



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:00 AM UTC

PDB ID : 5C41 / pdb_00005c41
Title : Crystal structure of human ribokinase in complex with AMPPCP in P21 space-group and with 4 protomers
Authors : Park, J.; Chakrabarti, J.; Singh, B.; Gupta, R.S.; Junop, M.S.
Deposited on : 2015-06-17
Resolution : 1.95 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

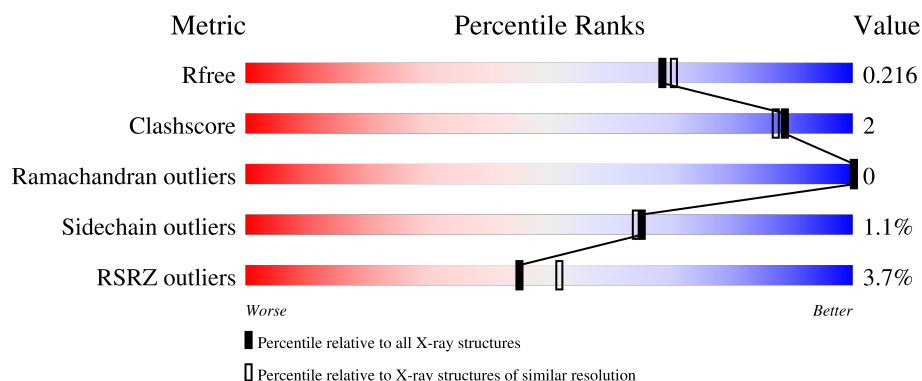
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	330	0% 90% 5% . .
1	B	330	2% 84% 9% . 6%
1	C	330	2% 90% 5% . .
1	D	330	8% 89% 6% . .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10589 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	7	0
			2412	1517	409	470	16			
1	B	310	Total	C	N	O	S	0	2	0
			2299	1452	382	451	14			
1	C	317	Total	C	N	O	S	0	5	0
			2378	1497	399	467	15			
1	D	316	Total	C	N	O	S	0	1	0
			2327	1468	391	454	14			

There are 32 discrepancies between the modelled and reference sequences:

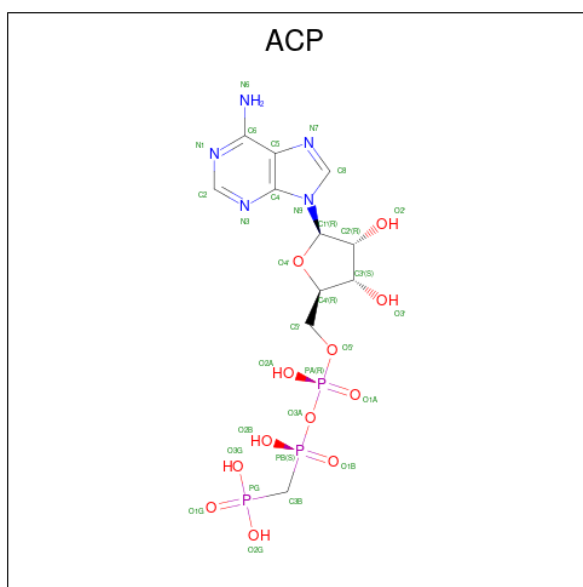
Chain	Residue	Modelled	Actual	Comment	Reference
A	323	LEU	-	expression tag	UNP Q9H477
A	324	GLU	-	expression tag	UNP Q9H477
A	325	HIS	-	expression tag	UNP Q9H477
A	326	HIS	-	expression tag	UNP Q9H477
A	327	HIS	-	expression tag	UNP Q9H477
A	328	HIS	-	expression tag	UNP Q9H477
A	329	HIS	-	expression tag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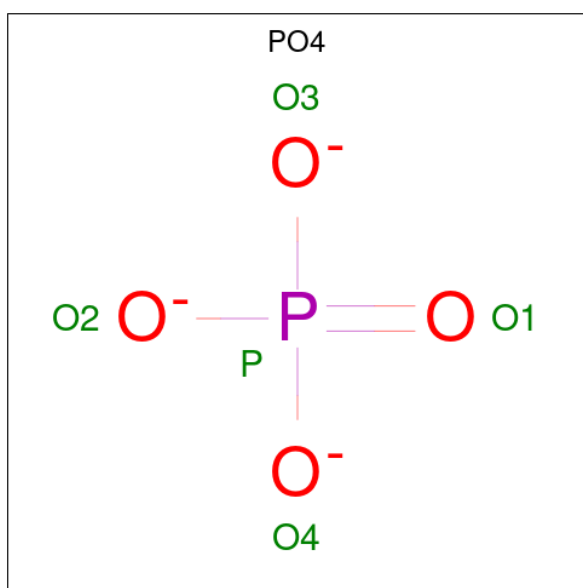
Chain	Residue	Modelled	Actual	Comment	Reference
C	328	HIS	-	expression tag	UNP Q9H477
C	329	HIS	-	expression tag	UNP Q9H477
C	330	HIS	-	expression tag	UNP Q9H477
D	323	LEU	-	expression tag	UNP Q9H477
D	324	GLU	-	expression tag	UNP Q9H477
D	325	HIS	-	expression tag	UNP Q9H477
D	326	HIS	-	expression tag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

- Molecule 2 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



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 PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	O	P	0	0
			5	4	1		

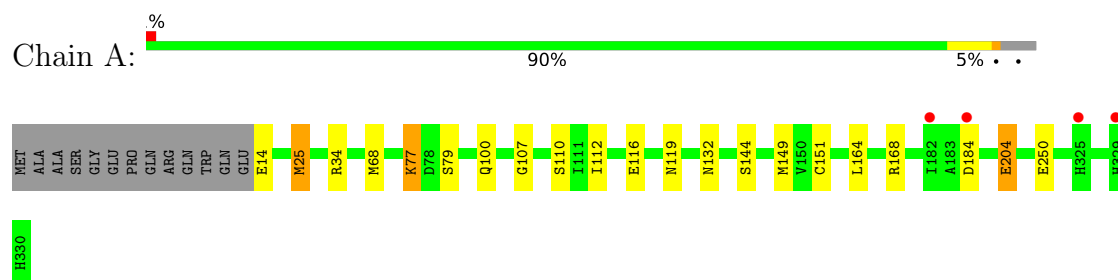
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	320	Total	O	0	1
			320	320		
5	B	259	Total	O	0	1
			260	260		
5	C	267	Total	O	0	0
			267	267		
5	D	158	Total	O	0	0
			158	158		

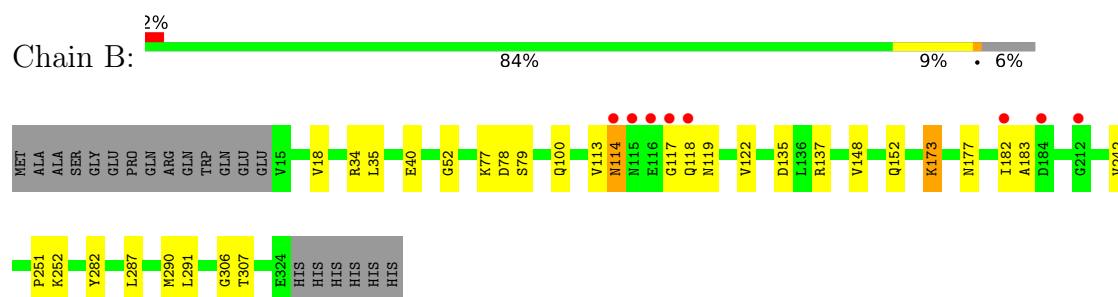
3 Residue-property plots [i](#)

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.

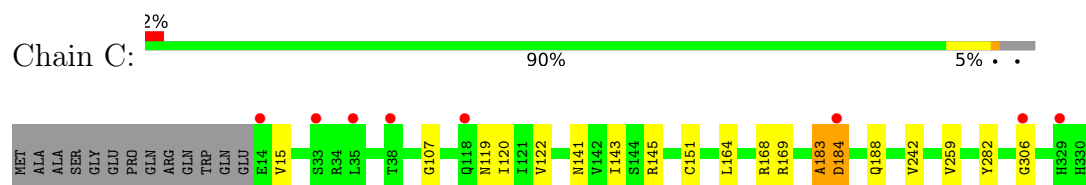
• Molecule 1: Ribokinase



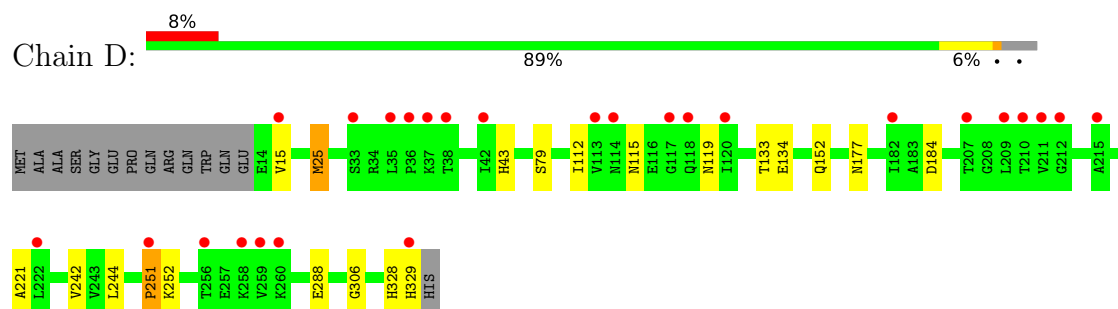
• Molecule 1: Ribokinase



• 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	51.95Å 89.19Å 144.40Å 90.00° 98.16° 90.00°	Depositor
Resolution (Å)	44.55 – 1.95 44.55 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.8 (44.55-1.95) 99.7 (44.55-1.95)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0123	Depositor
R, R_{free}	0.172 , 0.207 0.182 , 0.216	Depositor DCC
R_{free} test set	4824 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	21.9	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.025 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10589	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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: ACP, NA, PO4

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	1.38	4/2452 (0.2%)	1.11	4/3331 (0.1%)
1	B	1.45	12/2332 (0.5%)	1.17	4/3172 (0.1%)
1	C	1.33	4/2417 (0.2%)	1.12	7/3289 (0.2%)
1	D	1.16	3/2364 (0.1%)	1.08	7/3220 (0.2%)
All	All	1.33	23/9565 (0.2%)	1.12	22/13012 (0.2%)

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	D	0	2

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	114	ASN	N-CA	-10.18	1.33	1.46
1	B	52	GLY	N-CA	-8.77	1.37	1.44
1	B	306	GLY	C-O	7.77	1.33	1.23
1	B	307	THR	N-CA	-7.21	1.35	1.45
1	B	119	ASN	CA-C	-7.13	1.43	1.53
1	B	290	MET	SD-CE	6.86	1.96	1.79
1	A	204	GLU	CD-OE1	6.71	1.38	1.25
1	A	107	GLY	CA-C	6.31	1.57	1.52
1	C	282	TYR	CA-CB	6.14	1.60	1.53
1	B	182	ILE	CA-CB	5.95	1.61	1.54
1	C	107	GLY	CA-C	5.82	1.57	1.52
1	B	282	TYR	N-CA	5.80	1.53	1.46
1	A	144	SER	C-O	-5.75	1.16	1.24
1	B	113	VAL	CA-C	-5.49	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	329	HIS	N-CA	5.45	1.56	1.46
1	D	251	PRO	C-O	-5.43	1.17	1.23
1	C	259	VAL	N-CA	5.37	1.52	1.46
1	D	133	THR	CB-OG1	-5.36	1.35	1.43
1	B	78	ASP	N-CA	-5.36	1.39	1.45
1	A	110	SER	N-CA	-5.31	1.39	1.46
1	C	143	ILE	C-O	-5.16	1.18	1.24
1	B	135	ASP	CA-C	5.09	1.59	1.52
1	B	251	PRO	C-O	-5.01	1.18	1.23

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	119	ASN	N-CA-C	8.20	121.35	109.14
1	C	168	ARG	CG-CD-NE	6.67	126.68	112.00
1	C	183	ALA	N-CA-C	-6.33	102.18	110.53
1	B	114	ASN	N-CA-CB	-6.27	100.24	110.21
1	B	79	SER	CB-CA-C	-6.07	101.11	110.81
1	D	306	GLY	N-CA-C	5.91	124.77	115.08
1	A	25	MET	CG-SD-CE	-5.80	88.14	100.90
1	A	119	ASN	N-CA-C	5.79	117.77	109.14
1	A	34	ARG	NE-CZ-NH2	5.74	124.37	119.20
1	C	169	ARG	NE-CZ-NH2	5.69	124.33	119.20
1	B	137	ARG	CB-CG-CD	5.64	124.26	111.30
1	D	25	MET	CG-SD-CE	-5.61	88.55	100.90
1	D	79	SER	CB-CA-C	-5.45	102.32	110.88
1	D	119	ASN	N-CA-C	5.28	117.01	109.14
1	A	168	ARG	CB-CA-C	-5.25	102.07	110.79
1	C	15	VAL	N-CA-C	5.21	116.24	108.54
1	B	183	ALA	N-CA-C	5.12	118.62	112.38
1	C	184	ASP	N-CA-C	5.11	118.82	112.58
1	D	43	HIS	CA-CB-CG	5.11	118.91	113.80
1	D	115	ASN	N-CA-C	5.10	116.84	111.28
1	C	183	ALA	O-C-N	-5.09	116.99	122.79
1	D	15	VAL	N-CA-C	5.01	115.57	109.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	134	GLU	Sidechain
1	D	328	HIS	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	2412	0	2401	11	0
1	B	2299	0	2318	11	0
1	C	2378	0	2347	7	0
1	D	2327	0	2300	9	0
2	A	62	0	28	1	0
2	B	31	0	14	0	0
2	C	31	0	14	0	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	D	5	0	0	0	0
5	A	320	0	0	5	0
5	B	260	0	0	1	0
5	C	267	0	0	2	0
5	D	158	0	0	0	0
All	All	10589	0	9436	36	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 2.

All (36) 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:35:LEU:HD11	1:B:118:GLN:O	1.75	0.86
1:C:306[A]:GLY:O	5:C:501:HOH:O	2.02	0.78
1:B:117:GLY:O	5:B:501:HOH:O	2.03	0.75
2:A:401[B]:ACP:H3B2	5:A:621:HOH:O	1.94	0.66
1:D:221:ALA:CB	1:D:244:LEU:HD21	2.28	0.63
1:D:221:ALA:HB3	1:D:244:LEU:HD21	1.81	0.62
1:A:149[A]:MET:CE	1:A:164:LEU:HD23	2.33	0.59
1:A:149[A]:MET:HE1	1:A:151[A]:CYS:SG	2.43	0.58
1:A:151[B]:CYS:SG	1:A:164:LEU:HD21	2.47	0.55
1:C:151[B]:CYS:SG	1:C:164:LEU:HD21	2.47	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:GLU:OE1	5:A:502:HOH:O	2.18	0.54
1:C:122:VAL:HG21	1:D:112:ILE:HD13	1.90	0.54
1:A:112:ILE:HD13	1:B:122:VAL:HG21	1.90	0.53
1:B:77:LYS:HG2	1:B:100:GLN:HB3	1.91	0.51
1:A:149[A]:MET:SD	1:A:151[A]:CYS:SG	3.09	0.50
1:C:188:GLN:NE2	5:C:510:HOH:O	2.45	0.49
1:A:77:LYS:HG2	1:A:100:GLN:HB3	1.95	0.49
1:A:149[A]:MET:HE1	1:A:164:LEU:HD23	1.95	0.48
1:C:183:ALA:O	1:C:184:ASP:HB2	2.14	0.48
1:C:122:VAL:CG2	1:D:112:ILE:HD13	2.44	0.48
1:C:141:ASN:HD21	1:C:145:ARG:NE	2.12	0.47
1:A:250:GLU:OE1	5:A:503:HOH:O	2.20	0.47
1:B:18:VAL:HG22	1:B:148[B]:VAL:HG12	1.96	0.46
1:B:35:LEU:CD2	1:B:114:ASN:HB2	2.46	0.46
1:D:221:ALA:HB1	1:D:244:LEU:HD21	1.97	0.45
1:A:68:MET:HE3	5:A:547:HOH:O	2.17	0.44
1:D:244:LEU:HD22	1:D:251:PRO:HB3	2.00	0.43
1:D:252:LYS:HD3	1:D:288:GLU:OE2	2.19	0.43
1:B:173:LYS:HE2	1:B:173:LYS:HB2	1.85	0.42
1:D:242:VAL:HG23	1:D:252:LYS:O	2.19	0.42
1:B:287:LEU:O	1:B:291:LEU:HD13	2.20	0.42
1:B:34:ARG:NH2	1:B:40:GLU:OE1	2.51	0.41
1:A:132:ASN:HB2	5:A:622:HOH:O	2.21	0.41
1:B:152:GLN:HA	1:B:177:ASN:O	2.20	0.41
1:D:152:GLN:HA	1:D:177:ASN:O	2.21	0.41
1:B:242[A]:VAL:HG23	1:B:252:LYS:O	2.21	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	322/330 (98%)	317 (98%)	5 (2%)	0	100	100
1	B	310/330 (94%)	306 (99%)	4 (1%)	0	100	100
1	C	320/330 (97%)	316 (99%)	4 (1%)	0	100	100
1	D	315/330 (96%)	310 (98%)	5 (2%)	0	100	100
All	All	1267/1320 (96%)	1249 (99%)	18 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	262/266 (98%)	256 (98%)	6 (2%)	44	38
1	B	249/266 (94%)	248 (100%)	1 (0%)	84	85
1	C	254/266 (96%)	252 (99%)	2 (1%)	73	74
1	D	246/266 (92%)	244 (99%)	2 (1%)	73	74
All	All	1011/1064 (95%)	1000 (99%)	11 (1%)	65	64

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	GLU
1	A	25	MET
1	A	77	LYS
1	A	79	SER
1	A	116	GLU
1	A	184	ASP
1	B	173	LYS
1	C	120	ILE
1	C	242	VAL
1	D	25	MET
1	D	184	ASP

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	43	HIS
1	A	230	GLN
1	B	100	GLN
1	B	118	GLN
1	C	90	GLN
1	C	188	GLN
1	C	230	GLN
1	D	230	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 14 ligands modelled in this entry, 8 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ACP	A	401[A]	3	31,33,33	2.06	11 (35%)	47,52,52	1.89	12 (25%)
2	ACP	D	401	-	31,33,33	2.00	8 (25%)	47,52,52	1.96	12 (25%)
4	PO4	D	402	-	4,4,4	0.73	0	6,6,6	2.00	2 (33%)
2	ACP	B	401	-	31,33,33	2.35	11 (35%)	47,52,52	1.82	13 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ACP	A	401[B]	-	31,33,33	2.05	11 (35%)	47,52,52	2.01	15 (31%)
2	ACP	C	401	3	31,33,33	2.19	9 (29%)	47,52,52	1.98	13 (27%)

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	A	401[A]	3	-	4/19/38/38	0/3/3/3
2	ACP	D	401	-	-	3/19/38/38	0/3/3/3
2	ACP	B	401	-	-	2/19/38/38	0/3/3/3
2	ACP	A	401[B]	-	-	1/19/38/38	0/3/3/3
2	ACP	C	401	3	-	2/19/38/38	0/3/3/3

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	ACP	PB-O3A	7.72	1.67	1.58
2	B	401	ACP	PB-O3A	6.81	1.66	1.58
2	B	401	ACP	PG-O1G	6.72	1.63	1.50
2	D	401	ACP	PG-O1G	5.82	1.62	1.50
2	A	401[A]	ACP	PB-O3A	5.37	1.64	1.58
2	D	401	ACP	C5-C4	4.96	1.47	1.39
2	A	401[A]	ACP	C5-C4	4.57	1.47	1.39
2	C	401	ACP	C5-C4	4.54	1.47	1.39
2	A	401[B]	ACP	C5-C4	4.49	1.47	1.39
2	A	401[B]	ACP	PB-O1B	4.36	1.61	1.51
2	B	401	ACP	C5-C4	4.22	1.46	1.39
2	C	401	ACP	PG-O3G	3.79	1.63	1.55
2	D	401	ACP	PG-O2G	3.76	1.63	1.55
2	A	401[B]	ACP	PB-O2B	-3.75	1.47	1.56
2	A	401[A]	ACP	PB-O1B	3.72	1.60	1.51
2	A	401[A]	ACP	PB-O2B	-3.63	1.47	1.56
2	A	401[B]	ACP	PG-O2G	3.42	1.62	1.55
2	A	401[B]	ACP	PG-O3G	3.39	1.62	1.55
2	A	401[B]	ACP	PB-O3A	3.37	1.62	1.58
2	D	401	ACP	PB-O3A	3.31	1.62	1.58
2	C	401	ACP	PG-O2G	3.31	1.62	1.55
2	B	401	ACP	C4-N9	-3.29	1.30	1.37
2	B	401	ACP	PB-O2B	-2.79	1.49	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401[A]	ACP	C5-C6	2.71	1.48	1.41
2	C	401	ACP	C5-N7	-2.71	1.34	1.39
2	A	401[B]	ACP	C5-C6	2.65	1.48	1.41
2	A	401[A]	ACP	PG-O2G	2.63	1.60	1.55
2	A	401[B]	ACP	C4-N9	-2.62	1.32	1.37
2	A	401[B]	ACP	PA-O3A	2.58	1.62	1.59
2	A	401[A]	ACP	C4-N9	-2.57	1.32	1.37
2	C	401	ACP	PB-O2B	2.57	1.62	1.56
2	D	401	ACP	C5-C6	2.56	1.48	1.41
2	B	401	ACP	PG-O3G	2.54	1.60	1.55
2	C	401	ACP	C4-N9	-2.38	1.32	1.37
2	D	401	ACP	C8-N7	2.37	1.36	1.31
2	A	401[A]	ACP	C8-N7	2.35	1.36	1.31
2	A	401[B]	ACP	C8-N7	2.34	1.36	1.31
2	B	401	ACP	C5-N7	-2.34	1.34	1.39
2	B	401	ACP	PB-O1B	2.33	1.57	1.51
2	C	401	ACP	C8-N7	2.30	1.36	1.31
2	B	401	ACP	PA-O3A	2.29	1.62	1.59
2	A	401[A]	ACP	PG-O3G	2.25	1.60	1.55
2	D	401	ACP	C4-N9	-2.23	1.33	1.37
2	A	401[A]	ACP	PA-O3A	2.14	1.61	1.59
2	B	401	ACP	PA-O2A	-2.12	1.45	1.55
2	B	401	ACP	C8-N7	2.10	1.35	1.31
2	A	401[A]	ACP	C5-N7	-2.10	1.35	1.39
2	A	401[B]	ACP	C5-N7	-2.05	1.35	1.39
2	D	401	ACP	PG-O3G	-2.04	1.50	1.55
2	C	401	ACP	C2-N3	2.01	1.37	1.33

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	ACP	O1G-PG-C3B	-5.25	99.92	111.37
2	A	401[A]	ACP	C5-C4-N3	-5.18	119.58	126.72
2	D	401	ACP	C5-C4-N3	-5.05	119.76	126.72
2	A	401[B]	ACP	C5-C4-N3	-4.99	119.85	126.72
2	C	401	ACP	C5-C4-N3	-4.63	120.34	126.72
2	C	401	ACP	N3-C2-N1	-4.60	121.62	128.58
2	D	401	ACP	N3-C4-N9	4.50	134.82	127.17
2	A	401[B]	ACP	N3-C2-N1	-4.38	121.95	128.58
2	A	401[A]	ACP	N3-C2-N1	-4.37	121.96	128.58
2	C	401	ACP	N3-C4-N9	4.32	134.52	127.17
2	B	401	ACP	N3-C2-N1	-4.08	122.41	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401[A]	ACP	N3-C4-N9	4.05	134.05	127.17
2	A	401[B]	ACP	N3-C4-N9	3.96	133.90	127.17
2	D	401	ACP	N3-C2-N1	-3.92	122.64	128.58
2	A	401[B]	ACP	O3G-PG-C3B	3.91	115.89	106.40
2	A	401[A]	ACP	C2-N3-C4	3.82	121.16	111.83
2	D	401	ACP	O1B-PB-C3B	3.80	119.05	109.05
2	A	401[B]	ACP	C2-N3-C4	3.72	120.91	111.83
2	D	401	ACP	C2-N3-C4	3.69	120.85	111.83
2	D	401	ACP	O3G-PG-O1G	-3.69	102.85	112.39
2	D	401	ACP	O3G-PG-C3B	3.54	114.99	106.40
2	A	401[A]	ACP	O3G-PG-O2G	3.53	118.03	107.96
4	D	402	PO4	O4-P-O3	3.52	118.87	107.91
2	C	401	ACP	C4-N9-C8	3.44	109.35	105.74
2	B	401	ACP	O3A-PA-O1A	-3.43	100.38	110.70
2	A	401[B]	ACP	O2A-PA-O3A	3.34	116.30	107.27
2	B	401	ACP	O2B-PB-O1B	3.32	120.76	109.95
2	B	401	ACP	C2-N1-C6	3.31	124.17	118.73
2	B	401	ACP	O2A-PA-O1A	3.31	127.82	112.44
2	B	401	ACP	C2-N3-C4	3.13	119.47	111.83
2	B	401	ACP	C5-C4-N3	-3.13	122.41	126.72
2	C	401	ACP	C2-N3-C4	3.07	119.32	111.83
2	B	401	ACP	C6-C5-N7	3.00	137.88	132.09
2	D	401	ACP	C4-N9-C8	2.99	108.88	105.74
2	A	401[A]	ACP	C4-C5-N7	-2.97	107.19	110.58
2	A	401[B]	ACP	C4-N9-C8	2.94	108.83	105.74
2	C	401	ACP	C2-N1-C6	2.93	123.55	118.73
2	A	401[B]	ACP	C4-C5-N7	-2.90	107.27	110.58
2	A	401[B]	ACP	C2-N1-C6	2.82	123.36	118.73
2	B	401	ACP	C4-N9-C8	2.79	108.67	105.74
2	A	401[A]	ACP	C2-N1-C6	2.76	123.27	118.73
2	A	401[A]	ACP	C4-N9-C8	2.76	108.63	105.74
2	A	401[B]	ACP	O1B-PB-C3B	-2.75	101.80	109.05
2	A	401[A]	ACP	O3G-PG-C3B	-2.75	99.72	106.40
2	A	401[A]	ACP	O3G-PG-O1G	-2.74	105.31	112.39
2	C	401	ACP	O3A-PA-O1A	2.70	118.83	110.70
2	C	401	ACP	O3G-PG-C3B	2.69	112.93	106.40
2	B	401	ACP	O1G-PG-C3B	-2.68	105.53	111.37
2	B	401	ACP	C4-C5-N7	-2.66	107.54	110.58
2	A	401[B]	ACP	O2G-PG-O1G	-2.66	105.51	112.39
4	D	402	PO4	O3-P-O1	-2.63	101.65	110.95
2	D	401	ACP	O2A-PA-O1A	2.50	124.08	112.44
2	A	401[A]	ACP	C6-C5-N7	2.48	136.86	132.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401[B]	ACP	C6-C5-N7	2.46	136.83	132.09
2	A	401[B]	ACP	O2B-PB-C3B	2.39	116.62	106.73
2	B	401	ACP	N3-C4-N9	2.34	131.14	127.17
2	C	401	ACP	N9-C8-N7	-2.19	110.83	113.94
2	C	401	ACP	PB-O3A-PA	-2.17	125.29	132.37
2	D	401	ACP	O3G-PG-O2G	2.16	114.13	107.96
2	A	401[B]	ACP	O2A-PA-O1A	2.13	122.36	112.44
2	B	401	ACP	C4-N9-C1'	-2.12	121.67	126.63
2	A	401[B]	ACP	O3G-PG-O1G	-2.10	106.95	112.39
2	A	401[A]	ACP	PB-O3A-PA	-2.10	125.53	132.37
2	C	401	ACP	C4-C5-N7	-2.10	108.19	110.58
2	D	401	ACP	C4-C5-N7	-2.09	108.19	110.58
2	D	401	ACP	C2-N1-C6	2.08	122.14	118.73
2	C	401	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	A	401[A]	ACP	C5'-O5'-PA-O1A
2	A	401[A]	ACP	C5'-O5'-PA-O3A
2	C	401	ACP	C5'-O5'-PA-O3A
2	D	401	ACP	PB-C3B-PG-O1G
2	D	401	ACP	PB-C3B-PG-O3G
2	A	401[A]	ACP	PB-O3A-PA-O1A
2	B	401	ACP	O4'-C4'-C5'-O5'
2	D	401	ACP	PB-C3B-PG-O2G
2	A	401[A]	ACP	PB-O3A-PA-O2A
2	B	401	ACP	C3'-C4'-C5'-O5'
2	A	401[B]	ACP	PB-C3B-PG-O1G
2	C	401	ACP	PB-C3B-PG-O1G

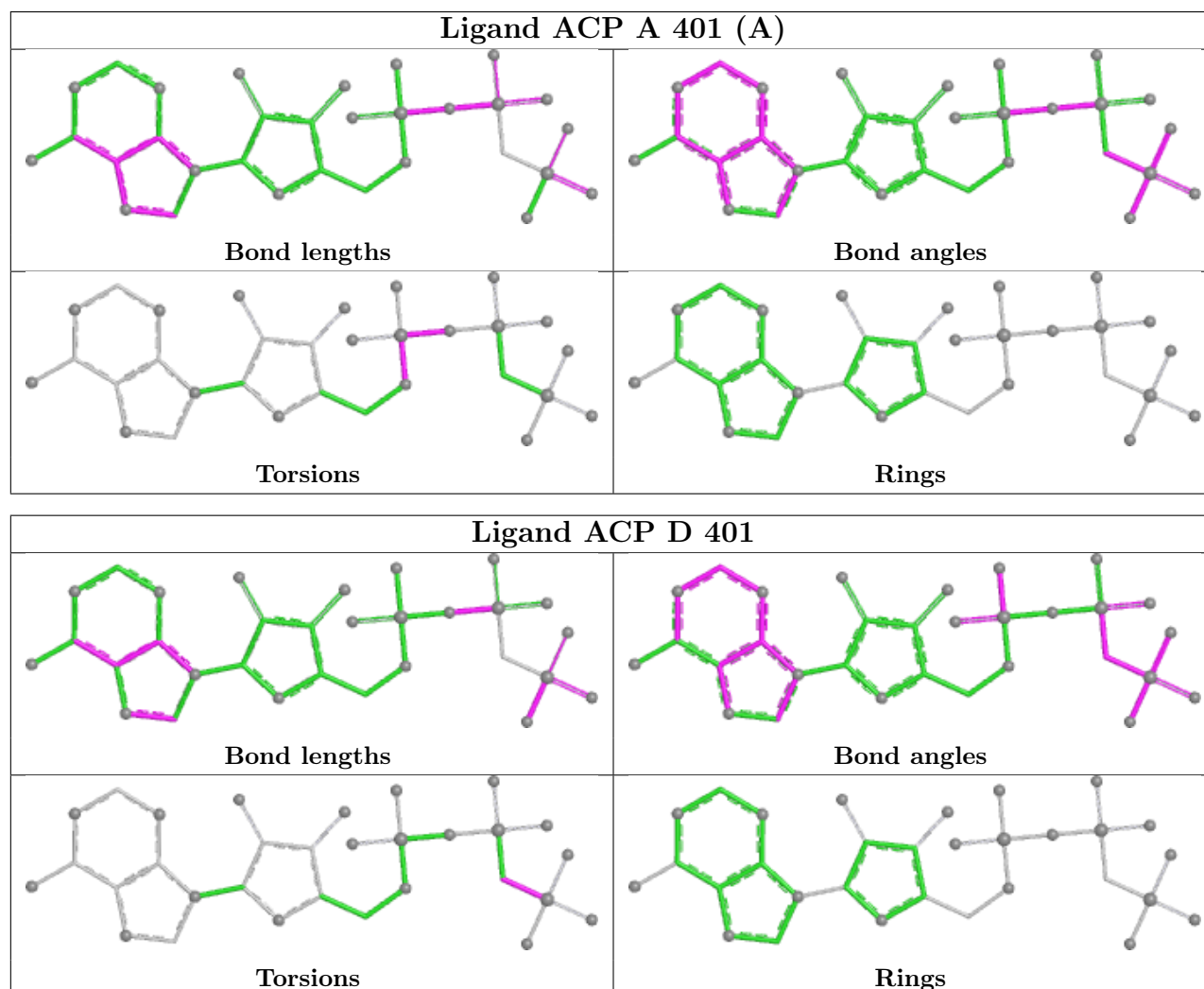
There are no ring outliers.

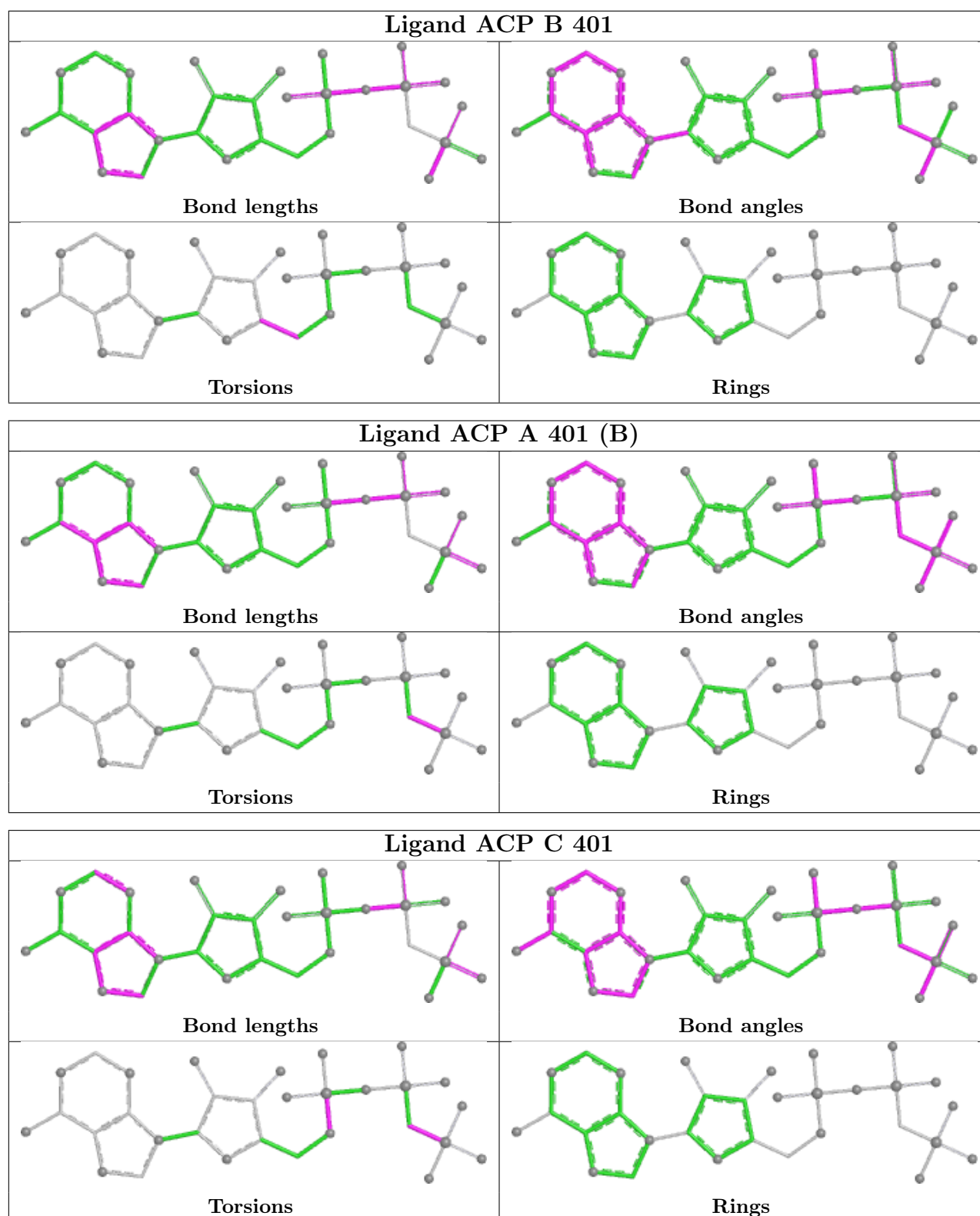
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401[B]	ACP	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 ⓘ

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	317/330 (96%)	-0.21	4 (1%) 75 81	7, 20, 46, 72	7 (2%)
1	B	310/330 (93%)	-0.11	8 (2%) 57 64	10, 25, 48, 61	2 (0%)
1	C	317/330 (96%)	-0.07	8 (2%) 58 65	7, 25, 50, 79	5 (1%)
1	D	316/330 (95%)	0.55	26 (8%) 17 20	15, 39, 77, 93	1 (0%)
All	All	1260/1320 (95%)	0.04	46 (3%) 45 52	7, 27, 63, 93	15 (1%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	306[A]	GLY	5.5
1	B	117	GLY	3.5
1	B	118	GLN	3.4
1	C	35	LEU	3.4
1	D	35	LEU	3.2
1	A	329	HIS	2.9
1	D	211	VAL	2.9
1	C	329	HIS	2.9
1	D	329	HIS	2.8
1	D	38	THR	2.8
1	D	15	VAL	2.8
1	B	212	GLY	2.7
1	D	209	LEU	2.7
1	D	215	ALA	2.7
1	D	210	THR	2.5
1	B	116	GLU	2.4
1	D	113	VAL	2.4
1	C	33	SER	2.4
1	D	37	LYS	2.4
1	A	182	ILE	2.4
1	B	182	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	325[A]	HIS	2.4
1	D	120	ILE	2.3
1	D	258	LYS	2.3
1	D	222	LEU	2.3
1	D	182	ILE	2.3
1	B	115	ASN	2.3
1	D	42	ILE	2.3
1	D	259	VAL	2.3
1	D	251	PRO	2.2
1	D	33	SER	2.2
1	D	256	THR	2.2
1	A	184	ASP	2.2
1	C	184	ASP	2.2
1	D	118	GLN	2.1
1	C	14	GLU	2.1
1	C	38	THR	2.1
1	D	207	THR	2.1
1	D	117	GLY	2.1
1	D	212	GLY	2.1
1	D	260	LYS	2.0
1	B	114	ASN	2.0
1	C	118	GLN	2.0
1	D	114	ASN	2.0
1	B	184	ASP	2.0
1	D	36	PRO	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

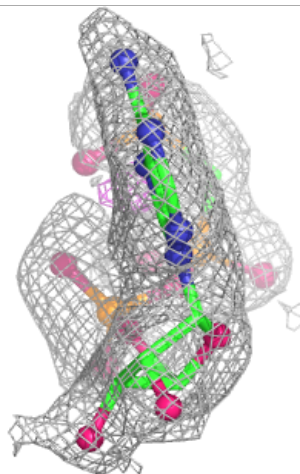
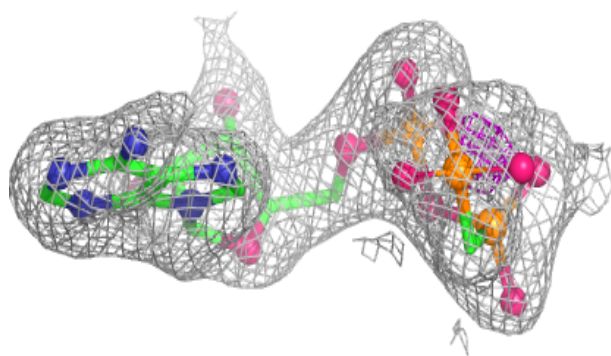
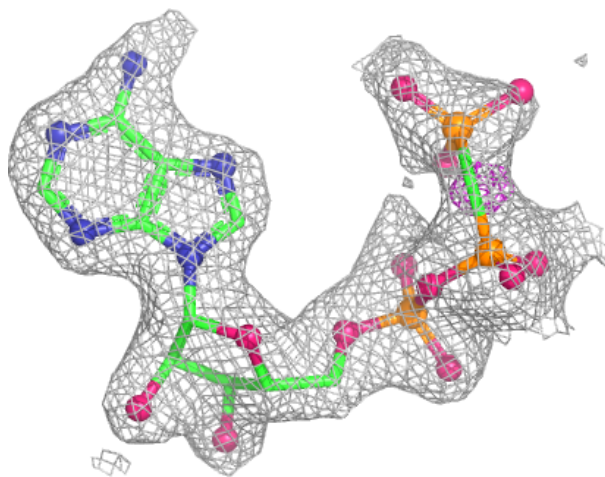
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NA	D	404	1/1	0.92	0.08	42,42,42,42	0
4	PO4	D	402	5/5	0.92	0.14	36,38,44,49	0
2	ACP	D	401	31/31	0.93	0.08	36,42,72,76	0
3	NA	D	403	1/1	0.96	0.07	35,35,35,35	0
2	ACP	A	401[A]	31/31	0.97	0.05	14,16,19,20	31
3	NA	B	402	1/1	0.97	0.05	17,17,17,17	0
2	ACP	A	401[B]	31/31	0.97	0.05	14,16,29,31	31
2	ACP	B	401	31/31	0.97	0.06	16,19,27,32	0
2	ACP	C	401	31/31	0.97	0.06	15,19,38,45	0
3	NA	C	403	1/1	0.98	0.08	22,22,22,22	0
3	NA	A	403	1/1	0.98	0.05	21,21,21,21	0
3	NA	B	403	1/1	0.98	0.06	23,23,23,23	0
3	NA	C	402	1/1	0.98	0.06	23,23,23,23	0
3	NA	A	402	1/1	0.99	0.05	18,18,18,18	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.

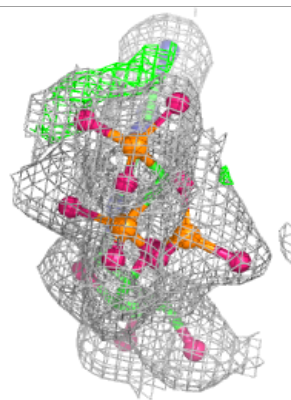
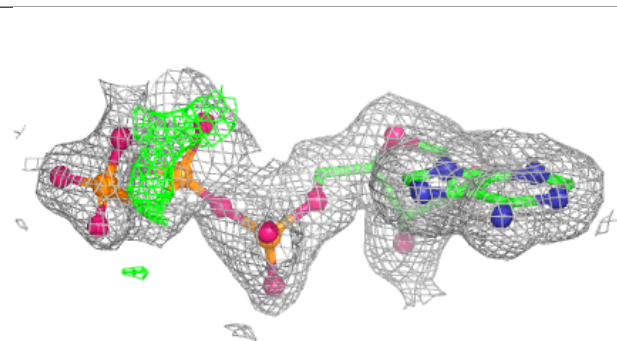
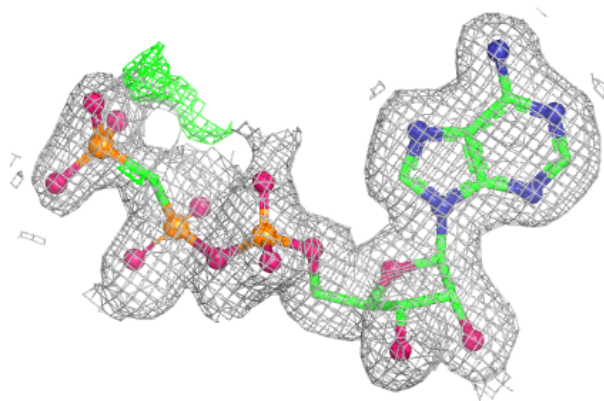
Electron density around ACP D 401:

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



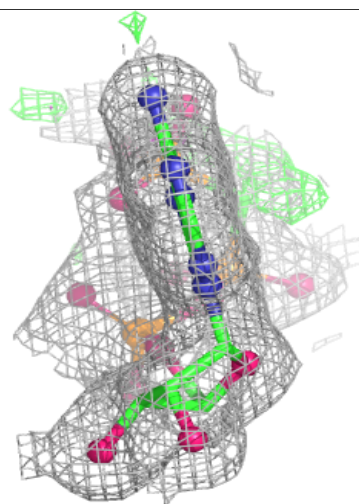
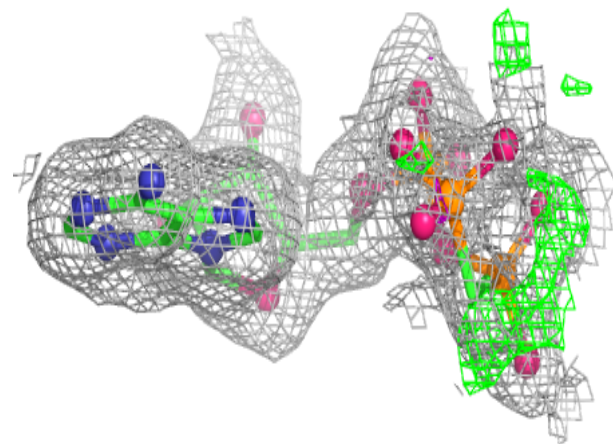
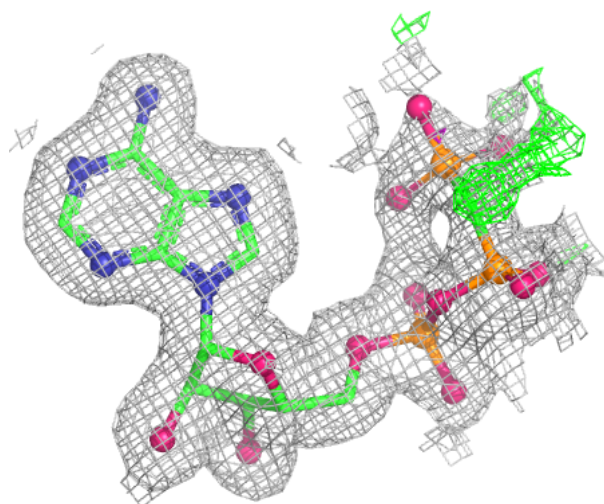
Electron density around ACP A 401 (A):

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



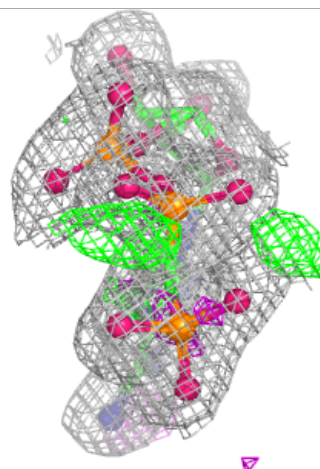
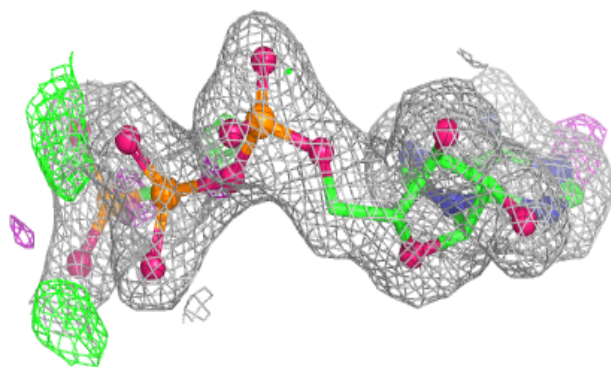
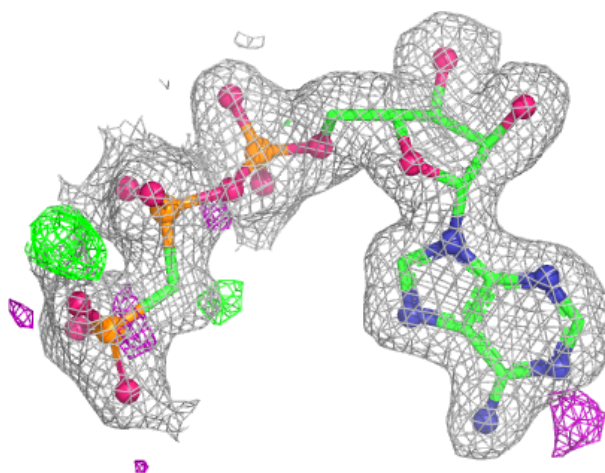
Electron density around ACP A 401 (B):

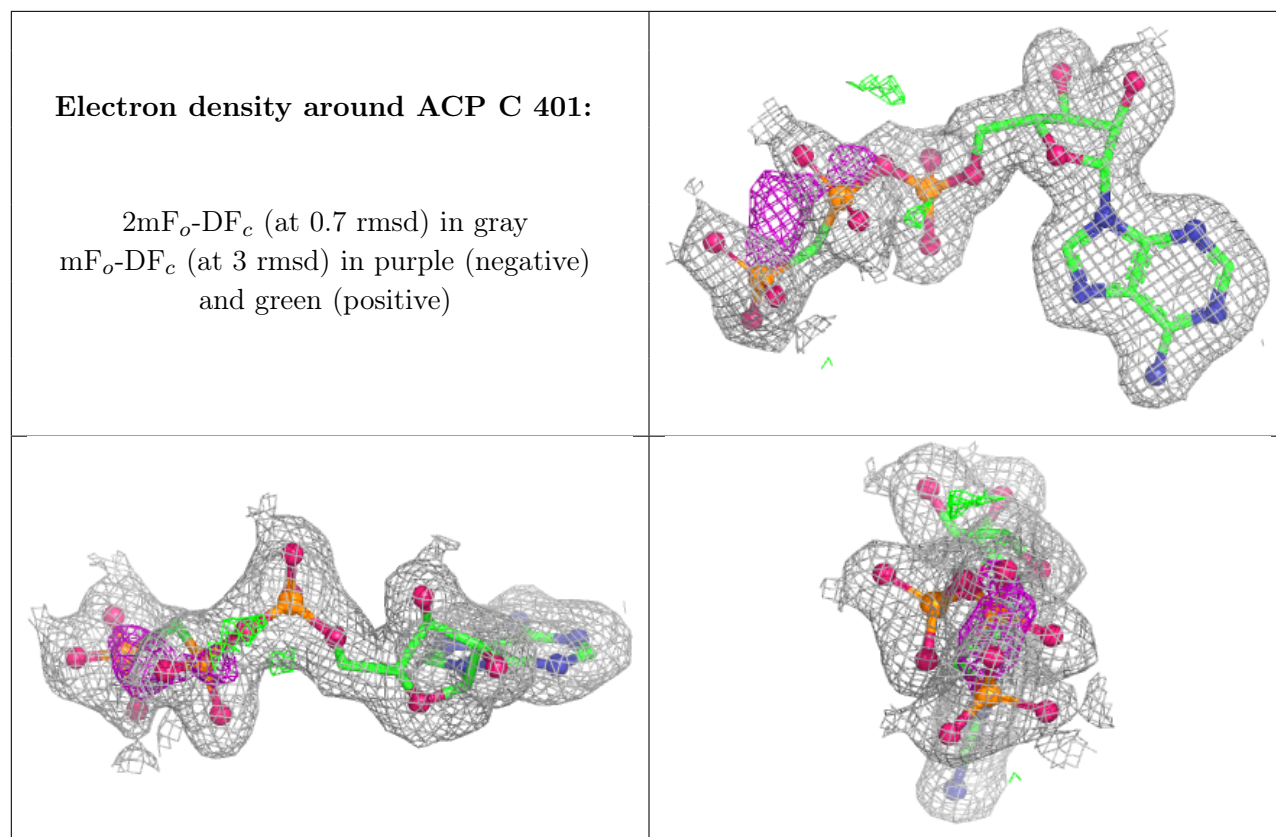
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ACP B 401:

$2mF_o-DF_c$ (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.