



# Full wwPDB X-ray Structure Validation Report i

Aug 29, 2023 – 03:23 AM EDT

PDB ID : 3OEH  
Title : Structure of four mutant forms of yeast F1 ATPase: beta-V279F  
Authors : Arsenieva, D.; Symersky, J.; Wang, Y.; Pagadala, V.; Mueller, D.M.  
Deposited on : 2010-08-12  
Resolution : 3.00 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 i symbol.

The types of validation reports are described at  
<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references](#) ①) 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 : 2.35  
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) : 2.35

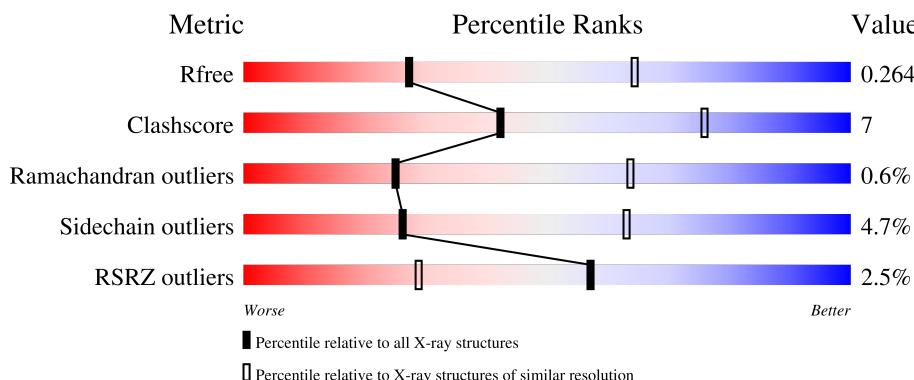
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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.



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Mol	Chain	Length	Quality of chain			
1	L	510	74%	19%	• 5%	
1	S	510	70%	23%	• 6%	
1	T	510	80%	13%	• 6%	
1	U	510	73%	21%	6%	
2	D	484	77%	19%	• •	
2	E	484	76%	19%	• •	
2	F	484	74%	21%	• •	
2	M	484	79%	17%	• •	
2	N	484	75%	21%	• •	
2	O	484	79%	17%	•	
2	V	484	75%	20%	• •	
2	W	484	78%	17%	• •	
2	X	484	83%	14%	• •	
3	G	278	69%	24%	• •	
3	P	278	68%	17%	• 12%	
3	Y	278	58%	13%	• 28%	
4	H	138	62%	17%	• 16%	
4	Q	138	57%	•	39%	
4	Z	138	12% •	88%		
5	I	61	43% •	56%		
5	R	61	56% •	20% 5% 20%		
5	1	61	15% •	44%		

## 2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 72707 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 3664	N 2314	O 648	S 699	3	0	0
1	B	483	Total	C 3669	N 2317	O 649	S 700	3	0	0
1	C	484	Total	C 3680	N 2325	O 650	S 702	3	0	0
1	J	481	Total	C 3655	N 2309	O 646	S 697	3	0	0
1	K	486	Total	C 3688	N 2327	O 652	S 706	3	0	0
1	L	482	Total	C 3664	N 2314	O 648	S 699	3	0	0
1	S	478	Total	C 3635	N 2297	O 643	S 692	3	0	0
1	T	479	Total	C 3642	N 2302	O 644	S 693	3	0	0
1	U	481	Total	C 3655	N 2308	O 646	S 698	3	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	470	Total	C 3549	N 2252	O 603	S 688	6	0	0
2	E	468	Total	C 3508	N 2227	O 598	S 677	6	0	0
2	F	469	Total	C 3531	N 2242	O 602	S 681	6	0	0
2	M	470	Total	C 3543	N 2249	O 600	S 688	6	0	0
2	N	470	Total	C 3545	N 2249	O 602	S 688	6	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	468	Total	C	N	O	S	0	0	0
			3538	2246	602	684	6			
2	V	470	Total	C	N	O	S	0	0	0
			3550	2251	604	689	6			
2	W	467	Total	C	N	O	S	0	0	0
			3535	2244	601	684	6			
2	X	469	Total	C	N	O	S	0	0	0
			3547	2251	603	687	6			

There are 81 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
D	279	PHE	VAL	engineered mutation	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
E	279	PHE	VAL	engineered mutation	UNP P00830
F	-5	ALA	-	expression tag	UNP P00830
F	-4	SER	-	expression tag	UNP P00830
F	-3	HIS	-	expression tag	UNP P00830
F	-2	HIS	-	expression tag	UNP P00830
F	-1	HIS	-	expression tag	UNP P00830
F	0	HIS	-	expression tag	UNP P00830
F	1	HIS	-	expression tag	UNP P00830
F	2	HIS	-	expression tag	UNP P00830
F	279	PHE	VAL	engineered mutation	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
M	279	PHE	VAL	engineered mutation	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
N	279	PHE	VAL	engineered mutation	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
O	279	PHE	VAL	engineered mutation	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
V	279	PHE	VAL	engineered mutation	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
W	279	PHE	VAL	engineered mutation	UNP P00830
X	-5	ALA	-	expression tag	UNP P00830

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Chain	Residue	Modelled	Actual	Comment	Reference
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
X	279	PHE	VAL	engineered mutation	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 2059 1293 359 397 10	0	0	0
3	P	246	Total C N O S 1872 1175 327 361 9	0	0	0
3	Y	201	Total C N O S 1523 947 274 293 9	0	0	0

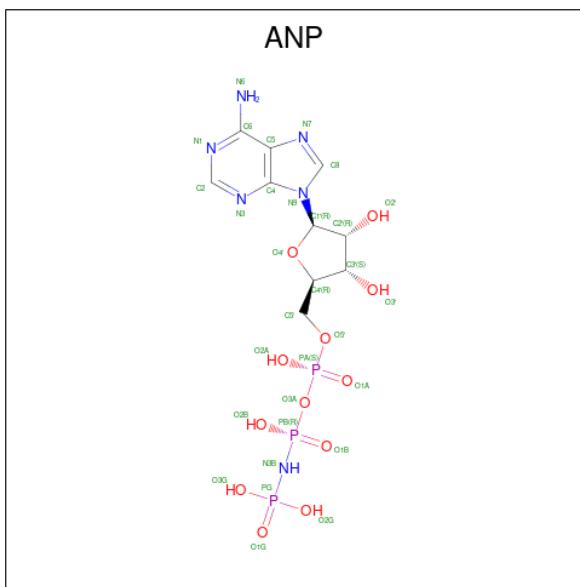
- Molecule 4 is a protein called ATP synthase subunit delta.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	H	116	Total C N O S 763 477 132 152 2	0	0	0
4	Q	84	Total C N O 454 277 89 88	0	0	0
4	Z	17	Total C N O 85 51 17 17	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	I	49	Total C N O 339 212 57 70	0	0	0
5	R	34	Total C N O 189 116 34 39	0	0	0
5	1	27	Total C N O 145 86 31 28	0	0	0

- 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
			Total	C	N	O	P		
6	A	1	31	10	6	12	3	0	0
6	B	1	31	10	6	12	3	0	0
6	C	1	31	10	6	12	3	0	0
6	D	1	31	10	6	12	3	0	0
6	F	1	31	10	6	12	3	0	0
6	J	1	31	10	6	12	3	0	0
6	K	1	31	10	6	12	3	0	0
6	L	1	31	10	6	12	3	0	0
6	M	1	31	10	6	12	3	0	0
6	O	1	31	10	6	12	3	0	0
6	S	1	31	10	6	12	3	0	0
6	T	1	31	10	6	12	3	0	0
6	U	1	31	10	6	12	3	0	0
6	V	1	31	10	6	12	3	0	0

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

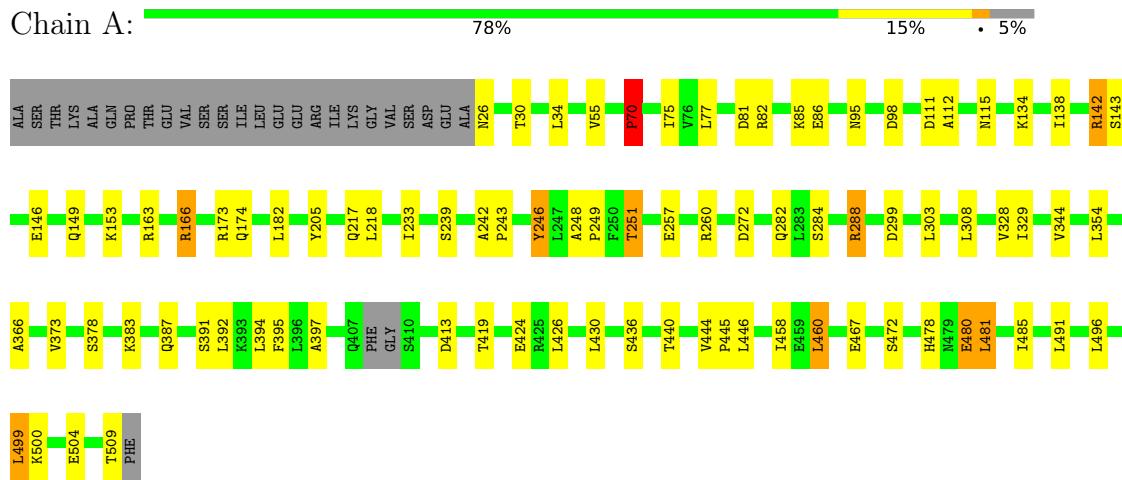
- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

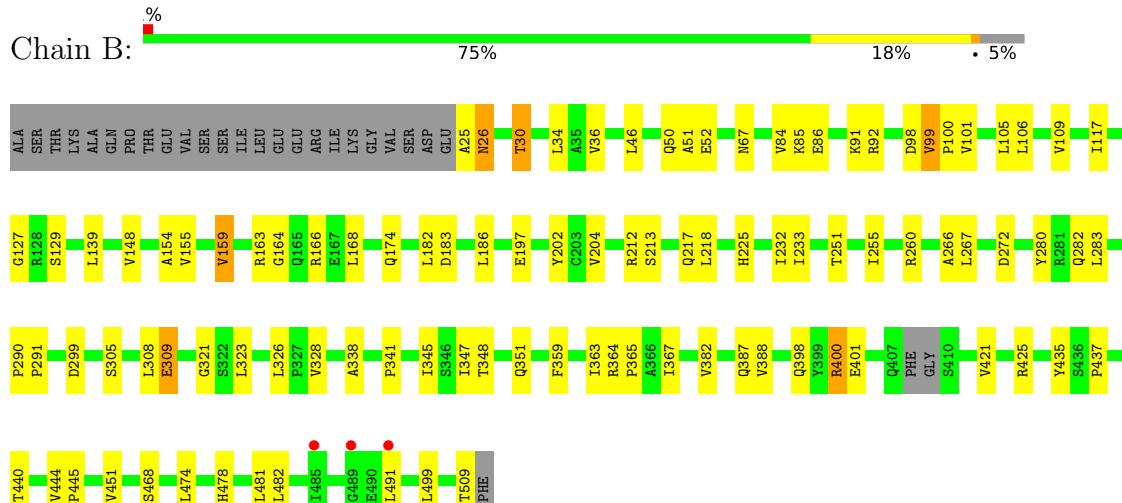
### 3 Residue-property plots

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

- Molecule 1: ATP synthase subunit alpha

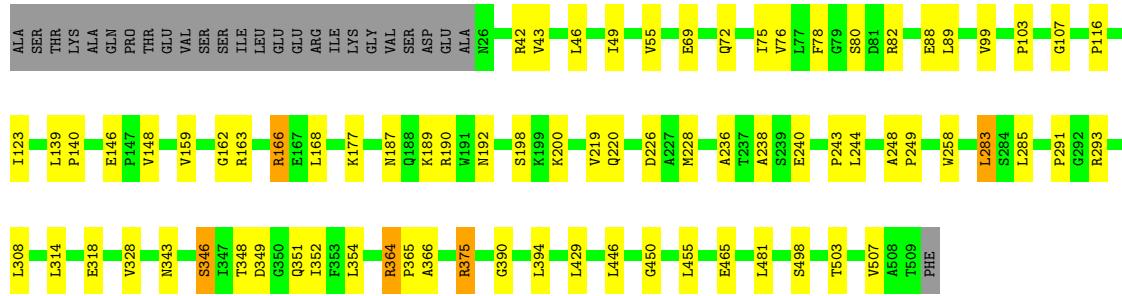


- Molecule 1: ATP synthase subunit alpha

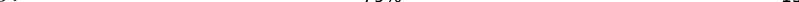


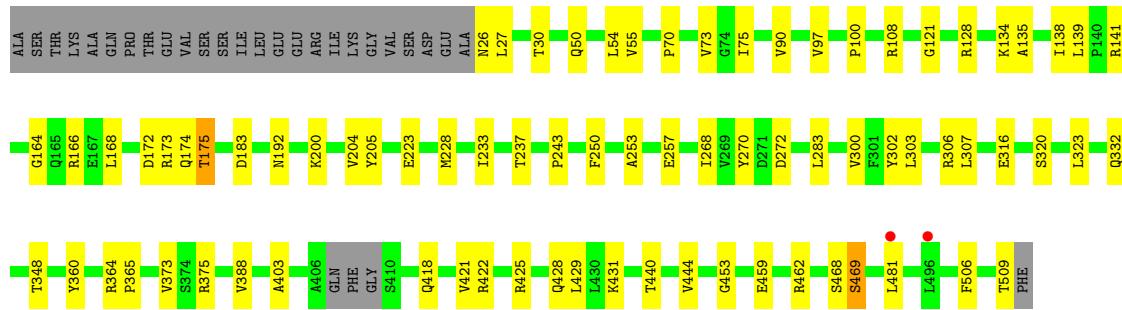
- Molecule 1: ATP synthase subunit alpha





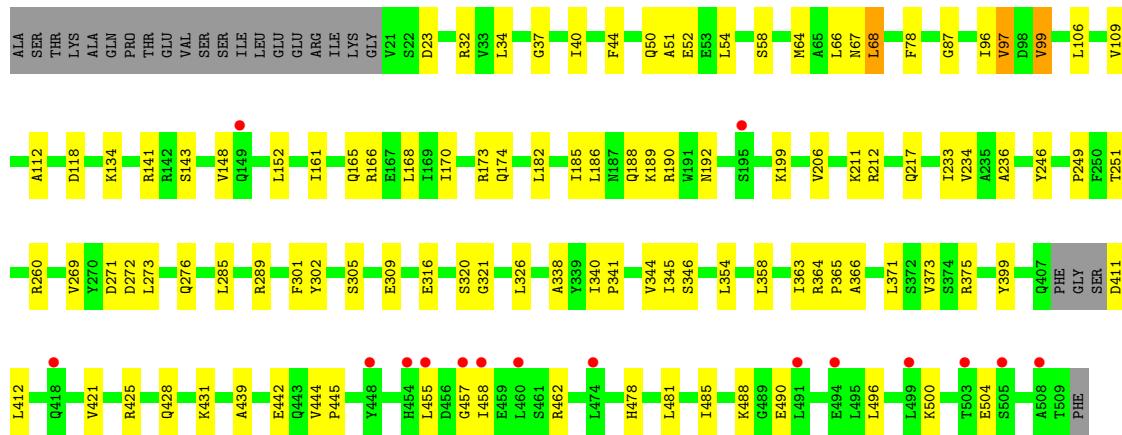
- Molecule 1: ATP synthase subunit alpha

Chain J:  79% 15% 6%



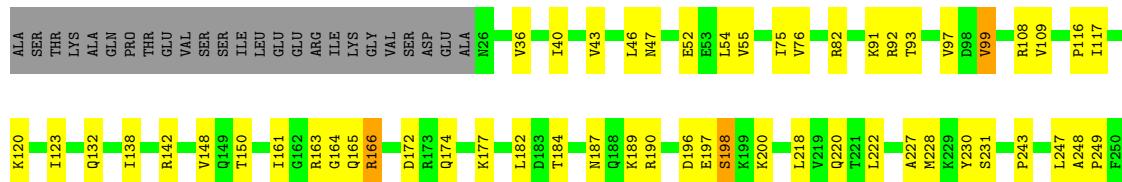
- Molecule 1: ATP synthase subunit alpha

Chain K: 3% • 74% • 21% • 5%



- Molecule 1: ATP synthase subunit alpha

Chain L:  74% 19% • 5%

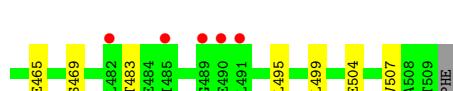
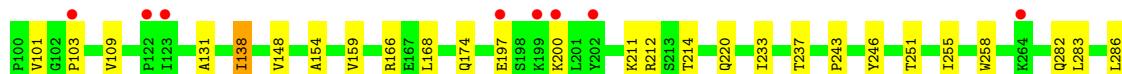
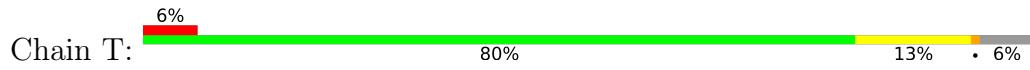




- Molecule 1: ATP synthase subunit alpha

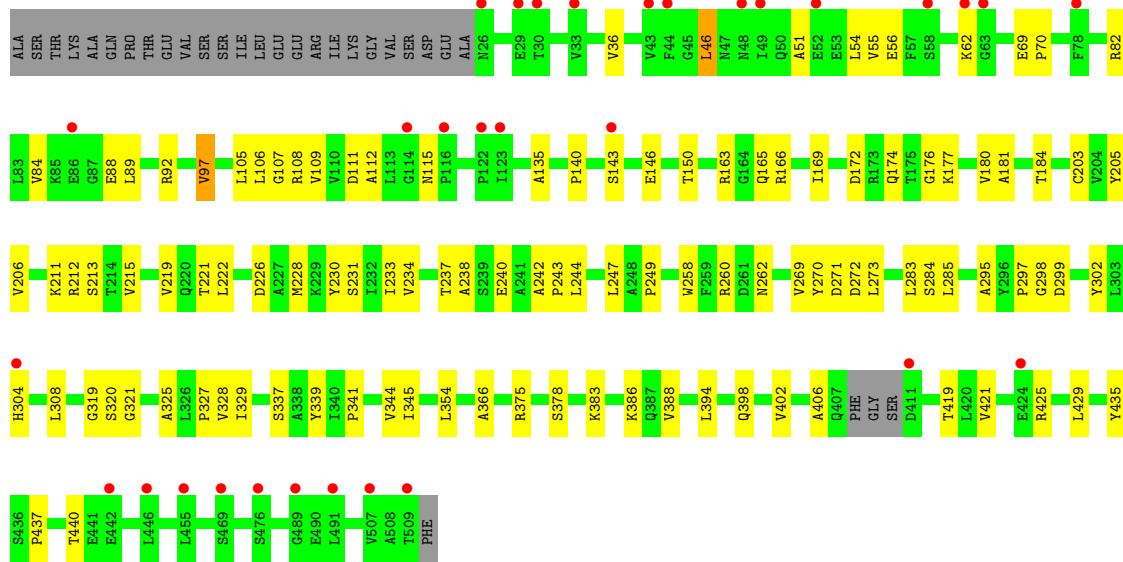


- Molecule 1: ATP synthase subunit alpha



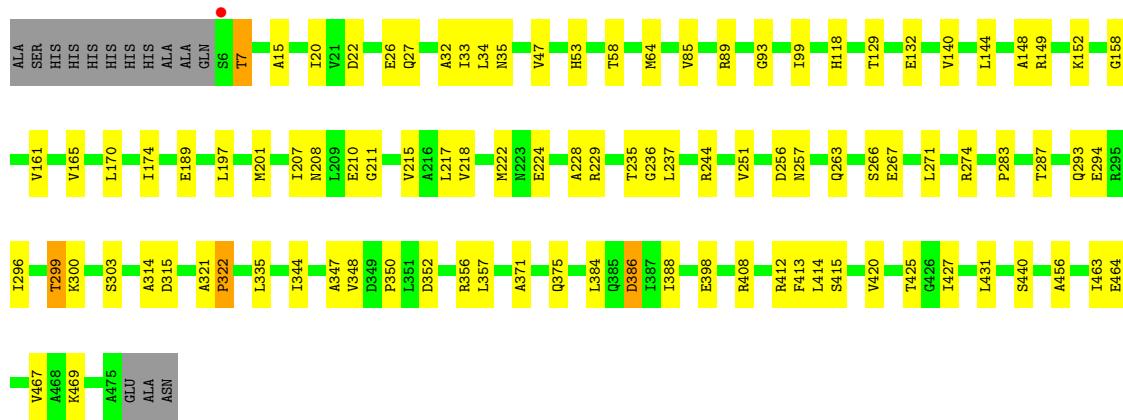
- Molecule 1: ATP synthase subunit alpha





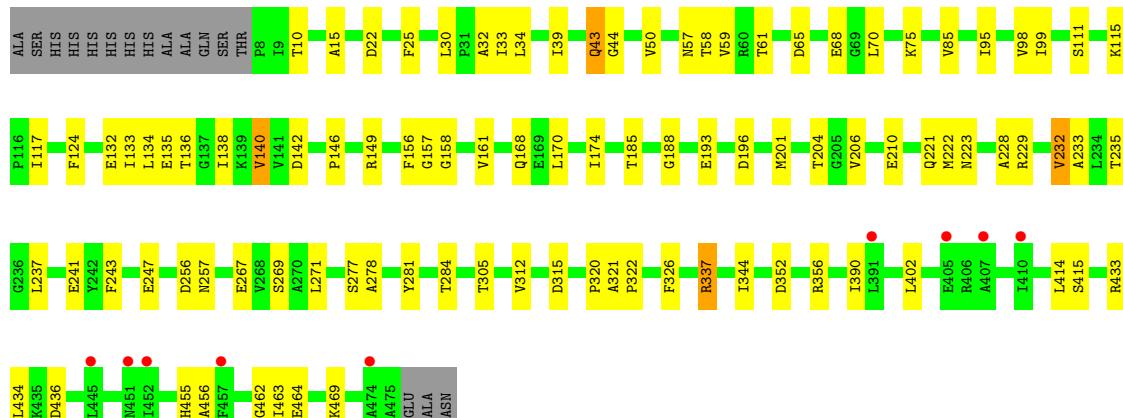
- Molecule 2: ATP synthase subunit beta

Chain D:



- Molecule 2: ATP synthase subunit beta

Chain E

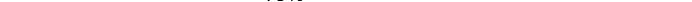


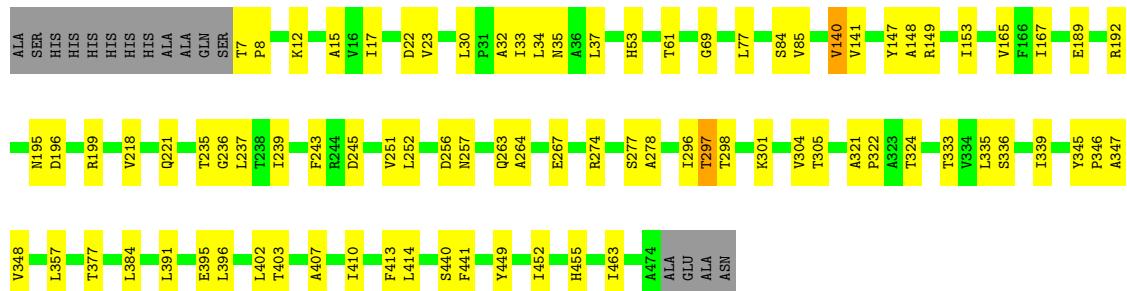
- Molecule 2: ATP synthase subunit beta

Chain F:  74% 21% • •

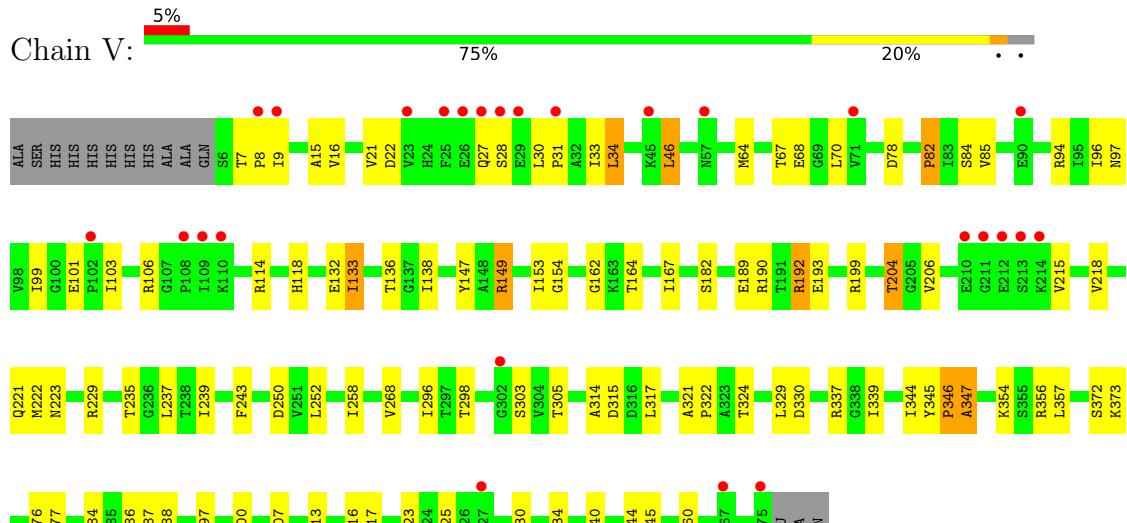


- Molecule 2: ATP synthase subunit beta

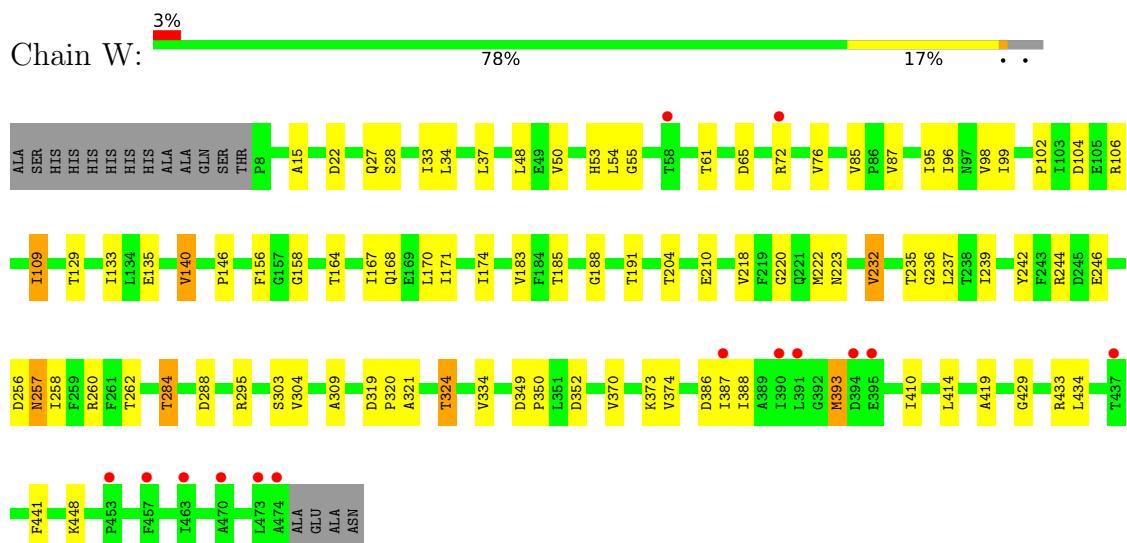
Chain O:  79% 17% •



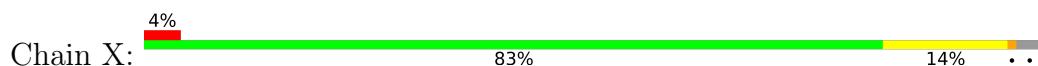
- Molecule 2: ATP synthase subunit beta

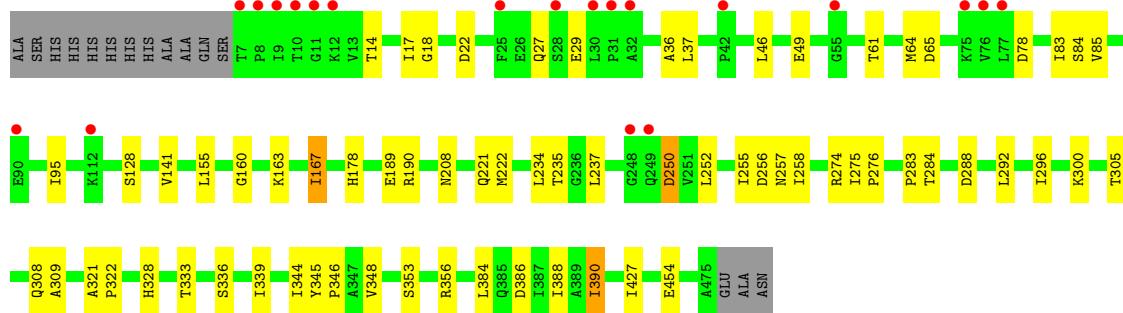


- Molecule 2: ATP synthase subunit beta



- Molecule 2: ATP synthase subunit beta

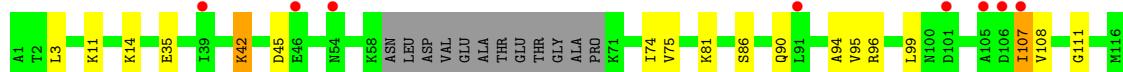




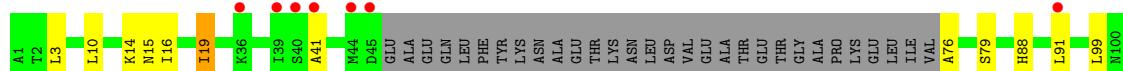
- Molecule 3: ATP synthase subunit gamma



- Molecule 3: ATP synthase subunit gamma

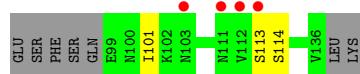


- Molecule 3: ATP synthase subunit gamma

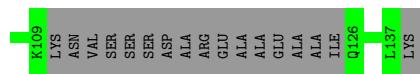




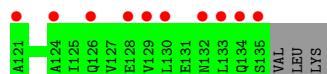
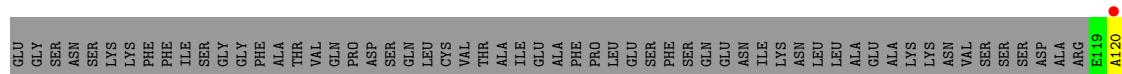
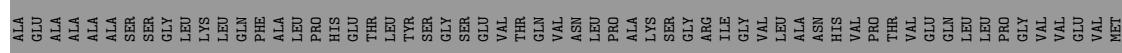
- Molecule 4: ATP synthase subunit delta



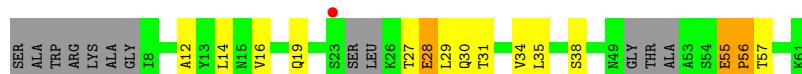
- Molecule 4: ATP synthase subunit delta



- Molecule 4: ATP synthase subunit delta



#### • Molecule 5: ATP synthase subunit epsilon

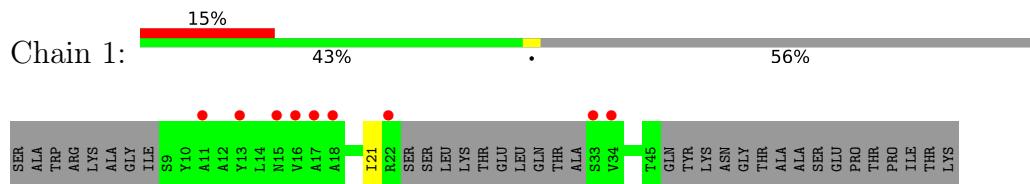


- Molecule 5: ATP synthase subunit epsilon





- Molecule 5: ATP synthase subunit epsilon



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.93Å 291.90Å 188.76Å 90.00° 101.91° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 49.39 – 3.00	Depositor EDS
% Data completeness (in resolution range)	88.8 (20.00-3.00) 88.6 (49.39-3.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$< I/\sigma(I) >$ <sup>1</sup>	2.29 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
$R$ , $R_{free}$	0.209 , 0.270 0.207 , 0.264	Depositor DCC
$R_{free}$ test set	4161 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	82.8	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 55.8	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.49$ , $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	72707	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% 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  $< |L| >$ ,  $< L^2 >$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ANP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.46	0/3718	0.65	0/5032
1	B	0.39	0/3723	0.59	0/5039
1	C	0.42	0/3736	0.62	1/5057 (0.0%)
1	J	0.36	0/3709	0.56	0/5020
1	K	0.35	0/3742	0.54	0/5065
1	L	0.43	0/3718	0.61	1/5032 (0.0%)
1	S	0.37	0/3689	0.54	0/4992
1	T	0.34	0/3696	0.50	0/5002
1	U	0.35	0/3709	0.54	0/5021
2	D	0.47	0/3606	0.61	0/4890
2	E	0.42	0/3565	0.58	0/4840
2	F	0.40	0/3588	0.58	0/4868
2	M	0.39	0/3600	0.58	0/4883
2	N	0.37	0/3602	0.53	1/4886 (0.0%)
2	O	0.37	0/3595	0.56	0/4875
2	V	0.37	0/3607	0.53	0/4891
2	W	0.36	0/3592	0.52	0/4869
2	X	0.36	0/3604	0.53	0/4887
3	G	0.39	0/2084	0.53	0/2803
3	P	0.36	0/1889	0.53	0/2537
3	Y	0.34	0/1533	0.51	0/2056
4	H	0.39	0/772	0.59	0/1058
4	Q	0.36	0/453	0.51	0/621
4	Z	0.35	0/84	0.45	0/116
5	1	0.30	0/143	0.42	0/195
5	I	0.42	0/343	0.59	0/470
5	R	0.39	0/189	0.50	0/261
All	All	0.39	0/73289	0.56	3/99266 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	283	LEU	CA-CB-CG	5.70	128.40	115.30
2	N	37	LEU	CA-CB-CG	5.34	127.57	115.30
1	C	283	LEU	CA-CB-CG	5.04	126.88	115.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3664	0	3747	59	0
1	B	3669	0	3752	59	0
1	C	3680	0	3763	40	0
1	J	3655	0	3739	43	0
1	K	3688	0	3763	63	0
1	L	3664	0	3747	54	0
1	S	3635	0	3724	70	0
1	T	3642	0	3733	36	0
1	U	3655	0	3734	62	0
2	D	3549	0	3614	59	0
2	E	3508	0	3550	51	0
2	F	3531	0	3592	58	0
2	M	3543	0	3603	49	0
2	N	3545	0	3604	63	0
2	O	3538	0	3606	47	0
2	V	3550	0	3611	64	0
2	W	3535	0	3605	47	0
2	X	3547	0	3615	39	0
3	G	2059	0	2127	43	0
3	P	1872	0	1917	34	0
3	Y	1523	0	1569	16	0
4	H	763	0	653	21	0
4	Q	454	0	259	2	0
4	Z	85	0	45	0	0
5	1	145	0	87	0	0
5	I	339	0	280	8	0
5	R	189	0	114	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	31	0	13	1	0
6	B	31	0	13	4	0
6	C	31	0	13	0	0
6	D	31	0	13	0	0
6	F	31	0	13	1	0
6	J	31	0	13	1	0
6	K	31	0	13	3	0
6	L	31	0	13	1	0
6	M	31	0	13	4	0
6	O	31	0	13	3	0
6	S	31	0	13	0	0
6	T	31	0	13	1	0
6	U	31	0	13	1	0
6	V	31	0	13	1	0
6	X	31	0	13	4	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
All	All	72707	0	73348	1008	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 7.

All (1008) 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:M:85:VAL:HG11	2:M:235:THR:HG23	1.30	1.12
2:D:85:VAL:HG11	2:D:235:THR:HG23	1.15	1.09
1:A:395:PHE:HZ	1:A:419:THR:HA	1.15	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:85:VAL:HG11	2:E:235:THR:HG23	1.38	1.01
1:B:174:GLN:HA	6:B:600:ANP:HNB1	1.28	0.97
1:A:395:PHE:CZ	1:A:419:THR:HA	2.00	0.96
1:A:77:LEU:HD12	1:A:81:ASP:HB3	1.49	0.95
3:P:205:VAL:H	3:P:206:PRO:HD2	1.30	0.94
2:M:160:GLY:H	6:M:600:ANP:HNB1	1.03	0.93
1:A:182:LEU:HD13	1:A:218:LEU:HD11	1.50	0.92
1:S:293:ARG:HD3	1:S:339:TYR:HD1	1.36	0.91
2:O:85:VAL:HG11	2:O:235:THR:HG23	1.51	0.91
1:K:67:ASN:HB3	2:O:17:ILE:HD13	1.55	0.89
1:L:182:LEU:HD13	1:L:218:LEU:HD11	1.55	0.87
2:M:142:ASP:HB3	2:M:434:LEU:HD12	1.55	0.86
5:I:55:GLU:CB	5:I:56:PRO:HD3	2.06	0.86
2:V:85:VAL:HG11	2:V:235:THR:HG23	1.56	0.86
2:D:85:VAL:CG1	2:D:235:THR:HG23	2.04	0.85
1:S:293:ARG:HD3	1:S:339:TYR:CD1	2.11	0.84
3:P:122:HIS:N	3:P:123:PRO:HD3	1.93	0.84
1:S:146:GLU:OE1	1:S:313:LYS:HE2	1.77	0.83
2:N:85:VAL:HG11	2:N:235:THR:HG23	1.60	0.82
1:T:99:VAL:HG11	1:T:251:THR:HB	1.62	0.82
2:M:182:SER:HB2	2:M:215:VAL:HG23	1.61	0.81
2:W:85:VAL:HG11	2:W:235:THR:HG23	1.61	0.81
3:P:205:VAL:N	3:P:206:PRO:HD2	1.97	0.80
1:C:192:ASN:HA	1:C:200:LYS:HG2	1.65	0.79
2:F:85:VAL:HG11	2:F:235:THR:HG23	1.64	0.78
3:G:23:MET:HG3	3:G:237:MET:HG3	1.66	0.78
1:S:112:ALA:O	1:S:251:THR:HG21	1.85	0.77
1:K:444:VAL:HG23	1:K:445:PRO:HD3	1.67	0.77
2:V:7:THR:HB	2:V:8:PRO:HD2	1.66	0.77
1:B:174:GLN:HA	6:B:600:ANP:N3B	2.00	0.76
2:D:371:ALA:O	2:D:375:GLN:HG3	1.86	0.75
1:U:166:ARG:HD3	1:U:308:LEU:O	1.87	0.75
1:J:469:SER:HB3	1:J:506:PHE:HZ	1.51	0.74
2:N:391:LEU:HB3	2:N:395:GLU:HG3	1.68	0.73
3:P:107:ILE:HG13	3:P:126:ILE:HA	1.71	0.73
1:T:346:SER:HA	6:X:600:ANP:O1G	1.89	0.73
3:G:89:SER:HA	3:G:117:GLN:HE21	1.53	0.73
1:K:364:ARG:HD3	6:K:600:ANP:C2	2.18	0.73
1:K:375:ARG:NH1	6:O:600:ANP:O2A	2.23	0.71
1:S:116:PRO:HB3	1:S:123:ILE:HD11	1.71	0.71
3:P:205:VAL:H	3:P:206:PRO:CD	2.03	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:236:ALA:HA	1:C:240:GLU:OE2	1.91	0.70
2:E:140:VAL:HG13	2:E:414:LEU:HB3	1.73	0.70
3:G:14:LYS:HA	3:G:248:ILE:HD11	1.73	0.70
3:P:155:LYS:O	3:P:155:LYS:HG2	1.89	0.70
2:V:154:GLY:HA3	2:V:329:LEU:HD13	1.71	0.70
1:C:343:ASN:O	1:C:346:SER:HB2	1.91	0.70
1:S:441:GLU:HG2	1:S:486:ARG:HB2	1.74	0.70
1:U:146:GLU:HB3	1:U:163:ARG:HD2	1.74	0.69
1:L:40:ILE:CD1	1:L:76:VAL:HG12	2.23	0.69
2:W:244:ARG:HD3	2:W:304:VAL:HG23	1.75	0.69
3:P:212:TYR:O	3:P:216:ASN:HB2	1.93	0.69
2:E:168:GLN:HE21	2:E:201:MET:HG3	1.58	0.69
1:L:52:GLU:OE1	2:M:68:GLU:HB3	1.92	0.69
2:V:440:SER:O	2:V:444:VAL:HG23	1.93	0.69
1:J:139:LEU:HD13	2:N:104:ASP:HA	1.75	0.68
2:O:391:LEU:HB3	2:O:395:GLU:HG3	1.74	0.68
1:A:149:GLN:OE1	1:A:440:THR:OG1	2.10	0.68
1:B:398:GLN:HA	1:B:401:GLU:HG2	1.75	0.68
3:G:23:MET:HA	3:G:26:VAL:HB	1.75	0.68
1:A:174:GLN:HA	6:A:600:ANP:HNB1	1.59	0.68
3:G:89:SER:HA	3:G:117:GLN:NE2	2.08	0.68
2:N:41:THR:HB	2:N:42:PRO:HD2	1.76	0.68
2:N:237:LEU:HD22	2:N:292:LEU:HD12	1.74	0.68
3:G:77:ILE:HG21	3:G:222:MET:HG2	1.75	0.68
2:X:163:LYS:N	6:X:600:ANP:O1B	2.27	0.68
2:D:7:THR:HG23	2:D:7:THR:O	1.94	0.67
2:N:279:PHE:HE1	3:P:263:ILE:HD12	1.59	0.67
2:O:377:THR:HG22	2:O:407:ALA:HB2	1.76	0.67
1:B:272:ASP:HB2	1:B:328:VAL:O	1.95	0.67
2:E:133:ILE:HD12	2:E:146:PRO:HB2	1.76	0.67
2:N:279:PHE:CE1	3:P:263:ILE:HD12	2.30	0.67
2:F:346:PRO:HB2	2:F:348:VAL:HG23	1.77	0.67
2:V:97:ASN:HD21	2:V:101:GLU:HB2	1.60	0.67
1:B:36:VAL:HG11	1:B:84:VAL:O	1.94	0.67
1:T:33:VAL:HB	1:T:87:GLY:H	1.60	0.66
2:X:128:SER:HB2	2:X:300:LYS:HG3	1.78	0.66
1:U:135:ALA:HB3	2:V:223:ASN:HD22	1.60	0.66
2:D:26:GLU:OE2	2:D:26:GLU:HA	1.96	0.65
1:J:192:ASN:HA	1:J:200:LYS:HG2	1.77	0.65
1:S:73:VAL:HG22	2:W:72:ARG:HH12	1.60	0.65
1:B:109:VAL:HG22	1:B:233:ILE:HB	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:358:LEU:HB2	1:K:366:ALA:HB1	1.79	0.65
1:K:99:VAL:HG11	1:K:251:THR:HB	1.79	0.65
1:S:349:ASP:O	1:S:375:ARG:HB2	1.96	0.65
1:B:166:ARG:HD3	1:B:308:LEU:O	1.96	0.65
1:S:107:GLY:HA2	1:S:228:MET:O	1.96	0.65
1:A:112:ALA:O	1:A:251:THR:HG21	1.97	0.64
1:C:168:LEU:HB2	1:C:348:THR:HG21	1.79	0.64
1:A:173:ARG:NH2	2:D:352:ASP:OD1	2.30	0.64
1:J:70:PRO:HD3	2:N:15:ALA:HB2	1.78	0.64
1:L:164:GLY:HA2	1:L:323:LEU:O	1.96	0.64
2:O:264:ALA:HA	2:O:267:GLU:HG3	1.79	0.64
1:T:101:VAL:HG12	1:T:255:ILE:HA	1.79	0.64
2:E:98:VAL:HB	2:E:232:VAL:HG13	1.79	0.64
2:N:405:GLU:HG2	2:N:409:LYS:HE2	1.80	0.64
2:E:158:GLY:O	2:E:161:VAL:HG22	1.98	0.64
1:A:329:ILE:HD11	1:A:344:VAL:HG21	1.80	0.64
3:G:15:ASN:O	3:G:19:ILE:HG12	1.98	0.64
1:L:290:PRO:HB2	2:M:270:ALA:HB1	1.79	0.64
1:U:111:ASP:OD1	1:U:115:ASN:HB2	1.98	0.64
2:F:41:THR:HB	2:F:42:PRO:HD2	1.79	0.63
2:O:252:LEU:HD23	2:O:305:THR:HB	1.80	0.63
2:F:15:ALA:HB3	2:F:22:ASP:HB2	1.81	0.63
1:J:375:ARG:HH22	2:N:190:ARG:NE	1.97	0.63
1:L:99:VAL:HG11	1:L:251:THR:HB	1.81	0.63
2:F:33:ILE:O	2:F:34:LEU:HB2	1.99	0.63
2:E:157:GLY:HA2	2:E:337:ARG:HH22	1.64	0.63
1:J:223:GLU:HG3	1:J:228:MET:HG3	1.79	0.63
3:P:42:LYS:O	3:P:42:LYS:HD3	1.99	0.63
1:T:504:GLU:HA	1:T:507:VAL:HB	1.81	0.63
1:U:176:GLY:O	1:U:180:VAL:HG23	1.98	0.63
2:V:84:SER:HB3	2:V:114:ARG:HE	1.62	0.63
2:V:189:GLU:O	2:V:222:MET:HG2	1.99	0.62
2:M:224:GLU:O	2:M:229:ARG:HD3	1.99	0.62
1:S:223:GLU:HG3	1:S:228:MET:HG3	1.81	0.62
3:P:122:HIS:N	3:P:123:PRO:CD	2.63	0.62
4:H:35:LYS:HD3	4:H:35:LYS:H	1.64	0.62
2:W:133:ILE:HD12	2:W:146:PRO:HB2	1.82	0.62
1:T:392:LEU:HD13	1:T:451:VAL:HG22	1.82	0.62
2:E:15:ALA:HB3	2:E:22:ASP:HB2	1.82	0.61
2:M:160:GLY:N	6:M:600:ANP:HNB1	1.87	0.61
1:U:212:ARG:HG2	1:U:237:THR:HG21	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:148:ALA:HB2	2:F:357:LEU:HD11	1.82	0.61
2:F:345:TYR:HA	2:F:346:PRO:C	2.18	0.61
1:J:302:TYR:O	1:J:306:ARG:HB2	2.00	0.61
2:N:244:ARG:HD3	2:N:304:VAL:HG23	1.81	0.61
2:X:160:GLY:H	6:X:600:ANP:HNB1	1.46	0.61
1:B:99:VAL:HG11	1:B:251:THR:HB	1.81	0.61
2:D:197:LEU:O	2:D:201:MET:HG2	2.01	0.61
1:J:469:SER:HB3	1:J:506:PHE:CZ	2.35	0.61
2:E:39:ILE:HD13	2:E:70:LEU:HD21	1.83	0.61
2:E:43:GLN:HG2	2:E:44:GLY:N	2.15	0.61
1:B:148:VAL:HG23	1:B:163:ARG:HG2	1.83	0.61
1:B:387:GLN:OE1	1:B:491:LEU:HB2	2.01	0.61
1:K:173:ARG:HH12	2:N:327:ALA:HA	1.66	0.61
2:N:458:TYR:HD2	2:N:459:MET:HG2	1.66	0.61
1:J:306:ARG:HA	2:N:223:ASN:HB2	1.83	0.60
2:V:252:LEU:HD23	2:V:305:THR:HB	1.83	0.60
2:X:386:ASP:O	2:X:390:ILE:HG12	2.01	0.60
2:W:15:ALA:HB3	2:W:22:ASP:HB2	1.83	0.60
6:F:600:ANP:O5'	6:F:600:ANP:H8	2.01	0.60
1:K:211:LYS:HD2	2:N:328:HIS:HA	1.83	0.60
1:U:97:VAL:HG11	1:U:247:LEU:HD11	1.83	0.60
3:G:115:LYS:O	3:G:119:LEU:HB2	2.01	0.60
2:N:255:ILE:HB	2:N:308:GLN:HG2	1.81	0.60
2:V:204:THR:HB	2:V:206:VAL:HG23	1.84	0.60
1:S:145:HIS:H	1:S:313:LYS:HZ3	1.50	0.60
1:L:116:PRO:HG3	1:L:123:ILE:HG12	1.84	0.60
3:G:49:GLN:HE21	3:G:217:GLN:NE2	1.99	0.60
3:G:205:VAL:O	3:G:209:LEU:HB2	2.02	0.59
1:K:346:SER:HA	6:O:600:ANP:O3G	2.02	0.59
1:T:220:GLN:HB2	2:W:129:THR:HB	1.84	0.59
3:P:81:LYS:HE3	3:P:135:LYS:HD2	1.84	0.59
1:J:173:ARG:HD2	1:J:174:GLN:HE21	1.66	0.59
1:C:116:PRO:HG3	1:C:123:ILE:HG12	1.85	0.59
1:L:248:ALA:HB3	1:L:249:PRO:HD3	1.85	0.59
2:N:23:VAL:HG11	2:N:76:VAL:HG21	1.84	0.59
1:A:77:LEU:CD1	1:A:81:ASP:HB3	2.29	0.59
2:D:208:ASN:ND2	2:D:211:GLY:HA3	2.18	0.59
2:M:234:LEU:CD2	2:M:292:LEU:HD13	2.33	0.59
2:V:94:ARG:NH2	2:V:106:ARG:HB2	2.18	0.59
2:M:371:ALA:O	2:M:375:GLN:HG3	2.03	0.59
2:D:344:ILE:HG23	2:D:415:SER:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:34:LEU:HD21	1:K:44:PHE:HB2	1.85	0.58
1:L:493:LYS:HA	1:L:496:LEU:HD12	1.85	0.58
3:P:168:ASP:HB2	3:P:178:SER:OG	2.03	0.58
2:V:64:MET:CE	2:V:99:ILE:HG22	2.33	0.58
5:I:12:ALA:O	5:I:16:VAL:HG23	2.03	0.58
1:A:239:SER:HB3	2:D:294:GLU:HG3	1.86	0.58
2:F:146:PRO:O	2:F:355:SER:OG	2.21	0.58
1:S:309:GLU:HG3	2:W:223:ASN:HB3	1.86	0.58
1:U:206:VAL:HG13	1:U:234:VAL:HB	1.84	0.58
2:X:384:LEU:O	2:X:388:ILE:HG12	2.04	0.58
2:V:164:THR:O	2:V:167:ILE:HG22	2.04	0.58
1:B:98:ASP:HB2	1:B:129:SER:O	2.04	0.58
1:K:260:ARG:O	1:K:321:GLY:HA3	2.04	0.58
1:K:364:ARG:HA	1:K:365:PRO:C	2.24	0.58
1:L:148:VAL:HG21	1:L:324:THR:HG21	1.85	0.58
2:O:449:TYR:HB3	2:O:452:ILE:HD12	1.86	0.58
3:P:169:PRO:HG3	3:P:227:ALA:HB3	1.84	0.58
3:Y:16:ILE:HA	3:Y:19:ILE:HG22	1.86	0.58
2:V:182:SER:O	2:V:215:VAL:HA	2.04	0.57
1:K:186:LEU:O	1:K:189:LYS:HE3	2.03	0.57
2:X:178:HIS:HE2	2:X:250:ASP:HB3	1.69	0.57
1:S:439:ALA:HB3	1:S:442:GLU:HG3	1.85	0.57
1:T:67:ASN:HB3	2:X:17:ILE:HG23	1.86	0.57
1:S:217:GLN:HG2	2:V:356:ARG:HH21	1.68	0.57
1:A:146:GLU:HB2	1:A:163:ARG:HG3	1.87	0.57
1:B:26:ASN:O	1:B:30:THR:HB	2.05	0.57
2:D:15:ALA:HB3	2:D:22:ASP:HB2	1.87	0.57
2:D:263:GLN:O	2:D:266:SER:HB3	2.05	0.57
1:S:166:ARG:HD3	1:S:308:LEU:O	2.05	0.57
1:U:243:PRO:HA	1:U:283:LEU:HD11	1.87	0.57
2:V:339:ILE:HG22	2:V:344:ILE:HB	1.86	0.57
2:F:26:GLU:OE1	2:F:26:GLU:HA	2.04	0.57
2:F:189:GLU:O	2:F:221:GLN:HB3	2.04	0.57
1:A:182:LEU:CD1	1:A:218:LEU:HD11	2.31	0.56
2:V:345:TYR:HA	2:V:346:PRO:C	2.25	0.56
2:V:162:GLY:HA2	6:V:600:ANP:H8	1.86	0.56
1:A:383:LYS:O	1:A:387:GLN:HG3	2.06	0.56
2:E:277:SER:OG	2:E:278:ALA:N	2.38	0.56
2:O:237:LEU:HD13	2:O:296:ILE:HG12	1.87	0.56
2:O:345:TYR:HA	2:O:346:PRO:C	2.24	0.56
2:W:319:ASP:HA	3:Y:260:GLN:HE22	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:85:VAL:HG11	2:X:235:THR:HG23	1.86	0.56
4:H:14:PHE:CB	4:H:22:TYR:HB2	2.35	0.56
2:N:96:ILE:HB	2:N:218:VAL:HG22	1.87	0.56
1:S:192:ASN:HA	1:S:200:LYS:HG2	1.88	0.56
1:S:284:SER:O	1:S:289:ARG:HB2	2.06	0.56
1:S:163:ARG:O	1:S:313:LYS:HE3	2.06	0.56
1:S:265:HIS:ND1	1:S:322:SER:HB2	2.21	0.56
4:H:14:PHE:CZ	4:H:70:ILE:HD11	2.40	0.56
2:M:229:ARG:NH2	2:M:267:GLU:OE1	2.37	0.56
1:A:55:VAL:HG21	1:A:75:ILE:HD13	1.87	0.56
1:J:364:ARG:HA	1:J:365:PRO:C	2.26	0.56
2:V:346:PRO:O	2:V:347:ALA:HB3	2.04	0.56
5:I:55:GLU:CB	5:I:56:PRO:CD	2.83	0.56
1:K:444:VAL:CG2	1:K:445:PRO:HD3	2.36	0.56
2:N:51:ALA:O	2:N:52:GLN:HG3	2.06	0.56
2:O:140:VAL:HG13	2:O:414:LEU:HB3	1.88	0.56
1:U:378:SER:HB3	1:U:386:LYS:HE2	1.88	0.56
1:C:450:GLY:HA2	1:C:455:LEU:HD12	1.87	0.55
4:H:14:PHE:HB3	4:H:22:TYR:HB2	1.88	0.55
1:K:488:LYS:HE3	1:K:490:GLU:HB2	1.88	0.55
1:U:237:THR:H	1:U:240:GLU:HG3	1.71	0.55
2:V:46:LEU:HD22	2:V:70:LEU:HD21	1.88	0.55
3:Y:108:VAL:HG12	3:Y:130:ILE:HG13	1.88	0.55
3:G:46:GLU:O	3:G:50:LEU:HB2	2.05	0.55
1:S:36:VAL:HG21	1:S:84:VAL:HB	1.88	0.55
1:S:484:GLU:HG2	1:S:495:LEU:HD11	1.87	0.55
1:B:260:ARG:O	1:B:321:GLY:HA3	2.06	0.55
1:U:169:ILE:HB	1:U:328:VAL:HG22	1.88	0.55
1:B:105:LEU:O	1:B:232:ILE:HG12	2.07	0.55
3:G:247:MET:HG3	3:G:250:ARG:HH21	1.71	0.55
1:L:344:VAL:HA	1:L:347:ILE:HD12	1.89	0.55
2:O:377:THR:HG23	2:O:403:THR:HG23	1.88	0.55
2:V:9:ILE:HB	2:V:78:ASP:HB3	1.89	0.55
2:V:192:ARG:NH1	2:V:193:GLU:HG2	2.22	0.55
2:D:144:LEU:HD22	2:D:375:GLN:HE21	1.72	0.55
1:L:306:ARG:HG2	1:L:307:LEU:N	2.21	0.55
2:N:220:GLY:HA3	2:N:232:VAL:HG11	1.89	0.55
3:P:111:GLY:HA2	3:P:133:ILE:HD11	1.88	0.55
1:A:500:LYS:O	1:A:504:GLU:HG3	2.06	0.55
4:H:72:GLY:O	4:H:87:ALA:HA	2.07	0.55
2:V:15:ALA:HB3	2:V:22:ASP:HB2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:52:GLN:HG2	2:F:60:ARG:HB3	1.89	0.55
2:O:324:THR:HG22	2:O:324:THR:O	2.07	0.55
1:T:67:ASN:HB2	2:X:17:ILE:HG12	1.89	0.55
1:B:444:VAL:HG22	1:B:445:PRO:HD3	1.88	0.54
1:C:503:THR:O	1:C:507:VAL:HG23	2.07	0.54
2:X:167:ILE:HD12	2:X:309:ALA:HB2	1.89	0.54
2:M:440:SER:OG	2:M:463:ILE:HG12	2.07	0.54
2:V:346:PRO:O	2:V:347:ALA:CB	2.55	0.54
2:X:258:ILE:HD13	2:X:308:GLN:OE1	2.07	0.54
1:L:222:LEU:HD12	1:L:228:MET:HE2	1.90	0.54
1:B:359:PHE:HZ	6:B:600:ANP:O4'	1.90	0.54
1:S:55:VAL:HG21	1:S:75:ILE:HD13	1.89	0.54
1:S:311:ALA:HA	1:S:323:LEU:HB3	1.90	0.54
1:T:282:GLN:O	1:T:286:LEU:HG	2.08	0.54
2:E:321:ALA:HB3	2:E:322:PRO:CD	2.37	0.54
1:L:196:ASP:OD1	1:L:198:SER:OG	2.23	0.54
1:L:174:GLN:HA	6:L:600:ANP:HNB1	1.73	0.54
2:N:169:GLU:HG2	2:N:418:PHE:CD1	2.42	0.54
3:P:205:VAL:N	3:P:206:PRO:CD	2.66	0.54
3:P:229:GLU:HG3	3:P:230:ILE:N	2.23	0.54
2:D:299:THR:OG1	2:D:300:LYS:N	2.41	0.54
3:G:118:LEU:HB3	3:G:126:ILE:HD11	1.90	0.54
5:I:19:GLN:HE22	5:I:38:SER:HB3	1.73	0.54
1:J:332:GLN:HB3	2:M:318:THR:HB	1.89	0.54
1:U:165:GLN:HG2	1:U:166:ARG:H	1.73	0.54
2:D:237:LEU:HD13	2:D:296:ILE:HG12	1.90	0.54
1:U:56:GLU:HG2	1:U:62:LYS:HG2	1.90	0.54
3:Y:91:LEU:HD12	3:Y:177:PRO:HB3	1.89	0.54
1:A:111:ASP:OD2	1:A:115:ASN:HB2	2.08	0.54
1:C:429:LEU:HD11	1:C:446:LEU:HB3	1.90	0.54
2:W:388:ILE:HD12	2:W:393:MET:HG2	1.90	0.54
3:P:86:SER:HB2	3:P:90:GLN:HG3	1.90	0.53
1:S:462:ARG:HH11	1:S:465:GLU:HG3	1.73	0.53
2:X:237:LEU:HD13	2:X:296:ILE:HG12	1.89	0.53
2:E:344:ILE:HG23	2:E:415:SER:HB3	1.89	0.53
2:M:321:ALA:HB3	2:M:322:PRO:CD	2.38	0.53
1:S:402:VAL:HA	1:S:405:PHE:HD1	1.73	0.53
2:X:345:TYR:HA	2:X:346:PRO:C	2.29	0.53
1:T:305:SER:HB2	2:X:222:MET:HB2	1.90	0.53
1:K:217:GLN:NE2	2:N:131:ALA:HB2	2.24	0.53
2:N:131:ALA:HB1	2:N:357:LEU:HD11	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:87:ILE:HG23	3:G:167:ASN:ND2	2.24	0.53
2:V:237:LEU:HD13	2:V:296:ILE:HG12	1.91	0.53
2:D:33:ILE:O	2:D:34:LEU:HB2	2.08	0.53
1:J:253:ALA:O	1:J:257:GLU:HG3	2.08	0.53
2:O:15:ALA:HB3	2:O:22:ASP:HB2	1.91	0.53
1:S:187:ASN:O	1:S:190:ARG:HG3	2.08	0.53
1:U:249:PRO:HB3	1:U:270:TYR:HD1	1.73	0.53
2:V:346:PRO:HD3	2:V:416:GLN:H	1.74	0.53
2:W:170:LEU:O	2:W:174:ILE:HG12	2.09	0.53
3:G:77:ILE:HD13	3:G:110:ILE:HD12	1.90	0.53
2:V:321:ALA:HB3	2:V:322:PRO:CD	2.39	0.53
4:H:57:VAL:CG2	4:H:70:ILE:HD12	2.38	0.53
2:E:228:ALA:O	2:E:232:VAL:HG22	2.09	0.53
1:K:301:PHE:CB	2:O:263:GLN:HE22	2.21	0.53
2:M:425:THR:CG2	6:M:600:ANP:H2	2.39	0.53
1:A:257:GLU:HG2	1:A:260:ARG:CZ	2.39	0.52
2:V:189:GLU:O	2:V:221:GLN:HB3	2.09	0.52
1:J:108:ARG:NH2	1:J:121:GLY:O	2.37	0.52
1:U:354:LEU:HA	1:U:366:ALA:O	2.08	0.52
1:K:148:VAL:HB	1:K:161:ILE:HB	1.91	0.52
3:P:133:ILE:O	3:P:135:LYS:N	2.35	0.52
1:S:118:ASP:OD1	1:S:120:LYS:HD2	2.09	0.52
1:U:54:LEU:HD21	1:U:97:VAL:HG13	1.90	0.52
1:L:54:LEU:O	1:L:93:THR:HB	2.10	0.52
2:M:336:SER:HB3	2:M:339:ILE:HG13	1.91	0.52
3:Y:79:SER:HB3	3:Y:88:HIS:HE1	1.73	0.52
2:N:384:LEU:O	2:N:388:ILE:HG12	2.08	0.52
2:V:192:ARG:HH11	2:V:193:GLU:HG2	1.74	0.52
1:C:43:VAL:HG21	1:C:75:ILE:HD12	1.90	0.52
2:D:158:GLY:O	2:D:161:VAL:HG22	2.09	0.52
2:O:221:GLN:HA	2:O:221:GLN:OE1	2.10	0.52
1:A:478:HIS:HB3	1:A:481:LEU:HD21	1.91	0.52
1:C:189:LYS:HE3	1:C:226:ASP:HB3	1.91	0.52
2:D:244:ARG:HD2	2:D:299:THR:HG22	1.91	0.52
3:G:49:GLN:HE21	3:G:217:GLN:HE22	1.57	0.52
2:N:98:VAL:HG13	2:N:99:ILE:HG23	1.90	0.52
2:N:152:LYS:HE2	2:N:293:GLN:O	2.10	0.52
2:N:184:PHE:HB3	2:N:217:LEU:HD23	1.90	0.52
1:S:311:ALA:HB1	1:S:323:LEU:O	2.10	0.52
1:C:103:PRO:HD3	1:C:258:TRP:CH2	2.45	0.51
2:E:136:THR:HG23	2:E:138:ILE:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:421:VAL:O	1:J:425:ARG:HD2	2.10	0.51
3:P:168:ASP:N	3:P:176:GLU:O	2.40	0.51
1:U:249:PRO:HB3	1:U:270:TYR:CD1	2.45	0.51
1:J:135:ALA:HB3	2:N:223:ASN:ND2	2.25	0.51
1:L:481:LEU:HD13	1:L:495:LEU:HD22	1.91	0.51
1:T:77:LEU:O	1:T:243:PRO:HG2	2.11	0.51
1:U:150:THR:HA	1:U:184:THR:HG23	1.91	0.51
1:U:211:LYS:HE3	1:U:213:SER:HB2	1.92	0.51
2:W:370:VAL:O	2:W:374:VAL:HG23	2.10	0.51
1:A:77:LEU:HD12	1:A:81:ASP:CB	2.33	0.51
1:K:269:VAL:HG22	1:K:326:LEU:HB2	1.91	0.51
1:L:187:ASN:O	1:L:190:ARG:HG3	2.09	0.51
2:F:176:LYS:HE2	2:F:204:THR:HB	1.93	0.51
4:H:33:PRO:HB3	4:H:38:ARG:NH1	2.26	0.51
1:J:174:GLN:HA	6:J:600:ANP:HNB1	1.74	0.51
1:K:66:LEU:HD21	1:K:289:ARG:HH22	1.75	0.51
1:K:354:LEU:HA	1:K:366:ALA:O	2.11	0.51
1:L:222:LEU:HD12	1:L:228:MET:CE	2.40	0.51
1:U:258:TRP:O	1:U:262:ASN:ND2	2.44	0.51
2:V:133:ILE:HD11	2:V:434:LEU:HD13	1.92	0.51
2:E:50:VAL:HA	2:E:61:THR:HG22	1.91	0.51
2:O:37:LEU:HD12	2:O:61:THR:HG21	1.91	0.51
1:S:99:VAL:HG21	1:S:251:THR:HG23	1.92	0.51
1:S:422:ARG:HH21	1:S:453:GLY:HA3	1.75	0.51
1:A:142:ARG:HD3	1:A:143:SER:O	2.11	0.51
1:A:153:LYS:NZ	1:A:467:GLU:OE1	2.42	0.51
1:A:391:SER:O	1:A:394:LEU:HB2	2.10	0.51
1:C:159:VAL:HG21	1:C:352:ILE:HG12	1.92	0.51
2:D:7:THR:O	2:D:7:THR:CG2	2.59	0.51
3:G:110:ILE:HA	3:G:130:ILE:HB	1.93	0.51
1:J:243:PRO:HD3	1:J:283:LEU:HD21	1.93	0.51
2:M:62:ILE:HD11	2:M:272:LEU:HD11	1.93	0.51
2:M:425:THR:HG23	6:M:600:ANP:H2	1.93	0.51
1:S:422:ARG:HE	1:S:453:GLY:HA2	1.76	0.51
3:G:165:PHE:CE2	3:G:179:GLU:HB2	2.46	0.51
2:W:220:GLY:HA3	2:W:232:VAL:HG11	1.92	0.51
2:D:64:MET:CE	2:D:228:ALA:HA	2.41	0.50
1:J:50:GLN:HB3	2:N:69:GLY:HA2	1.92	0.50
2:D:408:ARG:O	2:D:412:ARG:HD2	2.11	0.50
1:J:375:ARG:HH22	2:N:190:ARG:CZ	2.25	0.50
1:K:421:VAL:O	1:K:425:ARG:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:168:GLN:HE21	2:N:201:MET:HG2	1.77	0.50
2:V:82:PRO:HB3	2:V:118:HIS:HD2	1.76	0.50
2:V:298:THR:HG23	2:V:303:SER:HA	1.93	0.50
2:W:140:VAL:HG22	2:W:414:LEU:O	2.12	0.50
1:A:444:VAL:HG22	1:A:445:PRO:HD3	1.92	0.50
1:K:32:ARG:HD2	1:K:87:GLY:O	2.11	0.50
1:K:174:GLN:HA	6:K:600:ANP:N3B	2.27	0.50
2:D:20:ILE:HG13	2:D:271:LEU:HB3	1.93	0.50
2:D:148:ALA:HA	2:D:357:LEU:HD11	1.93	0.50
1:S:481:LEU:O	1:S:485:ILE:HG13	2.12	0.50
2:X:321:ALA:HB3	2:X:322:PRO:CD	2.42	0.50
1:B:421:VAL:O	1:B:425:ARG:HG2	2.12	0.50
1:C:107:GLY:HA2	1:C:228:MET:O	2.11	0.50
2:E:243:PHE:O	2:E:247:GLU:HB2	2.12	0.50
4:H:57:VAL:HG21	4:H:70:ILE:HD12	1.93	0.50
3:G:205:VAL:HB	3:G:206:PRO:HD3	1.93	0.50
2:M:20:ILE:HG13	2:M:271:LEU:HB3	1.94	0.50
1:A:282:GLN:HG3	2:D:283:PRO:O	2.11	0.50
1:S:248:ALA:HB3	1:S:249:PRO:HD3	1.92	0.50
2:W:242:TYR:CE1	2:W:246:GLU:HG3	2.47	0.50
2:W:284:THR:HB	2:W:288:ASP:OD1	2.12	0.50
1:C:219:VAL:HB	1:C:228:MET:HE3	1.94	0.49
3:P:162:ILE:HB	3:P:182:ILE:HB	1.94	0.49
1:S:287:LEU:HB2	1:S:289:ARG:HD2	1.94	0.49
3:Y:150:LEU:HA	3:Y:154:MET:HB2	1.93	0.49
1:B:168:LEU:HB2	1:B:348:THR:HG21	1.94	0.49
2:D:218:VAL:HG21	2:D:236:GLY:HA2	1.94	0.49
4:H:14:PHE:HZ	4:H:70:ILE:HD11	1.76	0.49
2:V:33:ILE:O	2:V:34:LEU:HB2	2.12	0.49
3:Y:263:ILE:O	3:Y:267:LEU:HB3	2.13	0.49
1:L:197:GLU:HA	1:L:200:LYS:HD2	1.95	0.49
2:W:419:ALA:HA	2:W:429:GLY:HA3	1.92	0.49
3:G:118:LEU:HA	3:G:121:THR:HG22	1.94	0.49
1:K:109:VAL:HG22	1:K:233:ILE:HB	1.93	0.49
1:K:273:LEU:HD22	1:K:276:GLN:OE1	2.13	0.49
2:N:253:LEU:O	2:N:306:SER:HA	2.13	0.49
2:D:201:MET:HE2	2:D:217:LEU:HD21	1.93	0.49
1:T:138:ILE:HD13	2:X:95:ILE:HG21	1.93	0.49
2:N:359:ASP:O	2:N:363:VAL:HG22	2.12	0.49
2:X:178:HIS:NE2	2:X:250:ASP:HB3	2.27	0.49
1:B:117:ILE:HD12	2:E:124:PHE:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:201:MET:HE1	2:D:215:VAL:HG11	1.94	0.49
2:F:140:VAL:HG12	2:F:414:LEU:HD22	1.94	0.49
1:L:166:ARG:HH21	1:L:349:ASP:CG	2.16	0.49
2:N:410:ILE:HG23	2:N:441:PHE:HE2	1.77	0.49
1:L:338:ALA:O	1:L:342:THR:OG1	2.31	0.49
2:M:152:LYS:HD3	2:M:328:HIS:O	2.12	0.49
2:N:220:GLY:CA	2:N:232:VAL:HG11	2.42	0.49
1:J:428:GLN:HA	1:J:431:LYS:HD2	1.94	0.49
1:L:441:GLU:OE2	1:L:486:ARG:HD3	2.13	0.49
1:L:484:GLU:HB3	1:L:495:LEU:HD11	1.95	0.49
3:P:150:LEU:HA	3:P:154:MET:HB2	1.95	0.49
1:T:103:PRO:HD3	1:T:258:TRP:CZ2	2.48	0.49
2:W:33:ILE:O	2:W:34:LEU:HB2	2.12	0.49
2:E:33:ILE:O	2:E:34:LEU:HB2	2.13	0.48
5:I:28:GLU:O	5:I:30:GLN:N	2.42	0.48
1:U:242:ALA:HB3	1:U:243:PRO:HD3	1.95	0.48
1:U:285:LEU:HD11	1:U:295:ALA:HB1	1.95	0.48
2:F:84:SER:HB2	2:F:114:ARG:HH11	1.78	0.48
1:S:39:GLY:HA2	1:S:77:LEU:HD12	1.94	0.48
1:S:441:GLU:CG	1:S:486:ARG:HB2	2.41	0.48
1:B:445:PRO:HB3	1:B:499:LEU:HD11	1.95	0.48
3:G:75:VAL:HB	3:G:164:ILE:HD13	1.95	0.48
1:J:173:ARG:HH11	1:J:174:GLN:HE21	1.60	0.48
1:L:161:ILE:HA	1:L:165:GLN:OE1	2.13	0.48
2:M:234:LEU:HD22	2:M:292:LEU:HD13	1.96	0.48
1:U:166:ARG:HG2	1:U:325:ALA:HB3	1.95	0.48
2:D:34:LEU:HD22	2:D:118:HIS:CE1	2.49	0.48
2:F:9:ILE:HG23	2:F:27:GLN:NE2	2.28	0.48
2:O:346:PRO:HB2	2:O:348:VAL:HG23	1.95	0.48
1:S:340:ILE:HB	1:S:341:PRO:HD3	1.95	0.48
2:D:384:LEU:O	2:D:388:ILE:HG12	2.13	0.48
2:E:456:ALA:HA	2:E:469:LYS:HD3	1.96	0.48
3:G:17:GLU:O	3:G:21:LYS:HB2	2.14	0.48
3:G:267:LEU:O	3:G:271:ILE:HG12	2.14	0.48
2:M:335:LEU:HA	2:M:347:ALA:O	2.13	0.48
1:A:394:LEU:O	1:A:397:ALA:HB3	2.13	0.48
1:C:88:GLU:HG3	1:C:89:LEU:N	2.28	0.48
1:K:51:ALA:O	1:K:52:GLU:HB2	2.13	0.48
2:O:165:VAL:HG23	6:O:600:ANP:O1A	2.13	0.48
1:C:481:LEU:HD21	1:C:498:SER:HB3	1.95	0.48
2:D:386:ASP:OD1	2:D:386:ASP:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:10:THR:HG21	2:E:75:LYS:HE2	1.96	0.48
1:K:478:HIS:HB3	1:K:481:LEU:HG	1.96	0.48
2:N:252:LEU:HA	2:N:305:THR:O	2.14	0.48
2:X:85:VAL:CG1	2:X:235:THR:HG23	2.44	0.48
1:A:134:LYS:HE2	2:E:65:ASP:OD1	2.13	0.48
4:H:88:ILE:HD11	5:I:14:LEU:HB3	1.95	0.48
1:K:152:LEU:HD22	1:K:365:PRO:HG3	1.96	0.48
2:V:190:ARG:HB2	2:V:193:GLU:HG3	1.96	0.48
1:B:345:ILE:HG12	1:B:351:GLN:HG2	1.94	0.48
1:L:172:ASP:O	1:L:177:LYS:NZ	2.47	0.48
2:M:143:LEU:O	2:M:367:HIS:HE1	1.97	0.48
1:S:47:ASN:HA	2:W:72:ARG:HH21	1.79	0.48
2:D:47:VAL:HG21	2:D:99:ILE:HG21	1.95	0.48
2:E:221:GLN:HB2	2:E:223:ASN:OD1	2.14	0.48
2:N:330:ASP:O	2:N:356:ARG:HD3	2.14	0.48
1:S:395:PHE:HE1	1:S:422:ARG:HH11	1.61	0.48
1:A:395:PHE:HZ	1:A:419:THR:CA	2.06	0.47
1:B:291:PRO:HG2	3:G:268:VAL:HG22	1.96	0.47
4:H:88:ILE:CD1	5:I:14:LEU:HB3	2.44	0.47
2:X:190:ARG:NH1	6:X:600:ANP:O3G	2.45	0.47
1:A:272:ASP:HB2	1:A:328:VAL:O	2.14	0.47
1:K:428:GLN:O	1:K:431:LYS:HB2	2.14	0.47
1:B:46:LEU:HD22	1:B:92:ARG:HG3	1.96	0.47
2:F:67:THR:HB	2:F:70:LEU:HD12	1.96	0.47
1:L:108:ARG:NH2	1:L:120:LYS:HB2	2.28	0.47
1:S:260:ARG:O	1:S:321:GLY:HA3	2.13	0.47
1:T:355:GLU:HB3	1:T:358:LEU:HD12	1.97	0.47
1:B:26:ASN:ND2	1:B:26:ASN:H	2.13	0.47
1:J:100:PRO:HD3	1:J:128:ARG:NH1	2.30	0.47
1:L:55:VAL:HG21	1:L:75:ILE:HD13	1.96	0.47
2:M:167:ILE:HD12	2:M:309:ALA:HB2	1.96	0.47
2:N:184:PHE:HA	2:N:254:PHE:HB2	1.96	0.47
1:T:413:ASP:O	1:T:417:LYS:HB2	2.15	0.47
2:V:397:SER:HB3	2:V:400:ASP:HB2	1.95	0.47
1:C:80:SER:OG	1:C:82:ARG:HG2	2.13	0.47
2:F:263:GLN:O	2:F:267:GLU:HG3	2.15	0.47
1:L:506:PHE:O	1:L:509:THR:HA	2.15	0.47
1:S:142:ARG:HG2	1:S:143:SER:N	2.29	0.47
1:B:213:SER:O	1:B:217:GLN:HG3	2.15	0.47
1:J:388:VAL:HG21	1:J:444:VAL:HB	1.96	0.47
1:K:271:ASP:HA	1:K:272:ASP:HA	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:416:GLN:HA	2:M:417:PRO:HD2	1.78	0.47
2:N:127:GLN:HE22	2:N:297:THR:HG21	1.80	0.47
3:P:136:ASP:OD2	3:P:136:ASP:N	2.48	0.47
1:C:364:ARG:HA	1:C:365:PRO:C	2.34	0.47
5:I:31:THR:HG22	5:I:34:VAL:HG23	1.97	0.47
1:L:280:TYR:CD2	1:L:303:LEU:HD22	2.50	0.47
1:S:309:GLU:OE1	2:W:191:THR:OG1	2.26	0.47
2:V:330:ASP:O	2:V:356:ARG:HG2	2.14	0.47
2:W:220:GLY:CA	2:W:232:VAL:HG11	2.45	0.47
3:Y:116:MET:HA	3:Y:119:LEU:HB2	1.95	0.47
1:A:354:LEU:HA	1:A:366:ALA:O	2.15	0.47
2:F:346:PRO:C	2:F:348:VAL:H	2.18	0.47
1:J:205:TYR:HB3	1:J:233:ILE:HD13	1.97	0.47
1:U:46:LEU:HD22	1:U:92:ARG:HG3	1.97	0.47
2:W:98:VAL:HG13	2:W:99:ILE:HG23	1.95	0.47
1:A:82:ARG:O	1:A:82:ARG:HG2	2.14	0.47
1:B:202:TYR:O	1:B:266:ALA:HA	2.15	0.47
1:C:187:ASN:O	1:C:190:ARG:HG3	2.14	0.47
2:D:189:GLU:O	2:D:222:MET:HG2	2.14	0.47
2:F:164:THR:O	2:F:168:GLN:HG3	2.15	0.47
3:G:81:LYS:HD2	3:G:134:GLY:O	2.14	0.47
2:M:158:GLY:O	2:M:163:LYS:NZ	2.48	0.47
1:S:168:LEU:HD12	1:S:327:PRO:O	2.15	0.47
2:F:289:MET:SD	2:F:324:THR:HG22	2.55	0.46
2:F:394:ASP:HB3	3:G:85:GLY:O	2.15	0.46
1:S:168:LEU:HD21	1:S:170:ILE:HD12	1.96	0.46
2:V:136:THR:HG21	2:V:147:TYR:CD2	2.49	0.46
2:V:315:ASP:OD2	2:V:337:ARG:NE	2.33	0.46
2:V:373:LYS:HG2	2:V:445:LEU:HD22	1.97	0.46
1:C:42:ARG:HE	1:C:72:GLN:HE22	1.61	0.46
2:E:136:THR:HG22	2:E:142:ASP:CG	2.36	0.46
2:E:188:GLY:O	2:E:222:MET:HG3	2.16	0.46
3:G:56:GLU:O	3:G:58:LYS:HD3	2.15	0.46
1:J:164:GLY:HA2	1:J:323:LEU:O	2.15	0.46
1:J:459:GLU:HG3	1:J:462:ARG:HG3	1.97	0.46
1:B:51:ALA:O	1:B:52:GLU:HB2	2.16	0.46
3:G:180:LYS:HZ1	3:G:220:THR:HB	1.80	0.46
1:J:270:TYR:O	1:J:272:ASP:HA	2.15	0.46
1:S:272:ASP:HB2	1:S:328:VAL:O	2.15	0.46
1:A:445:PRO:HB3	1:A:499:LEU:HD11	1.98	0.46
1:C:349:ASP:O	1:C:375:ARG:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:338:ALA:HB3	1:K:341:PRO:HG2	1.98	0.46
2:O:245:ASP:OD1	2:O:301:LYS:HD3	2.15	0.46
1:S:206:VAL:HG22	1:S:252:ALA:CB	2.46	0.46
2:V:96:ILE:HB	2:V:218:VAL:HG22	1.96	0.46
1:A:70:PRO:HD3	2:E:15:ALA:HB2	1.97	0.46
1:A:391:SER:O	1:A:394:LEU:N	2.49	0.46
2:D:256:ASP:OD1	2:D:257:ASN:HB2	2.15	0.46
4:H:56:VAL:HA	4:H:68:PHE:O	2.15	0.46
2:N:52:GLN:HB2	2:N:60:ARG:HB3	1.97	0.46
1:T:166:ARG:HH22	2:X:190:ARG:CD	2.28	0.46
1:U:106:LEU:HD22	1:U:230:TYR:HA	1.96	0.46
1:B:364:ARG:HA	1:B:365:PRO:C	2.35	0.46
2:M:84:SER:HB2	2:M:114:ARG:HH21	1.80	0.46
2:V:222:MET:HA	2:V:229:ARG:HD2	1.97	0.46
2:F:152:LYS:HZ1	2:F:293:GLN:HB3	1.81	0.46
2:N:187:VAL:HG11	2:N:261:PHE:HB2	1.97	0.46
2:O:336:SER:HB3	2:O:339:ILE:HD12	1.97	0.46
4:Q:16:LEU:HB2	4:Q:19:GLU:HB2	1.96	0.46
2:V:417:PRO:HG2	2:V:430:LYS:HB2	1.98	0.46
2:F:382:LYS:HA	2:F:385:GLN:HG2	1.97	0.46
3:G:13:ILE:HG22	3:G:248:ILE:HG13	1.98	0.46
1:K:64:MET:HB2	1:K:78:PHE:CE2	2.51	0.46
2:M:32:ALA:O	2:M:35:ASN:HB2	2.16	0.46
2:V:99:ILE:HD11	2:V:101:GLU:CD	2.36	0.46
2:E:30:LEU:HD11	2:E:57:ASN:HA	1.98	0.45
2:N:96:ILE:HG22	2:N:97:ASN:N	2.31	0.45
1:T:154:ALA:HB2	1:T:430:LEU:HB3	1.98	0.45
1:U:112:ALA:HB3	1:U:244:LEU:HD22	1.97	0.45
1:U:177:LYS:HG2	1:U:354:LEU:HD12	1.98	0.45
1:U:421:VAL:O	1:U:425:ARG:HD2	2.16	0.45
2:X:252:LEU:HD23	2:X:305:THR:HB	1.99	0.45
4:H:113:SER:N	4:H:114:SER:HA	2.30	0.45
1:J:30:THR:HA	1:J:90:VAL:O	2.15	0.45
2:E:134:LEU:HD22	2:E:305:THR:HG21	1.97	0.45
1:J:139:LEU:O	1:J:141:ARG:N	2.44	0.45
1:J:141:ARG:HB2	2:N:195:ASN:ND2	2.31	0.45
2:N:276:PRO:HD2	3:P:271:ILE:HD11	1.98	0.45
2:O:7:THR:HA	2:O:8:PRO:HD3	1.81	0.45
1:S:396:LEU:O	1:S:400:ARG:HG3	2.17	0.45
1:T:424:GLU:O	1:T:428:GLN:HB2	2.16	0.45
2:X:36:ALA:HB2	2:X:83:ILE:HG12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:VAL:HA	1:B:159:VAL:HG23	1.98	0.45
1:C:159:VAL:HG23	1:C:159:VAL:O	2.16	0.45
2:W:53:HIS:O	2:W:55:GLY:N	2.49	0.45
1:B:67:ASN:HB2	2:F:17:ILE:HG13	1.98	0.45
1:K:182:LEU:HA	1:K:185:ILE:HD12	1.99	0.45
2:N:23:VAL:CG1	2:N:76:VAL:HG21	2.46	0.45
1:K:188:GLN:HB3	1:K:192:ASN:ND2	2.31	0.45
1:L:97:VAL:HG11	1:L:247:LEU:HD21	1.98	0.45
1:L:227:ALA:HA	1:L:230:TYR:CE2	2.51	0.45
1:L:455:LEU:HA	1:L:458:ILE:HD12	1.99	0.45
2:N:144:LEU:HD22	2:N:375:GLN:HG3	1.98	0.45
2:O:384:LEU:HD22	2:O:396:LEU:HD21	1.99	0.45
1:S:146:GLU:H	1:S:313:LYS:NZ	2.14	0.45
1:T:77:LEU:HD21	1:T:84:VAL:HG21	1.99	0.45
1:U:181:ALA:HB1	1:U:269:VAL:HG21	1.97	0.45
1:U:205:TYR:HB3	1:U:233:ILE:HD13	1.99	0.45
3:Y:212:TYR:O	3:Y:216:ASN:HB2	2.15	0.45
1:A:217:GLN:HG2	2:D:356:ARG:HH21	1.82	0.45
1:A:446:LEU:CD2	1:A:467:GLU:HG3	2.47	0.45
1:B:435:TYR:C	1:B:437:PRO:HD3	2.37	0.45
3:Y:76:ALA:HB1	3:Y:109:THR:HG22	1.99	0.45
1:C:166:ARG:HD2	1:C:308:LEU:O	2.17	0.45
2:F:143:LEU:O	2:F:367:HIS:HE1	2.00	0.45
2:F:384:LEU:O	2:F:388:ILE:HG12	2.17	0.45
2:F:390:ILE:HD12	3:G:244:ALA:HA	1.99	0.45
4:H:71:SER:HB3	4:H:89:GLU:HB2	1.99	0.45
1:L:243:PRO:O	1:L:247:LEU:HB2	2.16	0.45
2:O:251:VAL:HB	2:O:304:VAL:HG22	1.99	0.45
1:T:148:VAL:HG21	1:T:324:THR:HG21	1.97	0.45
2:W:256:ASP:HA	2:W:257:ASN:HA	1.66	0.45
2:X:284:THR:O	2:X:288:ASP:HB2	2.16	0.45
1:A:424:GLU:HB3	1:A:460:LEU:HD21	1.98	0.45
2:O:189:GLU:O	2:O:221:GLN:HB3	2.17	0.45
1:T:243:PRO:HG3	1:T:283:LEU:HD21	1.99	0.45
1:A:446:LEU:HD22	1:A:467:GLU:HG3	1.99	0.45
1:B:474:LEU:HB3	1:B:482:LEU:HD11	2.00	0.45
1:C:78:PHE:HB3	1:C:244:LEU:HD21	1.98	0.45
2:E:170:LEU:O	2:E:174:ILE:HG12	2.17	0.45
2:M:144:LEU:O	2:M:358:LEU:HD22	2.17	0.45
1:S:161:ILE:HD11	1:S:352:ILE:HD11	1.98	0.45
2:D:425:THR:HB	2:D:427:ILE:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:21:VAL:O	2:F:61:THR:OG1	2.30	0.44
2:F:33:ILE:O	2:F:34:LEU:CB	2.64	0.44
2:F:277:SER:OG	2:F:278:ALA:N	2.50	0.44
1:J:360:TYR:OH	2:M:354:LYS:HE2	2.16	0.44
1:K:109:VAL:HB	1:K:118:ASP:HB3	1.98	0.44
2:M:33:ILE:O	2:M:34:LEU:HB2	2.17	0.44
2:N:96:ILE:HG22	2:N:97:ASN:O	2.18	0.44
2:O:32:ALA:O	2:O:35:ASN:HB2	2.17	0.44
2:O:196:ASP:OD1	2:O:199:ARG:NH2	2.49	0.44
2:O:277:SER:OG	2:O:278:ALA:N	2.50	0.44
1:A:205:TYR:HB3	1:A:233:ILE:HD13	1.99	0.44
1:A:288:ARG:HH11	1:A:288:ARG:HG2	1.83	0.44
1:B:290:PRO:HG2	2:F:270:ALA:HB2	1.98	0.44
2:D:229:ARG:NH2	2:D:267:GLU:OE1	2.48	0.44
2:D:456:ALA:HA	2:D:469:LYS:HD3	1.99	0.44
1:U:341:PRO:O	1:U:345:ILE:HG13	2.16	0.44
2:W:168:GLN:HA	2:W:171:ILE:HD12	1.99	0.44
2:D:152:LYS:NZ	2:D:293:GLN:HB3	2.32	0.44
2:D:321:ALA:HB3	2:D:322:PRO:CD	2.48	0.44
2:E:142:ASP:HB3	2:E:434:LEU:HD12	1.99	0.44
2:E:229:ARG:NH2	2:E:267:GLU:OE1	2.49	0.44
2:E:256:ASP:HA	2:E:257:ASN:HA	1.76	0.44
2:F:94:ARG:NH2	2:F:102:PRO:HB2	2.32	0.44
2:O:33:ILE:HG22	2:O:34:LEU:HG	1.99	0.44
1:S:146:GLU:H	1:S:313:LYS:HZ3	1.65	0.44
1:S:385:LEU:HD11	1:S:447:ILE:HD12	1.98	0.44
6:U:600:ANP:O2A	6:U:600:ANP:N3B	2.48	0.44
2:W:95:ILE:HB	2:W:104:ASP:HB3	1.98	0.44
2:W:102:PRO:HG3	2:W:109:ILE:HG13	2.00	0.44
2:W:185:THR:OG1	2:W:236:GLY:HA3	2.17	0.44
2:W:188:GLY:HA3	2:W:260:ARG:HD2	2.00	0.44
2:W:410:ILE:HG23	2:W:441:PHE:HE2	1.82	0.44
1:B:25:ALA:HB1	1:B:30:THR:HG21	1.99	0.44
1:B:50:GLN:HB3	2:F:69:GLY:HA2	1.99	0.44
1:C:55:VAL:HG21	1:C:75:ILE:HD13	1.99	0.44
3:G:9:ARG:HD2	3:G:251:TYR:HE2	1.81	0.44
1:L:40:ILE:HD11	1:L:76:VAL:HG12	2.00	0.44
2:N:45:LYS:HG3	2:N:45:LYS:O	2.18	0.44
1:T:168:LEU:HD12	1:T:327:PRO:O	2.17	0.44
1:U:211:LYS:O	1:U:215:VAL:HG23	2.16	0.44
1:U:219:VAL:HA	1:U:222:LEU:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:234:LEU:HD23	2:X:292:LEU:HD13	1.99	0.44
1:B:117:ILE:HD12	2:E:124:PHE:CB	2.48	0.44
2:E:117:ILE:HG22	2:E:235:THR:HA	1.99	0.44
2:F:104:ASP:C	2:F:106:ARG:H	2.21	0.44
2:F:182:SER:HA	2:F:252:LEU:O	2.17	0.44
4:H:35:LYS:HE2	4:H:37:GLY:H	1.83	0.44
1:L:187:ASN:OD1	1:L:190:ARG:NH1	2.47	0.44
1:L:426:LEU:HD21	1:L:450:GLY:HA3	1.99	0.44
2:M:314:ALA:O	2:M:315:ASP:HB2	2.18	0.44
3:P:42:LYS:HA	3:P:45:ASP:HB2	1.99	0.44
1:T:306:ARG:O	1:T:310:ARG:HD3	2.18	0.44
1:U:89:LEU:N	1:U:89:LEU:HD12	2.33	0.44
2:W:320:PRO:O	2:W:324:THR:OG1	2.28	0.44
2:X:141:VAL:HG22	2:X:333:THR:HG21	1.99	0.44
1:B:166:ARG:CD	1:B:308:LEU:O	2.65	0.44
2:D:314:ALA:O	2:D:315:ASP:HB2	2.18	0.44
1:K:112:ALA:HB2	1:K:236:ALA:HB2	1.98	0.44
1:L:150:THR:HA	1:L:184:THR:HG23	2.00	0.44
2:V:138:ILE:HA	2:V:416:GLN:OE1	2.18	0.44
1:A:248:ALA:HB3	1:A:249:PRO:HD3	1.99	0.44
2:N:150:GLY:HA2	2:N:304:VAL:O	2.18	0.44
3:Y:41:ALA:HB1	3:Y:220:THR:HA	2.00	0.44
1:A:426:LEU:O	1:A:430:LEU:HG	2.18	0.44
1:B:182:LEU:HD13	1:B:218:LEU:HD11	2.00	0.44
2:E:237:LEU:O	2:E:241:GLU:HG3	2.18	0.44
2:F:158:GLY:O	2:F:161:VAL:HG22	2.18	0.44
1:J:300:VAL:O	1:J:303:LEU:HB3	2.18	0.44
1:L:271:ASP:HA	1:L:272:ASP:HA	1.76	0.44
2:M:198:TYR:CZ	2:M:202:LYS:HE2	2.52	0.44
3:P:94:ALA:C	3:P:96:ARG:H	2.21	0.44
1:U:375:ARG:NH1	2:V:190:ARG:NH2	2.66	0.44
2:V:97:ASN:HD22	2:V:103:ILE:HG23	1.83	0.44
2:X:333:THR:HA	2:X:353:SER:HB3	2.00	0.44
1:B:34:LEU:O	1:B:86:GLU:HG3	2.18	0.44
1:B:164:GLY:HA2	1:B:323:LEU:O	2.18	0.44
3:G:133:ILE:HD13	3:G:133:ILE:HA	1.70	0.44
2:O:218:VAL:HG21	2:O:236:GLY:HA2	2.00	0.44
1:B:338:ALA:HB3	1:B:341:PRO:HG2	2.01	0.43
2:D:224:GLU:O	2:D:229:ARG:NH1	2.44	0.43
2:F:201:MET:HB2	2:F:207:ILE:HD12	2.00	0.43
1:T:131:ALA:HB2	1:T:251:THR:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:107:GLY:HA2	1:U:228:MET:HG3	1.98	0.43
1:U:299:ASP:HB2	1:U:302:TYR:HB3	2.00	0.43
1:U:329:ILE:HD11	1:U:344:VAL:HG21	2.00	0.43
2:W:37:LEU:HD13	2:W:76:VAL:HG11	2.00	0.43
2:W:258:ILE:HG22	2:W:309:ALA:O	2.18	0.43
1:B:400:ARG:HE	1:B:400:ARG:HB3	1.46	0.43
3:G:87:ILE:HG23	3:G:167:ASN:HD22	1.84	0.43
1:K:37:GLY:HA3	2:N:52:GLN:HG2	2.00	0.43
1:K:173:ARG:HH22	2:N:327:ALA:HB2	1.83	0.43
1:K:364:ARG:HD3	6:K:600:ANP:N1	2.31	0.43
1:K:455:LEU:HD23	1:K:458:ILE:HD12	1.99	0.43
1:L:177:LYS:HD2	1:L:328:VAL:HG13	2.00	0.43
1:L:480:GLU:H	1:L:480:GLU:HG3	1.67	0.43
1:T:495:LEU:O	1:T:499:LEU:HD13	2.18	0.43
1:A:77:LEU:CD1	1:A:81:ASP:CB	2.96	0.43
1:A:480:GLU:H	1:A:480:GLU:HG3	1.38	0.43
2:E:98:VAL:HG13	2:E:99:ILE:HG23	1.99	0.43
4:H:51:GLN:HG2	4:H:74:PHE:CZ	2.53	0.43
2:M:136:THR:HG21	2:M:147:TYR:CD2	2.53	0.43
2:M:342:LEU:HD13	2:M:344:ILE:HD12	2.01	0.43
1:A:392:LEU:HD13	1:A:426:LEU:HD22	2.00	0.43
1:C:354:LEU:HA	1:C:366:ALA:O	2.18	0.43
2:E:25:PHE:O	2:E:57:ASN:HB3	2.19	0.43
2:F:387:ILE:HG23	2:F:391:LEU:HD12	1.99	0.43
1:K:301:PHE:HB3	2:O:263:GLN:NE2	2.33	0.43
1:L:389:ALA:O	1:L:390:GLY:C	2.55	0.43
1:U:271:ASP:HA	1:U:272:ASP:HA	1.68	0.43
1:A:246:TYR:CE1	1:A:303:LEU:HD11	2.53	0.43
1:B:100:PRO:HA	1:B:127:GLY:O	2.19	0.43
1:C:46:LEU:O	1:C:49:ILE:HG22	2.18	0.43
2:D:64:MET:HE3	2:D:228:ALA:HA	2.00	0.43
1:L:99:VAL:CG1	1:L:251:THR:HB	2.49	0.43
1:A:217:GLN:OE1	2:D:129:THR:HB	2.19	0.43
1:C:238:ALA:O	2:F:290:GLY:HA3	2.18	0.43
2:D:149:ARG:HH11	2:D:149:ARG:HG2	1.83	0.43
2:F:38:GLU:HG2	2:F:45:LYS:HG2	2.00	0.43
2:F:395:GLU:HG3	3:G:83:LEU:HD23	1.99	0.43
1:J:55:VAL:HG21	1:J:75:ILE:HD13	2.01	0.43
1:J:422:ARG:HE	1:J:453:GLY:HA2	1.83	0.43
1:K:285:LEU:HD13	2:N:277:SER:HB3	2.00	0.43
1:L:109:VAL:HG12	1:L:117:ILE:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:435:TYR:C	1:U:437:PRO:HD3	2.39	0.43
2:E:22:ASP:HA	2:E:59:VAL:O	2.18	0.43
2:E:312:VAL:HG12	2:E:315:ASP:HA	2.01	0.43
1:K:444:VAL:HG21	1:K:485:ILE:HG21	2.01	0.43
1:L:36:VAL:HG12	2:O:53:HIS:HB2	2.01	0.43
2:O:141:VAL:HG22	2:O:333:THR:HG21	2.01	0.43
2:O:239:ILE:HG22	2:O:243:PHE:HE2	1.83	0.43
1:S:474:LEU:HD23	1:S:478:HIS:HB2	2.01	0.43
1:U:211:LYS:HB3	1:U:211:LYS:HE2	1.77	0.43
2:W:87:VAL:HG12	2:W:239:ILE:HA	2.00	0.43
1:B:388:VAL:O	1:B:451:VAL:HG21	2.18	0.43
1:C:146:GLU:O	1:C:162:GLY:HA2	2.19	0.43
2:F:142:ASP:HB3	2:F:434:LEU:HD12	2.01	0.43
3:G:151:LEU:HD23	3:G:156:ALA:HB3	2.00	0.43
2:W:164:THR:HA	2:W:167:ILE:HB	2.01	0.43
2:F:148:ALA:CB	2:F:357:LEU:HD11	2.49	0.43
2:F:377:THR:HG22	2:F:407:ALA:HB2	2.01	0.43
1:L:91:LYS:HG3	1:L:92:ARG:O	2.19	0.43
1:A:85:LYS:HG2	2:D:53:HIS:HE1	1.84	0.43
2:F:155:LEU:CD1	2:F:167:ILE:HG12	2.48	0.43
3:G:44:MET:HE2	4:H:86:THR:HB	2.00	0.43
2:M:241:GLU:HG2	2:M:244:ARG:NH2	2.33	0.43
2:O:12:LYS:O	2:O:23:VAL:HA	2.19	0.43
1:S:142:ARG:HG2	1:S:143:SER:H	1.84	0.43
1:S:246:TYR:CD2	1:S:247:LEU:HG	2.54	0.43
1:S:295:ALA:HB2	3:Y:270:ILE:HD13	2.01	0.43
1:S:446:LEU:HD21	1:S:467:GLU:HA	2.01	0.43
1:U:238:ALA:HB1	2:X:328:HIS:HE1	1.84	0.43
2:W:135:GLU:HG3	2:W:434:LEU:HB2	2.01	0.43
2:W:349:ASP:HA	2:W:350:PRO:HD3	1.86	0.43
2:X:256:ASP:HA	2:X:257:ASN:HA	1.79	0.43
1:A:34:LEU:O	1:A:86:GLU:HG3	2.19	0.42
1:C:148:VAL:HG22	1:C:163:ARG:HG3	2.00	0.42
2:E:132:GLU:OE2	2:E:149:ARG:NH1	2.52	0.42
3:G:150:LEU:HD12	3:G:150:LEU:HA	1.93	0.42
4:H:46:VAL:HA	4:H:47:PRO:HD3	1.94	0.42
1:J:172:ASP:O	1:J:175:THR:OG1	2.34	0.42
1:L:394:LEU:HD11	2:M:425:THR:HG22	2.01	0.42
2:N:97:ASN:HB3	2:N:103:ILE:HD13	2.01	0.42
3:P:74:ILE:HG23	3:P:165:PHE:HD2	1.84	0.42
1:U:143:SER:OG	2:V:199:ARG:NH2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:429:LEU:O	1:U:429:LEU:HG	2.18	0.42
2:V:30:LEU:HA	2:V:31:PRO:HD3	1.87	0.42
2:X:189:GLU:O	2:X:221:GLN:HB3	2.19	0.42
3:Y:99:LEU:HD23	3:Y:122:HIS:CE1	2.54	0.42
1:C:139:LEU:HB3	1:C:140:PRO:HD3	2.01	0.42
2:D:201:MET:HG2	2:D:201:MET:H	1.66	0.42
2:N:432:VAL:HG12	2:N:433:ARG:H	1.83	0.42
1:U:284:SER:HB2	1:U:297:PRO:HG3	2.00	0.42
1:U:319:GLY:O	1:U:320:SER:HB2	2.19	0.42
2:W:37:LEU:HD12	2:W:61:THR:HG21	2.01	0.42
2:W:37:LEU:HB2	2:W:48:LEU:HB2	2.02	0.42
2:W:96:ILE:O	2:W:218:VAL:HA	2.19	0.42
2:X:275:ILE:O	2:X:283:PRO:HG3	2.19	0.42
2:X:339:ILE:HG22	2:X:344:ILE:HB	2.00	0.42
2:F:145:ALA:HA	2:F:355:SER:HB2	2.01	0.42
2:F:244:ARG:HD3	2:F:304:VAL:HG23	2.00	0.42
2:M:155:LEU:HD12	2:M:167:ILE:HG13	2.01	0.42
2:D:256:ASP:HA	2:D:257:ASN:HA	1.88	0.42
4:H:35:LYS:HD3	4:H:35:LYS:N	2.33	0.42
1:K:96:ILE:O	1:K:97:VAL:C	2.58	0.42
1:K:170:ILE:HD11	1:K:341:PRO:HB3	2.01	0.42
1:L:43:VAL:HG21	1:L:75:ILE:HD12	2.00	0.42
2:N:432:VAL:HG12	2:N:433:ARG:N	2.34	0.42
2:O:140:VAL:CG1	2:O:414:LEU:HB3	2.49	0.42
2:O:256:ASP:HA	2:O:257:ASN:HA	1.71	0.42
3:P:164:ILE:HD11	3:P:182:ILE:HG13	2.01	0.42
1:U:273:LEU:HD11	1:U:327:PRO:HB3	2.01	0.42
1:B:305:SER:HB2	2:F:222:MET:HB2	2.02	0.42
2:D:170:LEU:O	2:D:174:ILE:HG12	2.19	0.42
2:E:281:TYR:CD2	2:E:320:PRO:HG2	2.55	0.42
2:F:256:ASP:HA	2:F:257:ASN:HA	1.78	0.42
2:F:443:ALA:O	2:F:448:LYS:HG3	2.19	0.42
1:J:204:VAL:O	1:J:268:ILE:HA	2.19	0.42
1:K:442:GLU:C	1:K:445:PRO:HD2	2.39	0.42
1:K:496:LEU:O	1:K:500:LYS:HB2	2.19	0.42
2:N:95:ILE:HD11	2:N:198:TYR:CG	2.55	0.42
2:O:239:ILE:HG22	2:O:243:PHE:CE2	2.55	0.42
1:U:105:LEU:O	1:U:108:ARG:HB2	2.19	0.42
1:B:478:HIS:HB3	1:B:481:LEU:HG	2.01	0.42
1:C:42:ARG:NE	1:C:72:GLN:HE22	2.17	0.42
3:G:189:GLU:HG2	3:G:206:PRO:HG2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:16:LEU:HB2	4:H:19:GLU:O	2.19	0.42
1:J:54:LEU:HD13	1:J:97:VAL:HG22	2.00	0.42
1:K:340:ILE:HB	1:K:341:PRO:HD3	2.01	0.42
1:K:363:ILE:HA	1:K:431:LYS:HE2	2.01	0.42
2:M:25:PHE:HB2	2:M:30:LEU:CD2	2.49	0.42
2:N:87:VAL:HG12	2:N:239:ILE:HA	2.02	0.42
1:U:203:CYS:O	1:U:231:SER:HA	2.20	0.42
1:U:221:THR:HG21	1:U:435:TYR:CE1	2.53	0.42
1:U:222:LEU:HB2	1:U:228:MET:HE1	2.02	0.42
1:U:272:ASP:HB3	1:U:328:VAL:HG12	2.01	0.42
1:A:485:ILE:HG12	1:A:491:LEU:HD21	2.01	0.42
1:B:280:TYR:OH	1:B:299:ASP:OD2	2.32	0.42
1:C:76:VAL:HB	1:C:243:PRO:HG2	2.01	0.42
1:C:103:PRO:HD3	1:C:258:TRP:CZ2	2.54	0.42
1:T:455:LEU:HA	1:T:458:ILE:HD13	2.02	0.42
1:U:55:VAL:HG12	1:U:92:ARG:HA	2.02	0.42
1:U:109:VAL:HG22	1:U:233:ILE:HB	2.01	0.42
2:V:15:ALA:O	2:V:21:VAL:HA	2.19	0.42
2:V:85:VAL:CG1	2:V:235:THR:HG23	2.39	0.42
2:X:49:GLU:O	2:X:61:THR:HA	2.20	0.42
1:A:26:ASN:HB3	1:A:30:THR:OG1	2.20	0.42
2:E:135:GLU:OE2	2:E:433:ARG:HD3	2.20	0.42
1:K:51:ALA:HB2	1:K:68:LEU:HD11	2.01	0.42
2:W:50:VAL:HA	2:W:61:THR:HG22	2.02	0.42
1:A:242:ALA:N	1:A:243:PRO:CD	2.83	0.42
1:B:174:GLN:CA	6:B:600:ANP:HN1	2.14	0.42
1:C:314:LEU:HB3	1:C:318:GLU:HB2	2.01	0.42
2:E:156:PHE:HZ	2:E:326:PHE:CZ	2.38	0.42
2:F:134:LEU:HD11	2:F:174:ILE:HG21	2.02	0.42
2:F:417:PRO:HG2	2:F:430:LYS:H	1.85	0.42
1:J:250:PHE:CE1	1:J:307:LEU:HB2	2.55	0.42
1:K:341:PRO:O	1:K:345:ILE:HG13	2.19	0.42
1:L:354:LEU:HA	1:L:366:ALA:O	2.20	0.42
1:T:197:GLU:HG3	1:T:200:LYS:HD2	2.00	0.42
1:T:364:ARG:HA	1:T:365:PRO:C	2.40	0.42
2:X:37:LEU:HD23	2:X:78:ASP:HA	2.02	0.42
3:Y:10:LEU:HG	3:Y:14:LYS:HE2	2.02	0.42
1:B:85:LYS:HE2	2:E:32:ALA:HB2	2.02	0.41
1:C:177:LYS:HD2	1:C:328:VAL:HG13	2.02	0.41
2:D:140:VAL:HA	2:D:414:LEU:HD22	2.01	0.41
2:M:344:ILE:HG23	2:M:415:SER:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:147:TYR:CE2	2:O:153:ILE:HG21	2.55	0.41
2:O:321:ALA:HB3	2:O:322:PRO:CD	2.49	0.41
2:O:335:LEU:HA	2:O:347:ALA:O	2.19	0.41
1:S:204:VAL:O	1:S:268:ILE:HA	2.20	0.41
2:V:384:LEU:O	2:V:388:ILE:HG12	2.20	0.41
1:C:168:LEU:HD23	1:C:351:GLN:HG2	2.03	0.41
1:C:285:LEU:HD21	1:C:291:PRO:HB3	2.02	0.41
2:D:32:ALA:O	2:D:35:ASN:HB2	2.19	0.41
2:F:290:GLY:O	2:F:294:GLU:HB2	2.20	0.41
2:M:97:ASN:HD22	2:M:103:ILE:HG23	1.86	0.41
2:M:237:LEU:HD23	2:M:292:LEU:HD12	2.02	0.41
2:M:324:THR:O	2:M:324:THR:HG22	2.20	0.41
3:P:188:ILE:O	3:P:188:ILE:HG22	2.21	0.41
1:S:145:HIS:H	1:S:313:LYS:NZ	2.16	0.41
1:T:212:ARG:HA	1:T:237:THR:HG21	2.02	0.41
2:W:262:THR:HG21	2:W:321:ALA:HB2	2.01	0.41
3:Y:233:ARG:O	3:Y:237:MET:HG2	2.21	0.41
2:M:417:PRO:HD2	2:M:460:VAL:O	2.20	0.41
2:O:297:THR:OG1	2:O:298:THR:N	2.54	0.41
4:Q:30:VAL:H	4:Q:41:VAL:HG12	1.85	0.41
1:B:154:ALA:HB3	1:B:367:ILE:HD12	2.03	0.41
3:G:258:THR:O	3:G:262:VAL:HG23	2.20	0.41
1:K:302:TYR:HA	1:K:305:SER:OG	2.20	0.41
2:O:148:ALA:HB2	2:O:357:LEU:HD11	2.02	0.41
1:A:138:ILE:HG21	2:E:95:ILE:HD13	2.02	0.41
1:C:219:VAL:HB	1:C:228:MET:CE	2.50	0.41
2:D:64:MET:HE1	2:D:228:ALA:HA	2.02	0.41
2:F:134:LEU:CD2	2:F:305:THR:HG21	2.50	0.41
1:J:73:VAL:HG12	1:J:75:ILE:HG13	2.02	0.41
3:P:141:GLN:HA	3:P:141:GLN:HE21	1.85	0.41
1:S:173:ARG:NH2	2:V:317:LEU:HD13	2.36	0.41
1:U:36:VAL:HG21	1:U:84:VAL:HB	2.03	0.41
2:V:16:VAL:HG12	2:V:21:VAL:HG22	2.02	0.41
2:X:255:ILE:HB	2:X:308:GLN:HG2	2.02	0.41
2:X:275:ILE:HA	2:X:276:PRO:HD3	1.95	0.41
1:B:186:LEU:HD22	1:B:225:HIS:CB	2.50	0.41
1:B:267:LEU:HD11	1:B:326:LEU:HG	2.02	0.41
2:D:152:LYS:HZ3	2:D:293:GLN:HB3	1.84	0.41
2:D:335:LEU:HA	2:D:347:ALA:O	2.21	0.41
2:F:266:SER:HB3	2:F:282:GLN:OE1	2.21	0.41
1:K:54:LEU:HG	1:K:97:VAL:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:356:ALA:HB1	1:S:360:TYR:OH	2.21	0.41
1:U:375:ARG:HH12	2:V:190:ARG:NH2	2.19	0.41
2:V:372:SER:O	2:V:376:GLU:HG3	2.20	0.41
2:W:156:PHE:HB2	2:W:334:VAL:HG22	2.02	0.41
2:X:64:MET:O	2:X:65:ASP:HB2	2.21	0.41
3:Y:3:LEU:HD11	3:Y:259:ARG:HD3	2.03	0.41
1:A:166:ARG:HD2	1:A:308:LEU:O	2.21	0.41
1:A:246:TYR:HE1	1:A:303:LEU:HD11	1.84	0.41
1:A:299:ASP:HB3	2:E:271:LEU:HD21	2.02	0.41
1:B:101:VAL:HG12	1:B:255:ILE:HA	2.03	0.41
2:M:266:SER:HB3	2:M:282:GLN:OE1	2.20	0.41
2:N:201:MET:HA	2:N:204:THR:HG22	2.03	0.41
3:P:14:LYS:HA	3:P:248:ILE:HD11	2.03	0.41
1:S:139:LEU:N	1:S:140:PRO:CD	2.84	0.41
1:S:139:LEU:N	1:S:140:PRO:HD2	2.36	0.41
2:D:165:VAL:HG13	2:D:420:VAL:HG12	2.03	0.41
2:F:134:LEU:HD22	2:F:305:THR:HG21	2.03	0.41
3:G:14:LYS:HA	3:G:248:ILE:CD1	2.48	0.41
1:K:190:ARG:NE	1:K:439:ALA:HB2	2.35	0.41
1:L:46:LEU:O	1:L:47:ASN:C	2.58	0.41
3:P:149:LYS:HA	3:P:152:SER:HB2	2.03	0.41
1:S:99:VAL:HG22	1:S:100:PRO:HD2	2.02	0.41
1:T:166:ARG:HH22	2:X:190:ARG:HD3	1.86	0.41
1:U:51:ALA:HB3	2:V:67:THR:O	2.20	0.41
1:U:398:GLN:O	1:U:402:VAL:HG23	2.21	0.41
2:W:237:LEU:HD21	2:W:295:ARG:HB2	2.03	0.41
2:X:346:PRO:HB2	2:X:348:VAL:HG23	2.03	0.41
1:A:98:ASP:C	1:A:98:ASP:OD1	2.58	0.41
1:B:308:LEU:HB2	1:B:347:ILE:HG21	2.03	0.41
1:B:309:GLU:HG3	2:F:222:MET:HG3	2.02	0.41
1:C:248:ALA:HB3	1:C:249:PRO:HD3	2.03	0.41
2:E:193:GLU:HA	2:E:196:ASP:HB2	2.03	0.41
1:J:138:ILE:HG22	1:J:139:LEU:HD12	2.02	0.41
1:L:138:ILE:HD12	2:M:191:THR:HG23	2.02	0.41
1:L:389:ALA:O	1:L:390:GLY:O	2.39	0.41
2:N:185:THR:OG1	2:N:236:GLY:HA3	2.21	0.41
2:O:440:SER:OG	2:O:463:ILE:HB	2.21	0.41
1:S:271:ASP:HA	1:S:272:ASP:HA	1.84	0.41
1:S:355:GLU:HB2	1:S:358:LEU:HD12	2.03	0.41
1:S:426:LEU:O	1:S:430:LEU:HG	2.21	0.41
1:T:168:LEU:HB2	1:T:348:THR:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:153:ILE:C	2:V:329:LEU:HD22	2.41	0.41
2:W:185:THR:HA	2:W:218:VAL:O	2.21	0.41
2:W:244:ARG:HG3	2:W:303:SER:N	2.36	0.41
1:A:142:ARG:HG3	1:A:142:ARG:HH11	1.86	0.41
2:D:201:MET:CE	2:D:215:VAL:HG11	2.50	0.41
2:E:462:GLY:O	2:E:464:GLU:N	2.54	0.41
1:J:316:GLU:HA	1:J:320:SER:OG	2.21	0.41
1:K:161:ILE:HD13	1:K:326:LEU:HD21	2.03	0.41
1:K:168:LEU:HD13	1:K:344:VAL:HG11	2.02	0.41
2:M:134:LEU:HD11	2:M:174:ILE:HD12	2.03	0.41
2:N:25:PHE:O	2:N:57:ASN:HB3	2.21	0.41
1:T:211:LYS:HB2	1:T:214:THR:OG1	2.20	0.41
2:V:97:ASN:ND2	2:V:101:GLU:HB2	2.34	0.41
2:V:132:GLU:HB3	2:V:149:ARG:HB2	2.03	0.41
2:V:377:THR:HG22	2:V:407:ALA:HB2	2.03	0.41
1:B:99:VAL:CG1	1:B:251:THR:HB	2.51	0.40
3:G:86:SER:O	3:G:90:GLN:HG2	2.21	0.40
1:K:141:ARG:HB2	2:O:195:ASN:ND2	2.36	0.40
1:K:206:VAL:HG13	1:K:234:VAL:HB	2.02	0.40
1:L:82:ARG:HG2	2:O:34:LEU:HD12	2.03	0.40
2:M:117:ILE:HD12	2:M:234:LEU:HB2	2.03	0.40
2:D:222:MET:HA	2:D:229:ARG:HD2	2.03	0.40
2:E:185:THR:HG21	2:E:233:ALA:HA	2.03	0.40
2:E:201:MET:HG2	2:E:206:VAL:CG2	2.51	0.40
1:K:249:PRO:HG2	1:K:276:GLN:NE2	2.36	0.40
1:L:329:ILE:HD11	1:L:344:VAL:HG21	2.03	0.40
2:N:168:GLN:HE21	2:N:201:MET:CG	2.35	0.40
1:S:96:ILE:HB	1:S:130:ARG:HD2	2.02	0.40
1:T:174:GLN:HA	6:T:600:ANP:HNB1	1.86	0.40
2:X:37:LEU:HD12	2:X:61:THR:HG21	2.02	0.40
1:A:491:LEU:HD13	1:A:496:LEU:HD23	2.03	0.40
2:D:93:GLY:HA2	2:D:207:ILE:HG12	2.03	0.40
2:D:440:SER:OG	2:D:463:ILE:HB	2.22	0.40
3:G:96:ARG:HE	3:G:121:THR:HG21	1.85	0.40
1:J:168:LEU:HB2	1:J:348:THR:HG21	2.03	0.40
1:K:161:ILE:HA	1:K:165:GLN:OE1	2.21	0.40
1:K:212:ARG:NH1	2:N:123:SER:HA	2.36	0.40
2:O:410:ILE:HG23	2:O:441:PHE:HE2	1.86	0.40
3:P:74:ILE:O	3:P:107:ILE:HA	2.21	0.40
3:P:75:VAL:HG22	3:P:108:VAL:HB	2.03	0.40
1:S:347:ILE:HA	2:W:222:MET:SD	2.62	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:53:GLU:HG2	1:T:54:LEU:H	1.87	0.40
1:T:109:VAL:HG13	1:T:233:ILE:HB	2.02	0.40
2:V:324:THR:HG22	2:V:324:THR:O	2.22	0.40
1:B:139:LEU:HD12	1:B:139:LEU:HA	1.83	0.40
1:B:382:VAL:HG11	1:B:440:THR:HG21	2.03	0.40
2:F:449:TYR:HB3	2:F:452:ILE:HD12	2.02	0.40
3:G:78:THR:HG23	3:G:91:LEU:HD23	2.03	0.40
4:H:14:PHE:HB2	4:H:22:TYR:HB2	2.02	0.40
1:K:50:GLN:NE2	2:O:69:GLY:HA2	2.37	0.40
2:N:32:ALA:O	2:N:35:ASN:HB2	2.22	0.40
1:S:237:THR:N	1:S:240:GLU:OE1	2.55	0.40
1:U:337:SER:HB3	2:V:314:ALA:HB1	2.02	0.40
2:V:239:ILE:O	2:V:243:PHE:HD2	2.05	0.40
1:B:282:GLN:OE1	2:E:284:THR:HA	2.21	0.40
2:D:348:VAL:O	2:D:350:PRO:HD3	2.21	0.40
2:M:237:LEU:CD2	2:M:292:LEU:HD12	2.51	0.40
1:S:49:ILE:HG23	1:S:68:LEU:HD22	2.04	0.40
1:U:69:GLU:HB3	1:U:70:PRO:HD2	2.03	0.40
1:U:260:ARG:O	1:U:321:GLY:HA3	2.22	0.40
2:V:258:ILE:HG13	2:V:258:ILE:O	2.21	0.40
2:W:183:VAL:HG11	2:W:236:GLY:O	2.21	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%)	454 (95%)	23 (5%)	1 (0%)	47 82
1	B	479/510 (94%)	448 (94%)	30 (6%)	1 (0%)	47 82
1	C	482/510 (94%)	453 (94%)	28 (6%)	1 (0%)	47 82
1	J	477/510 (94%)	460 (96%)	16 (3%)	1 (0%)	47 82

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	K	482/510 (94%)	442 (92%)	35 (7%)	5 (1%)	15 53
1	L	478/510 (94%)	450 (94%)	27 (6%)	1 (0%)	47 82
1	S	474/510 (93%)	447 (94%)	25 (5%)	2 (0%)	34 72
1	T	475/510 (93%)	438 (92%)	33 (7%)	4 (1%)	19 57
1	U	477/510 (94%)	432 (91%)	39 (8%)	6 (1%)	12 45
2	D	468/484 (97%)	439 (94%)	28 (6%)	1 (0%)	47 82
2	E	466/484 (96%)	436 (94%)	28 (6%)	2 (0%)	34 72
2	F	467/484 (96%)	435 (93%)	27 (6%)	5 (1%)	14 50
2	M	468/484 (97%)	437 (93%)	30 (6%)	1 (0%)	47 82
2	N	468/484 (97%)	431 (92%)	33 (7%)	4 (1%)	17 55
2	O	466/484 (96%)	442 (95%)	24 (5%)	0	100 100
2	V	468/484 (97%)	423 (90%)	38 (8%)	7 (2%)	10 42
2	W	465/484 (96%)	432 (93%)	30 (6%)	3 (1%)	25 64
2	X	467/484 (96%)	432 (92%)	33 (7%)	2 (0%)	34 72
3	G	262/278 (94%)	245 (94%)	17 (6%)	0	100 100
3	P	234/278 (84%)	210 (90%)	19 (8%)	5 (2%)	7 33
3	Y	189/278 (68%)	176 (93%)	13 (7%)	0	100 100
4	H	110/138 (80%)	89 (81%)	19 (17%)	2 (2%)	8 37
4	Q	74/138 (54%)	61 (82%)	13 (18%)	0	100 100
4	Z	15/138 (11%)	11 (73%)	3 (20%)	1 (7%)	1 6
5	1	23/61 (38%)	19 (83%)	3 (13%)	1 (4%)	2 15
5	I	43/61 (70%)	33 (77%)	6 (14%)	4 (9%)	0 3
5	R	30/61 (49%)	25 (83%)	5 (17%)	0	100 100
All	All	9485/10377 (91%)	8800 (93%)	625 (7%)	60 (1%)	25 64

All (60) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	H	101	ILE
5	I	55	GLU
1	L	390	GLY
2	N	221	GLN
2	V	347	ALA
2	W	54	LEU

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Mol	Chain	Res	Type
1	C	390	GLY
2	D	27	GLN
2	E	463	ILE
1	K	412	LEU
3	P	134	GLY
1	T	46	LEU
1	U	97	VAL
1	U	298	GLY
2	V	27	GLN
2	V	68	GLU
2	F	315	ASP
5	I	29	LEU
1	J	403	ALA
1	K	316	GLU
1	K	373	VAL
3	P	202	ASP
1	S	406	ALA
2	W	28	SER
1	B	363	ILE
2	F	34	LEU
2	F	83	ILE
2	F	105	GLU
1	K	457	GLY
1	T	59	SER
1	T	60	GLY
1	U	226	ASP
1	U	406	ALA
2	X	390	ILE
4	Z	120	ALA
2	E	455	HIS
4	H	36	SER
1	K	97	VAL
2	M	460	VAL
3	P	205	VAL
1	U	46	LEU
2	V	28	SER
2	V	34	LEU
2	W	158	GLY
1	A	70	PRO
2	F	347	ALA
5	I	28	GLU
1	U	140	PRO

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Mol	Chain	Res	Type
2	X	18	GLY
2	N	108	PRO
3	P	133	ILE
5	I	56	PRO
3	P	95	VAL
2	V	346	PRO
5	1	21	ILE
1	T	390	GLY
2	N	158	GLY
1	S	97	VAL
2	V	82	PRO
2	N	428	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%)	369 (95%)	19 (5%)	25 61
1	B	388/412 (94%)	373 (96%)	15 (4%)	32 69
1	C	390/412 (95%)	378 (97%)	12 (3%)	40 75
1	J	387/412 (94%)	372 (96%)	15 (4%)	32 69
1	K	390/412 (95%)	372 (95%)	18 (5%)	27 64
1	L	388/412 (94%)	365 (94%)	23 (6%)	19 54
1	S	385/412 (93%)	365 (95%)	20 (5%)	23 59
1	T	386/412 (94%)	371 (96%)	15 (4%)	32 69
1	U	387/412 (94%)	376 (97%)	11 (3%)	43 77
2	D	379/390 (97%)	362 (96%)	17 (4%)	27 64
2	E	370/390 (95%)	354 (96%)	16 (4%)	29 66
2	F	375/390 (96%)	358 (96%)	17 (4%)	27 64
2	M	378/390 (97%)	360 (95%)	18 (5%)	25 62
2	N	378/390 (97%)	357 (94%)	21 (6%)	21 56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	O	378/390 (97%)	366 (97%)	12 (3%)	39	74
2	V	379/390 (97%)	364 (96%)	15 (4%)	31	68
2	W	378/390 (97%)	360 (95%)	18 (5%)	25	62
2	X	379/390 (97%)	364 (96%)	15 (4%)	31	68
3	G	226/236 (96%)	210 (93%)	16 (7%)	14	46
3	P	200/236 (85%)	184 (92%)	16 (8%)	12	40
3	Y	164/236 (70%)	150 (92%)	14 (8%)	10	38
4	H	64/112 (57%)	54 (84%)	10 (16%)	2	13
4	Q	11/112 (10%)	9 (82%)	2 (18%)	1	9
5	1	2/48 (4%)	2 (100%)	0	100	100
5	I	28/48 (58%)	25 (89%)	3 (11%)	6	26
5	R	5/48 (10%)	4 (80%)	1 (20%)	1	7
All	All	7583/8294 (91%)	7224 (95%)	359 (5%)	26	63

All (359) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	PRO
1	A	95	ASN
1	A	142	ARG
1	A	166	ARG
1	A	246	TYR
1	A	251	THR
1	A	284	SER
1	A	288	ARG
1	A	373	VAL
1	A	378	SER
1	A	413	ASP
1	A	436	SER
1	A	458	ILE
1	A	460	LEU
1	A	472	SER
1	A	480	GLU
1	A	481	LEU
1	A	499	LEU
1	A	509	THR
1	B	26	ASN
1	B	30	THR

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Mol	Chain	Res	Type
1	B	91	LYS
1	B	99	VAL
1	B	106	LEU
1	B	159	VAL
1	B	183	ASP
1	B	197	GLU
1	B	204	VAL
1	B	212	ARG
1	B	283	LEU
1	B	309	GLU
1	B	400	ARG
1	B	468	SER
1	B	509	THR
1	C	69	GLU
1	C	99	VAL
1	C	166	ARG
1	C	198	SER
1	C	220	GLN
1	C	283	LEU
1	C	293	ARG
1	C	346	SER
1	C	364	ARG
1	C	375	ARG
1	C	394	LEU
1	C	465	GLU
2	D	7	THR
2	D	58	THR
2	D	89	ARG
2	D	132	GLU
2	D	210	GLU
2	D	251	VAL
2	D	274	ARG
2	D	287	THR
2	D	299	THR
2	D	303	SER
2	D	322	PRO
2	D	386	ASP
2	D	398	GLU
2	D	413	PHE
2	D	431	LEU
2	D	464	GLU
2	D	467	VAL

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Mol	Chain	Res	Type
2	E	43	GLN
2	E	58	THR
2	E	68	GLU
2	E	111	SER
2	E	115	LYS
2	E	140	VAL
2	E	204	THR
2	E	210	GLU
2	E	232	VAL
2	E	269	SER
2	E	337	ARG
2	E	352	ASP
2	E	356	ARG
2	E	390	ILE
2	E	402	LEU
2	E	436	ASP
2	F	27	GLN
2	F	28	SER
2	F	45	LYS
2	F	68	GLU
2	F	113	LEU
2	F	132	GLU
2	F	133	ILE
2	F	140	VAL
2	F	201	MET
2	F	208	ASN
2	F	297	THR
2	F	303	SER
2	F	336	SER
2	F	355	SER
2	F	403	THR
2	F	420	VAL
2	F	464	GLU
3	G	3	LEU
3	G	9	ARG
3	G	11	LYS
3	G	21	LYS
3	G	48	GLU
3	G	53	LYS
3	G	77	ILE
3	G	97	ARG
3	G	118	LEU

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Mol	Chain	Res	Type
3	G	133	ILE
3	G	150	LEU
3	G	153	VAL
3	G	235	ASN
3	G	239	ASN
3	G	252	SER
3	G	276	SER
4	H	14	PHE
4	H	20	THR
4	H	22	TYR
4	H	27	VAL
4	H	35	LYS
4	H	36	SER
4	H	39	ILE
4	H	46	VAL
4	H	48	THR
4	H	70	ILE
5	I	27	THR
5	I	35	LEU
5	I	57	THR
1	J	26	ASN
1	J	27	LEU
1	J	134	LYS
1	J	166	ARG
1	J	175	THR
1	J	183	ASP
1	J	237	THR
1	J	373	VAL
1	J	418	GLN
1	J	429	LEU
1	J	440	THR
1	J	468	SER
1	J	469	SER
1	J	481	LEU
1	J	509	THR
1	K	23	ASP
1	K	40	ILE
1	K	58	SER
1	K	68	LEU
1	K	99	VAL
1	K	106	LEU
1	K	134	LYS

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Mol	Chain	Res	Type
1	K	143	SER
1	K	166	ARG
1	K	199	LYS
1	K	246	TYR
1	K	309	GLU
1	K	320	SER
1	K	371	LEU
1	K	399	TYR
1	K	411	ASP
1	K	462	ARG
1	K	504	GLU
1	L	99	VAL
1	L	132	GLN
1	L	142	ARG
1	L	163	ARG
1	L	166	ARG
1	L	189	LYS
1	L	198	SER
1	L	220	GLN
1	L	231	SER
1	L	267	LEU
1	L	284	SER
1	L	293	ARG
1	L	342	THR
1	L	400	ARG
1	L	405	PHE
1	L	419	THR
1	L	436	SER
1	L	465	GLU
1	L	468	SER
1	L	469	SER
1	L	476	SER
1	L	480	GLU
1	L	481	LEU
2	M	57	ASN
2	M	89	ARG
2	M	90	GLU
2	M	132	GLU
2	M	182	SER
2	M	206	VAL
2	M	210	GLU
2	M	224	GLU

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Mol	Chain	Res	Type
2	M	250	ASP
2	M	261	PHE
2	M	342	LEU
2	M	359	ASP
2	M	385	GLN
2	M	386	ASP
2	M	394	ASP
2	M	413	PHE
2	M	434	LEU
2	M	460	VAL
2	N	68	GLU
2	N	113	LEU
2	N	126	GLU
2	N	130	SER
2	N	132	GLU
2	N	140	VAL
2	N	152	LYS
2	N	212	GLU
2	N	221	GLN
2	N	232	VAL
2	N	318	THR
2	N	330	ASP
2	N	376	GLU
2	N	386	ASP
2	N	387	ILE
2	N	393	MET
2	N	423	VAL
2	N	450	ASP
2	N	458	TYR
2	N	463	ILE
2	N	465	ASP
2	O	30	LEU
2	O	77	LEU
2	O	84	SER
2	O	140	VAL
2	O	149	ARG
2	O	167	ILE
2	O	192	ARG
2	O	274	ARG
2	O	297	THR
2	O	402	LEU
2	O	413	PHE

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Mol	Chain	Res	Type
2	O	455	HIS
3	P	3	LEU
3	P	11	LYS
3	P	35	GLU
3	P	42	LYS
3	P	99	LEU
3	P	107	ILE
3	P	130	ILE
3	P	133	ILE
3	P	136	ASP
3	P	141	GLN
3	P	155	LYS
3	P	178	SER
3	P	186	LYS
3	P	189	GLU
3	P	218	MET
3	P	220	THR
4	Q	39	ILE
4	Q	45	HIS
5	R	31	THR
1	S	32	ARG
1	S	105	LEU
1	S	111	ASP
1	S	115	ASN
1	S	123	ILE
1	S	124	ASP
1	S	134	LYS
1	S	139	LEU
1	S	189	LYS
1	S	267	LEU
1	S	318	GLU
1	S	360	TYR
1	S	373	VAL
1	S	383	LYS
1	S	441	GLU
1	S	459	GLU
1	S	490	GLU
1	S	496	LEU
1	S	504	GLU
1	S	505	SER
1	T	26	ASN
1	T	67	ASN

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Mol	Chain	Res	Type
1	T	95	ASN
1	T	99	VAL
1	T	138	ILE
1	T	159	VAL
1	T	246	TYR
1	T	371	LEU
1	T	373	VAL
1	T	401	GLU
1	T	427	THR
1	T	428	GLN
1	T	465	GLU
1	T	469	SER
1	T	483	THR
1	U	82	ARG
1	U	88	GLU
1	U	172	ASP
1	U	174	GLN
1	U	304	HIS
1	U	339	TYR
1	U	383	LYS
1	U	388	VAL
1	U	394	LEU
1	U	419	THR
1	U	440	THR
2	V	46	LEU
2	V	133	ILE
2	V	149	ARG
2	V	192	ARG
2	V	204	THR
2	V	250	ASP
2	V	268	VAL
2	V	354	LYS
2	V	357	LEU
2	V	386	ASP
2	V	387	ILE
2	V	413	PHE
2	V	423	VAL
2	V	425	THR
2	V	460	VAL
2	W	27	GLN
2	W	65	ASP
2	W	106	ARG

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Mol	Chain	Res	Type
2	W	109	ILE
2	W	140	VAL
2	W	204	THR
2	W	210	GLU
2	W	232	VAL
2	W	257	ASN
2	W	284	THR
2	W	324	THR
2	W	352	ASP
2	W	373	LYS
2	W	386	ASP
2	W	387	ILE
2	W	393	MET
2	W	433	ARG
2	W	448	LYS
2	X	14	THR
2	X	22	ASP
2	X	27	GLN
2	X	29	GLU
2	X	46	LEU
2	X	84	SER
2	X	155	LEU
2	X	167	ILE
2	X	208	ASN
2	X	250	ASP
2	X	274	ARG
2	X	336	SER
2	X	356	ARG
2	X	427	ILE
2	X	454	GLU
3	Y	15	ASN
3	Y	19	ILE
3	Y	101	ASP
3	Y	112	ASP
3	Y	119	LEU
3	Y	121	THR
3	Y	131	ASN
3	Y	136	ASP
3	Y	142	GLU
3	Y	162	ILE
3	Y	167	ASN
3	Y	216	ASN

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Mol	Chain	Res	Type
3	Y	267	LEU
3	Y	271	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	145	HIS
1	A	418	GLN
1	B	26	ASN
1	B	428	GLN
1	C	72	GLN
1	C	174	GLN
1	C	210	GLN
1	C	418	GLN
2	D	178	HIS
2	D	208	ASN
2	D	375	GLN
2	E	168	GLN
2	F	27	GLN
2	F	208	ASN
3	G	49	GLN
3	G	59	ASN
3	G	102	GLN
3	G	117	GLN
3	G	216	ASN
3	G	235	ASN
4	H	45	HIS
4	H	51	GLN
1	J	26	ASN
1	J	174	GLN
1	J	262	ASN
1	J	351	GLN
1	J	479	ASN
1	K	50	GLN
1	K	217	GLN
1	K	265	HIS
1	K	428	GLN
1	L	132	GLN
1	L	174	GLN
1	L	217	GLN
1	L	220	GLN
1	L	398	GLN

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Mol	Chain	Res	Type
2	M	195	ASN
2	M	367	HIS
2	M	375	GLN
2	N	168	GLN
2	O	27	GLN
2	O	208	ASN
2	O	328	HIS
3	P	88	HIS
3	P	141	GLN
4	Q	51	GLN
1	T	67	ASN
1	T	145	HIS
1	T	149	GLN
1	T	217	GLN
1	T	304	HIS
1	T	387	GLN
1	U	225	HIS
1	U	262	ASN
1	U	387	GLN
1	U	479	ASN
2	V	118	HIS
2	V	168	GLN
2	W	27	GLN
2	W	385	GLN
2	X	27	GLN
2	X	43	GLN
2	X	118	HIS
2	X	263	GLN
2	X	328	HIS
2	X	365	GLN
3	Y	100	ASN
3	Y	122	HIS
3	Y	260	GLN
3	Y	265	ASN

### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [\(i\)](#)

Of 30 ligands modelled in this entry, 15 are monoatomic - leaving 15 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	F	600	7	29,33,33	1.78	7 (24%)	31,52,52	1.95	8 (25%)
6	ANP	X	600	7	29,33,33	1.77	6 (20%)	31,52,52	2.17	8 (25%)
6	ANP	O	600	7	29,33,33	1.77	6 (20%)	31,52,52	1.97	7 (22%)
6	ANP	A	600	7	29,33,33	1.88	8 (27%)	31,52,52	1.87	5 (16%)
6	ANP	T	600	7	29,33,33	1.90	6 (20%)	31,52,52	1.97	8 (25%)
6	ANP	B	600	7	29,33,33	1.78	6 (20%)	31,52,52	1.93	6 (19%)
6	ANP	U	600	7	29,33,33	1.81	7 (24%)	31,52,52	2.15	8 (25%)
6	ANP	D	600	7	29,33,33	1.71	7 (24%)	31,52,52	1.77	8 (25%)
6	ANP	M	600	7	29,33,33	1.68	5 (17%)	31,52,52	2.21	6 (19%)
6	ANP	V	600	7	29,33,33	1.76	6 (20%)	31,52,52	2.10	8 (25%)
6	ANP	J	600	7	29,33,33	1.77	6 (20%)	31,52,52	1.97	7 (22%)
6	ANP	L	600	7	29,33,33	1.95	8 (27%)	31,52,52	1.86	7 (22%)
6	ANP	S	600	7	29,33,33	1.89	7 (24%)	31,52,52	1.93	8 (25%)
6	ANP	K	600	7	29,33,33	1.81	7 (24%)	31,52,52	2.12	9 (29%)
6	ANP	C	600	7	29,33,33	1.85	9 (31%)	31,52,52	2.01	8 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ANP	F	600	7	-	3/14/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ANP	X	600	7	-	8/14/38/38	0/3/3/3
6	ANP	O	600	7	-	3/14/38/38	0/3/3/3
6	ANP	A	600	7	-	2/14/38/38	0/3/3/3
6	ANP	T	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	U	600	7	-	4/14/38/38	0/3/3/3
6	ANP	D	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	V	600	7	-	7/14/38/38	0/3/3/3
6	ANP	J	600	7	-	2/14/38/38	0/3/3/3
6	ANP	L	600	7	-	2/14/38/38	0/3/3/3
6	ANP	S	600	7	-	4/14/38/38	0/3/3/3
6	ANP	K	600	7	-	9/14/38/38	0/3/3/3
6	ANP	C	600	7	-	3/14/38/38	0/3/3/3

All (101) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	S	600	ANP	PG-N3B	4.80	1.75	1.63
6	L	600	ANP	PG-N3B	4.79	1.75	1.63
6	T	600	ANP	PG-N3B	4.64	1.75	1.63
6	T	600	ANP	PB-N3B	4.55	1.75	1.63
6	X	600	ANP	PB-N3B	4.51	1.75	1.63
6	A	600	ANP	PG-N3B	4.47	1.75	1.63
6	S	600	ANP	PB-N3B	4.47	1.75	1.63
6	C	600	ANP	PB-N3B	4.41	1.74	1.63
6	C	600	ANP	PG-N3B	4.38	1.74	1.63
6	U	600	ANP	PB-N3B	4.37	1.74	1.63
6	L	600	ANP	PB-N3B	4.34	1.74	1.63
6	X	600	ANP	PG-N3B	4.22	1.74	1.63
6	J	600	ANP	PB-N3B	4.21	1.74	1.63
6	B	600	ANP	PG-N3B	4.19	1.74	1.63
6	V	600	ANP	PG-N3B	4.17	1.74	1.63
6	D	600	ANP	PG-N3B	4.16	1.74	1.63
6	F	600	ANP	PG-N3B	4.14	1.74	1.63
6	F	600	ANP	PB-N3B	4.12	1.74	1.63
6	D	600	ANP	PB-N3B	4.12	1.74	1.63
6	B	600	ANP	PB-N3B	4.08	1.74	1.63
6	J	600	ANP	PG-N3B	4.04	1.73	1.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	600	ANP	PB-N3B	4.04	1.73	1.63
6	U	600	ANP	PG-N3B	4.02	1.73	1.63
6	T	600	ANP	PG-O1G	4.00	1.52	1.46
6	O	600	ANP	PB-N3B	3.95	1.73	1.63
6	O	600	ANP	PG-N3B	3.93	1.73	1.63
6	K	600	ANP	PB-N3B	3.90	1.73	1.63
6	V	600	ANP	PB-N3B	3.89	1.73	1.63
6	M	600	ANP	PB-N3B	3.88	1.73	1.63
6	A	600	ANP	PB-O1B	3.62	1.51	1.46
6	K	600	ANP	PG-N3B	3.62	1.72	1.63
6	K	600	ANP	PB-O3A	3.48	1.63	1.59
6	S	600	ANP	PG-O1G	3.47	1.51	1.46
6	U	600	ANP	PG-O1G	3.46	1.51	1.46
6	M	600	ANP	PG-N3B	3.46	1.72	1.63
6	M	600	ANP	PB-O1B	3.46	1.51	1.46
6	A	600	ANP	PG-O1G	3.45	1.51	1.46
6	M	600	ANP	PG-O1G	3.34	1.51	1.46
6	B	600	ANP	PG-O1G	3.34	1.51	1.46
6	K	600	ANP	PG-O1G	3.32	1.51	1.46
6	C	600	ANP	PB-O1B	3.30	1.51	1.46
6	V	600	ANP	PB-O1B	3.28	1.51	1.46
6	T	600	ANP	PB-O1B	3.28	1.51	1.46
6	K	600	ANP	PB-O1B	3.26	1.51	1.46
6	J	600	ANP	PG-O1G	3.22	1.51	1.46
6	C	600	ANP	PG-O1G	3.21	1.51	1.46
6	D	600	ANP	PG-O1G	3.18	1.51	1.46
6	O	600	ANP	PG-O1G	3.17	1.51	1.46
6	F	600	ANP	PG-O1G	3.15	1.51	1.46
6	V	600	ANP	PG-O1G	3.13	1.51	1.46
6	U	600	ANP	PB-O1B	3.13	1.51	1.46
6	L	600	ANP	PB-O1B	3.10	1.51	1.46
6	X	600	ANP	PB-O1B	3.05	1.51	1.46
6	L	600	ANP	PB-O3A	3.02	1.62	1.59
6	O	600	ANP	PB-O3A	3.02	1.62	1.59
6	F	600	ANP	PB-O1B	2.99	1.50	1.46
6	S	600	ANP	PB-O1B	2.99	1.50	1.46
6	A	600	ANP	PB-O3A	2.98	1.62	1.59
6	L	600	ANP	PG-O1G	2.97	1.50	1.46
6	X	600	ANP	PG-O1G	2.86	1.50	1.46
6	B	600	ANP	PB-O1B	2.79	1.50	1.46
6	F	600	ANP	PB-O3A	2.78	1.62	1.59
6	K	600	ANP	C5-C4	2.78	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	X	600	ANP	C5-C4	2.76	1.48	1.40
6	J	600	ANP	PB-O3A	2.75	1.62	1.59
6	J	600	ANP	PB-O1B	2.72	1.50	1.46
6	B	600	ANP	C5-C4	2.70	1.48	1.40
6	L	600	ANP	PG-O2G	-2.65	1.49	1.56
6	L	600	ANP	C5-C4	2.62	1.47	1.40
6	T	600	ANP	C5-C4	2.61	1.47	1.40
6	O	600	ANP	PB-O1B	2.61	1.50	1.46
6	A	600	ANP	PG-O2G	-2.61	1.49	1.56
6	S	600	ANP	PB-O3A	2.59	1.62	1.59
6	F	600	ANP	C5-C4	2.56	1.47	1.40
6	U	600	ANP	PB-O3A	2.56	1.62	1.59
6	O	600	ANP	C5-C4	2.52	1.47	1.40
6	J	600	ANP	C5-C4	2.52	1.47	1.40
6	V	600	ANP	C5-C4	2.50	1.47	1.40
6	D	600	ANP	C5-C4	2.49	1.47	1.40
6	U	600	ANP	C5-C4	2.48	1.47	1.40
6	D	600	ANP	PB-O1B	2.45	1.50	1.46
6	C	600	ANP	C5-C4	2.42	1.47	1.40
6	S	600	ANP	C5-C4	2.42	1.47	1.40
6	S	600	ANP	C2-N3	2.39	1.35	1.32
6	V	600	ANP	C2-N3	2.31	1.35	1.32
6	T	600	ANP	PB-O3A	2.27	1.61	1.59
6	L	600	ANP	PG-O3G	-2.27	1.50	1.56
6	A	600	ANP	C5-C4	2.27	1.46	1.40
6	C	600	ANP	C2-N3	2.25	1.35	1.32
6	D	600	ANP	PB-O2B	-2.23	1.50	1.56
6	M	600	ANP	C5-C4	2.20	1.46	1.40
6	A	600	ANP	O4'-C1'	2.18	1.44	1.41
6	B	600	ANP	PB-O3A	2.17	1.61	1.59
6	X	600	ANP	PB-O3A	2.15	1.61	1.59
6	U	600	ANP	C2-N3	2.15	1.35	1.32
6	K	600	ANP	C2-N3	2.09	1.35	1.32
6	C	600	ANP	PG-O3G	-2.08	1.51	1.56
6	C	600	ANP	PG-O2G	-2.05	1.51	1.56
6	F	600	ANP	PG-O3G	-2.03	1.51	1.56
6	C	600	ANP	O4'-C1'	2.02	1.43	1.41
6	D	600	ANP	PG-O3G	-2.01	1.51	1.56

All (111) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	600	ANP	O1G-PG-N3B	-7.65	100.51	111.77
6	K	600	ANP	O1G-PG-N3B	-6.50	102.20	111.77
6	J	600	ANP	O1G-PG-N3B	-6.49	102.21	111.77
6	A	600	ANP	O1G-PG-N3B	-6.31	102.47	111.77
6	X	600	ANP	O1G-PG-N3B	-6.27	102.54	111.77
6	V	600	ANP	O1G-PG-N3B	-6.12	102.76	111.77
6	B	600	ANP	O1G-PG-N3B	-6.10	102.79	111.77
6	C	600	ANP	O2B-PB-O1B	5.98	122.45	109.92
6	M	600	ANP	O2B-PB-O1B	5.81	122.10	109.92
6	F	600	ANP	O1G-PG-N3B	-5.78	103.26	111.77
6	T	600	ANP	O1G-PG-N3B	-5.78	103.26	111.77
6	U	600	ANP	O1G-PG-N3B	-5.69	103.39	111.77
6	C	600	ANP	O1G-PG-N3B	-5.28	103.99	111.77
6	U	600	ANP	O2B-PB-O1B	5.28	120.98	109.92
6	O	600	ANP	O1G-PG-N3B	-5.15	104.18	111.77
6	L	600	ANP	O2B-PB-O1B	4.79	119.96	109.92
6	O	600	ANP	O1B-PB-N3B	-4.68	104.88	111.77
6	V	600	ANP	O2B-PB-O1B	4.67	119.72	109.92
6	F	600	ANP	O2B-PB-O1B	4.55	119.47	109.92
6	S	600	ANP	O1G-PG-N3B	-4.54	105.09	111.77
6	J	600	ANP	O2B-PB-O1B	4.51	119.38	109.92
6	L	600	ANP	O1G-PG-N3B	-4.49	105.16	111.77
6	X	600	ANP	O2B-PB-O1B	4.48	119.30	109.92
6	B	600	ANP	O2B-PB-O1B	4.47	119.30	109.92
6	U	600	ANP	O1B-PB-N3B	-4.42	105.26	111.77
6	A	600	ANP	O2B-PB-O1B	4.35	119.04	109.92
6	X	600	ANP	O1B-PB-N3B	-4.33	105.40	111.77
6	D	600	ANP	O1G-PG-N3B	-4.13	105.69	111.77
6	O	600	ANP	O2B-PB-O1B	4.10	118.53	109.92
6	T	600	ANP	O1B-PB-N3B	-4.10	105.73	111.77
6	T	600	ANP	O2B-PB-O1B	3.95	118.20	109.92
6	L	600	ANP	O1B-PB-N3B	-3.92	105.99	111.77
6	X	600	ANP	PB-O3A-PA	-3.81	119.22	132.62
6	S	600	ANP	O2B-PB-O1B	3.79	117.86	109.92
6	K	600	ANP	O2B-PB-O1B	3.71	117.69	109.92
6	B	600	ANP	N3-C2-N1	-3.69	122.91	128.68
6	S	600	ANP	PB-O3A-PA	-3.61	119.92	132.62
6	D	600	ANP	O2B-PB-O1B	3.61	117.48	109.92
6	D	600	ANP	N3-C2-N1	-3.60	123.05	128.68
6	D	600	ANP	O2G-PG-O3G	3.54	117.06	107.64
6	K	600	ANP	O1B-PB-N3B	-3.54	106.56	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	U	600	ANP	N3-C2-N1	-3.54	123.15	128.68
6	T	600	ANP	N3-C2-N1	-3.48	123.23	128.68
6	F	600	ANP	O1B-PB-N3B	-3.42	106.73	111.77
6	C	600	ANP	N3-C2-N1	-3.41	123.36	128.68
6	S	600	ANP	N3-C2-N1	-3.40	123.37	128.68
6	V	600	ANP	O1B-PB-N3B	-3.39	106.78	111.77
6	J	600	ANP	N3-C2-N1	-3.39	123.38	128.68
6	F	600	ANP	N3-C2-N1	-3.36	123.42	128.68
6	L	600	ANP	N3-C2-N1	-3.35	123.44	128.68
6	M	600	ANP	O1B-PB-N3B	-3.31	106.89	111.77
6	S	600	ANP	O1B-PB-N3B	-3.31	106.90	111.77
6	V	600	ANP	N3-C2-N1	-3.29	123.53	128.68
6	X	600	ANP	N3-C2-N1	-3.28	123.56	128.68
6	K	600	ANP	N3-C2-N1	-3.27	123.57	128.68
6	O	600	ANP	N3-C2-N1	-3.26	123.58	128.68
6	V	600	ANP	PB-O3A-PA	-3.21	121.30	132.62
6	A	600	ANP	N3-C2-N1	-3.20	123.67	128.68
6	X	600	ANP	C3'-C2'-C1'	3.17	105.75	100.98
6	S	600	ANP	O2G-PG-O3G	3.16	116.06	107.64
6	T	600	ANP	PB-O3A-PA	-3.06	121.84	132.62
6	K	600	ANP	O2B-PB-O3A	2.99	114.61	104.64
6	O	600	ANP	C3'-C2'-C1'	2.96	105.44	100.98
6	U	600	ANP	PB-O3A-PA	-2.94	122.26	132.62
6	X	600	ANP	O2G-PG-O3G	2.93	115.43	107.64
6	V	600	ANP	C3'-C2'-C1'	2.92	105.38	100.98
6	F	600	ANP	O2G-PG-O3G	2.88	115.30	107.64
6	B	600	ANP	O2G-PG-O3G	2.87	115.29	107.64
6	V	600	ANP	C4-C5-N7	-2.87	106.41	109.40
6	K	600	ANP	C3'-C2'-C1'	2.85	105.27	100.98
6	M	600	ANP	N3-C2-N1	-2.81	124.28	128.68
6	S	600	ANP	C3'-C2'-C1'	2.80	105.20	100.98
6	C	600	ANP	O2G-PG-O3G	2.80	115.08	107.64
6	D	600	ANP	PB-O3A-PA	-2.79	122.78	132.62
6	U	600	ANP	C4-C5-N7	-2.77	106.51	109.40
6	U	600	ANP	O2G-PG-O3G	2.76	115.00	107.64
6	J	600	ANP	C4-C5-N7	-2.74	106.55	109.40
6	K	600	ANP	C4-C5-N7	-2.71	106.58	109.40
6	M	600	ANP	C4-C5-N7	-2.70	106.59	109.40
6	C	600	ANP	PB-O3A-PA	-2.69	123.13	132.62
6	V	600	ANP	O2G-PG-O3G	2.69	114.80	107.64
6	U	600	ANP	C3'-C2'-C1'	2.69	105.02	100.98
6	K	600	ANP	PB-O3A-PA	-2.68	123.19	132.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	600	ANP	PB-O3A-PA	-2.57	123.56	132.62
6	O	600	ANP	C4-C5-N7	-2.55	106.74	109.40
6	A	600	ANP	C4-C5-N7	-2.52	106.78	109.40
6	D	600	ANP	C3'-C2'-C1'	2.52	104.77	100.98
6	L	600	ANP	C4-C5-N7	-2.51	106.79	109.40
6	K	600	ANP	O2G-PG-O3G	2.49	114.27	107.64
6	T	600	ANP	O2G-PG-O3G	2.48	114.23	107.64
6	B	600	ANP	C4-C5-N7	-2.47	106.83	109.40
6	M	600	ANP	C3'-C2'-C1'	2.45	104.67	100.98
6	F	600	ANP	O2B-PB-O3A	2.39	112.63	104.64
6	X	600	ANP	C4-C5-N7	-2.37	106.92	109.40
6	L	600	ANP	O2G-PG-O3G	2.33	113.84	107.64
6	C	600	ANP	C4-C5-N7	-2.32	106.98	109.40
6	J	600	ANP	O2G-PG-O3G	2.30	113.77	107.64
6	C	600	ANP	O1B-PB-N3B	-2.29	108.40	111.77
6	T	600	ANP	C4-C5-N7	-2.29	107.02	109.40
6	J	600	ANP	PB-O3A-PA	-2.29	124.56	132.62
6	S	600	ANP	C4-C5-N7	-2.23	107.08	109.40
6	F	600	ANP	PB-O3A-PA	-2.22	124.79	132.62
6	A	600	ANP	O1B-PB-N3B	-2.21	108.52	111.77
6	D	600	ANP	C4-C5-N7	-2.19	107.12	109.40
6	O	600	ANP	O2G-PG-O3G	2.15	113.37	107.64
6	C	600	ANP	O4'-C1'-C2'	-2.11	103.85	106.93
6	D	600	ANP	C2-N1-C6	2.10	122.35	118.75
6	L	600	ANP	O3A-PB-N3B	2.10	112.42	106.59
6	T	600	ANP	C3'-C2'-C1'	2.07	104.10	100.98
6	F	600	ANP	N6-C6-N1	2.06	122.85	118.57
6	J	600	ANP	C3'-C2'-C1'	2.04	104.05	100.98

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	600	ANP	PB-N3B-PG-O1G
6	A	600	ANP	PG-N3B-PB-O1B
6	B	600	ANP	PB-N3B-PG-O1G
6	B	600	ANP	PG-N3B-PB-O1B
6	C	600	ANP	PB-N3B-PG-O1G
6	C	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

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

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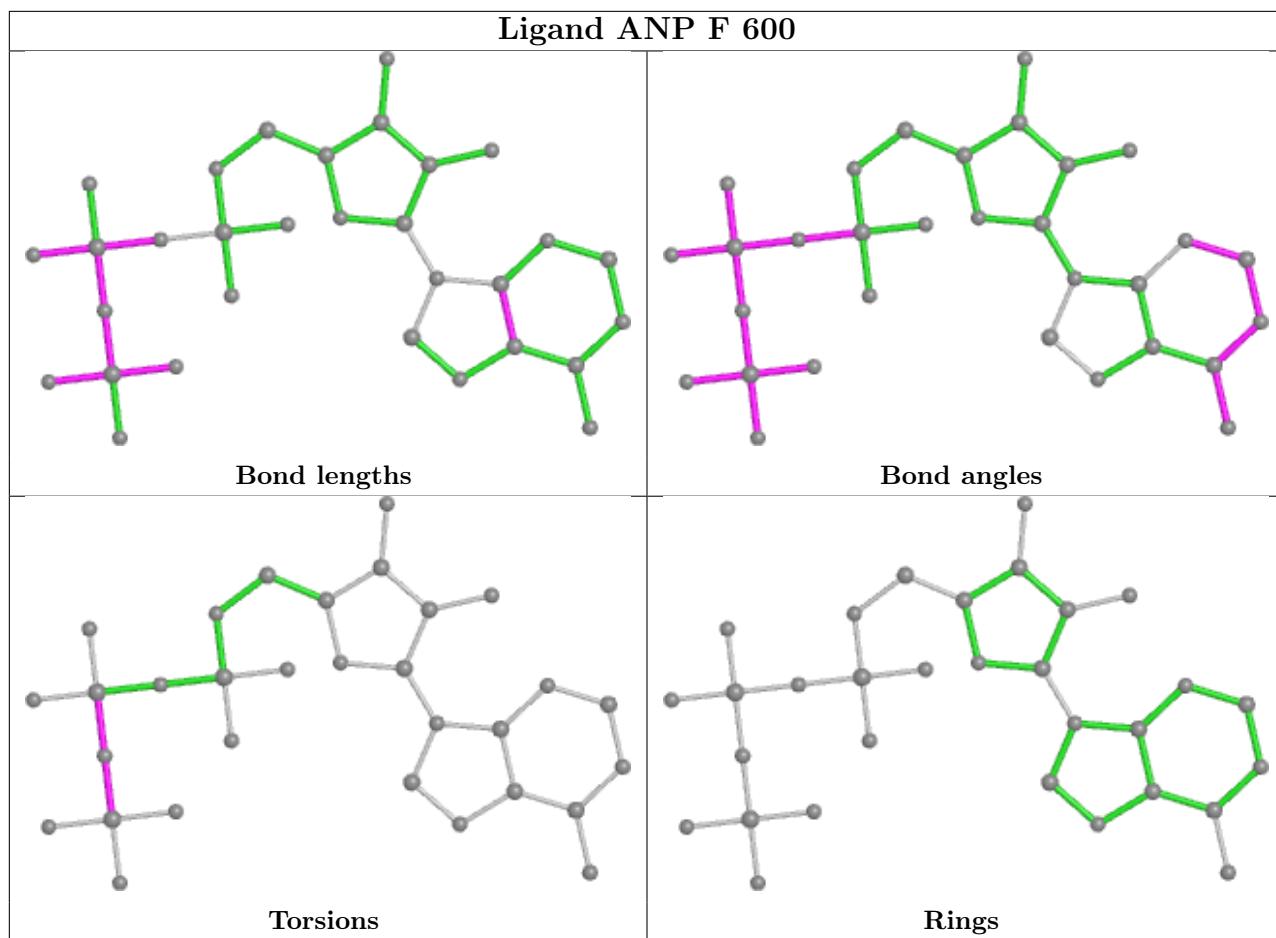
Mol	Chain	Res	Type	Atoms
6	K	600	ANP	C5'-O5'-PA-O1A
6	K	600	ANP	O4'-C4'-C5'-O5'
6	K	600	ANP	C3'-C4'-C5'-O5'
6	K	600	ANP	PB-O3A-PA-O2A
6	M	600	ANP	O4'-C4'-C5'-O5'
6	D	600	ANP	PA-O3A-PB-O2B
6	C	600	ANP	PB-O3A-PA-O1A
6	X	600	ANP	C5'-O5'-PA-O3A

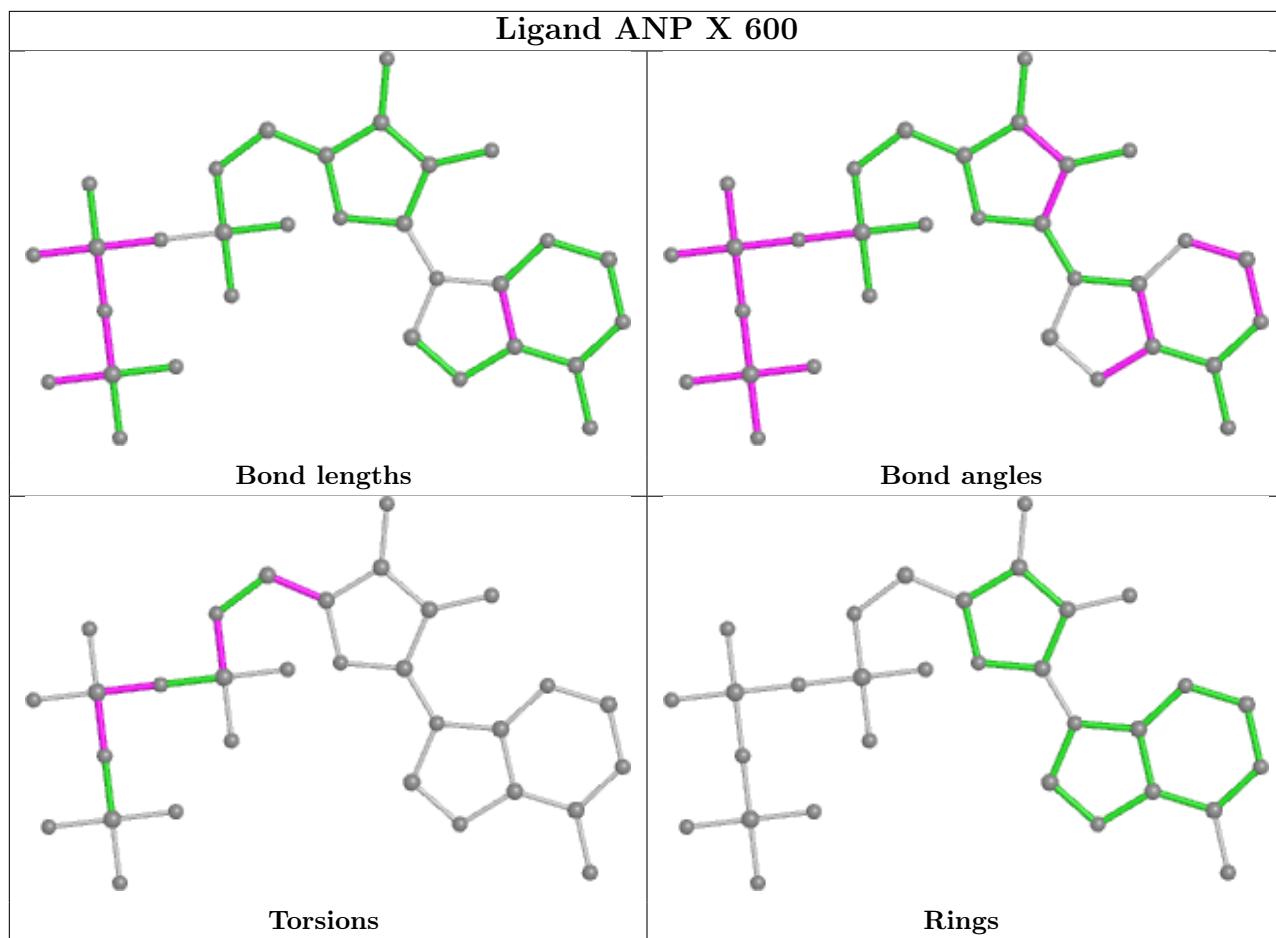
There are no ring outliers.

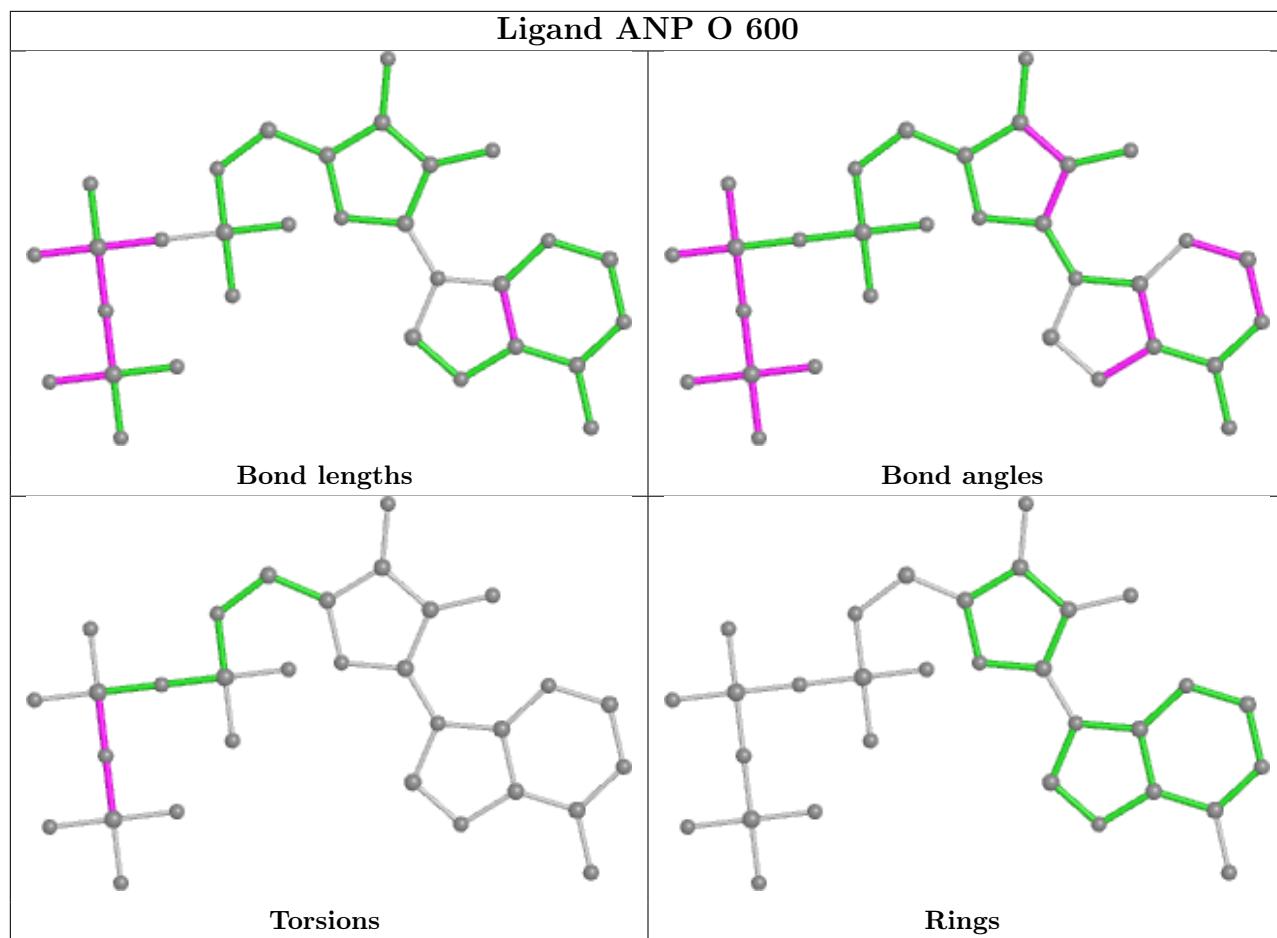
12 monomers are involved in 25 short contacts:

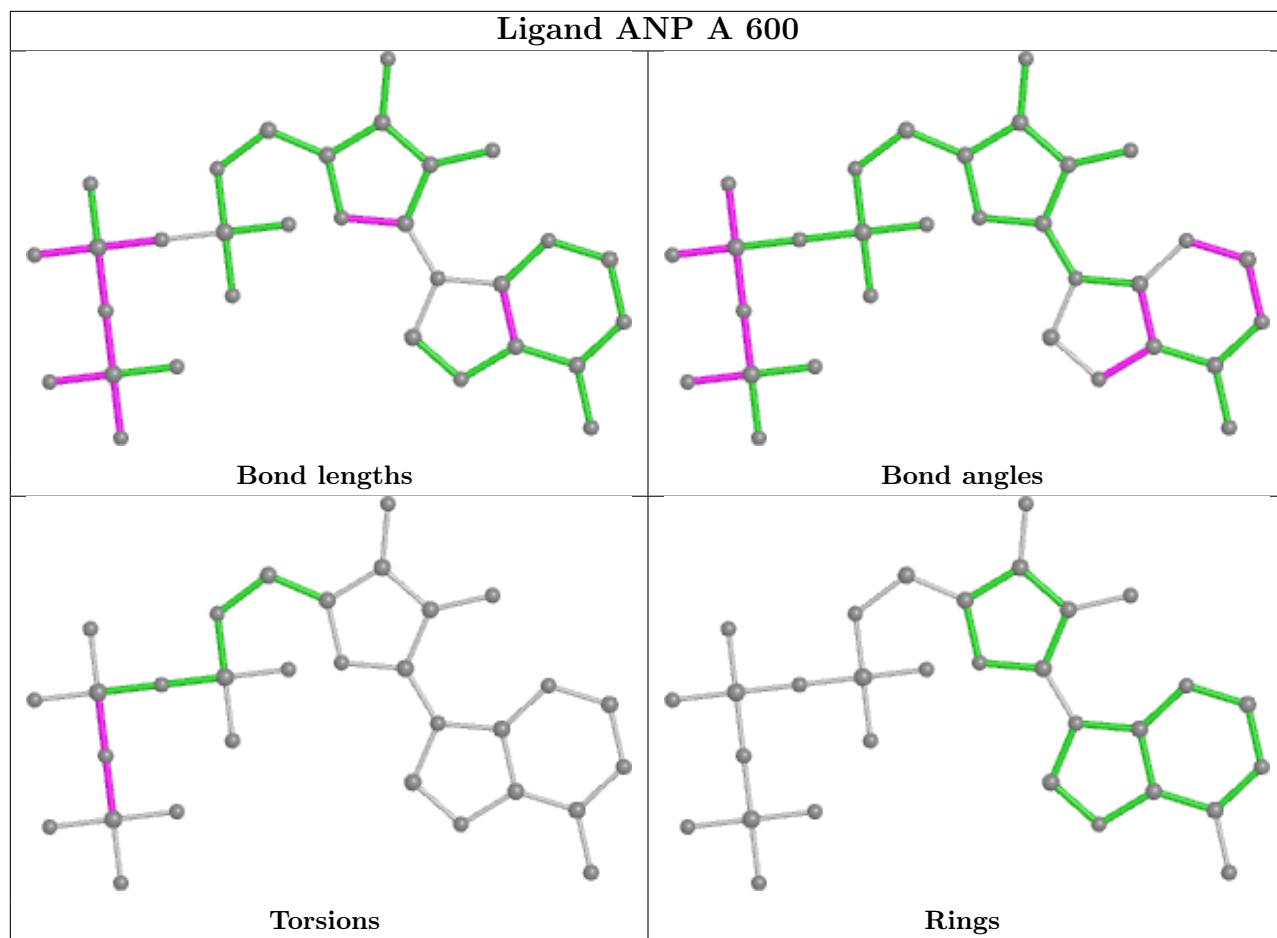
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	600	ANP	1	0
6	X	600	ANP	4	0
6	O	600	ANP	3	0
6	A	600	ANP	1	0
6	T	600	ANP	1	0
6	B	600	ANP	4	0
6	U	600	ANP	1	0
6	M	600	ANP	4	0
6	V	600	ANP	1	0
6	J	600	ANP	1	0
6	L	600	ANP	1	0
6	K	600	ANP	3	0

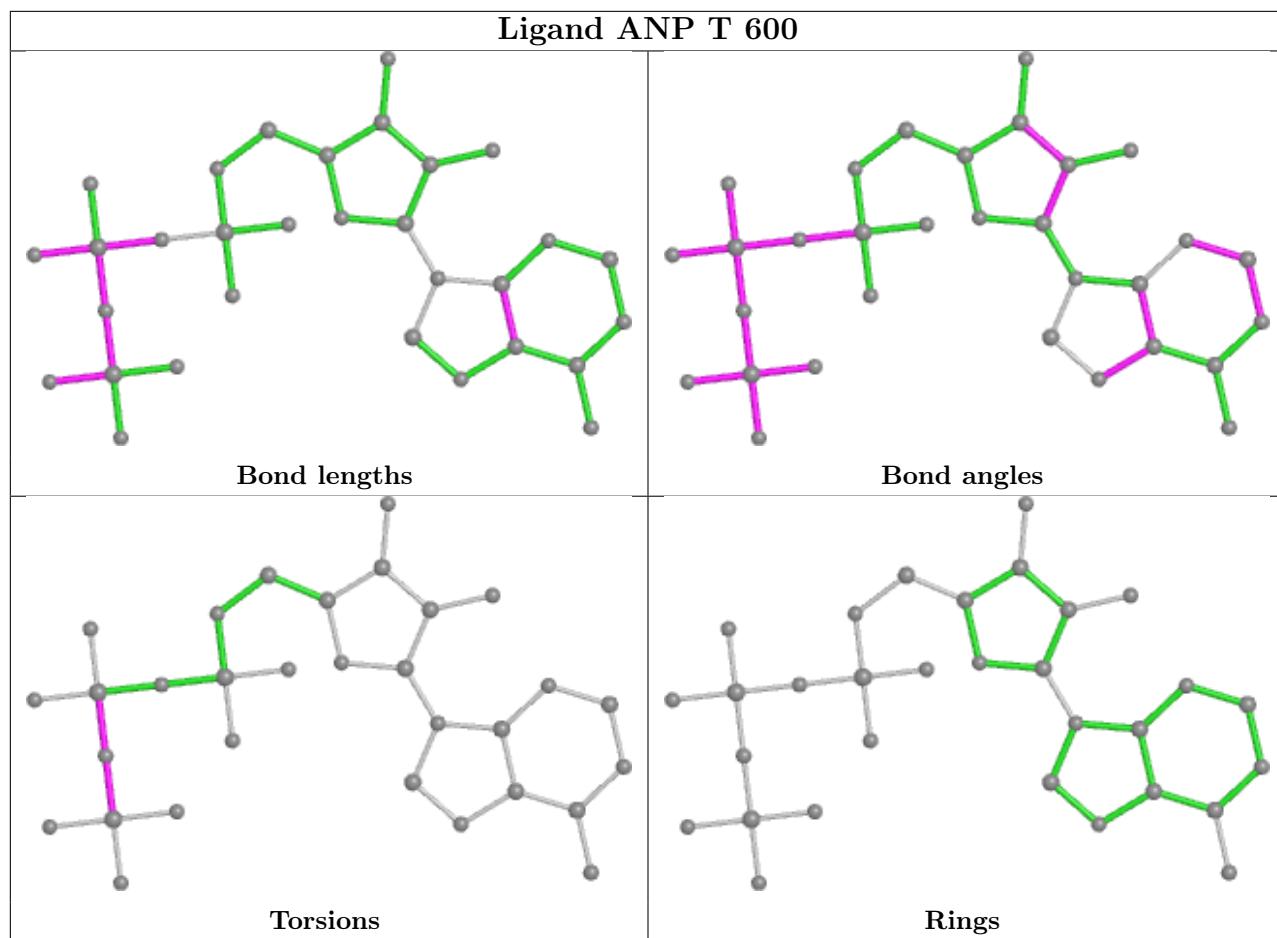
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

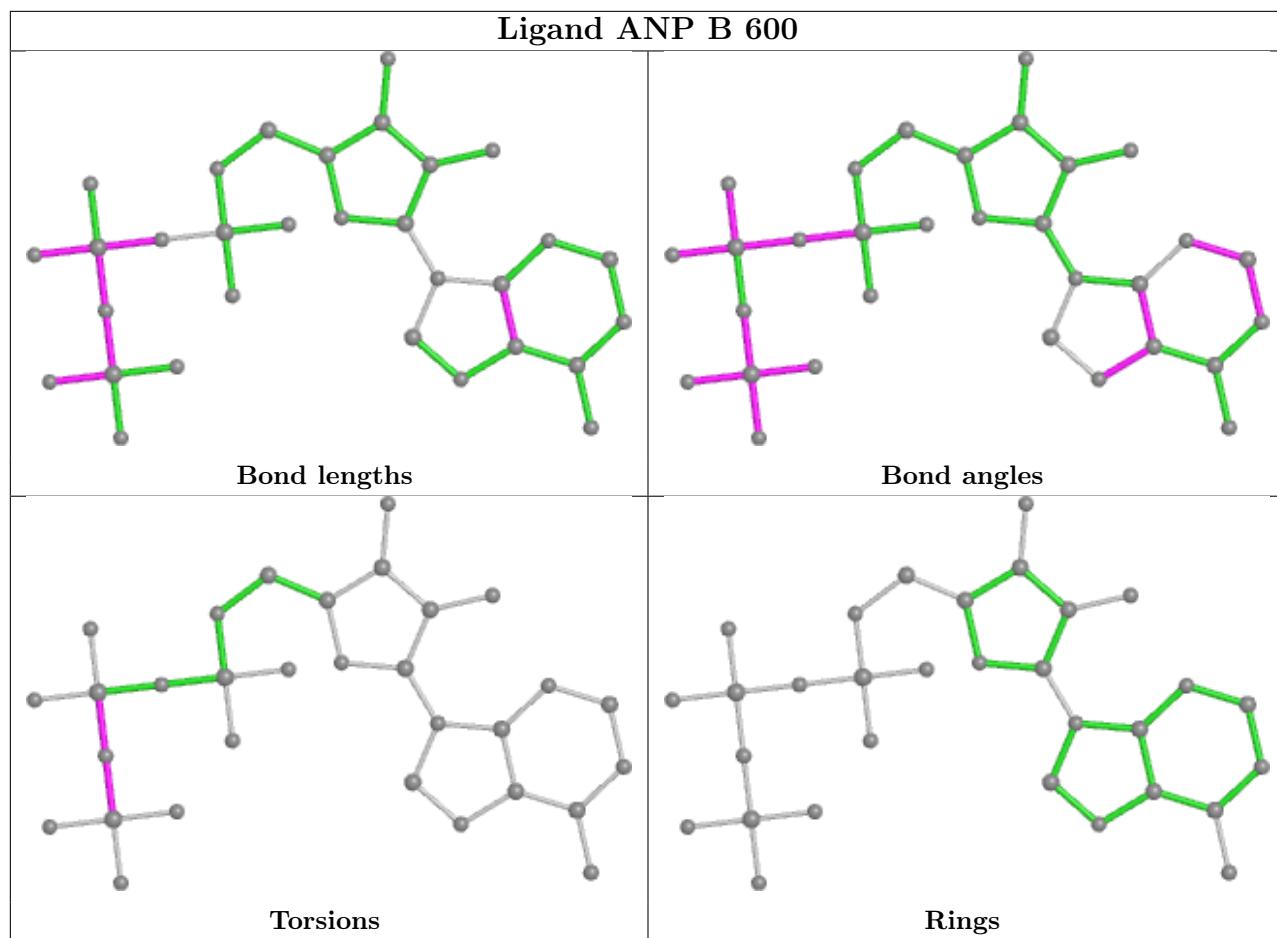


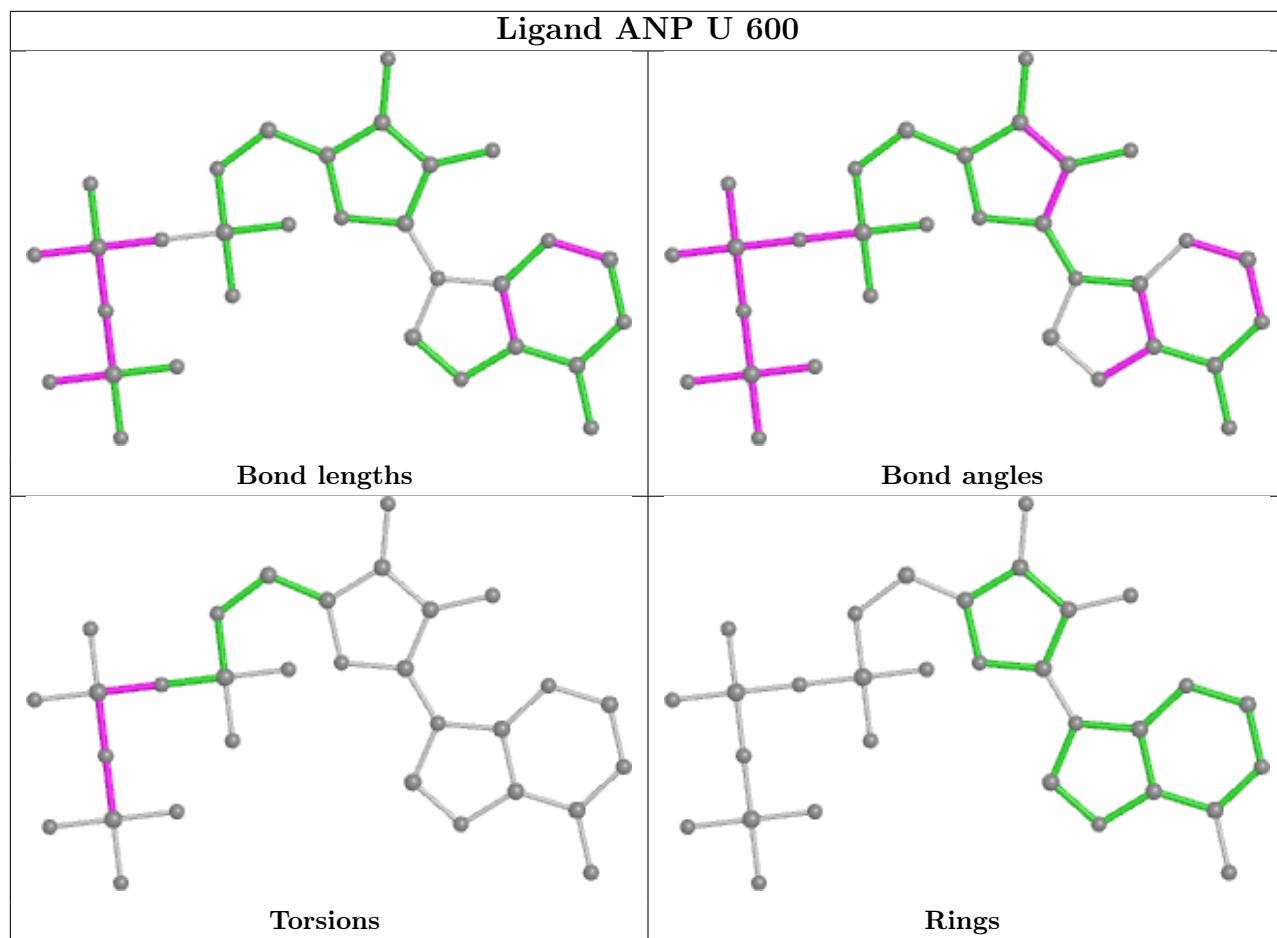


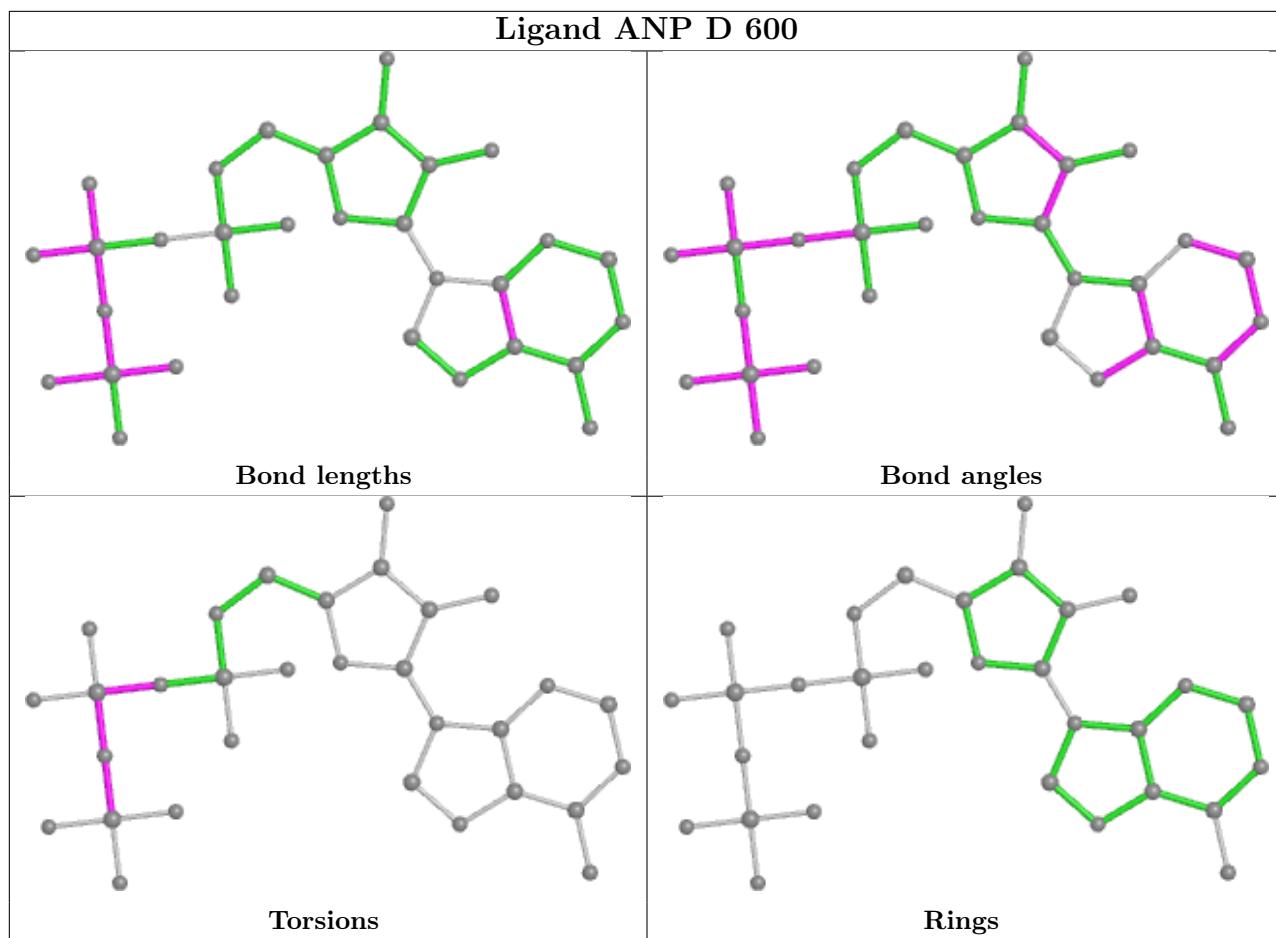


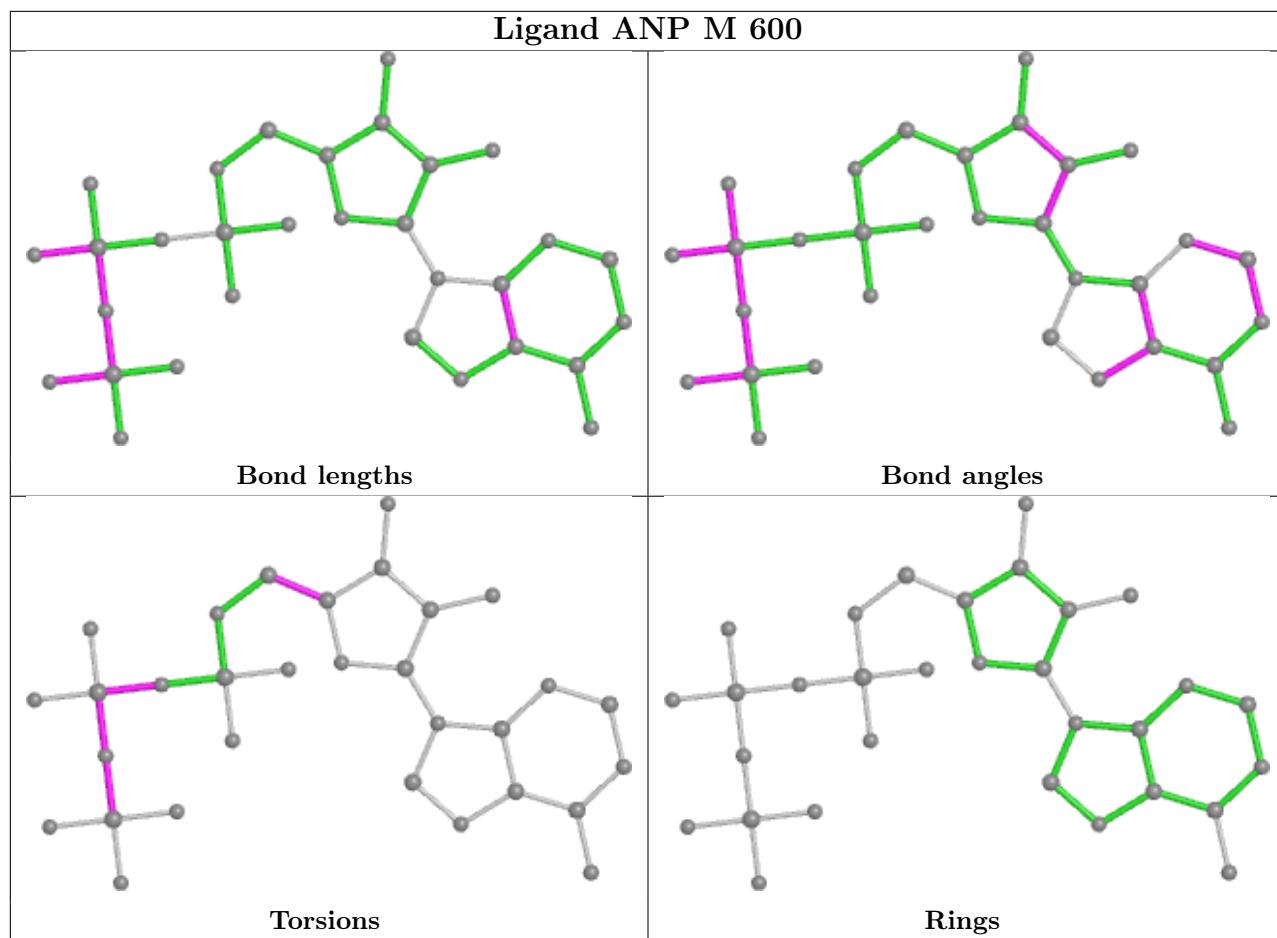


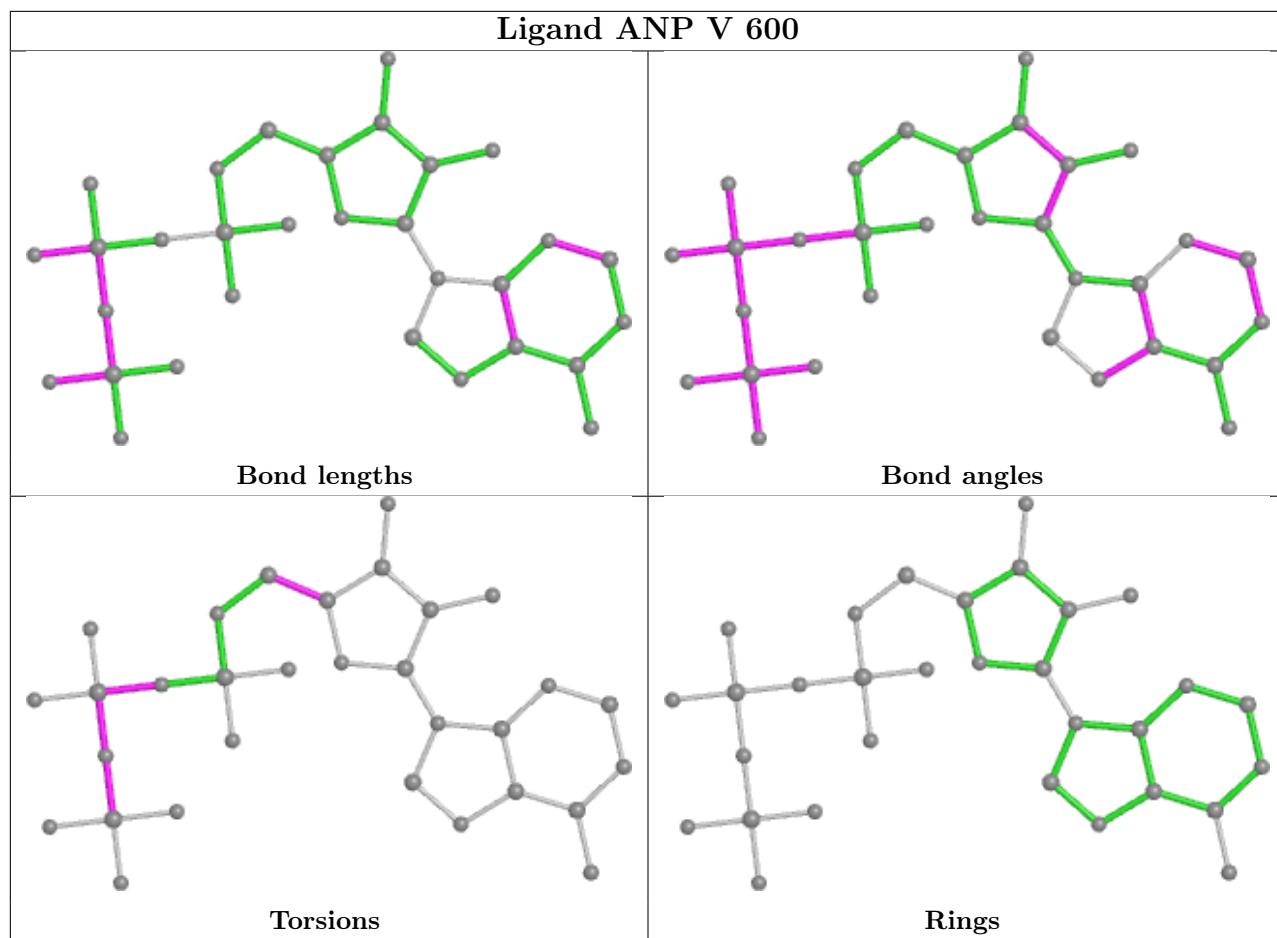


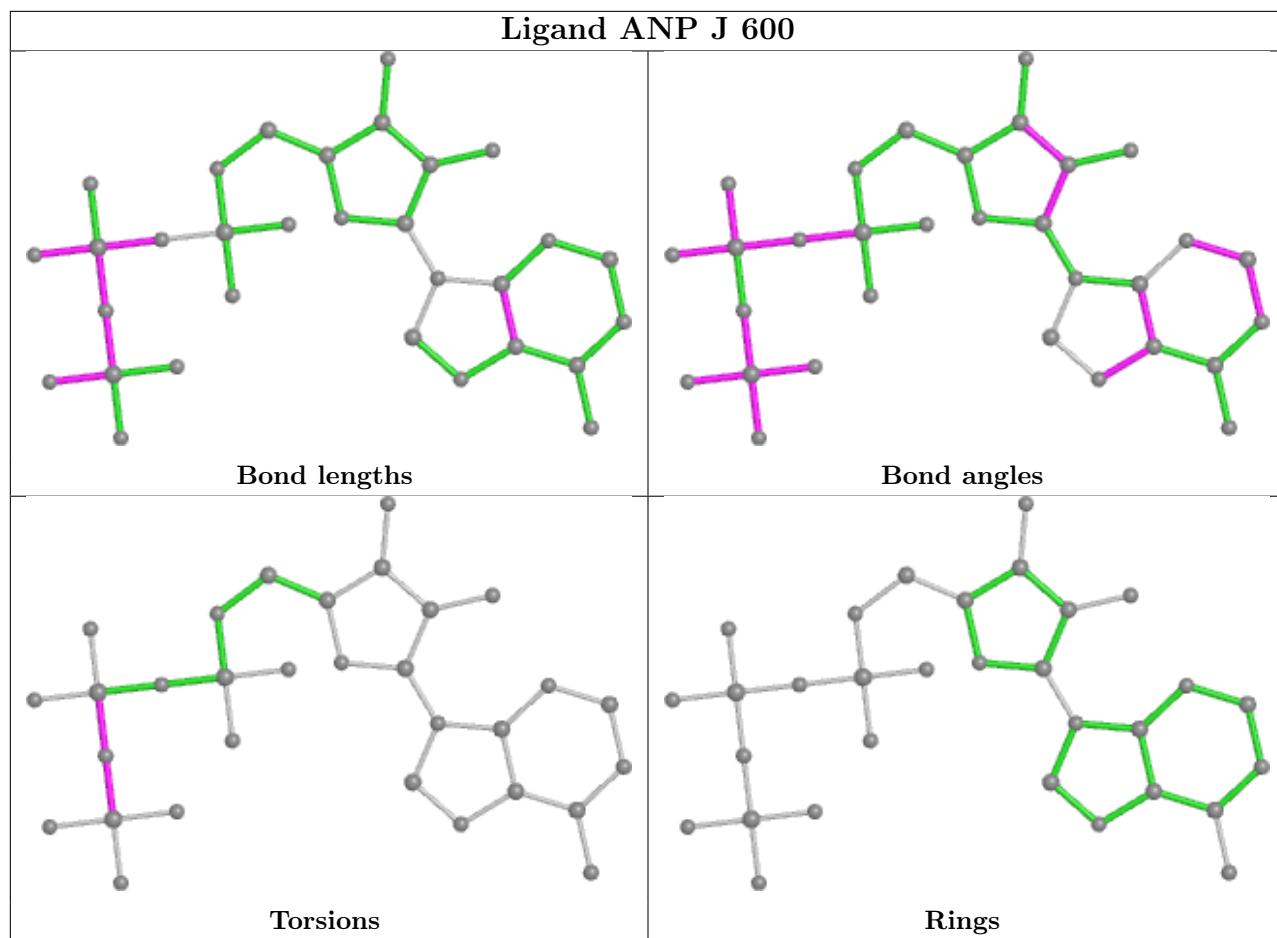


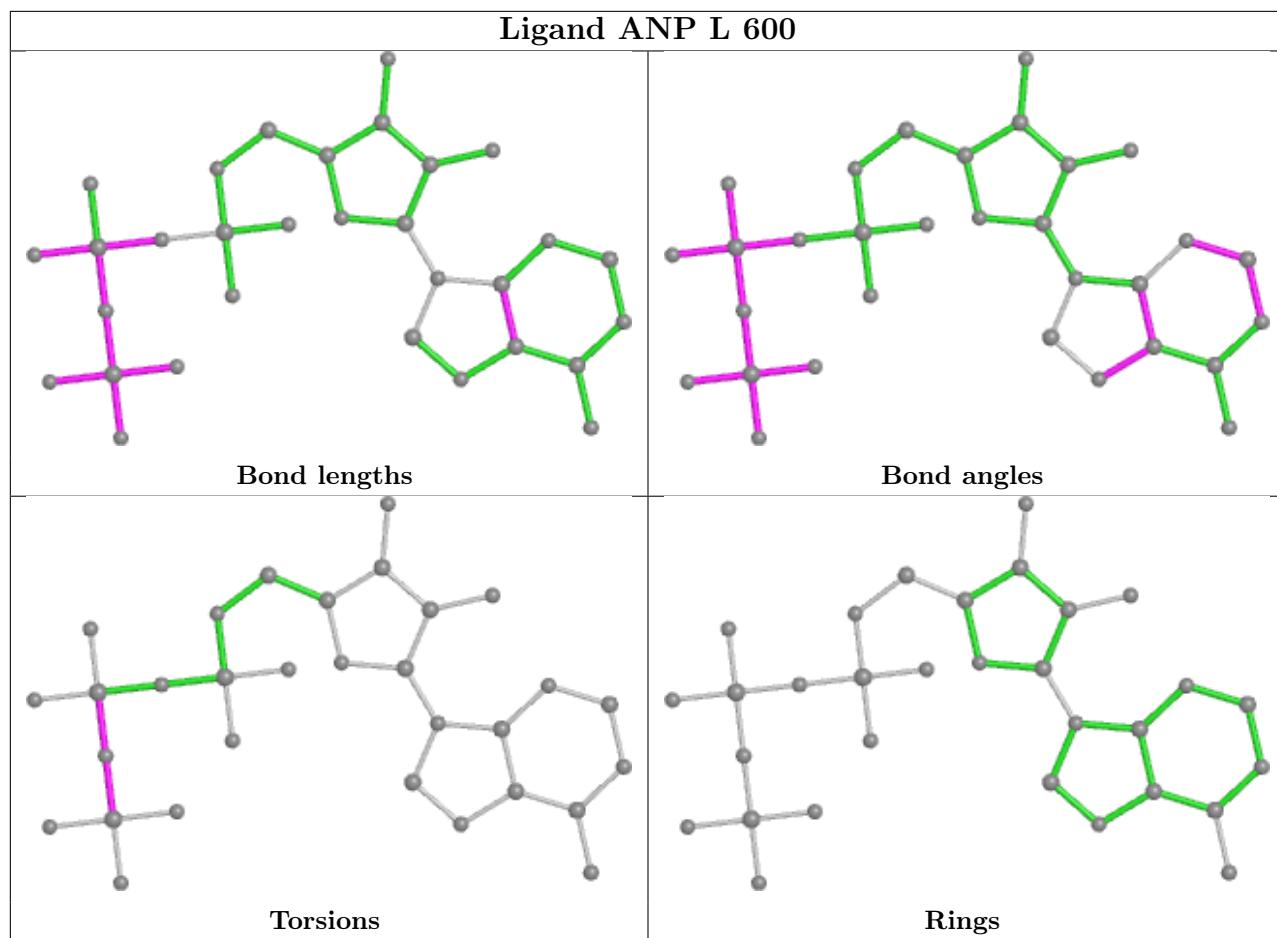


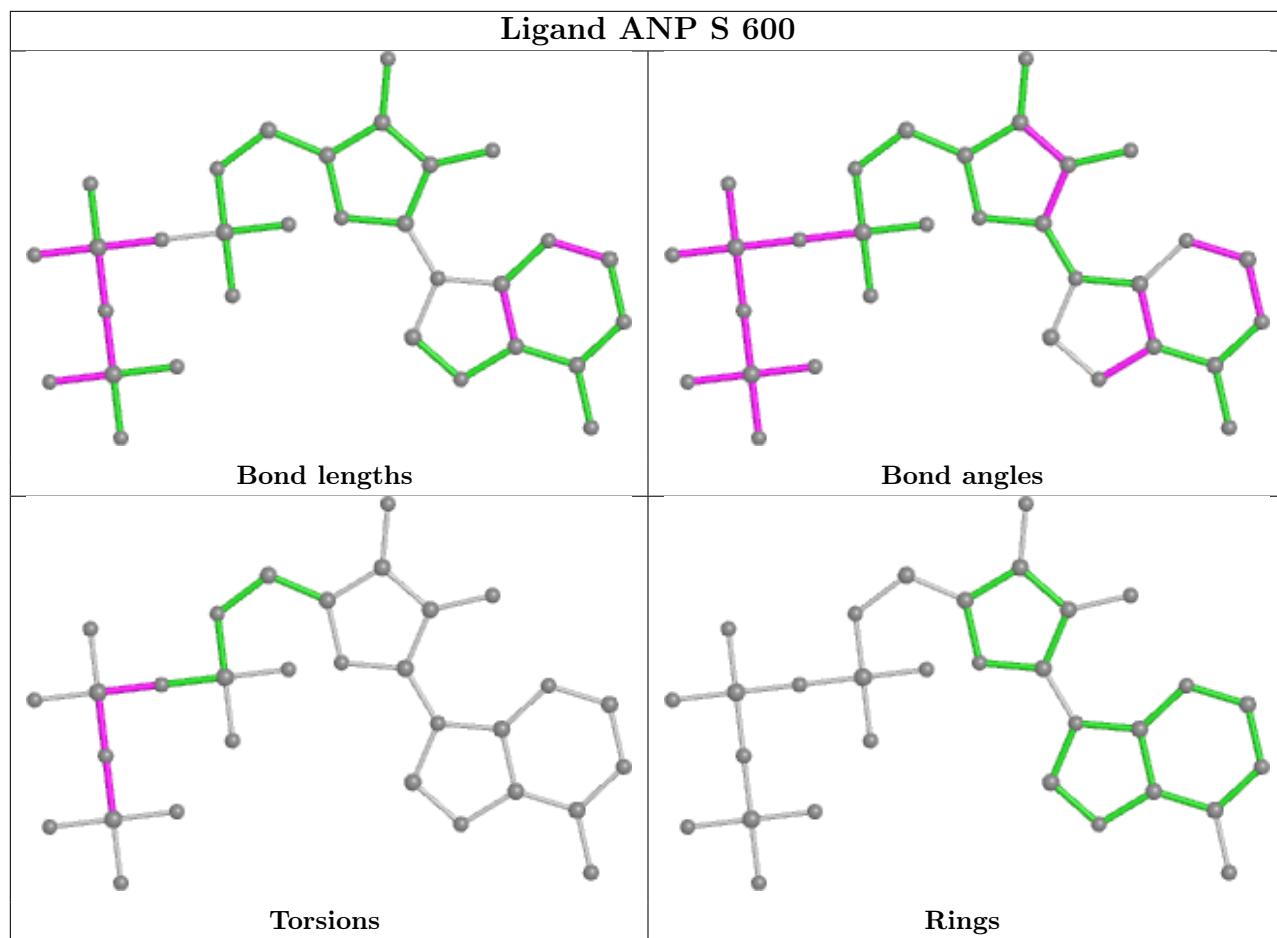


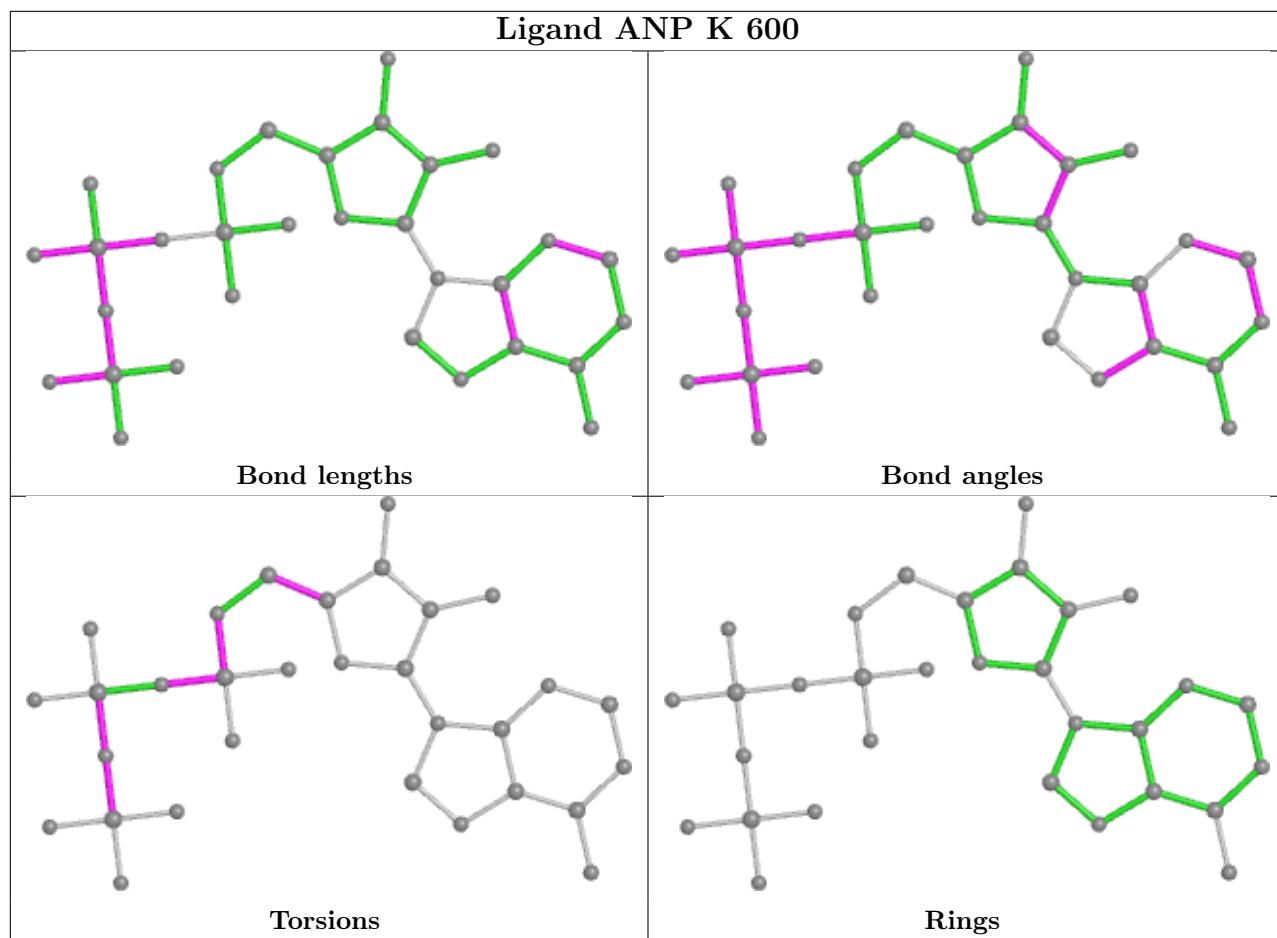


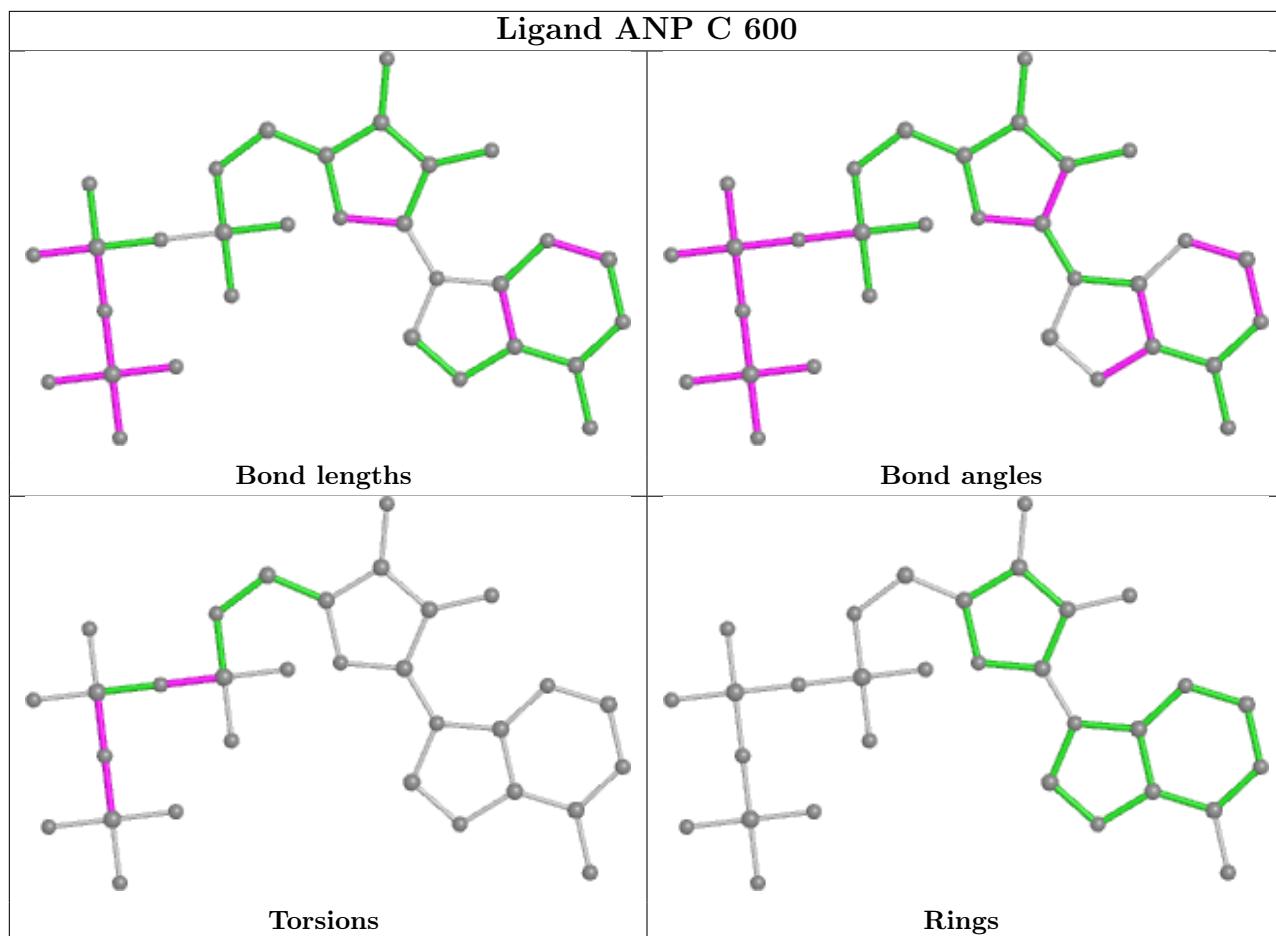












## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data (i)

### 6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.49	0	100	100	41, 63, 99, 156	0
1	B	483/510 (94%)	-0.23	3 (0%)	89	72	48, 92, 148, 188	0
1	C	484/510 (94%)	-0.41	0	100	100	43, 73, 129, 177	0
1	J	481/510 (94%)	-0.26	2 (0%)	92	79	60, 100, 149, 206	0
1	K	486/510 (95%)	-0.06	16 (3%)	46	20	78, 126, 187, 217	0
1	L	482/510 (94%)	-0.40	0	100	100	47, 68, 137, 194	0
1	S	478/510 (93%)	-0.21	8 (1%)	70	41	77, 109, 153, 179	0
1	T	479/510 (93%)	0.21	29 (6%)	21	7	103, 151, 186, 202	0
1	U	481/510 (94%)	0.19	31 (6%)	19	6	104, 150, 181, 217	0
2	D	470/484 (97%)	-0.44	1 (0%)	95	87	42, 70, 123, 181	0
2	E	468/484 (96%)	-0.23	9 (1%)	66	37	46, 86, 161, 211	0
2	F	469/484 (96%)	-0.31	0	100	100	48, 89, 128, 169	0
2	M	470/484 (97%)	-0.32	2 (0%)	92	79	55, 86, 134, 180	0
2	N	470/484 (97%)	0.06	18 (3%)	40	16	71, 133, 199, 229	0
2	O	468/484 (96%)	-0.30	0	100	100	54, 94, 141, 175	0
2	V	470/484 (97%)	0.10	26 (5%)	25	9	93, 138, 180, 210	0
2	W	467/484 (96%)	-0.07	14 (2%)	50	22	89, 117, 164, 189	0
2	X	469/484 (96%)	0.06	20 (4%)	35	13	93, 134, 185, 234	0
3	G	266/278 (95%)	-0.24	2 (0%)	86	65	63, 103, 140, 167	0
3	P	246/278 (88%)	0.22	13 (5%)	26	10	69, 131, 195, 237	0
3	Y	201/278 (72%)	0.43	19 (9%)	8	3	107, 146, 192, 232	0
4	H	116/138 (84%)	-0.05	6 (5%)	27	10	82, 127, 216, 236	0
4	Q	84/138 (60%)	0.01	3 (3%)	42	17	109, 150, 208, 214	0
4	Z	17/138 (12%)	2.21	11 (64%)	0	0	190, 210, 236, 245	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
5	1	27/61 (44%)	1.54	9 (33%) 0 0	159, 168, 187, 210	0
5	I	49/61 (80%)	-0.08	1 (2%) 65 36	97, 127, 178, 217	0
5	R	34/61 (55%)	-0.33	1 (2%) 51 23	108, 122, 187, 200	0
All	All	9597/10377 (92%)	-0.14	244 (2%) 57 29	41, 108, 176, 245	0

All (244) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	U	26	ASN	6.3
1	T	491	LEU	5.3
2	X	7	THR	5.2
5	1	33	SER	4.9
2	X	90	GLU	4.8
3	P	170	VAL	4.7
3	Y	140	PHE	4.7
1	U	63	GLY	4.4
2	W	474	ALA	4.4
2	N	387	ILE	4.4
3	Y	170	VAL	4.3
2	V	214	LYS	4.3
1	U	62	LYS	4.3
2	D	6	SER	4.2
2	X	30	LEU	4.2
1	T	27	LEU	4.1
4	Z	121	ALA	4.1
2	N	457	PHE	4.0
1	T	485	ILE	4.0
2	X	28	SER	3.9
2	V	213	SER	3.9
1	T	35	ALA	3.9
3	P	54	ASN	3.9
2	X	9	ILE	3.9
1	T	46	LEU	3.8
2	X	55	GLY	3.8
2	N	453	PRO	3.8
1	K	494	GLU	3.8
1	U	43	VAL	3.8
1	K	503	THR	3.7
2	N	6	SER	3.6
4	H	90	ALA	3.6
1	S	87	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
3	Y	41	ALA	3.5
1	B	491	LEU	3.5
2	X	8	PRO	3.5
3	P	169	PRO	3.5
2	V	110	LYS	3.5
2	N	475	ALA	3.4
1	T	202	TYR	3.4
2	V	57	ASN	3.4
2	E	457	PHE	3.4
2	N	23	VAL	3.4
2	V	28	SER	3.3
4	Q	81	SER	3.3
2	X	76	VAL	3.3
1	U	122	PRO	3.2
4	Z	135	SER	3.2
1	T	32	ARG	3.2
1	T	54	LEU	3.2
1	K	457	GLY	3.2
1	K	195	SER	3.1
5	1	11	ALA	3.1
2	X	249	GLN	3.1
2	V	9	ILE	3.1
2	E	391	LEU	3.1
1	U	489	GLY	3.1
1	U	446	LEU	3.1
4	H	111	ASN	3.1
1	T	55	VAL	3.1
1	K	454	HIS	3.1
1	T	26	ASN	3.0
3	Y	91	LEU	3.0
4	Z	128	GLU	3.0
1	U	52	GLU	3.0
5	1	22	ARG	3.0
1	S	89	LEU	3.0
1	T	30	THR	3.0
2	X	31	PRO	3.0
1	S	37	GLY	2.9
1	U	30	THR	2.9
2	V	108	PRO	2.9
1	T	314	LEU	2.9
2	W	470	ALA	2.9
4	Z	129	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
4	H	103	ASN	2.9
1	U	114	GLY	2.9
3	Y	45	ASP	2.9
2	X	11	GLY	2.9
2	X	77	LEU	2.9
1	U	491	LEU	2.9
1	U	455	LEU	2.8
2	V	27	GLN	2.8
3	P	105	ALA	2.8
4	Z	124	ALA	2.8
5	1	18	ALA	2.8
2	M	6	SER	2.8
2	V	210	GLU	2.8
2	N	8	PRO	2.8
2	W	437	THR	2.8
2	X	10	THR	2.8
2	V	102	PRO	2.8
1	B	485	ILE	2.7
4	Z	132	ASN	2.7
2	X	75	LYS	2.7
2	V	71	VAL	2.7
3	P	106	ASP	2.7
1	T	320	SER	2.7
2	W	390	ILE	2.7
1	S	30	THR	2.7
2	X	32	ALA	2.7
1	T	63	GLY	2.7
2	W	463	ILE	2.7
1	K	474	LEU	2.7
1	T	49	ILE	2.7
1	U	123	ILE	2.6
1	K	505	SER	2.6
5	1	15	ASN	2.6
2	W	394	ASP	2.6
2	V	475	ALA	2.6
4	Z	134	GLN	2.6
2	N	7	THR	2.6
2	N	302	GLY	2.6
2	N	409	LYS	2.6
4	H	113	SER	2.6
1	T	199	LYS	2.6
2	W	473	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
2	W	453	PRO	2.6
4	Z	130	LEU	2.6
1	T	321	GLY	2.6
1	U	442	GLU	2.6
5	I	23	SER	2.6
3	P	161	LYS	2.5
1	U	509	THR	2.5
1	T	489	GLY	2.5
2	W	395	GLU	2.5
1	U	507	VAL	2.5
2	N	445	LEU	2.5
1	T	412	LEU	2.5
3	Y	223	ALA	2.5
4	H	112	VAL	2.5
2	N	451	ASN	2.5
1	T	313	LYS	2.5
3	Y	165	PHE	2.5
1	U	143	SER	2.5
2	W	387	ILE	2.5
3	Y	124	ASN	2.5
2	V	31	PRO	2.5
3	P	39	ILE	2.5
3	Y	219	LEU	2.4
2	E	474	ALA	2.4
3	P	46	GLU	2.4
3	Y	141	GLN	2.4
2	N	402	LEU	2.4
5	R	27	THR	2.4
3	G	172	SER	2.4
1	T	200	LYS	2.4
2	V	29	GLU	2.4
3	P	164	ILE	2.4
3	Y	119	LEU	2.4
4	Q	80	ASP	2.3
1	T	197	GLU	2.3
1	U	424	GLU	2.3
4	Z	126	GLN	2.3
2	E	451	ASN	2.3
1	J	481	LEU	2.3
3	G	60	LEU	2.3
1	U	44	PHE	2.3
2	N	456	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
2	E	410	ILE	2.3
1	S	507	VAL	2.3
2	V	467	VAL	2.3
2	V	302	GLY	2.2
3	Y	39	ILE	2.2
2	E	405	GLU	2.2
1	T	122	PRO	2.2
1	B	489	GLY	2.2
2	V	212	GLU	2.2
3	Y	169	PRO	2.2
1	K	499	LEU	2.2
1	U	58	SER	2.2
1	K	491	LEU	2.2
4	H	49	VAL	2.2
1	U	48	ASN	2.2
1	U	476	SER	2.2
1	U	411	ASP	2.2
1	S	36	VAL	2.2
2	V	23	VAL	2.2
1	U	469	SER	2.2
2	E	407	ALA	2.2
1	U	304	HIS	2.2
2	V	90	GLU	2.2
1	T	482	LEU	2.2
2	V	8	PRO	2.2
2	V	427	ILE	2.2
5	1	16	VAL	2.2
2	X	248	GLY	2.2
5	1	13	TYR	2.2
3	Y	40	SER	2.2
1	K	418	GLN	2.2
1	U	29	GLU	2.2
2	N	395	GLU	2.2
2	E	445	LEU	2.1
1	K	149	GLN	2.1
3	P	91	LEU	2.1
1	U	33	VAL	2.1
2	N	390	ILE	2.1
4	Z	133	LEU	2.1
5	1	17	ALA	2.1
1	U	116	PRO	2.1
1	T	123	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	T	490	GLU	2.1
1	U	86	GLU	2.1
3	P	126	ILE	2.1
1	K	460	LEU	2.1
4	Q	97	SER	2.1
2	V	109	ILE	2.1
2	W	58	THR	2.1
1	T	264	LYS	2.1
1	S	44	PHE	2.1
2	X	42	PRO	2.1
1	K	508	ALA	2.1
3	Y	212	TYR	2.1
2	V	26	GLU	2.1
3	P	101	ASP	2.1
2	E	452	ILE	2.1
1	T	103	PRO	2.1
4	Z	120	ALA	2.1
1	K	458	ILE	2.1
2	W	72	ARG	2.1
2	V	211	GLY	2.1
2	X	112	LYS	2.1
2	W	391	LEU	2.1
3	Y	44	MET	2.1
1	T	48	ASN	2.1
2	V	45	LYS	2.1
5	1	34	VAL	2.1
2	M	27	GLN	2.0
2	N	394	ASP	2.0
1	K	448	TYR	2.0
1	J	496	LEU	2.0
2	N	11	GLY	2.0
3	Y	145	LEU	2.0
2	V	25	PHE	2.0
2	W	457	PHE	2.0
1	U	49	ILE	2.0
2	X	12	LYS	2.0
3	Y	224	GLN	2.0
1	K	455	LEU	2.0
3	P	107	ILE	2.0
3	Y	36	LYS	2.0
1	U	78	PHE	2.0
2	X	25	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	S	83	LEU	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 monosaccharides 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.

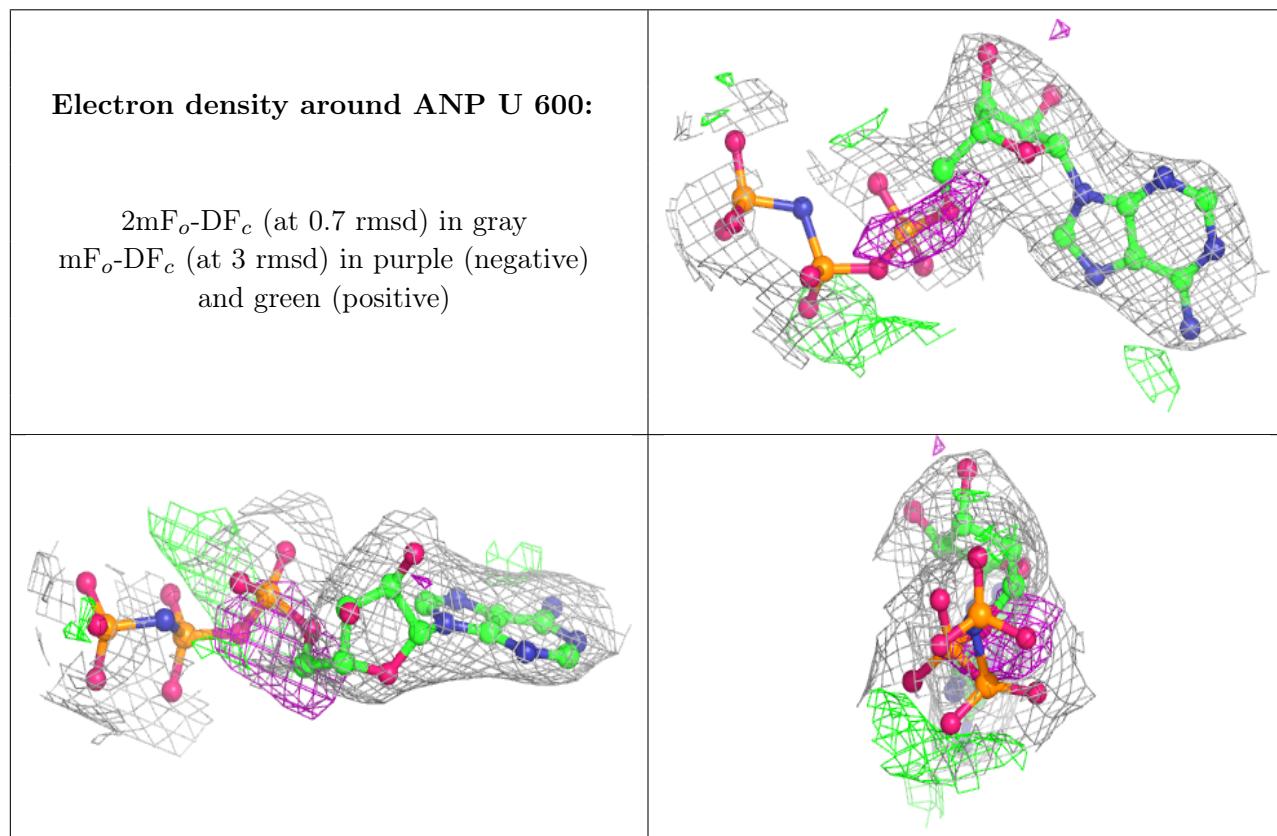
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
7	MG	J	700	1/1	0.88	0.24	51,51,51,51	0
6	ANP	U	600	31/31	0.89	0.20	73,79,82,82	0
6	ANP	K	600	31/31	0.91	0.19	79,96,100,101	0
6	ANP	T	600	31/31	0.92	0.17	81,102,107,108	0
7	MG	M	700	1/1	0.92	0.35	53,53,53,53	0
7	MG	T	700	1/1	0.93	0.28	62,62,62,62	0
7	MG	D	700	1/1	0.94	0.29	48,48,48,48	0
6	ANP	J	600	31/31	0.94	0.17	60,74,82,83	0
7	MG	L	700	1/1	0.95	0.33	48,48,48,48	0
6	ANP	B	600	31/31	0.95	0.16	66,79,81,82	0
7	MG	O	700	1/1	0.95	0.11	61,61,61,61	0
6	ANP	V	600	31/31	0.95	0.20	80,100,102,102	0
6	ANP	C	600	31/31	0.96	0.20	57,68,75,75	0
6	ANP	F	600	31/31	0.96	0.20	65,79,84,85	0
6	ANP	L	600	31/31	0.96	0.19	49,62,70,70	0
6	ANP	X	600	31/31	0.96	0.17	83,95,97,97	0
7	MG	S	700	1/1	0.96	0.27	53,53,53,53	0
6	ANP	S	600	31/31	0.96	0.14	64,78,80,80	0
7	MG	F	700	1/1	0.97	0.33	55,55,55,55	0
7	MG	C	700	1/1	0.97	0.37	52,52,52,52	0
7	MG	K	700	1/1	0.97	0.19	66,66,66,66	0
6	ANP	O	600	31/31	0.97	0.18	69,79,81,82	0

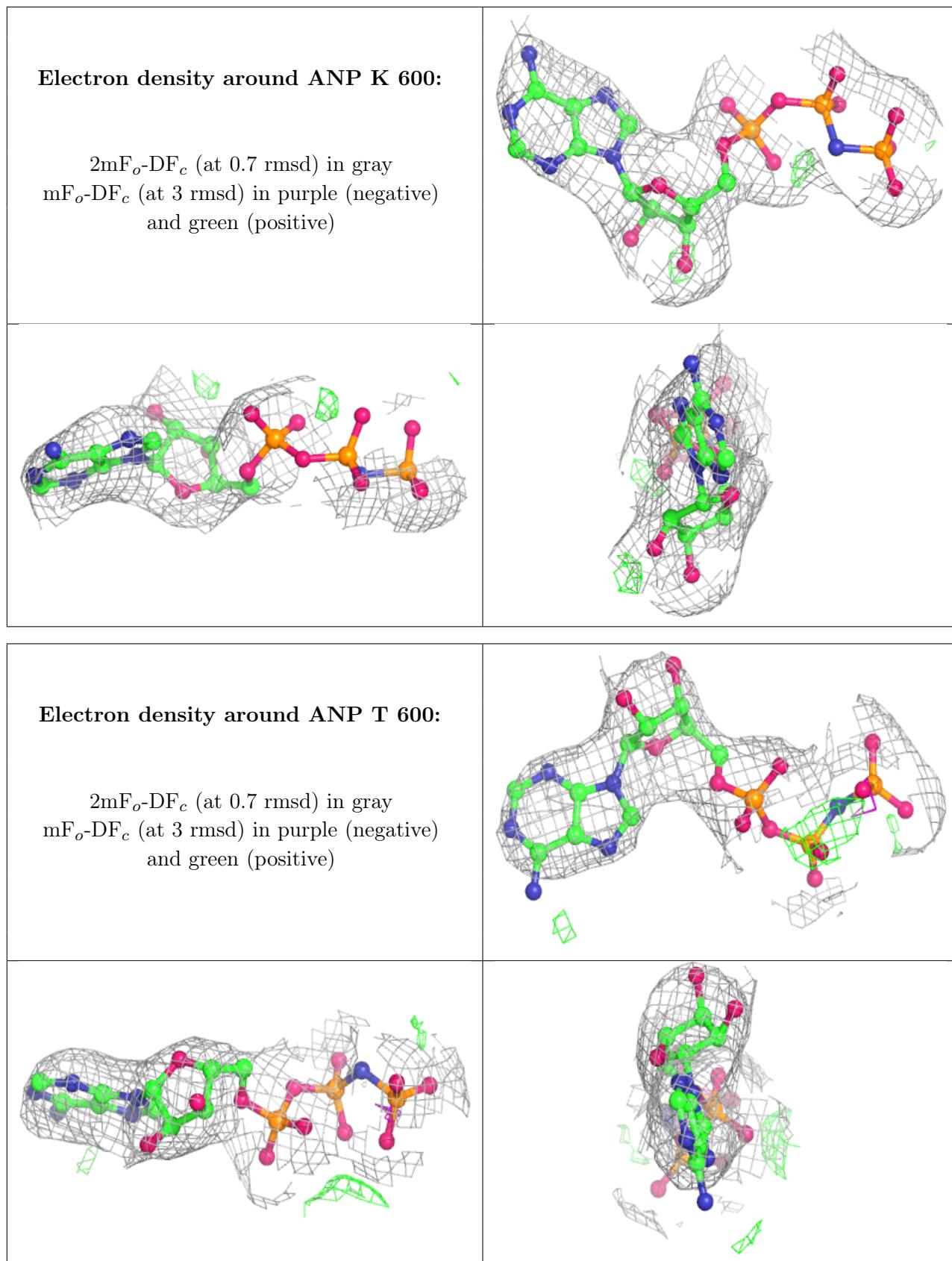
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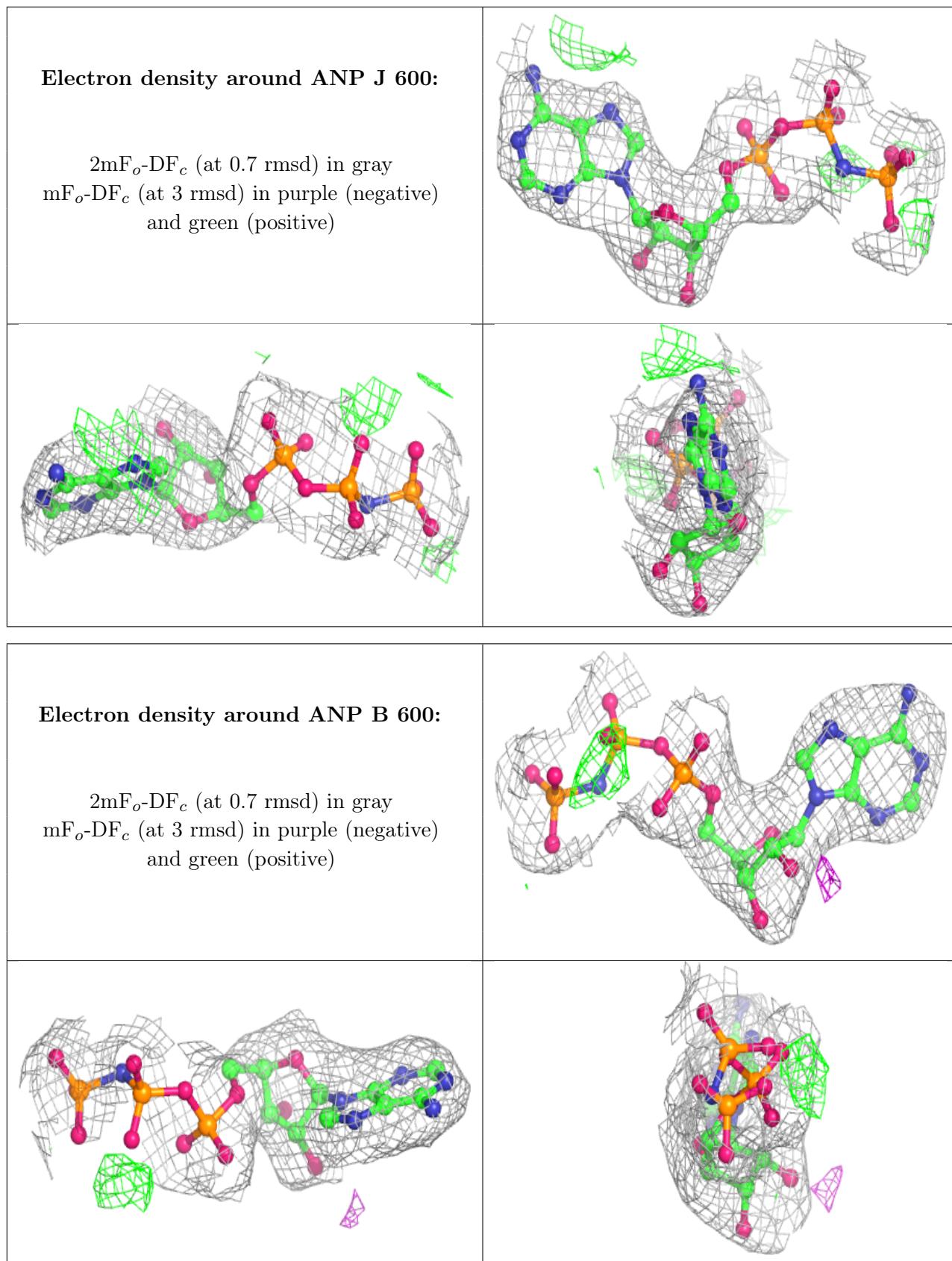
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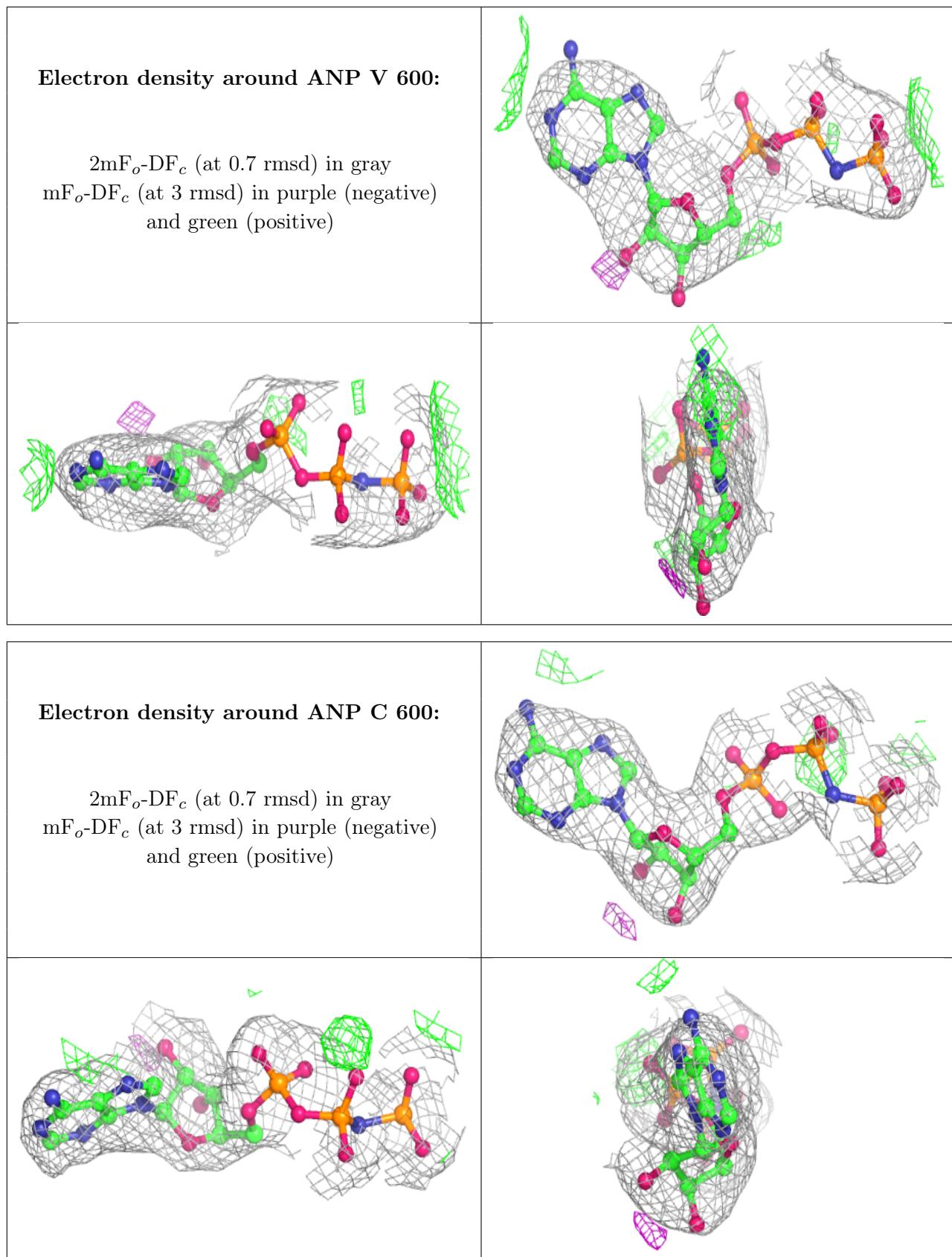
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
7	MG	V	700	1/1	0.97	0.21	61,61,61,61	0
6	ANP	D	600	31/31	0.98	0.19	55,65,68,69	0
6	ANP	M	600	31/31	0.98	0.20	60,70,73,74	0
7	MG	A	700	1/1	0.98	0.32	41,41,41,41	0
7	MG	B	700	1/1	0.98	0.32	57,57,57,57	0
6	ANP	A	600	31/31	0.98	0.19	44,57,61,63	0
7	MG	X	700	1/1	0.98	0.15	70,70,70,70	0
7	MG	U	700	1/1	0.99	0.30	61,61,61,61	0

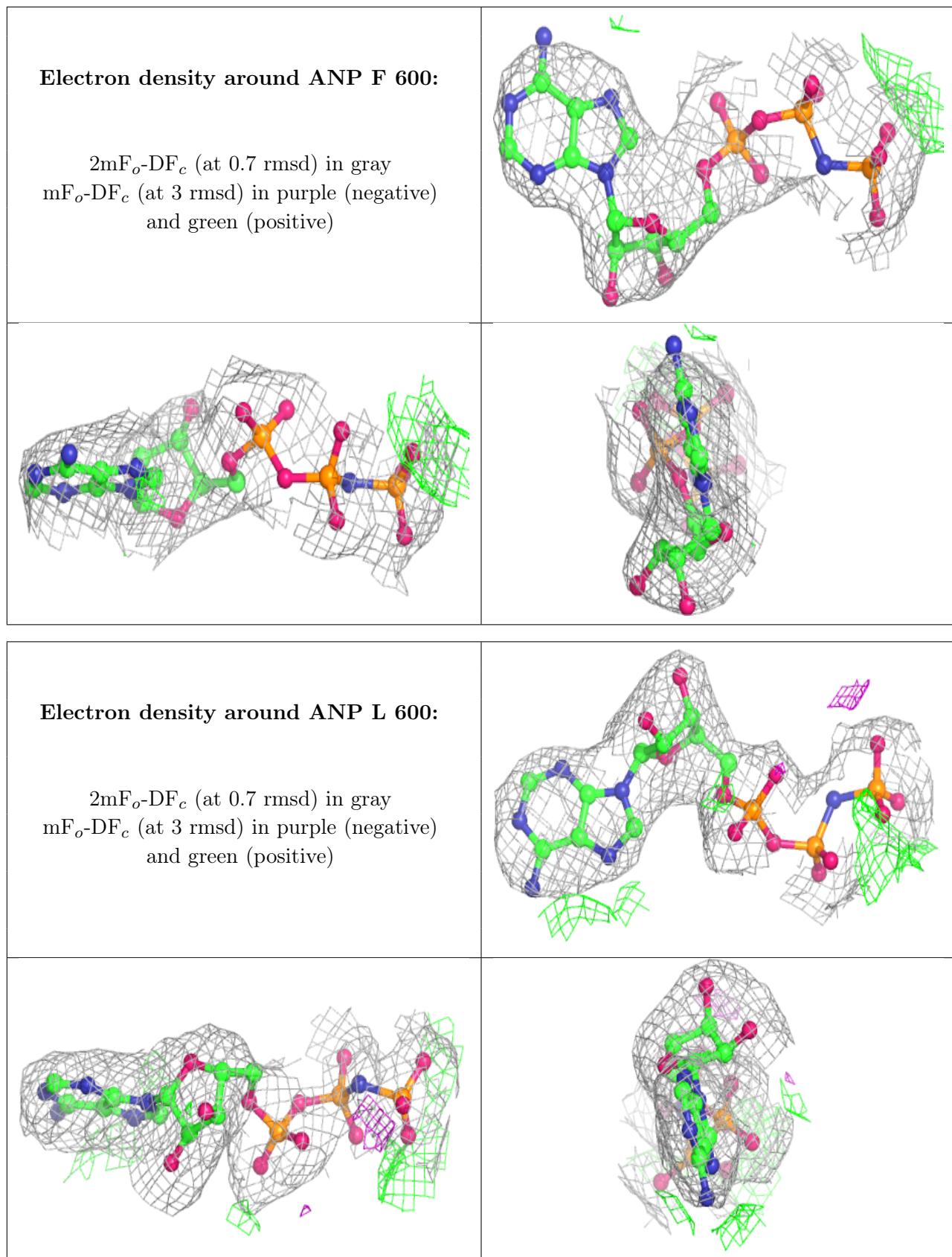
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

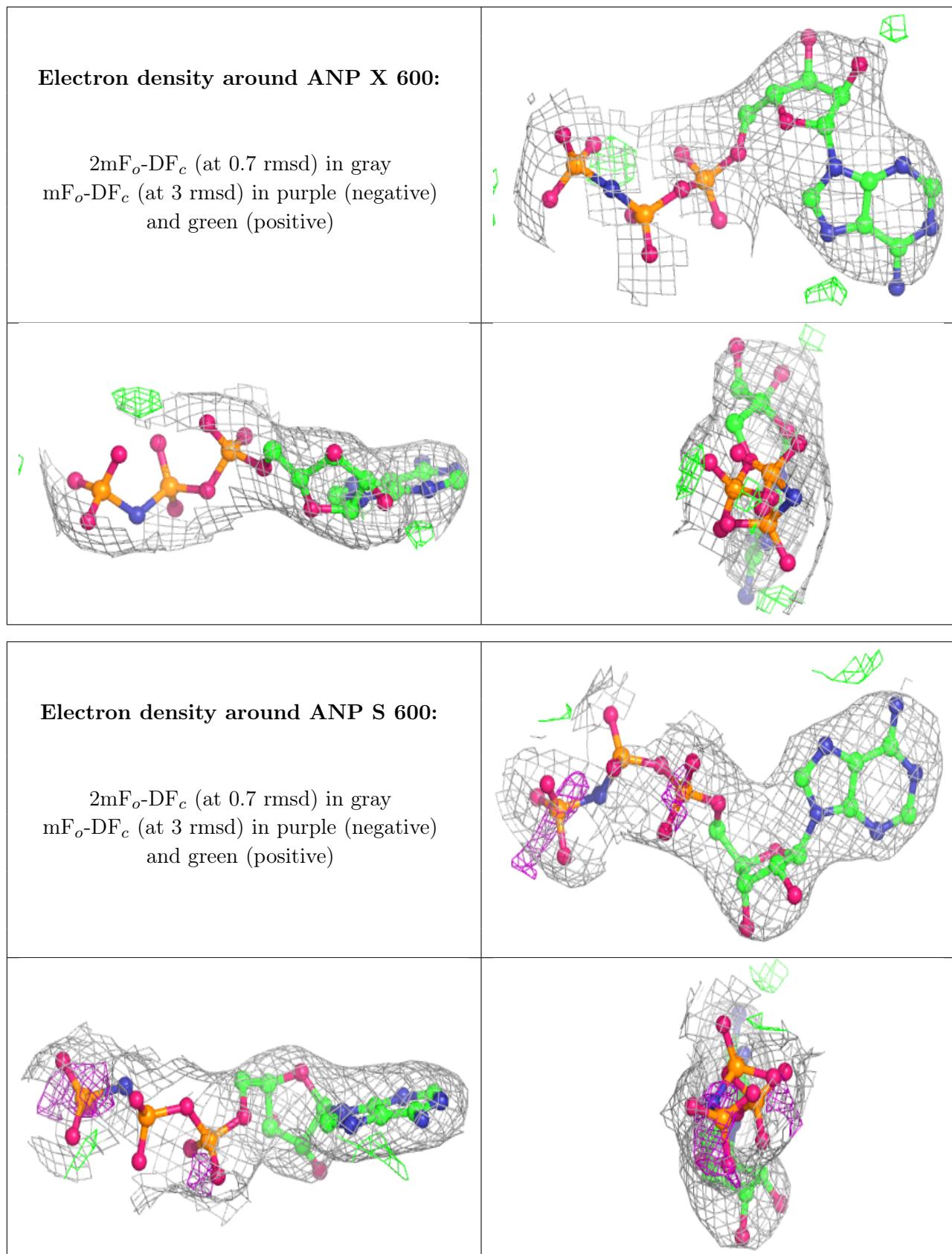


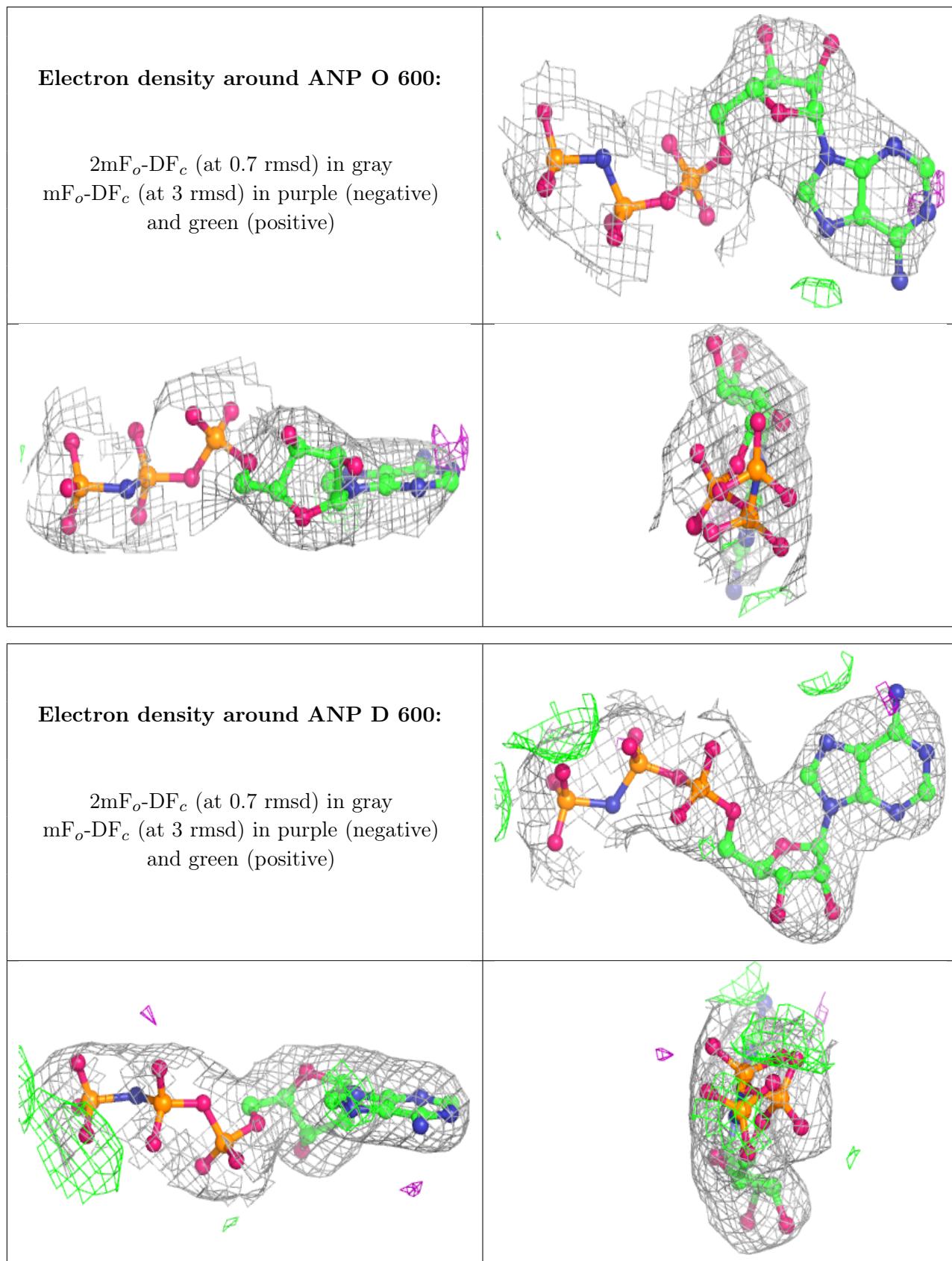


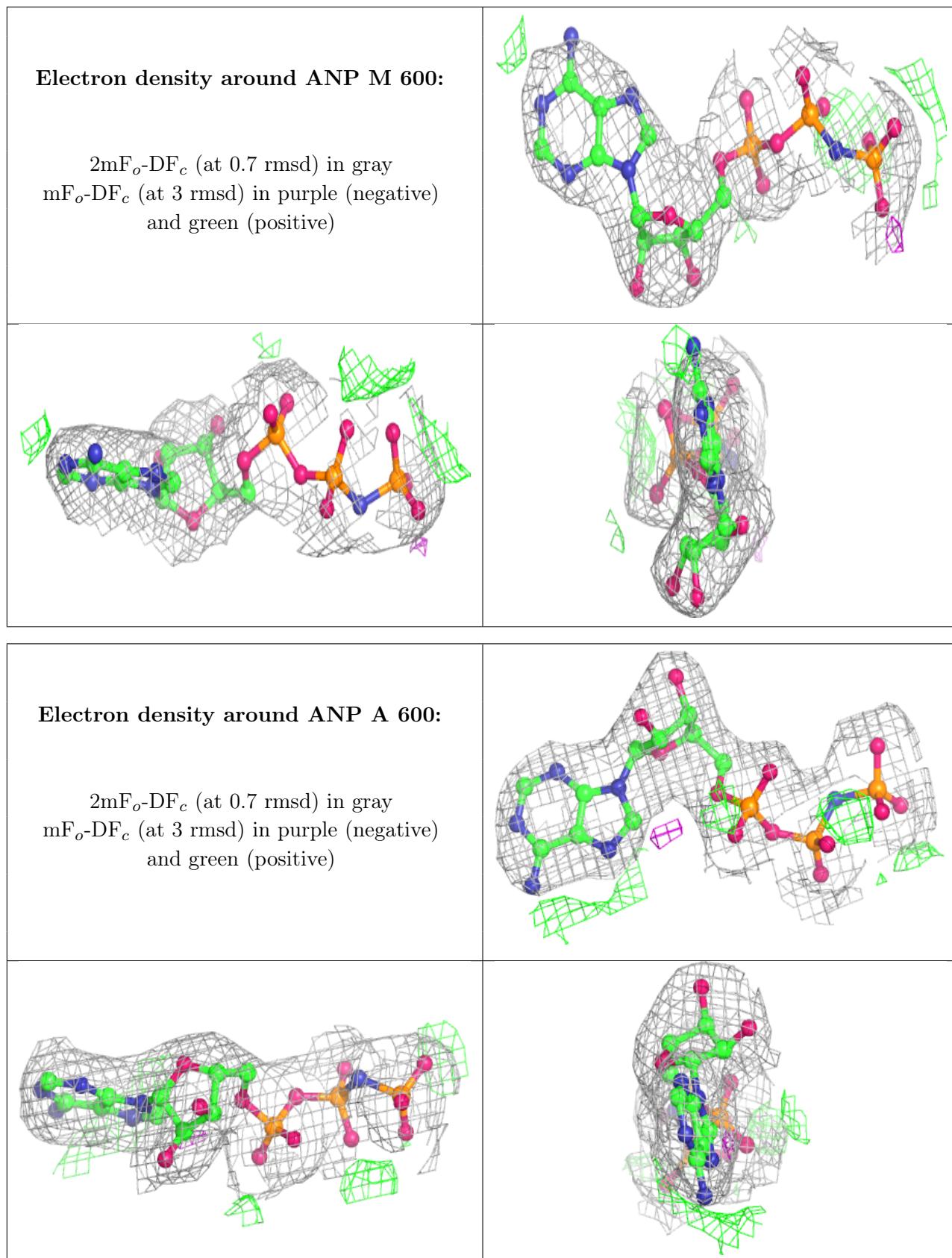












## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.