



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 09:17 am BST

PDB ID : 3OE7  
Title : Structure of four mutant forms of yeast f1 ATPase: gamma-I270T  
Authors : Arsenieva, D.; Symersky, J.; Wang, Y.; Pagadala, V.; Mueller, D.M.  
Deposited on : 2010-08-12  
Resolution : 3.19 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

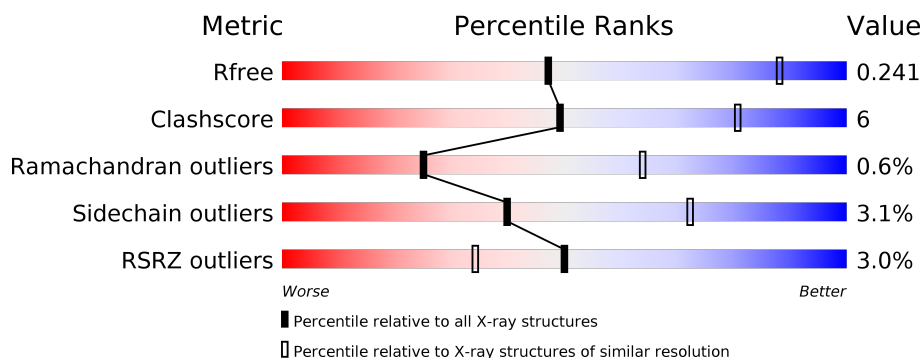
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.19 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	510	<div> <div>78%</div> <div>15%</div> <div>• 5%</div> </div>
1	B	510	<div> <div>4%</div> <div>80%</div> <div>14%</div> <div>• 5%</div> </div>
1	C	510	<div> <div>83%</div> <div>11%</div> <div>• 5%</div> </div>
1	J	510	<div> <div>80%</div> <div>14%</div> <div>• 6%</div> </div>
1	K	510	<div> <div>4%</div> <div>78%</div> <div>16%</div> <div>5%</div> </div>
1	L	510	<div> <div>79%</div> <div>15%</div> <div>• 5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	S	510	 % 82% 11% • 6%
1	T	510	 4% 76% 18% 6%
1	U	510	 6% 79% 15% 6%
2	D	484	 82% 14% •
2	E	484	 3% 80% 16% • •
2	F	484	 82% 15% • •
2	M	484	 % 80% 16% • •
2	N	484	 5% 79% 18% •
2	O	484	 % 83% 13% •
2	V	484	 6% 82% 14% • •
2	W	484	 3% 82% 13% • •
2	X	484	 4% 82% 14% • •
3	G	278	 74% 20% • 5%
3	P	278	 10% 59% 24% 5% 12%
3	Y	278	 8% 59% 12% 29%
4	H	137	 4% 71% 16% • 12%
4	Q	137	 13% 55% 6% • 39%
4	Z	137	 7% 10% • 89%
5	1	61	 15% 38% • • 59%
5	I	61	 61% 18% 21%
5	R	61	 46% 5% 49%

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 72533 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 ATP synthase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	482	Total	C	N	O	S	0	0	0
			3664	2314	648	699	3			
1	B	483	Total	C	N	O	S	0	0	0
			3669	2317	649	700	3			
1	C	484	Total	C	N	O	S	0	0	0
			3674	2319	650	702	3			
1	J	481	Total	C	N	O	S	0	0	0
			3655	2309	646	697	3			
1	K	486	Total	C	N	O	S	0	0	0
			3694	2331	652	708	3			
1	L	482	Total	C	N	O	S	0	0	0
			3664	2314	648	699	3			
1	S	480	Total	C	N	O	S	0	0	0
			3651	2307	645	696	3			
1	T	481	Total	C	N	O	S	0	0	0
			3659	2311	647	698	3			
1	U	481	Total	C	N	O	S	0	0	0
			3659	2311	647	698	3			

- Molecule 2 is a protein called ATP synthase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	470	Total	C	N	O	S	0	0	0
			3549	2250	604	689	6			
2	E	468	Total	C	N	O	S	0	0	0
			3536	2243	602	685	6			
2	F	469	Total	C	N	O	S	0	0	0
			3543	2247	603	687	6			
2	M	470	Total	C	N	O	S	0	0	0
			3549	2250	604	689	6			
2	N	470	Total	C	N	O	S	0	0	0
			3549	2250	604	689	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	468	Total	C	N	O	S	0	0	0
			3538	2244	602	686	6			
2	V	470	Total	C	N	O	S	0	0	0
			3549	2250	604	689	6			
2	W	467	Total	C	N	O	S	0	0	0
			3531	2240	601	684	6			
2	X	469	Total	C	N	O	S	0	0	0
			3543	2247	603	687	6			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-5	ALA	-	EXPRESSION TAG	UNP P00830
D	-4	SER	-	EXPRESSION TAG	UNP P00830
D	-3	HIS	-	EXPRESSION TAG	UNP P00830
D	-2	HIS	-	EXPRESSION TAG	UNP P00830
D	-1	HIS	-	EXPRESSION TAG	UNP P00830
D	0	HIS	-	EXPRESSION TAG	UNP P00830
D	1	HIS	-	EXPRESSION TAG	UNP P00830
D	2	HIS	-	EXPRESSION TAG	UNP P00830
E	-5	ALA	-	EXPRESSION TAG	UNP P00830
E	-4	SER	-	EXPRESSION TAG	UNP P00830
E	-3	HIS	-	EXPRESSION TAG	UNP P00830
E	-2	HIS	-	EXPRESSION TAG	UNP P00830
E	-1	HIS	-	EXPRESSION TAG	UNP P00830
E	0	HIS	-	EXPRESSION TAG	UNP P00830
E	1	HIS	-	EXPRESSION TAG	UNP P00830
E	2	HIS	-	EXPRESSION TAG	UNP P00830
F	-5	ALA	-	EXPRESSION TAG	UNP P00830
F	-4	SER	-	EXPRESSION TAG	UNP P00830
F	-3	HIS	-	EXPRESSION TAG	UNP P00830
F	-2	HIS	-	EXPRESSION TAG	UNP P00830
F	-1	HIS	-	EXPRESSION TAG	UNP P00830
F	0	HIS	-	EXPRESSION TAG	UNP P00830
F	1	HIS	-	EXPRESSION TAG	UNP P00830
F	2	HIS	-	EXPRESSION TAG	UNP P00830
M	-5	ALA	-	EXPRESSION TAG	UNP P00830
M	-4	SER	-	EXPRESSION TAG	UNP P00830
M	-3	HIS	-	EXPRESSION TAG	UNP P00830
M	-2	HIS	-	EXPRESSION TAG	UNP P00830
M	-1	HIS	-	EXPRESSION TAG	UNP P00830
M	0	HIS	-	EXPRESSION TAG	UNP P00830
M	1	HIS	-	EXPRESSION TAG	UNP P00830

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Chain	Residue	Modelled	Actual	Comment	Reference
M	2	HIS	-	EXPRESSION TAG	UNP P00830
N	-5	ALA	-	EXPRESSION TAG	UNP P00830
N	-4	SER	-	EXPRESSION TAG	UNP P00830
N	-3	HIS	-	EXPRESSION TAG	UNP P00830
N	-2	HIS	-	EXPRESSION TAG	UNP P00830
N	-1	HIS	-	EXPRESSION TAG	UNP P00830
N	0	HIS	-	EXPRESSION TAG	UNP P00830
N	1	HIS	-	EXPRESSION TAG	UNP P00830
N	2	HIS	-	EXPRESSION TAG	UNP P00830
O	-5	ALA	-	EXPRESSION TAG	UNP P00830
O	-4	SER	-	EXPRESSION TAG	UNP P00830
O	-3	HIS	-	EXPRESSION TAG	UNP P00830
O	-2	HIS	-	EXPRESSION TAG	UNP P00830
O	-1	HIS	-	EXPRESSION TAG	UNP P00830
O	0	HIS	-	EXPRESSION TAG	UNP P00830
O	1	HIS	-	EXPRESSION TAG	UNP P00830
O	2	HIS	-	EXPRESSION TAG	UNP P00830
V	-5	ALA	-	EXPRESSION TAG	UNP P00830
V	-4	SER	-	EXPRESSION TAG	UNP P00830
V	-3	HIS	-	EXPRESSION TAG	UNP P00830
V	-2	HIS	-	EXPRESSION TAG	UNP P00830
V	-1	HIS	-	EXPRESSION TAG	UNP P00830
V	0	HIS	-	EXPRESSION TAG	UNP P00830
V	1	HIS	-	EXPRESSION TAG	UNP P00830
V	2	HIS	-	EXPRESSION TAG	UNP P00830
W	-5	ALA	-	EXPRESSION TAG	UNP P00830
W	-4	SER	-	EXPRESSION TAG	UNP P00830
W	-3	HIS	-	EXPRESSION TAG	UNP P00830
W	-2	HIS	-	EXPRESSION TAG	UNP P00830
W	-1	HIS	-	EXPRESSION TAG	UNP P00830
W	0	HIS	-	EXPRESSION TAG	UNP P00830
W	1	HIS	-	EXPRESSION TAG	UNP P00830
W	2	HIS	-	EXPRESSION TAG	UNP P00830
X	-5	ALA	-	EXPRESSION TAG	UNP P00830
X	-4	SER	-	EXPRESSION TAG	UNP P00830
X	-3	HIS	-	EXPRESSION TAG	UNP P00830
X	-2	HIS	-	EXPRESSION TAG	UNP P00830
X	-1	HIS	-	EXPRESSION TAG	UNP P00830
X	0	HIS	-	EXPRESSION TAG	UNP P00830
X	1	HIS	-	EXPRESSION TAG	UNP P00830
X	2	HIS	-	EXPRESSION TAG	UNP P00830

- Molecule 3 is a protein called ATP synthase subunit gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	265	Total	C	N	O	S	0	0	0
			2042	1282	356	394	10			
3	P	244	Total	C	N	O	S	0	0	0
			1847	1159	322	357	9			
3	Y	198	Total	C	N	O	S	0	0	0
			1356	827	250	272	7			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	270	THR	ILE	ENGINEERED MUTATION	UNP P38077
P	270	THR	ILE	ENGINEERED MUTATION	UNP P38077
Y	270	THR	ILE	ENGINEERED MUTATION	UNP P38077

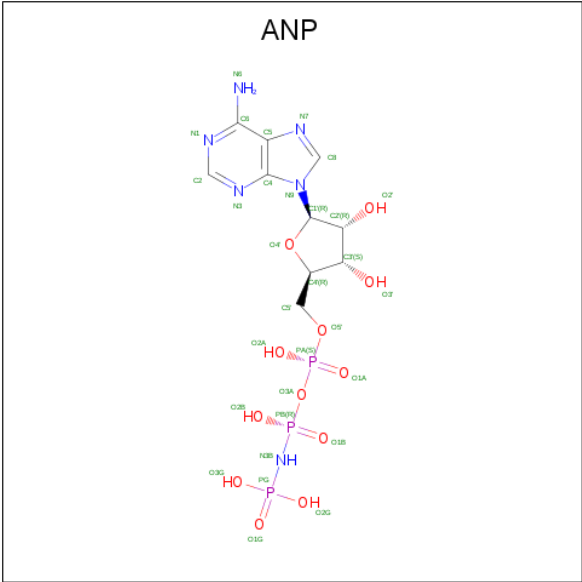
- Molecule 4 is a protein called ATP synthase subunit delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	120	Total	C	N	O	S	0	0	0
			775	484	135	154	2			
4	Q	84	Total	C	N	O		0	0	0
			449	271	88	90				
4	Z	15	Total	C	N	O		0	0	0
			75	45	15	15				

- Molecule 5 is a protein called ATP synthase subunit epsilon.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	48	Total	C	N	O	0	0	0
			330	204	59	67			
5	R	31	Total	C	N	O	0	0	0
			173	107	32	34			
5	1	25	Total	C	N	O	0	0	0
			125	75	25	25			

- Molecule 6 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>12</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	F	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	J	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	K	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	L	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	M	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	O	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	S	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	T	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	U	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	V	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

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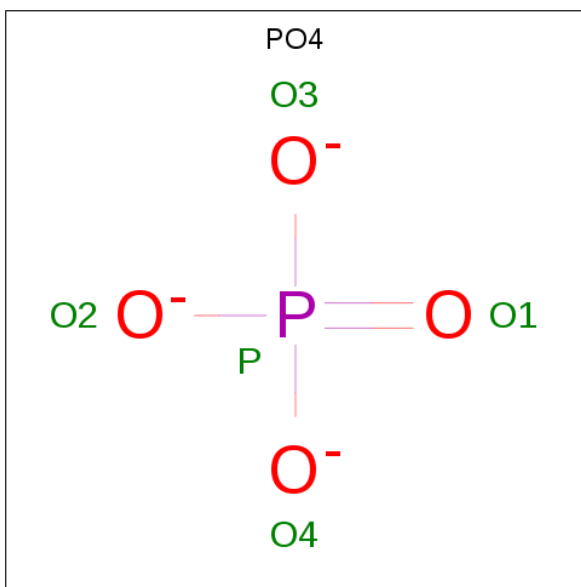
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	X	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	J	1	Total	Mg	0	0
			1	1		
7	D	1	Total	Mg	0	0
			1	1		
7	K	1	Total	Mg	0	0
			1	1		
7	B	1	Total	Mg	0	0
			1	1		
7	C	1	Total	Mg	0	0
			1	1		
7	V	1	Total	Mg	0	0
			1	1		
7	A	1	Total	Mg	0	0
			1	1		
7	T	1	Total	Mg	0	0
			1	1		
7	U	1	Total	Mg	0	0
			1	1		
7	X	1	Total	Mg	0	0
			1	1		
7	O	1	Total	Mg	0	0
			1	1		
7	L	1	Total	Mg	0	0
			1	1		
7	S	1	Total	Mg	0	0
			1	1		
7	F	1	Total	Mg	0	0
			1	1		
7	M	1	Total	Mg	0	0
			1	1		

- Molecule 8 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).

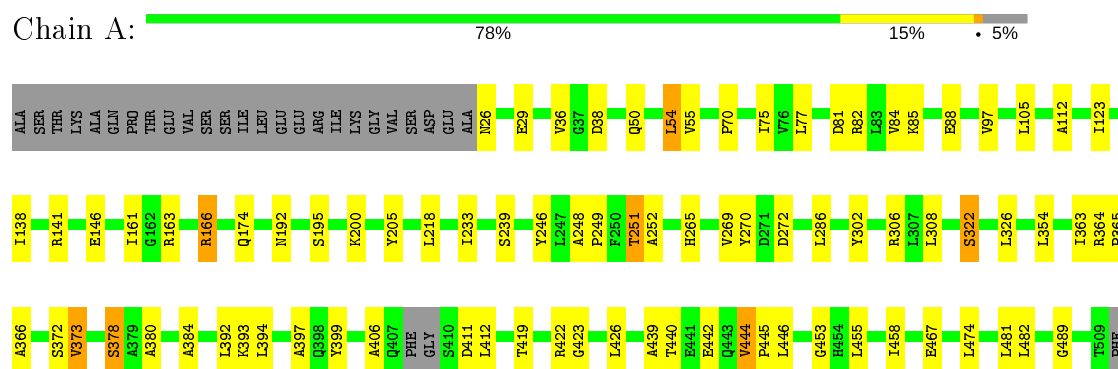


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	N	1	Total	O	P	0	0
			5	4	1		

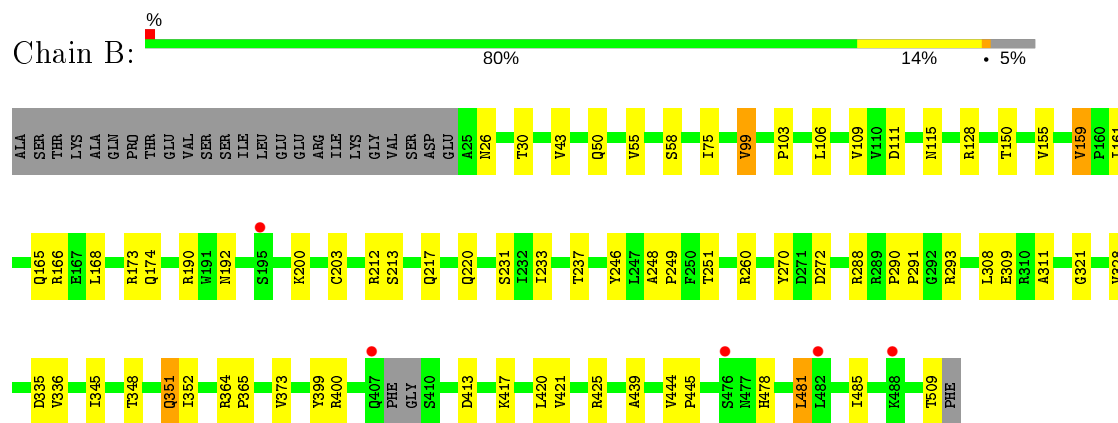
### 3 Residue-property plots

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

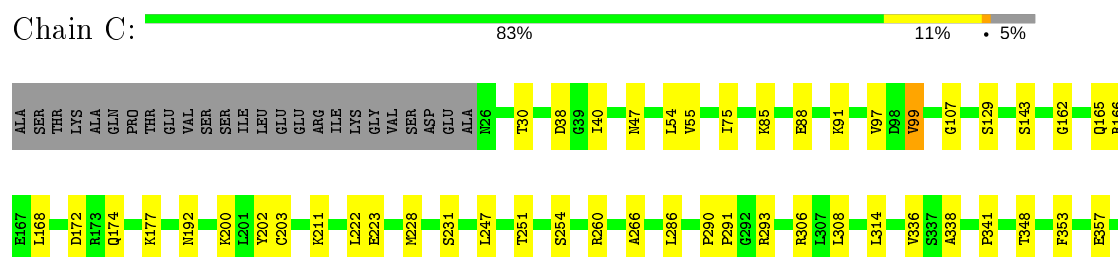
#### • Molecule 1: ATP synthase subunit alpha



#### • Molecule 1: ATP synthase subunit alpha



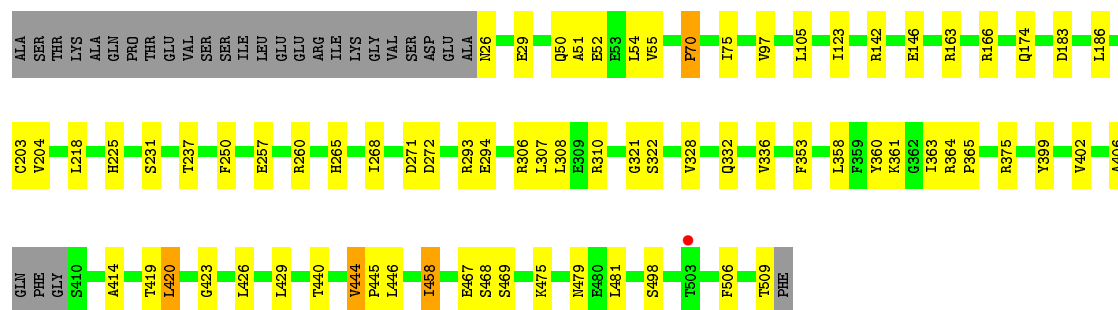
#### • Molecule 1: ATP synthase subunit alpha





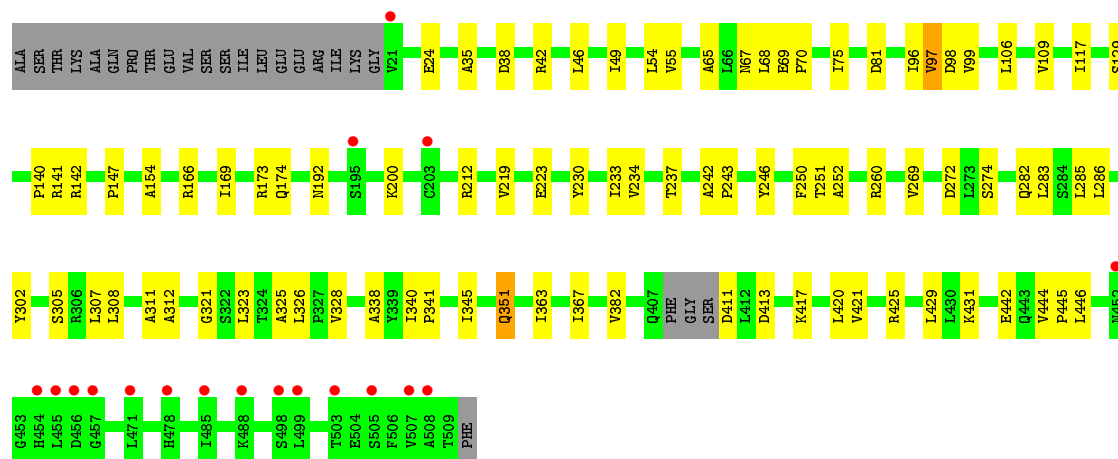
- Molecule 1: ATP synthase subunit alpha

Chain J: 80% 14% 6%



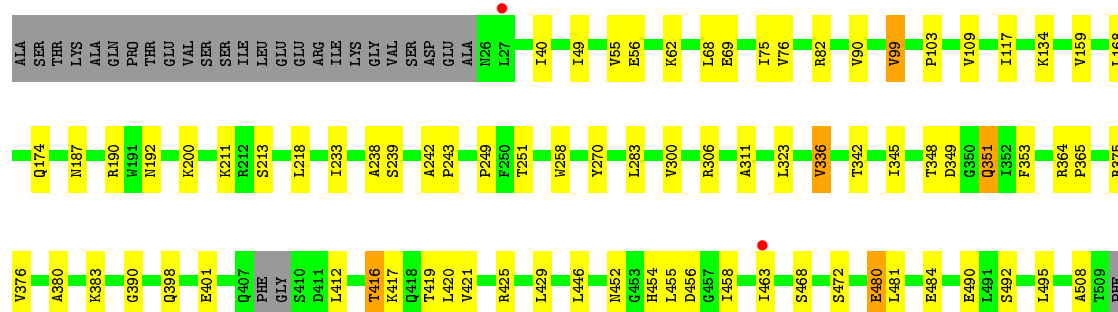
- Molecule 1: ATP synthase subunit alpha

Chain K: 4% 78% 16% 5%

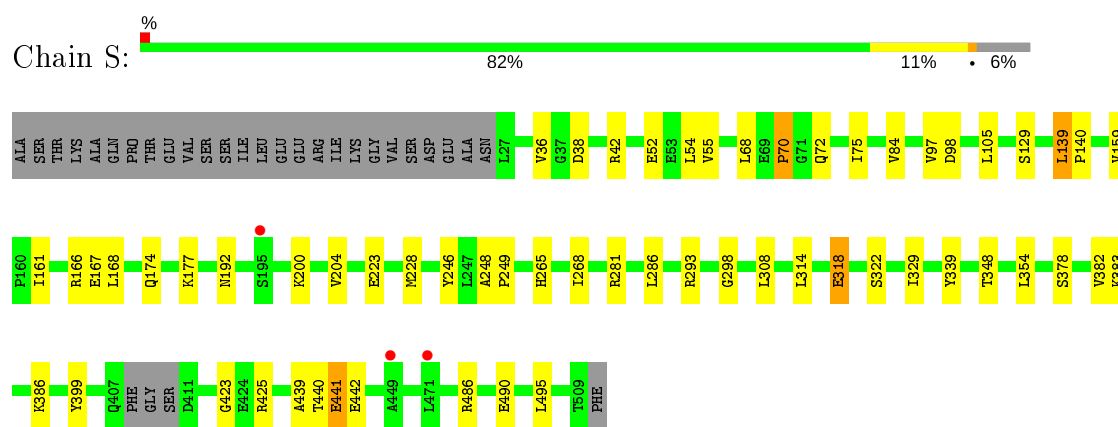


- Molecule 1: ATP synthase subunit alpha

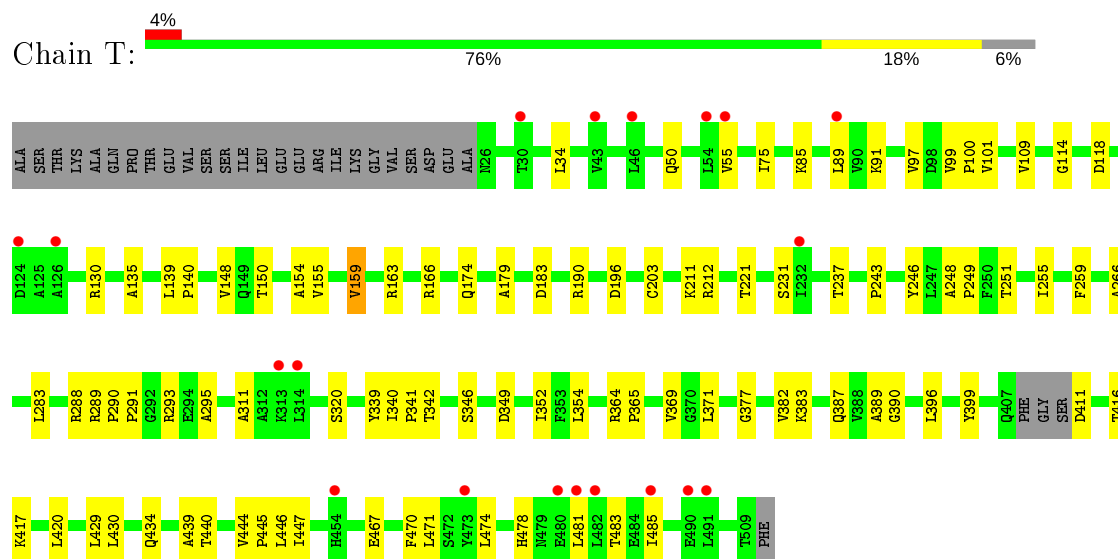
Chain L: 79% 15% 5%



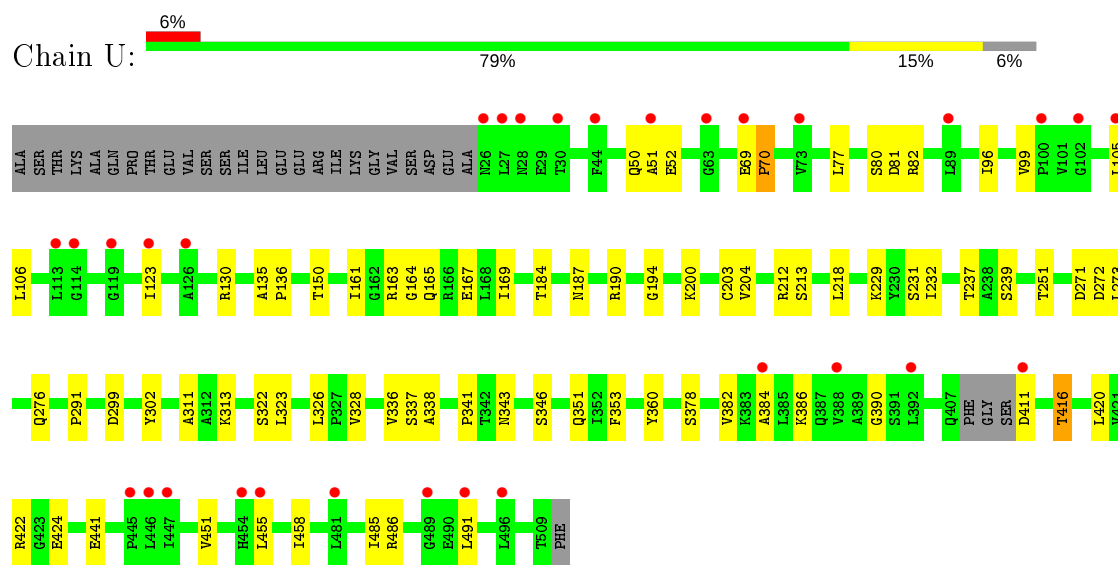
- Molecule 1: ATP synthase subunit alpha




• Molecule 1: ATP synthase subunit alpha

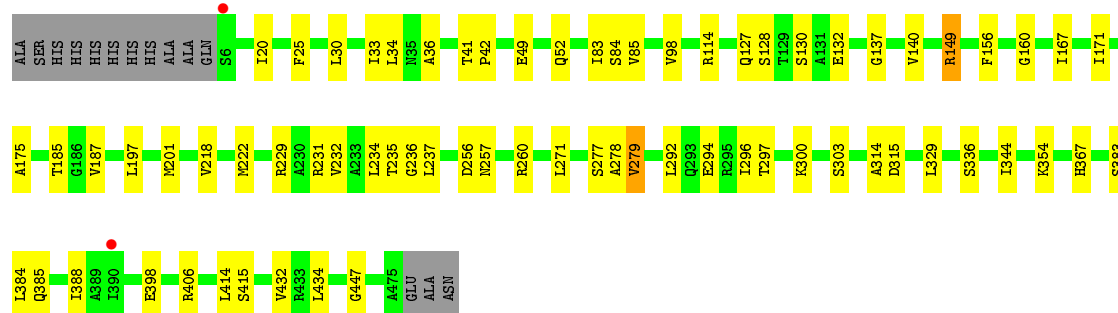


• Molecule 1: ATP synthase subunit alpha




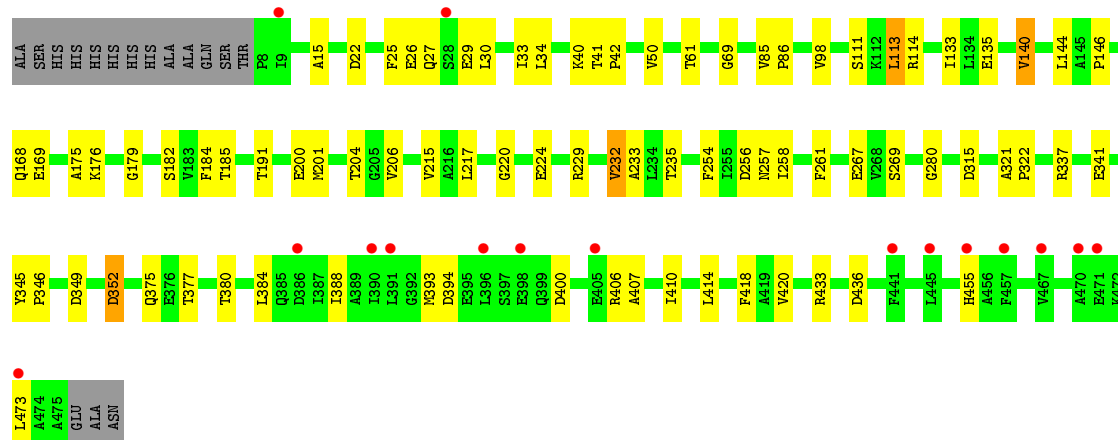
• Molecule 2: ATP synthase subunit beta

Chain D:  82% 14%




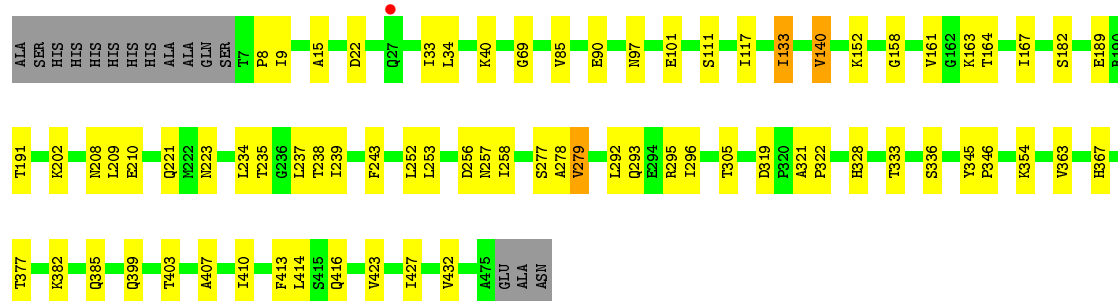
• Molecule 2: ATP synthase subunit beta

Chain E:  3% 80% 16%




• Molecule 2: ATP synthase subunit beta

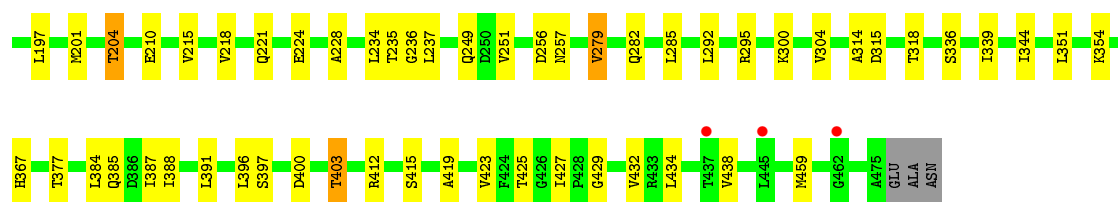
Chain F:  82% 15%



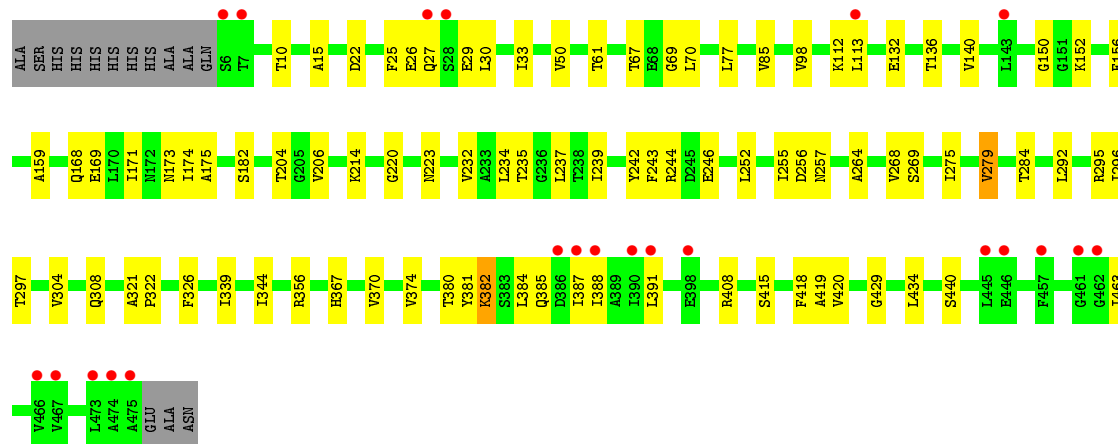
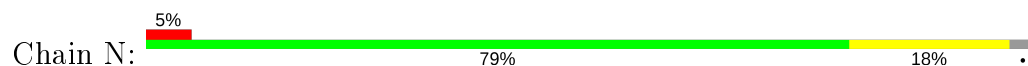
• Molecule 2: ATP synthase subunit beta

Chain M:  80% 16%

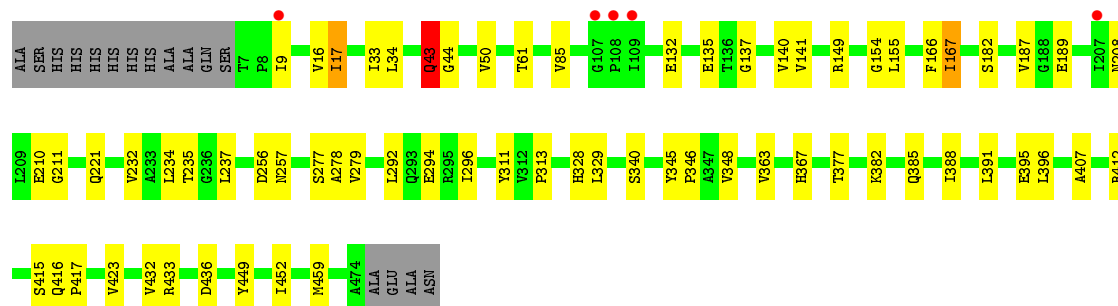
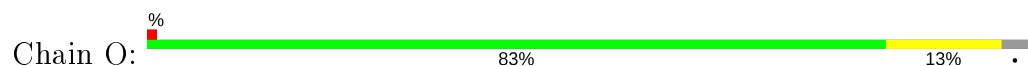




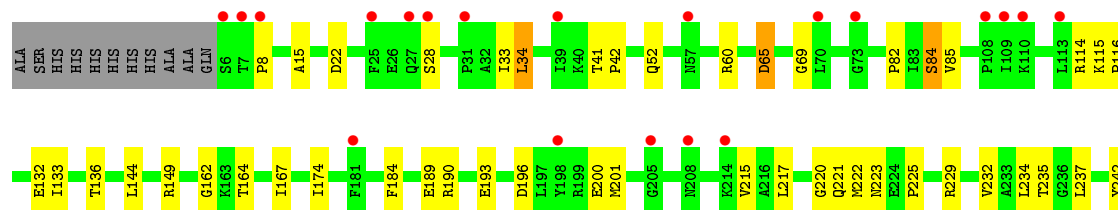
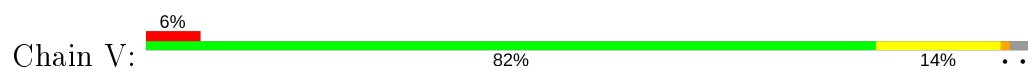
• Molecule 2: ATP synthase subunit beta

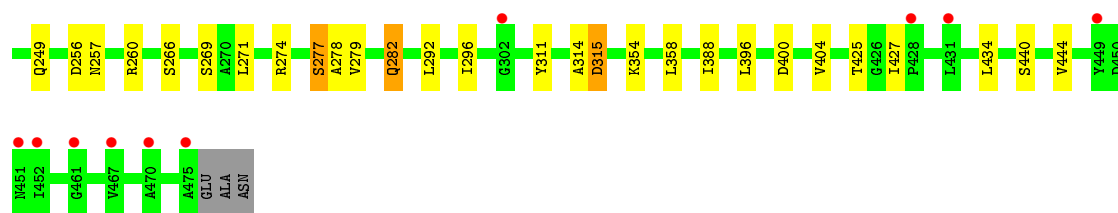


• Molecule 2: ATP synthase subunit beta

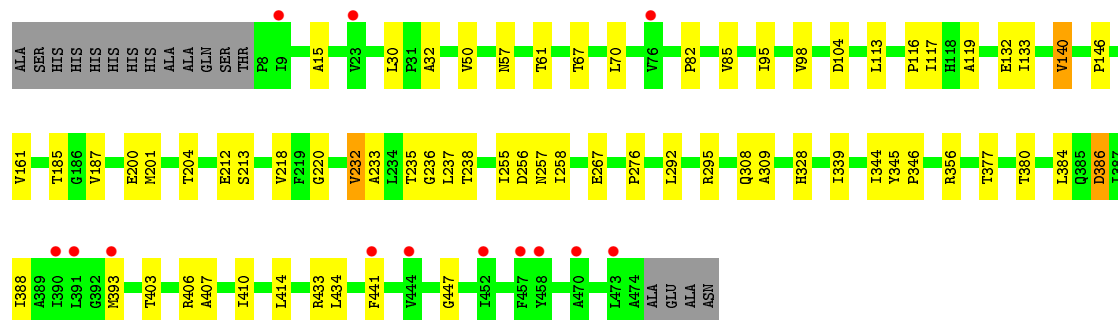
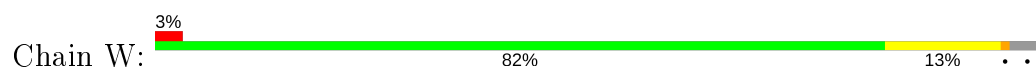


• Molecule 2: ATP synthase subunit beta

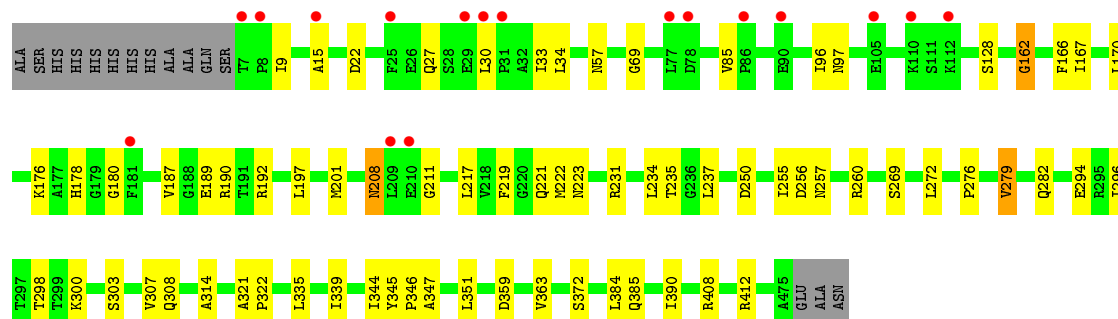
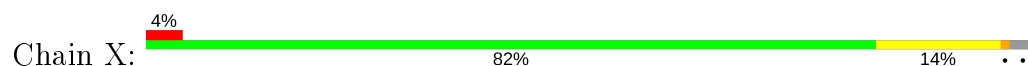




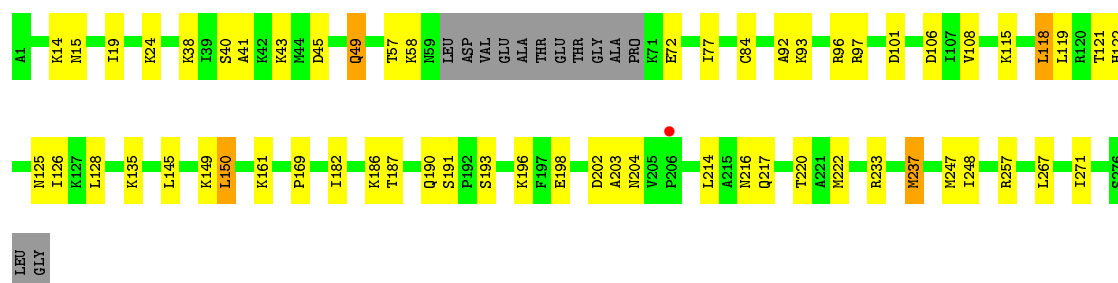
• Molecule 2: ATP synthase subunit beta



• Molecule 2: ATP synthase subunit beta



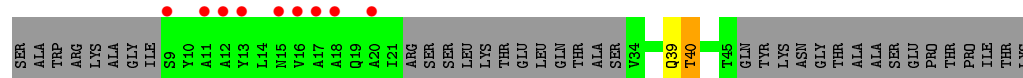
• Molecule 3: ATP synthase subunit gamma



• Molecule 3: ATP synthase subunit gamma







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	111.03Å 292.21Å 189.05Å 90.00° 101.82° 90.00°	Depositor
Resolution (Å)	20.00 – 3.19 49.47 – 3.19	Depositor EDS
% Data completeness (in resolution range)	95.4 (20.00-3.19) 95.4 (49.47-3.19)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.18 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.189 , 0.245 0.188 , 0.241	Depositor DCC
$R_{free}$ test set	9702 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	84.9	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 53.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	72533	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: PO4, ANP, MG

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	0.43	0/3718	0.60	0/5032
1	B	0.38	0/3723	0.56	0/5039
1	C	0.39	0/3729	0.56	0/5048
1	J	0.36	0/3709	0.54	0/5020
1	K	0.37	0/3748	0.53	0/5073
1	L	0.40	0/3718	0.57	0/5032
1	S	0.36	0/3705	0.54	0/5014
1	T	0.36	0/3713	0.51	0/5025
1	U	0.37	0/3713	0.52	0/5025
2	D	0.41	0/3605	0.58	0/4889
2	E	0.41	0/3592	0.56	1/4870 (0.0%)
2	F	0.39	0/3599	0.56	0/4881
2	M	0.40	0/3605	0.56	0/4889
2	N	0.38	0/3605	0.53	0/4889
2	O	0.37	0/3594	0.55	0/4874
2	V	0.37	0/3605	0.53	0/4889
2	W	0.37	0/3587	0.53	0/4863
2	X	0.37	0/3599	0.53	0/4881
3	G	0.39	0/2067	0.54	0/2782
3	P	0.36	0/1865	0.52	0/2508
3	Y	0.32	0/1361	0.46	0/1843
4	H	0.40	0/783	0.54	0/1072
4	Q	0.34	0/448	0.51	0/614
4	Z	0.31	0/74	0.44	0/102
5	1	0.32	0/123	0.50	0/169
5	I	0.44	0/332	0.59	0/452
5	R	0.38	0/173	0.53	0/238
All	All	0.38	0/73093	0.55	1/99013 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	113	LEU	CA-CB-CG	5.21	127.27	115.30

There are no chirality outliers.

There are no planarity outliers.

## 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	3664	0	3747	47	0
1	B	3669	0	3752	41	0
1	C	3674	0	3756	33	0
1	J	3655	0	3739	43	0
1	K	3694	0	3774	51	0
1	L	3664	0	3747	43	0
1	S	3651	0	3739	35	0
1	T	3659	0	3745	49	0
1	U	3659	0	3745	46	0
2	D	3549	0	3620	42	0
2	E	3536	0	3610	42	0
2	F	3543	0	3616	45	0
2	M	3549	0	3620	54	0
2	N	3549	0	3621	54	0
2	O	3538	0	3610	38	0
2	V	3549	0	3620	48	0
2	W	3531	0	3605	41	0
2	X	3543	0	3616	43	0
3	G	2042	0	2102	33	0
3	P	1847	0	1873	43	0
3	Y	1356	0	1262	15	0
4	H	775	0	640	19	0
4	Q	449	0	240	4	0
4	Z	75	0	38	0	0
5	1	125	0	66	1	0
5	I	330	0	260	8	0
5	R	173	0	101	0	0
6	A	31	0	13	1	0
6	B	31	0	13	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	31	0	13	1	0
6	D	31	0	13	4	0
6	F	31	0	13	0	0
6	J	31	0	13	0	0
6	K	31	0	13	0	0
6	L	31	0	13	1	0
6	M	31	0	13	2	0
6	O	31	0	13	0	0
6	S	31	0	13	0	0
6	T	31	0	13	2	0
6	U	31	0	13	0	0
6	V	31	0	13	1	0
6	X	31	0	13	2	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
7	F	1	0	0	0	0
7	J	1	0	0	0	0
7	K	1	0	0	0	0
7	L	1	0	0	0	0
7	M	1	0	0	0	0
7	O	1	0	0	0	0
7	S	1	0	0	0	0
7	T	1	0	0	0	0
7	U	1	0	0	0	0
7	V	1	0	0	0	0
7	X	1	0	0	0	0
8	N	5	0	0	0	0
All	All	72533	0	73059	852	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 6.

All (852) 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)
3:G:96:ARG:HE	3:G:121:THR:HG21	1.25	0.98
2:E:85:VAL:HG11	2:E:235:THR:HG23	1.47	0.96
3:P:180:LYS:HZ3	3:P:220:THR:HB	1.33	0.94
1:K:99:VAL:HG11	1:K:251:THR:HB	1.48	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:85:VAL:HG11	2:F:235:THR:HG23	1.51	0.92
2:M:85:VAL:HG11	2:M:235:THR:HG23	1.52	0.92
2:M:160:GLY:H	6:M:600:ANP:HNB1	1.08	0.91
1:L:99:VAL:HG11	1:L:251:THR:HB	1.54	0.88
2:D:85:VAL:HG11	2:D:235:THR:HG23	1.54	0.87
4:H:14:PHE:HZ	4:H:70:ILE:HD11	1.45	0.82
3:P:95:VAL:O	3:P:99:LEU:HB2	1.79	0.81
1:J:481:LEU:HD13	1:J:498:SER:HB3	1.63	0.79
1:A:239:SER:HB3	2:D:294:GLU:HG3	1.64	0.78
4:H:16:LEU:HD11	4:H:90:ALA:HB3	1.66	0.78
1:U:212:ARG:HG3	1:U:237:THR:HG21	1.67	0.77
5:I:33:SER:O	5:I:37:ARG:HG3	1.85	0.77
3:P:45:ASP:O	3:P:49:GLN:HB2	1.85	0.76
1:S:441:GLU:HG2	1:S:486:ARG:HB2	1.66	0.76
1:A:55:VAL:HG21	1:A:75:ILE:HD13	1.66	0.76
2:E:135:GLU:OE2	2:E:433:ARG:HD3	1.85	0.76
1:L:398:GLN:HE22	2:M:412:ARG:HE	1.33	0.76
2:W:85:VAL:HG11	2:W:235:THR:HG23	1.65	0.76
3:G:45:ASP:O	3:G:49:GLN:HB2	1.85	0.76
2:V:65:ASP:HA	2:V:225:PRO:HG3	1.68	0.75
3:P:31:LEU:O	3:P:35:GLU:HG2	1.87	0.75
1:S:223:GLU:HG3	1:S:228:MET:HG3	1.69	0.74
2:O:85:VAL:HG11	2:O:235:THR:HG23	1.68	0.74
1:J:70:PRO:HD3	2:N:15:ALA:HB2	1.70	0.74
1:B:444:VAL:HG23	1:B:445:PRO:HD3	1.70	0.73
1:B:413:ASP:O	1:B:417:LYS:HB2	1.90	0.72
3:P:180:LYS:NZ	3:P:220:THR:HB	2.02	0.72
1:S:425:ARG:HG2	1:S:425:ARG:HH11	1.55	0.72
2:M:388:ILE:HG12	2:M:396:LEU:HD21	1.73	0.71
1:B:26:ASN:O	1:B:30:THR:HB	1.90	0.71
3:Y:133:ILE:HD12	3:Y:134:GLY:H	1.55	0.70
3:G:72:GLU:HG3	3:G:161:LYS:HB3	1.73	0.70
2:D:41:THR:HB	2:D:42:PRO:HD2	1.73	0.70
1:B:212:ARG:HG2	1:B:237:THR:HG21	1.73	0.70
1:T:85:LYS:HE2	2:W:32:ALA:HB2	1.74	0.70
2:X:208:ASN:HD22	2:X:211:GLY:H	1.36	0.70
3:G:193:SER:HB3	3:G:196:LYS:HG3	1.73	0.70
3:G:43:LYS:HB2	4:H:20:THR:HG21	1.74	0.70
2:W:50:VAL:HA	2:W:61:THR:HG22	1.72	0.70
1:S:265:HIS:ND1	1:S:322:SER:HB2	2.07	0.69
4:H:45:HIS:HB3	4:H:77:VAL:HG11	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:14:PHE:CZ	4:H:70:ILE:HD11	2.28	0.69
1:J:469:SER:HB3	1:J:506:PHE:HZ	1.56	0.69
2:M:160:GLY:N	6:M:600:ANP:HNB1	1.87	0.68
2:D:234:LEU:CD2	2:D:292:LEU:HD13	2.23	0.68
2:D:218:VAL:HG21	2:D:236:GLY:HA2	1.74	0.68
1:U:77:LEU:HD13	1:U:81:ASP:HB3	1.76	0.68
1:K:212:ARG:HG2	1:K:237:THR:HG21	1.76	0.68
2:M:234:LEU:HD23	2:M:292:LEU:HD13	1.76	0.67
2:N:85:VAL:HG11	2:N:235:THR:HG23	1.77	0.67
2:N:419:ALA:HA	2:N:429:GLY:HA3	1.76	0.67
2:E:15:ALA:HB3	2:E:22:ASP:HB2	1.75	0.67
1:A:77:LEU:HD12	1:A:81:ASP:HB3	1.75	0.67
1:S:192:ASN:HA	1:S:200:LYS:HG2	1.76	0.66
2:V:33:ILE:O	2:V:34:LEU:HB2	1.94	0.66
3:G:93:LYS:HE3	3:G:97:ARG:HH12	1.60	0.66
2:M:384:LEU:HA	2:M:387:ILE:HD13	1.75	0.66
2:O:391:LEU:HB3	2:O:395:GLU:HG3	1.76	0.66
2:X:197:LEU:O	2:X:201:MET:HG2	1.96	0.66
1:K:444:VAL:HG23	1:K:445:PRO:HD3	1.76	0.65
1:L:55:VAL:HG21	1:L:75:ILE:HD13	1.77	0.65
1:J:336:VAL:HG11	1:J:353:PHE:HE1	1.61	0.65
1:K:54:LEU:HG	1:K:97:VAL:HG22	1.77	0.65
2:N:85:VAL:CG1	2:N:235:THR:HG23	2.26	0.65
2:V:41:THR:HB	2:V:42:PRO:HD2	1.77	0.65
1:J:265:HIS:ND1	1:J:322:SER:HB3	2.11	0.65
2:E:280:GLY:HA2	3:G:267:LEU:CD2	2.27	0.64
1:U:336:VAL:HG11	1:U:353:PHE:HE1	1.61	0.64
1:K:166:ARG:HD3	1:K:308:LEU:O	1.97	0.64
1:T:174:GLN:HA	6:T:600:ANP:HNB1	1.62	0.64
1:A:166:ARG:HD2	1:A:308:LEU:O	1.97	0.64
1:A:70:PRO:HD3	2:E:15:ALA:HB2	1.80	0.64
1:A:455:LEU:HA	1:A:458:ILE:HD12	1.79	0.64
1:L:383:LYS:HG2	1:L:490:GLU:HG3	1.79	0.64
1:T:99:VAL:HG11	1:T:251:THR:HB	1.79	0.63
2:D:171:ILE:O	2:D:175:ALA:HB3	1.98	0.63
3:P:110:ILE:HG22	3:P:133:ILE:HD13	1.81	0.63
3:P:78:THR:HG23	3:P:91:LEU:HD22	1.81	0.63
2:F:133:ILE:HD12	2:F:133:ILE:H	1.63	0.62
1:U:441:GLU:HG2	1:U:486:ARG:HB2	1.79	0.62
1:B:166:ARG:HD3	1:B:308:LEU:O	1.99	0.62
2:D:149:ARG:CG	2:D:149:ARG:HH11	2.12	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:387:ILE:HA	2:M:391:LEU:HD12	1.82	0.62
4:H:89:GLU:OE2	5:I:37:ARG:NH2	2.33	0.62
2:O:132:GLU:HB3	2:O:149:ARG:HB2	1.82	0.62
1:U:360:TYR:CE2	2:X:351:LEU:O	2.53	0.62
2:F:152:LYS:NZ	2:F:293:GLN:HG3	2.14	0.62
1:B:50:GLN:HB3	2:F:69:GLY:HA2	1.81	0.62
2:D:185:THR:HG23	2:D:218:VAL:HB	1.81	0.62
1:S:168:LEU:HB2	1:S:348:THR:HG21	1.82	0.62
1:L:68:LEU:HB3	2:M:72:ARG:HD3	1.81	0.61
2:W:133:ILE:HD12	2:W:146:PRO:HB2	1.81	0.61
2:D:160:GLY:HA2	6:D:600:ANP:HNB1	1.64	0.61
2:D:187:VAL:HG12	2:D:260:ARG:HB2	1.83	0.61
1:J:444:VAL:HG22	1:J:445:PRO:HD3	1.82	0.61
2:D:84:SER:HB3	2:D:114:ARG:HE	1.66	0.61
2:F:382:LYS:HA	2:F:385:GLN:HG2	1.83	0.61
1:U:336:VAL:HG11	1:U:353:PHE:CE1	2.36	0.61
2:V:84:SER:HB3	2:V:114:ARG:HE	1.66	0.61
1:A:439:ALA:HB3	1:A:442:GLU:HG3	1.83	0.61
1:L:492:SER:H	1:L:495:LEU:HD12	1.65	0.61
2:N:26:GLU:O	2:N:29:GLU:HB3	2.01	0.61
1:B:272:ASP:HB2	1:B:328:VAL:O	2.00	0.60
2:E:133:ILE:HD12	2:E:146:PRO:HB2	1.82	0.60
2:V:314:ALA:O	2:V:315:ASP:HB2	2.00	0.60
1:J:469:SER:HB3	1:J:506:PHE:CZ	2.35	0.60
1:K:81:ASP:HB3	2:N:33:ILE:HD12	1.83	0.60
1:S:55:VAL:HG21	1:S:75:ILE:HD13	1.83	0.60
3:Y:91:LEU:HD12	3:Y:177:PRO:HB3	1.82	0.60
1:K:38:ASP:HB3	1:K:286:LEU:HD22	1.84	0.60
2:N:244:ARG:HD3	2:N:304:VAL:HG23	1.84	0.60
1:T:243:PRO:HG3	1:T:283:LEU:HD21	1.84	0.60
1:U:69:GLU:HB3	1:U:70:PRO:HD2	1.84	0.59
1:B:111:ASP:OD2	1:B:115:ASN:HB2	2.02	0.59
1:J:250:PHE:CE1	1:J:307:LEU:HB2	2.38	0.59
1:A:192:ASN:HA	1:A:200:LYS:HG2	1.85	0.59
1:J:26:ASN:ND2	1:J:29:GLU:H	2.00	0.59
4:H:16:LEU:HD21	4:H:90:ALA:HB2	1.85	0.59
1:S:70:PRO:HD3	2:W:15:ALA:HB2	1.83	0.59
1:A:265:HIS:ND1	1:A:322:SER:HB3	2.17	0.59
1:K:169:ILE:O	1:K:328:VAL:HA	2.03	0.59
1:K:174:GLN:NE2	2:N:356:ARG:HD3	2.17	0.59
2:O:234:LEU:HD23	2:O:292:LEU:HD13	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:266:SER:HA	2:V:282:GLN:HG3	1.84	0.59
2:X:85:VAL:HG11	2:X:235:THR:HG23	1.85	0.59
1:A:174:GLN:HA	6:A:600:ANP:HNB1	1.67	0.58
2:E:220:GLY:HA3	2:E:232:VAL:HG11	1.86	0.58
3:P:30:ARG:HD2	3:P:230:ILE:HG12	1.84	0.58
1:T:248:ALA:HB3	1:T:249:PRO:HD3	1.84	0.58
1:K:69:GLU:HB2	1:K:70:PRO:HD2	1.83	0.58
1:C:97:VAL:HG11	1:C:247:LEU:HD21	1.86	0.58
2:V:85:VAL:HG11	2:V:235:THR:HG23	1.85	0.58
2:N:50:VAL:HA	2:N:61:THR:HG22	1.84	0.58
3:P:13:ILE:HG22	3:P:248:ILE:HG13	1.86	0.58
1:U:302:TYR:CE1	2:V:225:PRO:HA	2.39	0.58
1:B:260:ARG:O	1:B:321:GLY:HA3	2.03	0.57
3:P:91:LEU:O	3:P:95:VAL:HG23	2.04	0.57
1:S:425:ARG:CG	1:S:425:ARG:HH11	2.17	0.57
1:T:89:LEU:HD21	1:T:91:LYS:HE3	1.87	0.57
1:A:270:TYR:O	1:A:272:ASP:HA	2.04	0.57
2:O:382:LYS:HA	2:O:385:GLN:HG2	1.85	0.57
2:D:33:ILE:O	2:D:34:LEU:HB2	2.03	0.57
2:O:33:ILE:O	2:O:34:LEU:HB2	2.05	0.57
2:N:255:ILE:HB	2:N:308:GLN:HG2	1.86	0.57
2:O:137:GLY:HA2	2:O:432:VAL:O	2.05	0.57
1:T:139:LEU:N	1:T:140:PRO:HD2	2.19	0.57
1:C:174:GLN:HA	6:C:600:ANP:HNB1	1.69	0.57
3:G:15:ASN:O	3:G:19:ILE:HG12	2.04	0.56
3:Y:78:THR:HG23	3:Y:91:LEU:HD22	1.86	0.56
1:S:248:ALA:HB3	1:S:249:PRO:HD3	1.86	0.56
2:W:388:ILE:HD12	2:W:393:MET:HG2	1.87	0.56
3:P:258:THR:O	3:P:262:VAL:HG23	2.06	0.56
3:P:42:LYS:O	3:P:46:GLU:HG2	2.05	0.56
1:C:54:LEU:HD13	1:C:97:VAL:HG22	1.86	0.56
1:J:54:LEU:HD11	1:J:97:VAL:HG22	1.88	0.56
1:K:109:VAL:HG13	1:K:233:ILE:HB	1.87	0.56
2:O:363:VAL:HB	2:O:367:HIS:ND1	2.20	0.56
1:U:337:SER:HB3	2:V:314:ALA:HB1	1.87	0.56
1:K:413:ASP:O	1:K:417:LYS:HB2	2.05	0.56
2:F:33:ILE:O	2:F:34:LEU:HB2	2.05	0.56
2:F:97:ASN:HB2	2:F:101:GLU:H	1.70	0.56
3:Y:94:ALA:HA	3:Y:97:ARG:HD3	1.87	0.56
1:A:399:TYR:CD1	1:A:423:GLY:HA3	2.40	0.56
1:S:36:VAL:HG21	1:S:84:VAL:HB	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:156:PHE:HZ	2:N:326:PHE:HZ	1.53	0.55
1:U:346:SER:HB2	2:V:260:ARG:HH22	1.71	0.55
3:P:155:LYS:O	3:P:157:GLY:N	2.38	0.55
1:S:166:ARG:HD3	1:S:308:LEU:O	2.05	0.55
3:Y:31:LEU:O	3:Y:35:GLU:HG2	2.07	0.55
2:F:252:LEU:HD23	2:F:305:THR:HB	1.89	0.55
2:F:152:LYS:HZ3	2:F:293:GLN:HG3	1.70	0.55
1:L:242:ALA:HB3	1:L:243:PRO:HD3	1.89	0.55
1:K:141:ARG:NH1	1:K:312:ALA:HB2	2.22	0.55
1:K:363:ILE:HA	1:K:431:LYS:HE2	1.87	0.55
2:O:135:GLU:OE1	2:O:433:ARG:NH2	2.40	0.55
2:O:311:TYR:CE2	2:O:313:PRO:HA	2.42	0.55
1:U:299:ASP:HB2	1:U:302:TYR:HB3	1.89	0.55
1:B:166:ARG:HG2	1:B:311:ALA:HB3	1.88	0.55
2:D:160:GLY:H	6:D:600:ANP:HNB1	1.54	0.55
3:P:40:SER:O	3:P:44:MET:HB2	2.06	0.55
1:U:336:VAL:CG1	1:U:353:PHE:HE1	2.20	0.55
1:A:392:LEU:HD13	1:A:426:LEU:HD22	1.88	0.55
2:F:234:LEU:HD23	2:F:292:LEU:HD13	1.89	0.55
1:L:342:THR:HG21	2:M:314:ALA:HA	1.88	0.55
3:P:274:ALA:O	3:P:276:SER:N	2.40	0.55
2:V:196:ASP:O	2:V:200:GLU:HG2	2.07	0.54
2:D:160:GLY:CA	6:D:600:ANP:HNB1	2.20	0.54
3:G:182:ILE:HD11	3:G:217:GLN:HB2	1.90	0.54
2:M:221:GLN:OE1	2:M:221:GLN:HA	2.08	0.54
1:B:444:VAL:HG21	1:B:485:ILE:HG21	1.90	0.54
1:T:109:VAL:HB	1:T:118:ASP:HB3	1.89	0.54
5:I:28:GLU:O	5:I:29:LEU:HB2	2.07	0.54
2:N:242:TYR:CE1	2:N:246:GLU:HG3	2.43	0.54
1:U:51:ALA:O	1:U:52:GLU:HB2	2.08	0.54
2:W:220:GLY:CA	2:W:232:VAL:HG11	2.38	0.54
1:A:54:LEU:CD1	1:A:97:VAL:HG22	2.37	0.54
2:D:234:LEU:HD23	2:D:292:LEU:HD13	1.89	0.54
2:M:387:ILE:H	2:M:387:ILE:HD12	1.73	0.54
1:T:291:PRO:HB2	1:T:295:ALA:HA	1.89	0.54
2:X:9:ILE:HG23	2:X:27:GLN:HE21	1.71	0.54
2:E:280:GLY:HA2	3:G:267:LEU:HD21	1.90	0.54
2:M:128:SER:HB2	2:M:300:LYS:HG2	1.90	0.54
2:F:90:GLU:HG3	2:F:111:SER:HA	1.90	0.54
1:J:260:ARG:O	1:J:321:GLY:HA3	2.08	0.54
1:J:360:TYR:OH	2:M:354:LYS:HE2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:397:SER:HB3	2:M:400:ASP:OD2	2.08	0.54
2:N:156:PHE:HZ	2:N:326:PHE:CZ	2.25	0.54
4:Q:17:PRO:HD2	4:Q:88:ILE:O	2.08	0.54
1:B:168:LEU:HB2	1:B:348:THR:HG21	1.90	0.53
1:L:364:ARG:HA	1:L:365:PRO:C	2.29	0.53
1:A:302:TYR:O	1:A:306:ARG:HB2	2.07	0.53
3:P:109:THR:HB	3:P:114:ILE:HG23	1.89	0.53
1:S:382:VAL:HG11	1:S:440:THR:HG21	1.91	0.53
1:B:248:ALA:HB3	1:B:249:PRO:HD3	1.90	0.53
1:T:55:VAL:HG21	1:T:75:ILE:HD13	1.90	0.53
2:V:237:LEU:HD13	2:V:296:ILE:HG12	1.89	0.53
1:S:298:GLY:O	2:W:267:GLU:HG2	2.08	0.53
3:P:77:ILE:HG23	3:P:110:ILE:HB	1.90	0.53
2:E:204:THR:OG1	2:E:420:VAL:HB	2.08	0.53
1:K:166:ARG:HG2	1:K:325:ALA:HB3	1.90	0.53
1:L:192:ASN:HA	1:L:200:LYS:HG2	1.90	0.53
1:A:205:TYR:HB3	1:A:233:ILE:HD13	1.91	0.53
1:T:444:VAL:HG21	1:T:485:ILE:HG21	1.91	0.53
1:U:194:GLY:O	1:U:200:LYS:HE3	2.09	0.53
1:A:354:LEU:HA	1:A:366:ALA:O	2.09	0.53
1:C:166:ARG:HD2	1:C:308:LEU:O	2.09	0.53
2:E:204:THR:HG23	2:E:206:VAL:HG13	1.91	0.53
3:P:40:SER:HB3	4:Q:17:PRO:O	2.08	0.53
2:E:50:VAL:HA	2:E:61:THR:HG22	1.91	0.53
1:B:399:TYR:HE1	1:B:420:LEU:HD12	1.72	0.52
2:D:98:VAL:HG23	2:D:232:VAL:HA	1.91	0.52
2:F:237:LEU:HD21	2:F:295:ARG:HB2	1.92	0.52
1:J:406:ALA:HB2	1:J:420:LEU:HD21	1.92	0.52
1:J:426:LEU:HD23	1:J:429:LEU:HD12	1.91	0.52
2:W:255:ILE:HB	2:W:308:GLN:HG2	1.91	0.52
2:X:255:ILE:HD12	2:X:308:GLN:HG2	1.91	0.52
2:D:314:ALA:O	2:D:315:ASP:HB2	2.08	0.52
2:M:25:PHE:HB2	2:M:30:LEU:HD23	1.90	0.52
1:T:429:LEU:HD11	1:T:446:LEU:HB3	1.91	0.52
1:T:174:GLN:HA	6:T:600:ANP:N3B	2.23	0.52
2:W:30:LEU:HD21	2:W:57:ASN:HA	1.90	0.52
1:B:364:ARG:HA	1:B:365:PRO:C	2.29	0.52
2:V:133:ILE:HD11	2:V:434:LEU:HD13	1.90	0.52
2:D:160:GLY:N	6:D:600:ANP:HNB1	2.07	0.52
1:K:234:VAL:HG21	1:K:252:ALA:HB2	1.91	0.52
1:U:150:THR:HA	1:U:184:THR:HG23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:269:SER:HB2	2:X:282:GLN:HB3	1.90	0.52
3:Y:96:ARG:HA	3:Y:99:LEU:HB2	1.91	0.52
2:O:237:LEU:HD13	2:O:296:ILE:HG12	1.91	0.52
1:A:50:GLN:HB3	2:E:69:GLY:HA2	1.92	0.52
3:G:122:HIS:HB3	3:G:125:ASN:HD22	1.75	0.52
1:K:444:VAL:CG2	1:K:445:PRO:HD3	2.39	0.52
2:V:133:ILE:HD11	2:V:434:LEU:CD1	2.39	0.52
1:A:82:ARG:HG3	2:D:33:ILE:O	2.09	0.52
2:X:231:ARG:HD3	2:X:234:LEU:CD1	2.39	0.52
2:F:117:ILE:HA	2:F:238:THR:OG1	2.10	0.52
2:N:344:ILE:HG23	2:N:415:SER:HB3	1.92	0.52
1:T:203:CYS:HB2	1:T:231:SER:HB3	1.92	0.52
2:W:276:PRO:HD2	3:Y:271:ILE:HG12	1.92	0.52
1:B:103:PRO:O	1:B:106:LEU:HD13	2.10	0.52
2:E:168:GLN:HE21	2:E:201:MET:CG	2.23	0.52
2:E:168:GLN:HE22	2:E:200:GLU:HG2	1.74	0.52
1:U:422:ARG:NH1	1:U:451:VAL:O	2.42	0.52
2:X:30:LEU:HD21	2:X:57:ASN:HA	1.92	0.52
2:D:156:PHE:HE1	2:D:329:LEU:CD1	2.22	0.51
2:D:197:LEU:O	2:D:201:MET:HG2	2.10	0.51
2:E:321:ALA:HB3	2:E:322:PRO:CD	2.40	0.51
1:K:345:ILE:HG12	1:K:351:GLN:HG2	1.90	0.51
2:N:169:GLU:HG2	2:N:418:PHE:CD1	2.45	0.51
3:P:155:LYS:HA	3:P:155:LYS:HE3	1.92	0.51
2:W:377:THR:HG22	2:W:407:ALA:HB2	1.92	0.51
1:C:174:GLN:HB3	2:F:354:LYS:HE2	1.92	0.51
3:G:38:LYS:HD2	3:G:169:PRO:HG2	1.92	0.51
2:O:388:ILE:HD11	2:O:396:LEU:HD11	1.93	0.51
2:W:410:ILE:HG23	2:W:441:PHE:HE2	1.75	0.51
2:F:152:LYS:NZ	2:F:293:GLN:O	2.44	0.51
4:H:16:LEU:HB2	4:H:19:GLU:O	2.11	0.51
2:O:377:THR:HG22	2:O:407:ALA:HB2	1.93	0.51
1:T:135:ALA:HB3	2:X:223:ASN:HD22	1.76	0.51
1:A:36:VAL:HG21	1:A:84:VAL:HB	1.93	0.51
1:K:192:ASN:HA	1:K:200:LYS:HG2	1.92	0.51
3:P:99:LEU:HG	3:P:103:PRO:HA	1.93	0.51
2:V:279:VAL:O	2:V:279:VAL:HG12	2.11	0.51
4:H:70:ILE:HG23	4:H:72:GLY:H	1.76	0.51
1:L:109:VAL:HG22	1:L:233:ILE:HB	1.93	0.51
2:N:171:ILE:HG23	2:N:182:SER:HB2	1.93	0.51
2:N:25:PHE:HB2	2:N:30:LEU:HD23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:234:LEU:HD23	2:V:292:LEU:HD13	1.93	0.51
1:B:335:ASP:HB2	3:G:257:ARG:NH1	2.25	0.51
1:J:50:GLN:HB3	2:N:69:GLY:HA2	1.92	0.51
1:T:150:THR:HG21	1:T:155:VAL:HG11	1.92	0.51
2:X:187:VAL:HG12	2:X:260:ARG:HB2	1.93	0.50
1:C:364:ARG:HA	1:C:365:PRO:C	2.32	0.50
3:P:205:VAL:N	3:P:206:PRO:HD3	2.26	0.50
2:V:15:ALA:HB3	2:V:22:ASP:HB2	1.92	0.50
2:O:412:ARG:O	2:O:415:SER:OG	2.29	0.50
1:T:470:PHE:O	1:T:474:LEU:HG	2.11	0.50
1:B:270:TYR:O	1:B:272:ASP:HA	2.12	0.50
1:B:43:VAL:HG21	1:B:75:ILE:HD12	1.93	0.50
1:C:338:ALA:HB3	1:C:341:PRO:HG2	1.92	0.50
2:M:377:THR:HG23	2:M:403:THR:HG22	1.93	0.50
1:A:248:ALA:HB3	1:A:249:PRO:HD3	1.93	0.50
2:N:15:ALA:HB3	2:N:22:ASP:HB2	1.92	0.50
2:F:363:VAL:HB	2:F:367:HIS:HD1	1.77	0.50
1:J:51:ALA:O	1:J:52:GLU:HB2	2.11	0.50
1:B:444:VAL:CG2	1:B:445:PRO:HD3	2.40	0.50
2:D:20:ILE:HG13	2:D:271:LEU:HB3	1.92	0.50
2:D:367:HIS:CD2	2:D:434:LEU:HD21	2.47	0.50
2:F:377:THR:HG22	2:F:407:ALA:HB2	1.93	0.50
3:G:115:LYS:O	3:G:119:LEU:HB2	2.12	0.50
3:G:119:LEU:HD13	3:G:126:ILE:HD12	1.94	0.50
2:X:335:LEU:HA	2:X:347:ALA:O	2.12	0.50
2:N:264:ALA:O	2:N:268:VAL:HG23	2.12	0.49
1:T:389:ALA:HB2	1:T:447:ILE:HG21	1.94	0.49
1:T:444:VAL:HG23	1:T:445:PRO:HD3	1.93	0.49
1:A:422:ARG:HE	1:A:453:GLY:HA2	1.76	0.49
1:B:345:ILE:HG12	1:B:351:GLN:HG2	1.95	0.49
1:T:444:VAL:CG2	1:T:445:PRO:HD3	2.42	0.49
2:X:128:SER:HB2	2:X:300:LYS:HG2	1.94	0.49
2:D:222:MET:HA	2:D:229:ARG:HD2	1.93	0.49
2:F:140:VAL:HG13	2:F:414:LEU:HB3	1.94	0.49
5:I:20:ALA:C	5:I:22:ARG:H	2.16	0.49
1:J:402:VAL:O	1:J:402:VAL:CG1	2.59	0.49
1:S:68:LEU:O	2:W:15:ALA:HA	2.12	0.49
2:E:455:HIS:CD2	2:E:473:LEU:HD11	2.48	0.49
1:L:412:LEU:HB3	1:L:416:THR:CG2	2.42	0.49
1:J:332:GLN:HB3	2:M:318:THR:HB	1.95	0.49
1:B:421:VAL:O	1:B:425:ARG:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:168:LEU:HB2	1:C:348:THR:HG21	1.93	0.49
1:J:336:VAL:HG11	1:J:353:PHE:CE1	2.46	0.49
1:T:382:VAL:HG11	1:T:440:THR:HG21	1.95	0.49
1:A:138:ILE:HD13	2:E:191:THR:HG23	1.95	0.49
1:A:205:TYR:HB3	1:A:233:ILE:CD1	2.41	0.49
1:C:40:ILE:HG13	1:C:286:LEU:HB3	1.95	0.49
1:L:211:LYS:HE3	1:L:213:SER:OG	2.12	0.49
2:N:174:ILE:HG13	2:N:252:LEU:HD11	1.93	0.49
1:B:165:GLN:HG2	1:B:166:ARG:N	2.27	0.49
2:E:184:PHE:HA	2:E:254:PHE:HB2	1.94	0.49
4:H:88:ILE:HD11	5:I:14:LEU:HB3	1.93	0.49
1:K:154:ALA:HB1	1:K:367:ILE:HD12	1.94	0.49
3:P:186:LYS:C	3:P:188:ILE:H	2.16	0.49
1:K:65:ALA:HA	1:K:75:ILE:HG12	1.94	0.49
1:L:187:ASN:OD1	1:L:190:ARG:NH1	2.46	0.49
2:V:41:THR:HB	2:V:42:PRO:CD	2.43	0.49
1:J:257:GLU:CD	1:J:310:ARG:HH21	2.16	0.49
2:W:406:ARG:NH1	2:W:447:GLY:HA2	2.28	0.49
1:A:105:LEU:HD21	1:A:123:ILE:HG21	1.95	0.48
1:B:99:VAL:O	1:B:128:ARG:HA	2.13	0.48
1:B:309:GLU:OE1	2:F:223:ASN:HB3	2.13	0.48
1:J:203:CYS:O	1:J:231:SER:HA	2.12	0.48
1:K:429:LEU:HD11	1:K:446:LEU:HB3	1.95	0.48
1:U:187:ASN:OD1	1:U:190:ARG:NH1	2.46	0.48
2:X:359:ASP:O	2:X:363:VAL:HG22	2.13	0.48
1:C:222:LEU:HB2	1:C:228:MET:HE2	1.94	0.48
1:J:446:LEU:HD11	1:J:467:GLU:HG3	1.94	0.48
1:K:260:ARG:O	1:K:321:GLY:HA3	2.13	0.48
3:P:254:LEU:O	3:P:258:THR:OG1	2.30	0.48
1:C:192:ASN:HA	1:C:200:LYS:HG2	1.95	0.48
2:W:380:THR:O	2:W:384:LEU:HG	2.12	0.48
2:D:140:VAL:HG23	2:D:414:LEU:HD22	1.96	0.48
3:G:118:LEU:HA	3:G:121:THR:HG22	1.95	0.48
3:G:58:LYS:O	3:G:187:THR:CG2	2.62	0.48
1:S:166:ARG:CD	1:S:308:LEU:O	2.61	0.48
2:V:65:ASP:CA	2:V:225:PRO:HG3	2.42	0.48
2:E:384:LEU:O	2:E:388:ILE:HG12	2.12	0.48
4:H:16:LEU:HD11	4:H:90:ALA:CB	2.41	0.48
2:W:201:MET:HA	2:W:204:THR:HG22	1.95	0.48
2:W:386:ASP:OD1	2:W:386:ASP:N	2.47	0.48
1:K:46:LEU:O	1:K:49:ILE:HG22	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:82:ARG:HG2	2:O:34:LEU:HD12	1.95	0.48
2:V:136:THR:HA	2:V:174:ILE:HD11	1.95	0.48
2:D:85:VAL:CG1	2:D:235:THR:HG23	2.35	0.48
4:H:45:HIS:HD2	4:H:46:VAL:O	1.97	0.48
4:H:77:VAL:HG22	4:H:83:LEU:HD13	1.95	0.48
2:M:224:GLU:HB3	2:M:228:ALA:HB3	1.94	0.48
2:D:137:GLY:HA2	2:D:432:VAL:O	2.14	0.48
1:K:269:VAL:HG22	1:K:326:LEU:HB2	1.94	0.48
2:O:155:LEU:HD12	2:O:167:ILE:HG13	1.96	0.48
1:T:369:VAL:HG11	1:T:396:LEU:HB2	1.95	0.48
1:U:80:SER:OG	1:U:82:ARG:HG3	2.13	0.48
2:W:201:MET:HA	2:W:204:THR:CG2	2.44	0.48
2:D:36:ALA:HB2	2:D:83:ILE:HG13	1.95	0.48
1:L:455:LEU:HA	1:L:458:ILE:HD12	1.95	0.48
4:Q:34:ALA:H	4:Q:38:ARG:HA	1.77	0.48
1:J:174:GLN:HB3	2:M:354:LYS:HE3	1.96	0.48
1:J:375:ARG:HG2	2:N:159:ALA:CB	2.44	0.48
2:M:53:HIS:CD2	2:M:59:VAL:HG12	2.49	0.48
2:N:220:GLY:HA3	2:N:232:VAL:HG11	1.94	0.48
2:N:367:HIS:NE2	2:N:434:LEU:HD11	2.28	0.48
3:P:52:TYR:OH	3:P:213:THR:HG21	2.13	0.48
1:U:378:SER:HB2	1:U:386:LYS:HE2	1.95	0.48
2:M:53:HIS:HD2	2:M:59:VAL:HG12	1.79	0.47
2:E:258:ILE:O	2:E:261:PHE:HB3	2.14	0.47
2:E:41:THR:HB	2:E:42:PRO:HD2	1.95	0.47
1:S:52:GLU:O	1:S:97:VAL:HG23	2.14	0.47
1:T:416:THR:O	1:T:420:LEU:HB2	2.14	0.47
2:V:201:MET:SD	2:V:215:VAL:HG11	2.54	0.47
1:B:190:ARG:HE	1:B:439:ALA:HB2	1.80	0.47
2:N:237:LEU:HD22	2:N:292:LEU:HD12	1.95	0.47
2:N:152:LYS:HE3	2:N:296:ILE:HB	1.96	0.47
1:S:281:ARG:NH1	2:V:278:ALA:HB2	2.28	0.47
1:K:243:PRO:HG3	1:K:283:LEU:HD21	1.96	0.47
2:M:427:ILE:CD1	2:M:459:MET:HG2	2.43	0.47
2:X:298:THR:HG23	2:X:303:SER:HA	1.97	0.47
1:C:222:LEU:CB	1:C:228:MET:HE2	2.44	0.47
1:U:135:ALA:HB3	2:V:223:ASN:HD22	1.79	0.47
1:U:291:PRO:HG2	3:Y:273:GLY:HA2	1.97	0.47
2:F:253:LEU:HD23	2:F:296:ILE:HG23	1.96	0.47
1:J:458:ILE:HG13	1:J:458:ILE:H	1.50	0.47
1:J:55:VAL:HG21	1:J:75:ILE:HD13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:272:ASP:OD1	1:K:274:SER:HB2	2.14	0.47
2:N:237:LEU:HD21	2:N:295:ARG:HB2	1.95	0.47
2:E:201:MET:SD	2:E:217:LEU:HD21	2.55	0.47
1:K:272:ASP:HB2	1:K:328:VAL:O	2.15	0.47
2:O:208:ASN:HD22	2:O:211:GLY:H	1.63	0.47
2:W:220:GLY:HA3	2:W:232:VAL:HG11	1.96	0.47
2:X:321:ALA:HB3	2:X:322:PRO:CD	2.45	0.47
2:E:407:ALA:HA	2:E:410:ILE:HD12	1.95	0.47
1:B:293:ARG:NH2	2:F:319:ASP:OD2	2.46	0.47
1:L:187:ASN:O	1:L:190:ARG:HG3	2.14	0.47
3:P:35:GLU:O	3:P:39:ILE:HG12	2.14	0.47
1:U:69:GLU:HB3	1:U:70:PRO:CD	2.45	0.47
2:E:169:GLU:HG2	2:E:418:PHE:CD1	2.50	0.47
5:I:28:GLU:CD	5:I:29:LEU:H	2.19	0.47
2:O:388:ILE:CD1	2:O:396:LEU:HD11	2.45	0.47
2:D:344:ILE:HG23	2:D:415:SER:HB3	1.96	0.46
3:G:24:LYS:HB2	3:G:237:MET:HB3	1.97	0.46
1:K:338:ALA:HB3	1:K:341:PRO:HG2	1.97	0.46
3:P:205:VAL:N	3:P:206:PRO:CD	2.78	0.46
1:S:293:ARG:HG2	1:S:339:TYR:CD1	2.50	0.46
2:V:440:SER:O	2:V:444:VAL:HG23	2.15	0.46
2:X:384:LEU:O	2:X:385:GLN:C	2.53	0.46
1:C:481:LEU:HD13	1:C:495:LEU:HD23	1.97	0.46
1:T:364:ARG:HA	1:T:365:PRO:C	2.36	0.46
1:A:161:ILE:HD13	1:A:326:LEU:HD21	1.98	0.46
2:F:237:LEU:HD13	2:F:296:ILE:HG12	1.97	0.46
2:F:256:ASP:HA	2:F:257:ASN:HA	1.73	0.46
1:T:467:GLU:O	1:T:471:LEU:HG	2.15	0.46
1:U:203:CYS:O	1:U:231:SER:HA	2.16	0.46
2:W:256:ASP:HA	2:W:257:ASN:HA	1.65	0.46
2:W:406:ARG:HH12	2:W:447:GLY:HA2	1.81	0.46
1:A:112:ALA:O	1:A:251:THR:HG21	2.15	0.46
1:B:203:CYS:HB2	1:B:231:SER:HB3	1.97	0.46
2:M:7:THR:HA	2:M:8:PRO:HD3	1.80	0.46
2:O:449:TYR:HB3	2:O:452:ILE:HD12	1.98	0.46
1:T:211:LYS:HD2	2:W:328:HIS:HA	1.98	0.46
1:U:106:LEU:HB3	1:U:229:LYS:O	2.16	0.46
1:A:54:LEU:HD12	1:A:97:VAL:HG22	1.97	0.46
1:L:40:ILE:HD12	1:L:76:VAL:HG12	1.98	0.46
1:T:154:ALA:HB2	1:T:430:LEU:HB3	1.98	0.46
1:T:349:ASP:OD1	2:X:192:ARG:NE	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:GLN:HA	6:B:600:ANP:HNB1	1.81	0.46
3:P:80:ASP:HA	3:P:112:ASP:HB2	1.98	0.46
1:S:204:VAL:O	1:S:268:ILE:HA	2.16	0.46
1:U:105:LEU:HG	1:U:123:ILE:HG21	1.97	0.46
2:W:67:THR:HB	2:W:70:LEU:HD12	1.98	0.46
2:X:231:ARG:HA	2:X:234:LEU:HD12	1.97	0.46
2:E:220:GLY:CA	2:E:232:VAL:HG11	2.46	0.46
2:F:416:GLN:NE2	2:F:432:VAL:HG23	2.31	0.46
1:J:399:TYR:CD1	1:J:423:GLY:HA3	2.51	0.46
1:L:429:LEU:HD11	1:L:446:LEU:HD22	1.98	0.46
2:N:67:THR:HB	2:N:70:LEU:HD12	1.98	0.46
2:W:140:VAL:HG13	2:W:414:LEU:HB3	1.97	0.46
2:W:200:GLU:O	2:W:204:THR:HG22	2.15	0.46
1:A:302:TYR:CE1	1:A:306:ARG:HG3	2.51	0.46
2:E:229:ARG:NH2	2:E:267:GLU:OE1	2.47	0.46
3:G:108:VAL:HG11	3:G:150:LEU:HD11	1.98	0.46
1:K:35:ALA:HB3	1:K:42:ARG:NH1	2.31	0.46
2:M:137:GLY:HA2	2:M:432:VAL:O	2.16	0.46
2:W:98:VAL:HB	2:W:232:VAL:HG13	1.98	0.46
2:X:237:LEU:HD13	2:X:296:ILE:CG1	2.46	0.46
2:X:190:ARG:NH1	6:X:600:ANP:O3G	2.48	0.46
3:Y:213:THR:HA	3:Y:216:ASN:HB3	1.98	0.46
2:M:41:THR:HB	2:M:42:PRO:HD2	1.96	0.46
1:S:383:LYS:HG2	1:S:490:GLU:HG2	1.97	0.46
1:S:425:ARG:CG	1:S:425:ARG:NH1	2.78	0.46
2:F:377:THR:HG23	2:F:403:THR:HG22	1.98	0.45
2:V:425:THR:HB	2:V:427:ILE:HD12	1.97	0.45
2:W:218:VAL:HG21	2:W:236:GLY:HA2	1.98	0.45
2:X:178:HIS:CD2	2:X:180:GLY:H	2.33	0.45
2:F:293:GLN:HG2	2:F:328:HIS:HB3	1.98	0.45
3:G:14:LYS:HA	3:G:248:ILE:HD11	1.98	0.45
1:L:480:GLU:H	1:L:480:GLU:HG3	1.53	0.45
2:M:339:ILE:HG22	2:M:344:ILE:HB	1.98	0.45
2:M:434:LEU:O	2:M:438:VAL:HG23	2.16	0.45
1:U:164:GLY:HA3	1:U:313:LYS:HB2	1.99	0.45
1:U:455:LEU:HD23	1:U:458:ILE:HD12	1.97	0.45
2:W:119:ALA:O	2:W:295:ARG:HD2	2.16	0.45
2:W:345:TYR:HA	2:W:346:PRO:C	2.36	0.45
1:A:364:ARG:HA	1:A:365:PRO:C	2.35	0.45
1:C:203:CYS:O	1:C:231:SER:HA	2.17	0.45
4:H:14:PHE:HD1	4:H:15:ALA:N	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:484:GLU:HB3	1:L:495:LEU:HD21	1.97	0.45
2:M:182:SER:O	2:M:215:VAL:HA	2.16	0.45
2:N:239:ILE:O	2:N:243:PHE:HD2	1.99	0.45
2:N:234:LEU:HD23	2:N:292:LEU:HD13	1.98	0.45
2:N:29:GLU:O	2:N:29:GLU:HG2	2.16	0.45
2:E:140:VAL:HG13	2:E:414:LEU:HD22	1.97	0.45
1:J:446:LEU:CD1	1:J:467:GLU:HG3	2.46	0.45
2:M:387:ILE:O	2:M:391:LEU:HB2	2.16	0.45
3:P:150:LEU:O	3:P:154:MET:HB2	2.17	0.45
2:V:222:MET:HA	2:V:229:ARG:HD2	1.97	0.45
1:K:421:VAL:O	1:K:425:ARG:HG2	2.17	0.45
2:O:154:GLY:HA3	2:O:329:LEU:HD13	1.99	0.45
1:T:100:PRO:HD2	1:T:114:GLY:HA3	1.97	0.45
1:A:444:VAL:HG22	1:A:445:PRO:HD3	1.98	0.45
1:B:192:ASN:HA	1:B:200:LYS:HG2	1.97	0.45
1:C:129:SER:HB2	1:C:254:SER:HB3	1.98	0.45
2:E:349:ASP:HB3	2:E:352:ASP:HB2	1.99	0.45
1:L:109:VAL:HG12	1:L:117:ILE:HD11	1.98	0.45
3:P:24:LYS:HD2	3:P:238:ASP:OD1	2.16	0.45
1:T:179:ALA:CB	1:T:434:GLN:HE21	2.29	0.45
1:C:202:TYR:O	1:C:266:ALA:HA	2.17	0.45
3:G:108:VAL:HG22	3:G:128:LEU:HB3	1.99	0.45
1:K:219:VAL:O	1:K:223:GLU:HG3	2.17	0.45
2:N:98:VAL:HB	2:N:232:VAL:CG1	2.47	0.45
2:V:266:SER:HA	2:V:282:GLN:CG	2.47	0.45
1:C:260:ARG:HG2	1:C:314:LEU:HD12	1.98	0.45
2:E:168:GLN:HE21	2:E:201:MET:HG2	1.81	0.45
2:F:189:GLU:O	2:F:221:GLN:HB3	2.17	0.45
2:F:293:GLN:HG2	2:F:328:HIS:CG	2.52	0.45
1:J:204:VAL:O	1:J:268:ILE:HA	2.17	0.45
1:K:302:TYR:HA	1:K:305:SER:OG	2.17	0.45
2:M:95:ILE:HD12	2:M:104:ASP:HB3	1.99	0.45
1:S:168:LEU:HD11	1:S:329:ILE:HB	1.99	0.45
1:T:212:ARG:HG3	1:T:237:THR:HG21	1.98	0.45
2:V:269:SER:O	2:V:274:ARG:HB2	2.16	0.45
2:X:170:LEU:HD13	2:X:307:VAL:HG11	1.98	0.45
2:F:363:VAL:HB	2:F:367:HIS:ND1	2.32	0.45
3:G:145:LEU:O	3:G:149:LYS:HG2	2.17	0.45
1:J:146:GLU:HB2	1:J:163:ARG:HG3	1.99	0.45
2:M:176:LYS:HE2	2:M:204:THR:HG21	1.98	0.45
2:M:419:ALA:HA	2:M:429:GLY:HA3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:293:ARG:HD2	1:T:339:TYR:CD1	2.52	0.45
2:V:220:GLY:HA3	2:V:232:VAL:HG21	1.98	0.45
2:E:86:PRO:HD3	2:E:114:ARG:NH1	2.32	0.44
2:M:427:ILE:HD13	2:M:459:MET:HG2	1.97	0.44
2:N:279:VAL:HG12	2:N:279:VAL:O	2.17	0.44
2:O:140:VAL:HG21	2:O:348:VAL:HG21	2.00	0.44
1:T:190:ARG:HE	1:T:439:ALA:HB2	1.81	0.44
2:W:82:PRO:HG2	2:W:116:PRO:HB3	1.99	0.44
1:A:446:LEU:HD11	1:A:467:GLU:HG3	1.99	0.44
1:A:384:ALA:HB2	1:A:489:GLY:O	2.17	0.44
2:M:237:LEU:HD21	2:M:295:ARG:HB2	1.99	0.44
3:P:162:ILE:HB	3:P:182:ILE:HB	1.98	0.44
1:T:139:LEU:N	1:T:140:PRO:CD	2.80	0.44
2:X:190:ARG:O	2:X:221:GLN:NE2	2.50	0.44
1:A:372:SER:O	1:A:373:VAL:HG13	2.17	0.44
2:E:33:ILE:O	2:E:34:LEU:HB2	2.17	0.44
2:F:164:THR:O	2:F:167:ILE:HG22	2.18	0.44
2:V:132:GLU:HB3	2:V:149:ARG:HB3	2.00	0.44
2:V:189:GLU:O	2:V:221:GLN:HB3	2.17	0.44
2:D:25:PHE:HB2	2:D:30:LEU:HD23	2.00	0.44
1:L:417:LYS:O	1:L:421:VAL:HG23	2.17	0.44
1:S:38:ASP:O	1:S:286:LEU:HD13	2.17	0.44
1:T:101:VAL:HG12	1:T:255:ILE:HA	2.00	0.44
1:C:336:VAL:HG11	1:C:353:PHE:CE1	2.52	0.44
1:C:414:ALA:O	1:C:418:GLN:HB3	2.18	0.44
2:E:25:PHE:HB2	2:E:30:LEU:HD23	1.97	0.44
1:L:40:ILE:CD1	1:L:76:VAL:HG12	2.48	0.44
2:M:279:VAL:HG12	2:M:279:VAL:O	2.17	0.44
2:M:143:LEU:O	2:M:367:HIS:HE1	2.01	0.44
1:C:107:GLY:HA2	1:C:228:MET:O	2.17	0.44
2:D:128:SER:HB2	2:D:300:LYS:HG2	1.99	0.44
2:E:175:ALA:O	2:E:179:GLY:HA2	2.18	0.44
2:M:142:ASP:HB3	2:M:434:LEU:HD12	2.00	0.44
3:P:14:LYS:HA	3:P:248:ILE:HD11	1.99	0.44
2:V:33:ILE:O	2:V:34:LEU:CB	2.64	0.44
2:W:339:ILE:HG22	2:W:344:ILE:HB	1.99	0.44
1:J:293:ARG:HG2	1:J:294:GLU:HG3	2.00	0.44
1:K:147:PRO:HG3	1:K:382:VAL:HG23	1.99	0.44
1:L:68:LEU:HB2	2:M:16:VAL:H	1.82	0.44
2:N:384:LEU:O	2:N:388:ILE:HG12	2.18	0.44
2:O:50:VAL:HA	2:O:61:THR:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:184:PHE:HB3	2:V:217:LEU:HD23	2.00	0.44
2:V:257:ASN:HD21	2:V:311:TYR:N	2.16	0.44
2:W:237:LEU:HD22	2:W:292:LEU:HD12	1.99	0.44
3:Y:151:LEU:HA	3:Y:156:ALA:HB3	1.99	0.44
2:F:191:THR:HA	2:F:221:GLN:HG3	1.99	0.44
1:K:169:ILE:HB	1:K:328:VAL:HG22	2.00	0.44
1:U:273:LEU:HD22	1:U:276:GLN:OE1	2.18	0.44
2:X:408:ARG:O	2:X:412:ARG:HG3	2.18	0.44
2:F:256:ASP:OD1	2:F:257:ASN:HB2	2.18	0.43
3:G:77:ILE:HG21	3:G:222:MET:HG2	1.99	0.43
1:K:242:ALA:HB3	1:K:243:PRO:HD3	1.99	0.43
2:W:258:ILE:HG22	2:W:309:ALA:O	2.18	0.43
2:X:33:ILE:O	2:X:34:LEU:HB2	2.18	0.43
5:1:39:GLN:O	5:1:40:THR:CB	2.67	0.43
1:A:174:GLN:HB3	2:D:354:LYS:HD2	2.00	0.43
1:L:376:VAL:HG11	1:L:380:ALA:HB2	2.00	0.43
2:N:275:ILE:HG23	3:P:271:ILE:HD13	1.99	0.43
1:S:281:ARG:HH12	2:V:278:ALA:HB2	1.81	0.43
1:C:165:GLN:CG	1:C:166:ARG:N	2.81	0.43
2:E:377:THR:HG22	2:E:407:ALA:HB2	2.01	0.43
2:N:204:THR:OG1	2:N:420:VAL:HB	2.18	0.43
2:W:117:ILE:HG22	2:W:235:THR:HA	2.00	0.43
2:X:390:ILE:HD11	3:Y:247:MET:SD	2.58	0.43
2:D:406:ARG:HH21	2:D:447:GLY:HA3	1.82	0.43
1:L:455:LEU:HD13	1:L:463:ILE:HD12	1.99	0.43
2:N:156:PHE:CZ	2:N:326:PHE:HZ	2.35	0.43
1:U:311:ALA:HA	1:U:323:LEU:HB3	2.00	0.43
1:U:239:SER:HB3	2:X:294:GLU:HG3	2.01	0.43
1:T:342:THR:HG21	2:X:314:ALA:HA	2.00	0.43
1:A:440:THR:O	1:A:444:VAL:HG13	2.19	0.43
1:A:85:LYS:O	1:A:88:GLU:HB2	2.19	0.43
1:C:162:GLY:O	1:C:165:GLN:HB3	2.19	0.43
2:E:144:LEU:HD22	2:E:375:GLN:HG3	2.00	0.43
2:F:321:ALA:HB3	2:F:322:PRO:CD	2.49	0.43
3:G:182:ILE:HG21	3:G:214:LEU:HD13	2.00	0.43
2:M:218:VAL:HG21	2:M:236:GLY:HA2	2.00	0.43
3:P:74:ILE:HD11	3:P:98:HIS:HD2	1.83	0.43
1:T:346:SER:HA	6:X:600:ANP:O1G	2.19	0.43
2:W:187:VAL:HG21	2:W:233:ALA:HB2	2.01	0.43
2:X:256:ASP:HA	2:X:257:ASN:HA	1.81	0.43
1:B:55:VAL:HG21	1:B:75:ILE:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:277:SER:OG	2:D:278:ALA:N	2.51	0.43
2:M:191:THR:HA	2:M:221:GLN:HG3	2.00	0.43
2:M:344:ILE:HG23	2:M:415:SER:HB3	2.00	0.43
2:N:419:ALA:CA	2:N:429:GLY:HA3	2.46	0.43
2:O:155:LEU:HD13	2:O:166:PHE:HB3	2.00	0.43
1:U:169:ILE:HB	1:U:328:VAL:HG22	2.01	0.43
1:C:165:GLN:HG3	1:C:166:ARG:N	2.34	0.43
1:L:345:ILE:HG12	1:L:351:GLN:HG2	2.01	0.43
1:L:452:ASN:HB2	1:L:454:HIS:CE1	2.54	0.43
1:L:56:GLU:OE2	1:L:62:LYS:HE3	2.19	0.43
3:P:212:TYR:O	3:P:216:ASN:HB2	2.18	0.43
1:S:42:ARG:HE	1:S:72:GLN:HE22	1.67	0.43
1:T:383:LYS:HG2	1:T:387:GLN:HE21	1.84	0.43
1:U:50:GLN:HB3	2:V:69:GLY:HA2	2.00	0.43
3:Y:22:THR:HG22	3:Y:26:VAL:HG23	2.01	0.43
1:B:99:VAL:HG11	1:B:251:THR:HB	1.99	0.43
1:K:340:ILE:HB	1:K:341:PRO:HD3	2.01	0.43
2:O:140:VAL:HG23	2:O:141:VAL:H	1.84	0.43
1:B:290:PRO:HA	1:B:291:PRO:HD2	1.93	0.43
4:H:49:VAL:HG22	4:H:76:THR:HG22	2.01	0.43
2:N:150:GLY:O	2:N:297:THR:HA	2.19	0.43
1:L:238:ALA:HB1	2:O:328:HIS:HE1	1.84	0.43
1:S:98:ASP:HB2	1:S:129:SER:O	2.19	0.43
1:T:478:HIS:HB3	1:T:481:LEU:HG	2.01	0.43
1:U:313:LYS:HD2	1:U:322:SER:HB3	1.99	0.43
1:A:394:LEU:O	1:A:397:ALA:N	2.52	0.42
2:E:256:ASP:HA	2:E:257:ASN:HA	1.75	0.42
3:G:271:ILE:HA	3:G:271:ILE:HD13	1.92	0.42
4:H:78:GLN:HB3	4:H:79:PRO:HD2	2.01	0.42
2:M:197:LEU:O	2:M:201:MET:HG2	2.19	0.42
1:S:378:SER:HB3	1:S:386:LYS:HE3	2.00	0.42
1:U:167:GLU:O	1:U:326:LEU:HA	2.19	0.42
2:V:190:ARG:HB2	2:V:193:GLU:HG3	2.01	0.42
1:S:174:GLN:HB3	2:V:354:LYS:HD3	2.01	0.42
2:X:237:LEU:HD13	2:X:296:ILE:HG12	2.01	0.42
1:B:478:HIS:HB3	1:B:481:LEU:HG	2.00	0.42
3:G:84:CYS:HA	3:G:233:ARG:HA	2.01	0.42
1:J:166:ARG:CD	1:J:308:LEU:O	2.67	0.42
2:M:256:ASP:HA	2:M:257:ASN:HA	1.85	0.42
1:U:161:ILE:HD13	1:U:326:LEU:HD21	2.01	0.42
2:V:256:ASP:HA	2:V:257:ASN:HA	1.70	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:GLU:O	1:A:163:ARG:HG3	2.19	0.42
3:G:45:ASP:CG	3:G:220:THR:HG21	2.40	0.42
1:K:67:ASN:HB3	2:O:17:ILE:HG23	2.00	0.42
1:L:103:PRO:HD3	1:L:258:TRP:CZ2	2.54	0.42
2:N:339:ILE:HG22	2:N:344:ILE:HB	2.01	0.42
3:P:154:MET:C	3:P:156:ALA:H	2.22	0.42
1:S:161:ILE:HD11	1:S:167:GLU:HG2	2.01	0.42
1:U:485:ILE:HG12	1:U:491:LEU:HD21	2.02	0.42
1:T:290:PRO:HB3	2:X:276:PRO:HG3	2.01	0.42
1:B:190:ARG:NE	1:B:439:ALA:HB2	2.34	0.42
1:K:311:ALA:HA	1:K:323:LEU:HB3	2.01	0.42
1:L:425:ARG:HD3	1:L:456:ASP:HA	2.00	0.42
2:M:251:VAL:HB	2:M:304:VAL:HG22	2.00	0.42
2:X:339:ILE:CG2	2:X:344:ILE:HB	2.49	0.42
2:D:49:GLU:OE1	2:D:231:ARG:NE	2.44	0.42
2:F:158:GLY:O	2:F:163:LYS:NZ	2.53	0.42
2:F:202:LYS:HE3	2:F:209:LEU:HD11	2.02	0.42
2:F:239:ILE:O	2:F:243:PHE:HD2	2.02	0.42
1:K:250:PHE:CE1	1:K:307:LEU:HB2	2.55	0.42
2:O:311:TYR:HE2	2:O:313:PRO:HA	1.83	0.42
2:O:345:TYR:HA	2:O:346:PRO:C	2.39	0.42
1:A:26:ASN:HD21	1:A:29:GLU:HB2	1.84	0.42
2:E:98:VAL:HB	2:E:232:VAL:HG13	2.00	0.42
2:F:293:GLN:HG2	2:F:328:HIS:CB	2.50	0.42
3:G:186:LYS:HE3	3:G:190:GLN:HE22	1.85	0.42
1:J:272:ASP:HB2	1:J:328:VAL:O	2.20	0.42
1:J:475:LYS:O	1:J:479:ASN:HB2	2.19	0.42
1:K:417:LYS:HA	1:K:420:LEU:HD22	2.01	0.42
1:K:98:ASP:HB2	1:K:129:SER:O	2.19	0.42
1:S:139:LEU:N	1:S:140:PRO:HD2	2.34	0.42
1:U:204:VAL:HG22	1:U:232:ILE:HD12	2.01	0.42
1:U:271:ASP:HA	1:U:272:ASP:HA	1.79	0.42
1:C:422:ARG:NH1	1:C:453:GLY:HA2	2.35	0.42
3:P:78:THR:HG23	3:P:91:LEU:CD2	2.47	0.42
1:S:314:LEU:HB3	1:S:318:GLU:HB3	2.01	0.42
2:V:115:LYS:HE2	2:V:242:TYR:HD1	1.84	0.42
2:X:15:ALA:HB3	2:X:22:ASP:HB2	2.01	0.42
1:B:150:THR:HG21	1:B:155:VAL:HG11	2.01	0.42
1:B:217:GLN:O	1:B:220:GLN:HB3	2.20	0.42
2:F:258:ILE:HD13	2:F:293:GLN:HE22	1.85	0.42
2:F:410:ILE:O	2:F:414:LEU:HG	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:198:GLU:O	4:H:48:THR:HG23	2.20	0.42
3:G:92:ALA:O	3:G:96:ARG:HG3	2.20	0.42
1:J:105:LEU:HD23	1:J:123:ILE:HD12	2.01	0.42
1:K:141:ARG:NH1	1:K:312:ALA:CB	2.83	0.42
1:K:173:ARG:HG2	1:K:174:GLN:HG2	2.01	0.42
1:K:285:LEU:HD22	2:N:275:ILE:HG22	2.02	0.42
2:N:440:SER:OG	2:N:463:ILE:HB	2.19	0.42
2:V:388:ILE:HD13	2:V:396:LEU:HD21	2.01	0.42
2:V:400:ASP:O	2:V:404:VAL:HG23	2.20	0.42
3:Y:92:ALA:HB2	3:Y:117:GLN:HB3	2.02	0.42
1:C:99:VAL:HG11	1:C:251:THR:HB	2.02	0.42
1:C:30:THR:HG22	1:C:91:LYS:HA	2.02	0.42
4:H:69:PHE:O	4:H:90:ALA:HA	2.20	0.42
1:L:336:VAL:HG13	1:L:353:PHE:CE1	2.55	0.42
2:M:33:ILE:O	2:M:34:LEU:HB2	2.20	0.42
2:O:416:GLN:HA	2:O:417:PRO:HD3	1.94	0.42
1:T:340:ILE:HB	1:T:341:PRO:HD3	2.02	0.42
3:Y:86:SER:HB2	3:Y:89:SER:OG	2.20	0.42
2:D:279:VAL:HG12	2:D:279:VAL:O	2.20	0.42
1:K:96:ILE:O	1:K:97:VAL:C	2.58	0.42
2:M:425:THR:HB	2:M:427:ILE:HD12	2.01	0.42
2:X:189:GLU:O	2:X:222:MET:HG2	2.20	0.42
2:D:149:ARG:CG	2:D:149:ARG:NH1	2.75	0.41
2:F:345:TYR:HA	2:F:346:PRO:C	2.40	0.41
2:O:417:PRO:HG3	2:O:459:MET:HG3	2.01	0.41
2:W:117:ILE:HA	2:W:238:THR:OG1	2.20	0.41
1:A:269:VAL:HG22	1:A:326:LEU:HB2	2.02	0.41
1:B:159:VAL:HG21	1:B:352:ILE:HG12	2.02	0.41
2:D:149:ARG:HG3	2:D:149:ARG:NH1	2.33	0.41
4:H:22:TYR:O	4:H:23:SER:C	2.58	0.41
1:K:442:GLU:O	1:K:445:PRO:HD2	2.19	0.41
1:L:311:ALA:HA	1:L:323:LEU:HD23	2.00	0.41
2:M:27:GLN:O	2:M:29:GLU:N	2.53	0.41
4:Q:16:LEU:CB	4:Q:17:PRO:HD2	2.50	0.41
1:T:396:LEU:HA	1:T:399:TYR:HB3	2.02	0.41
2:W:276:PRO:HB2	3:Y:267:LEU:HD21	2.02	0.41
2:X:162:GLY:O	2:X:166:PHE:HB2	2.20	0.41
1:A:378:SER:C	1:A:380:ALA:H	2.23	0.41
1:C:500:LYS:HG2	1:C:504:GLU:OE2	2.20	0.41
3:G:41:ALA:O	3:G:45:ASP:HB2	2.20	0.41
5:I:20:ALA:C	5:I:22:ARG:N	2.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:28:GLU:C	5:I:30:GLN:H	2.22	0.41
1:J:306:ARG:HA	2:N:223:ASN:HB2	2.01	0.41
2:N:321:ALA:HB3	2:N:322:PRO:CD	2.50	0.41
2:O:43:GLN:HB2	2:O:44:GLY:H	1.63	0.41
1:B:109:VAL:HG22	1:B:233:ILE:HB	2.02	0.41
2:E:185:THR:HG21	2:E:233:ALA:HA	2.02	0.41
2:F:182:SER:HA	2:F:252:LEU:O	2.21	0.41
2:N:381:TYR:O	2:N:385:GLN:HG2	2.21	0.41
2:O:189:GLU:O	2:O:221:GLN:HB3	2.20	0.41
2:O:277:SER:OG	2:O:278:ALA:N	2.53	0.41
1:T:289:ARG:HA	1:T:290:PRO:HD3	1.93	0.41
1:T:166:ARG:HG2	1:T:311:ALA:HB3	2.02	0.41
1:U:96:ILE:HB	1:U:130:ARG:HD3	2.03	0.41
1:U:165:GLN:NE2	1:U:167:GLU:OE1	2.53	0.41
1:U:416:THR:O	1:U:420:LEU:HB2	2.20	0.41
2:V:82:PRO:HB2	2:V:116:PRO:HB3	2.02	0.41
2:X:345:TYR:HA	2:X:346:PRO:C	2.40	0.41
1:C:211:LYS:HD3	2:F:328:HIS:HA	2.02	0.41
2:E:26:GLU:O	2:E:29:GLU:HB3	2.21	0.41
2:F:158:GLY:O	2:F:161:VAL:HG22	2.20	0.41
1:J:358:LEU:HD22	1:J:363:ILE:HD12	2.03	0.41
1:J:360:TYR:CE2	2:M:351:LEU:O	2.74	0.41
2:N:387:ILE:HB	2:N:391:LEU:HD12	2.02	0.41
1:T:259:PHE:HB2	1:T:266:ALA:HB2	2.03	0.41
2:X:279:VAL:O	2:X:279:VAL:HG12	2.21	0.41
1:A:141:ARG:HH11	1:A:141:ARG:HD3	1.75	0.41
2:M:285:LEU:HD23	2:M:285:LEU:C	2.41	0.41
1:U:343:ASN:O	1:U:346:SER:OG	2.31	0.41
2:E:337:ARG:HG2	2:E:341:GLU:OE2	2.21	0.41
2:E:345:TYR:HA	2:E:346:PRO:C	2.40	0.41
1:J:271:ASP:HA	1:J:272:ASP:HA	1.72	0.41
1:J:481:LEU:CD1	1:J:498:SER:HB3	2.42	0.41
1:K:55:VAL:HG21	1:K:75:ILE:HD13	2.02	0.41
1:L:243:PRO:HA	1:L:283:LEU:HD11	2.02	0.41
1:L:249:PRO:HB3	1:L:270:TYR:CD1	2.55	0.41
3:P:133:ILE:O	3:P:135:LYS:N	2.53	0.41
1:S:177:LYS:HG2	1:S:354:LEU:HD12	2.02	0.41
1:T:159:VAL:HG21	1:T:352:ILE:HG12	2.02	0.41
2:V:144:LEU:O	2:V:358:LEU:HD22	2.19	0.41
1:A:251:THR:HG22	1:A:252:ALA:N	2.35	0.41
1:K:109:VAL:HG12	1:K:117:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:175:ALA:HB3	2:N:214:LYS:HD3	2.03	0.41
3:P:122:HIS:N	3:P:123:PRO:HD3	2.36	0.41
3:P:77:ILE:HG12	3:P:110:ILE:HD12	2.01	0.41
1:C:290:PRO:HA	1:C:291:PRO:HD3	1.96	0.41
2:E:182:SER:HB2	2:E:215:VAL:HG23	2.03	0.41
3:G:57:THR:HG23	3:G:191:SER:HB3	2.03	0.41
1:L:168:LEU:HB2	1:L:348:THR:HG21	2.03	0.41
1:L:49:ILE:HD11	1:L:55:VAL:CG1	2.51	0.41
1:L:69:GLU:O	2:M:72:ARG:NH1	2.53	0.41
2:N:136:THR:O	2:N:173:ASN:HB3	2.20	0.41
2:O:16:VAL:C	2:O:17:ILE:HG13	2.41	0.41
2:O:187:VAL:HG22	2:O:232:VAL:HG13	2.03	0.41
3:P:111:GLY:HA2	3:P:133:ILE:HD11	2.01	0.41
1:U:99:VAL:HG21	1:U:251:THR:HB	2.02	0.41
1:T:50:GLN:HB3	2:X:69:GLY:HA2	2.02	0.41
1:C:55:VAL:HG21	1:C:75:ILE:HD13	2.01	0.41
2:O:256:ASP:HA	2:O:257:ASN:HA	1.65	0.41
1:S:399:TYR:CD1	1:S:423:GLY:HA3	2.56	0.41
1:U:135:ALA:HA	1:U:136:PRO:HD2	1.84	0.41
2:V:162:GLY:HA2	6:V:600:ANP:H8	2.03	0.41
2:X:217:LEU:HB3	2:X:219:PHE:HE2	1.86	0.41
1:C:85:LYS:O	1:C:88:GLU:HB3	2.21	0.41
2:D:237:LEU:HD13	2:D:296:ILE:HG12	2.02	0.41
3:G:96:ARG:NE	3:G:121:THR:HG21	2.10	0.41
1:J:364:ARG:HA	1:J:365:PRO:C	2.41	0.41
2:W:185:THR:OG1	2:W:236:GLY:HA3	2.21	0.41
2:W:95:ILE:HD12	2:W:104:ASP:HB3	2.03	0.41
2:X:231:ARG:HD3	2:X:234:LEU:HD12	2.02	0.41
2:X:339:ILE:HG23	2:X:344:ILE:HB	2.03	0.41
1:A:474:LEU:HD13	1:A:482:LEU:HD21	2.02	0.40
1:C:407:GLN:C	1:C:409:GLY:H	2.25	0.40
2:D:127:GLN:O	2:D:300:LYS:HE3	2.21	0.40
2:D:256:ASP:HA	2:D:257:ASN:HA	1.78	0.40
1:J:166:ARG:HD2	1:J:308:LEU:O	2.21	0.40
1:L:174:GLN:HA	6:L:600:ANP:HNB1	1.86	0.40
2:N:168:GLN:NE2	2:N:204:THR:HG21	2.36	0.40
1:K:282:GLN:NE2	2:N:284:THR:HG22	2.36	0.40
2:N:370:VAL:O	2:N:374:VAL:HG23	2.22	0.40
2:V:164:THR:HA	2:V:167:ILE:HG22	2.02	0.40
2:V:52:GLN:HB2	2:V:60:ARG:HB3	2.03	0.40
1:A:77:LEU:CD1	1:A:81:ASP:HB3	2.44	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:ASP:CG	1:B:115:ASN:HB2	2.41	0.40
1:J:186:LEU:HD13	1:J:225:HIS:CD2	2.56	0.40
1:L:239:SER:HB3	2:O:294:GLU:HG3	2.03	0.40
2:O:43:GLN:H	2:O:43:GLN:HG2	1.65	0.40
3:P:133:ILE:H	3:P:133:ILE:HG13	1.76	0.40
1:S:439:ALA:HB3	1:S:442:GLU:HG3	2.02	0.40
1:U:338:ALA:HB3	1:U:341:PRO:HG2	2.03	0.40
1:A:38:ASP:HB3	1:A:286:LEU:HD13	2.02	0.40
1:B:161:ILE:HA	1:B:165:GLN:OE1	2.21	0.40
2:F:277:SER:OG	2:F:278:ALA:N	2.54	0.40
2:M:314:ALA:O	2:M:315:ASP:HB2	2.22	0.40
2:M:336:SER:HB3	2:M:339:ILE:CG1	2.52	0.40
2:N:382:LYS:HA	2:N:385:GLN:HG3	2.02	0.40
1:U:382:VAL:HG12	1:U:384:ALA:H	1.86	0.40
1:C:172:ASP:O	1:C:177:LYS:NZ	2.54	0.40
2:F:15:ALA:HB3	2:F:22:ASP:HB2	2.03	0.40
2:N:204:THR:HG23	2:N:206:VAL:H	1.87	0.40
2:N:256:ASP:HA	2:N:257:ASN:HA	1.84	0.40
1:T:148:VAL:HG22	1:T:163:ARG:HG2	2.03	0.40
1:T:85:LYS:CE	2:W:32:ALA:HB2	2.49	0.40
2:X:96:ILE:HG22	2:X:97:ASN:N	2.37	0.40
2:D:384:LEU:O	2:D:388:ILE:HG12	2.22	0.40
1:K:106:LEU:HD23	1:K:230:TYR:HA	2.03	0.40
1:L:349:ASP:HA	1:L:375:ARG:HD2	2.02	0.40
2:M:119:ALA:O	2:M:295:ARG:HD2	2.22	0.40
3:P:131:ASN:HB2	3:P:132:GLY:H	1.77	0.40
3:P:88:HIS:CD2	3:P:113:LYS:HB3	2.56	0.40
2:V:277:SER:OG	2:V:278:ALA:N	2.52	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	478/510 (94%)	456 (95%)	20 (4%)	2 (0%)	34	69
1	B	479/510 (94%)	457 (95%)	22 (5%)	0	100	100
1	C	482/510 (94%)	460 (95%)	21 (4%)	1 (0%)	47	79
1	J	477/510 (94%)	460 (96%)	15 (3%)	2 (0%)	34	69
1	K	482/510 (94%)	458 (95%)	21 (4%)	3 (1%)	25	64
1	L	478/510 (94%)	454 (95%)	22 (5%)	2 (0%)	34	69
1	S	476/510 (93%)	454 (95%)	21 (4%)	1 (0%)	47	79
1	T	477/510 (94%)	452 (95%)	22 (5%)	3 (1%)	25	64
1	U	477/510 (94%)	447 (94%)	28 (6%)	2 (0%)	34	69
2	D	468/484 (97%)	444 (95%)	22 (5%)	2 (0%)	34	69
2	E	466/484 (96%)	437 (94%)	29 (6%)	0	100	100
2	F	467/484 (96%)	436 (93%)	29 (6%)	2 (0%)	34	69
2	M	468/484 (97%)	442 (94%)	23 (5%)	3 (1%)	25	64
2	N	468/484 (97%)	437 (93%)	29 (6%)	2 (0%)	34	69
2	O	466/484 (96%)	441 (95%)	23 (5%)	2 (0%)	34	69
2	V	468/484 (97%)	424 (91%)	40 (8%)	4 (1%)	17	56
2	W	465/484 (96%)	442 (95%)	23 (5%)	0	100	100
2	X	467/484 (96%)	439 (94%)	25 (5%)	3 (1%)	25	64
3	G	261/278 (94%)	244 (94%)	13 (5%)	4 (2%)	10	44
3	P	232/278 (84%)	202 (87%)	22 (10%)	8 (3%)	3	24
3	Y	186/278 (67%)	173 (93%)	12 (6%)	1 (0%)	29	67
4	H	110/137 (80%)	100 (91%)	10 (9%)	0	100	100
4	Q	74/137 (54%)	58 (78%)	11 (15%)	5 (7%)	1	9
4	Z	13/137 (10%)	10 (77%)	2 (15%)	1 (8%)	1	6
5	1	21/61 (34%)	18 (86%)	2 (10%)	1 (5%)	2	17
5	I	42/61 (69%)	32 (76%)	7 (17%)	3 (7%)	1	8
5	R	27/61 (44%)	22 (82%)	3 (11%)	2 (7%)	1	7
All	All	9475/10374 (91%)	8899 (94%)	517 (6%)	59 (1%)	25	64

All (59) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	202	ASP

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Mol	Chain	Res	Type
1	J	414	ALA
2	M	28	SER
3	P	156	ALA
3	P	275	SER
4	Q	39	ILE
5	R	32	ALA
5	1	40	THR
1	C	47	ASN
3	G	204	ASN
2	M	27	GLN
2	N	27	GLN
2	O	43	GLN
3	P	134	GLY
3	P	201	THR
3	P	204	ASN
4	Q	88	ILE
1	T	377	GLY
1	U	390	GLY
2	V	34	LEU
2	X	176	LYS
1	K	24	GLU
4	Q	47	PRO
1	A	406	ALA
3	G	135	LYS
3	G	203	ALA
1	L	508	ALA
2	V	8	PRO
2	V	277	SER
4	Z	134	GLN
2	D	398	GLU
5	I	54	SER
5	I	56	PRO
1	J	70	PRO
1	L	390	GLY
4	Q	50	GLU
5	R	31	THR
1	U	70	PRO
2	V	28	SER
3	Y	172	SER
2	D	279	VAL
2	N	279	VAL
3	P	205	VAL

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Mol	Chain	Res	Type
4	Q	37	GLY
2	F	8	PRO
1	K	97	VAL
3	P	206	PRO
1	S	70	PRO
1	T	97	VAL
2	F	279	VAL
5	I	57	THR
2	O	279	VAL
3	P	157	GLY
1	T	390	GLY
1	A	363	ILE
1	K	140	PRO
2	X	279	VAL
2	M	279	VAL
2	X	162	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	388/412 (94%)	373 (96%)	15 (4%)	32	67
1	B	388/412 (94%)	375 (97%)	13 (3%)	37	70
1	C	389/412 (94%)	378 (97%)	11 (3%)	43	74
1	J	387/412 (94%)	375 (97%)	12 (3%)	40	72
1	K	392/412 (95%)	387 (99%)	5 (1%)	69	87
1	L	388/412 (94%)	371 (96%)	17 (4%)	28	64
1	S	387/412 (94%)	379 (98%)	8 (2%)	53	79
1	T	388/412 (94%)	374 (96%)	14 (4%)	35	69
1	U	388/412 (94%)	381 (98%)	7 (2%)	59	82
2	D	380/390 (97%)	370 (97%)	10 (3%)	46	76
2	E	378/390 (97%)	361 (96%)	17 (4%)	27	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	379/390 (97%)	366 (97%)	13 (3%)	37	70
2	M	380/390 (97%)	372 (98%)	8 (2%)	53	79
2	N	380/390 (97%)	370 (97%)	10 (3%)	46	76
2	O	379/390 (97%)	370 (98%)	9 (2%)	49	77
2	V	380/390 (97%)	374 (98%)	6 (2%)	62	84
2	W	378/390 (97%)	366 (97%)	12 (3%)	39	71
2	X	379/390 (97%)	374 (99%)	5 (1%)	69	87
3	G	223/236 (94%)	214 (96%)	9 (4%)	31	66
3	P	196/236 (83%)	172 (88%)	24 (12%)	5	22
3	Y	126/236 (53%)	117 (93%)	9 (7%)	14	47
4	H	62/112 (55%)	60 (97%)	2 (3%)	39	71
4	Q	9/112 (8%)	9 (100%)	0	100	100
5	I	24/48 (50%)	24 (100%)	0	100	100
5	R	3/48 (6%)	2 (67%)	1 (33%)	0	0
All	All	7551/8246 (92%)	7314 (97%)	237 (3%)	40	72

All (237) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	LEU
1	A	166	ARG
1	A	195	SER
1	A	218	LEU
1	A	246	TYR
1	A	251	THR
1	A	322	SER
1	A	373	VAL
1	A	378	SER
1	A	393	LYS
1	A	411	ASP
1	A	412	LEU
1	A	419	THR
1	A	444	VAL
1	A	481	LEU
1	B	58	SER
1	B	99	VAL
1	B	159	VAL

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Mol	Chain	Res	Type
1	B	173	ARG
1	B	213	SER
1	B	246	TYR
1	B	288	ARG
1	B	336	VAL
1	B	351	GLN
1	B	373	VAL
1	B	400	ARG
1	B	481	LEU
1	B	509	THR
1	C	38	ASP
1	C	99	VAL
1	C	143	SER
1	C	223	GLU
1	C	293	ARG
1	C	306	ARG
1	C	357	GLU
1	C	416	THR
1	C	418	GLN
1	C	481	LEU
1	C	495	LEU
2	D	52	GLN
2	D	130	SER
2	D	132	GLU
2	D	149	ARG
2	D	167	ILE
2	D	297	THR
2	D	303	SER
2	D	336	SER
2	D	383	SER
2	D	385	GLN
2	E	27	GLN
2	E	40	LYS
2	E	111	SER
2	E	113	LEU
2	E	140	VAL
2	E	176	LYS
2	E	224	GLU
2	E	232	VAL
2	E	269	SER
2	E	315	ASP
2	E	352	ASP

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Mol	Chain	Res	Type
2	E	380	THR
2	E	393	MET
2	E	394	ASP
2	E	400	ASP
2	E	406	ARG
2	E	436	ASP
2	F	9	ILE
2	F	40	LYS
2	F	133	ILE
2	F	140	VAL
2	F	208	ASN
2	F	210	GLU
2	F	279	VAL
2	F	333	THR
2	F	336	SER
2	F	399	GLN
2	F	413	PHE
2	F	423	VAL
2	F	427	ILE
3	G	40	SER
3	G	49	GLN
3	G	101	ASP
3	G	106	ASP
3	G	118	LEU
3	G	150	LEU
3	G	216	ASN
3	G	237	MET
3	G	247	MET
4	H	14	PHE
4	H	39	ILE
1	J	142	ARG
1	J	183	ASP
1	J	218	LEU
1	J	237	THR
1	J	361	LYS
1	J	419	THR
1	J	420	LEU
1	J	440	THR
1	J	444	VAL
1	J	458	ILE
1	J	468	SER
1	J	509	THR

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Mol	Chain	Res	Type
1	K	68	LEU
1	K	142	ARG
1	K	246	TYR
1	K	351	GLN
1	K	411	ASP
1	L	90	VAL
1	L	99	VAL
1	L	134	LYS
1	L	159	VAL
1	L	218	LEU
1	L	300	VAL
1	L	306	ARG
1	L	336	VAL
1	L	351	GLN
1	L	401	GLU
1	L	416	THR
1	L	419	THR
1	L	420	LEU
1	L	468	SER
1	L	472	SER
1	L	480	GLU
1	L	481	LEU
2	M	167	ILE
2	M	204	THR
2	M	210	GLU
2	M	249	GLN
2	M	282	GLN
2	M	385	GLN
2	M	403	THR
2	M	423	VAL
2	N	10	THR
2	N	77	LEU
2	N	112	LYS
2	N	113	LEU
2	N	132	GLU
2	N	140	VAL
2	N	269	SER
2	N	380	THR
2	N	382	LYS
2	N	408	ARG
2	O	9	ILE
2	O	17	ILE

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Mol	Chain	Res	Type
2	O	43	GLN
2	O	167	ILE
2	O	182	SER
2	O	210	GLU
2	O	340	SER
2	O	423	VAL
2	O	436	ASP
3	P	3	LEU
3	P	7	GLU
3	P	11	LYS
3	P	17	GLU
3	P	29	THR
3	P	44	MET
3	P	78	THR
3	P	97	ARG
3	P	107	ILE
3	P	113	LYS
3	P	130	ILE
3	P	131	ASN
3	P	133	ILE
3	P	136	ASP
3	P	148	ASP
3	P	150	LEU
3	P	155	LYS
3	P	202	ASP
3	P	214	LEU
3	P	216	ASN
3	P	226	TYR
3	P	229	GLU
3	P	242	LYS
3	P	258	THR
5	R	47	TYR
1	S	54	LEU
1	S	105	LEU
1	S	139	LEU
1	S	159	VAL
1	S	246	TYR
1	S	318	GLU
1	S	441	GLU
1	S	495	LEU
1	T	34	LEU
1	T	130	ARG

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Mol	Chain	Res	Type
1	T	159	VAL
1	T	183	ASP
1	T	196	ASP
1	T	221	THR
1	T	246	TYR
1	T	288	ARG
1	T	320	SER
1	T	354	LEU
1	T	371	LEU
1	T	411	ASP
1	T	417	LYS
1	T	483	THR
1	U	163	ARG
1	U	213	SER
1	U	218	LEU
1	U	351	GLN
1	U	411	ASP
1	U	416	THR
1	U	424	GLU
2	V	65	ASP
2	V	84	SER
2	V	249	GLN
2	V	271	LEU
2	V	282	GLN
2	V	315	ASP
2	W	113	LEU
2	W	132	GLU
2	W	140	VAL
2	W	161	VAL
2	W	212	GLU
2	W	213	SER
2	W	232	VAL
2	W	356	ARG
2	W	386	ASP
2	W	403	THR
2	W	433	ARG
2	W	434	LEU
2	X	167	ILE
2	X	208	ASN
2	X	250	ASP
2	X	272	LEU
2	X	372	SER

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Mol	Chain	Res	Type
3	Y	15	ASN
3	Y	80	ASP
3	Y	84	CYS
3	Y	98	HIS
3	Y	99	LEU
3	Y	101	ASP
3	Y	219	LEU
3	Y	235	ASN
3	Y	269	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	351	GLN
1	B	428	GLN
1	C	95	ASN
1	C	115	ASN
1	C	174	GLN
1	C	224	GLN
1	C	398	GLN
1	C	479	ASN
2	E	168	GLN
3	G	90	GLN
3	G	125	ASN
3	G	190	GLN
3	G	216	ASN
4	H	45	HIS
1	J	26	ASN
1	J	225	HIS
1	J	477	ASN
1	K	174	GLN
1	K	220	GLN
1	L	145	HIS
1	L	224	GLN
1	L	262	ASN
1	L	398	GLN
1	L	454	HIS
1	L	479	ASN
2	M	367	HIS
2	N	127	GLN
2	N	168	GLN

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Mol	Chain	Res	Type
2	O	52	GLN
2	O	208	ASN
2	O	328	HIS
3	P	54	ASN
3	P	88	HIS
3	P	122	HIS
3	P	216	ASN
1	S	407	GLN
1	T	50	GLN
1	T	387	GLN
1	T	434	GLN
1	U	217	GLN
1	U	479	ASN
2	V	282	GLN
2	X	27	GLN
2	X	52	GLN
2	X	178	HIS
2	X	208	ASN
2	X	379	GLN
2	X	455	HIS
3	Y	15	ASN
3	Y	117	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 31 ligands modelled in this entry, 15 are monoatomic - leaving 16 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	ANP	T	600	7	29,33,33	1.90	8 (27%)	31,52,52	1.88	8 (25%)
6	ANP	F	600	7	29,33,33	1.69	8 (27%)	31,52,52	1.77	7 (22%)
6	ANP	C	600	7	29,33,33	1.71	7 (24%)	31,52,52	1.85	7 (22%)
6	ANP	B	600	7	29,33,33	1.90	6 (20%)	31,52,52	1.96	6 (19%)
6	ANP	A	600	7	29,33,33	1.95	9 (31%)	31,52,52	1.70	8 (25%)
6	ANP	O	600	7	29,33,33	1.73	8 (27%)	31,52,52	1.89	9 (29%)
6	ANP	M	600	7	29,33,33	1.76	7 (24%)	31,52,52	2.03	6 (19%)
6	ANP	D	600	7	29,33,33	1.80	7 (24%)	31,52,52	1.76	8 (25%)
6	ANP	K	600	7	29,33,33	1.86	8 (27%)	31,52,52	1.91	8 (25%)
8	PO4	N	800	-	4,4,4	0.88	0	6,6,6	0.47	0
6	ANP	U	600	7	29,33,33	1.80	7 (24%)	31,52,52	2.01	8 (25%)
6	ANP	V	600	7	29,33,33	1.81	6 (20%)	31,52,52	2.03	8 (25%)
6	ANP	J	600	7	29,33,33	1.81	7 (24%)	31,52,52	2.00	6 (19%)
6	ANP	L	600	7	29,33,33	1.76	7 (24%)	31,52,52	1.94	9 (29%)
6	ANP	S	600	7	29,33,33	1.82	7 (24%)	31,52,52	1.95	8 (25%)
6	ANP	X	600	7	29,33,33	1.79	8 (27%)	31,52,52	2.04	8 (25%)

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
6	ANP	T	600	7	-	4/14/38/38	0/3/3/3
6	ANP	F	600	7	-	7/14/38/38	0/3/3/3
6	ANP	C	600	7	-	3/14/38/38	0/3/3/3
6	ANP	B	600	7	-	6/14/38/38	0/3/3/3
6	ANP	A	600	7	-	2/14/38/38	0/3/3/3
6	ANP	O	600	7	-	5/14/38/38	0/3/3/3
6	ANP	M	600	7	-	4/14/38/38	0/3/3/3
6	ANP	D	600	7	-	4/14/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ANP	K	600	7	-	5/14/38/38	0/3/3/3
6	ANP	J	600	7	-	3/14/38/38	0/3/3/3
6	ANP	V	600	7	-	6/14/38/38	0/3/3/3
6	ANP	U	600	7	-	4/14/38/38	0/3/3/3
6	ANP	L	600	7	-	3/14/38/38	0/3/3/3
6	ANP	S	600	7	-	3/14/38/38	0/3/3/3
6	ANP	X	600	7	-	9/14/38/38	0/3/3/3

All (110) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	600	ANP	PG-N3B	4.69	1.75	1.63
6	T	600	ANP	PB-N3B	4.54	1.75	1.63
6	S	600	ANP	PG-N3B	4.51	1.75	1.63
6	A	600	ANP	PB-N3B	4.50	1.75	1.63
6	V	600	ANP	PG-N3B	4.49	1.75	1.63
6	S	600	ANP	PB-N3B	4.46	1.75	1.63
6	T	600	ANP	PG-N3B	4.43	1.74	1.63
6	K	600	ANP	PB-N3B	4.42	1.74	1.63
6	B	600	ANP	PB-N3B	4.42	1.74	1.63
6	X	600	ANP	PB-N3B	4.40	1.74	1.63
6	M	600	ANP	PG-N3B	4.37	1.74	1.63
6	L	600	ANP	PG-N3B	4.33	1.74	1.63
6	L	600	ANP	PB-N3B	4.33	1.74	1.63
6	X	600	ANP	PG-N3B	4.29	1.74	1.63
6	V	600	ANP	PB-N3B	4.28	1.74	1.63
6	B	600	ANP	PG-N3B	4.25	1.74	1.63
6	J	600	ANP	PB-N3B	4.24	1.74	1.63
6	D	600	ANP	PG-N3B	4.22	1.74	1.63
6	K	600	ANP	PG-N3B	4.21	1.74	1.63
6	M	600	ANP	PB-N3B	4.11	1.74	1.63
6	D	600	ANP	PB-N3B	4.09	1.74	1.63
6	U	600	ANP	PG-N3B	4.07	1.74	1.63
6	J	600	ANP	PG-N3B	4.03	1.73	1.63
6	O	600	ANP	PB-N3B	3.93	1.73	1.63
6	U	600	ANP	PB-N3B	3.89	1.73	1.63
6	C	600	ANP	PG-N3B	3.85	1.73	1.63
6	O	600	ANP	PG-N3B	3.79	1.73	1.63
6	T	600	ANP	PG-O1G	3.77	1.52	1.46
6	C	600	ANP	PB-N3B	3.76	1.73	1.63
6	A	600	ANP	PG-O1G	3.76	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	600	ANP	PG-N3B	3.74	1.73	1.63
6	J	600	ANP	PG-O1G	3.70	1.52	1.46
6	F	600	ANP	PB-N3B	3.68	1.73	1.63
6	D	600	ANP	PG-O1G	3.65	1.51	1.46
6	B	600	ANP	PB-O1B	3.62	1.51	1.46
6	U	600	ANP	PG-O1G	3.50	1.51	1.46
6	K	600	ANP	PB-O1B	3.43	1.51	1.46
6	B	600	ANP	PG-O1G	3.35	1.51	1.46
6	M	600	ANP	PG-O1G	3.34	1.51	1.46
6	K	600	ANP	PG-O1G	3.34	1.51	1.46
6	A	600	ANP	PB-O1B	3.30	1.51	1.46
6	J	600	ANP	PB-O1B	3.30	1.51	1.46
6	T	600	ANP	PB-O1B	3.25	1.51	1.46
6	C	600	ANP	PG-O1G	3.25	1.51	1.46
6	V	600	ANP	PG-O1G	3.25	1.51	1.46
6	S	600	ANP	PB-O1B	3.21	1.51	1.46
6	C	600	ANP	PB-O1B	3.15	1.51	1.46
6	X	600	ANP	PB-O1B	3.11	1.51	1.46
6	F	600	ANP	PG-O1G	3.09	1.51	1.46
6	V	600	ANP	PB-O1B	2.97	1.50	1.46
6	O	600	ANP	PG-O1G	2.97	1.50	1.46
6	U	600	ANP	PB-O1B	2.97	1.50	1.46
6	L	600	ANP	PG-O1G	2.93	1.50	1.46
6	L	600	ANP	PB-O1B	2.92	1.50	1.46
6	O	600	ANP	PB-O1B	2.91	1.50	1.46
6	S	600	ANP	PG-O1G	2.87	1.50	1.46
6	M	600	ANP	PB-O1B	2.84	1.50	1.46
6	U	600	ANP	C5-C4	2.82	1.48	1.40
6	T	600	ANP	C5-C4	2.80	1.48	1.40
6	B	600	ANP	C5-C4	2.78	1.48	1.40
6	X	600	ANP	PG-O1G	2.71	1.50	1.46
6	B	600	ANP	PB-O3A	2.70	1.62	1.59
6	O	600	ANP	C5-C4	2.67	1.48	1.40
6	K	600	ANP	C5-C4	2.64	1.47	1.40
6	D	600	ANP	PB-O1B	2.63	1.50	1.46
6	F	600	ANP	PB-O1B	2.62	1.50	1.46
6	D	600	ANP	C5-C4	2.62	1.47	1.40
6	S	600	ANP	C5-C4	2.60	1.47	1.40
6	J	600	ANP	C5-C4	2.59	1.47	1.40
6	X	600	ANP	C5-C4	2.58	1.47	1.40
6	F	600	ANP	C5-C4	2.56	1.47	1.40
6	A	600	ANP	C5-C4	2.56	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	600	ANP	PG-O2G	-2.52	1.50	1.56
6	S	600	ANP	PG-O3G	-2.51	1.50	1.56
6	V	600	ANP	C5-C4	2.48	1.47	1.40
6	J	600	ANP	PG-O2G	-2.47	1.50	1.56
6	A	600	ANP	PB-O3A	2.45	1.62	1.59
6	A	600	ANP	PG-O3G	-2.44	1.50	1.56
6	C	600	ANP	C5-C4	2.41	1.47	1.40
6	C	600	ANP	PB-O3A	2.39	1.62	1.59
6	M	600	ANP	C5-C4	2.38	1.47	1.40
6	L	600	ANP	C5-C4	2.37	1.47	1.40
6	T	600	ANP	PB-O3A	2.36	1.62	1.59
6	U	600	ANP	C2-N3	2.29	1.35	1.32
6	F	600	ANP	PB-O2B	-2.25	1.50	1.56
6	X	600	ANP	PG-O3G	-2.22	1.50	1.56
6	M	600	ANP	PG-O2G	-2.19	1.50	1.56
6	K	600	ANP	C2-N3	2.19	1.35	1.32
6	L	600	ANP	PG-O3G	-2.18	1.50	1.56
6	F	600	ANP	C2-N3	2.17	1.35	1.32
6	X	600	ANP	O4'-C1'	2.14	1.44	1.41
6	O	600	ANP	PB-O3A	2.13	1.61	1.59
6	S	600	ANP	C2-N3	2.12	1.35	1.32
6	V	600	ANP	C2-N3	2.12	1.35	1.32
6	U	600	ANP	PB-O3A	2.10	1.61	1.59
6	D	600	ANP	PG-O3G	-2.09	1.51	1.56
6	J	600	ANP	PG-O3G	-2.09	1.51	1.56
6	O	600	ANP	PG-O3G	-2.07	1.51	1.56
6	X	600	ANP	C2-N3	2.07	1.35	1.32
6	C	600	ANP	PG-O3G	-2.06	1.51	1.56
6	D	600	ANP	C2-N3	2.05	1.35	1.32
6	F	600	ANP	PG-O3G	-2.03	1.51	1.56
6	A	600	ANP	C2-N3	2.02	1.35	1.32
6	M	600	ANP	PG-O3G	-2.02	1.51	1.56
6	T	600	ANP	O4'-C1'	2.02	1.43	1.41
6	L	600	ANP	PB-O2B	-2.02	1.51	1.56
6	O	600	ANP	PB-O2B	-2.02	1.51	1.56
6	T	600	ANP	PG-O3G	-2.01	1.51	1.56
6	K	600	ANP	PG-O3G	-2.01	1.51	1.56
6	K	600	ANP	O4'-C1'	2.00	1.43	1.41

All (114) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	X	600	ANP	O1G-PG-N3B	-6.32	102.46	111.77
6	J	600	ANP	O1G-PG-N3B	-6.02	102.90	111.77
6	B	600	ANP	O1G-PG-N3B	-6.00	102.94	111.77
6	V	600	ANP	O1G-PG-N3B	-5.95	103.00	111.77
6	M	600	ANP	O2B-PB-O1B	5.89	122.28	109.92
6	U	600	ANP	O1G-PG-N3B	-5.72	103.35	111.77
6	K	600	ANP	O1G-PG-N3B	-5.40	103.82	111.77
6	O	600	ANP	O1G-PG-N3B	-5.30	103.97	111.77
6	L	600	ANP	O2B-PB-O1B	5.25	120.93	109.92
6	M	600	ANP	O1G-PG-N3B	-5.24	104.06	111.77
6	B	600	ANP	O2B-PB-O1B	5.22	120.86	109.92
6	J	600	ANP	O2B-PB-O1B	5.15	120.72	109.92
6	L	600	ANP	O1G-PG-N3B	-5.03	104.36	111.77
6	C	600	ANP	O2B-PB-O1B	4.83	120.04	109.92
6	K	600	ANP	O2B-PB-O1B	4.79	119.97	109.92
6	S	600	ANP	O2B-PB-O1B	4.78	119.95	109.92
6	C	600	ANP	O1G-PG-N3B	-4.67	104.89	111.77
6	V	600	ANP	O2B-PB-O1B	4.65	119.67	109.92
6	D	600	ANP	O2B-PB-O1B	4.62	119.62	109.92
6	A	600	ANP	O2B-PB-O1B	4.54	119.45	109.92
6	F	600	ANP	O2B-PB-O1B	4.48	119.31	109.92
6	D	600	ANP	O1G-PG-N3B	-4.42	105.27	111.77
6	U	600	ANP	O2B-PB-O1B	4.39	119.14	109.92
6	T	600	ANP	O1G-PG-N3B	-4.38	105.33	111.77
6	M	600	ANP	O1B-PB-N3B	-4.34	105.37	111.77
6	F	600	ANP	O1G-PG-N3B	-4.29	105.45	111.77
6	O	600	ANP	O2B-PB-O1B	4.24	118.81	109.92
6	S	600	ANP	O1G-PG-N3B	-4.21	105.56	111.77
6	T	600	ANP	O2B-PB-O1B	4.17	118.67	109.92
6	X	600	ANP	O2B-PB-O1B	4.12	118.56	109.92
6	S	600	ANP	PA-O3A-PB	-3.98	118.59	132.62
6	K	600	ANP	N3-C2-N1	-3.60	123.06	128.68
6	S	600	ANP	N3-C2-N1	-3.59	123.06	128.68
6	A	600	ANP	O1G-PG-N3B	-3.58	106.50	111.77
6	L	600	ANP	N3-C2-N1	-3.56	123.11	128.68
6	T	600	ANP	O1B-PB-N3B	-3.56	106.53	111.77
6	V	600	ANP	PA-O3A-PB	-3.54	120.13	132.62
6	S	600	ANP	O1B-PB-N3B	-3.49	106.64	111.77
6	U	600	ANP	N3-C2-N1	-3.48	123.24	128.68
6	J	600	ANP	N3-C2-N1	-3.47	123.26	128.68
6	C	600	ANP	N3-C2-N1	-3.39	123.39	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	600	ANP	N3-C2-N1	-3.37	123.42	128.68
6	T	600	ANP	C3'-C2'-C1'	3.36	106.04	100.98
6	B	600	ANP	N3-C2-N1	-3.31	123.51	128.68
6	U	600	ANP	O1B-PB-N3B	-3.30	106.91	111.77
6	T	600	ANP	N3-C2-N1	-3.29	123.53	128.68
6	D	600	ANP	PA-O3A-PB	-3.28	121.07	132.62
6	X	600	ANP	PA-O3A-PB	-3.28	121.07	132.62
6	F	600	ANP	PA-O3A-PB	-3.27	121.10	132.62
6	M	600	ANP	N3-C2-N1	-3.26	123.58	128.68
6	O	600	ANP	N3-C2-N1	-3.22	123.64	128.68
6	X	600	ANP	N3-C2-N1	-3.22	123.65	128.68
6	L	600	ANP	PA-O3A-PB	-3.21	121.31	132.62
6	X	600	ANP	O1B-PB-N3B	-3.20	107.05	111.77
6	F	600	ANP	O3G-PG-O2G	3.18	116.11	107.64
6	X	600	ANP	C3'-C2'-C1'	3.12	105.68	100.98
6	V	600	ANP	C3'-C2'-C1'	3.11	105.66	100.98
6	V	600	ANP	N3-C2-N1	-3.09	123.86	128.68
6	C	600	ANP	O3G-PG-O2G	3.08	115.85	107.64
6	J	600	ANP	C3'-C2'-C1'	3.08	105.61	100.98
6	A	600	ANP	N3-C2-N1	-2.99	124.01	128.68
6	K	600	ANP	PA-O3A-PB	-2.98	122.14	132.62
6	V	600	ANP	C4-C5-N7	-2.98	106.30	109.40
6	U	600	ANP	C3'-C2'-C1'	2.94	105.40	100.98
6	O	600	ANP	O3G-PG-O2G	2.94	115.46	107.64
6	J	600	ANP	PA-O3A-PB	-2.93	122.30	132.62
6	O	600	ANP	PA-O3A-PB	-2.92	122.32	132.62
6	C	600	ANP	PA-O3A-PB	-2.92	122.32	132.62
6	D	600	ANP	C4-C5-N7	-2.91	106.36	109.40
6	D	600	ANP	O1B-PB-N3B	-2.91	107.49	111.77
6	T	600	ANP	PA-O3A-PB	-2.82	122.67	132.62
6	M	600	ANP	C4-C5-N7	-2.81	106.47	109.40
6	O	600	ANP	C4-C5-N7	-2.81	106.47	109.40
6	B	600	ANP	O3G-PG-O2G	2.79	115.07	107.64
6	A	600	ANP	PA-O3A-PB	-2.76	122.89	132.62
6	T	600	ANP	O3G-PG-O2G	2.72	114.88	107.64
6	V	600	ANP	O1B-PB-N3B	-2.71	107.78	111.77
6	D	600	ANP	N3-C2-N1	-2.67	124.51	128.68
6	K	600	ANP	C4-C5-N7	-2.67	106.62	109.40
6	S	600	ANP	O3G-PG-O2G	2.65	114.69	107.64
6	L	600	ANP	O3G-PG-O2G	2.63	114.65	107.64
6	B	600	ANP	C4-C5-N7	-2.63	106.66	109.40
6	L	600	ANP	C4-C5-N7	-2.61	106.67	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	600	ANP	O1B-PB-N3B	-2.60	107.94	111.77
6	K	600	ANP	O3G-PG-O2G	2.57	114.48	107.64
6	X	600	ANP	O3G-PG-O2G	2.55	114.42	107.64
6	U	600	ANP	O3G-PG-O2G	2.53	114.38	107.64
6	C	600	ANP	O1B-PB-N3B	-2.52	108.05	111.77
6	S	600	ANP	C4-C5-N7	-2.50	106.80	109.40
6	F	600	ANP	C4-C5-N7	-2.47	106.83	109.40
6	K	600	ANP	O1B-PB-N3B	-2.46	108.15	111.77
6	V	600	ANP	O3G-PG-O2G	2.43	114.11	107.64
6	A	600	ANP	O3G-PG-O2G	2.42	114.08	107.64
6	T	600	ANP	C4-C5-N7	-2.41	106.89	109.40
6	O	600	ANP	C3'-C2'-C1'	2.39	104.58	100.98
6	M	600	ANP	O3G-PG-O2G	2.34	113.86	107.64
6	X	600	ANP	C4-C5-N7	-2.31	107.00	109.40
6	U	600	ANP	C4-C5-N7	-2.27	107.03	109.40
6	J	600	ANP	C4-C5-N7	-2.25	107.06	109.40
6	U	600	ANP	PA-O3A-PB	-2.24	124.71	132.62
6	A	600	ANP	C4-C5-N7	-2.23	107.07	109.40
6	B	600	ANP	O1B-PB-N3B	-2.22	108.51	111.77
6	S	600	ANP	C3'-C2'-C1'	2.20	104.30	100.98
6	L	600	ANP	C2-N1-C6	2.19	122.50	118.75
6	C	600	ANP	C4-C5-N7	-2.14	107.17	109.40
6	O	600	ANP	O2B-PB-O3A	2.11	111.68	104.64
6	D	600	ANP	O3G-PG-O2G	2.09	113.22	107.64
6	A	600	ANP	C3'-C2'-C1'	2.09	104.12	100.98
6	K	600	ANP	C3'-C2'-C1'	2.09	104.12	100.98
6	L	600	ANP	O2A-PA-O1A	2.06	122.45	112.24
6	O	600	ANP	O1B-PB-N3B	-2.05	108.75	111.77
6	D	600	ANP	C3'-C2'-C1'	2.04	104.04	100.98
6	F	600	ANP	O2B-PB-O3A	2.02	111.40	104.64
6	A	600	ANP	O4'-C1'-C2'	-2.01	103.99	106.93

There are no chirality outliers.

All (68) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	F	600	ANP	PB-N3B-PG-O1G
6	F	600	ANP	PG-N3B-PB-O1B
6	F	600	ANP	C5'-O5'-PA-O2A
6	D	600	ANP	PB-N3B-PG-O1G
6	D	600	ANP	PG-N3B-PB-O1B
6	D	600	ANP	PA-O3A-PB-O1B

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Mol	Chain	Res	Type	Atoms
6	D	600	ANP	PA-O3A-PB-O2B
6	L	600	ANP	PB-N3B-PG-O1G
6	L	600	ANP	PG-N3B-PB-O1B
6	T	600	ANP	PB-N3B-PG-O1G
6	T	600	ANP	PG-N3B-PB-O1B
6	X	600	ANP	PB-N3B-PG-O1G
6	X	600	ANP	PG-N3B-PB-O1B
6	X	600	ANP	PA-O3A-PB-O1B
6	X	600	ANP	PA-O3A-PB-O2B
6	X	600	ANP	C5'-O5'-PA-O1A
6	X	600	ANP	C5'-O5'-PA-O2A
6	X	600	ANP	O4'-C4'-C5'-O5'
6	X	600	ANP	C3'-C4'-C5'-O5'
6	S	600	ANP	PB-N3B-PG-O1G
6	S	600	ANP	PG-N3B-PB-O1B
6	S	600	ANP	PG-N3B-PB-O3A
6	O	600	ANP	PB-N3B-PG-O1G
6	O	600	ANP	PG-N3B-PB-O1B
6	O	600	ANP	PG-N3B-PB-O3A
6	M	600	ANP	PB-N3B-PG-O1G
6	M	600	ANP	PG-N3B-PB-O1B
6	M	600	ANP	PA-O3A-PB-O1B
6	M	600	ANP	PA-O3A-PB-O2B
6	J	600	ANP	PB-N3B-PG-O1G
6	J	600	ANP	PG-N3B-PB-O1B
6	J	600	ANP	PG-N3B-PB-O3A
6	V	600	ANP	PB-N3B-PG-O1G
6	V	600	ANP	PG-N3B-PB-O1B
6	V	600	ANP	PA-O3A-PB-O1B
6	V	600	ANP	C5'-O5'-PA-O1A
6	V	600	ANP	C5'-O5'-PA-O2A
6	V	600	ANP	C5'-O5'-PA-O3A
6	U	600	ANP	PB-N3B-PG-O1G
6	U	600	ANP	PG-N3B-PB-O1B
6	C	600	ANP	PB-N3B-PG-O1G
6	C	600	ANP	PG-N3B-PB-O1B
6	B	600	ANP	PB-N3B-PG-O1G
6	B	600	ANP	PG-N3B-PB-O1B
6	B	600	ANP	C5'-O5'-PA-O2A
6	A	600	ANP	PB-N3B-PG-O1G
6	A	600	ANP	PG-N3B-PB-O1B
6	K	600	ANP	PB-N3B-PG-O1G

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Mol	Chain	Res	Type	Atoms
6	K	600	ANP	PG-N3B-PB-O1B
6	K	600	ANP	O4'-C4'-C5'-O5'
6	F	600	ANP	O4'-C4'-C5'-O5'
6	K	600	ANP	C3'-C4'-C5'-O5'
6	F	600	ANP	C5'-O5'-PA-O3A
6	B	600	ANP	C5'-O5'-PA-O3A
6	L	600	ANP	PG-N3B-PB-O3A
6	U	600	ANP	PB-O3A-PA-O2A
6	K	600	ANP	PB-O3A-PA-O1A
6	F	600	ANP	C3'-C4'-C5'-O5'
6	B	600	ANP	PB-O3A-PA-O1A
6	T	600	ANP	C5'-O5'-PA-O3A
6	X	600	ANP	C5'-O5'-PA-O3A
6	O	600	ANP	C5'-O5'-PA-O3A
6	F	600	ANP	C5'-O5'-PA-O1A
6	T	600	ANP	C5'-O5'-PA-O1A
6	O	600	ANP	C5'-O5'-PA-O2A
6	B	600	ANP	C5'-O5'-PA-O1A
6	U	600	ANP	PG-N3B-PB-O3A
6	C	600	ANP	PG-N3B-PB-O3A

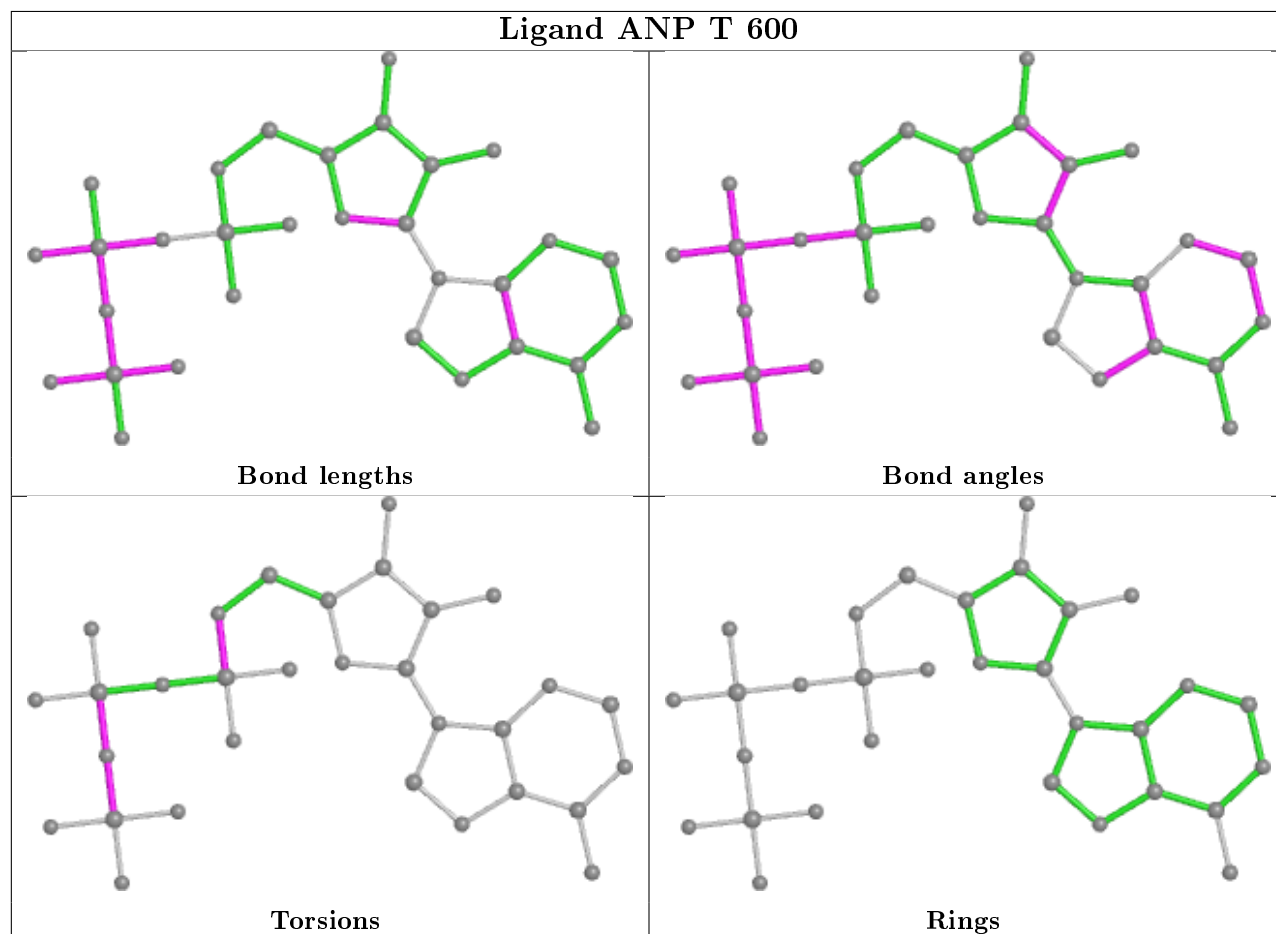
There are no ring outliers.

9 monomers are involved in 15 short contacts:

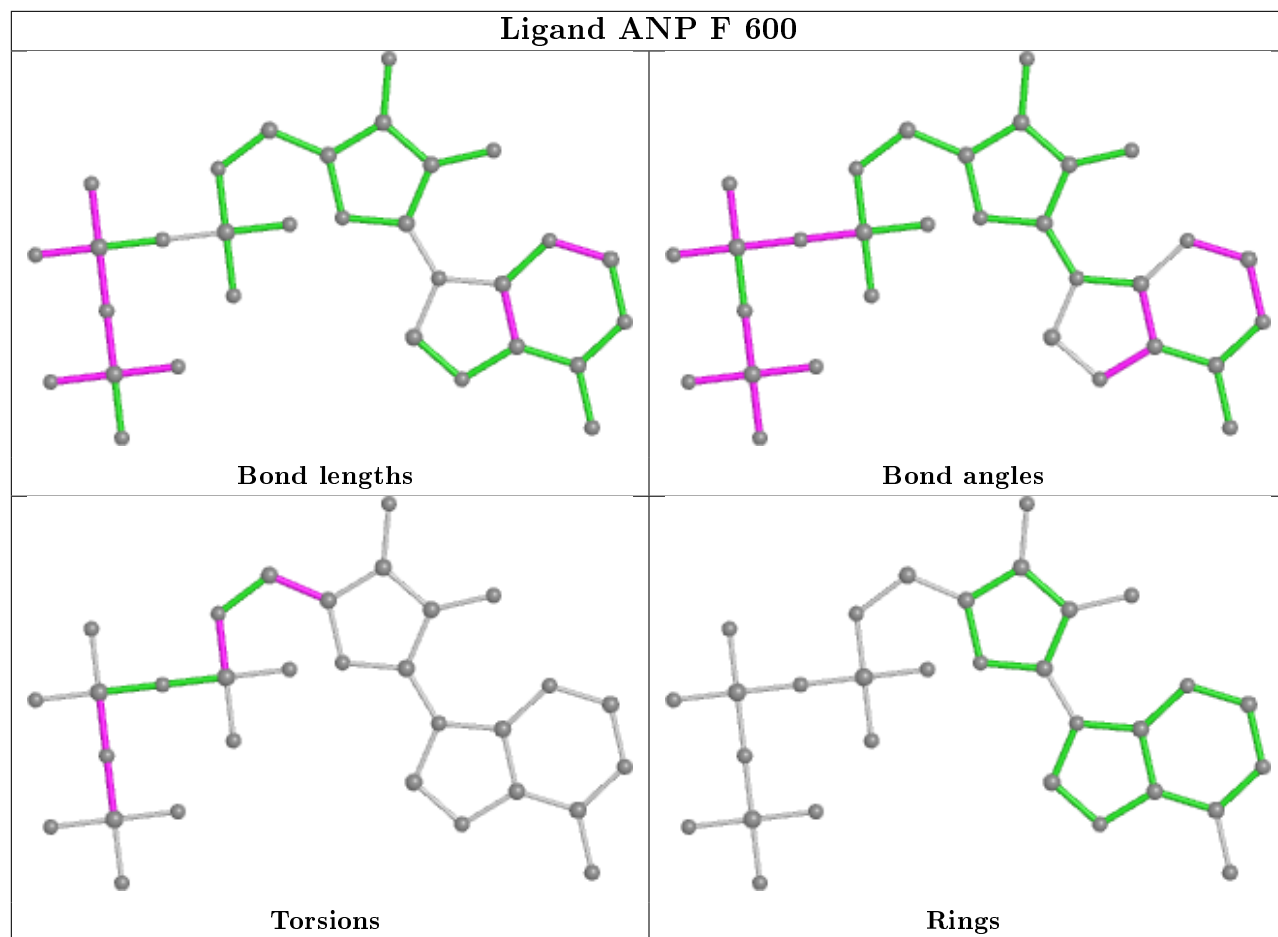
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	T	600	ANP	2	0
6	C	600	ANP	1	0
6	B	600	ANP	1	0
6	A	600	ANP	1	0
6	M	600	ANP	2	0
6	D	600	ANP	4	0
6	V	600	ANP	1	0
6	L	600	ANP	1	0
6	X	600	ANP	2	0

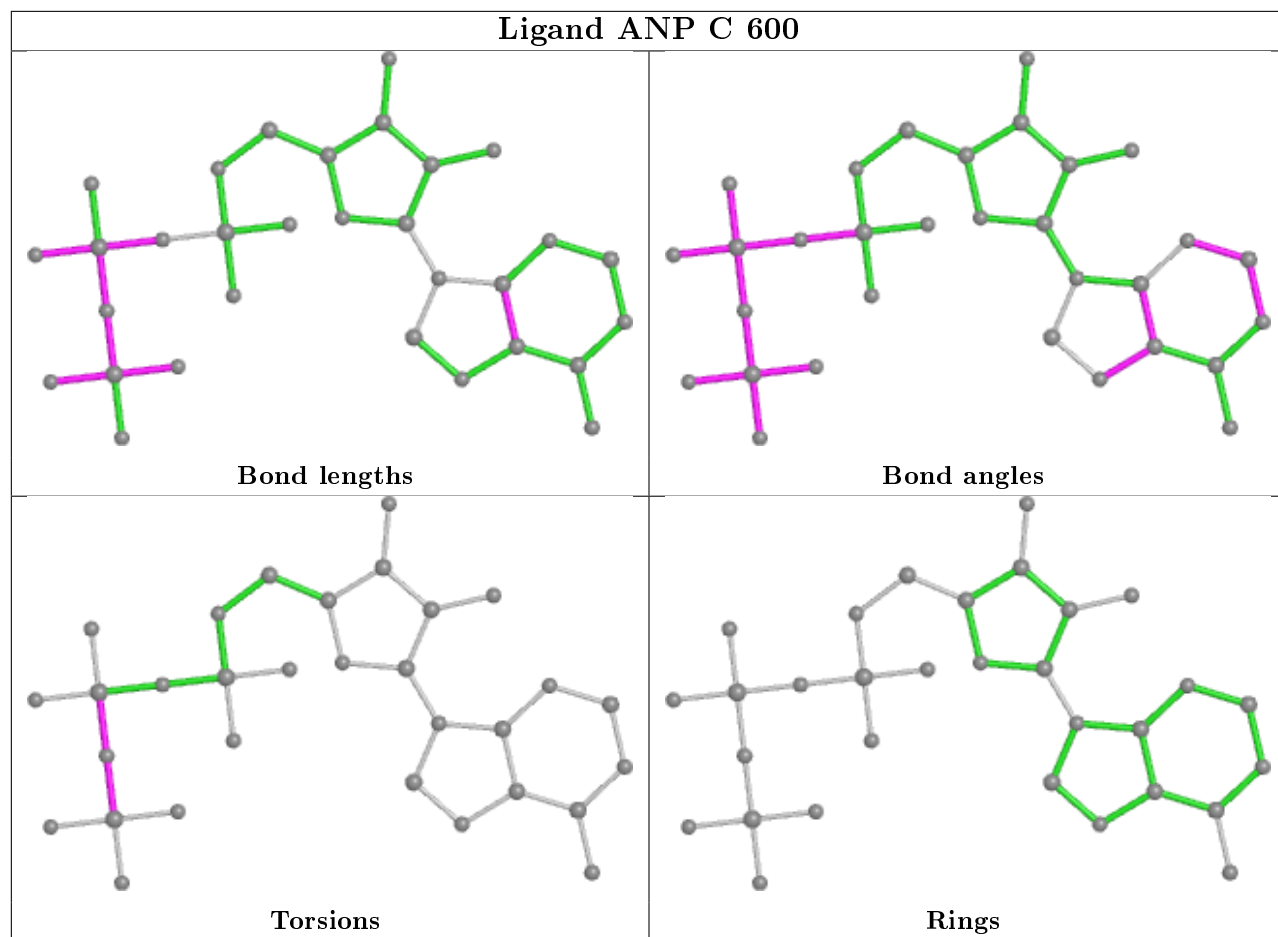
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

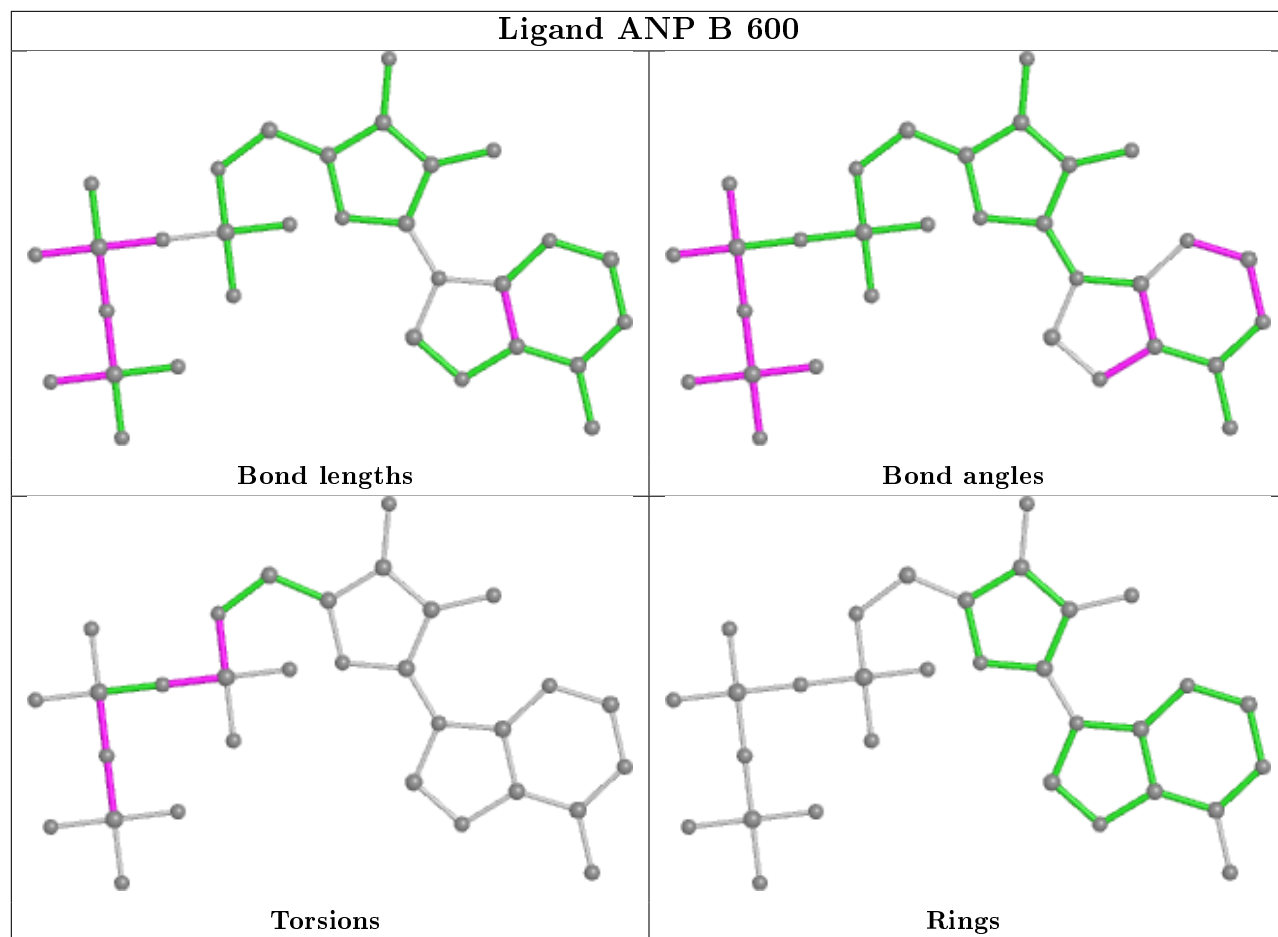
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

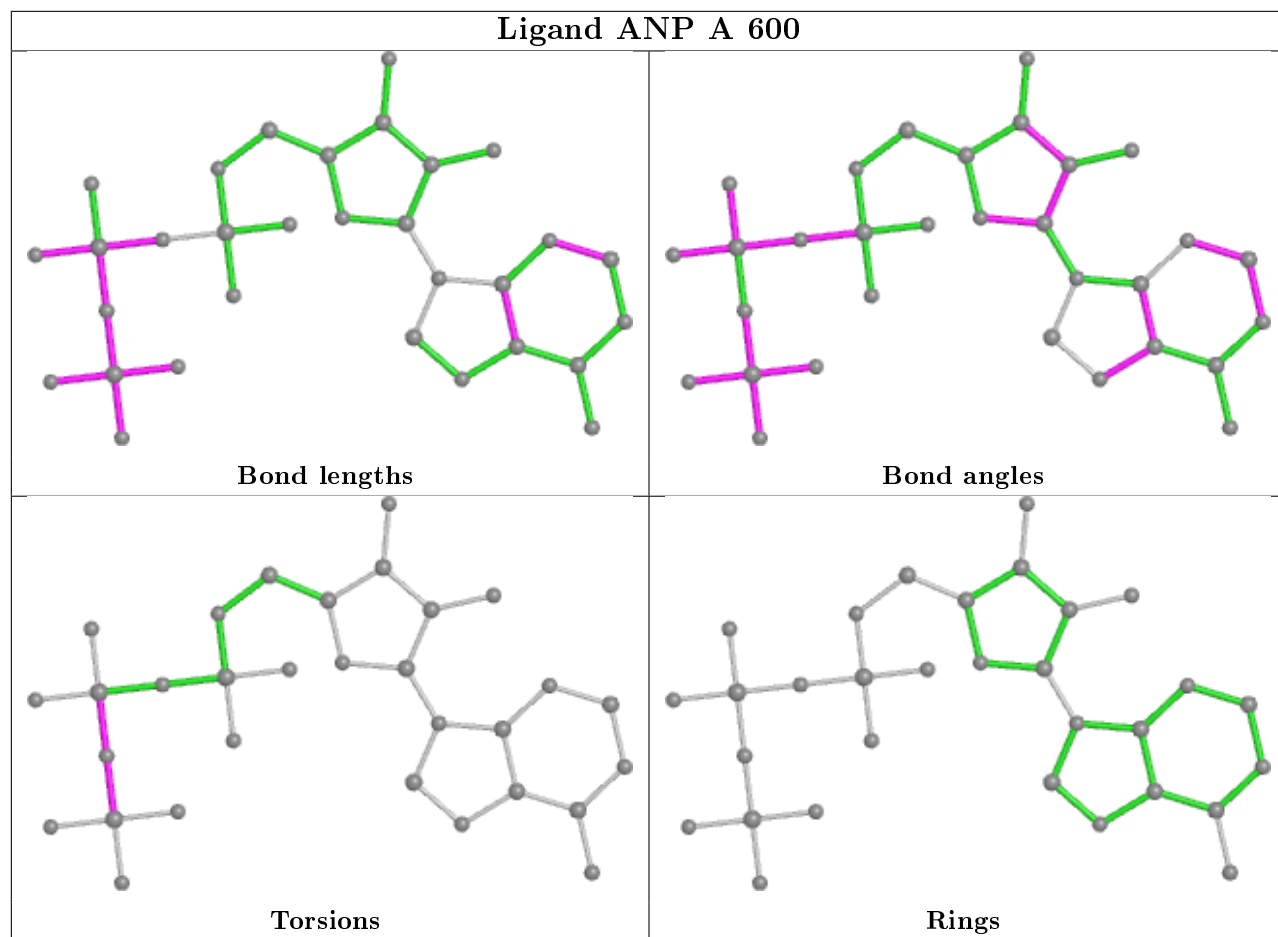


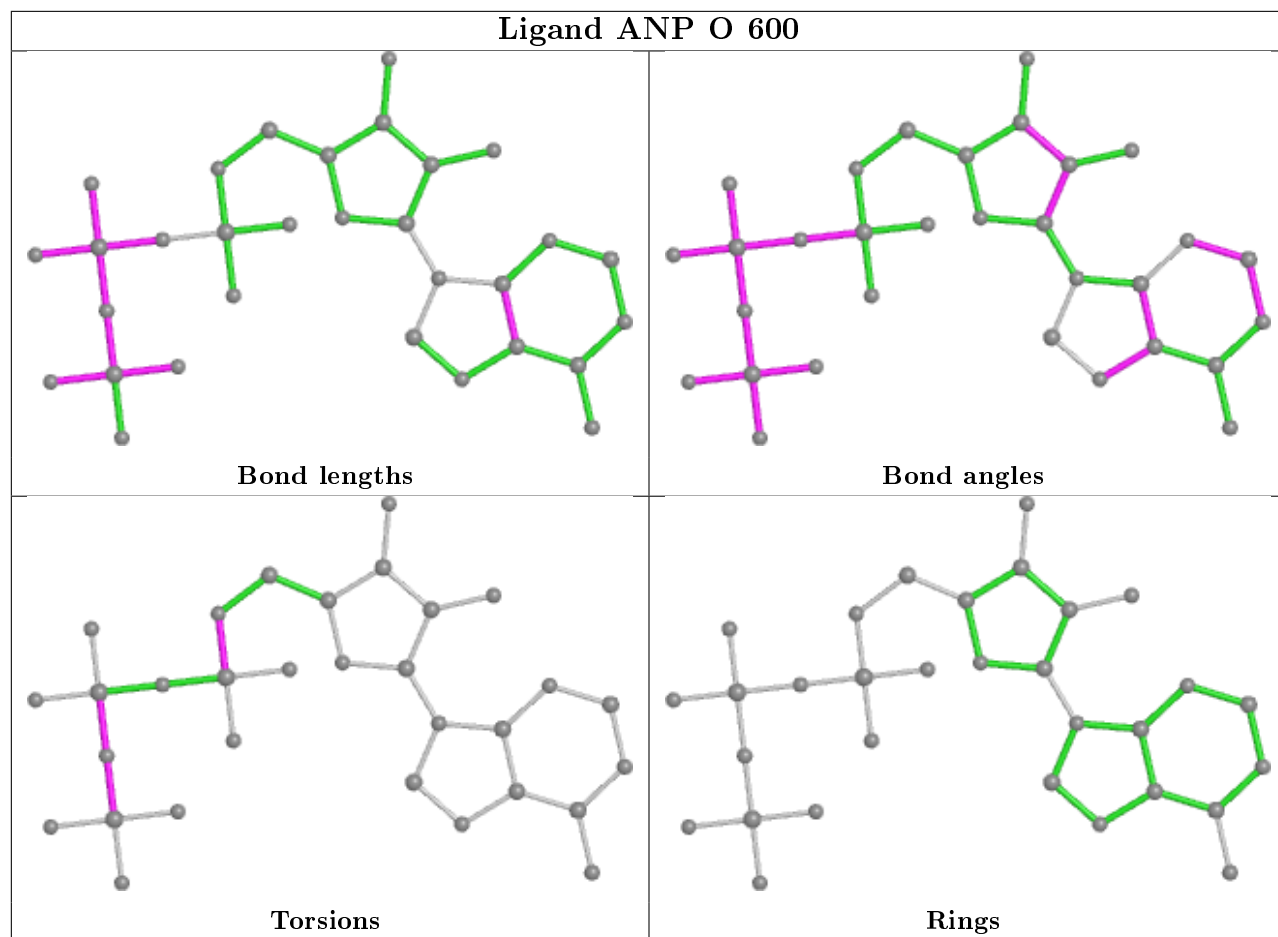


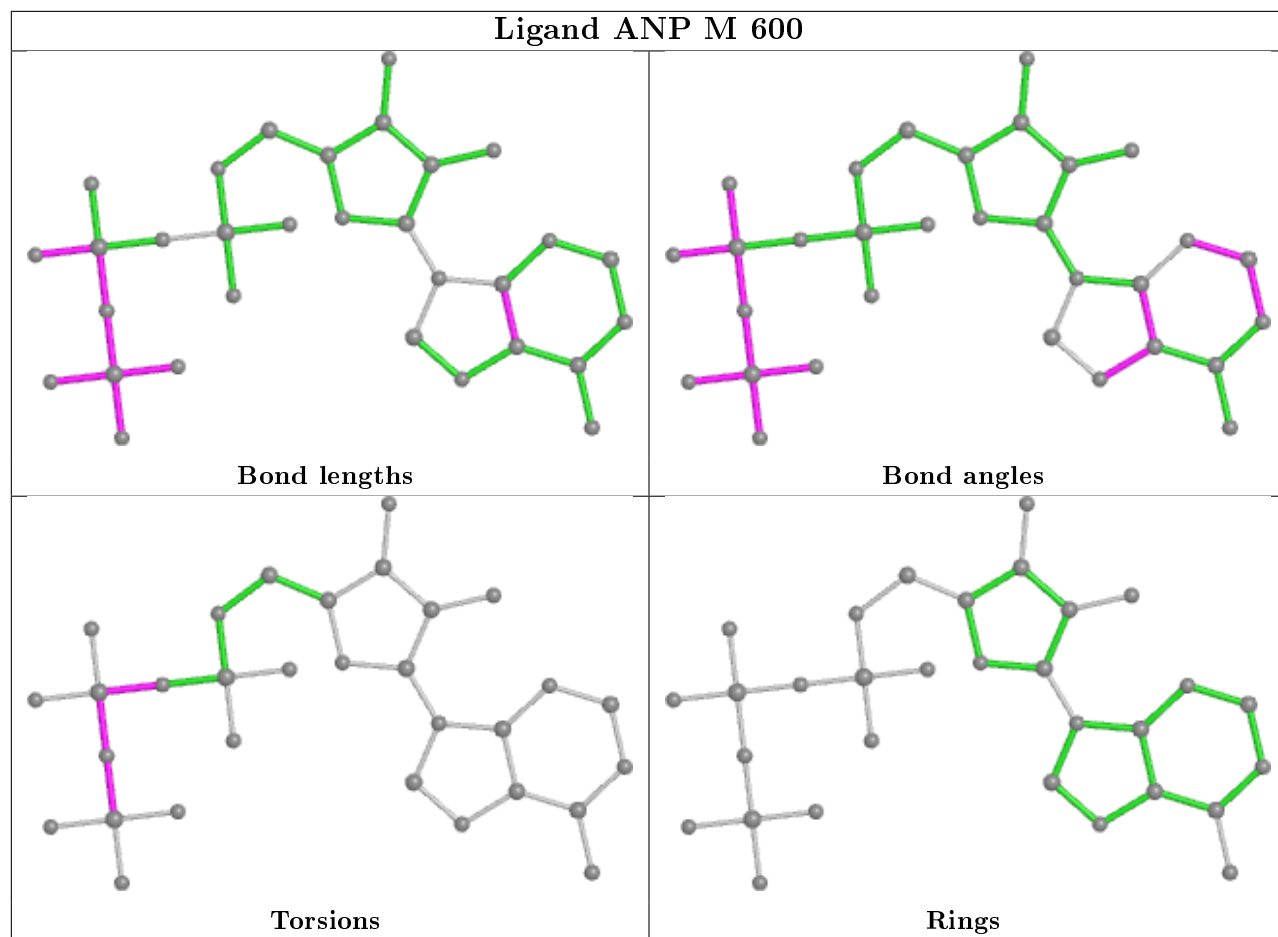


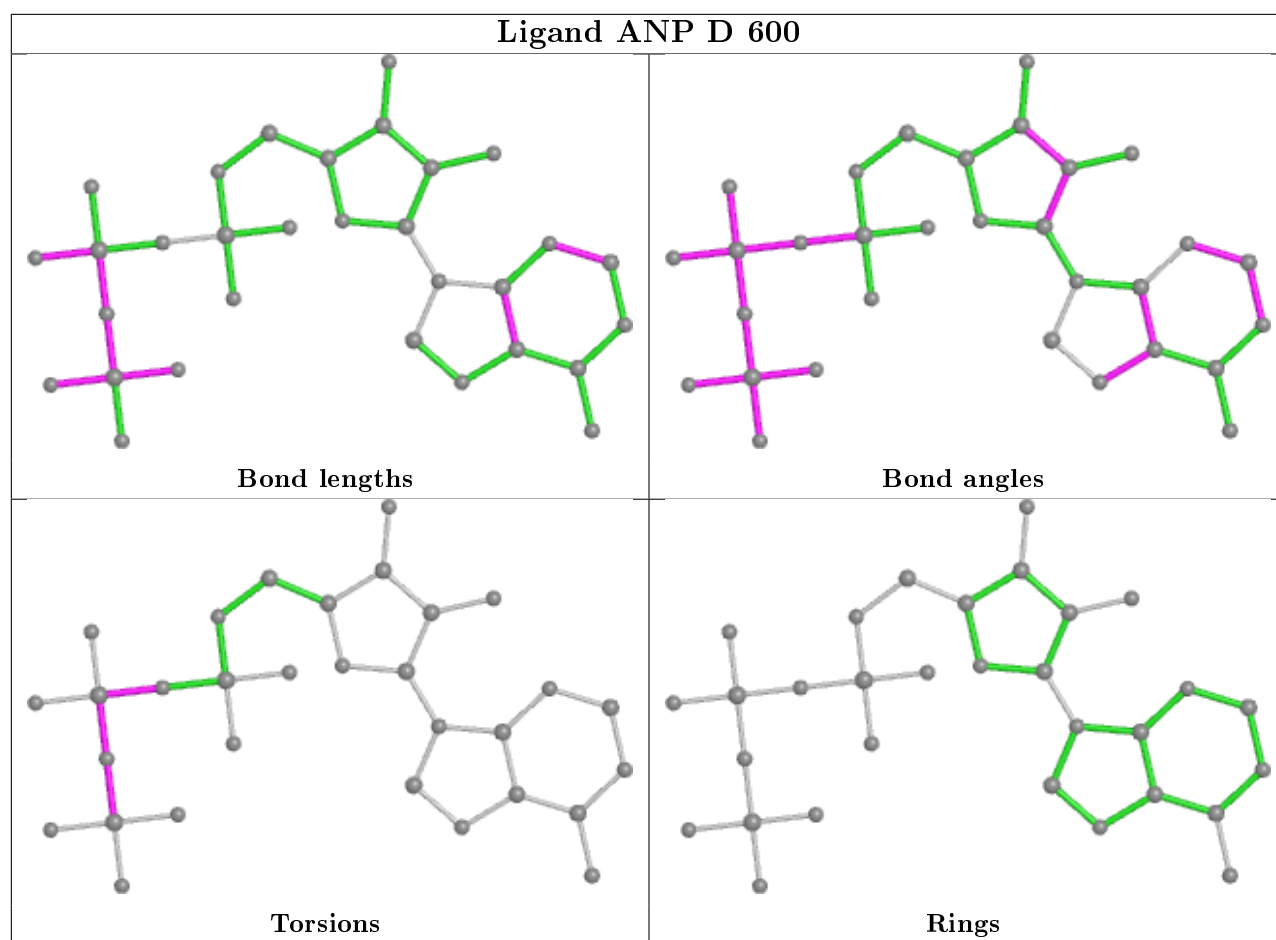


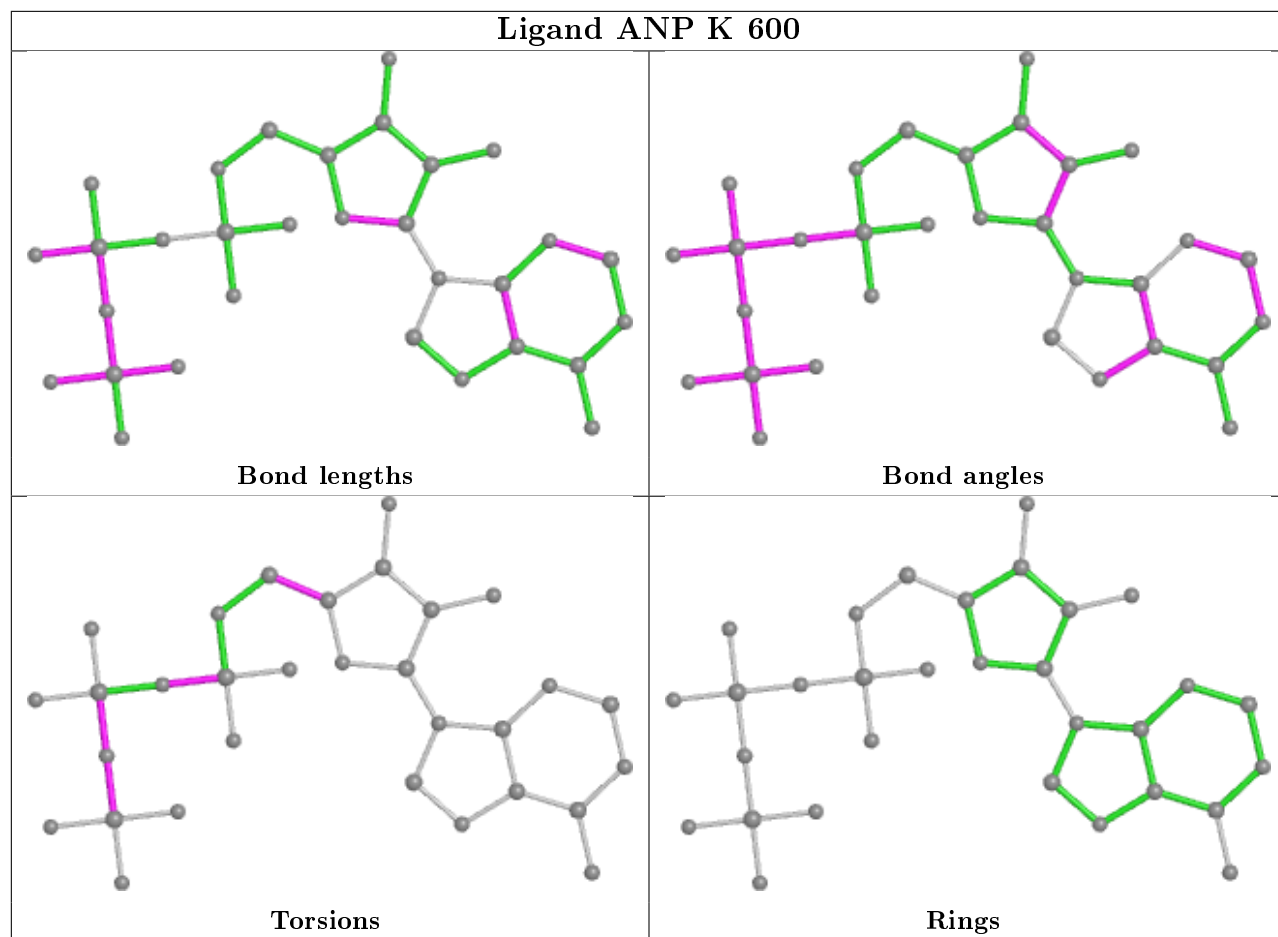




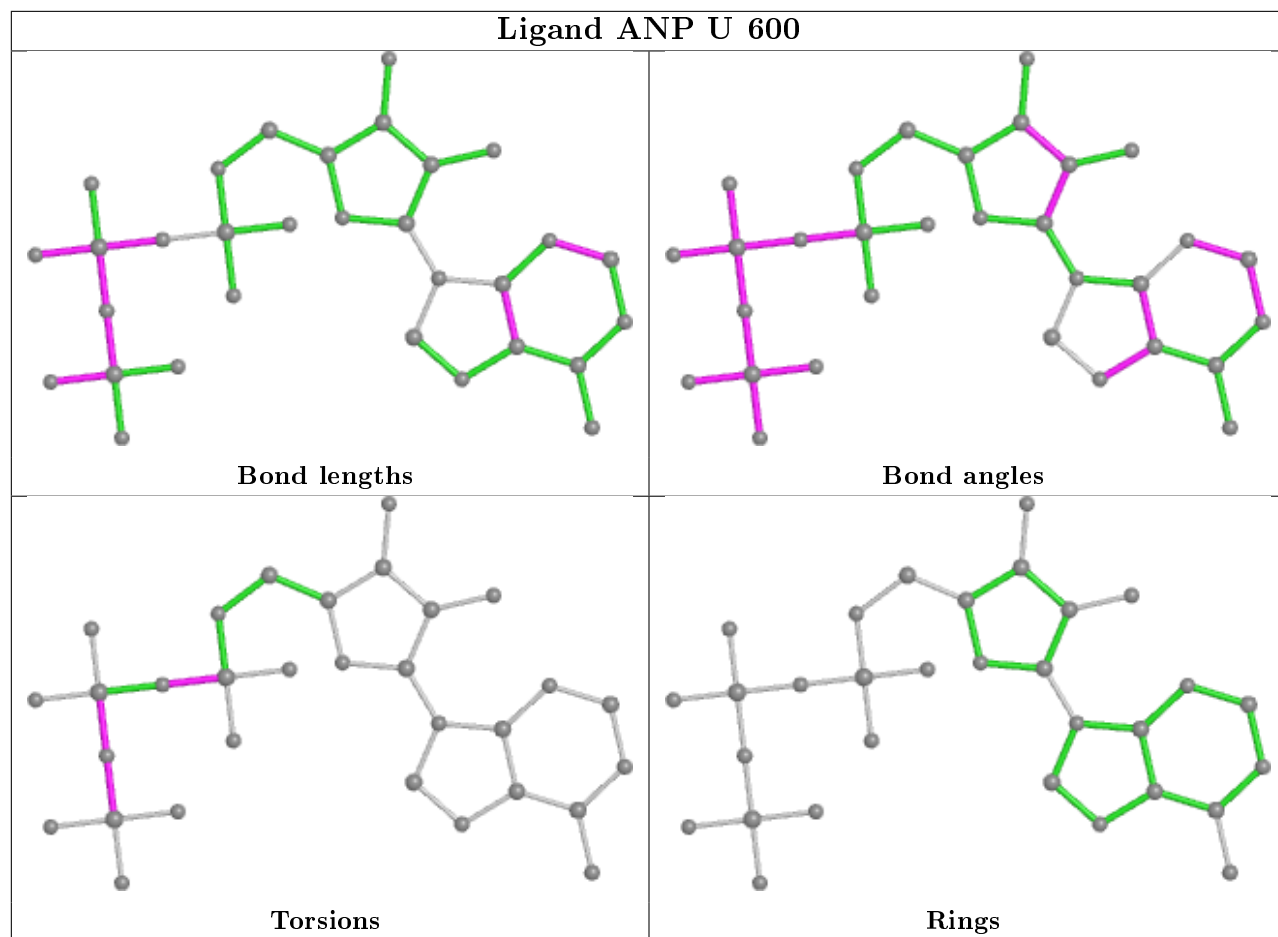


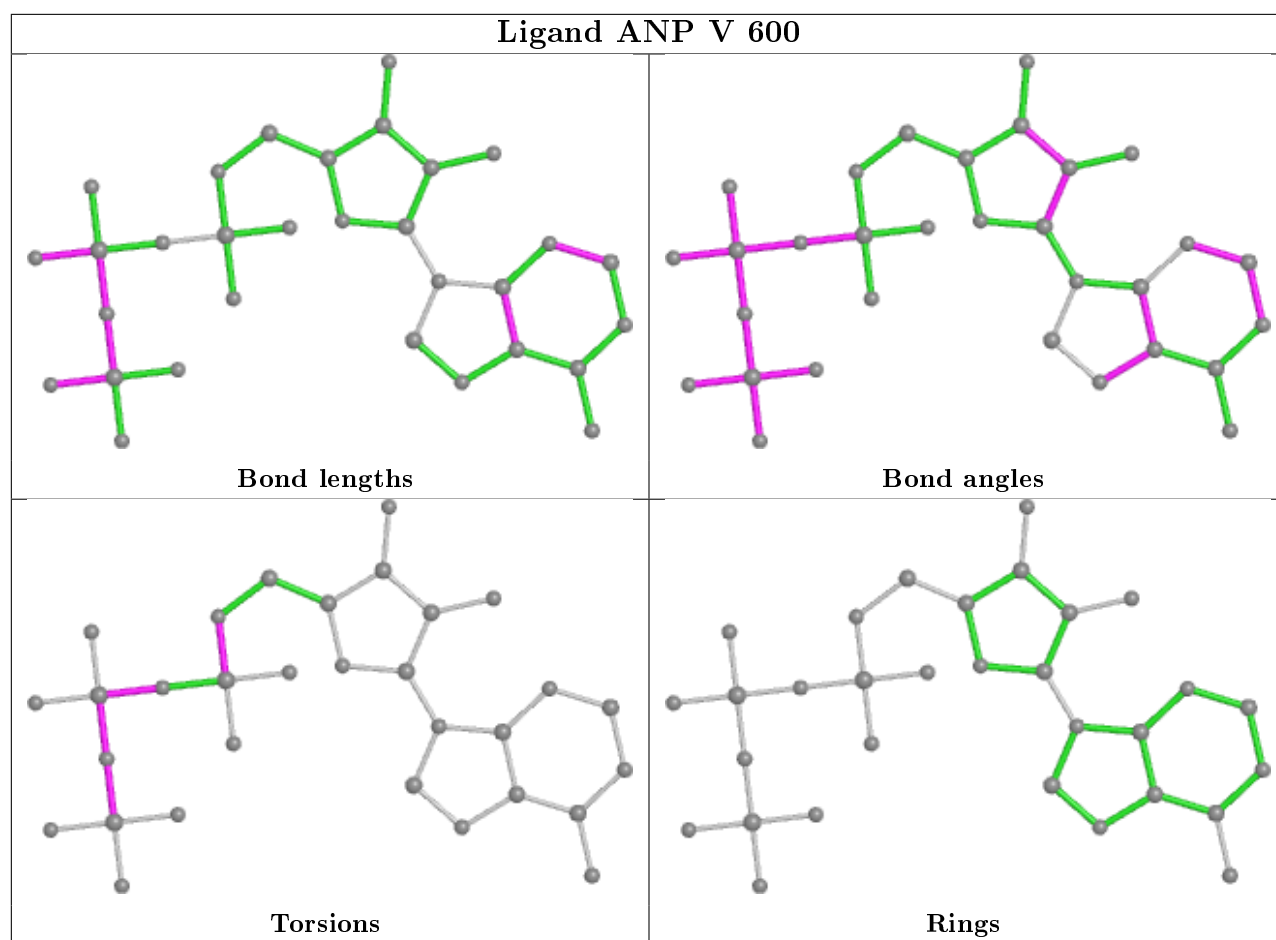




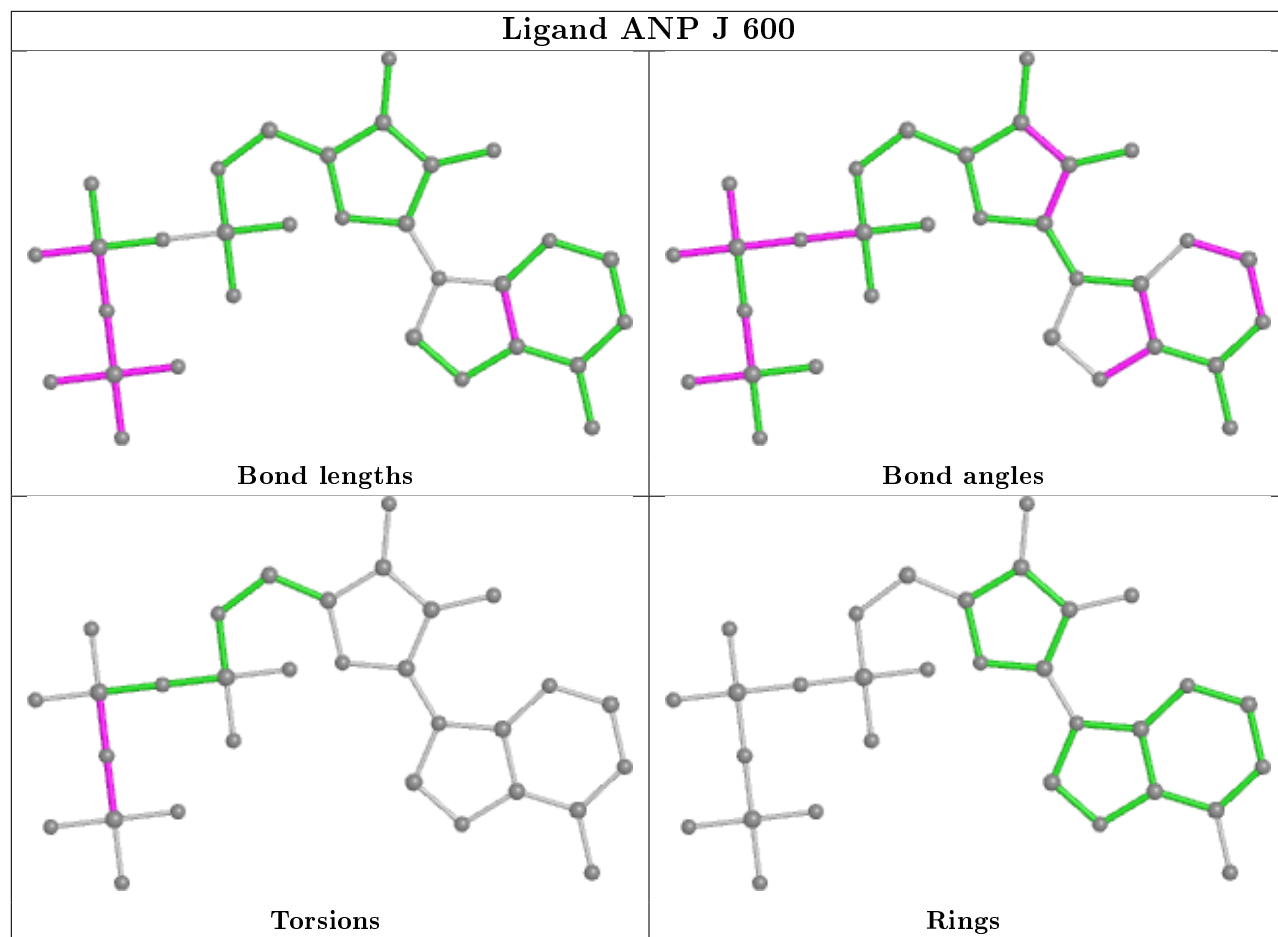


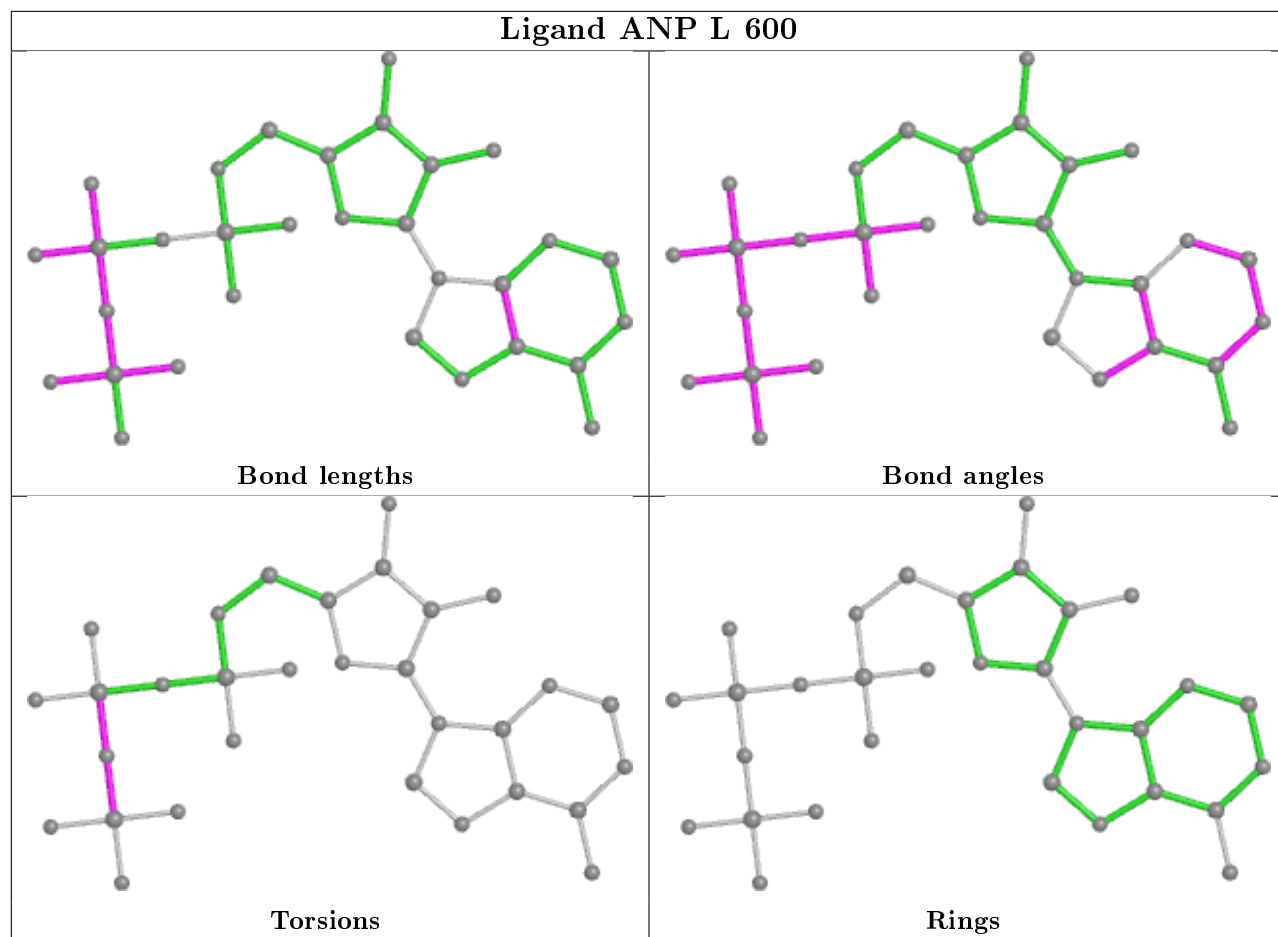


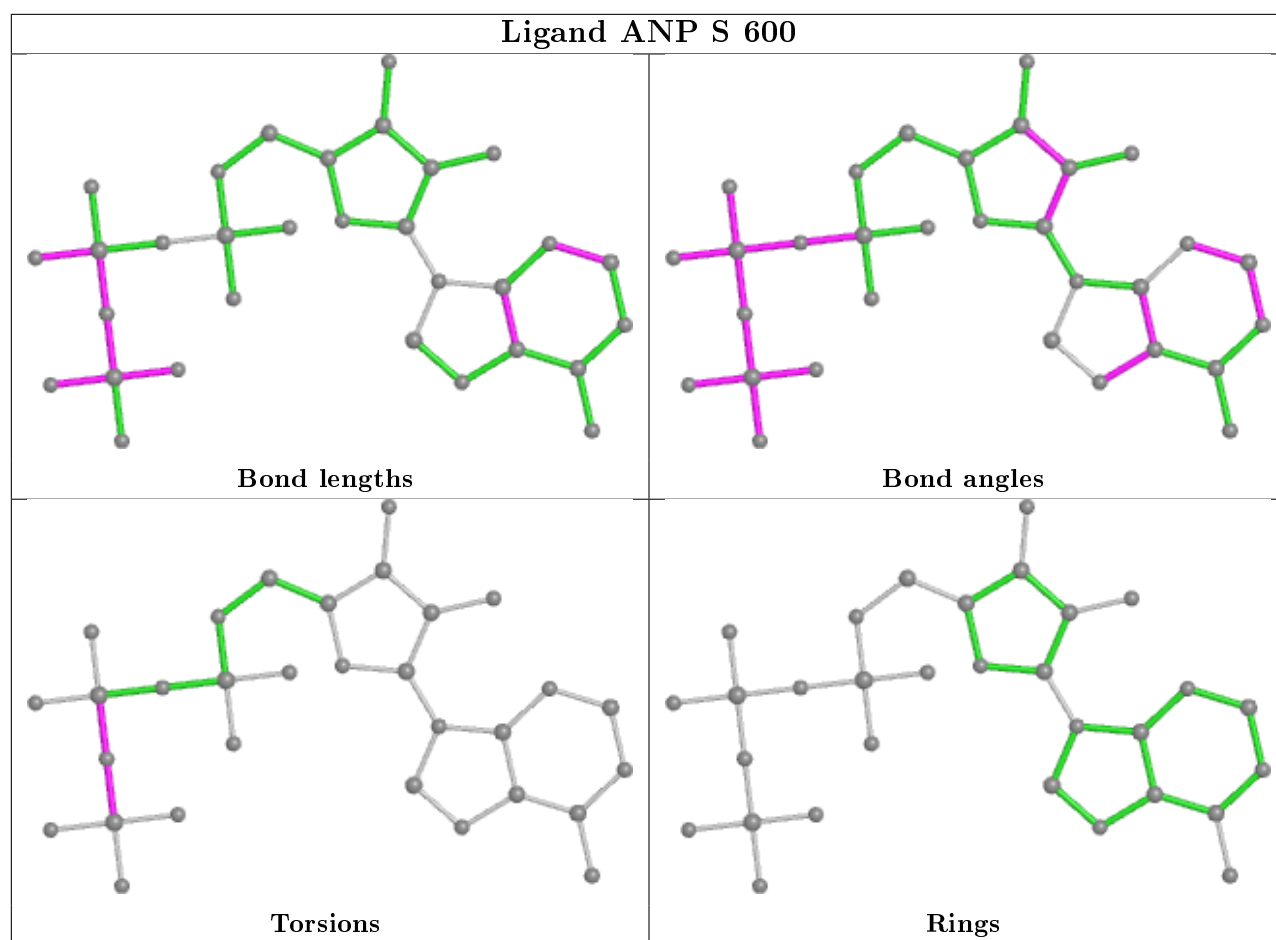


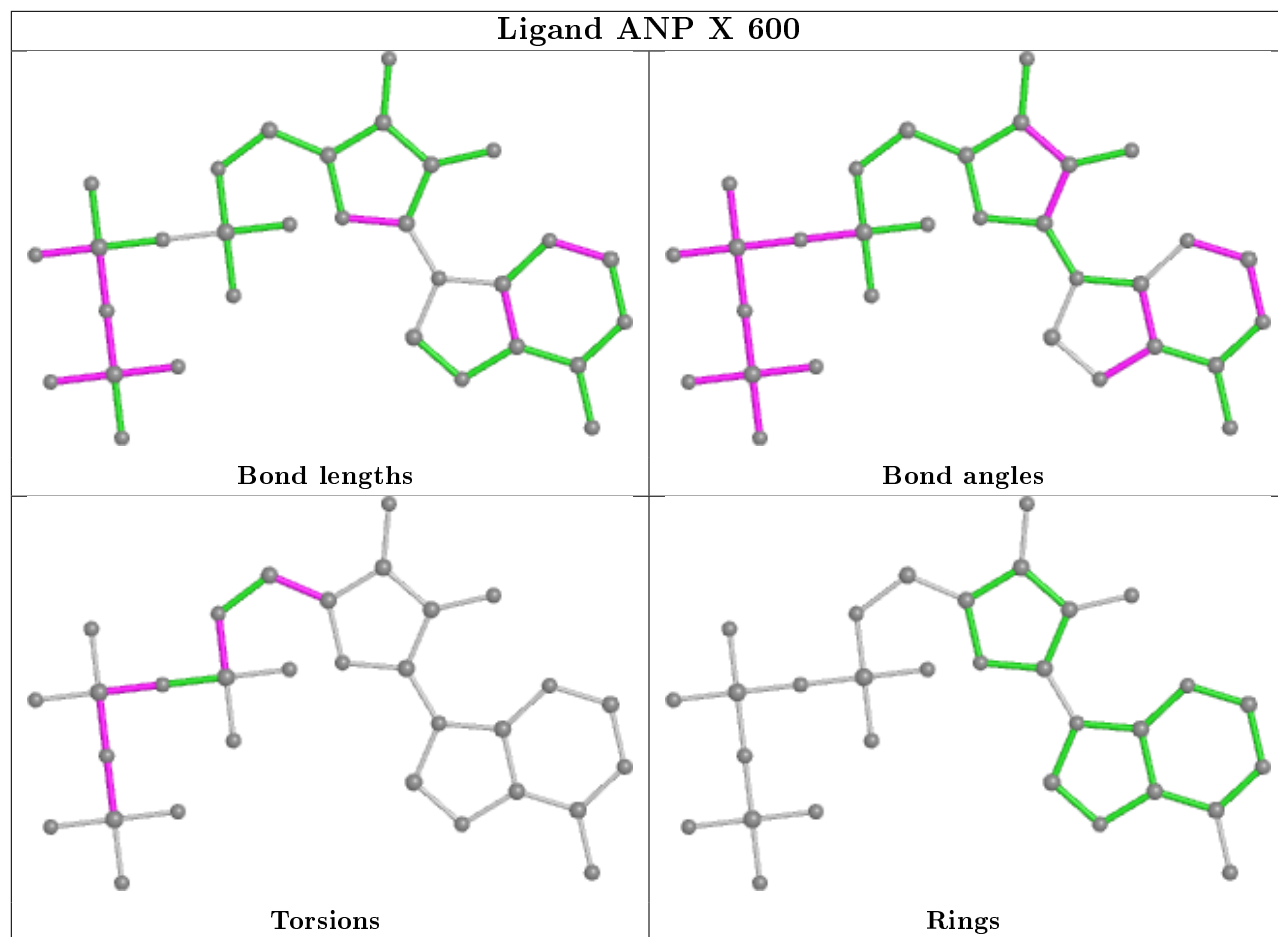


## Ligand ANP J 600









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	482/510 (94%)	-0.32	0 100 100	45, 64, 100, 166	0
1	B	483/510 (94%)	-0.06	5 (1%) 82 72	48, 92, 165, 195	0
1	C	484/510 (94%)	-0.18	2 (0%) 92 89	51, 75, 138, 181	0
1	J	481/510 (94%)	-0.14	1 (0%) 95 94	59, 93, 137, 181	0
1	K	486/510 (95%)	0.03	18 (3%) 41 26	61, 107, 166, 182	0
1	L	482/510 (94%)	-0.22	2 (0%) 92 89	47, 68, 123, 164	0
1	S	480/510 (94%)	-0.08	3 (0%) 89 83	72, 106, 140, 186	0
1	T	481/510 (94%)	0.21	19 (3%) 38 25	91, 131, 153, 165	0
1	U	481/510 (94%)	0.27	31 (6%) 19 11	93, 133, 166, 194	0
2	D	470/484 (97%)	-0.26	2 (0%) 92 89	46, 72, 121, 172	0
2	E	468/484 (96%)	-0.02	16 (3%) 45 29	48, 85, 147, 186	0
2	F	469/484 (96%)	-0.17	1 (0%) 95 94	48, 84, 117, 161	0
2	M	470/484 (97%)	-0.14	6 (1%) 77 65	57, 84, 131, 172	0
2	N	470/484 (97%)	0.09	22 (4%) 31 19	64, 110, 165, 188	0
2	O	468/484 (96%)	-0.14	5 (1%) 80 69	53, 92, 128, 153	0
2	V	470/484 (97%)	0.30	30 (6%) 19 11	93, 139, 171, 189	0
2	W	467/484 (96%)	0.01	13 (2%) 53 37	76, 101, 137, 171	0
2	X	469/484 (96%)	0.11	17 (3%) 42 27	85, 121, 162, 187	0
3	G	265/278 (95%)	-0.15	1 (0%) 92 89	56, 90, 117, 134	0
3	P	244/278 (87%)	0.59	27 (11%) 5 3	64, 139, 185, 209	0
3	Y	198/278 (71%)	0.55	22 (11%) 5 3	98, 147, 190, 214	0
4	H	120/137 (87%)	0.09	6 (5%) 28 16	86, 115, 166, 176	0
4	Q	84/137 (61%)	0.90	18 (21%) 0 1	138, 163, 187, 198	0
4	Z	15/137 (10%)	1.94	9 (60%) 0 0	192, 201, 222, 222	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
5	1	25/61 (40%)	1.41	9 (36%)	0	0	176, 183, 194, 202	0
5	I	48/61 (78%)	-0.30	0	100	100	92, 112, 140, 157	0
5	R	31/61 (50%)	0.08	0	100	100	136, 153, 167, 178	0
All	All	9591/10374 (92%)	0.00	285 (2%)	50	34	45, 100, 160, 222	0

All (285) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	83	LEU	5.4
2	M	6	SER	5.4
3	P	39	ILE	5.4
3	P	100	ASN	5.3
1	T	491	LEU	5.3
2	X	7	THR	5.1
3	P	46	GLU	5.0
3	P	54	ASN	4.9
4	Q	90	ALA	4.9
4	Q	71	SER	4.9
3	P	106	ASP	4.8
2	W	473	LEU	4.7
1	K	505	SER	4.7
3	P	47	ALA	4.5
1	B	195	SER	4.5
3	P	107	ILE	4.5
2	V	109	ILE	4.4
4	Q	54	PRO	4.3
3	P	154	MET	4.3
1	U	123	ILE	4.2
2	V	198	TYR	4.1
3	P	53	LYS	4.1
2	N	390	ILE	4.1
4	Z	128	GLU	3.9
1	U	454	HIS	3.9
2	E	398	GLU	3.9
2	V	181	PHE	3.8
1	T	454	HIS	3.8
4	Q	80	ASP	3.8
5	1	9	SER	3.8
2	X	78	ASP	3.8
1	K	499	LEU	3.8
2	N	6	SER	3.7

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Mol	Chain	Res	Type	RSRZ
3	P	126	ILE	3.7
2	V	70	LEU	3.7
2	X	77	LEU	3.7
2	V	461	GLY	3.6
1	K	503	THR	3.6
2	N	461	GLY	3.6
4	Z	133	LEU	3.6
3	P	108	VAL	3.5
5	1	18	ALA	3.5
2	N	446	GLU	3.5
2	N	462	GLY	3.5
1	K	471	LEU	3.5
2	N	473	LEU	3.5
3	Y	37	ALA	3.4
1	U	27	LEU	3.4
1	U	26	ASN	3.4
4	Q	15	ALA	3.4
1	T	46	LEU	3.4
2	M	27	GLN	3.4
4	Z	132	ASN	3.4
2	N	445	LEU	3.4
4	H	97	SER	3.4
1	U	63	GLY	3.4
2	V	7	THR	3.3
2	E	28	SER	3.3
1	U	44	PHE	3.3
1	U	446	LEU	3.3
3	Y	79	SER	3.2
1	T	54	LEU	3.2
3	P	95	VAL	3.2
2	W	470	ALA	3.2
4	Q	70	ILE	3.2
4	Q	84	CYS	3.2
1	U	445	PRO	3.2
1	T	314	LEU	3.1
2	N	386	ASP	3.1
4	Q	34	ALA	3.1
1	B	482	LEU	3.1
2	X	110	LYS	3.1
2	X	25	PHE	3.1
2	N	28	SER	3.1
2	W	444	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	U	30	THR	3.0
1	U	491	LEU	3.0
1	U	102	GLY	3.0
2	O	109	ILE	3.0
2	V	113	LEU	3.0
5	1	11	ALA	3.0
3	Y	91	LEU	3.0
5	1	15	ASN	3.0
5	1	13	TYR	3.0
1	K	455	LEU	2.9
2	V	110	LYS	2.9
5	1	16	VAL	2.9
1	U	481	LEU	2.9
2	E	391	LEU	2.9
2	N	7	THR	2.9
3	Y	36	LYS	2.9
1	K	456	ASP	2.9
1	T	89	LEU	2.9
1	K	507	VAL	2.8
4	Q	19	GLU	2.8
5	1	20	ALA	2.8
4	Q	82	GLN	2.8
2	V	428	PRO	2.8
3	P	183	PHE	2.8
1	K	488	LYS	2.8
2	M	437	THR	2.8
2	N	113	LEU	2.8
2	D	6	SER	2.8
2	X	15	ALA	2.8
3	P	161	LYS	2.8
2	V	73	GLY	2.8
2	N	475	ALA	2.8
2	V	8	PRO	2.8
2	N	457	PHE	2.8
1	C	414	ALA	2.8
1	T	482	LEU	2.8
3	P	74	ILE	2.8
3	P	99	LEU	2.8
1	U	119	GLY	2.8
2	W	23	VAL	2.7
3	P	51	PHE	2.7
3	Y	167	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
2	W	393	MET	2.7
2	V	431	LEU	2.7
2	V	451	ASN	2.7
1	T	490	GLU	2.7
2	V	39	ILE	2.7
2	W	391	LEU	2.7
1	T	30	THR	2.7
1	K	454	HIS	2.7
3	P	101	ASP	2.7
1	K	508	ALA	2.7
4	Q	55	GLY	2.6
3	Y	156	ALA	2.6
5	1	17	ALA	2.6
2	E	473	LEU	2.6
1	U	28	ASN	2.6
2	V	6	SER	2.6
2	V	27	GLN	2.6
2	V	452	ILE	2.6
1	K	21	VAL	2.6
1	L	463	ILE	2.6
2	N	387	ILE	2.6
3	P	98	HIS	2.6
1	K	478	HIS	2.6
2	V	475	ALA	2.5
4	H	90	ALA	2.5
3	Y	78	THR	2.5
2	N	398	GLU	2.5
3	Y	223	ALA	2.5
1	U	89	LEU	2.5
3	Y	108	VAL	2.5
1	B	476	SER	2.5
3	P	50	LEU	2.5
4	Q	137	LEU	2.5
1	T	313	LYS	2.5
1	U	114	GLY	2.5
3	Y	121	THR	2.5
2	V	28	SER	2.5
2	X	86	PRO	2.5
1	K	203	CYS	2.5
4	Z	131	GLU	2.5
1	U	105	LEU	2.5
3	P	170	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
4	Z	129	VAL	2.5
2	N	27	GLN	2.5
3	P	72	GLU	2.5
4	Q	49	VAL	2.4
2	E	390	ILE	2.4
3	Y	144	ALA	2.4
2	X	105	GLU	2.4
3	Y	216	ASN	2.4
3	Y	224	GLN	2.4
4	H	23	SER	2.4
1	U	388	VAL	2.4
2	E	405	GLU	2.4
1	U	447	ILE	2.4
1	S	195	SER	2.4
2	N	474	ALA	2.4
2	X	8	PRO	2.4
1	U	384	ALA	2.4
2	W	441	PHE	2.4
2	V	108	PRO	2.4
1	K	452	ASN	2.4
3	Y	100	ASN	2.4
2	E	457	PHE	2.3
2	X	31	PRO	2.3
1	U	455	LEU	2.3
1	T	43	VAL	2.3
2	O	107	GLY	2.3
2	W	76	VAL	2.3
2	N	391	LEU	2.3
3	P	25	ILE	2.3
2	M	462	GLY	2.3
1	T	126	ALA	2.3
1	U	496	LEU	2.3
2	V	467	VAL	2.3
2	W	457	PHE	2.3
2	X	29	GLU	2.3
1	T	232	ILE	2.3
2	E	467	VAL	2.3
1	U	69	GLU	2.3
2	E	471	GLU	2.3
2	X	209	LEU	2.3
1	U	392	LEU	2.3
2	X	112	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
3	P	141	GLN	2.2
1	K	195	SER	2.2
3	Y	214	LEU	2.2
2	E	386	ASP	2.2
2	V	57	ASN	2.2
1	U	51	ALA	2.2
4	Z	124	ALA	2.2
5	1	12	ALA	2.2
3	Y	148	ASP	2.2
1	B	488	LYS	2.2
3	Y	34	ALA	2.2
2	X	181	PHE	2.2
4	Z	134	GLN	2.2
4	Z	130	LEU	2.2
1	U	489	GLY	2.2
1	S	471	LEU	2.2
2	O	207	ILE	2.2
1	U	411	ASP	2.2
2	V	31	PRO	2.2
3	P	169	PRO	2.2
2	V	25	PHE	2.2
3	Y	130	ILE	2.2
2	V	470	ALA	2.2
2	X	30	LEU	2.2
1	U	100	PRO	2.2
4	Z	126	GLN	2.2
2	W	9	ILE	2.2
3	P	157	GLY	2.2
1	U	126	ALA	2.2
2	W	452	ILE	2.2
1	S	449	ALA	2.1
2	E	455	HIS	2.1
2	V	208	ASN	2.1
4	Q	32	LEU	2.1
1	K	457	GLY	2.1
1	L	27	LEU	2.1
2	N	143	LEU	2.1
1	U	113	LEU	2.1
2	N	466	VAL	2.1
2	N	467	VAL	2.1
2	X	210	GLU	2.1
2	V	302	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	T	473	TYR	2.1
1	K	485	ILE	2.1
1	U	73	VAL	2.1
2	F	27	GLN	2.1
4	Q	85	VAL	2.1
2	V	205	GLY	2.1
3	Y	138	PRO	2.1
3	P	94	ALA	2.1
2	V	214	LYS	2.1
3	Y	43	LYS	2.1
2	E	441	PHE	2.1
2	W	458	TYR	2.1
1	T	485	ILE	2.1
2	D	390	ILE	2.1
2	E	445	LEU	2.1
4	Q	72	GLY	2.1
2	E	396	LEU	2.1
1	T	55	VAL	2.1
1	B	407	GLN	2.1
3	Y	8	MET	2.1
4	H	106	ALA	2.1
2	O	9	ILE	2.1
2	W	390	ILE	2.1
4	H	72	GLY	2.1
1	T	124	ASP	2.1
2	V	449	TYR	2.0
2	M	7	THR	2.0
2	M	445	LEU	2.0
1	T	481	LEU	2.0
2	E	9	ILE	2.0
2	N	388	ILE	2.0
3	G	206	PRO	2.0
1	C	411	ASP	2.0
2	X	90	GLU	2.0
2	O	108	PRO	2.0
4	Q	29	GLN	2.0
1	K	498	SER	2.0
3	Y	98	HIS	2.0
2	E	470	ALA	2.0
4	H	32	LEU	2.0
1	J	503	THR	2.0
1	T	480	GLU	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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.

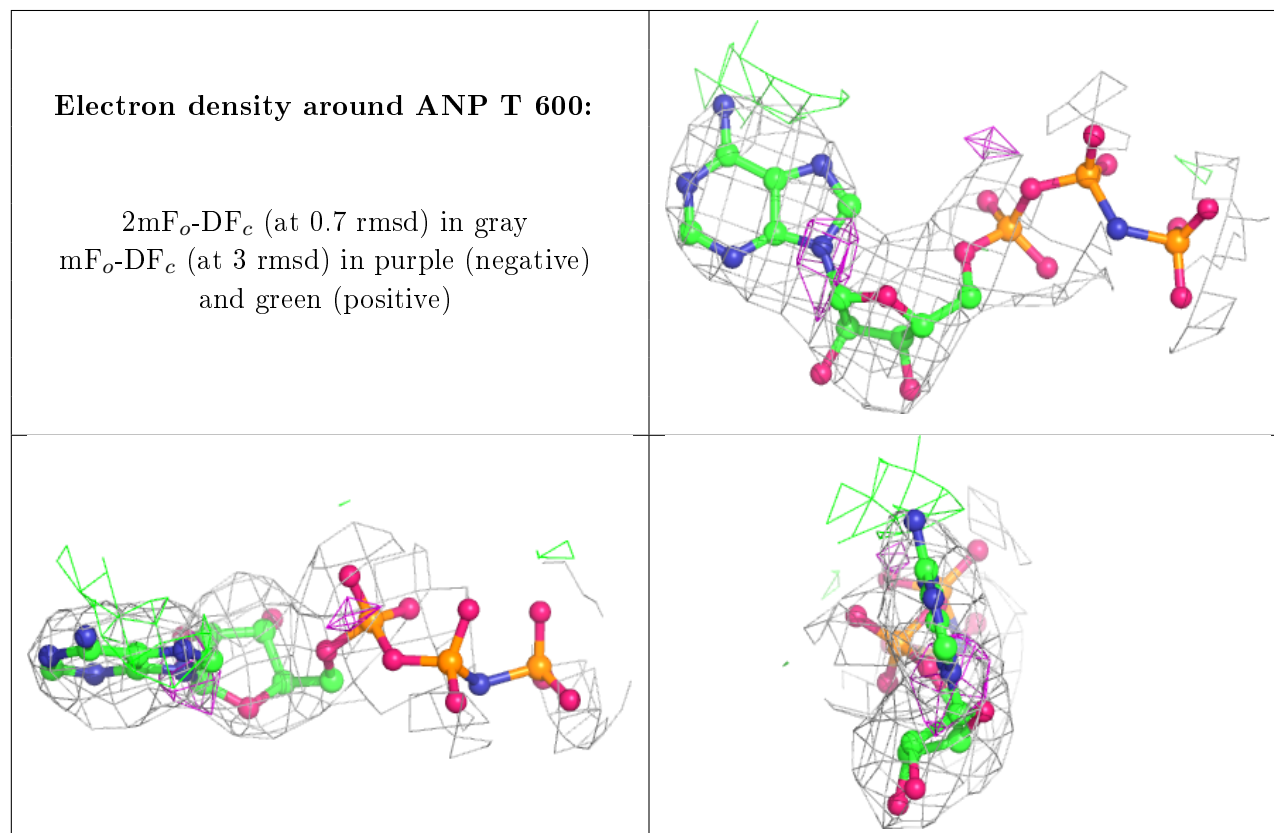
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	MG	T	700	1/1	0.83	0.52	91,91,91,91	0
6	ANP	T	600	31/31	0.91	0.22	91,101,106,106	0
6	ANP	B	600	31/31	0.92	0.20	71,82,85,85	0
8	PO4	N	800	5/5	0.92	0.24	131,131,131,132	0
6	ANP	U	600	31/31	0.92	0.21	84,89,90,91	0
7	MG	D	700	1/1	0.93	0.36	64,64,64,64	0
6	ANP	V	600	31/31	0.93	0.25	102,106,109,109	0
7	MG	F	700	1/1	0.94	0.44	65,65,65,65	0
6	ANP	J	600	31/31	0.94	0.20	67,73,80,81	0
7	MG	U	700	1/1	0.94	0.40	88,88,88,88	0
7	MG	A	700	1/1	0.94	0.43	48,48,48,48	0
6	ANP	X	600	31/31	0.94	0.24	93,94,96,97	0
6	ANP	K	600	31/31	0.94	0.17	90,97,99,100	0
7	MG	S	700	1/1	0.94	0.41	77,77,77,77	0
6	ANP	S	600	31/31	0.94	0.21	76,82,83,85	0
7	MG	K	700	1/1	0.94	0.35	90,90,90,90	0
6	ANP	C	600	31/31	0.95	0.22	58,64,68,70	0
6	ANP	F	600	31/31	0.95	0.26	66,70,78,78	0
7	MG	L	700	1/1	0.95	0.33	53,53,53,53	0
6	ANP	A	600	31/31	0.96	0.22	48,58,61,62	0
7	MG	M	700	1/1	0.96	0.42	64,64,64,64	0
7	MG	B	700	1/1	0.96	0.41	72,72,72,72	0
6	ANP	O	600	31/31	0.96	0.23	84,88,92,92	0
6	ANP	L	600	31/31	0.96	0.21	53,59,62,62	0
7	MG	X	700	1/1	0.97	0.43	96,96,96,96	0
6	ANP	M	600	31/31	0.97	0.24	64,68,70,71	0
6	ANP	D	600	31/31	0.97	0.22	62,65,68,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	MG	C	700	1/1	0.97	0.45	58,58,58,58	0
7	MG	J	700	1/1	0.97	0.46	67,67,67,67	0
7	MG	O	700	1/1	0.98	0.43	83,83,83,83	0
7	MG	V	700	1/1	0.98	0.35	107,107,107,107	0

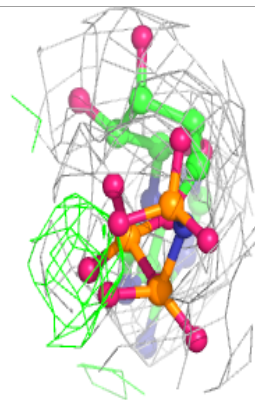
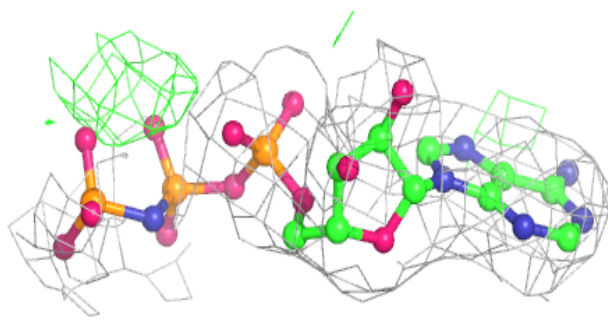
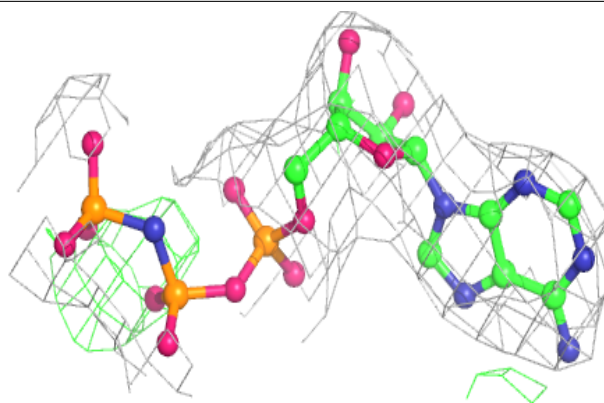
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



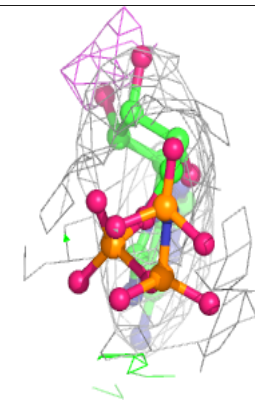
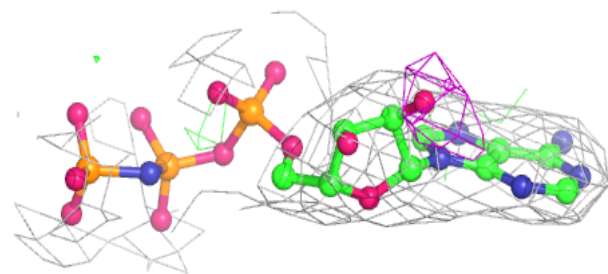
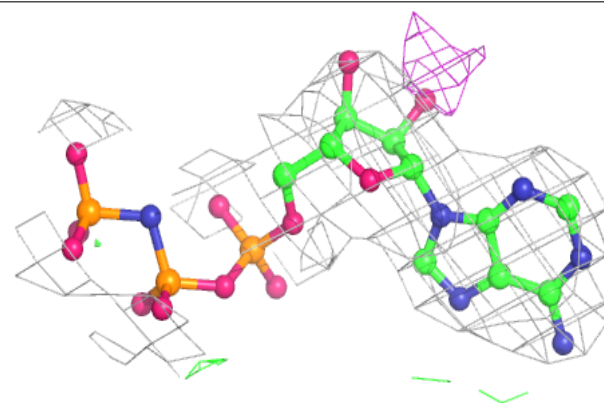


**Electron density around ANP B 600:**

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

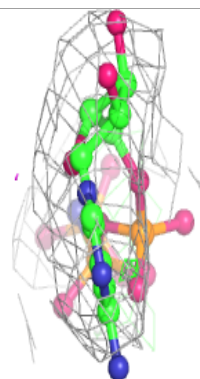
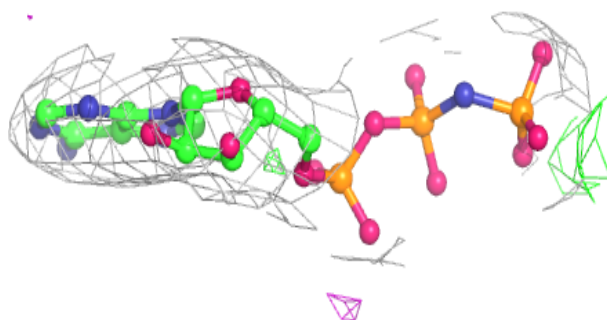
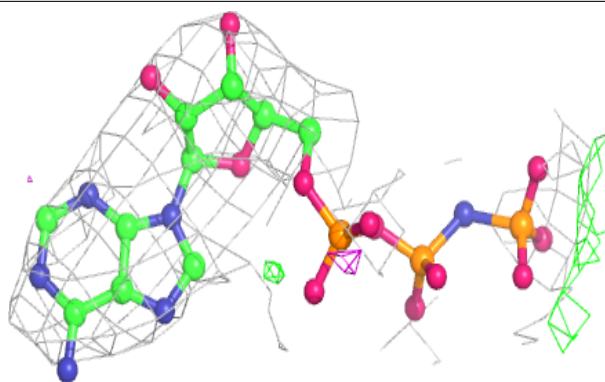
**Electron density around ANP U 600:**

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

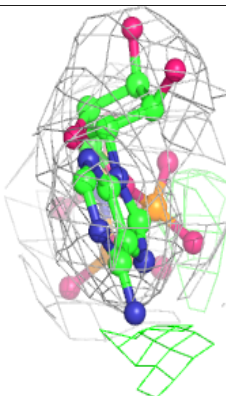
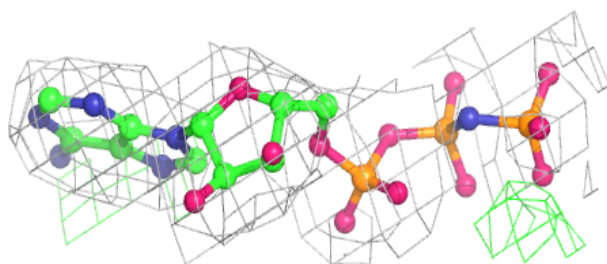
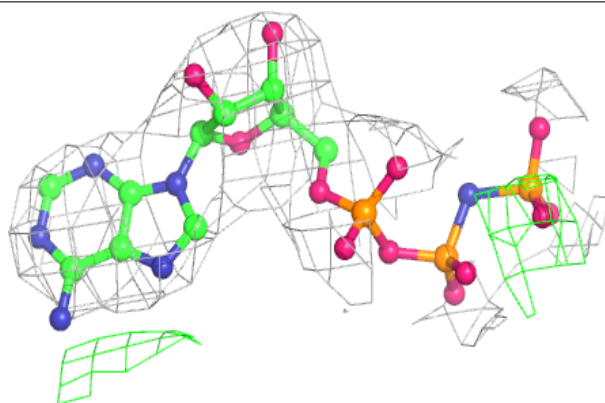


**Electron density around ANP V 600:**

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

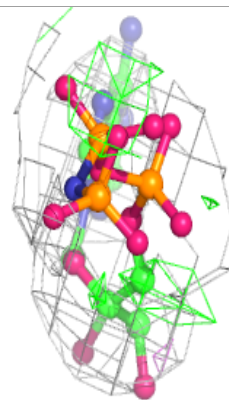
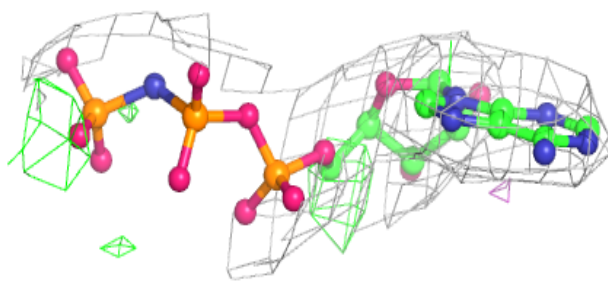
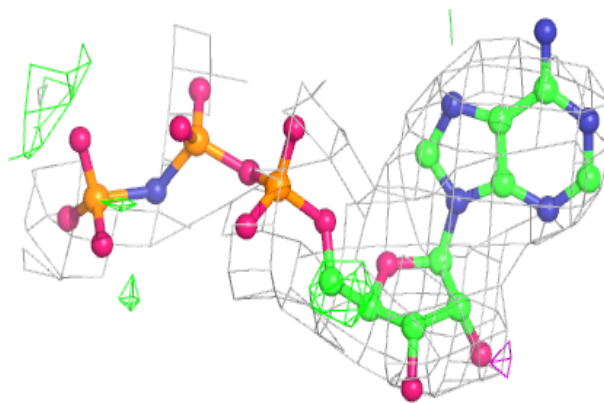
**Electron density around ANP J 600:**

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

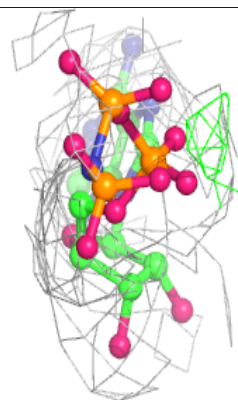
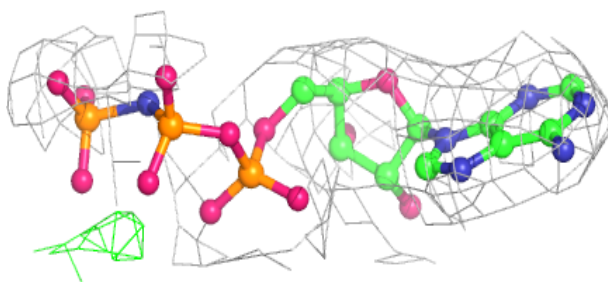
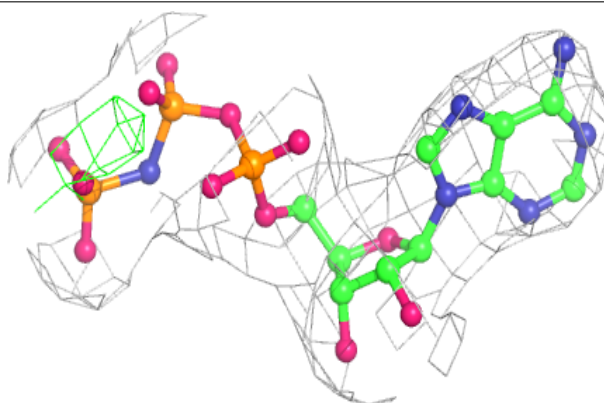


**Electron density around ANP X 600:**

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

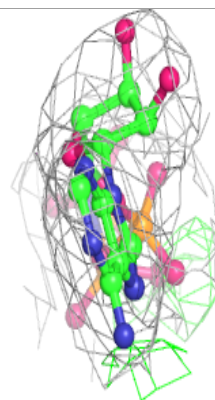
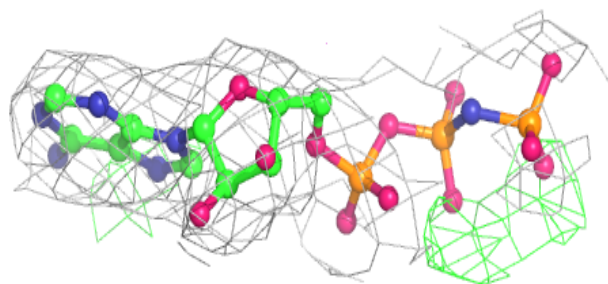
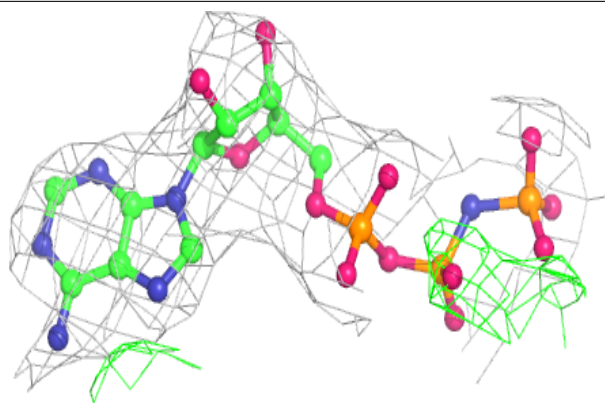
**Electron density around ANP K 600:**

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

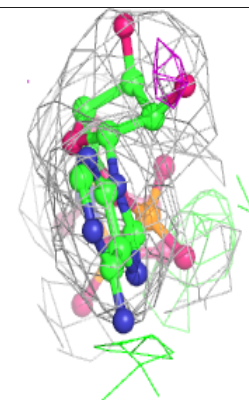
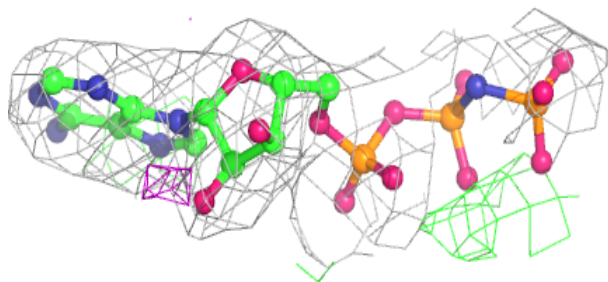
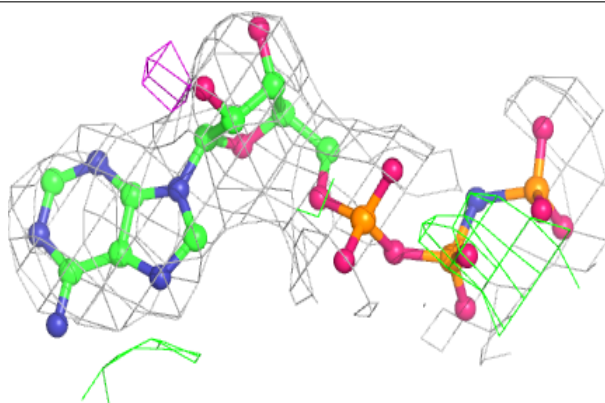


**Electron density around ANP S 600:**

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

**Electron density around ANP C 600:**

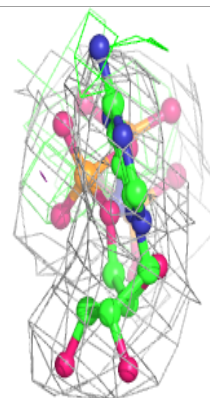
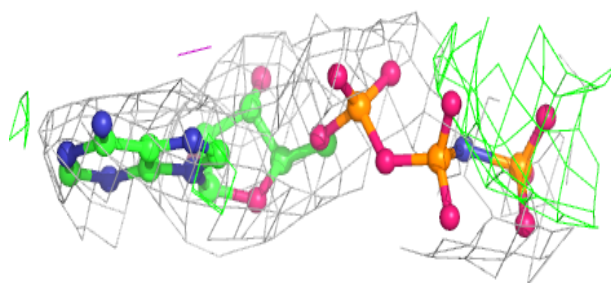
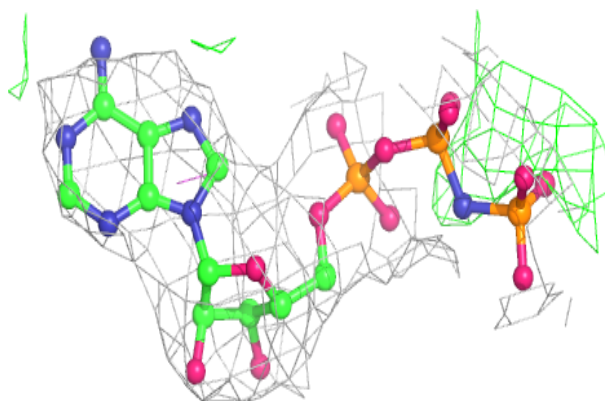
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



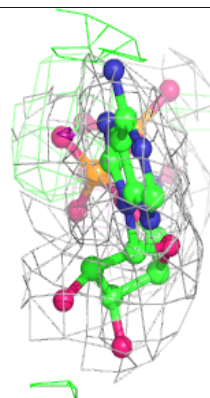
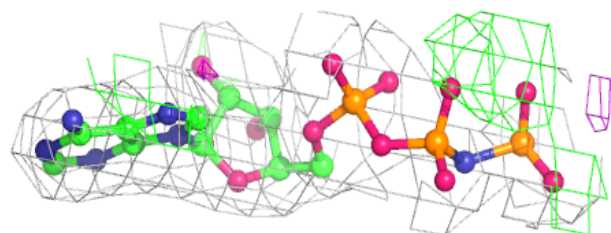
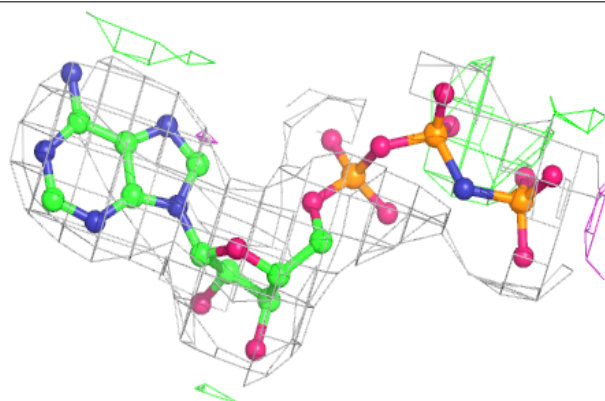


**Electron density around ANP F 600:**

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

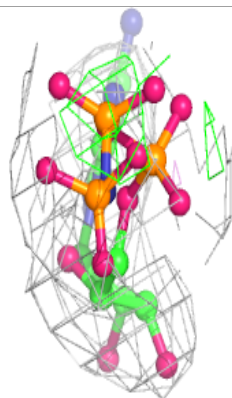
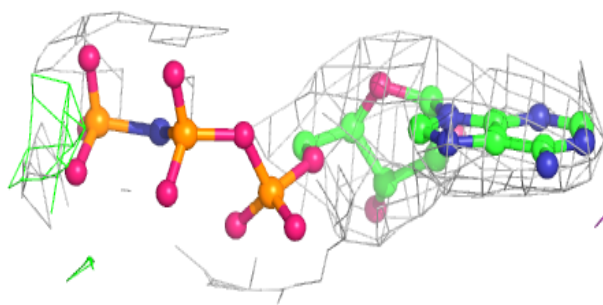
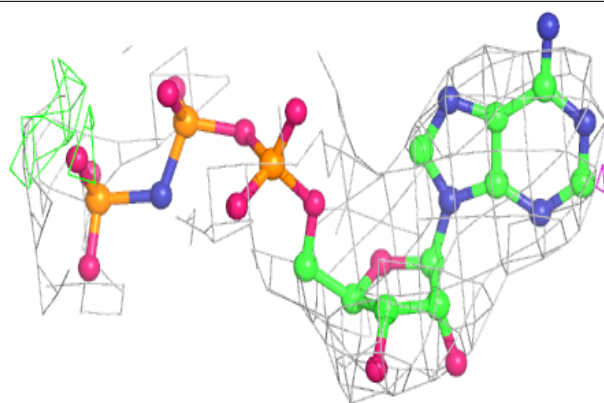
**Electron density around ANP A 600:**

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

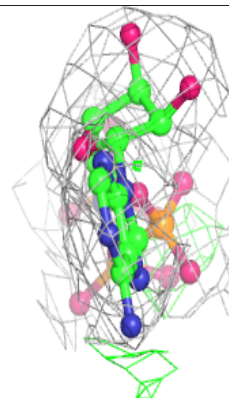
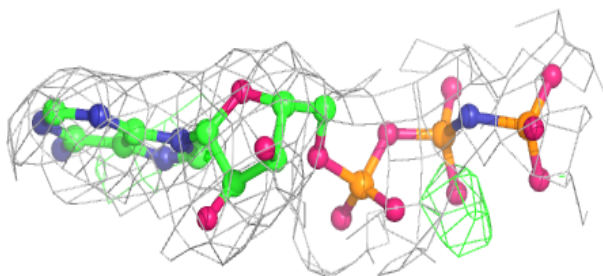
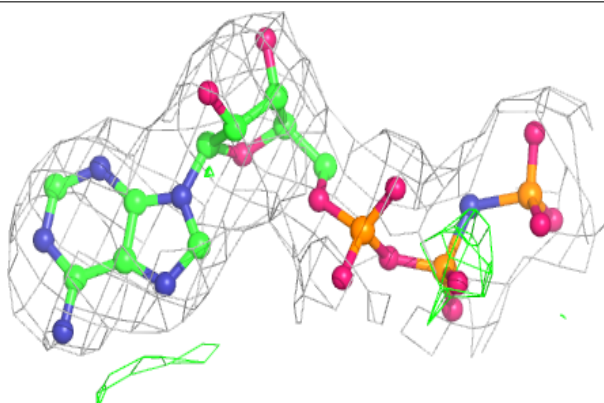


**Electron density around ANP O 600:**

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

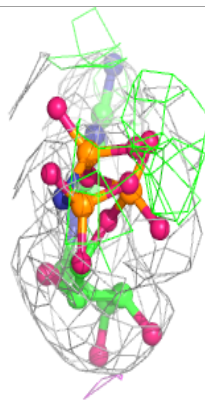
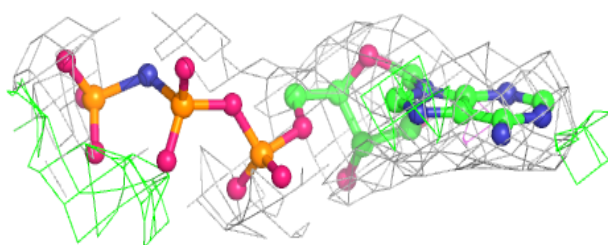
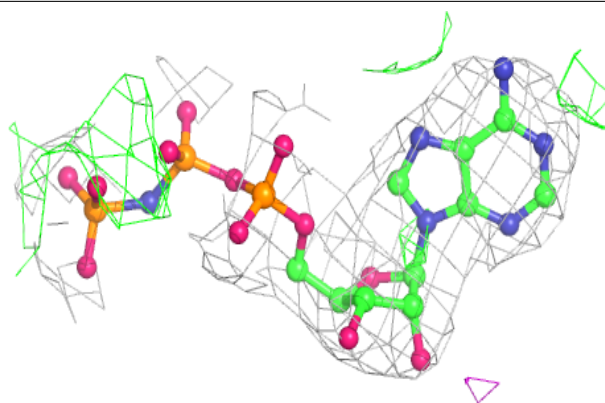
**Electron density around ANP L 600:**

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

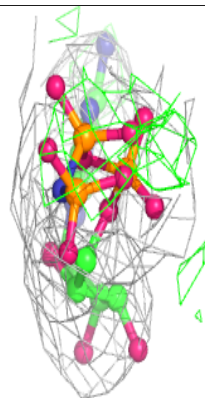
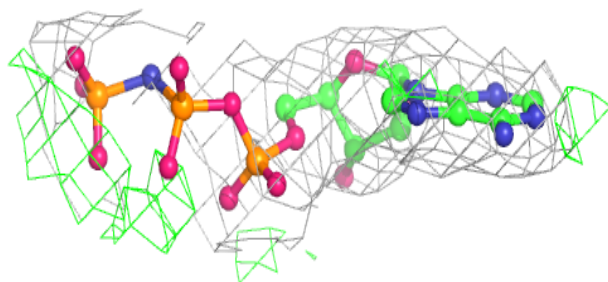
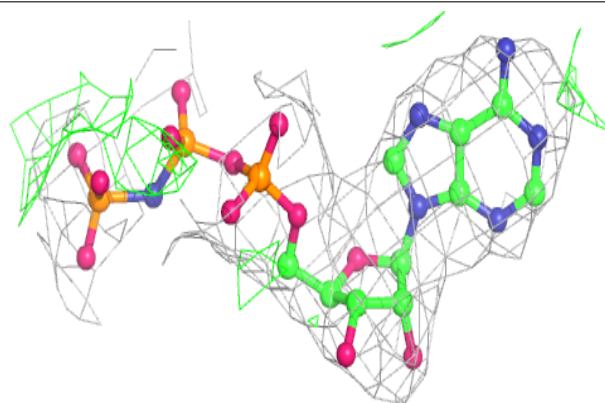


**Electron density around ANP M 600:**

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

**Electron density around ANP D 600:**

$2mF_o-DF_c$  (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.