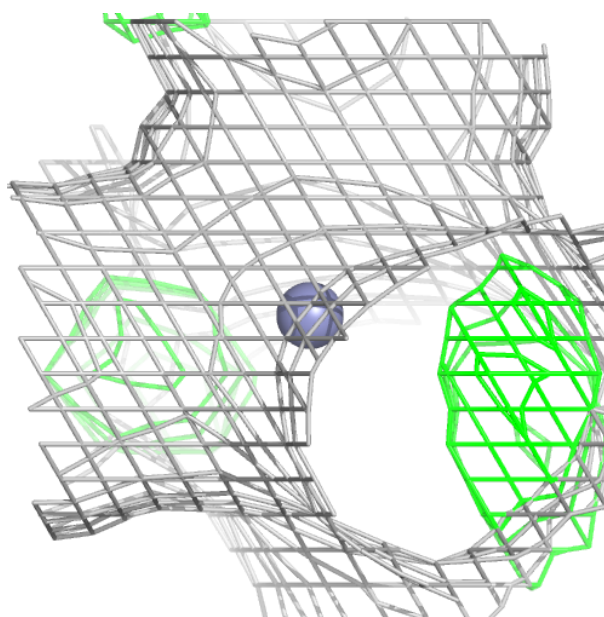
Electron density around ADP A 802:

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



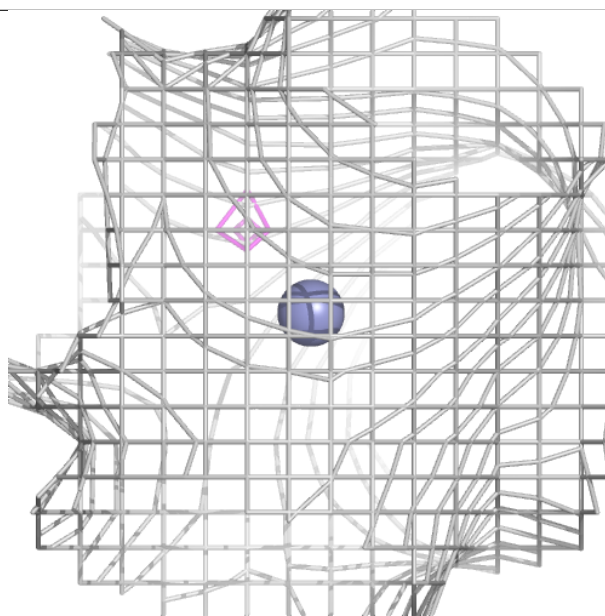
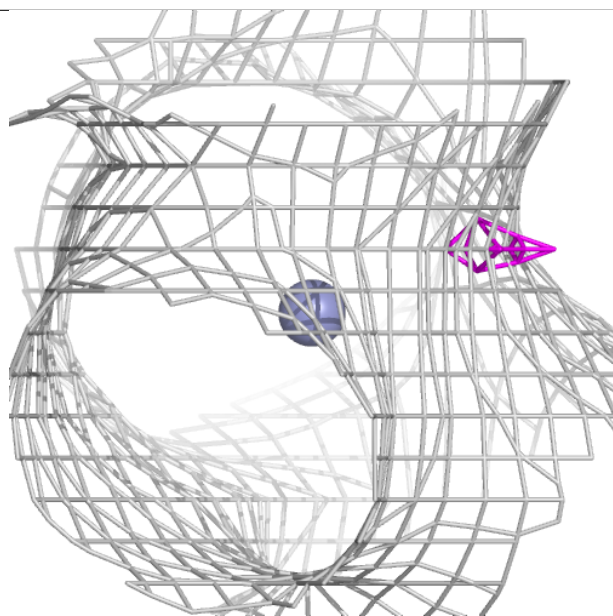
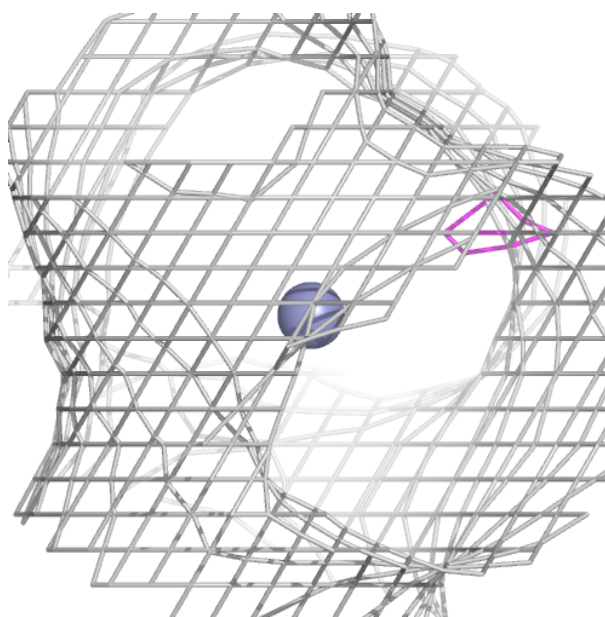
Electron density around ZN B 803:

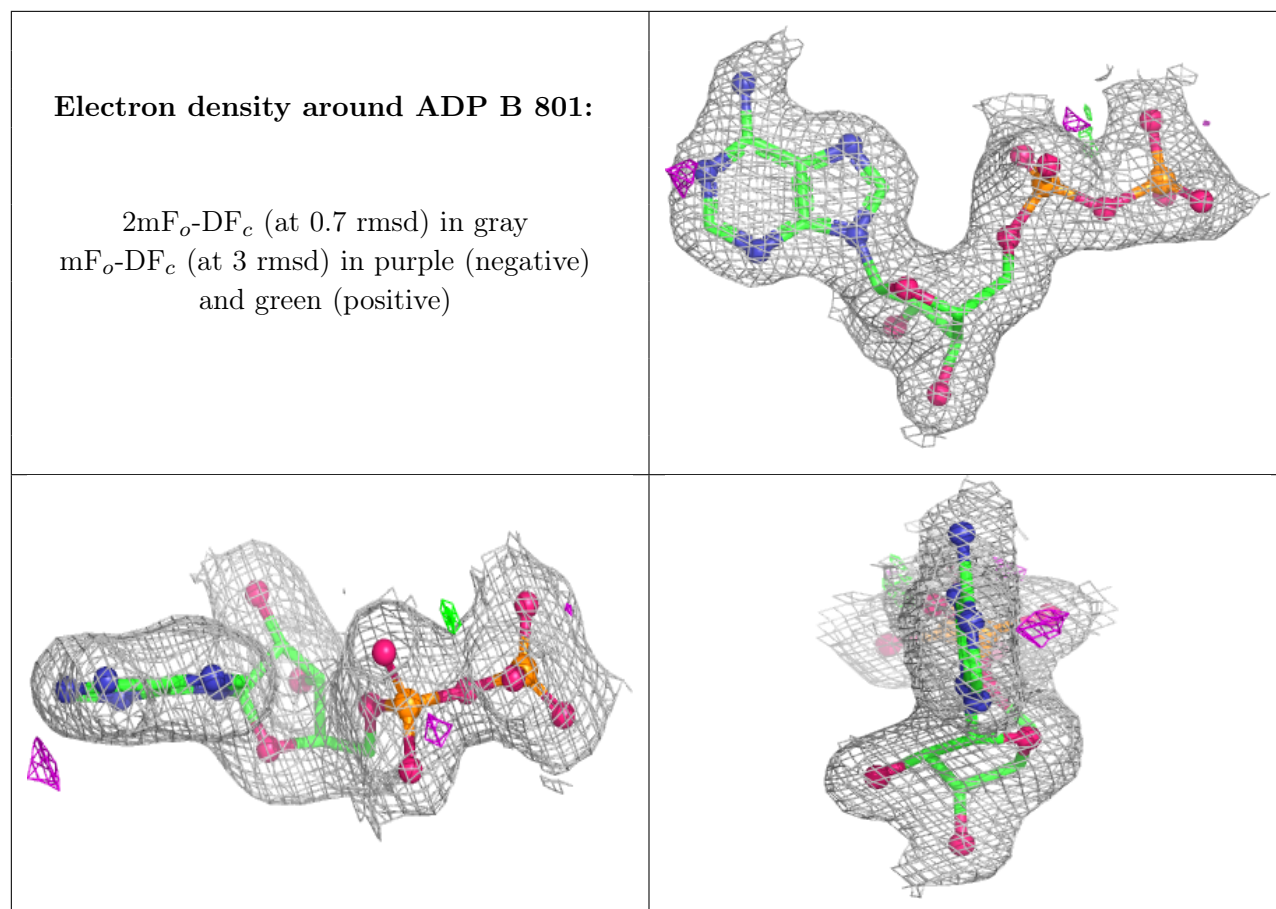
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZN B 804:

$2mF_o-DF_c$ (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.