Full wwPDB X-ray Structure Validation Report (i)

Sep 21, 2023 – 01:14 PM EDT

PDB ID	:	7UMB
Title	:	NanoBRET tracer Tram-bo bound to a KSR2-MEK1 complex
Authors	:	Marsiglia, W.M.; Khan, K.M.; Dar, A.C.
Deposited on	:	2022-04-06
Resolution	:	3.23 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 (i) 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 (i)) were used in the production of this report:

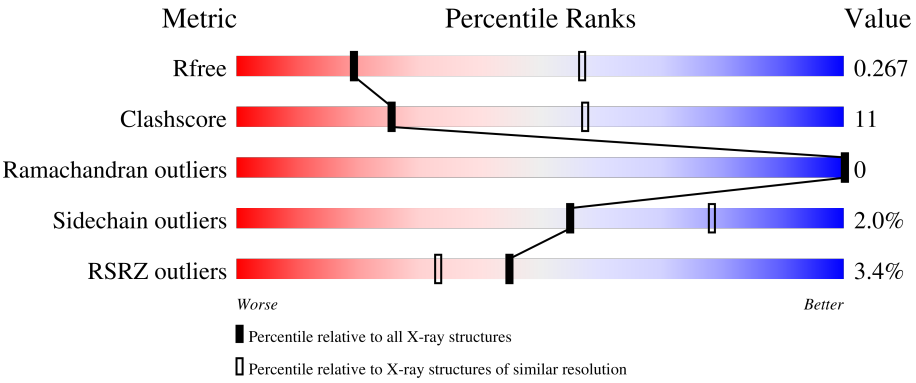
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

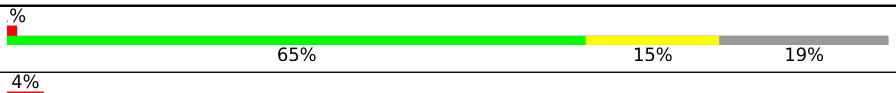
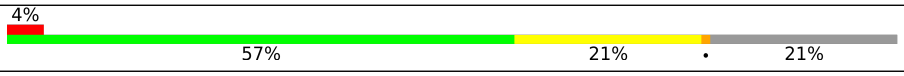
The reported resolution of this entry is 3.23 Å.

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	1619 (3.28-3.20)
Clashscore	141614	1755 (3.28-3.20)
Ramachandran outliers	138981	1728 (3.28-3.20)
Sidechain outliers	138945	1727 (3.28-3.20)
RSRZ outliers	127900	1567 (3.28-3.20)

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	B	342	
2	C	384	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	U9F	C	402	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4781 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 Kinase suppressor of Ras 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	277	2249	1448	386	402	13	0	0	0

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	609	MET	-	initiating methionine	UNP Q6VAB6
B	610	SER	-	expression tag	UNP Q6VAB6
B	611	TYR	-	expression tag	UNP Q6VAB6
B	612	TYR	-	expression tag	UNP Q6VAB6
B	613	HIS	-	expression tag	UNP Q6VAB6
B	614	HIS	-	expression tag	UNP Q6VAB6
B	615	HIS	-	expression tag	UNP Q6VAB6
B	616	HIS	-	expression tag	UNP Q6VAB6
B	617	HIS	-	expression tag	UNP Q6VAB6
B	618	HIS	-	expression tag	UNP Q6VAB6
B	619	ASP	-	expression tag	UNP Q6VAB6
B	620	TYR	-	expression tag	UNP Q6VAB6
B	621	ASP	-	expression tag	UNP Q6VAB6
B	622	ILE	-	expression tag	UNP Q6VAB6
B	623	PRO	-	expression tag	UNP Q6VAB6
B	624	THR	-	expression tag	UNP Q6VAB6
B	625	THR	-	expression tag	UNP Q6VAB6
B	626	GLU	-	expression tag	UNP Q6VAB6
B	627	ASN	-	expression tag	UNP Q6VAB6
B	628	LEU	-	expression tag	UNP Q6VAB6
B	629	TYR	-	expression tag	UNP Q6VAB6
B	630	PHE	-	expression tag	UNP Q6VAB6
B	631	GLN	-	expression tag	UNP Q6VAB6
B	632	GLY	-	expression tag	UNP Q6VAB6
B	633	ALA	-	expression tag	UNP Q6VAB6

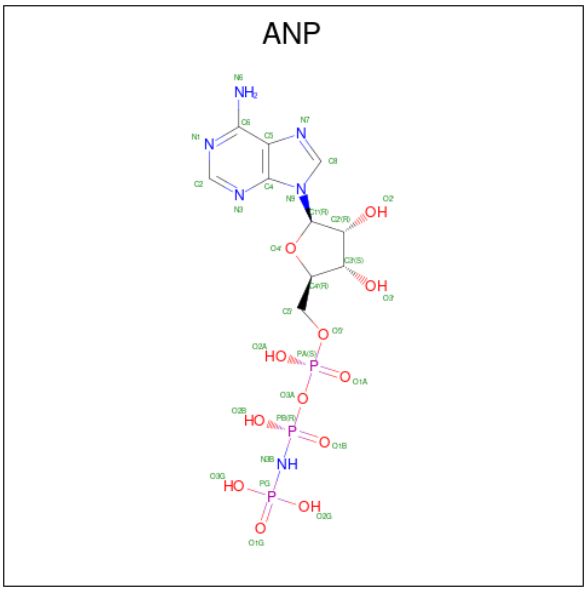
- Molecule 2 is a protein called Dual specificity mitogen-activated protein kinase kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	303	Total	C	N	O	S	0	0	0
			2402	1537	407	442	16			

There are 26 discrepancies between the modelled and reference sequences:

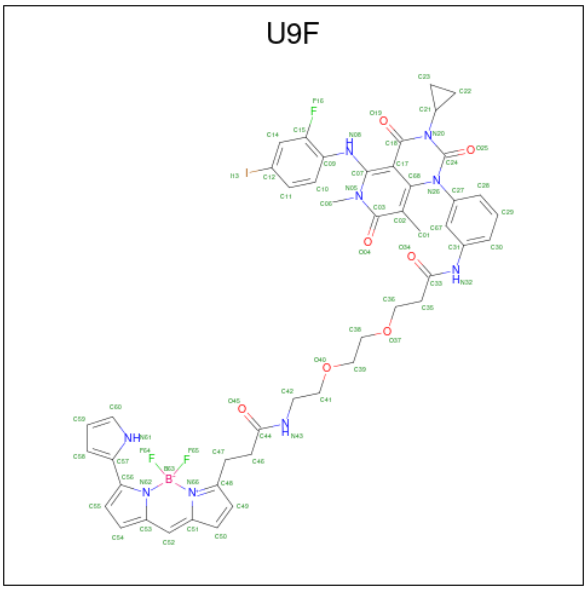
Chain	Residue	Modelled	Actual	Comment	Reference
C	10	MET	-	initiating methionine	UNP Q02750
C	11	SER	-	expression tag	UNP Q02750
C	12	TYR	-	expression tag	UNP Q02750
C	13	TYR	-	expression tag	UNP Q02750
C	14	HIS	-	expression tag	UNP Q02750
C	15	HIS	-	expression tag	UNP Q02750
C	16	HIS	-	expression tag	UNP Q02750
C	17	HIS	-	expression tag	UNP Q02750
C	18	HIS	-	expression tag	UNP Q02750
C	19	HIS	-	expression tag	UNP Q02750
C	20	ASP	-	expression tag	UNP Q02750
C	21	TYR	-	expression tag	UNP Q02750
C	22	ASP	-	expression tag	UNP Q02750
C	23	ILE	-	expression tag	UNP Q02750
C	24	PRO	-	expression tag	UNP Q02750
C	25	THR	-	expression tag	UNP Q02750
C	26	THR	-	expression tag	UNP Q02750
C	27	GLU	-	expression tag	UNP Q02750
C	28	ASN	-	expression tag	UNP Q02750
C	29	LEU	-	expression tag	UNP Q02750
C	30	TYR	-	expression tag	UNP Q02750
C	31	PHE	-	expression tag	UNP Q02750
C	32	GLN	-	expression tag	UNP Q02750
C	33	GLY	-	expression tag	UNP Q02750
C	34	ALA	-	expression tag	UNP Q02750
C	328	ALA	GLY	conflict	UNP Q02750

- Molecule 3 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
3	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 4 is {3-[(1M,2M)-2-{[(1S,2P)-1H,1'H-[2,2'-bipyrrol]-5-yl-kappaN 1]methylidene}-2H-pyrrol-5-yl-kappaN]-N-(2-{2-[3-({(3M)-3-[(4aM)-3-cyclopropyl-5-(2-fluoro-4-iodoanilino)-6,8-dimethyl-2,4,7-trioxo-3,4,6,7-tetrahydropyrido[4,3-d]pyrimidin-1(2H)-yl]phenyl}amino)-3-oxopropoxy]ethoxy}ethyl)propanamidato}(difluorido)boron (three-letter code: U9F) (formula: $C_{47}H_{46}BF_3IN_9O_7$) (labeled as "Ligand of Interest" by depositor).

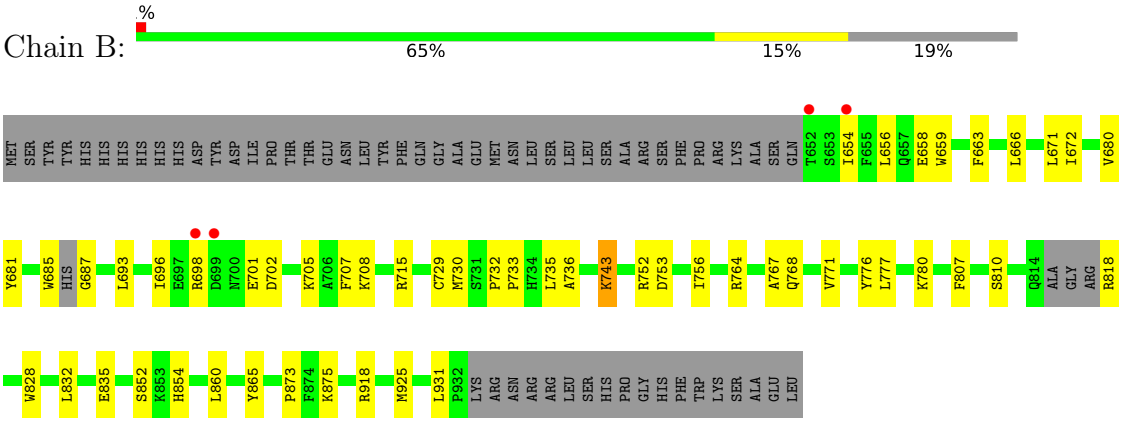


Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
			Total	B	C	F	I	N	O		
4	C	1	68	1	47	3	1	9	7	0	0

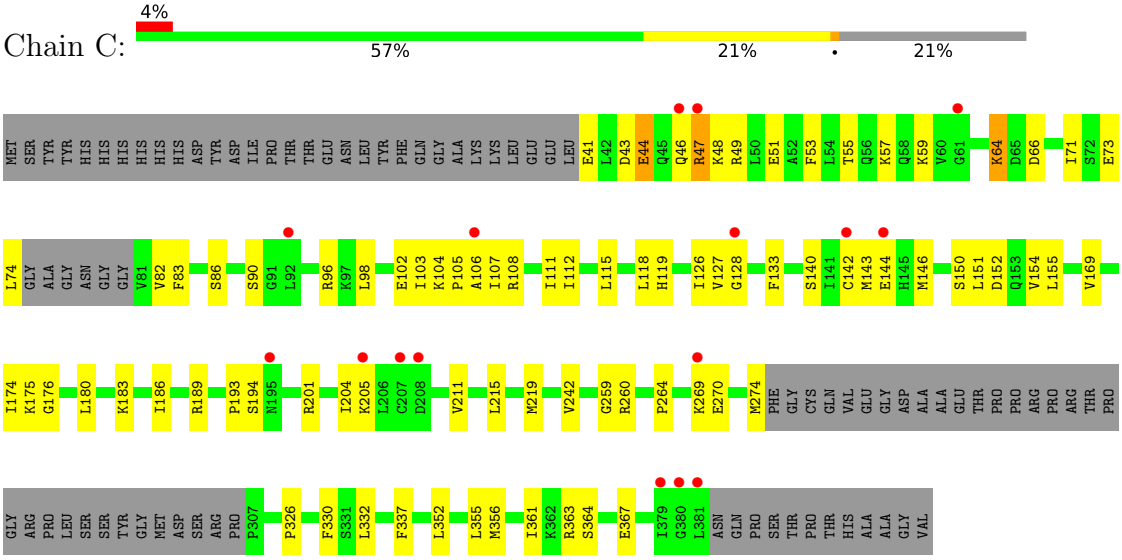
3 Residue-property plots (i)

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

• Molecule 1: Kinase suppressor of Ras 2



• Molecule 2: Dual specificity mitogen-activated protein kinase kinase 1



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	139.50Å 139.50Å 220.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.71 – 3.23 29.71 – 3.23	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.71-3.23) 100.0 (29.71-3.23)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.30 (at 3.24Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.229 , 0.268 0.228 , 0.267	Depositor DCC
R_{free} test set	1076 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å^2)	127.2	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 67.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4781	wwPDB-VP
Average B, all atoms (Å^2)	128.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: ANP, U9F

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	B	0.62	0/2299	0.79	1/3098 (0.0%)
2	C	0.49	0/2448	0.72	1/3295 (0.0%)
All	All	0.55	0/4747	0.75	2/6393 (0.0%)

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	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	687	GLY	N-CA-C	5.23	126.17	113.10
2	C	332	LEU	CB-CG-CD2	5.08	119.64	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	752	ARG	Sidechain

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	B	2249	0	2263	36	0
2	C	2402	0	2442	62	0
3	B	31	0	13	1	0
3	C	31	0	13	2	0
4	C	68	0	0	4	0
All	All	4781	0	4731	101	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 11.

All (101) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:74:LEU:HB2	2:C:82:VAL:HG23	1.64	0.80
3:B:1001:ANP:O2B	3:B:1001:ANP:O2A	2.00	0.79
2:C:146:MET:HE3	2:C:205:LYS:HD2	1.69	0.75
2:C:43:ASP:OD1	2:C:44:GLU:N	2.18	0.74
2:C:146:MET:CE	2:C:205:LYS:HD2	2.20	0.70
2:C:180:LEU:HD23	2:C:186:ILE:HD11	1.72	0.70
1:B:654:ILE:HD11	1:B:708:LYS:HG2	1.73	0.69
2:C:126:ILE:HD11	2:C:180:LEU:HD11	1.76	0.67
1:B:764:ARG:HD3	1:B:931:LEU:HB2	1.77	0.67
1:B:663:PHE:HE1	1:B:666:LEU:HB2	1.58	0.67
2:C:59:LYS:HD3	2:C:90:SER:HB3	1.78	0.66
2:C:73:GLU:HA	2:C:83:PHE:HD1	1.61	0.65
3:C:401:ANP:O1A	3:C:401:ANP:O3G	2.13	0.65
2:C:43:ASP:HB3	2:C:46:GLN:HG3	1.78	0.64
2:C:98:LEU:HD23	2:C:140:SER:HB3	1.79	0.62
1:B:696:ILE:HD11	1:B:732:PRO:HB3	1.81	0.62
2:C:64:LYS:HD2	2:C:66:ASP:H	1.64	0.62
2:C:260:ARG:NH2	2:C:264:PRO:O	2.29	0.62
2:C:356:MET:HA	2:C:361:ILE:HD11	1.82	0.61
2:C:71:ILE:HD11	2:C:86:SER:HB2	1.83	0.59
1:B:656:LEU:HG	1:B:729:CYS:HB3	1.85	0.59
2:C:111:ILE:O	2:C:115:LEU:HD12	2.02	0.59
2:C:105:PRO:HA	2:C:108:ARG:HG2	1.85	0.58
2:C:118:LEU:HD11	2:C:211:VAL:HG11	1.84	0.58
1:B:672:ILE:HD12	1:B:680:VAL:HG12	1.86	0.58
2:C:152:ASP:HB3	2:C:193:PRO:HB2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:44:GLU:O	2:C:48:LYS:HG2	2.06	0.56
2:C:127:VAL:HG13	4:C:402:U9F:I13	2.75	0.56
2:C:111:ILE:HG22	2:C:115:LEU:HD11	1.87	0.56
2:C:73:GLU:HA	2:C:83:PHE:CD1	2.40	0.56
2:C:242:VAL:HG21	2:C:352:LEU:HD11	1.88	0.56
2:C:176:GLY:O	2:C:180:LEU:HD12	2.05	0.55
2:C:215:LEU:O	2:C:219:MET:HG3	2.07	0.55
1:B:696:ILE:HD11	1:B:733:PRO:HA	1.88	0.55
1:B:768:GLN:HB3	1:B:925:MET:HE1	1.89	0.55
2:C:41:GLU:HA	2:C:175:LYS:NZ	2.21	0.55
1:B:658:GLU:O	1:B:715:ARG:NH1	2.39	0.54
2:C:169:VAL:HG12	2:C:204:ILE:HD13	1.89	0.54
2:C:57:LYS:NZ	2:C:119:HIS:HD2	2.05	0.54
2:C:103:ILE:HD13	2:C:107:ILE:HG21	1.91	0.53
1:B:656:LEU:O	1:B:659:TRP:HD1	1.92	0.52
2:C:44:GLU:HA	2:C:47:ARG:HB3	1.92	0.52
1:B:707:PHE:CZ	1:B:735:LEU:HD21	2.44	0.52
2:C:107:ILE:O	2:C:111:ILE:HG12	2.08	0.52
1:B:865:TYR:CD1	1:B:873:PRO:HG3	2.46	0.51
2:C:364:SER:HA	2:C:367:GLU:OE2	2.10	0.51
2:C:103:ILE:O	2:C:108:ARG:NH1	2.44	0.51
1:B:730:MET:HE1	1:B:735:LEU:HB2	1.93	0.51
2:C:108:ARG:O	2:C:112:ILE:HG12	2.10	0.50
1:B:743:LYS:N	1:B:743:LYS:HD3	2.26	0.50
1:B:656:LEU:HD23	1:B:659:TRP:CD1	2.47	0.50
1:B:753:ASP:HB3	1:B:756:ILE:HG13	1.94	0.49
2:C:269:LYS:HG2	2:C:270:GLU:N	2.26	0.49
1:B:663:PHE:HB2	1:B:685:TRP:CZ2	2.47	0.49
2:C:363:ARG:O	2:C:367:GLU:HG3	2.12	0.49
1:B:702:ASP:HA	1:B:705:LYS:HE2	1.94	0.48
1:B:767:ALA:O	1:B:771:VAL:HG23	2.13	0.48
2:C:337:PHE:CE1	2:C:355:LEU:HD22	2.49	0.48
2:C:155:LEU:HD11	2:C:259:GLY:HA2	1.96	0.47
1:B:828:TRP:CZ2	1:B:832:LEU:HD11	2.49	0.47
1:B:807:PHE:HA	1:B:810:SER:HB2	1.97	0.47
4:C:402:U9F:O19	4:C:402:U9F:N08	2.46	0.47
1:B:663:PHE:CE1	1:B:666:LEU:HB2	2.45	0.47
1:B:730:MET:CE	1:B:735:LEU:HB2	2.44	0.47
2:C:146:MET:HE1	2:C:205:LYS:HD2	1.96	0.47
1:B:656:LEU:HA	1:B:659:TRP:CD1	2.50	0.46
1:B:707:PHE:CE1	1:B:735:LEU:HD21	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:151:LEU:HA	2:C:154:VAL:HG22	1.98	0.46
1:B:852:SER:OG	1:B:854:HIS:N	2.49	0.45
2:C:126:ILE:N	2:C:205:LYS:HB3	2.32	0.45
2:C:194:SER:HB2	3:C:401:ANP:O1B	2.17	0.45
2:C:104:LYS:HE2	2:C:106:ALA:HB3	1.97	0.45
1:B:875:LYS:HZ2	1:B:875:LYS:HG2	1.64	0.44
1:B:818:ARG:HA	1:B:818:ARG:HD3	1.79	0.44
2:C:352:LEU:HD23	2:C:352:LEU:HA	1.61	0.44
2:C:143:MET:HG3	2:C:144:GLU:O	2.16	0.44
1:B:696:ILE:CD1	1:B:733:PRO:HA	2.45	0.44
2:C:96:ARG:HD2	2:C:140:SER:HB2	2.00	0.44
2:C:270:GLU:HG2	2:C:274:MET:HE2	2.00	0.44
2:C:57:LYS:NZ	2:C:119:HIS:CD2	2.86	0.44
1:B:835:GLU:CD	1:B:918:ARG:HH22	2.21	0.44
1:B:681:TYR:CE1	1:B:693:LEU:HD12	2.53	0.43
2:C:49:ARG:NE	2:C:201:ARG:HD3	2.33	0.43
2:C:189:ARG:NH2	4:C:402:U9F:O45	2.52	0.43
1:B:828:TRP:CE2	1:B:832:LEU:HD11	2.54	0.43
2:C:102:GLU:HA	2:C:102:GLU:OE1	2.17	0.43
2:C:53:PHE:CZ	2:C:128:GLY:HA3	2.54	0.43
2:C:127:VAL:HG22	2:C:144:GLU:HB3	2.00	0.42
1:B:681:TYR:HE1	1:B:693:LEU:HD12	1.85	0.41
2:C:127:VAL:CG1	4:C:402:U9F:I13	3.38	0.41
2:C:326:PRO:HG2	2:C:330:PHE:CE2	2.55	0.41
2:C:96:ARG:HH11	2:C:133:PHE:HZ	1.68	0.41
1:B:776:TYR:CZ	1:B:780:LYS:HD2	2.55	0.41
2:C:51:GLU:O	2:C:55:THR:HG23	2.20	0.41
1:B:735:LEU:HD12	1:B:736:ALA:H	1.86	0.41
2:C:174:ILE:HD13	2:C:174:ILE:HA	1.93	0.40
2:C:183:LYS:HA	2:C:183:LYS:HD3	1.90	0.40
2:C:326:PRO:HG2	2:C:330:PHE:HE2	1.87	0.40
2:C:356:MET:O	2:C:361:ILE:HD11	2.21	0.40
1:B:777:LEU:HD23	1:B:777:LEU:HA	1.83	0.40
2:C:201:ARG:HE	2:C:201:ARG:HB2	1.67	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	B	271/342 (79%)	256 (94%)	15 (6%)	0	100	100
2	C	297/384 (77%)	282 (95%)	15 (5%)	0	100	100
All	All	568/726 (78%)	538 (95%)	30 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	B	243/300 (81%)	238 (98%)	5 (2%)	53	77
2	C	268/333 (80%)	263 (98%)	5 (2%)	57	79
All	All	511/633 (81%)	501 (98%)	10 (2%)	55	78

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	671	LEU
1	B	698	ARG
1	B	701	GLU
1	B	743	LYS
1	B	860	LEU
2	C	44	GLU
2	C	47	ARG
2	C	64	LYS

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Mol	Chain	Res	Type
2	C	142	CYS
2	C	150	SER

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

Mol	Chain	Res	Type
1	B	768	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)

3 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
3	ANP	B	1001	-	29,33,33	1.18	3 (10%)	31,52,52	1.40	6 (19%)
4	U9F	C	402	-	74,76,76	3.91	26 (35%)	79,112,112	3.37	25 (31%)
3	ANP	C	401	-	29,33,33	1.14	3 (10%)	31,52,52	1.13	4 (12%)

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
3	ANP	B	1001	-	-	5/14/38/38	0/3/3/3
4	U9F	C	402	-	-	9/33/68/68	0/9/9/9
3	ANP	C	401	-	-	4/14/38/38	0/3/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	402	U9F	B63-F64	18.94	1.69	1.39
4	C	402	U9F	B63-F65	18.79	1.69	1.39
4	C	402	U9F	C68-C02	7.10	1.50	1.36
4	C	402	U9F	C44-N43	6.95	1.49	1.33
4	C	402	U9F	C09-N08	6.60	1.54	1.41
4	C	402	U9F	C33-N32	6.11	1.49	1.35
4	C	402	U9F	C07-N08	5.25	1.50	1.37
4	C	402	U9F	C27-N26	-5.24	1.36	1.44
3	B	1001	ANP	PB-O1B	3.81	1.52	1.46
4	C	402	U9F	C03-N05	-3.68	1.32	1.40
4	C	402	U9F	C52-C51	3.46	1.48	1.39
3	C	401	ANP	PG-N3B	3.28	1.71	1.63
4	C	402	U9F	C31-N32	3.05	1.47	1.41
4	C	402	U9F	C54-C53	3.02	1.45	1.39
4	C	402	U9F	C50-C49	2.97	1.41	1.35
3	C	401	ANP	PG-O1G	2.96	1.50	1.46
4	C	402	U9F	C47-C48	2.93	1.57	1.50
4	C	402	U9F	C22-C21	2.84	1.55	1.48
4	C	402	U9F	C17-C07	2.82	1.47	1.40
4	C	402	U9F	C46-C44	2.75	1.56	1.51
4	C	402	U9F	C67-C31	2.71	1.43	1.39
4	C	402	U9F	C14-C15	2.54	1.41	1.37
4	C	402	U9F	C35-C33	2.46	1.56	1.51
4	C	402	U9F	C23-C21	2.46	1.54	1.48
4	C	402	U9F	C09-C15	2.39	1.42	1.38
3	C	401	ANP	PB-N3B	2.38	1.69	1.63
4	C	402	U9F	C18-N20	-2.28	1.35	1.40
3	B	1001	ANP	PG-N3B	2.22	1.69	1.63
4	C	402	U9F	C68-N26	2.21	1.44	1.39
4	C	402	U9F	C53-C52	2.12	1.48	1.43
4	C	402	U9F	O19-C18	-2.04	1.18	1.23
3	B	1001	ANP	PB-O2B	2.01	1.62	1.56

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	402	U9F	C22-C21-N20	16.54	135.74	118.46
4	C	402	U9F	C67-C27-N26	15.41	138.18	119.12
4	C	402	U9F	C28-C27-N26	-11.41	105.95	119.64
4	C	402	U9F	C29-C28-C27	4.68	125.80	119.68
4	C	402	U9F	C11-C12-C14	-4.29	116.05	121.09
4	C	402	U9F	C18-N20-C24	-3.87	119.87	123.39
4	C	402	U9F	N26-C24-N20	3.68	121.14	115.79
4	C	402	U9F	C10-C09-C15	-3.59	113.56	117.17
3	B	1001	ANP	PB-O3A-PA	-3.55	120.13	132.62
4	C	402	U9F	C06-N05-C07	3.33	125.77	120.97
4	C	402	U9F	C23-C21-N20	3.21	121.81	118.46
3	C	401	ANP	O2G-PG-O1G	-3.16	105.51	113.45
3	B	1001	ANP	O2G-PG-O1G	-3.00	105.92	113.45
4	C	402	U9F	C06-N05-C03	-2.98	113.11	117.69
3	B	1001	ANP	O1G-PG-N3B	-2.97	107.40	111.77
4	C	402	U9F	F16-C15-C09	2.97	121.22	117.50
4	C	402	U9F	C15-C09-N08	2.93	124.00	118.44
4	C	402	U9F	F64-B63-N66	-2.85	106.09	110.03
4	C	402	U9F	C30-C31-C67	2.79	122.96	119.65
4	C	402	U9F	O19-C18-C17	-2.74	119.25	125.17
4	C	402	U9F	C60-N61-C57	2.70	111.51	104.44
3	B	1001	ANP	C5-C6-N6	2.64	124.36	120.35
4	C	402	U9F	C47-C48-C49	-2.48	124.46	129.41
4	C	402	U9F	O25-C24-N20	-2.40	116.82	121.68
3	B	1001	ANP	O1B-PB-N3B	-2.39	108.25	111.77
3	C	401	ANP	PB-O3A-PA	-2.34	124.38	132.62
4	C	402	U9F	C50-C51-C52	2.33	131.24	125.67
4	C	402	U9F	C46-C44-N43	2.32	120.32	116.42
4	C	402	U9F	C01-C02-C03	-2.30	109.74	116.20
4	C	402	U9F	C11-C10-C09	2.24	123.97	119.64
3	C	401	ANP	C5-C6-N6	2.21	123.71	120.35
4	C	402	U9F	C47-C48-N66	2.15	127.59	123.11
3	B	1001	ANP	O2A-PA-O1A	2.13	122.77	112.24
4	C	402	U9F	C56-N62-C53	2.12	109.43	106.78
3	C	401	ANP	O1G-PG-N3B	2.03	114.76	111.77

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1001	ANP	PB-N3B-PG-O1G

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Mol	Chain	Res	Type	Atoms
3	B	1001	ANP	PA-O3A-PB-O1B
3	B	1001	ANP	PA-O3A-PB-O2B
3	C	401	ANP	PG-N3B-PB-O1B
3	C	401	ANP	PG-N3B-PB-O3A
3	C	401	ANP	PA-O3A-PB-O2B
4	C	402	U9F	C22-C21-N20-C18
4	C	402	U9F	C22-C21-N20-C24
4	C	402	U9F	C23-C21-N20-C18
4	C	402	U9F	C23-C21-N20-C24
4	C	402	U9F	C44-C46-C47-C48
3	B	1001	ANP	PG-N3B-PB-O3A
3	B	1001	ANP	PB-O3A-PA-O2A
4	C	402	U9F	C38-C39-O40-C41
4	C	402	U9F	C35-C36-O37-C38
4	C	402	U9F	N05-C07-N08-C09
3	C	401	ANP	C5'-O5'-PA-O3A
4	C	402	U9F	O37-C38-C39-O40

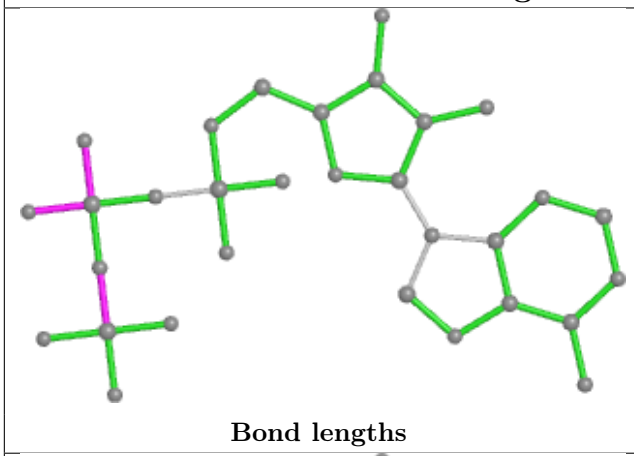
There are no ring outliers.

3 monomers are involved in 7 short contacts:

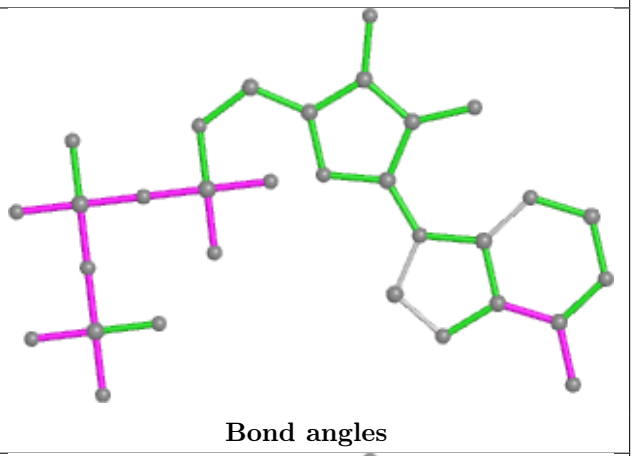
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1001	ANP	1	0
4	C	402	U9F	4	0
3	C	401	ANP	2	0

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

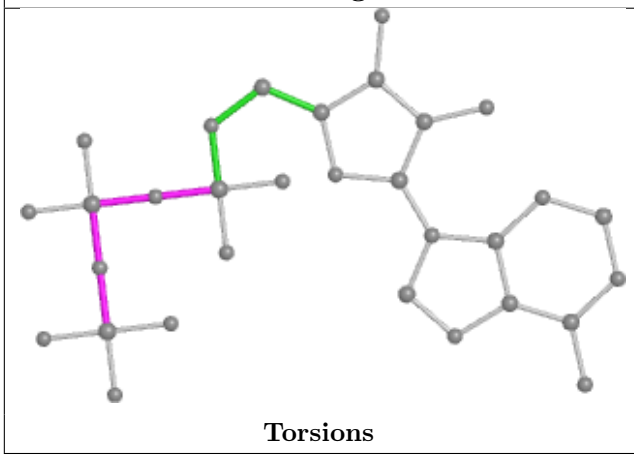
Ligand ANP B 1001



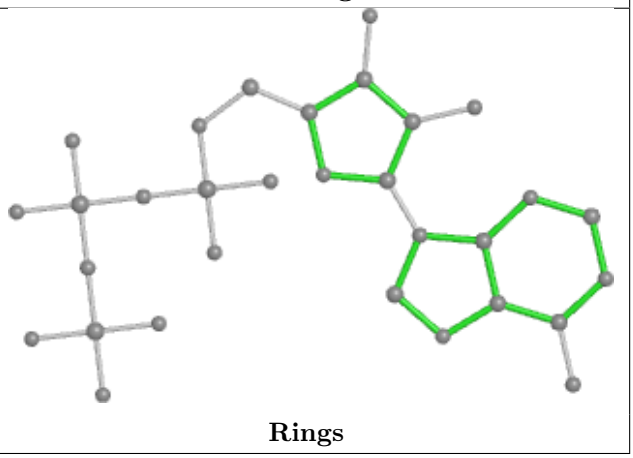
Bond lengths



Bond angles

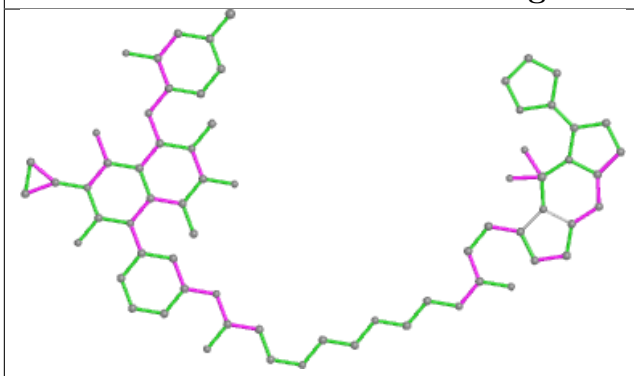


Torsions

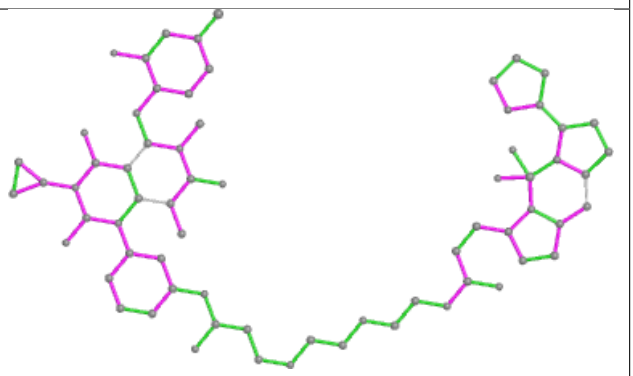


Rings

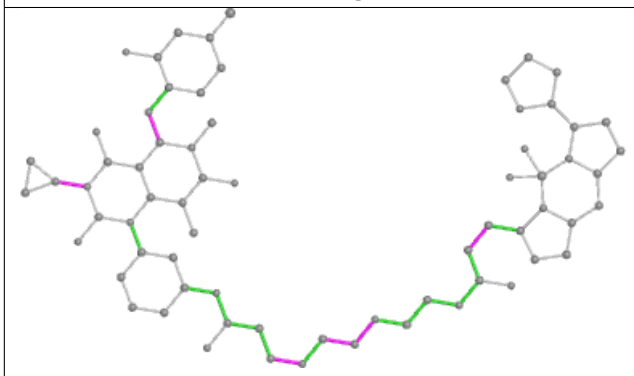
Ligand U9F C 402



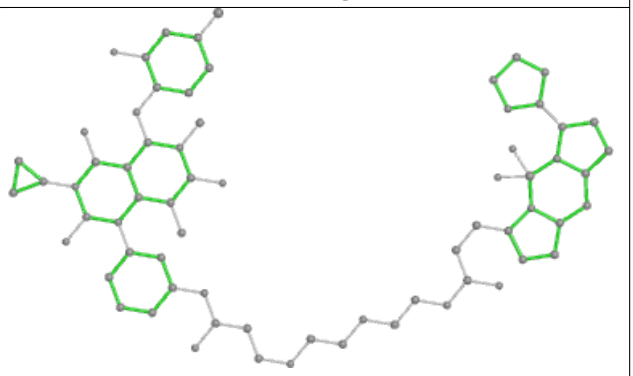
Bond lengths



Bond angles

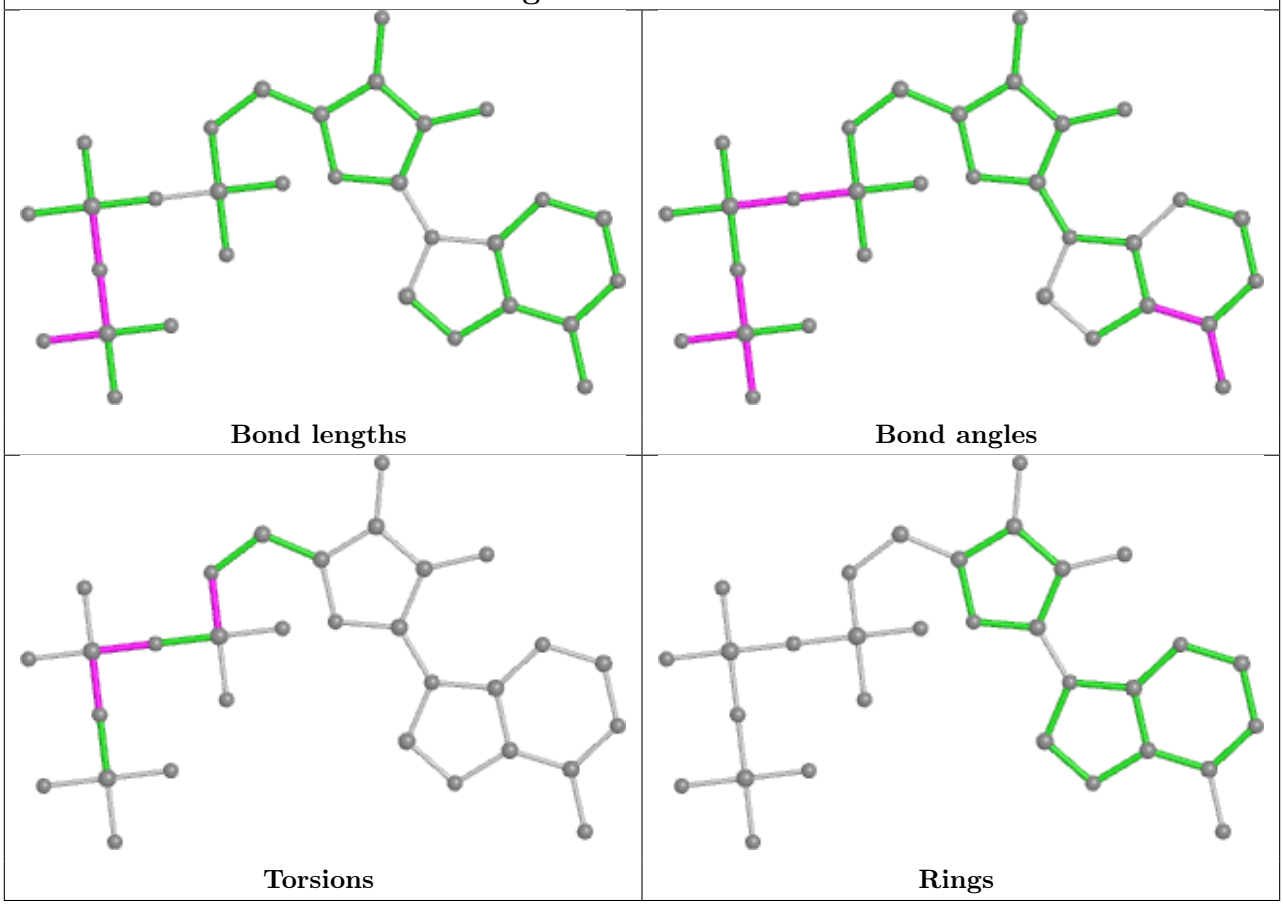


Torsions



Rings

Ligand ANP C 401



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	B	277/342 (80%)	-0.19	4 (1%)	75	66	77, 101, 154, 197	0
2	C	303/384 (78%)	0.24	16 (5%)	26	17	89, 147, 186, 206	0
All	All	580/726 (79%)	0.03	20 (3%)	45	33	77, 121, 183, 206	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	207	CYS	4.0
2	C	379	ILE	3.5
1	B	698	ARG	2.8
2	C	195	ASN	2.8
1	B	699	ASP	2.7
1	B	652	THR	2.6
2	C	144	GLU	2.6
2	C	208	ASP	2.6
2	C	128	GLY	2.6
2	C	61	GLY	2.4
2	C	92	LEU	2.4
2	C	106	ALA	2.4
2	C	46	GLN	2.4
2	C	142	CYS	2.4
2	C	205	LYS	2.4
1	B	654	ILE	2.2
2	C	381	LEU	2.2
2	C	380	GLY	2.1
2	C	47	ARG	2.0
2	C	269	LYS	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)

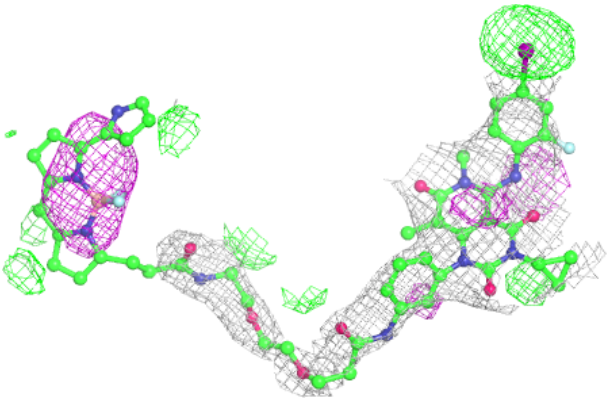
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

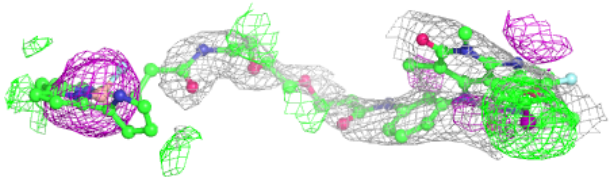
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	U9F	C	402	68/68	0.41	0.52	115,146,187,369	0
3	ANP	B	1001	31/31	0.92	0.23	76,88,96,101	0
3	ANP	C	401	31/31	0.93	0.32	139,152,171,186	0

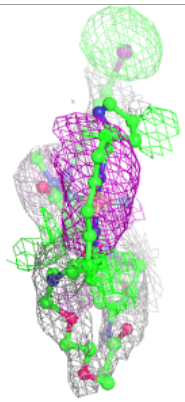
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around U9F C 402:

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

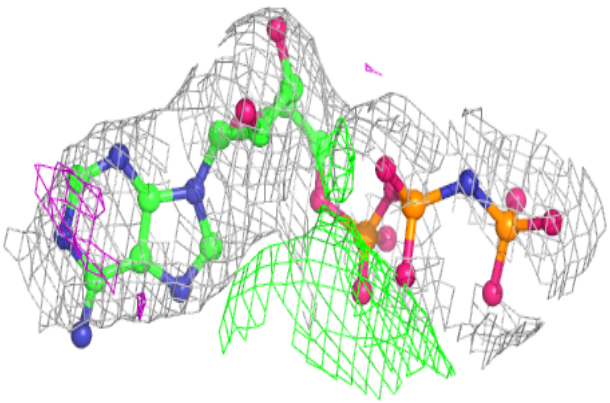


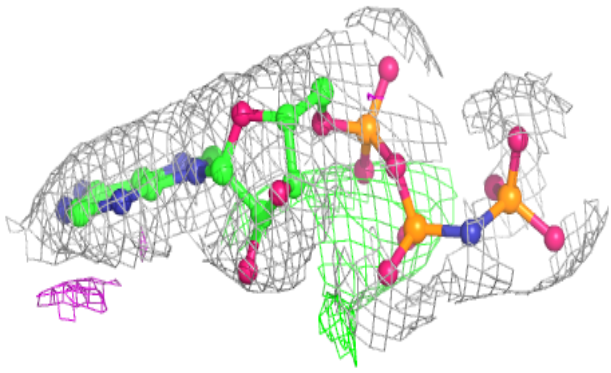


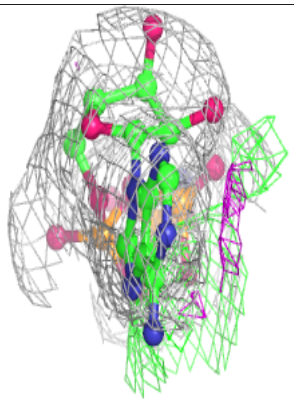


Electron density around ANP B 1001:

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

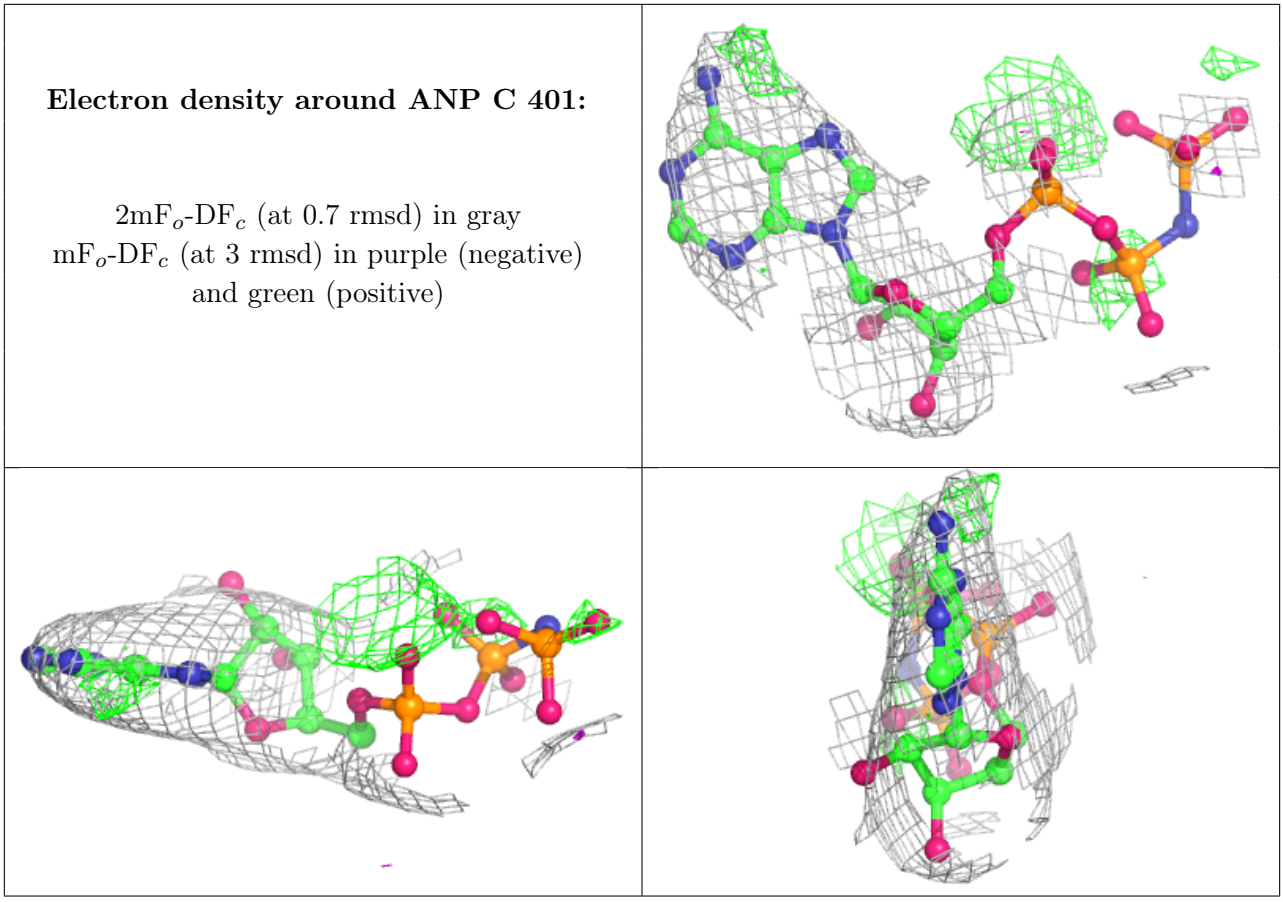






Electron density around ANP C 401:

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



6.5 Other polymers (i)

There are no such residues in this entry.