



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:01 AM UTC

PDB ID : 3OEH / pdb_00003oeh
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

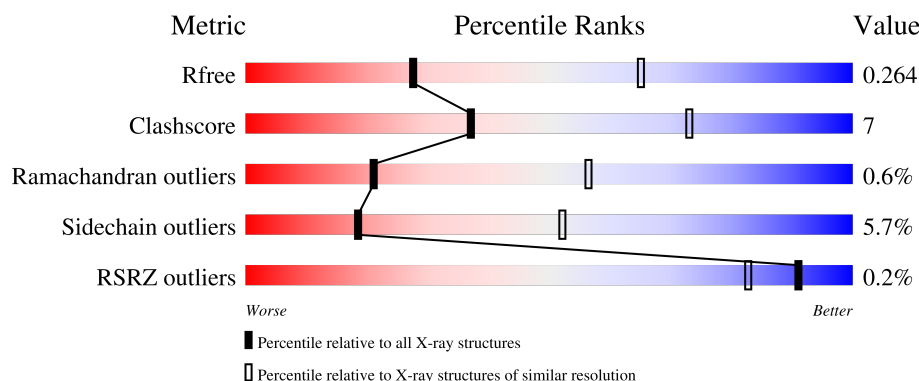
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

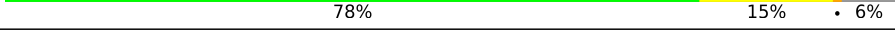
The reported resolution of this entry is 3.00 Å.

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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	510	
1	B	510	
1	C	510	
1	J	510	
1	K	510	

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

2 Entry composition [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	N	O	S	0	0	0
			3664	2314	648	699	3			
1	B	483	Total	C	N	O	S	0	0	0
			3669	2317	649	700	3			
1	C	484	Total	C	N	O	S	0	0	0
			3680	2325	650	702	3			
1	J	481	Total	C	N	O	S	0	0	0
			3655	2309	646	697	3			
1	K	486	Total	C	N	O	S	0	0	0
			3688	2327	652	706	3			
1	L	482	Total	C	N	O	S	0	0	0
			3664	2314	648	699	3			
1	S	478	Total	C	N	O	S	0	0	0
			3635	2297	643	692	3			
1	T	479	Total	C	N	O	S	0	0	0
			3642	2302	644	693	3			
1	U	481	Total	C	N	O	S	0	0	0
			3655	2308	646	698	3			

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

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

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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	0	0	0
			2059	1293	359	397	10			
3	P	246	Total	C	N	O	S	0	0	0
			1872	1175	327	361	9			
3	Y	201	Total	C	N	O	S	0	0	0
			1523	947	274	293	9			

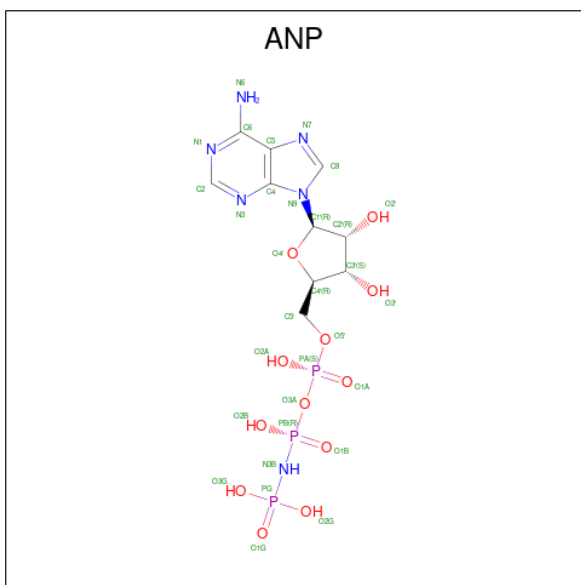
- Molecule 4 is a protein called ATP synthase subunit delta.

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

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

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

- Molecule 6 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



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

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

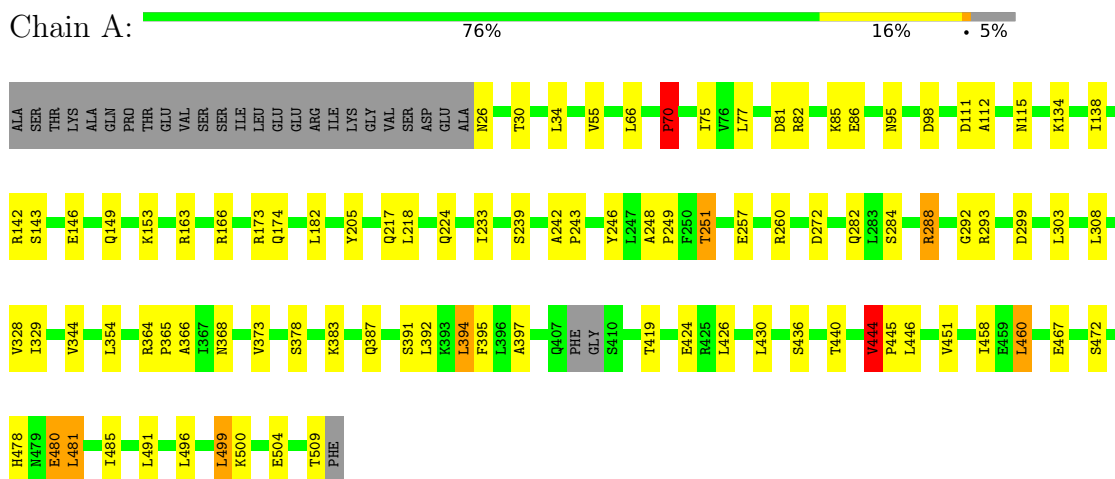
- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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		

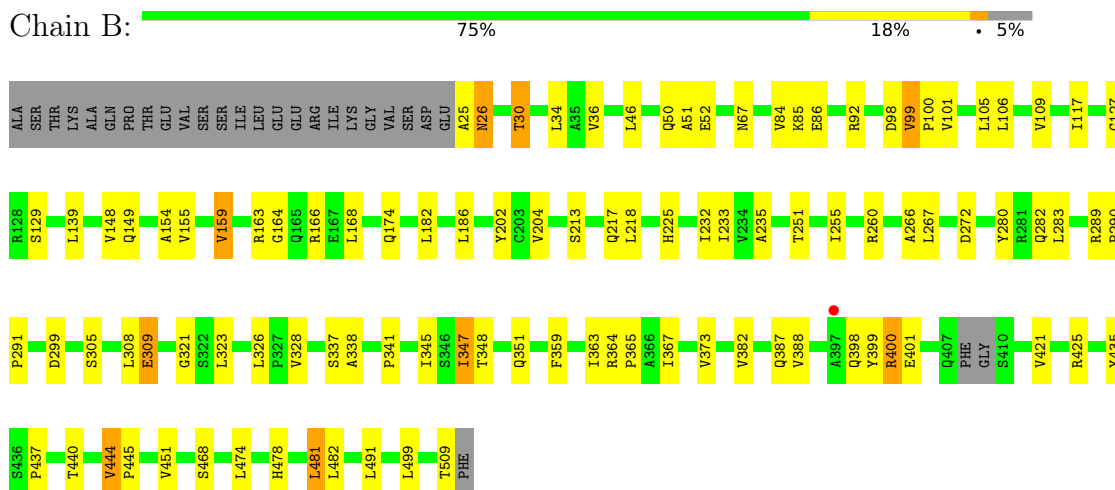
3 Residue-property plots

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.

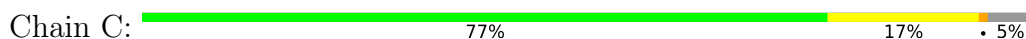
- Molecule 1: ATP synthase subunit alpha

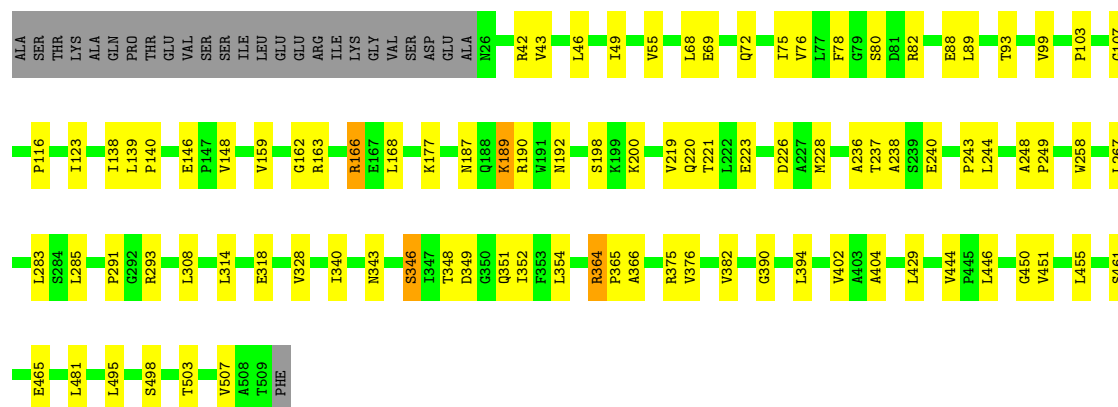


- Molecule 1: ATP synthase subunit alpha



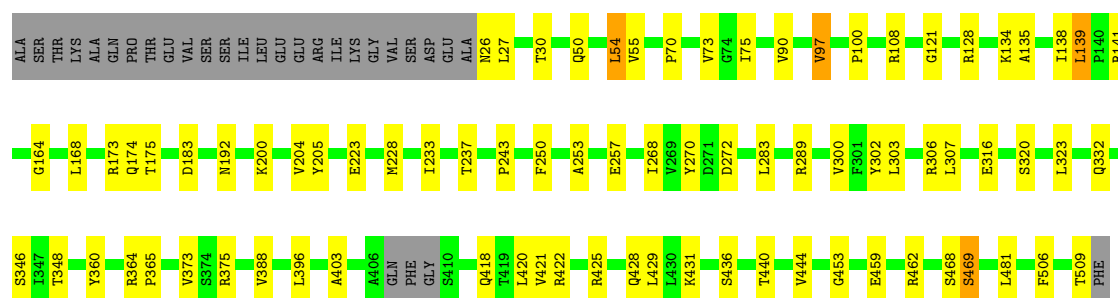
- Molecule 1: ATP synthase subunit alpha





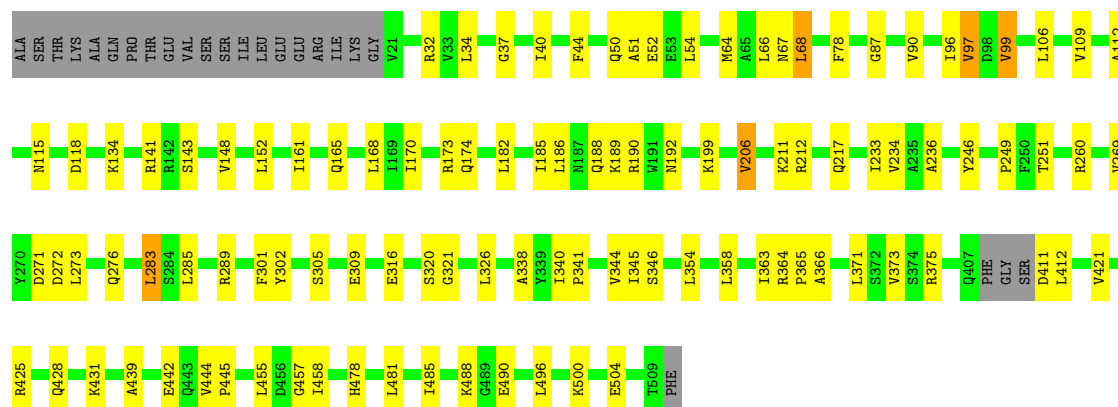
• Molecule 1: ATP synthase subunit alpha

Chain J: 78% 15% • 6%



• Molecule 1: ATP synthase subunit alpha

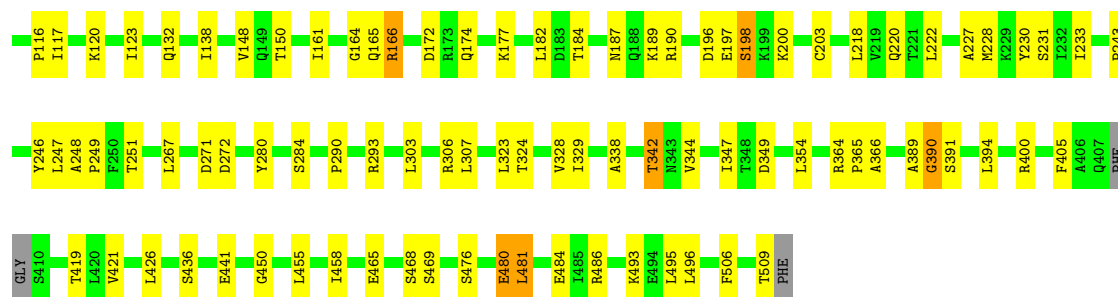
Chain K: 75% 20% • 5%



• Molecule 1: ATP synthase subunit alpha

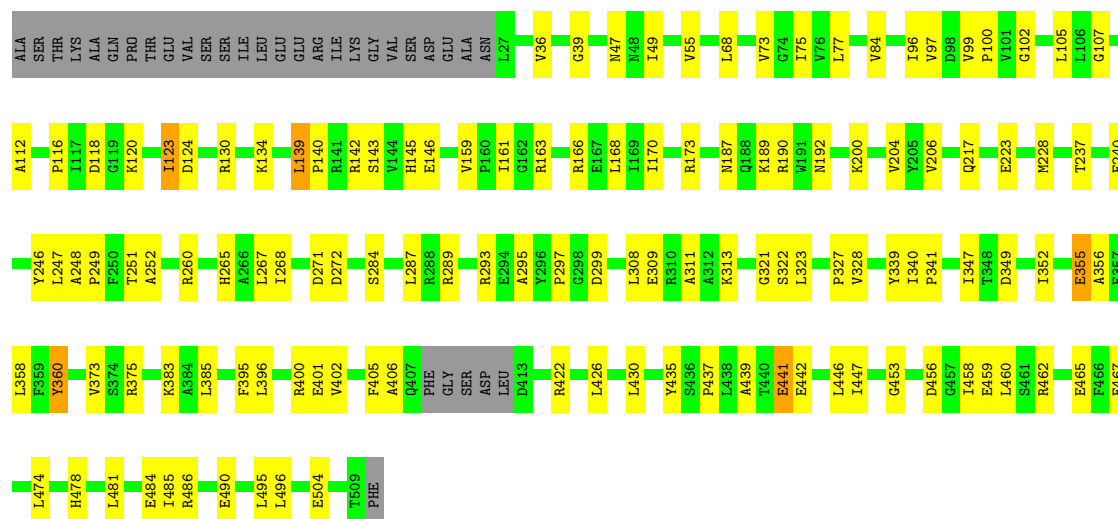
Chain L: 73% 20% • 5%





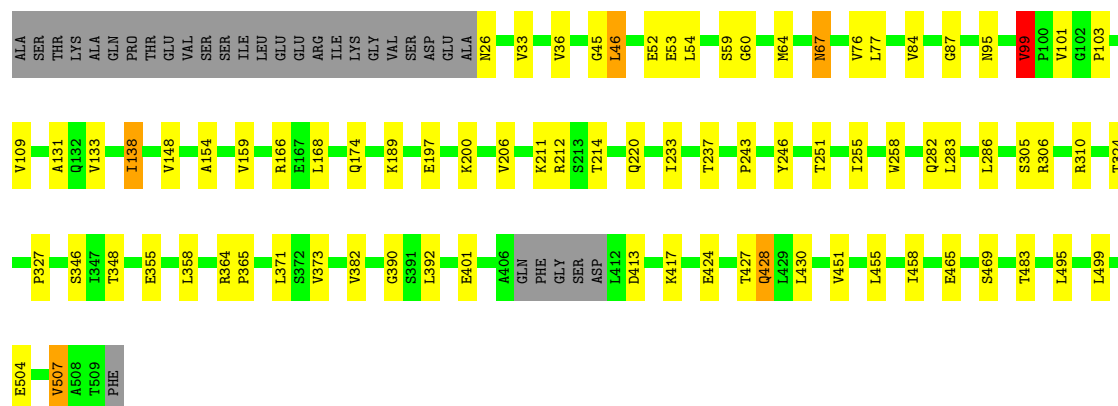
- Molecule 1: ATP synthase subunit alpha

Chain S: 69% 24% • 6%



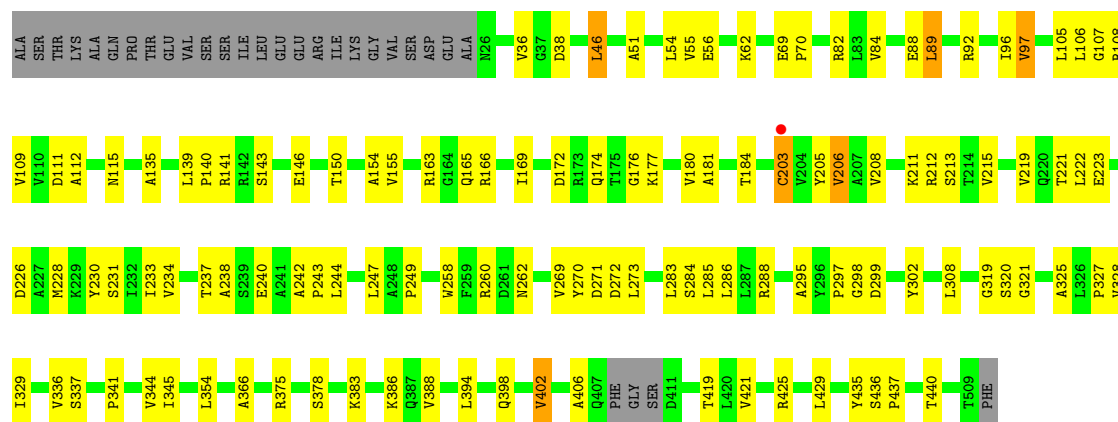
- Molecule 1: ATP synthase subunit alpha

Chain T: 78% 15% • 6%



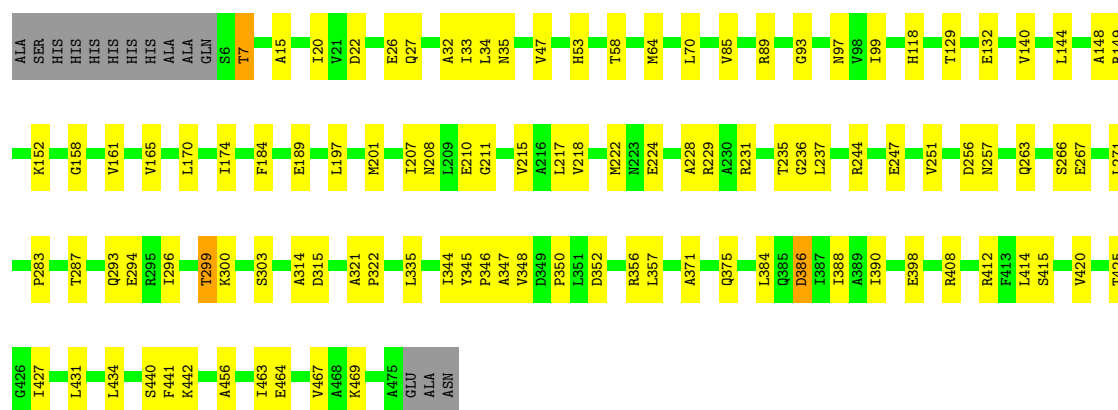
- Molecule 1: ATP synthase subunit alpha

Chain U: 71% 23% • 6%



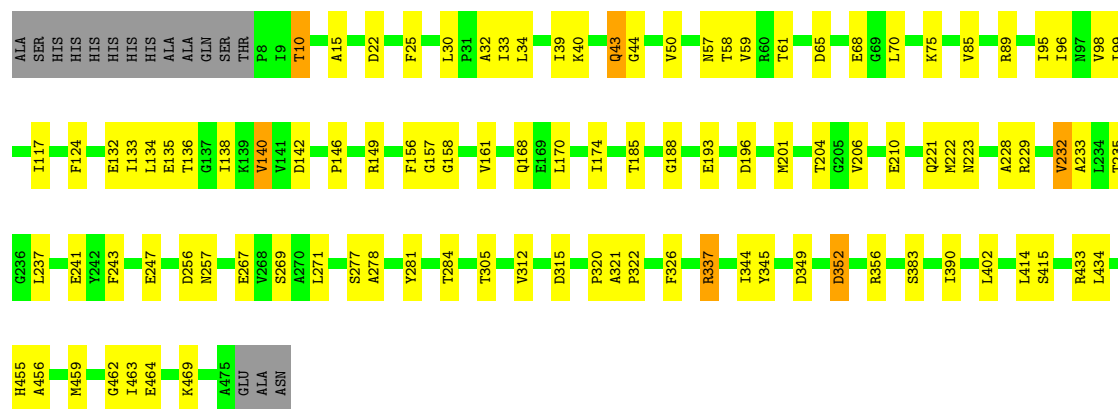
• Molecule 2: ATP synthase subunit beta

Chain D: 75% 21% ..



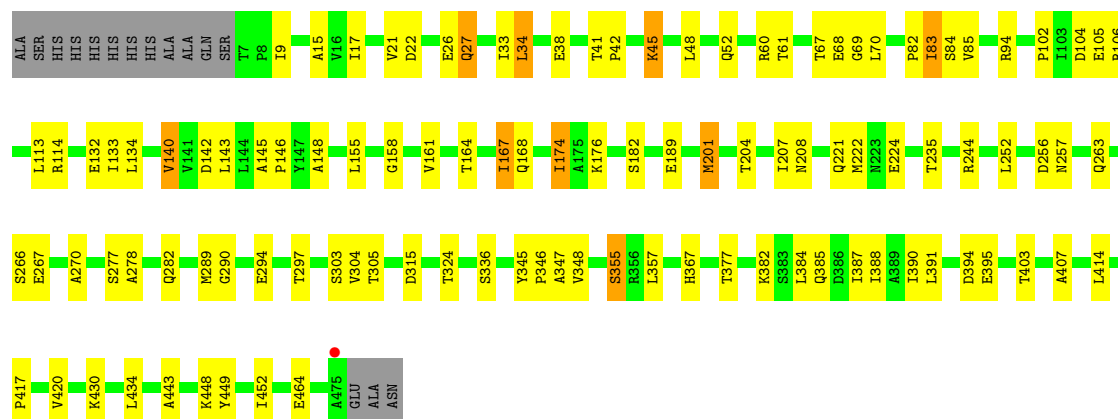
• Molecule 2: ATP synthase subunit beta

Chain E: 76% 20% ..



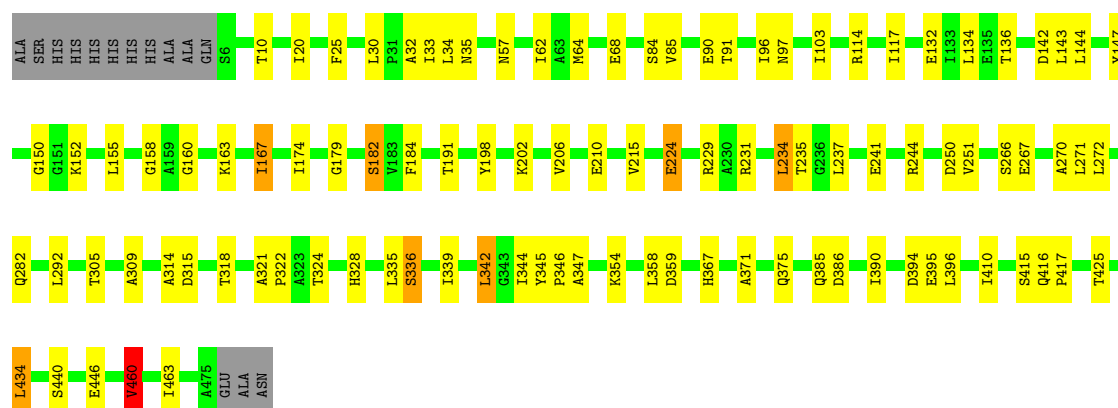
• Molecule 2: ATP synthase subunit beta

Chain F: 74% 21% ..



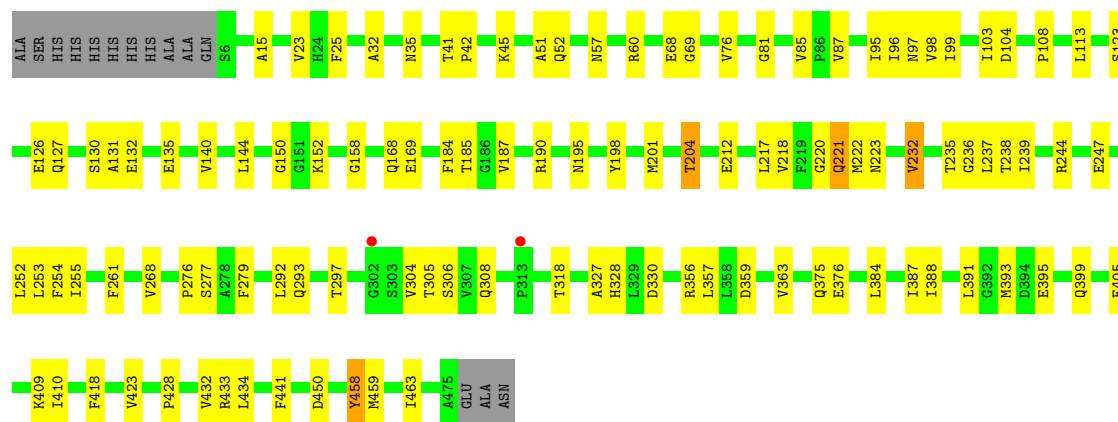
• Molecule 2: ATP synthase subunit beta

Chain M: 76% 19%



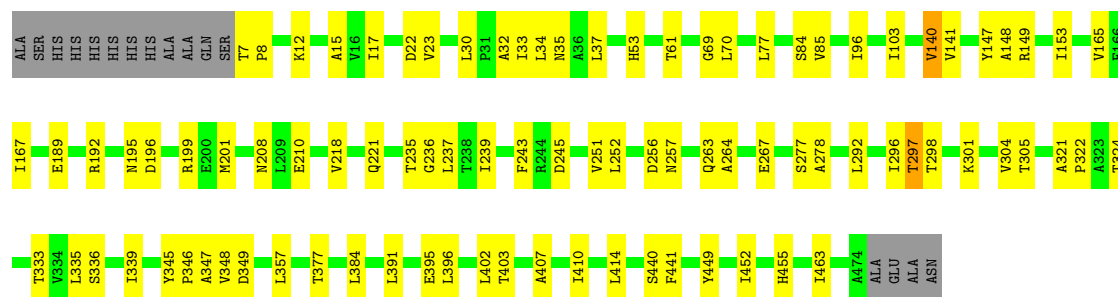
• Molecule 2: ATP synthase subunit beta

Chain N: 74% 22%



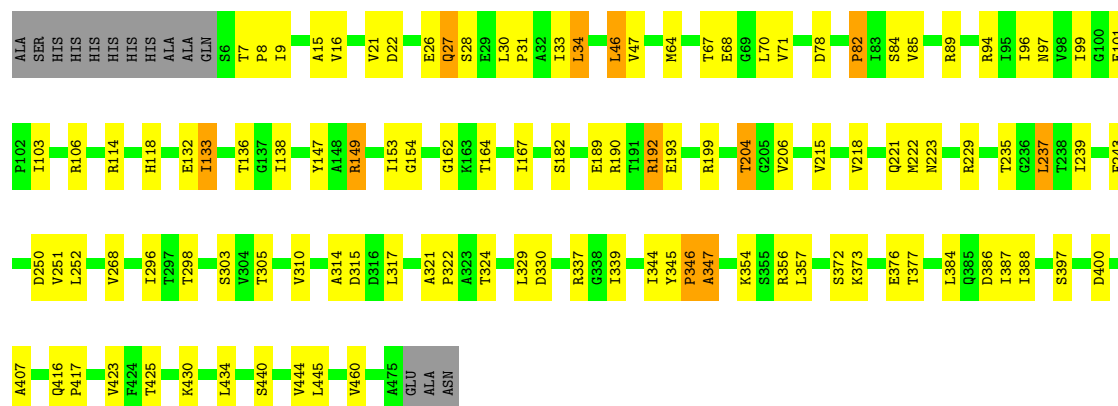
• Molecule 2: ATP synthase subunit beta

Chain O: 78% 18%



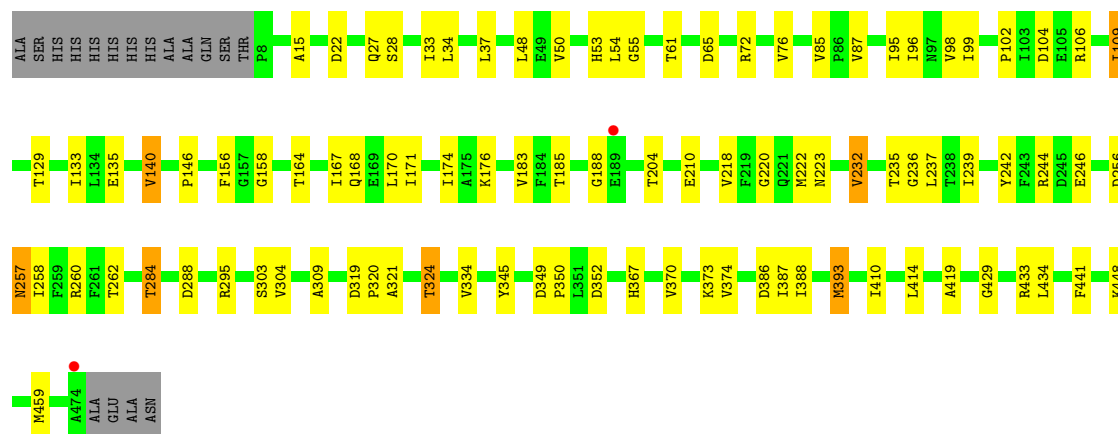
• Molecule 2: ATP synthase subunit beta

Chain V: 74% 21%



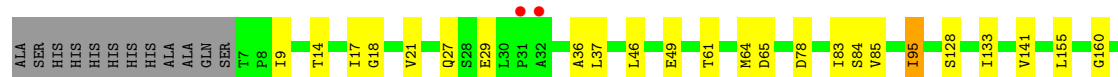
• Molecule 2: ATP synthase subunit beta

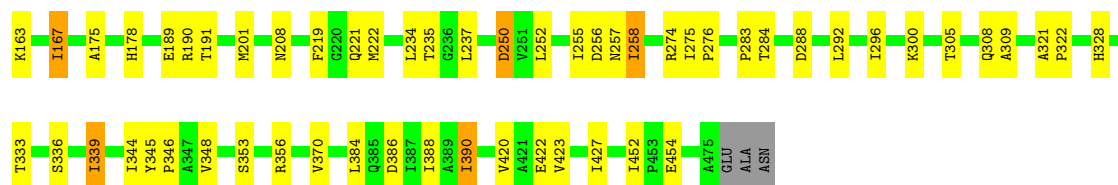
Chain W: 77% 18%



• Molecule 2: ATP synthase subunit beta

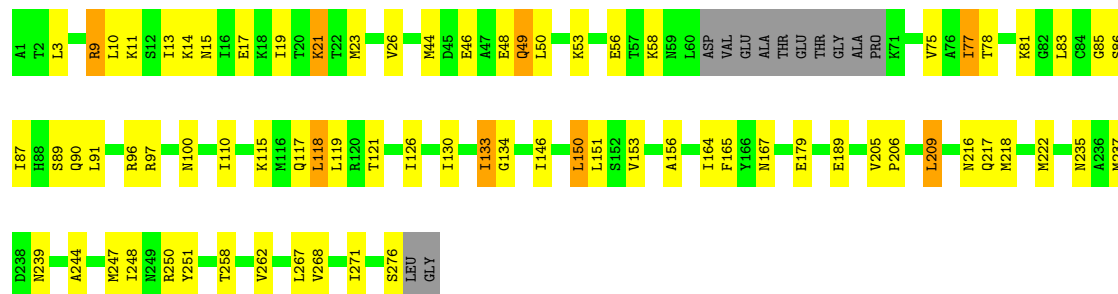
Chain X: 80% 15%



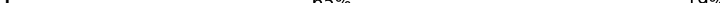


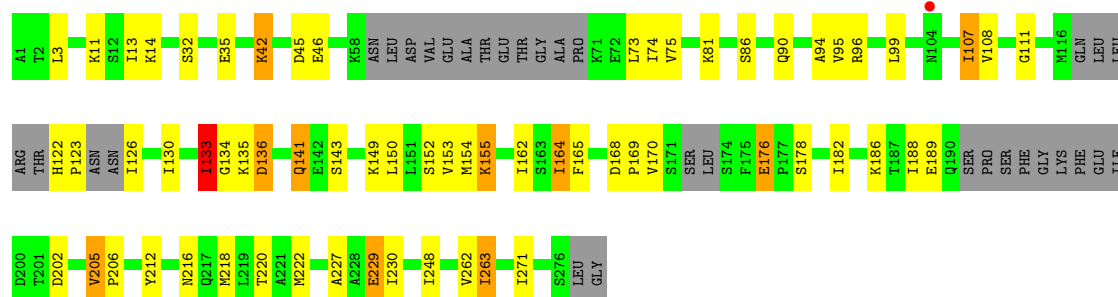
- Molecule 3: ATP synthase subunit gamma

Chain G: 69% 24% . .



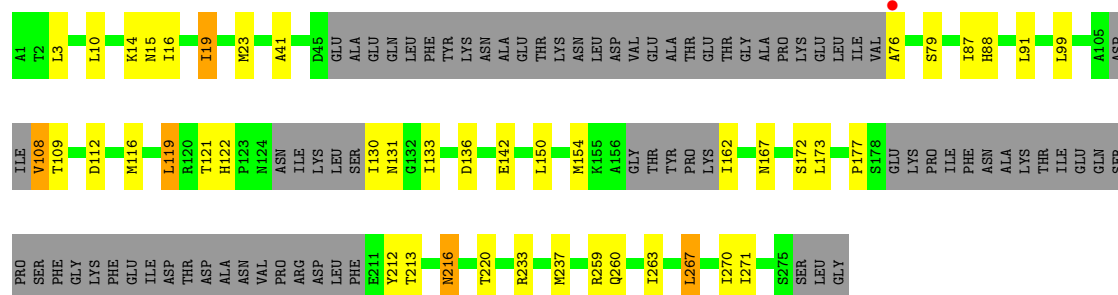
- Molecule 3: ATP synthase subunit gamma

Chain P:  65% 19% • 12%



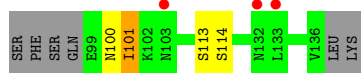
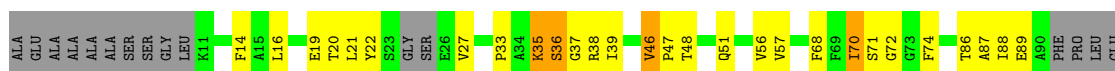
- Molecule 3: ATP synthase subunit gamma

Chain Y: 56% 14% 28%

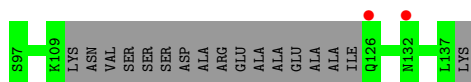


- Molecule 4: ATP synthase subunit delta

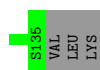
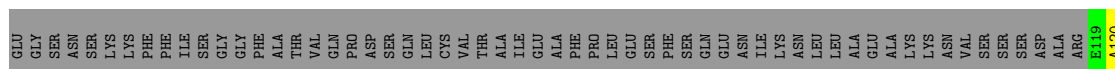
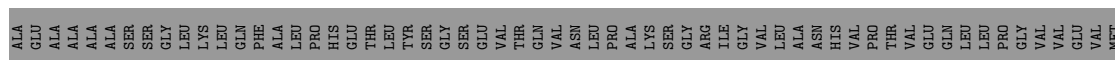
Chain H:



• Molecule 4: ATP synthase subunit delta



• Molecule 4: ATP synthase subunit delta



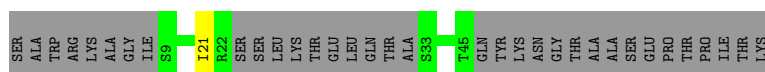
• Molecule 5: ATP synthase subunit epsilon



• Molecule 5: ATP synthase subunit epsilon



• Molecule 5: ATP synthase subunit epsilon



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	110.93Å 291.90Å 188.76Å 90.00° 101.91° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 20.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	88.8 (20.00-3.00) 88.6 (20.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 (1.77%)	wwPDB-VP
Wilson B-factor (Å ²)	82.8	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 69.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.59	0/3718	0.97	1/5032 (0.0%)
1	B	0.52	0/3723	0.88	3/5039 (0.1%)
1	C	0.56	2/3736 (0.1%)	0.93	2/5057 (0.0%)
1	J	0.48	0/3709	0.87	2/5020 (0.0%)
1	K	0.48	0/3742	0.84	0/5065
1	L	0.58	0/3718	0.91	2/5032 (0.0%)
1	S	0.51	0/3689	0.88	4/4992 (0.1%)
1	T	0.48	0/3696	0.82	1/5002 (0.0%)
1	U	0.49	0/3709	0.84	1/5021 (0.0%)
2	D	0.60	0/3606	0.92	1/4890 (0.0%)
2	E	0.55	0/3565	0.88	0/4840
2	F	0.53	0/3588	0.87	2/4868 (0.0%)
2	M	0.51	0/3600	0.89	4/4883 (0.1%)
2	N	0.49	0/3602	0.84	2/4886 (0.0%)
2	O	0.48	0/3595	0.86	0/4875
2	V	0.51	0/3607	0.86	0/4891
2	W	0.51	0/3592	0.84	0/4869
2	X	0.50	0/3604	0.86	2/4887 (0.0%)
3	G	0.52	0/2084	0.88	0/2803
3	P	0.49	0/1889	0.90	3/2537 (0.1%)
3	Y	0.47	0/1533	0.85	0/2056
4	H	0.56	0/772	0.91	1/1058 (0.1%)
4	Q	0.57	0/453	1.03	2/621 (0.3%)
4	Z	0.52	0/84	0.70	0/116
5	1	0.47	0/143	0.76	0/195
5	I	0.58	0/343	0.95	0/470
5	R	0.56	0/189	0.89	0/261
All	All	0.52	2/73289 (0.0%)	0.88	33/99266 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	340	ILE	CA-CB	5.66	1.57	1.53
1	C	444	VAL	CA-CB	5.39	1.56	1.54

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	444	VAL	N-CA-CB	9.73	116.63	110.50
1	S	460	LEU	N-CA-C	6.49	118.35	111.28
1	C	93	THR	N-CA-C	-6.39	106.02	113.88
4	Q	78	GLN	CA-C-N	6.27	127.68	119.84
4	Q	78	GLN	C-N-CA	6.27	127.68	119.84
2	D	247	GLU	N-CA-C	-6.09	105.85	113.28
3	P	32	SER	N-CA-C	-6.03	106.57	114.04
4	H	21	LEU	N-CA-C	6.01	118.74	111.40
2	M	395	GLU	N-CA-C	-5.98	106.11	113.41
1	S	355	GLU	N-CA-C	5.95	118.14	108.26
2	M	179	GLY	N-CA-C	5.93	120.36	112.77
2	F	224	GLU	CA-C-N	5.78	126.33	120.38
2	F	224	GLU	C-N-CA	5.78	126.33	120.38
1	T	99	VAL	N-CA-C	5.73	113.89	109.19
1	J	289	ARG	CA-C-N	5.66	126.21	120.38
1	J	289	ARG	C-N-CA	5.66	126.21	120.38
1	L	203	CYS	N-CA-C	5.61	117.54	108.34
1	B	347	ILE	N-CA-C	-5.46	107.31	111.62
1	B	399	TYR	N-CA-C	-5.44	105.51	111.82
3	P	73	LEU	N-CA-C	5.42	117.18	107.80
2	M	91	THR	N-CA-C	-5.38	106.71	113.28
2	M	336	SER	N-CA-C	5.38	117.86	108.76
1	U	203	CYS	N-CA-C	5.35	117.14	108.26
1	S	102	GLY	CA-C-N	5.33	125.65	119.47
1	S	102	GLY	C-N-CA	5.33	125.65	119.47
2	X	219	PHE	N-CA-C	5.25	116.95	108.34
1	L	72	GLN	N-CA-C	5.22	115.03	108.45
3	P	46	GLU	N-CA-C	-5.16	106.99	113.28
2	N	81	GLY	CA-C-N	5.14	125.86	120.11
2	N	81	GLY	C-N-CA	5.14	125.86	120.11
2	X	175	ALA	N-CA-C	5.14	117.28	111.11
1	B	235	ALA	N-CA-C	5.11	116.74	108.41
1	C	237	THR	N-CA-C	5.06	117.05	110.53

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3664	0	3747	63	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	66	0
1	L	3664	0	3747	58	0
1	S	3635	0	3724	71	0
1	T	3642	0	3733	38	0
1	U	3655	0	3734	66	0
2	D	3549	0	3614	62	0
2	E	3508	0	3550	54	0
2	F	3531	0	3592	58	0
2	M	3543	0	3603	53	0
2	N	3545	0	3604	65	0
2	O	3538	0	3606	48	0
2	V	3550	0	3611	65	0
2	W	3535	0	3605	48	0
2	X	3547	0	3615	38	0
3	G	2059	0	2127	43	0
3	P	1872	0	1917	35	0
3	Y	1523	0	1569	17	0
4	H	763	0	653	22	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1043	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 (1043) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:201:MET:HE2	2:D:217:LEU:HD21	1.72	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:W:345:TYR:HB2	2:W:459:MET:HE1	1.77	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
1:C:219:VAL:HB	1:C:228:MET:HE3	1.75	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
2:F:345:TYR:HA	2:F:346:PRO:C	2.18	0.66
1:U:135:ALA:HB3	2:V:223:ASN:HD22	1.60	0.66
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
2:D:26:GLU:OE2	2:D:26:GLU:HA	1.96	0.65
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:168:LEU:HB2	1:C:348:THR:HG21	1.79	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
3:G:44:MET:HE2	4:H:86:THR:HB	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
2:D:64:MET:HE3	2:D:228:ALA:HA	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
1:K:364:ARG:HA	1:K:365:PRO:C	2.24	0.62
2:M:224:GLU:O	2:M:229:ARG:HD3	1.99	0.62
1:J:346:SER:O	2:N:222:MET:HE1	1.98	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
2:F:148:ALA:HB2	2:F:357:LEU:HD11	1.82	0.61
1:J:302:TYR:O	1:J:306:ARG:HB2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:V:345:TYR:HA	2:V:346:PRO:C	2.25	0.61
2:E:39:ILE:HD13	2:E:70:LEU:HD21	1.83	0.61
1:S:145:HIS:H	1:S:313:LYS:HZ3	1.49	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
2:E:43:GLN:HG2	2:E:44:GLY:N	2.15	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: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
2:O:345:TYR:HA	2:O:346:PRO:C	2.24	0.60
3:G:205:VAL:O	3:G:209:LEU:HB2	2.02	0.59
2:M:64:MET:HE1	2:M:231:ARG:HB2	1.83	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
1:J:364:ARG:HA	1:J:365:PRO:C	2.26	0.59
2:M:371:ALA:O	2:M:375:GLN:HG3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:344:ILE:HG23	2:D:415:SER:HB3	1.85	0.58
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
2:X:345:TYR:HA	2:X:346:PRO:C	2.29	0.58
1:B:98:ASP:HB2	1:B:129:SER:O	2.04	0.58
2:E:345:TYR:HB2	2:E:459:MET:HE1	1.84	0.58
1:K:260:ARG:O	1:K:321:GLY:HA3	2.04	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
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: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:W:319:ASP:HA	3:Y:260:GLN:HE22	1.69	0.56
2:X:85:VAL:HG11	2:X:235:THR:HG23	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:201:MET:HE3	2:D:215:VAL:HG11	1.86	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
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:L:228:MET:HE1	1:L:233:ILE:HD11	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: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
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:L:166:ARG:HH21	1:L:349:ASP:CG	2.16	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
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
3:G:87:ILE:HG23	3:G:167:ASN:ND2	2.24	0.53
3:P:143:SER:HA	3:P:222:MET:HE1	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:299:THR:OG1	2:D:300:LYS:N	2.41	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
1:C:364:ARG:HA	1:C:365:PRO:C	2.34	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:136:THR:HG23	2:E:138:ILE:H	1.75	0.51
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:E:136:THR:HG22	2:E:142:ASP:CG	2.36	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:F:346:PRO:C	2:F:348:VAL:H	2.18	0.50
1:J:50:GLN:HB3	2:N:69:GLY:HA2	1.92	0.50
1:T:52:GLU:HG2	1:T:64:MET:HE3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:ARG:HA	1:B:365:PRO:C	2.35	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
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:64:MET:CE	2:D:228:ALA:HA	2.41	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:B:435:TYR:C	1:B:437:PRO:HD3	2.37	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
2:V:99:ILE:HD11	2:V:101:GLU:CD	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:253:LEU:O	2:N:306:SER:HA	2.13	0.49
2:X:178:HIS:NE2	2:X:250:ASP:HB3	2.27	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
1:B:117:ILE:HD12	2:E:124:PHE:HB3	1.95	0.49
2:F:140:VAL:HG12	2:F:414:LEU:HD22	1.94	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
2:F:104:ASP:C	2:F:106:ARG:H	2.21	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: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
3:P:94:ALA:C	3:P:96:ARG:H	2.21	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:W:33:ILE:O	2:W:34:LEU:HB2	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:L:389:ALA:O	1:L:390:GLY:C	2.55	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
2:F:21:VAL:O	2:F:61:THR:OG1	2.30	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
1:K:442:GLU:C	1:K:445:PRO:HD2	2.39	0.48
2:V:190:ARG:HB2	2:V:193:GLU:HG3	1.96	0.48
3:Y:23:MET:HE2	3:Y:23:MET:HA	1.95	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
1:U:435:TYR:C	1:U:437:PRO:HD3	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:96:ILE:O	1:K:97:VAL:C	2.58	0.47
1:K:271:ASP:HA	1:K:272:ASP:HA	1.62	0.47
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
2:D:386:ASP:OD1	2:D:386:ASP:N	2.46	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
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:459:GLU:HG3	1:J:462:ARG:HG3	1.97	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
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
2:M:84:SER:HB2	2:M:114:ARG:HH21	1.80	0.46
1:T:364:ARG:HA	1:T:365:PRO:C	2.40	0.46
2:V:222:MET:HA	2:V:229:ARG:HD2	1.97	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
1:L:46:LEU:O	1:L:47:ASN:C	2.58	0.46
2:M:32:ALA:O	2:M:35:ASN:HB2	2.16	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:V:189:GLU:HA	2:V:222:MET:HE3	1.97	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:V:153:ILE:C	2:V:329:LEU:HD22	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:98:ASP:C	1:A:98:ASP:OD1	2.58	0.45
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
1:K:302:TYR:HA	1:K:305:SER:HG	1.81	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
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:D:434:LEU:C	2:D:434:LEU:HD23	2.42	0.45
2:O:189:GLU:O	2:O:221:GLN:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:51:ALA:O	1:B:52:GLU:HB2	2.16	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:97:ASN:OD1	2:D:97:ASN:C	2.61	0.44
2:D:425:THR:HB	2:D:427:ILE:HD12	1.99	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:441:PHE:O	2:D:442:LYS:C	2.60	0.44
2:D:456:ALA:HA	2:D:469:LYS:HD3	1.99	0.44
2:E:349:ASP:CG	2:E:352:ASP:HB2	2.41	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
1:A:368:ASN:OD1	1:A:368:ASN:C	2.60	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
1:S:297:PRO:C	1:S:299:ASP:H	2.25	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
1:A:292:GLY:O	1:A:293:ARG:C	2.59	0.44
1:L:246:TYR:CD2	1:L:246:TYR:C	2.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:198:TYR:CZ	2:M:202:LYS:HE2	2.52	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
1:L:364:ARG:HA	1:L:365:PRO:C	2.42	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:S:146:GLU:H	1:S:313:LYS:HZ3	1.66	0.43
1:T:131:ALA:HB2	1:T:251:THR:HG22	2.00	0.43
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:184:PHE:CD1	2:M:184:PHE:C	2.96	0.43
2:M:342:LEU:HD13	2:M:344:ILE:HD12	2.01	0.43
2:W:367:HIS:ND1	2:W:367:HIS:C	2.76	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:E:136:THR:C	2:E:138:ILE:H	2.27	0.43
2:F:82:PRO:O	2:F:83:ILE:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:64:MET:HE1	2:D:231:ARG:HB2	2.01	0.43
2:D:149:ARG:HH11	2:D:149:ARG:HG2	1.83	0.43
2:D:345:TYR:HA	2:D:346:PRO:C	2.43	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
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
2:O:349:ASP:OD1	2:O:349:ASP:C	2.61	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:A:364:ARG:HA	1:A:365:PRO:C	2.42	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
1:L:228:MET:HE2	1:L:228:MET:HA	2.00	0.43
2:M:241:GLU:HG2	2:M:244:ARG:NH2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:U:223:GLU:HG3	1:U:228:MET:HE3	2.00	0.42
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:111:ASP:CG	1:A:115:ASN:HB2	2.45	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
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:M:345:TYR:HA	2:M:346:PRO:C	2.45	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: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
2:N:135:GLU:CD	2:N:434:LEU:HB2	2.45	0.42
1:T:45:GLY:O	1:T:46:LEU:C	2.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:U:139:LEU:C	1:U:141:ARG:H	2.28	0.42
1:U:286:LEU:C	1:U:288:ARG:H	2.28	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
4:H:100:ASN:O	4:H:101:ILE:C	2.63	0.42
2:V:26:GLU:O	2:V:27:GLN:C	2.62	0.42
1:B:174:GLN:CA	6:B:600:ANP:HNB1	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:188:GLN:C	1:K:190:ARG:H	2.27	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
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
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
1:U:96:ILE:O	1:U:97:VAL:C	2.63	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:402:VAL:C	1:C:404:ALA:H	2.27	0.41
2:F:134:LEU:CD2	2:F:305:THR:HG21	2.50	0.41
3:G:146:ILE:HG22	3:G:218:MET:HE1	2.02	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:190:ARG:NE	1:K:439:ALA:HB2	2.35	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: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:D:184:PHE:CD1	2:D:184:PHE:C	2.99	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:M:150:GLY:H	2:M:305:THR:HG1	1.68	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:S:435:TYR:C	1:S:437:PRO:HD3	2.46	0.41
1:T:168:LEU:HB2	1:T:348:THR:HG21	2.02	0.41
1:U:154:ALA:O	1:U:155:VAL:C	2.64	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:K:283:LEU:C	1:K:283:LEU:HD23	2.45	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
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
1:L:222:LEU:HD12	1:L:228:MET:HE1	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:188:ILE:O	3:P:188:ILE:HG22	2.21	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: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%)	43	76
1	B	479/510 (94%)	448 (94%)	30 (6%)	1 (0%)	43	76
1	C	482/510 (94%)	453 (94%)	28 (6%)	1 (0%)	43	76
1	J	477/510 (94%)	460 (96%)	16 (3%)	1 (0%)	43	76
1	K	482/510 (94%)	442 (92%)	35 (7%)	5 (1%)	12	45
1	L	478/510 (94%)	450 (94%)	27 (6%)	1 (0%)	43	76
1	S	474/510 (93%)	447 (94%)	25 (5%)	2 (0%)	30	65
1	T	475/510 (93%)	438 (92%)	33 (7%)	4 (1%)	16	50
1	U	477/510 (94%)	432 (91%)	39 (8%)	6 (1%)	9	38
2	D	468/484 (97%)	439 (94%)	28 (6%)	1 (0%)	43	76
2	E	466/484 (96%)	436 (94%)	28 (6%)	2 (0%)	30	65
2	F	467/484 (96%)	435 (93%)	27 (6%)	5 (1%)	11	43
2	M	468/484 (97%)	437 (93%)	30 (6%)	1 (0%)	43	76
2	N	468/484 (97%)	431 (92%)	33 (7%)	4 (1%)	14	48
2	O	466/484 (96%)	442 (95%)	24 (5%)	0	100	100
2	V	468/484 (97%)	423 (90%)	38 (8%)	7 (2%)	8	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	W	465/484 (96%)	432 (93%)	30 (6%)	3 (1%)	21	56
2	X	467/484 (96%)	432 (92%)	33 (7%)	2 (0%)	30	65
3	G	262/278 (94%)	245 (94%)	17 (6%)	0	100	100
3	P	234/278 (84%)	210 (90%)	19 (8%)	5 (2%)	5	27
3	Y	189/278 (68%)	176 (93%)	13 (7%)	0	100	100
4	H	110/138 (80%)	89 (81%)	19 (17%)	2 (2%)	6	31
4	Q	74/138 (54%)	61 (82%)	13 (18%)	0	100	100
4	Z	15/138 (11%)	11 (73%)	3 (20%)	1 (7%)	1	5
5	1	23/61 (38%)	19 (83%)	3 (13%)	1 (4%)	2	12
5	I	43/61 (70%)	33 (77%)	6 (14%)	4 (9%)	0	2
5	R	30/61 (49%)	25 (83%)	5 (17%)	0	100	100
All	All	9485/10377 (91%)	8800 (93%)	625 (7%)	60 (1%)	21	56

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
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

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Mol	Chain	Res	Type
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
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 ⓘ

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%)	368 (95%)	20 (5%)	21	55
1	B	388/412 (94%)	371 (96%)	17 (4%)	25	60
1	C	390/412 (95%)	368 (94%)	22 (6%)	19	52
1	J	387/412 (94%)	367 (95%)	20 (5%)	21	55
1	K	390/412 (95%)	373 (96%)	17 (4%)	25	60
1	L	388/412 (94%)	364 (94%)	24 (6%)	16	49
1	S	385/412 (93%)	366 (95%)	19 (5%)	22	56
1	T	386/412 (94%)	364 (94%)	22 (6%)	18	52
1	U	387/412 (94%)	371 (96%)	16 (4%)	27	61
2	D	379/390 (97%)	363 (96%)	16 (4%)	26	61
2	E	370/390 (95%)	352 (95%)	18 (5%)	22	56
2	F	375/390 (96%)	356 (95%)	19 (5%)	21	55
2	M	378/390 (97%)	354 (94%)	24 (6%)	16	48
2	N	378/390 (97%)	356 (94%)	22 (6%)	18	51
2	O	378/390 (97%)	361 (96%)	17 (4%)	24	59
2	V	379/390 (97%)	359 (95%)	20 (5%)	20	54
2	W	378/390 (97%)	359 (95%)	19 (5%)	22	56
2	X	379/390 (97%)	352 (93%)	27 (7%)	13	43
3	G	226/236 (96%)	206 (91%)	20 (9%)	9	35
3	P	200/236 (85%)	177 (88%)	23 (12%)	5	24
3	Y	164/236 (70%)	145 (88%)	19 (12%)	5	23
4	H	64/112 (57%)	56 (88%)	8 (12%)	4	20
4	Q	11/112 (10%)	8 (73%)	3 (27%)	0	2
5	1	2/48 (4%)	2 (100%)	0	100	100
5	I	28/48 (58%)	26 (93%)	2 (7%)	13	43
5	R	5/48 (10%)	4 (80%)	1 (20%)	1	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	7583/8294 (91%)	7148 (94%)	435 (6%)	18	52

All (435) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	LEU
1	A	70	PRO
1	A	95	ASN
1	A	224	GLN
1	A	251	THR
1	A	284	SER
1	A	288	ARG
1	A	373	VAL
1	A	378	SER
1	A	394	LEU
1	A	436	SER
1	A	444	VAL
1	A	451	VAL
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
1	B	99	VAL
1	B	106	LEU
1	B	149	GLN
1	B	159	VAL
1	B	204	VAL
1	B	283	LEU
1	B	289	ARG
1	B	309	GLU
1	B	337	SER
1	B	373	VAL
1	B	400	ARG
1	B	444	VAL
1	B	468	SER
1	B	481	LEU
1	B	509	THR

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Mol	Chain	Res	Type
1	C	68	LEU
1	C	69	GLU
1	C	99	VAL
1	C	138	ILE
1	C	166	ARG
1	C	189	LYS
1	C	198	SER
1	C	220	GLN
1	C	221	THR
1	C	223	GLU
1	C	267	LEU
1	C	283	LEU
1	C	293	ARG
1	C	346	SER
1	C	364	ARG
1	C	376	VAL
1	C	382	VAL
1	C	394	LEU
1	C	451	VAL
1	C	461	SER
1	C	465	GLU
1	C	495	LEU
2	D	7	THR
2	D	58	THR
2	D	70	LEU
2	D	89	ARG
2	D	132	GLU
2	D	210	GLU
2	D	251	VAL
2	D	287	THR
2	D	299	THR
2	D	303	SER
2	D	386	ASP
2	D	390	ILE
2	D	398	GLU
2	D	431	LEU
2	D	464	GLU
2	D	467	VAL
2	E	10	THR
2	E	40	LYS
2	E	43	GLN
2	E	58	THR

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Mol	Chain	Res	Type
2	E	68	GLU
2	E	89	ARG
2	E	96	ILE
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	383	SER
2	E	390	ILE
2	E	402	LEU
2	F	27	GLN
2	F	45	LYS
2	F	48	LEU
2	F	68	GLU
2	F	113	LEU
2	F	132	GLU
2	F	133	ILE
2	F	140	VAL
2	F	167	ILE
2	F	174	ILE
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	10	LEU
3	G	11	LYS
3	G	21	LYS
3	G	48	GLU
3	G	49	GLN
3	G	53	LYS
3	G	77	ILE

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Mol	Chain	Res	Type
3	G	97	ARG
3	G	100	ASN
3	G	118	LEU
3	G	133	ILE
3	G	150	LEU
3	G	153	VAL
3	G	209	LEU
3	G	216	ASN
3	G	235	ASN
3	G	239	ASN
3	G	276	SER
4	H	20	THR
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	57	THR
1	J	26	ASN
1	J	27	LEU
1	J	54	LEU
1	J	97	VAL
1	J	134	LYS
1	J	139	LEU
1	J	175	THR
1	J	183	ASP
1	J	237	THR
1	J	373	VAL
1	J	396	LEU
1	J	418	GLN
1	J	420	LEU
1	J	429	LEU
1	J	436	SER
1	J	440	THR
1	J	468	SER
1	J	469	SER
1	J	481	LEU
1	J	509	THR
1	K	40	ILE

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Mol	Chain	Res	Type
1	K	68	LEU
1	K	90	VAL
1	K	99	VAL
1	K	106	LEU
1	K	115	ASN
1	K	134	LYS
1	K	143	SER
1	K	199	LYS
1	K	206	VAL
1	K	246	TYR
1	K	283	LEU
1	K	309	GLU
1	K	320	SER
1	K	371	LEU
1	K	411	ASP
1	K	504	GLU
1	L	62	LYS
1	L	99	VAL
1	L	132	GLN
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	391	SER
1	L	400	ARG
1	L	405	PHE
1	L	419	THR
1	L	421	VAL
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	10	THR
2	M	57	ASN

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Mol	Chain	Res	Type
2	M	90	GLU
2	M	96	ILE
2	M	132	GLU
2	M	167	ILE
2	M	182	SER
2	M	206	VAL
2	M	210	GLU
2	M	224	GLU
2	M	234	LEU
2	M	250	ASP
2	M	251	VAL
2	M	342	LEU
2	M	359	ASP
2	M	385	GLN
2	M	386	ASP
2	M	390	ILE
2	M	394	ASP
2	M	396	LEU
2	M	410	ILE
2	M	434	LEU
2	M	446	GLU
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	204	THR
2	N	212	GLU
2	N	221	GLN
2	N	232	VAL
2	N	238	THR
2	N	247	GLU
2	N	268	VAL
2	N	318	THR
2	N	376	GLU
2	N	387	ILE
2	N	393	MET
2	N	399	GLN
2	N	423	VAL
2	N	450	ASP

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Mol	Chain	Res	Type
2	N	458	TYR
2	N	463	ILE
2	O	30	LEU
2	O	70	LEU
2	O	77	LEU
2	O	84	SER
2	O	96	ILE
2	O	103	ILE
2	O	140	VAL
2	O	149	ARG
2	O	167	ILE
2	O	192	ARG
2	O	201	MET
2	O	208	ASN
2	O	210	GLU
2	O	292	LEU
2	O	297	THR
2	O	402	LEU
2	O	455	HIS
3	P	3	LEU
3	P	11	LYS
3	P	13	ILE
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	153	VAL
3	P	155	LYS
3	P	164	ILE
3	P	170	VAL
3	P	176	GLU
3	P	186	LYS
3	P	189	GLU
3	P	218	MET
3	P	220	THR
3	P	229	GLU
3	P	262	VAL
3	P	263	ILE

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Mol	Chain	Res	Type
4	Q	39	ILE
4	Q	45	HIS
4	Q	51	GLN
5	R	31	THR
1	S	105	LEU
1	S	123	ILE
1	S	124	ASP
1	S	134	LYS
1	S	139	LEU
1	S	159	VAL
1	S	189	LYS
1	S	267	LEU
1	S	360	TYR
1	S	373	VAL
1	S	383	LYS
1	S	401	GLU
1	S	441	GLU
1	S	456	ASP
1	S	458	ILE
1	S	459	GLU
1	S	490	GLU
1	S	496	LEU
1	S	504	GLU
1	T	26	ASN
1	T	36	VAL
1	T	67	ASN
1	T	76	VAL
1	T	95	ASN
1	T	99	VAL
1	T	133	VAL
1	T	138	ILE
1	T	159	VAL
1	T	189	LYS
1	T	206	VAL
1	T	246	TYR
1	T	371	LEU
1	T	373	VAL
1	T	382	VAL
1	T	401	GLU
1	T	427	THR
1	T	428	GLN
1	T	465	GLU

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Mol	Chain	Res	Type
1	T	469	SER
1	T	483	THR
1	T	507	VAL
1	U	38	ASP
1	U	82	ARG
1	U	88	GLU
1	U	89	LEU
1	U	172	ASP
1	U	174	GLN
1	U	206	VAL
1	U	208	VAL
1	U	336	VAL
1	U	383	LYS
1	U	388	VAL
1	U	394	LEU
1	U	402	VAL
1	U	419	THR
1	U	436	SER
1	U	440	THR
2	V	46	LEU
2	V	47	VAL
2	V	71	VAL
2	V	89	ARG
2	V	133	ILE
2	V	149	ARG
2	V	192	ARG
2	V	204	THR
2	V	237	LEU
2	V	250	ASP
2	V	251	VAL
2	V	268	VAL
2	V	310	VAL
2	V	354	LYS
2	V	357	LEU
2	V	386	ASP
2	V	387	ILE
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	176	LYS
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	9	ILE
2	X	14	THR
2	X	21	VAL
2	X	27	GLN
2	X	29	GLU
2	X	46	LEU
2	X	84	SER
2	X	95	ILE
2	X	133	ILE
2	X	155	LEU
2	X	167	ILE
2	X	191	THR
2	X	201	MET
2	X	208	ASN
2	X	250	ASP
2	X	258	ILE
2	X	274	ARG
2	X	336	SER
2	X	339	ILE
2	X	356	ARG
2	X	370	VAL
2	X	420	VAL
2	X	422	GLU
2	X	423	VAL
2	X	427	ILE
2	X	452	ILE

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Mol	Chain	Res	Type
2	X	454	GLU
3	Y	15	ASN
3	Y	19	ILE
3	Y	87	ILE
3	Y	108	VAL
3	Y	112	ASP
3	Y	119	LEU
3	Y	121	THR
3	Y	131	ASN
3	Y	133	ILE
3	Y	136	ASP
3	Y	142	GLU
3	Y	162	ILE
3	Y	167	ASN
3	Y	172	SER
3	Y	173	LEU
3	Y	213	THR
3	Y	216	ASN
3	Y	267	LEU
3	Y	271	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (139) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	132	GLN
1	A	145	HIS
1	A	187	ASN
1	A	381	GLN
1	A	418	GLN
1	A	434	GLN
1	B	26	ASN
1	B	149	GLN
1	B	381	GLN
1	B	428	GLN
1	B	477	ASN
1	C	72	GLN
1	C	174	GLN
1	C	188	GLN
1	C	210	GLN
1	C	220	GLN
1	C	262	ASN
1	C	418	GLN

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Mol	Chain	Res	Type
1	C	428	GLN
2	D	168	GLN
2	D	178	HIS
2	D	208	ASN
2	D	293	GLN
2	D	308	GLN
2	D	375	GLN
2	E	52	GLN
2	E	168	GLN
2	E	328	HIS
2	E	385	GLN
2	E	411	GLN
2	F	27	GLN
2	F	168	GLN
2	F	379	GLN
3	G	49	GLN
3	G	59	ASN
3	G	90	GLN
3	G	100	ASN
3	G	117	GLN
3	G	141	GLN
3	G	190	GLN
3	G	216	ASN
3	G	224	GLN
4	H	51	GLN
5	I	36	ASN
1	J	26	ASN
1	J	28	ASN
1	J	47	ASN
1	J	149	GLN
1	J	174	GLN
1	J	217	GLN
1	J	225	HIS
1	J	351	GLN
1	J	428	GLN
1	K	26	ASN
1	K	47	ASN
1	K	50	GLN
1	K	72	GLN
1	K	188	GLN
1	K	217	GLN
1	K	245	GLN

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Mol	Chain	Res	Type
1	K	262	ASN
1	K	265	HIS
1	K	428	GLN
1	K	477	ASN
1	K	478	HIS
1	L	26	ASN
1	L	50	GLN
1	L	95	ASN
1	L	188	GLN
1	L	220	GLN
1	L	282	GLN
1	L	398	GLN
2	M	168	GLN
2	M	178	HIS
2	N	168	GLN
2	N	195	ASN
2	N	221	GLN
2	N	385	GLN
2	O	24	HIS
2	O	27	GLN
2	O	168	GLN
2	O	172	ASN
2	O	208	ASN
2	O	263	GLN
2	O	328	HIS
2	O	411	GLN
3	P	88	HIS
3	P	141	GLN
3	P	216	ASN
3	P	224	GLN
4	Q	51	GLN
1	S	28	ASN
1	S	145	HIS
1	S	332	GLN
1	S	443	GLN
1	S	479	ASN
1	T	47	ASN
1	T	50	GLN
1	T	67	ASN
1	T	145	HIS
1	T	149	GLN
1	T	217	GLN

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Mol	Chain	Res	Type
1	T	265	HIS
1	T	304	HIS
1	T	351	GLN
1	T	387	GLN
1	U	174	GLN
1	U	220	GLN
1	U	225	HIS
1	U	262	ASN
1	U	387	GLN
1	U	434	GLN
1	U	454	HIS
1	U	479	ASN
2	V	24	HIS
2	V	52	GLN
2	V	57	ASN
2	V	118	HIS
2	V	168	GLN
2	V	263	GLN
2	V	293	GLN
2	V	308	GLN
2	V	328	HIS
2	V	365	GLN
2	W	27	GLN
2	W	208	ASN
2	W	221	GLN
2	W	385	GLN
2	X	27	GLN
2	X	52	GLN
2	X	118	HIS
2	X	263	GLN
2	X	328	HIS
2	X	455	HIS
3	Y	117	GLN
3	Y	122	HIS
3	Y	141	GLN
3	Y	167	ASN
3	Y	260	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	L	600	7	33,33,33	2.13	12 (36%)	45,52,52	2.12	14 (31%)
6	ANP	C	600	7	33,33,33	2.00	9 (27%)	45,52,52	2.19	11 (24%)
6	ANP	D	600	7	33,33,33	1.89	11 (33%)	45,52,52	2.01	12 (26%)
6	ANP	U	600	7	33,33,33	2.06	10 (30%)	45,52,52	2.34	11 (24%)
6	ANP	M	600	7	33,33,33	1.88	10 (30%)	45,52,52	2.36	10 (22%)
6	ANP	F	600	7	33,33,33	1.99	11 (33%)	45,52,52	2.07	13 (28%)
6	ANP	S	600	7	33,33,33	2.07	10 (30%)	45,52,52	2.13	11 (24%)
6	ANP	B	600	7	33,33,33	2.00	10 (30%)	45,52,52	2.18	13 (28%)
6	ANP	O	600	7	33,33,33	2.03	12 (36%)	45,52,52	2.12	14 (31%)
6	ANP	J	600	7	33,33,33	2.01	10 (30%)	45,52,52	2.12	12 (26%)
6	ANP	K	600	7	33,33,33	2.05	10 (30%)	45,52,52	2.25	13 (28%)
6	ANP	A	600	7	33,33,33	2.06	11 (33%)	45,52,52	2.07	12 (26%)
6	ANP	V	600	7	33,33,33	1.91	9 (27%)	45,52,52	2.27	15 (33%)
6	ANP	X	600	7	33,33,33	1.97	9 (27%)	45,52,52	2.21	14 (31%)
6	ANP	T	600	7	33,33,33	2.08	9 (27%)	45,52,52	2.11	12 (26%)

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	L	600	7	-	3/18/38/38	0/3/3/3
6	ANP	C	600	7	-	3/18/38/38	0/3/3/3
6	ANP	D	600	7	-	4/18/38/38	0/3/3/3
6	ANP	U	600	7	-	4/18/38/38	0/3/3/3
6	ANP	M	600	7	-	4/18/38/38	0/3/3/3
6	ANP	F	600	7	-	3/18/38/38	0/3/3/3
6	ANP	S	600	7	-	4/18/38/38	0/3/3/3
6	ANP	B	600	7	-	2/18/38/38	0/3/3/3
6	ANP	O	600	7	-	3/18/38/38	0/3/3/3
6	ANP	J	600	7	-	2/18/38/38	0/3/3/3
6	ANP	K	600	7	-	9/18/38/38	0/3/3/3
6	ANP	A	600	7	-	2/18/38/38	0/3/3/3
6	ANP	V	600	7	-	7/18/38/38	0/3/3/3
6	ANP	X	600	7	-	7/18/38/38	0/3/3/3
6	ANP	T	600	7	-	2/18/38/38	0/3/3/3

All (153) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	K	600	ANP	C5-C4	5.15	1.48	1.39
6	X	600	ANP	C5-C4	5.13	1.48	1.39
6	B	600	ANP	C5-C4	5.04	1.48	1.39
6	L	600	ANP	C5-C4	4.92	1.47	1.39
6	T	600	ANP	C5-C4	4.91	1.47	1.39
6	F	600	ANP	C5-C4	4.83	1.47	1.39
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	O	600	ANP	C5-C4	4.77	1.47	1.39
6	J	600	ANP	C5-C4	4.77	1.47	1.39
6	V	600	ANP	C5-C4	4.74	1.47	1.39
6	D	600	ANP	C5-C4	4.72	1.47	1.39
6	U	600	ANP	C5-C4	4.71	1.47	1.39
6	T	600	ANP	PG-N3B	4.64	1.75	1.63
6	C	600	ANP	C5-C4	4.63	1.47	1.39
6	S	600	ANP	C5-C4	4.62	1.47	1.39
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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	A	600	ANP	C5-C4	4.40	1.46	1.39
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	M	600	ANP	C5-C4	4.29	1.46	1.39
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	T	600	ANP	PG-O1G	4.18	1.52	1.46
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
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	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	3.78	1.51	1.46
6	K	600	ANP	PG-N3B	3.62	1.72	1.63
6	S	600	ANP	PG-O1G	3.62	1.51	1.46
6	U	600	ANP	PG-O1G	3.61	1.51	1.46
6	M	600	ANP	PB-O1B	3.60	1.51	1.46
6	A	600	ANP	PG-O1G	3.59	1.51	1.46
6	K	600	ANP	PB-O3A	3.52	1.63	1.59
6	M	600	ANP	PG-O1G	3.48	1.51	1.46
6	B	600	ANP	PG-O1G	3.48	1.51	1.46
6	M	600	ANP	PG-N3B	3.46	1.72	1.63
6	K	600	ANP	PG-O1G	3.46	1.51	1.46
6	C	600	ANP	PB-O1B	3.44	1.51	1.46
6	V	600	ANP	PB-O1B	3.42	1.51	1.46
6	T	600	ANP	PB-O1B	3.42	1.51	1.46
6	K	600	ANP	PB-O1B	3.40	1.51	1.46
6	J	600	ANP	PG-O1G	3.36	1.51	1.46
6	O	600	ANP	PA-O3A	3.35	1.63	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	600	ANP	PG-O1G	3.35	1.51	1.46
6	D	600	ANP	PG-O1G	3.31	1.51	1.46
6	O	600	ANP	PG-O1G	3.31	1.51	1.46
6	U	600	ANP	PA-O3A	3.29	1.63	1.59
6	F	600	ANP	PG-O1G	3.28	1.51	1.46
6	V	600	ANP	PG-O1G	3.26	1.51	1.46
6	U	600	ANP	PB-O1B	3.26	1.51	1.46
6	L	600	ANP	PB-O1B	3.23	1.51	1.46
6	X	600	ANP	PB-O1B	3.17	1.51	1.46
6	F	600	ANP	PB-O1B	3.12	1.50	1.46
6	S	600	ANP	PB-O1B	3.11	1.50	1.46
6	L	600	ANP	PG-O1G	3.09	1.50	1.46
6	J	600	ANP	C5-C6	3.09	1.49	1.41
6	L	600	ANP	PB-O3A	3.06	1.62	1.59
6	M	600	ANP	C5-N7	-3.05	1.33	1.39
6	O	600	ANP	PB-O3A	3.05	1.62	1.59
6	A	600	ANP	PB-O3A	3.02	1.62	1.59
6	X	600	ANP	PG-O1G	2.97	1.50	1.46
6	J	600	ANP	PA-O3A	2.95	1.62	1.59
6	B	600	ANP	PB-O1B	2.90	1.50	1.46
6	K	600	ANP	C5-C6	2.85	1.48	1.41
6	U	600	ANP	C5-N7	-2.84	1.33	1.39
6	V	600	ANP	C5-C6	2.83	1.48	1.41
6	J	600	ANP	PB-O1B	2.83	1.50	1.46
6	X	600	ANP	C5-C6	2.82	1.48	1.41
6	F	600	ANP	PB-O3A	2.81	1.62	1.59
6	S	600	ANP	PA-O3A	2.80	1.62	1.59
6	J	600	ANP	PB-O3A	2.78	1.62	1.59
6	B	600	ANP	C5-C6	2.77	1.48	1.41
6	F	600	ANP	C5-N7	-2.75	1.34	1.39
6	T	600	ANP	C5-C6	2.74	1.48	1.41
6	C	600	ANP	C5-C6	2.73	1.48	1.41
6	O	600	ANP	PB-O1B	2.71	1.50	1.46
6	L	600	ANP	PG-O2G	-2.71	1.49	1.56
6	A	600	ANP	C5-N7	-2.70	1.34	1.39
6	S	600	ANP	C5-N7	-2.69	1.34	1.39
6	C	600	ANP	C5-N7	-2.69	1.34	1.39
6	O	600	ANP	C5-C6	2.66	1.48	1.41
6	A	600	ANP	PG-O2G	-2.66	1.49	1.56
6	S	600	ANP	PB-O3A	2.62	1.62	1.59
6	L	600	ANP	C5-C6	2.60	1.48	1.41
6	B	600	ANP	C8-N7	2.59	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	U	600	ANP	PB-O3A	2.58	1.62	1.59
6	K	600	ANP	C8-N7	2.56	1.36	1.31
6	O	600	ANP	C8-N7	2.55	1.36	1.31
6	B	600	ANP	PA-O3A	2.54	1.62	1.59
6	D	600	ANP	PB-O1B	2.54	1.50	1.46
6	D	600	ANP	C5-C6	2.54	1.48	1.41
6	L	600	ANP	PA-O3A	2.54	1.62	1.59
6	U	600	ANP	C5-C6	2.52	1.48	1.41
6	V	600	ANP	C8-N7	2.49	1.36	1.31
6	A	600	ANP	C5-C6	2.49	1.47	1.41
6	K	600	ANP	PA-O3A	2.48	1.62	1.59
6	K	600	ANP	C5-N7	-2.48	1.34	1.39
6	J	600	ANP	C8-N7	2.46	1.36	1.31
6	L	600	ANP	C8-N7	2.45	1.36	1.31
6	S	600	ANP	C5-C6	2.44	1.47	1.41
6	O	600	ANP	C5-N7	-2.44	1.34	1.39
6	T	600	ANP	C8-N7	2.39	1.36	1.31
6	X	600	ANP	C8-N7	2.39	1.36	1.31
6	D	600	ANP	C5-N7	-2.33	1.34	1.39
6	L	600	ANP	PG-O3G	-2.32	1.50	1.56
6	D	600	ANP	C8-N7	2.32	1.36	1.31
6	V	600	ANP	C5-N7	-2.30	1.34	1.39
6	U	600	ANP	C8-N7	2.30	1.36	1.31
6	L	600	ANP	C5-N7	-2.30	1.34	1.39
6	T	600	ANP	PB-O3A	2.29	1.61	1.59
6	D	600	ANP	PB-O2B	-2.28	1.50	1.56
6	F	600	ANP	C5-C6	2.28	1.47	1.41
6	B	600	ANP	C5-N7	-2.26	1.35	1.39
6	X	600	ANP	C5-N7	-2.25	1.35	1.39
6	M	600	ANP	C5-C6	2.23	1.47	1.41
6	F	600	ANP	PA-O3A	2.22	1.61	1.59
6	M	600	ANP	C8-N7	2.22	1.35	1.31
6	B	600	ANP	PB-O3A	2.19	1.61	1.59
6	X	600	ANP	PB-O3A	2.18	1.61	1.59
6	A	600	ANP	C8-N7	2.16	1.35	1.31
6	T	600	ANP	C5-N7	-2.16	1.35	1.39
6	A	600	ANP	C4-N9	-2.15	1.33	1.37
6	O	600	ANP	C4-N9	-2.15	1.33	1.37
6	J	600	ANP	C4-N9	-2.15	1.33	1.37
6	S	600	ANP	C8-N7	2.14	1.35	1.31
6	F	600	ANP	C8-N7	2.13	1.35	1.31
6	C	600	ANP	PG-O3G	-2.13	1.51	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	600	ANP	PG-O2G	-2.10	1.51	1.56
6	F	600	ANP	PG-O3G	-2.08	1.51	1.56
6	D	600	ANP	PG-O3G	-2.06	1.51	1.56
6	D	600	ANP	C4-N9	-2.06	1.33	1.37
6	O	600	ANP	PG-O2G	-2.03	1.51	1.56
6	M	600	ANP	PG-O2G	-2.03	1.51	1.56
6	M	600	ANP	PG-O3G	-2.02	1.51	1.56
6	V	600	ANP	PB-O2B	-2.01	1.51	1.56

All (187) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	600	ANP	O1G-PG-N3B	-7.65	100.51	111.77
6	U	600	ANP	C5-C4-N3	-6.51	117.75	126.72
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	M	600	ANP	C5-C4-N3	-6.31	118.02	126.72
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	S	600	ANP	C5-C4-N3	-6.19	118.19	126.72
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	K	600	ANP	C5-C4-N3	-6.06	118.38	126.72
6	B	600	ANP	C5-C4-N3	-5.94	118.54	126.72
6	C	600	ANP	C5-C4-N3	-5.89	118.61	126.72
6	C	600	ANP	O2B-PB-O1B	5.87	122.45	109.87
6	V	600	ANP	C5-C4-N3	-5.86	118.65	126.72
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	L	600	ANP	C5-C4-N3	-5.77	118.78	126.72
6	M	600	ANP	O2B-PB-O1B	5.70	122.10	109.87
6	U	600	ANP	O1G-PG-N3B	-5.69	103.39	111.77
6	X	600	ANP	C5-C4-N3	-5.68	118.90	126.72
6	A	600	ANP	C5-C4-N3	-5.68	118.90	126.72
6	J	600	ANP	C5-C4-N3	-5.53	119.10	126.72
6	D	600	ANP	C5-C4-N3	-5.52	119.12	126.72
6	T	600	ANP	C5-C4-N3	-5.46	119.20	126.72
6	O	600	ANP	C5-C4-N3	-5.32	119.40	126.72
6	C	600	ANP	O1G-PG-N3B	-5.28	103.99	111.77
6	F	600	ANP	C5-C4-N3	-5.23	119.52	126.72
6	U	600	ANP	O2B-PB-O1B	5.18	120.98	109.87
6	U	600	ANP	N3-C4-N9	5.18	135.98	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	O	600	ANP	O1G-PG-N3B	-5.15	104.18	111.77
6	S	600	ANP	N3-C4-N9	5.05	135.76	127.17
6	C	600	ANP	N3-C4-N9	4.85	135.42	127.17
6	M	600	ANP	N3-C4-N9	4.84	135.40	127.17
6	L	600	ANP	O2B-PB-O1B	4.70	119.96	109.87
6	O	600	ANP	O1B-PB-N3B	-4.68	104.88	111.77
6	B	600	ANP	N3-C4-N9	4.65	135.07	127.17
6	K	600	ANP	N3-C4-N9	4.62	135.02	127.17
6	D	600	ANP	N3-C4-N9	4.60	134.99	127.17
6	V	600	ANP	O2B-PB-O1B	4.59	119.72	109.87
6	L	600	ANP	N3-C4-N9	4.56	134.93	127.17
6	V	600	ANP	N3-C4-N9	4.56	134.92	127.17
6	X	600	ANP	N3-C4-N9	4.54	134.89	127.17
6	S	600	ANP	O1G-PG-N3B	-4.54	105.09	111.77
6	T	600	ANP	N3-C4-N9	4.53	134.88	127.17
6	F	600	ANP	N3-C4-N9	4.49	134.80	127.17
6	L	600	ANP	O1G-PG-N3B	-4.49	105.16	111.77
6	F	600	ANP	O2B-PB-O1B	4.48	119.47	109.87
6	J	600	ANP	O2B-PB-O1B	4.44	119.38	109.87
6	U	600	ANP	O1B-PB-N3B	-4.42	105.26	111.77
6	X	600	ANP	O2B-PB-O1B	4.40	119.30	109.87
6	B	600	ANP	O2B-PB-O1B	4.40	119.30	109.87
6	A	600	ANP	N3-C4-N9	4.33	134.53	127.17
6	X	600	ANP	O1B-PB-N3B	-4.33	105.40	111.77
6	A	600	ANP	O2B-PB-O1B	4.28	119.04	109.87
6	O	600	ANP	N3-C4-N9	4.21	134.32	127.17
6	J	600	ANP	N3-C4-N9	4.16	134.25	127.17
6	D	600	ANP	O1G-PG-N3B	-4.13	105.69	111.77
6	T	600	ANP	O1B-PB-N3B	-4.10	105.73	111.77
6	O	600	ANP	O2B-PB-O1B	4.04	118.53	109.87
6	L	600	ANP	O1B-PB-N3B	-3.92	105.99	111.77
6	U	600	ANP	C2-N3-C4	3.89	121.34	111.83
6	T	600	ANP	O2B-PB-O1B	3.89	118.20	109.87
6	B	600	ANP	C2-N3-C4	3.88	121.32	111.83
6	S	600	ANP	C2-N3-C4	3.87	121.28	111.83
6	K	600	ANP	C2-N3-C4	3.80	121.12	111.83
6	J	600	ANP	C2-N3-C4	3.80	121.12	111.83
6	V	600	ANP	C2-N3-C4	3.79	121.09	111.83
6	C	600	ANP	C2-N3-C4	3.79	121.08	111.83
6	B	600	ANP	N3-C2-N1	-3.75	122.91	128.58
6	S	600	ANP	O2B-PB-O1B	3.73	117.86	109.87
6	D	600	ANP	C2-N3-C4	3.69	120.84	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	T	600	ANP	C2-N3-C4	3.69	120.84	111.83
6	D	600	ANP	N3-C2-N1	-3.66	123.05	128.58
6	X	600	ANP	C2-N3-C4	3.66	120.76	111.83
6	L	600	ANP	C2-N3-C4	3.65	120.75	111.83
6	V	600	ANP	C4-C5-N7	-3.65	106.41	110.58
6	K	600	ANP	O2B-PB-O1B	3.65	117.69	109.87
6	M	600	ANP	C2-N3-C4	3.61	120.64	111.83
6	U	600	ANP	N3-C2-N1	-3.59	123.15	128.58
6	U	600	ANP	C4-C5-N7	-3.56	106.51	110.58
6	A	600	ANP	C2-N3-C4	3.56	120.53	111.83
6	D	600	ANP	O2B-PB-O1B	3.55	117.48	109.87
6	K	600	ANP	O1B-PB-N3B	-3.54	106.56	111.77
6	O	600	ANP	C2-N3-C4	3.54	120.47	111.83
6	T	600	ANP	N3-C2-N1	-3.53	123.23	128.58
6	J	600	ANP	C4-C5-N7	-3.53	106.55	110.58
6	D	600	ANP	O2G-PG-O3G	3.53	117.06	107.59
6	K	600	ANP	C4-C5-N7	-3.50	106.58	110.58
6	M	600	ANP	C4-C5-N7	-3.49	106.59	110.58
6	C	600	ANP	N3-C2-N1	-3.45	123.36	128.58
6	S	600	ANP	N3-C2-N1	-3.44	123.37	128.58
6	J	600	ANP	N3-C2-N1	-3.43	123.38	128.58
6	F	600	ANP	C2-N3-C4	3.43	120.21	111.83
6	F	600	ANP	O1B-PB-N3B	-3.42	106.73	111.77
6	B	600	ANP	O4'-C1'-N9	3.41	114.64	108.09
6	F	600	ANP	N3-C2-N1	-3.41	123.42	128.58
6	L	600	ANP	N3-C2-N1	-3.40	123.44	128.58
6	V	600	ANP	O1B-PB-N3B	-3.39	106.78	111.77
6	O	600	ANP	C4-C5-N7	-3.36	106.74	110.58
6	V	600	ANP	N3-C2-N1	-3.33	123.53	128.58
6	A	600	ANP	C4-C5-N7	-3.33	106.78	110.58
6	X	600	ANP	N3-C2-N1	-3.32	123.56	128.58
6	L	600	ANP	C4-C5-N7	-3.32	106.79	110.58
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	K	600	ANP	N3-C2-N1	-3.31	123.57	128.58
6	O	600	ANP	N3-C2-N1	-3.31	123.58	128.58
6	B	600	ANP	C4-C5-N7	-3.28	106.83	110.58
6	A	600	ANP	N3-C2-N1	-3.24	123.67	128.58
6	X	600	ANP	C4-C5-N7	-3.20	106.92	110.58
6	S	600	ANP	O2G-PG-O3G	3.15	116.06	107.59
6	C	600	ANP	C4-C5-N7	-3.15	106.98	110.58
6	T	600	ANP	C4-C5-N7	-3.12	107.02	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	S	600	ANP	C4-C5-N7	-3.06	107.08	110.58
6	D	600	ANP	C4-C5-N7	-3.03	107.12	110.58
6	K	600	ANP	O2B-PB-O3A	2.99	114.61	104.64
6	X	600	ANP	O2G-PG-O3G	2.92	115.43	107.59
6	D	600	ANP	C4-N9-C8	2.88	108.76	105.74
6	F	600	ANP	O2G-PG-O3G	2.87	115.30	107.59
6	B	600	ANP	O2G-PG-O3G	2.87	115.29	107.59
6	O	600	ANP	C4-N9-C8	2.86	108.74	105.74
6	M	600	ANP	N3-C2-N1	-2.84	124.28	128.58
6	T	600	ANP	C4-N9-C8	2.81	108.69	105.74
6	V	600	ANP	O4'-C1'-N9	2.80	113.48	108.09
6	C	600	ANP	O2G-PG-O3G	2.79	115.08	107.59
6	V	600	ANP	C5-N7-C8	2.77	107.81	103.45
6	U	600	ANP	C5-N7-C8	2.77	107.80	103.45
6	U	600	ANP	O2G-PG-O3G	2.76	115.00	107.59
6	V	600	ANP	O2G-PG-O3G	2.68	114.80	107.59
6	M	600	ANP	C5-N7-C8	2.66	107.64	103.45
6	V	600	ANP	C4-N9-C8	2.63	108.50	105.74
6	J	600	ANP	C4-N9-C8	2.54	108.41	105.74
6	S	600	ANP	C5-N7-C8	2.50	107.38	103.45
6	K	600	ANP	O2G-PG-O3G	2.49	114.27	107.59
6	T	600	ANP	O2G-PG-O3G	2.47	114.23	107.59
6	O	600	ANP	C5-N7-C8	2.44	107.28	103.45
6	C	600	ANP	C4-N9-C8	2.44	108.30	105.74
6	K	600	ANP	C5-N7-C8	2.40	107.22	103.45
6	F	600	ANP	O2B-PB-O3A	2.39	112.63	104.64
6	J	600	ANP	C6-C5-N7	2.38	136.69	132.09
6	C	600	ANP	C5-N7-C8	2.37	107.17	103.45
6	T	600	ANP	C5-N7-C8	2.36	107.17	103.45
6	L	600	ANP	C4-N9-C8	2.35	108.20	105.74
6	V	600	ANP	C6-C5-N7	2.33	136.58	132.09
6	L	600	ANP	O2G-PG-O3G	2.33	113.84	107.59
6	L	600	ANP	O4'-C1'-N9	2.32	112.55	108.09
6	F	600	ANP	C4-C5-N7	-2.31	107.94	110.58
6	S	600	ANP	C4-N9-C8	2.31	108.16	105.74
6	J	600	ANP	O2G-PG-O3G	2.30	113.77	107.59
6	J	600	ANP	C5-N7-C8	2.30	107.06	103.45
6	L	600	ANP	C5-N7-C8	2.29	107.05	103.45
6	C	600	ANP	O1B-PB-N3B	-2.29	108.40	111.77
6	X	600	ANP	C3'-C2'-C1'	2.27	105.75	101.46
6	B	600	ANP	C5-N7-C8	2.27	107.02	103.45
6	X	600	ANP	C4-N9-C8	2.24	108.09	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	X	600	ANP	C5-N7-C8	2.23	106.95	103.45
6	A	600	ANP	O1B-PB-N3B	-2.21	108.52	111.77
6	D	600	ANP	C2-N1-C6	2.21	122.35	118.73
6	A	600	ANP	C5-N7-C8	2.20	106.91	103.45
6	V	600	ANP	N9-C8-N7	-2.18	110.85	113.94
6	D	600	ANP	C5-N7-C8	2.17	106.86	103.45
6	U	600	ANP	C4-N9-C8	2.16	108.01	105.74
6	B	600	ANP	C6-C5-N7	2.16	136.25	132.09
6	O	600	ANP	O2G-PG-O3G	2.15	113.37	107.59
6	F	600	ANP	C4-N9-C8	2.14	107.99	105.74
6	M	600	ANP	C4-N9-C8	2.12	107.97	105.74
6	A	600	ANP	C6-C5-N7	2.12	136.18	132.09
6	T	600	ANP	C6-C5-N7	2.12	136.18	132.09
6	A	600	ANP	C4-N9-C8	2.11	107.95	105.74
6	O	600	ANP	N9-C8-N7	-2.10	110.96	113.94
6	O	600	ANP	C3'-C2'-C1'	2.10	105.44	101.46
6	L	600	ANP	O3A-PB-N3B	2.10	112.42	106.59
6	L	600	ANP	C6-C5-N7	2.09	136.12	132.09
6	B	600	ANP	C2-N1-C6	2.09	122.17	118.73
6	V	600	ANP	C3'-C2'-C1'	2.07	105.38	101.46
6	X	600	ANP	C2-N1-C6	2.06	122.11	118.73
6	D	600	ANP	C6-C5-N7	2.06	136.06	132.09
6	O	600	ANP	C6-C5-N7	2.05	136.04	132.09
6	A	600	ANP	C2-N1-C6	2.05	122.09	118.73
6	F	600	ANP	C2-N1-C6	2.04	122.08	118.73
6	B	600	ANP	C4-N9-C8	2.04	107.88	105.74
6	K	600	ANP	O3A-PA-O1A	-2.03	104.60	110.70
6	X	600	ANP	C6-C5-N7	2.02	135.99	132.09
6	K	600	ANP	C3'-C2'-C1'	2.01	105.27	101.46
6	J	600	ANP	C2-N1-C6	2.01	122.03	118.73
6	F	600	ANP	N6-C6-N1	2.01	122.85	118.38

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

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Mol	Chain	Res	Type	Atoms
6	D	600	ANP	PB-N3B-PG-O1G
6	D	600	ANP	PG-N3B-PB-O1B
6	D	600	ANP	PG-N3B-PB-O3A
6	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	K	600	ANP	C5'-O5'-PA-O3A
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	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-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	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-O2B
6	X	600	ANP	PG-N3B-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	C5'-O5'-PA-O3A
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	O4'-C4'-C5'-O5'

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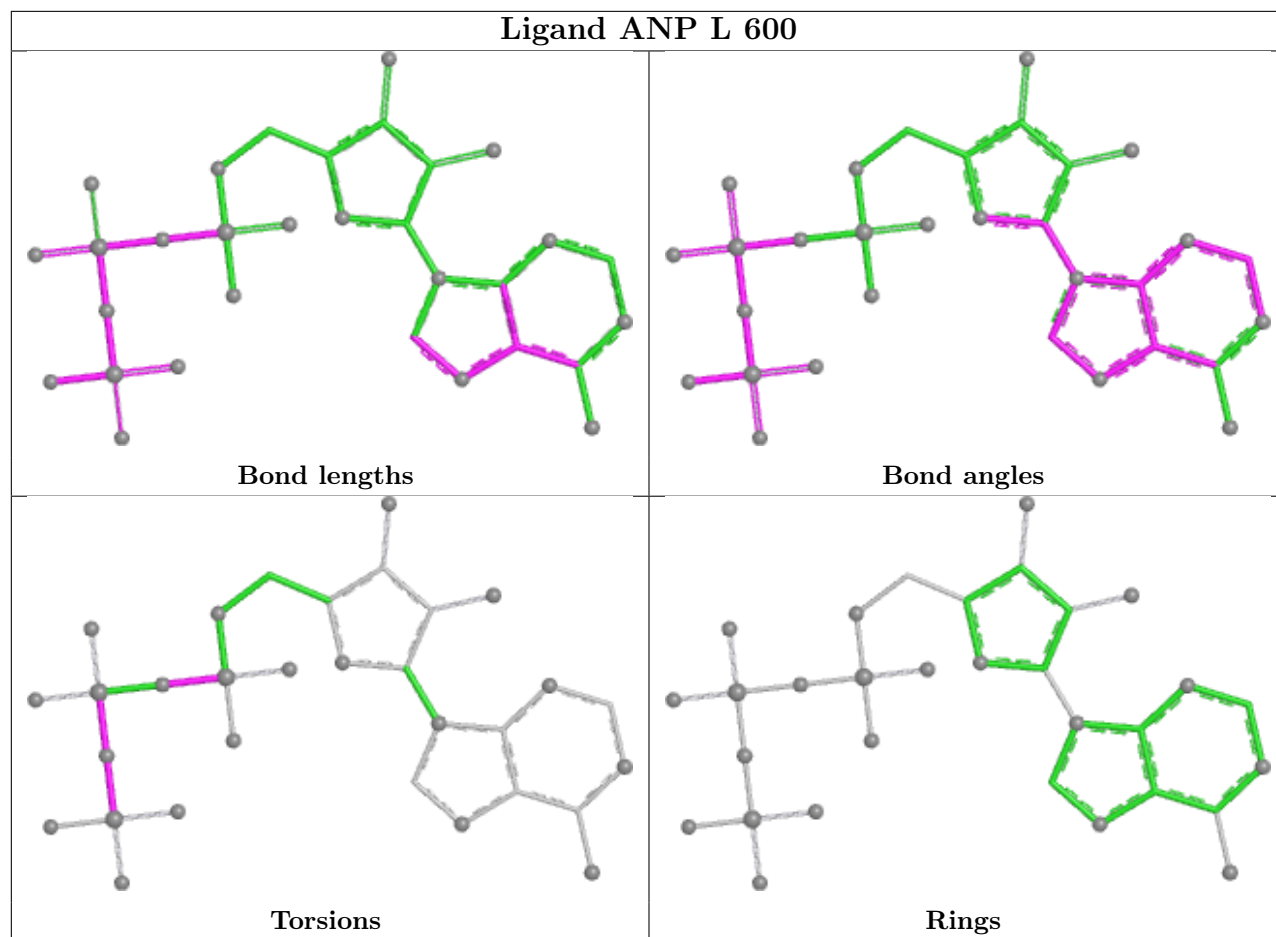
Mol	Chain	Res	Type	Atoms
6	K	600	ANP	C5'-O5'-PA-O1A
6	K	600	ANP	PB-O3A-PA-O2A
6	K	600	ANP	C3'-C4'-C5'-O5'
6	D	600	ANP	PA-O3A-PB-O2B
6	M	600	ANP	O4'-C4'-C5'-O5'
6	C	600	ANP	PB-O3A-PA-O1A
6	S	600	ANP	PA-O3A-PB-O1B
6	U	600	ANP	PA-O3A-PB-O1B
6	V	600	ANP	PA-O3A-PB-O1B
6	M	600	ANP	C3'-C4'-C5'-O5'
6	L	600	ANP	PB-O3A-PA-O1A

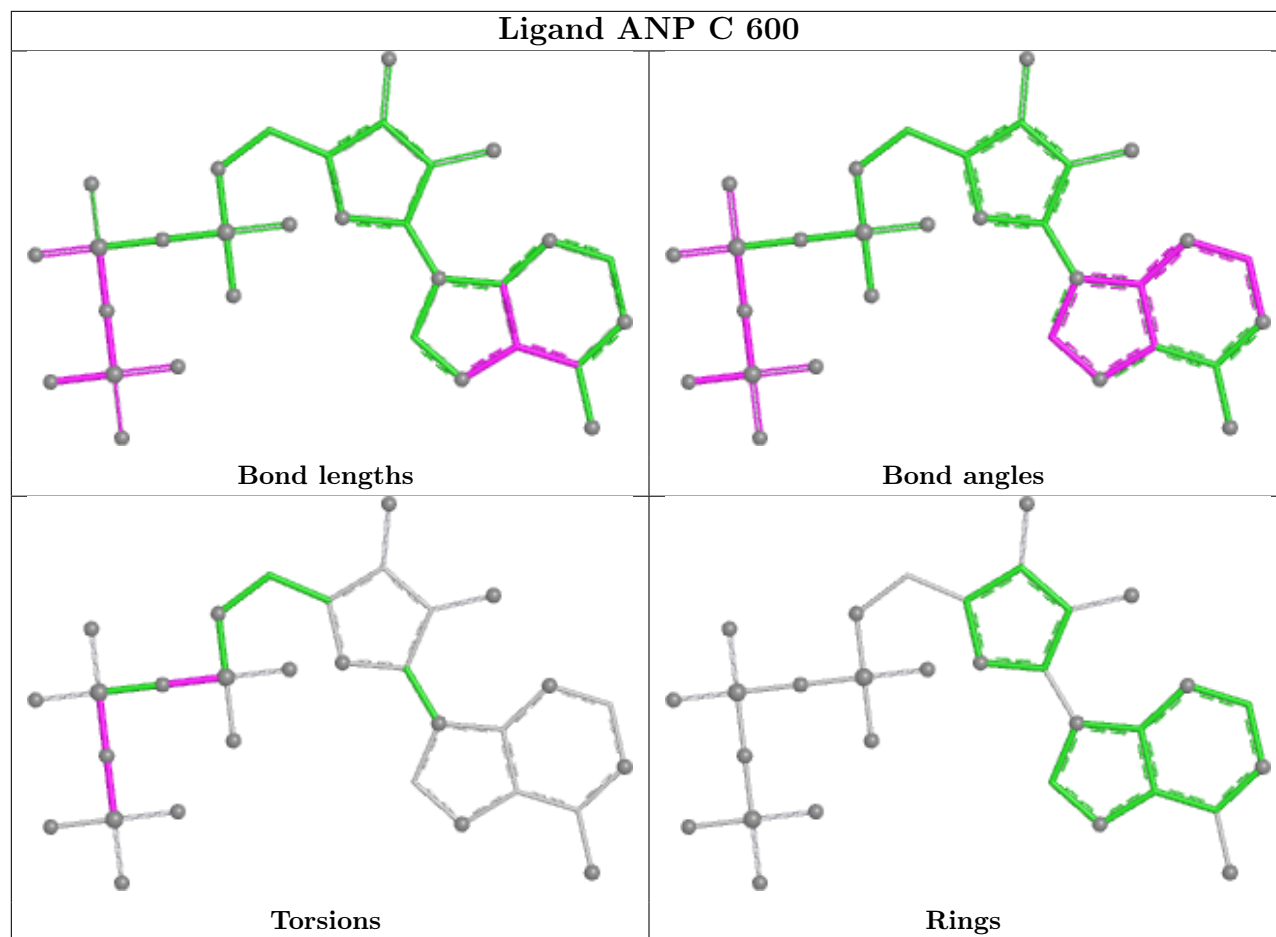
There are no ring outliers.

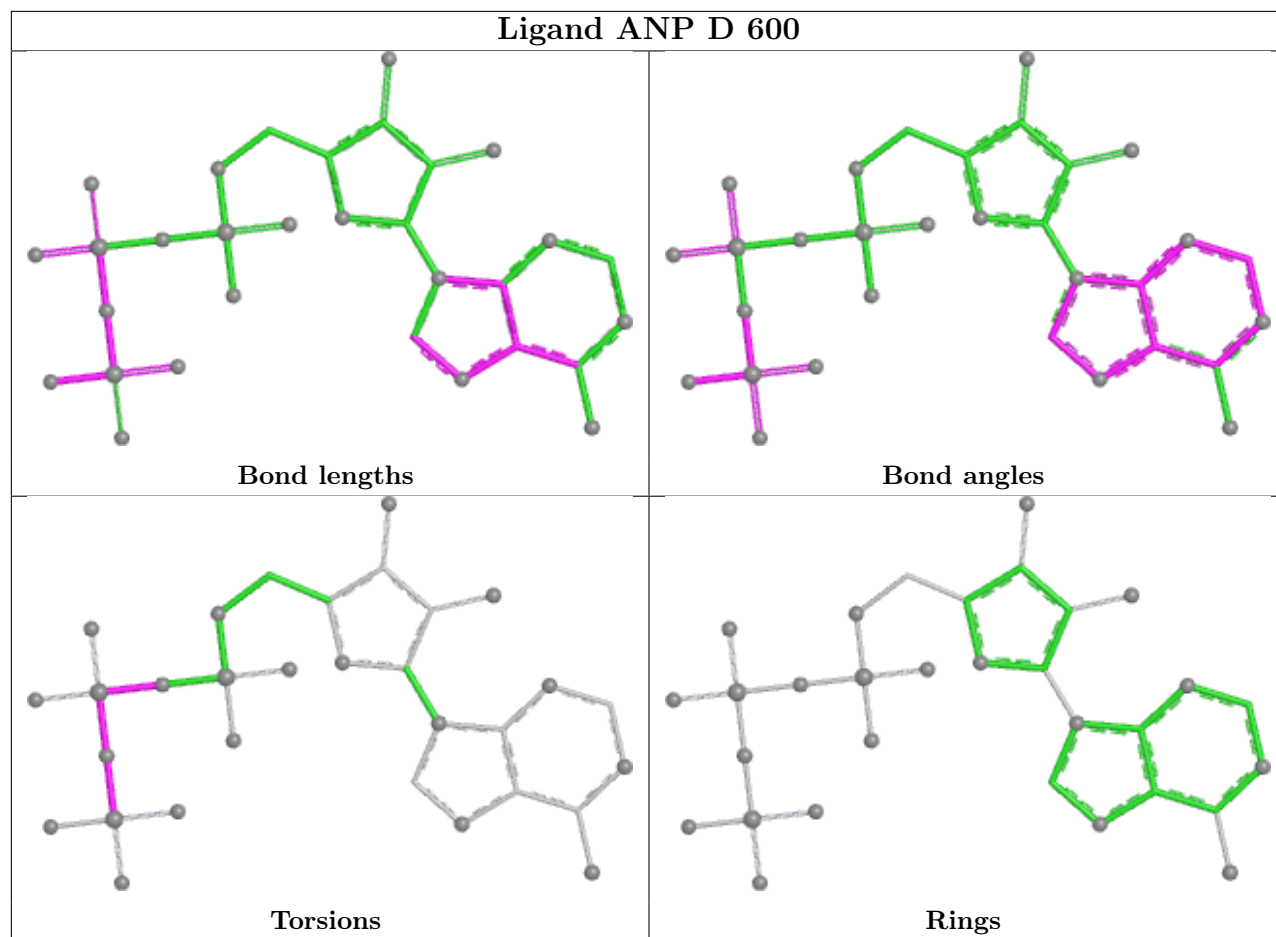
12 monomers are involved in 25 short contacts:

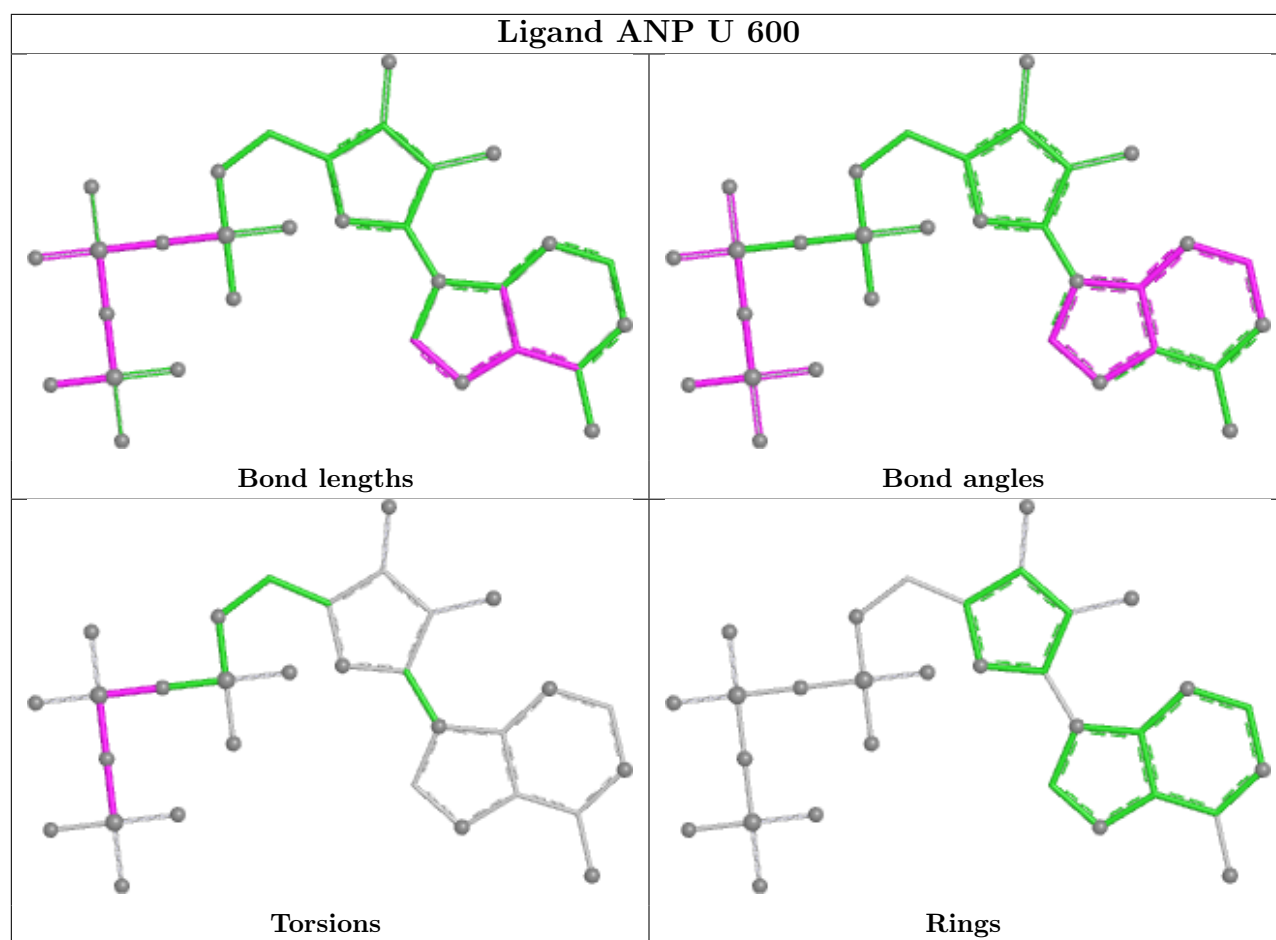
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L	600	ANP	1	0
6	U	600	ANP	1	0
6	M	600	ANP	4	0
6	F	600	ANP	1	0
6	B	600	ANP	4	0
6	O	600	ANP	3	0
6	J	600	ANP	1	0
6	K	600	ANP	3	0
6	A	600	ANP	1	0
6	V	600	ANP	1	0
6	X	600	ANP	4	0
6	T	600	ANP	1	0

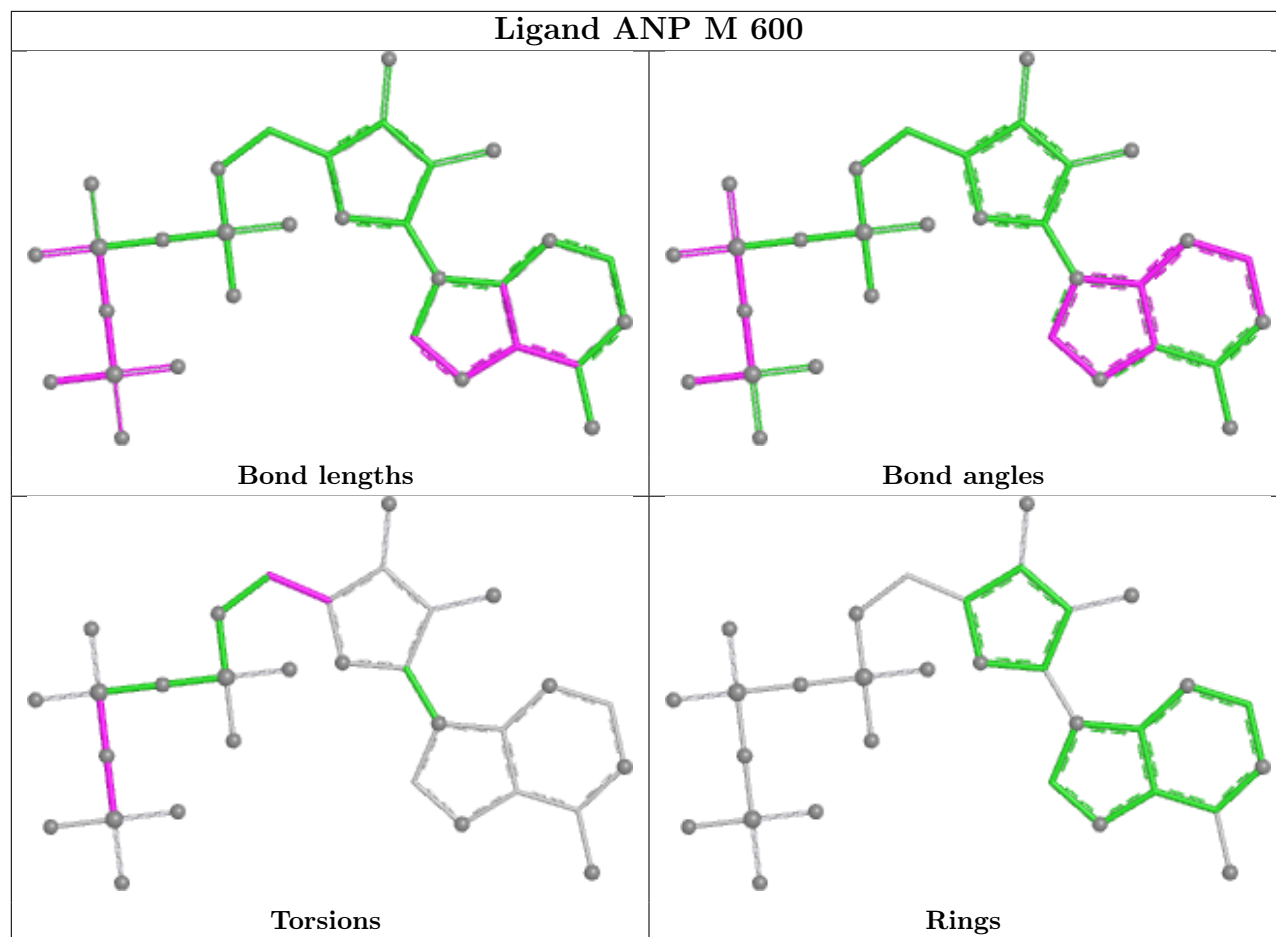
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

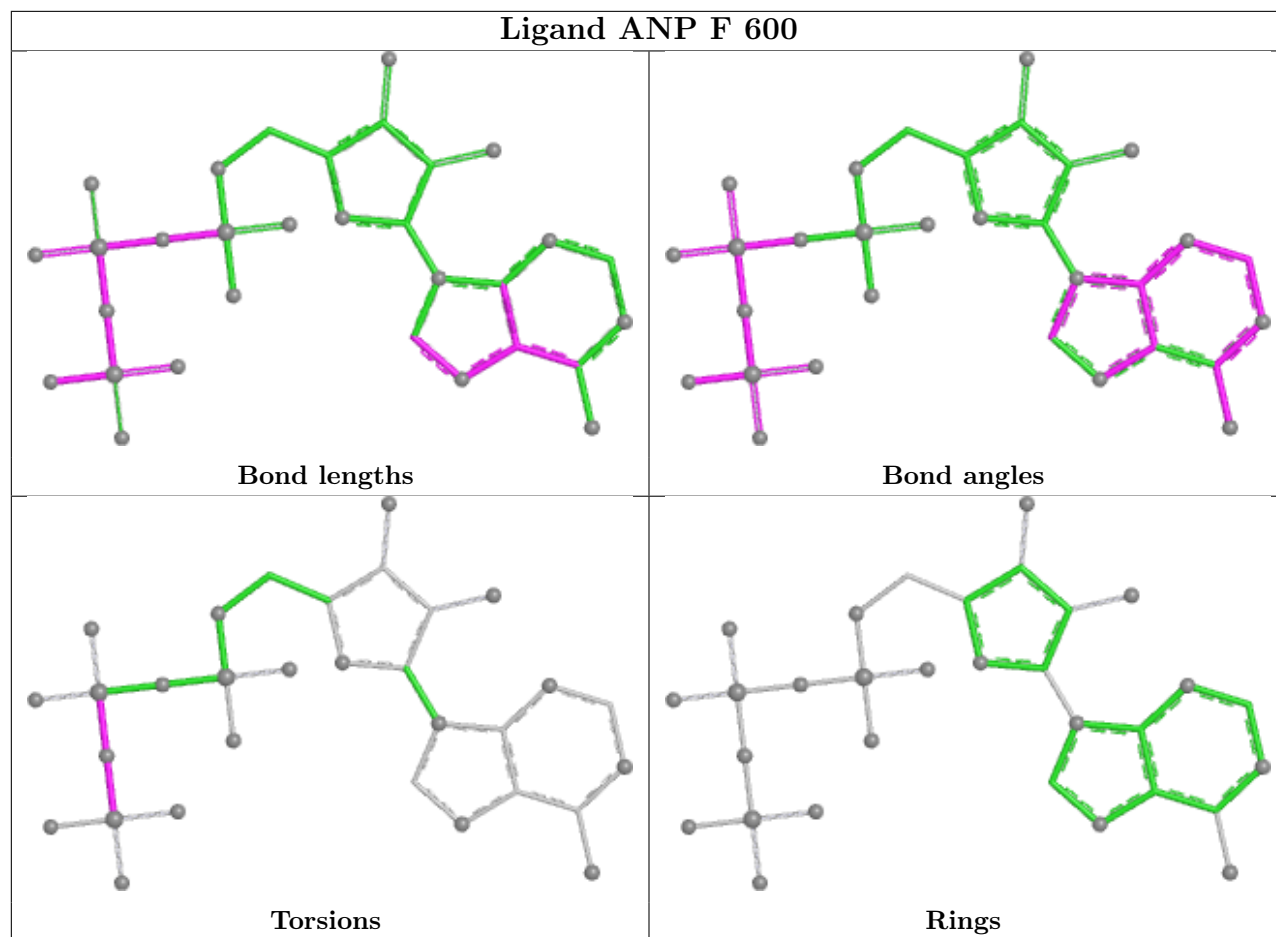


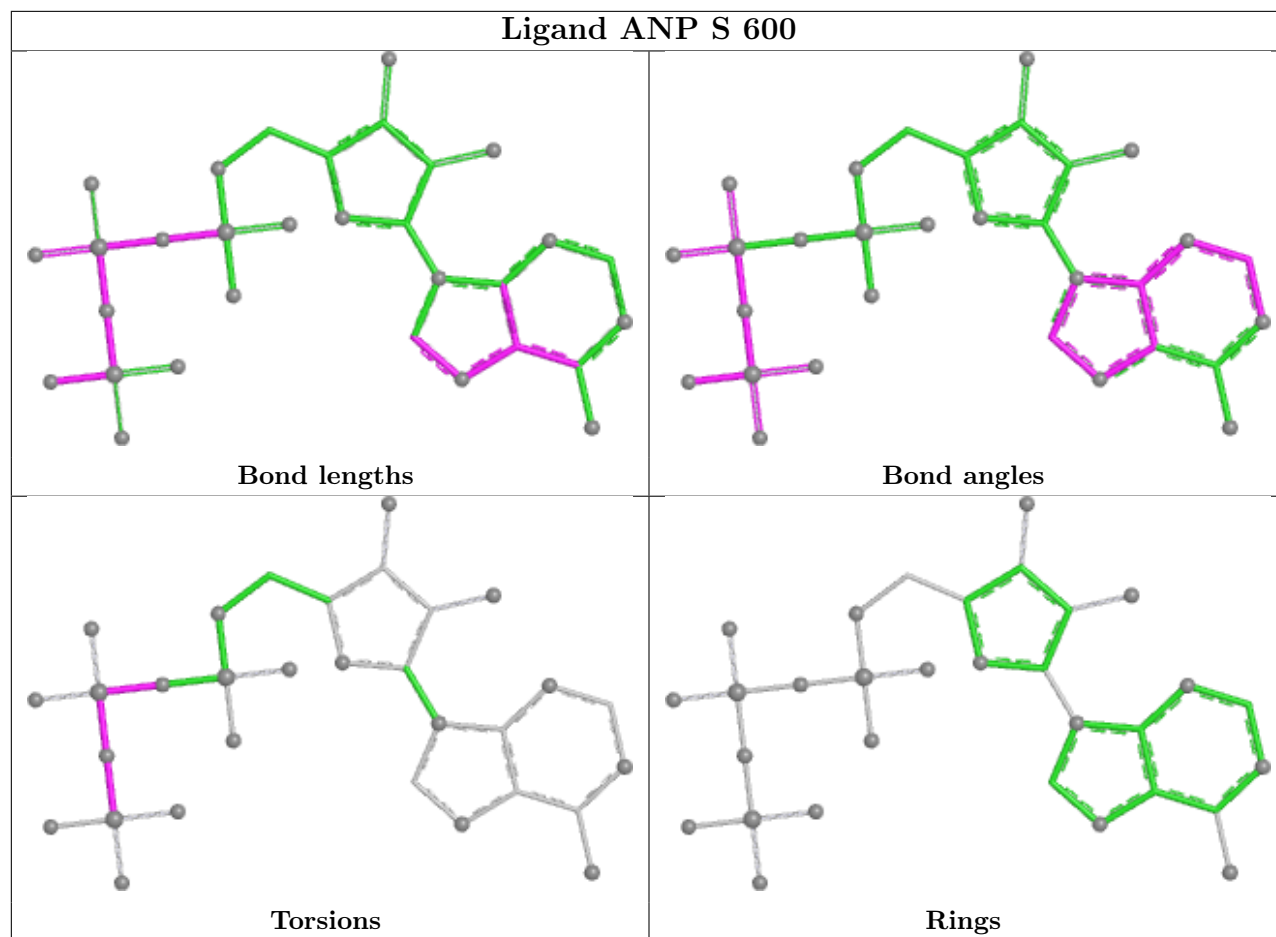


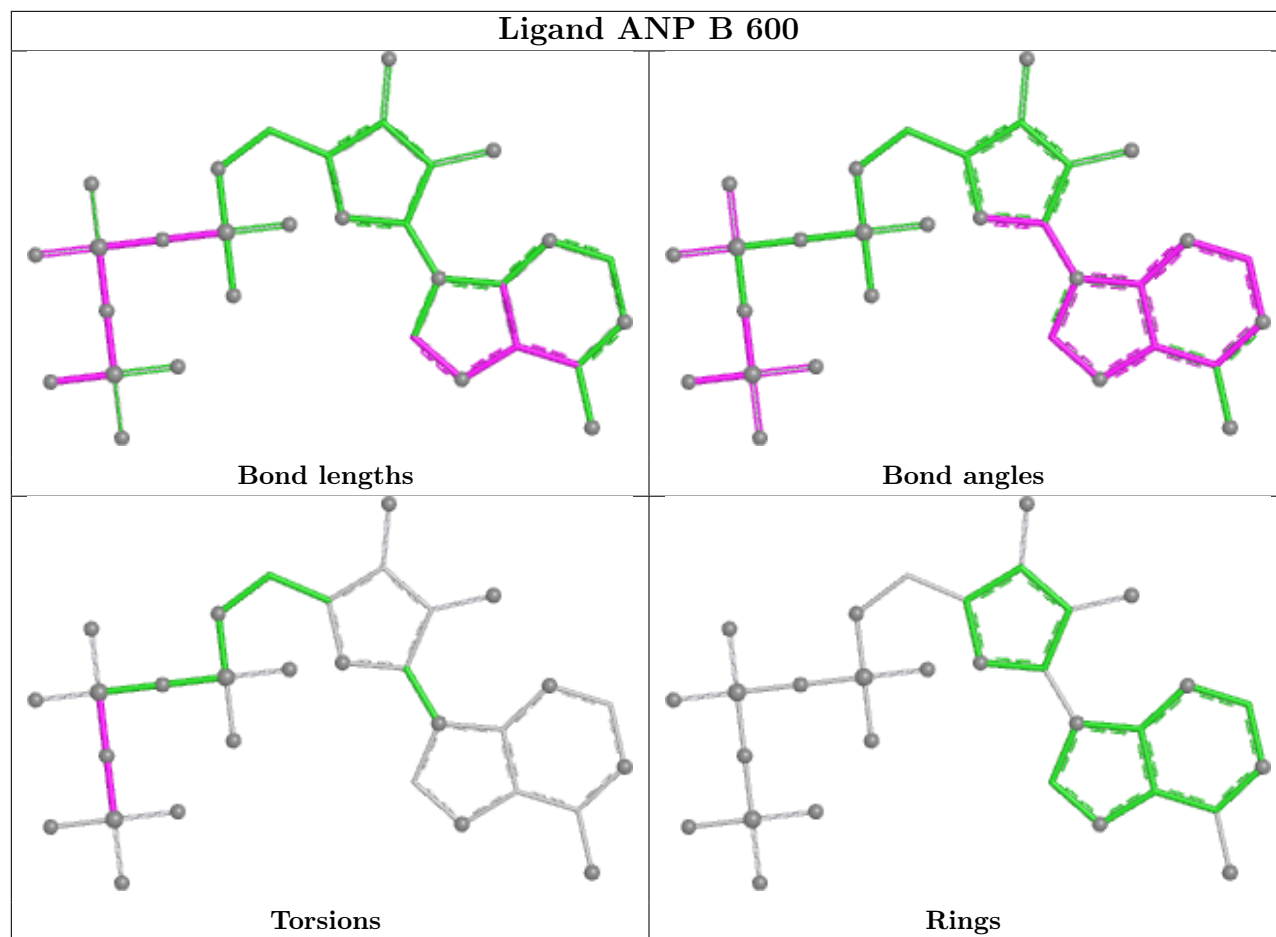


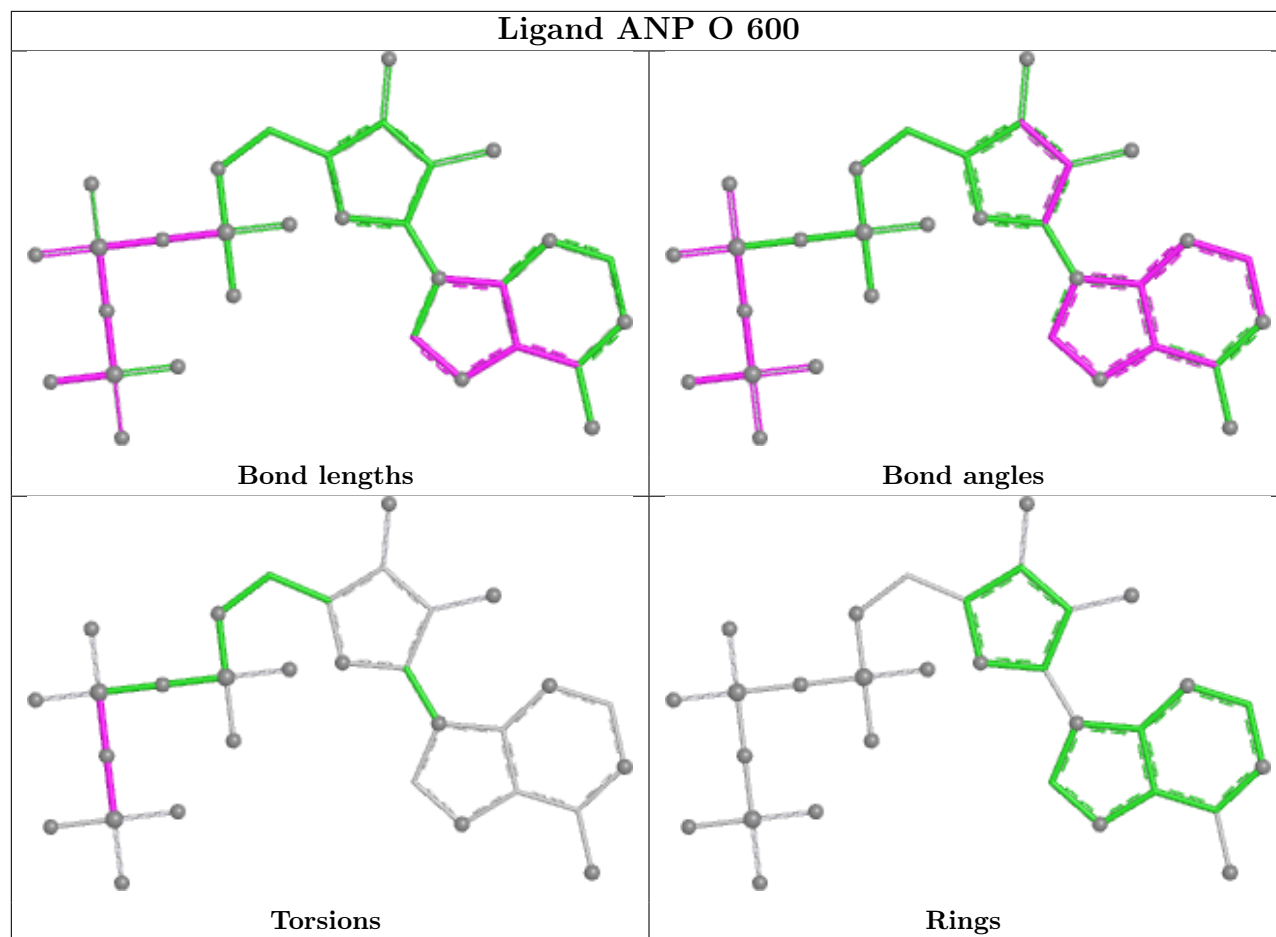




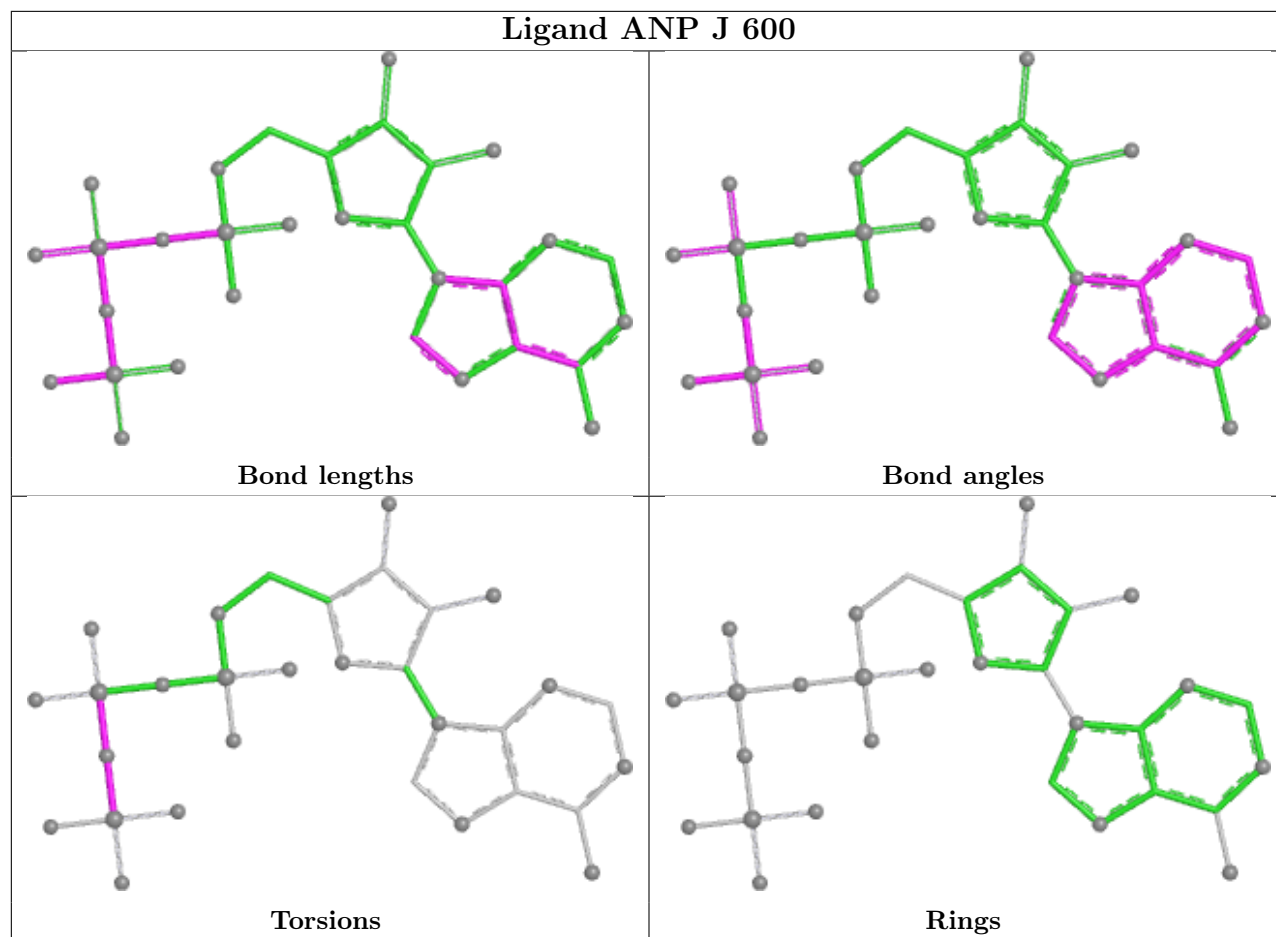


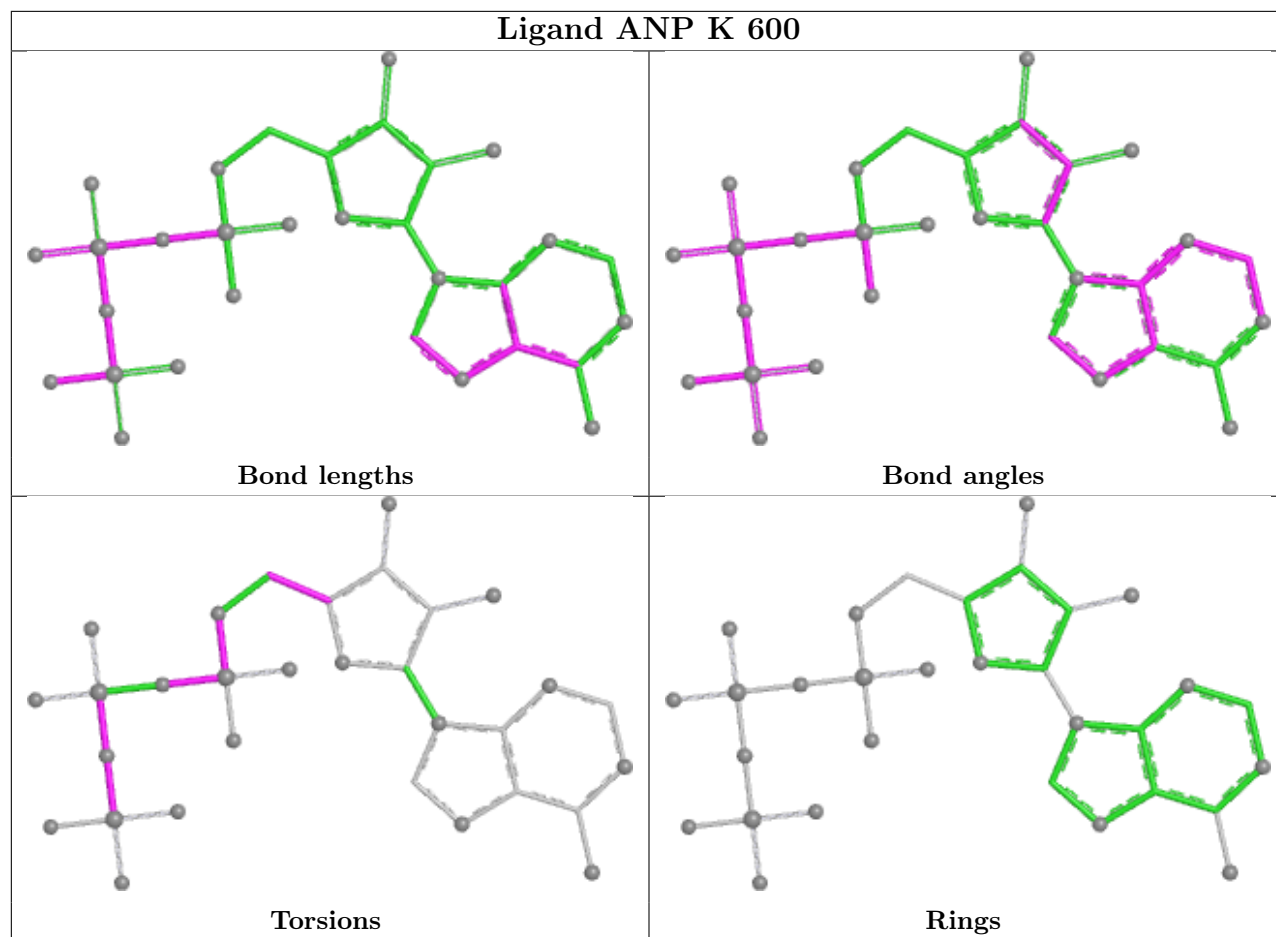


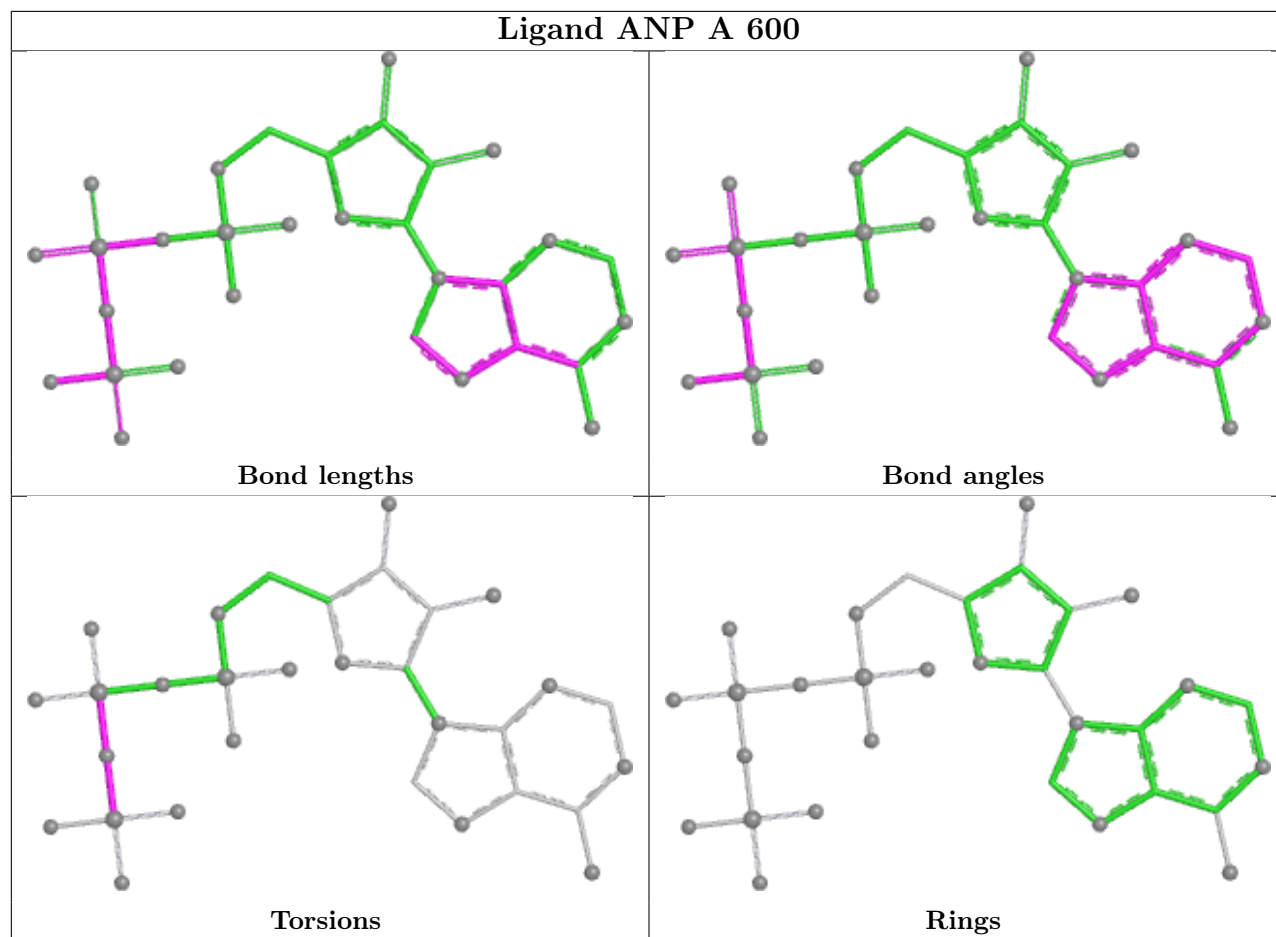


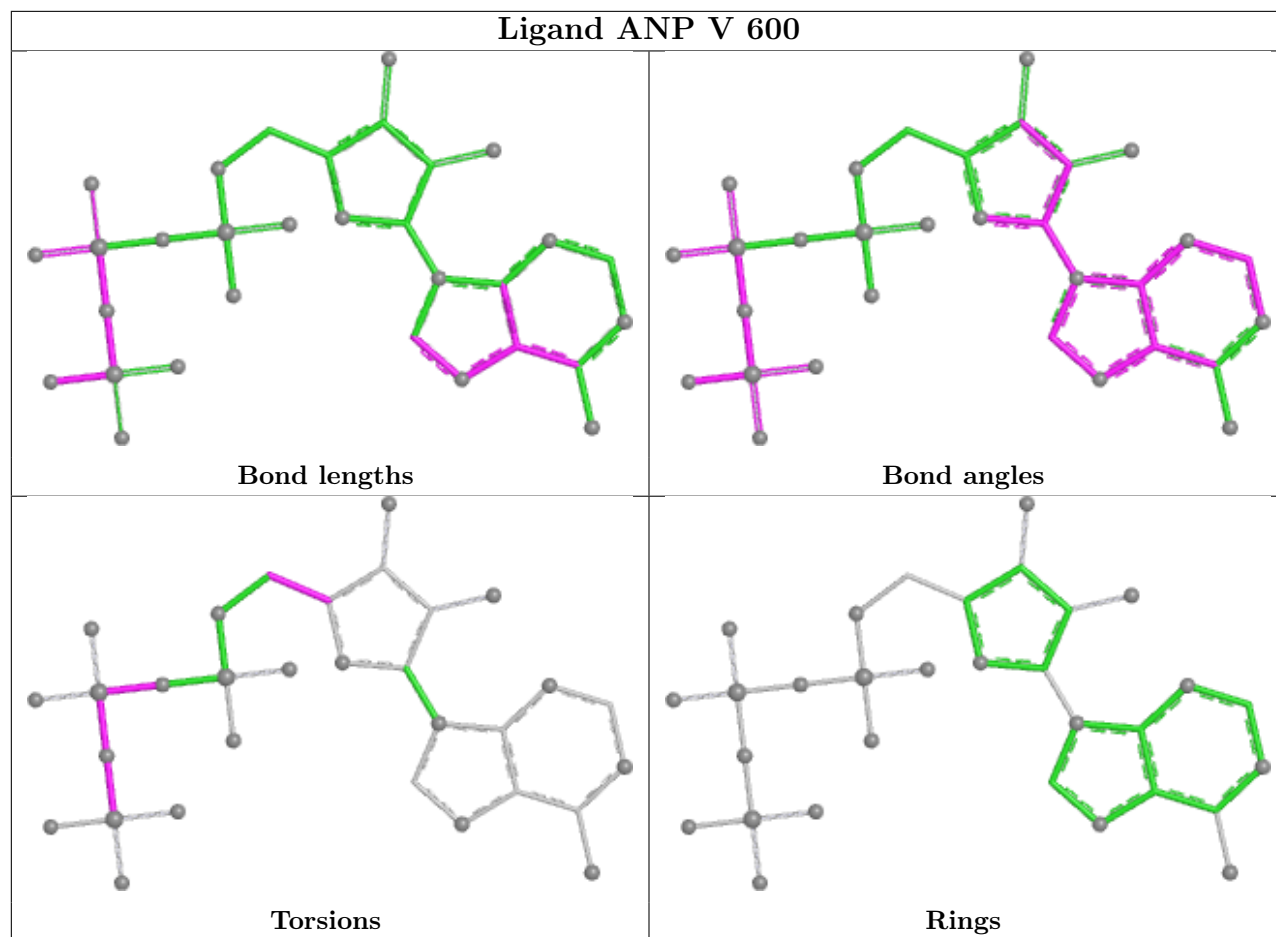


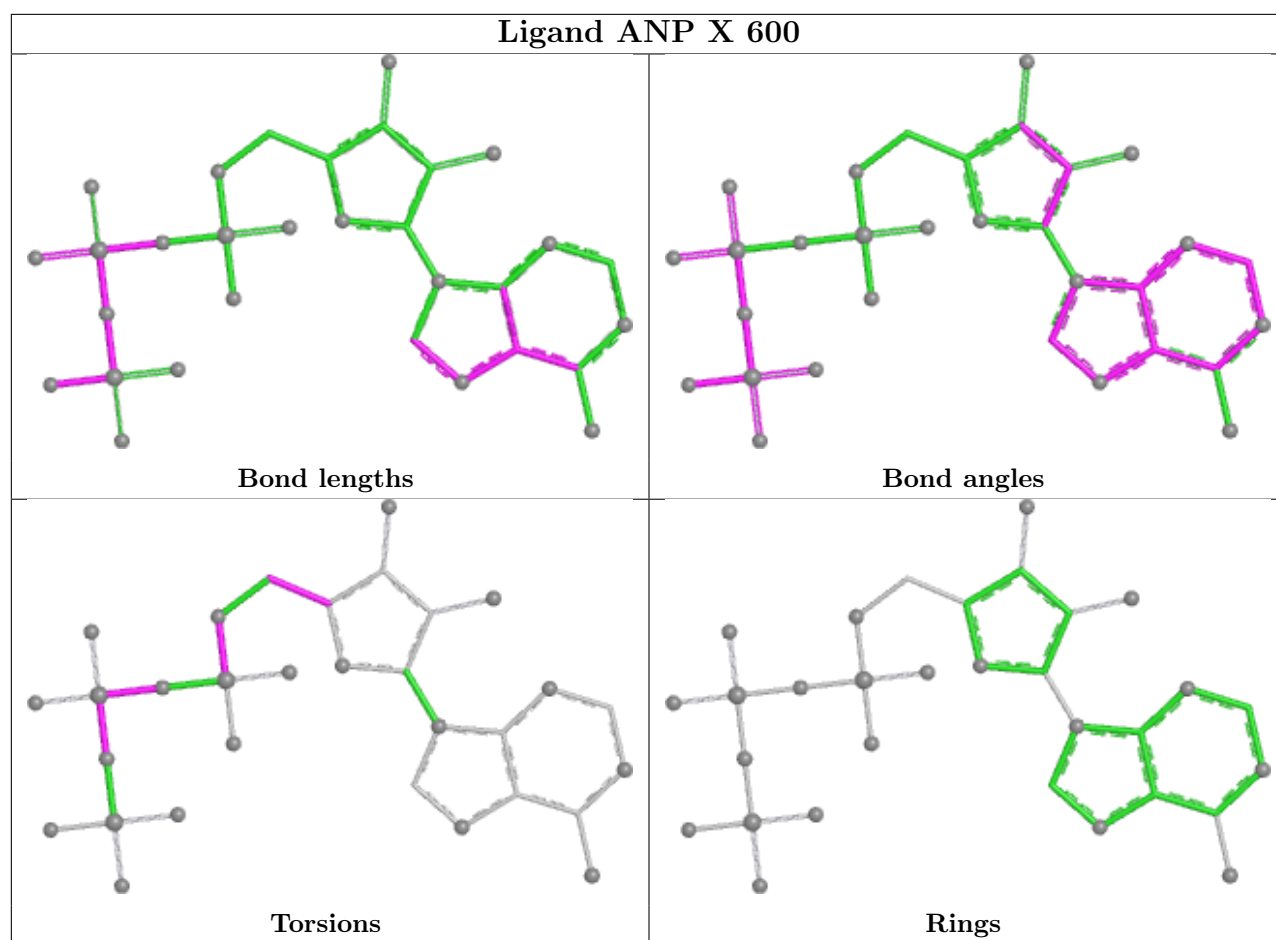
Ligand ANP J 600

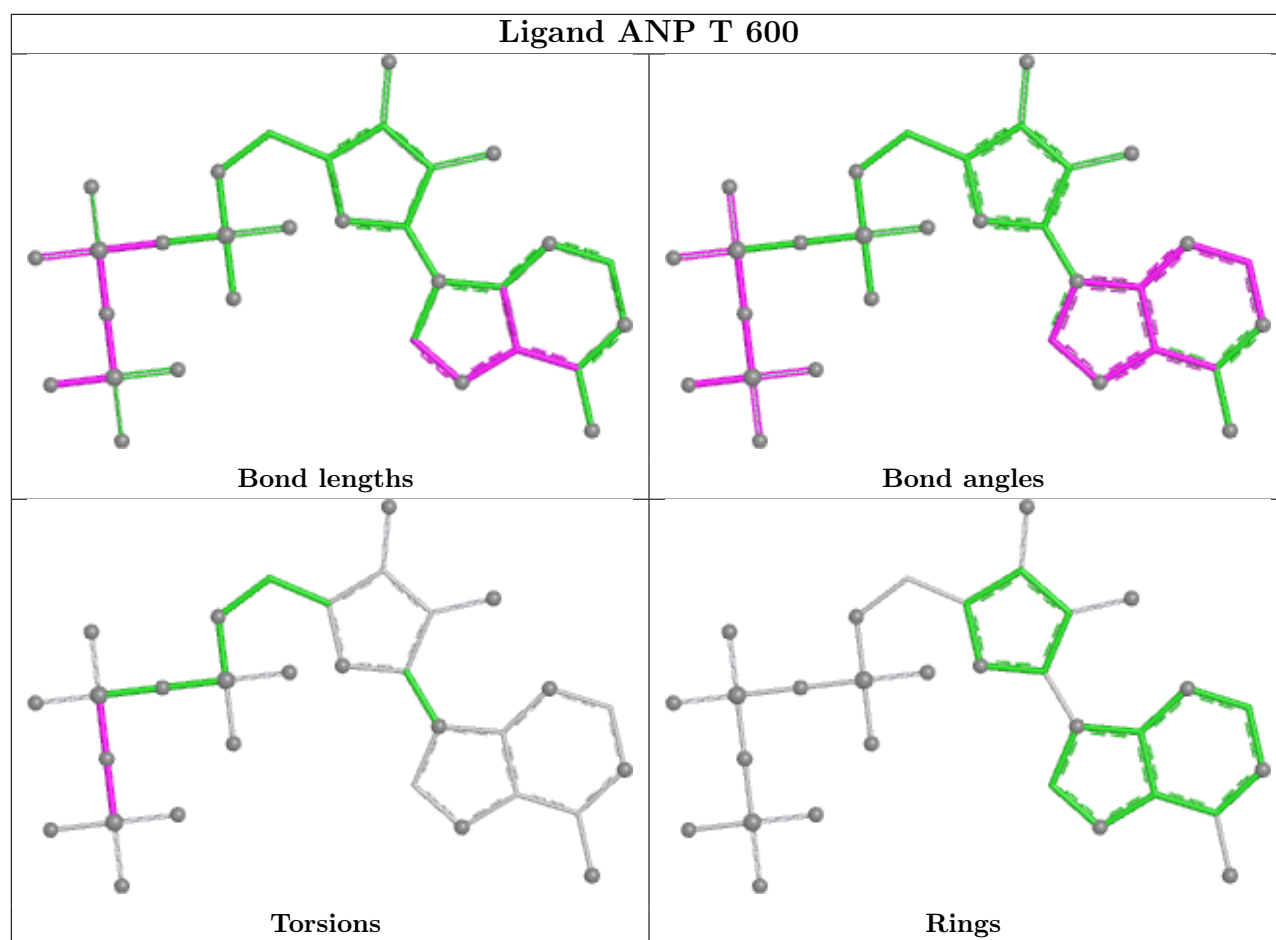












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	482/510 (94%)	-0.73	0 100 100	41, 63, 99, 156	0
1	B	483/510 (94%)	-0.52	1 (0%) 91 83	48, 92, 148, 188	0
1	C	484/510 (94%)	-0.71	0 100 100	43, 73, 129, 177	0
1	J	481/510 (94%)	-0.58	0 100 100	60, 100, 149, 206	0
1	K	486/510 (95%)	-0.41	0 100 100	78, 126, 187, 217	0
1	L	482/510 (94%)	-0.68	0 100 100	47, 68, 137, 194	0
1	S	478/510 (93%)	-0.48	0 100 100	77, 109, 153, 179	0
1	T	479/510 (93%)	-0.31	0 100 100	103, 151, 186, 202	0
1	U	481/510 (94%)	-0.14	1 (0%) 91 83	104, 150, 181, 217	0
2	D	470/484 (97%)	-0.69	0 100 100	42, 70, 123, 181	0
2	E	468/484 (96%)	-0.60	0 100 100	46, 86, 161, 211	0
2	F	469/484 (96%)	-0.61	1 (0%) 91 83	48, 89, 128, 169	0
2	M	470/484 (97%)	-0.58	0 100 100	55, 86, 134, 180	0
2	N	470/484 (97%)	-0.32	2 (0%) 88 76	71, 133, 199, 229	0
2	O	468/484 (96%)	-0.59	0 100 100	54, 94, 141, 175	0
2	V	470/484 (97%)	-0.30	0 100 100	93, 138, 180, 210	0
2	W	467/484 (96%)	-0.43	2 (0%) 88 76	89, 117, 164, 189	0
2	X	469/484 (96%)	-0.37	2 (0%) 88 76	93, 134, 185, 234	0
3	G	266/278 (95%)	-0.35	0 100 100	63, 103, 140, 167	0
3	P	246/278 (88%)	-0.07	1 (0%) 88 76	69, 131, 195, 237	0
3	Y	201/278 (72%)	-0.15	1 (0%) 87 72	107, 146, 192, 232	0
4	H	116/138 (84%)	0.06	3 (2%) 57 34	82, 127, 216, 236	0
4	Q	84/138 (60%)	0.24	2 (2%) 59 36	109, 150, 208, 214	0
4	Z	17/138 (12%)	0.11	0 100 100	190, 210, 236, 245	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
5	1	27/61 (44%)	0.13	0 100 100	159, 168, 187, 210	0
5	I	49/61 (80%)	0.21	3 (6%) 27 14	97, 127, 178, 217	0
5	R	34/61 (55%)	0.04	0 100 100	108, 122, 187, 200	0
All	All	9597/10377 (92%)	-0.46	19 (0%) 91 83	41, 108, 176, 245	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	103	ASN	3.7
4	Q	126	GLN	3.5
2	W	189	GLU	3.4
5	I	29	LEU	2.7
5	I	61	LYS	2.7
2	X	31	PRO	2.6
4	Q	132	ASN	2.6
1	U	203	CYS	2.5
2	N	313	PRO	2.4
2	F	475	ALA	2.3
2	N	302	GLY	2.3
3	Y	76	ALA	2.2
4	H	133	LEU	2.2
4	H	132	ASN	2.2
2	W	474	ALA	2.1
3	P	104	ASN	2.1
2	X	32	ALA	2.1
1	B	397	ALA	2.1
5	I	49	ASN	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

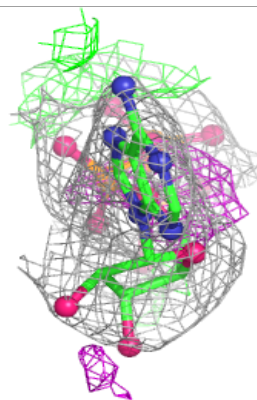
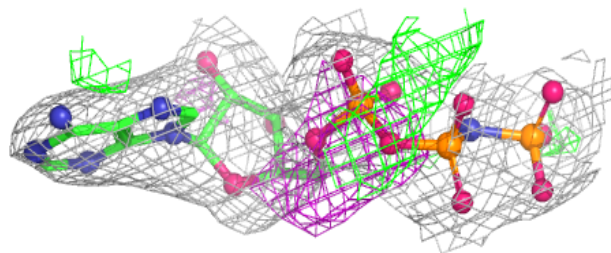
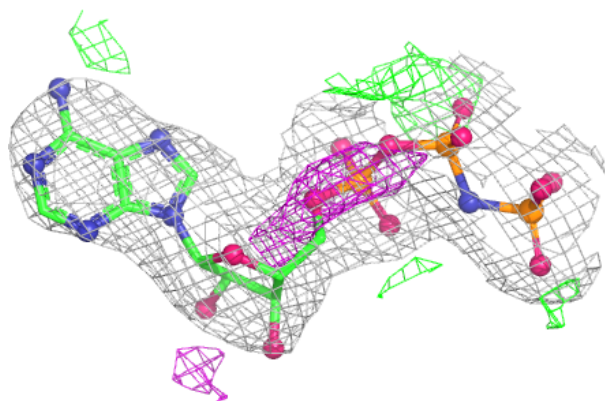
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	MG	K	700	1/1	0.80	0.08	66,66,66,66	0
7	MG	F	700	1/1	0.86	0.10	55,55,55,55	0
7	MG	C	700	1/1	0.87	0.14	52,52,52,52	0
6	ANP	U	600	31/31	0.88	0.10	73,79,82,82	0
7	MG	J	700	1/1	0.89	0.08	51,51,51,51	0
7	MG	S	700	1/1	0.89	0.10	53,53,53,53	0
6	ANP	V	600	31/31	0.90	0.10	80,100,102,102	0
7	MG	T	700	1/1	0.90	0.07	62,62,62,62	0
6	ANP	X	600	31/31	0.91	0.09	83,95,97,97	0
7	MG	M	700	1/1	0.92	0.15	53,53,53,53	0
6	ANP	T	600	31/31	0.92	0.07	81,102,107,108	0
7	MG	L	700	1/1	0.92	0.13	48,48,48,48	0
7	MG	X	700	1/1	0.92	0.08	70,70,70,70	0
7	MG	O	700	1/1	0.93	0.11	61,61,61,61	0
6	ANP	K	600	31/31	0.93	0.09	79,96,100,101	0
6	ANP	S	600	31/31	0.93	0.07	64,78,80,80	0
6	ANP	F	600	31/31	0.93	0.08	65,79,84,85	0
6	ANP	B	600	31/31	0.94	0.07	66,79,81,82	0
6	ANP	O	600	31/31	0.94	0.09	69,79,81,82	0
7	MG	D	700	1/1	0.94	0.12	48,48,48,48	0
7	MG	B	700	1/1	0.95	0.12	57,57,57,57	0
6	ANP	J	600	31/31	0.95	0.08	60,74,82,83	0
7	MG	A	700	1/1	0.95	0.11	41,41,41,41	0
6	ANP	C	600	31/31	0.96	0.06	57,68,75,75	0
6	ANP	M	600	31/31	0.96	0.07	60,70,73,74	0
7	MG	U	700	1/1	0.96	0.09	61,61,61,61	0
7	MG	V	700	1/1	0.96	0.06	61,61,61,61	0
6	ANP	D	600	31/31	0.96	0.06	55,65,68,69	0
6	ANP	A	600	31/31	0.97	0.06	44,57,61,63	0
6	ANP	L	600	31/31	0.97	0.06	49,62,70,70	0

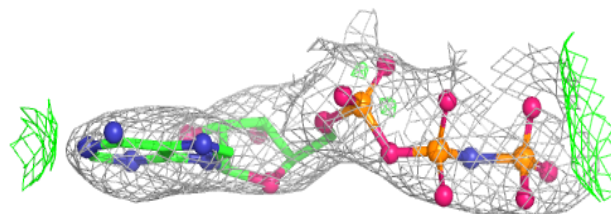
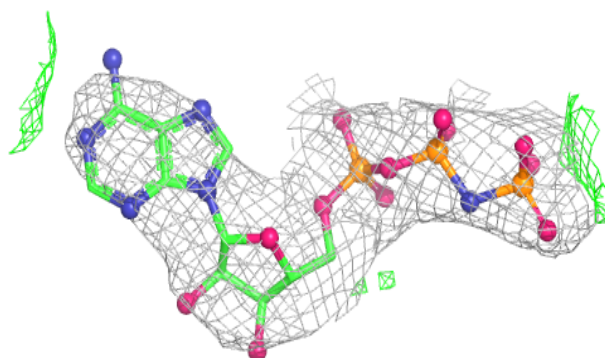
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ANP U 600:

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

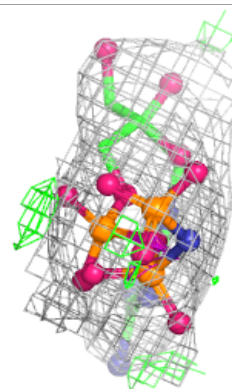
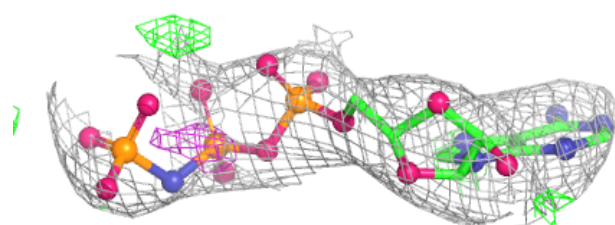
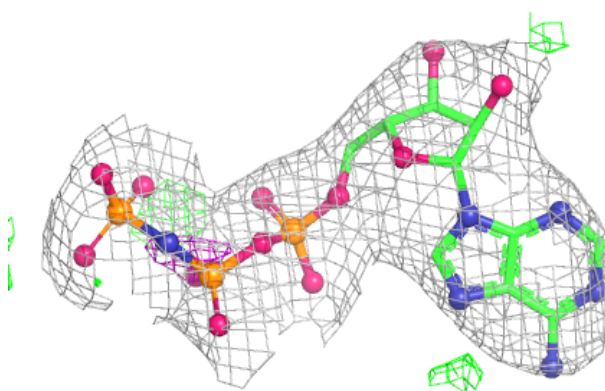
**Electron density around ANP V 600:**

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

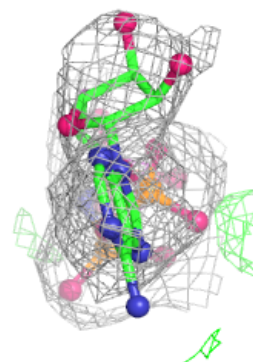
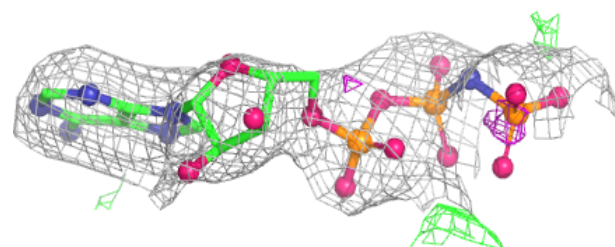
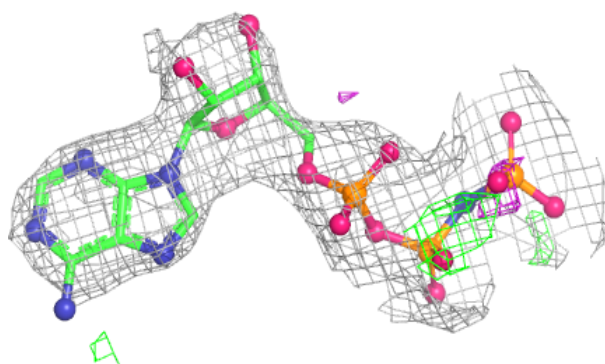


Electron density around ANP X 600:

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

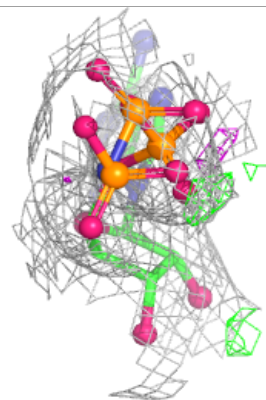
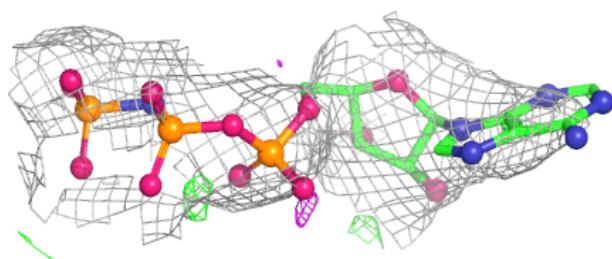
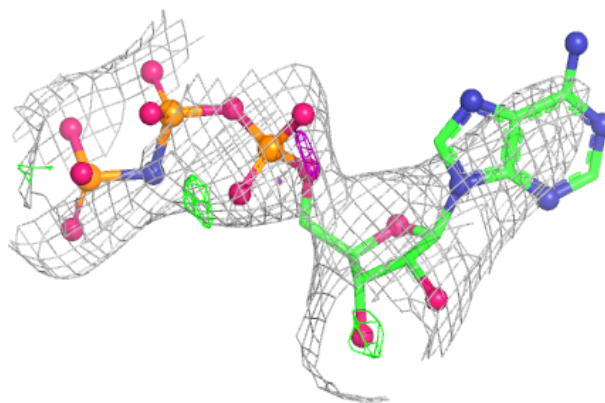
**Electron density around ANP T 600:**

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

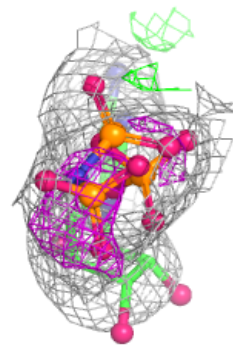
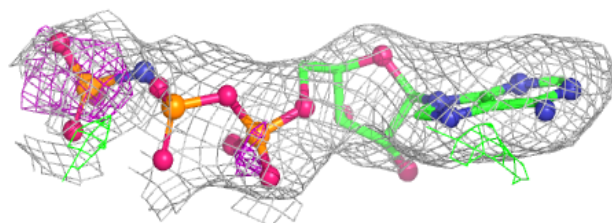
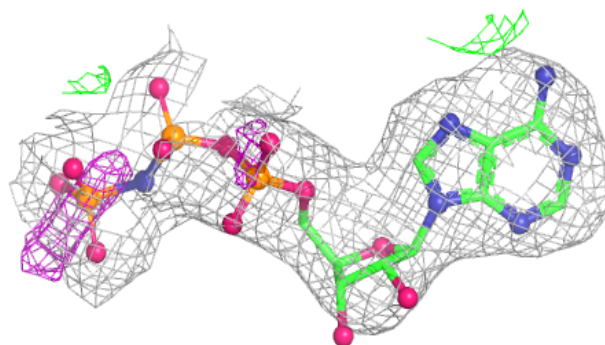


Electron density around ANP K 600:

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

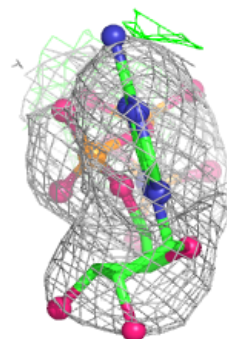
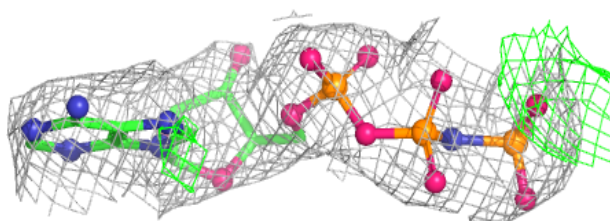
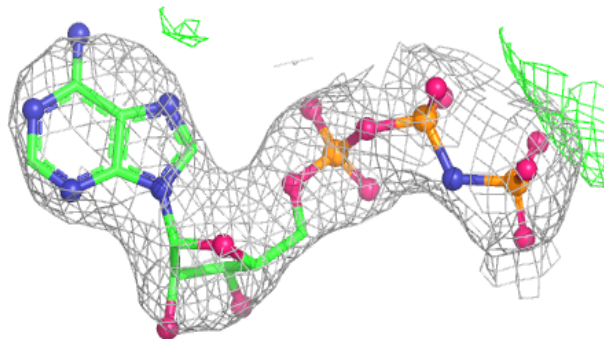
**Electron density around ANP S 600:**

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

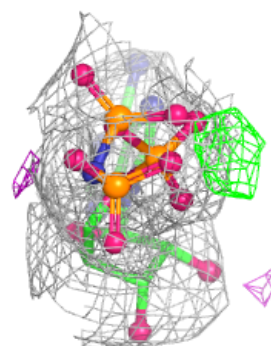
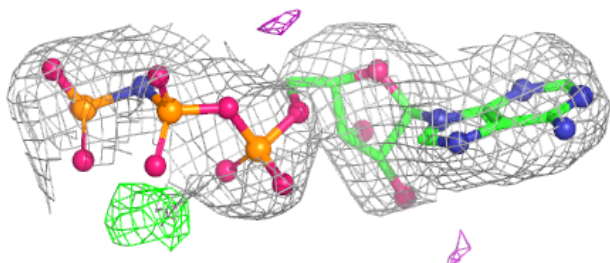
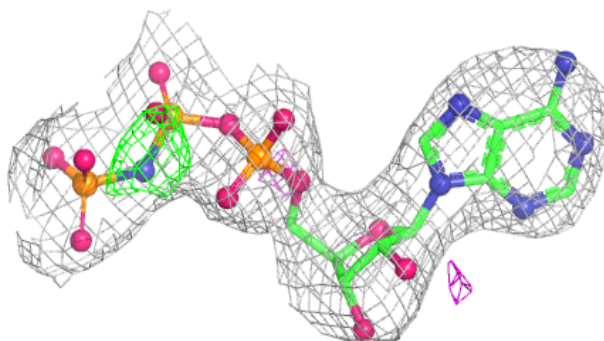


Electron density around ANP F 600:

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

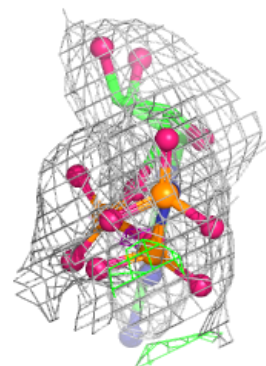
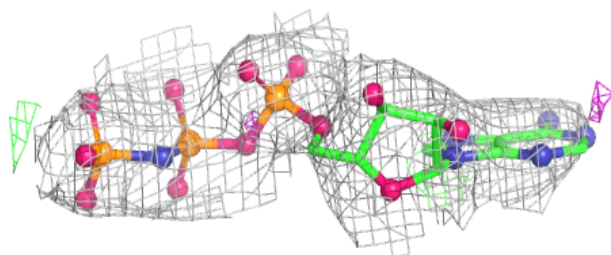
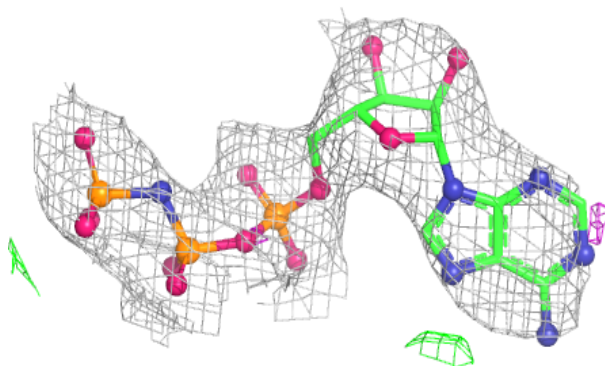
**Electron density around ANP B 600:**

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

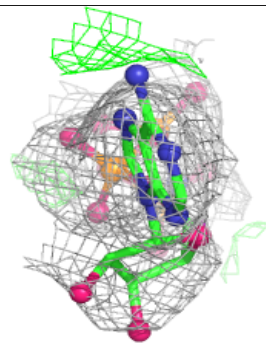
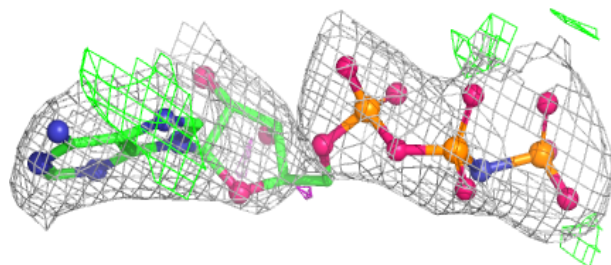
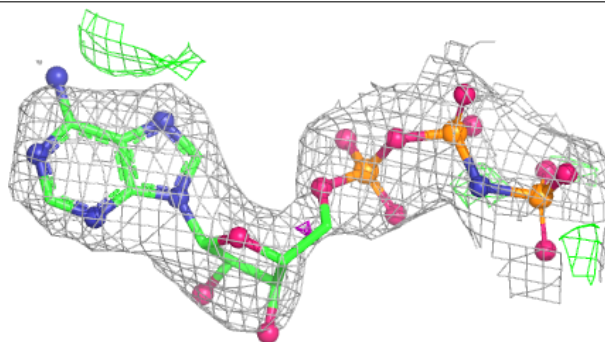


Electron density around ANP O 600:

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

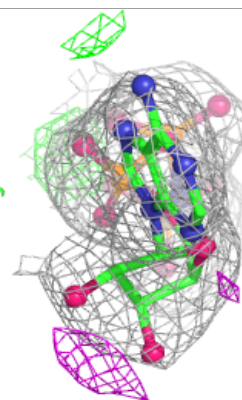
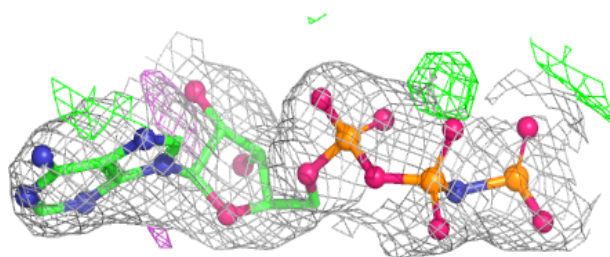
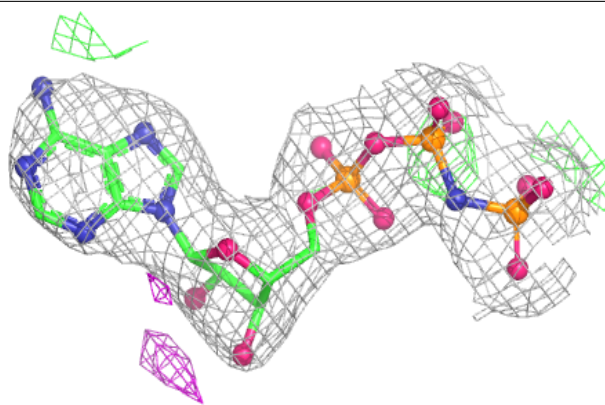
**Electron density around ANP J 600:**

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

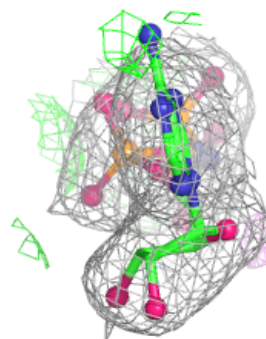
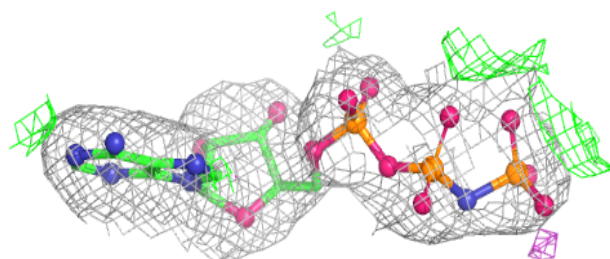
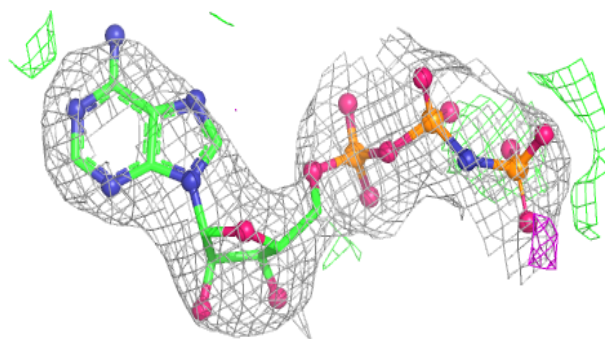


Electron density around ANP C 600:

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

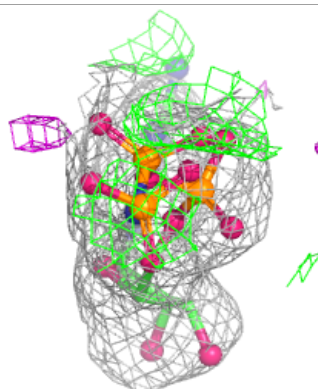
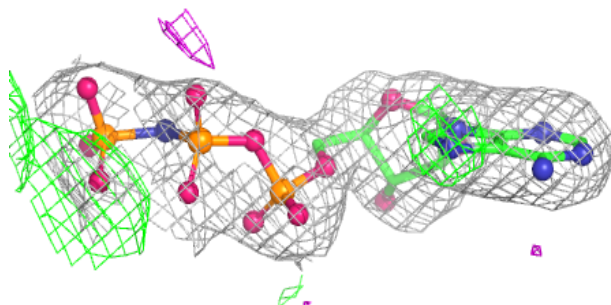
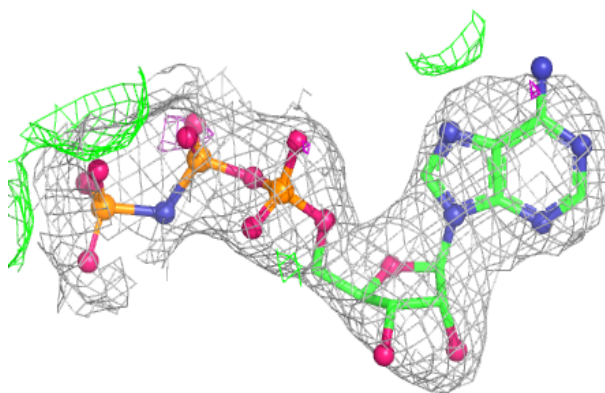
**Electron density around ANP M 600:**

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

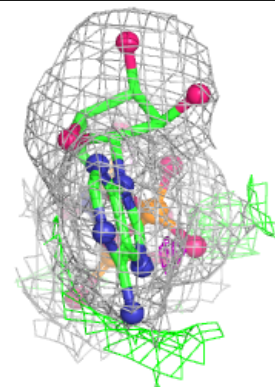
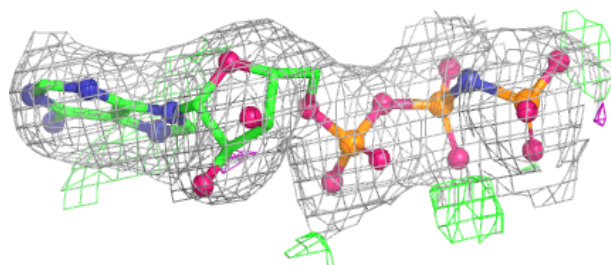
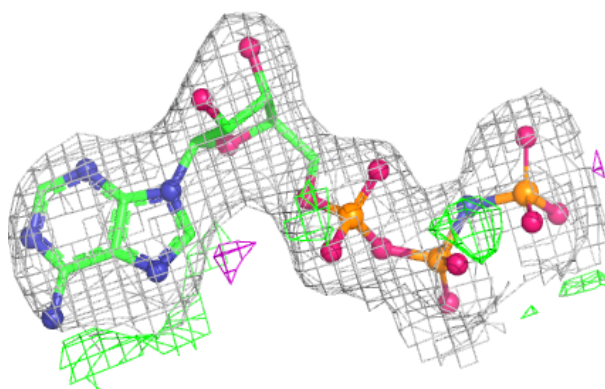


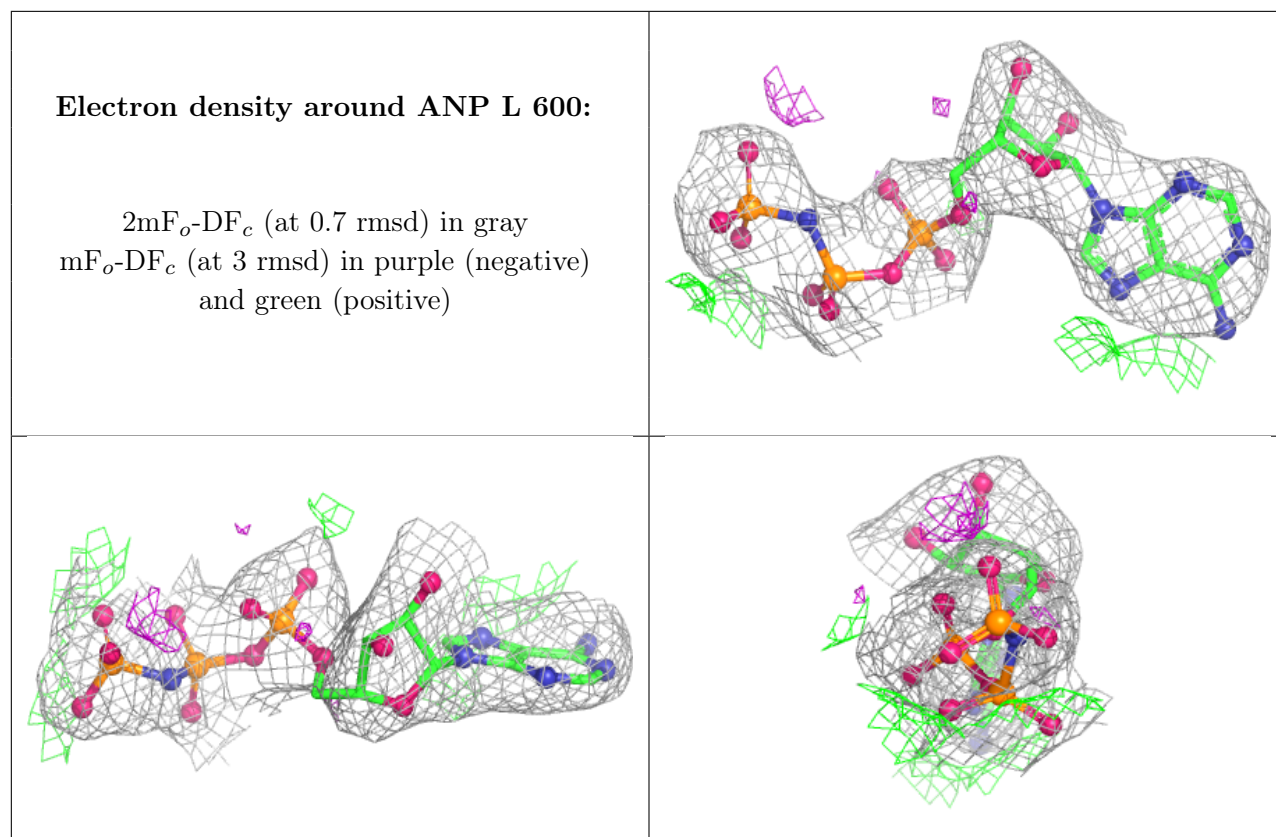
Electron density around ANP D 600:

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

**Electron density around ANP A 600:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.