



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:52 AM UTC

PDB ID : 5AKC / pdb_00005akc
Title : MutS in complex with the N-terminal domain of MutL - crystal form 2
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 : 6.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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

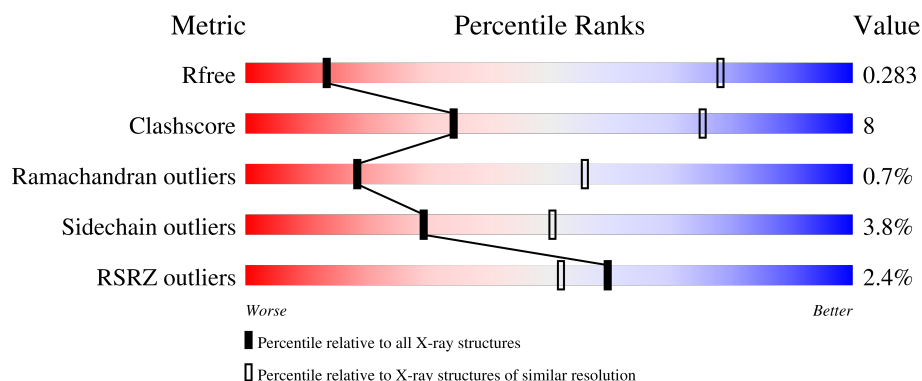
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.60 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	1162 (9.00-4.00)
Clashscore	190562	1000 (9.00-4.04)
Ramachandran outliers	187476	1050 (9.00-4.00)
Sidechain outliers	187428	1014 (9.00-4.00)
RSRZ outliers	180081	1155 (9.00-4.00)

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	 2% 73% 9% 17%
1	B	800	 2% 72% 10% 17%
1	E	800	 2% 72% 10% 17%
1	F	800	 2% 71% 11% 17%

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Mol	Chain	Length	Quality of chain
1	I	800	
1	J	800	
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	-

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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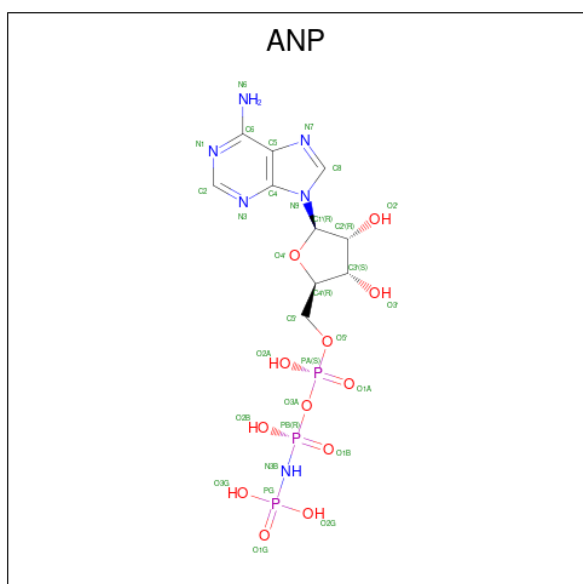
Chain	Residue	Modelled	Actual	Comment	Reference
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H	-8	SER	-	expression tag	UNP P23367
H	-7	GLY	-	expression tag	UNP P23367
H	-6	LEU	-	expression tag	UNP P23367
H	-5	VAL	-	expression tag	UNP P23367
H	-4	PRO	-	expression tag	UNP P23367
H	-3	ARG	-	expression 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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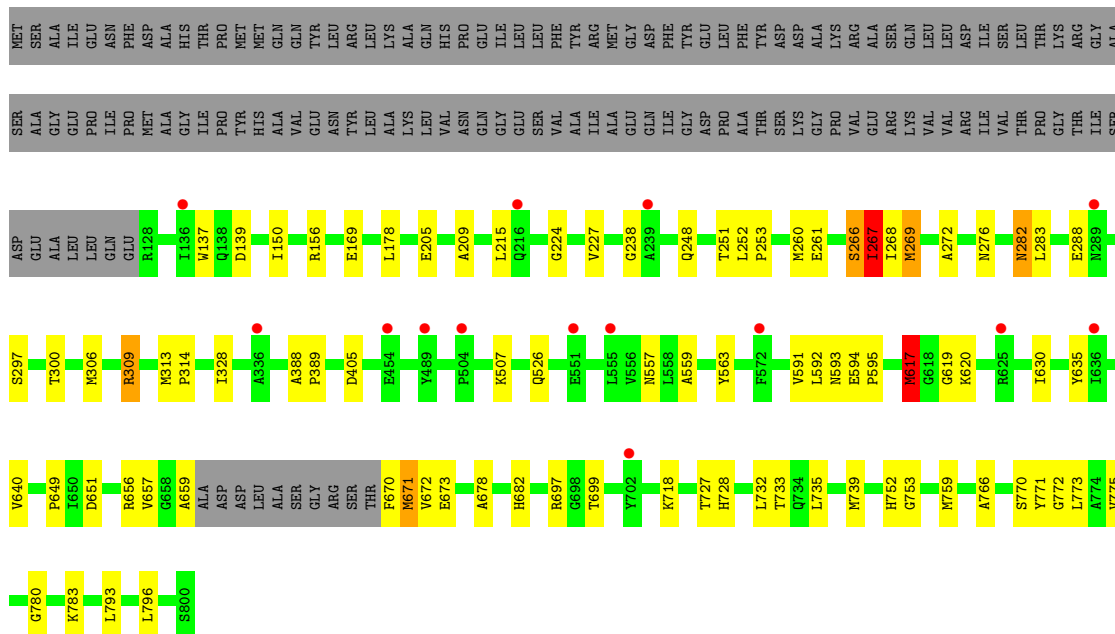
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L	-15	HIS	-	expression tag	UNP P23367
L	-14	HIS	-	expression tag	UNP P23367
L	-13	HIS	-	expression tag	UNP P23367
L	-12	HIS	-	expression tag	UNP P23367
L	-11	HIS	-	expression tag	UNP P23367
L	-10	HIS	-	expression tag	UNP P23367
L	-9	SER	-	expression 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).

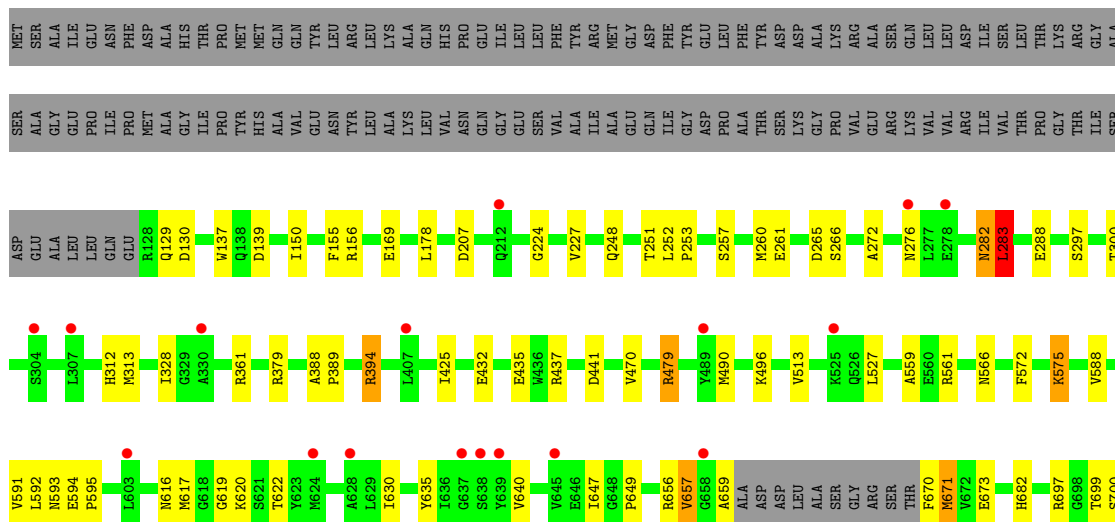


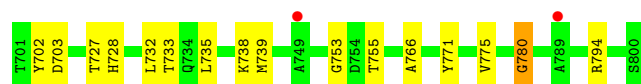
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	E	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	F	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	I	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	J	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 1: DNA MISMATCH REPAIR PROTEIN MUTS

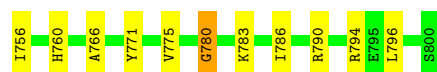
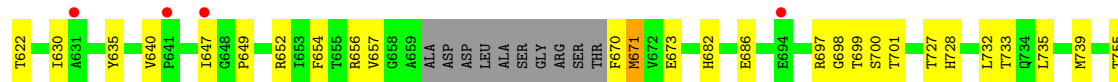
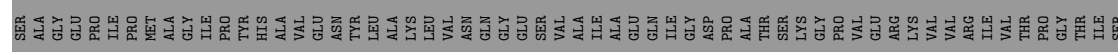
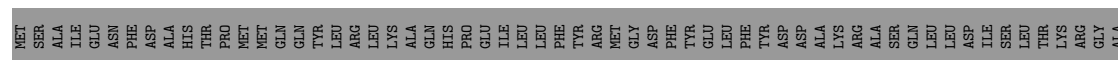


- Molecule 1: DNA MISMATCH REPAIR PROTEIN MUTS

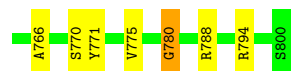
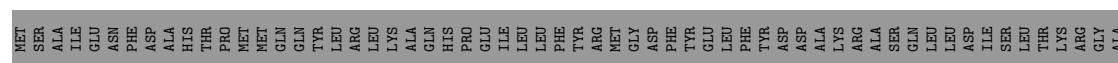




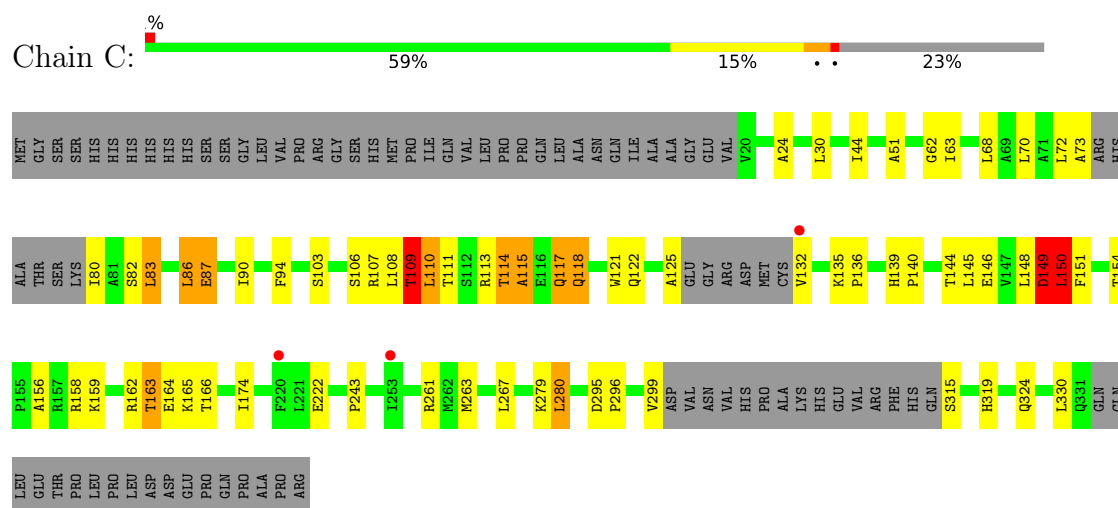
• Molecule 1: DNA MISMATCH REPAIR PROTEIN MUTS



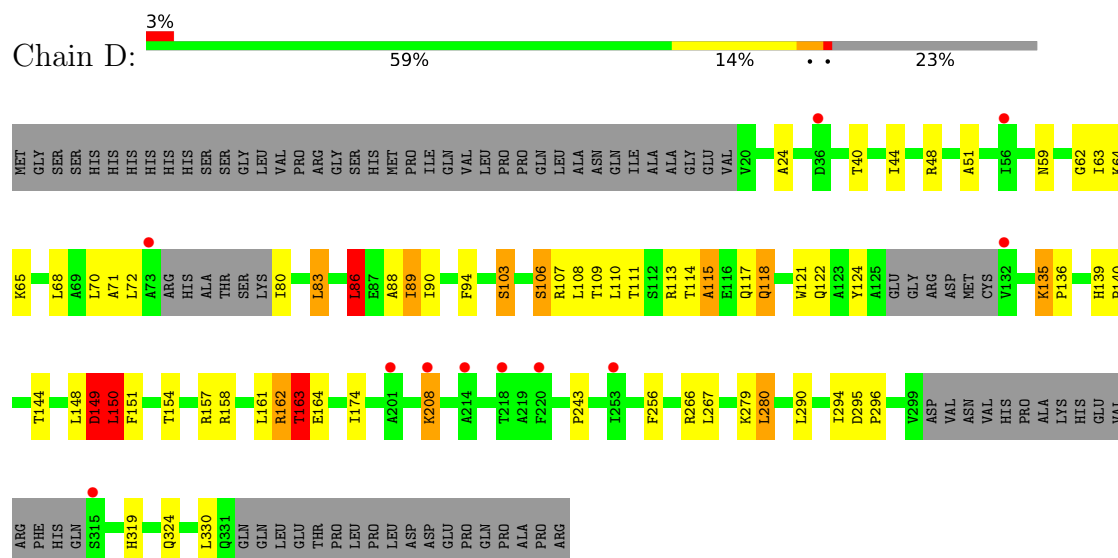
• Molecule 1: DNA MISMATCH REPAIR PROTEIN MUTS



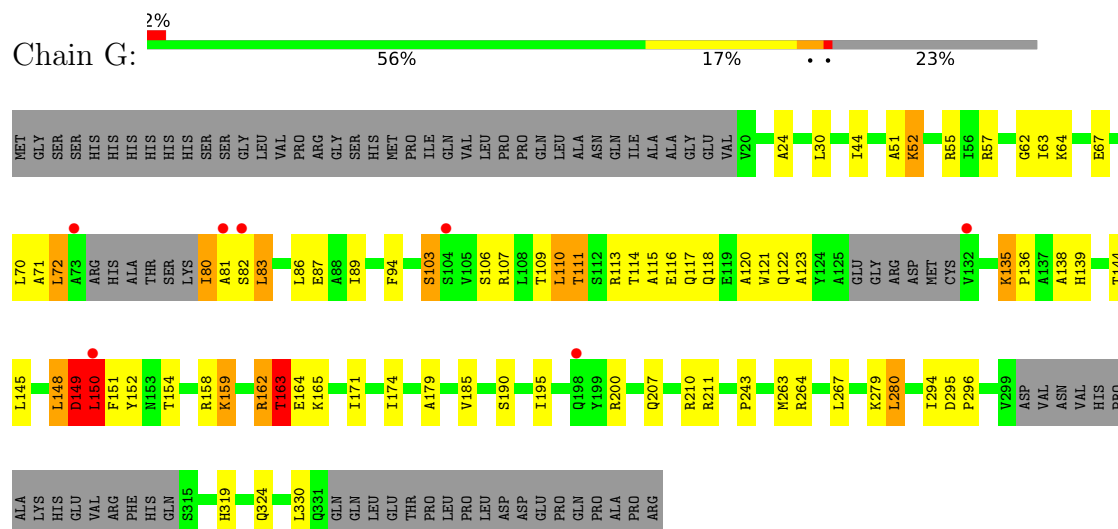
• Molecule 2: DNA MISMATCH REPAIR PROTEIN MUTL



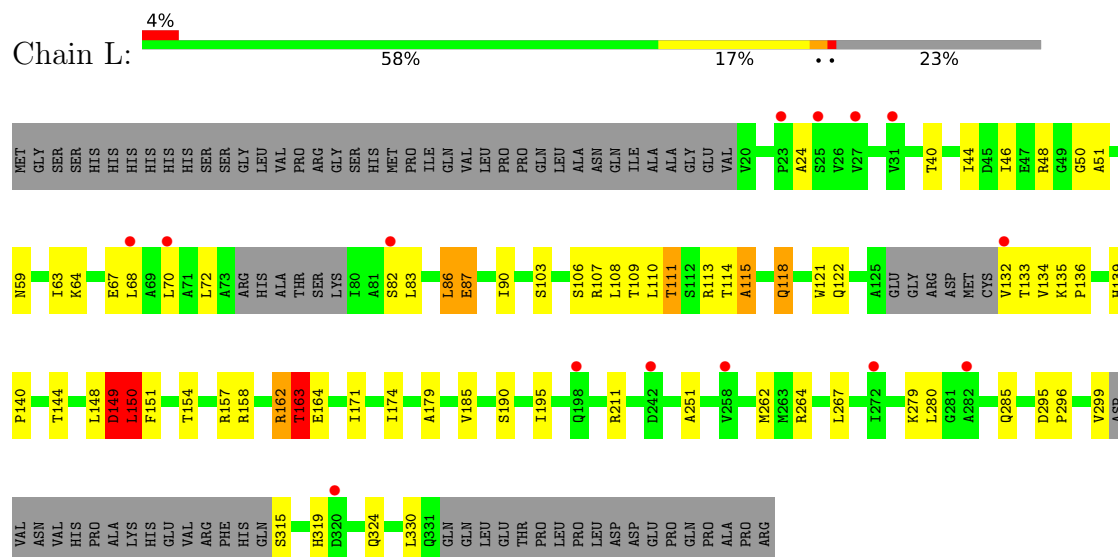
- Molecule 2: DNA MISMATCH REPAIR PROTEIN MUTL



- Molecule 2: DNA MISMATCH REPAIR PROTEIN MUTL



- Molecule 2: DNA MISMATCH REPAIR PROTEIN MUTL



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	380.63Å 126.46Å 243.35Å 90.00° 91.41° 90.00°	Depositor
Resolution (Å)	243.28 – 6.60 243.28 – 6.60	Depositor EDS
% Data completeness (in resolution range)	96.0 (243.28-6.60) 96.0 (243.28-6.60)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 6.68Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.259 , 0.291 0.261 , 0.283	Depositor DCC
R_{free} test set	1089 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	170.9	Xtriage
Anisotropy	0.989	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 342.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.095 for -h,-k,l	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	45054	wwPDB-VP
Average B, all atoms (Å ²)	253.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% 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	0.80	0/5311	0.97	7/7186 (0.1%)
1	B	0.80	4/5311 (0.1%)	0.99	9/7186 (0.1%)
1	E	0.83	2/5311 (0.0%)	0.98	4/7186 (0.1%)
1	F	0.83	2/5311 (0.0%)	0.99	4/7186 (0.1%)
1	I	0.76	2/5311 (0.0%)	0.95	4/7186 (0.1%)
1	J	0.76	0/5311	0.96	3/7186 (0.0%)
2	C	0.86	0/2288	1.06	9/3096 (0.3%)
2	D	0.97	1/2288 (0.0%)	1.09	7/3096 (0.2%)
2	G	0.85	1/2288 (0.0%)	1.05	7/3096 (0.2%)
2	H	0.94	2/2288 (0.1%)	1.09	11/3096 (0.4%)
2	K	0.87	0/2288	1.06	6/3096 (0.2%)
2	L	0.84	2/2288 (0.1%)	1.02	3/3096 (0.1%)
All	All	0.83	16/45594 (0.0%)	1.00	74/61692 (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	A	0	1
1	B	0	1
1	I	0	2
2	C	0	1
2	H	0	1
2	K	0	2
2	L	0	1
All	All	0	9

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	671	MET	CG-SD	13.90	2.15	1.80
2	D	208	LYS	CE-NZ	12.12	1.85	1.49
1	I	671	MET	SD-CE	-10.43	1.53	1.79
1	E	718	LYS	CD-CE	6.57	1.72	1.52
2	H	210	ARG	CD-NE	6.48	1.55	1.46
1	B	778	LEU	CB-CG	6.27	1.66	1.53
2	H	210	ARG	NE-CZ	6.01	1.39	1.33
1	E	671	MET	C-O	5.94	1.31	1.24
1	B	487	ILE	N-CA	-5.48	1.39	1.46
1	B	718	LYS	CA-C	5.43	1.58	1.53
1	I	671	MET	CG-SD	5.31	1.94	1.80
2	L	133	THR	CA-C	5.29	1.58	1.52
2	L	134	VAL	N-CA	5.12	1.52	1.46
1	B	576	PRO	C-O	-5.10	1.17	1.23
2	G	72	LEU	CA-C	5.04	1.58	1.52
1	F	588	VAL	C-O	-5.01	1.18	1.24

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	294	ILE	CA-C-N	9.58	137.09	121.57
2	H	294	ILE	C-N-CA	9.58	137.09	121.57
2	D	86	LEU	N-CA-C	-9.03	101.52	111.36
1	F	575	LYS	CB-CG-CD	8.65	131.19	111.30
2	C	162	ARG	N-CA-C	8.17	123.79	112.93
2	L	87	GLU	N-CA-C	8.16	122.14	110.14
2	K	87	GLU	N-CA-C	8.15	122.12	110.14
1	B	486	PRO	N-CA-C	-8.10	98.48	111.19
2	C	87	GLU	N-CA-C	7.93	121.80	110.14
1	F	283	LEU	CB-CG-CD2	-7.77	87.39	110.70
1	B	575	LYS	CB-CG-CD	7.50	128.54	111.30
1	I	130	ASP	N-CA-C	7.22	121.61	110.20
1	B	718	LYS	CB-CG-CD	6.93	127.24	111.30
1	E	783	LYS	CA-CB-CG	6.77	127.64	114.10
2	K	135	LYS	N-CA-C	6.74	114.07	108.07
1	B	283	LEU	CB-CG-CD2	-6.62	90.85	110.70
1	I	671	MET	CG-SD-CE	6.58	115.37	100.90
2	G	294	ILE	CA-C-N	6.49	131.41	121.03
2	G	294	ILE	C-N-CA	6.49	131.41	121.03
2	K	114	THR	N-CA-C	6.45	121.33	112.04
1	I	756	ILE	N-CA-C	6.42	117.36	108.12
1	B	591	VAL	CB-CA-C	-6.39	103.52	112.14
2	C	135	LYS	N-CA-C	6.29	113.67	108.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	294	ILE	CA-C-N	6.23	131.00	121.03
2	D	294	ILE	C-N-CA	6.23	131.00	121.03
2	H	210	ARG	CD-NE-CZ	6.19	133.07	124.40
2	H	84	ASP	N-CA-C	-6.18	104.63	111.36
2	C	94	PHE	N-CA-C	-6.15	105.78	113.28
1	F	129	GLN	CB-CG-CD	6.14	123.04	112.60
1	F	130	ASP	N-CA-C	6.13	119.14	110.50
1	E	507	LYS	CG-CD-CE	6.10	125.33	111.30
2	G	94	PHE	N-CA-C	-6.06	105.89	113.28
1	B	671	MET	CA-CB-CG	6.02	126.14	114.10
1	B	671	MET	CG-SD-CE	6.02	114.13	100.90
1	J	283	LEU	CB-CG-CD2	-6.00	92.70	110.70
1	J	671	MET	CB-CG-SD	5.96	130.58	112.70
2	G	111	THR	CB-CA-C	-5.93	99.31	110.16
2	G	135	LYS	N-CA-C	5.92	113.34	108.07
1	E	267	ILE	N-CA-C	5.88	121.58	109.34
1	A	756	ILE	N-CA-C	5.88	117.22	108.46
1	A	794	ARG	CB-CG-CD	5.87	124.81	111.30
1	B	487	ILE	CB-CA-C	5.86	120.90	111.29
2	D	94	PHE	N-CA-C	-5.79	106.22	113.28
2	G	110	LEU	CB-CA-C	-5.75	100.13	110.36
2	D	103	SER	N-CA-C	5.73	118.46	111.82
2	H	86	LEU	N-CA-C	5.66	120.21	112.68
2	C	110	LEU	CA-CB-CG	-5.65	96.51	116.30
2	K	263	MET	N-CA-C	-5.54	101.56	110.14
2	C	103	SER	N-CA-C	5.51	118.21	111.82
1	B	517	LYS	CB-CG-CD	-5.50	98.65	111.30
1	E	617	MET	CB-CG-SD	5.50	129.21	112.70
1	I	297	SER	N-CA-C	-5.50	104.12	111.87
2	G	103	SER	N-CA-C	5.47	118.17	111.82
1	A	718	LYS	CG-CD-CE	5.47	123.88	111.30
2	C	109	THR	N-CA-CB	-5.46	101.86	110.77
2	K	103	SER	N-CA-C	5.45	118.14	111.82
2	L	133	THR	N-CA-C	5.41	118.22	108.48
2	H	94	PHE	N-CA-C	-5.30	106.66	113.23
2	L	103	SER	N-CA-C	5.28	117.94	111.82
1	J	141	LYS	CD-CE-NZ	5.28	128.78	111.90
2	H	295	ASP	N-CA-CB	-5.20	103.12	110.04
1	A	129	GLN	N-CA-C	5.19	118.03	109.72
2	C	110	LEU	N-CA-C	5.18	117.87	109.06
1	A	297	SER	N-CA-C	-5.17	104.59	111.87
2	K	106	SER	N-CA-C	5.14	116.11	108.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	135	LYS	N-CA-C	5.13	112.64	108.07
2	H	251	ALA	N-CA-C	5.13	119.17	113.01
2	H	263	MET	N-CA-C	-5.10	102.64	110.14
2	H	103	SER	N-CA-C	5.09	117.72	111.82
2	H	106	SER	N-CA-C	5.07	116.01	108.60
1	A	676	GLU	N-CA-C	5.07	119.46	113.28
2	D	106	SER	N-CA-C	5.03	115.94	108.60
2	C	222	GLU	N-CA-C	5.01	116.74	111.28
1	A	313	MET	CA-CB-CG	5.00	124.11	114.10

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	752	HIS	Peptide
1	B	487	ILE	Peptide
2	C	86	LEU	Peptide
2	H	81	ALA	Peptide
1	I	129	GLN	Peptide
1	I	755	THR	Peptide
2	K	113	ARG	Peptide
2	K	86	LEU	Peptide
2	L	86	LEU	Peptide

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	54	0
1	B	5226	0	5283	60	0
1	E	5226	0	5283	80	0
1	F	5226	0	5283	74	0
1	I	5226	0	5283	86	0
1	J	5226	0	5283	88	0
2	C	2252	0	2272	74	0
2	D	2252	0	2272	57	0
2	G	2252	0	2271	62	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	2252	0	2272	60	0
2	K	2252	0	2272	69	0
2	L	2252	0	2272	52	0
3	A	31	0	13	2	0
3	B	31	0	13	2	0
3	E	31	0	13	9	0
3	F	31	0	13	4	0
3	I	31	0	13	5	0
3	J	31	0	13	5	0
All	All	45054	0	45407	687	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 8.

All (687) 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:D:208:LYS:NZ	2:D:208:LYS:CE	1.85	1.38
1:F:671:MET:SD	1:F:671:MET:CG	2.15	1.34
2:C:110:LEU:CD2	2:C:145:LEU:HA	1.64	1.26
3:I:1801:ANP:O1G	1:J:670:PHE:N	1.79	1.15
2:C:110:LEU:HD21	2:C:145:LEU:CA	1.76	1.14
2:G:83:LEU:HA	2:G:87:GLU:HA	1.18	1.13
2:H:97:GLU:HA	2:K:266:ARG:NH1	1.68	1.07
2:C:110:LEU:HD22	2:C:144:THR:O	1.56	1.05
2:C:62:GLY:C	2:C:114:THR:HG23	1.80	1.05
2:D:88:ALA:O	2:D:89:ILE:HG13	1.60	1.00
2:C:299:VAL:HG12	2:C:315:SER:OG	1.60	1.00
1:E:697:ARG:NH2	1:F:697:ARG:HB2	1.78	0.96
2:C:156:ALA:HA	2:C:159:LYS:HE3	1.48	0.96
1:E:267:ILE:HD11	1:E:314:PRO:HG2	1.49	0.95
1:E:670:PHE:N	3:F:1801:ANP:O1G	2.00	0.95
2:H:97:GLU:HA	2:K:266:ARG:HH12	1.29	0.95
2:H:70:LEU:HD22	2:H:86:LEU:HD21	1.48	0.94
2:H:266:ARG:NH2	2:K:90:ILE:HG21	1.84	0.93
1:A:670:PHE:N	3:B:1801:ANP:O1G	2.03	0.90
1:E:563:TYR:O	2:G:200:ARG:NH2	2.04	0.90
2:G:83:LEU:HA	2:G:87:GLU:CA	2.02	0.90
1:I:697:ARG:HB2	1:J:697:ARG:NH2	1.86	0.89
2:G:83:LEU:CA	2:G:87:GLU:HA	2.03	0.89
2:H:266:ARG:NH2	2:K:90:ILE:CG2	2.36	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:ALA:O	1:A:171:GLN:OE1	1.92	0.88
1:F:394:ARG:HG3	1:F:394:ARG:HH11	1.39	0.88
1:I:697:ARG:HH22	1:J:697:ARG:HB2	1.40	0.87
1:J:656:ARG:HG2	1:J:680:ILE:HD11	1.55	0.87
2:L:299:VAL:HG12	2:L:315:SER:OG	1.74	0.86
2:C:110:LEU:O	2:C:122:GLN:HA	1.75	0.86
2:H:97:GLU:HG2	2:K:266:ARG:HG3	1.58	0.85
2:K:110:LEU:O	2:K:122:GLN:HA	1.76	0.85
1:B:656:ARG:HG2	1:B:680:ILE:HD11	1.59	0.85
2:C:110:LEU:HD21	2:C:145:LEU:HA	0.86	0.83
1:I:617:MET:SD	1:J:671:MET:HA	2.17	0.83
2:D:110:LEU:O	2:D:122:GLN:HA	1.79	0.83
2:L:110:LEU:O	2:L:122:GLN:HA	1.78	0.83
1:I:780:GLY:O	1:J:678:ALA:HB1	1.79	0.82
1:A:752:HIS:CG	2:C:136:PRO:HG2	2.17	0.80
2:C:110:LEU:CD2	2:C:144:THR:O	2.29	0.80
2:H:70:LEU:HD22	2:H:86:LEU:CD2	2.11	0.79
1:E:267:ILE:HD11	1:E:314:PRO:CG	2.13	0.79
1:J:656:ARG:HG2	1:J:680:ILE:CD1	2.14	0.78
2:H:90:ILE:CG2	2:K:266:ARG:HH21	1.96	0.78
2:C:110:LEU:HD11	2:C:145:LEU:HD23	1.67	0.77
1:I:656:ARG:HH21	1:I:673:GLU:HA	1.48	0.77
2:D:117:GLN:OE1	1:E:405:ASP:OD1	2.02	0.77
2:C:299:VAL:CG1	2:C:315:SER:OG	2.32	0.77
1:F:620:LYS:NZ	3:F:1801:ANP:O1B	2.17	0.77
2:H:90:ILE:HG21	2:K:266:ARG:HH21	1.50	0.76
2:D:64:LYS:HD2	2:D:114:THR:HG21	1.68	0.76
2:L:299:VAL:CG1	2:L:315:SER:OG	2.34	0.76
1:I:656:ARG:NH2	1:I:673:GLU:HA	2.00	0.75
1:B:656:ARG:HG2	1:B:680:ILE:CD1	2.16	0.75
2:D:157:ARG:O	2:D:161:LEU:CD1	2.35	0.75
1:E:617:MET:HE3	3:E:1801:ANP:H4'	1.71	0.73
1:B:656:ARG:NE	1:B:676:GLU:HB3	2.04	0.73
1:A:656:ARG:HH21	1:A:673:GLU:HA	1.54	0.72
1:E:619:GLY:HA2	3:E:1801:ANP:H8	1.70	0.72
1:J:617:MET:HA	3:J:1801:ANP:H5'1	1.71	0.72
1:E:205:GLU:HG2	2:H:52:LYS:HZ3	1.54	0.72
1:E:617:MET:SD	1:F:671:MET:HB2	2.29	0.72
1:E:656:ARG:HH21	1:E:673:GLU:HA	1.53	0.72
2:H:64:LYS:HD2	2:H:114:THR:HG21	1.72	0.72
1:A:682:HIS:CE1	1:B:782:PRO:HD3	2.24	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:312:HIS:O	1:F:313:MET:HE2	1.90	0.71
1:I:796:LEU:HD13	1:J:702:TYR:HB3	1.73	0.71
1:I:697:ARG:NH2	1:J:697:ARG:HB2	2.05	0.71
1:E:267:ILE:CD1	1:E:314:PRO:HG2	2.20	0.71
1:A:656:ARG:NH2	1:A:673:GLU:HA	2.05	0.71
1:F:656:ARG:HH21	1:F:673:GLU:HA	1.56	0.70
1:F:432:GLU:O	1:F:435:GLU:HG2	1.92	0.70
1:I:697:ARG:HH22	1:J:697:ARG:CB	2.05	0.70
1:E:656:ARG:NH2	1:E:673:GLU:HA	2.06	0.70
1:F:394:ARG:HH11	1:F:394:ARG:CG	2.04	0.70
1:J:656:ARG:NE	1:J:676:GLU:HB3	2.06	0.70
2:H:266:ARG:HG3	2:K:97:GLU:HG2	1.75	0.69
1:F:656:ARG:NH2	1:F:673:GLU:HA	2.07	0.69
2:G:207:GLN:HG2	2:G:210:ARG:HG3	1.74	0.69
2:L:111:THR:HG23	2:L:122:GLN:HB2	1.75	0.69
2:C:299:VAL:C	2:C:315:SER:OG	2.35	0.69
2:L:107:ARG:HB3	2:L:148:LEU:HB2	1.73	0.69
1:E:620:LYS:NZ	3:E:1801:ANP:O1B	2.26	0.68
1:I:697:ARG:HB2	1:J:697:ARG:HH22	1.56	0.68
2:C:109:THR:O	2:C:110:LEU:HD23	1.92	0.68
2:C:62:GLY:CA	2:C:114:THR:HG23	2.23	0.67
1:B:479:ARG:NH1	1:B:499:GLU:OE1	2.27	0.67
2:K:162:ARG:O	2:K:163:THR:O	2.12	0.67
1:E:770:SER:HB3	1:F:700:SER:HB2	1.77	0.67
1:A:697:ARG:NH1	1:B:697:ARG:CZ	2.57	0.66
2:K:106:SER:HB3	2:K:150:LEU:HD22	1.77	0.66
2:H:90:ILE:CG2	2:K:266:ARG:NH2	2.58	0.66
2:H:106:SER:HB3	2:H:150:LEU:HD22	1.77	0.66
1:I:150:ILE:HG21	1:I:248:GLN:NE2	2.11	0.66
1:I:656:ARG:NH1	1:I:657:VAL:O	2.28	0.66
2:L:162:ARG:O	2:L:163:THR:O	2.14	0.66
1:A:699:THR:HA	1:B:728:HIS:ND1	2.11	0.66
1:B:630:ILE:HG23	1:B:640:VAL:HG11	1.78	0.66
2:G:162:ARG:O	2:G:163:THR:O	2.14	0.66
2:K:110:LEU:HD13	2:K:145:LEU:HG	1.78	0.66
2:C:163:THR:HB	2:C:166:THR:OG1	1.96	0.65
2:H:70:LEU:HD23	2:H:86:LEU:HD11	1.77	0.65
1:E:526:GLN:HE21	1:F:470:VAL:HG21	1.60	0.65
2:D:106:SER:HB3	2:D:150:LEU:HD22	1.79	0.65
2:H:162:ARG:O	2:H:163:THR:O	2.13	0.65
2:H:266:ARG:HH22	2:K:90:ILE:HG22	1.59	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:109:THR:O	2:C:110:LEU:CD2	2.44	0.65
1:I:780:GLY:O	1:J:678:ALA:CB	2.45	0.65
1:F:656:ARG:NH1	1:F:657:VAL:O	2.30	0.65
2:D:107:ARG:NH2	2:D:124:TYR:OH	2.30	0.65
1:I:699:THR:HA	1:J:728:HIS:ND1	2.12	0.65
1:A:656:ARG:NH1	1:A:657:VAL:O	2.30	0.65
1:E:630:ILE:HG23	1:E:640:VAL:HG11	1.78	0.65
1:F:630:ILE:HG23	1:F:640:VAL:HG11	1.80	0.64
2:D:162:ARG:O	2:D:163:THR:O	2.15	0.64
2:L:299:VAL:CB	2:L:315:SER:OG	2.45	0.64
1:J:630:ILE:HG23	1:J:640:VAL:HG11	1.78	0.64
1:A:615:PRO:HA	1:B:699:THR:HG21	1.80	0.64
2:D:88:ALA:O	2:D:89:ILE:CG1	2.41	0.64
2:D:256:PHE:CE2	2:D:290:LEU:HB2	2.33	0.64
2:G:64:LYS:HA	2:G:118:GLN:HE22	1.63	0.64
1:I:150:ILE:HD12	1:I:150:ILE:H	1.62	0.63
1:I:630:ILE:HG23	1:I:640:VAL:HG11	1.81	0.63
1:F:150:ILE:HD11	1:F:252:LEU:CD2	2.29	0.63
2:C:70:LEU:HB3	2:C:82:SER:HB2	1.78	0.63
2:H:266:ARG:NH2	2:K:90:ILE:HG22	2.13	0.63
2:G:106:SER:HB3	2:G:150:LEU:HD22	1.81	0.63
2:G:86:LEU:HB3	2:G:89:ILE:HD12	1.79	0.62
2:G:110:LEU:HD12	2:G:123:ALA:HB3	1.81	0.62
1:E:659:ALA:C	1:F:659:ALA:HB2	2.24	0.62
1:I:760:HIS:HB3	3:I:1801:ANP:N6	2.13	0.62
1:J:755:THR:HG21	2:L:135:LYS:NZ	2.15	0.62
1:I:671:MET:HA	1:J:617:MET:SD	2.39	0.62
2:L:106:SER:HB3	2:L:150:LEU:HD22	1.81	0.62
1:E:137:TRP:CH2	1:E:139:ASP:HB3	2.35	0.62
2:K:267:LEU:HD11	2:K:319:HIS:HB2	1.82	0.62
1:A:137:TRP:CH2	1:A:139:ASP:HB3	2.35	0.61
2:G:159:LYS:O	2:G:159:LYS:HG2	1.98	0.61
1:I:219:THR:HG22	1:J:780:GLY:HA2	1.81	0.61
1:A:630:ILE:HG23	1:A:640:VAL:HG11	1.81	0.61
1:I:137:TRP:CH2	1:I:139:ASP:HB3	2.35	0.61
1:J:727:THR:HG21	1:J:732:LEU:HD12	1.82	0.61
2:H:267:LEU:HD11	2:H:319:HIS:HB2	1.83	0.61
2:K:70:LEU:HB2	2:K:82:SER:HB2	1.82	0.61
1:B:137:TRP:CH2	1:B:139:ASP:HB3	2.35	0.61
1:E:617:MET:SD	1:F:671:MET:CG	2.89	0.61
1:E:770:SER:HB3	1:F:700:SER:CB	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:205:GLU:HG2	2:H:52:LYS:NZ	2.15	0.60
1:E:150:ILE:HD11	1:E:252:LEU:CD2	2.30	0.60
1:E:678:ALA:HB1	1:F:780:GLY:O	2.02	0.60
1:E:267:ILE:HA	1:E:651:ASP:O	2.01	0.60
1:I:616:ASN:ND2	1:J:670:PHE:CD2	2.70	0.60
2:C:106:SER:HB3	2:C:150:LEU:HD22	1.82	0.60
2:G:151:PHE:O	2:G:158:ARG:NH1	2.35	0.60
1:J:141:LYS:HD3	1:J:232:ARG:HH21	1.67	0.60
1:F:150:ILE:HG12	1:F:248:GLN:NE2	2.16	0.60
1:E:297:SER:OG	1:E:557:ASN:OD1	2.19	0.60
1:E:697:ARG:HH21	1:F:697:ARG:HB2	1.67	0.60
2:D:139:HIS:HE2	2:D:144:THR:HG1	1.50	0.59
2:C:151:PHE:O	2:C:158:ARG:NH1	2.35	0.59
2:C:299:VAL:CG1	2:C:315:SER:HG	2.13	0.59
1:J:137:TRP:CH2	1:J:139:ASP:HB3	2.37	0.59
2:K:110:LEU:HD12	2:K:144:THR:O	2.02	0.59
1:A:752:HIS:ND1	2:C:136:PRO:HG2	2.17	0.59
1:E:617:MET:SD	1:F:671:MET:CB	2.90	0.59
1:F:617:MET:SD	1:F:617:MET:N	2.76	0.59
1:I:697:ARG:HH22	1:J:697:ARG:CA	2.16	0.59
2:C:107:ARG:HB2	2:C:148:LEU:HB2	1.85	0.58
1:B:656:ARG:HE	1:B:676:GLU:HB3	1.67	0.58
2:G:24:ALA:HB1	2:G:174:ILE:HD12	1.84	0.58
3:A:1801:ANP:O1G	1:B:670:PHE:HB3	2.02	0.58
1:F:137:TRP:CH2	1:F:139:ASP:HB3	2.38	0.58
2:L:299:VAL:HB	2:L:315:SER:OG	2.04	0.58
2:D:157:ARG:O	2:D:161:LEU:HD13	2.02	0.58
1:F:727:THR:HG21	1:F:732:LEU:HD12	1.85	0.58
2:D:256:PHE:CD2	2:D:290:LEU:HB2	2.39	0.58
2:G:295:ASP:CG	2:G:296:PRO:HD2	2.29	0.58
2:L:24:ALA:HB1	2:L:174:ILE:HD12	1.85	0.58
2:D:83:LEU:CD1	2:D:90:ILE:HD12	2.33	0.58
2:C:299:VAL:HG12	2:C:315:SER:HG	1.69	0.58
1:F:593:ASN:O	2:H:55:ARG:NH2	2.37	0.57
2:D:295:ASP:CG	2:D:296:PRO:HD2	2.28	0.57
1:F:150:ILE:CD1	1:F:252:LEU:CD2	2.82	0.57
2:L:151:PHE:O	2:L:158:ARG:NH1	2.37	0.57
2:H:90:ILE:HG22	2:K:266:ARG:NH2	2.19	0.57
1:E:656:ARG:NH1	1:E:657:VAL:O	2.38	0.57
1:E:771:TYR:N	1:F:699:THR:OG1	2.35	0.57
2:H:295:ASP:CG	2:H:296:PRO:HD2	2.29	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:82:SER:O	2:K:87:GLU:HA	2.05	0.57
2:D:151:PHE:O	2:D:158:ARG:NH1	2.37	0.57
2:K:24:ALA:HB1	2:K:174:ILE:HD12	1.87	0.57
2:D:24:ALA:HB1	2:D:174:ILE:HD12	1.87	0.57
1:I:297:SER:OG	1:I:557:ASN:OD1	2.19	0.57
2:L:299:VAL:C	2:L:315:SER:OG	2.47	0.57
1:A:782:PRO:HD3	1:B:682:HIS:CE1	2.40	0.57
2:L:295:ASP:CG	2:L:296:PRO:HD2	2.30	0.57
2:L:82:SER:O	2:L:87:GLU:HA	2.05	0.57
1:J:656:ARG:HE	1:J:676:GLU:HB3	1.69	0.56
2:C:82:SER:O	2:C:87:GLU:HA	2.05	0.56
2:H:111:THR:HA	2:H:121:TRP:O	2.05	0.56
1:I:615:PRO:HA	1:J:699:THR:HG21	1.87	0.56
2:L:111:THR:HA	2:L:121:TRP:O	2.05	0.56
2:C:110:LEU:CD1	2:C:145:LEU:HD23	2.34	0.56
1:B:754:ASP:OD2	2:D:135:LYS:HE2	2.05	0.56
1:E:796:LEU:HD13	1:F:702:TYR:HB3	1.88	0.56
1:B:656:ARG:HH21	1:B:679:ASN:HB3	1.71	0.56
2:C:62:GLY:C	2:C:114:THR:CG2	2.68	0.56
1:F:635:TYR:OH	1:F:649:PRO:HA	2.06	0.56
1:E:266:SER:O	1:E:267:ILE:HG23	2.05	0.56
2:L:83:LEU:HD22	2:L:90:ILE:HG12	1.88	0.56
2:C:63:ILE:N	2:C:114:THR:HG23	2.19	0.55
1:E:306:MET:HA	1:E:309:ARG:NE	2.19	0.55
2:K:295:ASP:CG	2:K:296:PRO:HD2	2.32	0.55
1:E:595:PRO:HG3	2:G:57:ARG:HD2	1.88	0.55
2:H:279:LYS:HE2	2:H:330:LEU:HB3	1.87	0.55
1:J:264:GLN:HG2	1:J:264:GLN:O	2.06	0.55
1:J:656:ARG:HH21	1:J:679:ASN:HB3	1.71	0.55
2:H:151:PHE:O	2:H:158:ARG:NH1	2.39	0.55
1:E:617:MET:CE	3:E:1801:ANP:H4'	2.36	0.55
1:I:470:VAL:HG11	1:J:523:LEU:HD13	1.89	0.55
1:I:697:ARG:HH12	1:J:697:ARG:HB2	1.70	0.55
1:J:635:TYR:OH	1:J:649:PRO:HA	2.05	0.55
1:F:312:HIS:O	1:F:313:MET:CE	2.53	0.55
1:I:701:THR:HG1	1:J:729:TYR:HD1	1.53	0.55
1:A:635:TYR:OH	1:A:649:PRO:HA	2.06	0.55
1:E:635:TYR:OH	1:E:649:PRO:HA	2.07	0.55
1:E:727:THR:HG21	1:E:732:LEU:HD12	1.88	0.55
2:K:316:ARG:CG	2:K:317:LEU:N	2.69	0.55
1:J:617:MET:HA	3:J:1801:ANP:C5'	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:295:ASP:CG	2:C:296:PRO:HD2	2.32	0.55
2:D:113:ARG:NE	2:D:118:GLN:O	2.30	0.55
2:H:64:LYS:HB3	2:H:66:ASP:OD1	2.06	0.55
2:H:261:ARG:HD3	2:H:262:MET:H	1.72	0.55
1:I:469:ALA:HB1	1:J:522:ALA:HB1	1.89	0.55
2:K:107:ARG:HB2	2:K:148:LEU:HB2	1.88	0.55
2:C:24:ALA:HB1	2:C:174:ILE:HD12	1.88	0.54
1:E:150:ILE:HD11	1:E:252:LEU:HD21	1.90	0.54
2:K:316:ARG:HG3	2:K:317:LEU:N	2.21	0.54
1:I:635:TYR:OH	1:I:649:PRO:HA	2.07	0.54
1:E:697:ARG:HB2	1:F:697:ARG:NH2	2.21	0.54
1:E:671:MET:HG2	1:E:672:VAL:H	1.72	0.54
2:G:80:ILE:HG12	2:G:81:ALA:H	1.73	0.54
1:J:622:THR:OG1	3:J:1801:ANP:H8	2.07	0.54
2:C:111:THR:HA	2:C:121:TRP:O	2.08	0.54
2:G:83:LEU:HD23	2:G:87:GLU:O	2.07	0.54
1:I:227:VAL:HG12	1:I:260:MET:HB2	1.90	0.54
2:K:151:PHE:O	2:K:158:ARG:NH1	2.40	0.54
2:D:158:ARG:HA	2:D:161:LEU:HD13	1.89	0.54
2:K:139:HIS:HE2	2:K:144:THR:HG1	1.56	0.53
1:E:150:ILE:CD1	1:E:252:LEU:CD2	2.86	0.53
2:K:107:ARG:CZ	2:K:152:TYR:HD2	2.20	0.53
1:B:635:TYR:OH	1:B:649:PRO:HA	2.07	0.53
1:F:735:LEU:O	1:F:739:MET:N	2.38	0.53
2:K:279:LYS:HE2	2:K:330:LEU:HB3	1.90	0.53
2:D:107:ARG:HB2	2:D:148:LEU:HB2	1.90	0.53
2:L:279:LYS:HE2	2:L:330:LEU:HB3	1.90	0.53
2:C:279:LYS:HE2	2:C:330:LEU:HB3	1.90	0.53
2:L:299:VAL:HB	2:L:315:SER:HG	1.74	0.53
1:I:617:MET:HG3	1:J:671:MET:HB2	1.91	0.53
1:I:727:THR:HG21	1:I:732:LEU:HD12	1.89	0.53
1:A:616:ASN:CG	1:B:670:PHE:CD2	2.87	0.53
1:E:594:GLU:HB2	1:E:595:PRO:CD	2.39	0.53
2:D:279:LYS:HE2	2:D:330:LEU:HB3	1.89	0.52
2:G:111:THR:OG1	2:G:144:THR:HB	2.09	0.52
1:I:268:ILE:HG21	1:I:652:ARG:HH21	1.74	0.52
2:H:24:ALA:HB1	2:H:174:ILE:HD12	1.92	0.52
2:L:267:LEU:HD11	2:L:319:HIS:HB2	1.92	0.52
2:C:110:LEU:HD13	2:C:145:LEU:HG	1.92	0.52
1:E:593:ASN:O	2:G:55:ARG:CZ	2.58	0.52
2:G:64:LYS:HB2	2:G:67:GLU:HG3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:70:LEU:HD12	2:K:71:ALA:N	2.25	0.52
1:A:699:THR:HG21	1:B:615:PRO:HA	1.92	0.52
1:E:266:SER:C	1:E:267:ILE:HG23	2.35	0.52
2:D:72:LEU:HD23	2:D:103:SER:CB	2.39	0.52
2:D:72:LEU:HD23	2:D:103:SER:HB2	1.92	0.52
2:G:107:ARG:CZ	2:G:152:TYR:HD2	2.23	0.52
2:G:107:ARG:HB2	2:G:148:LEU:HB2	1.91	0.52
2:H:70:LEU:HD12	2:H:71:ALA:N	2.25	0.52
1:J:489:TYR:HD2	1:J:501:TYR:HB2	1.75	0.52
1:A:793:LEU:HD13	1:B:703:ASP:HA	1.92	0.51
2:D:151:PHE:O	2:D:158:ARG:CZ	2.58	0.51
1:E:759:MET:SD	2:G:138:ALA:HB1	2.50	0.51
1:B:754:ASP:HB2	2:D:135:LYS:NZ	2.25	0.51
2:C:299:VAL:CB	2:C:315:SER:OG	2.58	0.51
1:E:251:THR:O	1:E:252:LEU:HD23	2.10	0.51
2:H:107:ARG:HB2	2:H:148:LEU:HB2	1.91	0.51
1:F:150:ILE:HD11	1:F:252:LEU:HD21	1.91	0.51
2:C:267:LEU:HD11	2:C:319:HIS:HB2	1.93	0.51
2:K:164:GLU:HG3	2:K:165:LYS:N	2.25	0.51
1:I:670:PHE:HB3	3:J:1801:ANP:O1G	2.11	0.51
1:I:783:LYS:NZ	1:J:256:ARG:HB2	2.26	0.51
2:K:83:LEU:C	2:K:87:GLU:HB2	2.36	0.51
2:G:151:PHE:O	2:G:158:ARG:CZ	2.58	0.51
1:I:617:MET:SD	1:J:671:MET:CA	2.95	0.51
2:L:107:ARG:HG2	2:L:148:LEU:HD13	1.91	0.51
1:E:252:LEU:N	1:E:253:PRO:CD	2.74	0.51
1:F:394:ARG:HG3	1:F:394:ARG:NH1	2.12	0.51
2:G:82:SER:O	2:G:87:GLU:N	2.33	0.51
1:J:735:LEU:O	1:J:739:MET:N	2.38	0.51
2:L:83:LEU:C	2:L:87:GLU:HB2	2.35	0.51
2:H:164:GLU:HG2	2:H:165:LYS:N	2.26	0.51
1:J:755:THR:HG21	2:L:135:LYS:HZ2	1.76	0.51
1:A:264:GLN:O	1:A:264:GLN:HG2	2.10	0.50
2:C:72:LEU:C	2:C:72:LEU:HD12	2.36	0.50
3:E:1801:ANP:O2G	1:F:670:PHE:N	2.45	0.50
2:G:116:GLU:O	2:G:118:GLN:N	2.44	0.50
1:A:735:LEU:O	1:A:739:MET:N	2.39	0.50
2:K:179:ALA:HB1	2:K:211:ARG:HH12	1.76	0.50
3:E:1801:ANP:O1G	1:F:670:PHE:HB3	2.12	0.50
1:B:733:THR:HG21	1:B:766:ALA:HB1	1.93	0.50
1:A:617:MET:SD	1:B:671:MET:HA	2.52	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:264:ARG:HB2	2:L:264:ARG:CZ	2.41	0.50
1:J:252:LEU:N	1:J:253:PRO:CD	2.75	0.50
2:H:90:ILE:HG21	2:K:266:ARG:NH2	2.20	0.50
1:I:735:LEU:O	1:I:739:MET:N	2.38	0.50
2:D:267:LEU:HD11	2:D:319:HIS:HB2	1.94	0.50
1:E:772:GLY:HA3	1:F:703:ASP:OD2	2.12	0.50
1:F:394:ARG:CG	1:F:394:ARG:NH1	2.68	0.50
2:G:70:LEU:HD12	2:G:71:ALA:N	2.26	0.50
1:A:733:THR:HG21	1:A:766:ALA:HB1	1.93	0.50
2:H:70:LEU:CD2	2:H:86:LEU:HD11	2.40	0.50
2:H:72:LEU:C	2:H:72:LEU:HD12	2.36	0.50
1:J:251:THR:O	1:J:252:LEU:HD23	2.12	0.50
2:K:83:LEU:HD22	2:K:90:ILE:HG12	1.93	0.50
2:L:48:ARG:HG2	2:L:164:GLU:OE1	2.12	0.50
1:A:594:GLU:HB2	1:A:595:PRO:CD	2.42	0.49
2:C:72:LEU:HD13	2:C:125:ALA:HB2	1.93	0.49
1:I:388:ALA:HB3	1:I:389:PRO:HD3	1.94	0.49
1:F:594:GLU:HB2	1:F:595:PRO:CD	2.42	0.49
2:H:179:ALA:HB1	2:H:211:ARG:HH12	1.76	0.49
1:I:616:ASN:OD1	1:J:670:PHE:HB3	2.13	0.49
1:I:697:ARG:NH1	1:J:697:ARG:HB2	2.27	0.49
1:A:778:LEU:HD21	1:B:220:ARG:CZ	2.42	0.49
2:H:97:GLU:CA	2:K:266:ARG:HH12	2.14	0.49
1:I:700:SER:HB2	1:J:770:SER:HB3	1.94	0.49
1:F:733:THR:HG21	1:F:766:ALA:HB1	1.95	0.49
2:K:64:LYS:HD2	2:K:114:THR:HG21	1.93	0.49
2:L:72:LEU:HD12	2:L:72:LEU:C	2.38	0.49
1:E:619:GLY:HA2	3:E:1801:ANP:C8	2.39	0.49
1:J:156:ARG:HD2	1:J:261:GLU:HG3	1.94	0.49
2:K:82:SER:O	2:K:86:LEU:O	2.29	0.49
2:K:113:ARG:NE	2:K:118:GLN:O	2.30	0.49
1:A:251:THR:O	1:A:252:LEU:HD23	2.12	0.49
2:C:83:LEU:C	2:C:87:GLU:HB2	2.38	0.49
2:C:110:LEU:CD1	2:C:145:LEU:HG	2.42	0.49
2:C:151:PHE:O	2:C:158:ARG:CZ	2.61	0.49
2:D:70:LEU:O	2:D:80:ILE:HD11	2.12	0.49
1:F:252:LEU:N	1:F:253:PRO:CD	2.76	0.49
1:F:388:ALA:HB3	1:F:389:PRO:HD3	1.94	0.49
2:H:97:GLU:CG	2:K:266:ARG:HG3	2.35	0.49
1:A:202:TRP:CZ2	2:D:158:ARG:NH2	2.81	0.49
1:A:252:LEU:N	1:A:253:PRO:CD	2.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:ILE:HG23	1:A:559:ALA:HA	1.94	0.49
2:G:279:LYS:HE2	2:G:330:LEU:HB3	1.94	0.49
1:J:328:ILE:HG23	1:J:559:ALA:HA	1.93	0.49
1:A:727:THR:HG21	1:A:732:LEU:HD12	1.94	0.49
2:H:251:ALA:HB1	2:H:285:GLN:HB3	1.94	0.49
1:I:252:LEU:N	1:I:253:PRO:CD	2.75	0.49
1:I:622:THR:OG1	3:I:1801:ANP:C8	2.61	0.49
2:L:151:PHE:O	2:L:158:ARG:CZ	2.60	0.49
1:A:780:GLY:HA2	1:B:219:THR:HG22	1.94	0.49
2:C:30:LEU:HD22	2:C:145:LEU:HD22	1.94	0.49
1:E:150:ILE:HG12	1:E:248:GLN:NE2	2.27	0.49
1:E:594:GLU:HB2	1:E:595:PRO:HD3	1.95	0.49
1:F:150:ILE:HD13	1:F:248:GLN:HG3	1.94	0.49
2:C:164:GLU:HG2	2:C:165:LYS:N	2.27	0.48
1:E:735:LEU:O	1:E:739:MET:N	2.42	0.48
2:G:164:GLU:OE1	2:G:164:GLU:N	2.42	0.48
2:C:156:ALA:HA	2:C:159:LYS:HG2	1.95	0.48
1:F:251:THR:O	1:F:252:LEU:HD23	2.13	0.48
1:J:622:THR:HG21	3:J:1801:ANP:N7	2.28	0.48
2:K:110:LEU:CD1	2:K:144:THR:O	2.61	0.48
1:I:328:ILE:HG23	1:I:559:ALA:HA	1.94	0.48
1:I:616:ASN:CG	1:J:670:PHE:HB3	2.38	0.48
1:J:733:THR:HG21	1:J:766:ALA:HB1	1.94	0.48
2:L:63:ILE:N	2:L:114:THR:HG22	2.28	0.48
1:F:156:ARG:HD2	1:F:261:GLU:HG3	1.96	0.48
2:G:164:GLU:CD	2:G:165:LYS:H	2.21	0.48
1:A:671:MET:HA	1:B:617:MET:SD	2.53	0.48
1:I:251:THR:O	1:I:252:LEU:HD23	2.13	0.48
1:I:733:THR:HG21	1:I:766:ALA:HB1	1.96	0.48
1:A:793:LEU:HD13	1:B:706:SER:OG	2.13	0.48
2:H:151:PHE:O	2:H:158:ARG:CZ	2.61	0.48
1:I:268:ILE:HG21	1:I:652:ARG:NH2	2.28	0.48
1:B:487:ILE:C	1:B:489:TYR:N	2.71	0.48
2:H:266:ARG:HB3	2:K:80:ILE:HD11	1.96	0.48
2:G:263:MET:HG3	2:G:264:ARG:N	2.29	0.48
2:L:113:ARG:HD3	2:L:139:HIS:O	2.14	0.48
2:D:70:LEU:HD12	2:D:71:ALA:N	2.28	0.48
2:G:113:ARG:NE	2:G:118:GLN:O	2.31	0.48
1:I:701:THR:CG2	1:J:701:THR:HG23	2.44	0.48
1:A:793:LEU:CD1	1:B:706:SER:OG	2.62	0.47
2:L:139:HIS:HE2	2:L:144:THR:HG1	1.59	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:80:ILE:HG12	2:G:81:ALA:N	2.29	0.47
1:A:792:LYS:HE2	1:B:709:TRP:CE3	2.49	0.47
1:B:487:ILE:HA	1:B:489:TYR:H	1.80	0.47
1:J:282:ASN:O	1:J:283:LEU:C	2.57	0.47
2:C:110:LEU:CD1	2:C:145:LEU:CD2	2.92	0.47
2:C:113:ARG:NE	2:C:118:GLN:O	2.31	0.47
2:D:86:LEU:HD22	2:D:89:ILE:HD12	1.96	0.47
1:F:297:SER:OG	1:F:561:ARG:HD3	2.15	0.47
1:I:698:GLY:O	1:J:728:HIS:CG	2.67	0.47
2:D:83:LEU:HD11	2:D:90:ILE:CD1	2.44	0.47
2:K:63:ILE:C	2:K:114:THR:OG1	2.58	0.47
2:K:151:PHE:O	2:K:158:ARG:CZ	2.63	0.47
2:L:82:SER:O	2:L:86:LEU:O	2.31	0.47
1:A:776:ALA:HB2	1:B:674:MET:SD	2.55	0.47
1:B:252:LEU:N	1:B:253:PRO:CD	2.77	0.47
1:B:388:ALA:HB3	1:B:389:PRO:HD3	1.97	0.47
2:C:82:SER:O	2:C:86:LEU:O	2.32	0.47
2:D:83:LEU:HD11	2:D:90:ILE:HD12	1.96	0.47
2:D:149:ASP:OD1	2:D:149:ASP:N	2.47	0.47
1:E:227:VAL:HG12	1:E:260:MET:HB2	1.96	0.47
2:G:30:LEU:HD22	2:G:145:LEU:HD22	1.97	0.47
2:G:72:LEU:HD23	2:G:103:SER:CB	2.45	0.47
1:I:594:GLU:HB2	1:I:595:PRO:CD	2.45	0.47
1:I:728:HIS:ND1	1:J:699:THR:HA	2.28	0.47
2:K:62:GLY:HA3	2:K:114:THR:HA	1.97	0.47
1:I:282:ASN:O	1:I:283:LEU:C	2.58	0.47
2:L:251:ALA:HB1	2:L:285:GLN:HB3	1.97	0.47
1:E:282:ASN:O	1:E:283:LEU:C	2.58	0.47
2:G:110:LEU:O	2:G:122:GLN:HG2	2.15	0.47
1:I:786:ILE:HG22	1:I:790:ARG:HE	1.80	0.47
2:C:110:LEU:HD11	2:C:145:LEU:CD2	2.40	0.46
2:D:157:ARG:O	2:D:161:LEU:HD11	2.15	0.46
1:B:251:THR:O	1:B:252:LEU:HD23	2.13	0.46
2:C:113:ARG:HD3	2:C:139:HIS:O	2.16	0.46
1:F:282:ASN:O	1:F:283:LEU:C	2.58	0.46
1:F:328:ILE:HG23	1:F:559:ALA:HA	1.98	0.46
1:I:699:THR:HG21	1:J:615:PRO:HA	1.96	0.46
1:B:798:SER:HA	1:F:496:LYS:HZ1	1.80	0.46
2:G:113:ARG:HD3	2:G:139:HIS:O	2.16	0.46
2:G:267:LEU:HD11	2:G:319:HIS:HB2	1.98	0.46
1:J:771:TYR:O	1:J:775:VAL:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:68:LEU:CD1	2:D:121:TRP:HB2	2.46	0.46
1:E:678:ALA:CB	1:F:780:GLY:O	2.63	0.46
2:H:113:ARG:NE	2:H:118:GLN:O	2.31	0.46
1:J:272:ALA:O	1:J:276:ASN:HB2	2.16	0.46
1:J:425:ILE:CD1	1:J:527:LEU:HB2	2.45	0.46
1:A:156:ARG:HD2	1:A:261:GLU:HG3	1.98	0.46
2:C:109:THR:C	2:C:110:LEU:HG	2.41	0.46
2:D:48:ARG:HG2	2:D:164:GLU:OE1	2.16	0.46
1:I:616:ASN:CG	1:J:670:PHE:CD2	2.94	0.46
2:D:83:LEU:HD21	2:D:90:ILE:CD1	2.45	0.46
1:E:620:LYS:N	3:E:1801:ANP:O1A	2.49	0.46
1:B:297:SER:OG	1:B:561:ARG:HD3	2.16	0.46
1:E:388:ALA:HB3	1:E:389:PRO:HD3	1.97	0.46
1:E:617:MET:HA	3:E:1801:ANP:H5'1	1.98	0.46
2:H:113:ARG:HD3	2:H:139:HIS:O	2.16	0.46
1:I:219:THR:CG2	1:J:780:GLY:HA2	2.46	0.46
1:J:594:GLU:HB3	1:J:595:PRO:CD	2.46	0.46
1:A:697:ARG:HH12	1:B:697:ARG:CZ	2.27	0.46
2:C:109:THR:OG1	2:C:146:GLU:HB2	2.16	0.45
1:E:733:THR:HG21	1:E:766:ALA:HB1	1.97	0.45
2:H:97:GLU:HA	2:K:266:ARG:HH11	1.68	0.45
1:J:388:ALA:HB3	1:J:389:PRO:HD3	1.98	0.45
2:L:114:THR:OG1	2:L:118:GLN:OE1	2.35	0.45
1:A:702:TYR:HB3	1:B:796:LEU:HD13	1.97	0.45
1:B:282:ASN:O	1:B:283:LEU:C	2.60	0.45
2:K:30:LEU:HD22	2:K:145:LEU:HD22	1.99	0.45
2:K:149:ASP:OD1	2:K:149:ASP:N	2.49	0.45
1:A:388:ALA:HB3	1:A:389:PRO:HD3	1.99	0.45
1:B:156:ARG:HD2	1:B:261:GLU:HG3	1.97	0.45
2:G:149:ASP:OD1	2:G:149:ASP:N	2.49	0.45
1:I:425:ILE:CD1	1:I:527:LEU:HB2	2.47	0.45
1:B:150:ILE:C	1:B:150:ILE:HD12	2.42	0.45
1:E:617:MET:SD	1:F:671:MET:HG3	2.57	0.45
1:E:671:MET:HG2	1:E:672:VAL:N	2.31	0.45
2:G:72:LEU:HD23	2:G:103:SER:HB2	1.99	0.45
2:C:70:LEU:HD22	2:C:82:SER:HA	1.98	0.45
1:F:227:VAL:HG12	1:F:260:MET:HB2	1.99	0.45
1:J:656:ARG:HE	1:J:676:GLU:C	2.24	0.45
2:K:48:ARG:HG2	2:K:164:GLU:OE1	2.17	0.45
2:L:149:ASP:OD1	2:L:149:ASP:N	2.49	0.45
2:C:110:LEU:CD2	2:C:145:LEU:CA	2.58	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:698:GLY:O	1:J:728:HIS:CD2	2.70	0.45
1:I:771:TYR:O	1:I:775:VAL:HG23	2.17	0.45
1:A:778:LEU:HD21	1:B:220:ARG:NH1	2.32	0.45
1:I:224:GLY:O	1:I:682:HIS:ND1	2.50	0.45
2:K:113:ARG:HD3	2:K:139:HIS:O	2.17	0.45
1:B:771:TYR:O	1:B:775:VAL:HG23	2.16	0.45
2:D:113:ARG:HD3	2:D:139:HIS:O	2.16	0.45
2:G:64:LYS:HD2	2:G:114:THR:HG21	1.99	0.45
1:B:656:ARG:HE	1:B:676:GLU:C	2.25	0.44
1:B:727:THR:HG21	1:B:732:LEU:HD12	1.97	0.44
1:J:656:ARG:HE	1:J:676:GLU:CB	2.30	0.44
1:B:594:GLU:HB3	1:B:595:PRO:CD	2.48	0.44
1:E:526:GLN:NE2	1:F:470:VAL:HG21	2.28	0.44
1:E:670:PHE:CD2	1:F:616:ASN:ND2	2.85	0.44
1:E:772:GLY:N	1:F:699:THR:OG1	2.50	0.44
1:I:594:GLU:HB2	1:I:595:PRO:HD3	1.99	0.44
1:I:697:ARG:CZ	1:J:697:ARG:HB2	2.47	0.44
2:G:190:SER:HA	2:G:195:ILE:HA	2.00	0.44
2:L:113:ARG:NE	2:L:118:GLN:O	2.32	0.44
2:L:135:LYS:HB2	2:L:136:PRO:CD	2.48	0.44
1:A:780:GLY:HA2	1:B:219:THR:CG2	2.48	0.44
2:C:114:THR:O	2:C:115:ALA:C	2.60	0.44
1:I:272:ALA:O	1:I:276:ASN:HB2	2.17	0.44
2:L:190:SER:HA	2:L:195:ILE:HA	2.00	0.44
1:F:619:GLY:HA2	3:F:1801:ANP:C8	2.47	0.44
1:A:771:TYR:O	1:A:775:VAL:HG23	2.18	0.44
2:G:107:ARG:NH2	2:G:152:TYR:HD2	2.15	0.44
1:A:282:ASN:O	1:A:283:LEU:C	2.60	0.44
1:E:215:LEU:HD22	2:H:124:TYR:CE2	2.52	0.44
1:F:755:THR:HG21	2:H:135:LYS:HD2	2.00	0.44
2:H:68:LEU:CD1	2:H:121:TRP:HB2	2.48	0.44
1:J:297:SER:OG	1:J:561:ARG:HD3	2.17	0.44
2:K:107:ARG:NH2	2:K:152:TYR:HD2	2.14	0.44
2:K:111:THR:HA	2:K:121:TRP:O	2.18	0.44
1:E:656:ARG:HA	1:E:656:ARG:HD2	1.75	0.44
2:H:114:THR:O	2:H:115:ALA:C	2.60	0.44
2:D:114:THR:O	2:D:115:ALA:C	2.61	0.44
2:L:107:ARG:CG	2:L:148:LEU:HD13	2.47	0.44
2:G:70:LEU:HB2	2:G:82:SER:HB2	2.00	0.43
2:C:121:TRP:CZ3	2:C:136:PRO:HG3	2.54	0.43
2:C:149:ASP:N	2:C:149:ASP:OD1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:771:TYR:O	1:E:775:VAL:HG23	2.17	0.43
1:F:379:ARG:HG2	1:F:394:ARG:HH12	1.83	0.43
2:H:83:LEU:HD23	2:H:86:LEU:HD23	2.00	0.43
1:J:788:ARG:HD3	1:J:788:ARG:HA	1.82	0.43
1:E:156:ARG:HD2	1:E:261:GLU:HG3	2.00	0.43
1:B:328:ILE:HG23	1:B:559:ALA:HA	2.00	0.43
2:C:62:GLY:C	2:C:63:ILE:HG13	2.44	0.43
2:C:73:ALA:C	2:C:132:VAL:HG22	2.42	0.43
1:E:752:HIS:ND1	2:G:136:PRO:HG2	2.33	0.43
1:F:224:GLY:O	1:F:682:HIS:ND1	2.51	0.43
2:G:62:GLY:C	2:G:63:ILE:HG13	2.42	0.43
1:I:700:SER:HA	1:J:728:HIS:O	2.18	0.43
2:L:64:LYS:HB2	2:L:67:GLU:HG3	1.99	0.43
1:B:621:SER:OG	3:B:1801:ANP:O2B	2.30	0.43
1:B:798:SER:HA	1:F:496:LYS:CE	2.49	0.43
2:C:163:THR:CB	2:C:166:THR:OG1	2.63	0.43
2:D:86:LEU:C	2:D:88:ALA:H	2.25	0.43
1:E:267:ILE:CG1	1:E:314:PRO:HG2	2.47	0.43
1:F:566:ASN:OD1	2:H:200:ARG:NH2	2.51	0.43
2:G:179:ALA:HB1	2:G:211:ARG:HH12	1.83	0.43
2:K:80:ILE:O	2:K:80:ILE:HG23	2.19	0.43
2:D:108:LEU:HD11	2:D:110:LEU:HD23	2.01	0.43
1:E:328:ILE:HG23	1:E:559:ALA:HA	2.00	0.43
2:G:110:LEU:CD1	2:G:123:ALA:HB3	2.49	0.43
1:I:420:ARG:NH2	1:J:420:ARG:NH2	2.67	0.43
1:J:209:ALA:CB	1:J:238:GLY:HA3	2.49	0.43
1:A:425:ILE:CD1	1:A:527:LEU:HB2	2.49	0.43
2:H:110:LEU:CD1	2:H:145:LEU:HG	2.48	0.43
1:A:227:VAL:HG12	1:A:260:MET:HB2	2.00	0.43
1:A:656:ARG:HA	1:A:656:ARG:HD2	1.76	0.43
2:D:63:ILE:N	2:D:114:THR:HG22	2.33	0.43
1:F:425:ILE:CD1	1:F:527:LEU:HB2	2.49	0.43
2:G:111:THR:OG1	2:G:111:THR:O	2.37	0.43
1:B:425:ILE:CD1	1:B:527:LEU:HB2	2.49	0.43
2:C:299:VAL:CB	2:C:315:SER:HG	2.31	0.43
1:E:593:ASN:O	2:G:55:ARG:NE	2.52	0.43
1:F:155:PHE:HB3	1:F:257:SER:O	2.19	0.43
2:G:87:GLU:O	2:G:89:ILE:N	2.48	0.43
1:I:593:ASN:O	2:K:55:ARG:CZ	2.67	0.43
1:I:656:ARG:HA	1:I:656:ARG:HD2	1.72	0.43
2:L:114:THR:O	2:L:115:ALA:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:114:THR:OG1	2:D:118:GLN:OE1	2.37	0.43
1:I:150:ILE:HG21	1:I:248:GLN:CD	2.43	0.43
1:I:156:ARG:HD2	1:I:261:GLU:HG3	2.00	0.43
1:J:150:ILE:HD12	1:J:150:ILE:C	2.44	0.43
2:K:40:THR:HG22	2:K:59:ASN:HD21	1.84	0.43
2:C:149:ASP:O	2:C:150:LEU:C	2.62	0.42
1:F:771:TYR:O	1:F:775:VAL:HG23	2.19	0.42
2:G:164:GLU:CG	2:G:165:LYS:N	2.81	0.42
2:D:139:HIS:ND1	2:D:140:PRO:O	2.53	0.42
1:I:580:ILE:HD12	1:I:601:LEU:HD23	2.01	0.42
2:K:263:MET:HG3	2:K:264:ARG:N	2.34	0.42
2:C:299:VAL:HB	2:C:315:SER:HG	1.83	0.42
1:F:432:GLU:HA	1:F:435:GLU:HG2	2.02	0.42
2:K:189:LEU:HB3	2:K:197:ARG:HB2	2.02	0.42
2:L:179:ALA:HB1	2:L:211:ARG:HH12	1.83	0.42
2:C:156:ALA:O	2:C:159:LYS:HG2	2.20	0.42
2:C:108:LEU:HD13	2:C:109:THR:N	2.34	0.42
1:E:209:ALA:CB	1:E:238:GLY:HA3	2.49	0.42
1:E:224:GLY:O	1:E:682:HIS:ND1	2.51	0.42
1:J:615:PRO:HB2	1:J:758:PHE:HE1	1.83	0.42
2:C:80:ILE:HG23	2:C:80:ILE:O	2.19	0.42
2:C:109:THR:OG1	2:C:146:GLU:O	2.36	0.42
1:I:155:PHE:HB3	1:I:257:SER:O	2.19	0.42
1:I:620:LYS:NZ	3:I:1801:ANP:O1B	2.46	0.42
1:I:670:PHE:HB3	1:J:616:ASN:ND2	2.34	0.42
2:C:83:LEU:HD22	2:C:90:ILE:HG12	2.00	0.42
2:D:80:ILE:HG23	2:D:80:ILE:O	2.19	0.42
1:B:227:VAL:HG12	1:B:260:MET:HB2	2.02	0.42
1:F:272:ALA:O	1:F:276:ASN:HB2	2.20	0.42
1:F:572:PHE:HA	1:F:647:ILE:O	2.20	0.42
1:I:656:ARG:NH2	1:I:673:GLU:CA	2.78	0.42
2:L:68:LEU:CD1	2:L:121:TRP:HB2	2.49	0.42
2:C:68:LEU:CD1	2:C:121:TRP:HB2	2.50	0.42
2:K:135:LYS:HB2	2:K:136:PRO:CD	2.50	0.42
2:G:63:ILE:N	2:G:114:THR:HG22	2.34	0.42
2:G:243:PRO:HB2	2:G:280:LEU:HD21	2.02	0.42
1:I:671:MET:CA	1:J:617:MET:SD	3.08	0.42
2:C:243:PRO:HB2	2:C:280:LEU:HD21	2.01	0.41
2:D:111:THR:HA	2:D:121:TRP:O	2.20	0.41
2:G:121:TRP:CZ3	2:G:136:PRO:HG3	2.54	0.41
1:I:167:ALA:O	1:I:171:GLN:OE1	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:108:LEU:HD11	2:L:110:LEU:HD23	2.02	0.41
2:C:139:HIS:ND1	2:C:140:PRO:O	2.53	0.41
1:E:728:HIS:ND1	1:F:699:THR:HA	2.35	0.41
1:I:622:THR:OG1	3:I:1801:ANP:H8	2.20	0.41
1:A:212:GLN:CD	2:D:107:ARG:HH12	2.28	0.41
1:A:219:THR:CG2	1:B:780:GLY:HA2	2.51	0.41
1:B:656:ARG:NE	1:B:676:GLU:CB	2.81	0.41
1:B:656:ARG:HE	1:B:676:GLU:CB	2.31	0.41
2:C:110:LEU:CD2	2:C:145:LEU:HG	2.49	0.41
2:G:135:LYS:HB2	2:G:136:PRO:CD	2.50	0.41
2:G:149:ASP:O	2:G:150:LEU:C	2.63	0.41
1:J:224:GLY:O	1:J:682:HIS:ND1	2.51	0.41
1:J:572:PHE:HA	1:J:647:ILE:O	2.19	0.41
2:K:51:ALA:O	2:K:149:ASP:CG	2.64	0.41
2:L:82:SER:O	2:L:86:LEU:C	2.63	0.41
2:L:83:LEU:HA	2:L:87:GLU:HA	2.02	0.41
2:C:110:LEU:HD21	2:C:145:LEU:CB	2.48	0.41
2:H:135:LYS:HB2	2:H:136:PRO:CD	2.51	0.41
1:I:168:ALA:HA	1:I:171:GLN:OE1	2.20	0.41
2:D:62:GLY:C	2:D:63:ILE:HG13	2.46	0.41
2:G:51:ALA:O	2:G:149:ASP:CG	2.64	0.41
2:G:139:HIS:NE2	2:G:144:THR:OG1	2.54	0.41
2:H:90:ILE:HG22	2:K:266:ARG:HH21	1.73	0.41
1:A:224:GLY:O	1:A:682:HIS:ND1	2.53	0.41
2:G:185:VAL:O	2:G:211:ARG:NH2	2.53	0.41
1:I:572:PHE:HA	1:I:647:ILE:O	2.21	0.41
1:J:155:PHE:HB3	1:J:257:SER:O	2.20	0.41
2:K:82:SER:O	2:K:86:LEU:C	2.63	0.41
2:C:51:ALA:O	2:C:149:ASP:CG	2.64	0.41
2:D:83:LEU:CD2	2:D:90:ILE:HD12	2.51	0.41
2:D:243:PRO:HB2	2:D:280:LEU:HD21	2.03	0.41
2:H:40:THR:HG22	2:H:59:ASN:HD21	1.86	0.41
1:A:622:THR:HG21	3:A:1801:ANP:N7	2.35	0.41
1:E:671:MET:HG2	1:E:672:VAL:HG23	2.02	0.41
1:E:699:THR:HA	1:F:728:HIS:ND1	2.35	0.41
2:H:185:VAL:O	2:H:211:ARG:NH2	2.53	0.41
1:J:656:ARG:CG	1:J:680:ILE:CD1	2.95	0.41
2:L:262:MET:HE2	2:L:264:ARG:HH21	1.85	0.41
1:A:150:ILE:C	1:A:150:ILE:HD12	2.46	0.41
2:D:40:THR:HG22	2:D:59:ASN:HD21	1.86	0.41
2:D:51:ALA:O	2:D:149:ASP:CG	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:773:LEU:HD12	1:E:793:LEU:HD22	2.03	0.41
1:F:207:ASP:HB2	2:G:52:LYS:HE3	2.02	0.41
1:I:699:THR:OG1	1:J:771:TYR:N	2.47	0.41
2:L:139:HIS:ND1	2:L:140:PRO:O	2.54	0.41
1:A:437:ARG:O	1:A:441:ASP:N	2.47	0.41
1:B:202:TRP:CZ2	2:C:158:ARG:NH2	2.89	0.41
1:E:272:ALA:O	1:E:276:ASN:HB2	2.21	0.41
2:H:80:ILE:HG23	2:H:80:ILE:O	2.21	0.41
1:I:339:GLN:N	1:I:340:PRO:CD	2.84	0.41
1:I:783:LYS:HZ2	1:J:256:ARG:HB2	1.85	0.41
2:K:22:ARG:HE	2:K:167:GLU:CD	2.29	0.41
2:L:40:THR:HG22	2:L:59:ASN:HD21	1.86	0.41
1:B:155:PHE:HB3	1:B:257:SER:O	2.22	0.40
2:H:149:ASP:O	2:H:150:LEU:C	2.63	0.40
1:J:319:ARG:HA	1:J:319:ARG:HD3	1.74	0.40
1:J:486:PRO:HD2	1:J:489:TYR:CD1	2.56	0.40
1:B:735:LEU:O	1:B:739:MET:N	2.42	0.40
2:D:121:TRP:CZ3	2:D:136:PRO:HG3	2.56	0.40
1:F:437:ARG:O	1:F:441:ASP:N	2.48	0.40
1:F:622:THR:OG1	3:F:1801:ANP:C8	2.70	0.40
2:K:185:VAL:O	2:K:211:ARG:NH2	2.54	0.40
2:L:185:VAL:O	2:L:211:ARG:NH2	2.54	0.40
1:A:155:PHE:HB3	1:A:257:SER:O	2.22	0.40
1:A:219:THR:HG21	1:B:780:GLY:HA2	2.03	0.40
2:D:149:ASP:O	2:D:150:LEU:C	2.63	0.40
1:F:479:ARG:HD2	1:F:479:ARG:HA	1.69	0.40
2:H:66:ASP:OD1	2:H:66:ASP:N	2.55	0.40
1:I:652:ARG:CZ	1:I:654:PHE:HZ	2.34	0.40
1:I:671:MET:HB2	1:J:617:MET:HG3	2.03	0.40
1:J:227:VAL:HG12	1:J:260:MET:HB2	2.02	0.40
2:K:22:ARG:NE	2:K:167:GLU:OE2	2.55	0.40
2:K:111:THR:HG22	2:K:122:GLN:HB2	2.03	0.40
2:K:121:TRP:CZ3	2:K:136:PRO:HG3	2.56	0.40
2:K:243:PRO:HB2	2:K:280:LEU:HD21	2.03	0.40
2:L:46:ILE:HG13	2:L:50:GLY:HA2	2.03	0.40
1:B:670:PHE:C	1:B:672:VAL:N	2.79	0.40
1:E:268:ILE:C	1:E:269:MET:HG3	2.46	0.40
2:G:120:ALA:HB2	2:G:139:HIS:HB3	2.04	0.40
2:H:190:SER:HA	2:H:195:ILE:HA	2.02	0.40
1:I:179:LEU:HD23	1:I:197:ARG:HB2	2.03	0.40
2:L:149:ASP:O	2:L:150:LEU:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:51:ALA:O	2:C:149:ASP:CA	2.69	0.40
2:D:135:LYS:HB3	2:D:136:PRO:CD	2.51	0.40
2:H:86:LEU:HG	2:H:89:ILE:HD12	2.03	0.40
1:J:202:TRP:CZ2	2:K:158:ARG:NH2	2.90	0.40
1:J:475:ILE:HG21	1:J:489:TYR:HE2	1.87	0.40
2:K:110:LEU:HD12	2:K:111:THR:N	2.37	0.40
2:L:51:ALA:O	2:L:149:ASP:CA	2.69	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	A	659/800 (82%)	626 (95%)	31 (5%)	2 (0%)	36	72
1	B	659/800 (82%)	627 (95%)	30 (5%)	2 (0%)	36	72
1	E	659/800 (82%)	629 (95%)	27 (4%)	3 (0%)	24	63
1	F	659/800 (82%)	630 (96%)	26 (4%)	3 (0%)	24	63
1	I	659/800 (82%)	627 (95%)	31 (5%)	1 (0%)	43	78
1	J	659/800 (82%)	631 (96%)	25 (4%)	3 (0%)	24	63
2	C	277/369 (75%)	255 (92%)	18 (6%)	4 (1%)	9	40
2	D	277/369 (75%)	252 (91%)	20 (7%)	5 (2%)	6	34
2	G	277/369 (75%)	250 (90%)	22 (8%)	5 (2%)	6	34
2	H	277/369 (75%)	247 (89%)	25 (9%)	5 (2%)	6	34
2	K	277/369 (75%)	253 (91%)	21 (8%)	3 (1%)	11	46
2	L	277/369 (75%)	255 (92%)	18 (6%)	4 (1%)	9	40
All	All	5616/7014 (80%)	5282 (94%)	294 (5%)	40 (1%)	18	56

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	115	ALA
2	D	89	ILE
2	D	115	ALA
2	D	163	THR
2	G	115	ALA
2	G	163	THR
2	H	115	ALA
2	H	163	THR
2	K	163	THR
2	L	115	ALA
2	L	163	THR
2	C	149	ASP
2	D	149	ASP
2	D	150	LEU
1	E	267	ILE
2	G	117	GLN
2	G	149	ASP
2	H	149	ASP
2	H	150	LEU
2	K	149	ASP
2	K	150	LEU
2	L	149	ASP
2	L	150	LEU
2	C	150	LEU
1	F	283	LEU
2	G	150	LEU
1	J	283	LEU
1	A	283	LEU
2	H	111	THR
1	A	780	GLY
1	B	283	LEU
1	F	780	GLY
1	J	780	GLY
1	B	780	GLY
2	C	117	GLN
1	E	780	GLY
1	F	753	GLY
1	I	780	GLY
1	E	753	GLY
1	J	753	GLY

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%)	536 (98%)	14 (2%)	42	63
1	B	550/662 (83%)	533 (97%)	17 (3%)	35	56
1	E	550/662 (83%)	537 (98%)	13 (2%)	43	64
1	F	550/662 (83%)	531 (96%)	19 (4%)	32	53
1	I	550/662 (83%)	535 (97%)	15 (3%)	39	61
1	J	550/662 (83%)	536 (98%)	14 (2%)	42	63
2	C	235/308 (76%)	221 (94%)	14 (6%)	17	39
2	D	235/308 (76%)	221 (94%)	14 (6%)	17	39
2	G	235/308 (76%)	220 (94%)	15 (6%)	16	37
2	H	235/308 (76%)	219 (93%)	16 (7%)	14	36
2	K	235/308 (76%)	221 (94%)	14 (6%)	17	39
2	L	235/308 (76%)	220 (94%)	15 (6%)	16	37
All	All	4710/5820 (81%)	4530 (96%)	180 (4%)	29	50

All (180) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	169	GLU
1	A	178	LEU
1	A	265	ASP
1	A	275	ARG
1	A	282	ASN
1	A	288	GLU
1	A	313	MET
1	A	361	ARG
1	A	383	GLU
1	A	490	MET
1	A	513	VAL
1	A	591	VAL
1	A	592	LEU
1	A	794	ARG

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Mol	Chain	Res	Type
1	B	169	GLU
1	B	178	LEU
1	B	265	ASP
1	B	266	SER
1	B	282	ASN
1	B	283	LEU
1	B	288	GLU
1	B	300	THR
1	B	361	ARG
1	B	479	ARG
1	B	490	MET
1	B	575	LYS
1	B	591	VAL
1	B	592	LEU
1	B	657	VAL
1	B	783	LYS
1	B	794	ARG
2	C	44	ILE
2	C	83	LEU
2	C	109	THR
2	C	114	THR
2	C	117	GLN
2	C	118	GLN
2	C	149	ASP
2	C	150	LEU
2	C	154	THR
2	C	163	THR
2	C	261	ARG
2	C	263	MET
2	C	280	LEU
2	C	324	GLN
2	D	44	ILE
2	D	65	LYS
2	D	83	LEU
2	D	86	LEU
2	D	109	THR
2	D	118	GLN
2	D	149	ASP
2	D	150	LEU
2	D	154	THR
2	D	162	ARG
2	D	163	THR

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Mol	Chain	Res	Type
2	D	266	ARG
2	D	280	LEU
2	D	324	GLN
1	E	169	GLU
1	E	178	LEU
1	E	266	SER
1	E	267	ILE
1	E	269	MET
1	E	282	ASN
1	E	288	GLU
1	E	300	THR
1	E	309	ARG
1	E	313	MET
1	E	591	VAL
1	E	592	LEU
1	E	617	MET
1	F	169	GLU
1	F	178	LEU
1	F	265	ASP
1	F	266	SER
1	F	282	ASN
1	F	283	LEU
1	F	288	GLU
1	F	300	THR
1	F	361	ARG
1	F	394	ARG
1	F	479	ARG
1	F	490	MET
1	F	513	VAL
1	F	575	LYS
1	F	591	VAL
1	F	592	LEU
1	F	657	VAL
1	F	738	LYS
1	F	794	ARG
2	G	44	ILE
2	G	52	LYS
2	G	80	ILE
2	G	83	LEU
2	G	109	THR
2	G	148	LEU
2	G	149	ASP

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Mol	Chain	Res	Type
2	G	150	LEU
2	G	154	THR
2	G	159	LYS
2	G	162	ARG
2	G	163	THR
2	G	171	ILE
2	G	280	LEU
2	G	324	GLN
2	H	44	ILE
2	H	52	LYS
2	H	80	ILE
2	H	83	LEU
2	H	109	THR
2	H	111	THR
2	H	118	GLN
2	H	132	VAL
2	H	148	LEU
2	H	149	ASP
2	H	154	THR
2	H	162	ARG
2	H	163	THR
2	H	233	ASP
2	H	261	ARG
2	H	280	LEU
1	I	150	ILE
1	I	169	GLU
1	I	178	LEU
1	I	265	ASP
1	I	266	SER
1	I	282	ASN
1	I	288	GLU
1	I	300	THR
1	I	490	MET
1	I	530	GLU
1	I	575	LYS
1	I	591	VAL
1	I	592	LEU
1	I	686	GLU
1	I	794	ARG
1	J	140	SER
1	J	169	GLU
1	J	178	LEU

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Mol	Chain	Res	Type
1	J	265	ASP
1	J	266	SER
1	J	282	ASN
1	J	283	LEU
1	J	288	GLU
1	J	300	THR
1	J	323	GLU
1	J	333	ASP
1	J	591	VAL
1	J	730	PHE
1	J	794	ARG
2	K	44	ILE
2	K	72	LEU
2	K	109	THR
2	K	118	GLN
2	K	149	ASP
2	K	154	THR
2	K	162	ARG
2	K	163	THR
2	K	171	ILE
2	K	194	LYS
2	K	228	GLU
2	K	233	ASP
2	K	280	LEU
2	K	324	GLN
2	L	44	ILE
2	L	70	LEU
2	L	109	THR
2	L	111	THR
2	L	118	GLN
2	L	132	VAL
2	L	149	ASP
2	L	150	LEU
2	L	154	THR
2	L	157	ARG
2	L	162	ARG
2	L	163	THR
2	L	171	ILE
2	L	280	LEU
2	L	324	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (90) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	ASN
1	A	138	GLN
1	A	214	ASN
1	A	248	GLN
1	A	312	HIS
1	A	493	GLN
1	A	497	ASN
1	A	557	ASN
1	A	590	GLN
1	A	679	ASN
1	A	760	HIS
1	B	138	GLN
1	B	214	ASN
1	B	471	HIS
1	B	497	ASN
1	B	643	GLN
1	B	714	ASN
2	C	117	GLN
2	C	118	GLN
2	C	270	HIS
2	C	324	GLN
2	D	118	GLN
2	D	122	GLN
2	D	270	HIS
2	D	324	GLN
1	E	131	ASN
1	E	138	GLN
1	E	214	ASN
1	E	248	GLN
1	E	312	HIS
1	E	471	HIS
1	E	497	ASN
1	E	526	GLN
1	E	590	GLN
1	E	760	HIS
1	F	131	ASN
1	F	138	GLN
1	F	214	ASN
1	F	242	GLN
1	F	248	GLN
1	F	264	GLN
1	F	312	HIS
1	F	344	GLN

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Mol	Chain	Res	Type
1	F	370	HIS
1	F	471	HIS
1	F	526	GLN
1	F	590	GLN
1	F	643	GLN
2	G	118	GLN
2	G	122	GLN
2	G	324	GLN
2	H	118	GLN
2	H	122	GLN
2	H	270	HIS
2	H	319	HIS
2	H	324	GLN
1	I	131	ASN
1	I	138	GLN
1	I	214	ASN
1	I	248	GLN
1	I	312	HIS
1	I	344	GLN
1	I	370	HIS
1	I	471	HIS
1	I	526	GLN
1	I	590	GLN
1	I	679	ASN
1	I	752	HIS
1	I	763	GLN
1	J	131	ASN
1	J	138	GLN
1	J	214	ASN
1	J	312	HIS
1	J	344	GLN
1	J	370	HIS
1	J	471	HIS
1	J	497	ASN
1	J	590	GLN
1	J	616	ASN
1	J	643	GLN
1	J	744	ASN
1	J	760	HIS
1	J	791	GLN
2	K	118	GLN
2	K	319	HIS

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Mol	Chain	Res	Type
2	K	324	GLN
2	L	118	GLN
2	L	122	GLN
2	L	270	HIS
2	L	324	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	I	1801	-	33,33,33	2.20	11 (33%)	45,52,52	2.35	14 (31%)
3	ANP	J	1801	-	33,33,33	1.96	9 (27%)	45,52,52	2.26	15 (33%)
3	ANP	F	1801	-	33,33,33	2.17	12 (36%)	45,52,52	2.13	11 (24%)
3	ANP	E	1801	-	33,33,33	1.95	10 (30%)	45,52,52	2.08	14 (31%)
3	ANP	A	1801	-	33,33,33	2.23	13 (39%)	45,52,52	2.79	19 (42%)
3	ANP	B	1801	-	33,33,33	2.42	14 (42%)	45,52,52	2.49	13 (28%)

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	I	1801	-	-	6/18/38/38	0/3/3/3
3	ANP	J	1801	-	-	3/18/38/38	0/3/3/3
3	ANP	F	1801	-	-	4/18/38/38	0/3/3/3
3	ANP	E	1801	-	-	5/18/38/38	0/3/3/3
3	ANP	A	1801	-	-	9/18/38/38	0/3/3/3
3	ANP	B	1801	-	-	8/18/38/38	0/3/3/3

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1801	ANP	C5-C4	6.06	1.49	1.39
3	B	1801	ANP	C5-C4	5.94	1.49	1.39
3	I	1801	ANP	C5-C4	5.48	1.48	1.39
3	F	1801	ANP	C5-C4	5.19	1.48	1.39
3	F	1801	ANP	PG-N3B	5.10	1.76	1.63
3	I	1801	ANP	PG-N3B	4.92	1.76	1.63
3	J	1801	ANP	C5-C4	4.92	1.47	1.39
3	F	1801	ANP	PB-N3B	4.91	1.76	1.63
3	A	1801	ANP	PG-N3B	4.80	1.75	1.63
3	I	1801	ANP	PB-N3B	4.76	1.75	1.63
3	B	1801	ANP	PG-N3B	4.75	1.75	1.63
3	B	1801	ANP	PB-N3B	4.54	1.75	1.63
3	E	1801	ANP	C5-C4	4.50	1.47	1.39
3	E	1801	ANP	PB-N3B	4.48	1.75	1.63
3	J	1801	ANP	PB-N3B	4.29	1.74	1.63
3	B	1801	ANP	PB-O1B	3.91	1.52	1.46
3	E	1801	ANP	PG-N3B	3.72	1.73	1.63
3	B	1801	ANP	PA-O3A	3.68	1.63	1.59
3	B	1801	ANP	PB-O3A	3.63	1.63	1.59
3	E	1801	ANP	PG-O2G	-3.61	1.47	1.56
3	J	1801	ANP	PG-O2G	-3.55	1.47	1.56
3	B	1801	ANP	C5-C6	3.51	1.50	1.41
3	I	1801	ANP	PB-O2B	-3.38	1.47	1.56
3	F	1801	ANP	PG-O3G	-3.31	1.48	1.56
3	A	1801	ANP	C8-N7	3.28	1.38	1.31
3	A	1801	ANP	PB-N3B	3.23	1.71	1.63
3	E	1801	ANP	PG-O3G	-3.22	1.48	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	1801	ANP	PG-O3G	-3.21	1.48	1.56
3	J	1801	ANP	C8-N7	3.21	1.37	1.31
3	J	1801	ANP	PB-O2B	-3.19	1.48	1.56
3	F	1801	ANP	PB-O1B	3.08	1.50	1.46
3	J	1801	ANP	PG-O3G	-3.03	1.48	1.56
3	B	1801	ANP	PB-O2B	-3.00	1.48	1.56
3	A	1801	ANP	PB-O2B	-2.96	1.48	1.56
3	I	1801	ANP	C5-C6	2.94	1.49	1.41
3	A	1801	ANP	C5-C6	2.94	1.49	1.41
3	F	1801	ANP	PA-O3A	2.90	1.62	1.59
3	F	1801	ANP	C5-N7	-2.89	1.33	1.39
3	F	1801	ANP	C5-C6	2.82	1.48	1.41
3	I	1801	ANP	C5-N7	-2.82	1.33	1.39
3	I	1801	ANP	C8-N7	2.82	1.37	1.31
3	B	1801	ANP	C8-N7	2.81	1.37	1.31
3	J	1801	ANP	C5-C6	2.81	1.48	1.41
3	E	1801	ANP	PB-O2B	-2.78	1.49	1.56
3	B	1801	ANP	PG-O2G	-2.74	1.49	1.56
3	E	1801	ANP	C5-C6	2.74	1.48	1.41
3	B	1801	ANP	C1'-N9	2.68	1.53	1.46
3	J	1801	ANP	PG-N3B	2.68	1.70	1.63
3	B	1801	ANP	PG-O3G	-2.66	1.49	1.56
3	I	1801	ANP	PG-O2G	-2.64	1.49	1.56
3	A	1801	ANP	PG-O3G	-2.63	1.49	1.56
3	A	1801	ANP	PA-O3A	2.62	1.62	1.59
3	J	1801	ANP	C5-N7	-2.60	1.34	1.39
3	A	1801	ANP	C5-N7	-2.59	1.34	1.39
3	F	1801	ANP	PG-O2G	-2.57	1.50	1.56
3	I	1801	ANP	C1'-N9	2.38	1.52	1.46
3	B	1801	ANP	C2-N3	2.34	1.38	1.33
3	E	1801	ANP	C5-N7	-2.33	1.34	1.39
3	F	1801	ANP	C2-N3	2.31	1.38	1.33
3	A	1801	ANP	PG-O1G	2.26	1.49	1.46
3	A	1801	ANP	PB-O1B	2.26	1.49	1.46
3	A	1801	ANP	PG-O2G	-2.25	1.50	1.56
3	I	1801	ANP	PB-O1B	2.24	1.49	1.46
3	B	1801	ANP	C5-N7	-2.22	1.35	1.39
3	F	1801	ANP	PB-O2B	-2.16	1.51	1.56
3	E	1801	ANP	C4-N9	-2.12	1.33	1.37
3	E	1801	ANP	C8-N7	2.07	1.35	1.31
3	F	1801	ANP	C8-N7	2.03	1.35	1.31
3	A	1801	ANP	PB-O3A	2.00	1.61	1.59

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1801	ANP	O1G-PG-N3B	-8.65	99.03	111.77
3	B	1801	ANP	C5-C4-N3	-8.38	115.18	126.72
3	A	1801	ANP	C5-C4-N3	-8.01	115.69	126.72
3	I	1801	ANP	C5-C4-N3	-7.84	115.92	126.72
3	F	1801	ANP	C5-C4-N3	-6.75	117.42	126.72
3	J	1801	ANP	C5-C4-N3	-6.75	117.42	126.72
3	A	1801	ANP	N3-C4-N9	5.57	136.64	127.17
3	E	1801	ANP	C5-C4-N3	-5.55	119.08	126.72
3	J	1801	ANP	O1G-PG-N3B	-5.47	103.71	111.77
3	I	1801	ANP	N3-C4-N9	5.42	136.38	127.17
3	B	1801	ANP	N3-C4-N9	5.38	136.32	127.17
3	B	1801	ANP	O1G-PG-N3B	-5.30	103.97	111.77
3	B	1801	ANP	C4-C5-N7	-5.02	104.84	110.58
3	J	1801	ANP	O2B-PB-O1B	4.97	120.53	109.87
3	F	1801	ANP	N3-C4-N9	4.86	135.43	127.17
3	A	1801	ANP	O2B-PB-O1B	4.84	120.24	109.87
3	E	1801	ANP	N3-C4-N9	4.83	135.38	127.17
3	I	1801	ANP	O1G-PG-N3B	-4.76	104.76	111.77
3	J	1801	ANP	N3-C4-N9	4.60	135.00	127.17
3	F	1801	ANP	O1G-PG-N3B	-4.50	105.15	111.77
3	A	1801	ANP	C4-C5-N7	-4.44	105.51	110.58
3	B	1801	ANP	C2-N3-C4	4.40	122.58	111.83
3	I	1801	ANP	C2-N3-C4	4.36	122.49	111.83
3	E	1801	ANP	O2B-PB-O1B	4.32	119.14	109.87
3	J	1801	ANP	C2-N3-C4	4.22	122.13	111.83
3	A	1801	ANP	C2-N3-C4	3.96	121.49	111.83
3	B	1801	ANP	C3'-C2'-C1'	3.94	108.92	101.46
3	J	1801	ANP	C4-C5-N7	-3.93	106.08	110.58
3	F	1801	ANP	C4-C5-N7	-3.90	106.13	110.58
3	E	1801	ANP	C2-N3-C4	3.80	121.12	111.83
3	A	1801	ANP	O1B-PB-N3B	-3.78	106.20	111.77
3	E	1801	ANP	N3-C2-N1	-3.77	122.87	128.58
3	F	1801	ANP	C2-N3-C4	3.65	120.75	111.83
3	I	1801	ANP	C4-C5-N7	-3.58	106.49	110.58
3	I	1801	ANP	C3'-C2'-C1'	3.54	108.16	101.46
3	B	1801	ANP	C5-N7-C8	3.53	109.00	103.45
3	J	1801	ANP	N3-C2-N1	-3.42	123.40	128.58
3	A	1801	ANP	O5'-C5'-C4'	3.42	120.63	108.99
3	A	1801	ANP	C3'-C2'-C1'	3.37	107.83	101.46
3	I	1801	ANP	N3-C2-N1	-3.33	123.54	128.58
3	F	1801	ANP	N3-C2-N1	-3.20	123.74	128.58
3	F	1801	ANP	C3'-C2'-C1'	3.19	107.49	101.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1801	ANP	N3-C2-N1	-3.14	123.82	128.58
3	A	1801	ANP	C5-N7-C8	3.05	108.25	103.45
3	E	1801	ANP	C4-N9-C8	2.96	108.85	105.74
3	E	1801	ANP	O2G-PG-O3G	2.89	115.36	107.59
3	B	1801	ANP	N3-C2-N1	-2.88	124.22	128.58
3	E	1801	ANP	O1G-PG-N3B	-2.86	107.55	111.77
3	F	1801	ANP	C5-N7-C8	2.80	107.85	103.45
3	I	1801	ANP	O2B-PB-O1B	2.73	115.71	109.87
3	I	1801	ANP	C4'-O4'-C1'	2.69	115.40	109.47
3	A	1801	ANP	C1'-N9-C8	-2.68	121.15	127.09
3	E	1801	ANP	C4-C5-N7	-2.67	107.53	110.58
3	F	1801	ANP	O2B-PB-O1B	2.62	115.49	109.87
3	A	1801	ANP	C4-N9-C1'	2.60	132.72	126.63
3	I	1801	ANP	C4-N9-C1'	2.56	132.61	126.63
3	E	1801	ANP	C3'-C2'-C1'	2.54	106.27	101.46
3	J	1801	ANP	C3'-C2'-C1'	2.50	106.20	101.46
3	J	1801	ANP	O3A-PB-N3B	2.49	113.50	106.59
3	A	1801	ANP	C4'-O4'-C1'	2.47	114.93	109.47
3	B	1801	ANP	O3A-PA-O1A	-2.46	103.30	110.70
3	B	1801	ANP	O2G-PG-O3G	2.46	114.19	107.59
3	B	1801	ANP	C5-C4-N9	2.46	108.49	105.81
3	J	1801	ANP	C6-C5-N7	2.46	136.82	132.09
3	J	1801	ANP	C5-N7-C8	2.43	107.27	103.45
3	A	1801	ANP	C6-C5-C4	2.40	120.46	117.18
3	I	1801	ANP	C5-N7-C8	2.39	107.21	103.45
3	E	1801	ANP	N6-C6-N1	2.32	123.55	118.38
3	A	1801	ANP	O4'-C4'-C5'	2.30	116.71	109.33
3	B	1801	ANP	O4'-C1'-N9	2.30	112.51	108.09
3	J	1801	ANP	O2'-C2'-C1'	2.26	117.90	110.10
3	J	1801	ANP	O1B-PB-N3B	-2.26	108.44	111.77
3	J	1801	ANP	O2G-PG-O3G	2.25	113.64	107.59
3	B	1801	ANP	O2'-C2'-C3'	-2.24	104.64	111.82
3	I	1801	ANP	O2G-PG-O3G	2.23	113.59	107.59
3	A	1801	ANP	O2G-PG-O3G	2.23	113.59	107.59
3	A	1801	ANP	C2-N1-C6	2.18	122.31	118.73
3	F	1801	ANP	C2-N1-C6	2.18	122.30	118.73
3	E	1801	ANP	C5-C6-N6	-2.17	117.91	123.29
3	E	1801	ANP	O1B-PB-N3B	-2.14	108.62	111.77
3	I	1801	ANP	C1'-N9-C8	-2.13	122.36	127.09
3	A	1801	ANP	C2'-C3'-C4'	2.10	106.67	102.61
3	E	1801	ANP	C1'-N9-C8	-2.08	122.48	127.09
3	F	1801	ANP	O2'-C2'-C3'	-2.05	105.23	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	1801	ANP	O4'-C1'-N9	2.05	112.02	108.09
3	I	1801	ANP	O1B-PB-N3B	2.02	114.74	111.77

There are no chirality outliers.

All (35) torsion outliers are listed below:

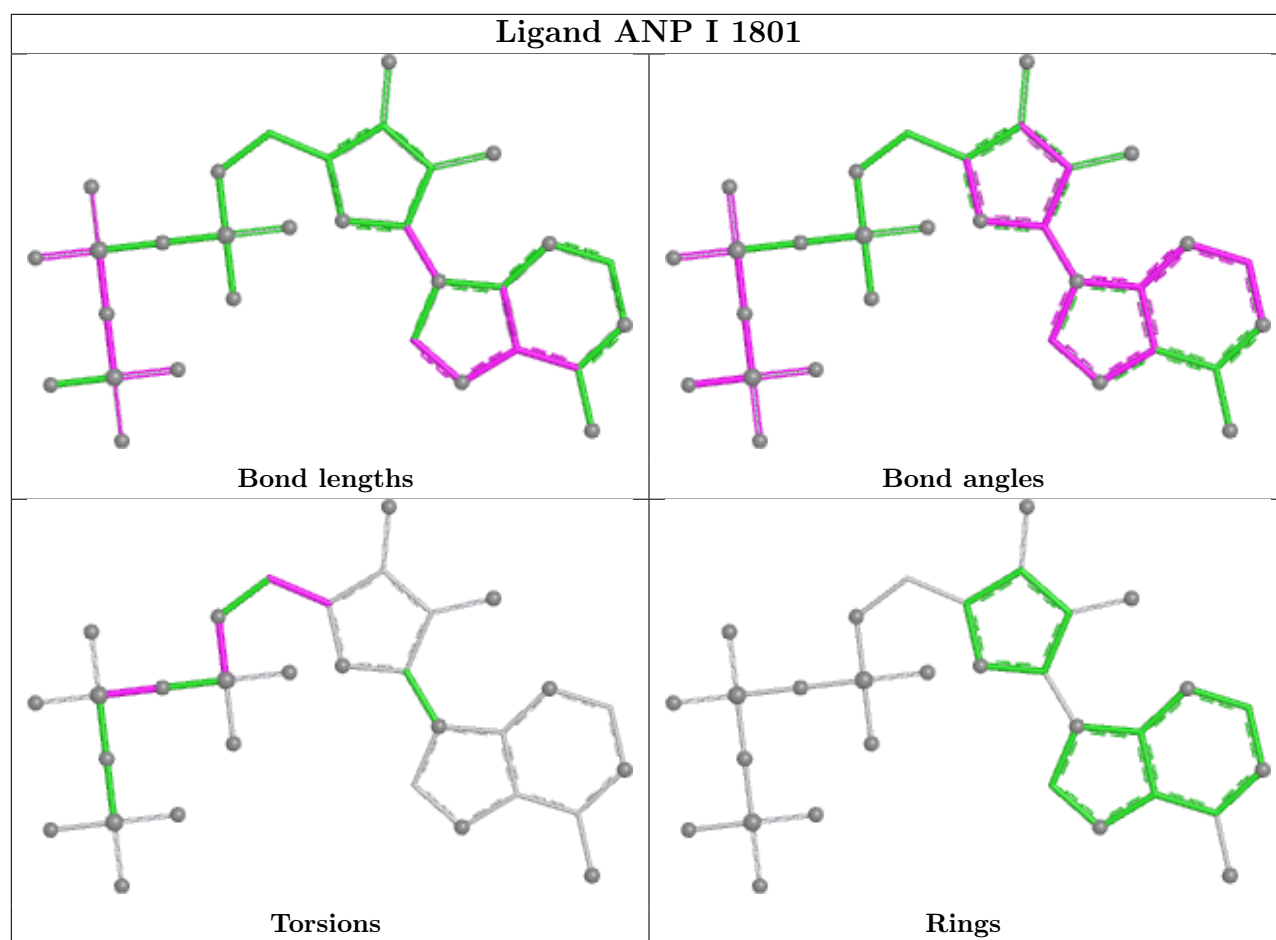
Mol	Chain	Res	Type	Atoms
3	A	1801	ANP	PB-N3B-PG-O1G
3	A	1801	ANP	PG-N3B-PB-O1B
3	A	1801	ANP	PA-O3A-PB-O2B
3	A	1801	ANP	C5'-O5'-PA-O2A
3	A	1801	ANP	C5'-O5'-PA-O3A
3	A	1801	ANP	O4'-C4'-C5'-O5'
3	B	1801	ANP	PA-O3A-PB-O2B
3	B	1801	ANP	C5'-O5'-PA-O1A
3	B	1801	ANP	C5'-O5'-PA-O2A
3	B	1801	ANP	C5'-O5'-PA-O3A
3	B	1801	ANP	O4'-C4'-C5'-O5'
3	E	1801	ANP	PB-N3B-PG-O1G
3	E	1801	ANP	PG-N3B-PB-O1B
3	E	1801	ANP	PA-O3A-PB-O2B
3	E	1801	ANP	O4'-C4'-C5'-O5'
3	F	1801	ANP	PA-O3A-PB-O2B
3	F	1801	ANP	C5'-O5'-PA-O2A
3	F	1801	ANP	O4'-C4'-C5'-O5'
3	I	1801	ANP	PA-O3A-PB-O2B
3	I	1801	ANP	C5'-O5'-PA-O3A
3	I	1801	ANP	O4'-C4'-C5'-O5'
3	J	1801	ANP	PB-N3B-PG-O1G
3	J	1801	ANP	PA-O3A-PB-O2B
3	J	1801	ANP	C5'-O5'-PA-O3A
3	A	1801	ANP	C3'-C4'-C5'-O5'
3	I	1801	ANP	C3'-C4'-C5'-O5'
3	E	1801	ANP	C3'-C4'-C5'-O5'
3	B	1801	ANP	C3'-C4'-C5'-O5'
3	F	1801	ANP	C3'-C4'-C5'-O5'
3	B	1801	ANP	PG-N3B-PB-O3A
3	A	1801	ANP	C5'-O5'-PA-O1A
3	I	1801	ANP	C5'-O5'-PA-O1A
3	A	1801	ANP	PA-O3A-PB-O1B
3	B	1801	ANP	PA-O3A-PB-O1B
3	I	1801	ANP	PA-O3A-PB-O1B

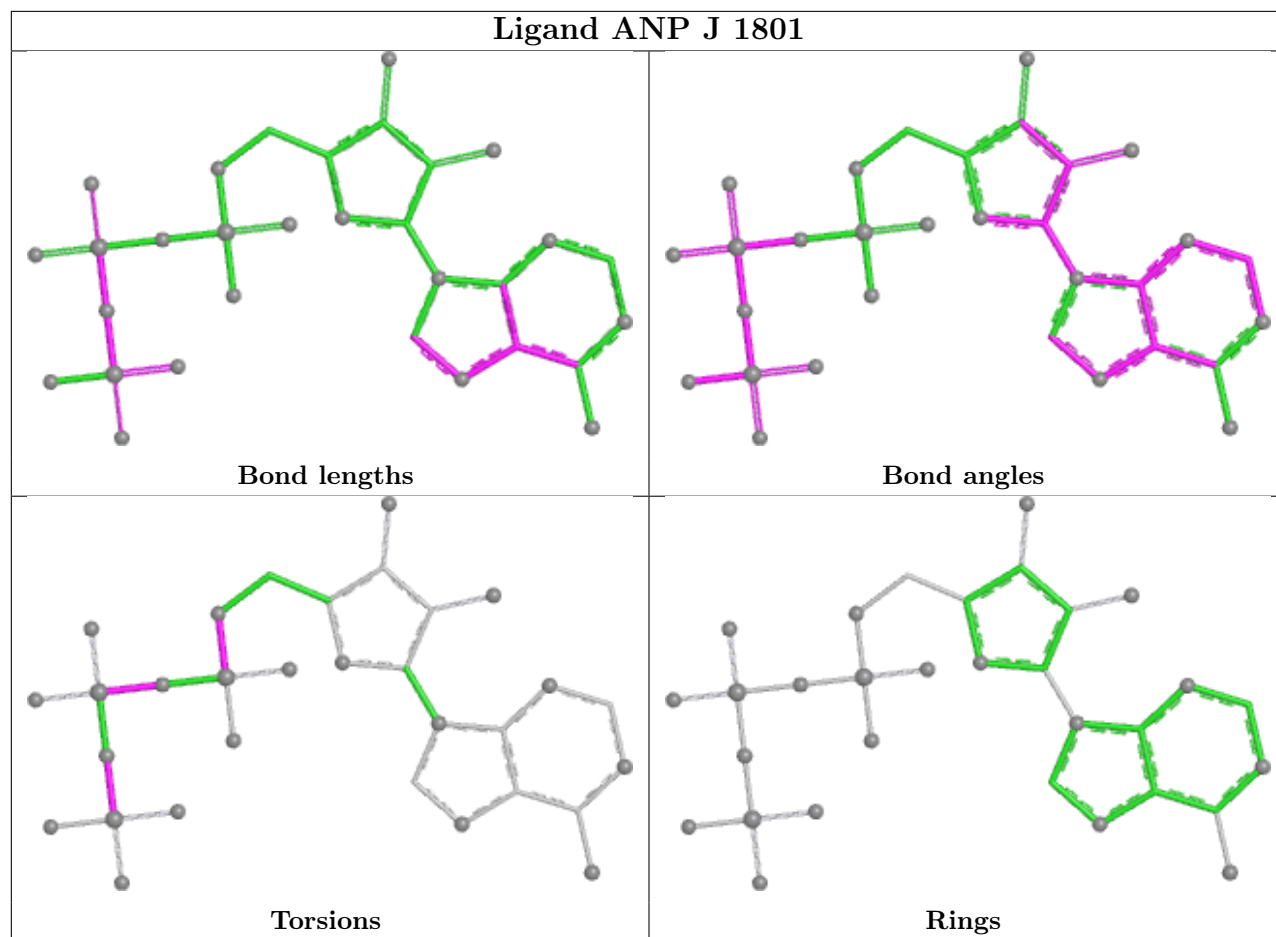
There are no ring outliers.

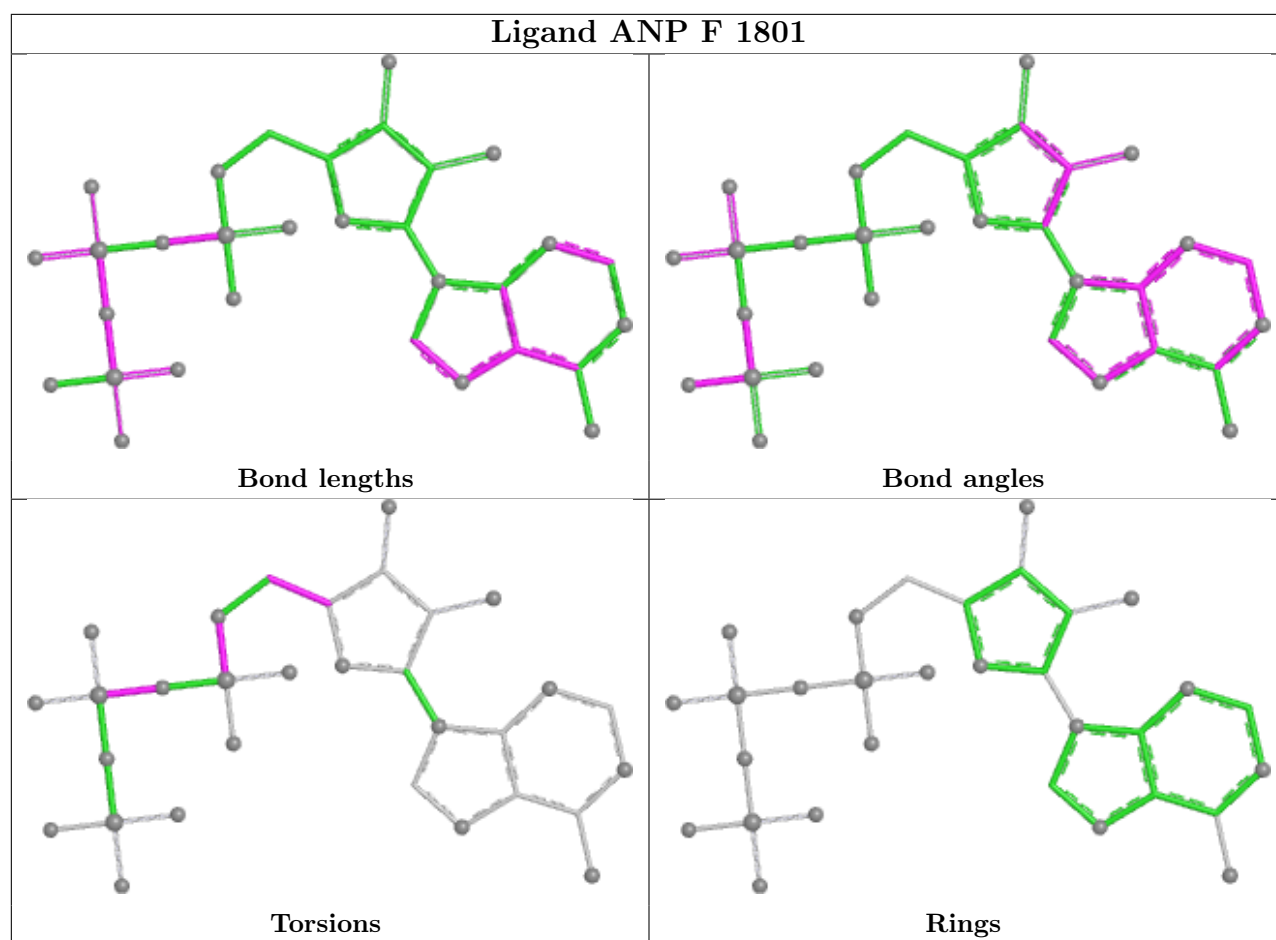
6 monomers are involved in 27 short contacts:

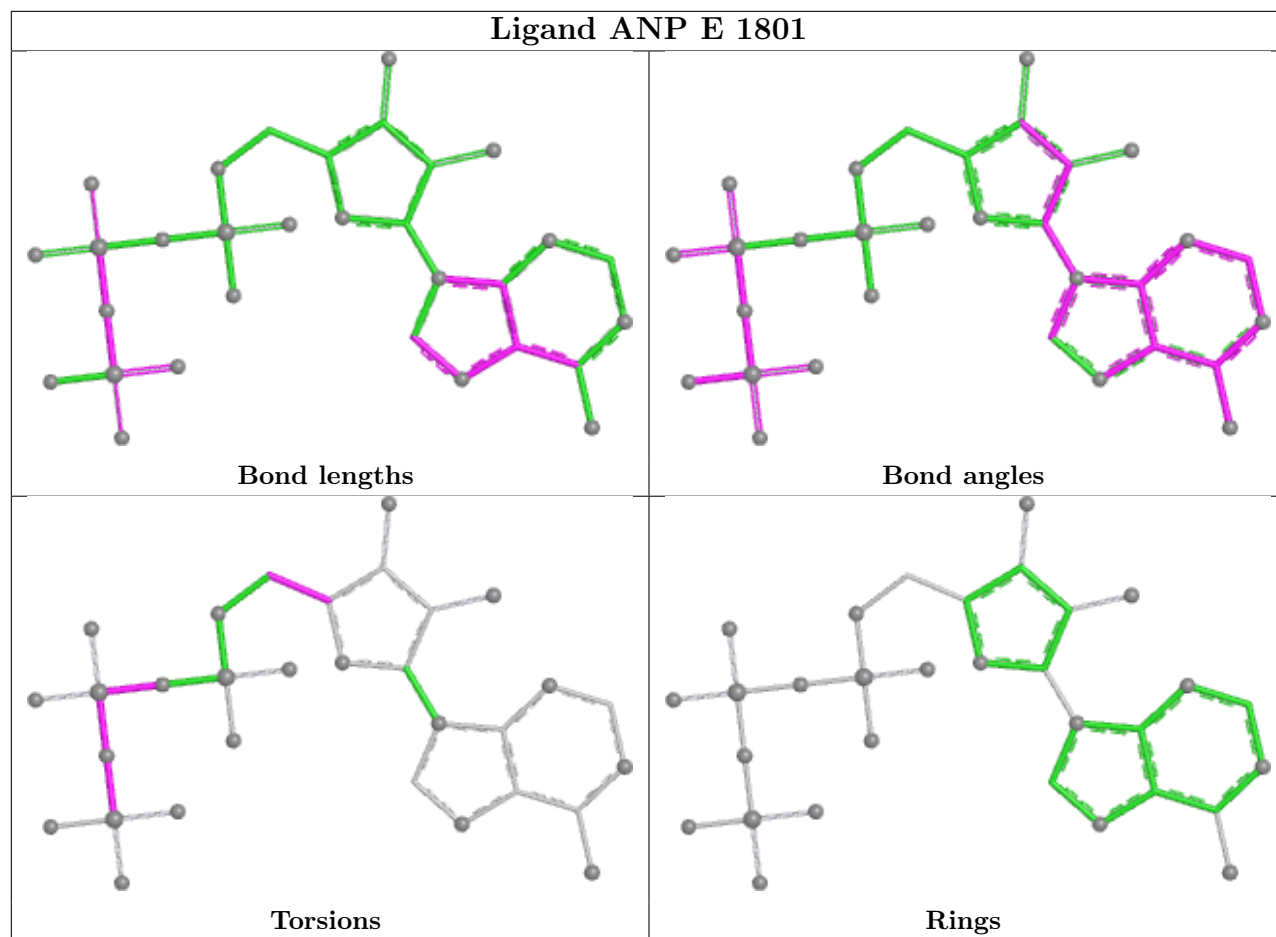
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	1801	ANP	5	0
3	J	1801	ANP	5	0
3	F	1801	ANP	4	0
3	E	1801	ANP	9	0
3	A	1801	ANP	2	0
3	B	1801	ANP	2	0

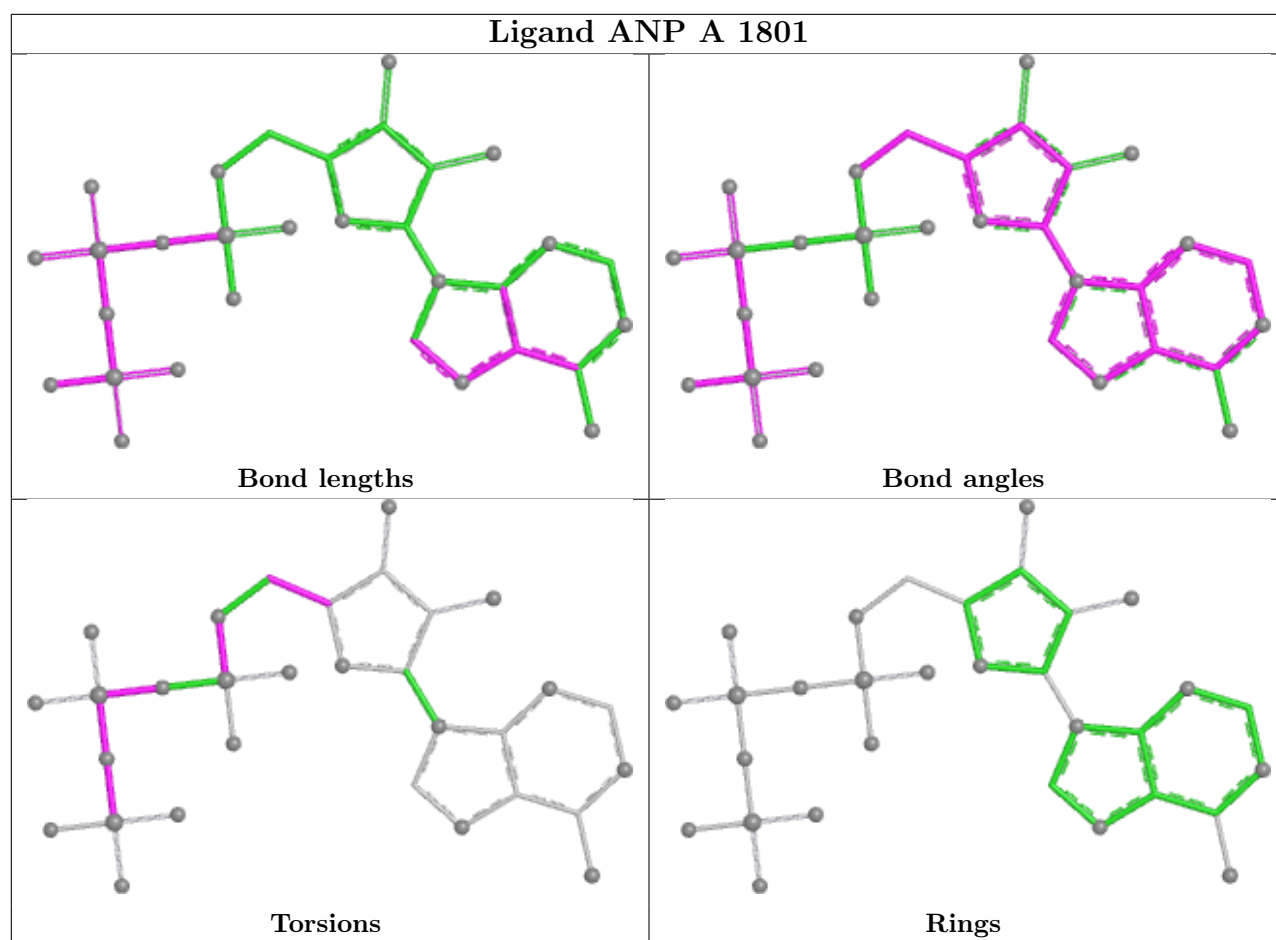
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

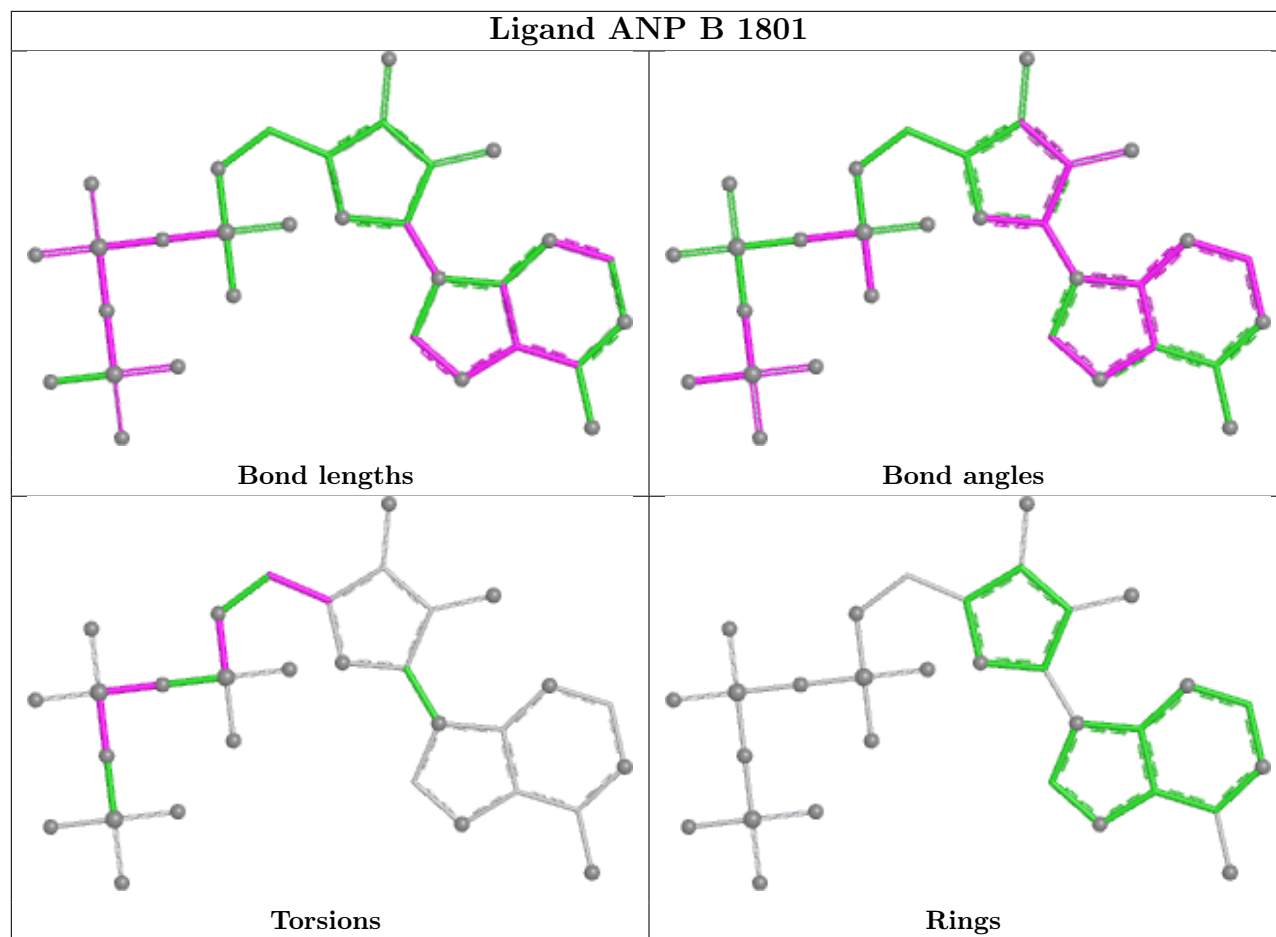












5.7 Other polymers [i](#)

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 ⓘ

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%)	0.13	14 (2%) 63 54	177, 220, 306, 373	0
1	B	663/800 (82%)	0.12	15 (2%) 61 53	196, 245, 311, 362	0
1	E	663/800 (82%)	0.07	14 (2%) 63 54	191, 224, 348, 398	0
1	F	663/800 (82%)	0.10	19 (2%) 53 47	181, 220, 296, 350	0
1	I	663/800 (82%)	0.13	10 (1%) 72 60	198, 244, 528, 643	0
1	J	663/800 (82%)	0.11	11 (1%) 69 59	213, 266, 510, 602	0
2	C	285/369 (77%)	0.19	3 (1%) 78 66	200, 237, 282, 323	0
2	D	285/369 (77%)	0.31	11 (3%) 43 42	193, 234, 273, 296	0
2	G	285/369 (77%)	0.27	7 (2%) 58 50	217, 239, 319, 347	0
2	H	285/369 (77%)	0.46	11 (3%) 43 42	210, 227, 268, 294	0
2	K	285/369 (77%)	0.30	10 (3%) 47 43	197, 233, 295, 329	0
2	L	285/369 (77%)	0.32	14 (4%) 35 36	233, 264, 336, 375	0
All	All	5688/7014 (81%)	0.17	139 (2%) 59 52	177, 237, 355, 643	0

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	49	GLY	11.2
2	H	49	GLY	8.6
2	L	82	SER	5.1
2	K	260	GLY	4.7
2	H	51	ALA	4.5
1	J	212	GLN	4.4
1	A	712	ALA	4.4
2	D	208	LYS	4.4
1	I	694	GLU	4.1
1	E	702	TYR	4.1
2	L	70	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
2	H	50	GLY	4.0
1	B	784	GLU	4.0
2	K	125	ALA	3.8
1	A	315	VAL	3.7
1	E	555	LEU	3.6
2	L	198	GLN	3.6
1	B	368	MET	3.4
2	L	132	VAL	3.4
2	L	31	VAL	3.4
1	B	628	ALA	3.4
2	D	36	ASP	3.4
2	D	201	ALA	3.3
2	G	81	ALA	3.3
2	G	150	LEU	3.2
1	F	304	SER	3.2
2	K	132	VAL	3.2
2	C	253	ILE	3.2
1	E	336	ALA	3.1
1	A	680	ILE	3.1
1	B	671	MET	3.1
2	D	218	THR	3.1
2	K	281	GLY	3.0
2	K	73	ALA	3.0
1	E	136	ILE	3.0
2	G	132	VAL	3.0
1	I	577	GLY	2.9
1	A	388	ALA	2.9
1	F	624	MET	2.9
2	D	73	ALA	2.9
1	A	514	LEU	2.9
1	F	637	GLY	2.8
1	F	603	LEU	2.8
1	E	625	ARG	2.8
2	K	95	ARG	2.8
1	I	647	ILE	2.7
2	H	125	ALA	2.7
2	D	315	SER	2.7
1	J	301	PRO	2.7
2	D	132	VAL	2.7
2	K	160	PHE	2.7
2	K	146	GLU	2.6
1	B	531	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	645	VAL	2.6
2	L	27	VAL	2.6
1	F	639	TYR	2.6
2	H	183	PHE	2.5
1	F	407	LEU	2.5
1	E	551	GLU	2.5
1	A	672	VAL	2.5
1	E	489	TYR	2.5
1	B	732	LEU	2.5
2	D	253	ILE	2.5
2	H	263	MET	2.5
1	B	759	MET	2.5
1	E	239	ALA	2.5
1	I	641	PRO	2.5
1	I	241	LEU	2.4
2	H	146	GLU	2.4
2	L	25	SER	2.4
2	L	23	PRO	2.4
1	F	307	LEU	2.4
1	F	749	ALA	2.4
2	D	220	PHE	2.4
1	F	525	LYS	2.4
1	J	152	SER	2.4
1	J	700	SER	2.4
2	L	282	ALA	2.4
2	L	320	ASP	2.4
1	F	628	ALA	2.4
1	I	279	ILE	2.4
2	H	162	ARG	2.4
1	A	458	THR	2.4
2	H	22	ARG	2.4
1	A	277	LEU	2.4
1	E	504	PRO	2.3
1	A	356	ALA	2.3
1	B	686	GLU	2.3
1	I	469	ALA	2.3
1	A	591	VAL	2.3
2	G	104	SER	2.3
2	L	68	LEU	2.3
2	D	214	ALA	2.3
1	B	201	LEU	2.3
1	A	469	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
2	G	73	ALA	2.3
1	E	289	ASN	2.3
1	J	480	GLY	2.3
1	J	533	ASP	2.3
1	I	131	ASN	2.2
1	F	489	TYR	2.2
1	F	276	ASN	2.2
1	F	330	ALA	2.2
1	I	584	ARG	2.2
1	F	789	ALA	2.2
1	B	206	ILE	2.2
1	E	216	GLN	2.2
2	G	198	GLN	2.2
1	F	658	GLY	2.2
1	B	730	PHE	2.2
1	J	333	ASP	2.2
1	E	636	ILE	2.2
1	A	368	MET	2.2
1	E	572	PHE	2.1
1	F	212	GLN	2.1
1	I	631	ALA	2.1
1	J	300	THR	2.1
2	G	82	SER	2.1
2	C	220	PHE	2.1
1	B	289	ASN	2.1
2	H	73	ALA	2.1
2	L	242	ASP	2.1
1	A	537	PRO	2.1
1	E	454	GLU	2.1
1	F	278	GLU	2.1
2	C	132	VAL	2.1
1	B	710	ALA	2.1
1	J	336	ALA	2.1
1	J	707	LEU	2.0
1	B	436	TRP	2.0
2	D	56	ILE	2.0
2	H	155	PRO	2.0
2	L	258	VAL	2.0
1	F	638	SER	2.0
2	L	272	ILE	2.0
1	J	337	GLY	2.0
1	A	359	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	490	MET	2.0
2	K	109	THR	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

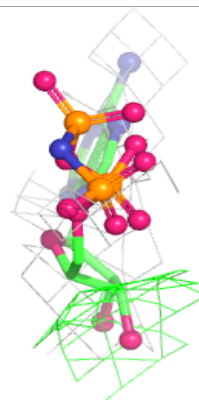
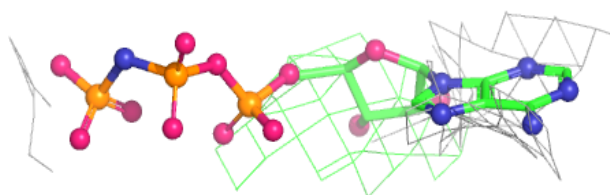
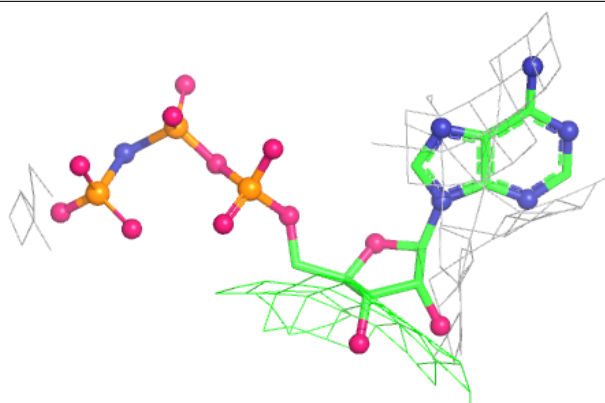
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ANP	B	1801	31/31	0.81	0.11	216,223,227,230	0
3	ANP	F	1801	31/31	0.83	0.11	195,202,206,209	0
3	ANP	I	1801	31/31	0.85	0.12	198,200,203,204	0
3	ANP	A	1801	31/31	0.91	0.10	198,206,212,215	0
3	ANP	J	1801	31/31	0.95	0.09	218,226,233,235	0
3	ANP	E	1801	31/31	0.96	0.11	198,201,206,207	0

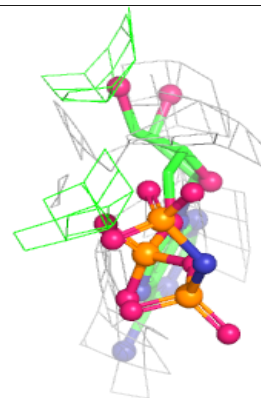
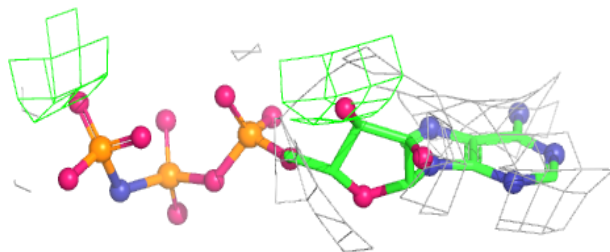
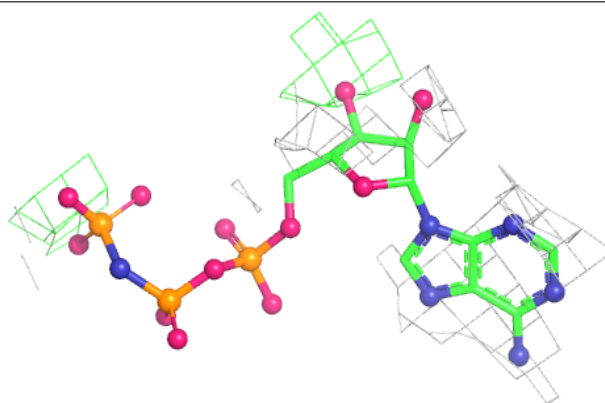
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ANP 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)

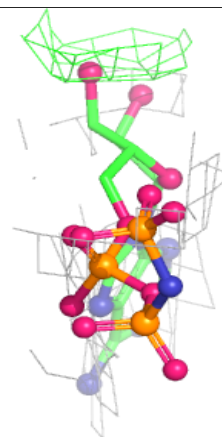
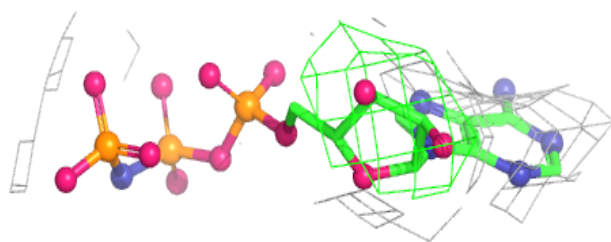
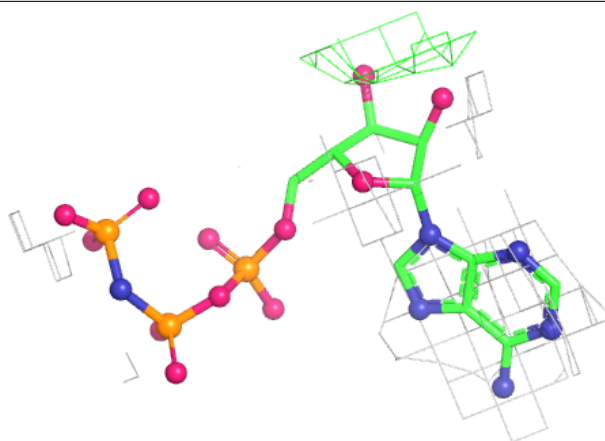
**Electron density around ANP F 1801:**

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



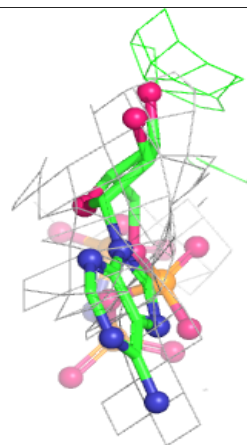
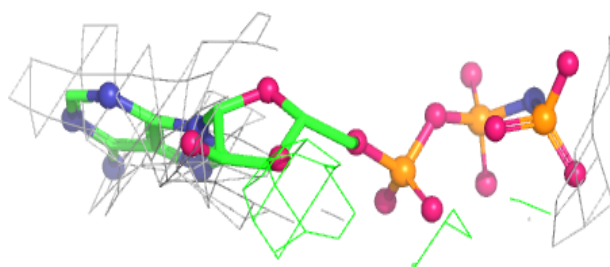
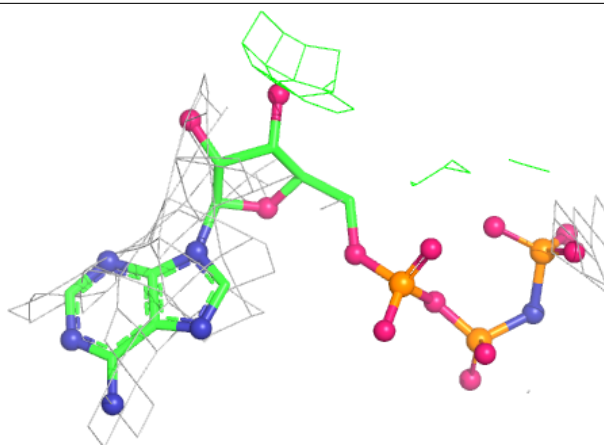
Electron density around ANP I 1801:

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

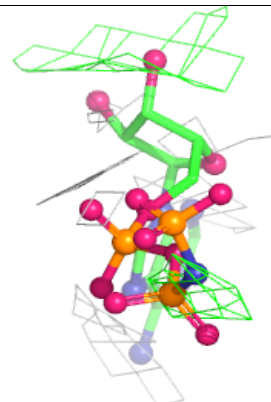
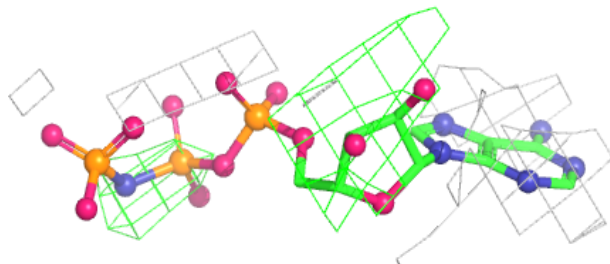
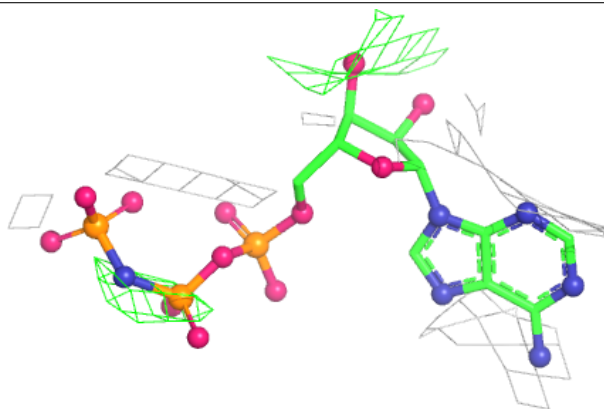


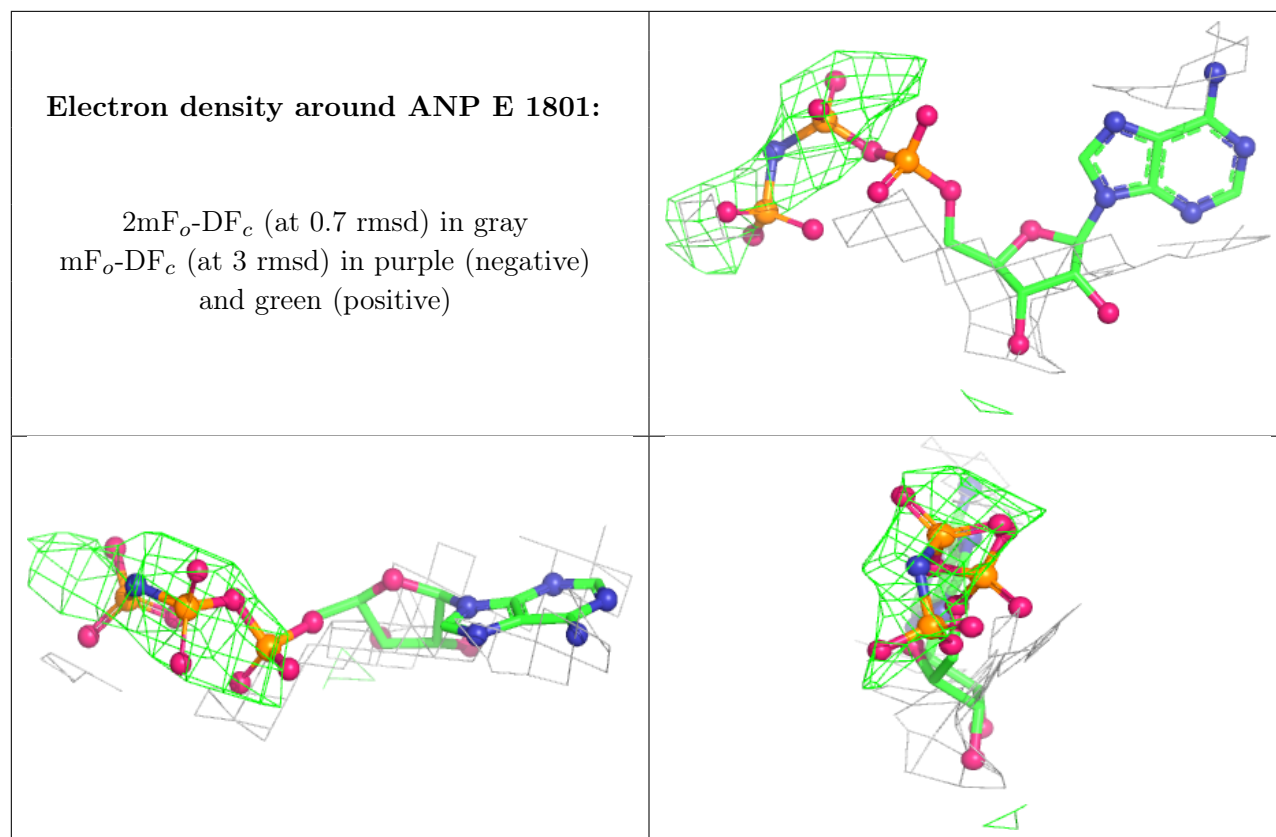
Electron density around ANP A 1801:

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

**Electron density around ANP J 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.