



wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2020 – 07:23 am BST

PDB ID : 5AKD
Title : MutS in complex with the N-terminal domain of MutL - crystal form 3
Authors : Groothuizen, F.S.; Winkler, I.; Cristovao, M.; Fish, A.; Winterwerp, H.H.K.; Reumer, A.; Marx, A.D.; Hermans, N.; Nicholls, R.A.; Murshudov, G.N.; Lebbink, J.H.G.; Friedhoff, P.; Sixma, T.K.
Deposited on : 2015-03-03
Resolution : 7.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 2.11
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) : 2.11

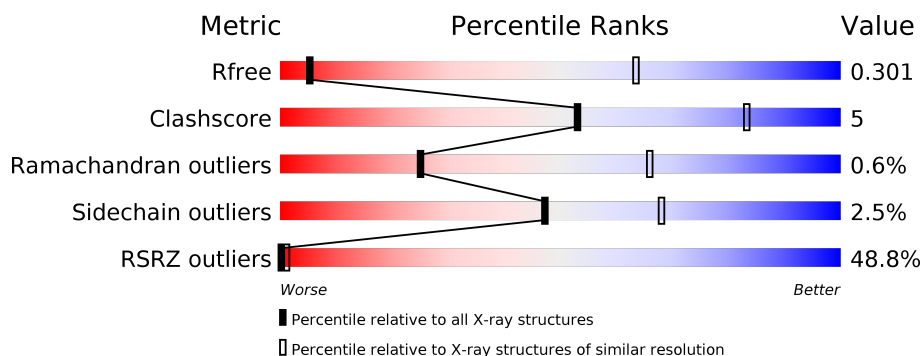
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 7.60 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	1004 (10.00-3.90)
Clashscore	141614	1069 (10.00-3.90)
Ramachandran outliers	138981	1002 (10.00-3.90)
Sidechain outliers	138945	1002 (10.00-3.86)
RSRZ outliers	127900	1004 (9.50-3.80)

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	800	<div> <div>39%</div> <div> <div>72%</div> <div>10%</div> <div>17%</div> </div> </div>
1	B	800	<div> <div>36%</div> <div> <div>73%</div> <div>9%</div> <div>17%</div> </div> </div>
1	E	800	<div> <div>43%</div> <div> <div>72%</div> <div>10%</div> <div>17%</div> </div> </div>
1	F	800	<div> <div>35%</div> <div> <div>73%</div> <div>10%</div> <div>17%</div> </div> </div>
1	I	800	<div> <div>41%</div> <div> <div>75%</div> <div>7%</div> <div>17%</div> </div> </div>
1	J	800	<div> <div>45%</div> <div> <div>74%</div> <div>9%</div> <div>17%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	C	369	
2	D	369	
2	G	369	
2	H	369	
2	K	369	
2	L	369	

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
3	ANP	E	1801	-	-	-	X
3	ANP	I	1801	-	-	-	X
3	ANP	J	1801	-	-	-	X

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 45054 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 DNA MISMATCH REPAIR PROTEIN MUTS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	663	Total	C	N	O	S	0	0	0
			5226	3284	938	984	20			
1	B	663	Total	C	N	O	S	0	0	0
			5226	3284	938	984	20			
1	E	663	Total	C	N	O	S	0	0	0
			5226	3284	938	984	20			
1	F	663	Total	C	N	O	S	0	0	0
			5226	3284	938	984	20			
1	I	663	Total	C	N	O	S	0	0	0
			5226	3284	938	984	20			
1	J	663	Total	C	N	O	S	0	0	0
			5226	3284	938	984	20			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	93	ALA	CYS	engineered mutation	UNP P23909
A	235	SER	CYS	engineered mutation	UNP P23909
A	239	ALA	CYS	engineered mutation	UNP P23909
A	246	CYS	ASP	engineered mutation	UNP P23909
A	297	SER	CYS	engineered mutation	UNP P23909
A	569	SER	CYS	engineered mutation	UNP P23909
A	711	VAL	CYS	engineered mutation	UNP P23909
B	93	ALA	CYS	engineered mutation	UNP P23909
B	235	SER	CYS	engineered mutation	UNP P23909
B	239	ALA	CYS	engineered mutation	UNP P23909
B	246	CYS	ASP	engineered mutation	UNP P23909
B	297	SER	CYS	engineered mutation	UNP P23909
B	569	SER	CYS	engineered mutation	UNP P23909
B	711	VAL	CYS	engineered mutation	UNP P23909
E	93	ALA	CYS	engineered mutation	UNP P23909
E	235	SER	CYS	engineered mutation	UNP P23909
E	239	ALA	CYS	engineered mutation	UNP P23909

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Chain	Residue	Modelled	Actual	Comment	Reference
E	246	CYS	ASP	engineered mutation	UNP P23909
E	297	SER	CYS	engineered mutation	UNP P23909
E	569	SER	CYS	engineered mutation	UNP P23909
E	711	VAL	CYS	engineered mutation	UNP P23909
F	93	ALA	CYS	engineered mutation	UNP P23909
F	235	SER	CYS	engineered mutation	UNP P23909
F	239	ALA	CYS	engineered mutation	UNP P23909
F	246	CYS	ASP	engineered mutation	UNP P23909
F	297	SER	CYS	engineered mutation	UNP P23909
F	569	SER	CYS	engineered mutation	UNP P23909
F	711	VAL	CYS	engineered mutation	UNP P23909
I	93	ALA	CYS	engineered mutation	UNP P23909
I	235	SER	CYS	engineered mutation	UNP P23909
I	239	ALA	CYS	engineered mutation	UNP P23909
I	246	CYS	ASP	engineered mutation	UNP P23909
I	297	SER	CYS	engineered mutation	UNP P23909
I	569	SER	CYS	engineered mutation	UNP P23909
I	711	VAL	CYS	engineered mutation	UNP P23909
J	93	ALA	CYS	engineered mutation	UNP P23909
J	235	SER	CYS	engineered mutation	UNP P23909
J	239	ALA	CYS	engineered mutation	UNP P23909
J	246	CYS	ASP	engineered mutation	UNP P23909
J	297	SER	CYS	engineered mutation	UNP P23909
J	569	SER	CYS	engineered mutation	UNP P23909
J	711	VAL	CYS	engineered mutation	UNP P23909

- Molecule 2 is a protein called DNA MISMATCH REPAIR PROTEIN MUTL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	285	Total	C	N	O	S	0	0	0
			2252	1423	409	418	2			
2	D	285	Total	C	N	O	S	0	0	0
			2252	1423	409	418	2			
2	G	285	Total	C	N	O	S	0	0	0
			2252	1423	409	418	2			
2	H	285	Total	C	N	O	S	0	0	0
			2252	1423	409	418	2			
2	K	285	Total	C	N	O	S	0	0	0
			2252	1423	409	418	2			
2	L	285	Total	C	N	O	S	0	0	0
			2252	1423	409	418	2			

There are 150 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-19	MET	-	expression tag	UNP P23367
C	-18	GLY	-	expression tag	UNP P23367
C	-17	SER	-	expression tag	UNP P23367
C	-16	SER	-	expression tag	UNP P23367
C	-15	HIS	-	expression tag	UNP P23367
C	-14	HIS	-	expression tag	UNP P23367
C	-13	HIS	-	expression tag	UNP P23367
C	-12	HIS	-	expression tag	UNP P23367
C	-11	HIS	-	expression tag	UNP P23367
C	-10	HIS	-	expression tag	UNP P23367
C	-9	SER	-	expression tag	UNP P23367
C	-8	SER	-	expression tag	UNP P23367
C	-7	GLY	-	expression tag	UNP P23367
C	-6	LEU	-	expression tag	UNP P23367
C	-5	VAL	-	expression tag	UNP P23367
C	-4	PRO	-	expression tag	UNP P23367
C	-3	ARG	-	expression tag	UNP P23367
C	-2	GLY	-	expression tag	UNP P23367
C	-1	SER	-	expression tag	UNP P23367
C	0	HIS	-	expression tag	UNP P23367
C	61	SER	CYS	engineered mutation	UNP P23367
C	131	CYS	ASN	engineered mutation	UNP P23367
C	216	LEU	CYS	engineered mutation	UNP P23367
C	256	PHE	CYS	engineered mutation	UNP P23367
C	276	TYR	CYS	engineered mutation	UNP P23367
D	-19	MET	-	expression tag	UNP P23367
D	-18	GLY	-	expression tag	UNP P23367
D	-17	SER	-	expression tag	UNP P23367
D	-16	SER	-	expression tag	UNP P23367
D	-15	HIS	-	expression tag	UNP P23367
D	-14	HIS	-	expression tag	UNP P23367
D	-13	HIS	-	expression tag	UNP P23367
D	-12	HIS	-	expression tag	UNP P23367
D	-11	HIS	-	expression tag	UNP P23367
D	-10	HIS	-	expression tag	UNP P23367
D	-9	SER	-	expression tag	UNP P23367
D	-8	SER	-	expression tag	UNP P23367
D	-7	GLY	-	expression tag	UNP P23367
D	-6	LEU	-	expression tag	UNP P23367
D	-5	VAL	-	expression tag	UNP P23367
D	-4	PRO	-	expression tag	UNP P23367
D	-3	ARG	-	expression tag	UNP P23367
D	-2	GLY	-	expression tag	UNP P23367

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	SER	-	expression tag	UNP P23367
D	0	HIS	-	expression tag	UNP P23367
D	61	SER	CYS	engineered mutation	UNP P23367
D	131	CYS	ASN	engineered mutation	UNP P23367
D	216	LEU	CYS	engineered mutation	UNP P23367
D	256	PHE	CYS	engineered mutation	UNP P23367
D	276	TYR	CYS	engineered mutation	UNP P23367
G	-19	MET	-	expression tag	UNP P23367
G	-18	GLY	-	expression tag	UNP P23367
G	-17	SER	-	expression tag	UNP P23367
G	-16	SER	-	expression tag	UNP P23367
G	-15	HIS	-	expression tag	UNP P23367
G	-14	HIS	-	expression tag	UNP P23367
G	-13	HIS	-	expression tag	UNP P23367
G	-12	HIS	-	expression tag	UNP P23367
G	-11	HIS	-	expression tag	UNP P23367
G	-10	HIS	-	expression tag	UNP P23367
G	-9	SER	-	expression tag	UNP P23367
G	-8	SER	-	expression tag	UNP P23367
G	-7	GLY	-	expression tag	UNP P23367
G	-6	LEU	-	expression tag	UNP P23367
G	-5	VAL	-	expression tag	UNP P23367
G	-4	PRO	-	expression tag	UNP P23367
G	-3	ARG	-	expression tag	UNP P23367
G	-2	GLY	-	expression tag	UNP P23367
G	-1	SER	-	expression tag	UNP P23367
G	0	HIS	-	expression tag	UNP P23367
G	61	SER	CYS	engineered mutation	UNP P23367
G	131	CYS	ASN	engineered mutation	UNP P23367
G	216	LEU	CYS	engineered mutation	UNP P23367
G	256	PHE	CYS	engineered mutation	UNP P23367
G	276	TYR	CYS	engineered mutation	UNP P23367
H	-19	MET	-	expression tag	UNP P23367
H	-18	GLY	-	expression tag	UNP P23367
H	-17	SER	-	expression tag	UNP P23367
H	-16	SER	-	expression tag	UNP P23367
H	-15	HIS	-	expression tag	UNP P23367
H	-14	HIS	-	expression tag	UNP P23367
H	-13	HIS	-	expression tag	UNP P23367
H	-12	HIS	-	expression tag	UNP P23367
H	-11	HIS	-	expression tag	UNP P23367
H	-10	HIS	-	expression tag	UNP P23367

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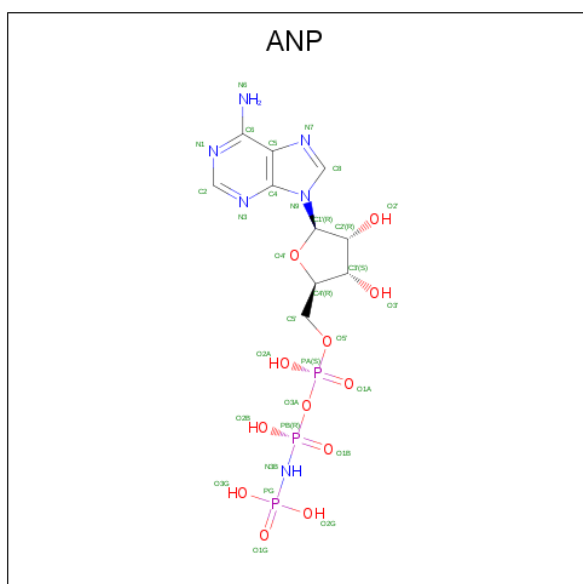
Chain	Residue	Modelled	Actual	Comment	Reference
H	-9	SER	-	expression tag	UNP P23367
H	-8	SER	-	expression tag	UNP P23367
H	-7	GLY	-	expression tag	UNP P23367
H	-6	LEU	-	expression tag	UNP P23367
H	-5	VAL	-	expression tag	UNP P23367
H	-4	PRO	-	expression tag	UNP P23367
H	-3	ARG	-	expression tag	UNP P23367
H	-2	GLY	-	expression tag	UNP P23367
H	-1	SER	-	expression tag	UNP P23367
H	0	HIS	-	expression tag	UNP P23367
H	61	SER	CYS	engineered mutation	UNP P23367
H	131	CYS	ASN	engineered mutation	UNP P23367
H	216	LEU	CYS	engineered mutation	UNP P23367
H	256	PHE	CYS	engineered mutation	UNP P23367
H	276	TYR	CYS	engineered mutation	UNP P23367
K	-19	MET	-	expression tag	UNP P23367
K	-18	GLY	-	expression tag	UNP P23367
K	-17	SER	-	expression tag	UNP P23367
K	-16	SER	-	expression tag	UNP P23367
K	-15	HIS	-	expression tag	UNP P23367
K	-14	HIS	-	expression tag	UNP P23367
K	-13	HIS	-	expression tag	UNP P23367
K	-12	HIS	-	expression tag	UNP P23367
K	-11	HIS	-	expression tag	UNP P23367
K	-10	HIS	-	expression tag	UNP P23367
K	-9	SER	-	expression tag	UNP P23367
K	-8	SER	-	expression tag	UNP P23367
K	-7	GLY	-	expression tag	UNP P23367
K	-6	LEU	-	expression tag	UNP P23367
K	-5	VAL	-	expression tag	UNP P23367
K	-4	PRO	-	expression tag	UNP P23367
K	-3	ARG	-	expression tag	UNP P23367
K	-2	GLY	-	expression tag	UNP P23367
K	-1	SER	-	expression tag	UNP P23367
K	0	HIS	-	expression tag	UNP P23367
K	61	SER	CYS	engineered mutation	UNP P23367
K	131	CYS	ASN	engineered mutation	UNP P23367
K	216	LEU	CYS	engineered mutation	UNP P23367
K	256	PHE	CYS	engineered mutation	UNP P23367
K	276	TYR	CYS	engineered mutation	UNP P23367
L	-19	MET	-	expression tag	UNP P23367
L	-18	GLY	-	expression tag	UNP P23367

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-17	SER	-	expression tag	UNP P23367
L	-16	SER	-	expression tag	UNP P23367
L	-15	HIS	-	expression tag	UNP P23367
L	-14	HIS	-	expression tag	UNP P23367
L	-13	HIS	-	expression tag	UNP P23367
L	-12	HIS	-	expression tag	UNP P23367
L	-11	HIS	-	expression tag	UNP P23367
L	-10	HIS	-	expression tag	UNP P23367
L	-9	SER	-	expression tag	UNP P23367
L	-8	SER	-	expression tag	UNP P23367
L	-7	GLY	-	expression tag	UNP P23367
L	-6	LEU	-	expression tag	UNP P23367
L	-5	VAL	-	expression tag	UNP P23367
L	-4	PRO	-	expression tag	UNP P23367
L	-3	ARG	-	expression tag	UNP P23367
L	-2	GLY	-	expression tag	UNP P23367
L	-1	SER	-	expression tag	UNP P23367
L	0	HIS	-	expression tag	UNP P23367
L	61	SER	CYS	engineered mutation	UNP P23367
L	131	CYS	ASN	engineered mutation	UNP P23367
L	216	LEU	CYS	engineered mutation	UNP P23367
L	256	PHE	CYS	engineered mutation	UNP P23367
L	276	TYR	CYS	engineered mutation	UNP P23367

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).

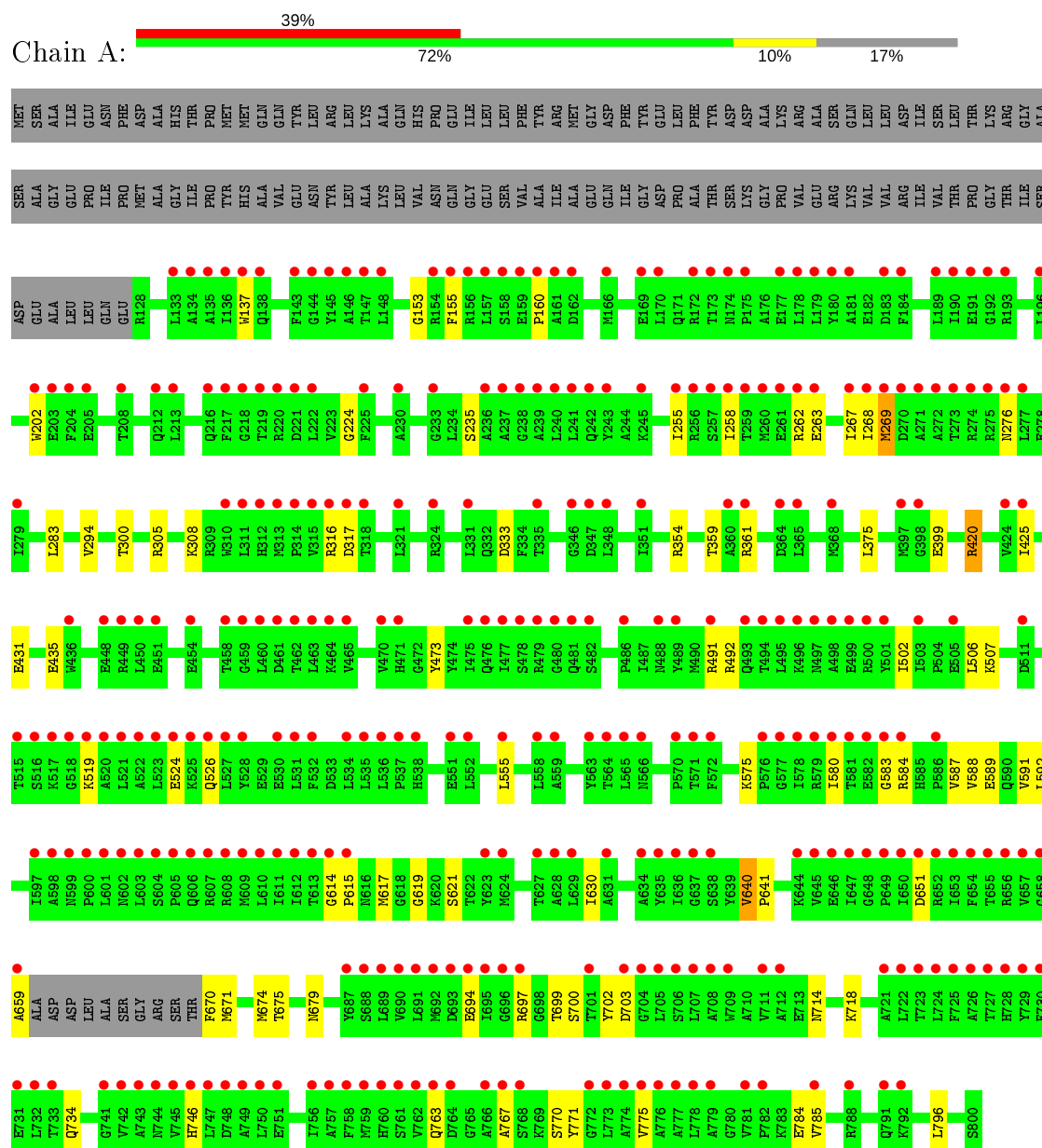


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 31	C 10	N 6	O 12	P 3	0	0
3	B	1	Total 31	C 10	N 6	O 12	P 3	0	0
3	E	1	Total 31	C 10	N 6	O 12	P 3	0	0
3	F	1	Total 31	C 10	N 6	O 12	P 3	0	0
3	I	1	Total 31	C 10	N 6	O 12	P 3	0	0
3	J	1	Total 31	C 10	N 6	O 12	P 3	0	0

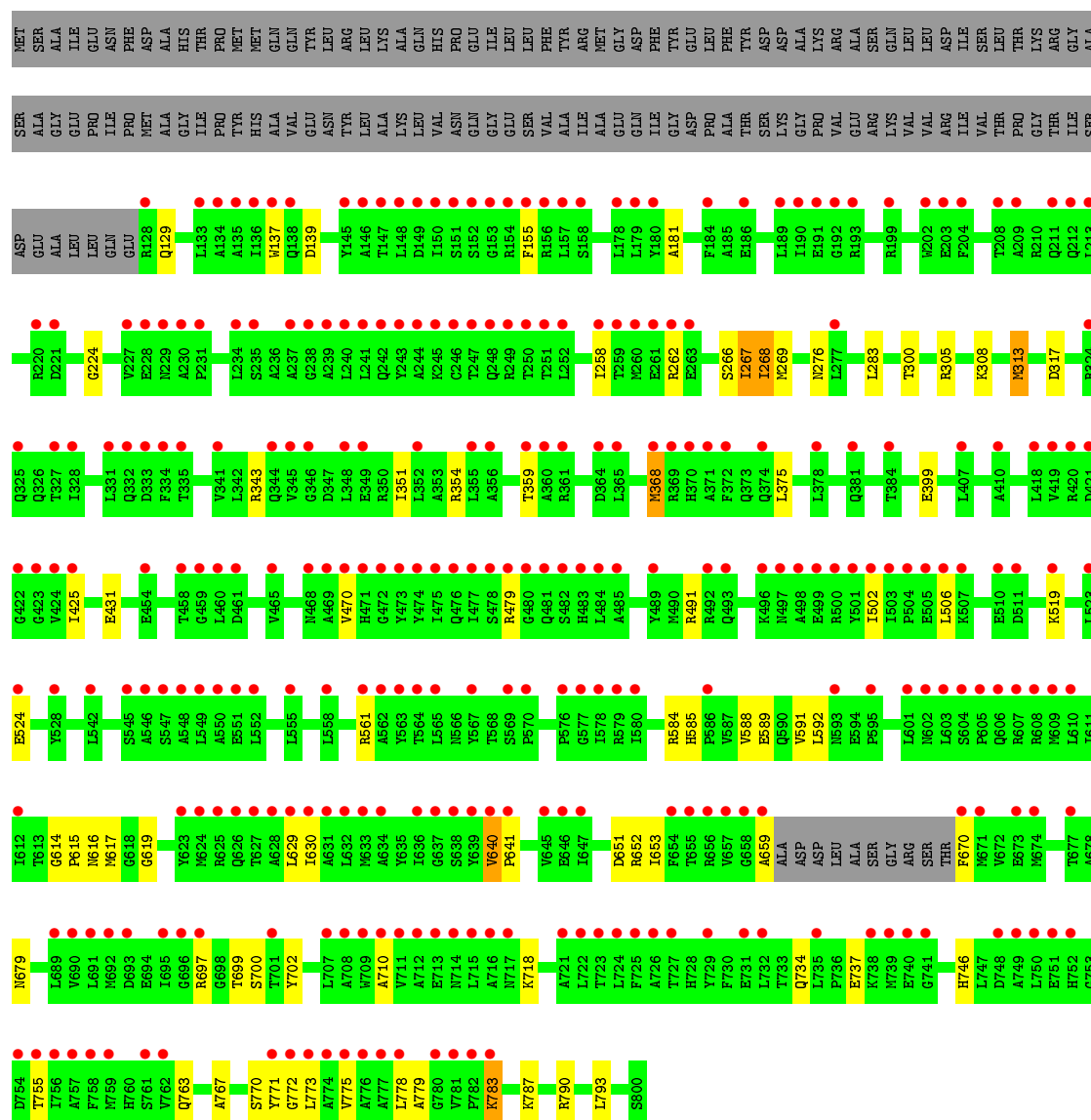
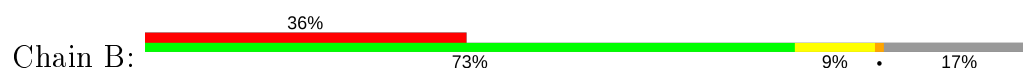
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

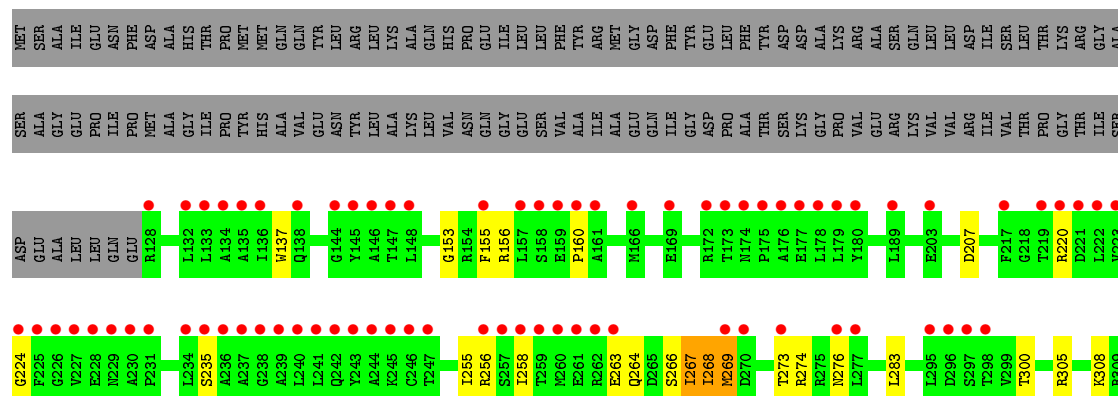
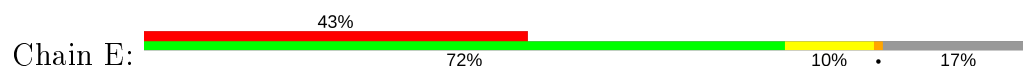
• Molecule 1: DNA MISMATCH REPAIR PROTEIN MUTS

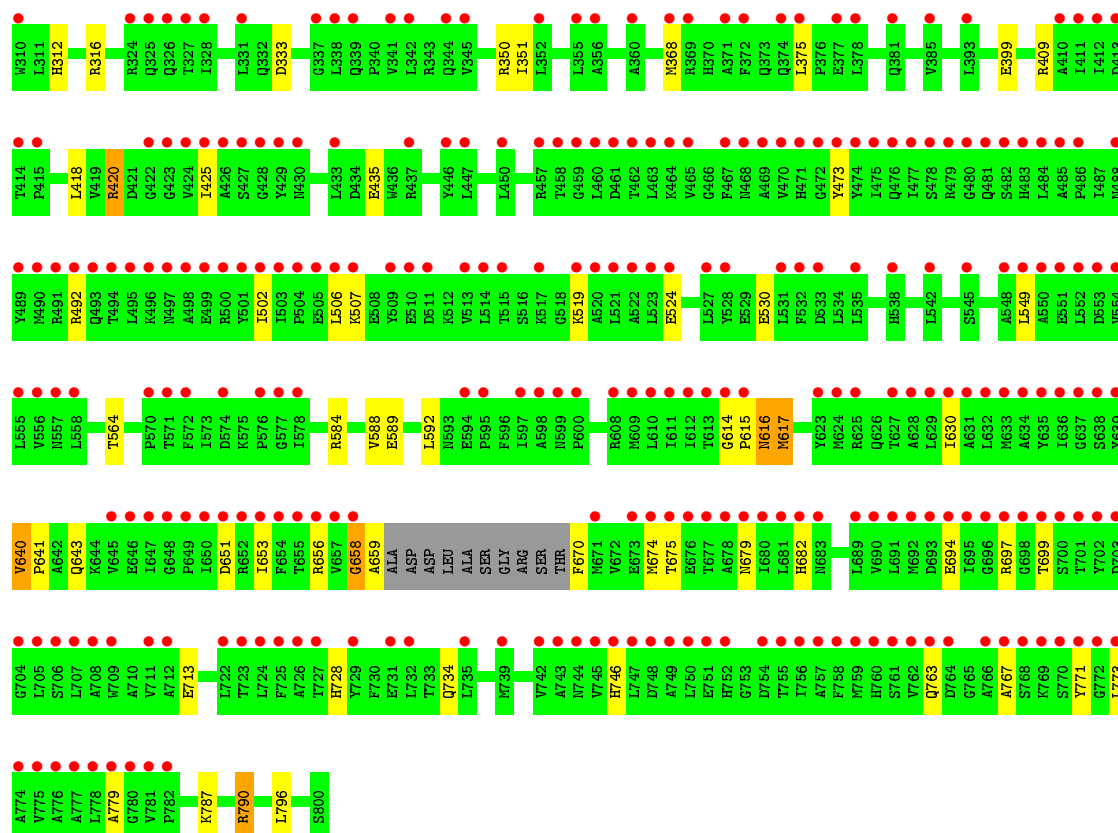


• Molecule 1: DNA MISMATCH REPAIR PROTEIN MUTS

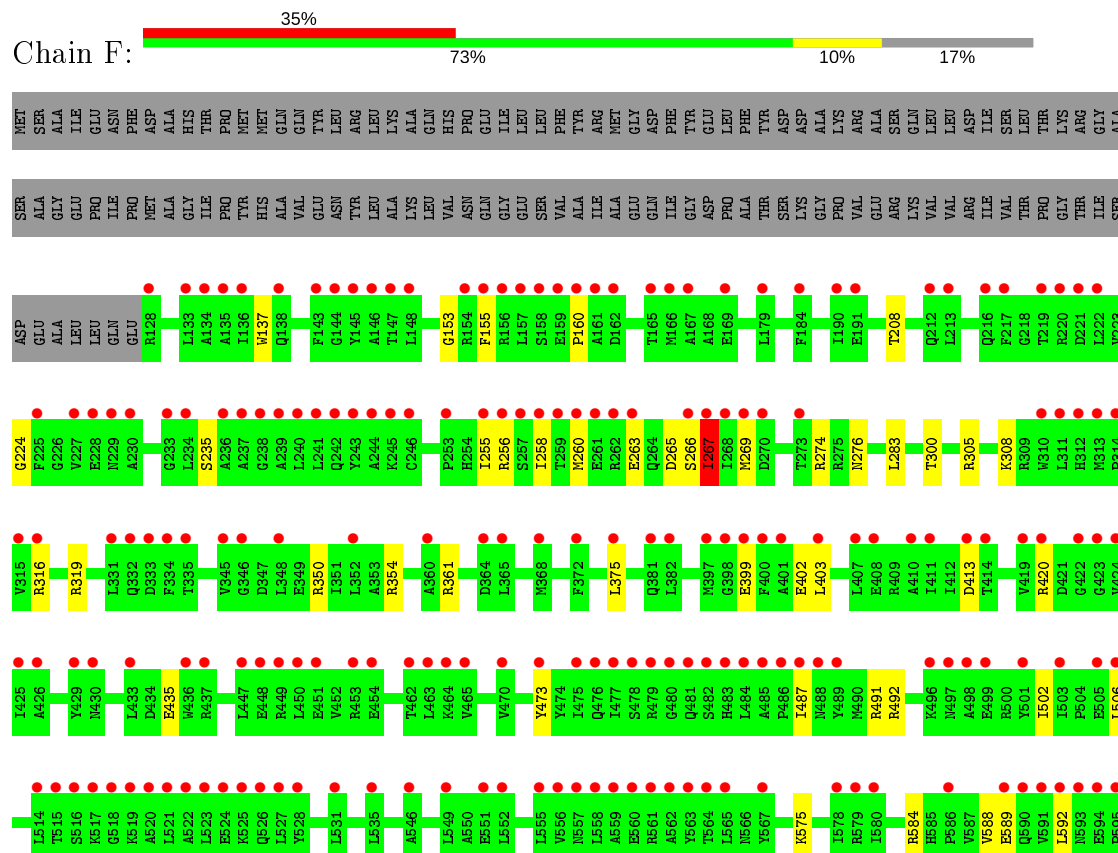


• Molecule 1: DNA MISMATCH REPAIR PROTEIN MUTS





● Molecule 1: DNA MISMATCH REPAIR PROTEIN MUTS





Chain J: 45% 74% 9% 17%

The visualization displays a sequence of 100 nodes, labeled from Q763 to W762, arranged in a grid. Each node is represented by a colored square (red or green) and a label. The nodes are connected by lines, forming a complex network. The visualization is divided into four quadrants by a vertical line at node W762. The top half of the grid shows a dense network of connections, while the bottom half shows a sparser network. The nodes are labeled with letters and numbers, and the colors of the squares indicate a binary state for each node.

Chain C:

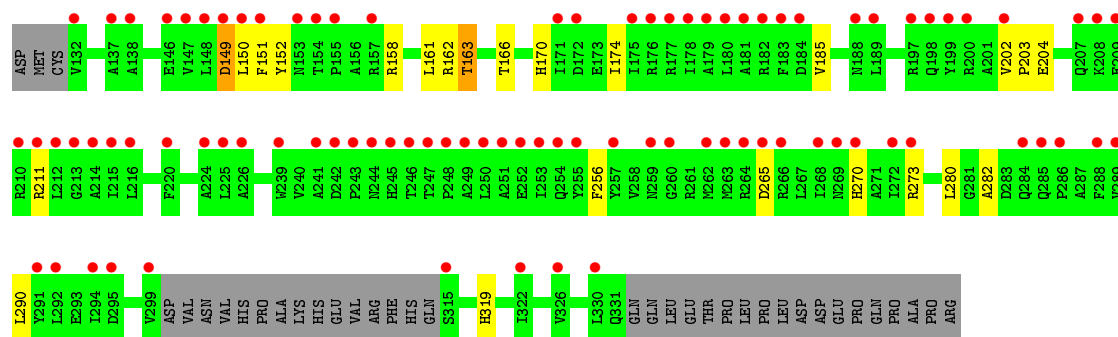
37%

64%

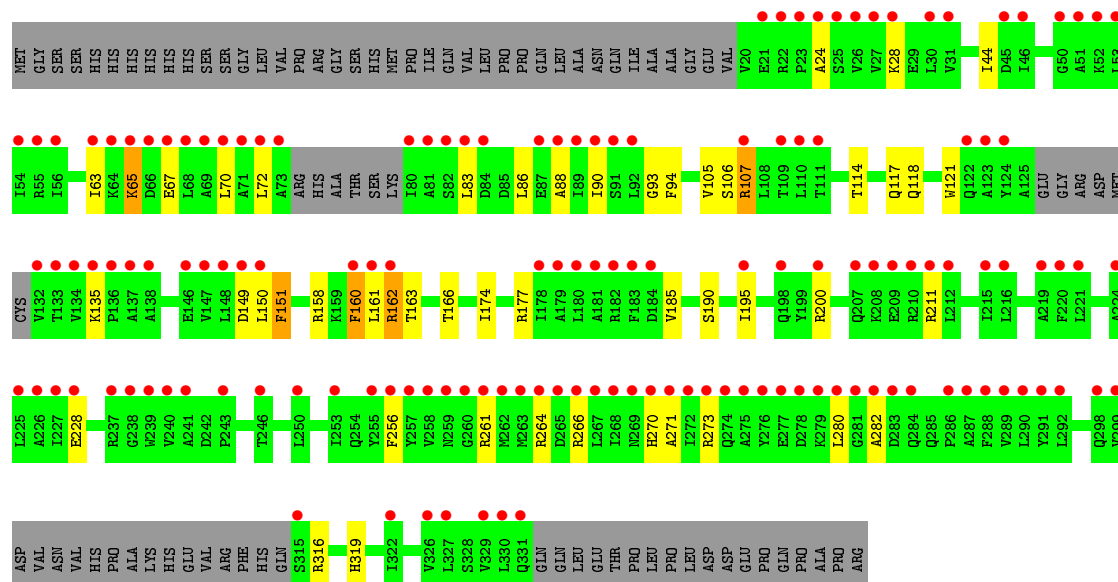
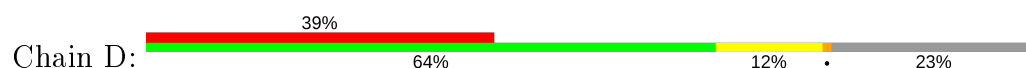
12%

23%

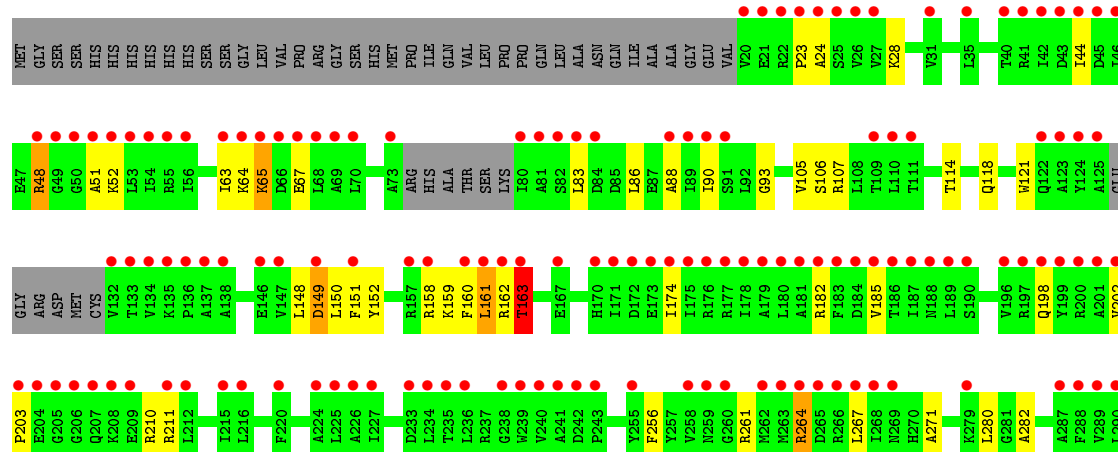
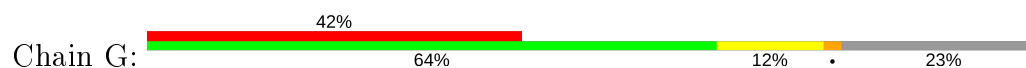
MET GLY SER SER HIS HIS HIS HIS HIS HIS HIS SER SER SER GLY LEU VAL PRO ARG ARG GLY SER SER MET PRO ILE ILE GLN VAL LEU PRO PRO GLN LEU ALA ASN GLN ILE ALA ALA GLY GLU VAL V20 E21 R22 A23 A24 K28 V31 L35 I44 R48 G49 G50 A51 K52 L53 F54 I63 K64 K65 D66 E67 L68 A69 L70 A71 L72 A73 A75 HIS HIS ALA THR SER LYS I80 A81 S82 L83 D84 D85 L86 E87 A88 I89 I90 S91 L92 G93 F94 R95 G96 E97 V105 S106 R107 L108 T109 L110 R113 T114 A115 E116 Q117 Q118 E119 A120 W121 Q122 Y123 A124 A125 GLU GLY P126

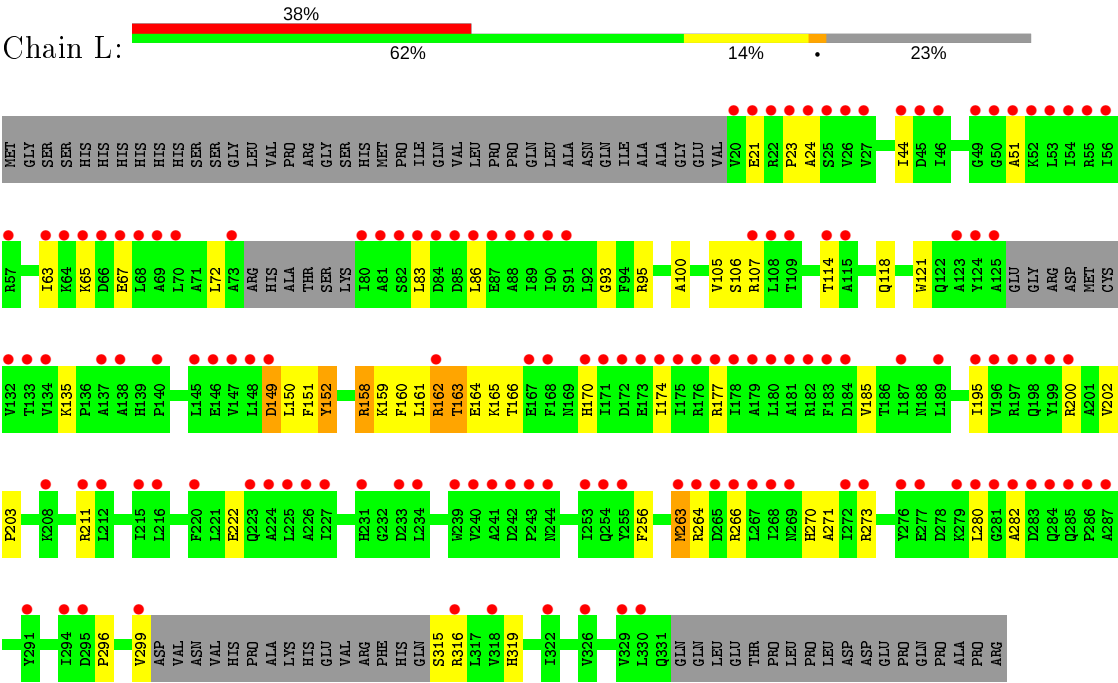


• Molecule 2: DNA MISMATCH REPAIR PROTEIN MUTL



• Molecule 2: DNA MISMATCH REPAIR PROTEIN MUTL





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	193.02Å 109.76Å 275.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	275.84 – 7.60 49.30 – 7.60	Depositor EDS
% Data completeness (in resolution range)	80.1 (275.84-7.60) 80.5 (49.30-7.60)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 7.37Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.264 , 0.306 0.260 , 0.301	Depositor DCC
R_{free} test set	585 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	441.7	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 500.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	0.090 for h,-k,-l	Xtriage
F_o, F_c correlation	0.79	EDS
Total number of atoms	45054	wwPDB-VP
Average B, all atoms (Å ²)	231.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.81% 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: ANP

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	0.66	1/5311 (0.0%)	0.80	9/7186 (0.1%)
1	B	0.66	0/5311	0.80	10/7186 (0.1%)
1	E	0.65	3/5311 (0.1%)	0.84	16/7186 (0.2%)
1	F	0.64	0/5311	0.77	13/7186 (0.2%)
1	I	0.62	0/5311	0.74	2/7186 (0.0%)
1	J	0.70	3/5311 (0.1%)	0.86	11/7186 (0.2%)
2	C	0.72	1/2288 (0.0%)	0.79	2/3096 (0.1%)
2	D	0.82	2/2288 (0.1%)	0.85	6/3096 (0.2%)
2	G	0.71	0/2288	0.81	4/3096 (0.1%)
2	H	0.71	1/2288 (0.0%)	0.84	8/3096 (0.3%)
2	K	0.90	3/2288 (0.1%)	1.03	8/3096 (0.3%)
2	L	0.71	0/2288	0.82	5/3096 (0.2%)
All	All	0.69	14/45594 (0.0%)	0.82	94/61692 (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	B	0	2
2	K	0	1
All	All	0	3

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	157	ARG	CD-NE	17.42	1.76	1.46
2	K	157	ARG	NE-CZ	17.13	1.55	1.33
1	J	787	LYS	CE-NZ	15.77	1.88	1.49
1	J	249	ARG	NE-CZ	13.73	1.50	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	228	GLU	CD-OE1	11.54	1.38	1.25

The worst 5 of 94 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	157	ARG	NE-CZ-NH1	31.56	136.08	120.30
1	J	249	ARG	NE-CZ-NH1	29.02	134.81	120.30
1	J	249	ARG	NE-CZ-NH2	-20.07	110.27	120.30
1	E	156	ARG	NE-CZ-NH2	16.87	128.74	120.30
1	E	420	ARG	NE-CZ-NH1	13.33	126.97	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	129	GLN	Peptide
1	B	268	ILE	Peptide
2	K	157	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	A	5226	0	5283	64	0
1	B	5226	0	5283	74	1
1	E	5226	0	5283	86	0
1	F	5226	0	5283	61	1
1	I	5226	0	5283	46	1
1	J	5226	0	5283	42	0
2	C	2252	0	2272	29	0
2	D	2252	0	2272	37	0
2	G	2252	0	2272	38	0
2	H	2252	0	2272	41	0
2	K	2252	0	2272	29	1
2	L	2252	0	2272	39	0
3	A	31	0	13	5	0
3	B	31	0	13	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	31	0	13	2	0
3	F	31	0	13	3	0
3	I	31	0	13	6	0
3	J	31	0	13	2	0
All	All	45054	0	45408	488	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 488 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:28:LYS:NZ	2:C:28:LYS:CE	1.71	1.50
2:K:157:ARG:NE	2:K:157:ARG:CD	1.76	1.46
1:J:787:LYS:CE	1:J:787:LYS:NZ	1.88	1.35
1:E:269:MET:SD	1:E:653:ILE:HB	1.69	1.31
2:D:105:VAL:O	2:D:150:LEU:CD1	1.90	1.20

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:737:GLU:OE2	1:F:491:ARG:NH1[2_544]	1.87	0.33
1:I:488:ASN:ND2	2:K:117:GLN:OE1[1_545]	1.91	0.29

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	659/800 (82%)	636 (96%)	23 (4%)	0	100	100
1	B	659/800 (82%)	638 (97%)	21 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	659/800 (82%)	632 (96%)	24 (4%)	3 (0%)	29	69
1	F	659/800 (82%)	634 (96%)	23 (4%)	2 (0%)	41	77
1	I	659/800 (82%)	635 (96%)	22 (3%)	2 (0%)	41	77
1	J	659/800 (82%)	639 (97%)	18 (3%)	2 (0%)	41	77
2	C	277/369 (75%)	258 (93%)	15 (5%)	4 (1%)	11	46
2	D	277/369 (75%)	260 (94%)	13 (5%)	4 (1%)	11	46
2	G	277/369 (75%)	261 (94%)	13 (5%)	3 (1%)	14	52
2	H	277/369 (75%)	260 (94%)	13 (5%)	4 (1%)	11	46
2	K	277/369 (75%)	262 (95%)	11 (4%)	4 (1%)	11	46
2	L	277/369 (75%)	261 (94%)	12 (4%)	4 (1%)	11	46
All	All	5616/7014 (80%)	5376 (96%)	208 (4%)	32 (1%)	25	66

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	163	THR
2	D	151	PHE
1	F	267	ILE
2	G	163	THR
2	H	163	THR

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	550/662 (83%)	539 (98%)	11 (2%)	55	74
1	B	550/662 (83%)	541 (98%)	9 (2%)	62	79
1	E	550/662 (83%)	539 (98%)	11 (2%)	55	74
1	F	550/662 (83%)	541 (98%)	9 (2%)	62	79
1	I	550/662 (83%)	538 (98%)	12 (2%)	52	71
1	J	550/662 (83%)	541 (98%)	9 (2%)	62	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	235/308 (76%)	228 (97%)	7 (3%)	41	63
2	D	235/308 (76%)	225 (96%)	10 (4%)	29	53
2	G	235/308 (76%)	227 (97%)	8 (3%)	37	60
2	H	235/308 (76%)	223 (95%)	12 (5%)	24	48
2	K	235/308 (76%)	227 (97%)	8 (3%)	37	60
2	L	235/308 (76%)	224 (95%)	11 (5%)	26	51
All	All	4710/5820 (81%)	4593 (98%)	117 (2%)	47	68

5 of 117 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	616	ASN
2	H	21	GLU
2	L	72	LEU
1	F	697	ARG
2	G	48	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	319	HIS
1	F	212	GLN
1	I	585	HIS
1	E	214	ASN
1	E	585	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

6 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	J	1801	-	29,33,33	1.88	9 (31%)	31,52,52	1.87	7 (22%)
3	ANP	F	1801	-	29,33,33	1.75	9 (31%)	31,52,52	2.06	10 (32%)
3	ANP	E	1801	-	29,33,33	1.96	10 (34%)	31,52,52	2.09	8 (25%)
3	ANP	A	1801	-	29,33,33	1.99	7 (24%)	31,52,52	2.03	8 (25%)
3	ANP	I	1801	-	29,33,33	1.85	8 (27%)	31,52,52	1.83	7 (22%)
3	ANP	B	1801	-	29,33,33	1.80	7 (24%)	31,52,52	2.10	9 (29%)

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	J	1801	-	-	2/14/38/38	0/3/3/3
3	ANP	F	1801	-	-	5/14/38/38	0/3/3/3
3	ANP	E	1801	-	-	7/14/38/38	0/3/3/3
3	ANP	A	1801	-	-	5/14/38/38	0/3/3/3
3	ANP	I	1801	-	-	3/14/38/38	0/3/3/3
3	ANP	B	1801	-	-	8/14/38/38	0/3/3/3

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	1801	ANP	PG-N3B	4.96	1.76	1.63
3	A	1801	ANP	PG-N3B	4.86	1.76	1.63
3	A	1801	ANP	PB-N3B	4.74	1.75	1.63
3	J	1801	ANP	PB-N3B	4.42	1.74	1.63
3	I	1801	ANP	PB-N3B	4.28	1.74	1.63

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1801	ANP	O1G-PG-N3B	-6.82	101.73	111.77
3	F	1801	ANP	O1G-PG-N3B	-6.64	101.99	111.77
3	J	1801	ANP	O1G-PG-N3B	-5.55	103.59	111.77
3	E	1801	ANP	O1G-PG-N3B	-5.23	104.07	111.77
3	E	1801	ANP	C3'-C2'-C1'	5.03	108.55	100.98

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

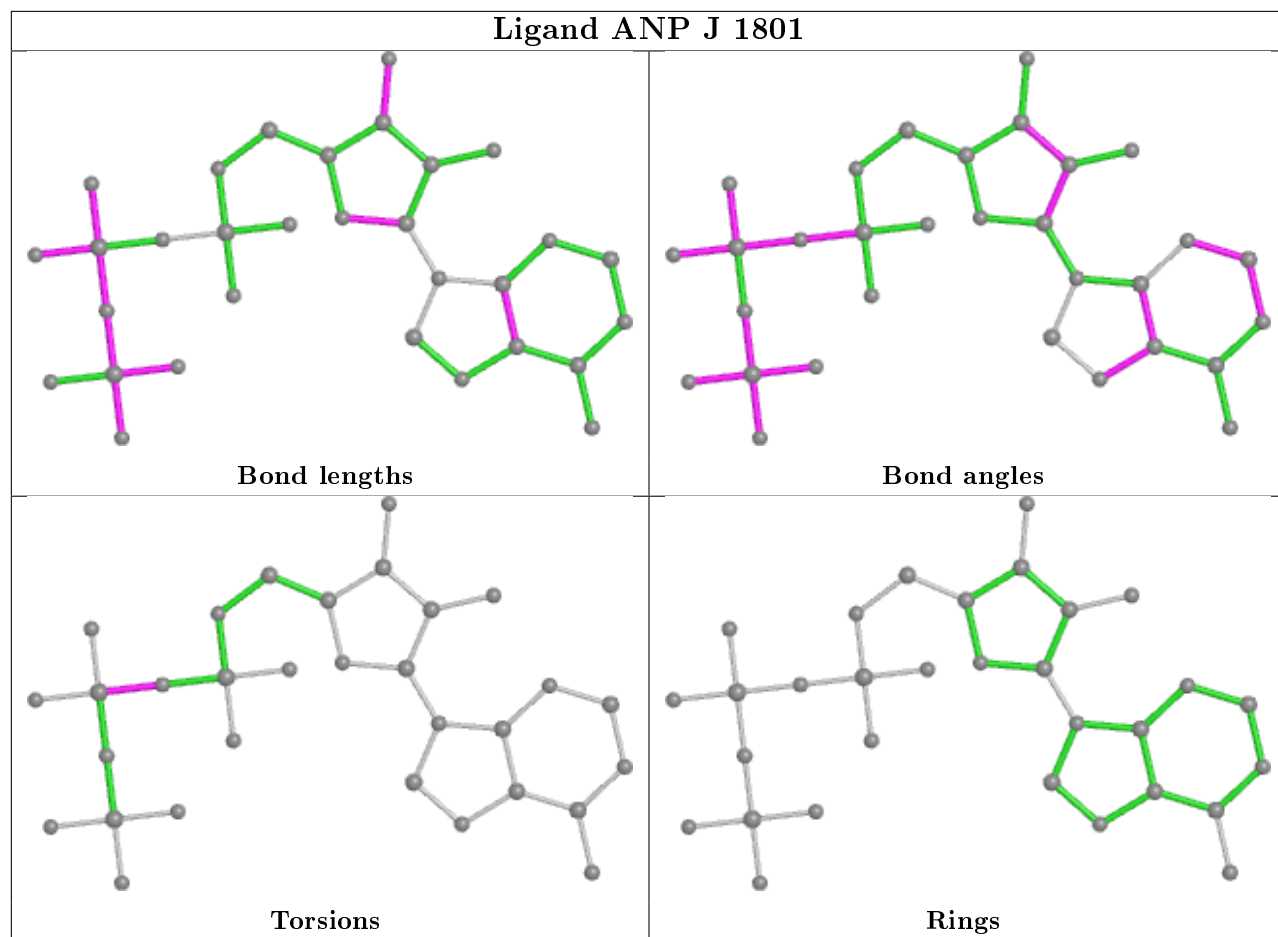
Mol	Chain	Res	Type	Atoms
3	J	1801	ANP	PA-O3A-PB-O1B
3	J	1801	ANP	PA-O3A-PB-O2B
3	F	1801	ANP	PG-N3B-PB-O1B
3	F	1801	ANP	PA-O3A-PB-O1B
3	F	1801	ANP	PA-O3A-PB-O2B

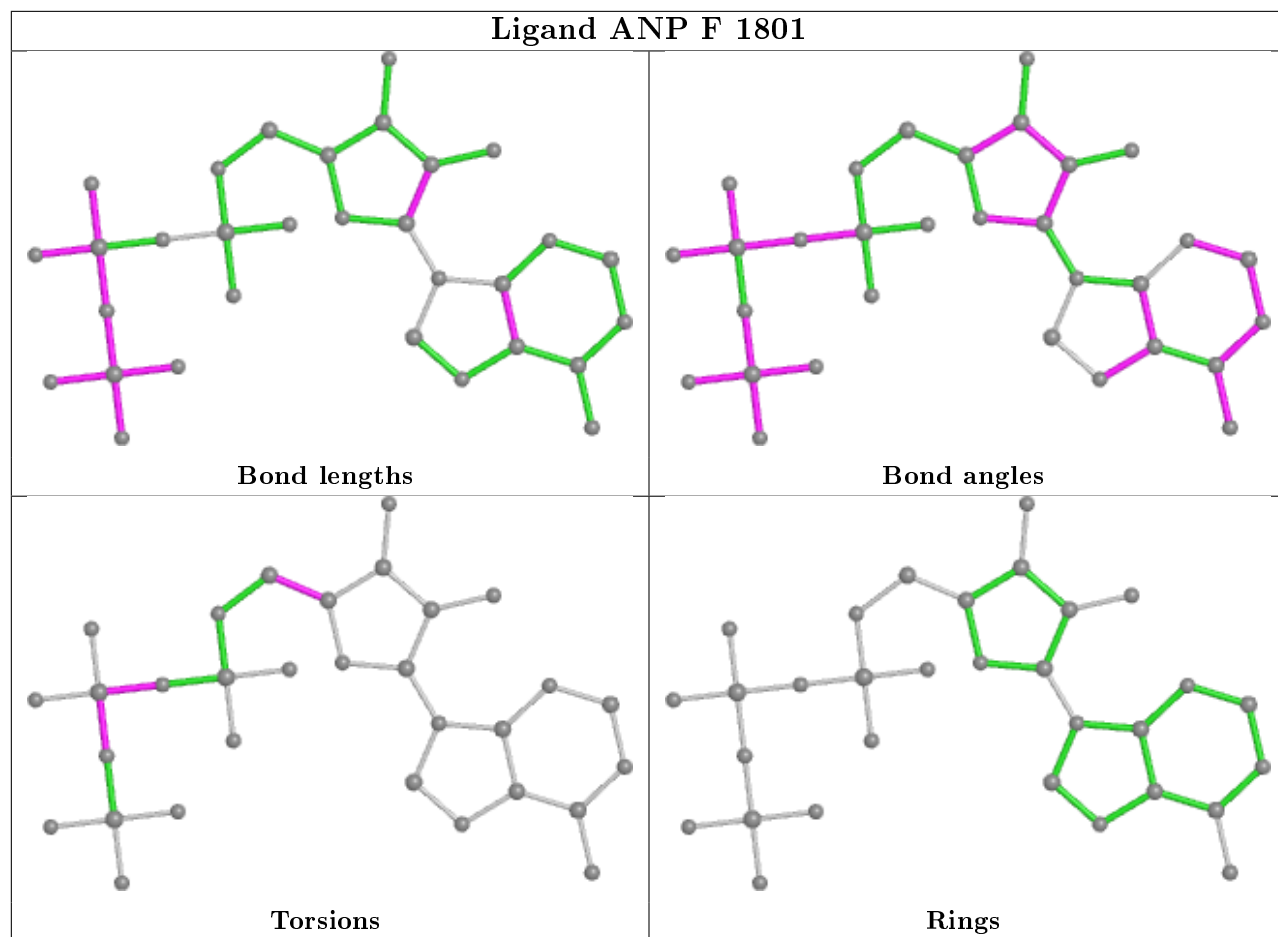
There are no ring outliers.

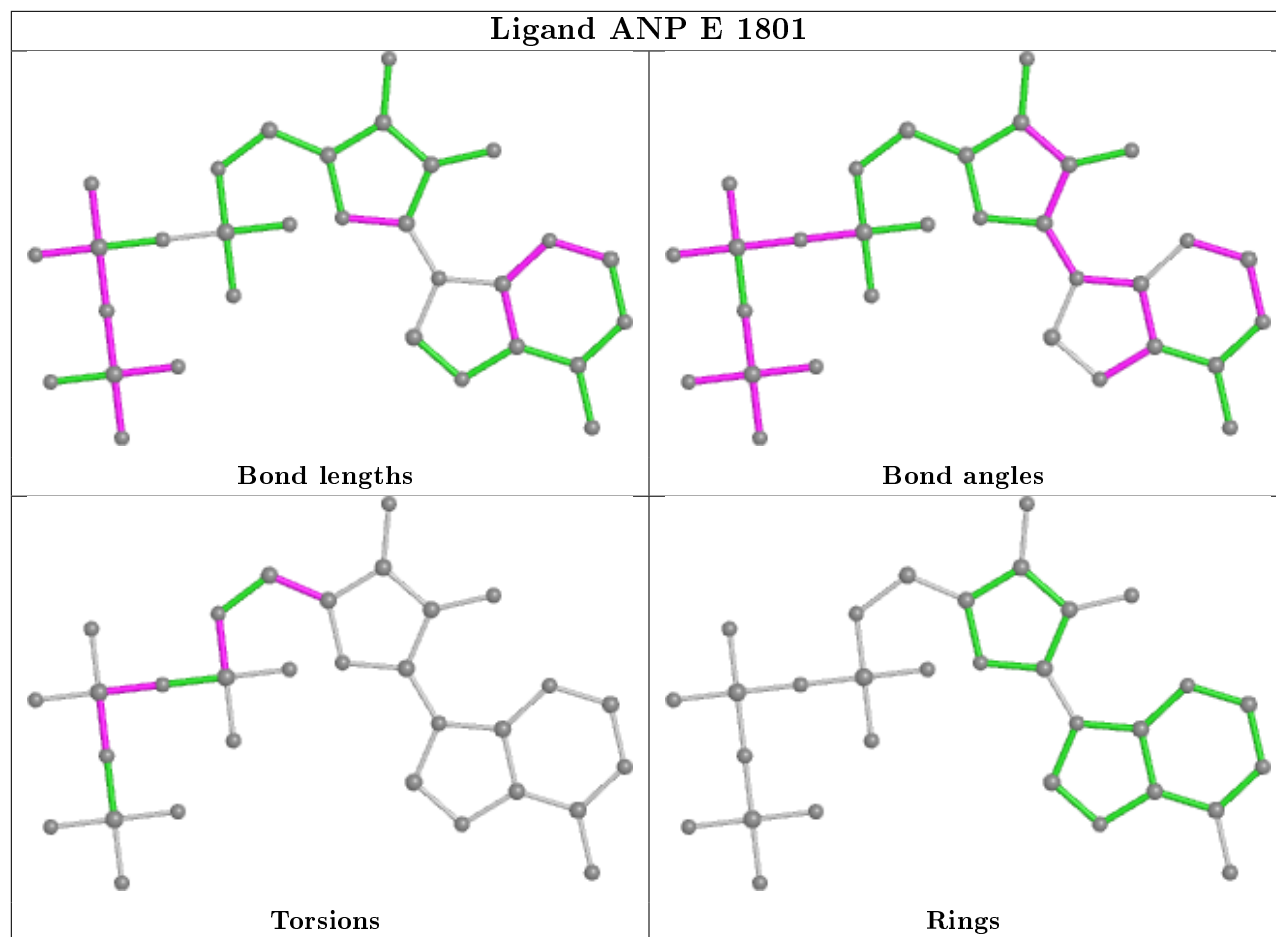
6 monomers are involved in 22 short contacts:

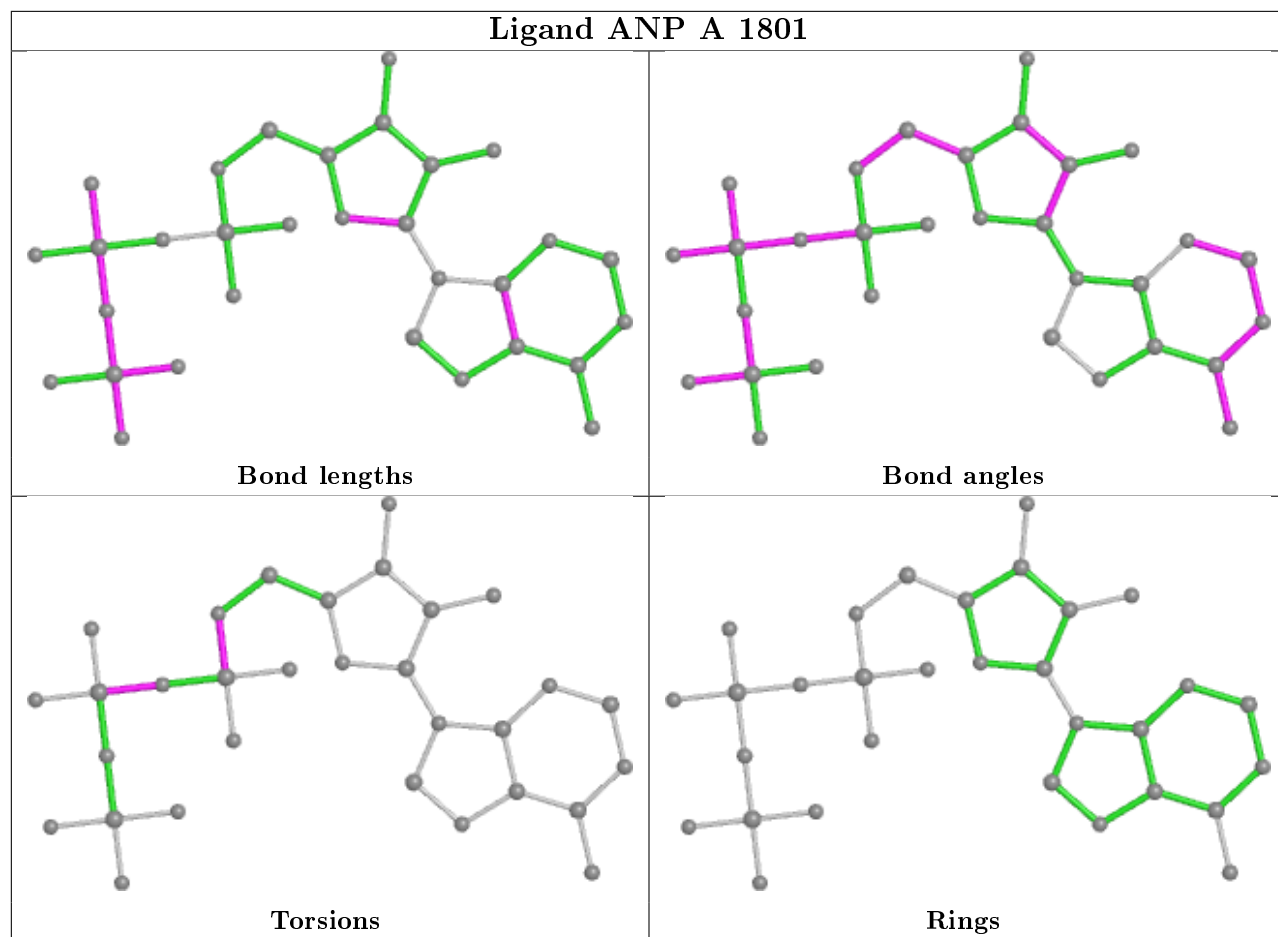
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	1801	ANP	2	0
3	F	1801	ANP	3	0
3	E	1801	ANP	2	0
3	A	1801	ANP	5	0
3	I	1801	ANP	6	0
3	B	1801	ANP	4	0

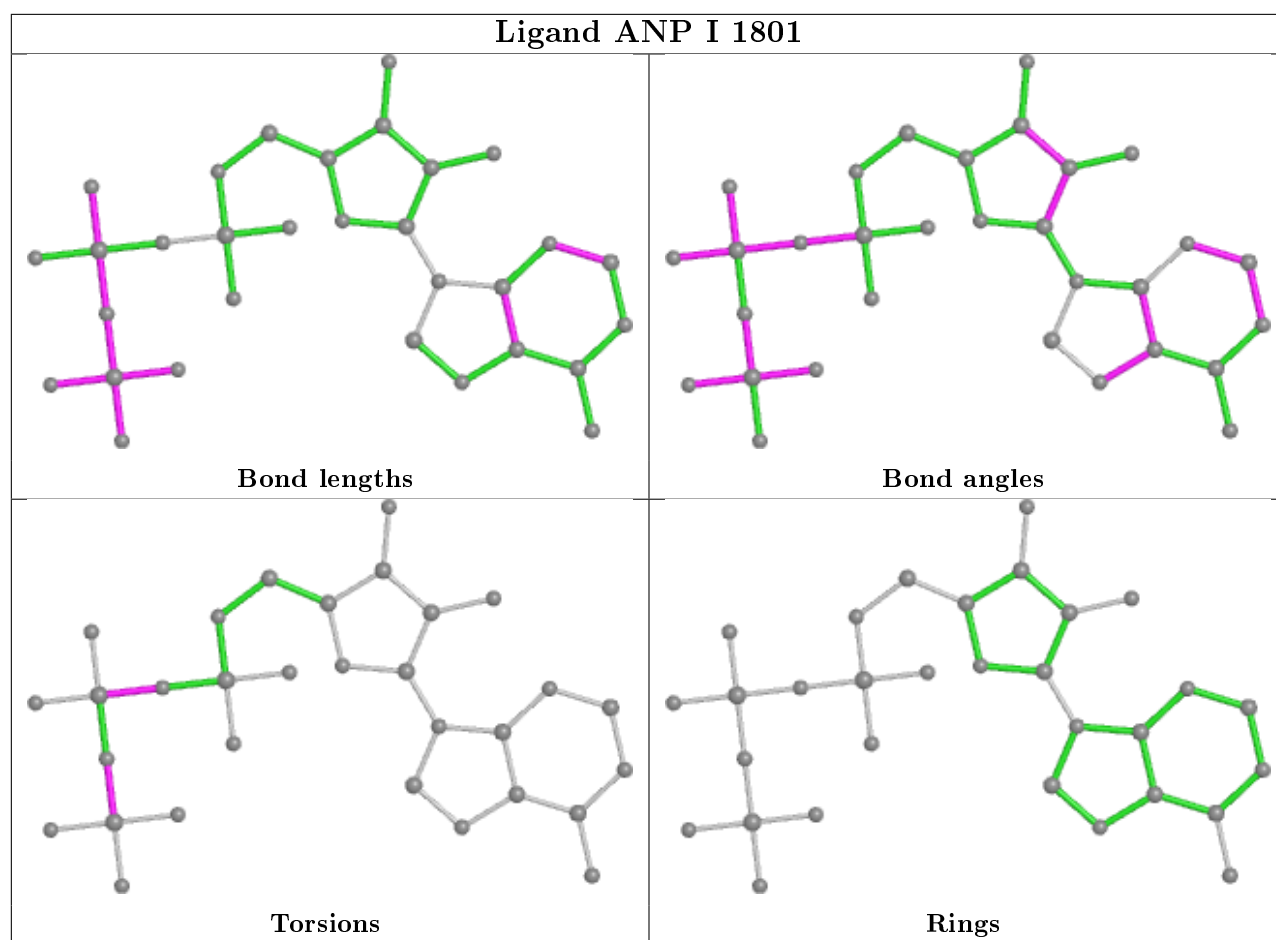
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

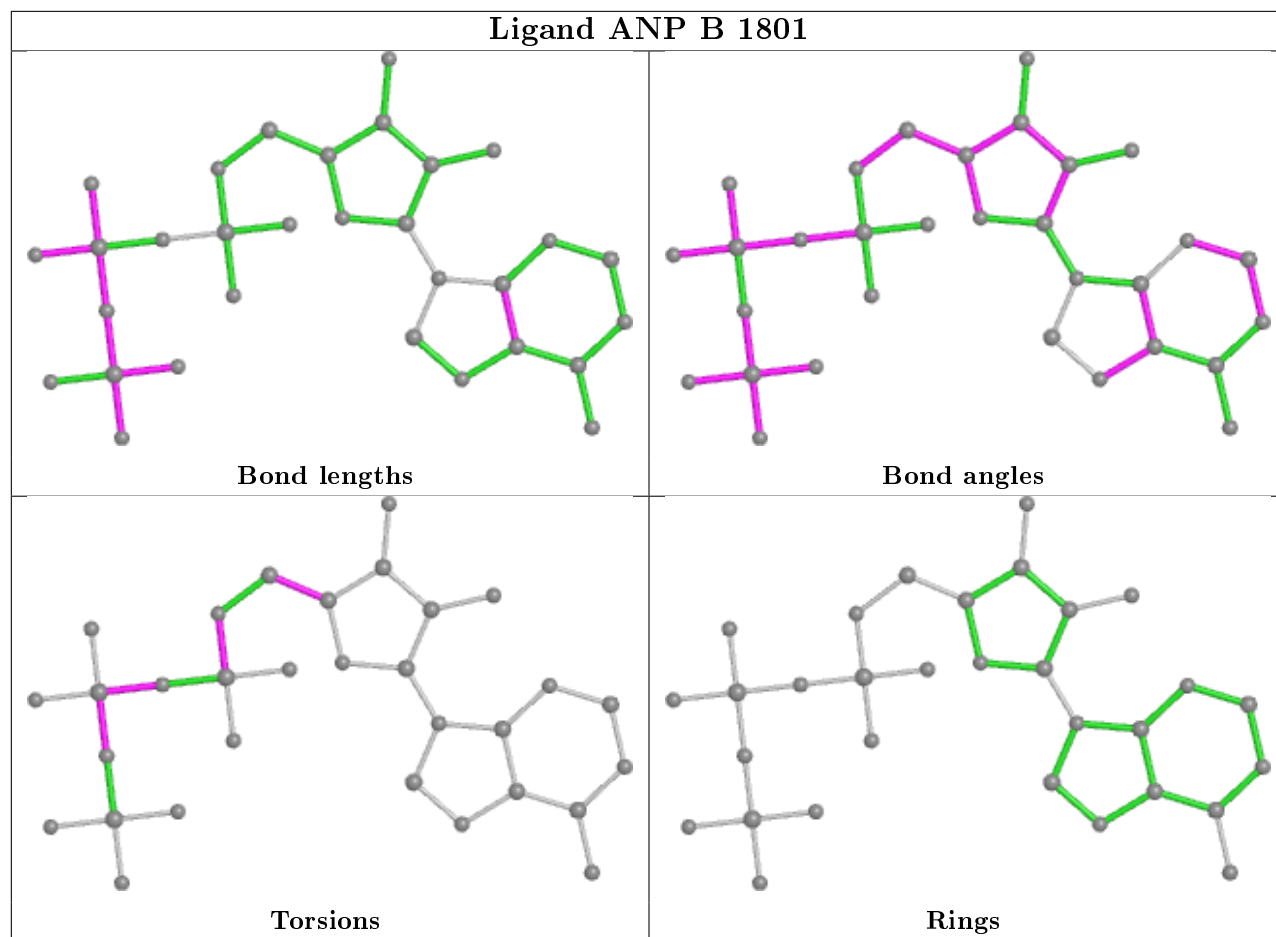












5.7 Other polymers [i](#)

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, 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	663/800 (82%)	2.23	315 (47%) 0 1	120, 187, 361, 469	0
1	B	663/800 (82%)	2.06	289 (43%) 0 1	125, 203, 272, 321	0
1	E	663/800 (82%)	2.67	343 (51%) 0 1	170, 262, 510, 665	0
1	F	663/800 (82%)	2.01	276 (41%) 0 1	127, 197, 351, 463	0
1	I	663/800 (82%)	2.38	325 (49%) 0 1	174, 224, 402, 487	0
1	J	663/800 (82%)	2.73	363 (54%) 0 1	172, 231, 378, 460	0
2	C	285/369 (77%)	2.04	136 (47%) 0 1	178, 213, 254, 293	0
2	D	285/369 (77%)	2.37	144 (50%) 0 1	170, 201, 273, 306	0
2	G	285/369 (77%)	2.38	155 (54%) 0 1	204, 224, 251, 265	0
2	H	285/369 (77%)	2.60	159 (55%) 0 1	154, 218, 301, 389	0
2	K	285/369 (77%)	2.12	130 (45%) 0 1	185, 220, 264, 283	0
2	L	285/369 (77%)	2.31	139 (48%) 0 1	210, 231, 253, 269	0
All	All	5688/7014 (81%)	2.33	2774 (48%) 0 1	120, 220, 361, 665	0

The worst 5 of 2774 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	749	ALA	21.6
1	E	757	ALA	19.1
1	J	147	THR	16.8
1	E	134	ALA	14.9
1	A	135	ALA	14.7

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

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

6.3 Carbohydrates [i](#)

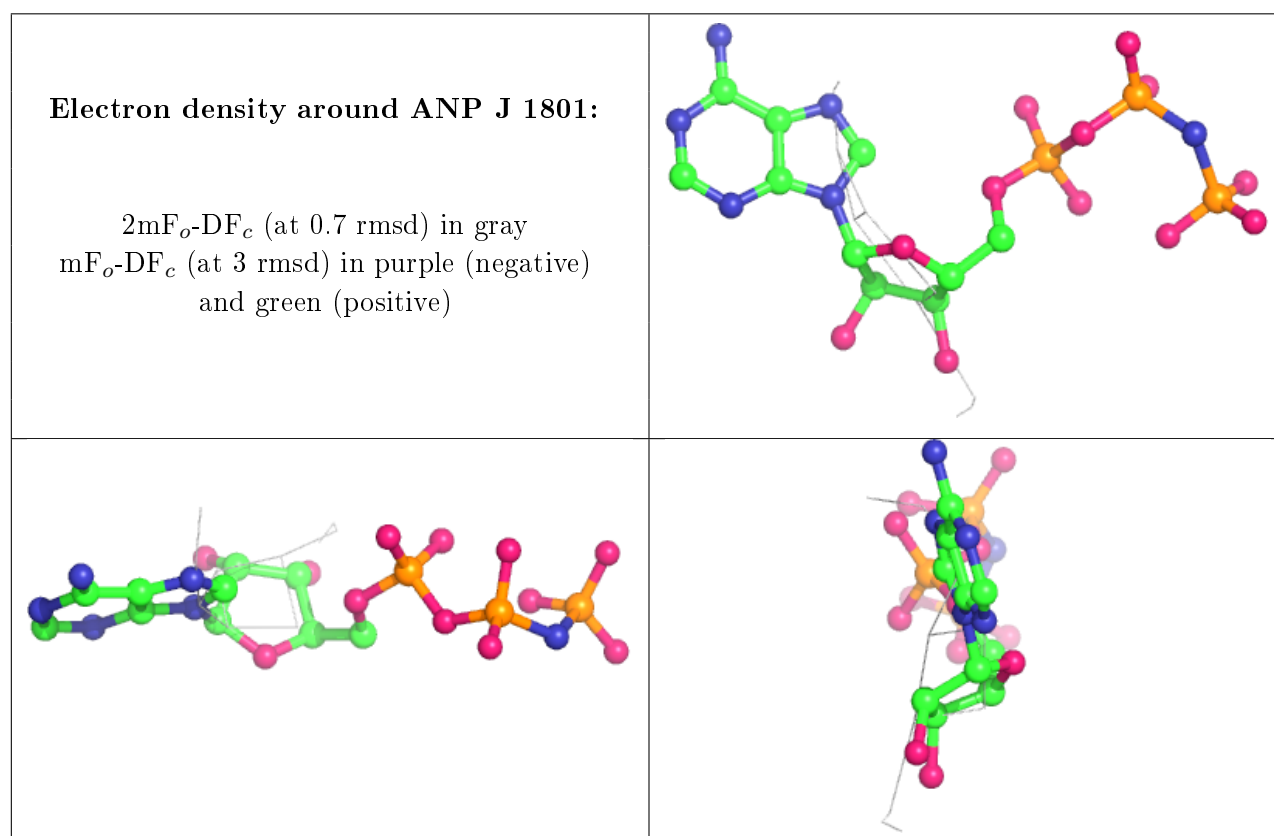
There are no carbohydrates in this entry.

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.

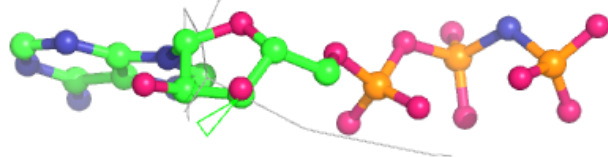
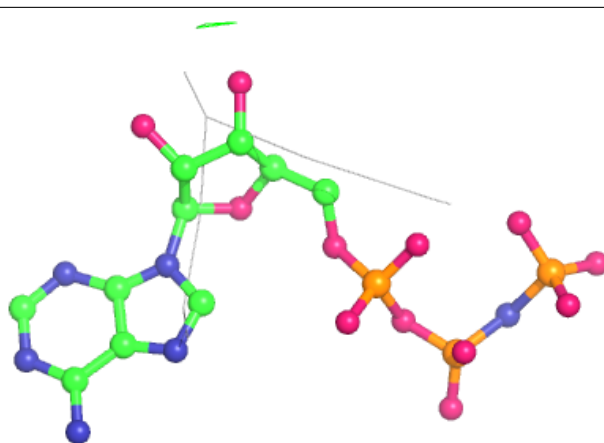
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	ANP	J	1801	31/31	0.64	0.49	193,199,212,213	0
3	ANP	E	1801	31/31	0.70	0.51	204,216,227,232	0
3	ANP	I	1801	31/31	0.70	0.41	177,180,186,187	0
3	ANP	B	1801	31/31	0.72	0.31	165,174,179,181	0
3	ANP	A	1801	31/31	0.81	0.51	156,164,170,171	0
3	ANP	F	1801	31/31	0.85	0.30	154,162,169,174	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.

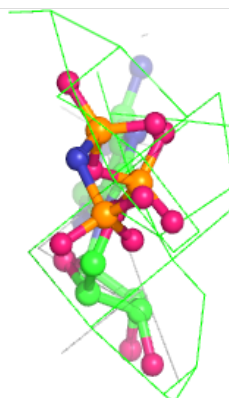
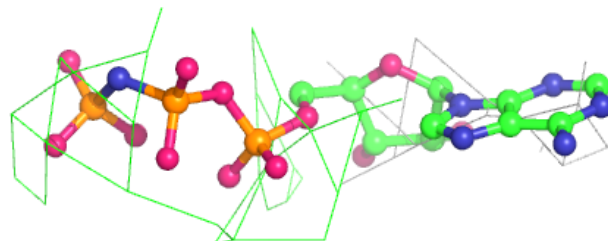
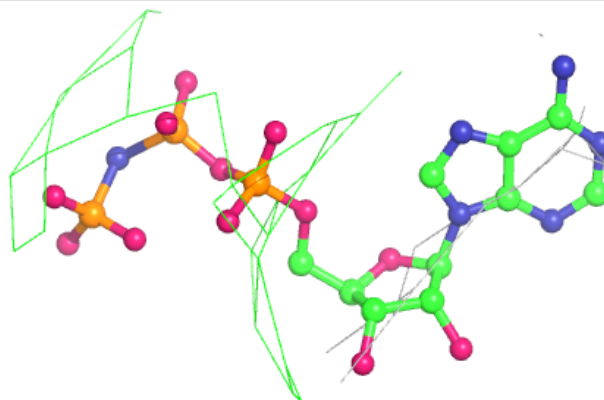


Electron density around ANP E 1801:

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

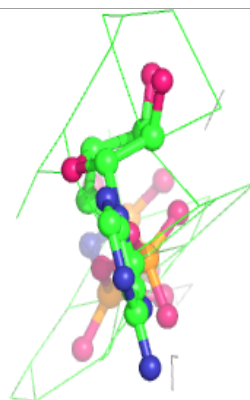
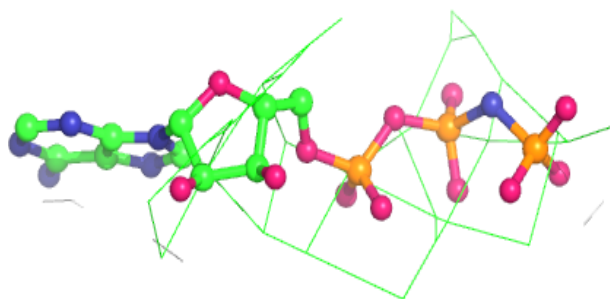
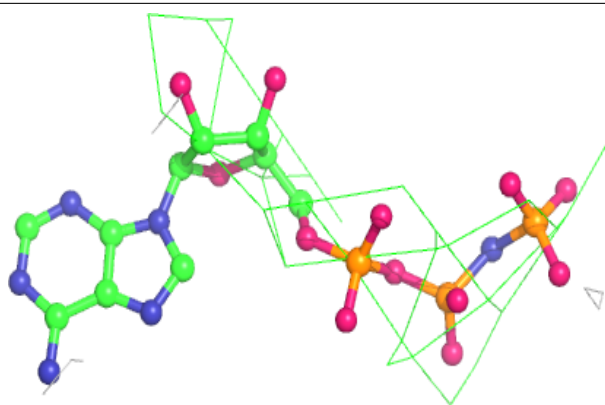
**Electron density around ANP I 1801:**

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

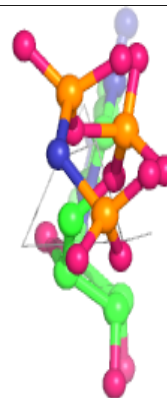
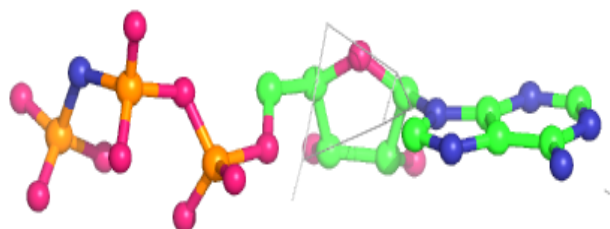
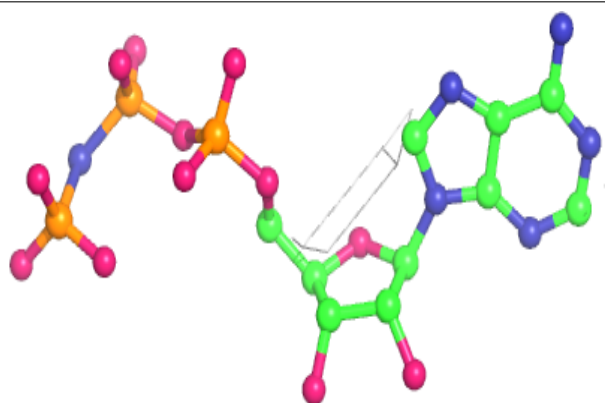


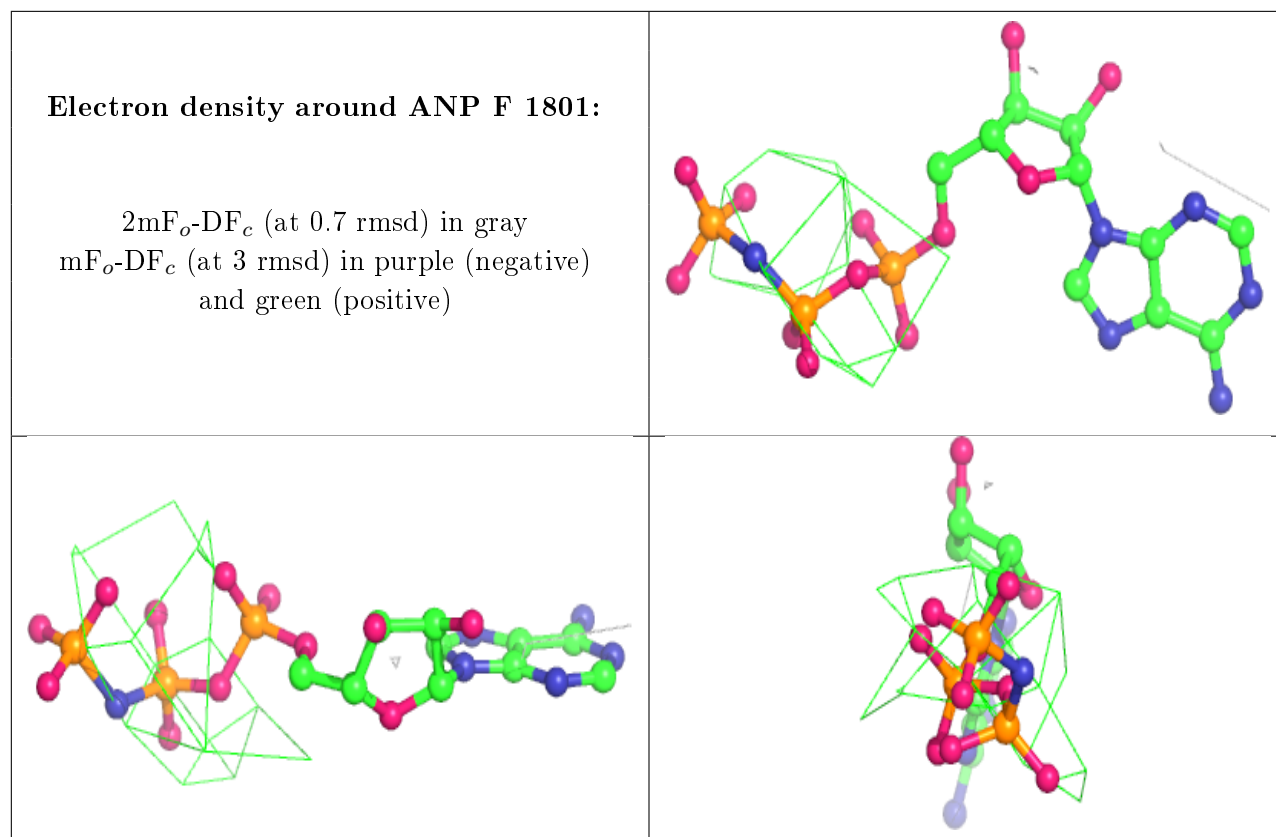
Electron density around ANP B 1801:

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

**Electron density around ANP A 1801:**

$2mF_o-DF_c$ (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.