Full wwPDB X-ray Structure Validation Report (i)

Feb 22, 2021 – 02:22 PM GMT

PDB ID	:	7B94
Title	:	MEK1 in complex with compound 6
Authors	:	Kack, H.; Oster, L.
Deposited on	:	2020-12-14
Resolution	:	2.00 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

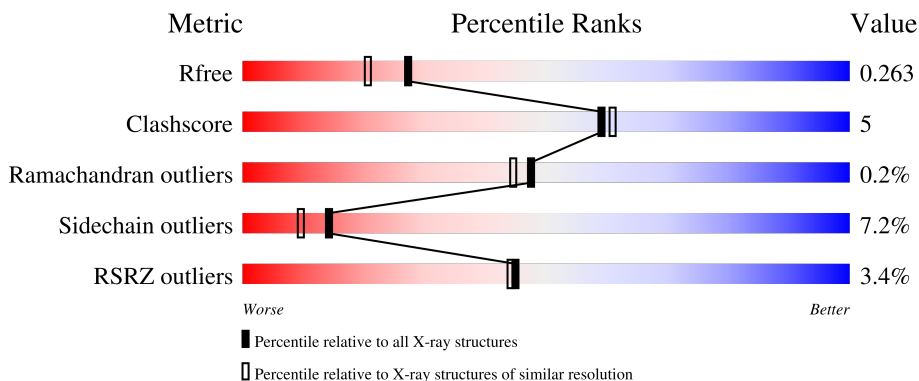|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.17.1.dev1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.17.1.dev1

1 Overall quality at a glance (i)

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	Percentile Ranks	Value
Rfree		0.263
Clashscore		5
Ramachandran outliers		0.2%
Sidechain outliers		7.2%
RSRZ outliers		3.4%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 <=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	326	2% 77% 15% 8%
1	B	326	4% 77% 13% • 10%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 5073 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 Dual specificity mitogen-activated protein kinase kinase 1,Dual specificity mitogen-activated protein kinase kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	301	Total 2380	C 1519	N 406	O 440	S 15	0	0	0
1	B	295	Total 2316	C 1475	N 399	O 427	S 15	0	0	0

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	MET	-	initiating methionine	UNP Q02750
A	21	ALA	-	expression tag	UNP Q02750
A	22	HIS	-	expression tag	UNP Q02750
A	23	HIS	-	expression tag	UNP Q02750
A	24	HIS	-	expression tag	UNP Q02750
A	25	HIS	-	expression tag	UNP Q02750
A	26	HIS	-	expression tag	UNP Q02750
A	27	HIS	-	expression tag	UNP Q02750
A	28	ALA	-	expression tag	UNP Q02750
A	29	ALA	-	expression tag	UNP Q02750
A	30	ALA	-	expression tag	UNP Q02750
A	31	GLU	-	expression tag	UNP Q02750
A	32	ASN	-	expression tag	UNP Q02750
A	33	LEU	-	expression tag	UNP Q02750
A	34	TYR	-	expression tag	UNP Q02750
A	35	PHE	-	expression tag	UNP Q02750
A	36	GLN	-	expression tag	UNP Q02750
A	302	GLY	-	linker	UNP Q02750
A	303	SER	-	linker	UNP Q02750
A	304	GLY	-	linker	UNP Q02750
A	305	SER	-	linker	UNP Q02750
A	306	GLY	-	linker	UNP Q02750
A	307	SER	-	linker	UNP Q02750
B	20	MET	-	initiating methionine	UNP Q02750

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Chain	Residue	Modelled	Actual	Comment	Reference
B	21	ALA	-	expression tag	UNP Q02750
B	22	HIS	-	expression tag	UNP Q02750
B	23	HIS	-	expression tag	UNP Q02750
B	24	HIS	-	expression tag	UNP Q02750
B	25	HIS	-	expression tag	UNP Q02750
B	26	HIS	-	expression tag	UNP Q02750
B	27	HIS	-	expression tag	UNP Q02750
B	28	ALA	-	expression tag	UNP Q02750
B	29	ALA	-	expression tag	UNP Q02750
B	30	ALA	-	expression tag	UNP Q02750
B	31	GLU	-	expression tag	UNP Q02750
B	32	ASN	-	expression tag	UNP Q02750
B	33	LEU	-	expression tag	UNP Q02750
B	34	TYR	-	expression tag	UNP Q02750
B	35	PHE	-	expression tag	UNP Q02750
B	36	GLN	-	expression tag	UNP Q02750
B	264	GLY	-	linker	UNP Q02750
B	303	SER	-	linker	UNP Q02750
B	304	GLY	-	linker	UNP Q02750
B	305	SER	-	linker	UNP Q02750
B	306	GLY	-	linker	UNP Q02750
B	307	SER	-	linker	UNP Q02750

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).
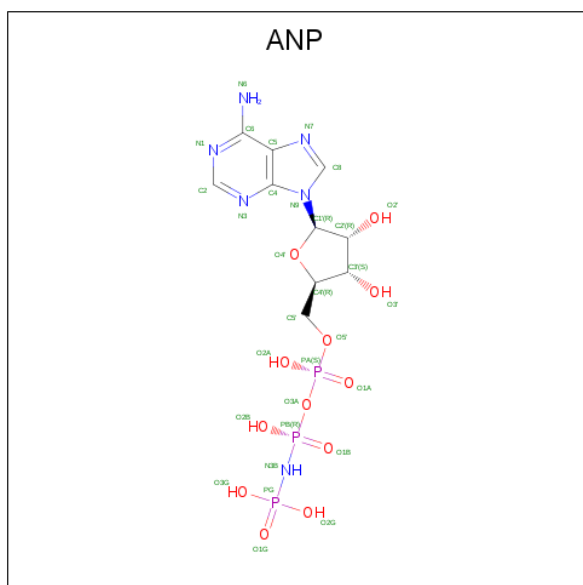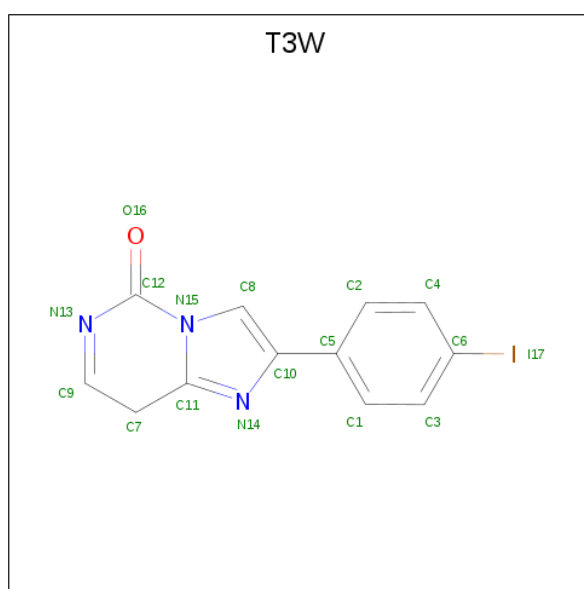
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is 2-(4-iodophenyl)-8 {H}-imidazo[1,2-c]pyrimidin-5-one (three-letter code: T3W) (formula: $C_{12}H_8IN_3O$) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	I	N	O	0	0
			17	12	1	3	1		
4	B	1	Total	C	I	N	O	0	0
			17	12	1	3	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
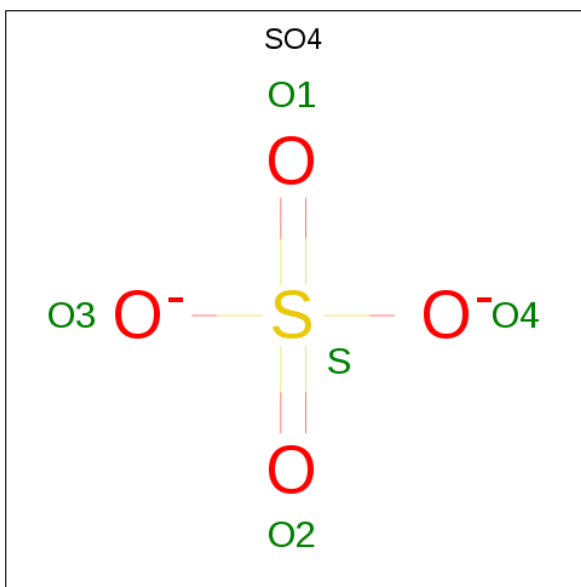
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 5	O 4	S 1	0	0
5	B	1	Total 5	O 4	S 1	0	0

- Molecule 6 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	135	Total 135	O 135	0	0
6	B	134	Total 134	O 134	0	0

3 Residue-property plots ⓘ

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

• Molecule 1: Dual specificity mitogen-activated protein kinase kinase 1,Dual specificity mitogen-activated protein kinase kinase 1
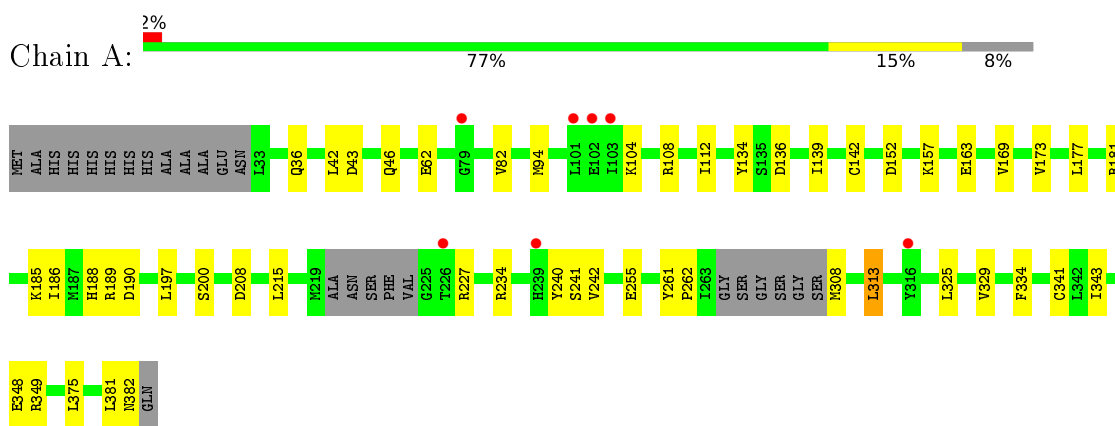
• Molecule 1: Dual specificity mitogen-activated protein kinase kinase 1,Dual specificity mitogen-activated protein kinase kinase 1
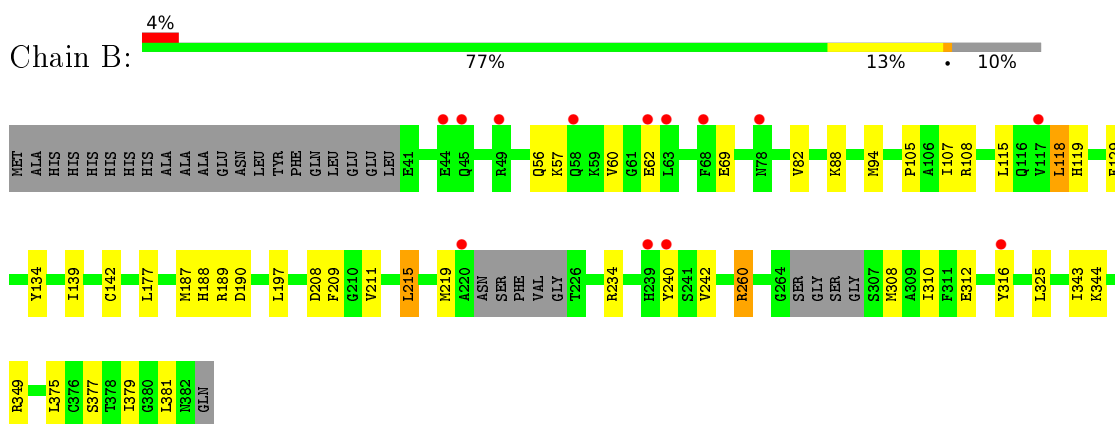
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	57.28Å 71.75Å 157.80Å	Depositor
a, b, c, α, β, γ	90.00° 90.00° 90.00°	
Resolution (Å)	78.90 – 2.00	Depositor
	78.90 – 2.00	EDS
% Data completeness	96.7 (78.90-2.00)	Depositor
(in resolution range)	96.7 (78.90-2.00)	EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.27 (at 2.00Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.216 , 0.265	Depositor
	0.213 , 0.263	DCC
R_{free} test set	2115 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	37.8	Xtriage
Anisotropy	0.400	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 54.8	EDS
L-test for twinning[2]	$< |L| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5073	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.61% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: T3W, MG, ANP, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$>5	RMSZ	#$|Z|$>5
1	A	0.52	0/2423	0.69	0/3257
1	B	0.50	0/2357	0.70	0/3168
All	All	0.51	0/4780	0.69	0/6425

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2380	0	2406	21	0
1	B	2316	0	2350	24	0
2	A	31	0	13	0	0
2	B	31	0	13	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	17	0	0	1	0
4	B	17	0	0	1	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
6	A	135	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	134	0	0	0	0
All	All	5073	0	4782	45	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 5.

All (45) 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:A:94:MET:CE	1:A:142:CYS:HB3	1.93	0.98
1:A:188:HIS:HD2	1:A:190:ASP:H	1.23	0.85
1:B:343:ILE:O	1:B:349:ARG:HD3	1.83	0.78
1:A:343:ILE:O	1:A:349:ARG:HD3	1.90	0.70
1:A:94:MET:HE2	1:A:142:CYS:HB3	1.72	0.70
1:B:188:HIS:HD2	1:B:190:ASP:H	1.40	0.70
1:A:227:ARG:HE	1:A:261:TYR:HB2	1.58	0.69
1:A:112:ILE:HD11	1:A:134:TYR:HB2	1.77	0.66
1:A:43:ASP:H	1:A:46:GLN:HE21	1.45	0.65
1:A:94:MET:HE1	1:A:142:CYS:HB3	1.79	0.61
1:B:234:ARG:HD3	1:B:240:TYR:HD1	1.65	0.61
1:B:234:ARG:HD3	1:B:240:TYR:CD1	2.37	0.60
1:A:343:ILE:HG21	1:A:348:GLU:HB3	1.83	0.59
1:B:115:LEU:O	1:B:118:LEU:HB2	2.05	0.57
1:B:118:LEU:HD13	1:B:211:VAL:HG21	1.89	0.54
1:B:57:LYS:NZ	1:B:119:HIS:HD2	2.06	0.54
1:A:261:TYR:HE2	1:A:313:LEU:HD11	1.73	0.53
1:B:260:ARG:HH11	1:B:260:ARG:HG2	1.74	0.53
1:B:343:ILE:O	1:B:349:ARG:CD	2.56	0.52
1:B:189:ARG:HA	1:B:240:TYR:CZ	2.45	0.51
1:A:255:GLU:HB2	1:A:262:PRO:HD3	1.93	0.51
1:A:341:CYS:O	1:A:349:ARG:HD2	2.11	0.51
1:B:118:LEU:HB3	1:B:129:PHE:CD2	2.46	0.50
1:B:310:ILE:H	1:B:310:ILE:HD12	1.76	0.50
1:A:181:ARG:HD2	1:A:242:VAL:HG11	1.95	0.49
1:A:188:HIS:HD2	1:A:190:ASP:N	2.01	0.48
1:B:57:LYS:O	1:B:60:VAL:HG22	2.12	0.48
1:A:189:ARG:HA	1:A:240:TYR:CZ	2.50	0.46
1:A:241:SER:HB3	6:A:546:HOH:O	2.16	0.46
1:A:188:HIS:CD2	1:A:190:ASP:H	2.15	0.46
1:B:308:MET:CE	1:B:316:TYR:CD2	2.99	0.46
1:B:69:GLU:HB2	1:B:88:LYS:HE2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:379:ILE:HD11	1:B:381:LEU:HD12	1.99	0.43
1:A:200:SER:HB3	1:A:381:LEU:HD13	1.99	0.43
1:B:208:ASP:HA	4:B:403:T3W:C5	2.49	0.42
1:B:188:HIS:ND1	1:B:209:PHE:HB3	2.34	0.42
1:B:105:PRO:HA	1:B:108:ARG:HG2	2.01	0.42
1:B:312:GLU:O	1:B:316:TYR:HD2	2.03	0.42
1:A:169:VAL:O	1:A:173:VAL:HG23	2.20	0.41
1:B:94:MET:CE	1:B:142:CYS:HB3	2.50	0.41
1:B:215:LEU:O	1:B:219:MET:HG2	2.20	0.41
1:A:163:GLU:HG3	1:A:334:PHE:CD2	2.55	0.41
1:B:108:ARG:HD3	1:B:134:TYR:CD1	2.56	0.41
1:B:118:LEU:HB3	1:B:129:PHE:CG	2.56	0.40
1:A:208:ASP:HA	4:A:403:T3W:C5	2.52	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	295/326 (90%)	285 (97%)	9 (3%)	1 (0%)	41	37
1	B	289/326 (89%)	281 (97%)	8 (3%)	0	100	100
All	All	584/652 (90%)	566 (97%)	17 (3%)	1 (0%)	47	44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	LEU

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	262/280 (94%)	241 (92%)	21 (8%)	12	7
1	B	255/280 (91%)	239 (94%)	16 (6%)	18	13
All	All	517/560 (92%)	480 (93%)	37 (7%)	14	9

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	62	GLU
1	A	82	VAL
1	A	104	LYS
1	A	108	ARG
1	A	136	ASP
1	A	139	ILE
1	A	152	ASP
1	A	157	LYS
1	A	177	LEU
1	A	185	LYS
1	A	186	ILE
1	A	197	LEU
1	A	215	LEU
1	A	234	ARG
1	A	308	MET
1	A	313	LEU
1	A	325	LEU
1	A	329	VAL
1	A	375	LEU
1	A	382	ASN
1	B	56	GLN
1	B	62	GLU
1	B	82	VAL
1	B	107	ILE
1	B	118	LEU
1	B	139	ILE

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Mol	Chain	Res	Type
1	B	177	LEU
1	B	187	MET
1	B	197	LEU
1	B	215	LEU
1	B	242	VAL
1	B	260	ARG
1	B	325	LEU
1	B	344	LYS
1	B	375	LEU
1	B	377	SER

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	46	GLN
1	A	164	GLN
1	A	188	HIS
1	A	354	GLN
1	B	119	HIS
1	B	164	GLN
1	B	188	HIS
1	B	354	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 8 ligands modelled in this entry, 2 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	T3W	B	403	-	15,19,19	0.81	0	17,27,27	1.45	4 (23%)
2	ANP	B	401	3	29,33,33	0.56	0	31,52,52	1.00	3 (9%)
2	ANP	A	401	3	29,33,33	0.68	0	31,52,52	1.03	4 (12%)
4	T3W	A	403	-	15,19,19	0.87	0	17,27,27	1.61	4 (23%)
5	SO4	B	404	-	4,4,4	0.17	0	6,6,6	0.06	0
5	SO4	A	404	-	4,4,4	0.14	0	6,6,6	0.15	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	T3W	B	403	-	-	0/4/14/14	0/2/3/3
2	ANP	B	401	3	-	3/14/38/38	0/3/3/3
2	ANP	A	401	3	-	2/14/38/38	0/3/3/3
4	T3W	A	403	-	-	0/4/14/14	0/2/3/3

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	403	T3W	C7-C11-N15	-3.64	120.59	123.34
4	B	403	T3W	C7-C11-N15	-3.11	121.00	123.34
4	A	403	T3W	O16-C12-N15	2.88	123.59	118.16
4	B	403	T3W	O16-C12-N15	2.72	123.29	118.16
2	A	401	ANP	O2G-PG-O1G	-2.58	106.97	113.45
4	A	403	T3W	C8-C10-C5	-2.57	123.34	129.15
2	A	401	ANP	O1G-PG-N3B	2.55	115.52	111.77
2	A	401	ANP	O3G-PG-O1G	-2.51	107.14	113.45
4	A	403	T3W	C7-C11-N14	2.31	127.57	122.17
2	B	401	ANP	C5-C6-N6	2.23	123.74	120.35
4	B	403	T3W	C7-C11-N14	2.19	127.28	122.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	403	T3W	C8-C10-C5	-2.16	124.28	129.15
2	B	401	ANP	O1B-PB-N3B	2.10	114.87	111.77
2	B	401	ANP	O3G-PG-O1G	-2.05	108.30	113.45
2	A	401	ANP	C5-C6-N6	2.05	123.46	120.35

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	ANP	PB-N3B-PG-O1G
2	A	401	ANP	PG-N3B-PB-O3A
2	B	401	ANP	PB-N3B-PG-O1G
2	B	401	ANP	PA-O3A-PB-O1B
2	B	401	ANP	PA-O3A-PB-O2B

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	403	T3W	1	0
4	A	403	T3W	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 then 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 T3W B 403

Bond lengths

Bond angles

Torsions

Rings

Ligand ANP B 401

Bond lengths

Bond angles

Torsions

Rings

Ligand ANP A 401

Bond lengths

Bond angles

Torsions

Rings

Ligand T3W A 403

Bond lengths

Bond angles

Torsions

Rings
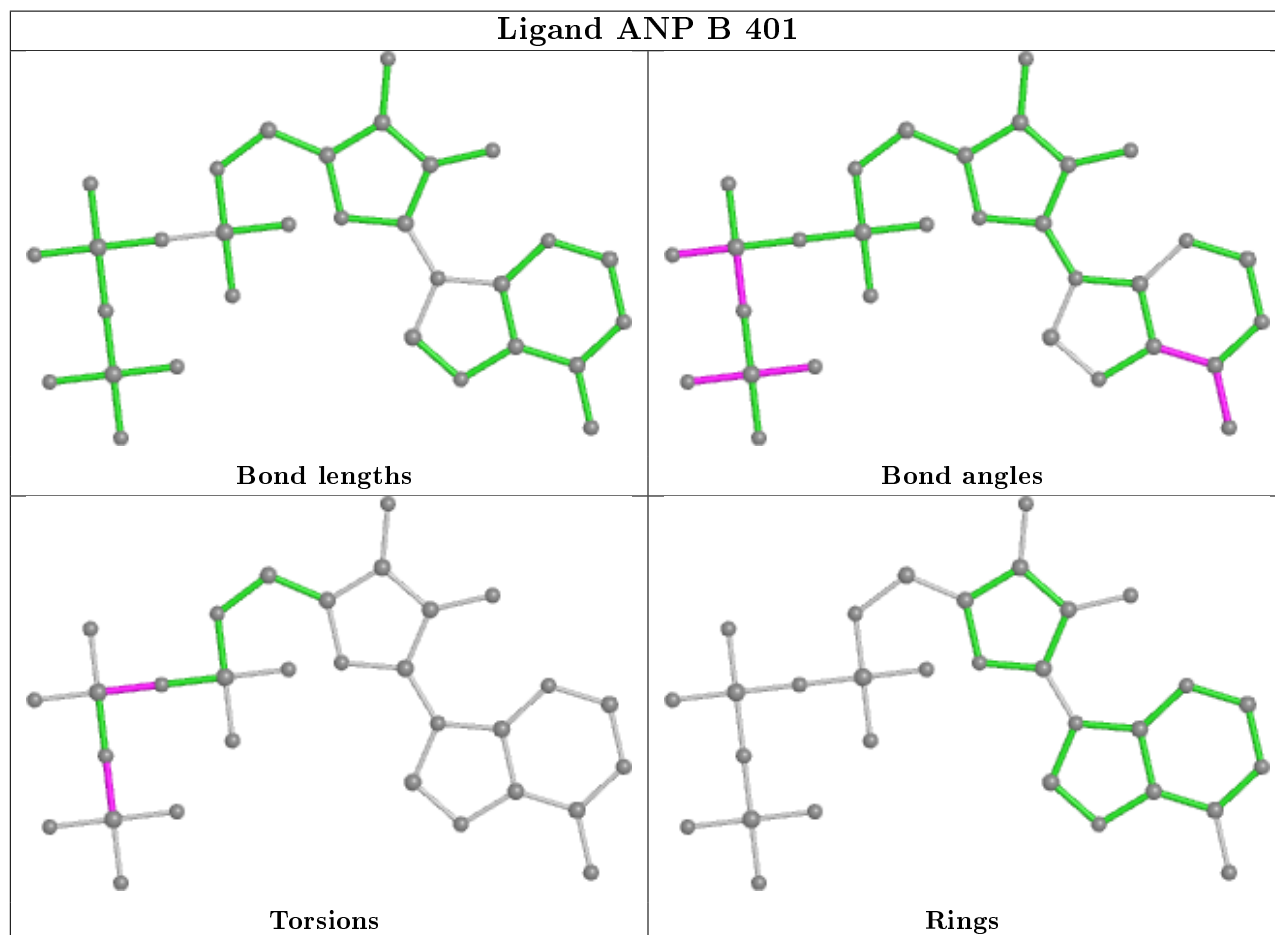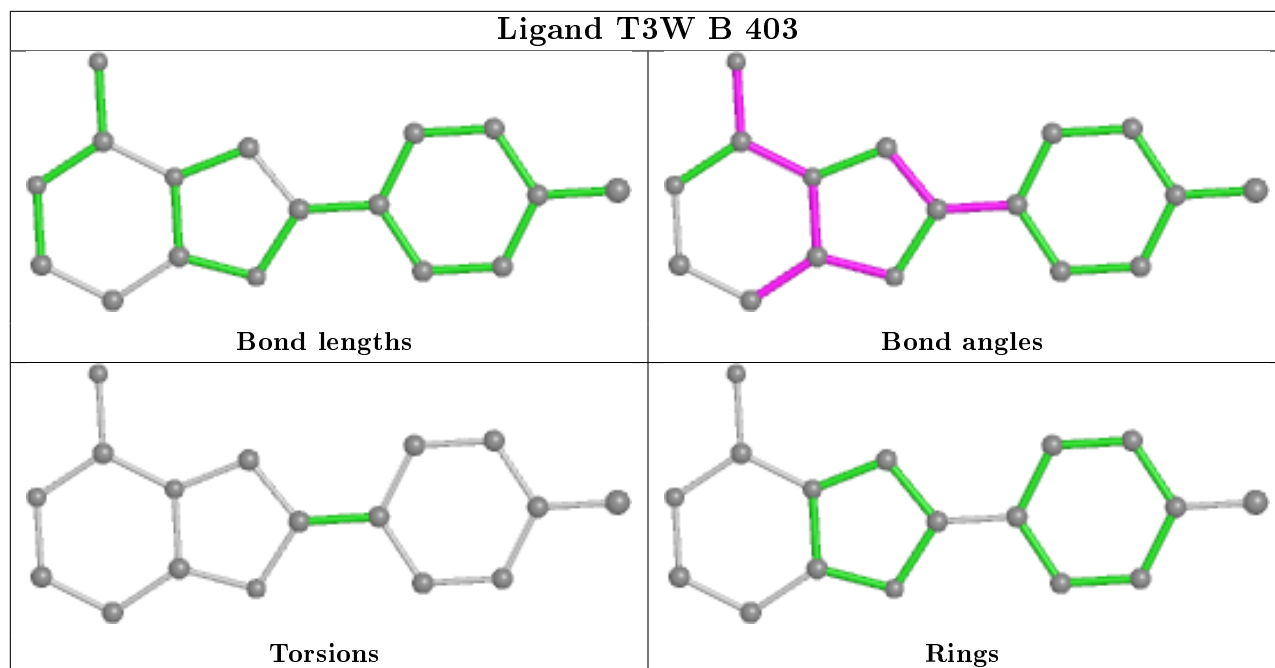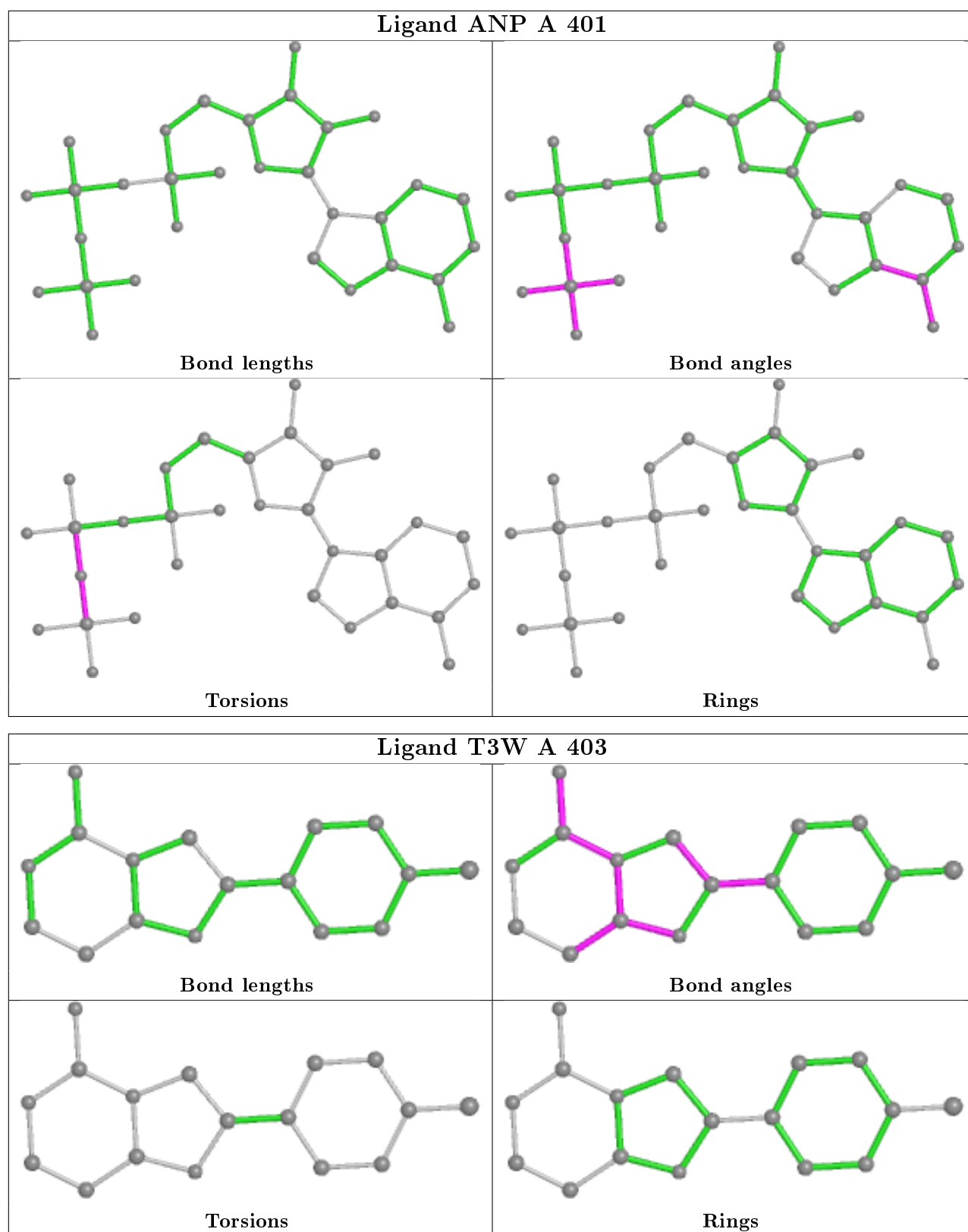
5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	301/326 (92%)	0.14	7 (2%)	60	59	31, 45, 74, 114	0
1	B	295/326 (90%)	0.27	13 (4%)	34	33	29, 50, 91, 112	0
All	All	596/652 (91%)	0.20	20 (3%)	45	44	29, 48, 83, 114	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	102	GLU	6.3
1	A	226	THR	4.8
1	A	101	LEU	4.4
1	B	63	LEU	3.0
1	B	239	HIS	3.0
1	A	103	ILE	2.9
1	B	49	ARG	2.8
1	B	240	TYR	2.7
1	B	45	GLN	2.7
1	A	79	GLY	2.7
1	B	68	PHE	2.7
1	A	239	HIS	2.6
1	B	220	ALA	2.5
1	A	316	TYR	2.5
1	B	78	ASN	2.5
1	B	44	GLU	2.4
1	B	117	VAL	2.3
1	B	316	TYR	2.2
1	B	62	GLU	2.2
1	B	58	GLN	2.2

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(Å^2)	Q<0.9
5	SO4	B	404	5/5	0.84	0.22	143,143,144,144	0
4	T3W	B	403	17/17	0.89	0.23	91,96,111,117	0
5	SO4	A	404	5/5	0.94	0.13	83,85,86,88	0
4	T3W	A	403	17/17	0.94	0.21	61,66,84,93	0
2	ANP	A	401	31/31	0.96	0.10	32,43,58,61	0
3	MG	A	402	1/1	0.97	0.05	44,44,44,44	0
3	MG	B	402	1/1	0.97	0.04	38,38,38,38	0
2	ANP	B	401	31/31	0.97	0.10	34,46,59,62	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 T3W B 403:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
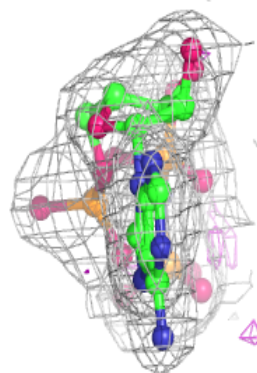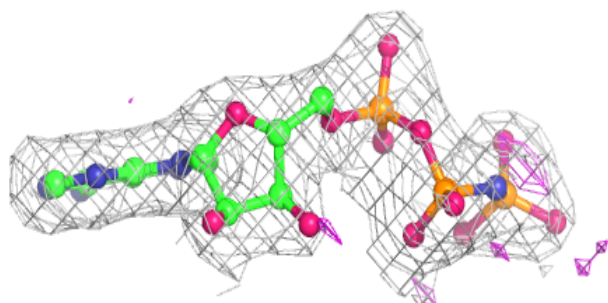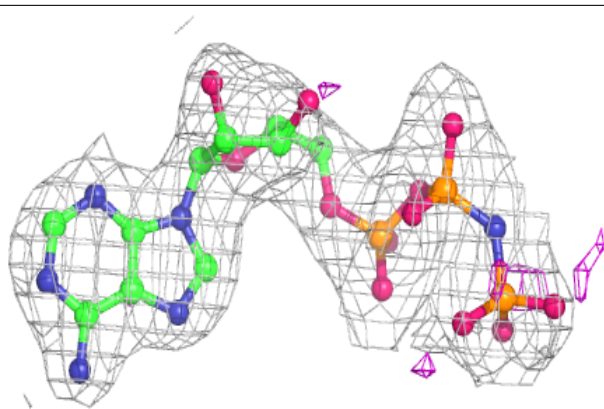and green (positive)
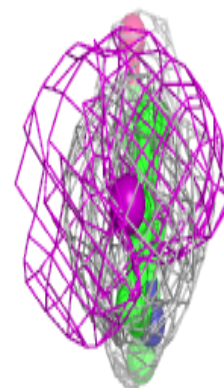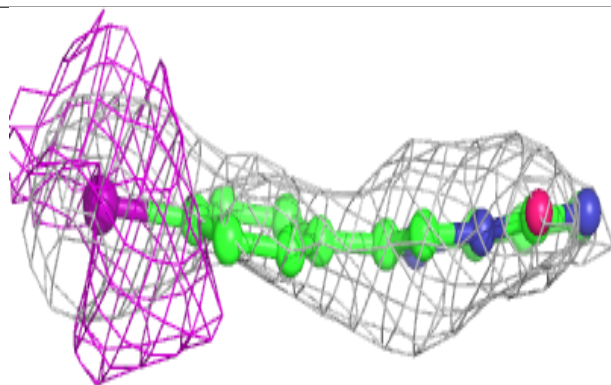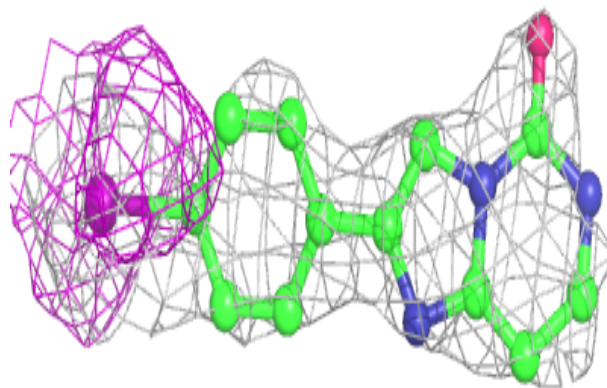
Electron density around T3W A 403:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
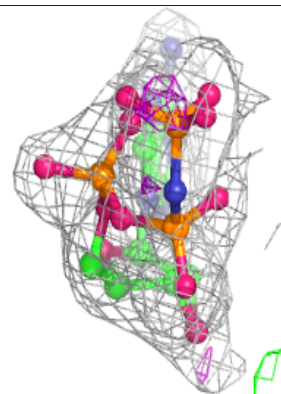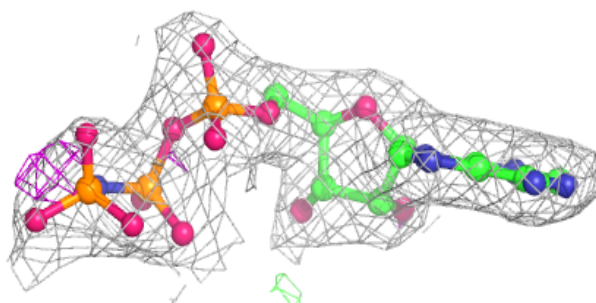mF_o-DF_c (at 3 rmsd) in purple (negative)
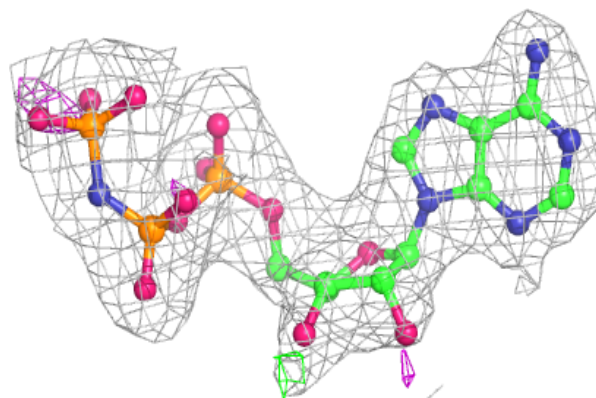and green (positive)
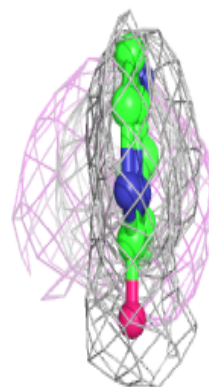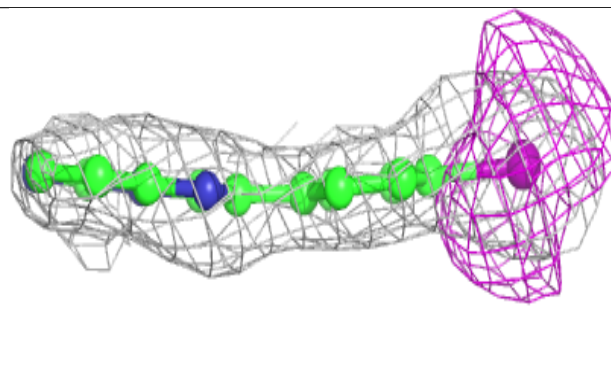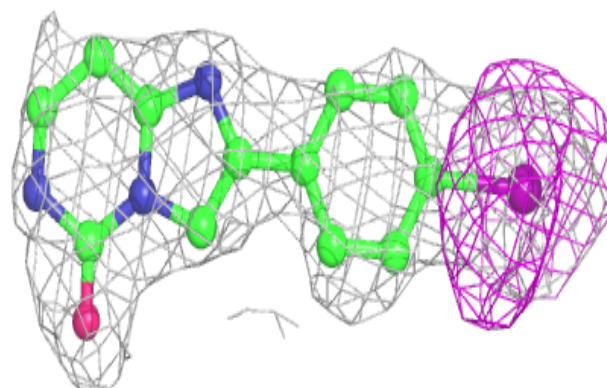
Electron density around ANP A 401:

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

Electron density around ANP 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.