



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:31 AM UTC

PDB ID : 6WK0 / pdb_00006wk0
Title : Crystal structure of human ribokinase in complex with AMPPCP and ribose
Authors : Park, J.
Deposited on : 2020-04-15
Resolution : 2.00 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

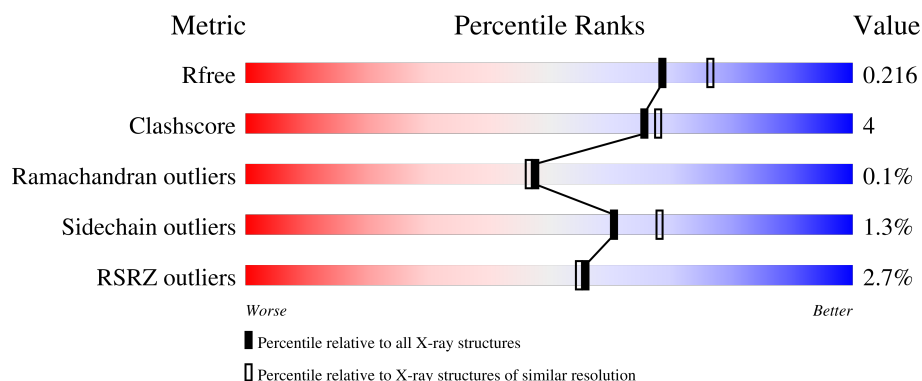
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	317	8% 90% 9%
1	B	317	8% 89% 8% ..
1	C	317	91% 9%
1	D	317	8% 91% 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10510 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 Ribokinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	317	Total	C	N	O	S	0	5	0
			2384	1502	403	462	17			
1	B	311	Total	C	N	O	S	0	3	0
			2307	1457	384	452	14			
1	C	317	Total	C	N	O	S	0	1	0
			2334	1472	391	456	15			
1	D	316	Total	C	N	O	S	0	2	0
			2324	1467	391	452	14			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	323	LEU	-	expression tag	UNP Q9H477
A	324	GLU	-	expression tag	UNP Q9H477
A	325	HIS	-	expression tag	UNP Q9H477
A	326	HIS	-	expression tag	UNP Q9H477
A	327	HIS	-	expression tag	UNP Q9H477
A	328	HIS	-	expression tag	UNP Q9H477
A	329	HIS	-	expression tag	UNP Q9H477
A	330	HIS	-	expression tag	UNP Q9H477
B	323	LEU	-	expression tag	UNP Q9H477
B	324	GLU	-	expression tag	UNP Q9H477
B	325	HIS	-	expression tag	UNP Q9H477
B	326	HIS	-	expression tag	UNP Q9H477
B	327	HIS	-	expression tag	UNP Q9H477
B	328	HIS	-	expression tag	UNP Q9H477
B	329	HIS	-	expression tag	UNP Q9H477
B	330	HIS	-	expression tag	UNP Q9H477
C	323	LEU	-	expression tag	UNP Q9H477
C	324	GLU	-	expression tag	UNP Q9H477
C	325	HIS	-	expression tag	UNP Q9H477
C	326	HIS	-	expression tag	UNP Q9H477
C	327	HIS	-	expression tag	UNP Q9H477

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Chain	Residue	Modelled	Actual	Comment	Reference
C	328	HIS	-	expression tag	UNP Q9H477
C	329	HIS	-	expression tag	UNP Q9H477
C	330	HIS	-	expression tag	UNP Q9H477
D	323	LEU	-	expression tag	UNP Q9H477
D	324	GLU	-	expression tag	UNP Q9H477
D	325	HIS	-	expression tag	UNP Q9H477
D	326	HIS	-	expression tag	UNP Q9H477
D	327	HIS	-	expression tag	UNP Q9H477
D	328	HIS	-	expression tag	UNP Q9H477
D	329	HIS	-	expression tag	UNP Q9H477
D	330	HIS	-	expression tag	UNP Q9H477

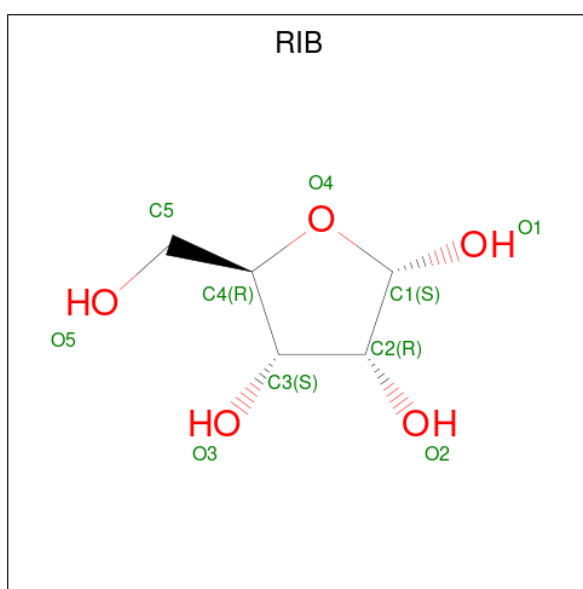
- # ACP
-
- The chemical structure of Adenosine 3'-phosphate (ACP) is shown. It consists of an adenosine moiety (adenine base and ribose sugar) linked to a triphosphate group. The structure includes atom labels (N1, N3, N7, N9, C2, C4, C5, C6, C8, C10, O1, O2, O3, O4, O5, O6, O7, O8, O9, O10, O11, O12, O13, O14, O15, O16, O17, O18, O19, O20, O21, O22, O23, O24, O25, O26, O27, O28, O29, O30, O31, O32, O33, O34, O35, O36, O37, O38, O39, O40, O41, O42, O43, O44, O45, O46, O47, O48, O49, O50, O51, O52, O53, O54, O55, O56, O57, O58, O59, O60, O61, O62, O63, O64, O65, O66, O67, O68, O69, O70, O71, O72, O73, O74, O75, O76, O77, O78, O79, O80, O81, O82, O83, O84, O85, O86, O87, O88, O89, O90, O91, O92, O93, O94, O95, O96, O97, O98, O99, O100) and bond types (single, double, triple, aromatic, coordinate).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 31	C 11	N 5	O 12	P 3	0	0
2	B	1	Total 62	C 22	N 10	O 24	P 6	0	1
2	C	1	Total 31	C 11	N 5	O 12	P 3	0	0
2	D	1	Total 31	C 11	N 5	O 12	P 3	0	0

- 
- WORLD WIDE
PDB
PROTEIN DATA BANK

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Na	0	0
			2	2		
3	B	2	Total	Na	0	0
			2	2		
3	C	2	Total	Na	0	0
			2	2		
3	D	2	Total	Na	0	0
			2	2		

- Molecule 4 is alpha-D-ribofuranose (CCD ID: RIB) (formula: $C_5H_{10}O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			10	5	5		
4	C	1	Total	C	O	0	0
			10	5	5		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	368	Total	O	0	0
			368	368		
5	B	248	Total	O	0	0
			248	248		
5	C	253	Total	O	0	0
			253	253		

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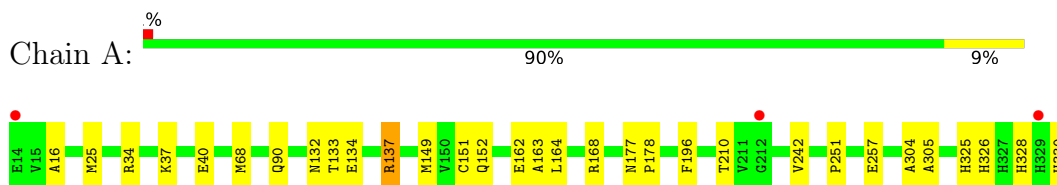
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	109	Total 109	O 109	0	0

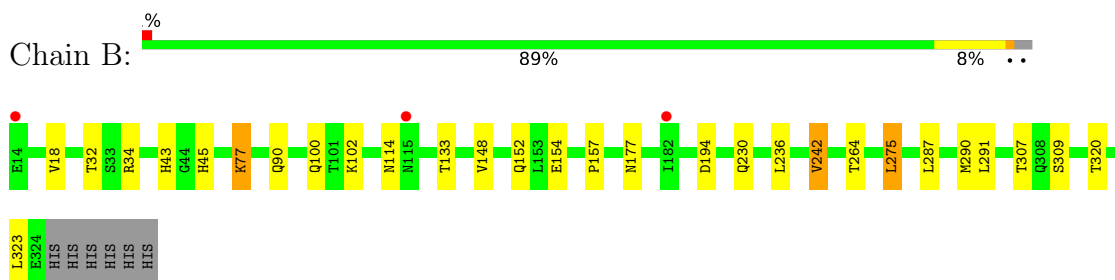
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

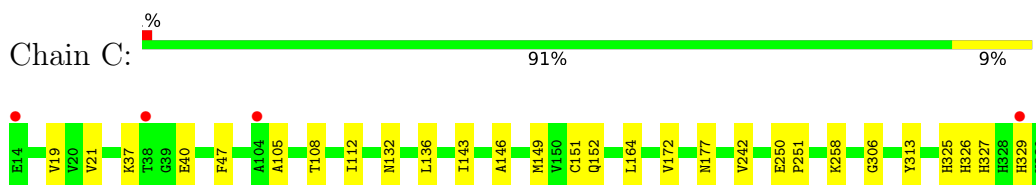
- Molecule 1: Ribokinase



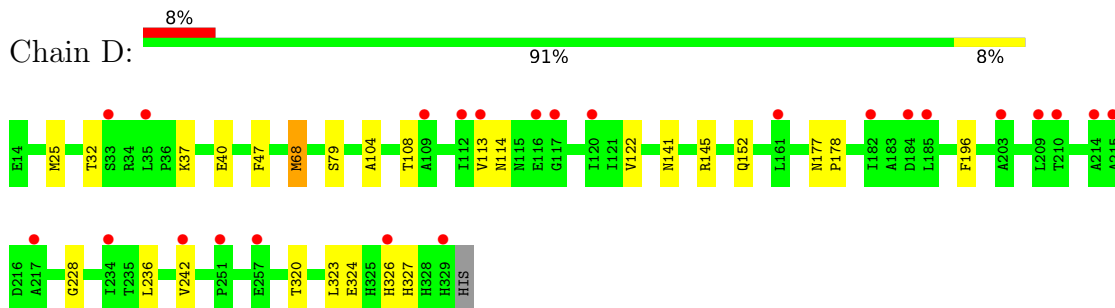
- Molecule 1: Ribokinase



- Molecule 1: Ribokinase



- Molecule 1: Ribokinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	52.02Å 89.35Å 144.70Å 90.00° 98.61° 90.00°	Depositor
Resolution (Å)	51.43 – 2.00 51.43 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.6 (51.43-2.00) 98.6 (51.43-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.197 , 0.239 (Not available) , 0.216	Depositor DCC
R_{free} test set	4355 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	28.7	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 37.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.025 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10510	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% 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: RIB, ACP, NA

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	1.23	7/2423 (0.3%)	1.37	3/3294 (0.1%)
1	B	1.19	3/2340 (0.1%)	1.37	1/3184 (0.0%)
1	C	1.20	7/2373 (0.3%)	1.38	2/3231 (0.1%)
1	D	1.21	8/2361 (0.3%)	1.33	1/3216 (0.0%)
All	All	1.21	25/9497 (0.3%)	1.36	7/12925 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	326	HIS	ND1-CE1	11.02	1.43	1.32
1	D	326	HIS	CG-CD2	9.52	1.46	1.35
1	D	326	HIS	CB-CG	8.85	1.62	1.50
1	C	326	HIS	CE1-NE2	7.57	1.40	1.32
1	D	326	HIS	C-O	6.70	1.31	1.23
1	B	45	HIS	CE1-NE2	6.68	1.39	1.32
1	A	326	HIS	CE1-NE2	6.58	1.39	1.32
1	D	326	HIS	CA-CB	6.37	1.63	1.53
1	A	330	HIS	CE1-NE2	5.97	1.38	1.32
1	C	306	GLY	C-O	5.89	1.32	1.23
1	A	325	HIS	CE1-NE2	5.88	1.38	1.32
1	D	326	HIS	CA-C	5.82	1.60	1.52
1	A	328	HIS	CE1-NE2	5.71	1.38	1.32
1	A	16	ALA	C-O	5.66	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	105	ALA	N-CA	5.63	1.53	1.45
1	A	251	PRO	C-O	-5.57	1.17	1.23
1	C	327	HIS	CE1-NE2	5.41	1.38	1.32
1	C	329	HIS	CE1-NE2	5.38	1.38	1.32
1	D	324	GLU	C-O	5.22	1.31	1.23
1	C	325	HIS	CE1-NE2	5.20	1.37	1.32
1	B	77	LYS	C-O	5.19	1.31	1.23
1	A	304	ALA	C-O	5.17	1.30	1.23
1	C	251	PRO	C-O	-5.10	1.18	1.23
1	D	104	ALA	CA-C	5.03	1.58	1.52
1	B	43	HIS	CD2-NE2	-5.02	1.32	1.37

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	326	HIS	CA-CB-CG	-8.69	105.11	113.80
1	A	257	GLU	CB-CG-CD	5.88	122.59	112.60
1	A	168	ARG	CG-CD-NE	-5.22	100.53	112.00
1	B	133	THR	CA-CB-OG1	-5.21	101.78	109.60
1	A	133	THR	CA-CB-OG1	-5.17	101.84	109.60
1	C	132	ASN	CA-C-N	5.16	127.15	120.44
1	C	132	ASN	C-N-CA	5.16	127.15	120.44

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	305	ALA	Peptide

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	2384	0	2369	23	0
1	B	2307	0	2321	13	0
1	C	2334	0	2297	17	0
1	D	2324	0	2291	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	31	0	14	2	0
2	B	62	0	28	5	0
2	C	31	0	14	1	0
2	D	31	0	14	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	B	10	0	0	1	0
4	C	10	0	0	0	0
5	A	368	0	0	13	2
5	B	248	0	0	6	0
5	C	253	0	0	5	1
5	D	109	0	0	5	0
All	All	10510	0	9348	71	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (71) 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:402[B]:ACP:H3B1	5:B:570:HOH:O	1.62	0.97
1:C:313:TYR:OH	5:C:501:HOH:O	2.00	0.79
1:B:264:THR:O	2:B:402[B]:ACP:H3B2	1.83	0.77
1:D:236:LEU:HD11	1:D:242:VAL:HG23	1.68	0.76
1:A:151[B]:CYS:SG	1:A:164:LEU:HD21	2.26	0.76
1:A:149[A]:MET:HE1	1:A:164:LEU:HD23	1.67	0.76
1:D:141:ASN:HD21	1:D:145:ARG:HH21	1.35	0.75
2:B:402[A]:ACP:O2A	5:B:504:HOH:O	2.10	0.69
1:A:162:GLU:OE2	5:A:501:HOH:O	2.11	0.68
1:A:134:GLU:CD	1:A:137:ARG:HH22	2.02	0.67
1:A:132:ASN:HB2	5:A:718:HOH:O	1.96	0.65
1:C:250:GLU:OE2	5:C:502:HOH:O	2.15	0.64
2:A:401:ACP:O2B	5:A:502:HOH:O	2.16	0.63
1:A:68[A]:MET:HG3	5:A:528:HOH:O	2.00	0.61
1:C:108:THR:HG21	1:D:47:PHE:CD1	2.36	0.61
1:C:108:THR:HG21	1:D:47:PHE:CG	2.35	0.61
1:C:112:ILE:HD12	1:D:122:VAL:HG21	1.84	0.60
1:D:68:MET:HE2	5:D:573:HOH:O	2.02	0.59
1:B:18:VAL:HG22	1:B:148[B]:VAL:CG1	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68[A]:MET:HE2	5:A:528:HOH:O	2.04	0.58
1:A:134:GLU:HG2	5:A:766:HOH:O	2.06	0.56
1:A:90:GLN:CG	5:A:627:HOH:O	2.54	0.55
2:C:402:ACP:O3G	5:C:503:HOH:O	2.18	0.53
1:A:68[A]:MET:CE	5:A:528:HOH:O	2.57	0.52
1:B:77:LYS:HE2	5:B:717:HOH:O	2.09	0.52
1:A:37:LYS:O	1:A:40:GLU:HB2	2.12	0.50
1:C:151[B]:CYS:SG	1:C:164:LEU:HD21	2.51	0.50
1:A:134:GLU:OE2	1:A:137:ARG:NH2	2.45	0.49
1:B:236:LEU:HD11	1:B:242[B]:VAL:HG13	1.94	0.49
2:A:401:ACP:O2A	5:A:503:HOH:O	2.19	0.49
1:D:37:LYS:O	1:D:40:GLU:HB2	2.13	0.49
1:C:37:LYS:O	1:C:40:GLU:HB2	2.12	0.49
1:A:149[A]:MET:CE	1:A:164:LEU:HD23	2.40	0.48
1:B:152:GLN:HA	1:B:177:ASN:O	2.14	0.48
1:C:152:GLN:HA	1:C:177:ASN:O	2.13	0.48
1:D:152:GLN:HA	1:D:177:ASN:O	2.13	0.48
1:B:275:LEU:HD23	1:B:290:MET:SD	2.54	0.48
1:C:21:VAL:HG11	1:C:136:LEU:HD21	1.94	0.48
1:C:108:THR:HG22	5:D:559:HOH:O	2.13	0.48
1:A:68[B]:MET:HE3	5:A:791:HOH:O	2.15	0.47
1:A:210:THR:HG23	5:A:562:HOH:O	2.15	0.46
1:B:90:GLN:HG3	5:B:703:HOH:O	2.15	0.46
1:B:287:LEU:O	1:B:291:LEU:HG	2.14	0.46
1:A:149[A]:MET:HE3	1:A:149[A]:MET:HB3	1.80	0.46
1:C:47:PHE:CD2	1:D:108:THR:HG21	2.51	0.46
1:C:47:PHE:CG	1:D:108:THR:HG21	2.51	0.46
1:A:152:GLN:HA	1:A:177:ASN:O	2.16	0.45
1:A:134:GLU:CD	1:A:137:ARG:NH2	2.74	0.45
1:A:90:GLN:HG3	5:A:627:HOH:O	2.16	0.44
1:B:77:LYS:HG2	1:B:100:GLN:HB3	2.00	0.44
1:C:143:ILE:O	1:C:172:VAL:HG21	2.18	0.44
1:A:149[A]:MET:SD	1:A:151[A]:CYS:SG	3.15	0.44
2:B:402[B]:ACP:C3B	5:B:570:HOH:O	2.42	0.44
1:D:178:PRO:HG3	1:D:196:PHE:CZ	2.53	0.43
1:A:34:ARG:HD3	5:A:790:HOH:O	2.19	0.43
1:D:228:GLY:O	5:D:501:HOH:O	2.21	0.43
1:B:320:THR:HA	1:B:323:LEU:HD12	2.00	0.43
2:B:402[A]:ACP:O2G	5:B:505:HOH:O	2.21	0.43
1:C:258:LYS:HD3	5:C:716:HOH:O	2.19	0.42
1:C:40:GLU:HA	5:C:532:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:113:VAL:HG12	5:D:502:HOH:O	2.18	0.42
1:B:154:GLU:OE2	4:B:401:RIB:O1	2.38	0.42
1:D:32:THR:O	1:D:114:ASN:HA	2.20	0.42
1:A:149[A]:MET:HE2	1:A:163:ALA:O	2.19	0.41
1:A:178:PRO:HG3	1:A:196:PHE:CZ	2.55	0.41
1:B:32:THR:O	1:B:114:ASN:HA	2.20	0.41
1:C:149:MET:HE2	1:C:149:MET:HB2	1.85	0.41
1:D:327:HIS:HA	5:D:547:HOH:O	2.20	0.41
1:D:320:THR:HA	1:D:323:LEU:HD12	2.03	0.41
1:C:19:VAL:HG23	1:C:146:ALA:HB2	2.03	0.41
1:B:194:ASP:O	1:B:230:GLN:HB2	2.22	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:699:HOH:O	5:C:688:HOH:O[1_455]	2.15	0.05
5:A:842:HOH:O	5:A:867:HOH:O[1_455]	2.16	0.04

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	320/317 (101%)	313 (98%)	7 (2%)	0	100	100
1	B	312/317 (98%)	308 (99%)	3 (1%)	1 (0%)	36	35
1	C	316/317 (100%)	311 (98%)	5 (2%)	0	100	100
1	D	316/317 (100%)	310 (98%)	6 (2%)	0	100	100
All	All	1264/1268 (100%)	1242 (98%)	21 (2%)	1 (0%)	48	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	307	THR

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	256/256 (100%)	253 (99%)	3 (1%)	63	70
1	B	249/256 (97%)	242 (97%)	7 (3%)	38	41
1	C	247/256 (96%)	246 (100%)	1 (0%)	84	89
1	D	244/256 (95%)	241 (99%)	3 (1%)	63	70
All	All	996/1024 (97%)	982 (99%)	14 (1%)	61	66

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	MET
1	A	137	ARG
1	A	242	VAL
1	B	34	ARG
1	B	102	LYS
1	B	157	PRO
1	B	242[A]	VAL
1	B	242[B]	VAL
1	B	275	LEU
1	B	309	SER
1	C	242	VAL
1	D	25	MET
1	D	68	MET
1	D	79	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	HIS
1	C	43	HIS

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Mol	Chain	Res	Type
1	C	141	ASN
1	C	328	HIS
1	C	329	HIS
1	D	118	GLN
1	D	141	ASN

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, 8 are monoatomic - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ACP	D	401	3	31,33,33	1.67	7 (22%)	47,52,52	1.81	9 (19%)
4	RIB	C	401	-	10,10,10	0.64	0	13,14,14	1.39	2 (15%)
2	ACP	B	402[A]	3	31,33,33	1.64	8 (25%)	47,52,52	1.65	10 (21%)
2	ACP	B	402[B]	-	31,33,33	1.92	8 (25%)	47,52,52	1.52	9 (19%)
2	ACP	C	402	3	31,33,33	1.86	10 (32%)	47,52,52	2.06	11 (23%)
4	RIB	B	401	-	10,10,10	0.76	0	13,14,14	2.13	2 (15%)
2	ACP	A	401	3	31,33,33	2.15	8 (25%)	47,52,52	2.03	12 (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	ACP	D	401	3	-	2/19/38/38	0/3/3/3
4	RIB	C	401	-	-	0/2/18/18	0/1/1/1
2	ACP	B	402[A]	3	-	1/19/38/38	0/3/3/3
2	ACP	B	402[B]	-	-	3/19/38/38	0/3/3/3
2	ACP	C	402	3	-	2/19/38/38	0/3/3/3
4	RIB	B	401	-	-	0/2/18/18	0/1/1/1
2	ACP	A	401	3	-	4/19/38/38	0/3/3/3

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	ACP	PB-O3A	6.56	1.65	1.58
2	B	402[B]	ACP	PB-O3A	5.98	1.65	1.58
2	C	402	ACP	PB-O3A	5.26	1.64	1.58
2	D	401	ACP	C5-C4	4.68	1.47	1.39
2	A	401	ACP	PG-O2G	4.64	1.65	1.55
2	C	402	ACP	C5-C4	4.35	1.46	1.39
2	D	401	ACP	PG-O3G	4.16	1.64	1.55
2	B	402[A]	ACP	C5-C4	4.09	1.46	1.39
2	B	402[B]	ACP	C5-C4	4.03	1.46	1.39
2	C	402	ACP	PG-O2G	3.87	1.63	1.55
2	A	401	ACP	C5-C4	3.81	1.45	1.39
2	A	401	ACP	PG-O3G	3.67	1.63	1.55
2	B	402[A]	ACP	PB-O3A	3.46	1.62	1.58
2	B	402[B]	ACP	PA-O3A	3.22	1.63	1.59
2	B	402[B]	ACP	C4-N9	-3.15	1.31	1.37
2	A	401	ACP	PA-O3A	-3.15	1.56	1.59
2	B	402[B]	ACP	PG-O3G	3.15	1.62	1.55
2	B	402[A]	ACP	C4-N9	-3.15	1.31	1.37
2	A	401	ACP	C5-C6	3.13	1.49	1.41
2	A	401	ACP	PB-O1B	2.95	1.58	1.51
2	D	401	ACP	PG-O2G	2.93	1.61	1.55
2	B	402[B]	ACP	PG-O2G	2.88	1.61	1.55
2	B	402[A]	ACP	PG-O3G	2.86	1.61	1.55
2	D	401	ACP	C5-N7	-2.70	1.34	1.39
2	C	402	ACP	PB-O2B	2.62	1.62	1.56
2	C	402	ACP	PG-O3G	2.55	1.60	1.55
2	D	401	ACP	C5-C6	2.52	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	402[B]	ACP	C5-N7	-2.40	1.34	1.39
2	C	402	ACP	C8-N7	2.40	1.36	1.31
2	B	402[A]	ACP	C5-N7	-2.39	1.34	1.39
2	B	402[A]	ACP	PB-O2B	2.31	1.62	1.56
2	C	402	ACP	PA-O3A	-2.25	1.57	1.59
2	D	401	ACP	PB-O3A	2.18	1.60	1.58
2	C	402	ACP	C5-C6	2.16	1.47	1.41
2	B	402[A]	ACP	PG-O2G	2.14	1.59	1.55
2	C	402	ACP	C4-N9	-2.13	1.33	1.37
2	D	401	ACP	C8-N7	2.10	1.35	1.31
2	C	402	ACP	C5-N7	-2.08	1.35	1.39
2	A	401	ACP	C8-N7	2.02	1.35	1.31
2	B	402[A]	ACP	C5-C6	2.01	1.46	1.41
2	B	402[B]	ACP	C5-C6	2.00	1.46	1.41

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	ACP	C5-C4-N3	-6.51	117.75	126.72
4	B	401	RIB	O1-C1-O4	-6.33	103.05	111.12
2	D	401	ACP	C5-C4-N3	-5.84	118.67	126.72
2	C	402	ACP	C5-C4-N3	-5.50	119.14	126.72
2	A	401	ACP	N3-C4-N9	5.38	136.32	127.17
2	C	402	ACP	N3-C4-N9	4.88	135.47	127.17
2	D	401	ACP	N3-C4-N9	4.69	135.14	127.17
2	C	402	ACP	O2G-PG-C3B	4.32	116.88	106.40
2	A	401	ACP	C2-N3-C4	4.29	122.30	111.83
2	C	402	ACP	N3-C2-N1	-4.09	122.40	128.58
2	C	402	ACP	C2-N3-C4	4.08	121.81	111.83
2	B	402[A]	ACP	C5-C4-N3	-3.90	121.35	126.72
2	A	401	ACP	O2A-PA-O3A	3.84	117.65	107.27
2	D	401	ACP	C2-N3-C4	3.80	121.12	111.83
2	B	402[B]	ACP	C5-C4-N3	-3.80	121.48	126.72
2	D	401	ACP	N3-C2-N1	-3.77	122.87	128.58
2	B	402[A]	ACP	N3-C2-N1	-3.67	123.03	128.58
2	B	402[B]	ACP	N3-C2-N1	-3.64	123.08	128.58
4	C	401	RIB	O1-C1-O4	-3.63	106.50	111.12
2	B	402[A]	ACP	N3-C4-N9	3.54	133.19	127.17
2	B	402[A]	ACP	C4-N9-C8	3.47	109.38	105.74
2	A	401	ACP	O3A-PA-O1A	-3.45	100.33	110.70
2	B	402[B]	ACP	N3-C4-N9	3.43	133.00	127.17
2	B	402[B]	ACP	C4-N9-C8	3.38	109.28	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	401	RIB	O4-C1-C2	3.29	109.24	104.67
2	C	402	ACP	O2A-PA-O3A	3.23	116.01	107.27
2	C	402	ACP	C4-N9-C8	3.16	109.06	105.74
2	A	401	ACP	N3-C2-N1	-3.05	123.96	128.58
2	C	402	ACP	O1G-PG-C3B	-3.04	104.75	111.37
2	D	401	ACP	C4-C5-N7	-3.03	107.12	110.58
2	B	402[A]	ACP	C2-N3-C4	2.92	118.96	111.83
2	A	401	ACP	PB-O3A-PA	-2.90	122.91	132.37
2	C	402	ACP	O2G-PG-O1G	-2.86	104.98	112.39
2	B	402[B]	ACP	C2-N3-C4	2.84	118.78	111.83
2	B	402[B]	ACP	C2-N1-C6	2.72	123.20	118.73
2	A	401	ACP	O1G-PG-C3B	-2.68	105.53	111.37
2	B	402[A]	ACP	C2-N1-C6	2.67	123.12	118.73
2	B	402[A]	ACP	O3G-PG-C3B	2.67	112.88	106.40
2	A	401	ACP	C4-N9-C8	2.59	108.46	105.74
2	A	401	ACP	C4-C5-N7	-2.54	107.67	110.58
2	D	401	ACP	C5-N7-C8	2.47	107.34	103.45
4	C	401	RIB	O4-C1-C2	2.45	108.07	104.67
2	C	402	ACP	N9-C8-N7	-2.41	110.51	113.94
2	B	402[A]	ACP	O2B-PB-C3B	2.41	116.69	106.73
2	D	401	ACP	PB-O3A-PA	-2.40	124.54	132.37
2	B	402[B]	ACP	O1B-PB-C3B	2.27	115.02	109.05
2	D	401	ACP	C4-N9-C8	2.26	108.11	105.74
2	C	402	ACP	C5-C6-N6	-2.24	117.74	123.29
2	A	401	ACP	O3G-PG-O2G	2.20	114.24	107.96
2	D	401	ACP	C2-N1-C6	2.20	122.35	118.73
2	B	402[A]	ACP	N9-C8-N7	-2.20	110.82	113.94
2	B	402[B]	ACP	N9-C8-N7	-2.16	110.88	113.94
2	A	401	ACP	C5-C6-N6	-2.09	118.11	123.29
2	B	402[B]	ACP	N6-C6-N1	2.09	123.02	118.38
2	B	402[A]	ACP	N6-C6-N1	2.07	122.98	118.38

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	402[B]	ACP	O4'-C4'-C5'-O5'
2	B	402[B]	ACP	C3'-C4'-C5'-O5'
2	D	401	ACP	O4'-C4'-C5'-O5'
2	D	401	ACP	C3'-C4'-C5'-O5'
2	A	401	ACP	C5'-O5'-PA-O1A
2	B	402[B]	ACP	PG-C3B-PB-O2B

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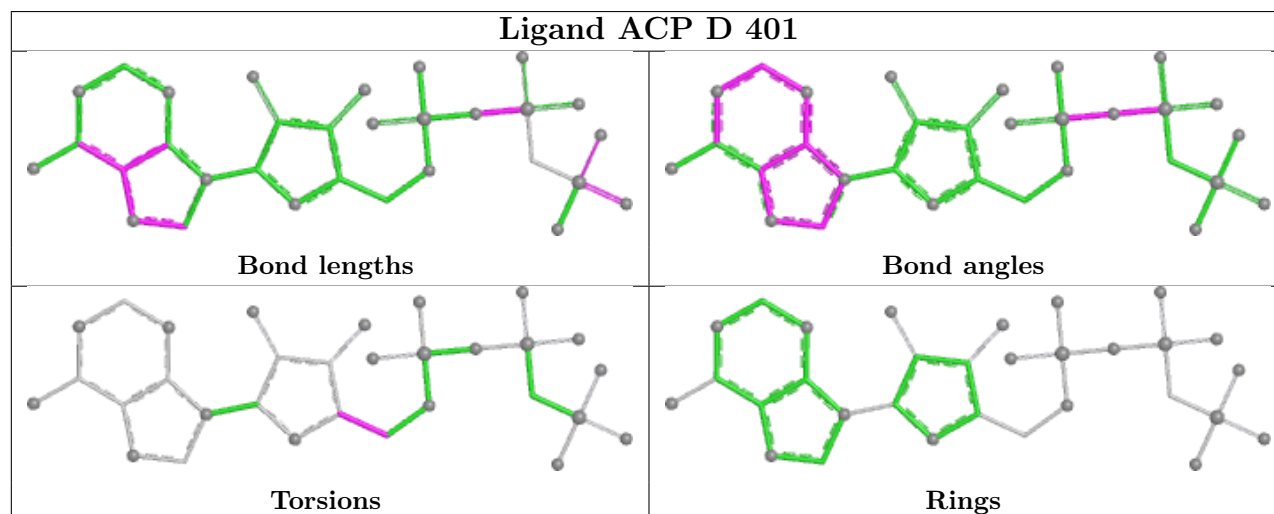
Mol	Chain	Res	Type	Atoms
2	C	402	ACP	C5'-O5'-PA-O1A
2	A	401	ACP	PB-O3A-PA-O1A
2	A	401	ACP	PB-O3A-PA-O2A
2	C	402	ACP	PB-O3A-PA-O2A
2	B	402[A]	ACP	PG-C3B-PB-O1B
2	A	401	ACP	PB-C3B-PG-O1G

There are no ring outliers.

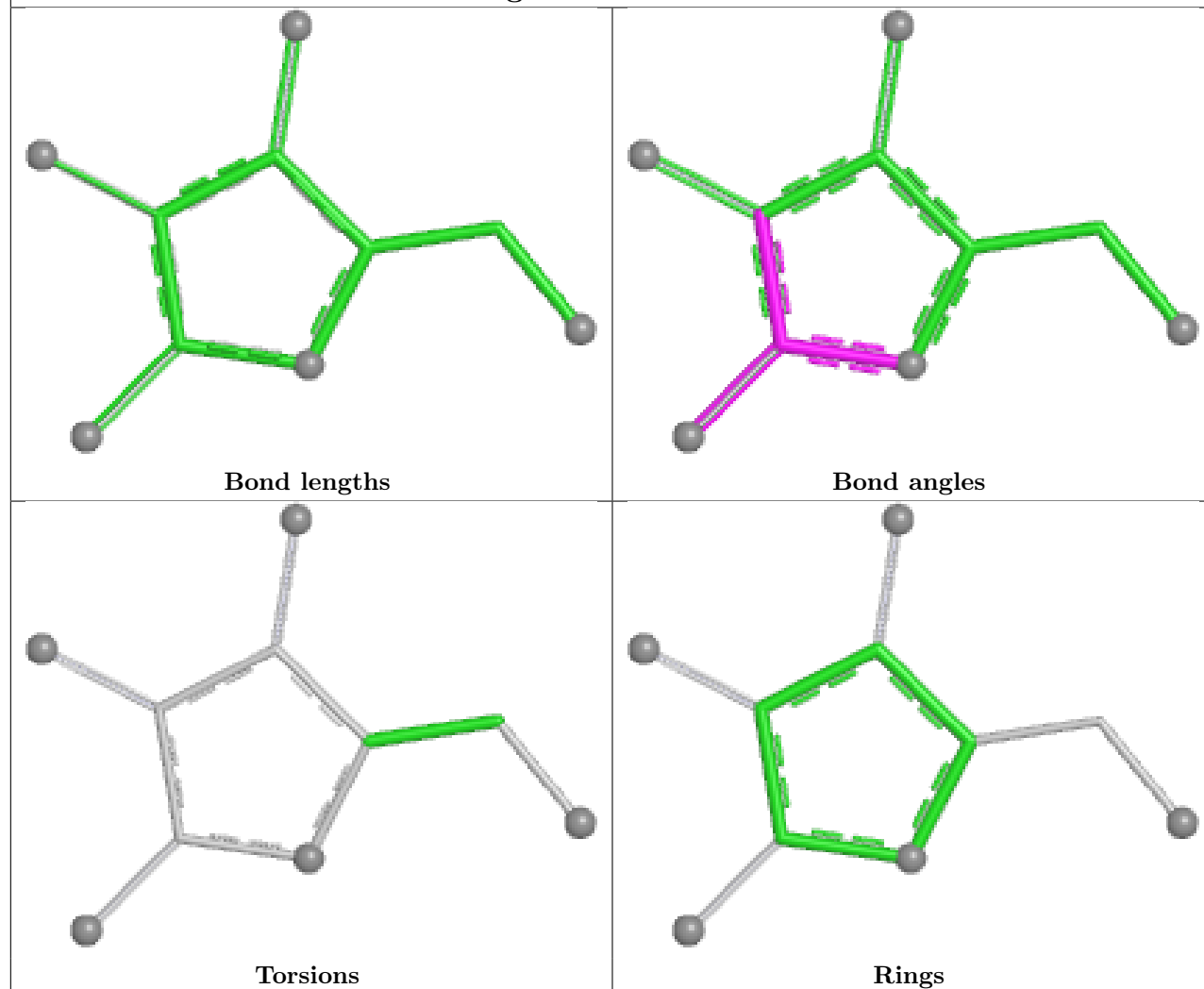
5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	402[A]	ACP	2	0
2	B	402[B]	ACP	3	0
2	C	402	ACP	1	0
4	B	401	RIB	1	0
2	A	401	ACP	2	0

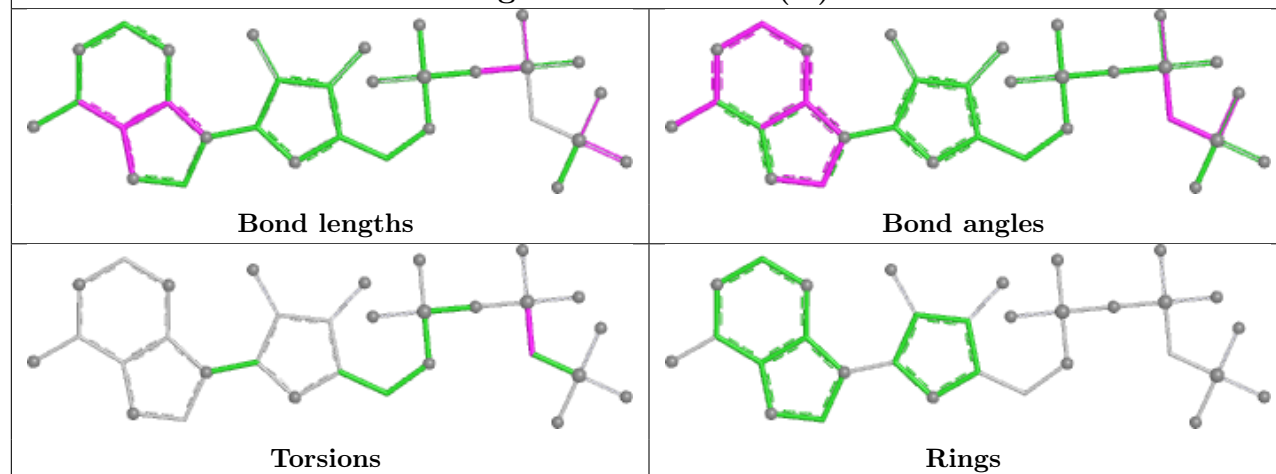
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



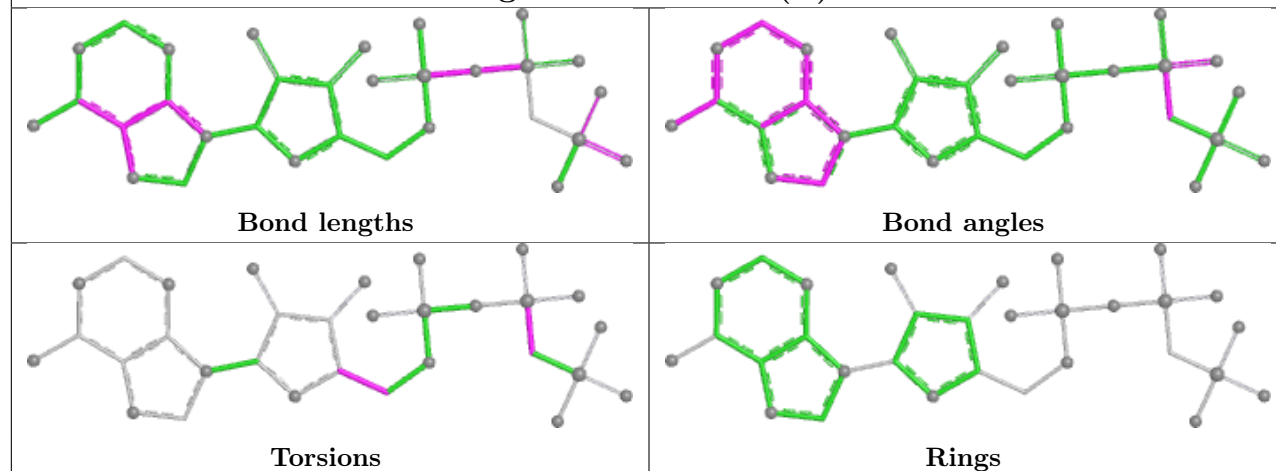
Ligand RIB C 401



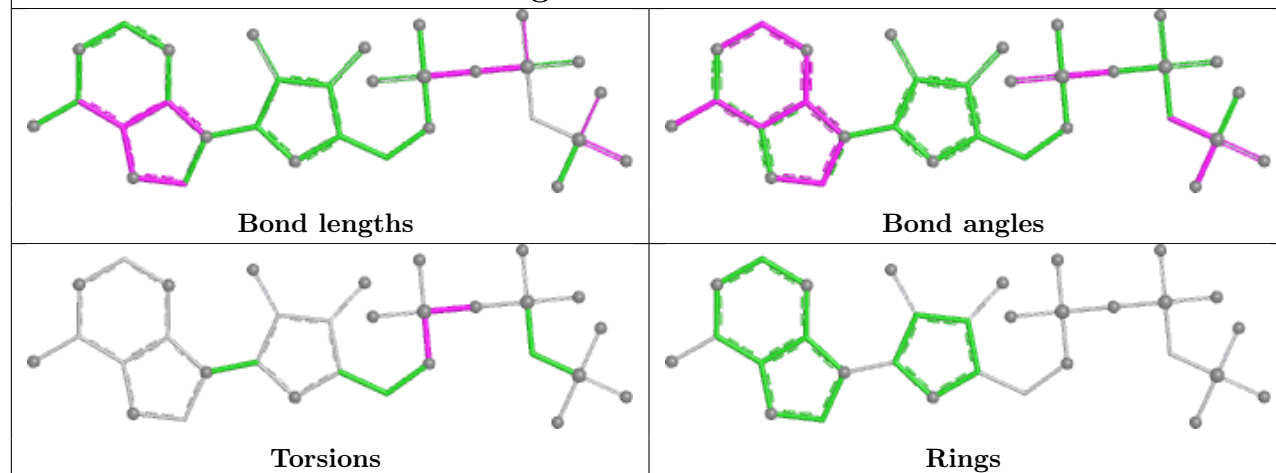
Ligand ACP B 402 (A)

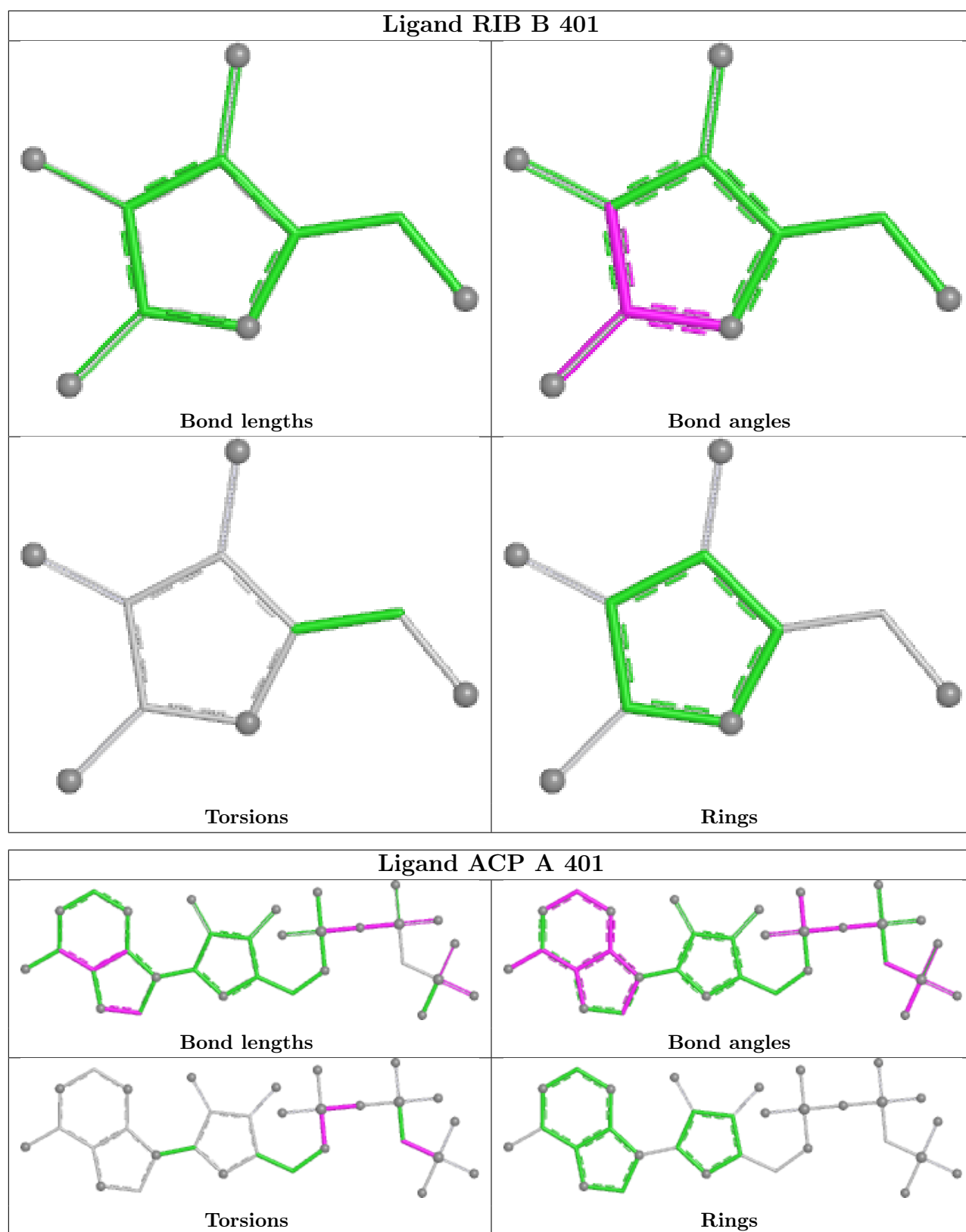


Ligand ACP B 402 (B)



Ligand ACP C 402





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	317/317 (100%)	-0.15	3 (0%) 81 80	12, 30, 54, 80	5 (1%)
1	B	311/317 (98%)	-0.06	3 (0%) 79 79	16, 34, 57, 70	3 (0%)
1	C	317/317 (100%)	0.01	4 (1%) 75 74	13, 35, 61, 86	1 (0%)
1	D	316/317 (99%)	0.74	24 (7%) 20 18	23, 57, 102, 121	2 (0%)
All	All	1261/1268 (99%)	0.14	34 (2%) 56 55	12, 38, 78, 121	11 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	120	ILE	3.8
1	D	329	HIS	3.5
1	D	112	ILE	3.5
1	D	203	ALA	2.9
1	D	214	ALA	2.7
1	D	234	ILE	2.7
1	D	210	THR	2.7
1	A	212	GLY	2.6
1	D	184	ASP	2.6
1	D	185	LEU	2.6
1	D	242	VAL	2.5
1	D	257	GLU	2.5
1	D	113	VAL	2.4
1	A	329	HIS	2.4
1	D	209	LEU	2.4
1	D	251	PRO	2.4
1	D	217	ALA	2.4
1	B	182	ILE	2.3
1	C	104	ALA	2.3
1	D	35	LEU	2.3
1	D	326	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	14	GLU	2.2
1	C	14	GLU	2.2
1	D	33	SER	2.2
1	D	117	GLY	2.2
1	C	38	THR	2.2
1	D	182	ILE	2.1
1	D	215	ALA	2.1
1	D	161	LEU	2.1
1	C	329	HIS	2.1
1	D	116	GLU	2.1
1	B	115	ASN	2.1
1	D	109	ALA	2.1
1	B	14	GLU	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.

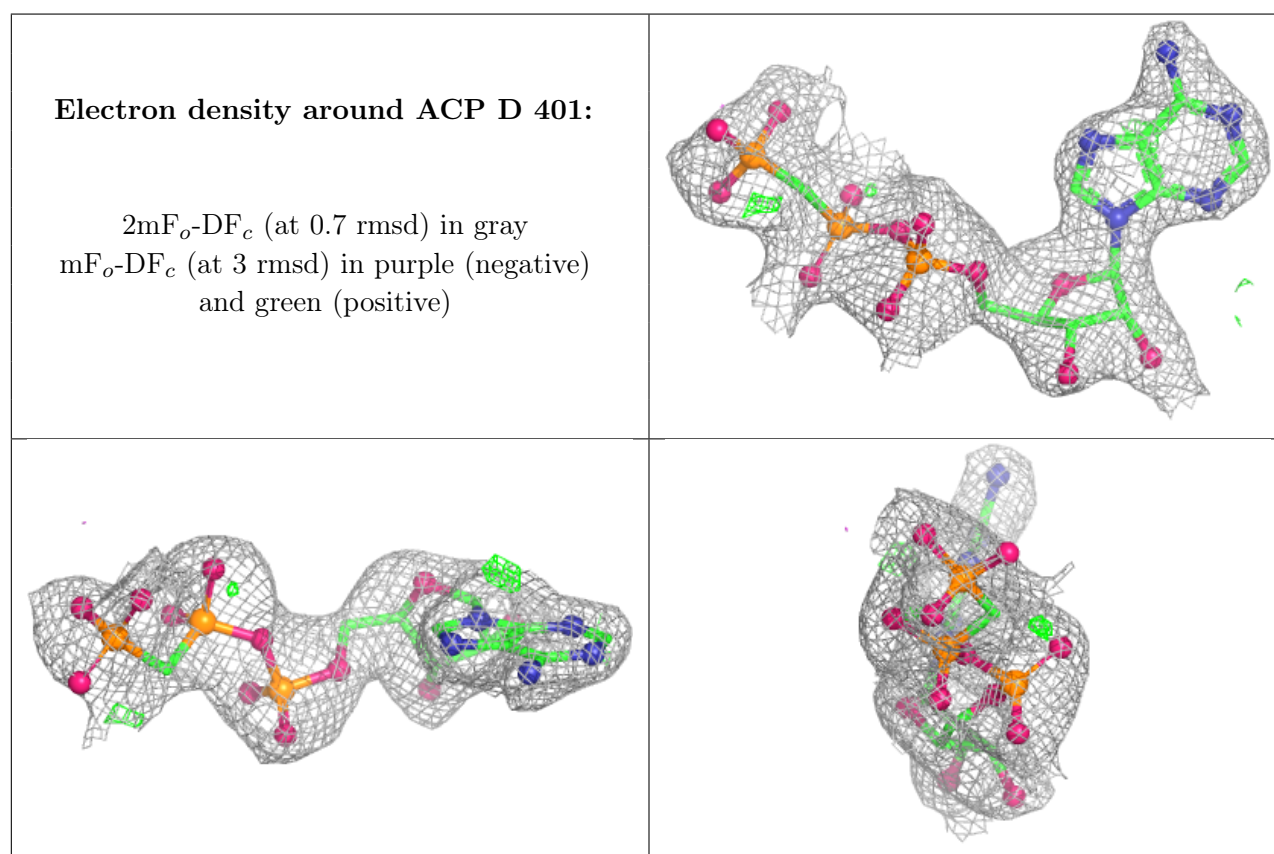
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ACP	D	401	31/31	0.90	0.09	54,70,79,92	0
3	NA	D	402	1/1	0.91	0.07	55,55,55,55	0
3	NA	B	404	1/1	0.92	0.09	48,48,48,48	0
2	ACP	B	402[B]	31/31	0.94	0.07	25,28,40,51	31
2	ACP	B	402[A]	31/31	0.94	0.07	25,28,38,42	31
3	NA	D	403	1/1	0.94	0.07	54,54,54,54	0
2	ACP	A	401	31/31	0.95	0.06	21,27,40,47	0
2	ACP	C	402	31/31	0.95	0.07	24,29,48,48	0
4	RIB	B	401	10/10	0.95	0.07	23,26,30,33	0
4	RIB	C	401	10/10	0.95	0.07	25,29,31,31	0

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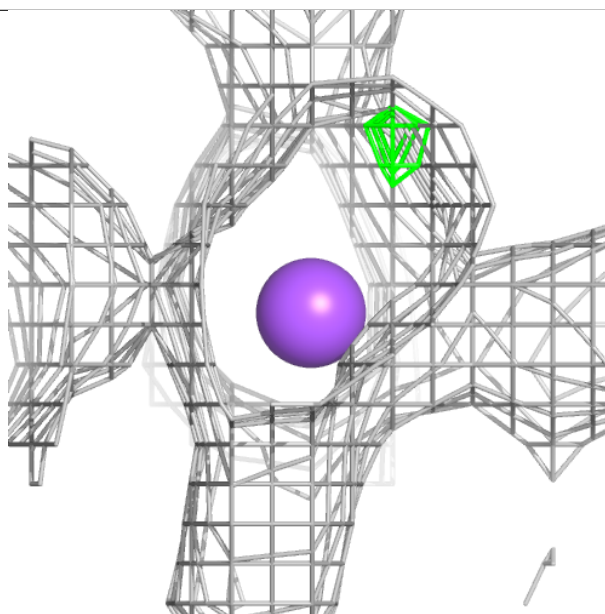
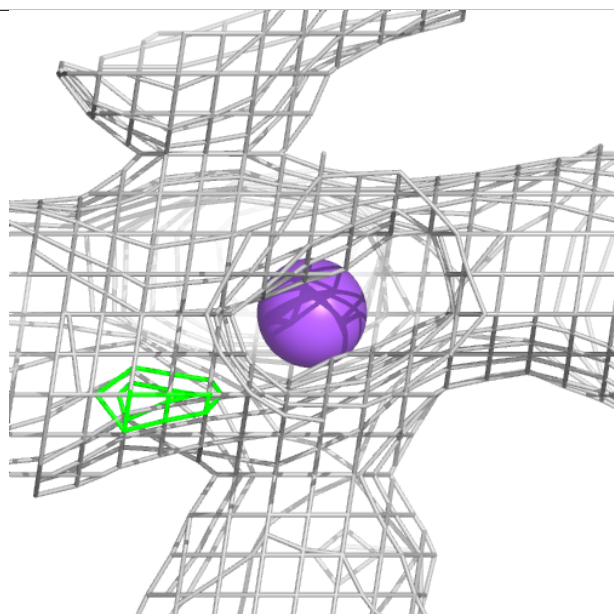
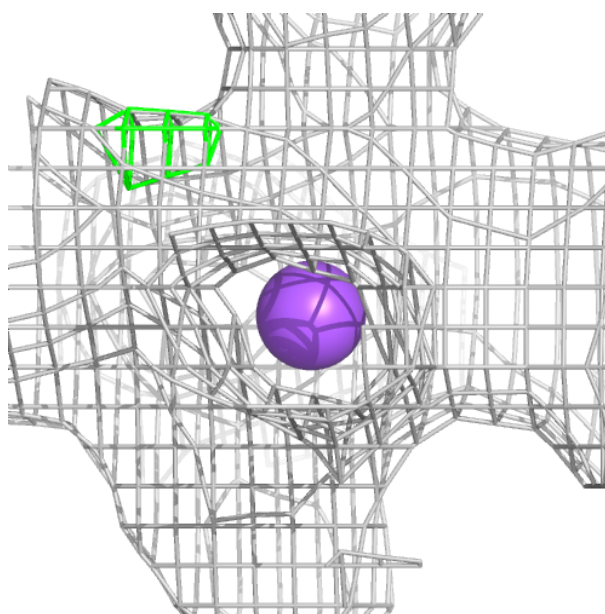
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NA	B	403	1/1	0.96	0.04	26,26,26,26	0
3	NA	A	403	1/1	0.96	0.07	29,29,29,29	0
3	NA	C	403	1/1	0.97	0.08	30,30,30,30	0
3	NA	A	402	1/1	0.98	0.06	26,26,26,26	0
3	NA	C	404	1/1	0.98	0.06	34,34,34,34	0

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.



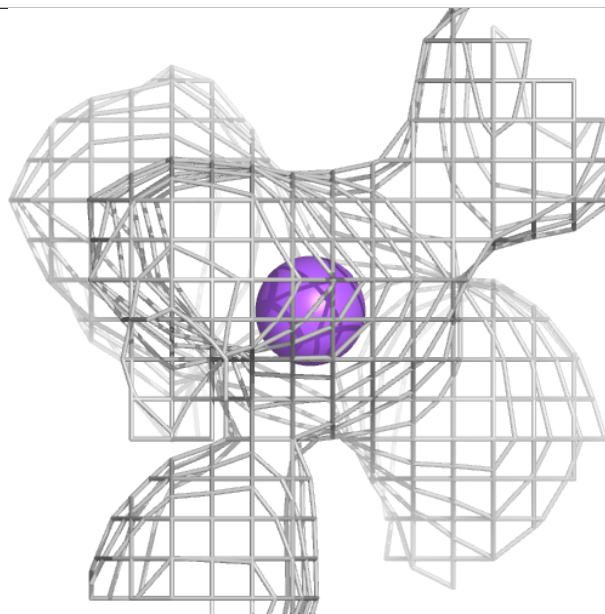
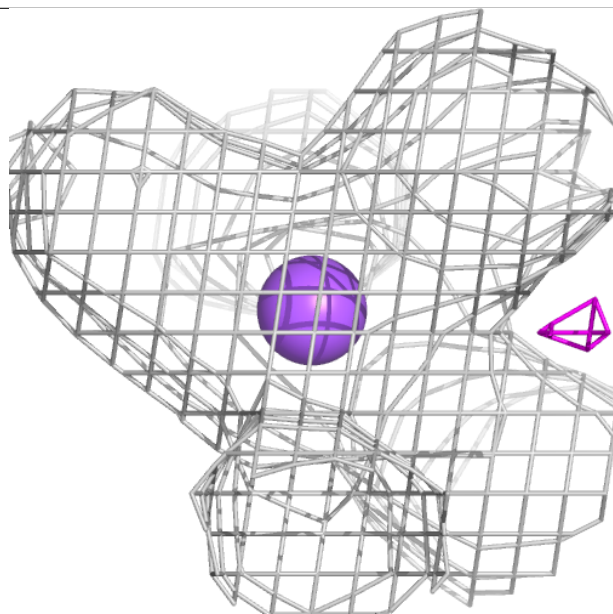
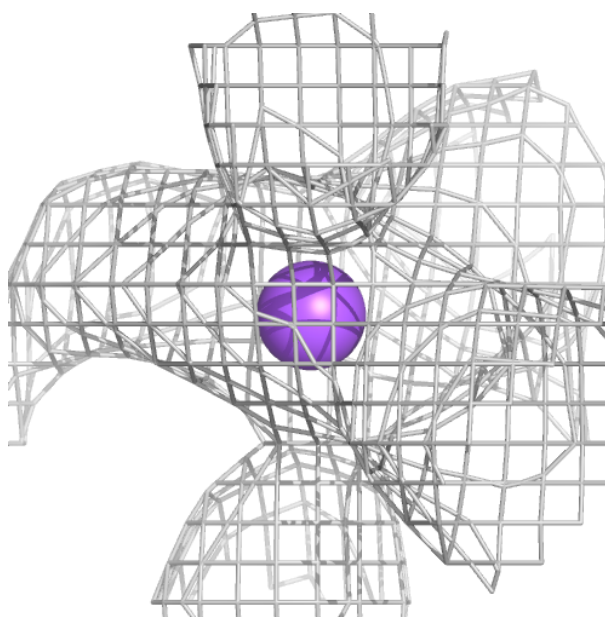
Electron density around NA D 402:

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



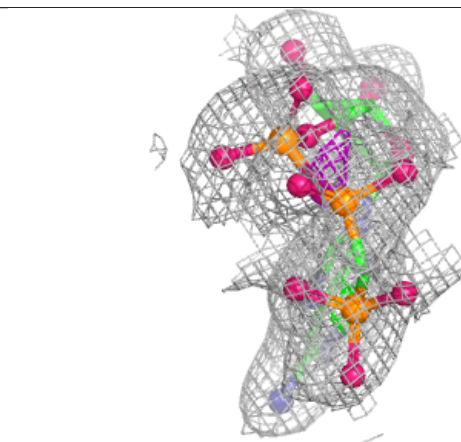
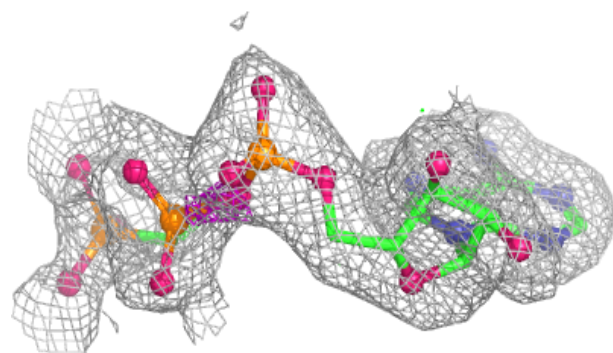
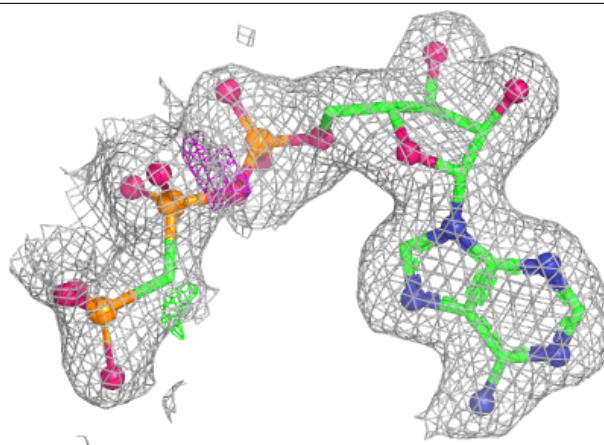
Electron density around NA B 404:

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

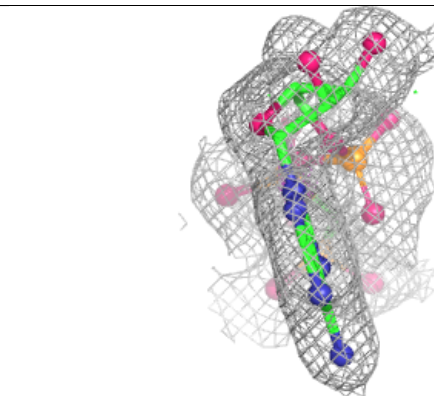
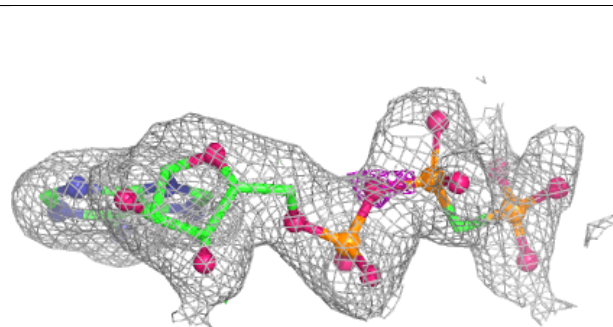
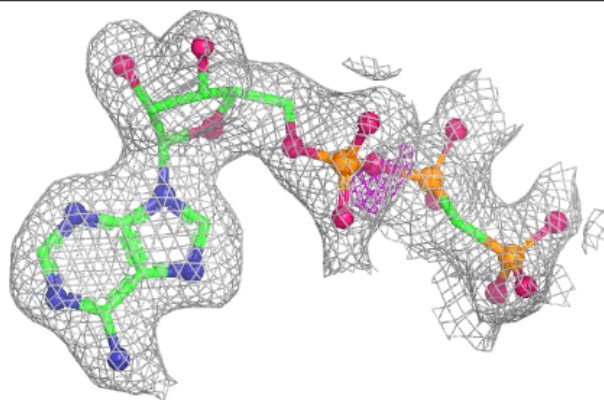


Electron density around ACP B 402 (B):

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

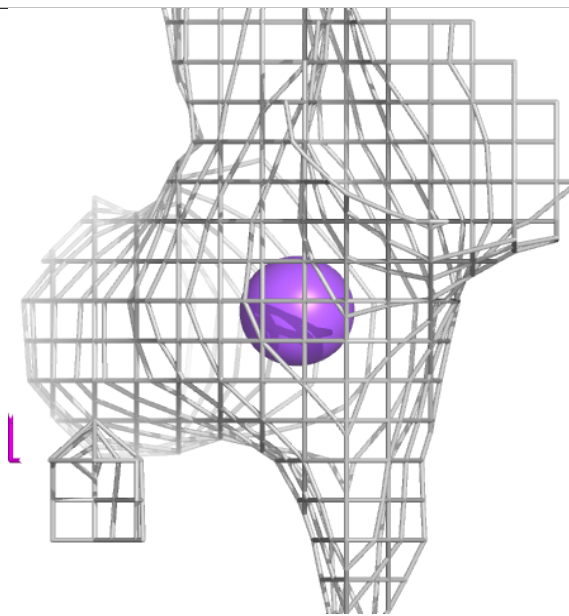
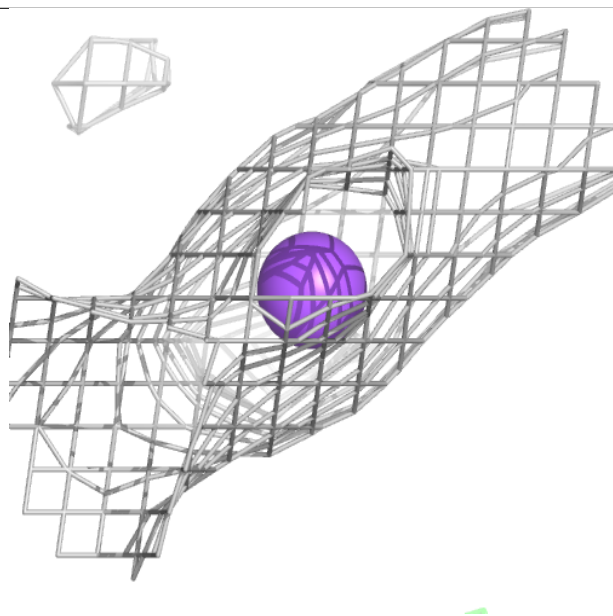
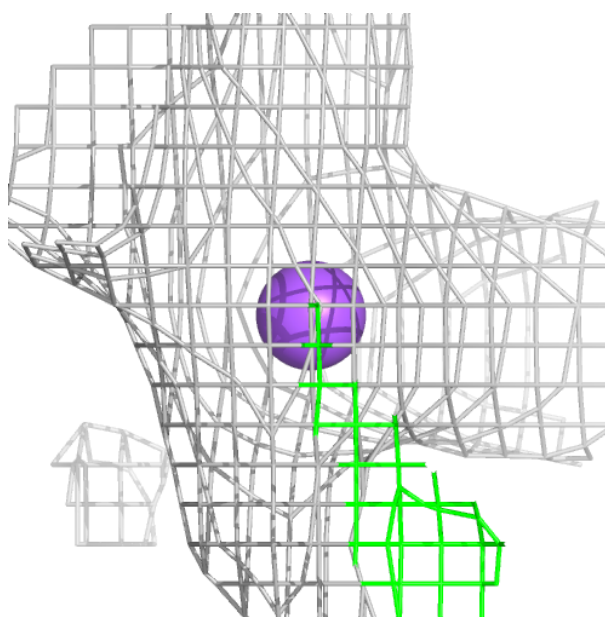
**Electron density around ACP B 402 (A):**

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



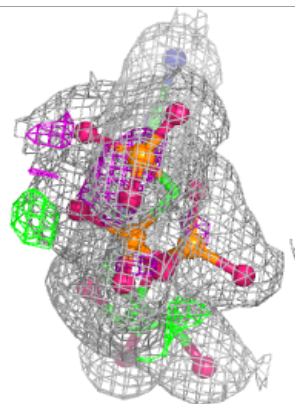
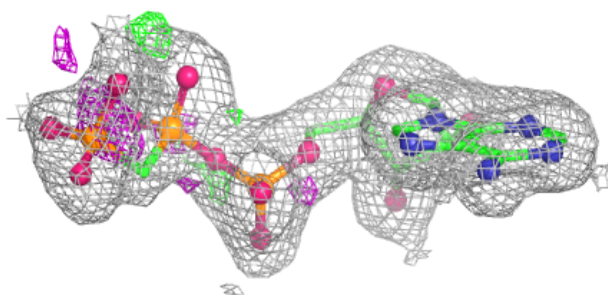
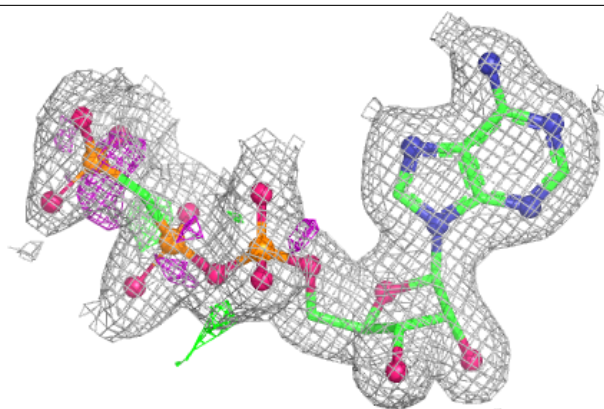
Electron density around NA D 403:

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

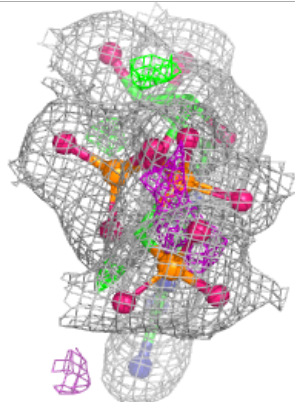
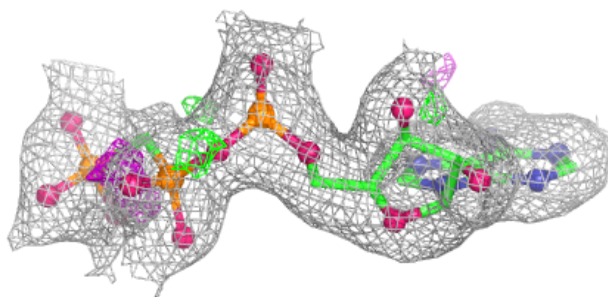
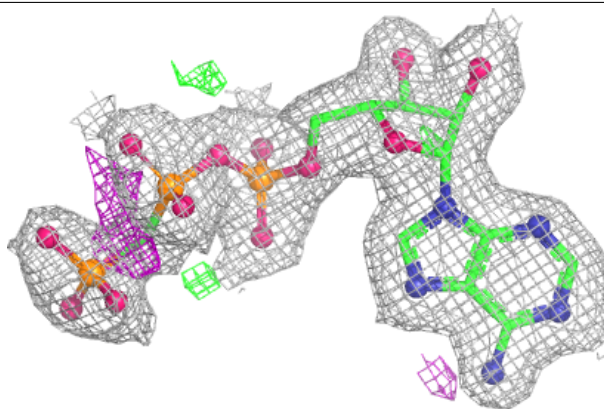


Electron density around ACP A 401:

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

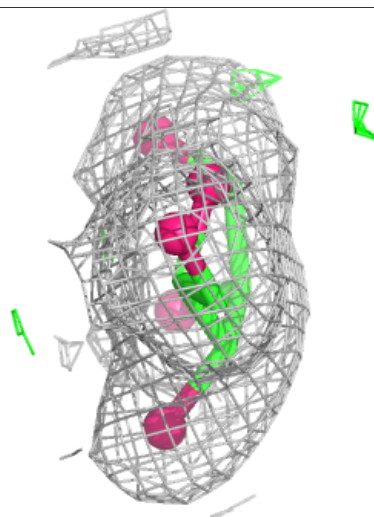
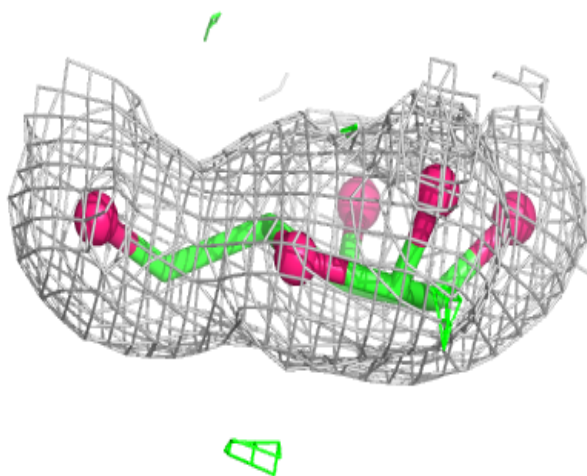
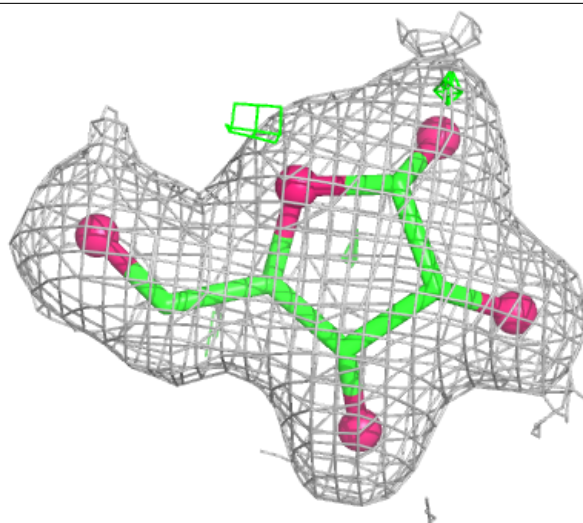
**Electron density around ACP C 402:**

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



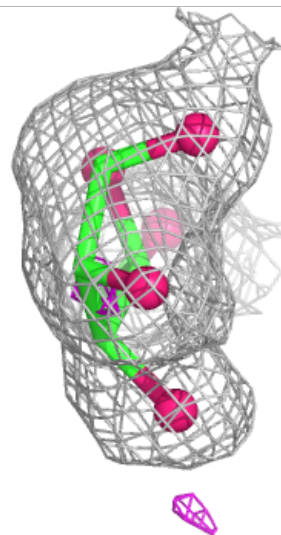
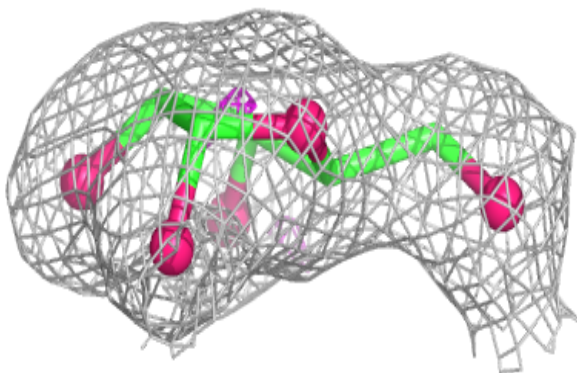
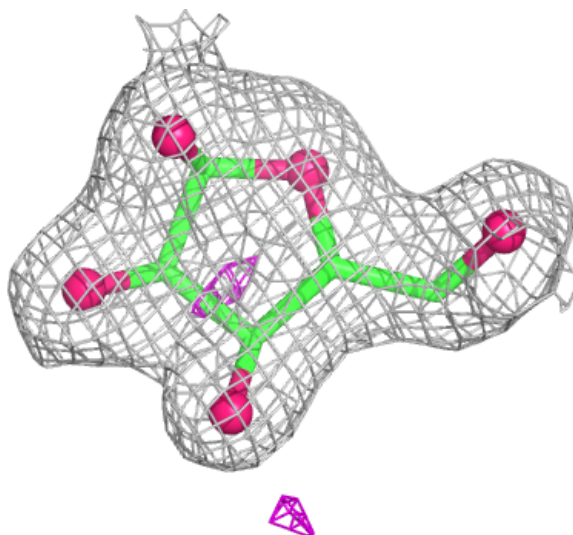
Electron density around RIB B 401:

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



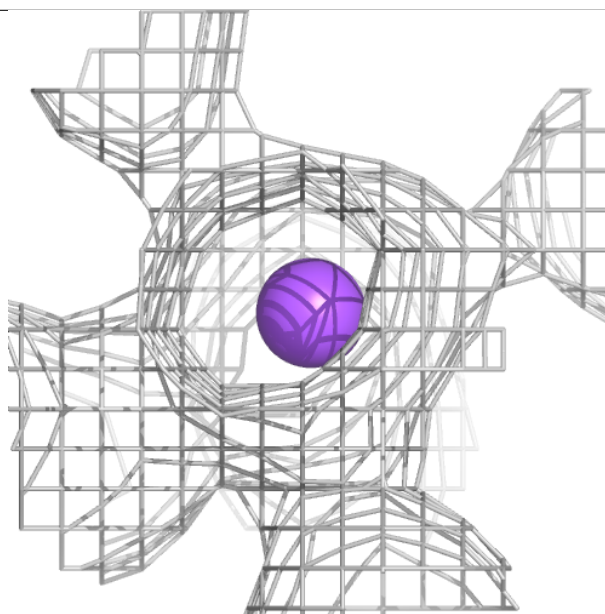
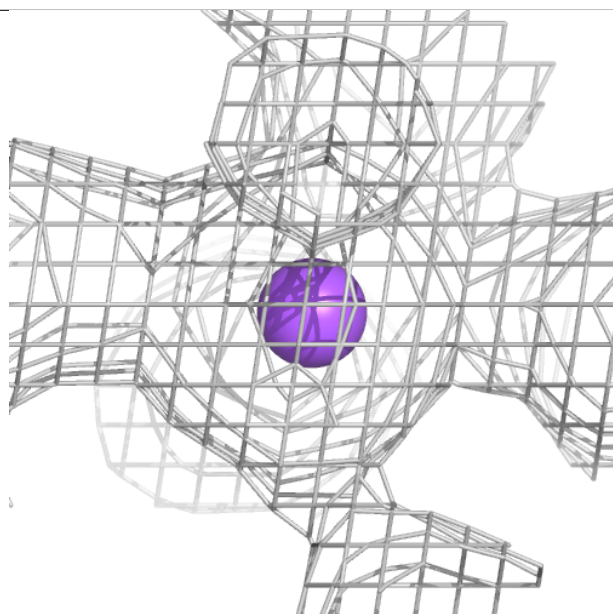
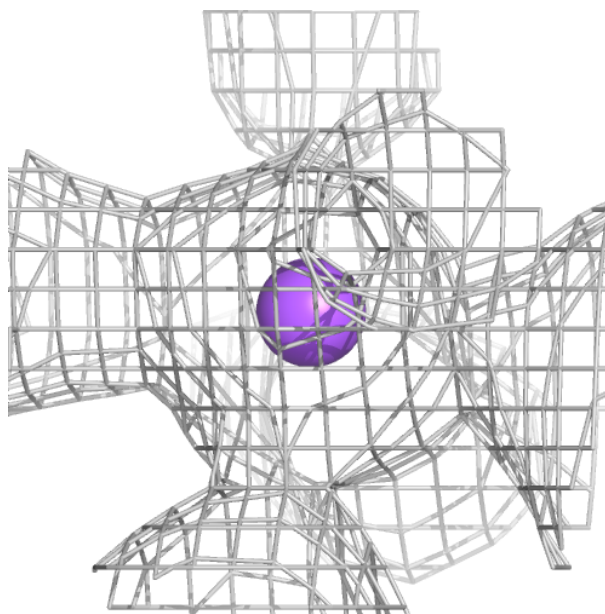
Electron density around RIB C 401:

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



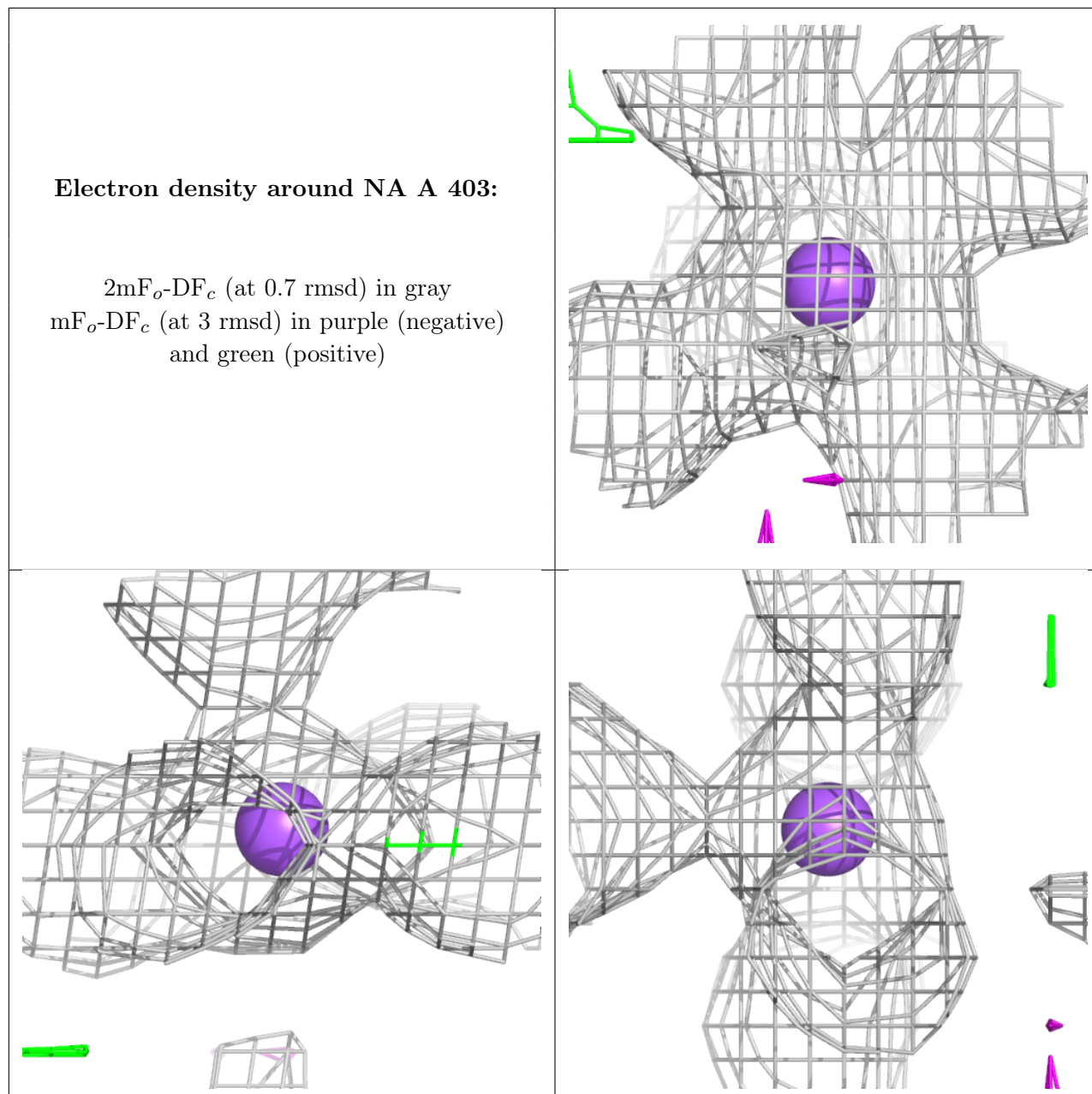
Electron density around NA B 403:

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



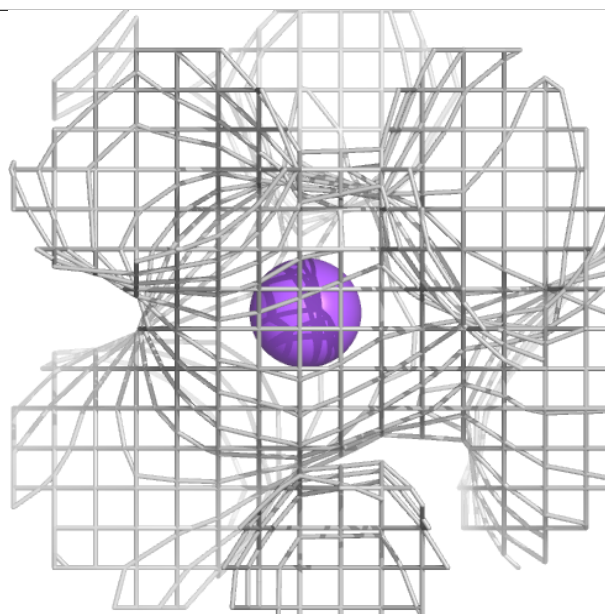
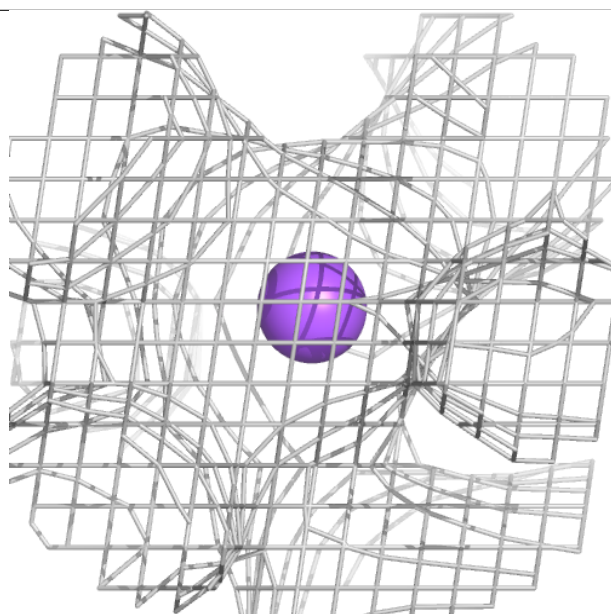
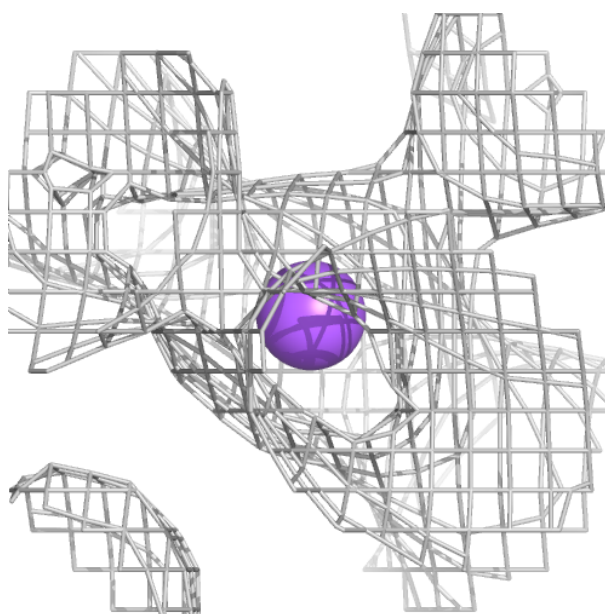
Electron density around NA A 403:

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



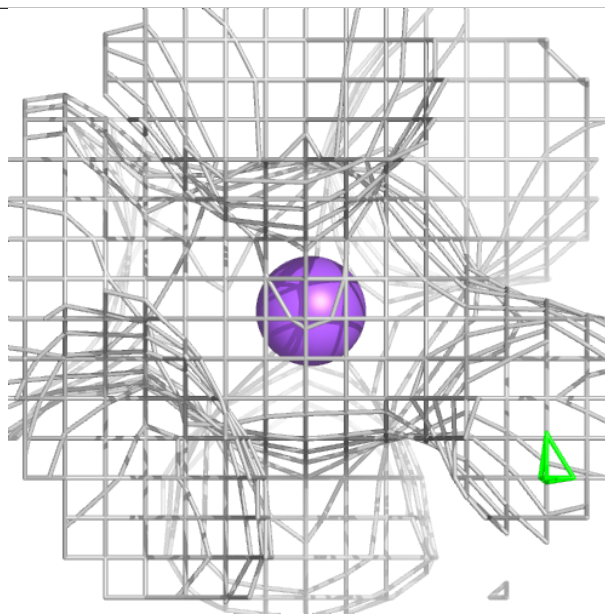
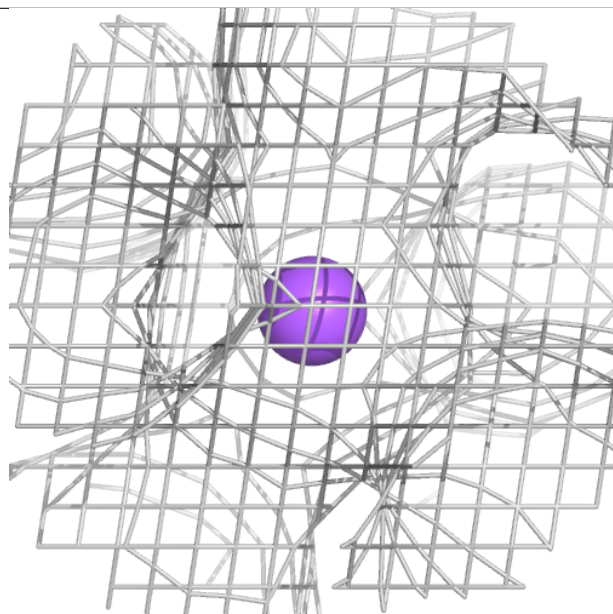
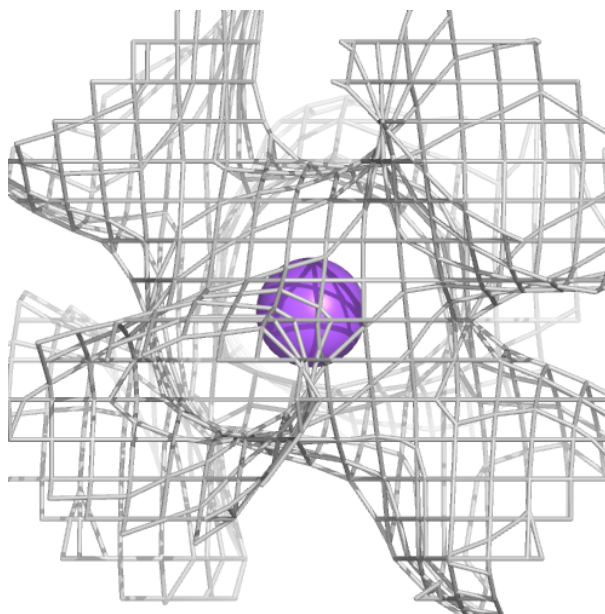
Electron density around NA C 403:

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



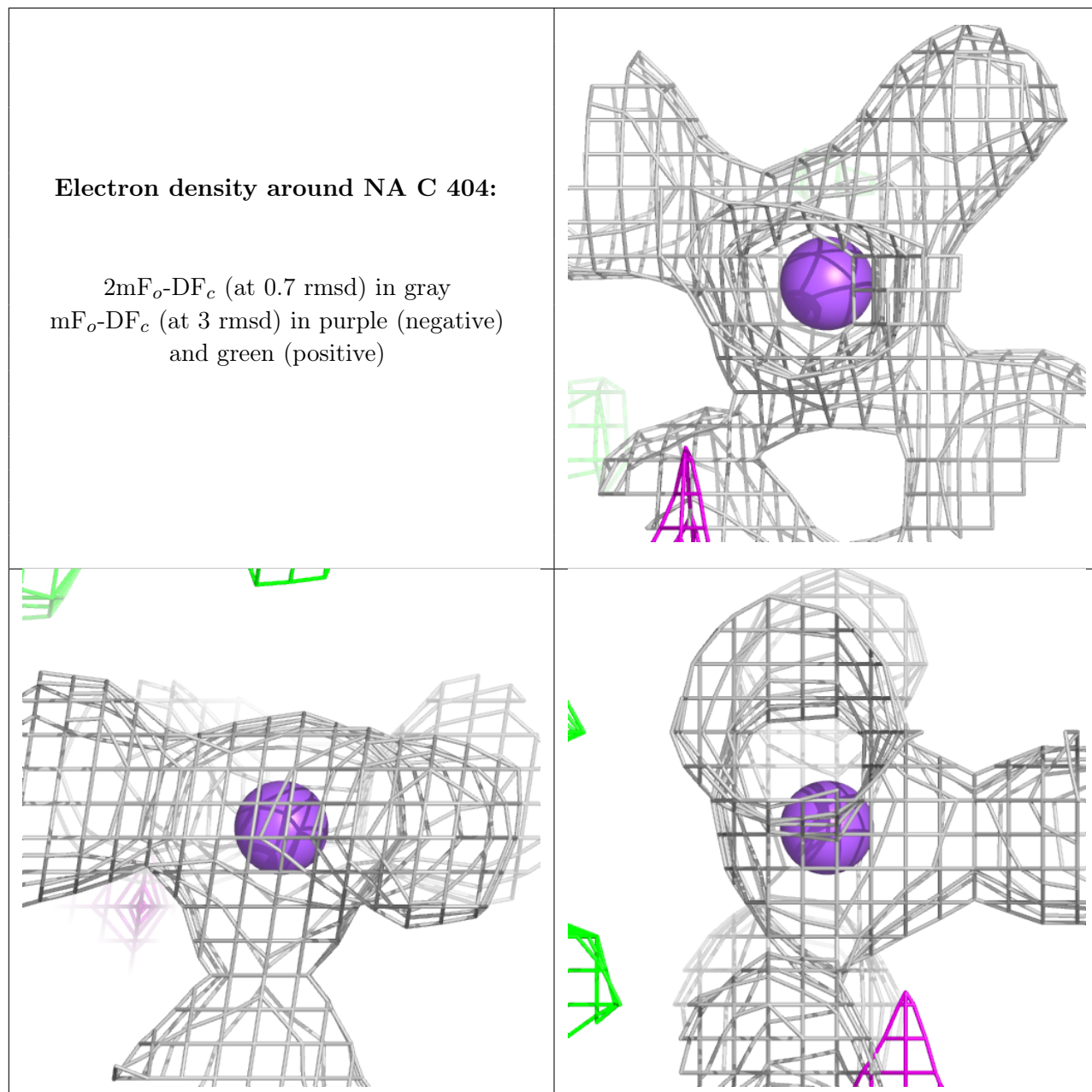
Electron density around NA A 402:

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



Electron density around NA C 404:

$2mF_o-DF_c$ (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.