



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 14, 2026 – 10:02 PM UTC

PDB ID : 5AKD / pdb_00005akd
Title : MutS in complex with the N-terminal domain of MutL - crystal form 3
Authors : Grootuizen, 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

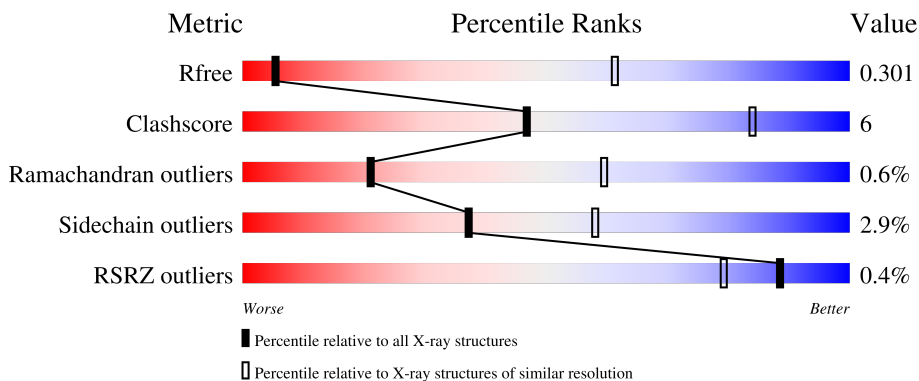
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1167 (10.00-4.00)
Clashscore	190562	1000 (10.00-4.06)
Ramachandran outliers	187476	1054 (10.00-4.00)
Sidechain outliers	187428	1017 (10.00-4.00)
RSRZ outliers	180081	1161 (10.00-4.00)

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 $\leq 5\%$. 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	
1	B	800	
1	E	800	
1	F	800	

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Mol	Chain	Length	Quality of chain
1	I	800	 75% 8% 17%
1	J	800	 74% 8% 17%
2	C	369	 63% 12% 23%
2	D	369	 64% 11% 23%
2	G	369	 63% 12% 23%
2	H	369	 62% 13% 23%
2	K	369	 64% 11% 23%
2	L	369	 61% 15% 23%

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
			Total	C	N	O	S			
1	A	663	5226	3284	938	984	20	0	0	0
1	B	663	5226	3284	938	984	20	0	0	0
1	E	663	5226	3284	938	984	20	0	0	0
1	F	663	5226	3284	938	984	20	0	0	0
1	I	663	5226	3284	938	984	20	0	0	0
1	J	663	5226	3284	938	984	20	0	0	0

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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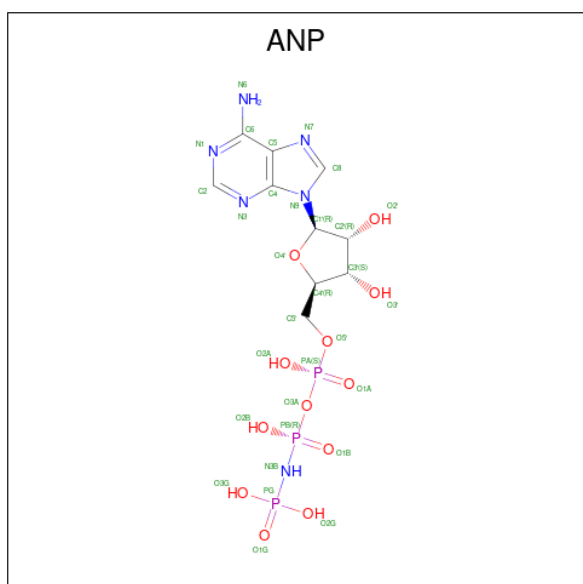
Chain	Residue	Modelled	Actual	Comment	Reference
H	-9	SER	-	expression tag	UNP P23367
H	-8	SER	-	expression tag	UNP P23367
H	-7	GLY	-	expression tag	UNP P23367
H	-6	LEU	-	expression tag	UNP P23367
H	-5	VAL	-	expression tag	UNP P23367
H	-4	PRO	-	expression tag	UNP P23367
H	-3	ARG	-	expression tag	UNP P23367
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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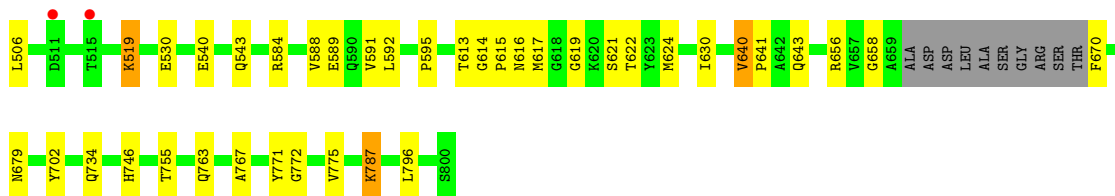
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Chain	Residue	Modelled	Actual	Comment	Reference
L	-17	SER	-	expression tag	UNP P23367
L	-16	SER	-	expression tag	UNP P23367
L	-15	HIS	-	expression tag	UNP P23367
L	-14	HIS	-	expression tag	UNP P23367
L	-13	HIS	-	expression tag	UNP P23367
L	-12	HIS	-	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

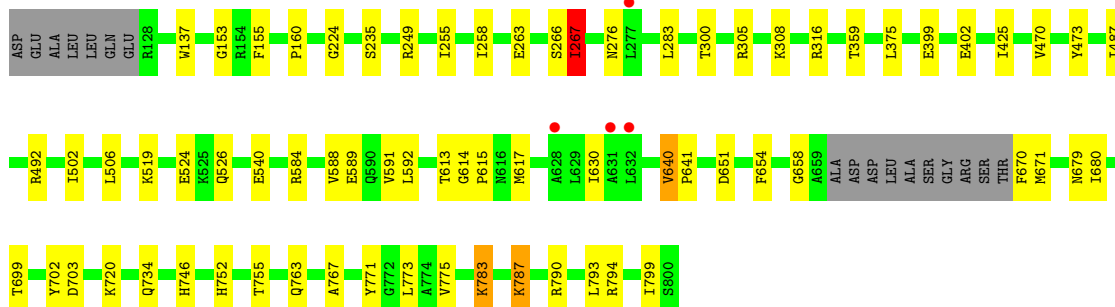
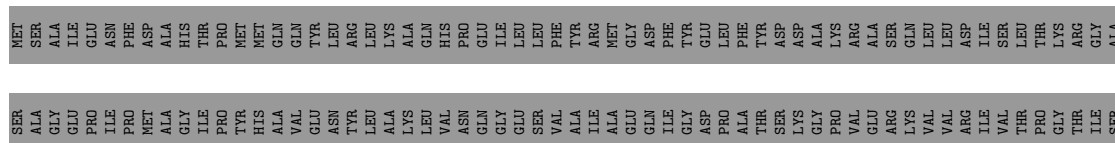
- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



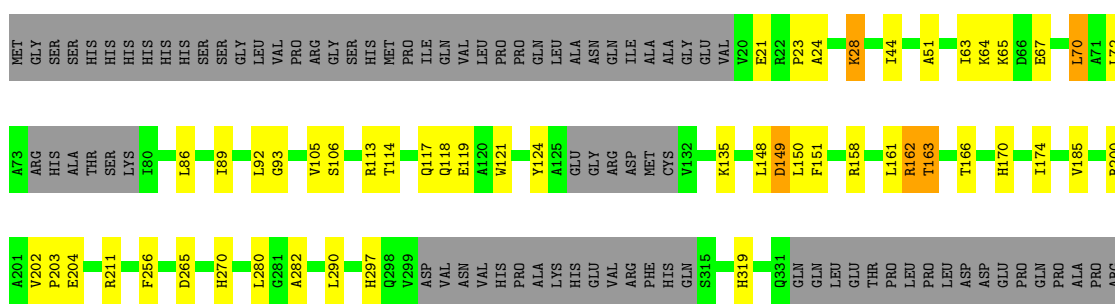
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	Total 31	C 10	N 6	O 12	P 3	0	0
3	B	1	Total 31	C 10	N 6	O 12	P 3	0	0
3	E	1	Total 31	C 10	N 6	O 12	P 3	0	0
3	F	1	Total 31	C 10	N 6	O 12	P 3	0	0
3	I	1	Total 31	C 10	N 6	O 12	P 3	0	0
3	J	1	Total 31	C 10	N 6	O 12	P 3	0	0



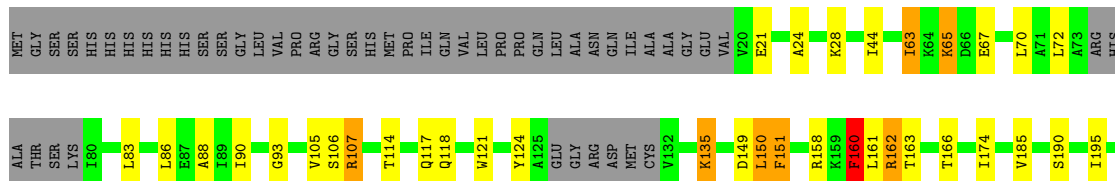
• Molecule 1: DNA MISMATCH REPAIR PROTEIN MUTS

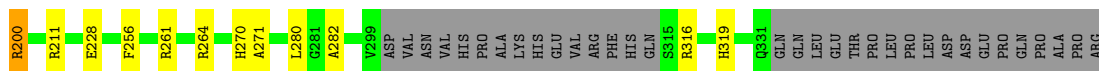


• Molecule 2: DNA MISMATCH REPAIR PROTEIN MUTL

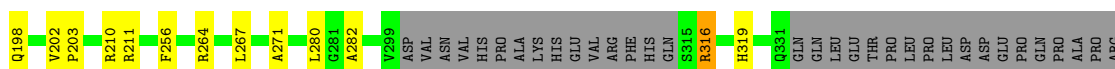
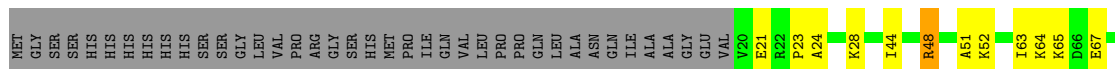


• Molecule 2: DNA MISMATCH REPAIR PROTEIN MUTL

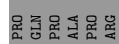
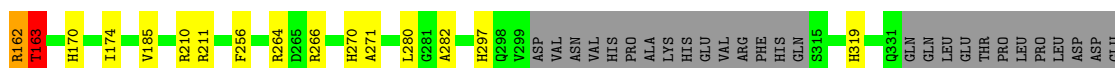
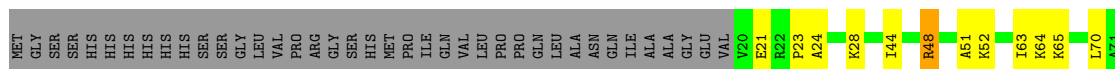




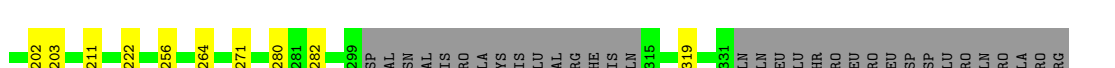
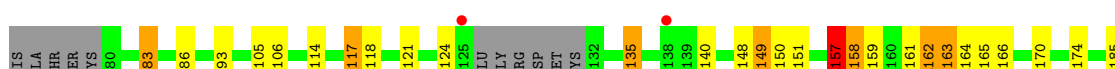
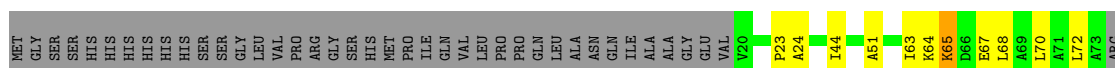
• Molecule 2: DNA MISMATCH REPAIR PROTEIN MUTL



• Molecule 2: DNA MISMATCH REPAIR PROTEIN MUTL

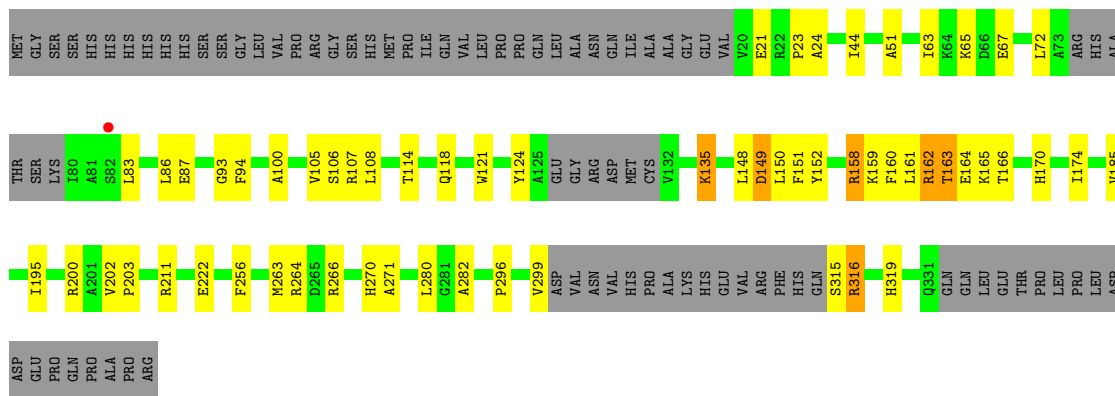


• Molecule 2: DNA MISMATCH REPAIR PROTEIN MUTL



• Molecule 2: DNA MISMATCH REPAIR PROTEIN MUTL





4 Data and refinement statistics i

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 – 7.60 275.84 – 7.60	Depositor EDS
% Data completeness (in resolution range)	80.1 (275.84-7.60) 80.1 (275.84-7.60)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 7.37Å)	Xtrriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.264 , 0.306 0.260 , 0.301	Depositor DCC
R_{free} test set	586 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	441.7	Xtrriage
Anisotropy	0.279	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 583.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.19$	Xtrriage
Estimated twinning fraction	0.090 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	45054	wwPDB-VP
Average B, all atoms (Å ²)	231.0	wwPDB-VP

Xtrriage'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 i

5.1 Standard geometry i

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	0.81	0/5311	0.98	4/7186 (0.1%)
1	B	0.84	0/5311	0.99	5/7186 (0.1%)
1	E	0.80	2/5311 (0.0%)	0.99	9/7186 (0.1%)
1	F	0.80	1/5311 (0.0%)	0.96	2/7186 (0.0%)
1	I	0.78	2/5311 (0.0%)	0.94	3/7186 (0.0%)
1	J	0.85	2/5311 (0.0%)	0.99	7/7186 (0.1%)
2	C	0.93	4/2288 (0.2%)	1.00	2/3096 (0.1%)
2	D	0.99	2/2288 (0.1%)	1.06	6/3096 (0.2%)
2	G	0.91	0/2288	1.00	3/3096 (0.1%)
2	H	0.96	5/2288 (0.2%)	1.06	6/3096 (0.2%)
2	K	1.13	3/2288 (0.1%)	1.08	7/3096 (0.2%)
2	L	0.91	0/2288	1.02	6/3096 (0.2%)
All	All	0.86	21/45594 (0.0%)	0.99	60/61692 (0.1%)

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 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	157	ARG	CD-NE	21.30	1.76	1.46
2	K	157	ARG	NE-CZ	20.25	1.55	1.33
1	J	249	ARG	NE-CZ	16.22	1.50	1.33
1	J	787	LYS	CE-NZ	13.04	1.88	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	157	ARG	CZ-NH1	8.19	1.44	1.32

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	157	ARG	NE-CZ-NH1	14.58	136.08	121.50
1	J	249	ARG	NE-CZ-NH1	13.31	134.81	121.50
2	H	297	HIS	N-CA-C	11.56	126.60	109.95
2	K	157	ARG	CD-NE-CZ	11.52	140.52	124.40
1	E	156	ARG	NE-CZ-NH2	10.60	128.74	119.20

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 [i](#)

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	65	0
1	B	5226	0	5283	79	1
1	E	5226	0	5283	86	0
1	F	5226	0	5283	63	1
1	I	5226	0	5283	52	1
1	J	5226	0	5283	44	0
2	C	2252	0	2272	31	0
2	D	2252	0	2272	37	0
2	G	2252	0	2272	40	0
2	H	2252	0	2272	43	0
2	K	2252	0	2272	31	1
2	L	2252	0	2272	41	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	4	0
3	I	31	0	13	8	0
3	J	31	0	13	2	0
All	All	45054	0	45408	511	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 6.

The worst 5 of 511 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:CE	2:C:28:LYS:NZ	1.71	1.50
2:K:157:ARG:CD	2:K:157:ARG:NE	1.76	1.46
1:J:787:LYS:NZ	1:J:787:LYS:CE	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

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	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%)	24	63
1	F	659/800 (82%)	634 (96%)	23 (4%)	2 (0%)	36	72
1	I	659/800 (82%)	635 (96%)	22 (3%)	2 (0%)	36	72
1	J	659/800 (82%)	639 (97%)	18 (3%)	2 (0%)	36	72
2	C	277/369 (75%)	258 (93%)	15 (5%)	4 (1%)	9	40
2	D	277/369 (75%)	260 (94%)	13 (5%)	4 (1%)	9	40
2	G	277/369 (75%)	261 (94%)	13 (5%)	3 (1%)	11	46
2	H	277/369 (75%)	260 (94%)	13 (5%)	4 (1%)	9	40
2	K	277/369 (75%)	262 (95%)	11 (4%)	4 (1%)	9	40
2	L	277/369 (75%)	261 (94%)	12 (4%)	4 (1%)	9	40
All	All	5616/7014 (80%)	5376 (96%)	208 (4%)	32 (1%)	21	59

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 [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	550/662 (83%)	539 (98%)	11 (2%)	48	66
1	B	550/662 (83%)	537 (98%)	13 (2%)	43	64
1	E	550/662 (83%)	536 (98%)	14 (2%)	42	63
1	F	550/662 (83%)	538 (98%)	12 (2%)	45	64
1	I	550/662 (83%)	538 (98%)	12 (2%)	45	64
1	J	550/662 (83%)	539 (98%)	11 (2%)	48	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	235/308 (76%)	227 (97%)	8 (3%)	32	54
2	D	235/308 (76%)	222 (94%)	13 (6%)	19	41
2	G	235/308 (76%)	225 (96%)	10 (4%)	26	47
2	H	235/308 (76%)	221 (94%)	14 (6%)	17	39
2	K	235/308 (76%)	228 (97%)	7 (3%)	36	57
2	L	235/308 (76%)	224 (95%)	11 (5%)	23	45
All	All	4710/5820 (81%)	4574 (97%)	136 (3%)	37	58

5 of 136 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	734	GLN
2	K	72	LEU
2	L	159	LYS
1	E	420	ARG
1	E	333	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 90 such sidechains are listed below:

Mol	Chain	Res	Type
2	G	319	HIS
1	I	746	HIS
2	H	270	HIS
1	I	339	GLN
1	J	214	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	A	1801	-	33,33,33	2.13	9 (27%)	45,52,52	2.20	13 (28%)
3	ANP	F	1801	-	33,33,33	2.04	13 (39%)	45,52,52	2.05	14 (31%)
3	ANP	E	1801	-	33,33,33	2.19	13 (39%)	45,52,52	2.43	12 (26%)
3	ANP	I	1801	-	33,33,33	2.07	13 (39%)	45,52,52	1.88	12 (26%)
3	ANP	B	1801	-	33,33,33	2.09	12 (36%)	45,52,52	2.15	15 (33%)
3	ANP	J	1801	-	33,33,33	2.06	12 (36%)	45,52,52	2.06	10 (22%)

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	A	1801	-	-	5/18/38/38	0/3/3/3
3	ANP	F	1801	-	-	4/18/38/38	0/3/3/3
3	ANP	E	1801	-	-	7/18/38/38	0/3/3/3
3	ANP	I	1801	-	-	2/18/38/38	0/3/3/3
3	ANP	B	1801	-	-	7/18/38/38	0/3/3/3
3	ANP	J	1801	-	-	2/18/38/38	0/3/3/3

The worst 5 of 72 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1801	ANP	C5-C4	5.60	1.49	1.39
3	E	1801	ANP	C5-C4	5.48	1.48	1.39
3	I	1801	ANP	C5-C4	5.16	1.48	1.39
3	J	1801	ANP	C5-C4	5.15	1.48	1.39
3	J	1801	ANP	PG-N3B	4.96	1.76	1.63

The worst 5 of 76 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1801	ANP	C5-C4-N3	-8.16	115.48	126.72
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	A	1801	ANP	C5-C4-N3	-6.25	118.12	126.72
3	J	1801	ANP	C5-C4-N3	-6.18	118.21	126.72

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

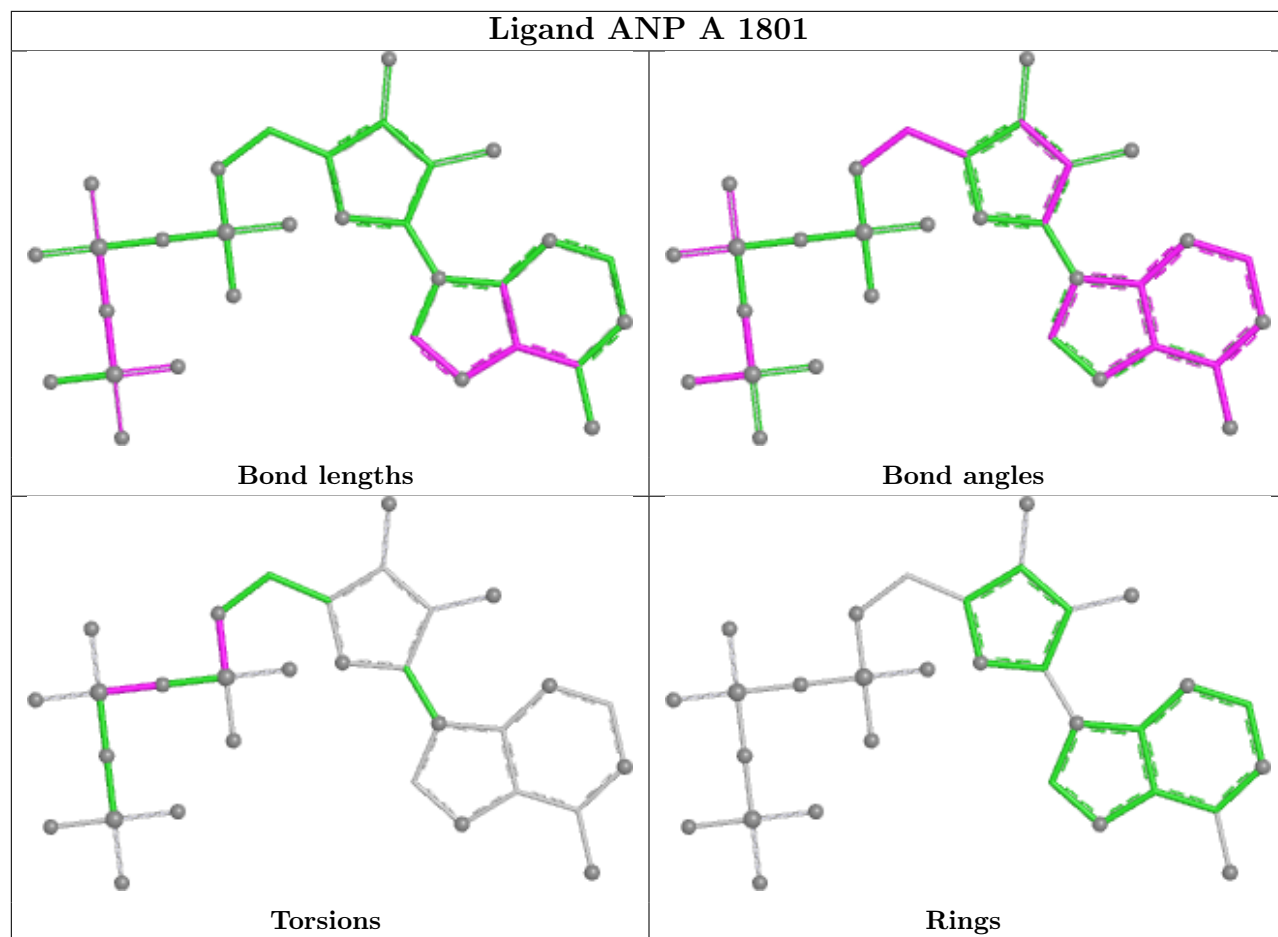
Mol	Chain	Res	Type	Atoms
3	A	1801	ANP	PA-O3A-PB-O2B
3	A	1801	ANP	C5'-O5'-PA-O1A
3	A	1801	ANP	C5'-O5'-PA-O2A
3	B	1801	ANP	PG-N3B-PB-O1B
3	B	1801	ANP	PA-O3A-PB-O2B

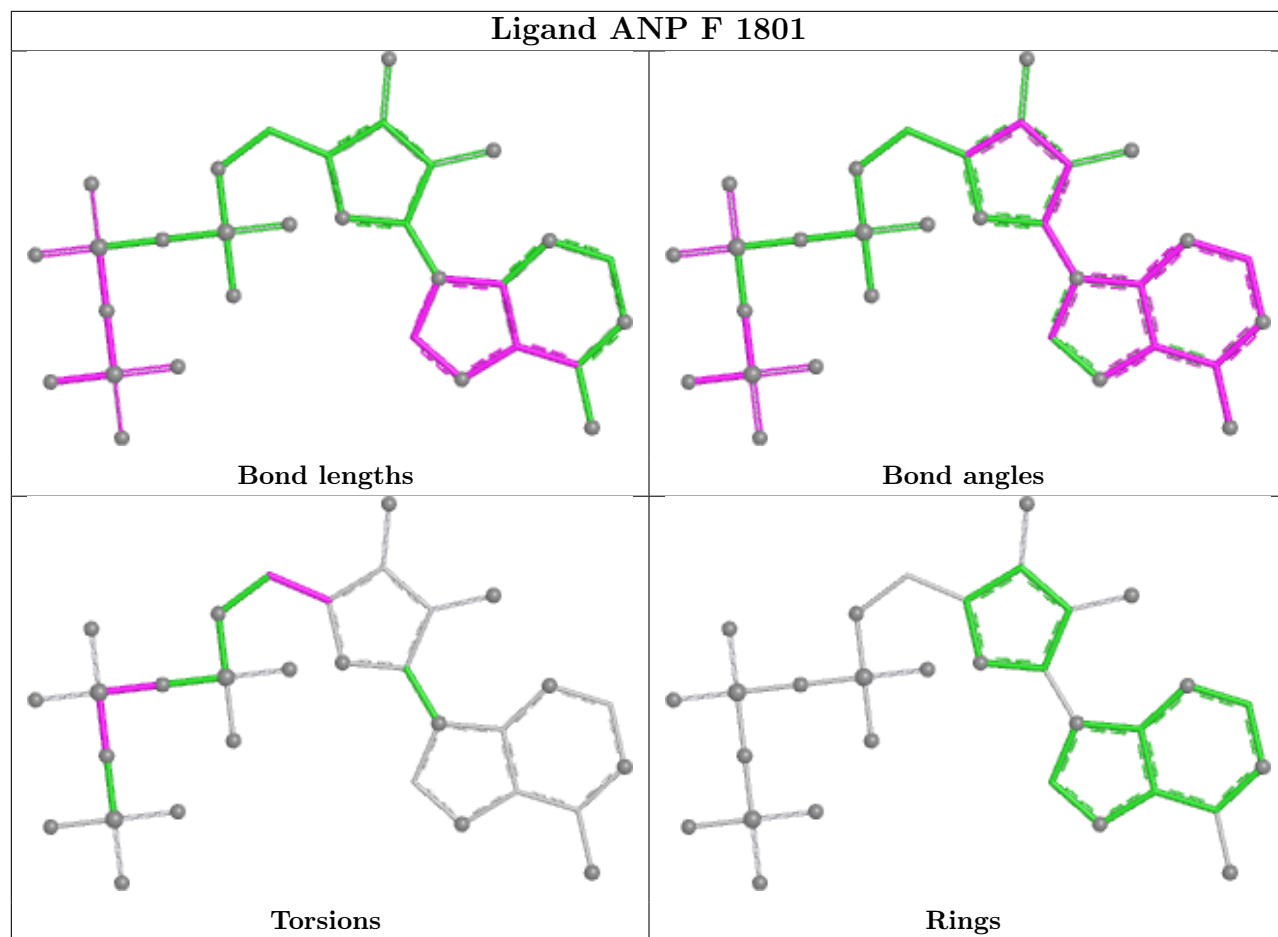
There are no ring outliers.

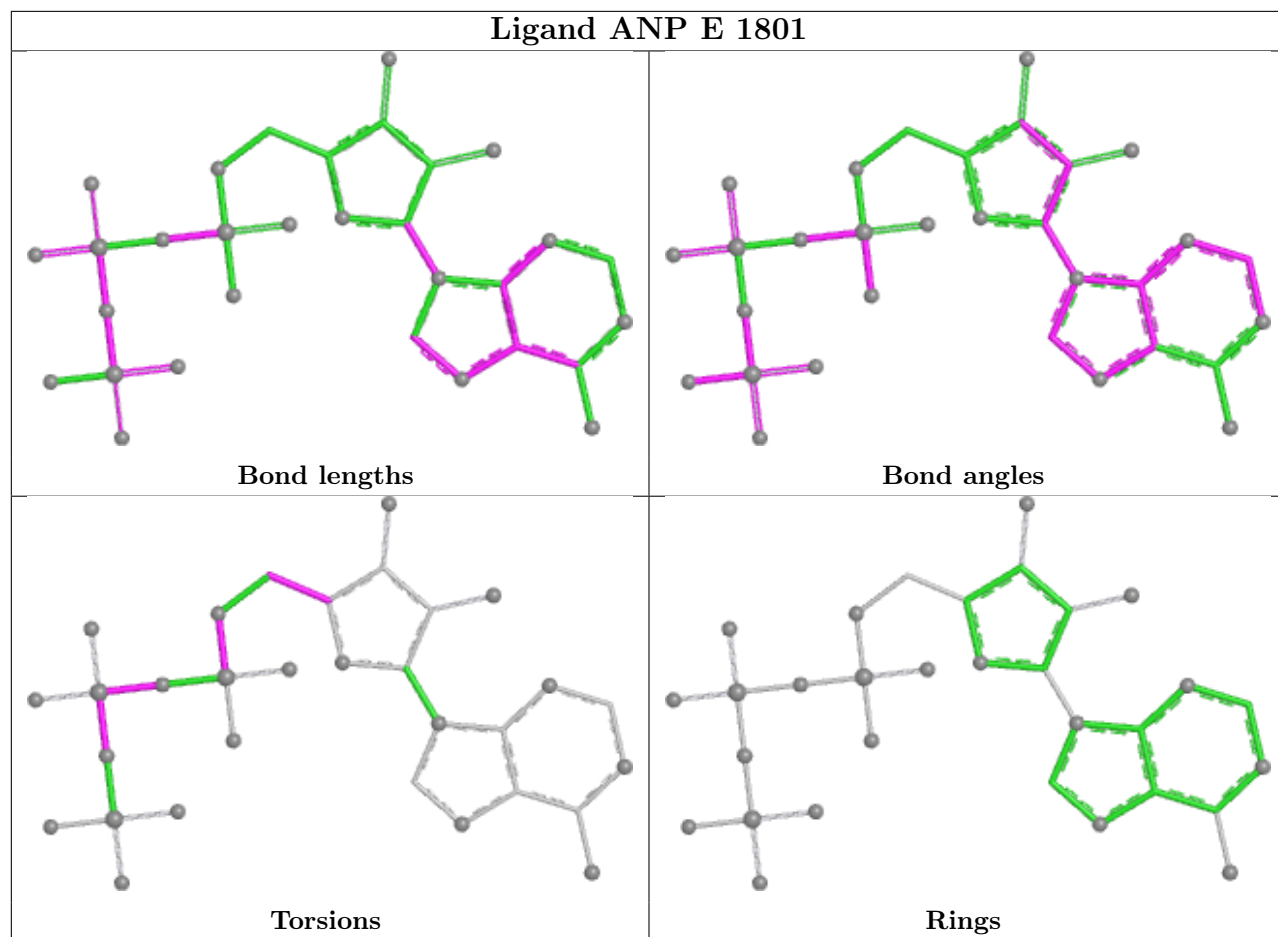
6 monomers are involved in 25 short contacts:

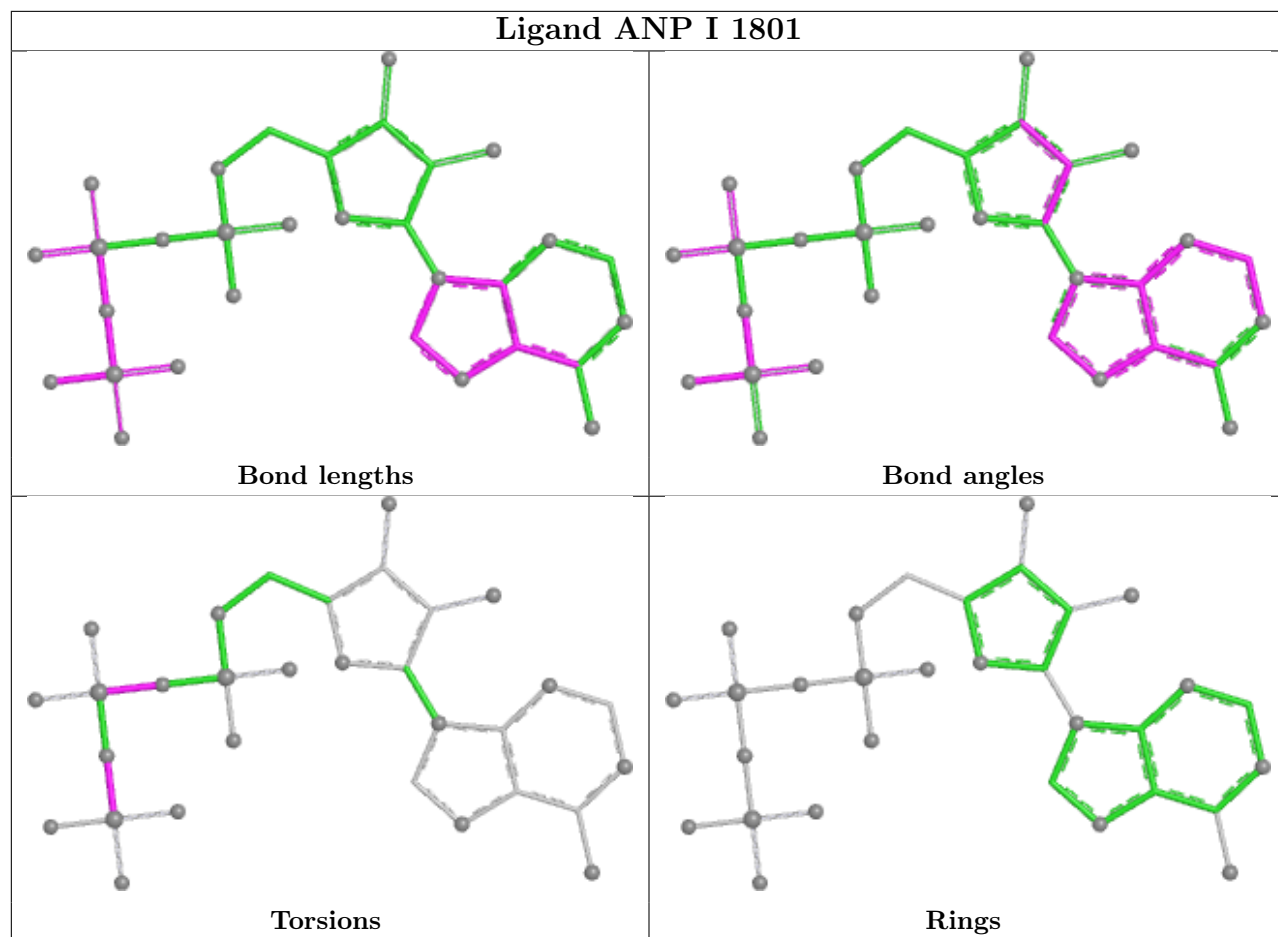
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1801	ANP	5	0
3	F	1801	ANP	4	0
3	E	1801	ANP	2	0
3	I	1801	ANP	8	0
3	B	1801	ANP	4	0
3	J	1801	ANP	2	0

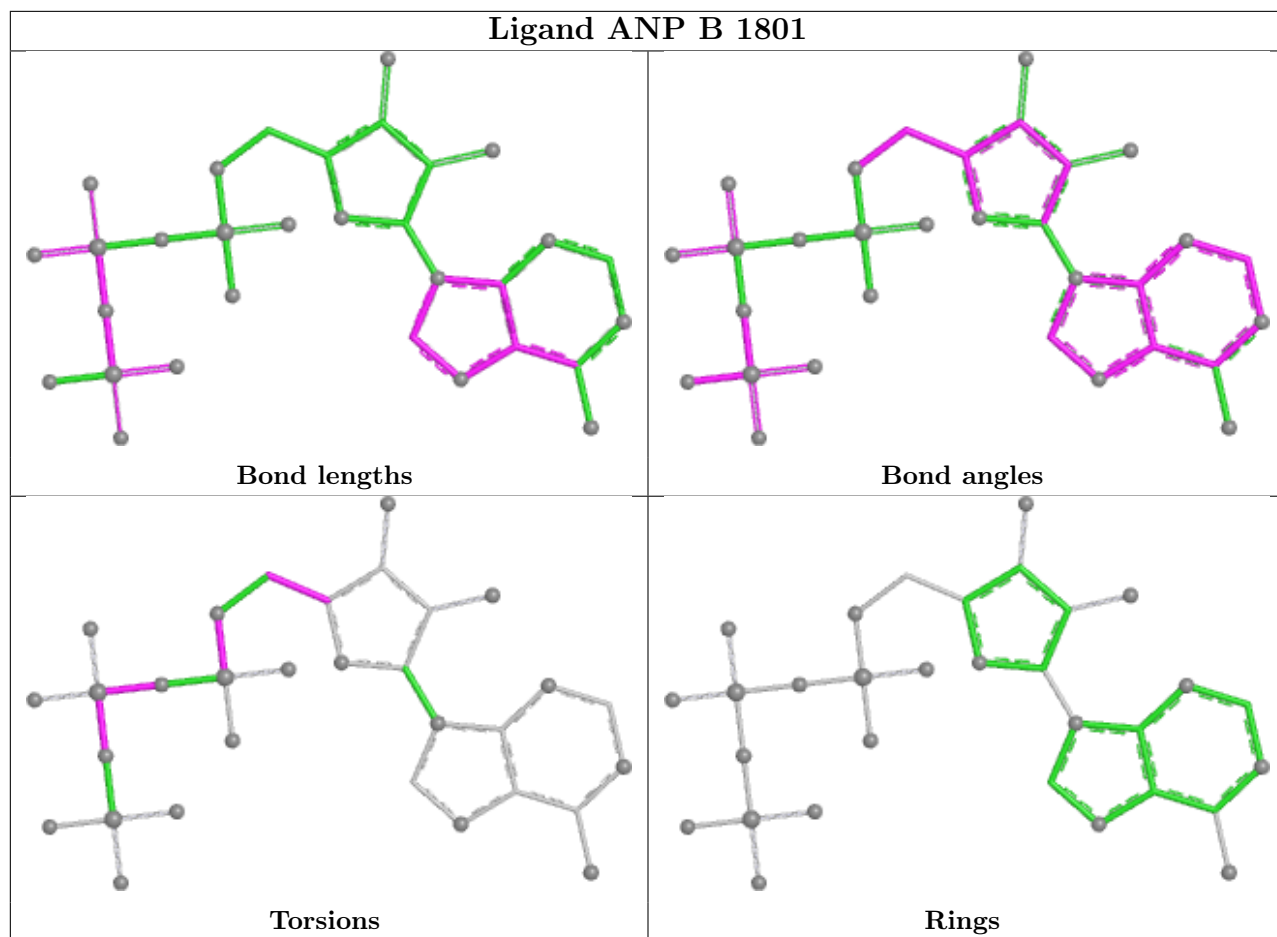
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

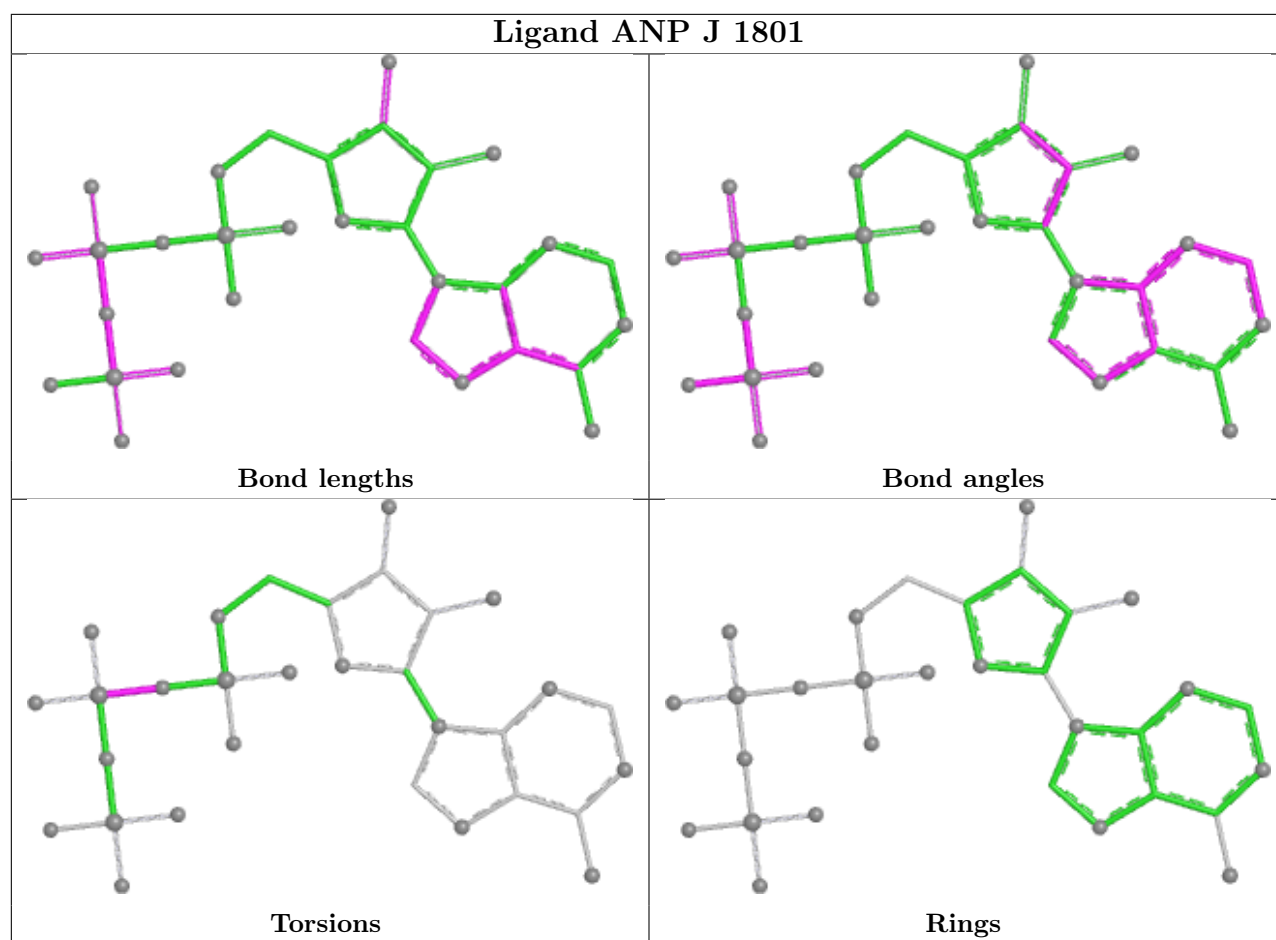












5.7 Other polymers [i](#)

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 [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	663/800 (82%)	-0.73	3 (0%) 87 78	120, 187, 361, 469	0
1	B	663/800 (82%)	-0.79	1 (0%) 91 84	125, 203, 272, 321	0
1	E	663/800 (82%)	-0.71	5 (0%) 82 72	170, 262, 510, 665	0
1	F	663/800 (82%)	-0.72	5 (0%) 82 72	127, 197, 351, 463	0
1	I	663/800 (82%)	-0.77	3 (0%) 87 78	174, 224, 402, 487	0
1	J	663/800 (82%)	-0.69	4 (0%) 85 76	172, 231, 378, 460	0
2	C	285/369 (77%)	-0.80	0 100 100	178, 213, 254, 293	0
2	D	285/369 (77%)	-0.71	0 100 100	170, 201, 273, 306	0
2	G	285/369 (77%)	-0.78	0 100 100	204, 224, 251, 265	0
2	H	285/369 (77%)	-0.86	0 100 100	154, 218, 301, 389	0
2	K	285/369 (77%)	-0.75	2 (0%) 84 74	185, 220, 264, 283	0
2	L	285/369 (77%)	-0.86	1 (0%) 88 79	210, 231, 253, 269	0
All	All	5688/7014 (81%)	-0.75	24 (0%) 88 79	120, 220, 361, 665	0

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	628	ALA	3.6
1	F	240	LEU	3.5
1	F	244	ALA	3.2
1	E	631	ALA	3.2
1	B	563	TYR	3.0

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](#)

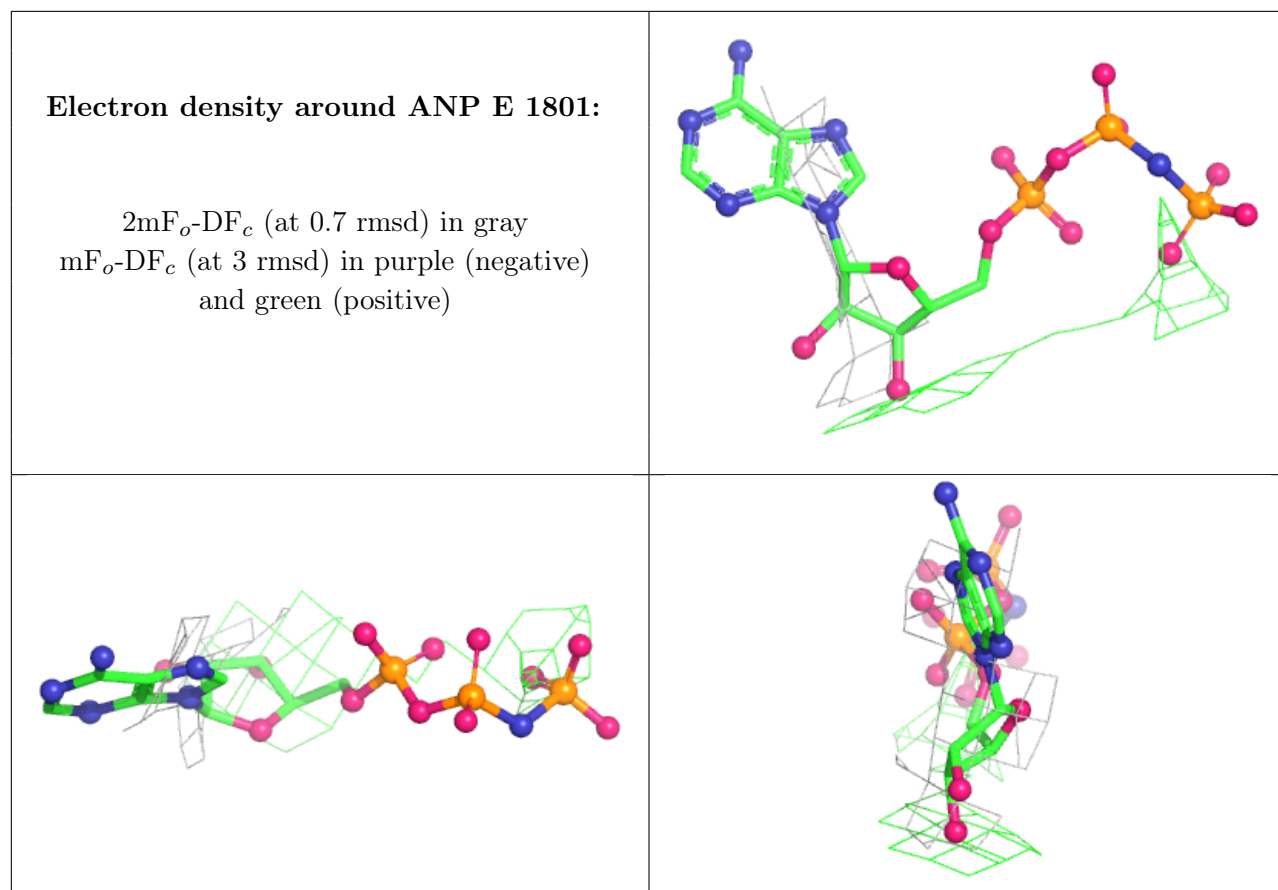
There are no oligosaccharides in this entry.

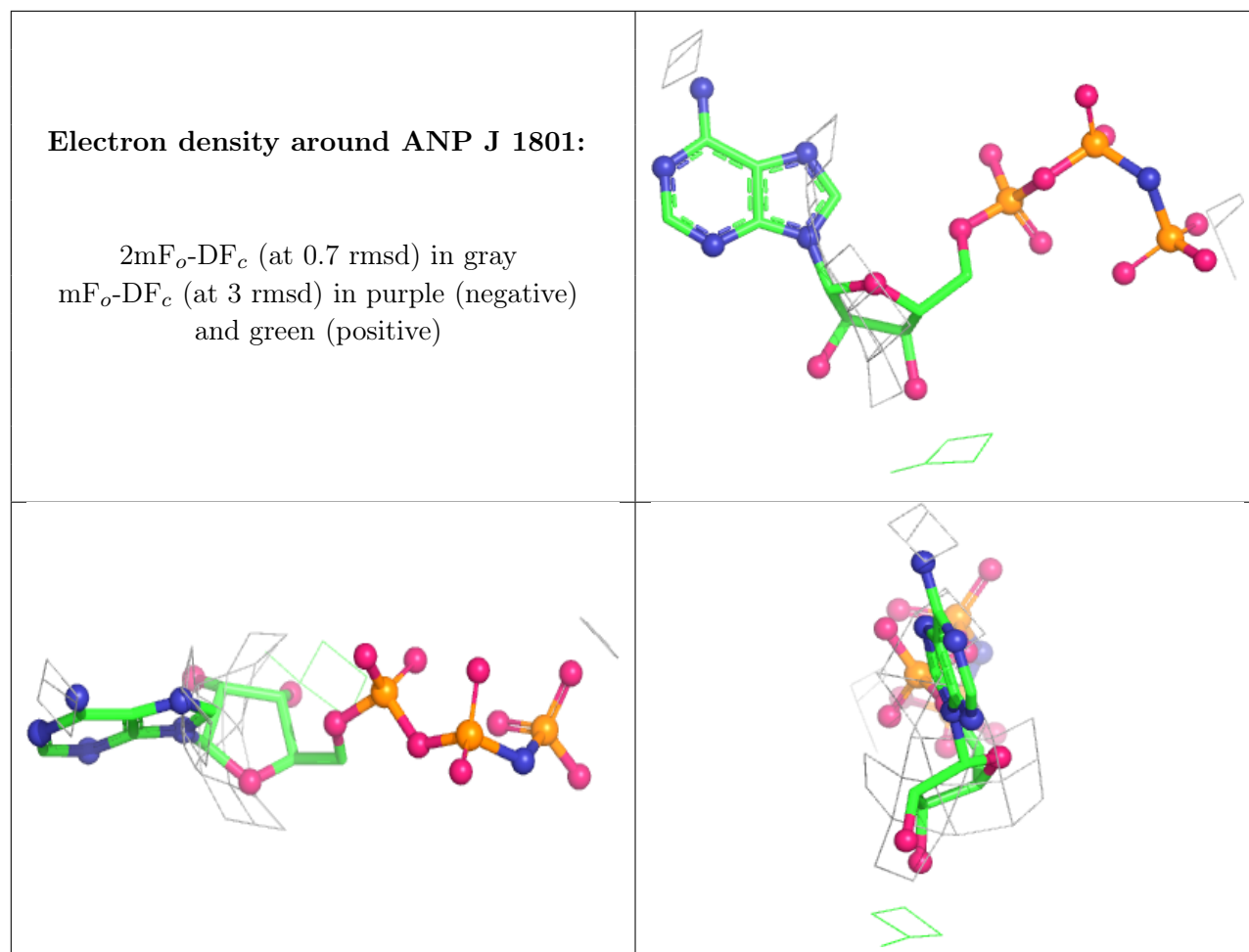
6.4 Ligands [i](#)

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	E	1801	31/31	0.69	0.11	204,216,227,232	0
3	ANP	J	1801	31/31	0.84	0.07	193,199,212,213	0
3	ANP	A	1801	31/31	0.87	0.09	156,164,170,171	0
3	ANP	I	1801	31/31	0.92	0.09	177,180,186,187	0
3	ANP	B	1801	31/31	0.92	0.07	165,174,179,181	0
3	ANP	F	1801	31/31	0.95	0.07	154,162,169,174	0

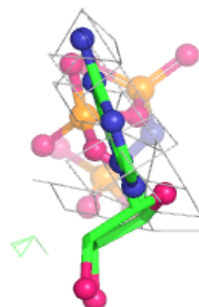
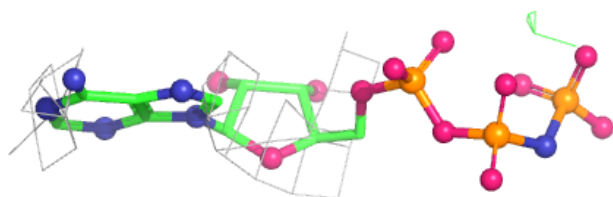
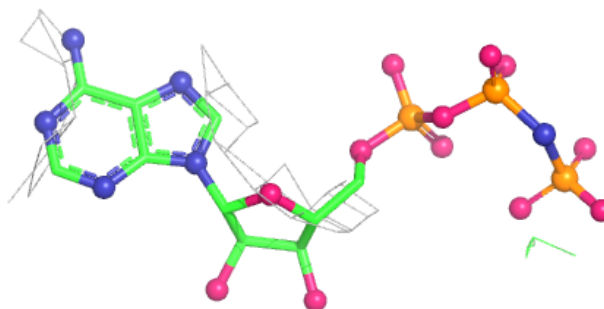
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



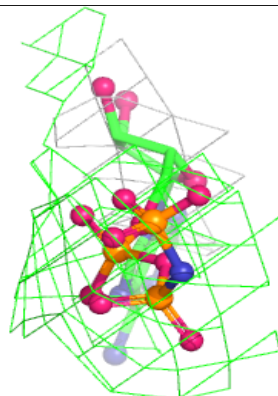
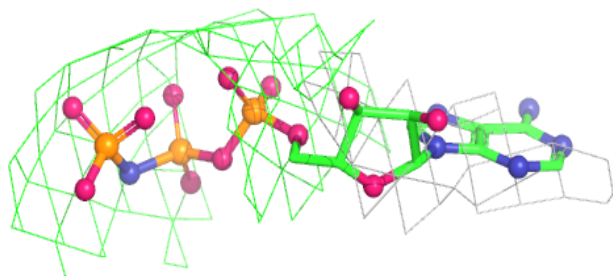
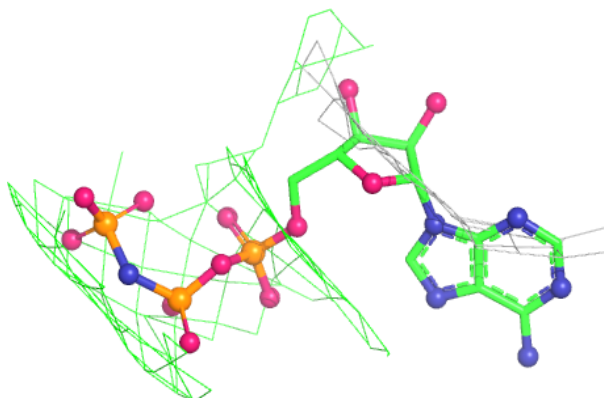


Electron density around ANP A 1801:

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

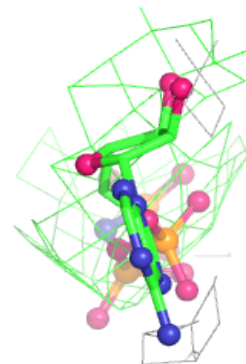
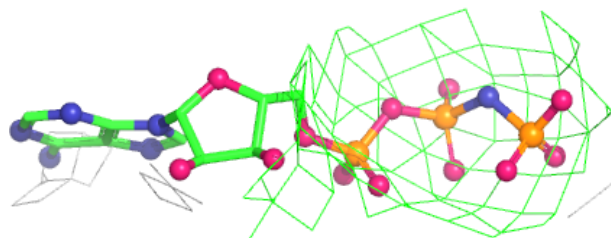
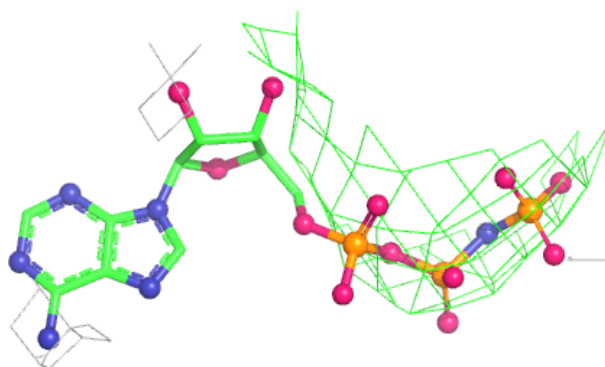
**Electron density around ANP I 1801:**

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

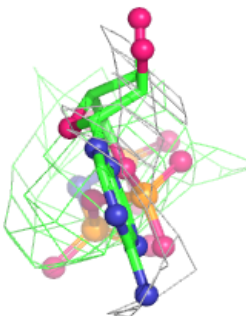
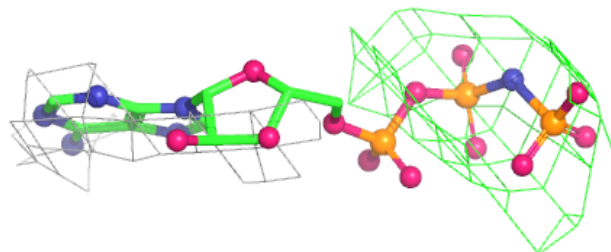
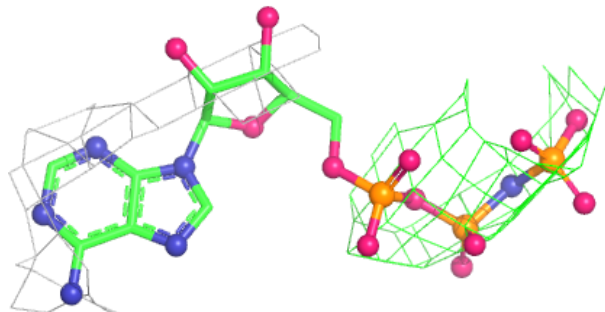


Electron density around ANP B 1801:

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

**Electron density around ANP F 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.