



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 02:45 PM BST

PDB ID : 5C41
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

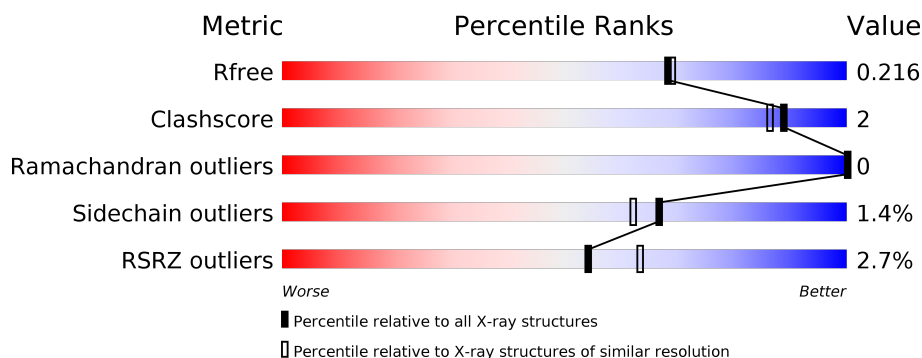
1 Overall quality at a glance

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}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (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 on 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	<div> <div>8%</div> <div> <div></div> <div>89%</div> <div>6%</div> <div>• •</div> </div> </div>
1	B	330	<div> <div></div> <div> <div></div> <div>84%</div> <div>9%</div> <div>• 6%</div> </div> </div>
1	C	330	<div> <div></div> <div> <div></div> <div>90%</div> <div>6%</div> <div>•</div> </div> </div>
1	D	330	<div> <div>8%</div> <div> <div></div> <div>90%</div> <div>5%</div> <div>• •</div> </div> </div>

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:

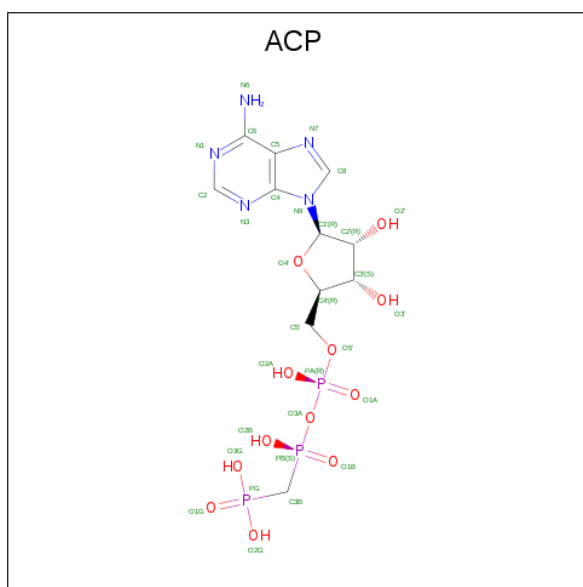
Chain	Residue	Modelled	Actual	Comment	Reference
A	323	LEU	-	expression tag	UNP Q9H477
A	324	GLU	-	expression tag	UNP Q9H477
A	325	HIS	-	expression tag	UNP Q9H477
A	326	HIS	-	expression tag	UNP Q9H477
A	327	HIS	-	expression tag	UNP Q9H477
A	328	HIS	-	expression tag	UNP Q9H477
A	329	HIS	-	expression tag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

Continued on next page...

Continued from previous page...

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 (three-letter code: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).

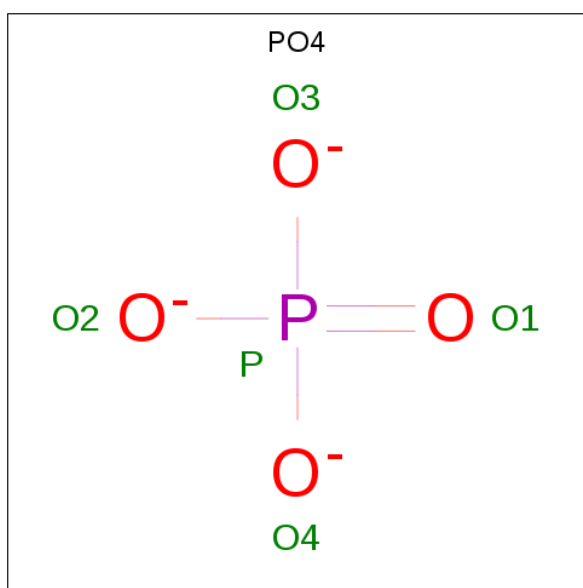


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	1
			62	22	10	24	6		
2	B	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
2	C	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
2	D	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

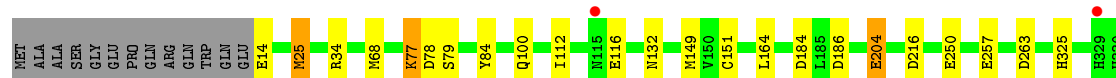
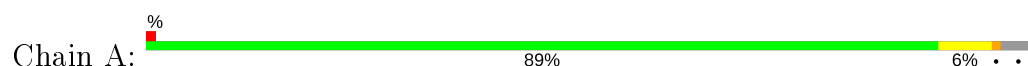
- Molecule 5 is water.

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		

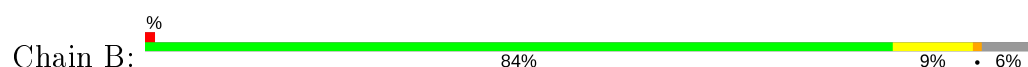
3 Residue-property plots [i](#)

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.

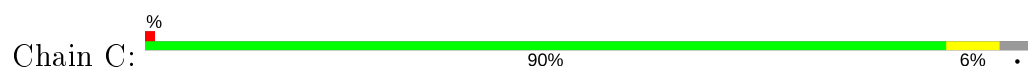
• Molecule 1: Ribokinase



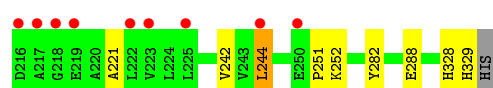
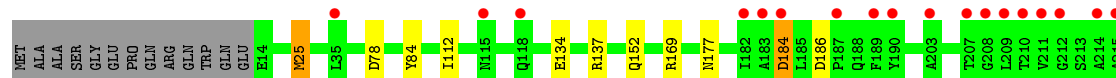
• Molecule 1: Ribokinase



• 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) 99.8 (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)	0.34 , 48.3	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: NA, PO4, ACP

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	1.07	2/2452 (0.1%)	0.99	9/3331 (0.3%)
1	B	1.09	8/2332 (0.3%)	1.02	7/3172 (0.2%)
1	C	1.03	3/2417 (0.1%)	0.98	7/3289 (0.2%)
1	D	0.88	3/2364 (0.1%)	0.93	7/3220 (0.2%)
All	All	1.02	16/9565 (0.2%)	0.98	30/13012 (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 (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	204	GLU	CD-OE1	11.31	1.38	1.25
1	A	257	GLU	CD-OE1	8.06	1.34	1.25
1	B	79	SER	CB-OG	-7.57	1.32	1.42
1	B	306	GLY	C-O	6.47	1.33	1.23
1	B	114	ASN	N-CA	-6.25	1.33	1.46
1	C	200	GLU	CD-OE1	5.93	1.32	1.25
1	B	52	GLY	N-CA	-5.61	1.37	1.46
1	D	184	ASP	CB-CG	-5.61	1.40	1.51
1	B	86	GLU	CG-CD	5.58	1.60	1.51
1	B	250	GLU	CD-OE1	5.58	1.31	1.25
1	C	324	GLU	CG-CD	5.58	1.60	1.51
1	B	162	GLU	CD-OE1	5.56	1.31	1.25
1	C	33	SER	CB-OG	-5.40	1.35	1.42
1	B	307	THR	N-CA	-5.22	1.35	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	329	HIS	N-CA	5.12	1.56	1.46
1	D	282	TYR	CG-CD1	5.04	1.45	1.39

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	34	ARG	NE-CZ-NH2	8.14	124.37	120.30
1	C	169	ARG	NE-CZ-NH2	8.05	124.33	120.30
1	A	25	MET	CG-SD-CE	-7.54	88.14	100.20
1	D	25	MET	CG-SD-CE	-7.28	88.55	100.20
1	A	186	ASP	CB-CG-OD1	7.26	124.84	118.30
1	C	168	ARG	CG-CD-NE	7.09	126.68	111.80
1	D	137	ARG	NE-CZ-NH2	-6.93	116.83	120.30
1	C	186	ASP	CB-CG-OD1	6.71	124.34	118.30
1	B	186	ASP	CB-CG-OD1	6.69	124.32	118.30
1	D	137	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	C	103	ASP	CB-CG-OD2	6.48	124.13	118.30
1	D	184	ASP	CB-CG-OD2	-6.17	112.74	118.30
1	C	216	ASP	CB-CG-OD1	6.08	123.77	118.30
1	A	78	ASP	CB-CG-OD2	6.06	123.75	118.30
1	D	186	ASP	CB-CG-OD1	5.97	123.68	118.30
1	C	263	ASP	CB-CG-OD1	5.96	123.66	118.30
1	D	169	ARG	NE-CZ-NH2	5.95	123.27	120.30
1	B	114	ASN	N-CA-CB	-5.75	100.24	110.60
1	B	263	ASP	CB-CG-OD1	5.68	123.41	118.30
1	B	78	ASP	CB-CG-OD2	5.61	123.35	118.30
1	B	130	LEU	CB-CG-CD1	5.49	120.33	111.00
1	A	34	ARG	CD-NE-CZ	5.38	131.14	123.60
1	A	263	ASP	CB-CG-OD1	5.20	122.98	118.30
1	D	78	ASP	CB-CG-OD2	5.09	122.88	118.30
1	B	216	ASP	CB-CG-OD1	5.08	122.87	118.30
1	C	78	ASP	CB-CG-OD2	5.07	122.86	118.30
1	A	325[A]	HIS	CB-CA-C	5.04	120.47	110.40
1	A	325[B]	HIS	CB-CA-C	5.04	120.47	110.40
1	B	137	ARG	CG-CD-NE	-5.04	101.22	111.80
1	A	216	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	134	GLU	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
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	10	0
1	B	2299	0	2318	11	0
1	C	2378	0	2347	9	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	4	0
5	D	158	0	0	0	0
All	All	10589	0	9436	37	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 (37) 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
1:C:306[B]:GLY:O	5:C:502:HOH:O	2.06	0.73
2:A:401[B]:ACP:H3B2	5:A:621:HOH:O	1.94	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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:A:149[A]:MET:HE3	1:A:164:LEU:HD23	1.97	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: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:C:46:LYS:NZ	5:C:516:HOH:O	2.51	0.42
1:B:287:LEU:O	1:B:291:LEU:HD13	2.20	0.42
1:A:68:MET:HE3	5:A:547:HOH:O	2.20	0.41
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

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	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%)	255 (97%)	7 (3%)	44	34
1	B	249/266 (94%)	247 (99%)	2 (1%)	81	80
1	C	254/266 (96%)	253 (100%)	1 (0%)	91	90
1	D	246/266 (92%)	242 (98%)	4 (2%)	62	58
All	All	1011/1064 (95%)	997 (99%)	14 (1%)	67	62

All (14) 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	84	TYR
1	A	116	GLU
1	A	184	ASP
1	B	84	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	173	LYS
1	C	84	TYR
1	D	25	MET
1	D	84	TYR
1	D	184	ASP
1	D	244	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	188	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 monosaccharides 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	$\# Z > 2$
4	PO4	D	402	-	4,4,4	0.69	0	6,6,6	1.93	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ACP	A	401[B]	-	27,33,33	1.89	7 (25%)	32,52,52	1.73	9 (28%)
2	ACP	A	401[A]	3	27,33,33	1.91	7 (25%)	32,52,52	1.58	7 (21%)
2	ACP	B	401	-	27,33,33	2.18	7 (25%)	32,52,52	1.63	6 (18%)
2	ACP	C	401	3	27,33,33	2.10	6 (22%)	32,52,52	1.73	7 (21%)
2	ACP	D	401	-	27,33,33	1.85	6 (22%)	32,52,52	1.73	7 (21%)

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	B	401	-	-	2/15/38/38	0/3/3/3
2	ACP	C	401	3	-	2/15/38/38	0/3/3/3
2	ACP	D	401	-	-	3/15/38/38	0/3/3/3
2	ACP	A	401[B]	-	-	1/15/38/38	0/3/3/3
2	ACP	A	401[A]	3	-	5/15/38/38	0/3/3/3

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	ACP	PB-O3A	7.73	1.67	1.58
2	B	401	ACP	PB-O3A	6.82	1.66	1.58
2	B	401	ACP	PG-O1G	6.50	1.63	1.50
2	D	401	ACP	PG-O1G	5.62	1.62	1.50
2	A	401[A]	ACP	PB-O3A	5.39	1.64	1.58
2	A	401[B]	ACP	PB-O1B	4.27	1.61	1.51
2	A	401[B]	ACP	PB-O2B	-3.90	1.47	1.56
2	A	401[A]	ACP	PB-O2B	-3.77	1.47	1.56
2	C	401	ACP	PG-O3G	3.72	1.63	1.54
2	D	401	ACP	PG-O2G	3.70	1.63	1.54
2	A	401[A]	ACP	PB-O1B	3.65	1.60	1.51
2	A	401[B]	ACP	PB-O3A	3.40	1.62	1.58
2	A	401[B]	ACP	PG-O2G	3.36	1.62	1.54
2	C	401	ACP	C2-N3	3.36	1.37	1.32
2	D	401	ACP	PB-O3A	3.33	1.62	1.58
2	A	401[B]	ACP	PG-O3G	3.33	1.62	1.54
2	C	401	ACP	PG-O2G	3.25	1.62	1.54
2	B	401	ACP	PB-O2B	-2.90	1.49	1.56
2	D	401	ACP	O4'-C1'	2.73	1.44	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	ACP	PB-O2B	2.68	1.62	1.56
2	D	401	ACP	C5-C4	2.65	1.47	1.40
2	A	401[A]	ACP	PG-O2G	2.59	1.60	1.54
2	B	401	ACP	PG-O3G	2.50	1.60	1.54
2	A	401[A]	ACP	C5-C4	2.39	1.47	1.40
2	C	401	ACP	C5-C4	2.36	1.47	1.40
2	A	401[A]	ACP	O4'-C1'	2.34	1.44	1.41
2	A	401[B]	ACP	C5-C4	2.33	1.47	1.40
2	B	401	ACP	PB-O1B	2.28	1.57	1.51
2	D	401	ACP	C2-N3	2.26	1.35	1.32
2	A	401[B]	ACP	O4'-C1'	2.24	1.44	1.41
2	A	401[A]	ACP	PG-O3G	2.21	1.60	1.54
2	B	401	ACP	C5-C4	2.15	1.46	1.40
2	B	401	ACP	PA-O2A	-2.09	1.45	1.55

All (38) 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	111.24
2	C	401	ACP	N3-C2-N1	-4.52	121.62	128.68
2	A	401[B]	ACP	N3-C2-N1	-4.31	121.95	128.68
2	A	401[A]	ACP	N3-C2-N1	-4.30	121.96	128.68
2	B	401	ACP	N3-C2-N1	-4.01	122.41	128.68
2	A	401[B]	ACP	O3G-PG-C3B	3.91	115.89	106.40
2	D	401	ACP	N3-C2-N1	-3.86	122.64	128.68
2	D	401	ACP	O1B-PB-C3B	3.77	119.05	109.07
2	D	401	ACP	O3G-PG-O1G	-3.61	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	3.41	118.03	108.08
4	D	402	PO4	O4-P-O3	3.40	118.87	107.97
2	B	401	ACP	O2B-PB-O1B	3.20	120.76	110.07
2	B	401	ACP	C2-N1-C6	3.17	124.17	118.75
2	B	401	ACP	O2A-PA-O1A	3.15	127.82	112.24
2	B	401	ACP	C1'-N9-C4	-2.83	121.67	126.64
2	C	401	ACP	C2-N1-C6	2.80	123.55	118.75
2	A	401[A]	ACP	O3G-PG-C3B	-2.75	99.72	106.40
2	A	401[B]	ACP	O1B-PB-C3B	-2.75	101.80	109.07
2	A	401[B]	ACP	C2-N1-C6	2.70	123.36	118.75
2	C	401	ACP	O3G-PG-C3B	2.69	112.93	106.40
2	A	401[A]	ACP	O3G-PG-O1G	-2.68	105.31	112.39
2	B	401	ACP	O1G-PG-C3B	-2.65	105.53	111.24
2	A	401[A]	ACP	C2-N1-C6	2.64	123.27	118.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	ACP	C1'-N9-C4	-2.61	122.05	126.64
2	A	401[B]	ACP	O2G-PG-O1G	-2.60	105.51	112.39
4	D	402	PO4	O3-P-O1	-2.53	101.65	110.89
2	A	401[B]	ACP	O2B-PB-C3B	2.45	116.62	106.58
2	D	401	ACP	O2A-PA-O1A	2.39	124.08	112.24
2	C	401	ACP	PA-O3A-PB	-2.29	125.29	132.56
2	A	401[A]	ACP	PA-O3A-PB	-2.22	125.53	132.56
2	D	401	ACP	C3'-C2'-C1'	2.18	104.26	100.98
2	C	401	ACP	N6-C6-N1	2.12	122.98	118.57
2	A	401[A]	ACP	C4-C5-N7	-2.12	107.19	109.40
2	D	401	ACP	O3G-PG-O2G	2.07	114.13	108.08
2	A	401[B]	ACP	O3G-PG-O1G	-2.05	106.95	112.39
2	A	401[B]	ACP	O2A-PA-O1A	2.05	122.36	112.24
2	A	401[B]	ACP	C4-C5-N7	-2.04	107.27	109.40

There are no chirality outliers.

All (13) 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	A	401[B]	ACP	PB-C3B-PG-O1G
2	C	401	ACP	PB-C3B-PG-O1G
2	B	401	ACP	C3'-C4'-C5'-O5'
2	A	401[A]	ACP	C5'-O5'-PA-O2A

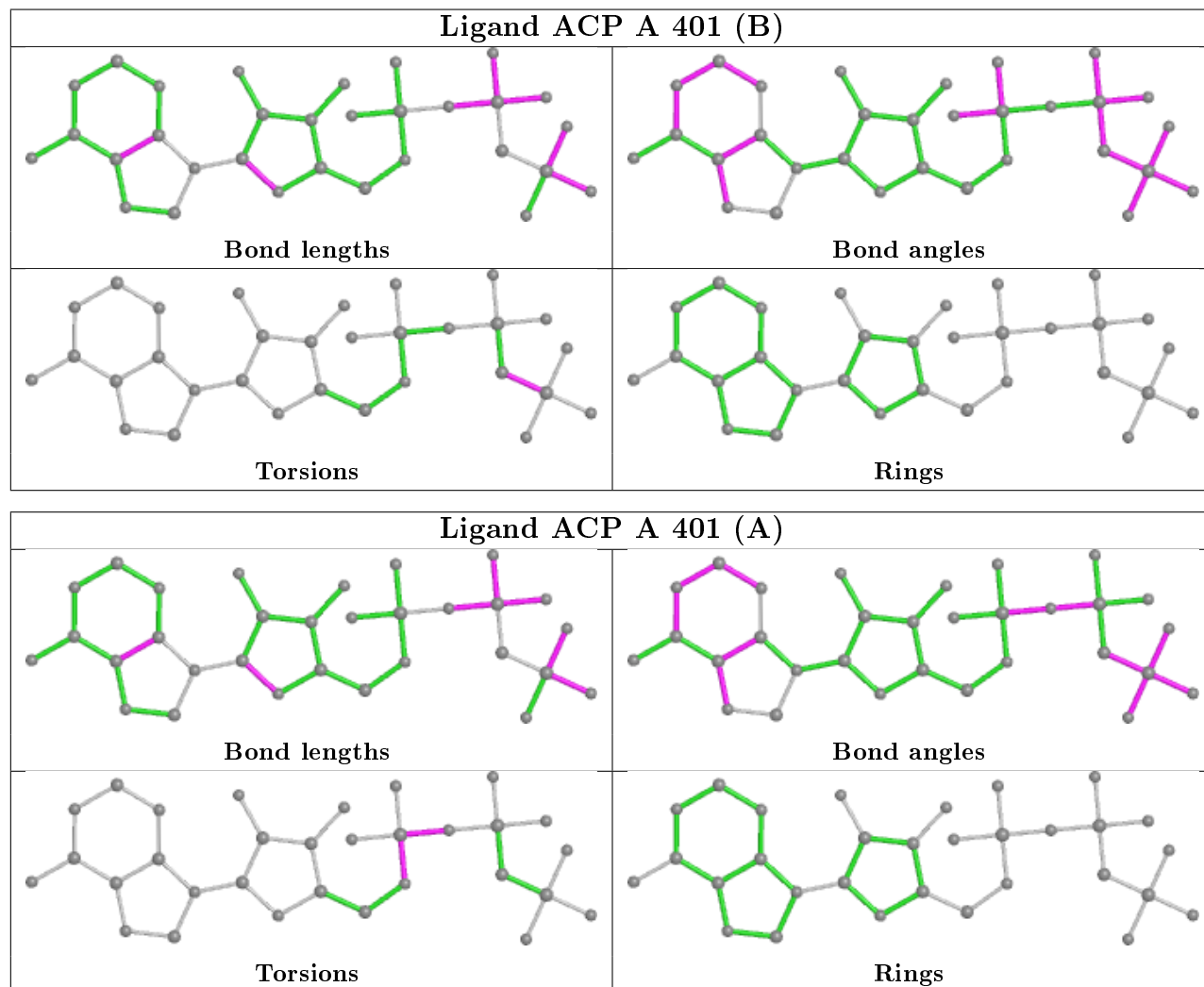
There are no ring outliers.

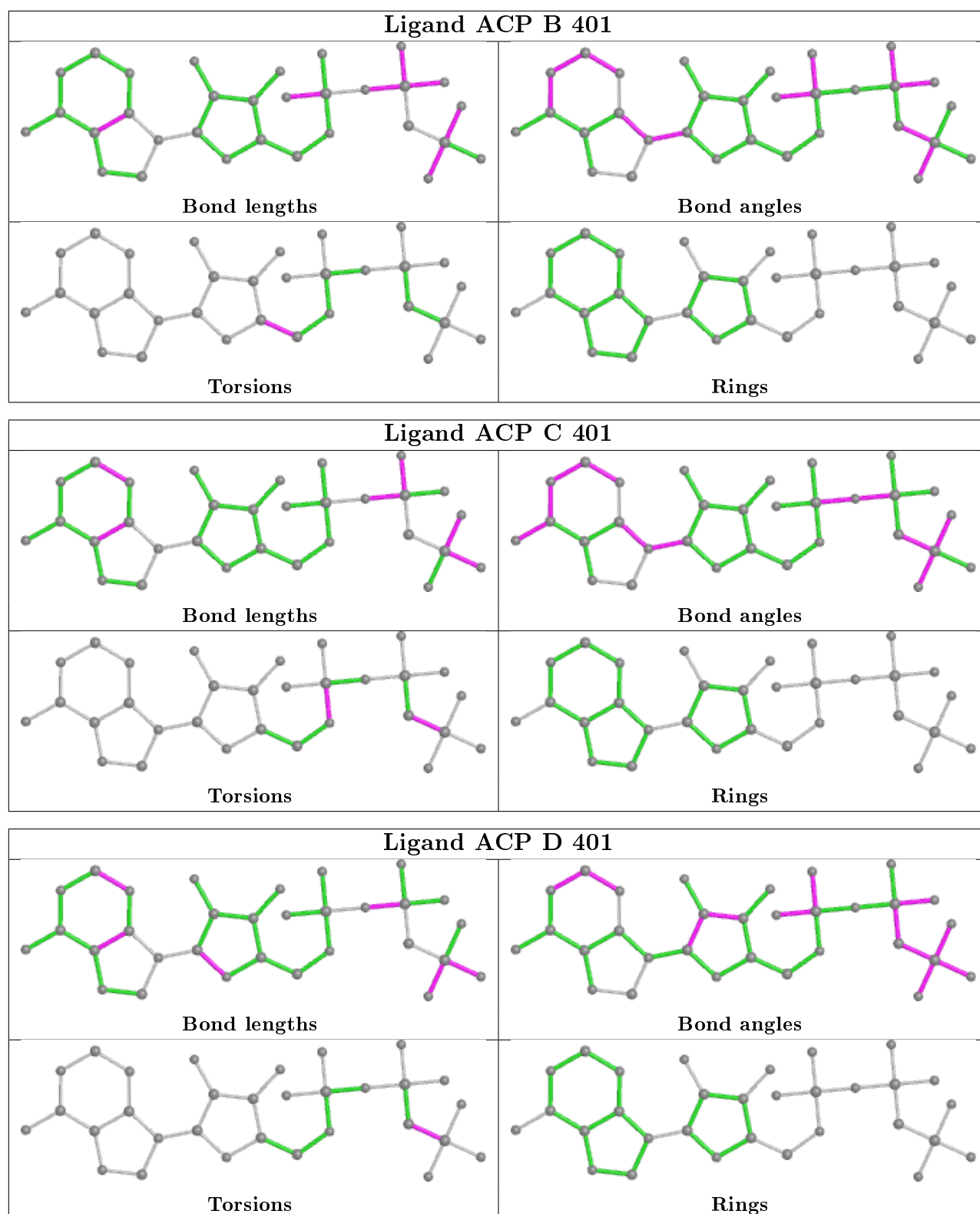
1 monomer is involved in 1 short contact:

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%)	-0.22	2 (0%) 89 93	11, 20, 49, 72	0
1	B	310/330 (93%)	-0.21	2 (0%) 89 93	13, 25, 48, 61	0
1	C	317/330 (96%)	-0.14	3 (0%) 84 89	13, 26, 50, 79	0
1	D	316/330 (95%)	0.44	27 (8%) 10 17	23, 39, 77, 93	0
All	All	1260/1320 (95%)	-0.03	34 (2%) 54 63	11, 27, 63, 93	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	211	VAL	6.2
1	D	209	LEU	5.1
1	D	183	ALA	4.5
1	D	210	THR	4.4
1	D	222	LEU	4.1
1	D	182	ILE	3.9
1	D	214	ALA	3.9
1	D	207	THR	3.6
1	D	215	ALA	3.5
1	D	217	ALA	3.3
1	D	223	VAL	3.3
1	B	118	GLN	3.3
1	D	218	GLY	3.1
1	D	187	PRO	3.0
1	D	184	ASP	2.9
1	D	190	TYR	2.8
1	D	35	LEU	2.7
1	D	208	GLY	2.7
1	D	212	GLY	2.7
1	C	34	ARG	2.6
1	D	115	ASN	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	216	ASP	2.4
1	A	329	HIS	2.4
1	D	244	LEU	2.3
1	D	250	GLU	2.3
1	D	118	GLN	2.3
1	D	203	ALA	2.2
1	A	115	ASN	2.2
1	D	189	PHE	2.2
1	D	225	LEU	2.2
1	D	219	GLU	2.1
1	C	306[A]	GLY	2.1
1	B	212	GLY	2.1
1	C	33	SER	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 monosaccharides 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.

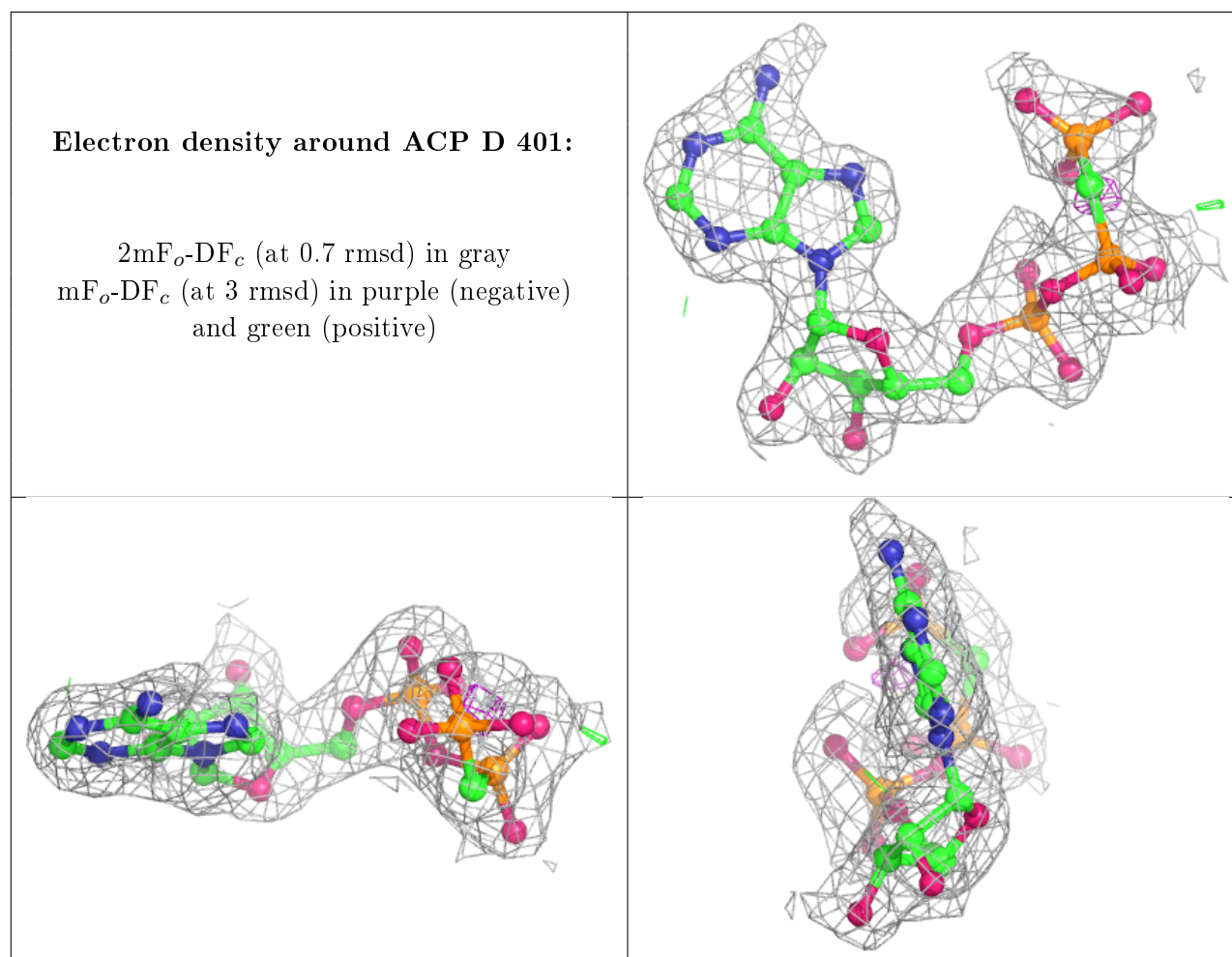
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NA	D	404	1/1	0.92	0.22	42,42,42,42	0
4	PO4	D	402	5/5	0.94	0.19	36,38,44,49	0
2	ACP	D	401	31/31	0.95	0.12	36,42,72,76	0
2	ACP	B	401	31/31	0.96	0.09	16,19,27,32	0
2	ACP	C	401	31/31	0.96	0.10	15,19,38,45	0
3	NA	D	403	1/1	0.96	0.09	35,35,35,35	0
2	ACP	A	401[B]	31/31	0.97	0.10	14,16,29,31	31
2	ACP	A	401[A]	31/31	0.97	0.10	14,16,19,20	31
3	NA	C	403	1/1	0.98	0.06	22,22,22,22	0
3	NA	A	403	1/1	0.99	0.07	21,21,21,21	0

Continued on next page...

Continued from previous page...

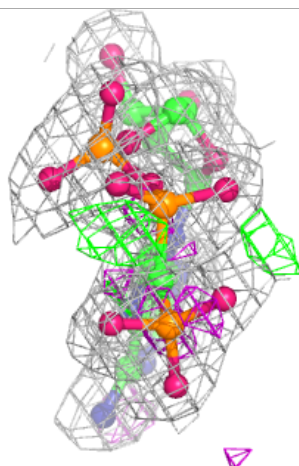
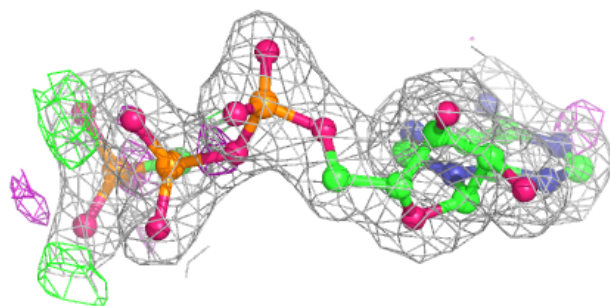
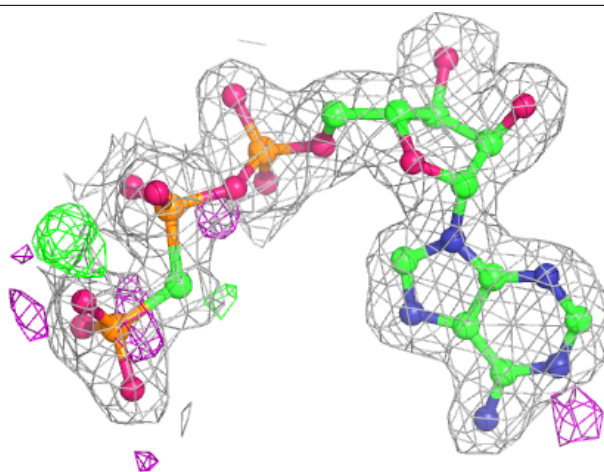
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NA	B	402	1/1	0.99	0.07	17,17,17,17	0
3	NA	A	402	1/1	0.99	0.06	18,18,18,18	0
3	NA	B	403	1/1	0.99	0.05	23,23,23,23	0
3	NA	C	402	1/1	0.99	0.07	23,23,23,23	0

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.



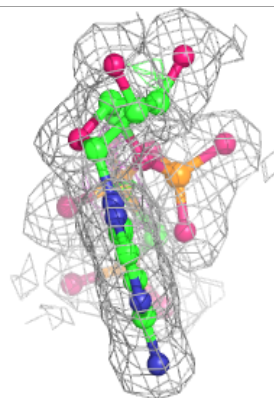
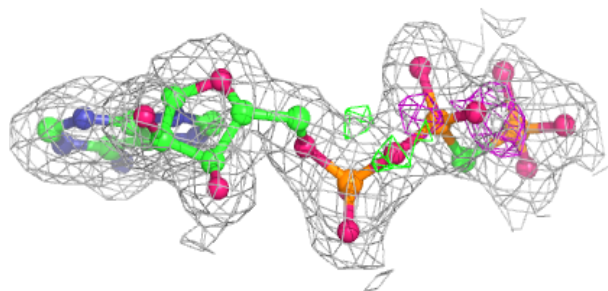
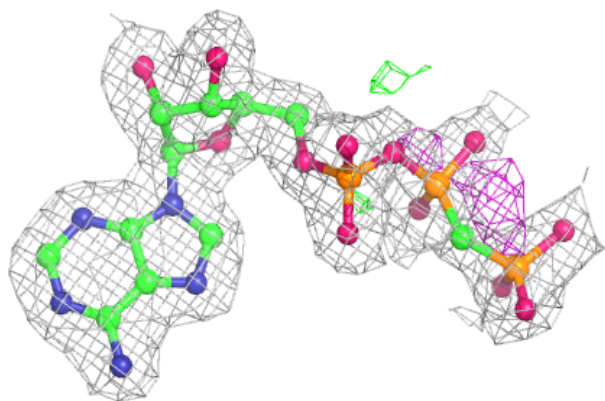
Electron density around ACP B 401:

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



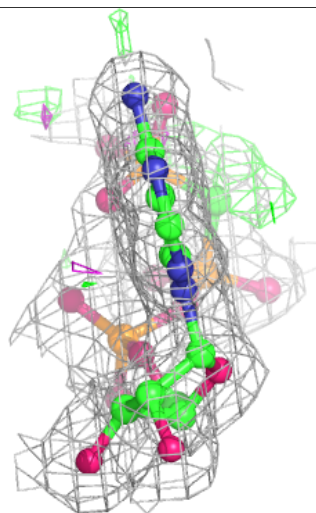
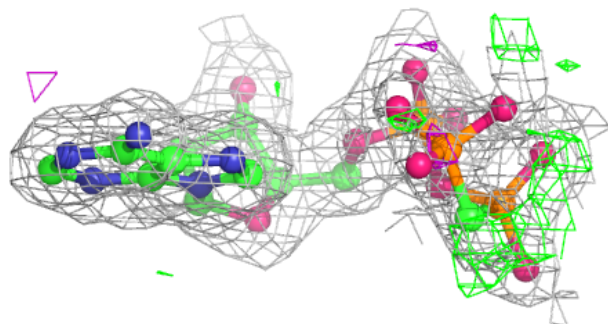
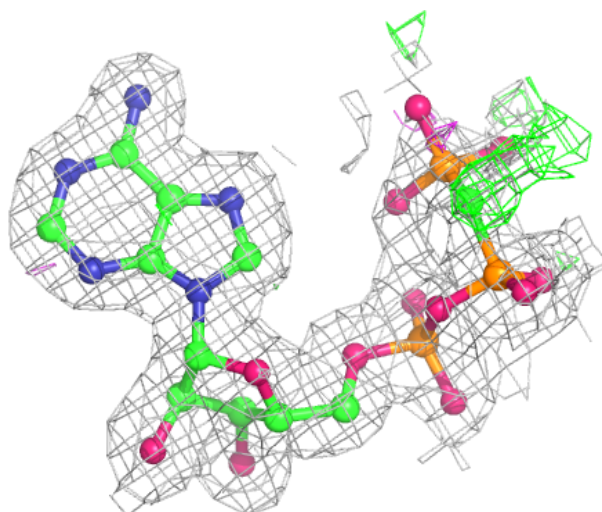
Electron density around ACP C 401:

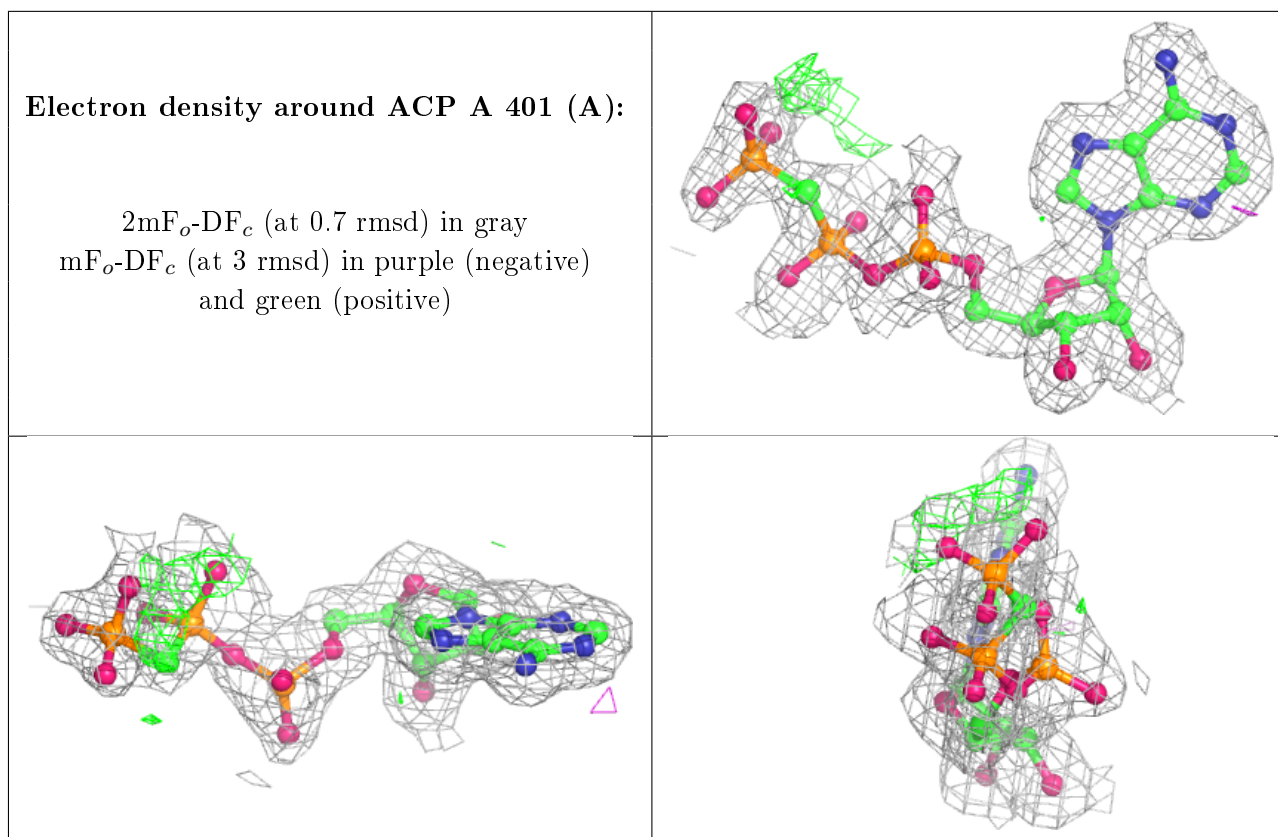
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.