



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 10:14 pm BST

PDB ID : 3OEE  
Title : Structure of four mutant forms of yeast F1 ATPase: alpha-F405S  
Authors : Arsenieva, D.; Symersky, J.; Wang, Y.; Pagadala, V.; Mueller, D.M.  
Deposited on : 2010-08-12  
Resolution : 2.74 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.

---

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

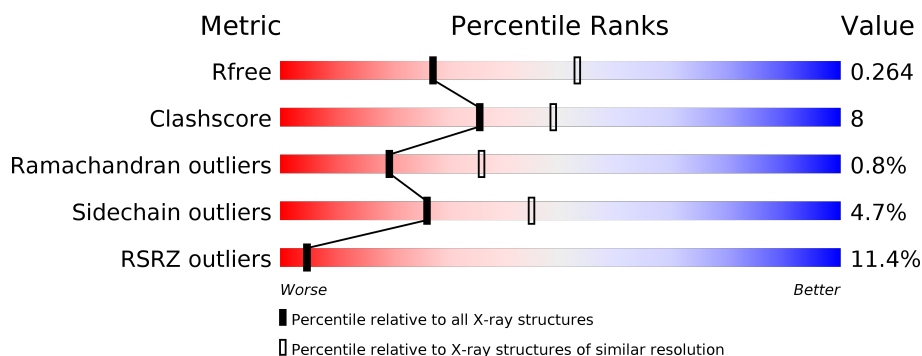
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.74 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	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (2.76-2.72)

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>76%</div> <div>17%</div> <div>• 5%</div> </div>
1	B	510	<div> <div>2%</div> <div>77%</div> <div>17%</div> <div>• 5%</div> </div>
1	C	510	<div> <div>2%</div> <div>76%</div> <div>18%</div> <div>• 5%</div> </div>
1	J	510	<div> <div>2%</div> <div>76%</div> <div>17%</div> <div>• 6%</div> </div>
1	K	510	<div> <div>2%</div> <div>74%</div> <div>20%</div> <div>• 5%</div> </div>
1	L	510	<div> <div>2%</div> <div>76%</div> <div>17%</div> <div>• 5%</div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	S	510	
1	T	510	
1	U	510	
2	D	484	
2	E	484	
2	F	484	
2	M	484	
2	N	484	
2	O	484	
2	V	484	
2	W	484	
2	X	484	
3	G	278	
3	P	278	
3	Y	278	
4	H	138	
4	Q	138	
4	Z	138	
5	1	61	
5	I	61	
5	R	61	

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 72675 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
			3659	2308	648	700	3			
1	B	483	Total	C	N	O	S	0	0	0
			3664	2311	649	701	3			
1	C	484	Total	C	N	O	S	0	0	0
			3675	2319	650	703	3			
1	J	481	Total	C	N	O	S	0	0	0
			3650	2303	646	698	3			
1	K	486	Total	C	N	O	S	0	0	0
			3679	2320	652	704	3			
1	L	482	Total	C	N	O	S	0	0	0
			3659	2308	648	700	3			
1	S	477	Total	C	N	O	S	0	0	0
			3622	2287	642	690	3			
1	T	478	Total	C	N	O	S	0	0	0
			3632	2293	643	693	3			
1	U	481	Total	C	N	O	S	0	0	0
			3650	2302	646	699	3			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	405	SER	PHE	ENGINEERED MUTATION	UNP P07251
B	405	SER	PHE	ENGINEERED MUTATION	UNP P07251
C	405	SER	PHE	ENGINEERED MUTATION	UNP P07251
J	405	SER	PHE	ENGINEERED MUTATION	UNP P07251
K	405	SER	PHE	ENGINEERED MUTATION	UNP P07251
L	405	SER	PHE	ENGINEERED MUTATION	UNP P07251
S	405	SER	PHE	ENGINEERED MUTATION	UNP P07251
T	405	SER	PHE	ENGINEERED MUTATION	UNP P07251
U	405	SER	PHE	ENGINEERED MUTATION	UNP P07251

- 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
			3545	2248	603	688	6			
2	E	468	Total	C	N	O	S	0	0	0
			3504	2223	598	677	6			
2	F	469	Total	C	N	O	S	0	0	0
			3527	2238	602	681	6			
2	M	470	Total	C	N	O	S	0	0	0
			3535	2243	600	686	6			
2	N	470	Total	C	N	O	S	0	0	0
			3541	2245	602	688	6			
2	O	468	Total	C	N	O	S	0	0	0
			3534	2242	602	684	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

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
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
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

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
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	266	Total	C	N	O	S	0	0	0
			2055	1291	359	395	10			
3	P	244	Total	C	N	O	S	0	0	0
			1850	1162	323	356	9			
3	Y	200	Total	C	N	O	S	0	0	0
			1517	944	273	291	9			

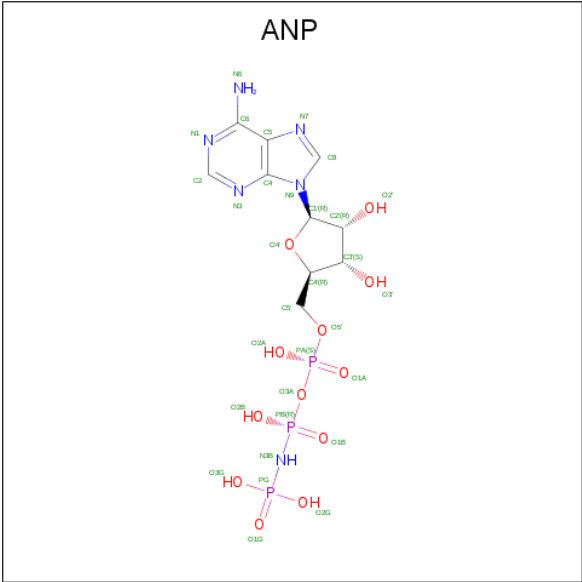
- Molecule 4 is a protein called ATP synthase subunit delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	122	Total	C	N	O	S	0	0	0
			795	497	138	158	2			
4	Q	83	Total	C	N	O		0	0	0
			441	267	88	86				
4	Z	17	Total	C	N	O		0	0	0
			85	51	17	17				

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	49	Total	C	N	O	0	0	0
			339	212	57	70			
5	R	34	Total	C	N	O	0	0	0
			175	104	34	37			
5	1	27	Total	C	N	O	0	0	0
			145	86	31	28			

- 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		

Continued on next page...



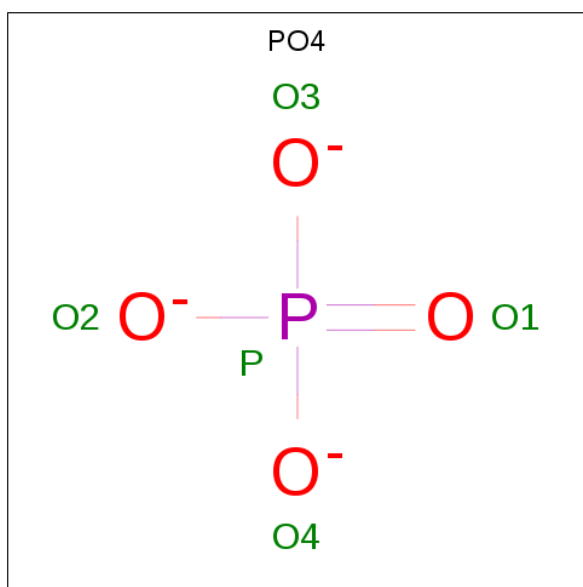
*Continued from previous page...*

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	E	1	Total	O	P	0	0
			5	4	1		
8	N	1	Total	O	P	0	0
			5	4	1		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	10	Total	O	0	0
			10	10		
9	B	9	Total	O	0	0
			9	9		
9	C	3	Total	O	0	0
			3	3		
9	D	11	Total	O	0	0
			11	11		
9	E	10	Total	O	0	0
			10	10		
9	F	8	Total	O	0	0
			8	8		
9	G	2	Total	O	0	0
			2	2		
9	J	3	Total	O	0	0
			3	3		
9	K	5	Total	O	0	0
			5	5		
9	L	8	Total	O	0	0
			8	8		

*Continued on next page...*

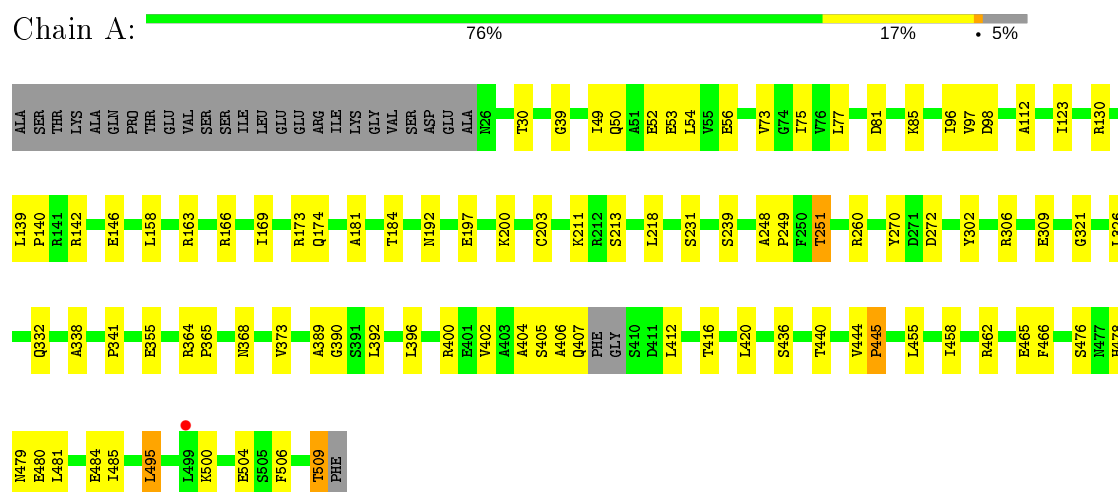
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	M	4	Total 4	O 4	0	0
9	N	3	Total 3	O 3	0	0
9	O	5	Total 5	O 5	0	0
9	P	2	Total 2	O 2	0	0
9	X	1	Total 1	O 1	0	0

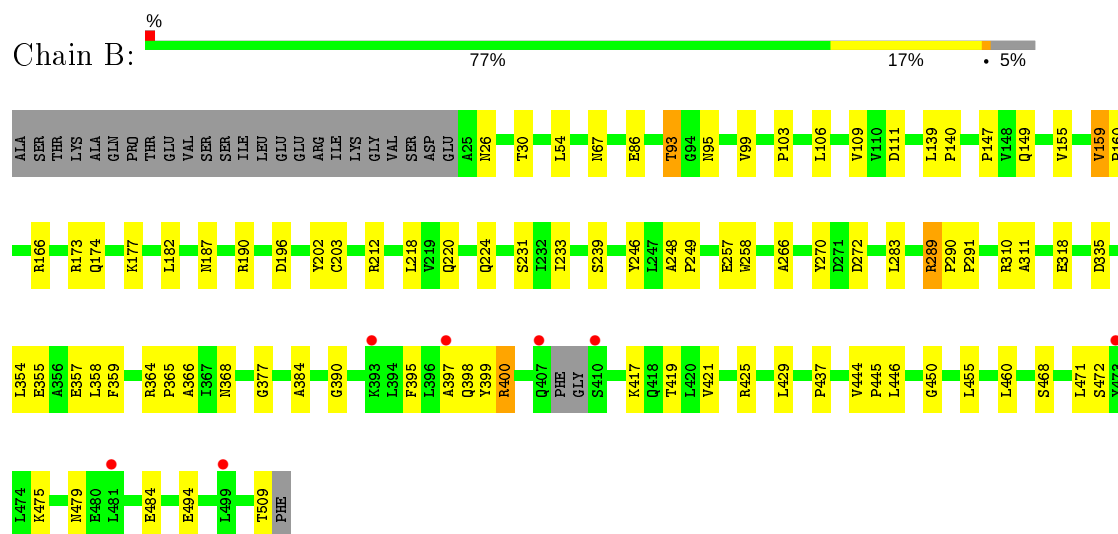
### 3 Residue-property plots

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

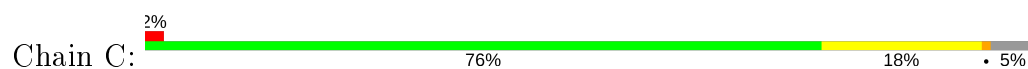
#### • Molecule 1: ATP synthase subunit alpha

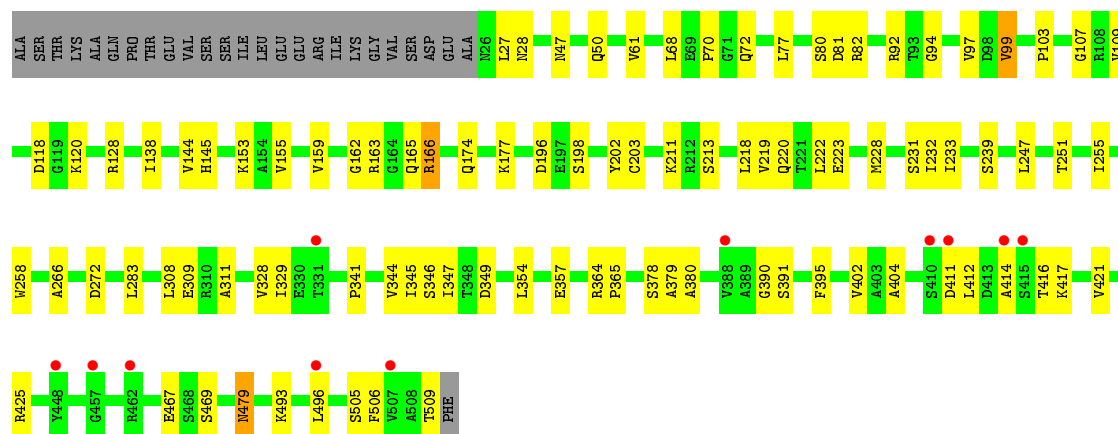


#### • Molecule 1: ATP synthase subunit alpha



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

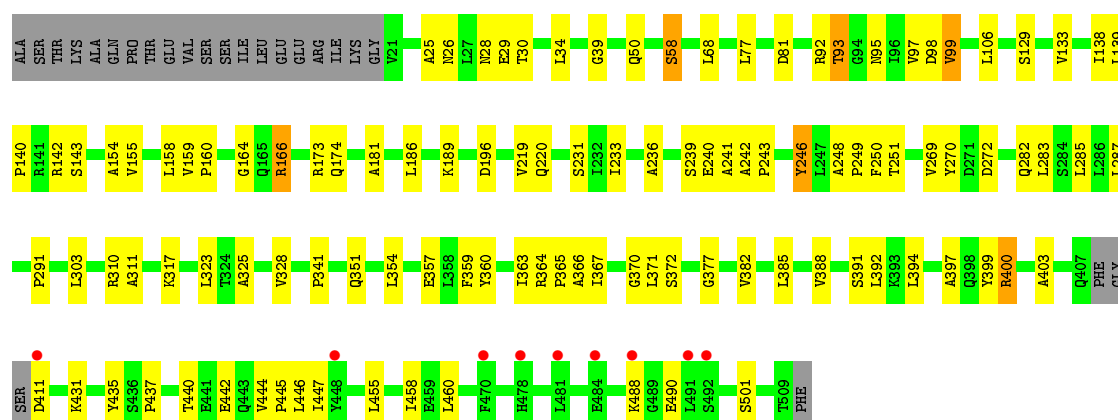
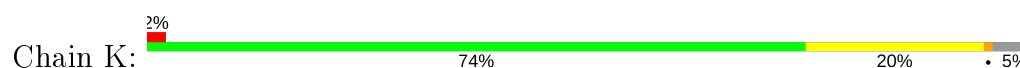




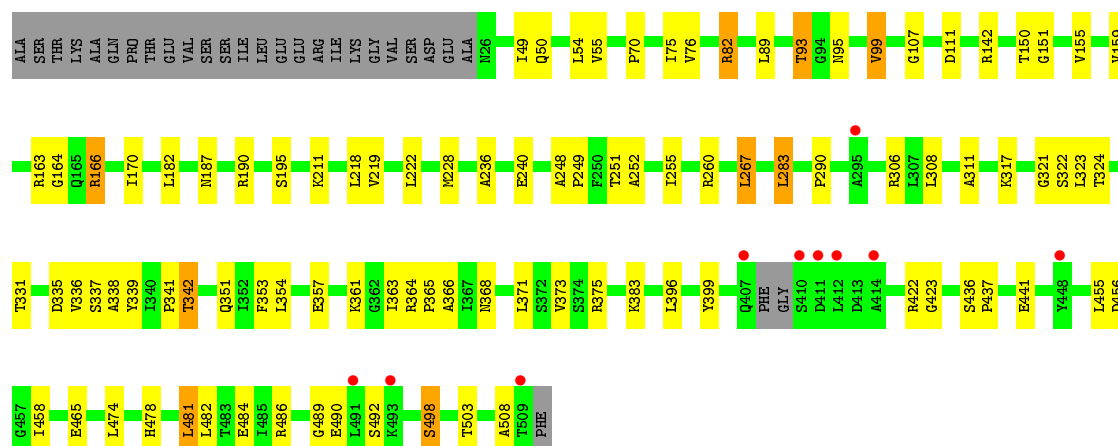
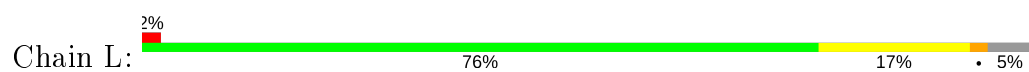
• Molecule 1: ATP synthase subunit alpha



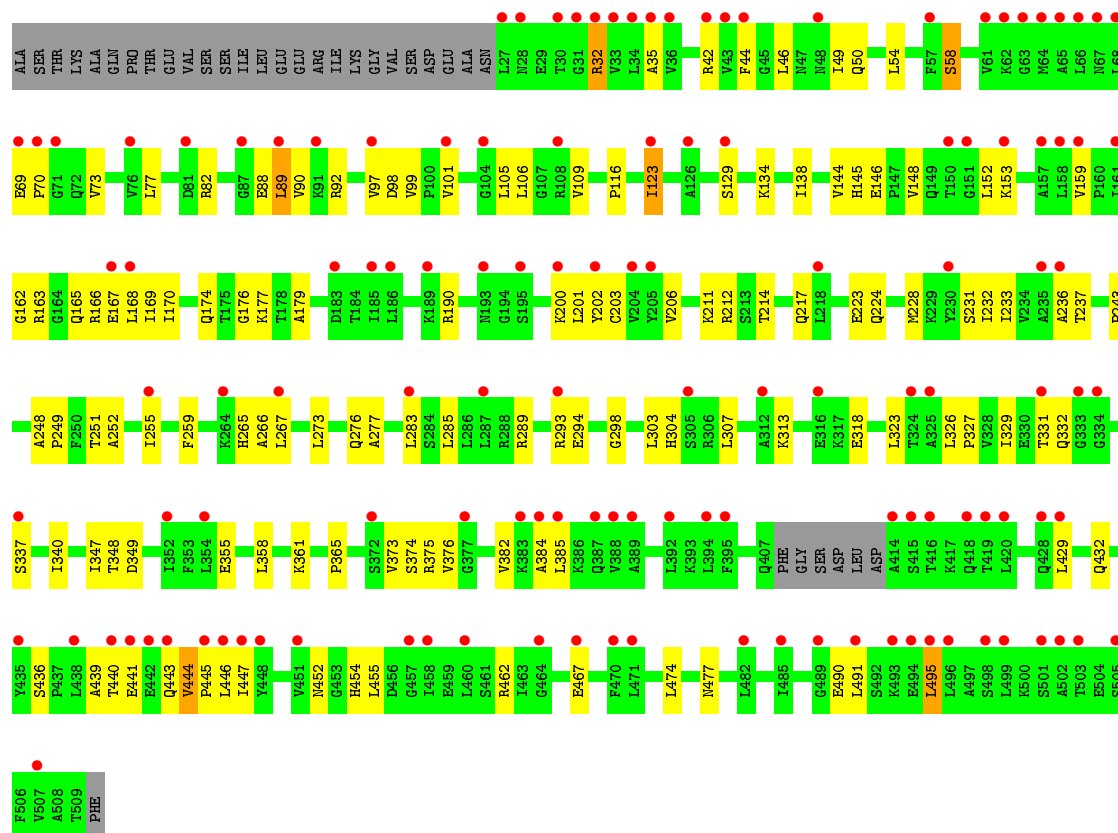
• Molecule 1: ATP synthase subunit alpha



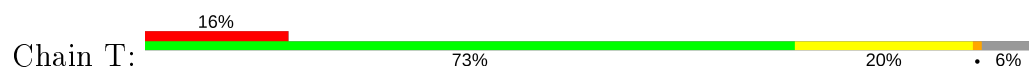
• Molecule 1: ATP synthase subunit alpha

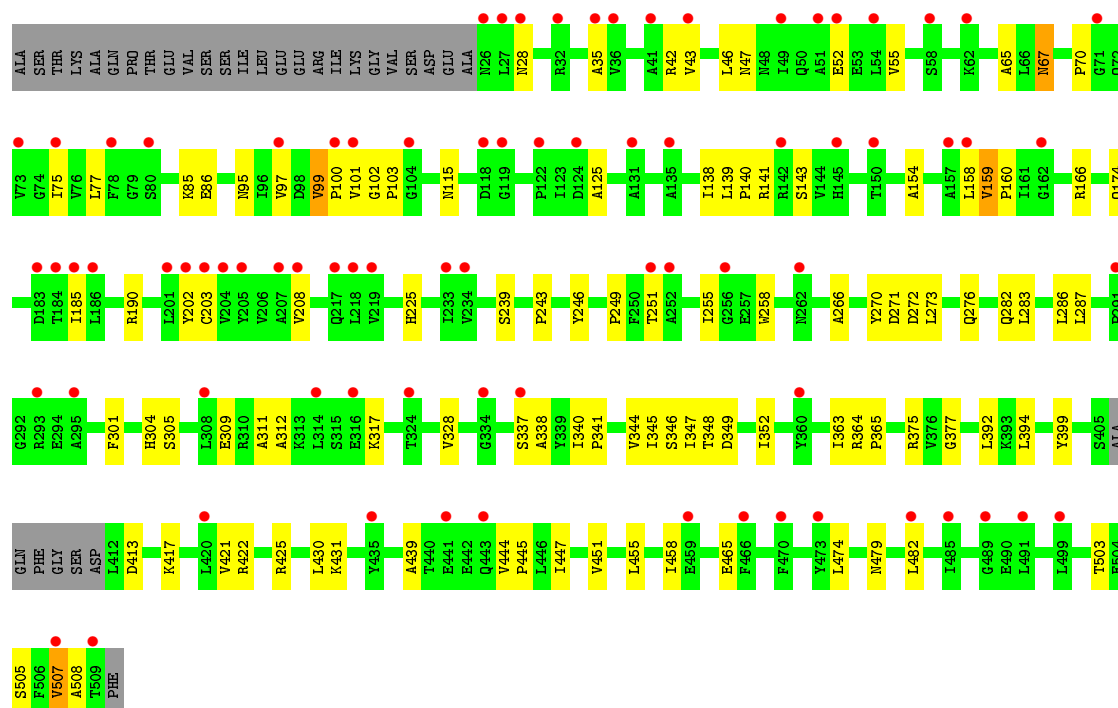


• Molecule 1: ATP synthase subunit alpha

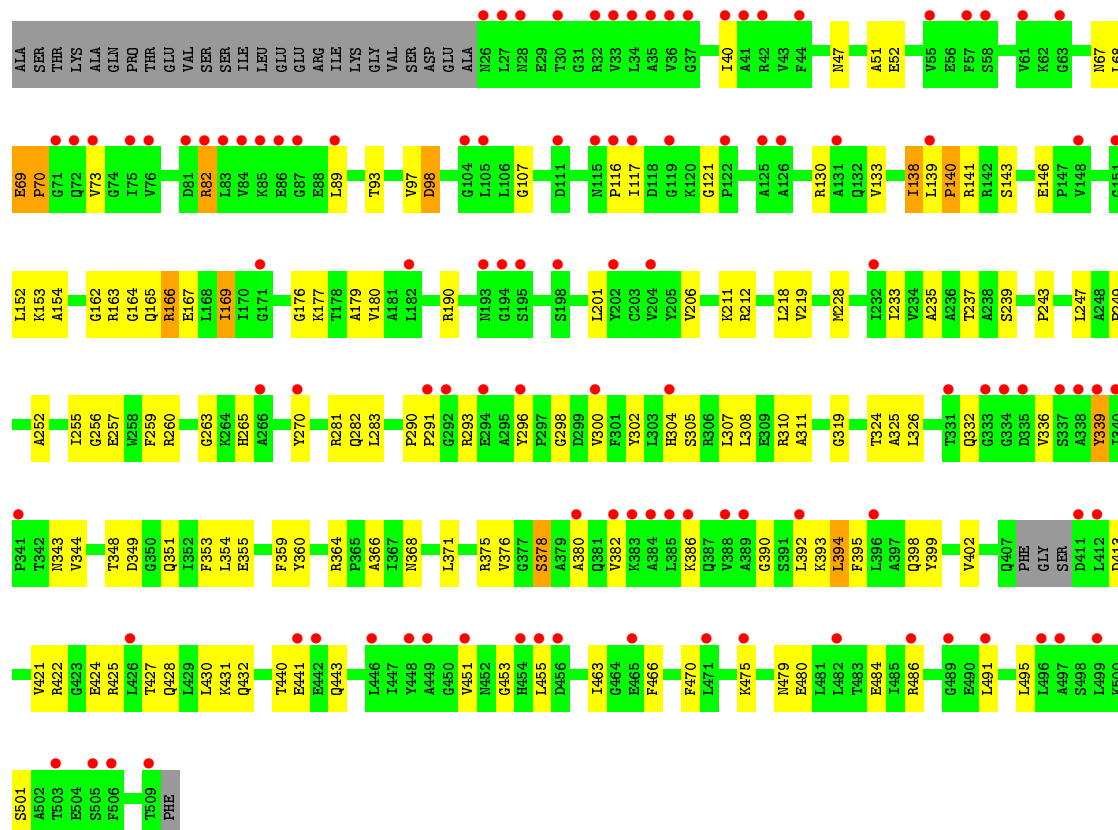


• Molecule 1: ATP synthase subunit alpha

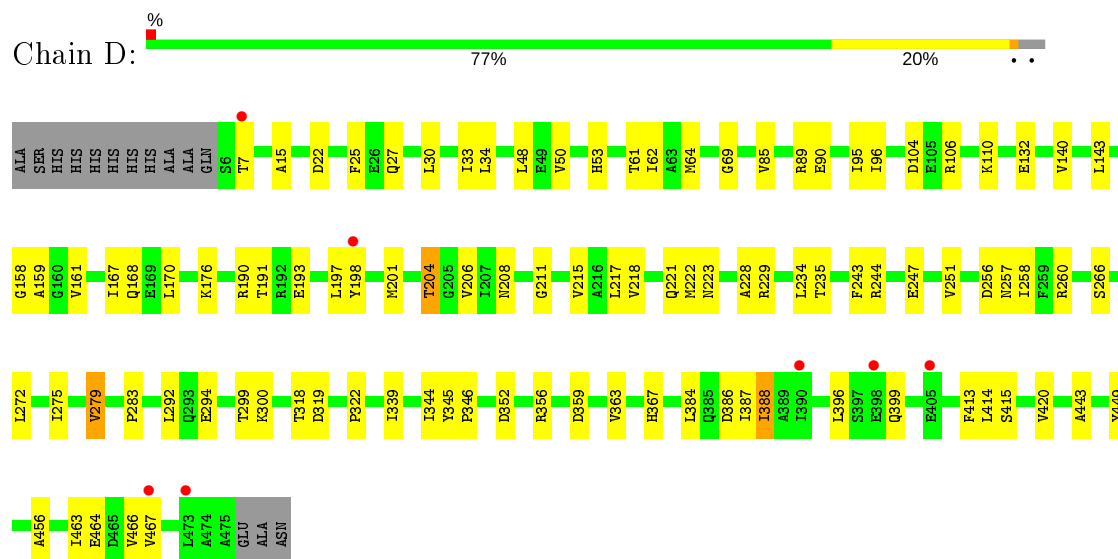




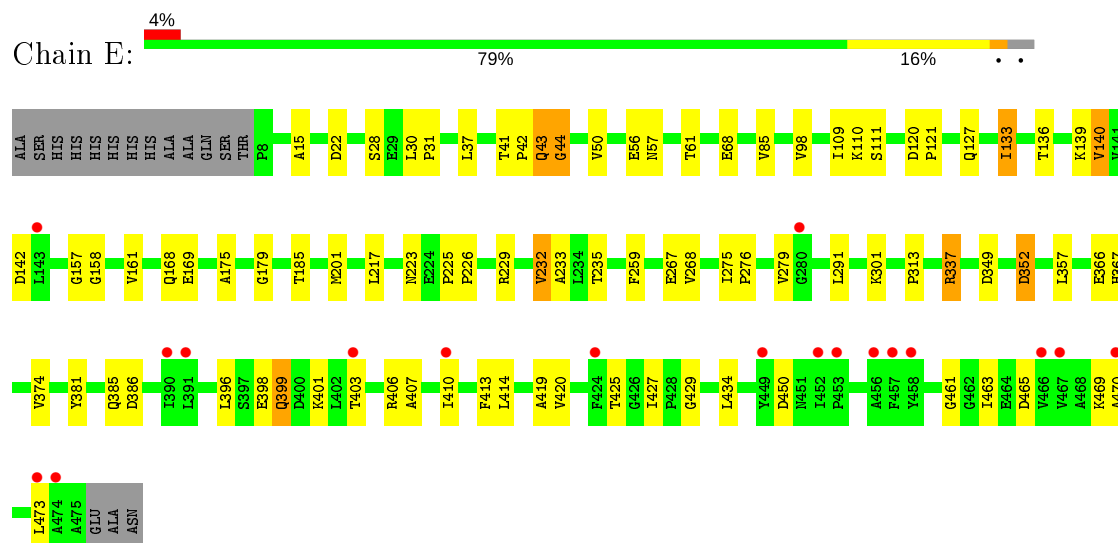
• Molecule 1: ATP synthase subunit alpha



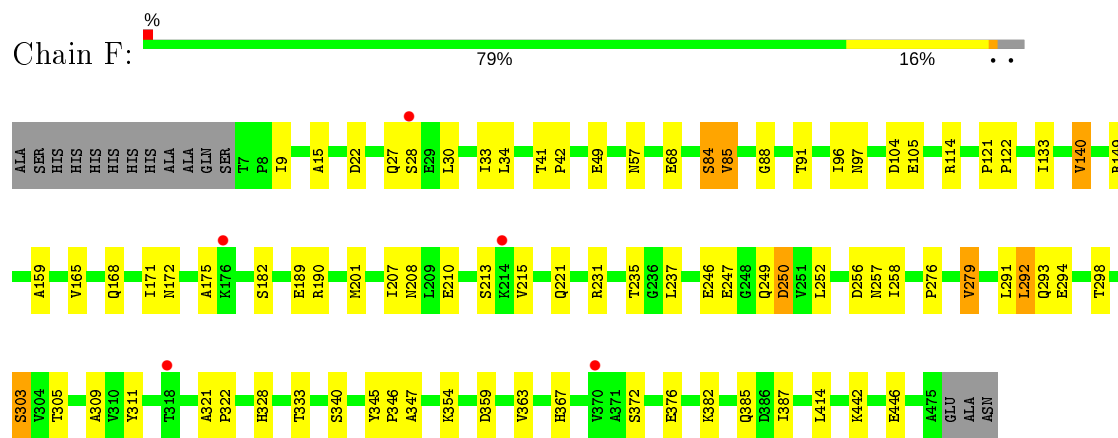
• Molecule 2: ATP synthase subunit beta



• Molecule 2: ATP synthase subunit beta

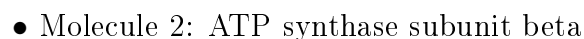


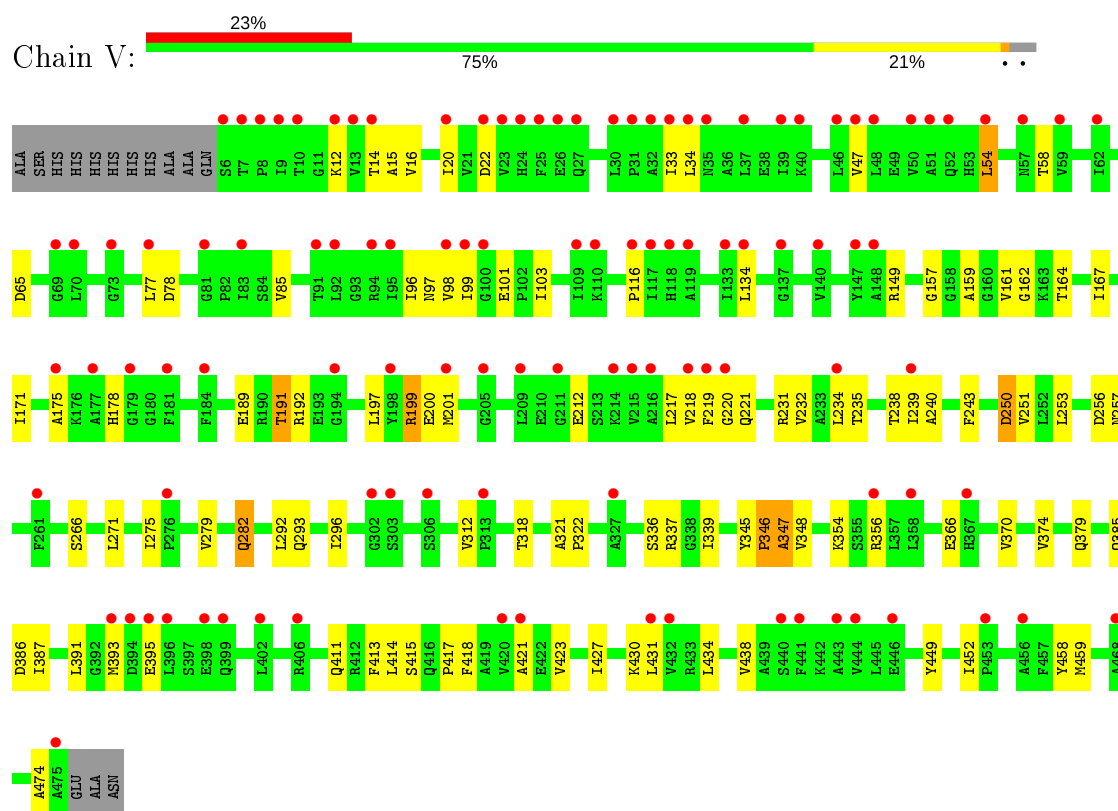
• Molecule 2: ATP synthase subunit beta



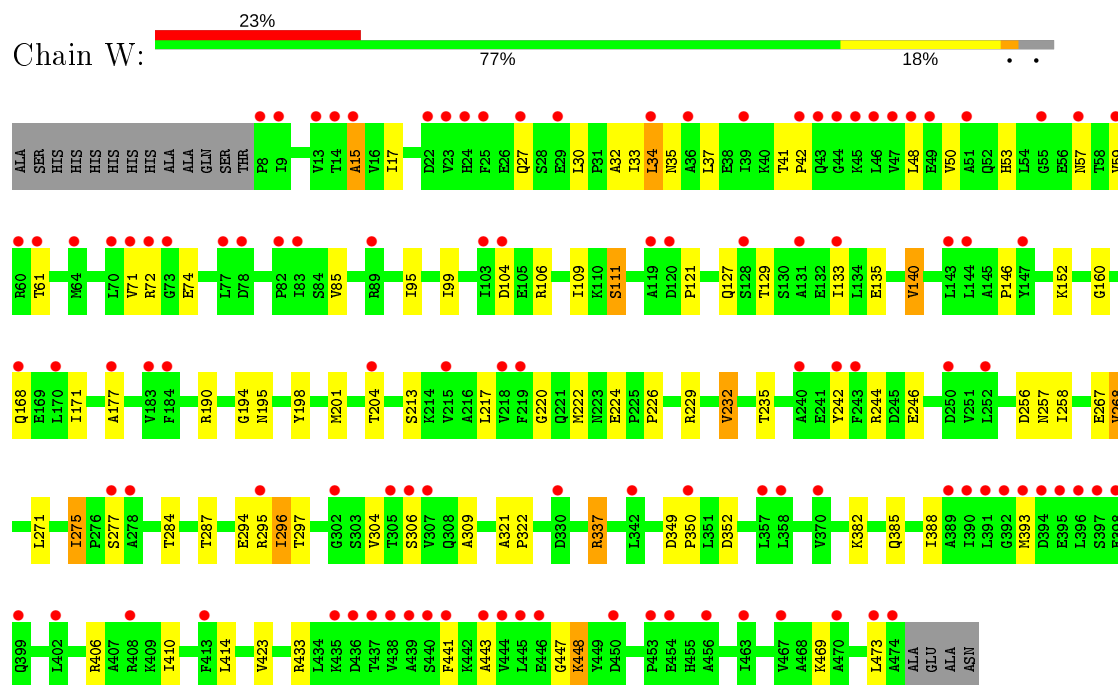
• Molecule 2: ATP synthase subunit beta







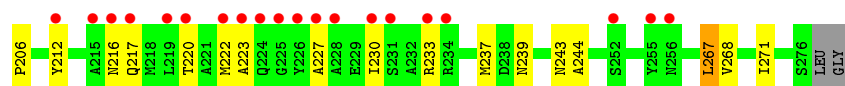
• Molecule 2: ATP synthase subunit beta



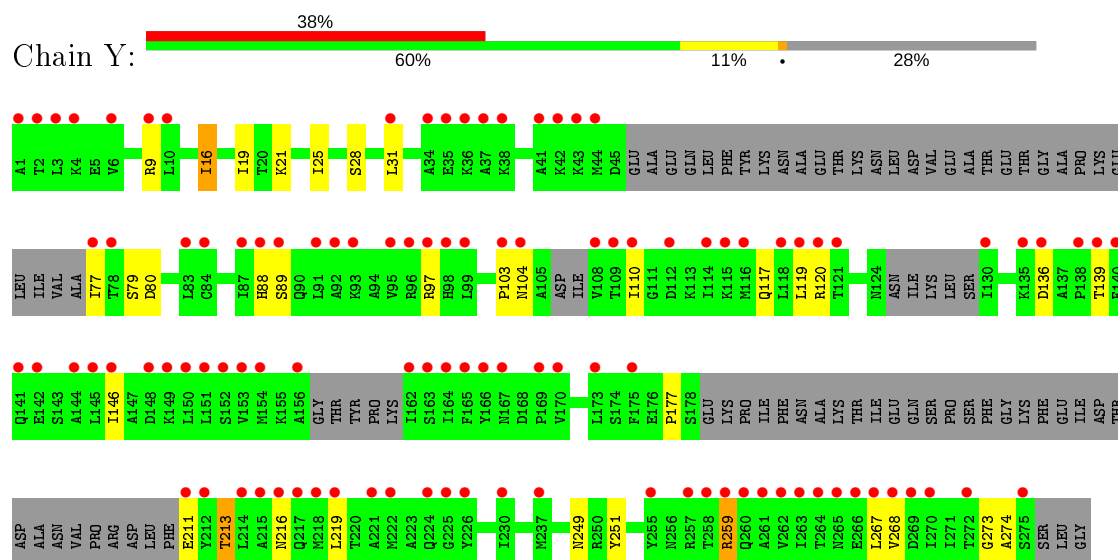
• Molecule 2: ATP synthase subunit beta



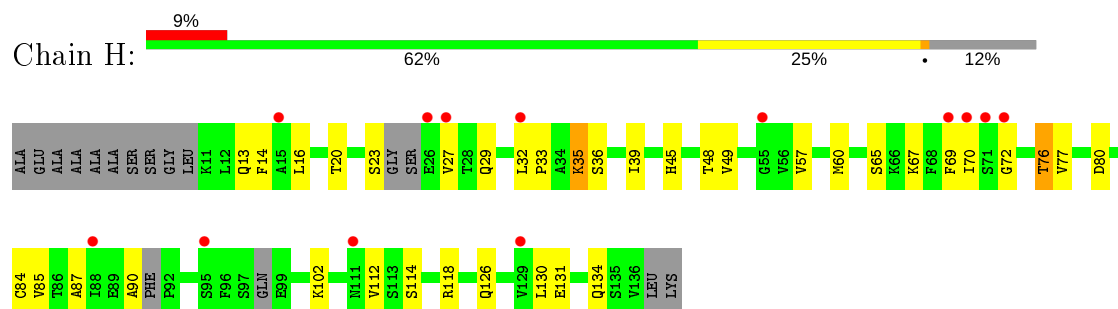




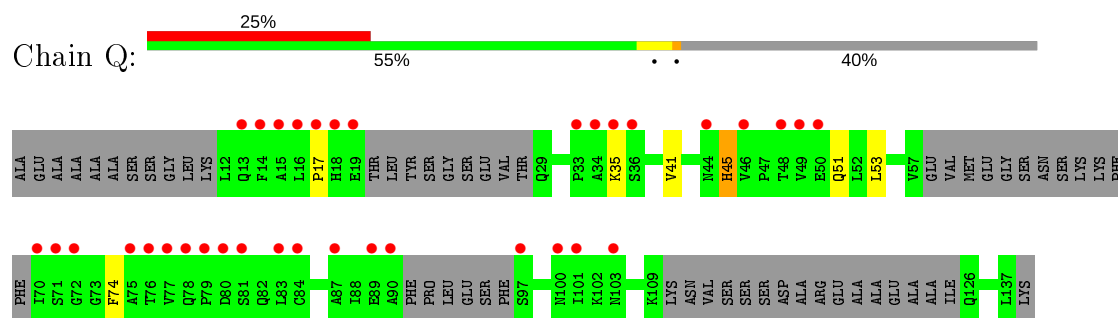
• Molecule 3: ATP synthase subunit gamma



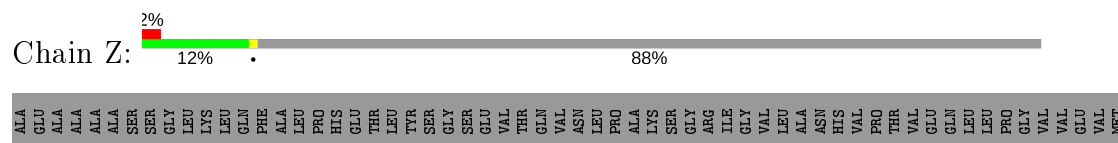
• Molecule 4: ATP synthase subunit delta

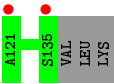
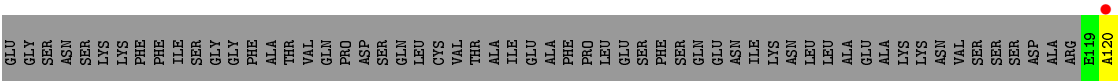


• Molecule 4: ATP synthase subunit delta

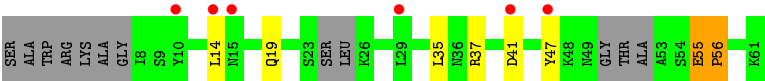


• Molecule 4: ATP synthase subunit delta

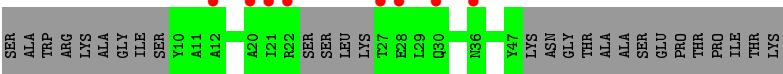




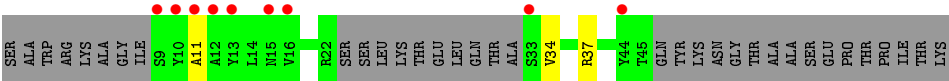
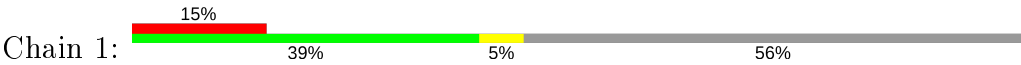
• Molecule 5: ATP synthase subunit epsilon



• Molecule 5: ATP synthase subunit epsilon



• Molecule 5: ATP synthase subunit epsilon



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.43Å 288.58Å 187.17Å 90.00° 101.37° 90.00°	Depositor
Resolution (Å)	20.00 – 2.74 67.14 – 2.74	Depositor EDS
% Data completeness (in resolution range)	98.6 (20.00-2.74) 98.6 (67.14-2.74)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.72 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.212 , 0.259 0.215 , 0.264	Depositor DCC
$R_{free}$ test set	5983 reflections (2.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	66.2	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 48.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	72675	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.20% 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	0.52	0/3712	0.67	0/5024
1	B	0.51	0/3717	0.66	1/5031 (0.0%)
1	C	0.43	0/3730	0.61	0/5049
1	J	0.43	0/3703	0.61	0/5012
1	K	0.46	0/3732	0.63	0/5052
1	L	0.45	0/3712	0.62	1/5024 (0.0%)
1	S	0.40	0/3675	0.57	0/4973
1	T	0.40	0/3685	0.55	0/4987
1	U	0.41	0/3703	0.58	0/5013
2	D	0.48	0/3601	0.65	0/4884
2	E	0.51	0/3560	0.65	0/4834
2	F	0.44	0/3583	0.63	0/4862
2	M	0.42	0/3591	0.61	0/4872
2	N	0.50	0/3597	0.64	0/4880
2	O	0.47	0/3590	0.65	0/4869
2	V	0.40	0/3605	0.57	0/4889
2	W	0.43	0/3587	0.56	0/4863
2	X	0.40	0/3599	0.56	0/4881
3	G	0.39	0/2080	0.55	0/2798
3	P	0.40	0/1867	0.54	0/2509
3	Y	0.38	0/1527	0.53	0/2048
4	H	0.40	0/804	0.58	0/1101
4	Q	0.39	0/440	0.50	0/603
4	Z	0.43	0/84	0.59	0/116
5	1	0.36	0/143	0.53	0/195
5	I	0.46	0/343	0.58	0/470
5	R	0.41	0/173	0.52	0/239
All	All	0.45	0/73143	0.61	2/99078 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	283	LEU	CA-CB-CG	6.71	130.74	115.30
1	B	111	ASP	CB-CG-OD1	5.54	123.28	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3659	0	3743	54	0
1	B	3664	0	3748	50	0
1	C	3675	0	3759	53	0
1	J	3650	0	3735	41	0
1	K	3679	0	3754	71	0
1	L	3659	0	3743	52	0
1	S	3622	0	3716	90	0
1	T	3632	0	3724	72	0
1	U	3650	0	3730	99	0
2	D	3545	0	3614	64	0
2	E	3504	0	3550	53	0
2	F	3527	0	3592	49	0
2	M	3535	0	3599	66	0
2	N	3541	0	3604	63	0
2	O	3534	0	3606	52	0
2	V	3549	0	3620	75	0
2	W	3531	0	3605	59	0
2	X	3543	0	3615	92	0
3	G	2055	0	2123	44	0
3	P	1850	0	1892	49	0
3	Y	1517	0	1561	20	0
4	H	795	0	670	19	0
4	Q	441	0	234	3	0
4	Z	85	0	45	0	0
5	1	145	0	87	2	0
5	I	339	0	280	4	0
5	R	175	0	100	0	0
6	A	31	0	13	1	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	31	0	13	2	0
6	C	31	0	13	0	0
6	D	31	0	13	1	0
6	F	31	0	13	2	0
6	J	31	0	13	0	0
6	K	31	0	13	1	0
6	L	31	0	13	0	0
6	M	31	0	13	5	0
6	O	31	0	13	0	0
6	S	31	0	13	4	0
6	T	31	0	13	1	0
6	U	31	0	13	4	0
6	V	31	0	13	4	0
6	X	31	0	13	6	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	E	5	0	0	0	0
8	N	5	0	0	0	0
9	A	10	0	0	0	0
9	B	9	0	0	0	0
9	C	3	0	0	0	0
9	D	11	0	0	0	0
9	E	10	0	0	0	0
9	F	8	0	0	0	0
9	G	2	0	0	1	0
9	J	3	0	0	0	0
9	K	5	0	0	0	0
9	L	8	0	0	0	0
9	M	4	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	N	3	0	0	0	0
9	O	5	0	0	0	0
9	P	2	0	0	0	0
9	X	1	0	0	0	0
All	All	72675	0	73244	1182	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (1182) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:85:VAL:HG11	2:D:235:THR:HG23	1.24	1.08
2:O:84:SER:HB3	2:O:114:ARG:HH11	1.18	1.07
1:L:336:VAL:HG11	1:L:353:PHE:HE2	1.23	1.03
1:A:112:ALA:O	1:A:251:THR:HG21	1.61	1.01
2:X:95:ILE:HD12	2:X:104:ASP:HB3	1.43	1.01
3:P:88:HIS:CD2	3:P:113:LYS:HB2	1.97	0.98
2:E:85:VAL:HG11	2:E:235:THR:HG23	1.46	0.97
5:I:55:GLU:CB	5:I:56:PRO:HD3	1.95	0.96
2:O:84:SER:CB	2:O:114:ARG:HH11	1.79	0.95
2:W:85:VAL:HG11	2:W:235:THR:HG23	1.52	0.92
2:M:160:GLY:H	6:M:600:ANP:HNB1	1.15	0.90
2:O:85:VAL:HG11	2:O:235:THR:HG23	1.54	0.90
2:V:449:TYR:HD1	2:V:452:ILE:HD11	1.39	0.88
1:K:186:LEU:O	1:K:189:LYS:HE3	1.73	0.88
1:C:97:VAL:HG11	1:C:247:LEU:HD21	1.56	0.87
2:V:47:VAL:HG21	2:V:99:ILE:HG21	1.55	0.87
1:U:69:GLU:HB3	1:U:70:PRO:HD2	1.55	0.86
2:M:25:PHE:HB2	2:M:30:LEU:HD23	1.56	0.84
1:L:336:VAL:HG11	1:L:353:PHE:CE2	2.12	0.83
2:W:27:GLN:HG3	2:W:57:ASN:HD21	1.42	0.83
2:F:41:THR:HB	2:F:42:PRO:HD2	1.60	0.83
1:B:26:ASN:O	1:B:30:THR:HB	1.78	0.83
1:A:444:VAL:HG22	1:A:445:PRO:HD3	1.62	0.82
2:X:258:ILE:HD13	2:X:308:GLN:OE1	1.80	0.81
1:B:93:THR:HG22	1:B:95:ASN:H	1.45	0.81
3:G:110:ILE:HG12	3:G:130:ILE:HG13	1.62	0.81
3:P:88:HIS:HD2	3:P:113:LYS:HB2	1.40	0.81
1:U:212:ARG:HG2	1:U:237:THR:HG21	1.63	0.81
2:X:160:GLY:H	6:X:600:ANP:HNB1	1.29	0.81

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:246:TYR:CE2	1:K:283:LEU:CD1	2.64	0.80
2:M:85:VAL:HG11	2:M:235:THR:HG23	1.63	0.80
1:U:354:LEU:HA	1:U:366:ALA:O	1.80	0.80
2:F:363:VAL:HB	2:F:367:HIS:CD2	2.16	0.79
1:S:98:ASP:HB2	1:S:129:SER:O	1.82	0.79
2:D:176:LYS:HD3	2:D:204:THR:HG22	1.64	0.79
2:O:84:SER:CB	2:O:114:ARG:NH1	2.45	0.79
1:S:212:ARG:HG3	1:S:237:THR:HG21	1.63	0.79
1:S:444:VAL:HG23	1:S:445:PRO:HD3	1.65	0.78
3:G:89:SER:HA	3:G:117:GLN:HE21	1.48	0.78
1:C:138:ILE:HD12	2:D:191:THR:HG23	1.65	0.77
1:T:143:SER:H	2:X:199:ARG:HH22	1.33	0.77
3:P:95:VAL:O	3:P:99:LEU:HB2	1.84	0.77
1:T:239:SER:HB3	2:W:294:GLU:HG3	1.66	0.76
1:L:93:THR:HG22	1:L:95:ASN:H	1.50	0.76
1:J:211:LYS:HE3	1:J:213:SER:OG	1.86	0.76
3:G:108:VAL:HG22	3:G:128:LEU:HB3	1.67	0.76
2:N:384:LEU:O	2:N:388:ILE:HG12	1.86	0.75
2:F:363:VAL:HB	2:F:367:HIS:HD2	1.51	0.75
1:B:147:PRO:HB2	1:B:149:GLN:HE21	1.49	0.75
1:U:441:GLU:HG2	1:U:486:ARG:HB2	1.70	0.74
2:N:85:VAL:CG1	2:N:235:THR:HG23	2.18	0.74
1:L:290:PRO:HB2	2:M:270:ALA:HB1	1.71	0.73
2:F:85:VAL:HG11	2:F:235:THR:HG23	1.70	0.73
2:N:85:VAL:HG11	2:N:235:THR:HG23	1.70	0.73
2:X:85:VAL:HG11	2:X:235:THR:HG23	1.71	0.72
3:Y:16:ILE:HA	3:Y:19:ILE:HG22	1.69	0.72
2:E:136:THR:HG22	2:E:142:ASP:OD1	1.89	0.72
1:C:341:PRO:O	1:C:345:ILE:HG13	1.89	0.72
2:D:234:LEU:HD23	2:D:292:LEU:HD13	1.70	0.72
3:Y:79:SER:HB3	3:Y:88:HIS:HE1	1.53	0.72
4:H:126:GLN:O	4:H:130:LEU:HG	1.90	0.71
2:E:133:ILE:HD13	2:E:357:LEU:HD12	1.72	0.71
1:A:302:TYR:O	1:A:306:ARG:HB2	1.90	0.71
1:C:239:SER:HB3	2:F:294:GLU:HG3	1.73	0.71
1:S:166:ARG:HH22	2:W:190:ARG:HD3	1.55	0.71
3:P:180:LYS:NZ	3:P:220:THR:HB	2.06	0.71
1:L:481:LEU:HD21	1:L:498:SER:HB3	1.73	0.70
2:O:9:ILE:HG23	2:O:27:GLN:HE21	1.56	0.70
3:P:88:HIS:CD2	3:P:113:LYS:CB	2.74	0.70
1:C:92:ARG:HH21	1:C:94:GLY:HA2	1.55	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:97:ASN:HD21	2:V:101:GLU:HB2	1.57	0.70
2:M:371:ALA:O	2:M:375:GLN:HG3	1.92	0.70
1:L:54:LEU:O	1:L:93:THR:HB	1.92	0.69
2:M:50:VAL:HA	2:M:61:THR:HG22	1.74	0.69
2:V:77:LEU:HG	2:V:78:ASP:H	1.58	0.69
2:W:226:PRO:HB2	2:W:268:VAL:HG23	1.75	0.69
1:C:107:GLY:HA2	1:C:228:MET:O	1.92	0.69
2:N:229:ARG:NH2	2:N:267:GLU:OE1	2.26	0.69
2:D:244:ARG:HD2	2:D:299:THR:HG22	1.75	0.69
1:L:383:LYS:HG2	1:L:490:GLU:HG3	1.73	0.69
1:J:309:GLU:HG3	2:N:223:ASN:HB3	1.75	0.69
2:V:178:HIS:CE1	2:V:250:ASP:HB3	2.28	0.68
2:O:84:SER:HB2	2:O:114:ARG:NH1	2.07	0.68
1:S:148:VAL:HG23	1:S:163:ARG:HG2	1.76	0.68
2:O:9:ILE:HD12	2:O:9:ILE:H	1.58	0.68
1:T:35:ALA:HB3	1:T:42:ARG:NH1	2.09	0.68
1:T:77:LEU:O	1:T:243:PRO:HG2	1.94	0.68
5:I:55:GLU:CB	5:I:56:PRO:CD	2.70	0.67
1:A:481:LEU:O	1:A:485:ILE:HG13	1.94	0.67
2:V:85:VAL:HG11	2:V:235:THR:HG23	1.75	0.67
2:F:250:ASP:OD1	2:F:303:SER:HB3	1.94	0.67
2:X:321:ALA:HB3	2:X:322:PRO:HD2	1.77	0.67
3:P:187:THR:O	3:P:188:ILE:HG13	1.94	0.67
1:J:260:ARG:O	1:J:321:GLY:HA3	1.94	0.67
2:M:160:GLY:N	6:M:600:ANP:HNB1	1.92	0.67
2:N:142:ASP:HB3	2:N:434:LEU:HD12	1.77	0.66
1:T:138:ILE:HD13	2:X:95:ILE:HG21	1.75	0.66
1:K:138:ILE:HD12	1:K:138:ILE:N	2.11	0.66
1:C:412:LEU:HB3	1:C:416:THR:OG1	1.96	0.66
2:X:208:ASN:HD22	2:X:210:GLU:H	1.44	0.66
2:D:456:ALA:O	2:D:466:VAL:HG13	1.96	0.66
1:U:378:SER:HB3	1:U:386:LYS:HG3	1.78	0.66
2:D:197:LEU:O	2:D:201:MET:HG2	1.96	0.65
1:K:388:VAL:HG12	1:K:447:ILE:HG22	1.78	0.65
2:X:160:GLY:N	6:X:600:ANP:HNB1	1.95	0.65
1:A:174:GLN:HA	6:A:600:ANP:HNB1	1.60	0.65
2:E:168:GLN:HE21	2:E:201:MET:HG2	1.61	0.65
2:F:140:VAL:HG13	2:F:414:LEU:HD22	1.79	0.65
3:G:77:ILE:HG21	3:G:222:MET:HG2	1.77	0.65
2:O:9:ILE:HG23	2:O:27:GLN:NE2	2.11	0.65
2:V:47:VAL:HG21	2:V:99:ILE:HD13	1.77	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:465:ASP:O	2:E:469:LYS:HB2	1.97	0.65
2:V:15:ALA:HB3	2:V:22:ASP:HB2	1.79	0.65
2:V:162:GLY:HA2	6:V:600:ANP:O1A	1.97	0.65
4:H:35:LYS:HG2	4:H:36:SER:H	1.62	0.64
1:K:98:ASP:HB2	1:K:129:SER:O	1.97	0.64
1:U:349:ASP:O	1:U:375:ARG:HB2	1.97	0.64
2:V:275:ILE:HG23	3:Y:274:ALA:HB2	1.79	0.64
1:L:187:ASN:OD1	1:L:190:ARG:NH1	2.30	0.64
4:H:48:THR:H	4:H:77:VAL:HB	1.62	0.64
2:X:321:ALA:HB3	2:X:322:PRO:CD	2.27	0.64
2:D:319:ASP:O	2:D:322:PRO:HD2	1.97	0.64
1:K:93:THR:HG22	1:K:95:ASN:H	1.63	0.64
2:X:384:LEU:O	2:X:388:ILE:HG12	1.97	0.64
1:B:140:PRO:HB3	1:B:318:GLU:HG3	1.79	0.63
1:L:422:ARG:HG3	1:L:456:ASP:OD1	1.98	0.63
2:O:140:VAL:HG13	2:O:414:LEU:HD22	1.80	0.63
3:P:138:PRO:HG3	3:P:223:ALA:HA	1.80	0.63
1:U:263:GLY:HA2	1:U:319:GLY:O	1.98	0.63
2:V:449:TYR:HD1	2:V:452:ILE:CD1	2.10	0.63
2:M:90:GLU:HG3	2:M:111:SER:CB	2.28	0.63
1:J:26:ASN:O	1:J:27:LEU:HB2	1.99	0.63
1:S:69:GLU:HG2	1:S:70:PRO:HD2	1.79	0.63
1:B:54:LEU:O	1:B:93:THR:HB	1.99	0.63
2:N:30:LEU:HD11	2:N:57:ASN:HA	1.80	0.63
1:S:177:LYS:HB2	6:S:600:ANP:O1B	1.99	0.63
1:U:153:LYS:HE2	1:U:432:GLN:HB2	1.81	0.63
3:G:118:LEU:HA	3:G:121:THR:HG22	1.81	0.62
1:T:479:ASN:HA	1:T:482:LEU:HD12	1.81	0.62
2:E:168:GLN:HE21	2:E:201:MET:CG	2.12	0.62
2:M:234:LEU:CD2	2:M:292:LEU:HD13	2.29	0.62
1:T:455:LEU:HA	1:T:458:ILE:HD13	1.80	0.62
1:T:85:LYS:HE2	2:W:32:ALA:HB2	1.80	0.62
2:N:33:ILE:O	2:N:34:LEU:HB2	1.99	0.62
2:N:425:THR:O	2:N:427:ILE:HD12	1.99	0.62
3:P:26:VAL:O	3:P:30:ARG:HD2	1.99	0.62
1:U:166:ARG:HD3	1:U:308:LEU:O	1.99	0.62
1:L:338:ALA:O	1:L:342:THR:OG1	2.18	0.62
1:U:281:ARG:HH12	2:X:278:ALA:HB2	1.65	0.62
1:C:166:ARG:HD2	1:C:308:LEU:O	2.00	0.62
3:G:189:GLU:OE2	3:G:206:PRO:HG2	2.00	0.62
1:B:355:GLU:HG3	1:B:368:ASN:HD22	1.63	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:55:VAL:HG21	1:J:75:ILE:HD13	1.82	0.61
1:S:355:GLU:HB2	1:S:358:LEU:HD12	1.82	0.61
1:U:212:ARG:CG	1:U:237:THR:HG21	2.29	0.61
2:D:258:ILE:HD11	2:D:292:LEU:HD21	1.81	0.61
1:K:246:TYR:CE2	1:K:283:LEU:HD12	2.35	0.61
2:D:221:GLN:HA	2:D:221:GLN:OE1	2.01	0.61
3:G:193:SER:HB3	3:G:196:LYS:HG3	1.81	0.61
1:K:246:TYR:HE2	1:K:283:LEU:CD1	2.11	0.61
2:N:296:ILE:HD13	2:N:306:SER:HB2	1.82	0.61
2:V:47:VAL:CG2	2:V:99:ILE:HD13	2.29	0.61
3:G:180:LYS:NZ	3:G:220:THR:HG22	2.15	0.61
3:P:239:ASN:O	3:P:243:ASN:ND2	2.32	0.61
1:B:109:VAL:HG13	1:B:233:ILE:HB	1.83	0.61
1:S:349:ASP:O	1:S:375:ARG:HB2	2.01	0.61
2:D:25:PHE:HB2	2:D:30:LEU:HD23	1.82	0.61
3:Y:213:THR:HA	3:Y:216:ASN:HB3	1.82	0.61
1:S:266:ALA:O	1:S:323:LEU:HA	2.00	0.61
2:V:189:GLU:HG3	2:V:221:GLN:OE1	2.00	0.61
2:O:85:VAL:CG1	2:O:235:THR:HG23	2.30	0.61
3:P:150:LEU:O	3:P:154:MET:HB2	2.01	0.61
1:S:243:PRO:HG3	1:S:283:LEU:HD21	1.81	0.61
1:U:466:PHE:O	1:U:470:PHE:HB2	2.01	0.61
1:U:176:GLY:HA2	6:U:600:ANP:O5'	2.00	0.61
2:F:33:ILE:O	2:F:34:LEU:HB2	2.01	0.60
1:J:358:LEU:HB2	1:J:366:ALA:HB1	1.83	0.60
1:L:375:ARG:HH12	2:M:160:GLY:HA2	1.65	0.60
2:W:160:GLY:HA3	2:W:337:ARG:NH2	2.16	0.60
1:B:290:PRO:HB3	2:F:276:PRO:HG3	1.83	0.60
2:O:168:GLN:HB3	2:O:420:VAL:HG11	1.84	0.60
1:T:101:VAL:HG12	1:T:255:ILE:HA	1.83	0.60
1:U:69:GLU:HB3	1:U:70:PRO:CD	2.28	0.60
2:N:310:VAL:HG11	2:N:326:PHE:HE1	1.67	0.60
2:M:144:LEU:O	2:M:358:LEU:HD22	2.01	0.60
2:E:226:PRO:HB2	2:E:268:VAL:HG23	1.83	0.60
2:O:84:SER:HB3	2:O:114:ARG:NH1	2.00	0.60
1:J:265:HIS:ND1	1:J:322:SER:HB3	2.17	0.60
1:L:368:ASN:ND2	1:L:371:LEU:HD12	2.17	0.60
1:K:382:VAL:HG11	1:K:440:THR:HG21	1.84	0.59
2:V:220:GLY:HA3	2:V:232:VAL:HG11	1.84	0.59
2:F:165:VAL:HG23	6:F:600:ANP:O1A	2.01	0.59
1:L:441:GLU:OE2	1:L:486:ARG:HD3	2.01	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:213:THR:HG23	3:G:217:GLN:HE21	1.68	0.59
1:K:243:PRO:HA	1:K:246:TYR:CD2	2.37	0.59
1:S:249:PRO:HB2	1:S:307:LEU:HD21	1.84	0.59
1:U:304:HIS:CE1	1:U:343:ASN:HB3	2.37	0.59
2:W:48:LEU:HB3	2:W:61:THR:HB	1.85	0.59
2:X:87:VAL:HG22	2:X:113:LEU:O	2.02	0.59
1:L:76:VAL:HG11	1:L:283:LEU:HG	1.84	0.59
2:N:98:VAL:HB	2:N:232:VAL:HG13	1.83	0.59
3:P:122:HIS:N	3:P:123:PRO:HD3	2.17	0.59
1:J:143:SER:OG	2:N:199:ARG:NH1	2.36	0.59
2:M:33:ILE:O	2:M:34:LEU:HB2	2.03	0.59
2:N:220:GLY:HA3	2:N:232:VAL:HG11	1.84	0.59
1:T:458:ILE:H	1:T:458:ILE:HD12	1.68	0.59
2:O:242:TYR:CE1	2:O:246:GLU:HG3	2.36	0.59
2:O:417:PRO:HG3	2:O:459:MET:HG3	1.84	0.58
2:W:388:ILE:HD12	2:W:393:MET:HG2	1.85	0.58
3:G:91:LEU:HD23	3:G:114:ILE:HD13	1.86	0.58
2:M:197:LEU:O	2:M:201:MET:HG2	2.02	0.58
2:M:344:ILE:HG23	2:M:415:SER:HB3	1.84	0.58
1:S:46:LEU:HG	1:S:49:ILE:HB	1.85	0.58
1:U:359:PHE:CE1	1:U:364:ARG:HD3	2.39	0.58
2:N:220:GLY:CA	2:N:232:VAL:HG11	2.33	0.58
2:O:122:PRO:HG2	2:O:297:THR:HG21	1.84	0.58
2:O:391:LEU:HB3	2:O:395:GLU:HG3	1.86	0.58
1:T:346:SER:HA	6:X:600:ANP:O1G	2.04	0.58
1:C:144:VAL:CG1	1:C:162:GLY:HA3	2.32	0.58
2:D:204:THR:HB	2:D:206:VAL:HG23	1.85	0.58
3:Y:9:ARG:HD3	3:Y:251:TYR:HE1	1.69	0.58
1:K:138:ILE:H	1:K:138:ILE:HD12	1.67	0.58
1:B:358:LEU:HB2	1:B:366:ALA:HB1	1.86	0.58
2:D:143:LEU:O	2:D:367:HIS:HE1	1.87	0.58
2:F:293:GLN:HA	2:F:293:GLN:OE1	2.04	0.58
2:M:148:ALA:HB2	2:M:357:LEU:HD11	1.84	0.58
1:U:302:TYR:HA	1:U:305:SER:OG	2.03	0.58
2:N:15:ALA:HB3	2:N:22:ASP:HB2	1.86	0.58
2:X:325:THR:O	2:X:328:HIS:HB2	2.03	0.57
1:U:360:TYR:CZ	2:X:351:LEU:O	2.57	0.57
2:D:234:LEU:CD2	2:D:292:LEU:HD13	2.34	0.57
1:L:364:ARG:HA	1:L:365:PRO:C	2.24	0.57
2:W:168:GLN:HE21	2:W:201:MET:HG2	1.69	0.57
2:F:140:VAL:CG1	2:F:414:LEU:HD22	2.34	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:208:VAL:HG11	1:T:276:GLN:HB2	1.86	0.57
1:A:478:HIS:HB3	1:A:481:LEU:HG	1.86	0.57
2:N:359:ASP:O	2:N:363:VAL:HG22	2.03	0.57
1:C:144:VAL:HG11	1:C:162:GLY:HA3	1.86	0.57
2:W:177:ALA:HB1	2:W:433:ARG:HH22	1.68	0.57
2:E:406:ARG:HD3	2:E:450:ASP:OD1	2.05	0.57
2:F:293:GLN:HG3	2:F:328:HIS:CG	2.39	0.57
1:K:154:ALA:HB1	1:K:367:ILE:HD12	1.86	0.57
1:U:375:ARG:NH1	6:V:600:ANP:HNB1	2.02	0.57
1:L:187:ASN:O	1:L:190:ARG:HG3	2.05	0.57
1:U:51:ALA:O	1:U:52:GLU:HB2	2.05	0.57
3:G:95:VAL:O	3:G:99:LEU:HB3	2.05	0.56
4:H:29:GLN:O	4:H:60:MET:HB2	2.05	0.56
2:W:95:ILE:HB	2:W:104:ASP:HB3	1.86	0.56
1:K:236:ALA:HA	1:K:240:GLU:OE1	2.05	0.56
2:N:405:GLU:HG2	2:N:409:LYS:HE2	1.87	0.56
1:T:305:SER:HB2	2:X:222:MET:HB2	1.87	0.56
2:F:345:TYR:HA	2:F:346:PRO:C	2.25	0.56
2:N:381:TYR:O	2:N:385:GLN:HG2	2.04	0.56
2:N:85:VAL:HG11	2:N:235:THR:CG2	2.35	0.56
4:H:16:LEU:HD11	4:H:90:ALA:HB3	1.87	0.56
1:K:364:ARG:HA	1:K:365:PRO:C	2.25	0.56
1:S:249:PRO:HG2	1:S:276:GLN:NE2	2.21	0.56
2:V:346:PRO:O	2:V:347:ALA:HB3	2.04	0.56
1:A:270:TYR:O	1:A:272:ASP:HA	2.05	0.56
2:D:33:ILE:O	2:D:34:LEU:HB2	2.05	0.56
3:Y:79:SER:HB3	3:Y:88:HIS:CE1	2.39	0.56
1:B:147:PRO:HB2	1:B:149:GLN:NE2	2.19	0.56
1:K:99:VAL:HG11	1:K:251:THR:HB	1.87	0.56
2:O:206:VAL:HG12	2:O:215:VAL:HG12	1.88	0.56
2:N:84:SER:O	2:N:114:ARG:NH1	2.39	0.56
2:O:30:LEU:HD21	2:O:57:ASN:HA	1.88	0.56
3:P:40:SER:HB3	4:Q:17:PRO:O	2.06	0.56
1:B:395:PHE:HE1	1:B:419:THR:HG22	1.71	0.56
2:E:425:THR:HB	2:E:427:ILE:HD12	1.86	0.56
2:V:266:SER:N	2:V:282:GLN:HE21	2.02	0.56
1:B:139:LEU:HD22	2:F:104:ASP:HA	1.88	0.56
2:E:157:GLY:HA2	2:E:337:ARG:HH22	1.71	0.56
1:S:217:GLN:OE1	2:V:356:ARG:NH2	2.39	0.56
1:S:289:ARG:HE	2:W:17:ILE:HG22	1.70	0.56
3:P:168:ASP:N	3:P:176:GLU:O	2.28	0.56

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:68:LEU:O	2:O:15:ALA:HA	2.06	0.56
2:O:197:LEU:O	2:O:201:MET:HG2	2.06	0.56
1:B:166:ARG:HD3	1:B:311:ALA:HB3	1.87	0.55
2:D:50:VAL:HA	2:D:61:THR:HG22	1.86	0.55
1:K:138:ILE:H	1:K:138:ILE:CD1	2.20	0.55
2:M:170:LEU:O	2:M:174:ILE:HG12	2.07	0.55
1:U:166:ARG:CD	1:U:308:LEU:O	2.54	0.55
3:Y:9:ARG:HD3	3:Y:251:TYR:CE1	2.41	0.55
1:B:212:ARG:HG2	2:E:127:GLN:HG3	1.88	0.55
2:D:222:MET:HA	2:D:229:ARG:HD2	1.88	0.55
4:H:69:PHE:O	4:H:90:ALA:HA	2.06	0.55
2:N:32:ALA:O	2:N:35:ASN:HB2	2.07	0.55
3:P:180:LYS:HZ3	3:P:220:THR:HB	1.72	0.55
1:U:336:VAL:HG11	1:U:353:PHE:HE1	1.71	0.55
2:X:162:GLY:HA2	6:X:600:ANP:O1A	2.06	0.55
2:M:64:MET:CE	2:M:228:ALA:HA	2.37	0.55
2:W:41:THR:HB	2:W:42:PRO:CD	2.37	0.55
2:O:75:LYS:NZ	2:X:177:ALA:HB1	2.21	0.55
2:X:33:ILE:HG22	2:X:34:LEU:HG	1.87	0.55
1:A:309:GLU:HG3	2:E:223:ASN:HB3	1.88	0.55
2:O:204:THR:OG1	2:O:206:VAL:HG23	2.06	0.55
1:S:236:ALA:HB2	1:S:248:ALA:HB2	1.89	0.55
1:U:441:GLU:CG	1:U:486:ARG:HB2	2.36	0.55
1:A:462:ARG:HD2	1:A:465:GLU:OE2	2.06	0.55
2:D:339:ILE:HG22	2:D:344:ILE:HB	1.86	0.55
2:D:7:THR:HG23	2:D:7:THR:O	2.06	0.55
3:G:162:ILE:HB	3:G:182:ILE:HB	1.88	0.55
3:G:49:GLN:HA	3:G:52:TYR:HD1	1.72	0.55
1:U:68:LEU:HD13	1:U:73:VAL:HG13	1.88	0.55
1:C:309:GLU:HG3	2:D:223:ASN:HB3	1.87	0.55
2:E:175:ALA:O	2:E:179:GLY:HA2	2.07	0.55
1:K:220:GLN:HB2	2:N:129:THR:HB	1.87	0.55
1:T:70:PRO:HD3	2:X:15:ALA:HB2	1.87	0.55
1:J:212:ARG:HG3	1:J:237:THR:HG21	1.89	0.55
1:S:70:PRO:HD3	2:W:15:ALA:HB2	1.88	0.55
3:G:180:LYS:HE3	3:G:217:GLN:HB3	1.89	0.54
1:U:378:SER:HB2	1:U:386:LYS:HE2	1.90	0.54
2:O:75:LYS:HZ1	2:X:177:ALA:HB1	1.73	0.54
2:M:134:LEU:HD13	2:M:149:ARG:HH12	1.73	0.54
1:T:447:ILE:O	1:T:451:VAL:HG23	2.07	0.54
2:V:345:TYR:HA	2:V:347:ALA:N	2.22	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:253:LEU:HD23	2:V:296:ILE:HG23	1.89	0.54
1:U:475:LYS:HA	1:U:479:ASN:HD22	1.72	0.54
2:X:191:THR:HA	2:X:221:GLN:HG3	1.90	0.54
2:D:388:ILE:HG22	2:D:388:ILE:O	2.08	0.54
2:N:226:PRO:HB2	2:N:268:VAL:HG23	1.89	0.54
2:X:168:GLN:HA	2:X:171:ILE:HD12	1.89	0.54
2:X:442:LYS:HG2	2:X:446:GLU:OE2	2.07	0.54
1:B:357:GLU:HA	1:B:357:GLU:OE1	2.08	0.54
3:P:97:ARG:HA	3:P:100:ASN:HD22	1.72	0.54
3:P:233:ARG:O	3:P:237:MET:HG2	2.08	0.54
1:S:101:VAL:HG12	1:S:255:ILE:HG12	1.89	0.54
1:T:166:ARG:HH22	2:X:190:ARG:HD3	1.73	0.54
1:K:173:ARG:HG3	1:K:173:ARG:HH11	1.72	0.54
1:S:159:VAL:HG12	1:S:374:SER:HB2	1.90	0.54
2:X:367:HIS:HD2	2:X:367:HIS:O	1.91	0.54
1:T:138:ILE:CD1	2:X:95:ILE:HG21	2.38	0.54
1:J:77:LEU:CD1	1:J:81:ASP:HB3	2.37	0.54
1:K:154:ALA:CB	1:K:367:ILE:HD12	2.38	0.54
2:O:382:LYS:HA	2:O:385:GLN:HG2	1.88	0.54
2:X:133:ILE:HD12	2:X:133:ILE:H	1.73	0.54
1:B:203:CYS:HB2	1:B:231:SER:HB3	1.89	0.53
2:F:30:LEU:HD11	2:F:57:ASN:OD1	2.08	0.53
1:A:389:ALA:O	1:A:390:GLY:C	2.47	0.53
1:S:361:LYS:HE3	2:V:379:GLN:HG3	1.90	0.53
2:V:434:LEU:O	2:V:438:VAL:HG23	2.09	0.53
2:X:237:LEU:HD21	2:X:295:ARG:HB2	1.89	0.53
1:A:484:GLU:HG2	1:A:495:LEU:HD11	1.91	0.53
1:B:450:GLY:HA2	1:B:455:LEU:HD12	1.89	0.53
1:C:346:SER:HB3	2:D:260:ARG:HH22	1.74	0.53
1:S:89:LEU:HG	1:S:90:VAL:N	2.23	0.53
1:T:344:VAL:HA	1:T:347:ILE:HD12	1.90	0.53
1:S:332:GLN:HB3	2:V:318:THR:HB	1.90	0.53
2:W:133:ILE:HD12	2:W:146:PRO:HB2	1.89	0.53
1:L:222:LEU:CB	1:L:228:MET:HE2	2.38	0.53
1:L:99:VAL:HG11	1:L:251:THR:HB	1.90	0.53
1:T:301:PHE:HB3	2:X:263:GLN:HE22	1.73	0.53
3:G:184:ASN:HA	3:G:210:PHE:CD1	2.44	0.53
4:H:13:GLN:HG2	4:H:23:SER:HA	1.89	0.53
1:T:103:PRO:HD3	1:T:258:TRP:CH2	2.43	0.53
1:U:117:ILE:HD11	1:U:235:ALA:HB3	1.91	0.53
2:W:109:ILE:HG22	2:W:111:SER:HB2	1.90	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:436:ASP:O	2:M:440:SER:N	2.38	0.53
2:M:90:GLU:HG3	2:M:111:SER:HB3	1.89	0.53
1:S:200:LYS:HD2	1:S:202:TYR:OH	2.08	0.53
2:W:35:ASN:O	2:W:50:VAL:HG23	2.09	0.53
2:D:89:ARG:NH1	2:D:247:GLU:OE2	2.41	0.53
3:G:87:ILE:HG23	3:G:167:ASN:HD22	1.73	0.53
2:M:406:ARG:HH21	2:M:447:GLY:HA3	1.74	0.53
1:T:100:PRO:HB3	1:T:125:ALA:HB2	1.90	0.53
1:T:337:SER:O	2:X:314:ALA:HA	2.09	0.53
1:S:50:GLN:HG2	2:W:71:VAL:HG22	1.91	0.53
2:V:266:SER:HA	2:V:282:GLN:HG3	1.90	0.53
2:W:127:GLN:HE22	2:W:297:THR:HG21	1.74	0.53
1:T:35:ALA:HB1	2:W:53:HIS:O	2.09	0.53
4:H:57:VAL:O	4:H:67:LYS:HA	2.08	0.52
2:M:136:THR:HB	2:M:138:ILE:HD12	1.91	0.52
2:N:237:LEU:HD22	2:N:292:LEU:HD12	1.91	0.52
1:S:169:ILE:HD11	1:S:326:LEU:HB3	1.90	0.52
1:A:54:LEU:HD13	1:A:97:VAL:HG22	1.91	0.52
1:K:250:PHE:HZ	1:K:303:LEU:HD12	1.75	0.52
2:W:406:ARG:NH1	2:W:447:GLY:HA2	2.25	0.52
2:E:158:GLY:H	2:E:337:ARG:HH12	1.56	0.52
1:K:29:GLU:OE2	1:K:92:ARG:NH1	2.42	0.52
2:N:243:PHE:HB2	2:N:251:VAL:HG21	1.92	0.52
1:S:249:PRO:HG2	1:S:276:GLN:HE21	1.75	0.52
1:A:444:VAL:HG22	1:A:445:PRO:CD	2.37	0.52
1:A:500:LYS:O	1:A:504:GLU:HG3	2.09	0.52
2:M:15:ALA:HB3	2:M:22:ASP:HB2	1.90	0.52
1:T:102:GLY:HA2	1:T:258:TRP:CE2	2.44	0.52
3:G:259:ARG:HD2	9:G:279:HOH:O	2.10	0.52
2:M:25:PHE:HB2	2:M:30:LEU:CD2	2.34	0.52
1:S:298:GLY:HA3	2:W:271:LEU:HG	1.92	0.52
3:P:72:GLU:HG3	3:P:161:LYS:HB3	1.91	0.52
1:T:340:ILE:HB	1:T:341:PRO:HD3	1.92	0.52
2:D:206:VAL:HG12	2:D:215:VAL:HG12	1.90	0.52
1:L:236:ALA:HA	1:L:240:GLU:OE2	2.10	0.52
1:S:174:GLN:HB3	2:V:354:LYS:HD3	1.92	0.52
3:G:89:SER:HA	3:G:117:GLN:NE2	2.22	0.52
1:T:166:ARG:O	1:T:348:THR:HB	2.10	0.52
3:G:139:THR:HG21	5:I:37:ARG:HA	1.91	0.52
1:S:293:ARG:O	1:S:294:GLU:HB2	2.09	0.52
2:V:164:THR:O	2:V:167:ILE:HG22	2.10	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:VAL:HA	1:B:159:VAL:HG23	1.92	0.51
1:L:50:GLN:HB3	2:M:69:GLY:HA2	1.92	0.51
1:C:28:ASN:HA	1:C:47:ASN:HB2	1.92	0.51
1:T:138:ILE:CD1	2:X:95:ILE:HD13	2.39	0.51
1:A:85:LYS:HG2	2:D:53:HIS:HE1	1.75	0.51
2:E:403:THR:O	2:E:407:ALA:N	2.43	0.51
2:E:169:GLU:OE1	2:E:420:VAL:HG22	2.09	0.51
2:F:189:GLU:O	2:F:221:GLN:HB3	2.09	0.51
1:J:302:TYR:O	1:J:306:ARG:HB2	2.10	0.51
1:K:166:ARG:HG3	1:K:325:ALA:HB3	1.92	0.51
1:K:370:GLY:H	1:K:400:ARG:NH1	2.09	0.51
1:L:151:GLY:HA3	1:L:437:PRO:HB2	1.93	0.51
1:A:39:GLY:HA2	1:A:77:LEU:HD12	1.90	0.51
1:B:202:TYR:O	1:B:266:ALA:HA	2.10	0.51
1:C:174:GLN:HB3	2:F:354:LYS:HD3	1.92	0.51
1:C:166:ARG:HD3	1:C:311:ALA:HB3	1.91	0.51
2:E:349:ASP:HB3	2:E:352:ASP:HB2	1.92	0.51
1:S:152:LEU:HA	1:S:432:GLN:OE1	2.09	0.51
1:T:349:ASP:HA	1:T:375:ARG:HD2	1.91	0.51
1:T:507:VAL:HG12	1:T:508:ALA:N	2.26	0.51
1:U:336:VAL:HG11	1:U:353:PHE:CE1	2.46	0.51
1:B:160:PRO:O	1:B:377:GLY:HA3	2.09	0.51
2:O:345:TYR:HA	2:O:346:PRO:C	2.31	0.51
2:W:410:ILE:HG23	2:W:441:PHE:HE2	1.75	0.51
1:A:173:ARG:NH2	2:D:352:ASP:OD1	2.44	0.51
2:E:37:LEU:HD12	2:E:61:THR:HG21	1.93	0.51
1:J:223:GLU:HG3	1:J:228:MET:HG3	1.93	0.51
1:U:399:TYR:OH	1:U:424:GLU:HG3	2.10	0.51
2:W:321:ALA:HB3	2:W:322:PRO:CD	2.40	0.51
2:W:469:LYS:O	2:W:473:LEU:HG	2.10	0.51
2:V:20:ILE:HG13	2:V:271:LEU:HB2	1.93	0.51
2:D:363:VAL:HB	2:D:367:HIS:CD2	2.45	0.51
1:J:77:LEU:HD12	1:J:81:ASP:HB3	1.92	0.51
1:K:435:TYR:C	1:K:437:PRO:HD3	2.30	0.51
1:S:159:VAL:CG1	1:S:374:SER:HB2	2.41	0.51
1:C:344:VAL:HA	1:C:347:ILE:HD12	1.93	0.51
2:E:470:ALA:HA	2:E:473:LEU:HD12	1.93	0.51
3:G:204:ASN:N	3:G:204:ASN:OD1	2.42	0.51
1:S:144:VAL:HG11	1:S:162:GLY:HA3	1.91	0.51
1:U:139:LEU:C	1:U:141:ARG:H	2.14	0.51
1:U:152:LEU:HA	1:U:432:GLN:OE1	2.11	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:475:LYS:O	1:B:479:ASN:HB2	2.12	0.51
1:S:384:ALA:O	1:S:491:LEU:HD12	2.11	0.51
1:U:375:ARG:CZ	6:V:600:ANP:HNB1	2.24	0.51
2:X:157:GLY:O	2:X:163:LYS:HD3	2.11	0.51
2:D:104:ASP:O	2:D:106:ARG:HG3	2.12	0.50
2:N:201:MET:HG2	2:N:206:VAL:CG2	2.41	0.50
1:S:82:ARG:HB2	2:V:34:LEU:HD12	1.93	0.50
2:V:98:VAL:HG13	2:V:99:ILE:HG23	1.91	0.50
1:A:402:VAL:O	1:A:405:SER:HB2	2.11	0.50
2:F:298:THR:HG23	2:F:303:SER:HA	1.92	0.50
1:T:99:VAL:HG11	1:T:251:THR:HB	1.93	0.50
3:G:253:ILE:HG22	3:G:257:ARG:NH1	2.26	0.50
1:K:219:VAL:HG22	1:K:233:ILE:HG13	1.93	0.50
1:L:150:THR:HG21	1:L:155:VAL:HG11	1.92	0.50
1:T:444:VAL:HG22	1:T:445:PRO:HD3	1.93	0.50
1:U:164:GLY:N	1:U:324:THR:OG1	2.43	0.50
2:D:279:VAL:HG12	2:D:279:VAL:O	2.11	0.50
2:E:30:LEU:HD21	2:E:57:ASN:HA	1.93	0.50
3:G:161:LYS:HE2	3:G:163:SER:OG	2.11	0.50
1:K:158:LEU:HD21	1:K:392:LEU:HG	1.93	0.50
2:O:140:VAL:HG13	2:O:414:LEU:HB3	1.94	0.50
1:U:97:VAL:HG11	1:U:247:LEU:HD21	1.93	0.50
3:G:247:MET:HG2	3:G:250:ARG:NH2	2.26	0.50
1:K:138:ILE:CD1	1:K:138:ILE:N	2.75	0.50
2:O:14:THR:HG21	2:O:24:HIS:HB2	1.92	0.50
2:X:256:ASP:HA	2:X:309:ALA:HB3	1.93	0.50
2:D:90:GLU:HG3	2:D:110:LYS:O	2.11	0.50
2:E:374:VAL:HG13	2:E:410:ILE:HG21	1.93	0.50
1:S:211:LYS:HE3	1:S:214:THR:OG1	2.11	0.50
1:S:277:ALA:HB2	1:S:304:HIS:HE1	1.77	0.50
1:S:385:LEU:HD11	1:S:447:ILE:HD12	1.92	0.50
1:S:446:LEU:HD21	1:S:467:GLU:HA	1.94	0.50
1:C:109:VAL:HG13	1:C:233:ILE:HB	1.94	0.50
2:F:442:LYS:HG2	2:F:446:GLU:OE2	2.11	0.50
2:M:381:TYR:O	2:M:385:GLN:HG3	2.12	0.50
2:N:85:VAL:HG13	2:N:235:THR:HG23	1.92	0.50
2:D:208:ASN:ND2	2:D:211:GLY:HA3	2.27	0.50
2:E:109:ILE:C	2:E:111:SER:H	2.14	0.50
1:L:375:ARG:HH11	6:M:600:ANP:C5'	2.24	0.50
2:O:384:LEU:O	2:O:388:ILE:HG12	2.12	0.50
1:S:101:VAL:HA	1:S:105:LEU:HD11	1.93	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:28:SER:O	3:Y:31:LEU:HB3	2.12	0.50
1:A:239:SER:HB3	2:D:294:GLU:HG3	1.94	0.50
1:J:399:TYR:CD1	1:J:423:GLY:HA3	2.46	0.50
2:M:377:THR:HG22	2:M:407:ALA:HB2	1.94	0.50
3:Y:89:SER:HA	3:Y:117:GLN:HE21	1.77	0.50
1:C:203:CYS:O	1:C:231:SER:HA	2.12	0.49
1:K:30:THR:HG23	2:X:464:GLU:OE2	2.12	0.49
2:M:143:LEU:O	2:M:367:HIS:HE1	1.95	0.49
1:S:165:GLN:NE2	1:S:374:SER:OG	2.44	0.49
1:T:283:LEU:O	1:T:287:LEU:HD12	2.12	0.49
1:T:166:ARG:NH2	2:X:190:ARG:HD3	2.27	0.49
1:A:405:SER:C	1:A:407:GLN:H	2.16	0.49
1:B:429:LEU:HD21	1:B:446:LEU:O	2.12	0.49
1:K:166:ARG:CD	1:K:311:ALA:HB3	2.42	0.49
2:N:224:GLU:O	2:N:229:ARG:NH1	2.41	0.49
1:B:248:ALA:HB3	1:B:249:PRO:HD3	1.94	0.49
2:E:425:THR:HB	2:E:427:ILE:CD1	2.42	0.49
2:F:96:ILE:HG22	2:F:97:ASN:N	2.27	0.49
2:M:97:ASN:C	2:M:97:ASN:OD1	2.51	0.49
2:D:15:ALA:HB3	2:D:22:ASP:HB2	1.94	0.49
2:E:15:ALA:HB3	2:E:22:ASP:HB2	1.94	0.49
2:M:335:LEU:HA	2:M:347:ALA:O	2.12	0.49
2:O:140:VAL:CG1	2:O:414:LEU:HD22	2.42	0.49
1:T:208:VAL:HG21	1:T:249:PRO:HD3	1.94	0.49
3:G:77:ILE:HG12	3:G:165:PHE:O	2.12	0.49
4:H:131:GLU:HA	4:H:134:GLN:HE21	1.77	0.49
1:L:331:THR:HG21	1:L:336:VAL:HG12	1.95	0.49
3:P:107:ILE:HG13	3:P:126:ILE:HA	1.94	0.49
2:W:53:HIS:CD2	2:W:59:VAL:HG12	2.47	0.49
2:F:15:ALA:HB3	2:F:22:ASP:HB2	1.95	0.49
3:G:149:LYS:HA	3:G:152:SER:HB2	1.94	0.49
1:T:421:VAL:O	1:T:425:ARG:HG2	2.13	0.49
1:C:77:LEU:HD12	1:C:81:ASP:HB3	1.95	0.49
2:E:98:VAL:HG23	2:E:232:VAL:HA	1.93	0.49
1:S:99:VAL:HG21	1:S:251:THR:HG23	1.95	0.49
1:U:68:LEU:HB2	2:V:16:VAL:HG23	1.95	0.49
2:W:242:TYR:CE1	2:W:246:GLU:HG3	2.47	0.49
1:A:197:GLU:HA	1:A:200:LYS:HD2	1.95	0.49
1:A:364:ARG:HA	1:A:365:PRO:C	2.33	0.49
4:H:35:LYS:H	4:H:35:LYS:HD3	1.77	0.49
1:K:138:ILE:O	2:O:195:ASN:ND2	2.45	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:387:ILE:HG23	2:M:391:LEU:HD12	1.94	0.49
3:P:212:TYR:O	3:P:216:ASN:HB2	2.13	0.49
1:U:332:GLN:HB3	2:X:318:THR:HG21	1.94	0.49
2:X:344:ILE:HG23	2:X:415:SER:HB3	1.94	0.49
3:G:42:LYS:O	3:G:46:GLU:HG2	2.13	0.49
3:P:267:LEU:O	3:P:271:ILE:HD12	2.13	0.49
3:P:74:ILE:HG23	3:P:165:PHE:CD2	2.47	0.49
1:S:347:ILE:HA	2:W:222:MET:SD	2.53	0.49
2:X:52:GLN:HE22	2:X:60:ARG:HH11	1.61	0.49
2:M:138:ILE:HG12	2:M:418:PHE:CE1	2.47	0.48
1:T:444:VAL:CG2	1:T:445:PRO:HD3	2.41	0.48
1:C:232:ILE:HD13	1:C:255:ILE:CG2	2.42	0.48
2:D:176:LYS:HD3	2:D:204:THR:CG2	2.40	0.48
1:K:155:VAL:HA	1:K:159:VAL:HG23	1.95	0.48
1:K:455:LEU:HA	1:K:458:ILE:HD12	1.94	0.48
1:A:158:LEU:HD21	1:A:392:LEU:HG	1.94	0.48
1:C:222:LEU:HB2	1:C:228:MET:HE2	1.94	0.48
2:E:396:LEU:HB3	2:E:401:LYS:HB3	1.95	0.48
1:S:145:HIS:H	1:S:313:LYS:HZ3	1.62	0.48
1:S:429:LEU:HD11	1:S:455:LEU:HD12	1.95	0.48
1:S:166:ARG:NH2	2:W:190:ARG:HD3	2.27	0.48
1:B:220:GLN:HG3	1:B:224:GLN:NE2	2.29	0.48
2:D:190:ARG:O	2:D:193:GLU:HB2	2.13	0.48
2:D:345:TYR:HA	2:D:346:PRO:C	2.33	0.48
2:E:185:THR:HG21	2:E:233:ALA:HA	1.96	0.48
3:G:34:ALA:HB2	3:G:226:TYR:HE2	1.79	0.48
3:P:86:SER:HB2	3:P:90:GLN:HG3	1.96	0.48
1:U:455:LEU:HD22	1:U:463:ILE:HD12	1.96	0.48
2:X:218:VAL:HG21	2:X:236:GLY:CA	2.43	0.48
1:C:145:HIS:HA	1:C:379:ALA:O	2.13	0.48
2:D:64:MET:CE	2:D:228:ALA:HA	2.43	0.48
2:X:52:GLN:HE22	2:X:60:ARG:NH1	2.11	0.48
1:A:455:LEU:HD21	1:A:466:PHE:CE1	2.48	0.48
1:B:384:ALA:HB1	1:B:444:VAL:HG11	1.96	0.48
1:S:106:LEU:HD21	1:S:259:PHE:CZ	2.49	0.48
1:T:43:VAL:HG21	1:T:75:ILE:HD12	1.95	0.48
1:B:335:ASP:HB2	3:G:257:ARG:NH1	2.29	0.48
1:K:285:LEU:CD1	2:N:277:SER:HB3	2.44	0.48
2:O:237:LEU:O	2:O:237:LEU:HD12	2.14	0.48
2:O:432:VAL:HG12	2:O:433:ARG:H	1.79	0.48
1:K:50:GLN:HB3	2:O:69:GLY:HA2	1.95	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:153:LYS:HG2	1:S:443:GLN:HG2	1.96	0.48
1:U:392:LEU:HD13	1:U:451:VAL:HG22	1.96	0.48
2:V:293:GLN:HA	2:V:296:ILE:HD12	1.96	0.48
1:C:99:VAL:HG11	1:C:251:THR:HB	1.96	0.48
2:V:157:GLY:HA3	2:V:161:VAL:HG21	1.94	0.48
2:V:279:VAL:HG12	2:V:279:VAL:O	2.14	0.48
1:U:332:GLN:HB3	2:X:318:THR:CG2	2.44	0.48
1:A:484:GLU:HB3	1:A:495:LEU:HD21	1.95	0.47
1:L:211:LYS:HD3	2:O:328:HIS:HA	1.95	0.47
2:V:391:LEU:HG	3:Y:19:ILE:HD11	1.96	0.47
1:U:282:GLN:CD	2:X:284:THR:HA	2.34	0.47
1:J:202:TYR:O	1:J:266:ALA:HA	2.14	0.47
1:L:55:VAL:HG21	1:L:75:ILE:HD13	1.96	0.47
1:T:86:GLU:HB3	2:W:30:LEU:HD13	1.95	0.47
1:B:187:ASN:OD1	1:B:437:PRO:HB2	2.14	0.47
3:G:213:THR:CG2	3:G:217:GLN:HE21	2.26	0.47
2:N:279:VAL:HG12	2:N:279:VAL:O	2.14	0.47
1:K:291:PRO:HG2	3:P:268:VAL:HG22	1.97	0.47
6:S:600:ANP:O2A	6:S:600:ANP:N3B	2.46	0.47
1:U:428:GLN:HA	1:U:431:LYS:HE3	1.96	0.47
2:X:224:GLU:HB3	2:X:228:ALA:HB3	1.96	0.47
1:A:260:ARG:O	1:A:321:GLY:HA3	2.14	0.47
3:G:110:ILE:HD11	3:G:146:ILE:HG21	1.96	0.47
1:J:139:LEU:HD13	2:N:104:ASP:HA	1.97	0.47
1:U:293:ARG:HB3	1:U:339:TYR:CE2	2.48	0.47
1:B:444:VAL:N	1:B:445:PRO:CD	2.77	0.47
2:D:190:ARG:HB2	2:D:193:GLU:HG3	1.96	0.47
2:D:258:ILE:HD11	2:D:292:LEU:CD2	2.44	0.47
1:J:424:GLU:HB3	1:J:460:LEU:CD1	2.45	0.47
1:L:375:ARG:NH1	6:M:600:ANP:H5'1	2.30	0.47
2:N:68:GLU:CD	2:N:68:GLU:H	2.17	0.47
2:O:9:ILE:HB	2:O:78:ASP:HB3	1.95	0.47
3:P:166:TYR:HE1	3:P:180:LYS:HG2	1.80	0.47
1:S:146:GLU:H	1:S:313:LYS:HZ3	1.62	0.47
1:T:270:TYR:O	1:T:272:ASP:HA	2.15	0.47
1:U:290:PRO:HA	1:U:291:PRO:HD3	1.80	0.47
1:U:296:TYR:CD2	1:U:300:VAL:HG21	2.50	0.47
2:V:240:ALA:HB2	2:V:253:LEU:HD13	1.96	0.47
2:V:346:PRO:O	2:V:347:ALA:CB	2.62	0.47
2:W:140:VAL:HG22	2:W:414:LEU:O	2.15	0.47
2:X:163:LYS:H	6:X:600:ANP:PB	2.38	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:344:ILE:HG23	2:D:415:SER:HB3	1.97	0.47
3:G:55:ALA:HA	3:G:193:SER:HB2	1.96	0.47
2:O:67:THR:HB	2:O:70:LEU:HD12	1.96	0.47
1:T:338:ALA:HB3	1:T:341:PRO:HG2	1.96	0.47
1:T:474:LEU:HD13	1:T:482:LEU:HD21	1.97	0.47
1:S:174:GLN:HB3	2:V:354:LYS:CD	2.44	0.47
2:X:217:LEU:HB3	2:X:219:PHE:HE2	1.79	0.47
1:J:43:VAL:HG21	1:J:75:ILE:HD12	1.97	0.47
1:K:174:GLN:HA	6:K:600:ANP:HNB1	1.80	0.47
2:M:96:ILE:HG22	2:M:97:ASN:O	2.15	0.47
2:N:152:LYS:HE3	2:N:296:ILE:HB	1.97	0.47
3:P:227:ALA:HA	3:P:230:ILE:HG22	1.96	0.47
1:S:32:ARG:HD2	1:S:89:LEU:HD12	1.96	0.47
2:V:346:PRO:HG3	2:V:418:PHE:CZ	2.50	0.47
2:X:321:ALA:CB	2:X:322:PRO:CD	2.92	0.47
2:X:65:ASP:CG	2:X:66:GLY:H	2.18	0.47
2:M:64:MET:HE1	2:M:228:ALA:HA	1.97	0.47
1:T:52:GLU:HA	1:T:65:ALA:O	2.14	0.47
2:V:97:ASN:ND2	2:V:101:GLU:HB2	2.27	0.47
1:A:396:LEU:O	1:A:400:ARG:HG3	2.15	0.47
2:N:30:LEU:HD22	2:N:59:VAL:HG13	1.97	0.47
1:S:232:ILE:HG21	1:S:255:ILE:HG21	1.96	0.47
1:S:382:VAL:HG11	1:S:440:THR:HG21	1.97	0.47
2:V:191:THR:HA	2:V:221:GLN:HG3	1.96	0.47
1:J:397:ALA:HA	1:J:400:ARG:NH2	2.30	0.47
2:M:198:TYR:CZ	2:M:202:LYS:HE2	2.50	0.47
1:T:474:LEU:HB3	1:T:482:LEU:HD11	1.96	0.47
1:T:174:GLN:HA	6:T:600:ANP:HNB1	1.80	0.47
2:V:189:GLU:HG2	2:V:256:ASP:O	2.15	0.47
1:U:394:LEU:HD11	2:V:458:TYR:OH	2.15	0.47
2:W:220:GLY:HA3	2:W:232:VAL:HG21	1.97	0.47
1:A:77:LEU:CD1	1:A:81:ASP:HB3	2.44	0.47
2:D:62:ILE:HD11	2:D:272:LEU:HD11	1.96	0.47
2:E:30:LEU:HA	2:E:31:PRO:HD2	1.72	0.47
2:M:132:GLU:HG2	2:M:149:ARG:HG3	1.97	0.47
2:N:471:GLU:HA	2:N:474:ALA:HB2	1.97	0.47
3:P:17:GLU:HB2	3:P:244:ALA:HB1	1.97	0.47
1:S:452:ASN:HB3	1:S:454:HIS:HE1	1.80	0.47
1:S:32:ARG:HH11	1:S:89:LEU:HB2	1.79	0.46
1:U:166:ARG:HD3	1:U:311:ALA:HB3	1.96	0.46
1:U:260:ARG:NH1	1:U:310:ARG:O	2.49	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:LEU:HD23	1:A:458:ILE:HD12	1.98	0.46
1:A:96:ILE:CG2	2:E:68:GLU:OE2	2.63	0.46
2:F:182:SER:O	2:F:215:VAL:HA	2.15	0.46
2:N:133:ILE:HD12	2:N:146:PRO:HB2	1.97	0.46
1:S:179:ALA:CB	6:S:600:ANP:H8	2.45	0.46
1:S:491:LEU:HD23	1:S:495:LEU:HB3	1.96	0.46
2:N:150:GLY:HA2	2:N:304:VAL:O	2.15	0.46
1:T:166:ARG:HG2	1:T:311:ALA:HB3	1.96	0.46
2:V:346:PRO:HB2	2:V:348:VAL:HG23	1.97	0.46
2:W:95:ILE:HD11	2:W:198:TYR:CD1	2.50	0.46
2:X:178:HIS:NE2	2:X:250:ASP:O	2.48	0.46
2:X:217:LEU:HB3	2:X:219:PHE:CE2	2.50	0.46
2:X:360:ALA:O	2:X:364:GLY:N	2.46	0.46
1:A:169:ILE:HD11	1:A:326:LEU:HD13	1.97	0.46
1:A:338:ALA:HB3	1:A:341:PRO:HD2	1.98	0.46
2:F:171:ILE:O	2:F:175:ALA:HB3	2.16	0.46
1:J:428:GLN:HA	1:J:431:LYS:HG3	1.97	0.46
1:T:160:PRO:O	1:T:377:GLY:HA3	2.16	0.46
1:U:252:ALA:HA	1:U:255:ILE:HD12	1.98	0.46
2:W:135:GLU:OE2	2:W:433:ARG:HD3	2.16	0.46
2:X:279:VAL:O	2:X:279:VAL:HG12	2.15	0.46
2:F:321:ALA:HB3	2:F:322:PRO:CD	2.46	0.46
1:K:142:ARG:HG2	1:K:143:SER:N	2.30	0.46
1:K:160:PRO:O	1:K:377:GLY:HA3	2.15	0.46
2:M:449:TYR:HD1	2:M:452:ILE:CD1	2.28	0.46
2:M:30:LEU:HD22	2:M:59:VAL:HG13	1.97	0.46
1:S:54:LEU:HD13	1:S:97:VAL:HG22	1.98	0.46
1:U:291:PRO:HD2	3:Y:273:GLY:HA2	1.98	0.46
2:D:167:ILE:HA	2:D:170:LEU:HD12	1.98	0.46
4:H:112:VAL:C	4:H:114:SER:HB3	2.36	0.46
1:U:153:LYS:HA	1:U:443:GLN:OE1	2.15	0.46
2:W:296:ILE:HG21	2:W:306:SER:HB2	1.98	0.46
1:A:405:SER:O	1:A:407:GLN:N	2.49	0.46
1:B:364:ARG:HA	1:B:365:PRO:C	2.35	0.46
3:P:180:LYS:HZ1	3:P:220:THR:HB	1.78	0.46
1:S:138:ILE:HD12	2:W:194:GLY:HA3	1.96	0.46
1:T:185:ILE:HG12	1:T:203:CYS:SG	2.56	0.46
1:A:211:LYS:HE3	1:A:213:SER:OG	2.16	0.46
1:B:187:ASN:OD1	1:B:190:ARG:NH1	2.49	0.46
1:B:270:TYR:O	1:B:272:ASP:HA	2.15	0.46
1:A:96:ILE:HG21	2:E:68:GLU:CD	2.36	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:GLU:HB2	2:E:68:GLU:HG3	1.98	0.46
1:A:96:ILE:HG21	2:E:68:GLU:OE2	2.16	0.46
1:J:270:TYR:O	1:J:272:ASP:HA	2.16	0.46
2:M:337:ARG:HG2	2:M:341:GLU:OE2	2.16	0.46
2:M:30:LEU:HD11	2:M:57:ASN:HA	1.98	0.46
1:T:35:ALA:HB3	1:T:42:ARG:HH12	1.80	0.46
1:U:166:ARG:HD2	1:U:308:LEU:HB3	1.97	0.46
1:U:368:ASN:ND2	1:U:371:LEU:HD12	2.31	0.46
1:A:192:ASN:HA	1:A:200:LYS:HG2	1.97	0.46
1:B:421:VAL:HG13	1:B:425:ARG:HH12	1.81	0.46
1:A:407:GLN:HE21	2:D:384:LEU:HD21	1.81	0.46
1:K:242:ALA:N	1:K:243:PRO:CD	2.79	0.46
1:L:455:LEU:HA	1:L:458:ILE:HD12	1.98	0.46
3:P:171:SER:HG	3:P:174:SER:N	2.13	0.46
3:P:17:GLU:HB2	3:P:244:ALA:CB	2.46	0.46
1:T:139:LEU:HB3	1:T:140:PRO:HD3	1.97	0.46
1:T:345:ILE:HG22	2:X:159:ALA:HB1	1.97	0.46
1:U:349:ASP:HB3	2:V:192:ARG:HH21	1.80	0.46
2:W:321:ALA:HB3	2:W:322:PRO:HD3	1.97	0.46
2:X:13:VAL:O	2:X:73:GLY:N	2.47	0.46
2:D:299:THR:OG1	2:D:300:LYS:N	2.49	0.46
2:E:41:THR:HB	2:E:42:PRO:HD2	1.98	0.46
2:F:257:ASN:HD21	2:F:311:TYR:N	2.14	0.46
1:J:166:ARG:HD2	1:J:308:LEU:O	2.16	0.46
1:J:46:LEU:O	1:J:49:ILE:HG22	2.16	0.46
1:K:363:ILE:HA	1:K:431:LYS:HE2	1.98	0.46
2:M:90:GLU:CG	2:M:111:SER:HB3	2.45	0.46
3:P:77:ILE:HD13	3:P:222:MET:HG3	1.97	0.46
1:S:223:GLU:HG3	1:S:228:MET:HG3	1.98	0.46
1:S:77:LEU:O	1:S:243:PRO:HG2	2.16	0.46
1:T:138:ILE:HD12	2:X:95:ILE:HD13	1.97	0.46
1:U:177:LYS:NZ	6:U:600:ANP:O1B	2.43	0.46
2:V:134:LEU:HB2	2:V:149:ARG:HG3	1.98	0.46
2:X:312:VAL:HG11	2:X:317:LEU:HD23	1.98	0.46
1:K:243:PRO:HA	1:K:246:TYR:HD2	1.81	0.45
3:P:77:ILE:HG21	3:P:222:MET:HG2	1.98	0.45
1:U:344:VAL:O	1:U:348:THR:HG23	2.16	0.45
2:X:43:GLN:HA	2:X:43:GLN:HE21	1.82	0.45
1:B:86:GLU:HB3	2:E:30:LEU:HD13	1.98	0.45
1:L:363:ILE:O	1:L:366:ALA:HA	2.15	0.45
2:N:310:VAL:HG11	2:N:326:PHE:CE1	2.49	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:133:ILE:HD11	2:O:362:VAL:HG12	1.98	0.45
2:O:33:ILE:O	2:O:34:LEU:HB2	2.16	0.45
1:T:273:LEU:HD22	1:T:304:HIS:CD2	2.51	0.45
2:D:140:VAL:HG23	2:D:414:LEU:HD22	1.97	0.45
2:E:396:LEU:HD13	2:E:401:LYS:HA	1.98	0.45
2:O:182:SER:O	2:O:215:VAL:HA	2.16	0.45
1:S:82:ARG:HH11	2:V:34:LEU:HB2	1.81	0.45
1:C:165:GLN:HG3	1:C:349:ASP:HB2	1.98	0.45
1:C:211:LYS:HE3	1:C:213:SER:OG	2.16	0.45
2:E:140:VAL:HG13	2:E:414:LEU:HB3	1.98	0.45
1:T:309:GLU:CG	2:X:222:MET:HG3	2.47	0.45
1:U:107:GLY:HA2	1:U:228:MET:HG3	1.99	0.45
1:B:103:PRO:HD3	1:B:258:TRP:CH2	2.51	0.45
1:K:283:LEU:CD2	1:K:287:LEU:HD12	2.46	0.45
1:L:375:ARG:HH11	6:M:600:ANP:H5'2	1.81	0.45
1:S:168:LEU:HB2	1:S:348:THR:HG21	1.98	0.45
1:U:201:LEU:HA	1:U:265:HIS:O	2.16	0.45
2:W:34:LEU:H	2:W:50:VAL:HB	1.80	0.45
1:U:282:GLN:OE1	2:X:284:THR:HA	2.16	0.45
1:U:239:SER:HB3	2:X:290:GLY:O	2.16	0.45
1:C:329:ILE:HA	1:C:329:ILE:HD13	1.88	0.45
2:D:168:GLN:HB3	2:D:420:VAL:HG11	1.98	0.45
2:F:159:ALA:HA	6:F:600:ANP:O1G	2.16	0.45
3:G:23:MET:O	3:G:27:ALA:HB2	2.17	0.45
1:J:353:PHE:CE2	1:J:355:GLU:HG3	2.51	0.45
1:K:283:LEU:CD2	1:K:287:LEU:CD1	2.95	0.45
2:M:90:GLU:CG	2:M:111:SER:CB	2.93	0.45
1:S:201:LEU:HA	1:S:265:HIS:O	2.17	0.45
1:J:421:VAL:O	1:J:425:ARG:HD2	2.17	0.45
1:L:357:GLU:OE2	1:L:361:LYS:NZ	2.47	0.45
2:N:317:LEU:HD22	2:N:326:PHE:HE2	1.81	0.45
2:W:33:ILE:O	2:W:34:LEU:HB2	2.16	0.45
1:C:364:ARG:HA	1:C:365:PRO:C	2.37	0.45
1:C:92:ARG:NH2	1:C:94:GLY:HA2	2.26	0.45
2:D:96:ILE:O	2:D:218:VAL:HA	2.16	0.45
1:J:167:GLU:O	1:J:326:LEU:HA	2.16	0.45
2:N:242:TYR:CE1	2:N:246:GLU:HG3	2.51	0.45
1:U:176:GLY:HA2	6:U:600:ANP:PA	2.57	0.45
1:U:206:VAL:HG11	1:U:249:PRO:HA	1.98	0.45
1:U:339:TYR:HE1	1:U:343:ASN:HD21	1.65	0.45
1:U:375:ARG:NH1	6:V:600:ANP:N3B	2.65	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:PHE:O	1:A:509:THR:HG22	2.17	0.45
1:B:471:LEU:O	1:B:475:LYS:HG3	2.17	0.45
3:G:87:ILE:HG23	3:G:167:ASN:ND2	2.31	0.45
1:L:478:HIS:HB3	1:L:481:LEU:HB2	1.99	0.45
3:P:74:ILE:HG21	3:P:95:VAL:HG13	1.99	0.45
1:S:109:VAL:HG22	1:S:233:ILE:HB	1.99	0.45
1:T:503:THR:O	1:T:507:VAL:HG23	2.16	0.45
2:V:33:ILE:O	2:V:34:LEU:HB2	2.17	0.45
1:A:203:CYS:O	1:A:231:SER:HA	2.17	0.45
1:L:248:ALA:HB3	1:L:249:PRO:HD3	1.99	0.45
1:S:165:GLN:NE2	1:S:167:GLU:OE1	2.50	0.45
1:T:375:ARG:NH2	2:X:160:GLY:HA2	2.32	0.45
1:U:139:LEU:O	1:U:141:ARG:N	2.47	0.45
2:X:359:ASP:O	2:X:363:VAL:HG22	2.17	0.45
1:L:252:ALA:HA	1:L:255:ILE:HD12	1.99	0.44
2:V:197:LEU:HA	2:V:200:GLU:HG2	2.00	0.44
1:C:174:GLN:CB	2:F:354:LYS:HD3	2.48	0.44
1:K:400:ARG:HA	1:K:403:ALA:HB3	1.99	0.44
2:M:93:GLY:HA2	2:M:207:ILE:HG12	1.99	0.44
3:P:204:ASN:C	3:P:206:PRO:HD2	2.38	0.44
1:U:69:GLU:CB	1:U:70:PRO:HD2	2.36	0.44
1:A:98:ASP:HA	1:A:130:ARG:HA	2.00	0.44
2:D:201:MET:CE	2:D:217:LEU:HD21	2.48	0.44
2:F:359:ASP:O	2:F:363:VAL:HG22	2.18	0.44
2:F:41:THR:HB	2:F:42:PRO:CD	2.39	0.44
1:K:155:VAL:HA	1:K:159:VAL:CG2	2.48	0.44
1:L:383:LYS:HB3	1:L:489:GLY:O	2.17	0.44
1:U:382:VAL:HG21	1:U:440:THR:HG21	1.99	0.44
2:W:382:LYS:HA	2:W:385:GLN:HG3	1.99	0.44
2:X:388:ILE:HD11	2:X:396:LEU:HD11	1.99	0.44
1:C:395:PHE:CD1	1:C:395:PHE:C	2.90	0.44
1:J:201:LEU:HD11	1:J:267:LEU:HB2	1.98	0.44
1:K:181:ALA:HB1	1:K:269:VAL:HG21	1.99	0.44
4:Q:51:GLN:HG3	4:Q:74:PHE:CE2	2.52	0.44
1:U:98:ASP:HB3	1:U:130:ARG:HA	1.99	0.44
2:X:163:LYS:HE2	2:X:163:LYS:HB2	1.82	0.44
2:X:274:ARG:NH2	2:X:284:THR:OG1	2.50	0.44
2:O:257:ASN:HD21	2:O:311:TYR:N	2.15	0.44
3:P:133:ILE:HD12	3:P:134:GLY:N	2.32	0.44
4:Q:41:VAL:HG23	4:Q:45:HIS:HB2	2.00	0.44
1:S:152:LEU:HD22	1:S:365:PRO:HG3	2.00	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:162:GLY:N	1:S:165:GLN:OE1	2.50	0.44
1:A:455:LEU:HA	1:A:458:ILE:HD12	1.99	0.44
1:B:220:GLN:HE21	1:B:224:GLN:HE21	1.66	0.44
1:B:290:PRO:HA	1:B:291:PRO:HD2	1.90	0.44
1:J:484:GLU:HB3	1:J:495:LEU:HD21	1.99	0.44
1:K:442:GLU:C	1:K:445:PRO:HD2	2.38	0.44
2:M:140:VAL:HA	2:M:414:LEU:HD22	1.99	0.44
2:M:54:LEU:HD11	2:M:60:ARG:HB2	1.98	0.44
2:N:237:LEU:HD21	2:N:295:ARG:HB2	1.99	0.44
2:N:33:ILE:O	2:N:34:LEU:CB	2.65	0.44
1:C:155:VAL:HG13	1:C:159:VAL:HG23	1.99	0.44
2:E:225:PRO:O	2:E:226:PRO:C	2.56	0.44
1:K:488:LYS:HB3	1:K:490:GLU:H	1.81	0.44
2:M:89:ARG:HH11	2:M:181:PHE:HZ	1.64	0.44
1:S:203:CYS:O	1:S:231:SER:HA	2.17	0.44
1:U:270:TYR:CE1	1:U:307:LEU:HD11	2.53	0.44
2:W:242:TYR:CD1	2:W:246:GLU:HG3	2.53	0.44
2:E:139:LYS:NZ	2:E:413:PHE:O	2.49	0.44
2:F:182:SER:HA	2:F:252:LEU:O	2.17	0.44
4:H:45:HIS:HD2	4:H:77:VAL:HG21	1.82	0.44
2:N:296:ILE:HD13	2:N:306:SER:CB	2.45	0.44
1:S:452:ASN:HB3	1:S:454:HIS:CE1	2.53	0.44
1:U:395:PHE:O	1:U:398:GLN:HB2	2.18	0.44
2:W:121:PRO:HG3	2:W:295:ARG:HG3	2.00	0.44
2:W:37:LEU:HD12	2:W:61:THR:HG21	1.99	0.44
2:X:367:HIS:CD2	2:X:367:HIS:O	2.71	0.44
1:B:166:ARG:CD	1:B:311:ALA:HB3	2.47	0.44
2:D:48:LEU:HD13	2:D:61:THR:OG1	2.17	0.44
2:F:190:ARG:HH11	2:F:190:ARG:HG3	1.83	0.44
3:G:204:ASN:HB2	3:G:207:ARG:HB3	1.98	0.44
3:G:143:SER:OG	3:G:215:ALA:O	2.34	0.44
3:G:213:THR:CG2	3:G:217:GLN:NE2	2.81	0.44
4:H:57:VAL:HG21	4:H:70:ILE:HD12	2.00	0.44
1:K:34:LEU:O	2:N:55:GLY:HA2	2.17	0.44
1:K:77:LEU:O	1:K:243:PRO:HG2	2.18	0.44
2:M:279:VAL:HG12	2:M:279:VAL:O	2.18	0.44
2:N:168:GLN:HE21	2:N:201:MET:HG3	1.82	0.44
2:N:26:GLU:O	2:N:29:GLU:HB2	2.18	0.44
2:N:92:LEU:HD11	2:N:181:PHE:CE2	2.53	0.44
3:P:75:VAL:HB	3:P:164:ILE:HD13	2.00	0.44
2:V:231:ARG:HD2	2:V:234:LEU:HD12	1.99	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:337:SER:HB3	3:Y:259:ARG:HH11	1.83	0.44
3:Y:211:GLU:O	5:1:11:ALA:HB2	2.18	0.43
1:C:68:LEU:O	2:D:15:ALA:HA	2.17	0.43
2:F:247:GLU:CB	2:F:249:GLN:HG2	2.48	0.43
3:G:95:VAL:O	3:G:99:LEU:CB	2.64	0.43
1:K:164:GLY:HA2	1:K:323:LEU:O	2.18	0.43
1:T:190:ARG:HE	1:T:439:ALA:HB2	1.83	0.43
1:T:202:TYR:O	1:T:266:ALA:HA	2.18	0.43
1:U:139:LEU:N	1:U:140:PRO:CD	2.80	0.43
3:Y:77:ILE:HA	3:Y:110:ILE:HB	2.00	0.43
1:B:421:VAL:O	1:B:425:ARG:HG2	2.18	0.43
1:C:414:ALA:HA	1:C:417:LYS:HE2	1.99	0.43
2:D:191:THR:HA	2:D:221:GLN:HG3	1.99	0.43
2:E:43:GLN:HG2	2:E:44:GLY:N	2.33	0.43
2:F:258:ILE:HD11	2:F:292:LEU:HD21	2.00	0.43
4:H:32:LEU:HD21	4:H:85:VAL:HG22	2.00	0.43
4:H:35:LYS:HG2	4:H:36:SER:N	2.31	0.43
1:K:397:ALA:HA	1:K:400:ARG:HD2	1.99	0.43
1:S:148:VAL:HG12	1:S:148:VAL:O	2.18	0.43
2:X:293:GLN:HA	2:X:296:ILE:HD12	2.00	0.43
1:C:493:LYS:H	1:C:493:LYS:HD2	1.83	0.43
2:D:64:MET:HE1	2:D:228:ALA:HA	2.00	0.43
2:E:419:ALA:HA	2:E:429:GLY:HA3	2.00	0.43
2:M:252:LEU:HD23	2:M:305:THR:HB	1.99	0.43
1:S:138:ILE:O	2:W:195:ASN:ND2	2.44	0.43
1:S:385:LEU:HD12	1:S:444:VAL:HG13	1.99	0.43
1:S:58:SER:HB2	1:S:88:GLU:HG3	2.00	0.43
1:U:165:GLN:NE2	1:U:167:GLU:OE1	2.50	0.43
1:U:154:ALA:HA	1:U:430:LEU:HD22	2.01	0.43
2:V:159:ALA:O	2:V:337:ARG:NH2	2.45	0.43
2:V:96:ILE:HB	2:V:218:VAL:HG22	1.99	0.43
1:C:202:TYR:O	1:C:266:ALA:HA	2.18	0.43
1:K:139:LEU:HB3	1:K:140:PRO:HD3	2.01	0.43
2:M:277:SER:OG	2:M:278:ALA:N	2.50	0.43
2:X:182:SER:HB2	2:X:215:VAL:HB	1.99	0.43
1:C:219:VAL:HB	1:C:228:MET:CE	2.48	0.43
1:C:177:LYS:HG2	1:C:354:LEU:HD12	2.00	0.43
1:C:80:SER:OG	1:C:82:ARG:HG2	2.18	0.43
2:E:367:HIS:CD2	2:E:434:LEU:HD11	2.53	0.43
2:E:31:PRO:HB2	2:E:50:VAL:HG21	2.00	0.43
1:L:107:GLY:HA2	1:L:228:MET:O	2.19	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:166:ARG:HD2	1:L:308:LEU:O	2.17	0.43
2:V:417:PRO:HD2	2:V:430:LYS:HB2	2.00	0.43
2:W:71:VAL:O	2:W:74:GLU:HB2	2.18	0.43
1:C:421:VAL:HG13	1:C:425:ARG:NH1	2.33	0.43
1:L:311:ALA:HA	1:L:323:LEU:HB3	1.99	0.43
1:U:146:GLU:O	1:U:162:GLY:HA2	2.19	0.43
1:B:174:GLN:HA	6:B:600:ANP:HNB1	1.82	0.43
1:K:249:PRO:HB3	1:K:270:TYR:CD1	2.54	0.43
2:M:64:MET:HE3	2:M:228:ALA:HA	2.00	0.43
2:O:388:ILE:CD1	2:O:396:LEU:HD11	2.49	0.43
1:U:116:PRO:HG3	1:U:121:GLY:O	2.19	0.43
2:V:199:ARG:CZ	2:V:199:ARG:HB3	2.48	0.43
2:V:201:MET:SD	2:V:217:LEU:HD21	2.59	0.43
2:X:121:PRO:HA	2:X:122:PRO:HD2	1.84	0.43
2:X:41:THR:HB	2:X:42:PRO:HD2	2.00	0.43
3:Y:139:THR:HG21	5:1:37:ARG:HA	2.00	0.43
3:G:135:LYS:HB2	3:G:135:LYS:HE2	1.74	0.43
1:L:182:LEU:HD13	1:L:218:LEU:HD11	2.00	0.43
1:L:219:VAL:HG22	1:L:228:MET:HE1	2.00	0.43
1:U:211:LYS:HD3	2:X:328:HIS:O	2.18	0.43
2:X:382:LYS:HA	2:X:385:GLN:HG2	1.99	0.43
2:E:275:ILE:HA	2:E:276:PRO:HD3	1.86	0.43
1:J:188:GLN:CD	1:J:201:LEU:HD23	2.39	0.43
1:K:272:ASP:HB2	1:K:328:VAL:O	2.19	0.43
2:M:366:GLU:O	2:M:370:VAL:HG23	2.19	0.43
3:P:106:ASP:HB3	3:P:127:LYS:HG3	2.01	0.43
1:T:159:VAL:HG21	1:T:352:ILE:HG12	2.01	0.43
1:C:479:ASN:O	1:C:479:ASN:ND2	2.49	0.42
3:G:203:ALA:O	3:G:205:VAL:N	2.52	0.42
1:K:93:THR:HG22	1:K:95:ASN:N	2.31	0.42
2:M:24:HIS:CE1	2:M:25:PHE:O	2.72	0.42
2:N:357:LEU:HD13	2:N:362:VAL:HG11	2.01	0.42
2:N:440:SER:O	2:N:444:VAL:HG23	2.19	0.42
2:O:206:VAL:HG12	2:O:215:VAL:CG1	2.48	0.42
2:O:374:VAL:HG13	2:O:410:ILE:HG21	2.01	0.42
1:S:105:LEU:HD23	1:S:123:ILE:HG21	2.00	0.42
1:U:133:VAL:HB	1:U:310:ARG:NH2	2.34	0.42
1:K:442:GLU:O	1:K:446:LEU:HG	2.19	0.42
1:J:239:SER:HB3	2:M:294:GLU:HG3	2.00	0.42
1:U:441:GLU:CD	1:U:486:ARG:HD3	2.40	0.42
2:W:244:ARG:HD3	2:W:304:VAL:HG23	2.00	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:LEU:N	1:A:140:PRO:HD2	2.34	0.42
1:C:272:ASP:HB2	1:C:328:VAL:O	2.20	0.42
2:E:120:ASP:HA	2:E:121:PRO:HD3	1.92	0.42
1:J:389:ALA:O	1:J:390:GLY:C	2.58	0.42
1:U:422:ARG:NH1	1:U:453:GLY:HA3	2.33	0.42
2:V:321:ALA:HB3	2:V:322:PRO:CD	2.49	0.42
2:W:256:ASP:HA	2:W:257:ASN:HA	1.85	0.42
1:C:239:SER:HB2	2:F:291:LEU:HD23	2.02	0.42
2:F:372:SER:O	2:F:376:GLU:HG3	2.19	0.42
2:F:49:GLU:CD	2:F:231:ARG:HE	2.22	0.42
1:K:139:LEU:HD12	1:K:139:LEU:HA	1.86	0.42
2:M:172:ASN:ND2	2:M:419:ALA:HB3	2.34	0.42
2:O:351:LEU:HD23	2:O:375:GLN:HG2	2.01	0.42
2:V:387:ILE:HG23	2:V:391:LEU:HD12	2.00	0.42
1:U:360:TYR:OH	2:X:351:LEU:O	2.31	0.42
2:X:472:LYS:HD2	2:X:472:LYS:HA	1.81	0.42
3:Y:79:SER:OG	3:Y:80:ASP:N	2.53	0.42
1:A:248:ALA:HB3	1:A:249:PRO:HD3	2.00	0.42
1:B:67:ASN:O	1:B:67:ASN:OD1	2.37	0.42
1:J:424:GLU:HB3	1:J:460:LEU:HD11	2.01	0.42
2:M:209:LEU:O	2:M:210:GLU:HG3	2.20	0.42
1:J:52:GLU:CD	2:N:68:GLU:HG3	2.40	0.42
3:P:49:GLN:HG3	3:P:217:GLN:NE2	2.34	0.42
2:X:351:LEU:HD12	2:X:382:LYS:HE3	2.01	0.42
2:D:275:ILE:O	2:D:283:PRO:HG3	2.20	0.42
2:F:256:ASP:HA	2:F:309:ALA:HB3	2.02	0.42
4:H:72:GLY:HA3	5:I:14:LEU:HD21	1.99	0.42
1:J:474:LEU:HD13	1:J:482:LEU:HD21	2.01	0.42
2:M:221:GLN:OE1	2:M:221:GLN:HA	2.19	0.42
2:M:373:LYS:O	2:M:377:THR:OG1	2.38	0.42
3:P:180:LYS:HA	3:P:181:PRO:HD3	1.77	0.42
1:S:176:GLY:HA2	6:S:600:ANP:O5'	2.18	0.42
2:V:239:ILE:O	2:V:243:PHE:HD2	2.01	0.42
2:X:189:GLU:O	2:X:221:GLN:HB3	2.19	0.42
2:X:25:PHE:CZ	2:X:31:PRO:HG3	2.55	0.42
3:G:75:VAL:HA	3:G:108:VAL:O	2.19	0.42
1:J:297:PRO:HD2	1:J:300:VAL:HB	2.02	0.42
1:J:50:GLN:HB3	2:N:69:GLY:HA2	2.02	0.42
3:P:166:TYR:CE1	3:P:180:LYS:HG2	2.54	0.42
1:S:206:VAL:HG22	1:S:252:ALA:CB	2.49	0.42
1:S:144:VAL:HB	1:S:376:VAL:HG11	2.01	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:363:ILE:HA	1:T:431:LYS:HE2	2.00	0.42
1:U:257:GLU:HG2	1:U:260:ARG:CZ	2.50	0.42
2:V:77:LEU:CG	2:V:78:ASP:H	2.23	0.42
2:X:218:VAL:HG21	2:X:236:GLY:HA2	2.02	0.42
1:A:355:GLU:OE2	1:A:368:ASN:ND2	2.44	0.42
1:C:118:ASP:CG	1:C:120:LYS:HG3	2.40	0.42
2:D:158:GLY:O	2:D:161:VAL:HG22	2.18	0.42
2:F:88:GLY:O	2:F:91:THR:OG1	2.34	0.42
2:N:458:TYR:CE2	2:N:459:MET:HG2	2.55	0.42
2:O:252:LEU:HD23	2:O:305:THR:HB	2.02	0.42
1:U:428:GLN:O	1:U:431:LYS:HB2	2.20	0.42
2:V:171:ILE:O	2:V:175:ALA:HB3	2.19	0.42
2:X:320:PRO:O	2:X:324:THR:OG1	2.34	0.42
1:A:440:THR:O	1:A:444:VAL:HG13	2.20	0.42
2:D:243:PHE:O	2:D:247:GLU:HB3	2.20	0.42
2:M:84:SER:HB2	2:M:114:ARG:NH2	2.35	0.42
2:O:189:GLU:O	2:O:221:GLN:HB3	2.19	0.42
3:P:74:ILE:HB	3:P:107:ILE:HG22	2.02	0.42
2:W:258:ILE:HG22	2:W:309:ALA:O	2.20	0.42
2:W:160:GLY:HA3	2:W:337:ARG:HH22	1.82	0.42
2:E:50:VAL:HA	2:E:61:THR:HG22	2.01	0.42
2:F:9:ILE:HG23	2:F:27:GLN:NE2	2.34	0.42
1:J:391:SER:O	1:J:394:LEU:N	2.51	0.42
1:J:501:SER:O	1:J:505:SER:HB2	2.20	0.42
1:L:222:LEU:HB3	1:L:228:MET:HE2	2.01	0.42
1:L:399:TYR:CD1	1:L:423:GLY:HA3	2.55	0.42
3:P:12:SER:O	3:P:15:ASN:HB2	2.20	0.42
1:U:293:ARG:HB3	1:U:339:TYR:HE2	1.85	0.42
1:U:491:LEU:HA	1:U:495:LEU:HD12	2.01	0.42
2:V:415:SER:HB2	2:V:459:MET:H	1.85	0.42
1:B:182:LEU:HD13	1:B:218:LEU:HD11	2.01	0.41
2:D:463:ILE:O	2:D:467:VAL:HG23	2.19	0.41
2:F:84:SER:HB3	2:F:114:ARG:HH11	1.85	0.41
1:K:241:ALA:HB1	1:K:243:PRO:HD2	2.02	0.41
1:K:354:LEU:HA	1:K:366:ALA:O	2.20	0.41
1:K:39:GLY:HA2	1:K:81:ASP:OD1	2.19	0.41
1:L:49:ILE:HD11	1:L:55:VAL:CG1	2.49	0.41
2:O:33:ILE:HG22	2:O:34:LEU:HG	2.02	0.41
2:O:432:VAL:HG12	2:O:433:ARG:N	2.34	0.41
1:S:168:LEU:HD12	1:S:327:PRO:O	2.20	0.41
1:S:285:LEU:HD22	2:V:275:ILE:HG22	2.02	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:271:ASP:HA	1:T:272:ASP:HA	1.66	0.41
1:U:138:ILE:HD13	2:V:103:ILE:HD12	2.02	0.41
2:V:345:TYR:HA	2:V:346:PRO:C	2.41	0.41
1:K:282:GLN:NE2	2:N:284:THR:HG22	2.34	0.41
1:L:474:LEU:HB3	1:L:482:LEU:HD21	2.02	0.41
3:P:91:LEU:HD11	3:P:165:PHE:HB3	2.02	0.41
1:S:106:LEU:HD21	1:S:259:PHE:HZ	1.84	0.41
1:U:153:LYS:HB2	1:U:153:LYS:HE3	1.88	0.41
1:U:480:GLU:O	1:U:484:GLU:HB2	2.20	0.41
1:T:143:SER:N	2:X:199:ARG:HH22	2.09	0.41
3:Y:21:LYS:O	3:Y:25:ILE:HG12	2.20	0.41
1:B:239:SER:HB2	2:E:291:LEU:HD23	2.01	0.41
2:F:382:LYS:HA	2:F:385:GLN:HG2	2.02	0.41
3:G:111:GLY:O	3:G:114:ILE:HG22	2.21	0.41
1:K:246:TYR:CE2	1:K:283:LEU:HD13	2.53	0.41
1:U:169:ILE:HD11	1:U:326:LEU:HB3	2.02	0.41
1:U:179:ALA:N	6:U:600:ANP:O1A	2.52	0.41
2:V:418:PHE:HB2	2:V:421:ALA:CB	2.50	0.41
2:X:231:ARG:HA	2:X:234:LEU:HD12	2.02	0.41
1:A:146:GLU:O	1:A:163:ARG:HG3	2.20	0.41
1:A:49:ILE:HG13	1:A:53:GLU:CD	2.41	0.41
1:B:257:GLU:OE2	1:B:310:ARG:NE	2.34	0.41
1:B:398:GLN:C	1:B:400:ARG:N	2.72	0.41
2:D:256:ASP:HA	2:D:257:ASN:HA	1.81	0.41
3:G:47:ALA:HB1	4:H:84:CYS:HB3	2.03	0.41
2:M:84:SER:HB2	2:M:114:ARG:HH21	1.85	0.41
2:N:85:VAL:HG22	2:N:117:ILE:HG22	2.03	0.41
2:V:411:GLN:HA	2:V:414:LEU:HD12	2.02	0.41
1:A:181:ALA:O	1:A:184:THR:HB	2.20	0.41
1:A:332:GLN:HB3	2:D:318:THR:HB	2.02	0.41
1:A:455:LEU:HD21	1:A:466:PHE:CZ	2.55	0.41
1:C:378:SER:C	1:C:380:ALA:H	2.24	0.41
1:J:150:THR:HG21	1:J:155:VAL:HG11	2.02	0.41
1:L:267:LEU:HB2	1:L:324:THR:HB	2.01	0.41
2:M:158:GLY:O	2:M:163:LYS:NZ	2.54	0.41
3:P:77:ILE:HG12	3:P:110:ILE:HB	2.01	0.41
1:S:35:ALA:HB3	1:S:42:ARG:HH11	1.86	0.41
1:U:166:ARG:HG2	1:U:325:ALA:HB3	2.01	0.41
2:W:267:GLU:O	2:W:271:LEU:N	2.52	0.41
1:T:46:LEU:O	2:X:72:ARG:NH2	2.53	0.41
2:D:159:ALA:HA	6:D:600:ANP:O1G	2.20	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:443:ALA:HB1	2:D:449:TYR:HE2	1.86	0.41
3:G:16:ILE:O	3:G:20:THR:HG23	2.19	0.41
4:H:72:GLY:O	4:H:87:ALA:HA	2.20	0.41
1:K:25:ALA:O	1:K:28:ASN:ND2	2.54	0.41
1:L:170:ILE:HD11	1:L:341:PRO:HB3	2.03	0.41
1:L:164:GLY:HA2	1:L:323:LEU:O	2.21	0.41
1:L:354:LEU:HA	1:L:366:ALA:O	2.21	0.41
1:L:396:LEU:HA	1:L:399:TYR:HB3	2.02	0.41
2:N:54:LEU:HD21	2:N:60:ARG:HB2	2.02	0.41
1:T:158:LEU:HD21	1:T:392:LEU:HG	2.02	0.41
1:T:28:ASN:HA	1:T:47:ASN:H	1.86	0.41
2:W:201:MET:SD	2:W:217:LEU:HD21	2.61	0.41
1:T:67:ASN:HB2	2:X:17:ILE:HG12	2.02	0.41
2:E:399:GLN:O	2:E:403:THR:HG23	2.20	0.41
2:F:27:GLN:HG2	2:F:27:GLN:H	1.67	0.41
2:F:340:SER:HB3	2:F:347:ALA:CB	2.51	0.41
1:J:364:ARG:HA	1:J:365:PRO:C	2.40	0.41
2:N:208:ASN:ND2	2:N:211:GLY:HA3	2.36	0.41
2:O:90:GLU:O	2:O:109:ILE:HG23	2.21	0.41
1:T:364:ARG:HA	1:T:365:PRO:C	2.41	0.41
1:U:176:GLY:O	1:U:180:VAL:HG23	2.19	0.41
1:U:398:GLN:O	1:U:402:VAL:HG23	2.21	0.41
1:U:82:ARG:HG3	1:U:82:ARG:H	1.49	0.41
2:W:220:GLY:N	2:W:232:VAL:HG11	2.35	0.41
2:X:154:GLY:HA3	2:X:329:LEU:HD13	2.01	0.41
2:E:201:MET:SD	2:E:217:LEU:HD21	2.61	0.41
2:E:381:TYR:O	2:E:385:GLN:HG2	2.21	0.41
2:E:398:GLU:HA	2:E:401:LYS:HE2	2.02	0.41
2:F:168:GLN:O	2:F:172:ASN:HB2	2.20	0.41
2:F:207:ILE:HA	2:F:213:SER:HB3	2.01	0.41
3:P:205:VAL:N	3:P:206:PRO:CD	2.84	0.41
1:S:73:VAL:HG23	2:W:72:ARG:HH22	1.86	0.41
1:T:141:ARG:NH1	1:T:312:ALA:HB2	2.36	0.41
2:V:116:PRO:O	2:V:238:THR:HG21	2.21	0.41
1:C:144:VAL:HG22	1:C:163:ARG:O	2.21	0.41
1:L:219:VAL:HG13	1:L:228:MET:HE3	2.03	0.41
2:N:377:THR:HG22	2:N:407:ALA:HB2	2.01	0.41
3:P:187:THR:C	3:P:188:ILE:HG13	2.41	0.41
1:T:272:ASP:HB3	1:T:328:VAL:HB	2.02	0.41
2:V:256:ASP:HA	2:V:257:ASN:HA	1.73	0.41
2:V:385:GLN:C	2:V:387:ILE:H	2.24	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:418:PHE:HB2	2:V:421:ALA:HB3	2.02	0.41
2:W:275:ILE:HG12	2:W:275:ILE:H	1.55	0.41
2:W:443:ALA:O	2:W:448:LYS:HB2	2.21	0.41
2:X:345:TYR:HB3	6:X:600:ANP:C6	2.50	0.41
1:B:359:PHE:HZ	6:B:600:ANP:O4'	2.04	0.41
1:B:417:LYS:O	1:B:421:VAL:HG23	2.21	0.41
2:D:359:ASP:OD1	2:D:359:ASP:C	2.59	0.41
3:G:95:VAL:HG11	3:G:118:LEU:HD21	2.03	0.41
1:K:26:ASN:O	2:X:464:GLU:OE1	2.39	0.41
1:K:250:PHE:CZ	1:K:303:LEU:HD12	2.55	0.41
2:N:113:LEU:HD22	2:N:113:LEU:HA	1.78	0.41
2:N:276:PRO:HD2	3:P:271:ILE:HD11	2.02	0.41
1:S:329:ILE:HD12	1:S:340:ILE:HG22	2.03	0.41
1:T:154:ALA:HB2	1:T:430:LEU:HB3	2.03	0.41
1:U:256:GLY:HA2	1:U:259:PHE:HD2	1.85	0.41
2:X:30:LEU:HD21	2:X:57:ASN:HA	2.03	0.41
1:A:50:GLN:HB2	1:A:53:GLU:HB2	2.02	0.41
1:B:289:ARG:HA	1:B:290:PRO:HD3	1.92	0.41
1:C:219:VAL:HB	1:C:228:MET:HE1	2.03	0.41
1:C:402:VAL:C	1:C:404:ALA:H	2.25	0.41
1:C:50:GLN:HB3	2:D:69:GLY:HA2	2.03	0.41
2:E:229:ARG:NH2	2:E:267:GLU:OE1	2.48	0.41
1:L:260:ARG:O	1:L:321:GLY:HA3	2.21	0.41
2:M:164:THR:O	2:M:167:ILE:HG22	2.21	0.41
2:M:393:MET:O	2:M:401:LYS:HE2	2.21	0.41
1:K:239:SER:HB2	2:N:291:LEU:HD23	2.03	0.41
2:N:374:VAL:HG13	2:N:410:ILE:HG21	2.02	0.41
2:O:319:ASP:O	2:O:320:PRO:C	2.59	0.41
3:P:138:PRO:HG3	3:P:222:MET:O	2.21	0.41
1:S:293:ARG:HA	3:Y:267:LEU:HD12	2.03	0.41
2:W:349:ASP:HA	2:W:350:PRO:HD2	1.92	0.41
2:X:190:ARG:O	2:X:221:GLN:NE2	2.51	0.41
2:X:398:GLU:HG3	3:Y:120:ARG:HE	1.85	0.41
1:B:177:LYS:HG2	1:B:354:LEU:HD12	2.03	0.40
1:C:493:LYS:HA	1:C:496:LEU:HD12	2.03	0.40
2:F:121:PRO:HA	2:F:122:PRO:HD3	1.86	0.40
1:K:248:ALA:HB3	1:K:249:PRO:HD3	2.02	0.40
2:M:184:PHE:HB3	2:M:217:LEU:HD23	2.02	0.40
2:M:90:GLU:HG3	2:M:111:SER:CA	2.50	0.40
1:T:413:ASP:O	1:T:417:LYS:HB2	2.22	0.40
1:U:421:VAL:O	1:U:425:ARG:HD2	2.20	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:157:GLY:H	2:V:312:VAL:HG23	1.86	0.40
2:V:336:SER:HB3	2:V:339:ILE:HG13	2.02	0.40
2:V:54:LEU:HD13	2:V:58:THR:HG22	2.04	0.40
2:W:48:LEU:HB3	2:W:61:THR:CB	2.50	0.40
2:X:33:ILE:O	2:X:34:LEU:HB2	2.21	0.40
1:C:103:PRO:HD3	1:C:258:TRP:CZ2	2.56	0.40
1:C:153:LYS:NZ	1:C:467:GLU:OE1	2.51	0.40
2:D:201:MET:HE2	2:D:217:LEU:HD21	2.03	0.40
1:L:111:ASP:C	1:L:111:ASP:OD1	2.60	0.40
2:M:26:GLU:O	2:M:27:GLN:C	2.59	0.40
2:O:92:LEU:HB3	2:O:213:SER:O	2.22	0.40
1:S:273:LEU:HD13	1:S:304:HIS:CD2	2.55	0.40
1:U:219:VAL:HB	1:U:228:MET:CE	2.51	0.40
1:U:376:VAL:HG11	1:U:380:ALA:HB2	2.02	0.40
2:V:197:LEU:HD23	2:V:219:PHE:HZ	1.86	0.40
2:V:395:GLU:HG3	2:V:395:GLU:O	2.21	0.40
2:X:10:THR:HA	2:X:76:VAL:O	2.20	0.40
1:A:73:VAL:HG12	1:A:75:ILE:HG13	2.04	0.40
1:C:99:VAL:O	1:C:128:ARG:HA	2.22	0.40
1:C:469:SER:HB3	1:C:506:PHE:HZ	1.86	0.40
2:D:95:ILE:HD11	2:D:198:TYR:CE1	2.56	0.40
1:J:28:ASN:HA	1:J:47:ASN:HB2	2.04	0.40
1:K:133:VAL:H	1:K:310:ARG:NH1	2.20	0.40
1:K:444:VAL:N	1:K:445:PRO:CD	2.84	0.40
2:N:182:SER:HA	2:N:252:LEU:O	2.20	0.40
2:O:183:VAL:HG11	2:O:236:GLY:O	2.21	0.40
1:S:170:ILE:HG12	1:S:331:THR:HG23	2.02	0.40
1:T:282:GLN:O	1:T:286:LEU:HG	2.21	0.40
1:T:55:VAL:HG21	1:T:75:ILE:HD13	2.03	0.40
1:U:243:PRO:HA	1:U:283:LEU:HD11	2.03	0.40
1:U:68:LEU:HB2	2:V:16:VAL:CG2	2.51	0.40
2:W:168:GLN:HA	2:W:171:ILE:HD12	2.03	0.40
2:X:189:GLU:O	2:X:222:MET:HG2	2.21	0.40
3:Y:110:ILE:HD11	3:Y:146:ILE:HG21	2.02	0.40
2:E:109:ILE:O	2:E:111:SER:N	2.47	0.40
2:E:259:PHE:CE1	2:E:313:PRO:HG3	2.56	0.40
4:H:49:VAL:HG22	4:H:76:THR:HB	2.03	0.40
2:M:244:ARG:HD3	2:M:304:VAL:HG23	2.03	0.40
1:S:116:PRO:HB3	1:S:123:ILE:HD11	2.04	0.40
1:S:190:ARG:CZ	1:S:439:ALA:HB2	2.51	0.40
1:U:355:GLU:OE2	1:U:368:ASN:ND2	2.54	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:370:VAL:O	2:V:374:VAL:HG23	2.21	0.40
1:B:139:LEU:HD23	2:F:105:GLU:OE2	2.22	0.40
2:F:252:LEU:HD23	2:F:305:THR:HB	2.04	0.40
3:P:79:SER:HB2	3:P:134:GLY:HA3	2.04	0.40
3:P:163:SER:HB3	3:P:179:GLU:HG3	2.02	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%)	19 (4%)	3 (1%)	25	44
1	B	479/510 (94%)	455 (95%)	21 (4%)	3 (1%)	25	44
1	C	482/510 (94%)	448 (93%)	31 (6%)	3 (1%)	25	44
1	J	477/510 (94%)	449 (94%)	23 (5%)	5 (1%)	15	28
1	K	482/510 (94%)	446 (92%)	32 (7%)	4 (1%)	19	36
1	L	478/510 (94%)	451 (94%)	23 (5%)	4 (1%)	19	36
1	S	473/510 (93%)	434 (92%)	39 (8%)	0	100	100
1	T	474/510 (93%)	430 (91%)	42 (9%)	2 (0%)	34	55
1	U	477/510 (94%)	423 (89%)	48 (10%)	6 (1%)	12	21
2	D	468/484 (97%)	435 (93%)	30 (6%)	3 (1%)	25	44
2	E	466/484 (96%)	429 (92%)	30 (6%)	7 (2%)	10	18
2	F	467/484 (96%)	432 (92%)	34 (7%)	1 (0%)	47	69
2	M	468/484 (97%)	431 (92%)	32 (7%)	5 (1%)	14	26
2	N	468/484 (97%)	438 (94%)	27 (6%)	3 (1%)	25	44
2	O	466/484 (96%)	430 (92%)	34 (7%)	2 (0%)	34	55
2	V	468/484 (97%)	433 (92%)	31 (7%)	4 (1%)	17	32

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	W	465/484 (96%)	425 (91%)	36 (8%)	4 (1%)	17	32
2	X	467/484 (96%)	419 (90%)	45 (10%)	3 (1%)	25	44
3	G	262/278 (94%)	240 (92%)	19 (7%)	3 (1%)	14	26
3	P	232/278 (84%)	210 (90%)	20 (9%)	2 (1%)	17	32
3	Y	188/278 (68%)	173 (92%)	13 (7%)	2 (1%)	14	26
4	H	114/138 (83%)	91 (80%)	20 (18%)	3 (3%)	5	8
4	Q	73/138 (53%)	61 (84%)	9 (12%)	3 (4%)	3	3
4	Z	15/138 (11%)	10 (67%)	4 (27%)	1 (7%)	1	1
5	1	23/61 (38%)	18 (78%)	4 (17%)	1 (4%)	2	3
5	I	43/61 (70%)	39 (91%)	2 (5%)	2 (5%)	2	2
5	R	30/61 (49%)	21 (70%)	9 (30%)	0	100	100
All	All	9483/10377 (91%)	8727 (92%)	677 (7%)	79 (1%)	19	36

All (79) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	152	SER
3	G	204	ASN
4	H	118	ARG
5	I	55	GLU
5	I	56	PRO
1	J	392	LEU
1	T	507	VAL
1	U	298	GLY
1	A	406	ALA
1	B	196	ASP
1	C	390	GLY
2	E	279	VAL
2	E	366	GLU
4	H	102	LYS
1	J	27	LEU
1	J	390	GLY
1	J	403	ALA
1	K	196	ASP
1	L	82	ARG
2	M	250	ASP
3	P	134	GLY
1	T	97	VAL

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	U	390	GLY
2	V	347	ALA
2	X	28	SER
3	Y	103	PRO
1	A	479	ASN
3	G	135	LYS
1	L	335	ASP
1	L	508	ALA
2	M	27	GLN
2	M	279	VAL
3	P	152	SER
4	Q	35	LYS
1	U	70	PRO
2	V	474	ALA
1	B	397	ALA
2	D	388	ILE
2	E	110	LYS
1	K	58	SER
2	M	463	ILE
2	N	421	ALA
1	U	140	PRO
2	W	277	SER
2	W	284	THR
4	Z	120	ALA
1	A	404	ALA
2	D	27	GLN
2	E	28	SER
4	H	33	PRO
1	K	359	PHE
1	L	339	TYR
2	M	175	ALA
2	N	279	VAL
4	Q	45	HIS
2	V	212	GLU
2	W	15	ALA
2	W	34	LEU
1	C	196	ASP
2	N	158	GLY
2	E	461	GLY
2	E	463	ILE
1	U	69	GLU
2	X	248	GLY

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	F	279	VAL
2	O	279	VAL
2	O	461	GLY
4	Q	53	LEU
2	X	100	GLY
3	Y	177	PRO
1	B	390	GLY
1	K	97	VAL
1	C	70	PRO
2	D	279	VAL
1	U	138	ILE
5	1	34	VAL
2	E	44	GLY
1	J	70	PRO
2	V	346	PRO

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	388/412 (94%)	371 (96%)	17 (4%)	28	47
1	B	388/412 (94%)	372 (96%)	16 (4%)	30	50
1	C	390/412 (95%)	374 (96%)	16 (4%)	30	50
1	J	387/412 (94%)	366 (95%)	21 (5%)	22	38
1	K	388/412 (94%)	366 (94%)	22 (6%)	20	36
1	L	388/412 (94%)	363 (94%)	25 (6%)	17	31
1	S	384/412 (93%)	364 (95%)	20 (5%)	23	39
1	T	386/412 (94%)	373 (97%)	13 (3%)	37	58
1	U	387/412 (94%)	365 (94%)	22 (6%)	20	36
2	D	379/390 (97%)	368 (97%)	11 (3%)	42	62
2	E	370/390 (95%)	359 (97%)	11 (3%)	41	61
2	F	375/390 (96%)	357 (95%)	18 (5%)	25	44

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	M	377/390 (97%)	362 (96%)	15 (4%)	31	52
2	N	378/390 (97%)	356 (94%)	22 (6%)	20	35
2	O	378/390 (97%)	364 (96%)	14 (4%)	34	54
2	V	380/390 (97%)	363 (96%)	17 (4%)	27	47
2	W	378/390 (97%)	359 (95%)	19 (5%)	24	42
2	X	379/390 (97%)	365 (96%)	14 (4%)	34	54
3	G	225/236 (95%)	209 (93%)	16 (7%)	14	26
3	P	197/236 (84%)	191 (97%)	6 (3%)	41	61
3	Y	163/236 (69%)	153 (94%)	10 (6%)	18	32
4	H	65/112 (58%)	57 (88%)	8 (12%)	4	7
4	Q	8/112 (7%)	8 (100%)	0	100	100
5	1	2/48 (4%)	2 (100%)	0	100	100
5	I	28/48 (58%)	24 (86%)	4 (14%)	3	4
5	R	3/48 (6%)	3 (100%)	0	100	100
All	All	7571/8294 (91%)	7214 (95%)	357 (5%)	26	45

All (357) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	THR
1	A	56	GLU
1	A	123	ILE
1	A	142	ARG
1	A	166	ARG
1	A	218	LEU
1	A	251	THR
1	A	373	VAL
1	A	412	LEU
1	A	416	THR
1	A	420	LEU
1	A	436	SER
1	A	445	PRO
1	A	476	SER
1	A	480	GLU
1	A	495	LEU
1	A	509	THR
1	B	93	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	99	VAL
1	B	106	LEU
1	B	159	VAL
1	B	173	ARG
1	B	246	TYR
1	B	283	LEU
1	B	289	ARG
1	B	399	TYR
1	B	400	ARG
1	B	460	LEU
1	B	468	SER
1	B	472	SER
1	B	484	GLU
1	B	494	GLU
1	B	509	THR
1	C	27	LEU
1	C	61	VAL
1	C	72	GLN
1	C	99	VAL
1	C	166	ARG
1	C	198	SER
1	C	218	LEU
1	C	220	GLN
1	C	223	GLU
1	C	283	LEU
1	C	357	GLU
1	C	391	SER
1	C	411	ASP
1	C	479	ASN
1	C	505	SER
1	C	509	THR
2	D	132	GLU
2	D	204	THR
2	D	251	VAL
2	D	266	SER
2	D	356	ARG
2	D	386	ASP
2	D	387	ILE
2	D	396	LEU
2	D	399	GLN
2	D	413	PHE
2	D	464	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	E	43	GLN
2	E	56	GLU
2	E	133	ILE
2	E	140	VAL
2	E	161	VAL
2	E	232	VAL
2	E	301	LYS
2	E	337	ARG
2	E	352	ASP
2	E	386	ASP
2	E	399	GLN
2	F	28	SER
2	F	68	GLU
2	F	84	SER
2	F	85	VAL
2	F	133	ILE
2	F	140	VAL
2	F	149	ARG
2	F	201	MET
2	F	208	ASN
2	F	210	GLU
2	F	237	LEU
2	F	246	GLU
2	F	250	ASP
2	F	279	VAL
2	F	292	LEU
2	F	303	SER
2	F	333	THR
2	F	387	ILE
3	G	23	MET
3	G	77	ILE
3	G	81	LYS
3	G	86	SER
3	G	97	ARG
3	G	102	GLN
3	G	130	ILE
3	G	153	VAL
3	G	204	ASN
3	G	205	VAL
3	G	210	PHE
3	G	216	ASN
3	G	220	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	G	231	SER
3	G	234	ARG
3	G	254	LEU
4	H	14	PHE
4	H	20	THR
4	H	27	VAL
4	H	35	LYS
4	H	39	ILE
4	H	65	SER
4	H	76	THR
4	H	80	ASP
5	I	19	GLN
5	I	35	LEU
5	I	41	ASP
5	I	47	TYR
1	J	30	THR
1	J	67	ASN
1	J	90	VAL
1	J	134	LYS
1	J	139	LEU
1	J	163	ARG
1	J	166	ARG
1	J	183	ASP
1	J	231	SER
1	J	246	TYR
1	J	322	SER
1	J	373	VAL
1	J	411	ASP
1	J	418	GLN
1	J	420	LEU
1	J	436	SER
1	J	444	VAL
1	J	465	GLU
1	J	468	SER
1	J	480	GLU
1	J	487	GLU
1	K	58	SER
1	K	93	THR
1	K	99	VAL
1	K	106	LEU
1	K	166	ARG
1	K	231	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	K	246	TYR
1	K	317	LYS
1	K	341	PRO
1	K	351	GLN
1	K	357	GLU
1	K	360	TYR
1	K	371	LEU
1	K	372	SER
1	K	385	LEU
1	K	391	SER
1	K	394	LEU
1	K	399	TYR
1	K	400	ARG
1	K	411	ASP
1	K	460	LEU
1	K	501	SER
1	L	70	PRO
1	L	82	ARG
1	L	89	LEU
1	L	93	THR
1	L	99	VAL
1	L	142	ARG
1	L	159	VAL
1	L	163	ARG
1	L	166	ARG
1	L	195	SER
1	L	267	LEU
1	L	306	ARG
1	L	317	LYS
1	L	322	SER
1	L	337	SER
1	L	342	THR
1	L	351	GLN
1	L	373	VAL
1	L	436	SER
1	L	465	GLU
1	L	481	LEU
1	L	484	GLU
1	L	492	SER
1	L	498	SER
1	L	503	THR
2	M	10	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	M	113	LEU
2	M	134	LEU
2	M	149	ARG
2	M	206	VAL
2	M	251	VAL
2	M	336	SER
2	M	386	ASP
2	M	390	ILE
2	M	394	ASP
2	M	397	SER
2	M	422	GLU
2	M	435	LYS
2	M	436	ASP
2	M	450	ASP
2	N	9	ILE
2	N	10	THR
2	N	85	VAL
2	N	113	LEU
2	N	130	SER
2	N	140	VAL
2	N	161	VAL
2	N	164	THR
2	N	176	LYS
2	N	204	THR
2	N	212	GLU
2	N	232	VAL
2	N	356	ARG
2	N	357	LEU
2	N	366	GLU
2	N	372	SER
2	N	376	GLU
2	N	380	THR
2	N	393	MET
2	N	394	ASP
2	N	398	GLU
2	N	399	GLN
2	O	29	GLU
2	O	85	VAL
2	O	140	VAL
2	O	200	GLU
2	O	201	MET
2	O	208	ASN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	O	210	GLU
2	O	237	LEU
2	O	274	ARG
2	O	306	SER
2	O	333	THR
2	O	336	SER
2	O	399	GLN
2	O	464	GLU
3	P	19	ILE
3	P	84	CYS
3	P	112	ASP
3	P	142	GLU
3	P	143	SER
3	P	267	LEU
1	S	32	ARG
1	S	44	PHE
1	S	58	SER
1	S	89	LEU
1	S	92	ARG
1	S	123	ILE
1	S	134	LYS
1	S	224	GLN
1	S	267	LEU
1	S	303	LEU
1	S	318	GLU
1	S	373	VAL
1	S	436	SER
1	S	441	GLU
1	S	444	VAL
1	S	462	ARG
1	S	474	LEU
1	S	477	ASN
1	S	490	GLU
1	S	495	LEU
1	T	67	ASN
1	T	95	ASN
1	T	99	VAL
1	T	115	ASN
1	T	159	VAL
1	T	225	HIS
1	T	246	TYR
1	T	317	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	T	394	LEU
1	T	399	TYR
1	T	422	ARG
1	T	465	GLU
1	T	505	SER
1	U	40	ILE
1	U	47	ASN
1	U	67	ASN
1	U	82	ARG
1	U	89	LEU
1	U	93	THR
1	U	98	ASP
1	U	143	SER
1	U	163	ARG
1	U	166	ARG
1	U	169	ILE
1	U	190	ARG
1	U	218	LEU
1	U	233	ILE
1	U	339	TYR
1	U	351	GLN
1	U	378	SER
1	U	393	LYS
1	U	394	LEU
1	U	413	ASP
1	U	427	THR
1	U	501	SER
2	V	12	LYS
2	V	14	THR
2	V	54	LEU
2	V	65	ASP
2	V	191	THR
2	V	199	ARG
2	V	250	ASP
2	V	251	VAL
2	V	282	GLN
2	V	292	LEU
2	V	366	GLU
2	V	386	ASP
2	V	393	MET
2	V	413	PHE
2	V	423	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	V	427	ILE
2	V	431	LEU
2	W	99	ILE
2	W	106	ARG
2	W	111	SER
2	W	129	THR
2	W	140	VAL
2	W	152	LYS
2	W	204	THR
2	W	213	SER
2	W	224	GLU
2	W	229	ARG
2	W	232	VAL
2	W	268	VAL
2	W	275	ILE
2	W	287	THR
2	W	296	ILE
2	W	337	ARG
2	W	352	ASP
2	W	423	VAL
2	W	448	LYS
2	X	43	GLN
2	X	68	GLU
2	X	95	ILE
2	X	98	VAL
2	X	129	THR
2	X	133	ILE
2	X	208	ASN
2	X	238	THR
2	X	250	ASP
2	X	274	ARG
2	X	324	THR
2	X	382	LYS
2	X	412	ARG
2	X	413	PHE
3	Y	16	ILE
3	Y	97	ARG
3	Y	104	ASN
3	Y	119	LEU
3	Y	136	ASP
3	Y	213	THR
3	Y	219	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	Y	249	ASN
3	Y	259	ARG
3	Y	268	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	418	GLN
1	A	452	ASN
1	B	149	GLN
1	B	224	GLN
1	B	368	ASN
1	B	454	HIS
1	C	145	HIS
1	C	174	GLN
2	D	52	GLN
2	D	178	HIS
2	D	195	ASN
2	D	208	ASN
2	D	367	HIS
2	E	168	GLN
2	E	399	GLN
2	F	43	GLN
2	F	208	ASN
2	F	367	HIS
3	G	54	ASN
3	G	59	ASN
3	G	117	GLN
3	G	217	GLN
4	H	45	HIS
4	H	134	GLN
5	I	19	GLN
1	J	145	HIS
1	K	28	ASN
1	K	149	GLN
1	K	428	GLN
1	L	132	GLN
1	L	145	HIS
1	L	225	HIS
2	M	195	ASN
2	M	328	HIS
2	M	367	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	M	379	GLN
2	M	385	GLN
2	N	168	GLN
2	O	27	GLN
2	O	52	GLN
2	O	328	HIS
3	P	88	HIS
3	P	100	ASN
3	P	216	ASN
3	P	239	ASN
3	P	243	ASN
1	S	387	GLN
1	S	443	GLN
1	S	454	HIS
1	T	28	ASN
1	T	47	ASN
1	T	48	ASN
1	T	67	ASN
1	T	428	GLN
1	U	220	GLN
1	U	265	HIS
1	U	407	GLN
1	U	479	ASN
2	V	282	GLN
2	W	57	ASN
2	W	127	GLN
2	W	168	GLN
2	W	221	GLN
2	X	43	GLN
2	X	52	GLN
2	X	208	ASN
2	X	263	GLN
3	Y	102	GLN
3	Y	117	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 15 are monoatomic - leaving 17 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	2.01	8 (27%)	31,52,52	1.94	7 (22%)
8	PO4	N	800	-	4,4,4	0.80	0	6,6,6	0.56	0
6	ANP	J	600	7	29,33,33	1.73	8 (27%)	31,52,52	1.87	5 (16%)
6	ANP	M	600	7	29,33,33	1.79	9 (31%)	31,52,52	1.85	8 (25%)
6	ANP	L	600	7	29,33,33	1.71	8 (27%)	31,52,52	1.91	5 (16%)
6	ANP	O	600	7	29,33,33	1.75	9 (31%)	31,52,52	1.96	8 (25%)
6	ANP	V	600	7	29,33,33	1.87	8 (27%)	31,52,52	1.91	8 (25%)
6	ANP	K	600	7	29,33,33	1.71	7 (24%)	31,52,52	1.66	6 (19%)
6	ANP	B	600	7	29,33,33	1.83	9 (31%)	31,52,52	1.73	6 (19%)
8	PO4	E	800	-	4,4,4	0.62	0	6,6,6	0.75	0
6	ANP	D	600	7	29,33,33	1.74	7 (24%)	31,52,52	1.83	8 (25%)
6	ANP	A	600	7	29,33,33	1.69	8 (27%)	31,52,52	2.23	9 (29%)
6	ANP	C	600	7	29,33,33	1.80	7 (24%)	31,52,52	1.91	7 (22%)
6	ANP	F	600	7	29,33,33	1.74	7 (24%)	31,52,52	2.08	8 (25%)
6	ANP	S	600	7	29,33,33	2.00	9 (31%)	31,52,52	2.03	5 (16%)
6	ANP	X	600	7	29,33,33	1.86	7 (24%)	31,52,52	1.80	7 (22%)
6	ANP	U	600	7	29,33,33	1.72	7 (24%)	31,52,52	2.16	10 (32%)

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	-	7/14/38/38	0/3/3/3
6	ANP	S	600	7	-	6/14/38/38	0/3/3/3
6	ANP	J	600	7	-	4/14/38/38	0/3/3/3
6	ANP	M	600	7	-	4/14/38/38	0/3/3/3
6	ANP	L	600	7	-	2/14/38/38	0/3/3/3
6	ANP	O	600	7	-	4/14/38/38	0/3/3/3
6	ANP	V	600	7	-	9/14/38/38	0/3/3/3
6	ANP	K	600	7	-	2/14/38/38	0/3/3/3
6	ANP	B	600	7	-	2/14/38/38	0/3/3/3
6	ANP	D	600	7	-	5/14/38/38	0/3/3/3
6	ANP	A	600	7	-	2/14/38/38	0/3/3/3
6	ANP	C	600	7	-	3/14/38/38	0/3/3/3
6	ANP	F	600	7	-	8/14/38/38	0/3/3/3
6	ANP	X	600	7	-	5/14/38/38	0/3/3/3
6	ANP	U	600	7	-	4/14/38/38	0/3/3/3

All (118) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	T	600	ANP	PG-N3B	4.98	1.76	1.63
6	T	600	ANP	PB-N3B	4.95	1.76	1.63
6	S	600	ANP	PB-N3B	4.62	1.75	1.63
6	S	600	ANP	PG-N3B	4.57	1.75	1.63
6	X	600	ANP	PB-N3B	4.44	1.75	1.63
6	B	600	ANP	PB-N3B	4.42	1.74	1.63
6	X	600	ANP	PG-N3B	4.36	1.74	1.63
6	V	600	ANP	PG-N3B	4.28	1.74	1.63
6	S	600	ANP	PG-O1G	4.27	1.52	1.46
6	V	600	ANP	PB-N3B	4.27	1.74	1.63
6	B	600	ANP	PG-N3B	4.24	1.74	1.63
6	M	600	ANP	PB-N3B	4.15	1.74	1.63
6	C	600	ANP	PG-N3B	4.14	1.74	1.63
6	T	600	ANP	PG-O1G	4.11	1.52	1.46
6	U	600	ANP	PG-N3B	4.09	1.74	1.63
6	K	600	ANP	PG-N3B	4.07	1.74	1.63
6	D	600	ANP	PB-N3B	4.04	1.73	1.63
6	L	600	ANP	PB-N3B	4.02	1.73	1.63
6	L	600	ANP	PG-N3B	3.97	1.73	1.63
6	D	600	ANP	PG-N3B	3.95	1.73	1.63
6	K	600	ANP	PB-N3B	3.92	1.73	1.63

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	600	ANP	PB-N3B	3.90	1.73	1.63
6	J	600	ANP	PB-N3B	3.83	1.73	1.63
6	O	600	ANP	PG-N3B	3.81	1.73	1.63
6	J	600	ANP	PG-N3B	3.80	1.73	1.63
6	X	600	ANP	PG-O1G	3.80	1.52	1.46
6	F	600	ANP	PG-N3B	3.79	1.73	1.63
6	F	600	ANP	PB-N3B	3.77	1.73	1.63
6	O	600	ANP	PB-N3B	3.75	1.73	1.63
6	C	600	ANP	PG-O1G	3.71	1.52	1.46
6	M	600	ANP	PG-N3B	3.71	1.73	1.63
6	A	600	ANP	PB-N3B	3.68	1.73	1.63
6	U	600	ANP	PB-N3B	3.68	1.73	1.63
6	S	600	ANP	PB-O1B	3.60	1.51	1.46
6	A	600	ANP	PG-N3B	3.55	1.72	1.63
6	V	600	ANP	PG-O1G	3.37	1.51	1.46
6	X	600	ANP	PB-O1B	3.27	1.51	1.46
6	J	600	ANP	PG-O1G	3.26	1.51	1.46
6	T	600	ANP	PB-O1B	3.20	1.51	1.46
6	M	600	ANP	PG-O1G	3.19	1.51	1.46
6	C	600	ANP	PB-O1B	3.15	1.51	1.46
6	V	600	ANP	PB-O1B	3.14	1.51	1.46
6	K	600	ANP	PG-O2G	-3.11	1.48	1.56
6	M	600	ANP	PB-O1B	3.06	1.51	1.46
6	F	600	ANP	PB-O1B	3.04	1.51	1.46
6	D	600	ANP	PG-O1G	2.98	1.50	1.46
6	A	600	ANP	PG-O2G	-2.94	1.48	1.56
6	X	600	ANP	C5-C4	2.94	1.48	1.40
6	L	600	ANP	PG-O1G	2.88	1.50	1.46
6	F	600	ANP	PG-O1G	2.86	1.50	1.46
6	O	600	ANP	C5-C4	2.86	1.48	1.40
6	F	600	ANP	PG-O2G	-2.85	1.49	1.56
6	U	600	ANP	PG-O1G	2.81	1.50	1.46
6	M	600	ANP	C5-C4	2.77	1.48	1.40
6	U	600	ANP	C5-C4	2.77	1.48	1.40
6	B	600	ANP	PG-O3G	-2.77	1.49	1.56
6	K	600	ANP	PG-O3G	-2.73	1.49	1.56
6	J	600	ANP	PB-O1B	2.72	1.50	1.46
6	U	600	ANP	PB-O3A	2.72	1.62	1.59
6	D	600	ANP	PB-O1B	2.70	1.50	1.46
6	B	600	ANP	PB-O1B	2.70	1.50	1.46
6	T	600	ANP	C5-C4	2.69	1.48	1.40
6	S	600	ANP	C5-C4	2.69	1.48	1.40

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	600	ANP	C5-C4	2.68	1.48	1.40
6	O	600	ANP	PG-O1G	2.68	1.50	1.46
6	S	600	ANP	C2-N3	2.66	1.36	1.32
6	A	600	ANP	C5-C4	2.65	1.47	1.40
6	F	600	ANP	C5-C4	2.62	1.47	1.40
6	T	600	ANP	PB-O3A	2.61	1.62	1.59
6	L	600	ANP	PG-O2G	-2.60	1.49	1.56
6	V	600	ANP	C5-C4	2.60	1.47	1.40
6	B	600	ANP	C5-C4	2.57	1.47	1.40
6	O	600	ANP	PG-O2G	-2.54	1.49	1.56
6	U	600	ANP	PB-O1B	2.54	1.50	1.46
6	L	600	ANP	PB-O1B	2.54	1.50	1.46
6	B	600	ANP	PG-O2G	-2.53	1.50	1.56
6	J	600	ANP	C5-C4	2.51	1.47	1.40
6	K	600	ANP	PB-O1B	2.50	1.50	1.46
6	K	600	ANP	C5-C4	2.50	1.47	1.40
6	L	600	ANP	PG-O3G	-2.46	1.50	1.56
6	B	600	ANP	PG-O1G	2.46	1.50	1.46
6	A	600	ANP	PG-O3G	-2.45	1.50	1.56
6	V	600	ANP	PB-O3A	2.44	1.62	1.59
6	C	600	ANP	PB-O3A	2.42	1.62	1.59
6	M	600	ANP	C2-N3	2.41	1.36	1.32
6	O	600	ANP	PB-O1B	2.40	1.50	1.46
6	T	600	ANP	C2-N3	2.39	1.35	1.32
6	D	600	ANP	PG-O3G	-2.39	1.50	1.56
6	J	600	ANP	PG-O2G	-2.34	1.50	1.56
6	A	600	ANP	PB-O1B	2.34	1.49	1.46
6	S	600	ANP	O4'-C1'	2.34	1.44	1.41
6	V	600	ANP	C2-N3	2.33	1.35	1.32
6	C	600	ANP	C5-C4	2.31	1.47	1.40
6	V	600	ANP	O4'-C1'	2.31	1.44	1.41
6	J	600	ANP	PB-O2B	-2.30	1.50	1.56
6	F	600	ANP	PG-O3G	-2.30	1.50	1.56
6	T	600	ANP	O4'-C1'	2.29	1.44	1.41
6	D	600	ANP	PG-O2G	-2.29	1.50	1.56
6	S	600	ANP	PB-O3A	2.28	1.61	1.59
6	O	600	ANP	PB-O3A	2.25	1.61	1.59
6	B	600	ANP	PB-O2B	-2.25	1.50	1.56
6	M	600	ANP	PB-O3A	2.24	1.61	1.59
6	K	600	ANP	PG-O1G	2.23	1.49	1.46
6	J	600	ANP	O4'-C1'	2.23	1.44	1.41
6	A	600	ANP	PG-O1G	2.19	1.49	1.46

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	U	600	ANP	C2-N3	2.19	1.35	1.32
6	C	600	ANP	PG-O2G	-2.15	1.51	1.56
6	M	600	ANP	PG-O2G	-2.14	1.51	1.56
6	L	600	ANP	C5-C4	2.13	1.46	1.40
6	O	600	ANP	C2-N3	2.10	1.35	1.32
6	O	600	ANP	PG-O3G	-2.10	1.51	1.56
6	A	600	ANP	PB-O3A	2.07	1.61	1.59
6	X	600	ANP	C2-N3	2.06	1.35	1.32
6	M	600	ANP	PG-O3G	-2.06	1.51	1.56
6	S	600	ANP	PG-O3G	-2.04	1.51	1.56
6	X	600	ANP	PB-O3A	2.03	1.61	1.59
6	L	600	ANP	PB-O3A	2.00	1.61	1.59
6	B	600	ANP	C2-N3	2.00	1.35	1.32

All (107) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	600	ANP	O1G-PG-N3B	-7.52	100.69	111.77
6	V	600	ANP	O1G-PG-N3B	-6.70	101.90	111.77
6	S	600	ANP	PA-O3A-PB	-6.58	109.44	132.62
6	L	600	ANP	O1G-PG-N3B	-6.56	102.11	111.77
6	F	600	ANP	O1G-PG-N3B	-6.29	102.50	111.77
6	J	600	ANP	O1G-PG-N3B	-6.16	102.70	111.77
6	U	600	ANP	O1G-PG-N3B	-5.74	103.31	111.77
6	U	600	ANP	O1B-PB-N3B	-5.22	104.08	111.77
6	C	600	ANP	O1G-PG-N3B	-5.15	104.19	111.77
6	B	600	ANP	O1G-PG-N3B	-5.12	104.23	111.77
6	F	600	ANP	O2B-PB-O1B	5.03	120.48	109.92
6	A	600	ANP	O2B-PB-O1B	5.03	120.47	109.92
6	S	600	ANP	O1G-PG-N3B	-4.98	104.44	111.77
6	M	600	ANP	O2B-PB-O1B	4.94	120.28	109.92
6	T	600	ANP	O1G-PG-N3B	-4.75	104.77	111.77
6	J	600	ANP	O2B-PB-O1B	4.75	119.89	109.92
6	D	600	ANP	O1G-PG-N3B	-4.71	104.83	111.77
6	C	600	ANP	O2B-PB-O1B	4.63	119.64	109.92
6	O	600	ANP	O2B-PB-O1B	4.53	119.43	109.92
6	X	600	ANP	O1G-PG-N3B	-4.48	105.17	111.77
6	O	600	ANP	O1G-PG-N3B	-4.21	105.57	111.77
6	L	600	ANP	O2B-PB-O1B	4.18	118.69	109.92
6	T	600	ANP	PA-O3A-PB	-4.12	118.11	132.62
6	M	600	ANP	O1G-PG-N3B	-4.11	105.72	111.77
6	S	600	ANP	O2B-PB-O1B	4.03	118.38	109.92

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	U	600	ANP	O2B-PB-O1B	4.02	118.35	109.92
6	A	600	ANP	O1B-PB-N3B	-4.01	105.87	111.77
6	D	600	ANP	O2B-PB-O1B	3.96	118.23	109.92
6	X	600	ANP	O2B-PB-O1B	3.86	118.02	109.92
6	K	600	ANP	O2B-PB-O1B	3.73	117.75	109.92
6	L	600	ANP	N3-C2-N1	-3.72	122.86	128.68
6	T	600	ANP	O2B-PB-O1B	3.71	117.69	109.92
6	D	600	ANP	N3-C2-N1	-3.70	122.90	128.68
6	K	600	ANP	O1G-PG-N3B	-3.69	106.34	111.77
6	O	600	ANP	O3G-PG-O2G	3.67	117.41	107.64
6	O	600	ANP	O2B-PB-O3A	3.65	116.82	104.64
6	T	600	ANP	C3'-C2'-C1'	3.62	106.43	100.98
6	C	600	ANP	N3-C2-N1	-3.59	123.07	128.68
6	F	600	ANP	O2B-PB-O3A	3.56	116.53	104.64
6	T	600	ANP	O1B-PB-N3B	-3.54	106.56	111.77
6	B	600	ANP	O2B-PB-O1B	3.48	117.22	109.92
6	K	600	ANP	N3-C2-N1	-3.42	123.33	128.68
6	U	600	ANP	PA-O3A-PB	-3.41	120.59	132.62
6	X	600	ANP	C3'-C2'-C1'	3.34	106.01	100.98
6	T	600	ANP	N3-C2-N1	-3.31	123.51	128.68
6	M	600	ANP	O3G-PG-O2G	3.29	116.41	107.64
6	J	600	ANP	N3-C2-N1	-3.27	123.56	128.68
6	B	600	ANP	N3-C2-N1	-3.19	123.70	128.68
6	V	600	ANP	N3-C2-N1	-3.18	123.70	128.68
6	A	600	ANP	N3-C2-N1	-3.15	123.75	128.68
6	S	600	ANP	N3-C2-N1	-3.09	123.85	128.68
6	F	600	ANP	N3-C2-N1	-3.07	123.88	128.68
6	M	600	ANP	N3-C2-N1	-3.06	123.89	128.68
6	O	600	ANP	N3-C2-N1	-3.06	123.89	128.68
6	O	600	ANP	C4-C5-N7	-3.01	106.27	109.40
6	A	600	ANP	C4-C5-N7	-3.00	106.27	109.40
6	A	600	ANP	O2B-PB-O3A	2.98	114.60	104.64
6	X	600	ANP	PA-O3A-PB	-2.98	122.12	132.62
6	J	600	ANP	C4-C5-N7	-2.90	106.38	109.40
6	O	600	ANP	O1B-PB-N3B	-2.87	107.54	111.77
6	F	600	ANP	O3G-PG-O2G	2.86	115.25	107.64
6	K	600	ANP	C3'-C2'-C1'	2.85	105.26	100.98
6	X	600	ANP	C4-C5-N7	-2.82	106.46	109.40
6	C	600	ANP	O2B-PB-O3A	2.82	114.04	104.64
6	V	600	ANP	PA-O3A-PB	-2.81	122.73	132.62
6	B	600	ANP	C3'-C2'-C1'	2.80	105.20	100.98
6	C	600	ANP	C4-C5-N7	-2.79	106.49	109.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	U	600	ANP	C3'-C2'-C1'	2.78	105.17	100.98
6	V	600	ANP	C4-C5-N7	-2.78	106.50	109.40
6	V	600	ANP	O2B-PB-O1B	2.73	115.65	109.92
6	V	600	ANP	O3G-PG-O2G	2.71	114.86	107.64
6	D	600	ANP	C2-N1-C6	2.69	123.36	118.75
6	U	600	ANP	N3-C2-N1	-2.68	124.48	128.68
6	M	600	ANP	C3'-C2'-C1'	2.66	104.98	100.98
6	M	600	ANP	O2B-PB-O3A	2.63	113.43	104.64
6	X	600	ANP	N3-C2-N1	-2.62	124.58	128.68
6	S	600	ANP	O3G-PG-O2G	2.59	114.55	107.64
6	F	600	ANP	PA-O3A-PB	-2.58	123.52	132.62
6	D	600	ANP	PA-O3A-PB	-2.58	123.55	132.62
6	C	600	ANP	O3G-PG-O2G	2.56	114.45	107.64
6	U	600	ANP	O3A-PB-N3B	2.55	113.66	106.59
6	X	600	ANP	O1B-PB-N3B	-2.52	108.05	111.77
6	U	600	ANP	O3G-PG-O2G	2.51	114.31	107.64
6	D	600	ANP	O3G-PG-O2G	2.50	114.30	107.64
6	V	600	ANP	C3'-C2'-C1'	2.50	104.74	100.98
6	U	600	ANP	C4-C5-N7	-2.49	106.80	109.40
6	D	600	ANP	O2B-PB-O3A	2.45	112.82	104.64
6	C	600	ANP	C3'-C2'-C1'	2.45	104.66	100.98
6	T	600	ANP	O3G-PG-O2G	2.37	113.95	107.64
6	O	600	ANP	C3'-C2'-C1'	2.35	104.52	100.98
6	K	600	ANP	C4-C5-N7	-2.35	106.95	109.40
6	K	600	ANP	O3G-PG-O2G	2.35	113.89	107.64
6	D	600	ANP	C3'-C2'-C1'	2.30	104.44	100.98
6	A	600	ANP	C2-N1-C6	2.24	122.58	118.75
6	M	600	ANP	O1B-PB-N3B	-2.18	108.57	111.77
6	L	600	ANP	O2B-PB-O3A	2.15	111.82	104.64
6	U	600	ANP	O5'-C5'-C4'	2.13	116.32	108.99
6	B	600	ANP	C4-C5-N7	-2.12	107.19	109.40
6	F	600	ANP	O4'-C1'-C2'	-2.09	103.87	106.93
6	L	600	ANP	O1B-PB-N3B	-2.09	108.70	111.77
6	M	600	ANP	O2A-PA-O1A	2.08	122.52	112.24
6	A	600	ANP	C3'-C2'-C1'	2.08	104.11	100.98
6	V	600	ANP	O1B-PB-N3B	-2.07	108.72	111.77
6	B	600	ANP	O2A-PA-O1A	2.06	122.43	112.24
6	F	600	ANP	C4-C5-N7	-2.04	107.27	109.40
6	A	600	ANP	O3G-PG-O1G	2.03	118.56	113.45
6	J	600	ANP	C3'-C2'-C1'	2.01	104.00	100.98

There are no chirality outliers.

All (67) torsion outliers are listed below:

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

*Continued on next page...*

*Continued from previous page...*

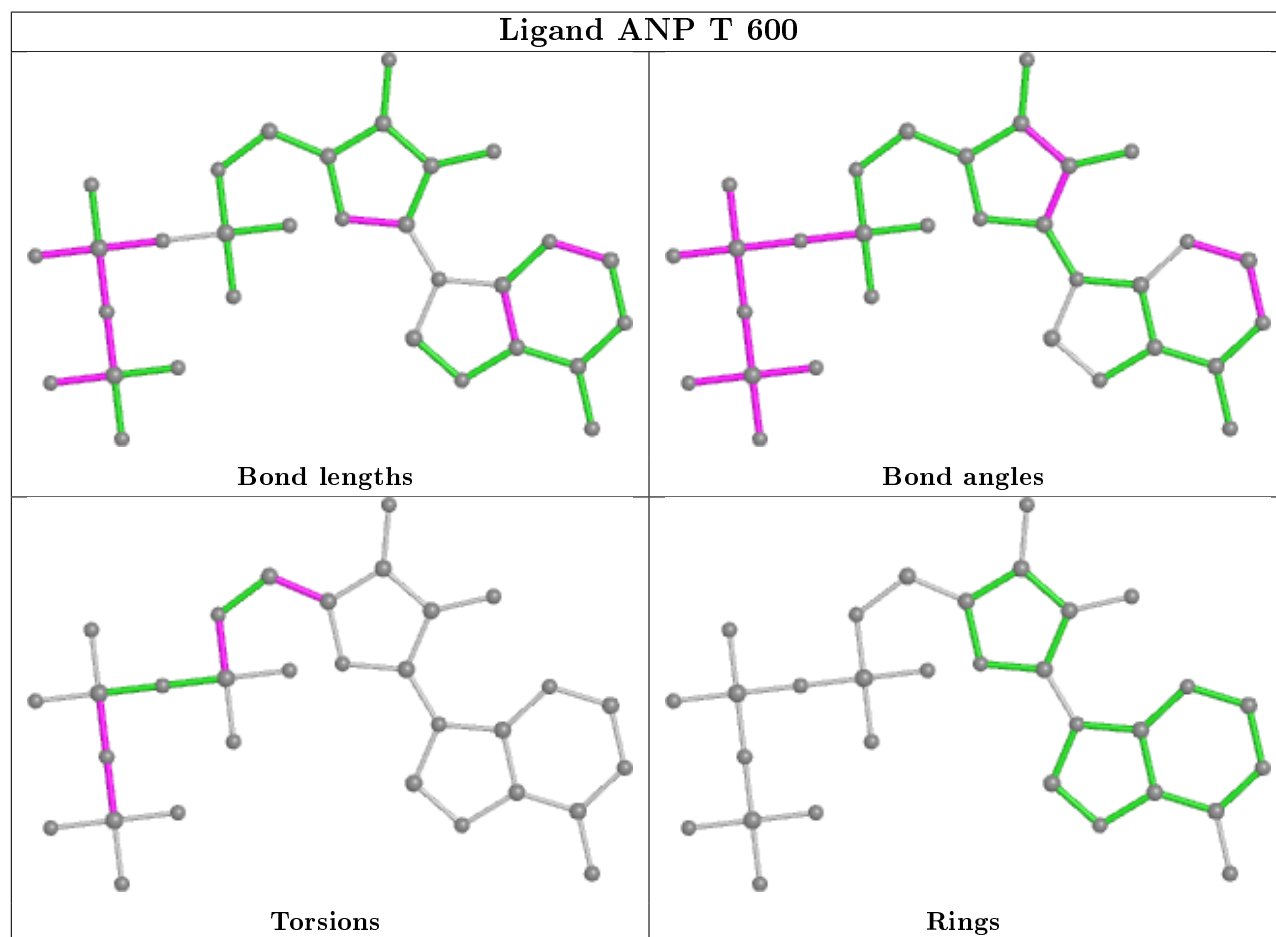
Mol	Chain	Res	Type	Atoms
6	D	600	ANP	PA-O3A-PB-O2B
6	A	600	ANP	PB-N3B-PG-O1G
6	A	600	ANP	PG-N3B-PB-O1B
6	X	600	ANP	PG-N3B-PB-O1B
6	X	600	ANP	PA-O3A-PB-O1B
6	X	600	ANP	PA-O3A-PB-O2B
6	F	600	ANP	O4'-C4'-C5'-O5'
6	T	600	ANP	C3'-C4'-C5'-O5'
6	S	600	ANP	O4'-C4'-C5'-O5'
6	S	600	ANP	C3'-C4'-C5'-O5'
6	F	600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

There are no ring outliers.

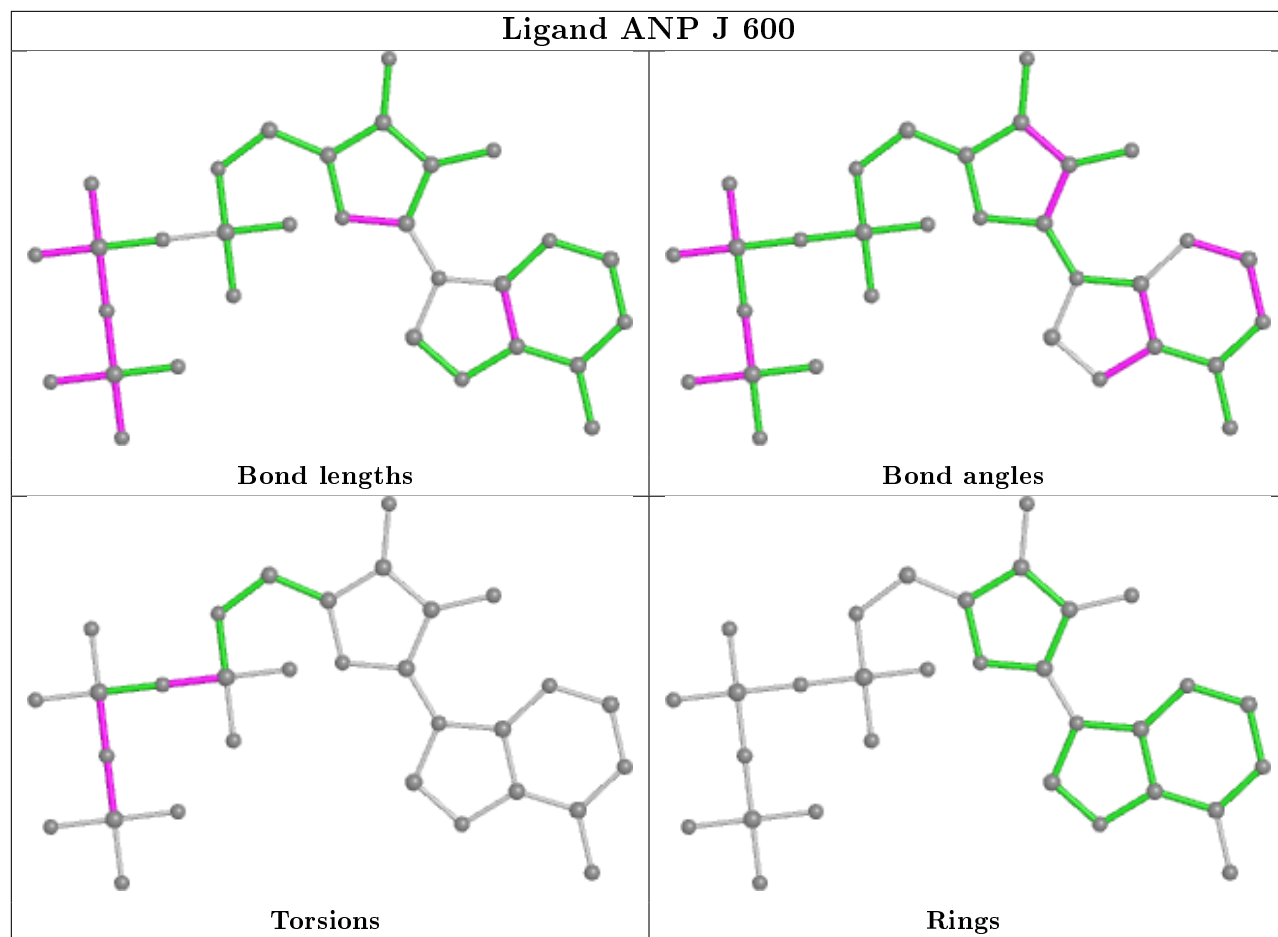
11 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	T	600	ANP	1	0
6	M	600	ANP	5	0
6	V	600	ANP	4	0
6	K	600	ANP	1	0
6	B	600	ANP	2	0
6	D	600	ANP	1	0
6	A	600	ANP	1	0
6	F	600	ANP	2	0
6	S	600	ANP	4	0
6	X	600	ANP	6	0
6	U	600	ANP	4	0

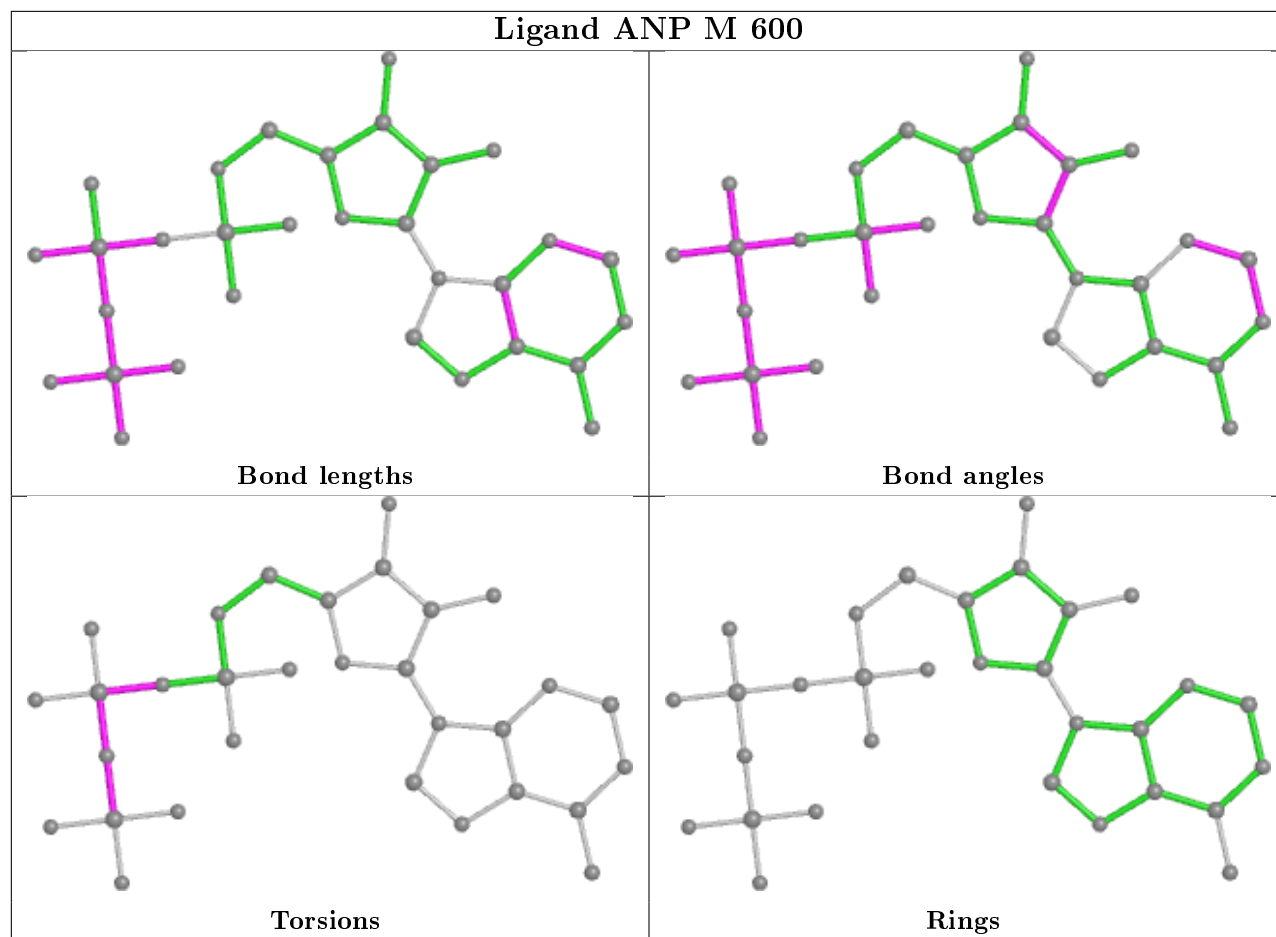
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

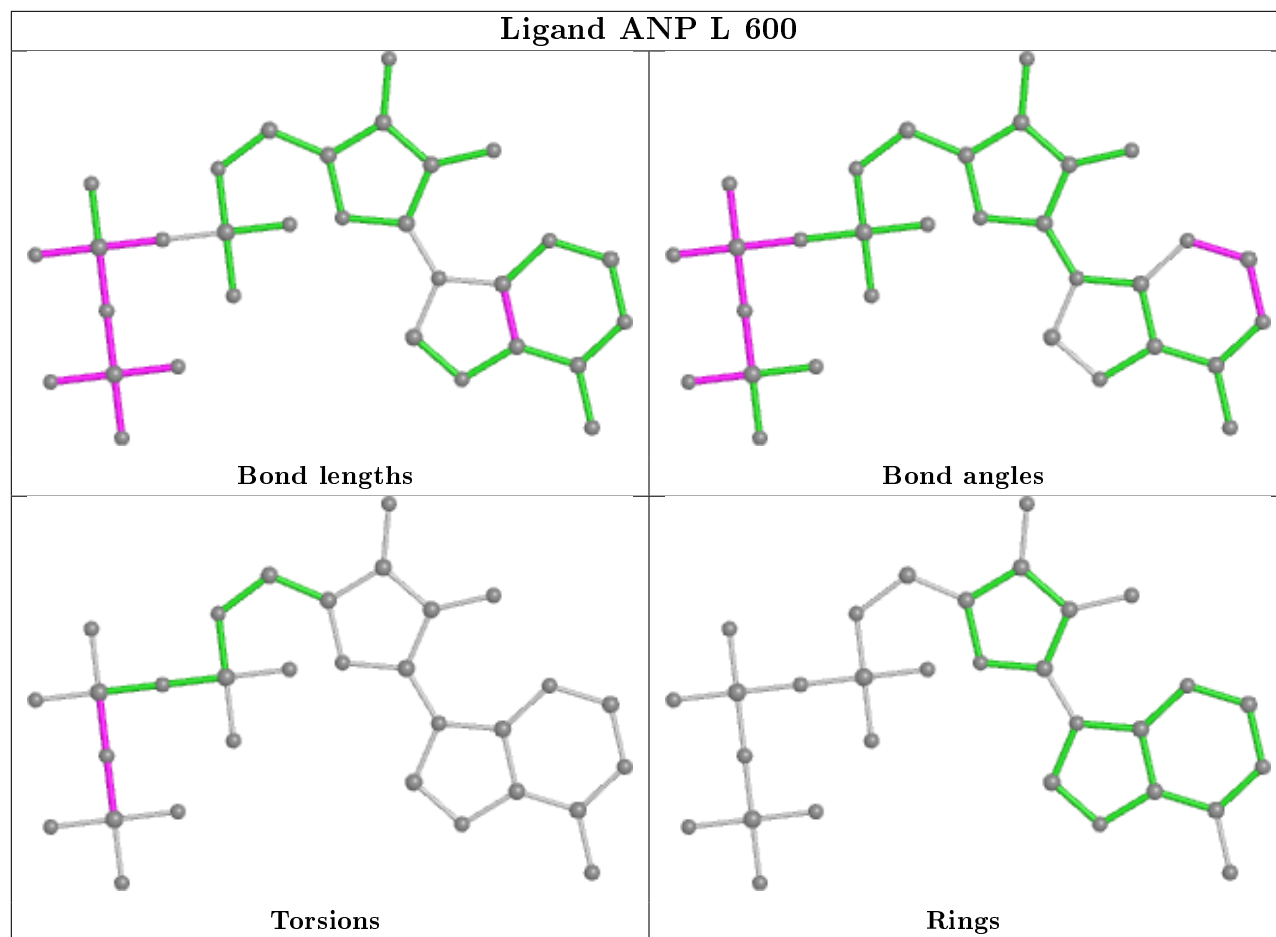


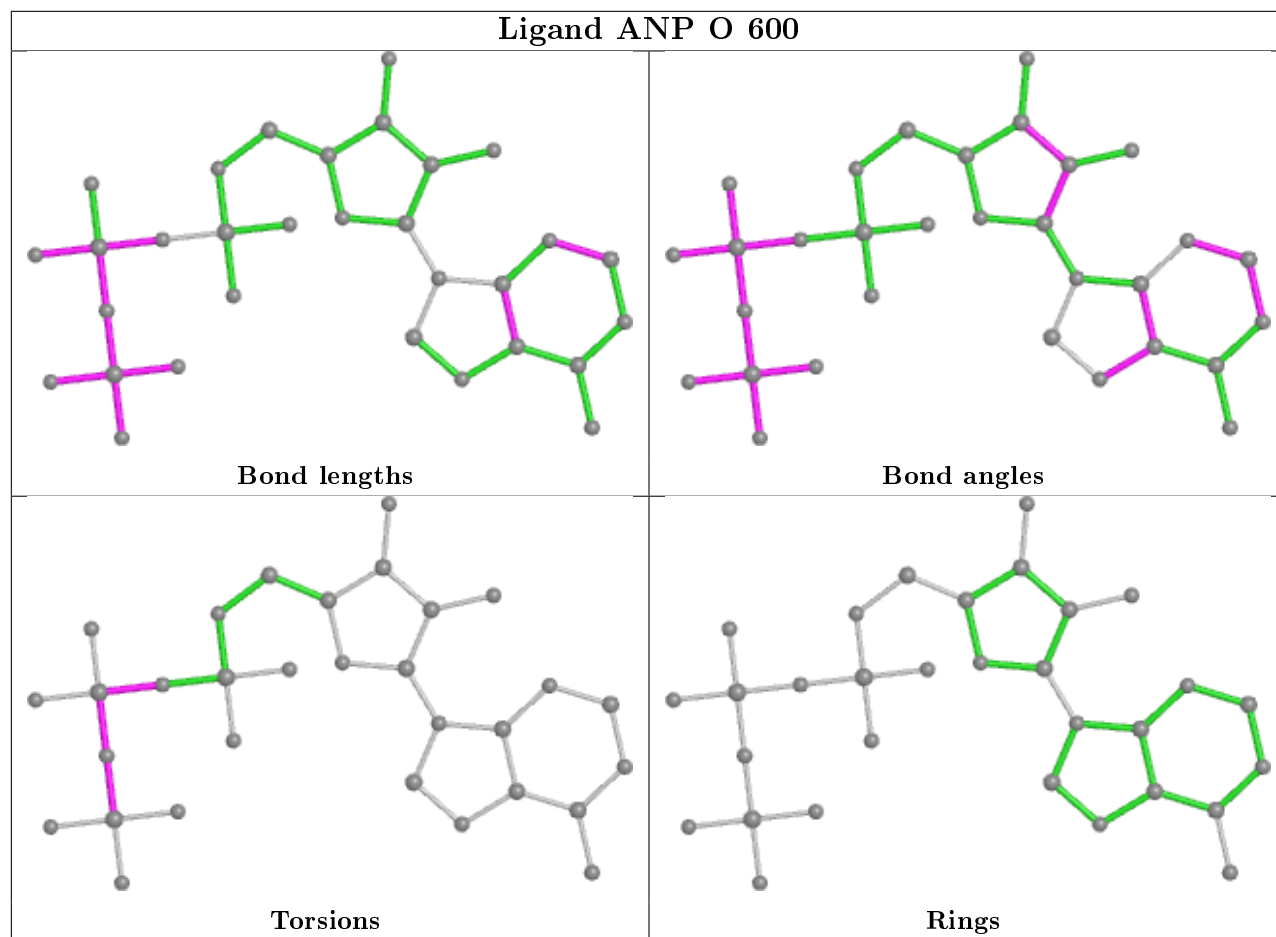
## Ligand ANP J 600

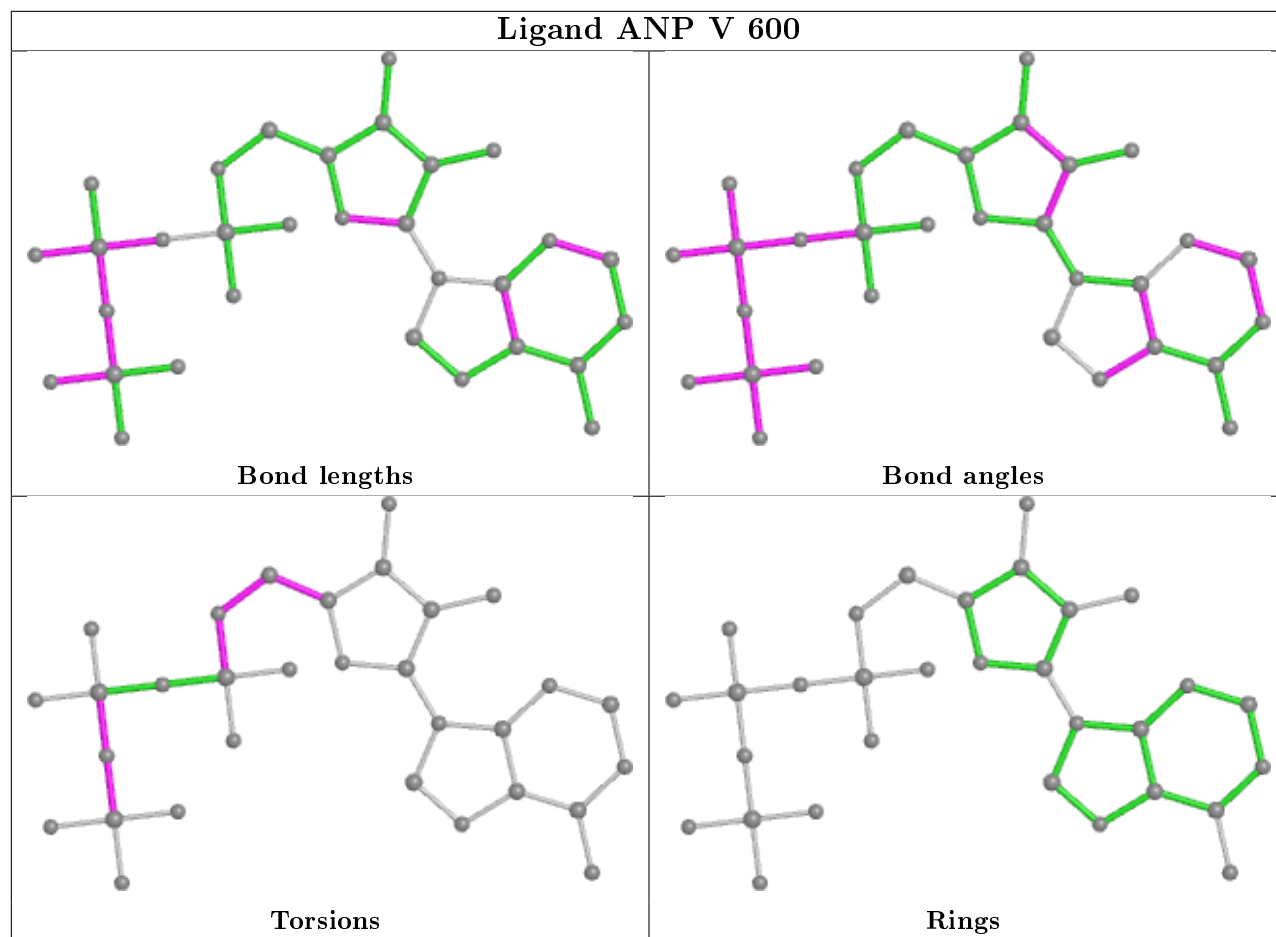


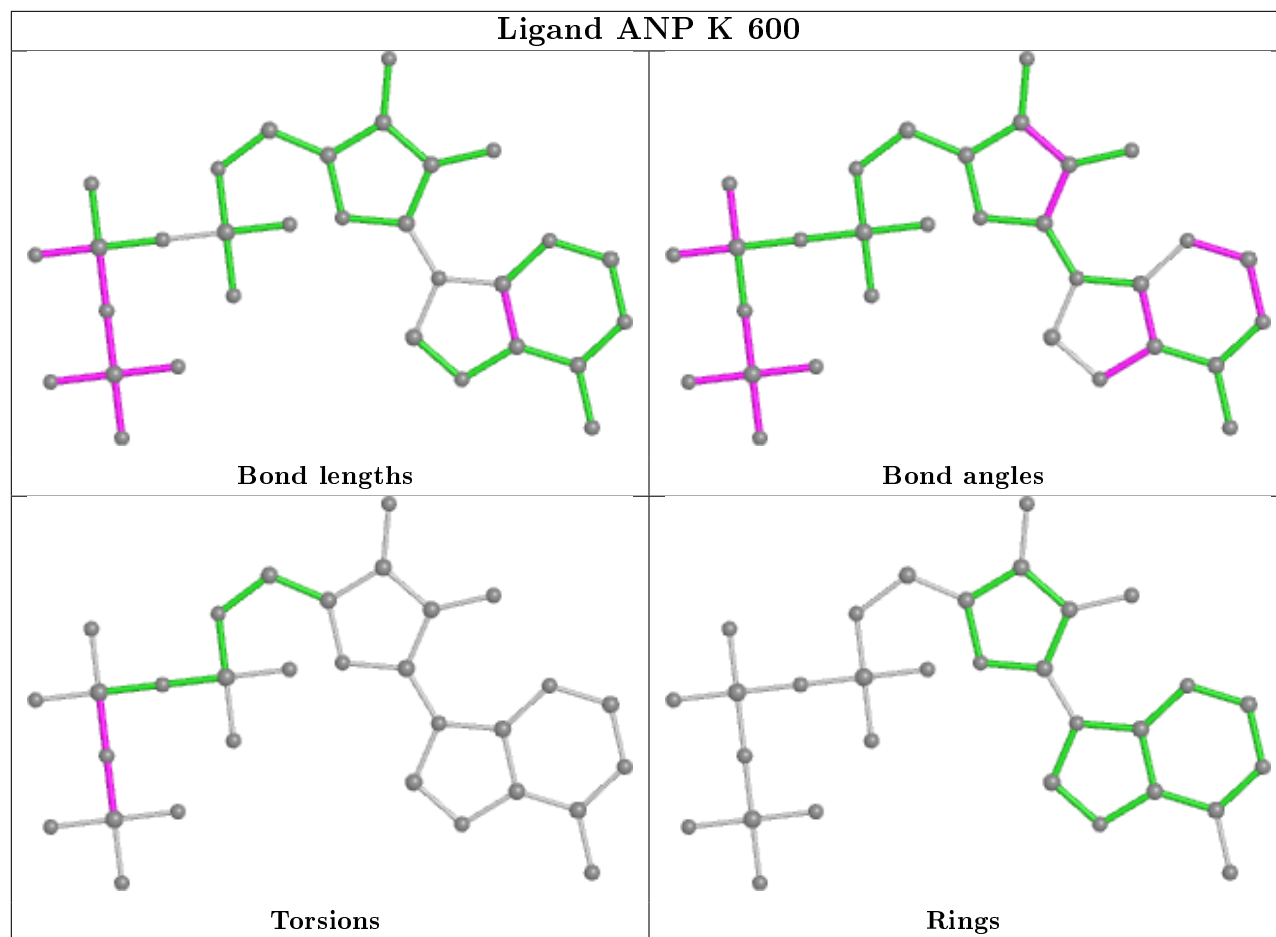


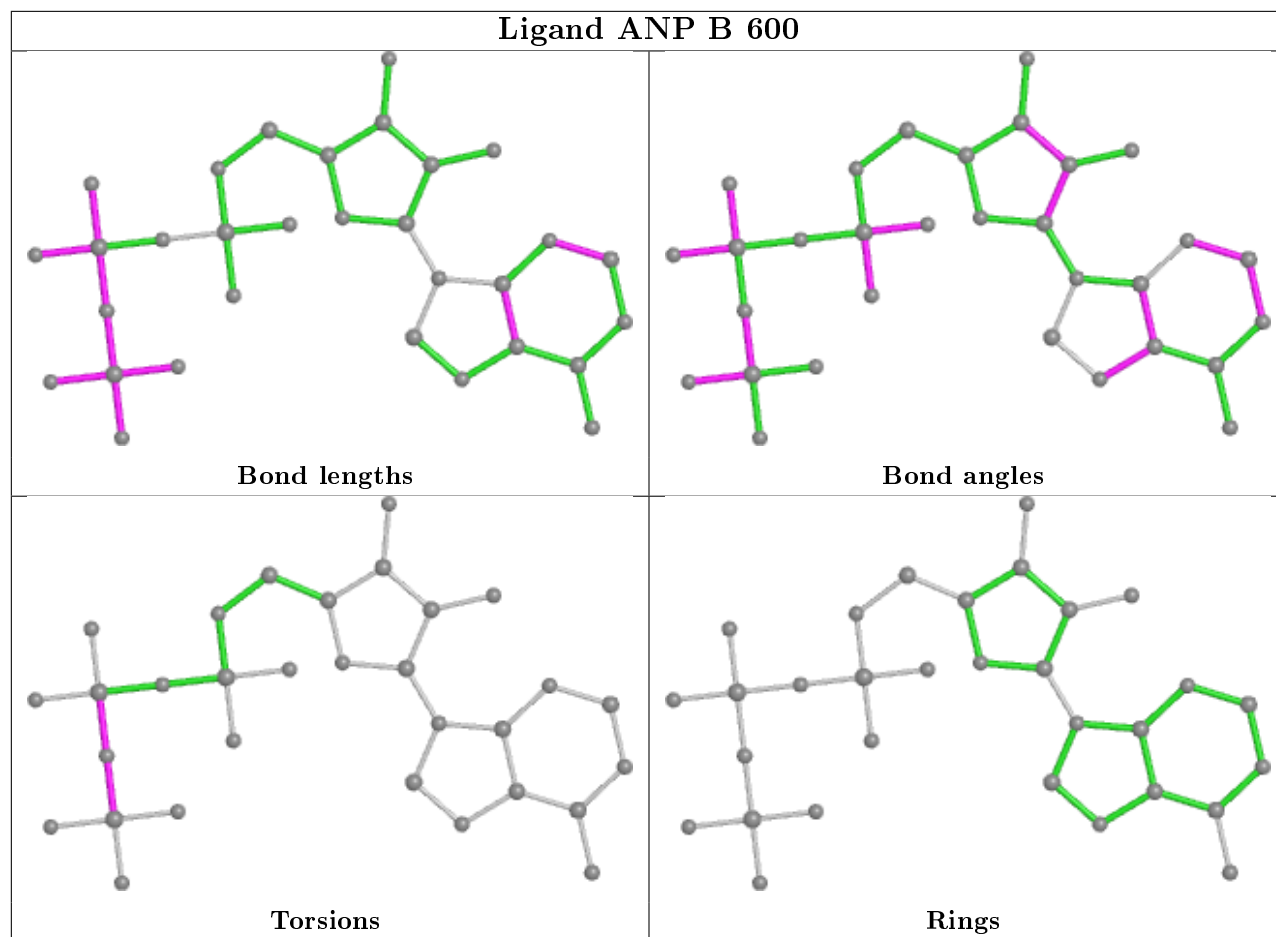


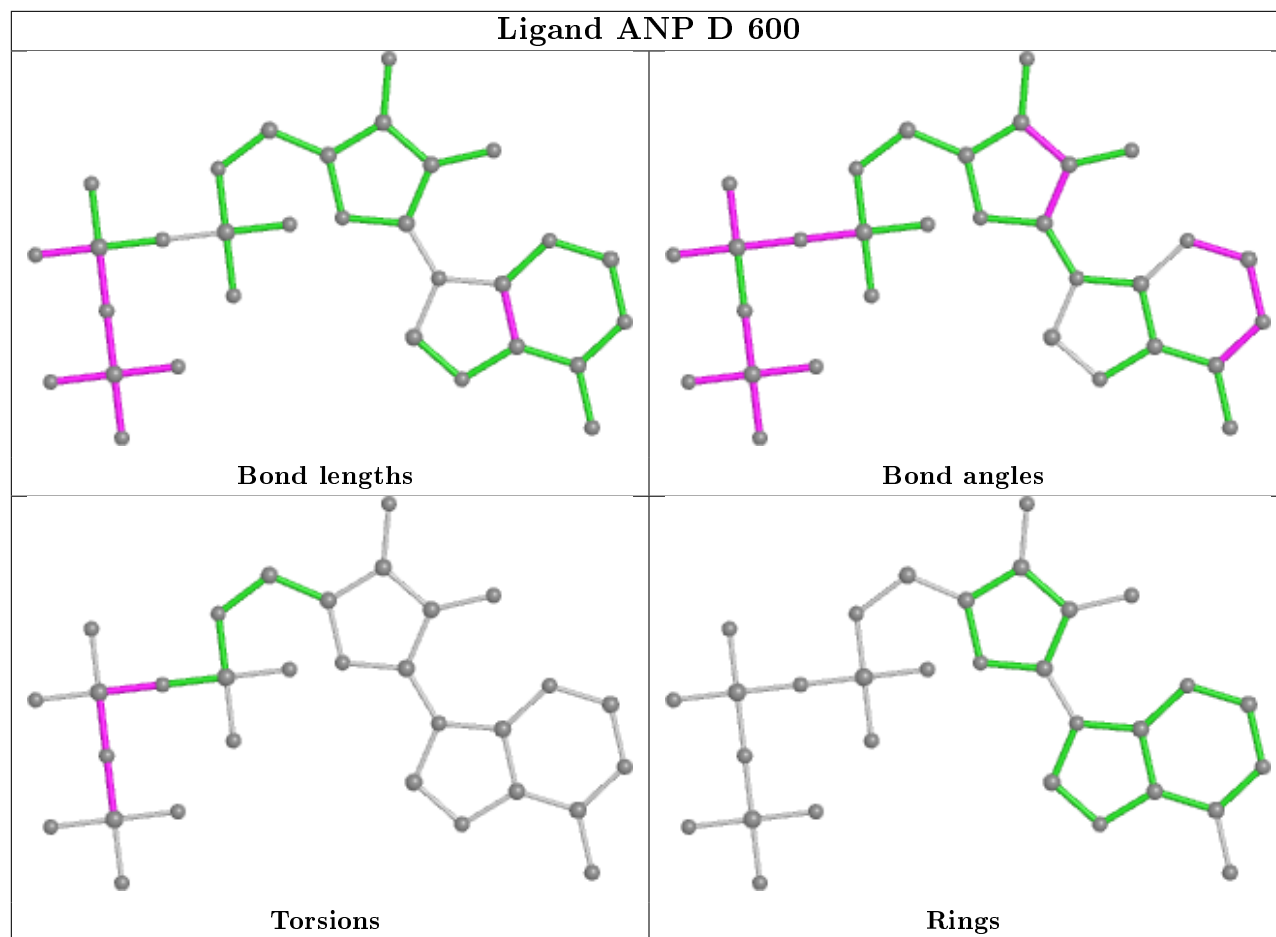


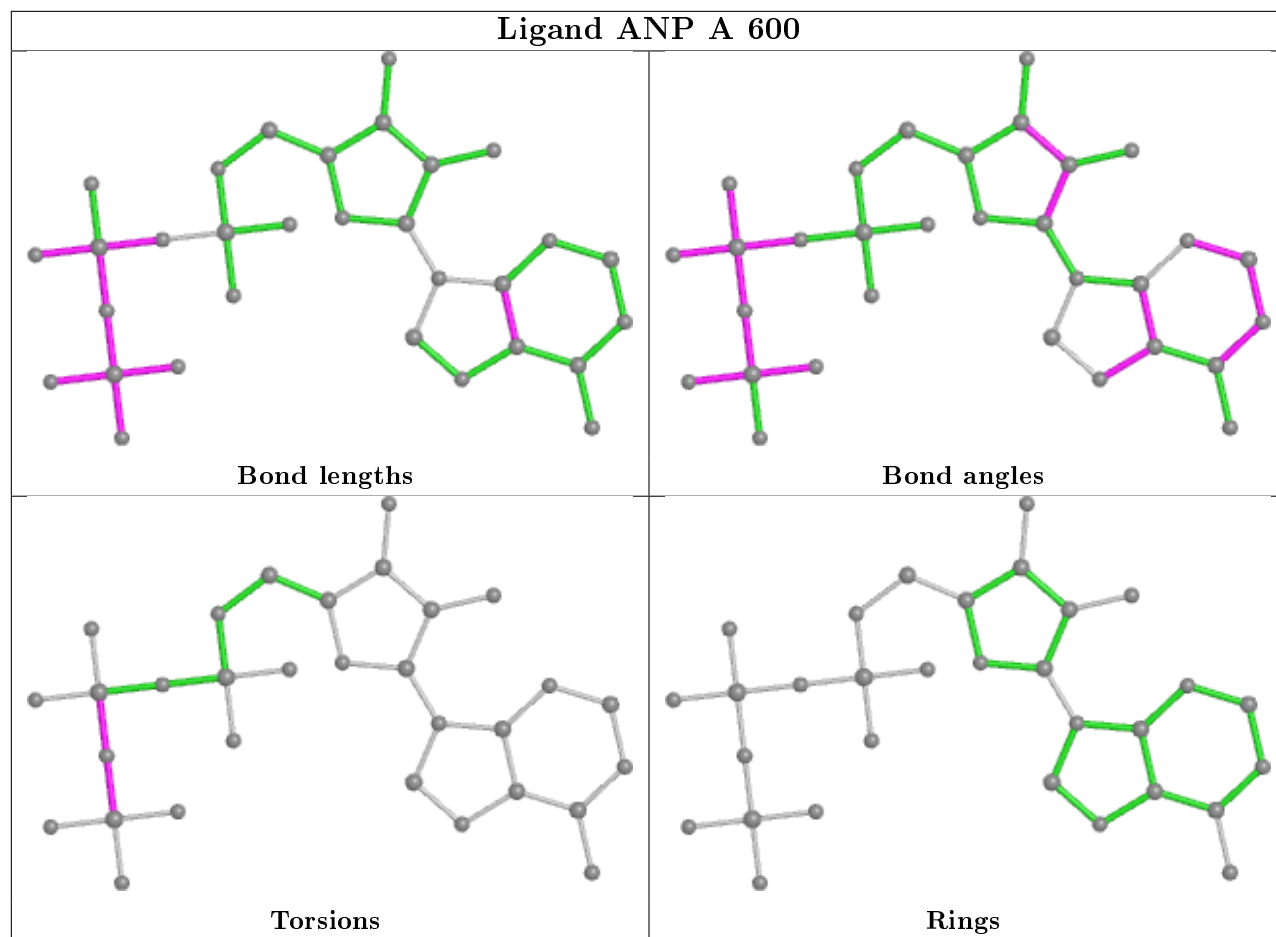




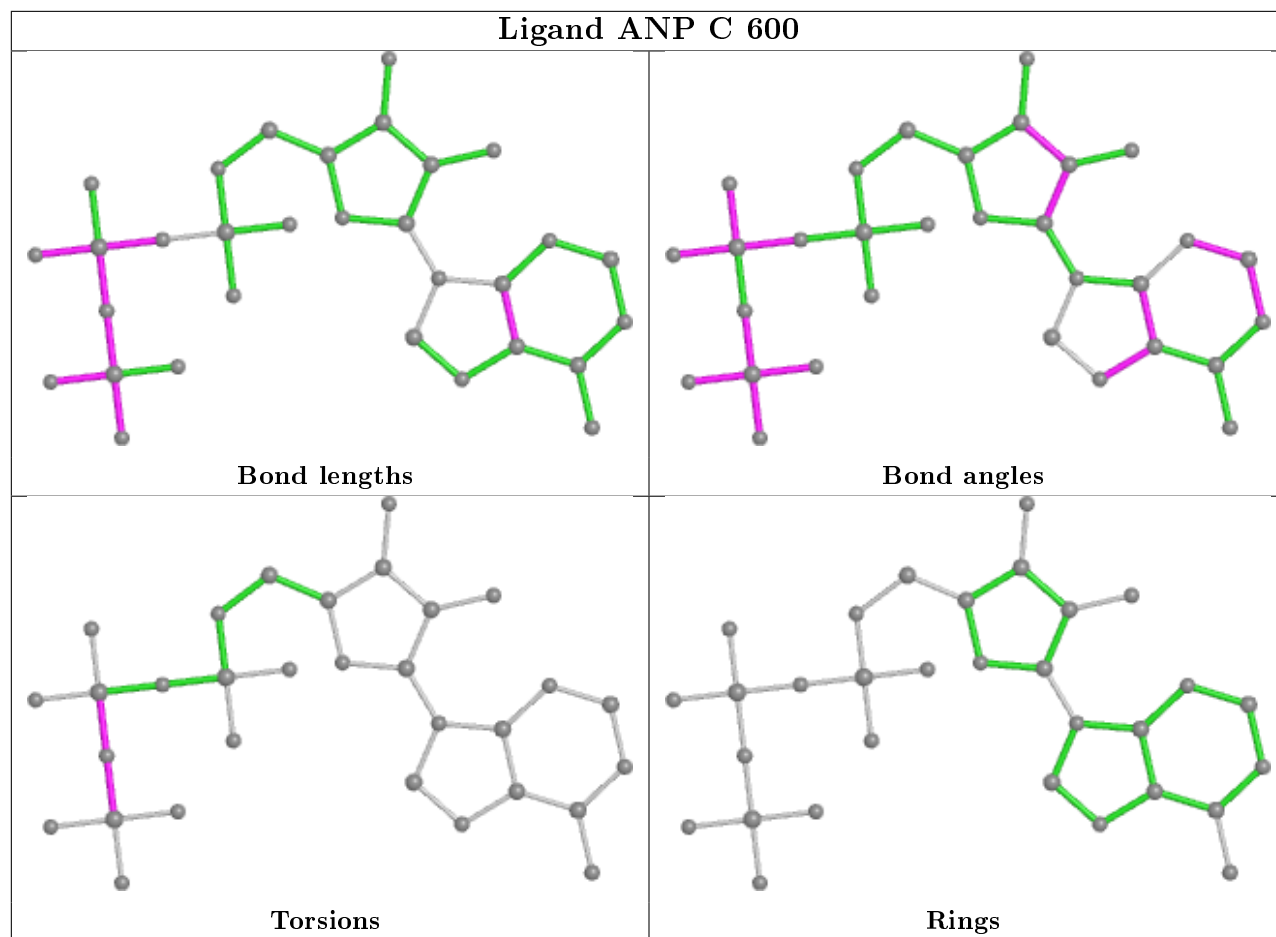


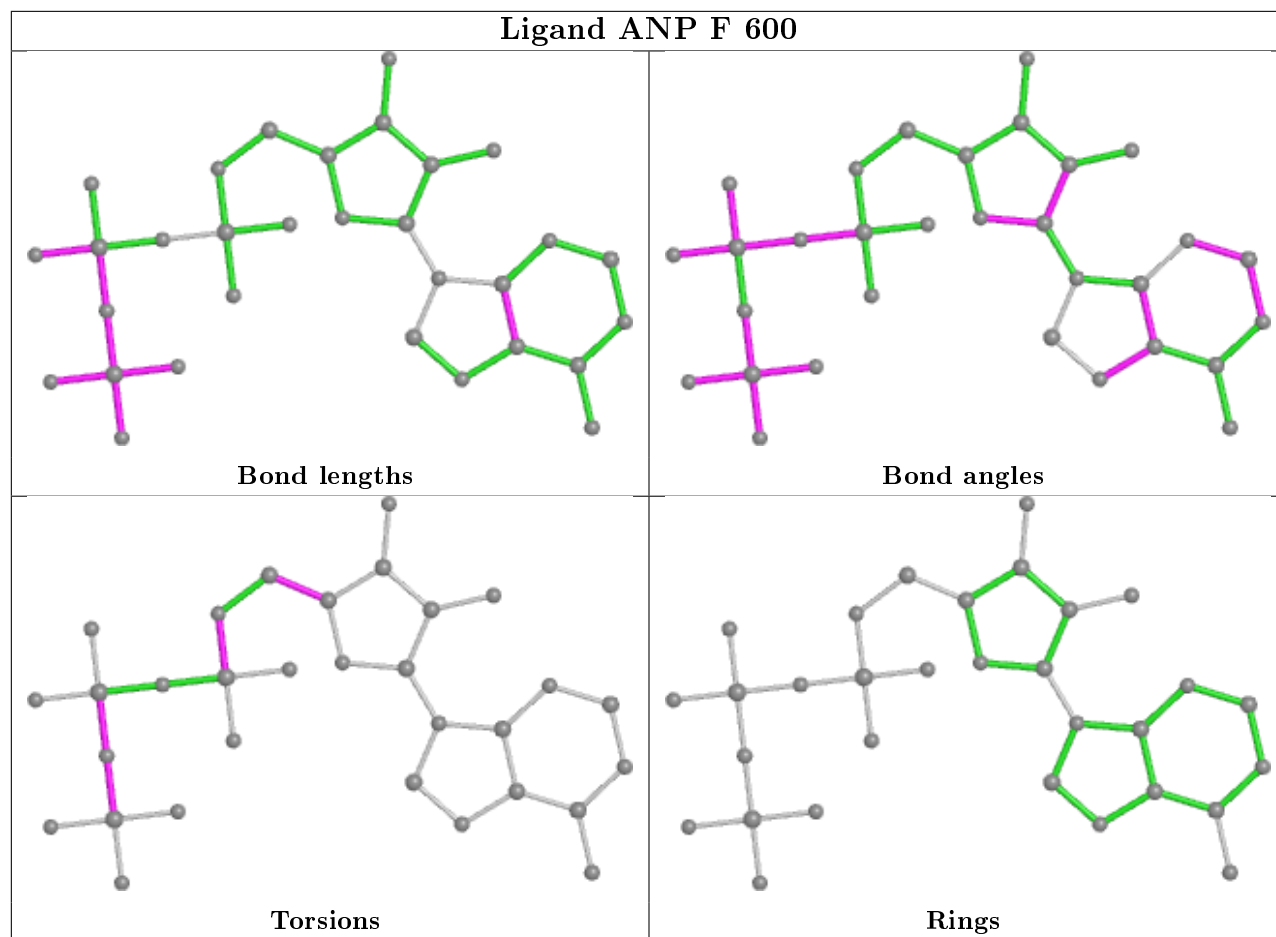




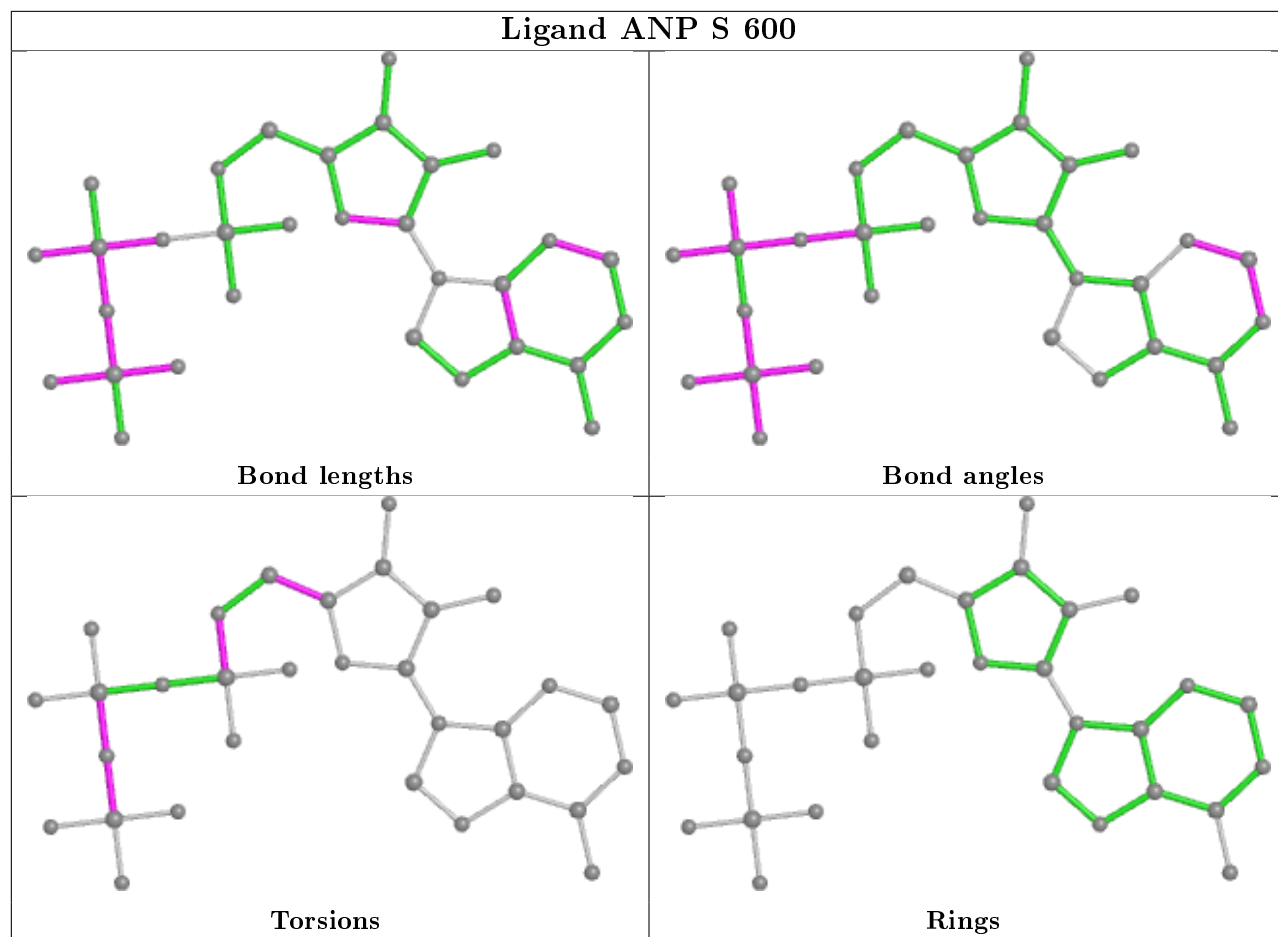


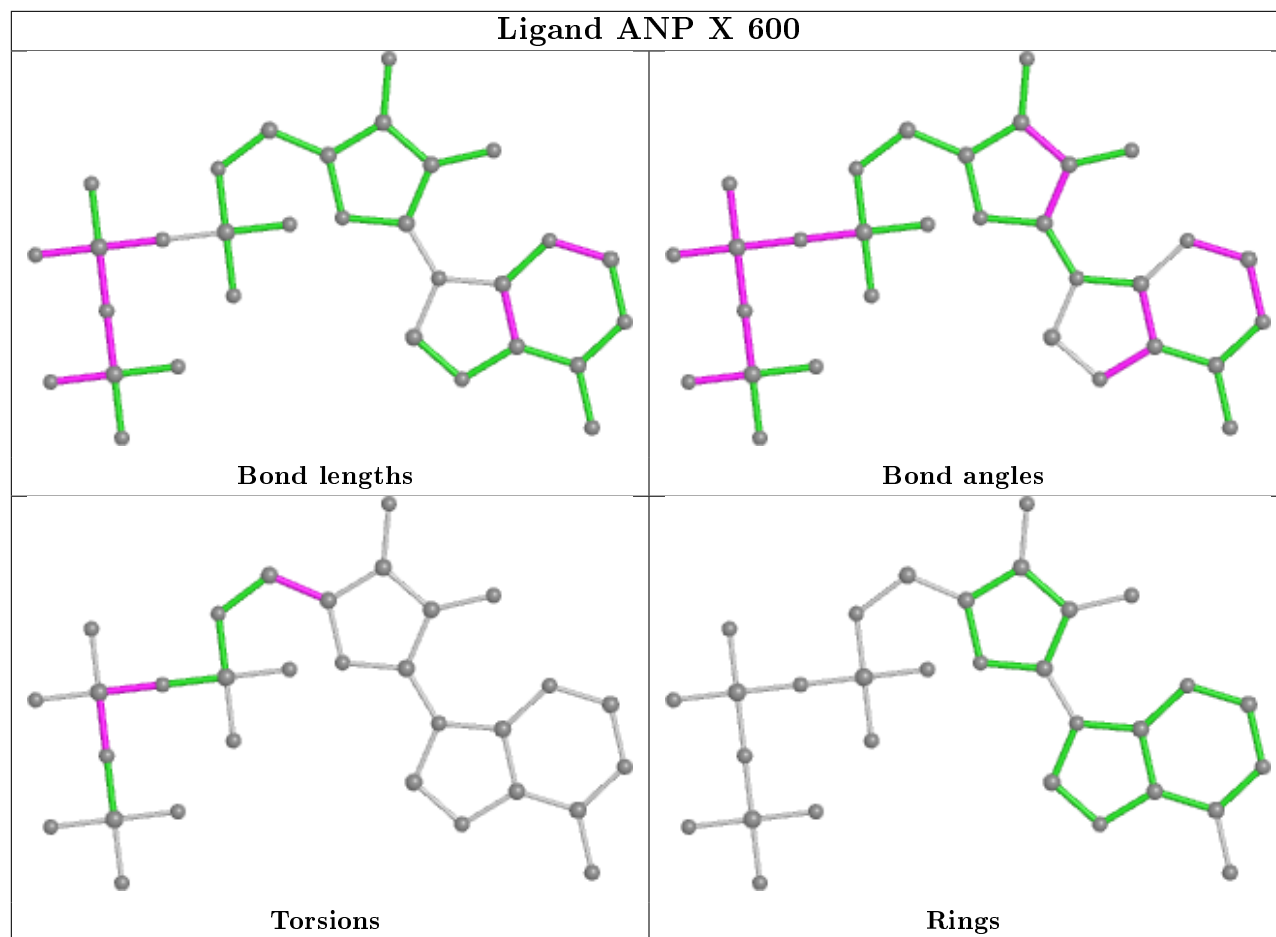


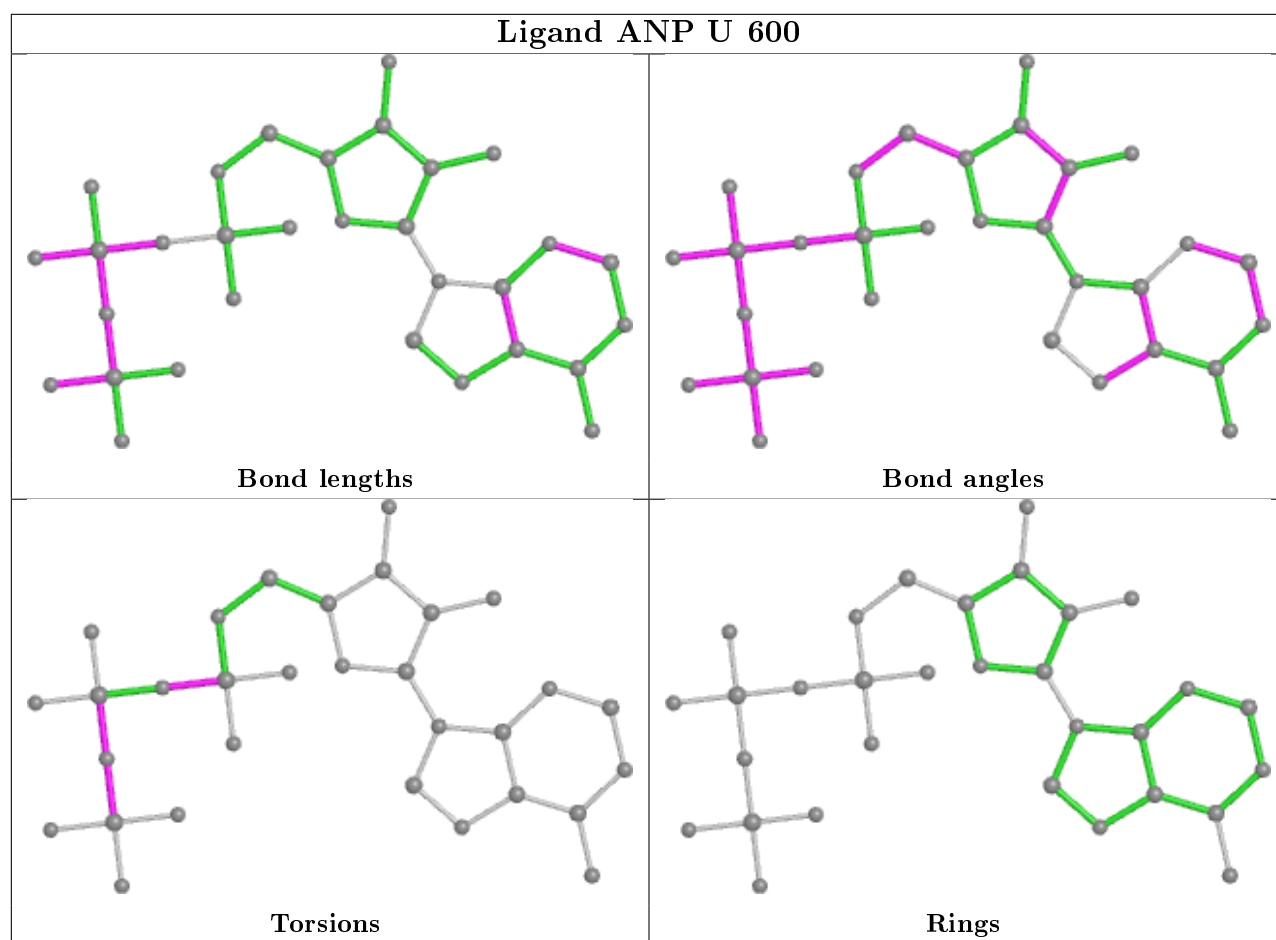




## Ligand ANP S 600







## 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%)	-0.00	1 (0%) 95 97	37, 55, 89, 139	0
1	B	483/510 (94%)	0.12	7 (1%) 75 80	35, 58, 109, 138	0
1	C	484/510 (94%)	0.16	11 (2%) 60 67	47, 74, 127, 169	0
1	J	481/510 (94%)	0.14	12 (2%) 57 64	45, 72, 114, 155	0
1	K	486/510 (95%)	0.13	9 (1%) 66 73	41, 64, 116, 150	0
1	L	482/510 (94%)	0.14	10 (2%) 63 70	46, 62, 113, 162	0
1	S	477/510 (93%)	1.31	129 (27%) 0 0	95, 123, 165, 179	0
1	T	478/510 (93%)	0.88	80 (16%) 1 1	93, 120, 148, 167	0
1	U	481/510 (94%)	1.28	108 (22%) 0 0	85, 120, 151, 163	0
2	D	470/484 (97%)	0.15	7 (1%) 73 79	43, 66, 102, 136	0
2	E	468/484 (96%)	0.19	18 (3%) 40 44	36, 61, 129, 168	0
2	F	469/484 (96%)	0.01	5 (1%) 80 85	42, 75, 98, 120	0
2	M	470/484 (97%)	0.41	31 (6%) 18 20	51, 81, 139, 168	0
2	N	470/484 (97%)	0.05	6 (1%) 77 82	42, 62, 117, 157	0
2	O	468/484 (96%)	0.16	12 (2%) 56 63	44, 70, 103, 129	0
2	V	470/484 (97%)	1.20	109 (23%) 0 0	85, 123, 151, 172	0
2	W	467/484 (96%)	1.16	109 (23%) 0 0	92, 107, 138, 156	0
2	X	469/484 (96%)	1.41	129 (27%) 0 0	66, 125, 158, 176	0
3	G	266/278 (95%)	0.70	26 (9%) 7 7	49, 102, 128, 137	0
3	P	244/278 (87%)	1.75	92 (37%) 0 0	50, 117, 137, 152	0
3	Y	200/278 (71%)	2.31	106 (53%) 0 0	89, 116, 141, 152	0
4	H	122/138 (88%)	0.64	13 (10%) 6 5	96, 126, 153, 160	0
4	Q	83/138 (60%)	1.89	35 (42%) 0 0	113, 135, 153, 156	0
4	Z	17/138 (12%)	0.53	3 (17%) 1 1	134, 138, 144, 146	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
5	1	27/61 (44%)	1.36	9 (33%) 0 0	119, 126, 131, 136	0
5	I	49/61 (80%)	0.43	6 (12%) 4 4	98, 111, 131, 143	0
5	R	34/61 (55%)	1.00	8 (23%) 0 0	107, 118, 147, 152	0
All	All	9597/10377 (92%)	0.59	1091 (11%) 5 5	35, 90, 146, 179	0

All (1091) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	X	37	LEU	11.7
1	S	43	VAL	10.8
2	X	83	ILE	10.4
2	X	217	LEU	9.8
1	T	203	CYS	9.3
1	T	36	VAL	9.1
1	U	36	VAL	8.8
2	X	209	LEU	8.8
1	U	37	GLY	8.4
1	U	388	VAL	8.4
2	X	32	ALA	8.3
4	Q	15	ALA	8.3
3	P	53	LYS	8.3
2	X	30	LEU	8.2
4	Q	49	VAL	8.2
2	X	77	LEU	8.2
2	E	457	PHE	8.1
2	X	39	ILE	8.1
1	U	499	LEU	7.8
2	X	46	LEU	7.7
1	U	392	LEU	7.7
1	S	44	PHE	7.7
3	Y	108	VAL	7.6
2	V	432	VAL	7.6
3	P	47	ALA	7.6
1	S	385	LEU	7.6
2	X	7	THR	7.5
3	Y	95	VAL	7.4
2	X	31	PRO	7.4
2	M	467	VAL	7.3
2	V	46	LEU	7.3
4	Q	83	LEU	7.2
3	Y	164	ILE	7.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	X	63	ALA	7.2
4	Q	84	CYS	7.0
1	T	207	ALA	7.0
3	P	126	ILE	6.9
2	X	210	GLU	6.8
2	X	54	LEU	6.8
1	U	27	LEU	6.8
1	T	202	TYR	6.7
3	Y	212	TYR	6.7
3	P	95	VAL	6.7
1	U	35	ALA	6.7
4	Q	77	VAL	6.6
2	W	59	VAL	6.6
2	M	457	PHE	6.5
1	U	34	LEU	6.5
3	Y	146	ILE	6.5
3	Y	145	LEU	6.5
3	P	36	LYS	6.5
4	Q	90	ALA	6.5
1	S	388	VAL	6.4
1	T	124	ASP	6.4
2	V	33	ILE	6.4
1	U	125	ALA	6.4
1	U	266	ALA	6.3
3	P	93	LYS	6.3
1	U	85	LYS	6.3
1	S	447	ILE	6.3
2	V	198	TYR	6.2
3	P	164	ILE	6.2
1	U	384	ALA	6.2
2	X	23	VAL	6.1
1	U	30	THR	6.1
2	X	28	SER	6.1
1	U	32	ARG	6.1
3	P	29	THR	6.1
2	W	444	VAL	6.1
3	P	25	ILE	6.0
1	S	81	ASP	6.0
2	W	305	THR	6.0
3	Y	36	LYS	6.0
2	X	53	HIS	6.0
2	X	43	GLN	5.9

*Continued on next page...*



*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	X	87	VAL	5.9
3	Y	110	ILE	5.9
1	S	414	ALA	5.9
1	U	84	VAL	5.9
2	V	52	GLN	5.8
3	Y	165	PHE	5.8
1	J	499	LEU	5.8
3	P	39	ILE	5.8
1	S	446	LEU	5.8
2	W	391	LEU	5.7
2	X	8	PRO	5.7
2	W	389	ALA	5.7
4	Q	72	GLY	5.7
2	W	23	VAL	5.7
1	T	491	LEU	5.6
2	W	143	LEU	5.6
2	V	22	ASP	5.6
1	S	61	VAL	5.6
4	Q	48	THR	5.6
1	S	457	GLY	5.5
2	W	9	ILE	5.5
1	T	205	TYR	5.5
1	S	448	TYR	5.5
5	R	21	ILE	5.5
2	X	246	GLU	5.5
3	Y	78	THR	5.4
3	P	34	ALA	5.4
1	U	131	ALA	5.4
1	U	89	LEU	5.4
3	Y	91	LEU	5.4
3	P	100	ASN	5.4
1	S	460	LEU	5.3
2	V	9	ILE	5.3
2	X	238	THR	5.3
1	U	75	ILE	5.3
2	W	83	ILE	5.3
2	V	6	SER	5.3
2	W	47	VAL	5.3
1	S	68	LEU	5.3
2	M	466	VAL	5.2
3	Y	261	ALA	5.2
1	U	26	ASN	5.2

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	W	82	PRO	5.2
3	Y	99	LEU	5.2
1	S	352	ILE	5.2
2	X	304	VAL	5.2
2	V	116	PRO	5.2
2	X	24	HIS	5.2
1	S	438	LEU	5.2
1	T	26	ASN	5.2
3	Y	120	ARG	5.2
2	X	29	GLU	5.2
3	P	182	ILE	5.2
1	U	194	GLY	5.1
5	R	30	GLN	5.1
4	H	72	GLY	5.1
2	V	7	THR	5.1
2	W	133	ILE	5.1
2	W	342	LEU	5.1
2	X	207	ILE	5.1
3	Y	211	GLU	5.1
2	V	34	LEU	5.1
2	V	39	ILE	5.1
2	V	175	ALA	5.1
2	W	119	ALA	5.1
2	X	239	ILE	5.1
2	W	103	ILE	5.0
3	Y	83	LEU	5.0
2	W	395	GLU	5.0
4	H	129	VAL	5.0
1	U	482	LEU	5.0
2	V	179	GLY	5.0
2	W	394	ASP	5.0
1	S	503	THR	5.0
1	U	454	HIS	5.0
2	W	219	PHE	5.0
1	S	33	VAL	5.0
1	S	491	LEU	5.0
2	V	134	LEU	5.0
2	V	30	LEU	4.9
1	S	389	ALA	4.9
1	S	493	LYS	4.9
3	Y	140	PHE	4.9
2	W	390	ILE	4.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	U	61	VAL	4.9
2	X	181	PHE	4.9
2	W	473	LEU	4.9
2	X	76	VAL	4.9
2	V	94	ARG	4.9
1	T	150	THR	4.9
2	W	77	LEU	4.8
2	X	70	LEU	4.8
2	V	62	ILE	4.8
2	W	8	PRO	4.8
2	X	184	PHE	4.8
3	Y	266	GLU	4.8
1	U	509	THR	4.8
3	Y	150	LEU	4.8
1	S	418	GLN	4.8
2	N	387	ILE	4.8
2	X	48	LEU	4.8
3	Y	230	ILE	4.8
2	W	437	THR	4.7
3	G	165	PHE	4.7
3	Y	130	ILE	4.7
2	W	306	SER	4.7
2	V	32	ALA	4.7
2	W	440	SER	4.7
2	V	393	MET	4.7
2	X	79	THR	4.6
2	V	25	PHE	4.6
3	P	91	LEU	4.6
1	S	202	TYR	4.6
1	U	41	ALA	4.6
1	U	83	LEU	4.6
2	X	36	ALA	4.6
3	P	46	GLU	4.6
1	S	499	LEU	4.6
1	U	44	PHE	4.6
2	D	467	VAL	4.6
2	X	38	GLU	4.6
1	S	70	PRO	4.6
1	U	71	GLY	4.6
1	T	234	VAL	4.6
3	Y	153	VAL	4.6
2	V	91	THR	4.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	X	180	GLY	4.6
5	1	9	SER	4.6
1	S	34	LEU	4.5
2	W	57	ASN	4.5
2	V	81	GLY	4.5
2	W	474	ALA	4.5
1	S	167	GLU	4.5
2	V	99	ILE	4.5
1	S	392	LEU	4.5
4	Q	50	GLU	4.5
1	S	387	GLN	4.5
1	B	410	SER	4.4
3	Y	265	ASN	4.4
4	Q	79	PRO	4.4
2	V	83	ILE	4.4
2	X	27	GLN	4.4
2	W	55	GLY	4.4
1	U	122	PRO	4.4
2	V	10	THR	4.4
3	Y	264	THR	4.4
3	Y	148	ASP	4.4
2	X	254	PHE	4.4
2	V	50	VAL	4.4
4	Z	135	SER	4.4
3	Y	2	THR	4.4
3	Y	166	TYR	4.4
2	W	46	LEU	4.4
1	U	232	ILE	4.4
2	M	387	ILE	4.4
1	U	119	GLY	4.3
2	V	100	GLY	4.3
2	X	50	VAL	4.3
2	X	391	LEU	4.3
4	Q	70	ILE	4.3
2	V	118	HIS	4.3
3	P	171	SER	4.3
2	W	34	LEU	4.3
1	S	324	THR	4.3
3	Y	103	PRO	4.3
1	U	126	ALA	4.3
2	O	7	THR	4.3
2	V	440	SER	4.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	U	385	LEU	4.2
2	X	75	LYS	4.2
1	S	57	PHE	4.2
4	H	70	ILE	4.2
1	K	411	ASP	4.2
2	V	117	ILE	4.2
1	S	485	ILE	4.2
1	C	457	GLY	4.2
1	S	27	LEU	4.2
2	E	466	VAL	4.2
2	V	218	VAL	4.2
1	T	35	ALA	4.2
2	W	413	PHE	4.2
4	H	88	ILE	4.2
1	S	204	VAL	4.2
3	Y	151	LEU	4.2
1	U	72	GLN	4.2
1	U	380	ALA	4.2
1	S	502	ALA	4.1
3	P	37	ALA	4.1
3	Y	156	ALA	4.1
3	P	133	ILE	4.1
1	K	488	LYS	4.1
1	S	157	ALA	4.1
3	Y	37	ALA	4.1
2	W	22	ASP	4.1
1	T	54	LEU	4.1
2	V	443	ALA	4.1
1	S	420	LEU	4.1
2	V	13	VAL	4.1
3	Y	269	ASP	4.1
2	W	144	LEU	4.1
1	U	195	SER	4.1
3	Y	175	PHE	4.1
1	S	63	GLY	4.0
1	U	87	GLY	4.0
3	Y	225	GLY	4.0
4	H	95	SER	4.0
2	X	183	VAL	4.0
2	X	35	ASN	4.0
1	T	204	VAL	4.0
4	Q	89	GLU	4.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	Y	92	ALA	4.0
3	Y	96	ARG	4.0
2	X	78	ASP	4.0
2	W	307	VAL	4.0
2	M	445	LEU	4.0
4	Q	17	PRO	4.0
2	X	14	THR	4.0
2	W	71	VAL	4.0
4	H	15	ALA	4.0
2	E	473	LEU	4.0
3	Y	87	ILE	4.0
4	Q	34	ALA	4.0
1	S	419	THR	3.9
2	X	147	TYR	3.9
2	V	98	VAL	3.9
3	Y	104	ASN	3.9
3	Y	170	VAL	3.9
1	U	57	PHE	3.9
4	Q	71	SER	3.9
2	D	390	ILE	3.9
2	W	398	GLU	3.9
3	P	31	LEU	3.9
1	S	205	TYR	3.9
2	X	71	VAL	3.9
1	T	218	LEU	3.9
1	T	51	ALA	3.9
2	W	131	ALA	3.9
1	U	496	LEU	3.9
2	X	88	GLY	3.9
3	Y	114	ILE	3.9
1	S	429	LEU	3.8
2	W	45	LYS	3.8
3	P	234	ARG	3.8
2	V	303	SER	3.8
4	H	26	GLU	3.8
4	Q	103	ASN	3.8
3	P	76	ALA	3.8
3	Y	141	GLN	3.8
2	V	8	PRO	3.8
1	U	441	GLU	3.8
2	X	113	LEU	3.8
3	G	76	ALA	3.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	T	49	ILE	3.8
1	U	338	ALA	3.8
2	M	391	LEU	3.8
2	W	15	ALA	3.8
2	X	16	VAL	3.8
1	U	63	GLY	3.8
2	X	9	ILE	3.8
2	X	92	LEU	3.8
2	X	314	ALA	3.8
2	W	358	LEU	3.7
3	Y	42	LYS	3.7
3	P	128	LEU	3.7
2	V	394	ASP	3.7
2	W	51	ALA	3.7
1	U	76	VAL	3.7
3	Y	1	ALA	3.7
2	M	462	GLY	3.7
4	H	32	LEU	3.7
2	X	279	VAL	3.7
1	U	42	ARG	3.7
3	P	35	GLU	3.7
2	W	397	SER	3.7
2	V	421	ALA	3.7
3	Y	263	ILE	3.7
2	V	31	PRO	3.7
2	V	453	PRO	3.7
3	G	258	THR	3.7
1	S	195	SER	3.7
2	M	441	PHE	3.7
1	T	142	ARG	3.7
1	U	40	ILE	3.7
1	U	270	TYR	3.7
1	T	27	LEU	3.7
1	T	186	LEU	3.7
3	P	48	GLU	3.7
1	S	32	ARG	3.7
2	W	128	SER	3.7
2	X	68	GLU	3.7
1	S	482	LEU	3.6
1	U	148	VAL	3.6
1	U	55	VAL	3.6
2	V	14	THR	3.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	U	33	VAL	3.6
1	U	503	THR	3.6
3	Y	77	ILE	3.6
3	P	220	THR	3.6
3	P	174	SER	3.6
2	V	70	LEU	3.6
2	X	302	GLY	3.6
3	Y	262	VAL	3.6
3	P	185	ALA	3.6
5	1	12	ALA	3.6
1	S	415	SER	3.6
2	V	140	VAL	3.6
4	H	27	VAL	3.6
2	X	219	PHE	3.5
1	S	62	LYS	3.5
3	P	108	VAL	3.5
1	L	509	THR	3.5
1	T	183	ASP	3.5
2	W	64	MET	3.5
3	Y	222	MET	3.5
2	W	445	LEU	3.5
3	Y	173	LEU	3.5
2	W	240	ALA	3.5
2	D	473	LEU	3.5
1	U	82	ARG	3.5
2	X	42	PRO	3.5
2	X	69	GLY	3.5
3	P	228	ALA	3.5
3	Y	275	SER	3.5
2	V	69	GLY	3.5
1	S	435	TYR	3.5
2	V	367	HIS	3.5
2	M	439	ALA	3.5
1	T	184	THR	3.5
2	N	388	ILE	3.5
2	E	474	ALA	3.5
3	Y	218	MET	3.5
5	1	11	ALA	3.5
2	X	82	PRO	3.5
2	W	43	GLN	3.5
3	P	32	SER	3.4
2	X	249	GLN	3.4

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	U	117	ILE	3.4
3	P	87	ILE	3.4
1	S	151	GLY	3.4
2	X	51	ALA	3.4
1	S	443	GLN	3.4
2	V	27	GLN	3.4
2	V	57	ASN	3.4
4	Q	35	LYS	3.4
5	R	22	ARG	3.4
1	U	139	LEU	3.4
2	X	171	ILE	3.4
1	S	64	MET	3.4
1	U	455	LEU	3.4
3	Y	116	MET	3.4
3	P	30	ARG	3.4
2	W	396	LEU	3.4
3	Y	118	LEU	3.4
2	W	39	ILE	3.4
2	V	181	PHE	3.4
1	U	296	TYR	3.4
2	X	215	VAL	3.4
4	Q	46	VAL	3.4
2	V	219	PHE	3.4
1	U	86	GLU	3.4
2	M	438	VAL	3.4
2	W	25	PHE	3.3
2	X	117	ILE	3.3
3	P	223	ALA	3.3
4	Q	75	ALA	3.3
3	Y	260	GLN	3.3
2	V	12	LYS	3.3
3	Y	93	LYS	3.3
2	W	120	ASP	3.3
2	X	26	GLU	3.3
3	Y	215	ALA	3.3
3	Y	268	VAL	3.3
1	U	505	SER	3.3
2	V	148	ALA	3.3
2	V	475	ALA	3.3
3	P	227	ALA	3.3
1	U	291	PRO	3.3
3	Y	119	LEU	3.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	G	262	VAL	3.3
2	X	109	ILE	3.3
2	X	243	PHE	3.3
3	Y	217	GLN	3.3
1	T	135	ALA	3.3
1	T	489	GLY	3.3
1	S	66	LEU	3.3
1	T	420	LEU	3.3
2	V	396	LEU	3.3
2	W	42	PRO	3.3
3	P	175	PHE	3.3
3	P	77	ILE	3.3
2	V	395	GLU	3.3
3	P	23	MET	3.3
3	Y	214	LEU	3.3
1	T	473	TYR	3.2
2	X	21	VAL	3.2
2	V	446	GLU	3.2
2	X	317	LEU	3.2
3	P	151	LEU	3.2
1	S	150	THR	3.2
2	X	81	GLY	3.2
5	1	13	TYR	3.2
1	S	495	LEU	3.2
1	U	335	ASP	3.2
1	S	498	SER	3.2
4	H	55	GLY	3.2
2	W	370	VAL	3.2
1	K	484	GLU	3.2
1	S	89	LEU	3.2
2	V	398	GLU	3.2
3	Y	35	GLU	3.2
1	S	65	ALA	3.2
2	X	108	PRO	3.2
3	Y	88	HIS	3.2
3	Y	97	ARG	3.2
1	T	78	PHE	3.2
3	Y	109	THR	3.2
2	W	29	GLU	3.2
2	V	119	ALA	3.2
3	P	81	LYS	3.2
2	E	467	VAL	3.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	Y	6	VAL	3.2
1	T	158	LEU	3.2
1	U	337	SER	3.2
1	U	341	PRO	3.2
3	Y	3	LEU	3.2
2	X	148	ALA	3.1
2	E	453	PRO	3.1
5	1	15	ASN	3.1
2	V	444	VAL	3.1
1	T	75	ILE	3.1
3	P	54	ASN	3.1
3	Y	138	PRO	3.1
2	D	7	THR	3.1
2	W	89	ARG	3.1
2	W	168	GLN	3.1
3	Y	149	LYS	3.1
1	S	489	GLY	3.1
1	U	446	LEU	3.1
2	X	99	ILE	3.1
3	Y	144	ALA	3.1
1	T	509	THR	3.1
3	Y	142	GLU	3.1
1	U	396	LEU	3.1
2	W	450	ASP	3.1
1	J	471	LEU	3.1
2	X	130	SER	3.1
3	G	50	LEU	3.1
2	X	33	ILE	3.1
2	V	356	ARG	3.1
3	P	180	LYS	3.1
3	Y	154	MET	3.1
1	S	235	ALA	3.1
1	S	236	ALA	3.1
1	S	496	LEU	3.1
3	G	146	ILE	3.1
5	1	44	TYR	3.0
3	P	225	GLY	3.0
2	M	403	THR	3.0
2	V	23	VAL	3.0
1	T	314	LEU	3.0
2	V	54	LEU	3.0
2	W	250	ASP	3.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	P	73	LEU	3.0
1	S	71	GLY	3.0
1	T	119	GLY	3.0
2	V	261	PHE	3.0
2	W	14	THR	3.0
4	Q	76	THR	3.0
1	L	412	LEU	3.0
2	V	216	ALA	3.0
3	P	231	SER	3.0
1	J	447	ILE	3.0
2	E	458	TYR	3.0
1	T	208	VAL	3.0
2	M	394	ASP	3.0
2	W	436	ASP	3.0
1	S	255	ILE	3.0
2	X	242	TYR	3.0
4	Q	78	GLN	3.0
1	S	183	ASP	3.0
2	W	277	SER	3.0
1	T	131	ALA	3.0
2	V	214	LYS	3.0
1	T	122	PRO	3.0
2	V	73	GLY	3.0
2	V	220	GLY	3.0
2	X	276	PRO	3.0
2	E	390	ILE	3.0
2	O	398	GLU	3.0
2	W	27	GLN	3.0
3	G	2	THR	3.0
3	P	86	SER	3.0
2	X	323	ALA	3.0
3	P	105	ALA	3.0
1	S	470	PHE	3.0
3	Y	38	LYS	3.0
2	X	47	VAL	3.0
3	P	136	ASP	2.9
2	X	213	SER	2.9
1	U	105	LEU	2.9
2	V	194	GLY	2.9
3	P	219	LEU	2.9
1	S	153	LYS	2.9
1	U	411	ASP	2.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	W	24	HIS	2.9
1	U	442	GLU	2.9
2	W	70	LEU	2.9
3	P	50	LEU	2.9
1	S	383	LYS	2.9
2	X	361	ALA	2.9
2	V	441	PHE	2.9
1	S	30	THR	2.9
2	V	327	ALA	2.9
1	S	69	GLU	2.9
2	W	104	ASP	2.9
2	V	48	LEU	2.9
2	X	85	VAL	2.9
5	1	16	VAL	2.9
2	V	51	ALA	2.9
1	T	118	ASP	2.9
3	P	230	ILE	2.9
1	S	287	LEU	2.9
2	W	147	TYR	2.9
2	V	110	LYS	2.9
1	S	337	SER	2.9
3	Y	162	ILE	2.9
2	W	357	LEU	2.9
2	X	10	THR	2.9
2	V	215	VAL	2.9
2	E	456	ALA	2.9
1	U	115	ASN	2.9
2	X	313	PRO	2.9
1	U	151	GLY	2.9
2	X	275	ILE	2.9
1	U	383	LYS	2.9
2	W	48	LEU	2.9
1	S	384	ALA	2.9
2	O	320	PRO	2.9
4	Q	14	PHE	2.8
1	T	41	ALA	2.8
3	Y	226	TYR	2.8
5	I	10	TYR	2.8
1	S	87	GLY	2.8
2	W	302	GLY	2.8
2	X	12	LYS	2.8
3	G	98	HIS	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
4	Q	36	SER	2.8
2	W	60	ARG	2.8
2	V	399	GLN	2.8
2	X	318	THR	2.8
2	M	443	ALA	2.8
2	M	468	ALA	2.8
2	V	177	ALA	2.8
3	P	42	LYS	2.8
3	P	216	ASN	2.8
2	W	242	TYR	2.8
1	S	42	ARG	2.8
2	W	184	PHE	2.8
3	P	51	PHE	2.8
1	S	186	LEU	2.8
3	P	150	LEU	2.8
3	Y	219	LEU	2.8
5	R	28	GLU	2.8
1	S	104	GLY	2.8
1	U	489	GLY	2.8
4	Q	87	ALA	2.8
1	C	410	SER	2.8
1	B	499	LEU	2.8
5	I	15	ASN	2.8
2	X	59	VAL	2.8
1	U	304	HIS	2.8
3	Y	163	SER	2.8
2	V	26	GLU	2.8
2	M	143	LEU	2.8
2	X	305	THR	2.8
2	V	201	MET	2.8
1	S	129	SER	2.8
1	U	465	GLU	2.8
5	1	10	TYR	2.8
2	W	78	ASP	2.8
2	V	302	GLY	2.8
1	S	445	PRO	2.8
2	X	102	PRO	2.8
5	I	47	TYR	2.8
2	V	209	LEU	2.8
2	W	441	PHE	2.8
2	X	95	ILE	2.8
1	S	67	ASN	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	P	43	LYS	2.8
2	W	36	ALA	2.7
1	U	412	LEU	2.7
1	S	36	VAL	2.7
2	X	121	PRO	2.7
2	W	435	LYS	2.7
2	X	316	ASP	2.7
1	U	182	LEU	2.7
3	G	1	ALA	2.7
1	B	473	TYR	2.7
1	K	481	LEU	2.7
2	V	37	LEU	2.7
3	P	233	ARG	2.7
4	H	111	ASN	2.7
2	W	463	ILE	2.7
3	Y	270	ILE	2.7
1	J	507	VAL	2.7
2	W	467	VAL	2.7
2	X	98	VAL	2.7
1	S	293	ARG	2.7
3	Y	259	ARG	2.7
1	J	470	PHE	2.7
3	P	183	PHE	2.7
3	Y	224	GLN	2.7
2	X	96	ILE	2.7
3	P	74	ILE	2.7
2	W	456	ALA	2.7
3	G	261	ALA	2.7
1	C	462	ARG	2.7
1	S	168	LEU	2.7
1	T	360	TYR	2.7
3	G	133	ILE	2.7
1	S	316	GLU	2.7
3	P	252	SER	2.7
1	T	256	GLY	2.7
2	V	211	GLY	2.7
1	A	499	LEU	2.7
2	V	35	ASN	2.7
2	V	95	ILE	2.7
2	X	240	ALA	2.7
3	P	156	ALA	2.7
1	T	101	VAL	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	Y	31	LEU	2.7
2	W	446	GLU	2.7
2	X	153	ILE	2.7
3	G	77	ILE	2.7
3	P	212	TYR	2.7
1	S	200	LYS	2.7
2	W	204	THR	2.7
1	B	397	ALA	2.6
1	L	407	GLN	2.6
1	T	157	ALA	2.6
2	X	55	GLY	2.6
3	P	169	PRO	2.6
1	S	76	VAL	2.6
1	S	189	LYS	2.6
2	W	72	ARG	2.6
1	S	185	ILE	2.6
2	V	147	TYR	2.6
3	P	255	TYR	2.6
3	Y	139	THR	2.6
3	Y	258	THR	2.6
1	T	295	ALA	2.6
1	U	389	ALA	2.6
2	W	439	ALA	2.6
2	X	321	ALA	2.6
2	X	118	HIS	2.6
1	S	218	LEU	2.6
1	U	491	LEU	2.6
2	W	295	ARG	2.6
3	P	217	GLN	2.6
1	T	185	ILE	2.6
1	T	233	ILE	2.6
3	Y	89	SER	2.6
2	W	392	GLY	2.6
2	X	236	GLY	2.6
1	S	312	ALA	2.6
1	S	193	ASN	2.6
2	X	49	GLU	2.6
3	P	7	GLU	2.6
2	N	391	LEU	2.6
4	H	69	PHE	2.6
2	O	467	VAL	2.6
2	V	234	LEU	2.6

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	S	91	LYS	2.6
1	S	442	GLU	2.6
2	O	430	LYS	2.6
2	X	11	GLY	2.6
1	U	193	ASN	2.6
3	G	268	VAL	2.6
3	P	75	VAL	2.6
1	S	267	LEU	2.6
2	F	318	THR	2.6
2	X	86	PRO	2.6
2	V	24	HIS	2.6
1	B	407	GLN	2.6
1	U	204	VAL	2.6
2	O	396	LEU	2.6
2	M	393	MET	2.6
1	L	448	TYR	2.6
1	U	448	TYR	2.6
2	X	131	ALA	2.6
3	P	256	ASN	2.6
2	X	319	ASP	2.6
1	T	71	GLY	2.6
1	S	505	SER	2.6
1	S	48	ASN	2.5
3	P	90	GLN	2.5
4	Z	121	ALA	2.5
1	J	481	LEU	2.5
1	S	507	VAL	2.5
1	U	300	VAL	2.5
1	T	32	ARG	2.5
2	F	214	LYS	2.5
1	S	123	ILE	2.5
3	P	215	ALA	2.5
2	V	47	VAL	2.5
2	W	73	GLY	2.5
1	B	393	LYS	2.5
2	M	6	SER	2.5
3	Y	4	LYS	2.5
1	S	494	GLU	2.5
3	P	179	GLU	2.5
1	J	508	ALA	2.5
2	O	207	ILE	2.5
1	S	471	LEU	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	N	280	GLY	2.5
2	W	44	GLY	2.5
1	T	62	LYS	2.5
4	Q	80	ASP	2.5
2	X	278	ALA	2.5
1	S	158	LEU	2.5
1	S	394	LEU	2.5
2	N	393	MET	2.5
3	P	41	ALA	2.5
2	X	277	SER	2.5
3	Y	152	SER	2.5
2	X	202	LYS	2.5
3	Y	135	LYS	2.5
1	C	411	ASP	2.5
2	X	89	ARG	2.5
1	C	414	ALA	2.5
1	U	334	GLY	2.5
1	U	449	ALA	2.5
1	S	467	GLU	2.5
1	U	471	LEU	2.5
1	T	219	VAL	2.5
3	P	135	LYS	2.5
1	T	162	GLY	2.5
2	X	167	ILE	2.5
3	Y	267	LEU	2.5
1	T	262	ASN	2.5
1	U	28	ASN	2.5
3	Y	9	ARG	2.5
4	Q	44	ASN	2.5
1	T	100	PRO	2.4
1	S	264	LYS	2.4
2	W	443	ALA	2.4
1	L	491	LEU	2.4
1	S	354	LEU	2.4
2	V	92	LEU	2.4
4	Q	101	ILE	2.4
2	X	149	ARG	2.4
1	S	333	GLY	2.4
4	Q	18	HIS	2.4
1	J	482	LEU	2.4
2	M	431	LEU	2.4
3	G	188	ILE	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	L	410	SER	2.4
4	H	71	SER	2.4
1	S	395	PHE	2.4
3	Y	237	MET	2.4
4	Q	13	GLN	2.4
2	V	276	PRO	2.4
1	T	485	ILE	2.4
1	C	415	SER	2.4
2	V	306	SER	2.4
3	Y	43	LYS	2.4
1	S	440	THR	2.4
2	M	406	ARG	2.4
2	M	396	LEU	2.4
2	V	77	LEU	2.4
1	U	506	PHE	2.4
3	Y	41	ALA	2.4
3	Y	84	CYS	2.4
4	Q	16	LEU	2.4
3	P	224	GLN	2.4
5	1	33	SER	2.4
2	W	183	VAL	2.4
3	Y	167	ASN	2.4
3	Y	255	TYR	2.4
2	M	398	GLU	2.4
2	W	453	PRO	2.4
1	S	325	ALA	2.4
2	V	109	ILE	2.4
1	S	334	GLY	2.4
1	S	97	VAL	2.4
3	P	140	PHE	2.4
1	S	230	TYR	2.4
4	Q	33	PRO	2.4
1	T	482	LEU	2.4
1	U	58	SER	2.4
2	W	61	THR	2.4
2	X	182	SER	2.4
4	Z	120	ALA	2.4
5	R	27	THR	2.4
3	G	107	ILE	2.4
1	T	43	VAL	2.4
2	W	49	GLU	2.4
1	K	492	SER	2.3

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	T	251	THR	2.3
1	U	198	SER	2.3
2	X	394	ASP	2.3
2	X	110	LYS	2.3
3	P	40	SER	2.3
3	Y	121	THR	2.3
2	V	137	GLY	2.3
1	T	316	GLU	2.3
1	U	382	VAL	2.3
2	V	420	VAL	2.3
1	S	428	GLN	2.3
1	U	294	GLU	2.3
3	G	272	THR	2.3
3	Y	257	ARG	2.3
1	T	291	PRO	2.3
2	V	313	PRO	2.3
1	J	484	GLU	2.3
1	K	491	LEU	2.3
2	V	431	LEU	2.3
2	W	402	LEU	2.3
2	O	318	THR	2.3
3	P	78	THR	2.3
1	U	386	LYS	2.3
2	W	215	VAL	2.3
2	W	399	GLN	2.3
2	M	8	PRO	2.3
2	E	403	THR	2.3
2	V	468	ALA	2.3
5	R	20	ALA	2.3
1	T	443	GLN	2.3
2	W	13	VAL	2.3
2	M	400	ASP	2.3
2	O	394	ASP	2.3
2	E	143	LEU	2.3
3	G	118	LEU	2.3
3	G	150	LEU	2.3
3	Y	34	ALA	2.3
2	V	184	PHE	2.3
1	U	292	GLY	2.3
2	X	322	PRO	2.3
3	P	222	MET	2.3
5	I	29	LEU	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	S	458	ILE	2.3
3	P	9	ARG	2.3
1	T	104	GLY	2.3
2	M	435	LYS	2.3
2	V	205	GLY	2.3
2	X	303	SER	2.3
2	X	393	MET	2.3
3	P	154	MET	2.3
5	R	12	ALA	2.3
2	W	454	GLU	2.3
1	K	470	PHE	2.3
1	L	411	ASP	2.3
1	U	81	ASP	2.3
2	X	401	LYS	2.3
1	T	499	LEU	2.2
1	U	426	LEU	2.2
3	P	167	ASN	2.2
1	T	52	GLU	2.2
2	D	398	GLU	2.2
3	P	2	THR	2.2
2	V	133	ILE	2.2
1	T	58	SER	2.2
4	Q	97	SER	2.2
2	E	391	LEU	2.2
1	S	108	ARG	2.2
1	U	497	ALA	2.2
2	X	15	ALA	2.2
1	C	448	TYR	2.2
3	P	226	TYR	2.2
1	S	464	GLY	2.2
1	T	466	PHE	2.2
2	X	25	PHE	2.2
2	X	315	ASP	2.2
2	E	452	ILE	2.2
2	M	9	ILE	2.2
1	T	308	LEU	2.2
2	F	176	LYS	2.2
1	L	414	ALA	2.2
1	T	324	THR	2.2
1	U	104	GLY	2.2
1	U	202	TYR	2.2
2	M	469	LYS	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	V	59	VAL	2.2
1	T	252	ALA	2.2
2	W	330	ASP	2.2
1	U	475	LYS	2.2
2	E	410	ILE	2.2
2	V	20	ILE	2.2
1	S	28	ASN	2.2
5	I	14	LEU	2.2
1	S	331	THR	2.2
2	X	90	GLU	2.2
2	X	281	TYR	2.2
1	S	451	VAL	2.2
3	P	161	LYS	2.2
1	L	295	ALA	2.2
1	T	293	ARG	2.2
1	T	337	SER	2.2
1	U	73	VAL	2.2
1	L	493	LYS	2.2
1	T	459	GLU	2.2
2	O	453	PRO	2.2
2	W	252	LEU	2.2
1	S	377	GLY	2.2
2	W	470	ALA	2.2
2	M	380	THR	2.2
1	S	161	ILE	2.1
1	S	501	SER	2.1
3	Y	115	LYS	2.1
2	M	395	GLU	2.1
1	J	454	HIS	2.1
1	S	283	LEU	2.1
3	Y	169	PRO	2.1
1	S	31	GLY	2.1
1	S	126	ALA	2.1
2	W	408	ARG	2.1
3	Y	44	MET	2.1
2	E	424	PHE	2.1
1	K	448	TYR	2.1
1	T	80	SER	2.1
1	T	73	VAL	2.1
2	D	198	TYR	2.1
2	F	28	SER	2.1
2	M	381	TYR	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	V	239	ILE	2.1
3	G	19	ILE	2.1
2	V	358	LEU	2.1
3	Y	112	ASP	2.1
2	V	456	ALA	2.1
2	X	58	THR	2.1
1	T	441	GLU	2.1
1	J	466	PHE	2.1
2	N	390	ILE	2.1
2	W	218	VAL	2.1
2	E	470	ALA	2.1
3	P	55	ALA	2.1
1	C	331	THR	2.1
3	G	22	THR	2.1
3	Y	216	ASN	2.1
1	B	481	LEU	2.1
1	C	496	LEU	2.1
1	T	97	VAL	2.1
2	F	370	VAL	2.1
2	V	406	ARG	2.1
2	W	438	VAL	2.1
5	I	41	ASP	2.1
3	P	88	HIS	2.1
2	O	175	ALA	2.1
3	Y	221	ALA	2.1
1	J	503	THR	2.1
3	G	260	GLN	2.1
3	Y	272	THR	2.1
1	S	372	SER	2.1
1	T	470	PHE	2.1
1	U	111	ASP	2.1
1	U	456	ASP	2.1
1	S	101	VAL	2.1
2	E	280	GLY	2.1
3	G	259	ARG	2.1
3	P	6	VAL	2.1
4	Q	19	GLU	2.1
1	T	28	ASN	2.1
1	T	334	GLY	2.1
3	G	273	GLY	2.1
1	T	507	VAL	2.1
2	O	384	LEU	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	Y	98	HIS	2.1
2	E	449	TYR	2.1
2	W	350	PRO	2.1
2	X	216	ALA	2.1
3	P	94	ALA	2.1
3	P	104	ASN	2.1
1	S	305	SER	2.1
1	C	388	VAL	2.1
2	M	434	LEU	2.1
2	V	402	LEU	2.1
3	G	3	LEU	2.1
3	Y	10	LEU	2.1
1	U	116	PRO	2.1
1	U	340	ILE	2.1
3	P	107	ILE	2.1
2	W	278	ALA	2.1
3	G	124	ASN	2.1
2	W	393	MET	2.1
1	U	171	GLY	2.1
1	K	478	HIS	2.0
3	P	98	HIS	2.0
3	P	130	ILE	2.0
1	T	435	TYR	2.0
1	S	441	GLU	2.0
2	D	405	GLU	2.0
4	Q	100	ASN	2.0
1	S	416	THR	2.0
1	U	333	GLY	2.0
2	X	306	SER	2.0
1	T	201	LEU	2.0
2	W	170	LEU	2.0
1	S	159	VAL	2.0
1	U	486	ARG	2.0
2	M	321	ALA	2.0
2	W	177	ALA	2.0
1	U	331	THR	2.0
2	V	40	LYS	2.0
3	Y	136	ASP	2.0
2	W	243	PHE	2.0
1	T	145	HIS	2.0
1	C	507	VAL	2.0
1	S	35	ALA	2.0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	U	339	TYR	2.0
3	G	53	LYS	2.0
5	R	36	ASN	2.0
3	P	134	GLY	2.0
1	T	217	GLN	2.0
4	Q	81	SER	2.0
1	U	451	VAL	2.0
2	X	320	PRO	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(Å <sup>2</sup> )	Q<0.9
8	PO4	E	800	5/5	0.83	0.15	101,101,102,103	0
7	MG	T	700	1/1	0.87	0.07	65,65,65,65	0
6	ANP	S	600	31/31	0.88	0.16	74,79,82,83	0
7	MG	S	700	1/1	0.89	0.08	64,64,64,64	0
7	MG	B	700	1/1	0.91	0.35	50,50,50,50	0
7	MG	F	700	1/1	0.91	0.28	56,56,56,56	0
7	MG	U	700	1/1	0.92	0.23	75,75,75,75	0
7	MG	X	700	1/1	0.92	0.20	65,65,65,65	0
7	MG	O	700	1/1	0.93	0.25	55,55,55,55	0
6	ANP	V	600	31/31	0.93	0.16	77,85,87,88	0
6	ANP	U	600	31/31	0.93	0.21	71,74,77,79	0
8	PO4	N	800	5/5	0.94	0.14	96,97,97,97	0
7	MG	C	700	1/1	0.94	0.33	56,56,56,56	0
6	ANP	T	600	31/31	0.94	0.12	75,82,84,85	0
6	ANP	J	600	31/31	0.95	0.20	58,73,81,82	0

*Continued on next page...*

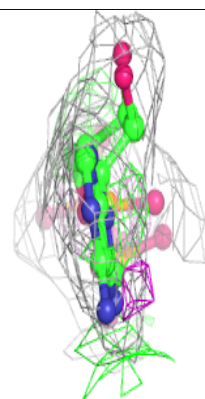
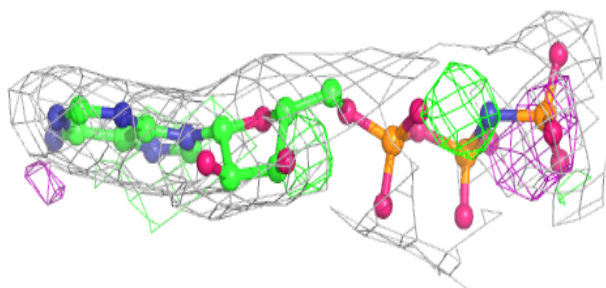
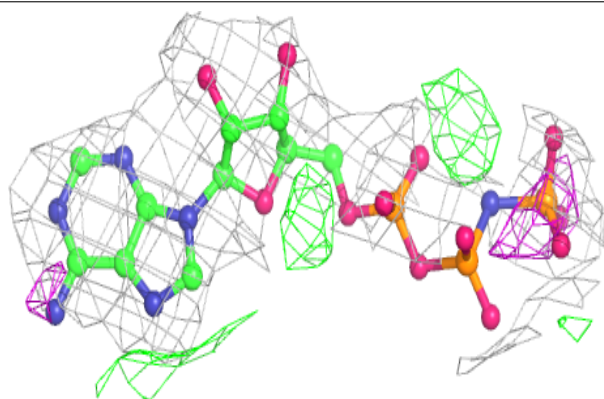
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	MG	D	700	1/1	0.95	0.32	57,57,57,57	0
6	ANP	C	600	31/31	0.95	0.21	60,70,72,73	0
6	ANP	M	600	31/31	0.95	0.20	64,77,78,78	0
6	ANP	O	600	31/31	0.96	0.21	58,62,72,72	0
7	MG	K	700	1/1	0.96	0.36	47,47,47,47	0
6	ANP	B	600	31/31	0.96	0.23	53,63,65,65	0
6	ANP	A	600	31/31	0.96	0.22	50,60,62,62	0
6	ANP	X	600	31/31	0.96	0.15	75,79,83,85	0
7	MG	V	700	1/1	0.97	0.10	67,67,67,67	0
7	MG	J	700	1/1	0.97	0.38	52,52,52,52	0
7	MG	M	700	1/1	0.97	0.28	57,57,57,57	0
6	ANP	K	600	31/31	0.97	0.22	51,60,62,63	0
6	ANP	D	600	31/31	0.97	0.20	62,66,69,71	0
6	ANP	F	600	31/31	0.97	0.19	58,65,69,70	0
6	ANP	L	600	31/31	0.97	0.23	57,61,63,64	0
7	MG	A	700	1/1	0.98	0.40	47,47,47,47	0
7	MG	L	700	1/1	0.98	0.44	52,52,52,52	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.

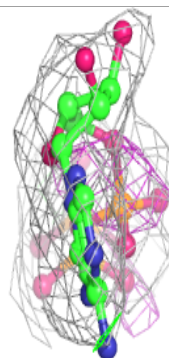
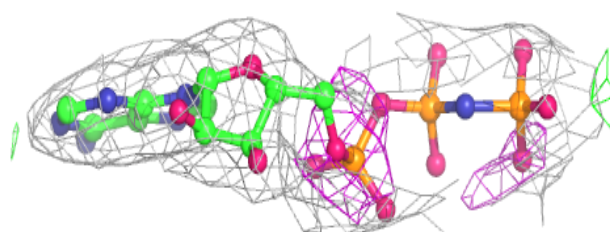
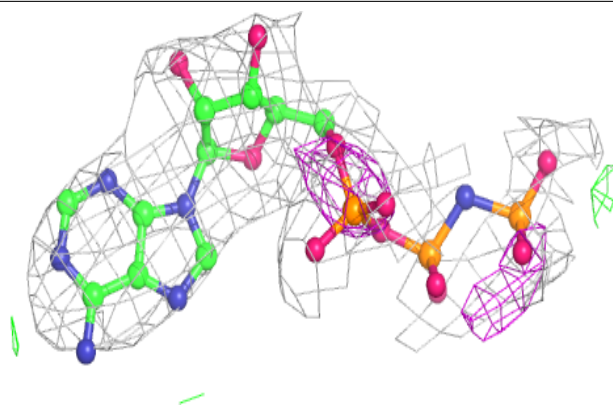
#### Electron density around ANP S 600:

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

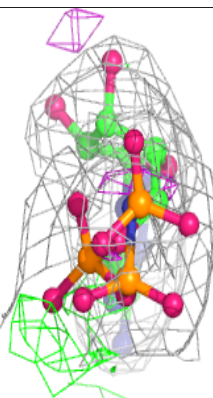
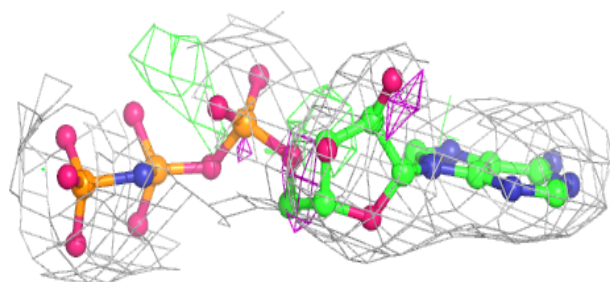
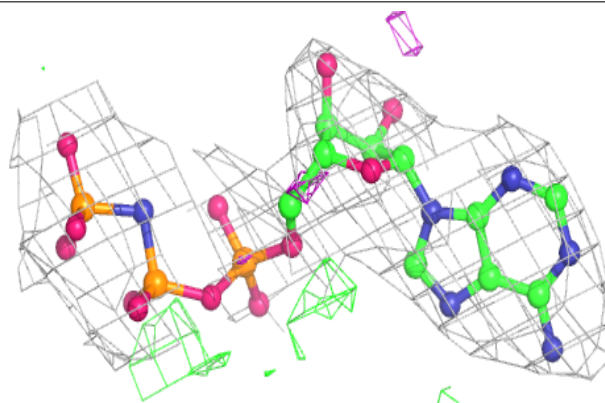


**Electron density around ANP V 600:**

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

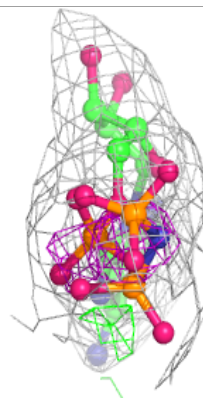
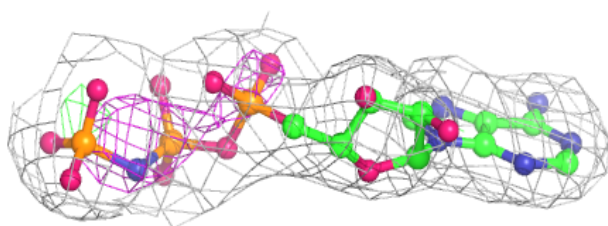
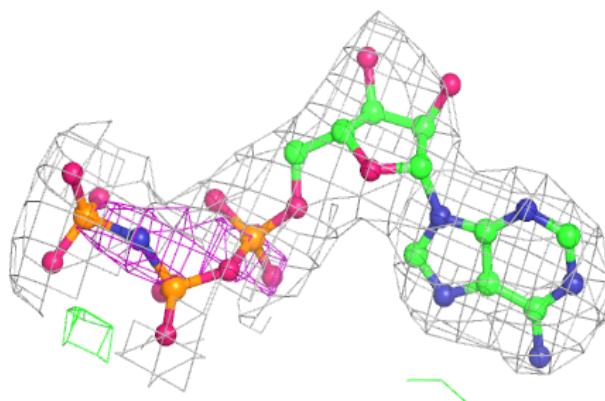
**Electron density around ANP U 600:**

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

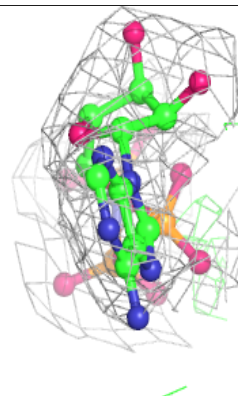
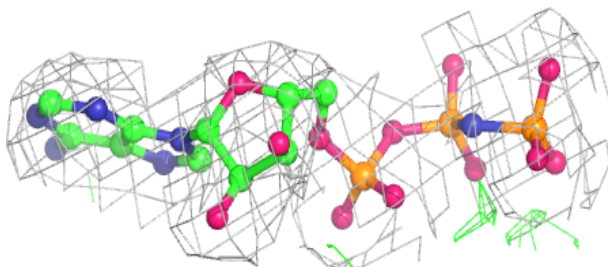
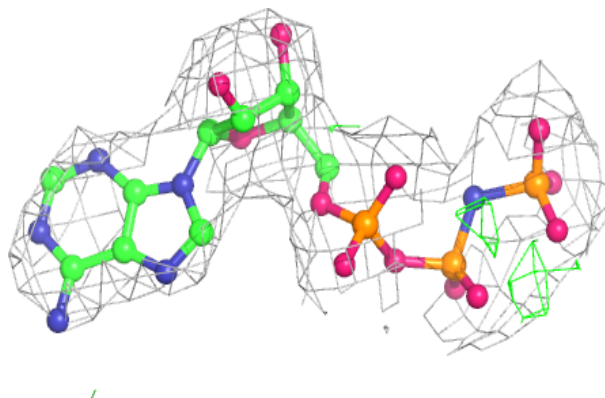


**Electron density around ANP T 600:**

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

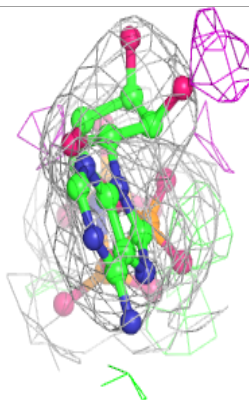
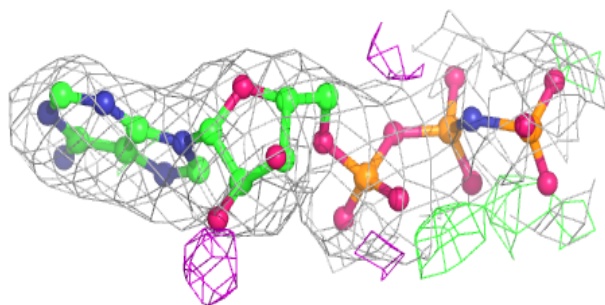
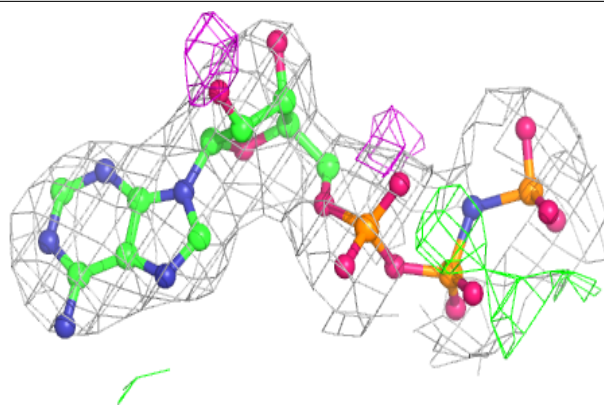
**Electron density around ANP J 600:**

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

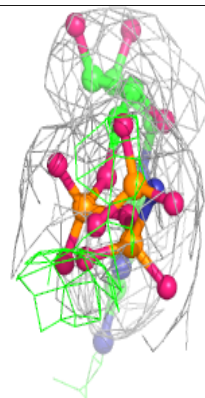
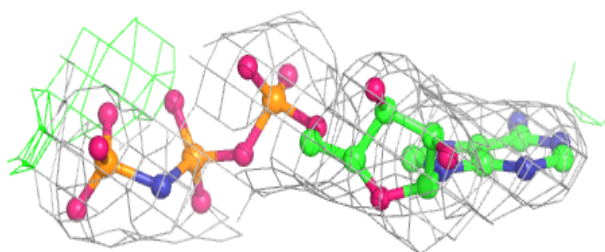
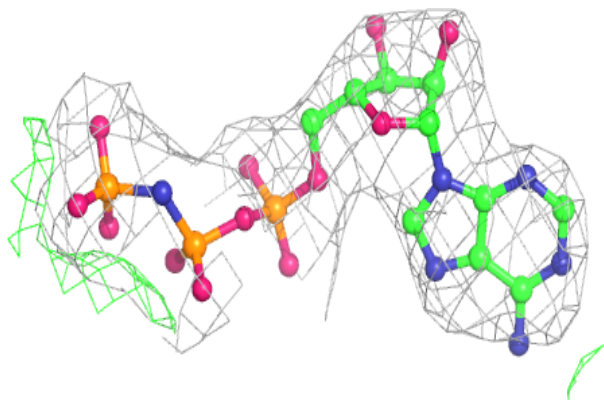


**Electron density around ANP C 600:**

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

**Electron density around ANP M 600:**

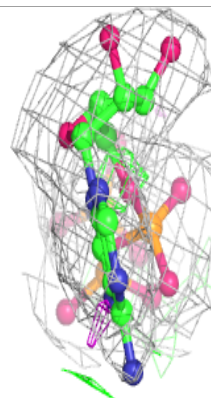
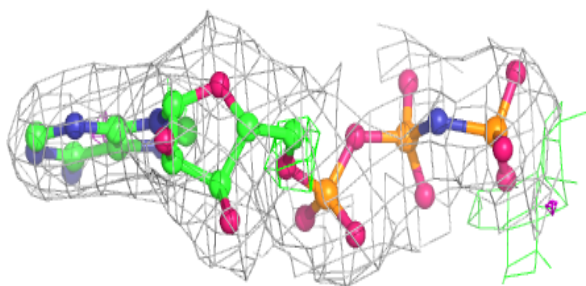
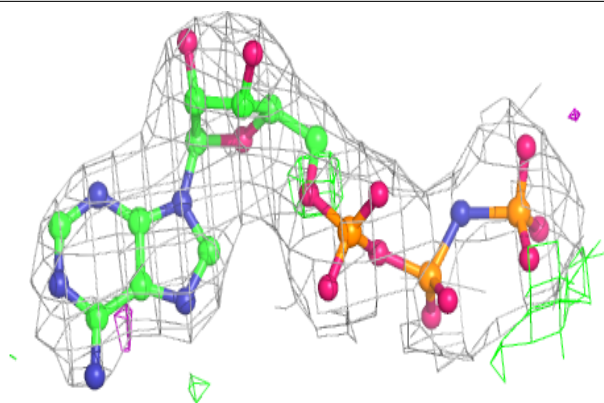
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



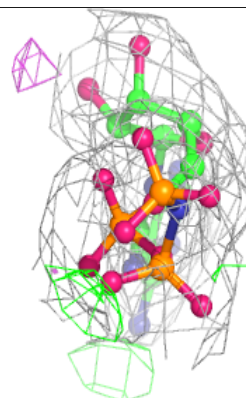
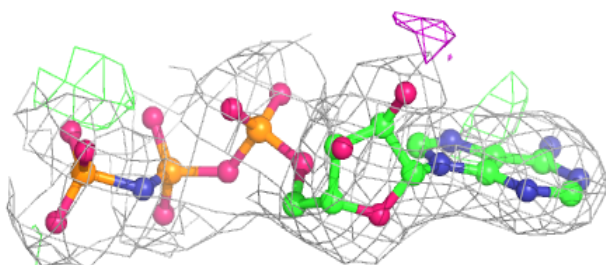
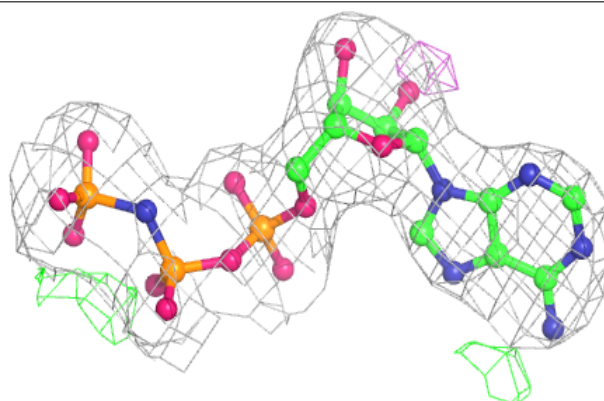


**Electron density around ANP O 600:**

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

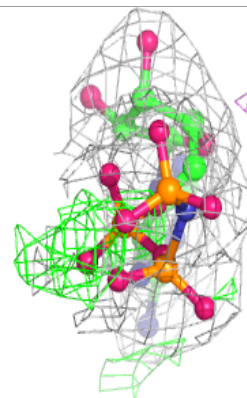
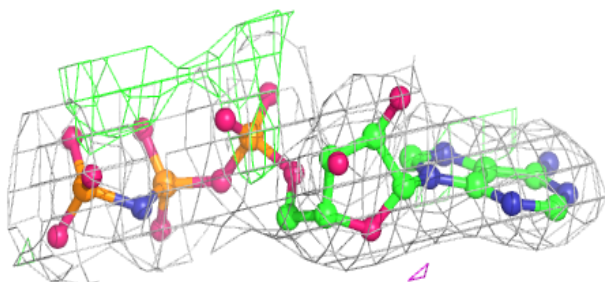
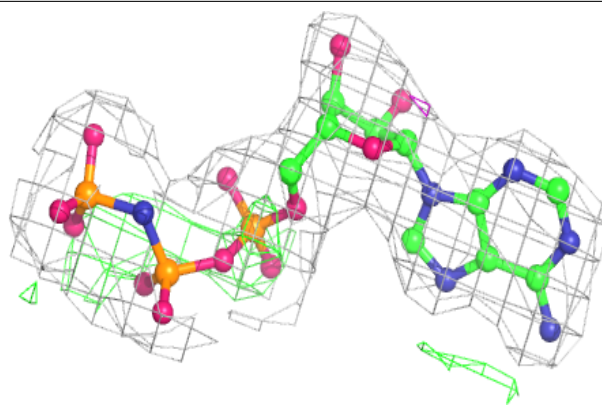
**Electron density around ANP B 600:**

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

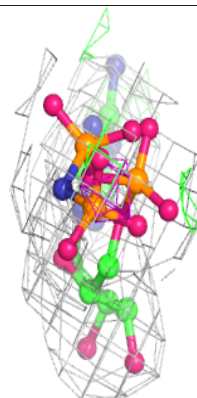
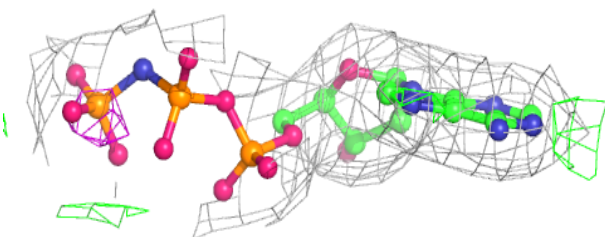
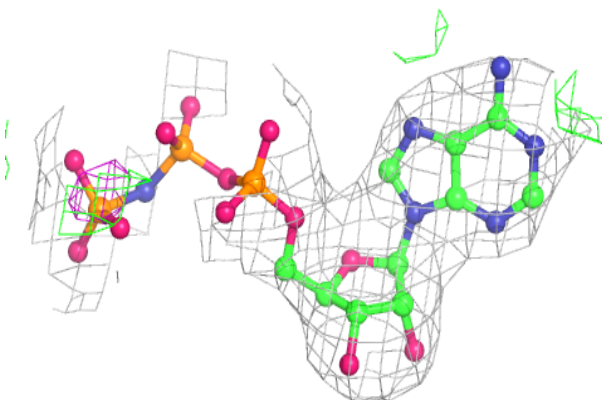


**Electron density around ANP A 600:**

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

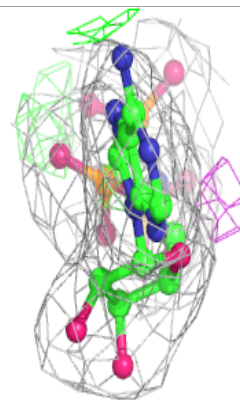
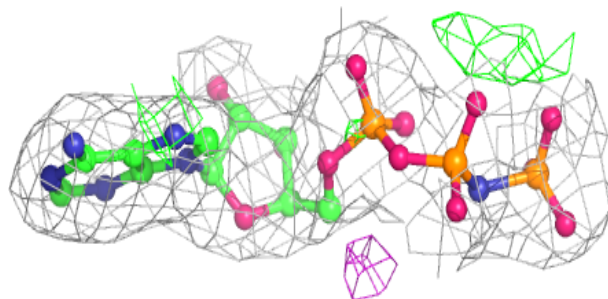
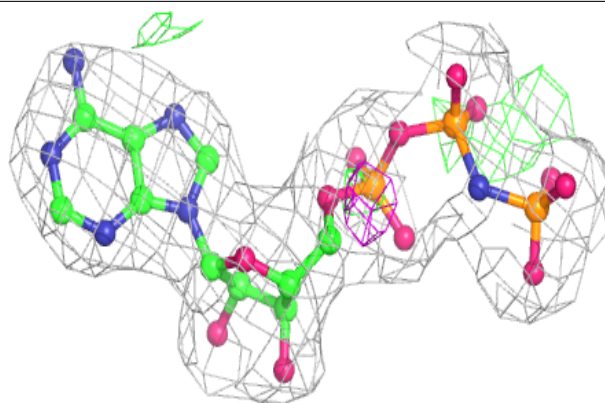
**Electron density around ANP X 600:**

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

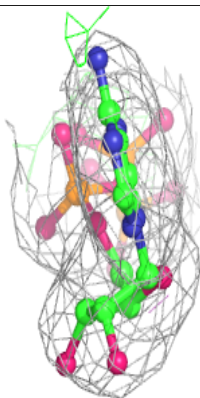
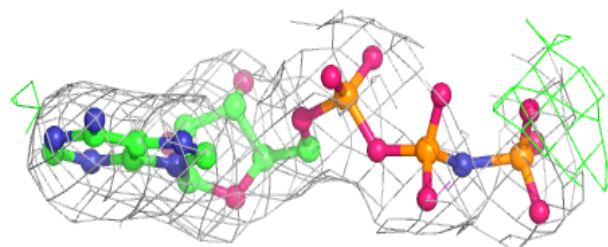
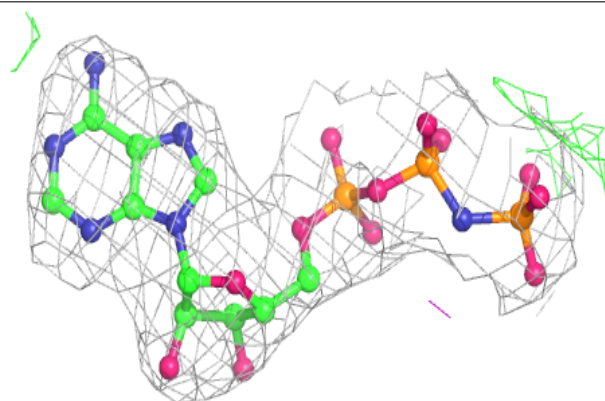


**Electron density around ANP K 600:**

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

**Electron density around ANP D 600:**

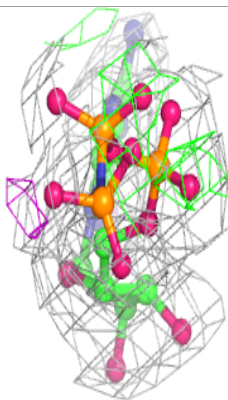
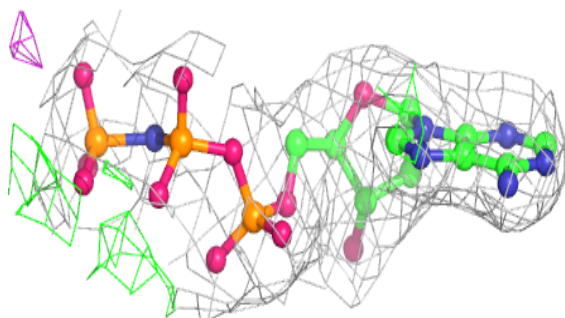
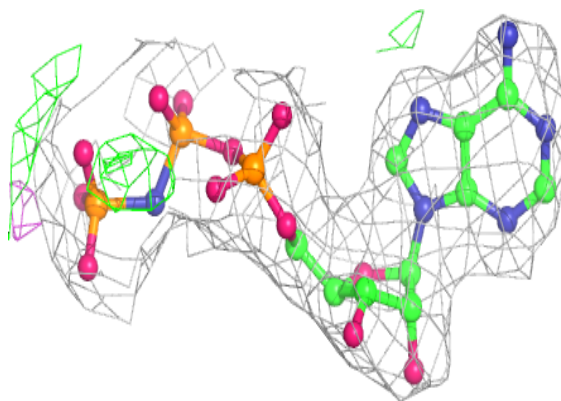
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



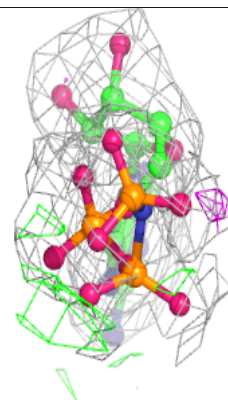
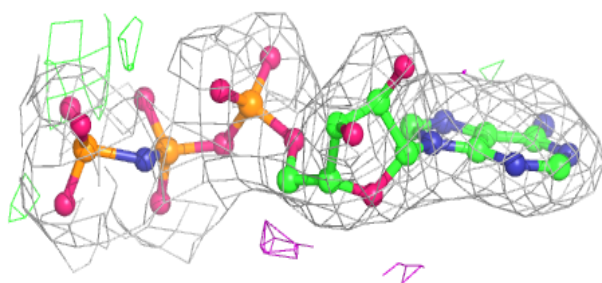
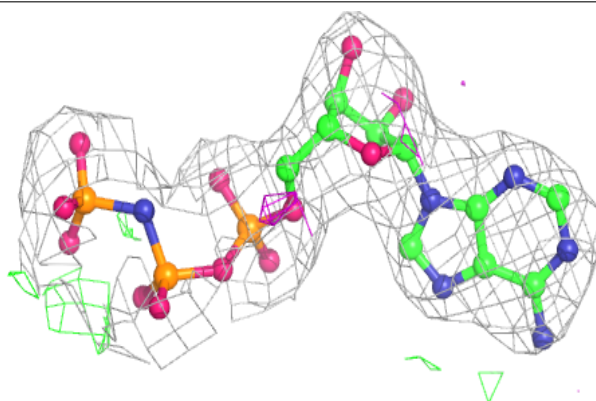


**Electron density around ANP F 600:**

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

**Electron density around ANP 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)



## 6.5 Other polymers

There are no such residues in this entry.