



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 03:34 PM UTC

PDB ID : 3OFN / pdb_00003ofn
Title : Structure of four mutant forms of yeast F1 ATPase: alpha-N67I
Authors : Arsenieva, D.; Symersky, J.; Wang, Y.; Pagadala, V.; Mueller, D.M.
Deposited on : 2010-08-15
Resolution : 3.20 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

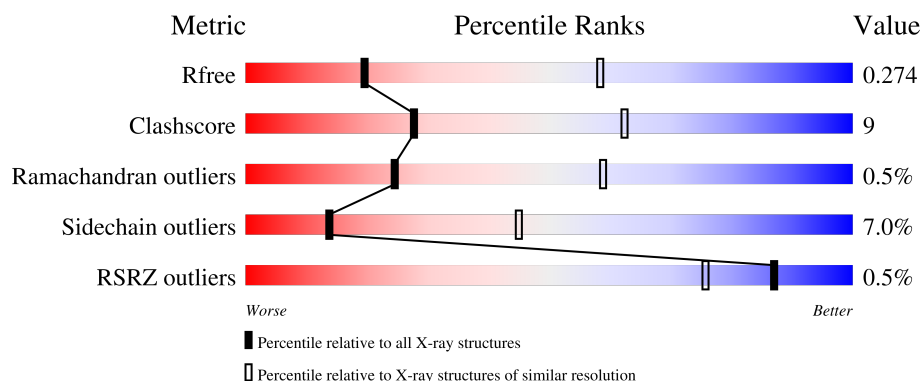
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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.



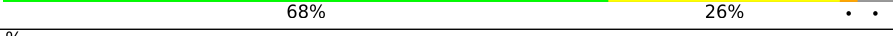
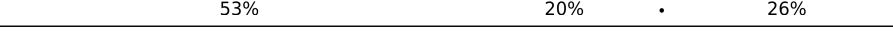
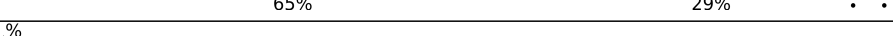
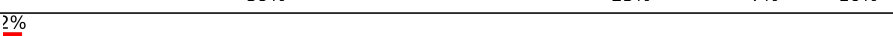
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	 69% 23% • 5%
1	B	510	 72% 22% • 5%
1	C	510	 77% 16% • 5%
1	J	510	 73% 21% • 5%
1	K	510	 73% 21% • 5%

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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	
5	I	61	
5	R	61	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 70481 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	485	Total	C	N	O	S	0	0	0
			3691	2336	650	702	3			
1	B	486	Total	C	N	O	S	0	0	0
			3690	2336	648	703	3			
1	C	484	Total	C	N	O	S	0	0	0
			3680	2327	649	701	3			
1	J	482	Total	C	N	O	S	0	0	0
			3664	2316	647	698	3			
1	K	483	Total	C	N	O	S	0	0	0
			3578	2255	634	686	3			
1	L	479	Total	C	N	O	S	0	0	0
			3608	2282	637	686	3			
1	S	483	Total	C	N	O	S	0	0	0
			3642	2302	640	697	3			
1	T	484	Total	C	N	O	S	0	0	0
			3639	2296	642	698	3			
1	U	485	Total	C	N	O	S	0	0	0
			3511	2205	619	684	3			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	ILE	ASN	engineered mutation	UNP P07251
B	67	ILE	ASN	engineered mutation	UNP P07251
C	67	ILE	ASN	engineered mutation	UNP P07251
J	67	ILE	ASN	engineered mutation	UNP P07251
K	67	ILE	ASN	engineered mutation	UNP P07251
L	67	ILE	ASN	engineered mutation	UNP P07251
S	67	ILE	ASN	engineered mutation	UNP P07251
T	67	ILE	ASN	engineered mutation	UNP P07251
U	67	ILE	ASN	engineered mutation	UNP P07251

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	470	Total	C	N	O	S	0	0	0
			3545	2248	603	688	6			
2	E	469	Total	C	N	O	S	0	0	0
			3511	2226	598	681	6			
2	F	469	Total	C	N	O	S	0	0	0
			3539	2245	603	685	6			
2	M	460	Total	C	N	O	S	0	0	0
			3436	2180	584	667	5			
2	N	463	Total	C	N	O	S	0	0	0
			3403	2160	573	665	5			
2	O	469	Total	C	N	O	S	0	0	0
			3449	2191	581	671	6			
2	V	360	Total	C	N	O	S	0	0	0
			2582	1625	439	515	3			
2	W	468	Total	C	N	O	S	0	0	0
			3468	2198	590	674	6			
2	X	469	Total	C	N	O	S	0	0	0
			3447	2181	588	673	5			

There are 72 discrepancies between the modelled and reference sequences:

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

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Chain	Residue	Modelled	Actual	Comment	Reference
F	1	HIS	-	expression tag	UNP P00830
F	2	HIS	-	expression tag	UNP P00830
M	-5	ALA	-	expression tag	UNP P00830
M	-4	SER	-	expression tag	UNP P00830
M	-3	HIS	-	expression tag	UNP P00830
M	-2	HIS	-	expression tag	UNP P00830
M	-1	HIS	-	expression tag	UNP P00830
M	0	HIS	-	expression tag	UNP P00830
M	1	HIS	-	expression tag	UNP P00830
M	2	HIS	-	expression tag	UNP P00830
N	-5	ALA	-	expression tag	UNP P00830
N	-4	SER	-	expression tag	UNP P00830
N	-3	HIS	-	expression tag	UNP P00830
N	-2	HIS	-	expression tag	UNP P00830
N	-1	HIS	-	expression tag	UNP P00830
N	0	HIS	-	expression tag	UNP P00830
N	1	HIS	-	expression tag	UNP P00830
N	2	HIS	-	expression tag	UNP P00830
O	-5	ALA	-	expression tag	UNP P00830
O	-4	SER	-	expression tag	UNP P00830
O	-3	HIS	-	expression tag	UNP P00830
O	-2	HIS	-	expression tag	UNP P00830
O	-1	HIS	-	expression tag	UNP P00830
O	0	HIS	-	expression tag	UNP P00830
O	1	HIS	-	expression tag	UNP P00830
O	2	HIS	-	expression tag	UNP P00830
V	-5	ALA	-	expression tag	UNP P00830
V	-4	SER	-	expression tag	UNP P00830
V	-3	HIS	-	expression tag	UNP P00830
V	-2	HIS	-	expression tag	UNP P00830
V	-1	HIS	-	expression tag	UNP P00830
V	0	HIS	-	expression tag	UNP P00830
V	1	HIS	-	expression tag	UNP P00830
V	2	HIS	-	expression tag	UNP P00830
W	-5	ALA	-	expression tag	UNP P00830
W	-4	SER	-	expression tag	UNP P00830
W	-3	HIS	-	expression tag	UNP P00830
W	-2	HIS	-	expression tag	UNP P00830
W	-1	HIS	-	expression tag	UNP P00830
W	0	HIS	-	expression tag	UNP P00830
W	1	HIS	-	expression tag	UNP P00830
W	2	HIS	-	expression tag	UNP P00830

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Chain	Residue	Modelled	Actual	Comment	Reference
X	-5	ALA	-	expression tag	UNP P00830
X	-4	SER	-	expression tag	UNP P00830
X	-3	HIS	-	expression tag	UNP P00830
X	-2	HIS	-	expression tag	UNP P00830
X	-1	HIS	-	expression tag	UNP P00830
X	0	HIS	-	expression tag	UNP P00830
X	1	HIS	-	expression tag	UNP P00830
X	2	HIS	-	expression tag	UNP P00830

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	268	Total	C	N	O	S	0	0	0
			2064	1297	358	399	10			
3	P	268	Total	C	N	O	S	0	0	0
			1869	1163	320	380	6			
3	Y	115	Total	C	N	O	S	0	0	0
			790	482	141	163	4			

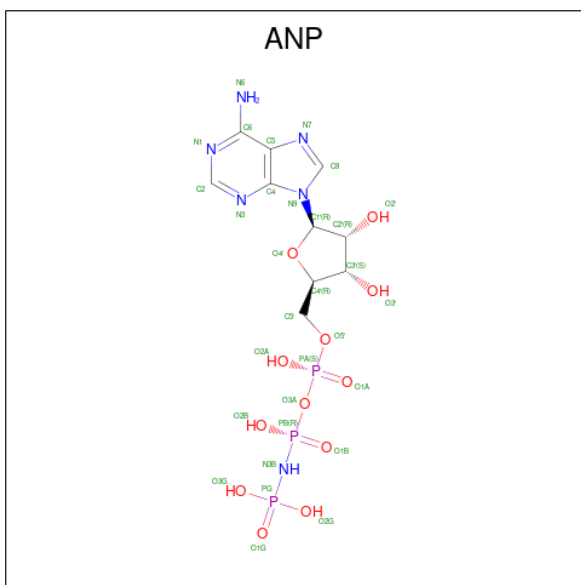
- Molecule 4 is a protein called ATP synthase subunit delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	122	Total	C	N	O	S	0	0	0
			815	513	139	161	2			
4	Q	101	Total	C	N	O	S	0	0	0
			625	389	110	125	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	55	Total	C	N	O	0	0	0
			388	242	68	78			
5	R	55	Total	C	N	O	0	0	0
			367	227	66	74			

- 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).

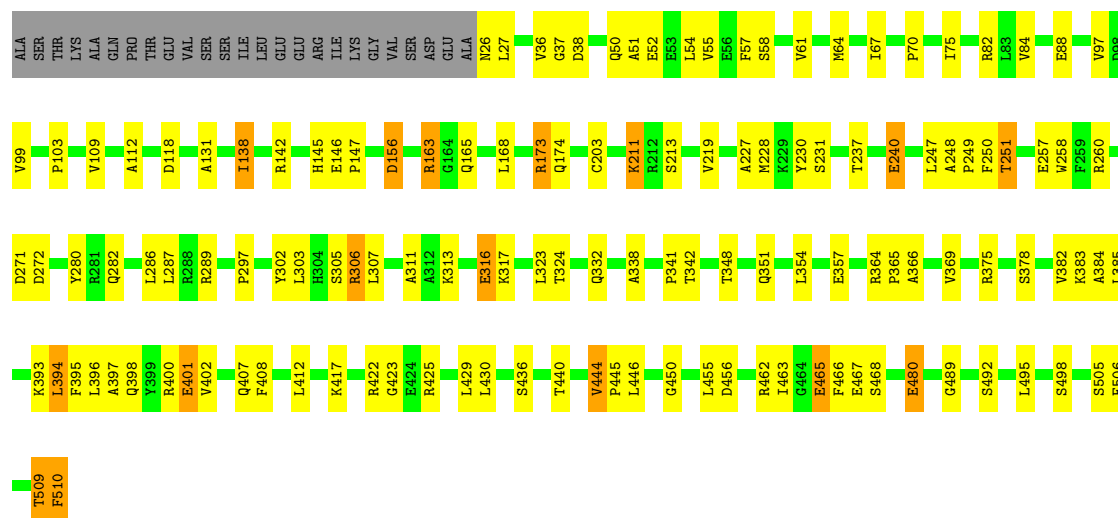
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Mg	0	0
			1	1		
7	B	1	Total	Mg	0	0
			1	1		
7	C	1	Total	Mg	0	0
			1	1		
7	D	1	Total	Mg	0	0
			1	1		
7	F	1	Total	Mg	0	0
			1	1		
7	J	1	Total	Mg	0	0
			1	1		
7	K	1	Total	Mg	0	0
			1	1		
7	L	1	Total	Mg	0	0
			1	1		
7	M	1	Total	Mg	0	0
			1	1		
7	O	1	Total	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 [i](#)

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.

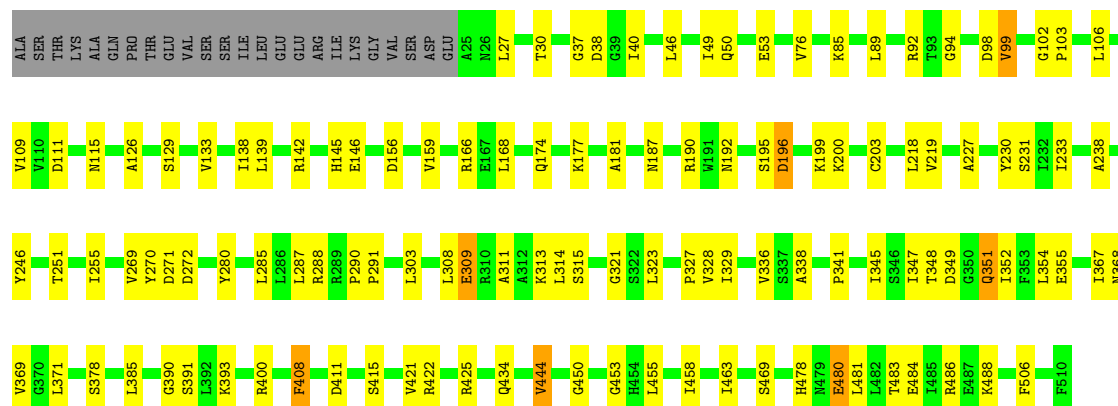
- Molecule 1: ATP synthase subunit alpha

Chain A: 



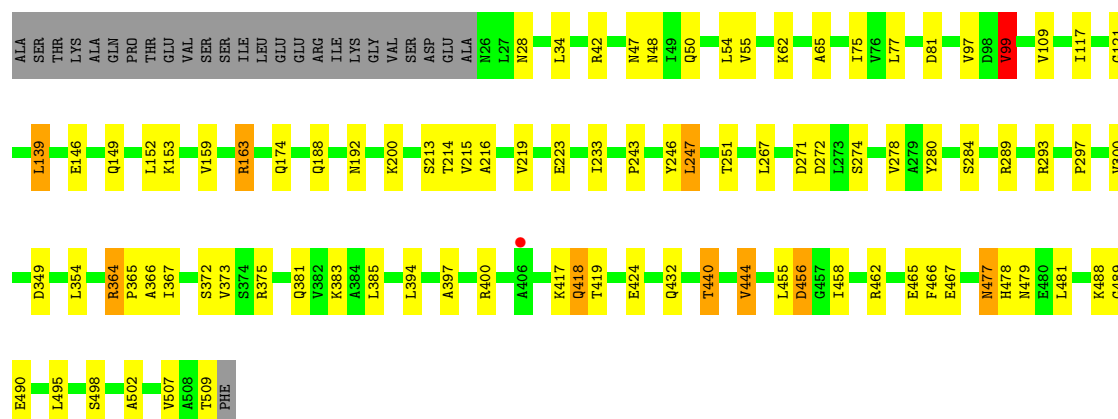
- Molecule 1: ATP synthase subunit alpha

Chain B: 



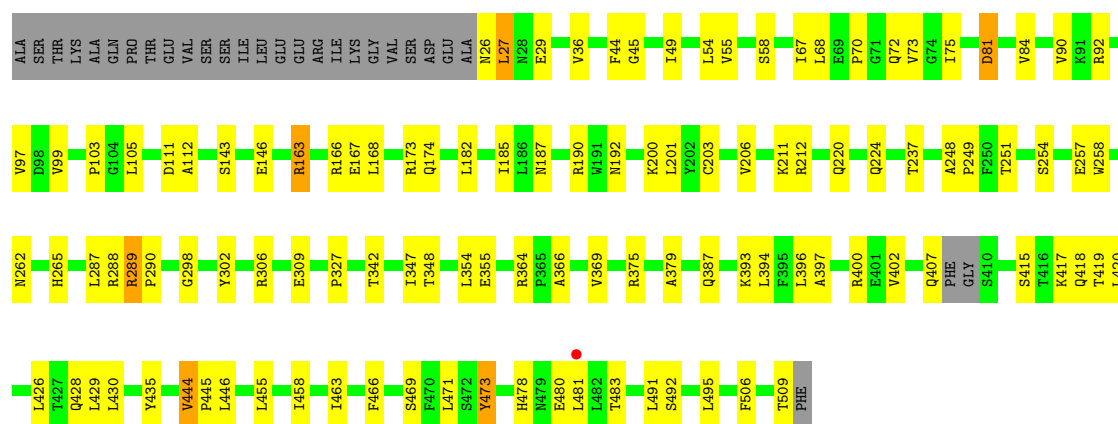
- Molecule 1: ATP synthase subunit alpha

Chain C:  77% 16% 5%



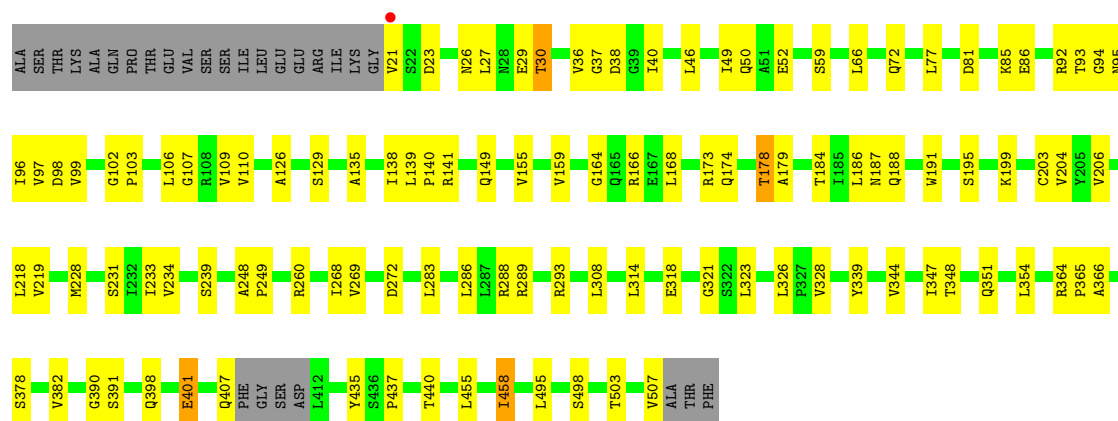
• Molecule 1: ATP synthase subunit alpha

Chain J:  73% 21% 5%



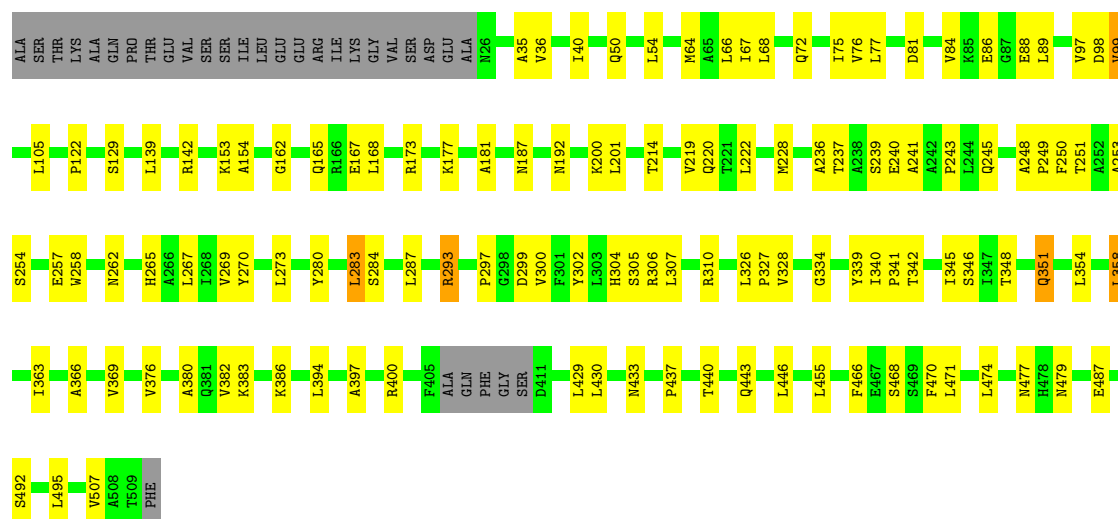
• Molecule 1: ATP synthase subunit alpha

Chain K:  73% 21% 5%



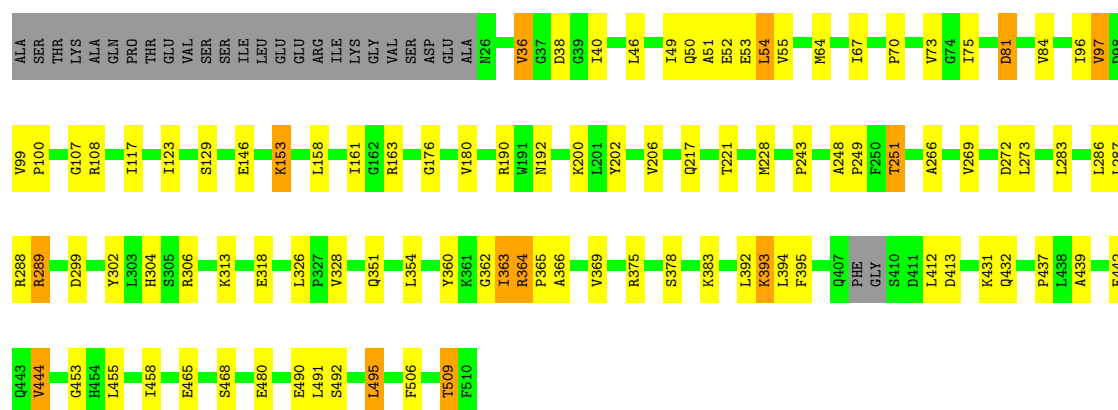
• Molecule 1: ATP synthase subunit alpha

Chain L:  70% 23% • 6%



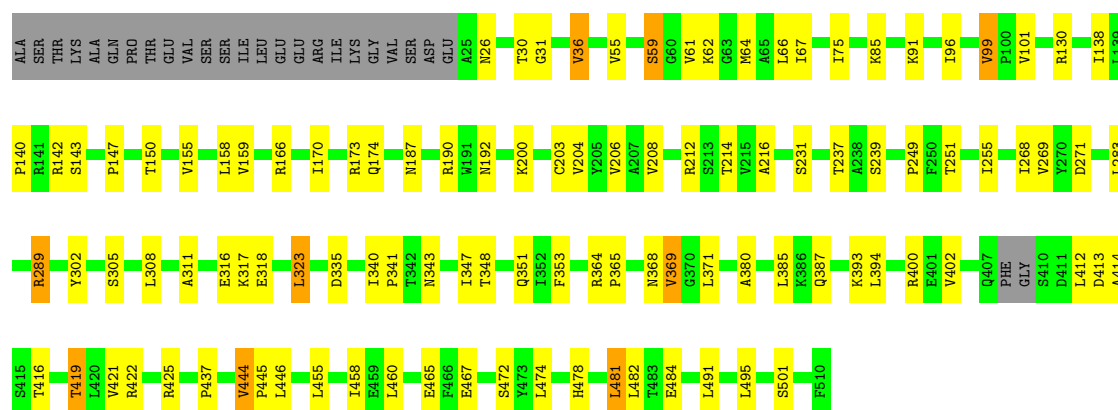
• Molecule 1: ATP synthase subunit alpha

Chain S:  75% 17% • 5%



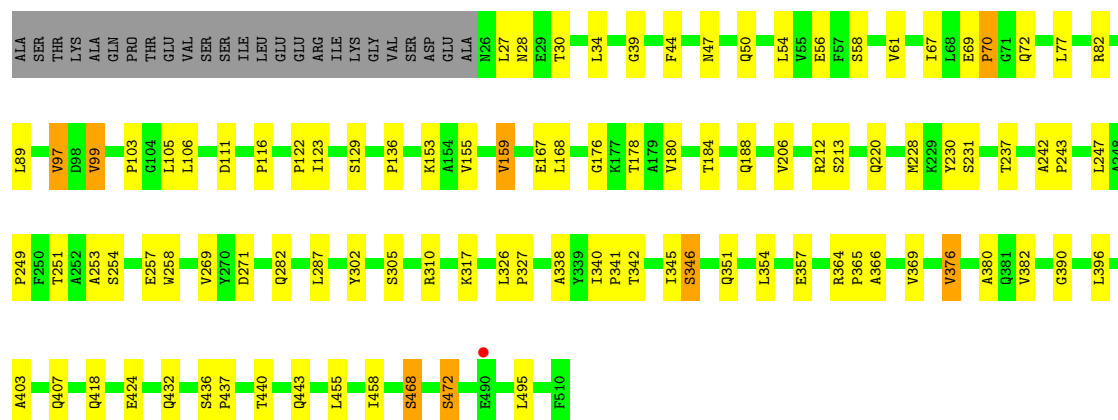
• Molecule 1: ATP synthase subunit alpha

Chain T:  74% 19% • 5%



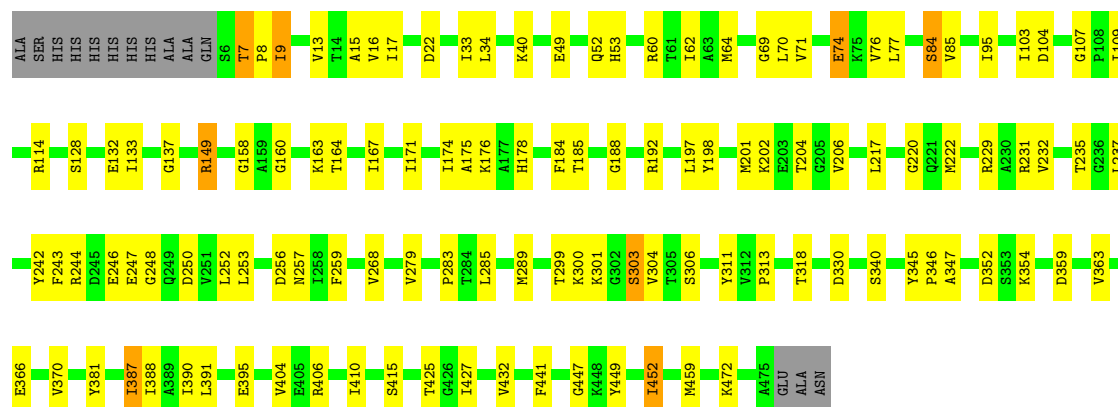
• Molecule 1: ATP synthase subunit alpha

Chain U:  76% 18% 5%



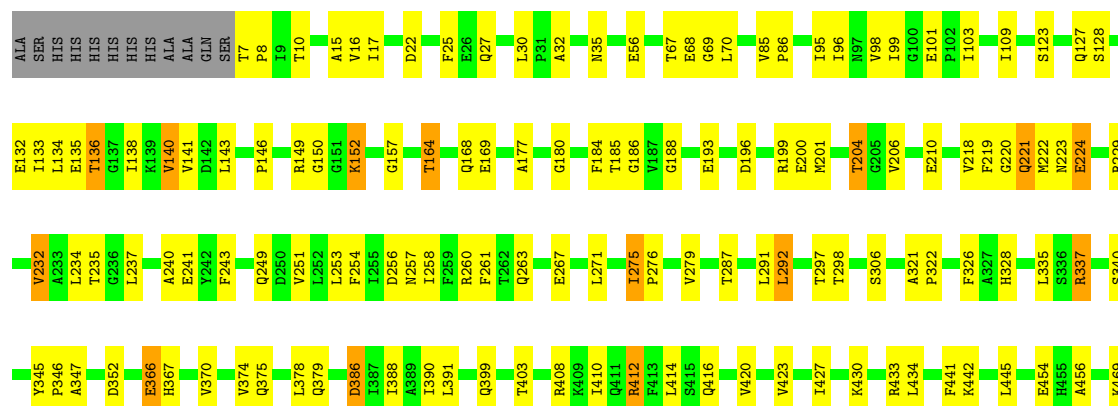
• Molecule 2: ATP synthase subunit beta

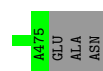
Chain D:  72% 23% 5%



• Molecule 2: ATP synthase subunit beta

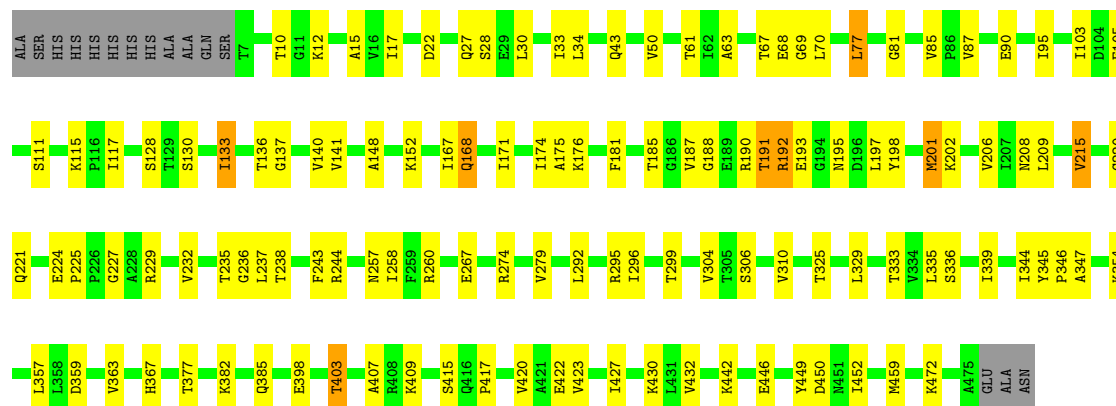
Chain E:  69% 25% 6%





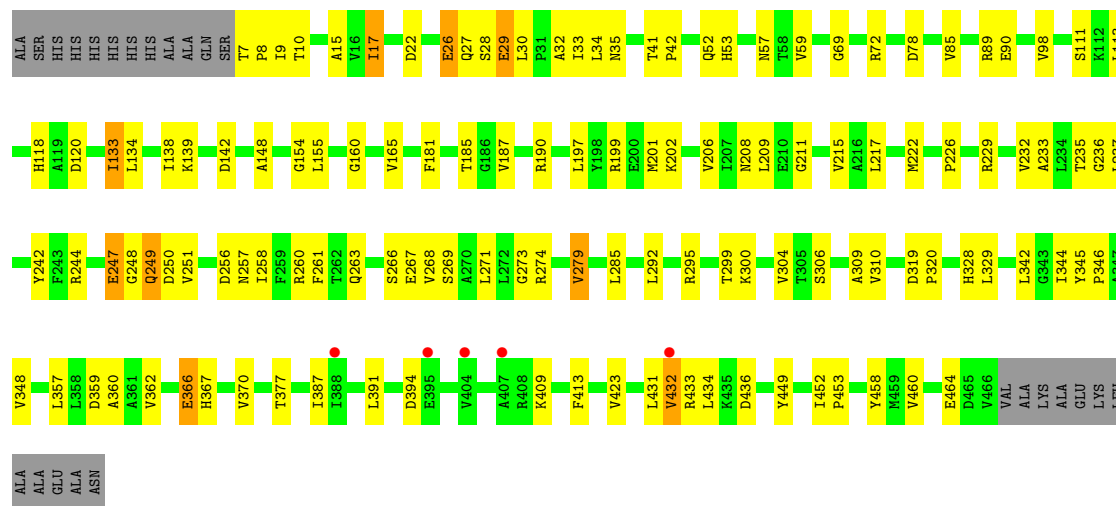
• Molecule 2: ATP synthase subunit beta

Chain F: 71% 24%



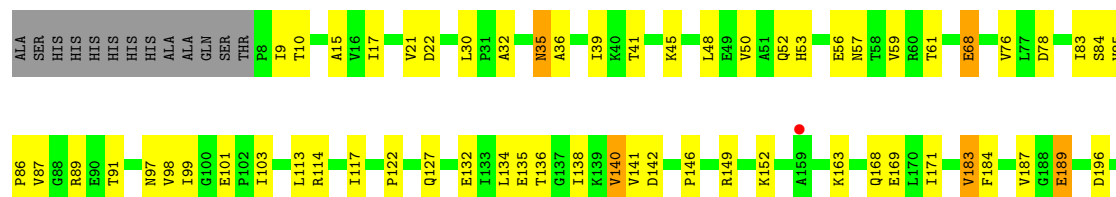
• Molecule 2: ATP synthase subunit beta

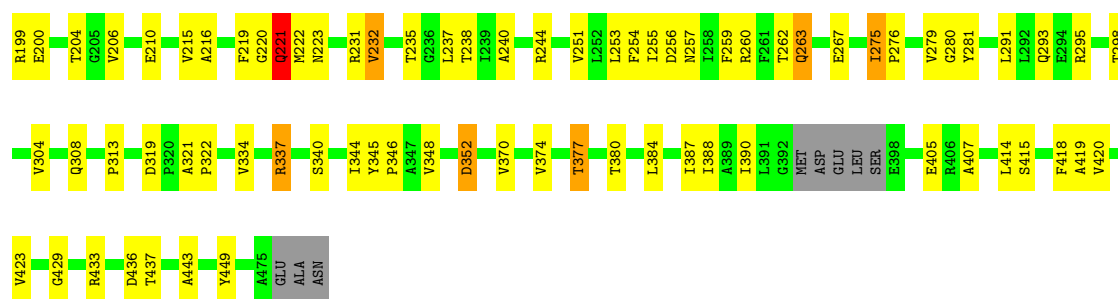
Chain M: 68% 25% 5%



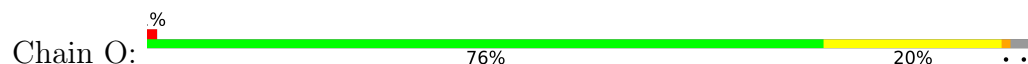
• Molecule 2: ATP synthase subunit beta

Chain N: 68% 26%

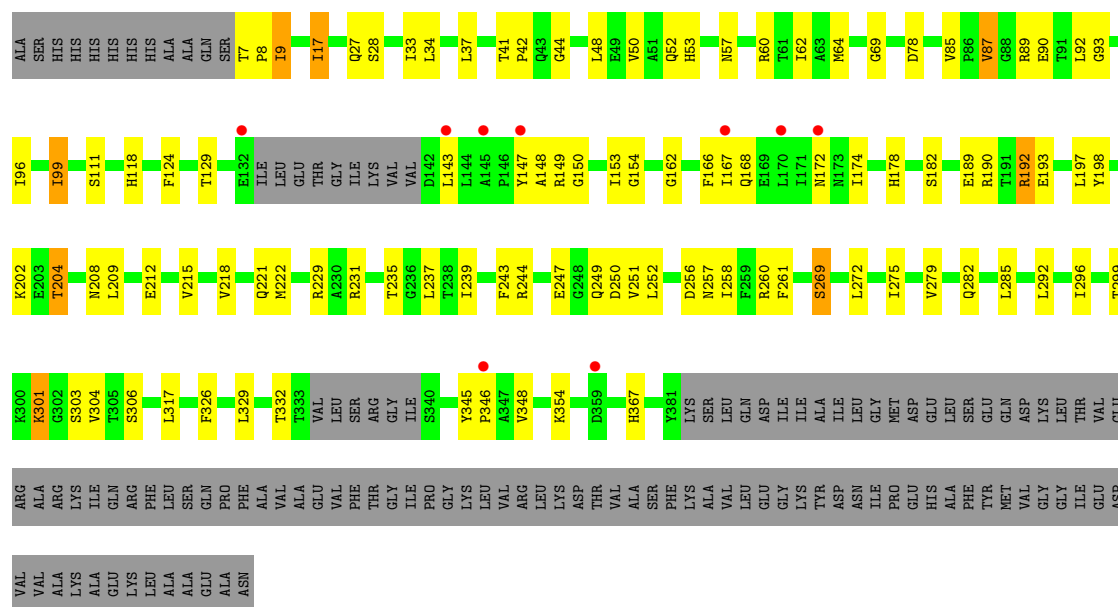




• Molecule 2: ATP synthase subunit beta

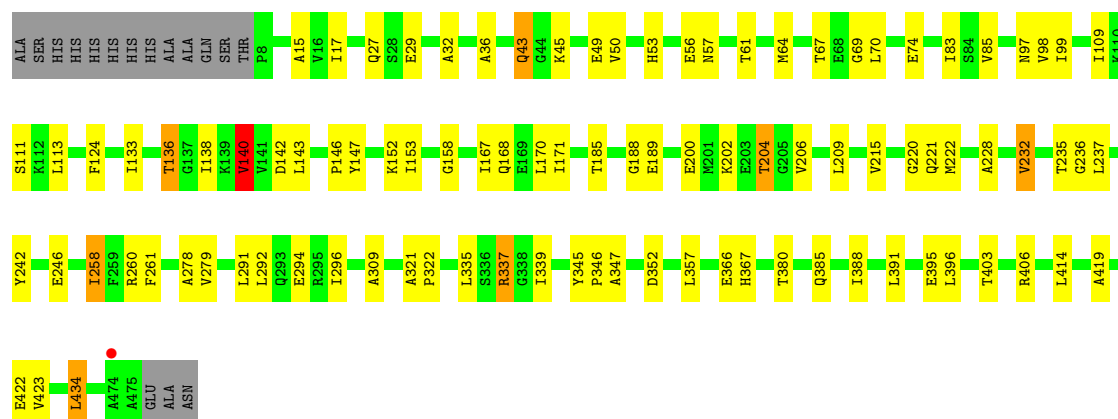


• Molecule 2: ATP synthase subunit beta

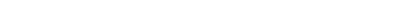


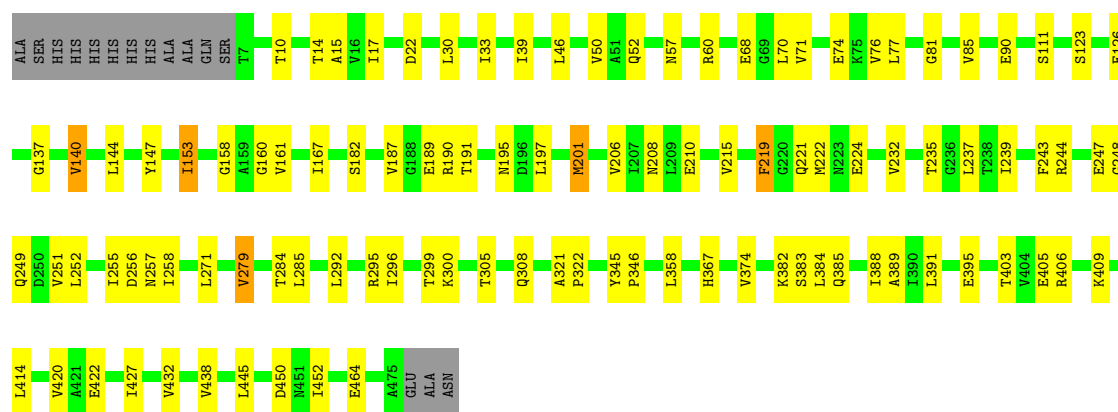
• Molecule 2: ATP synthase subunit beta

Chain W:  77% 18% ..

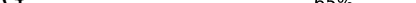


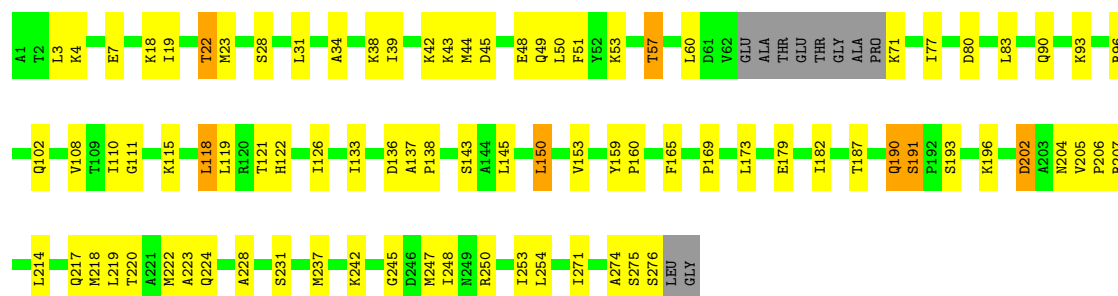
- Molecule 2: ATP synthase subunit beta

Chain X:  75% 21% ..

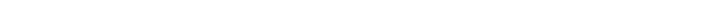


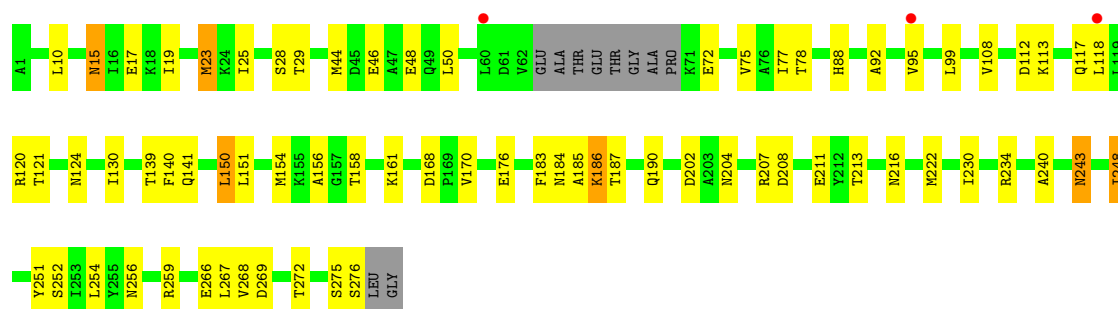
- Molecule 3: ATP synthase subunit gamma

Chain G:  65% 29% . .

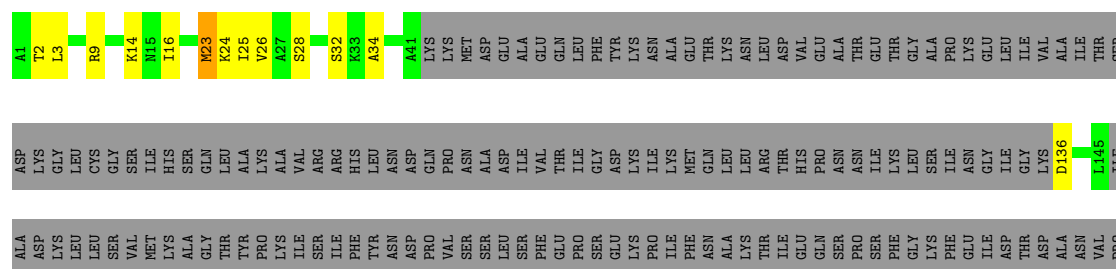


- Molecule 3: ATP synthase subunit gamma

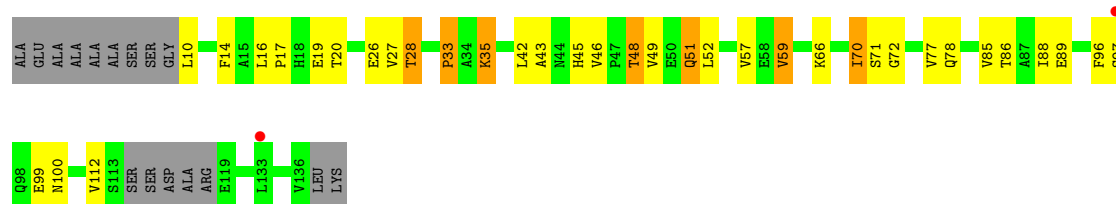
Chain P:  %



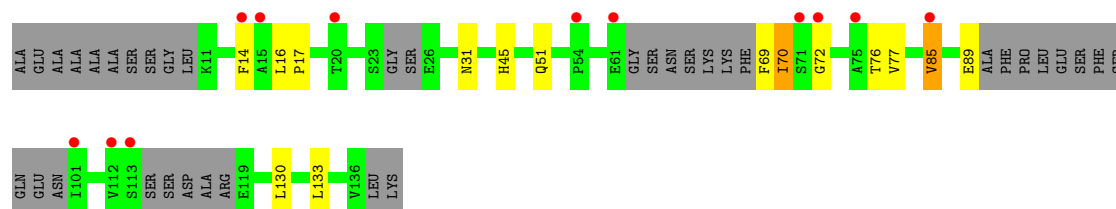
- Molecule 3: ATP synthase subunit gamma



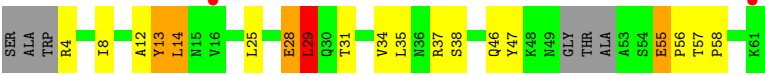
- Molecule 4: ATP synthase subunit delta



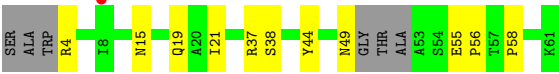
- Molecule 4: ATP synthase subunit delta



- 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	112.02Å 290.62Å 188.47Å 90.00° 102.34° 90.00°	Depositor
Resolution (Å)	50.00 – 3.20 50.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	91.2 (50.00-3.20) 91.4 (50.00-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.4.0066	Depositor
R, R_{free}	0.210 , 0.276 0.211 , 0.274	Depositor DCC
R_{free} test set	3557 reflections (1.84%)	wwPDB-VP
Wilson B-factor (Å ²)	90.9	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 60.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	70481	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% 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	0.55	0/3748	0.89	0/5073
1	B	0.56	1/3747 (0.0%)	0.88	4/5073 (0.1%)
1	C	0.54	1/3736 (0.0%)	0.89	4/5057 (0.1%)
1	J	0.51	0/3718	0.86	1/5032 (0.0%)
1	K	0.52	0/3630	0.86	5/4926 (0.1%)
1	L	0.53	0/3662	0.88	1/4963 (0.0%)
1	S	0.55	1/3696 (0.0%)	0.90	2/5008 (0.0%)
1	T	0.54	0/3693	0.86	1/5006 (0.0%)
1	U	0.54	1/3564 (0.0%)	0.85	0/4850
2	D	0.55	0/3601	0.90	6/4884 (0.1%)
2	E	0.58	0/3567	0.91	0/4846
2	F	0.55	0/3595	0.93	3/4876 (0.1%)
2	M	0.56	0/3492	0.90	4/4747 (0.1%)
2	N	0.54	0/3457	0.88	2/4708 (0.0%)
2	O	0.53	0/3505	0.88	1/4774 (0.0%)
2	V	0.59	0/2623	0.88	0/3585
2	W	0.58	0/3524	0.92	4/4796 (0.1%)
2	X	0.55	0/3503	0.88	3/4774 (0.1%)
3	G	0.52	0/2089	0.94	4/2812 (0.1%)
3	P	0.55	0/1892	0.88	0/2586
3	Y	0.59	0/791	0.93	0/1077
4	H	0.59	0/827	0.99	3/1133 (0.3%)
4	Q	0.64	0/629	0.87	0/866
5	I	0.66	0/393	1.07	1/537 (0.2%)
5	R	0.66	0/372	0.85	0/510
All	All	0.55	4/71054 (0.0%)	0.89	49/96499 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	444	VAL	CA-CB	9.18	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S	444	VAL	CA-CB	8.34	1.59	1.53
1	U	340	ILE	CA-CB	6.97	1.58	1.54
1	C	444	VAL	CA-CB	5.33	1.57	1.54

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	444	VAL	N-CA-CB	7.39	115.16	110.50
4	H	97	SER	N-CA-C	7.36	119.71	107.20
1	B	444	VAL	N-CA-CB	6.84	114.81	110.50
5	I	29	LEU	N-CA-C	6.45	118.37	109.54
1	S	392	LEU	N-CA-C	6.22	117.86	111.14
1	C	99	VAL	N-CA-C	6.22	114.29	109.19
2	N	215	VAL	N-CA-C	6.09	115.86	108.06
2	F	215	VAL	N-CA-C	5.96	116.66	107.78
3	G	159	TYR	CA-C-N	5.95	125.66	119.05
3	G	159	TYR	C-N-CA	5.95	125.66	119.05
2	X	81	GLY	CA-C-N	5.92	127.24	119.84
2	X	81	GLY	C-N-CA	5.92	127.24	119.84
2	F	81	GLY	CA-C-N	5.90	126.23	119.92
2	F	81	GLY	C-N-CA	5.90	126.23	119.92
2	X	219	PHE	N-CA-C	5.90	119.08	109.06
2	O	96	ILE	N-CA-C	5.88	116.59	108.12
3	G	137	ALA	CA-C-N	5.88	125.84	119.78
3	G	137	ALA	C-N-CA	5.88	125.84	119.78
2	N	219	PHE	N-CA-C	5.86	118.44	108.02
2	D	452	ILE	CA-C-N	5.84	127.14	119.84
2	D	452	ILE	C-N-CA	5.84	127.14	119.84
2	D	330	ASP	N-CA-C	-5.77	106.28	113.55
1	B	102	GLY	CA-C-N	5.71	125.33	119.56
1	B	102	GLY	C-N-CA	5.71	125.33	119.56
1	C	121	GLY	CA-C-N	5.70	125.65	119.78
1	C	121	GLY	C-N-CA	5.70	125.65	119.78
2	M	120	ASP	CA-C-N	5.62	123.76	119.66
2	M	120	ASP	C-N-CA	5.62	123.76	119.66
1	K	102	GLY	CA-C-N	5.57	124.92	118.85
1	K	102	GLY	C-N-CA	5.57	124.92	118.85
2	D	133	ILE	N-CA-C	5.44	116.55	108.23
2	M	432	VAL	N-CA-C	5.33	116.28	109.30
4	H	28	THR	N-CA-C	5.23	117.89	111.82
1	J	355	GLU	N-CA-C	5.21	117.91	108.69
1	L	334	GLY	N-CA-C	-5.21	108.13	115.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	289	ARG	CA-C-N	5.17	125.71	120.38
1	K	289	ARG	C-N-CA	5.17	125.71	120.38
2	W	339	ILE	N-CA-C	-5.17	106.64	111.45
1	K	72	GLN	N-CA-C	5.15	116.89	109.07
2	W	29	GLU	N-CA-C	-5.13	105.38	113.02
4	H	26	GLU	N-CA-C	5.12	116.94	107.73
1	B	238	ALA	N-CA-C	5.11	117.59	111.71
2	M	10	THR	N-CA-C	5.07	117.71	109.24
2	D	107	GLY	CA-C-N	5.06	125.05	119.89
2	D	107	GLY	C-N-CA	5.06	125.05	119.89
1	T	237	THR	N-CA-C	5.04	117.04	110.53
2	W	215	VAL	N-CA-C	5.03	115.72	108.48
1	C	47	ASN	N-CA-C	5.03	117.41	111.33
2	W	140	VAL	CB-CA-C	-5.01	105.48	112.04

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	3691	0	3777	87	0
1	B	3690	0	3771	67	0
1	C	3680	0	3768	48	0
1	J	3664	0	3752	71	0
1	K	3578	0	3577	61	0
1	L	3608	0	3668	69	0
1	S	3642	0	3697	62	0
1	T	3639	0	3673	65	0
1	U	3511	0	3411	49	0
2	D	3545	0	3614	67	0
2	E	3511	0	3549	82	0
2	F	3539	0	3611	69	0
2	M	3436	0	3459	83	0
2	N	3403	0	3385	78	0
2	O	3449	0	3435	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	V	2582	0	2492	66	0
2	W	3468	0	3463	61	0
2	X	3447	0	3402	62	0
3	G	2064	0	2125	46	0
3	P	1869	0	1710	36	0
3	Y	790	0	735	20	0
4	H	815	0	712	26	0
4	Q	625	0	501	6	0
5	I	388	0	344	19	0
5	R	367	0	301	8	0
6	A	31	0	13	0	0
6	B	31	0	13	2	0
6	C	31	0	13	3	0
6	D	31	0	13	2	0
6	F	31	0	13	3	0
6	J	31	0	13	3	0
6	K	31	0	13	1	0
6	L	31	0	13	0	0
6	M	31	0	13	3	0
6	O	31	0	13	0	0
6	S	31	0	13	0	0
6	T	31	0	13	2	0
6	U	31	0	13	0	0
6	V	31	0	13	2	0
6	X	31	0	13	2	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
7	F	1	0	0	0	0
7	J	1	0	0	0	0
7	K	1	0	0	0	0
7	L	1	0	0	0	0
7	M	1	0	0	0	0
7	O	1	0	0	0	0
7	S	1	0	0	0	0
7	T	1	0	0	0	0
7	U	1	0	0	0	0
7	V	1	0	0	0	0
7	X	1	0	0	0	0
All	All	70481	0	70127	1260	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 9.

All (1260) 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)
6:F:600:ANP:H5'1	6:F:600:ANP:H8	1.26	1.16
3:G:96:ARG:HE	3:G:121:THR:HG21	1.25	1.01
2:D:85:VAL:HG11	2:D:235:THR:HG23	1.42	1.00
5:I:31:THR:HG22	5:I:34:VAL:HG23	1.45	0.98
1:T:289:ARG:HG2	1:T:289:ARG:HH11	1.23	0.98
2:E:85:VAL:HG11	2:E:235:THR:HG23	1.46	0.96
2:V:85:VAL:HG11	2:V:235:THR:HG23	1.47	0.95
4:H:72:GLY:HA3	5:I:14:LEU:HD21	1.47	0.95
2:M:85:VAL:HG11	2:M:235:THR:HG23	1.48	0.95
1:A:397:ALA:HA	1:A:400:ARG:NE	1.81	0.94
2:F:192:ARG:HG2	2:F:192:ARG:HH11	1.31	0.92
2:M:160:GLY:H	6:M:600:ANP:HNB1	1.11	0.92
2:W:168:GLN:NE2	2:W:204:THR:HG21	1.84	0.92
3:G:19:ILE:HG22	3:G:23:MET:HE2	1.53	0.90
2:W:168:GLN:HE21	2:W:204:THR:HG21	1.34	0.89
2:N:68:GLU:HG2	2:N:68:GLU:O	1.69	0.89
5:I:46:GLN:HB3	5:I:56:PRO:HG2	1.55	0.89
1:A:112:ALA:O	1:A:251:THR:HG21	1.71	0.88
2:F:15:ALA:HB3	2:F:22:ASP:HB2	1.56	0.88
1:A:397:ALA:HA	1:A:400:ARG:CZ	2.04	0.87
2:X:85:VAL:HG11	2:X:235:THR:HG23	1.54	0.87
4:H:35:LYS:HD2	4:H:51:GLN:HG3	1.55	0.86
2:D:160:GLY:H	6:D:600:ANP:HNB1	1.22	0.86
2:W:85:VAL:HG11	2:W:235:THR:HG23	1.57	0.86
1:A:142:ARG:HA	2:E:199:ARG:HH12	1.40	0.85
2:X:197:LEU:O	2:X:201:MET:HG2	1.77	0.85
4:H:14:PHE:HZ	4:H:70:ILE:HD11	1.41	0.84
1:S:369:VAL:HG13	1:S:393:LYS:HD3	1.60	0.84
1:J:289:ARG:HD3	1:J:290:PRO:HD2	1.59	0.83
2:F:50:VAL:HA	2:F:61:THR:HG22	1.62	0.82
2:E:15:ALA:HB3	2:E:22:ASP:HB2	1.60	0.82
2:D:244:ARG:HD3	2:D:304:VAL:HG23	1.60	0.81
1:A:146:GLU:HB2	1:A:163:ARG:HG3	1.63	0.81
2:N:85:VAL:HG11	2:N:235:THR:HG23	1.62	0.80
2:D:149:ARG:NH2	2:D:178:HIS:NE2	2.30	0.80
1:A:142:ARG:HG2	2:E:199:ARG:HH22	1.47	0.79
3:G:219:LEU:HD21	4:H:17:PRO:HB3	1.64	0.79
2:M:249:GLN:HE21	2:M:249:GLN:HA	1.48	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:212:ARG:HG3	1:U:237:THR:HG21	1.62	0.79
2:F:344:ILE:HG23	2:F:415:SER:HB3	1.66	0.78
1:J:174:GLN:HA	6:J:600:ANP:HNB1	1.46	0.78
1:T:369:VAL:HG12	1:T:393:LYS:HD2	1.64	0.77
1:S:190:ARG:NH1	1:S:439:ALA:HB2	1.99	0.77
1:T:174:GLN:HA	6:T:600:ANP:HNB1	1.49	0.77
1:T:289:ARG:HG2	1:T:289:ARG:NH1	1.97	0.77
2:M:160:GLY:N	6:M:600:ANP:HNB1	1.81	0.77
1:A:351:GLN:HE22	1:A:375:ARG:HH12	1.31	0.76
1:K:495:LEU:HA	1:K:498:SER:HB3	1.66	0.76
3:P:72:GLU:HG3	3:P:161:LYS:HB3	1.66	0.76
2:M:449:TYR:HD1	2:M:452:ILE:HD12	1.50	0.76
1:A:282:GLN:HG3	2:D:283:PRO:O	1.86	0.76
2:D:299:THR:HG23	2:D:301:LYS:H	1.51	0.76
2:O:174:ILE:HG22	2:O:178:HIS:HB2	1.69	0.75
1:A:219:VAL:HG13	1:A:228:MET:HE3	1.69	0.75
1:S:289:ARG:HH11	1:S:289:ARG:HA	1.52	0.75
2:E:221:GLN:HB2	2:E:223:ASN:OD1	1.87	0.74
1:J:44:PHE:HD2	1:J:45:GLY:N	1.85	0.74
1:C:97:VAL:HG11	1:C:247:LEU:HD21	1.70	0.74
1:L:64:MET:HE3	1:L:97:VAL:HG21	1.70	0.74
5:I:55:GLU:CB	5:I:56:PRO:HD3	2.17	0.74
2:N:39:ILE:HD11	2:N:48:LEU:HD11	1.68	0.74
2:F:85:VAL:HG11	2:F:235:THR:HG23	1.69	0.74
5:I:4:ARG:HG3	5:I:13:TYR:CE2	2.23	0.73
2:F:190:ARG:HB2	2:F:193:GLU:HG3	1.69	0.73
2:V:190:ARG:HB2	2:V:193:GLU:HG3	1.71	0.73
2:X:391:LEU:HB3	2:X:395:GLU:HG3	1.70	0.73
2:W:189:GLU:HA	2:W:260:ARG:HH21	1.54	0.73
1:B:455:LEU:HD23	1:B:458:ILE:HD12	1.71	0.72
5:I:28:GLU:O	5:I:29:LEU:HD13	1.88	0.72
1:A:394:LEU:O	1:A:397:ALA:HB3	1.90	0.72
2:D:7:THR:HG23	2:D:8:PRO:HD3	1.70	0.72
1:T:187:ASN:OD1	1:T:190:ARG:NH1	2.22	0.72
2:F:382:LYS:HA	2:F:385:GLN:HG2	1.72	0.72
2:N:337:ARG:HA	2:N:340:SER:HB3	1.71	0.72
3:P:230:ILE:O	3:P:234:ARG:HG2	1.89	0.72
2:D:222:MET:HA	2:D:229:ARG:HD2	1.72	0.71
5:I:31:THR:HG22	5:I:34:VAL:CG2	2.19	0.71
2:F:202:LYS:HE3	2:F:209:LEU:HD11	1.72	0.71
2:O:189:GLU:O	2:O:221:GLN:HB3	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:25:ILE:HA	3:Y:28:SER:HB2	1.71	0.71
2:O:237:LEU:HD21	2:O:295:ARG:HB2	1.73	0.71
1:B:287:LEU:O	1:B:288:ARG:HB2	1.91	0.71
2:F:192:ARG:HG2	2:F:192:ARG:NH1	2.02	0.71
1:U:99:VAL:HG11	1:U:251:THR:HB	1.72	0.71
1:S:36:VAL:HG12	2:V:53:HIS:HB2	1.72	0.71
2:F:148:ALA:HA	2:F:357:LEU:HD11	1.71	0.70
2:V:154:GLY:HA3	2:V:329:LEU:HD13	1.72	0.70
1:B:174:GLN:HA	6:B:600:ANP:HNB1	1.56	0.70
2:E:140:VAL:HG13	2:E:414:LEU:HD22	1.74	0.70
1:L:397:ALA:HA	1:L:400:ARG:CZ	2.20	0.70
2:M:197:LEU:O	2:M:201:MET:HG2	1.91	0.70
1:B:85:LYS:HE2	2:E:32:ALA:HB2	1.73	0.69
2:F:221:GLN:OE1	2:F:221:GLN:HA	1.92	0.69
3:G:57:THR:HA	3:G:191:SER:HB3	1.72	0.69
2:F:377:THR:HG22	2:F:407:ALA:HB2	1.75	0.69
2:W:242:TYR:CZ	2:W:246:GLU:HG2	2.27	0.69
2:N:419:ALA:HA	2:N:429:GLY:HA3	1.75	0.69
3:P:118:LEU:HA	3:P:121:THR:HG22	1.73	0.69
2:X:158:GLY:O	2:X:161:VAL:HG22	1.91	0.69
1:L:305:SER:HB2	2:M:222:MET:HB2	1.75	0.69
1:K:187:ASN:HB2	1:K:437:PRO:HB3	1.75	0.68
5:I:46:GLN:HB3	5:I:56:PRO:CG	2.22	0.68
1:A:369:VAL:HB	1:A:400:ARG:NH1	2.09	0.68
1:L:239:SER:HB3	2:O:294:GLU:HG3	1.76	0.68
2:N:220:GLY:HA3	2:N:232:VAL:HG21	1.74	0.68
2:N:384:LEU:HD22	2:N:387:ILE:HD11	1.74	0.68
1:S:383:LYS:HD3	1:S:490:GLU:OE2	1.94	0.67
1:L:187:ASN:OD1	1:L:437:PRO:HB2	1.94	0.67
3:G:51:PHE:CE1	4:H:49:VAL:HG21	2.29	0.67
2:F:398:GLU:HA	2:F:398:GLU:OE1	1.94	0.67
1:A:397:ALA:O	1:A:400:ARG:HG3	1.95	0.67
2:O:85:VAL:HG11	2:O:235:THR:HG23	1.76	0.67
2:N:244:ARG:HD3	2:N:304:VAL:HG23	1.77	0.66
2:V:9:ILE:HB	2:V:78:ASP:HB3	1.77	0.66
2:E:169:GLU:OE1	2:E:420:VAL:HG22	1.95	0.66
1:L:98:ASP:HB2	1:L:129:SER:O	1.95	0.66
2:M:249:GLN:HG3	2:M:250:ASP:H	1.61	0.66
2:N:189:GLU:OE2	2:N:221:GLN:HA	1.96	0.66
2:W:202:LYS:HD3	2:W:209:LEU:HD11	1.78	0.66
1:J:168:LEU:HD12	1:J:327:PRO:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:92:ARG:HH21	1:K:94:GLY:HA2	1.60	0.66
2:W:50:VAL:HA	2:W:61:THR:HG22	1.77	0.66
2:D:250:ASP:OD2	2:D:303:SER:HB2	1.96	0.65
3:G:45:ASP:OD1	3:G:220:THR:HG21	1.96	0.65
1:B:422:ARG:HH21	1:B:453:GLY:HA3	1.61	0.65
2:V:244:ARG:HD3	2:V:304:VAL:HG23	1.77	0.65
1:J:44:PHE:CD2	1:J:45:GLY:N	2.65	0.65
2:M:133:ILE:HG12	2:M:134:LEU:N	2.10	0.65
2:M:15:ALA:HB3	2:M:22:ASP:HB2	1.78	0.65
2:X:237:LEU:HD13	2:X:296:ILE:HG12	1.77	0.65
1:B:203:CYS:HB2	1:B:231:SER:HB3	1.78	0.65
1:T:364:ARG:HA	1:T:365:PRO:C	2.22	0.65
2:O:398:GLU:HB2	3:P:120:ARG:HD3	1.79	0.65
2:F:115:LYS:HE3	2:F:238:THR:HG22	1.78	0.64
2:D:9:ILE:HD12	2:D:9:ILE:H	1.61	0.64
2:D:160:GLY:N	6:D:600:ANP:HNB1	1.91	0.64
3:P:141:GLN:HG3	5:R:15:ASN:HD21	1.62	0.64
2:O:41:THR:HB	2:O:42:PRO:HD2	1.79	0.64
1:T:64:MET:HE3	1:T:66:LEU:HD13	1.79	0.64
1:U:69:GLU:HB3	1:U:70:PRO:HD2	1.78	0.64
2:N:53:HIS:HD2	2:N:59:VAL:HG12	1.62	0.64
2:N:204:THR:OG1	2:N:420:VAL:HB	1.97	0.64
5:I:46:GLN:O	5:I:56:PRO:HD2	1.97	0.64
2:X:30:LEU:HD21	2:X:57:ASN:HA	1.78	0.64
2:V:174:ILE:O	2:V:178:HIS:HB2	1.98	0.63
1:T:239:SER:HB2	2:W:291:LEU:HD23	1.80	0.63
1:T:416:THR:HA	1:T:419:THR:HG23	1.80	0.63
1:L:369:VAL:HB	1:L:400:ARG:HH12	1.63	0.63
2:W:142:ASP:HB3	2:W:434:LEU:HD12	1.79	0.63
3:Y:9:ARG:HD3	3:Y:251:TYR:CE1	2.32	0.63
1:A:168:LEU:HB2	1:A:348:THR:HG21	1.79	0.63
1:S:243:PRO:HG3	1:S:283:LEU:HD21	1.80	0.63
1:B:142:ARG:HB2	1:B:315:SER:HA	1.80	0.63
1:K:166:ARG:HD3	1:K:308:LEU:O	1.99	0.63
1:K:248:ALA:HB3	1:K:249:PRO:HD3	1.81	0.63
2:E:221:GLN:H	2:E:221:GLN:HE21	1.47	0.63
1:B:369:VAL:H	1:B:400:ARG:HH12	1.47	0.62
1:K:455:LEU:HA	1:K:458:ILE:HD12	1.79	0.62
1:T:174:GLN:HA	6:T:600:ANP:N3B	2.14	0.62
1:B:338:ALA:HB3	1:B:341:PRO:HG2	1.81	0.62
1:A:109:VAL:HB	1:A:118:ASP:HB3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:237:LEU:HD21	2:M:295:ARG:HB2	1.81	0.62
2:E:152:LYS:HD3	2:E:328:HIS:O	1.99	0.62
2:O:47:VAL:HG21	2:O:99:ILE:HG21	1.81	0.62
2:E:98:VAL:HG23	2:E:232:VAL:HA	1.80	0.62
2:F:377:THR:HG23	2:F:403:THR:HG22	1.81	0.62
2:W:258:ILE:HG22	2:W:309:ALA:O	2.00	0.62
1:J:393:LYS:O	1:J:397:ALA:HB2	1.99	0.62
1:L:222:LEU:HB2	1:L:228:MET:HE2	1.80	0.62
1:J:248:ALA:HB3	1:J:249:PRO:HD3	1.80	0.62
2:W:188:GLY:C	2:W:260:ARG:HE	2.07	0.62
2:V:243:PHE:HB3	2:V:249:GLN:HE21	1.64	0.62
2:W:158:GLY:H	2:W:337:ARG:HH12	1.47	0.62
4:H:16:LEU:HD12	4:H:19:GLU:HB3	1.82	0.62
1:A:174:GLN:HB3	2:D:354:LYS:HD2	1.82	0.61
2:N:390:ILE:HG21	3:P:28:SER:HB3	1.82	0.61
2:O:387:ILE:HG23	2:O:391:LEU:HD12	1.80	0.61
3:P:130:ILE:HD13	5:R:44:TYR:HB3	1.81	0.61
6:F:600:ANP:H8	6:F:600:ANP:C5'	2.18	0.61
2:M:7:THR:N	2:M:8:PRO:HD3	2.15	0.61
2:X:160:GLY:H	6:X:600:ANP:HNB1	1.47	0.61
2:M:367:HIS:CD2	2:M:434:LEU:HD21	2.35	0.61
1:U:153:LYS:HG2	1:U:432:GLN:OE1	2.00	0.61
2:M:346:PRO:HB2	2:M:348:VAL:HG23	1.83	0.61
2:N:344:ILE:HG23	2:N:415:SER:HB3	1.81	0.61
1:U:67:ILE:HD12	1:U:287:LEU:HD22	1.81	0.61
1:U:364:ARG:HA	1:U:365:PRO:C	2.25	0.61
1:L:369:VAL:HB	1:L:400:ARG:NH1	2.15	0.61
2:X:382:LYS:HA	2:X:385:GLN:HG2	1.82	0.61
2:N:135:GLU:OE2	2:N:433:ARG:HD3	2.01	0.61
3:Y:136:ASP:HB3	3:Y:226:TYR:HE1	1.65	0.61
2:D:128:SER:HB2	2:D:300:LYS:HG2	1.83	0.61
2:E:185:THR:HA	2:E:218:VAL:O	2.01	0.61
2:N:255:ILE:HB	2:N:308:GLN:HG2	1.82	0.61
1:J:469:SER:O	1:J:473:TYR:HB3	2.02	0.60
3:P:184:ASN:HD21	3:P:186:LYS:HD3	1.65	0.60
2:F:141:VAL:HG22	2:F:333:THR:HG21	1.82	0.60
2:M:229:ARG:NH2	2:M:267:GLU:OE1	2.28	0.60
2:E:337:ARG:HA	2:E:340:SER:HB3	1.83	0.60
2:X:147:TYR:CE1	2:X:153:ILE:HG21	2.36	0.60
1:B:174:GLN:HA	6:B:600:ANP:N3B	2.16	0.60
2:E:168:GLN:NE2	2:E:201:MET:HA	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:382:LYS:HA	2:O:385:GLN:HG2	1.82	0.60
4:H:52:LEU:HD11	4:H:85:VAL:HG13	1.82	0.60
2:V:243:PHE:HA	2:V:247:GLU:HG3	1.84	0.60
1:U:455:LEU:HA	1:U:458:ILE:HD12	1.82	0.60
2:X:244:ARG:O	2:X:248:GLY:HA2	2.01	0.60
1:U:345:ILE:HG12	1:U:351:GLN:HG2	1.83	0.60
1:A:145:HIS:CD2	1:A:146:GLU:HG3	2.37	0.59
3:G:60:LEU:HD23	3:G:187:THR:HA	1.84	0.59
1:S:40:ILE:HD12	1:S:287:LEU:HG	1.83	0.59
2:V:143:LEU:HA	2:V:367:HIS:CE1	2.37	0.59
2:W:136:THR:HG23	2:W:138:ILE:H	1.67	0.59
2:O:242:TYR:CE1	2:O:246:GLU:HG3	2.37	0.59
2:N:98:VAL:HG13	2:N:99:ILE:HG23	1.84	0.59
2:N:86:PRO:HD3	2:N:114:ARG:NH1	2.18	0.59
1:U:67:ILE:HG12	2:V:17:ILE:HG23	1.83	0.59
2:E:204:THR:CG2	2:E:206:VAL:HG22	2.32	0.59
1:A:26:ASN:O	1:A:27:LEU:HB2	2.02	0.59
1:B:483:THR:HG23	1:B:486:ARG:HH12	1.66	0.59
1:U:354:LEU:HA	1:U:366:ALA:O	2.02	0.59
1:J:26:ASN:O	1:J:27:LEU:HB2	2.02	0.59
1:J:44:PHE:HD2	1:J:45:GLY:H	1.50	0.59
1:U:376:VAL:HG11	1:U:380:ALA:HB3	1.84	0.59
6:F:600:ANP:H5'1	6:F:600:ANP:C8	2.17	0.59
2:N:334:VAL:HG21	2:N:352:ASP:HB3	1.85	0.59
2:E:229:ARG:NH2	2:E:267:GLU:OE1	2.36	0.59
5:I:55:GLU:CB	5:I:56:PRO:CD	2.80	0.59
2:M:201:MET:HE3	2:M:217:LEU:HD21	1.85	0.59
1:S:54:LEU:HD12	1:S:64:MET:HB3	1.85	0.59
1:A:425:ARG:HD3	1:A:456:ASP:HA	1.84	0.58
4:H:27:VAL:CG1	4:H:59:VAL:HG13	2.33	0.58
1:L:382:VAL:HG11	1:L:440:THR:HG21	1.85	0.58
1:T:478:HIS:HB3	1:T:481:LEU:HG	1.84	0.58
2:X:384:LEU:O	2:X:388:ILE:HG12	2.02	0.58
1:B:92:ARG:HH21	1:B:94:GLY:HA2	1.67	0.58
1:C:55:VAL:HG21	1:C:75:ILE:HD13	1.86	0.58
2:F:152:LYS:HD2	2:F:296:ILE:O	2.02	0.58
2:F:336:SER:HB3	2:F:339:ILE:HD12	1.83	0.58
2:X:140:VAL:HG13	2:X:414:LEU:HD22	1.84	0.58
2:V:269:SER:OG	2:V:282:GLN:HB3	2.03	0.58
2:V:299:THR:HG23	2:V:301:LYS:H	1.67	0.58
2:W:345:TYR:HA	2:W:346:PRO:C	2.28	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:50:GLN:HB3	2:D:69:GLY:HA2	1.86	0.58
1:C:354:LEU:HA	1:C:366:ALA:O	2.04	0.58
1:T:455:LEU:HA	1:T:458:ILE:HD12	1.86	0.58
2:V:172:ASN:OD1	2:V:204:THR:HG21	2.03	0.58
2:E:86:PRO:HG2	2:E:109:ILE:HD13	1.85	0.58
3:G:44:MET:HE3	4:H:86:THR:HB	1.85	0.58
2:X:221:GLN:HA	2:X:221:GLN:OE1	2.04	0.58
1:B:159:VAL:HG21	1:B:352:ILE:HG12	1.86	0.58
1:C:146:GLU:HB2	1:C:163:ARG:HD2	1.86	0.58
1:C:174:GLN:HA	6:C:600:ANP:HNB1	1.68	0.58
2:F:171:ILE:O	2:F:175:ALA:HB3	2.02	0.58
1:S:192:ASN:HA	1:S:200:LYS:HG2	1.86	0.58
1:U:382:VAL:HG11	1:U:440:THR:HG21	1.86	0.58
2:E:133:ILE:HD12	2:E:146:PRO:HB2	1.85	0.58
2:N:50:VAL:HA	2:N:61:THR:HG22	1.85	0.58
1:T:96:ILE:HG13	1:T:130:ARG:NH2	2.18	0.58
1:B:46:LEU:O	1:B:49:ILE:HG22	2.03	0.58
1:C:99:VAL:HG11	1:C:251:THR:HB	1.85	0.58
2:M:201:MET:CE	2:M:217:LEU:HD21	2.34	0.58
2:V:202:LYS:NZ	2:V:209:LEU:HD21	2.19	0.58
2:W:98:VAL:HG13	2:W:99:ILE:HG23	1.86	0.58
2:D:95:ILE:HG22	2:D:103:ILE:HG13	1.86	0.57
1:K:85:LYS:HG2	2:N:53:HIS:HE1	1.68	0.57
1:L:429:LEU:HD21	1:L:446:LEU:O	2.04	0.57
2:V:202:LYS:HZ2	2:V:209:LEU:HD21	1.68	0.57
1:A:396:LEU:O	1:A:400:ARG:HG3	2.04	0.57
1:B:272:ASP:HB2	1:B:328:VAL:O	2.04	0.57
2:E:168:GLN:HE21	2:E:201:MET:HA	1.68	0.57
1:L:284:SER:OG	1:L:297:PRO:HG3	2.04	0.57
2:N:39:ILE:HG12	2:N:76:VAL:HG22	1.86	0.57
2:W:419:ALA:O	2:W:422:GLU:HB2	2.04	0.57
2:N:168:GLN:HA	2:N:171:ILE:HD12	1.86	0.57
1:B:49:ILE:HG13	1:B:53:GLU:CD	2.30	0.57
1:J:81:ASP:HB2	2:M:33:ILE:HD12	1.87	0.57
1:L:345:ILE:HG23	1:L:351:GLN:HG2	1.85	0.57
2:O:208:ASN:ND2	2:O:211:GLY:H	2.03	0.57
5:I:46:GLN:C	5:I:56:PRO:HD2	2.30	0.57
1:J:492:SER:HB2	1:J:495:LEU:H	1.69	0.57
1:L:358:LEU:HB2	1:L:366:ALA:HB1	1.85	0.57
2:O:197:LEU:O	2:O:201:MET:HG2	2.04	0.57
1:A:305:SER:HB2	2:E:222:MET:HG2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:VAL:CG1	1:A:393:LYS:HG3	2.35	0.57
4:H:14:PHE:CZ	4:H:70:ILE:HD11	2.32	0.57
4:H:27:VAL:HG11	4:H:59:VAL:HG13	1.86	0.57
2:M:367:HIS:HD2	2:M:434:LEU:HD21	1.68	0.57
2:X:345:TYR:HA	2:X:346:PRO:C	2.30	0.57
1:A:302:TYR:O	1:A:306:ARG:HB2	2.04	0.56
1:A:369:VAL:HG12	1:A:393:LYS:HG3	1.86	0.56
1:T:368:ASN:OD1	1:T:368:ASN:C	2.48	0.56
3:G:96:ARG:HG2	3:G:122:HIS:HE1	1.70	0.56
2:M:28:SER:C	2:M:30:LEU:H	2.12	0.56
1:A:50:GLN:HB3	2:E:69:GLY:HA2	1.87	0.56
2:D:204:THR:HB	2:D:206:VAL:HG23	1.88	0.56
2:D:366:GLU:O	2:D:370:VAL:HG23	2.05	0.56
3:G:44:MET:CE	4:H:86:THR:HB	2.36	0.56
2:M:90:GLU:HG3	2:M:111:SER:HA	1.88	0.56
1:S:38:ASP:HB3	1:S:286:LEU:HD22	1.86	0.56
3:G:45:ASP:CG	3:G:220:THR:HG21	2.29	0.56
1:L:302:TYR:O	1:L:306:ARG:HG2	2.06	0.56
2:N:15:ALA:HB3	2:N:22:ASP:HB2	1.87	0.56
2:V:243:PHE:HA	2:V:247:GLU:CG	2.35	0.56
3:Y:23:MET:HA	3:Y:23:MET:HE3	1.87	0.56
2:D:201:MET:CE	2:D:217:LEU:HD21	2.34	0.56
3:G:50:LEU:HG	4:H:78:GLN:NE2	2.20	0.56
2:V:258:ILE:O	2:V:261:PHE:HB3	2.05	0.56
2:D:201:MET:HE3	2:D:217:LEU:HD21	1.87	0.56
2:O:234:LEU:HD23	2:O:292:LEU:HD13	1.86	0.56
1:L:273:LEU:HB3	1:L:304:HIS:NE2	2.21	0.56
2:M:142:ASP:HB3	2:M:434:LEU:HD12	1.87	0.56
3:G:34:ALA:O	3:G:38:LYS:HB2	2.06	0.56
1:K:138:ILE:HD13	2:O:103:ILE:HD12	1.88	0.56
2:M:148:ALA:HA	2:M:357:LEU:HD11	1.88	0.56
1:S:51:ALA:HB3	2:W:69:GLY:H	1.70	0.56
2:V:154:GLY:HA3	2:V:329:LEU:CD1	2.36	0.56
1:T:99:VAL:HG11	1:T:251:THR:HB	1.87	0.56
2:M:258:ILE:HG22	2:M:310:VAL:HG22	1.88	0.55
2:E:95:ILE:HG22	2:E:103:ILE:HG13	1.88	0.55
1:L:192:ASN:HA	1:L:200:LYS:HG2	1.87	0.55
1:L:297:PRO:HB2	1:L:299:ASP:OD1	2.07	0.55
1:S:36:VAL:HG13	2:V:33:ILE:HD11	1.88	0.55
1:U:105:LEU:HG	1:U:123:ILE:HG21	1.87	0.55
2:V:143:LEU:HA	2:V:367:HIS:HE1	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:133:ILE:HD12	2:W:146:PRO:HB2	1.89	0.55
2:O:41:THR:HB	2:O:42:PRO:CD	2.37	0.55
3:P:272:THR:O	3:P:275:SER:HB2	2.06	0.55
1:T:85:LYS:HE2	2:W:32:ALA:HB2	1.88	0.55
1:J:302:TYR:O	1:J:306:ARG:HB2	2.06	0.55
2:D:415:SER:HB2	2:D:459:MET:H	1.71	0.55
2:E:164:THR:HB	2:E:200:GLU:OE1	2.06	0.55
1:K:85:LYS:HE2	2:N:32:ALA:HB2	1.89	0.55
1:A:97:VAL:HG11	1:A:247:LEU:HD13	1.89	0.55
1:J:81:ASP:OD1	1:J:81:ASP:N	2.36	0.55
1:L:397:ALA:HA	1:L:400:ARG:NH2	2.21	0.55
2:M:366:GLU:O	2:M:370:VAL:HG23	2.07	0.55
2:N:337:ARG:H	2:N:337:ARG:HE	1.54	0.55
3:P:140:PHE:HE2	3:P:216:ASN:HD22	1.55	0.55
1:U:69:GLU:HB3	1:U:70:PRO:CD	2.37	0.55
2:D:171:ILE:O	2:D:175:ALA:HB3	2.07	0.55
2:E:234:LEU:HD23	2:E:292:LEU:HD12	1.89	0.55
1:B:109:VAL:HG22	1:B:233:ILE:HB	1.88	0.55
3:G:138:PRO:HG3	3:G:223:ALA:HA	1.89	0.55
1:T:343:ASN:O	1:T:347:ILE:HG13	2.07	0.55
2:F:237:LEU:HD13	2:F:296:ILE:HG12	1.88	0.55
1:J:288:ARG:NH2	2:M:273:GLY:O	2.39	0.55
2:E:243:PHE:HB2	2:E:251:VAL:HG21	1.88	0.54
1:S:455:LEU:CD2	1:S:458:ILE:HD12	2.37	0.54
1:U:346:SER:HB3	2:V:260:ARG:HH12	1.72	0.54
1:A:401:GLU:HG3	1:A:402:VAL:N	2.22	0.54
2:E:188:GLY:HA3	2:E:260:ARG:HD2	1.88	0.54
1:L:142:ARG:HA	2:M:199:ARG:NH2	2.21	0.54
2:M:433:ARG:O	2:M:436:ASP:HB2	2.07	0.54
1:K:46:LEU:O	1:K:49:ILE:HG22	2.07	0.54
1:K:293:ARG:HD2	1:K:339:TYR:CD1	2.42	0.54
1:L:68:LEU:HB3	2:M:72:ARG:HD3	1.89	0.54
1:T:192:ASN:HA	1:T:200:LYS:HG2	1.90	0.54
1:A:57:PHE:HB2	1:A:61:VAL:HG12	1.89	0.54
1:K:260:ARG:O	1:K:321:GLY:HA3	2.08	0.54
1:L:250:PHE:CD1	1:L:307:LEU:HD13	2.41	0.54
2:M:89:ARG:NH1	2:M:247:GLU:OE1	2.40	0.54
1:T:308:LEU:HD12	1:T:347:ILE:HG21	1.90	0.54
2:F:90:GLU:HG3	2:F:111:SER:HA	1.89	0.54
1:J:455:LEU:HD23	1:J:458:ILE:HD12	1.88	0.54
1:C:153:LYS:NZ	1:C:467:GLU:OE1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:174:GLN:HB2	2:F:354:LYS:HE2	1.90	0.54
2:O:285:LEU:HD23	2:O:285:LEU:C	2.33	0.54
1:S:52:GLU:O	1:S:97:VAL:HG23	2.08	0.54
1:T:348:THR:O	2:X:190:ARG:NH2	2.40	0.54
1:A:174:GLN:CB	2:D:354:LYS:HD2	2.38	0.54
3:G:28:SER:HA	3:G:31:LEU:HB2	1.90	0.54
2:N:321:ALA:HB3	2:N:322:PRO:CD	2.38	0.54
2:E:16:VAL:HG21	2:E:70:LEU:HB3	1.88	0.54
3:G:205:VAL:N	3:G:206:PRO:CD	2.71	0.54
1:L:470:PHE:CE2	1:L:474:LEU:HD11	2.42	0.54
2:M:244:ARG:HD3	2:M:304:VAL:HG23	1.90	0.54
1:A:369:VAL:HB	1:A:400:ARG:HH12	1.72	0.53
2:D:184:PHE:CD1	2:D:184:PHE:C	2.85	0.53
1:B:166:ARG:NH2	1:B:349:ASP:OD1	2.41	0.53
1:J:174:GLN:HA	6:J:600:ANP:N3B	2.20	0.53
1:J:387:GLN:NE2	1:J:491:LEU:HB2	2.23	0.53
2:D:95:ILE:HG22	2:D:103:ILE:CG1	2.39	0.53
1:K:50:GLN:HB3	2:O:69:GLY:HA2	1.89	0.53
2:V:89:ARG:HG2	2:V:92:LEU:HD12	1.91	0.53
1:J:29:GLU:O	1:J:92:ARG:HG3	2.09	0.53
2:V:87:VAL:HG12	2:V:239:ILE:HA	1.90	0.53
2:V:198:TYR:O	2:V:202:LYS:HG2	2.08	0.53
1:J:397:ALA:HA	1:J:400:ARG:NH2	2.24	0.53
1:K:38:ASP:HB3	1:K:286:LEU:HD22	1.89	0.53
1:L:293:ARG:HD2	1:L:339:TYR:CD2	2.43	0.53
2:M:89:ARG:HH11	2:M:181:PHE:HZ	1.54	0.53
1:B:355:GLU:HG3	1:B:368:ASN:HB2	1.90	0.53
1:C:77:LEU:CD1	1:C:81:ASP:HB3	2.38	0.53
1:S:364:ARG:HA	1:S:365:PRO:C	2.33	0.53
1:T:101:VAL:HG12	1:T:255:ILE:HA	1.91	0.53
1:T:142:ARG:NH1	1:T:143:SER:O	2.41	0.53
1:C:481:LEU:HD21	1:C:498:SER:HB3	1.91	0.53
2:D:64:MET:HE1	2:D:231:ARG:HB2	1.91	0.53
2:F:87:VAL:HG11	2:F:115:LYS:HE2	1.89	0.53
3:G:218:MET:O	3:G:222:MET:HG3	2.08	0.53
2:W:189:GLU:CA	2:W:260:ARG:HH21	2.20	0.53
2:D:242:TYR:CE1	2:D:246:GLU:HG3	2.44	0.53
5:R:55:GLU:CB	5:R:56:PRO:CD	2.86	0.53
2:W:49:GLU:HB2	2:W:64:MET:HE3	1.90	0.53
5:I:4:ARG:HG3	5:I:13:TYR:CD2	2.44	0.53
1:K:364:ARG:HA	1:K:365:PRO:C	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:381:GLN:HE21	1:C:385:LEU:HG	1.74	0.52
1:L:358:LEU:HB3	1:L:363:ILE:HD12	1.89	0.52
3:P:88:HIS:CE1	3:P:113:LYS:HB2	2.43	0.52
2:X:52:GLN:HG2	2:X:60:ARG:HB3	1.90	0.52
2:X:126:GLU:O	2:X:299:THR:HA	2.08	0.52
1:L:280:TYR:CE2	1:L:297:PRO:HG2	2.45	0.52
2:N:84:SER:O	2:N:114:ARG:NH2	2.41	0.52
2:V:41:THR:HB	2:V:42:PRO:CD	2.39	0.52
2:E:136:THR:HG21	2:E:141:VAL:HB	1.91	0.52
2:M:9:ILE:HB	2:M:78:ASP:HB3	1.91	0.52
3:Y:14:LYS:HA	3:Y:248:ILE:HD11	1.91	0.52
2:D:33:ILE:O	2:D:34:LEU:HB2	2.09	0.52
1:K:203:CYS:HB2	1:K:231:SER:HA	1.91	0.52
1:L:201:LEU:HD21	1:L:267:LEU:HB2	1.90	0.52
1:A:364:ARG:HA	1:A:365:PRO:C	2.34	0.52
2:D:243:PHE:HD1	2:D:247:GLU:HG3	1.75	0.52
2:E:123:SER:O	2:E:127:GLN:HG2	2.09	0.52
1:J:298:GLY:O	2:N:267:GLU:HG2	2.09	0.52
1:L:40:ILE:CD1	1:L:76:VAL:HG12	2.40	0.52
2:X:39:ILE:HG12	2:X:76:VAL:HG22	1.91	0.52
2:X:206:VAL:HG12	2:X:215:VAL:HG12	1.92	0.52
1:C:109:VAL:HG13	1:C:233:ILE:HB	1.91	0.52
1:L:341:PRO:O	1:L:345:ILE:HG13	2.09	0.52
2:W:391:LEU:HD22	2:W:395:GLU:HG3	1.92	0.52
1:B:450:GLY:HA2	1:B:455:LEU:HD12	1.91	0.52
1:J:473:TYR:CE2	1:J:506:PHE:HB2	2.45	0.52
2:V:33:ILE:O	2:V:34:LEU:HB2	2.08	0.52
2:W:36:ALA:HB2	2:W:83:ILE:HG13	1.91	0.52
2:W:237:LEU:HD22	2:W:292:LEU:HD12	1.91	0.52
1:A:173:ARG:NH2	2:D:352:ASP:OD1	2.43	0.52
4:H:72:GLY:CA	5:I:14:LEU:HD21	2.32	0.52
2:O:417:PRO:HG2	2:O:430:LYS:HG2	1.91	0.52
3:G:49:GLN:HE21	3:G:217:GLN:HE22	1.56	0.52
2:O:384:LEU:O	2:O:388:ILE:HG12	2.09	0.52
2:V:174:ILE:HG22	2:V:252:LEU:HD11	1.92	0.52
2:D:259:PHE:CE1	2:D:313:PRO:HG3	2.45	0.51
5:I:31:THR:CG2	5:I:34:VAL:HG23	2.30	0.51
1:J:289:ARG:HH11	1:J:289:ARG:HA	1.76	0.51
1:J:309:GLU:HG3	2:N:223:ASN:HB3	1.91	0.51
2:M:279:VAL:O	2:M:279:VAL:HG12	2.09	0.51
1:B:227:ALA:HA	1:B:230:TYR:CE2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:197:LEU:O	2:D:201:MET:HG2	2.10	0.51
1:L:250:PHE:CE1	1:L:307:LEU:HB2	2.45	0.51
1:B:168:LEU:HB2	1:B:348:THR:HG21	1.92	0.51
1:L:50:GLN:HB3	2:M:69:GLY:HA2	1.93	0.51
2:V:189:GLU:O	2:V:221:GLN:HB3	2.10	0.51
2:V:192:ARG:HH11	2:V:193:GLU:HG2	1.75	0.51
1:A:444:VAL:N	1:A:445:PRO:HD2	2.26	0.51
2:V:96:ILE:O	2:V:218:VAL:HA	2.10	0.51
2:W:97:ASN:OD1	2:W:97:ASN:C	2.54	0.51
2:X:367:HIS:CD2	2:X:438:VAL:HG21	2.45	0.51
1:K:390:GLY:O	1:K:391:SER:HB2	2.11	0.51
2:M:345:TYR:HA	2:M:346:PRO:C	2.34	0.51
1:S:354:LEU:HA	1:S:366:ALA:O	2.11	0.51
3:Y:24:LYS:HG3	3:Y:238:ASP:HB2	1.93	0.51
1:B:166:ARG:CD	1:B:308:LEU:O	2.59	0.51
1:J:166:ARG:O	1:J:348:THR:HB	2.11	0.51
2:X:239:ILE:O	2:X:243:PHE:HD2	1.94	0.51
1:C:397:ALA:HA	1:C:400:ARG:NH2	2.26	0.51
1:J:396:LEU:O	1:J:400:ARG:HG3	2.11	0.51
2:M:98:VAL:HG23	2:M:232:VAL:HA	1.93	0.51
3:P:240:ALA:HA	3:P:243:ASN:HB3	1.93	0.51
1:T:311:ALA:HA	1:T:323:LEU:HB3	1.92	0.51
2:W:143:LEU:O	2:W:367:HIS:HE1	1.93	0.51
2:W:335:LEU:HA	2:W:347:ALA:O	2.11	0.51
1:A:248:ALA:HB3	1:A:249:PRO:HD3	1.93	0.51
2:D:137:GLY:HA2	2:D:432:VAL:O	2.11	0.51
2:E:456:ALA:HA	2:E:469:LYS:HD3	1.91	0.51
3:P:168:ASP:HB3	3:P:176:GLU:O	2.11	0.51
2:W:200:GLU:O	2:W:204:THR:HB	2.11	0.51
2:F:133:ILE:HD11	2:F:363:VAL:HG12	1.92	0.50
1:J:146:GLU:HB2	1:J:163:ARG:HG3	1.93	0.50
1:J:347:ILE:HA	2:N:222:MET:HE1	1.92	0.50
1:L:248:ALA:HB3	1:L:249:PRO:HD3	1.93	0.50
2:V:182:SER:HB2	2:V:215:VAL:HG23	1.92	0.50
2:E:253:LEU:O	2:E:306:SER:HA	2.11	0.50
2:F:67:THR:HB	2:F:70:LEU:HD12	1.93	0.50
1:T:26:ASN:O	1:T:30:THR:HB	2.11	0.50
2:X:255:ILE:HD12	2:X:308:GLN:HG2	1.93	0.50
1:B:453:GLY:C	1:B:455:LEU:H	2.18	0.50
1:J:201:LEU:HA	1:J:265:HIS:O	2.11	0.50
2:M:185:THR:OG1	2:M:236:GLY:HA3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:48:GLU:OE1	3:P:213:THR:HA	2.11	0.50
1:S:70:PRO:HD3	2:W:15:ALA:HB2	1.93	0.50
1:B:422:ARG:NH2	1:B:453:GLY:HA3	2.24	0.50
2:N:321:ALA:HB3	2:N:322:PRO:HD3	1.94	0.50
1:S:50:GLN:HB2	1:S:53:GLU:HB2	1.94	0.50
1:U:82:ARG:HA	2:X:33:ILE:HB	1.94	0.50
3:Y:215:ALA:HA	3:Y:218:MET:HE3	1.93	0.50
2:D:220:GLY:HA3	2:D:232:VAL:HG11	1.93	0.50
1:L:167:GLU:O	1:L:327:PRO:HD2	2.12	0.50
2:O:398:GLU:HB2	3:P:120:ARG:CD	2.40	0.50
1:S:67:ILE:HG12	2:W:17:ILE:HG23	1.93	0.50
1:S:146:GLU:HB2	1:S:163:ARG:HG3	1.94	0.50
2:F:237:LEU:HD21	2:F:295:ARG:HB2	1.93	0.50
1:J:444:VAL:N	1:J:445:PRO:HD2	2.27	0.50
2:M:357:LEU:HB3	2:M:362:VAL:HG11	1.94	0.50
2:N:9:ILE:HB	2:N:78:ASP:HB3	1.94	0.50
2:W:189:GLU:HA	2:W:260:ARG:NH2	2.25	0.50
1:C:455:LEU:HA	1:C:458:ILE:HD12	1.94	0.50
1:K:149:GLN:HG3	1:K:191:TRP:CH2	2.46	0.50
2:N:36:ALA:HB2	2:N:83:ILE:HG13	1.94	0.50
1:S:176:GLY:O	1:S:180:VAL:HG23	2.12	0.50
1:S:369:VAL:CG1	1:S:393:LYS:HD3	2.39	0.50
1:J:167:GLU:O	1:J:327:PRO:HD2	2.11	0.50
2:M:155:LEU:HB2	2:M:309:ALA:HA	1.93	0.50
2:V:222:MET:HA	2:V:229:ARG:HD2	1.94	0.50
2:F:367:HIS:C	2:F:367:HIS:HD1	2.19	0.50
3:G:50:LEU:HG	4:H:78:GLN:HE21	1.77	0.50
1:U:242:ALA:HB3	1:U:243:PRO:HD3	1.94	0.50
1:A:316:GLU:CD	1:A:316:GLU:H	2.20	0.49
3:G:108:VAL:HG11	3:G:150:LEU:HD11	1.94	0.49
4:H:78:GLN:HA	4:H:78:GLN:OE1	2.12	0.49
2:O:417:PRO:HG2	2:O:430:LYS:CG	2.42	0.49
1:S:302:TYR:O	1:S:306:ARG:HB2	2.12	0.49
1:B:181:ALA:HB1	1:B:269:VAL:HG11	1.94	0.49
2:E:136:THR:HG23	2:E:138:ILE:H	1.77	0.49
2:M:319:ASP:OD1	2:M:320:PRO:HD2	2.12	0.49
1:T:59:SER:HB2	1:T:61:VAL:HG12	1.93	0.49
2:V:345:TYR:HA	2:V:346:PRO:C	2.36	0.49
2:D:410:ILE:HG23	2:D:441:PHE:HE2	1.77	0.49
2:E:237:LEU:O	2:E:241:GLU:HG3	2.13	0.49
2:F:63:ALA:O	2:F:227:GLY:HA3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:67:ILE:HG12	2:M:17:ILE:HG23	1.94	0.49
2:O:234:LEU:CD2	2:O:292:LEU:HD13	2.43	0.49
2:W:188:GLY:O	2:W:222:MET:HG3	2.11	0.49
2:F:137:GLY:HA2	2:F:432:VAL:O	2.12	0.49
1:J:212:ARG:HG3	1:J:237:THR:HG21	1.95	0.49
1:J:289:ARG:HE	2:N:17:ILE:CG2	2.24	0.49
1:L:253:ALA:O	1:L:257:GLU:HG3	2.11	0.49
2:M:202:LYS:NZ	2:M:209:LEU:HD11	2.27	0.49
1:T:239:SER:HB3	2:W:294:GLU:HG3	1.93	0.49
1:U:282:GLN:NE2	2:X:284:THR:HA	2.28	0.49
2:V:37:LEU:HB2	2:V:48:LEU:HB2	1.95	0.49
2:W:168:GLN:HA	2:W:171:ILE:HD12	1.94	0.49
2:D:381:TYR:HD1	2:D:404:VAL:HG22	1.76	0.49
2:M:249:GLN:HG3	2:M:250:ASP:N	2.28	0.49
2:N:168:GLN:HG2	2:N:206:VAL:HG21	1.95	0.49
1:T:421:VAL:O	1:T:425:ARG:HG2	2.13	0.49
1:U:403:ALA:O	1:U:407:GLN:HG2	2.11	0.49
2:X:10:THR:HG22	2:X:77:LEU:HA	1.94	0.49
1:A:338:ALA:HB3	1:A:341:PRO:HG2	1.94	0.49
2:M:258:ILE:CG2	2:M:310:VAL:HG22	2.42	0.49
2:N:97:ASN:HD21	2:N:101:GLU:HB2	1.78	0.49
2:W:147:TYR:CE1	2:W:153:ILE:HG21	2.48	0.49
1:K:138:ILE:N	1:K:138:ILE:HD12	2.27	0.49
1:S:248:ALA:HB3	1:S:249:PRO:HD3	1.94	0.49
2:V:52:GLN:HE22	2:V:60:ARG:HD2	1.78	0.49
1:A:311:ALA:HA	1:A:323:LEU:HD23	1.94	0.49
2:E:427:ILE:H	2:E:427:ILE:HD12	1.78	0.49
3:G:274:ALA:C	3:G:276:SER:H	2.21	0.49
1:K:239:SER:HB2	2:N:291:LEU:HD23	1.93	0.49
1:S:99:VAL:HG21	1:S:251:THR:HG23	1.94	0.49
6:V:600:ANP:O5'	6:V:600:ANP:H8	2.12	0.49
1:A:38:ASP:O	1:A:286:LEU:HD13	2.13	0.49
2:D:244:ARG:O	2:D:248:GLY:HA2	2.13	0.49
2:D:406:ARG:HH21	2:D:447:GLY:HA3	1.77	0.49
2:O:185:THR:OG1	2:O:236:GLY:HA3	2.13	0.49
1:T:413:ASP:HB3	1:T:416:THR:OG1	2.13	0.49
3:Y:213:THR:HG22	3:Y:217:GLN:HG2	1.95	0.49
2:F:237:LEU:HD22	2:F:292:LEU:HD12	1.95	0.49
1:J:182:LEU:HA	1:J:185:ILE:HD12	1.94	0.49
3:P:183:PHE:HB3	3:P:187:THR:HB	1.95	0.49
2:V:90:GLU:HB2	2:V:111:SER:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:374:VAL:HG23	2:X:445:LEU:HD11	1.94	0.49
1:K:293:ARG:HD2	1:K:339:TYR:CG	2.48	0.48
1:L:99:VAL:CG1	1:L:251:THR:HB	2.43	0.48
2:N:384:LEU:O	2:N:388:ILE:HG12	2.12	0.48
1:S:491:LEU:HD23	1:S:495:LEU:HD13	1.94	0.48
2:W:27:GLN:HA	2:W:57:ASN:ND2	2.28	0.48
2:D:174:ILE:O	2:D:178:HIS:HB2	2.13	0.48
2:E:140:VAL:CG1	2:E:414:LEU:HD22	2.41	0.48
1:K:164:GLY:HA2	1:K:323:LEU:O	2.13	0.48
2:M:391:LEU:HD21	3:P:23:MET:SD	2.52	0.48
3:P:150:LEU:O	3:P:154:MET:HB2	2.13	0.48
1:B:111:ASP:OD1	1:B:111:ASP:C	2.56	0.48
1:C:28:ASN:HB3	1:C:48:ASN:ND2	2.29	0.48
1:L:177:LYS:HD2	1:L:328:VAL:HG13	1.94	0.48
1:L:201:LEU:HA	1:L:265:HIS:O	2.12	0.48
4:Q:69:PHE:CZ	4:Q:133:LEU:HA	2.47	0.48
2:V:221:GLN:HA	2:V:221:GLN:OE1	2.12	0.48
2:D:359:ASP:O	2:D:363:VAL:HG22	2.13	0.48
2:E:370:VAL:HG13	2:E:445:LEU:HD12	1.95	0.48
2:E:375:GLN:O	2:E:379:GLN:HB2	2.14	0.48
2:F:168:GLN:HB3	2:F:420:VAL:HG11	1.96	0.48
2:F:188:GLY:O	2:F:260:ARG:HG3	2.14	0.48
2:F:345:TYR:HA	2:F:346:PRO:C	2.38	0.48
1:U:155:VAL:HG13	1:U:159:VAL:HG23	1.94	0.48
1:B:168:LEU:HD11	1:B:329:ILE:HB	1.94	0.48
2:F:191:THR:HA	2:F:221:GLN:HG3	1.94	0.48
3:G:245:GLY:HA2	3:G:248:ILE:HD12	1.96	0.48
2:N:256:ASP:HA	2:N:257:ASN:HA	1.63	0.48
2:O:374:VAL:HG23	2:O:445:LEU:HD11	1.95	0.48
1:B:99:VAL:HG11	1:B:251:THR:HB	1.95	0.48
1:B:345:ILE:HG12	1:B:351:GLN:HG2	1.95	0.48
3:G:42:LYS:HE3	3:G:224:GLN:OE1	2.14	0.48
2:M:90:GLU:HG3	2:M:111:SER:CA	2.44	0.48
3:P:15:ASN:O	3:P:19:ILE:HG12	2.13	0.48
1:S:36:VAL:HG21	1:S:84:VAL:HB	1.94	0.48
2:X:187:VAL:HG22	2:X:232:VAL:HG13	1.95	0.48
1:A:332:GLN:HB3	2:D:318:THR:CG2	2.43	0.48
2:D:49:GLU:CD	2:D:231:ARG:HE	2.21	0.48
2:E:143:LEU:HD21	2:E:374:VAL:HG21	1.94	0.48
1:J:55:VAL:HG21	1:J:75:ILE:HD13	1.95	0.48
1:J:258:TRP:O	1:J:262:ASN:ND2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:173:ARG:HH11	1:T:173:ARG:HB3	1.78	0.48
1:U:58:SER:HB3	1:U:89:LEU:HB3	1.94	0.48
2:W:388:ILE:HD11	2:W:396:LEU:HD11	1.96	0.48
1:A:37:GLY:O	1:A:38:ASP:HB2	2.13	0.48
1:B:166:ARG:HD3	1:B:308:LEU:O	2.13	0.48
2:F:359:ASP:O	2:F:363:VAL:HG22	2.14	0.48
1:J:103:PRO:HD3	1:J:258:TRP:CZ2	2.48	0.48
1:J:354:LEU:HA	1:J:366:ALA:O	2.13	0.48
1:K:186:LEU:HD11	1:K:435:TYR:HD1	1.79	0.48
2:M:185:THR:HG21	2:M:233:ALA:HA	1.96	0.48
2:M:208:ASN:ND2	2:M:211:GLY:HA3	2.28	0.48
2:N:136:THR:HG23	2:N:138:ILE:H	1.79	0.48
1:S:453:GLY:C	1:S:455:LEU:H	2.22	0.48
1:A:317:LYS:O	1:A:317:LYS:HG2	2.13	0.48
1:A:480:GLU:CD	1:A:480:GLU:H	2.20	0.48
1:B:192:ASN:HA	1:B:200:LYS:HG2	1.94	0.48
4:H:16:LEU:HB2	4:H:19:GLU:O	2.13	0.48
1:J:402:VAL:HG12	1:J:402:VAL:O	2.14	0.48
1:L:236:ALA:CB	1:L:245:GLN:HA	2.44	0.48
1:C:418:GLN:HG3	1:C:419:THR:N	2.29	0.47
4:H:33:PRO:HD2	4:H:52:LEU:HD22	1.95	0.47
1:L:153:LYS:HG2	1:L:443:GLN:HG2	1.96	0.47
2:O:98:VAL:HG23	2:O:232:VAL:HA	1.96	0.47
1:S:54:LEU:HD13	1:S:97:VAL:HG22	1.96	0.47
1:S:107:GLY:HA2	1:S:228:MET:O	2.14	0.47
1:U:436:SER:N	1:U:437:PRO:HD3	2.29	0.47
2:D:109:ILE:HG22	2:D:109:ILE:O	2.14	0.47
2:E:150:GLY:HA3	2:E:298:THR:OG1	2.14	0.47
3:G:193:SER:HB3	3:G:196:LYS:CE	2.44	0.47
1:J:168:LEU:HB2	1:J:348:THR:HG21	1.96	0.47
2:O:174:ILE:O	2:O:178:HIS:N	2.39	0.47
1:S:299:ASP:HB2	1:S:302:TYR:HB3	1.95	0.47
1:T:36:VAL:HG13	2:W:53:HIS:HB2	1.95	0.47
1:A:446:LEU:HD21	1:A:467:GLU:HA	1.96	0.47
1:C:477:ASN:OD1	1:C:477:ASN:N	2.47	0.47
1:L:77:LEU:HD12	1:L:81:ASP:HB3	1.95	0.47
1:A:395:PHE:CZ	1:A:422:ARG:HB3	2.49	0.47
1:B:115:ASN:H	1:B:115:ASN:ND2	2.12	0.47
2:D:164:THR:HA	2:D:167:ILE:HG22	1.95	0.47
2:V:275:ILE:HG23	3:Y:274:ALA:HB2	1.97	0.47
2:W:136:THR:HG22	2:W:142:ASP:OD1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:MET:SD	1:A:97:VAL:HG21	2.54	0.47
2:D:40:LYS:O	2:D:40:LYS:HG3	2.13	0.47
3:G:96:ARG:HG2	3:G:122:HIS:CE1	2.50	0.47
1:S:351:GLN:HE22	1:S:375:ARG:HH12	1.63	0.47
1:U:376:VAL:CG1	1:U:380:ALA:HB3	2.45	0.47
2:V:41:THR:HB	2:V:42:PRO:HD2	1.96	0.47
3:Y:25:ILE:HA	3:Y:28:SER:CB	2.40	0.47
2:E:180:GLY:HA2	2:E:249:GLN:NE2	2.30	0.47
3:G:193:SER:HB3	3:G:196:LYS:HE2	1.97	0.47
1:L:154:ALA:HA	1:L:430:LEU:HD22	1.96	0.47
1:L:167:GLU:O	1:L:326:LEU:HA	2.14	0.47
1:L:237:THR:HB	1:L:240:GLU:HG3	1.97	0.47
2:O:335:LEU:HA	2:O:347:ALA:O	2.14	0.47
3:P:46:GLU:O	3:P:50:LEU:CB	2.62	0.47
2:W:167:ILE:O	2:W:170:LEU:HB2	2.14	0.47
2:X:71:VAL:O	2:X:74:GLU:HB2	2.14	0.47
1:A:412:LEU:HB3	1:A:417:LYS:HB2	1.97	0.47
1:A:462:ARG:HD2	1:A:465:GLU:OE2	2.13	0.47
1:B:177:LYS:HG2	1:B:354:LEU:HD12	1.95	0.47
2:E:204:THR:HG22	2:E:206:VAL:HG22	1.96	0.47
2:F:10:THR:N	2:F:27:GLN:HE22	2.13	0.47
2:F:10:THR:HG22	2:F:77:LEU:HA	1.97	0.47
1:T:67:ILE:HG12	2:X:17:ILE:HG23	1.97	0.47
1:T:166:ARG:HH22	2:X:190:ARG:HD3	1.80	0.47
1:U:97:VAL:HG11	1:U:247:LEU:HD21	1.97	0.47
2:X:160:GLY:N	6:X:600:ANP:HNB1	2.11	0.47
4:H:10:LEU:HB2	4:H:43:ALA:HA	1.96	0.47
4:H:45:HIS:HD2	4:H:77:VAL:HG21	1.79	0.47
2:N:117:ILE:HA	2:N:238:THR:OG1	2.15	0.47
1:T:55:VAL:HG21	1:T:75:ILE:HD13	1.96	0.47
1:T:491:LEU:HA	1:T:495:LEU:HD23	1.97	0.47
1:A:138:ILE:HD11	2:E:221:GLN:CG	2.45	0.47
1:B:368:ASN:ND2	1:B:371:LEU:HD22	2.29	0.47
1:C:243:PRO:O	1:C:247:LEU:HB2	2.14	0.47
2:D:13:VAL:HG23	2:D:76:VAL:CG2	2.45	0.47
2:E:157:GLY:HA2	2:E:337:ARG:HH22	1.80	0.47
3:G:165:PHE:CE2	3:G:179:GLU:HB2	2.49	0.47
2:X:90:GLU:HB2	2:X:111:SER:HB3	1.96	0.47
2:E:135:GLU:OE2	2:E:433:ARG:HD3	2.15	0.47
1:K:29:GLU:O	1:K:92:ARG:HB2	2.15	0.47
1:L:346:SER:HB3	2:M:260:ARG:HH22	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:413:ASP:CG	1:T:414:ALA:H	2.23	0.47
2:V:62:ILE:HD11	2:V:272:LEU:HD11	1.97	0.47
1:A:38:ASP:HB3	1:A:286:LEU:HD22	1.96	0.46
1:A:450:GLY:HA2	1:A:455:LEU:HD12	1.97	0.46
2:E:220:GLY:HA3	2:E:232:VAL:HG21	1.97	0.46
2:F:257:ASN:HB3	2:F:260:ARG:HG2	1.97	0.46
1:K:382:VAL:HG11	1:K:440:THR:HG21	1.97	0.46
2:N:134:LEU:HD13	2:N:149:ARG:HG3	1.96	0.46
2:N:187:VAL:HG13	2:N:232:VAL:HG23	1.96	0.46
2:O:154:GLY:HA3	2:O:329:LEU:HD13	1.97	0.46
3:Y:32:SER:C	3:Y:34:ALA:H	2.22	0.46
3:G:83:LEU:HD22	3:G:237:MET:HE1	1.97	0.46
3:G:182:ILE:HD12	3:G:214:LEU:HA	1.96	0.46
1:K:354:LEU:HB3	1:K:366:ALA:HB3	1.97	0.46
2:N:32:ALA:O	2:N:35:ASN:HB2	2.16	0.46
2:N:237:LEU:HD21	2:N:295:ARG:HB2	1.96	0.46
2:O:37:LEU:HB2	2:O:48:LEU:HB2	1.96	0.46
2:O:237:LEU:HD21	2:O:295:ARG:CB	2.43	0.46
4:Q:89:GLU:CB	5:R:21:ILE:HD11	2.44	0.46
1:T:269:VAL:HG12	1:T:271:ASP:HB2	1.97	0.46
1:B:478:HIS:HB3	1:B:481:LEU:HG	1.96	0.46
1:C:300:VAL:HG22	1:C:300:VAL:O	2.15	0.46
5:R:19:GLN:NE2	5:R:38:SER:HB3	2.30	0.46
1:A:99:VAL:HG21	1:A:251:THR:HG23	1.97	0.46
1:A:397:ALA:CA	1:A:400:ARG:CZ	2.86	0.46
1:C:456:ASP:OD1	1:C:456:ASP:N	2.47	0.46
1:K:204:VAL:O	1:K:268:ILE:HA	2.15	0.46
2:N:152:LYS:HE2	2:N:293:GLN:HB3	1.98	0.46
1:U:34:LEU:HG	1:U:44:PHE:HB2	1.98	0.46
1:C:215:VAL:O	1:C:219:VAL:HG13	2.16	0.46
1:K:109:VAL:HG13	1:K:233:ILE:HB	1.97	0.46
1:U:50:GLN:HB3	2:V:69:GLY:HA2	1.97	0.46
2:E:240:ALA:HB1	2:E:251:VAL:HG11	1.97	0.46
2:E:367:HIS:CD2	2:E:434:LEU:HD11	2.51	0.46
1:K:344:VAL:HA	1:K:347:ILE:HD12	1.98	0.46
2:N:98:VAL:HG21	2:N:231:ARG:HB2	1.97	0.46
1:U:302:TYR:HA	1:U:305:SER:HG	1.81	0.46
1:U:338:ALA:HB3	1:U:341:PRO:HG2	1.97	0.46
1:A:203:CYS:O	1:A:231:SER:HA	2.16	0.46
1:C:28:ASN:HB3	1:C:48:ASN:HD22	1.80	0.46
2:E:177:ALA:HB1	2:E:433:ARG:HH12	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:181:PHE:HD2	2:F:243:PHE:CD1	2.34	0.46
1:J:143:SER:H	2:N:199:ARG:NH1	2.13	0.46
2:O:384:LEU:HB3	2:O:388:ILE:HD11	1.97	0.46
1:S:99:VAL:HG23	1:S:100:PRO:HD2	1.96	0.46
1:U:369:VAL:HG11	1:U:396:LEU:CB	2.45	0.46
2:V:296:ILE:HG21	2:V:306:SER:HB3	1.97	0.46
1:A:302:TYR:CZ	1:A:306:ARG:HG3	2.51	0.46
1:A:395:PHE:HE2	1:A:423:GLY:HA2	1.81	0.46
4:H:96:PHE:O	5:I:25:LEU:HA	2.16	0.46
2:M:26:GLU:H	2:M:29:GLU:HG2	1.81	0.46
2:N:168:GLN:NE2	2:N:200:GLU:O	2.47	0.46
1:T:140:PRO:HB3	1:T:318:GLU:HG3	1.98	0.46
2:V:64:MET:HE1	2:V:231:ARG:HB2	1.98	0.46
2:X:389:ALA:O	3:Y:243:ASN:ND2	2.49	0.46
1:B:285:LEU:HD22	2:E:275:ILE:CG2	2.46	0.46
1:C:440:THR:O	1:C:444:VAL:HG23	2.16	0.46
2:F:325:THR:HG22	2:F:329:LEU:HD11	1.98	0.46
1:K:96:ILE:O	1:K:97:VAL:C	2.59	0.46
1:K:138:ILE:HG13	2:O:191:THR:HG23	1.97	0.46
1:L:492:SER:H	1:L:495:LEU:HD12	1.81	0.46
2:O:10:THR:HG21	2:O:75:LYS:HD3	1.98	0.46
2:X:321:ALA:HB3	2:X:322:PRO:CD	2.46	0.46
1:A:396:LEU:O	1:A:400:ARG:CG	2.63	0.46
2:D:449:TYR:HD1	2:D:452:ILE:HD12	1.80	0.46
2:F:417:PRO:HG2	2:F:430:LYS:HG3	1.97	0.46
3:G:96:ARG:NE	3:G:121:THR:HG21	2.09	0.46
1:J:211:LYS:HD3	2:M:328:HIS:HA	1.97	0.46
1:L:249:PRO:HB3	1:L:270:TYR:CD1	2.51	0.46
2:M:53:HIS:CD2	2:M:59:VAL:HG12	2.51	0.46
1:T:474:LEU:HD13	1:T:482:LEU:HD21	1.98	0.46
1:U:116:PRO:HG3	1:U:122:PRO:HA	1.98	0.46
2:X:382:LYS:O	2:X:385:GLN:HG2	2.16	0.46
1:C:478:HIS:CE1	1:C:502:ALA:HB2	2.52	0.45
2:X:70:LEU:HD23	2:X:70:LEU:HA	1.83	0.45
1:B:46:LEU:HD22	1:B:92:ARG:HG3	1.97	0.45
1:J:67:ILE:HD12	1:J:287:LEU:HD22	1.98	0.45
2:M:244:ARG:O	2:M:248:GLY:HA2	2.15	0.45
1:S:153:LYS:HG2	1:S:432:GLN:OE1	2.16	0.45
2:X:147:TYR:CZ	2:X:153:ILE:HG21	2.52	0.45
2:E:370:VAL:HG21	2:E:442:LYS:HB2	1.98	0.45
2:F:335:LEU:HA	2:F:347:ALA:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:187:ASN:O	1:J:190:ARG:HG3	2.16	0.45
1:J:289:ARG:HH21	2:N:17:ILE:CG2	2.29	0.45
2:M:387:ILE:HG23	2:M:391:LEU:HD22	1.98	0.45
1:T:170:ILE:HG23	1:T:353:PHE:HA	1.98	0.45
1:T:335:ASP:HB2	3:Y:257:ARG:NH1	2.31	0.45
2:W:152:LYS:HE3	2:W:296:ILE:HB	1.98	0.45
2:W:170:LEU:HD23	2:W:170:LEU:HA	1.87	0.45
2:X:406:ARG:NH2	2:X:450:ASP:OD2	2.50	0.45
3:Y:218:MET:HB3	3:Y:222:MET:HE2	1.98	0.45
1:B:484:GLU:O	1:B:488:LYS:HB2	2.17	0.45
2:E:221:GLN:NE2	2:E:224:GLU:OE2	2.49	0.45
1:K:107:GLY:HA2	1:K:228:MET:O	2.17	0.45
1:K:179:ALA:HB2	6:K:600:ANP:H8	1.98	0.45
1:L:241:ALA:HB1	1:L:243:PRO:HD2	1.99	0.45
2:N:45:LYS:HE3	2:N:99:ILE:HD12	1.96	0.45
4:Q:14:PHE:HA	4:Q:85:VAL:HB	1.99	0.45
1:B:290:PRO:HA	1:B:291:PRO:HD2	1.90	0.45
4:H:48:THR:H	4:H:77:VAL:HB	1.81	0.45
1:J:49:ILE:HA	1:J:92:ARG:HE	1.81	0.45
2:N:281:TYR:OH	2:N:321:ALA:HB2	2.16	0.45
3:P:10:LEU:HD13	3:P:251:TYR:HB3	1.98	0.45
3:P:75:VAL:HA	3:P:108:VAL:O	2.17	0.45
2:V:7:THR:N	2:V:8:PRO:HD3	2.31	0.45
2:X:15:ALA:HB3	2:X:22:ASP:HB2	1.98	0.45
2:E:99:ILE:HG13	2:E:101:GLU:HG3	1.98	0.45
1:J:428:GLN:HG2	1:J:463:ILE:HB	1.98	0.45
1:K:30:THR:HB	2:X:464:GLU:OE2	2.16	0.45
1:U:111:ASP:OD1	1:U:111:ASP:C	2.60	0.45
2:D:256:ASP:HA	2:D:257:ASN:HA	1.66	0.45
1:K:155:VAL:HA	1:K:159:VAL:HG23	1.99	0.45
1:K:272:ASP:C	1:K:272:ASP:OD1	2.58	0.45
1:L:284:SER:CB	1:L:297:PRO:HG3	2.46	0.45
1:S:272:ASP:HB2	1:S:328:VAL:O	2.17	0.45
2:V:34:LEU:HD22	2:V:118:HIS:CE1	2.52	0.45
1:A:103:PRO:HD3	1:A:258:TRP:CH2	2.52	0.45
1:C:488:LYS:C	1:C:490:GLU:H	2.25	0.45
1:J:44:PHE:CD2	1:J:44:PHE:C	2.95	0.45
1:J:220:GLN:HG2	1:J:224:GLN:HE21	1.82	0.45
1:J:455:LEU:HD21	1:J:466:PHE:CE1	2.52	0.45
1:K:503:THR:O	1:K:507:VAL:HG23	2.17	0.45
2:N:89:ARG:C	2:N:91:THR:H	2.22	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:248:ILE:O	3:P:252:SER:HB2	2.17	0.45
2:V:33:ILE:HA	2:V:50:VAL:HB	1.99	0.45
2:V:93:GLY:N	2:V:215:VAL:O	2.50	0.45
2:V:247:GLU:HB2	2:V:249:GLN:HG2	1.98	0.45
2:W:220:GLY:HA3	2:W:232:VAL:HG21	1.97	0.45
1:B:196:ASP:OD2	1:B:199:LYS:HG3	2.16	0.45
2:D:95:ILE:CG2	2:D:103:ILE:HG13	2.47	0.45
1:L:168:LEU:HB2	1:L:348:THR:HG21	1.99	0.45
1:L:302:TYR:HA	1:L:305:SER:OG	2.17	0.45
1:L:468:SER:HA	1:L:471:LEU:HD12	1.99	0.45
2:N:345:TYR:HA	2:N:346:PRO:C	2.41	0.45
2:O:201:MET:HE2	2:O:201:MET:HA	1.99	0.45
1:T:147:PRO:HB3	1:T:380:ALA:O	2.17	0.45
1:B:138:ILE:O	2:F:195:ASN:ND2	2.50	0.45
1:B:187:ASN:OD1	1:B:190:ARG:NH1	2.50	0.45
2:D:391:LEU:HD22	2:D:395:GLU:HG2	1.99	0.45
2:F:187:VAL:HG22	2:F:232:VAL:HG13	1.99	0.45
1:K:95:ASN:ND2	1:K:98:ASP:OD2	2.49	0.45
1:L:254:SER:OG	1:L:310:ARG:NH2	2.49	0.45
2:M:32:ALA:O	2:M:35:ASN:HB2	2.16	0.45
1:U:39:GLY:HA2	1:U:77:LEU:HD12	1.99	0.45
1:C:216:ALA:O	1:C:219:VAL:HG22	2.17	0.44
2:F:33:ILE:HG22	2:F:34:LEU:HG	1.99	0.44
1:K:103:PRO:HD2	1:K:126:ALA:HB2	1.99	0.44
1:L:77:LEU:CD1	1:L:81:ASP:HB3	2.47	0.44
1:L:348:THR:O	2:M:190:ARG:NH2	2.45	0.44
2:O:321:ALA:HB3	2:O:322:PRO:CD	2.47	0.44
1:T:385:LEU:HG	1:T:444:VAL:HG12	1.99	0.44
2:V:256:ASP:HA	2:V:257:ASN:HA	1.72	0.44
2:W:185:THR:OG1	2:W:236:GLY:HA3	2.18	0.44
2:X:252:LEU:HD23	2:X:305:THR:HB	1.97	0.44
2:E:410:ILE:HG23	2:E:441:PHE:HE2	1.82	0.44
5:I:46:GLN:HG3	5:I:47:TYR:H	1.81	0.44
1:K:93:THR:HG22	1:K:95:ASN:HB2	1.99	0.44
1:K:110:VAL:CG2	1:K:234:VAL:HG22	2.47	0.44
1:K:173:ARG:HG2	1:K:174:GLN:HG2	1.99	0.44
2:M:256:ASP:HA	2:M:257:ASN:HA	1.76	0.44
2:O:90:GLU:HB2	2:O:111:SER:CB	2.47	0.44
1:S:117:ILE:O	2:V:124:PHE:HD2	2.00	0.44
1:S:360:TYR:C	1:S:362:GLY:H	2.25	0.44
1:U:302:TYR:HA	1:U:305:SER:OG	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:244:ARG:HD3	2:F:304:VAL:HG23	1.98	0.44
3:G:250:ARG:HA	3:G:253:ILE:HD12	2.00	0.44
1:J:364:ARG:HB3	6:J:600:ANP:N6	2.31	0.44
1:K:314:LEU:HB2	1:K:321:GLY:O	2.17	0.44
1:K:435:TYR:O	1:K:437:PRO:HD3	2.17	0.44
2:M:258:ILE:O	2:M:261:PHE:HB3	2.17	0.44
3:P:208:ASP:HA	3:P:211:GLU:HB2	1.98	0.44
4:Q:70:ILE:HG22	4:Q:72:GLY:H	1.81	0.44
1:U:269:VAL:HG22	1:U:326:LEU:HD12	1.99	0.44
1:C:149:GLN:O	1:C:188:GLN:NE2	2.50	0.44
1:C:365:PRO:HB2	1:C:367:ILE:HG13	1.98	0.44
1:J:185:ILE:HG23	1:J:203:CYS:SG	2.57	0.44
1:K:37:GLY:HA3	2:N:52:GLN:HG2	1.98	0.44
2:M:30:LEU:HD11	2:M:57:ASN:HA	1.99	0.44
2:N:259:PHE:CE1	2:N:313:PRO:HG3	2.53	0.44
2:O:179:GLY:H	2:O:214:LYS:NZ	2.15	0.44
2:X:17:ILE:HG22	2:X:271:LEU:HD22	1.98	0.44
3:Y:230:ILE:HD13	3:Y:233:ARG:HH12	1.82	0.44
1:B:156:ASP:O	1:B:385:LEU:HD13	2.18	0.44
1:J:36:VAL:HG21	1:J:84:VAL:HB	1.99	0.44
2:O:90:GLU:HB2	2:O:111:SER:HB3	1.99	0.44
1:S:46:LEU:O	1:S:49:ILE:HG22	2.18	0.44
1:S:190:ARG:NH2	1:S:437:PRO:O	2.51	0.44
1:T:216:ALA:HA	2:W:124:PHE:CE1	2.52	0.44
2:F:258:ILE:HD11	2:F:292:LEU:HD21	1.99	0.44
1:L:258:TRP:O	1:L:262:ASN:ND2	2.50	0.44
2:M:458:TYR:O	2:M:460:VAL:HG13	2.18	0.44
2:N:163:LYS:NZ	2:N:256:ASP:OD2	2.50	0.44
1:S:480:GLU:CD	1:S:480:GLU:H	2.26	0.44
1:T:335:ASP:HB2	3:Y:257:ARG:HH11	1.83	0.44
1:A:67:ILE:HD12	1:A:287:LEU:HD22	2.00	0.44
1:A:510:PHE:C	1:A:510:PHE:CD2	2.95	0.44
1:B:50:GLN:HB3	2:F:69:GLY:HA2	1.98	0.44
1:J:417:LYS:O	1:J:417:LYS:HG2	2.16	0.44
2:O:359:ASP:O	2:O:363:VAL:HG22	2.17	0.44
2:W:67:THR:HB	2:W:70:LEU:HD12	1.99	0.44
2:W:168:GLN:NE2	2:W:204:THR:CG2	2.69	0.44
2:D:22:ASP:OD2	2:D:60:ARG:NH2	2.51	0.44
2:E:256:ASP:HA	2:E:257:ASN:HA	1.76	0.44
1:K:269:VAL:HG22	1:K:326:LEU:HB2	1.99	0.44
2:N:136:THR:HG21	2:N:141:VAL:HG11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:260:ARG:HA	2:N:263:GLN:HG2	1.98	0.44
2:O:193:GLU:HA	2:O:196:ASP:HB2	2.00	0.44
3:P:92:ALA:HB1	3:P:118:LEU:HD11	2.00	0.44
4:Q:16:LEU:HB3	4:Q:17:PRO:HD2	2.00	0.44
1:S:96:ILE:O	1:S:97:VAL:C	2.61	0.44
2:V:168:GLN:HG2	2:V:197:LEU:CD1	2.48	0.44
1:A:146:GLU:CB	1:A:163:ARG:HG3	2.43	0.44
1:B:280:TYR:CD2	1:B:303:LEU:HD22	2.53	0.44
3:P:151:LEU:HD23	3:P:156:ALA:HB3	1.99	0.44
2:V:27:GLN:HA	2:V:57:ASN:HD21	1.83	0.44
2:V:208:ASN:HB3	2:V:212:GLU:O	2.18	0.44
2:V:317:LEU:HD22	2:V:326:PHE:HE2	1.83	0.44
1:A:36:VAL:HG21	1:A:84:VAL:HB	1.99	0.43
1:A:51:ALA:O	1:A:52:GLU:HB2	2.18	0.43
2:M:139:LYS:HG3	2:M:432:VAL:HG21	1.99	0.43
2:M:242:TYR:CD2	2:M:242:TYR:C	2.95	0.43
2:O:95:ILE:C	2:O:96:ILE:HG13	2.42	0.43
1:T:212:ARG:HG2	2:W:124:PHE:HA	2.00	0.43
1:T:289:ARG:NH1	1:T:289:ARG:CG	2.70	0.43
2:D:16:VAL:HG21	2:D:70:LEU:HB3	2.00	0.43
2:D:345:TYR:HA	2:D:346:PRO:C	2.43	0.43
2:E:335:LEU:HA	2:E:347:ALA:O	2.18	0.43
3:G:80:ASP:OD1	3:G:111:GLY:HA2	2.18	0.43
1:K:178:THR:O	1:K:179:ALA:C	2.61	0.43
1:S:190:ARG:HH12	1:S:439:ALA:HB2	1.77	0.43
1:U:167:GLU:O	1:U:327:PRO:HD2	2.18	0.43
1:A:394:LEU:HD13	1:A:398:GLN:NE2	2.33	0.43
5:I:29:LEU:HD12	5:I:29:LEU:HA	1.79	0.43
1:K:166:ARG:CD	1:K:308:LEU:O	2.64	0.43
2:M:249:GLN:HA	2:M:249:GLN:NE2	2.26	0.43
2:M:452:ILE:HG23	2:M:453:PRO:HD2	2.00	0.43
1:S:108:ARG:NH1	1:S:123:ILE:HD13	2.33	0.43
1:A:280:TYR:CE2	1:A:297:PRO:CG	3.01	0.43
2:D:84:SER:HB3	2:D:114:ARG:HB3	1.99	0.43
2:O:140:VAL:HA	2:O:414:LEU:HD22	2.00	0.43
1:S:81:ASP:OD1	1:S:81:ASP:N	2.52	0.43
1:S:506:PHE:O	1:S:509:THR:HG22	2.19	0.43
2:W:220:GLY:HA3	2:W:232:VAL:HG11	2.00	0.43
2:D:15:ALA:HB3	2:D:22:ASP:HB2	1.99	0.43
2:D:425:THR:HB	2:D:427:ILE:HD12	2.00	0.43
2:F:409:LYS:HE3	2:F:450:ASP:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:90:GLN:HA	3:G:93:LYS:HG2	2.01	0.43
1:S:273:LEU:HD22	1:S:304:HIS:CD2	2.54	0.43
1:S:439:ALA:HB3	1:S:442:GLU:HG3	2.01	0.43
1:T:302:TYR:HA	1:T:305:SER:OG	2.18	0.43
1:T:446:LEU:HD11	1:T:467:GLU:HG3	2.00	0.43
2:W:140:VAL:HG13	2:W:414:LEU:HB3	2.01	0.43
2:E:186:GLY:HA3	2:E:219:PHE:CD1	2.53	0.43
2:E:321:ALA:HB3	2:E:322:PRO:HD3	2.00	0.43
1:J:446:LEU:HD11	1:J:471:LEU:HD11	2.00	0.43
3:P:77:ILE:HG21	3:P:222:MET:HA	2.00	0.43
1:T:166:ARG:HG2	1:T:311:ALA:HB3	2.00	0.43
3:Y:267:LEU:O	3:Y:271:ILE:HG12	2.18	0.43
1:A:156:ASP:HB3	1:A:385:LEU:HD21	1.99	0.43
1:A:271:ASP:HA	1:A:272:ASP:HA	1.77	0.43
2:E:267:GLU:O	2:E:271:LEU:HG	2.19	0.43
1:J:289:ARG:HD3	1:J:290:PRO:CD	2.40	0.43
2:M:187:VAL:HG22	2:M:232:VAL:HG13	2.00	0.43
2:N:280:GLY:HA2	3:P:267:LEU:CD2	2.48	0.43
3:P:17:GLU:HG3	3:P:248:ILE:HD12	2.01	0.43
1:C:280:TYR:CD2	1:C:297:PRO:HG2	2.53	0.43
1:C:364:ARG:HB3	6:C:600:ANP:N6	2.34	0.43
2:D:425:THR:C	2:D:427:ILE:H	2.26	0.43
2:E:32:ALA:O	2:E:35:ASN:HB2	2.19	0.43
2:E:168:GLN:HE21	2:E:201:MET:HG2	1.84	0.43
2:E:199:ARG:HE	2:E:199:ARG:HB2	1.50	0.43
2:F:15:ALA:HB3	2:F:22:ASP:CB	2.38	0.43
1:J:174:GLN:O	1:J:174:GLN:HG3	2.18	0.43
1:K:139:LEU:C	1:K:141:ARG:H	2.26	0.43
1:L:181:ALA:HB1	1:L:269:VAL:HG21	2.01	0.43
2:M:226:PRO:HB2	2:M:268:VAL:HG13	2.00	0.43
2:N:140:VAL:HG22	2:N:414:LEU:HB3	2.00	0.43
1:S:269:VAL:HG22	1:S:326:LEU:HB2	2.01	0.43
1:T:208:VAL:HG21	1:T:249:PRO:HG3	2.01	0.43
1:U:167:GLU:HB3	1:U:326:LEU:HD23	2.01	0.43
2:X:144:LEU:O	2:X:358:LEU:HD22	2.19	0.43
2:X:258:ILE:HD11	2:X:292:LEU:HD21	1.99	0.43
1:B:103:PRO:HD2	1:B:126:ALA:HB2	2.01	0.43
2:E:7:THR:N	2:E:8:PRO:HD3	2.34	0.43
3:G:83:LEU:HB3	3:G:237:MET:CE	2.49	0.43
1:K:36:VAL:HG23	1:K:40:ILE:O	2.19	0.43
1:L:67:ILE:HD12	1:L:287:LEU:HD22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:222:LEU:CB	1:L:228:MET:HE2	2.47	0.43
1:U:176:GLY:O	1:U:180:VAL:HG23	2.18	0.43
2:W:228:ALA:O	2:W:232:VAL:HG22	2.18	0.43
1:A:227:ALA:HA	1:A:230:TYR:CE2	2.54	0.43
2:D:158:GLY:O	2:D:163:LYS:NZ	2.52	0.43
2:F:427:ILE:HD13	2:F:459:MET:HG2	2.00	0.43
3:G:18:LYS:O	3:G:22:THR:OG1	2.27	0.43
3:G:77:ILE:CD1	3:G:110:ILE:HD12	2.49	0.43
2:M:160:GLY:CA	6:M:600:ANP:HNB1	2.32	0.43
2:N:370:VAL:O	2:N:374:VAL:HG23	2.19	0.43
2:O:63:ALA:O	2:O:227:GLY:HA3	2.19	0.43
2:X:256:ASP:HA	2:X:257:ASN:HA	1.86	0.43
1:A:354:LEU:HA	1:A:366:ALA:O	2.19	0.42
1:B:37:GLY:O	1:B:38:ASP:HB2	2.19	0.42
1:B:219:VAL:HG22	1:B:233:ILE:HG13	2.01	0.42
1:J:192:ASN:HA	1:J:200:LYS:HG2	2.01	0.42
1:J:473:TYR:CZ	1:J:506:PHE:HB2	2.54	0.42
1:K:23:ASP:HB3	1:K:26:ASN:HD22	1.84	0.42
1:S:455:LEU:HD23	1:S:458:ILE:HD12	2.00	0.42
1:U:103:PRO:HD3	1:U:258:TRP:CZ2	2.54	0.42
1:U:106:LEU:HD22	1:U:230:TYR:HA	2.00	0.42
1:C:243:PRO:HA	1:C:246:TYR:HB3	2.01	0.42
2:F:220:GLY:HA3	2:F:232:VAL:HG11	2.00	0.42
1:K:140:PRO:HB3	1:K:318:GLU:HG3	2.01	0.42
3:P:124:ASN:HA	5:R:49:ASN:HA	2.00	0.42
1:S:161:ILE:HD13	1:S:326:LEU:HD21	2.00	0.42
2:X:247:GLU:O	2:X:249:GLN:HG3	2.19	0.42
1:B:139:LEU:CD2	2:F:105:GLU:HB2	2.49	0.42
1:B:314:LEU:HB2	1:B:321:GLY:O	2.19	0.42
1:C:159:VAL:HG11	1:C:372:SER:HB3	2.01	0.42
2:D:174:ILE:HG22	2:D:252:LEU:HD11	2.01	0.42
2:E:150:GLY:O	2:E:297:THR:HA	2.19	0.42
3:G:247:MET:HG2	3:G:250:ARG:NH2	2.35	0.42
4:H:57:VAL:HB	4:H:70:ILE:HD12	2.01	0.42
1:J:103:PRO:C	1:J:105:LEU:H	2.28	0.42
2:M:285:LEU:HD23	2:M:285:LEU:C	2.44	0.42
2:M:299:THR:OG1	2:M:300:LYS:N	2.52	0.42
3:P:139:THR:HG21	5:R:37:ARG:HA	2.02	0.42
1:S:363:ILE:HA	1:S:431:LYS:HE2	2.01	0.42
2:X:39:ILE:HD12	2:X:46:LEU:HD23	2.01	0.42
2:E:345:TYR:HA	2:E:346:PRO:C	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:71:LYS:O	3:G:160:PRO:HD2	2.18	0.42
1:K:27:LEU:CD2	1:K:30:THR:HG22	2.49	0.42
1:S:73:VAL:HG12	1:S:75:ILE:HG13	2.01	0.42
2:V:237:LEU:HD22	2:V:292:LEU:HD12	2.01	0.42
2:X:52:GLN:CG	2:X:60:ARG:HB3	2.49	0.42
1:A:82:ARG:HA	2:D:33:ILE:HB	2.02	0.42
1:C:174:GLN:HA	6:C:600:ANP:N3B	2.33	0.42
4:H:88:ILE:HD11	5:I:14:LEU:HD13	2.00	0.42
1:L:64:MET:H	1:L:75:ILE:HG23	1.85	0.42
2:M:41:THR:HB	2:M:42:PRO:CD	2.49	0.42
2:O:346:PRO:HG3	2:O:418:PHE:CZ	2.55	0.42
1:S:455:LEU:HD22	1:S:458:ILE:HD12	2.02	0.42
1:A:55:VAL:HG21	1:A:75:ILE:HD13	2.01	0.42
1:A:407:GLN:HB3	2:D:387:ILE:HD11	2.02	0.42
2:E:322:PRO:O	2:E:326:PHE:HD1	2.03	0.42
2:F:95:ILE:HG22	2:F:103:ILE:HG13	2.01	0.42
1:J:426:LEU:O	1:J:430:LEU:HG	2.19	0.42
2:N:377:THR:HG22	2:N:407:ALA:HB2	2.01	0.42
1:S:492:SER:HB2	1:S:495:LEU:HB2	2.01	0.42
2:E:135:GLU:CD	2:E:433:ARG:HD3	2.44	0.42
3:G:90:GLN:HA	3:G:93:LYS:CG	2.50	0.42
1:J:478:HIS:HB3	1:J:481:LEU:HG	2.02	0.42
1:K:398:GLN:HA	1:K:401:GLU:HG3	2.02	0.42
1:S:146:GLU:CB	1:S:163:ARG:HG3	2.50	0.42
2:V:166:PHE:CE2	2:V:346:PRO:HB2	2.55	0.42
2:X:237:LEU:CD2	2:X:292:LEU:HD12	2.50	0.42
1:A:131:ALA:O	1:A:250:PHE:HB3	2.19	0.42
2:D:71:VAL:O	2:D:74:GLU:HB2	2.20	0.42
1:K:77:LEU:HD12	1:K:81:ASP:HA	2.02	0.42
1:L:35:ALA:HB1	2:O:53:HIS:O	2.20	0.42
2:N:319:ASP:O	2:N:322:PRO:HD2	2.20	0.42
2:O:187:VAL:HG22	2:O:232:VAL:HG13	2.02	0.42
2:O:460:VAL:HB	2:O:465:ASP:HB3	2.02	0.42
1:U:253:ALA:O	1:U:257:GLU:HG3	2.19	0.42
2:V:162:GLY:HA2	6:V:600:ANP:O1A	2.20	0.42
2:X:197:LEU:O	2:X:201:MET:CG	2.60	0.42
2:X:237:LEU:HD21	2:X:295:ARG:HB2	2.00	0.42
1:B:145:HIS:CD2	1:B:146:GLU:HG3	2.55	0.42
1:C:274:SER:O	1:C:278:VAL:HG23	2.20	0.42
2:E:408:ARG:O	2:E:412:ARG:HD2	2.19	0.42
2:F:185:THR:OG1	2:F:236:GLY:HA3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:99:VAL:HG21	1:J:251:THR:HG23	2.01	0.42
1:J:415:SER:O	1:J:418:GLN:HB2	2.20	0.42
1:K:168:LEU:HB2	1:K:348:THR:HG21	2.02	0.42
2:N:122:PRO:HB2	2:N:127:GLN:HE21	1.84	0.42
2:N:169:GLU:HG2	2:N:418:PHE:CD1	2.55	0.42
2:O:84:SER:HB3	2:O:114:ARG:HB3	2.02	0.42
1:S:146:GLU:OE1	1:S:313:LYS:HE2	2.20	0.42
2:W:258:ILE:O	2:W:261:PHE:HB3	2.20	0.42
1:A:36:VAL:HG12	2:D:53:HIS:HB2	2.02	0.42
1:B:348:THR:O	2:F:190:ARG:NH2	2.53	0.42
2:E:184:PHE:CD2	2:E:254:PHE:HB2	2.55	0.42
2:E:258:ILE:O	2:E:261:PHE:HB3	2.19	0.42
2:E:408:ARG:NH1	2:E:454:GLU:OE1	2.50	0.42
2:F:50:VAL:CA	2:F:61:THR:HG22	2.41	0.42
2:N:183:VAL:HG13	2:N:216:ALA:HB3	2.01	0.42
2:O:388:ILE:HD12	2:O:396:LEU:HD11	2.02	0.42
4:Q:45:HIS:O	4:Q:77:VAL:HG11	2.20	0.42
1:S:360:TYR:C	1:S:362:GLY:N	2.78	0.42
2:X:406:ARG:HH21	2:X:450:ASP:CG	2.28	0.42
1:B:309:GLU:OE1	2:F:191:THR:OG1	2.38	0.41
1:C:109:VAL:HG12	1:C:117:ILE:HD11	2.01	0.41
1:C:146:GLU:CB	1:C:163:ARG:HD2	2.50	0.41
1:C:349:ASP:O	1:C:375:ARG:HB2	2.20	0.41
2:E:204:THR:OG1	2:E:420:VAL:HB	2.20	0.41
2:E:386:ASP:OD1	2:E:386:ASP:N	2.52	0.41
2:F:117:ILE:HG22	2:F:235:THR:HA	2.01	0.41
1:J:68:LEU:HD23	1:J:73:VAL:HG13	2.02	0.41
5:R:55:GLU:CB	5:R:56:PRO:HD3	2.50	0.41
1:T:305:SER:HB2	2:X:222:MET:HB2	2.02	0.41
2:W:43:GLN:NE2	2:W:45:LYS:O	2.53	0.41
2:X:422:GLU:HG3	2:X:427:ILE:O	2.20	0.41
1:A:163:ARG:O	1:A:313:LYS:HB2	2.20	0.41
1:A:466:PHE:O	1:A:467:GLU:C	2.62	0.41
1:B:142:ARG:HB3	1:B:313:LYS:HG3	2.02	0.41
2:D:311:TYR:CE2	2:D:313:PRO:HA	2.55	0.41
2:D:340:SER:HB3	2:D:347:ALA:HB2	2.00	0.41
2:E:25:PHE:HB2	2:E:30:LEU:HD23	2.01	0.41
2:F:197:LEU:O	2:F:201:MET:HG2	2.19	0.41
2:F:449:TYR:HD1	2:F:452:ILE:HD12	1.85	0.41
1:J:111:ASP:C	1:J:111:ASP:OD1	2.62	0.41
1:K:135:ALA:HB3	2:O:223:ASN:HD22	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:380:THR:O	2:N:384:LEU:HG	2.21	0.41
1:T:138:ILE:CD1	2:X:219:PHE:CD2	3.02	0.41
1:T:150:THR:HG21	1:T:155:VAL:HG11	2.02	0.41
1:U:28:ASN:HA	1:U:47:ASN:HB2	2.02	0.41
1:U:206:VAL:HG11	1:U:249:PRO:HA	2.01	0.41
2:W:385:GLN:H	2:W:385:GLN:HG2	1.71	0.41
1:B:98:ASP:HB2	1:B:129:SER:O	2.20	0.41
1:B:270:TYR:HB2	1:B:327:PRO:HA	2.01	0.41
1:B:347:ILE:O	2:F:190:ARG:NE	2.51	0.41
1:C:455:LEU:HD21	1:C:466:PHE:CZ	2.55	0.41
2:E:321:ALA:HB3	2:E:322:PRO:CD	2.50	0.41
2:F:229:ARG:HH22	2:F:267:GLU:CD	2.27	0.41
3:G:118:LEU:HB3	3:G:126:ILE:HD11	2.02	0.41
5:I:12:ALA:C	5:I:14:LEU:H	2.28	0.41
1:J:112:ALA:O	1:J:251:THR:HG21	2.20	0.41
1:K:184:THR:O	1:K:188:GLN:HG2	2.20	0.41
1:K:272:ASP:HB2	1:K:328:VAL:O	2.21	0.41
1:U:178:THR:HG23	1:U:271:ASP:OD2	2.19	0.41
1:B:408:PHE:CD2	1:B:411:ASP:HB3	2.56	0.41
1:B:421:VAL:O	1:B:425:ARG:HG2	2.21	0.41
1:C:152:LEU:HA	1:C:432:GLN:OE1	2.21	0.41
3:G:60:LEU:HD21	3:G:190:GLN:HB2	2.02	0.41
1:L:162:GLY:CA	1:L:380:ALA:HB1	2.51	0.41
3:P:25:ILE:HA	3:P:28:SER:OG	2.19	0.41
1:S:217:GLN:HA	2:V:129:THR:HG21	2.02	0.41
1:T:173:ARG:HB3	1:T:173:ARG:NH1	2.36	0.41
1:T:368:ASN:CG	1:T:371:LEU:HB2	2.45	0.41
2:V:99:ILE:H	2:V:99:ILE:HG12	1.63	0.41
2:X:137:GLY:HA2	2:X:432:VAL:O	2.21	0.41
2:X:191:THR:HA	2:X:221:GLN:HG3	2.01	0.41
1:A:165:GLN:O	1:A:324:THR:HG23	2.20	0.41
1:A:382:VAL:O	1:A:383:LYS:C	2.64	0.41
1:C:364:ARG:HA	1:C:365:PRO:C	2.45	0.41
2:D:253:LEU:O	2:D:306:SER:HA	2.20	0.41
2:E:416:GLN:NE2	2:E:430:LYS:O	2.54	0.41
1:J:309:GLU:CB	2:N:223:ASN:HB3	2.50	0.41
2:N:275:ILE:HA	2:N:276:PRO:HD3	1.90	0.41
2:N:443:ALA:HB1	2:N:449:TYR:HE2	1.85	0.41
1:S:243:PRO:CG	1:S:283:LEU:HD21	2.48	0.41
1:T:203:CYS:HB2	1:T:231:SER:HB3	2.01	0.41
1:T:204:VAL:O	1:T:268:ILE:HA	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:153:LYS:HA	1:U:443:GLN:OE1	2.20	0.41
1:U:468:SER:O	1:U:472:SER:HB2	2.21	0.41
2:V:296:ILE:HG23	2:V:304:VAL:HG12	2.01	0.41
2:W:85:VAL:HG11	2:W:235:THR:CG2	2.39	0.41
3:Y:9:ARG:HD3	3:Y:251:TYR:HE1	1.82	0.41
1:B:285:LEU:HD22	2:E:275:ILE:HG21	2.03	0.41
1:L:354:LEU:HA	1:L:366:ALA:O	2.21	0.41
1:L:383:LYS:HE3	1:L:386:LYS:HD3	2.02	0.41
2:M:359:ASP:O	2:M:360:ALA:C	2.63	0.41
1:S:55:VAL:HG21	1:S:75:ILE:HD13	2.01	0.41
1:U:184:THR:O	1:U:188:GLN:HG2	2.21	0.41
1:A:146:GLU:HA	1:A:147:PRO:HD3	1.94	0.41
3:G:169:PRO:HB3	3:G:228:ALA:HB2	2.03	0.41
1:J:182:LEU:HD21	1:J:435:TYR:HE1	1.86	0.41
1:K:191:TRP:HD1	1:K:199:LYS:HB3	1.85	0.41
2:M:138:ILE:O	2:M:139:LYS:C	2.64	0.41
1:T:387:GLN:HE22	1:T:491:LEU:H	1.68	0.41
1:U:168:LEU:CD2	1:U:345:ILE:HG13	2.51	0.41
2:V:52:GLN:NE2	2:V:60:ARG:HD2	2.35	0.41
2:W:133:ILE:HD13	2:W:357:LEU:HD12	2.03	0.41
1:A:384:ALA:HB2	1:A:489:GLY:C	2.46	0.41
1:C:65:ALA:HA	1:C:75:ILE:HG12	2.02	0.41
1:C:462:ARG:O	1:C:465:GLU:HG2	2.21	0.41
2:F:85:VAL:HG11	2:F:235:THR:CG2	2.44	0.41
3:G:115:LYS:O	3:G:119:LEU:HB2	2.21	0.41
1:L:86:GLU:C	1:L:88:GLU:H	2.29	0.41
2:M:34:LEU:HD13	2:M:118:HIS:CG	2.56	0.41
2:M:269:SER:O	2:M:274:ARG:HB2	2.21	0.41
1:T:30:THR:CG2	1:T:31:GLY:N	2.83	0.41
2:V:148:ALA:O	2:V:150:GLY:N	2.53	0.41
2:V:250:ASP:OD2	2:V:303:SER:HB3	2.21	0.41
2:X:405:GLU:O	2:X:409:LYS:HG3	2.20	0.41
3:Y:253:ILE:HG22	3:Y:257:ARG:NH1	2.36	0.41
1:A:440:THR:O	1:A:444:VAL:HG13	2.20	0.41
1:A:463:ILE:O	1:A:466:PHE:HB3	2.20	0.41
1:B:271:ASP:HA	1:B:272:ASP:HA	1.68	0.41
1:B:311:ALA:HA	1:B:323:LEU:HB3	2.03	0.41
1:B:469:SER:HB3	1:B:506:PHE:HZ	1.86	0.41
1:C:139:LEU:HD13	2:D:104:ASP:HA	2.02	0.41
2:E:134:LEU:HB2	2:E:149:ARG:HB2	2.03	0.41
2:F:95:ILE:HD11	2:F:198:TYR:CG	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:50:LEU:CG	4:H:78:GLN:HE21	2.33	0.41
4:H:71:SER:HB2	4:H:89:GLU:HB2	2.01	0.41
1:J:254:SER:O	1:J:257:GLU:HB2	2.20	0.41
1:L:455:LEU:HD21	1:L:466:PHE:CE1	2.56	0.41
2:M:26:GLU:HB2	2:M:29:GLU:CD	2.45	0.41
2:M:409:LYS:O	2:M:413:PHE:HB2	2.20	0.41
2:N:346:PRO:HB2	2:N:348:VAL:HG23	2.02	0.41
2:O:186:GLY:HA2	2:O:256:ASP:O	2.20	0.41
1:S:158:LEU:HD22	1:S:393:LYS:HG2	2.03	0.41
1:T:138:ILE:O	2:X:195:ASN:ND2	2.53	0.41
1:T:340:ILE:N	1:T:341:PRO:CD	2.84	0.41
1:U:136:PRO:HD2	1:U:310:ARG:HA	2.02	0.41
2:V:168:GLN:HG2	2:V:197:LEU:HD13	2.03	0.41
2:W:278:ALA:HA	3:Y:264:THR:HG23	2.02	0.41
2:W:321:ALA:HB3	2:W:322:PRO:CD	2.50	0.41
2:X:33:ILE:HA	2:X:50:VAL:HG12	2.03	0.41
2:X:182:SER:O	2:X:215:VAL:HA	2.21	0.41
1:A:237:THR:N	1:A:240:GLU:HG3	2.36	0.41
1:C:192:ASN:HA	1:C:200:LYS:HG2	2.02	0.41
1:C:455:LEU:HD21	1:C:466:PHE:CE1	2.55	0.41
2:D:198:TYR:O	2:D:202:LYS:HG3	2.21	0.41
2:E:96:ILE:HB	2:E:218:VAL:HG22	2.03	0.41
2:E:276:PRO:HD2	3:G:271:ILE:HG13	2.02	0.41
2:E:287:THR:O	2:E:291:LEU:HG	2.21	0.41
1:K:86:GLU:OE1	2:N:30:LEU:HD11	2.20	0.41
2:M:9:ILE:H	2:M:9:ILE:HD12	1.85	0.41
2:M:52:GLN:HE21	2:M:52:GLN:HB2	1.68	0.41
2:M:154:GLY:HA3	2:M:329:LEU:HD13	2.03	0.41
2:M:263:GLN:O	2:M:266:SER:HB3	2.21	0.41
2:N:142:ASP:HA	2:N:146:PRO:HB3	2.01	0.41
1:S:202:TYR:O	1:S:266:ALA:HA	2.21	0.41
1:T:444:VAL:HG22	1:T:445:PRO:HD3	2.03	0.41
2:V:147:TYR:CD2	2:V:153:ILE:HD13	2.56	0.41
1:B:166:ARG:HD2	1:B:308:LEU:O	2.21	0.40
1:B:369:VAL:HG13	1:B:393:LYS:HD2	2.03	0.40
2:E:67:THR:HB	2:E:70:LEU:HD12	2.02	0.40
2:F:136:THR:HA	2:F:174:ILE:HD11	2.03	0.40
2:F:258:ILE:HG22	2:F:310:VAL:HG22	2.02	0.40
2:N:240:ALA:HB2	2:N:253:LEU:HD13	2.04	0.40
1:T:444:VAL:N	1:T:445:PRO:CD	2.84	0.40
2:W:204:THR:HG22	2:W:206:VAL:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:LEU:HD23	1:A:430:LEU:HA	1.91	0.40
1:A:506:PHE:O	1:A:509:THR:HG22	2.21	0.40
1:B:480:GLU:CD	1:B:480:GLU:H	2.27	0.40
1:C:271:ASP:HA	1:C:272:ASP:HA	1.79	0.40
2:E:193:GLU:O	2:E:196:ASP:HB2	2.21	0.40
2:M:237:LEU:HD21	2:M:295:ARG:CB	2.49	0.40
2:N:184:PHE:HA	2:N:254:PHE:HB2	2.03	0.40
3:P:95:VAL:O	3:P:99:LEU:HB2	2.21	0.40
3:P:108:VAL:HG21	3:P:150:LEU:HD11	2.04	0.40
1:A:250:PHE:CE1	1:A:307:LEU:HB2	2.56	0.40
1:C:34:LEU:N	1:C:42:ARG:O	2.52	0.40
2:F:224:GLU:HA	2:F:225:PRO:HD3	1.94	0.40
1:L:36:VAL:HG21	1:L:84:VAL:HB	2.02	0.40
2:M:41:THR:HB	2:M:42:PRO:HD2	2.03	0.40
2:O:33:ILE:HG22	2:O:34:LEU:HG	2.03	0.40
1:T:158:LEU:HB3	1:T:393:LYS:HD3	2.04	0.40
2:W:202:LYS:C	2:W:204:THR:H	2.29	0.40
2:X:189:GLU:O	2:X:222:MET:HG2	2.21	0.40
1:A:257:GLU:HG2	1:A:260:ARG:CZ	2.52	0.40
1:A:280:TYR:CE2	1:A:297:PRO:HG2	2.56	0.40
3:G:39:ILE:O	3:G:43:LYS:HB2	2.22	0.40
1:L:340:ILE:HB	1:L:341:PRO:HD3	2.04	0.40
2:O:141:VAL:HG22	2:O:333:THR:HG21	2.02	0.40
3:P:185:ALA:HB2	3:P:207:ARG:HA	2.02	0.40
3:P:256:ASN:HA	3:P:259:ARG:HB3	2.02	0.40
1:T:187:ASN:OD1	1:T:437:PRO:HB2	2.21	0.40
1:U:228:MET:HA	1:U:231:SER:HB2	2.04	0.40
2:W:109:ILE:HG22	2:W:111:SER:HB2	2.02	0.40
1:A:211:LYS:HE3	1:A:213:SER:OG	2.21	0.40
2:F:442:LYS:O	2:F:446:GLU:HG3	2.22	0.40
1:J:289:ARG:HH21	2:N:17:ILE:HG21	1.87	0.40
1:L:165:GLN:HB2	1:L:376:VAL:HG21	2.03	0.40
2:N:98:VAL:HB	2:N:232:VAL:HG13	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	483/510 (95%)	457 (95%)	25 (5%)	1 (0%)	43	73
1	B	484/510 (95%)	455 (94%)	25 (5%)	4 (1%)	16	50
1	C	482/510 (94%)	458 (95%)	23 (5%)	1 (0%)	43	73
1	J	478/510 (94%)	443 (93%)	32 (7%)	3 (1%)	21	56
1	K	479/510 (94%)	442 (92%)	37 (8%)	0	100	100
1	L	475/510 (93%)	442 (93%)	31 (6%)	2 (0%)	30	62
1	S	479/510 (94%)	458 (96%)	20 (4%)	1 (0%)	43	73
1	T	480/510 (94%)	454 (95%)	26 (5%)	0	100	100
1	U	483/510 (95%)	450 (93%)	31 (6%)	2 (0%)	30	62
2	D	468/484 (97%)	440 (94%)	26 (6%)	2 (0%)	30	62
2	E	467/484 (96%)	437 (94%)	28 (6%)	2 (0%)	30	62
2	F	467/484 (96%)	443 (95%)	24 (5%)	0	100	100
2	M	458/484 (95%)	421 (92%)	34 (7%)	3 (1%)	18	52
2	N	459/484 (95%)	422 (92%)	34 (7%)	3 (1%)	18	52
2	O	467/484 (96%)	433 (93%)	33 (7%)	1 (0%)	43	73
2	V	354/484 (73%)	318 (90%)	31 (9%)	5 (1%)	9	39
2	W	466/484 (96%)	435 (93%)	30 (6%)	1 (0%)	43	73
2	X	467/484 (96%)	430 (92%)	35 (8%)	2 (0%)	30	62
3	G	264/278 (95%)	249 (94%)	14 (5%)	1 (0%)	30	62
3	P	264/278 (95%)	243 (92%)	19 (7%)	2 (1%)	16	50
3	Y	109/278 (39%)	102 (94%)	7 (6%)	0	100	100
4	H	118/138 (86%)	98 (83%)	17 (14%)	3 (2%)	4	27
4	Q	91/138 (66%)	81 (89%)	10 (11%)	0	100	100
5	I	51/61 (84%)	44 (86%)	3 (6%)	4 (8%)	1	5
5	R	51/61 (84%)	43 (84%)	7 (14%)	1 (2%)	6	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	9344/10178 (92%)	8698 (93%)	602 (6%)	44 (0%)	24	59

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	H	99	GLU
5	I	55	GLU
2	M	27	GLN
5	R	58	PRO
4	H	33	PRO
5	I	13	TYR
2	M	279	VAL
3	P	170	VAL
1	S	97	VAL
1	B	27	LEU
2	E	366	GLU
4	H	100	ASN
1	U	390	GLY
2	V	28	SER
1	B	390	GLY
1	B	415	SER
5	I	58	PRO
1	J	379	ALA
2	M	29	GLU
1	U	70	PRO
1	A	70	PRO
3	G	202	ASP
5	I	8	ILE
1	J	70	PRO
1	L	283	LEU
3	P	243	ASN
2	V	149	ARG
2	V	354	LYS
2	X	123	SER
1	B	367	ILE
2	N	221	GLN
1	C	489	GLY
2	D	188	GLY
2	V	279	VAL
2	D	279	VAL
2	E	279	VAL
2	O	108	PRO

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Mol	Chain	Res	Type
2	N	279	VAL
1	J	97	VAL
1	L	122	PRO
2	N	87	VAL
2	W	279	VAL
2	V	44	GLY
2	X	279	VAL

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	391/412 (95%)	359 (92%)	32 (8%)	10	39
1	B	390/412 (95%)	368 (94%)	22 (6%)	19	52
1	C	390/412 (95%)	363 (93%)	27 (7%)	14	45
1	J	388/412 (94%)	365 (94%)	23 (6%)	18	50
1	K	366/412 (89%)	346 (94%)	20 (6%)	19	52
1	L	378/412 (92%)	355 (94%)	23 (6%)	17	49
1	S	382/412 (93%)	358 (94%)	24 (6%)	16	48
1	T	379/412 (92%)	351 (93%)	28 (7%)	13	43
1	U	348/412 (84%)	325 (93%)	23 (7%)	15	47
2	D	379/390 (97%)	357 (94%)	22 (6%)	18	51
2	E	371/390 (95%)	340 (92%)	31 (8%)	10	38
2	F	378/390 (97%)	350 (93%)	28 (7%)	13	43
2	M	363/390 (93%)	342 (94%)	21 (6%)	18	51
2	N	352/390 (90%)	323 (92%)	29 (8%)	10	39
2	O	357/390 (92%)	330 (92%)	27 (8%)	12	42
2	V	261/390 (67%)	248 (95%)	13 (5%)	22	55
2	W	361/390 (93%)	343 (95%)	18 (5%)	22	55
2	X	354/390 (91%)	337 (95%)	17 (5%)	23	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	G	226/236 (96%)	201 (89%)	25 (11%)	6	25
3	P	178/236 (75%)	159 (89%)	19 (11%)	6	27
3	Y	72/236 (30%)	61 (85%)	11 (15%)	3	14
4	H	71/112 (63%)	60 (84%)	11 (16%)	2	14
4	Q	46/112 (41%)	40 (87%)	6 (13%)	4	20
5	I	34/48 (71%)	27 (79%)	7 (21%)	1	7
5	R	28/48 (58%)	27 (96%)	1 (4%)	31	63
All	All	7243/8246 (88%)	6735 (93%)	508 (7%)	14	45

All (508) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	LEU
1	A	58	SER
1	A	88	GLU
1	A	138	ILE
1	A	156	ASP
1	A	163	ARG
1	A	173	ARG
1	A	211	LYS
1	A	240	GLU
1	A	251	THR
1	A	289	ARG
1	A	303	LEU
1	A	306	ARG
1	A	316	GLU
1	A	342	THR
1	A	357	GLU
1	A	378	SER
1	A	394	LEU
1	A	401	GLU
1	A	408	PHE
1	A	429	LEU
1	A	436	SER
1	A	444	VAL
1	A	465	GLU
1	A	468	SER
1	A	480	GLU
1	A	492	SER
1	A	495	LEU

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Mol	Chain	Res	Type
1	A	498	SER
1	A	505	SER
1	A	509	THR
1	A	510	PHE
1	B	30	THR
1	B	40	ILE
1	B	76	VAL
1	B	89	LEU
1	B	99	VAL
1	B	106	LEU
1	B	133	VAL
1	B	195	SER
1	B	196	ASP
1	B	218	LEU
1	B	246	TYR
1	B	255	ILE
1	B	309	GLU
1	B	336	VAL
1	B	351	GLN
1	B	378	SER
1	B	391	SER
1	B	408	PHE
1	B	434	GLN
1	B	444	VAL
1	B	463	ILE
1	B	480	GLU
1	C	54	LEU
1	C	62	LYS
1	C	99	VAL
1	C	139	LEU
1	C	163	ARG
1	C	213	SER
1	C	214	THR
1	C	223	GLU
1	C	247	LEU
1	C	267	LEU
1	C	284	SER
1	C	289	ARG
1	C	293	ARG
1	C	364	ARG
1	C	373	VAL
1	C	383	LYS

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Mol	Chain	Res	Type
1	C	394	LEU
1	C	417	LYS
1	C	418	GLN
1	C	424	GLU
1	C	440	THR
1	C	456	ASP
1	C	477	ASN
1	C	479	ASN
1	C	495	LEU
1	C	507	VAL
1	C	509	THR
2	D	7	THR
2	D	9	ILE
2	D	17	ILE
2	D	52	GLN
2	D	62	ILE
2	D	74	GLU
2	D	77	LEU
2	D	84	SER
2	D	132	GLU
2	D	149	ARG
2	D	176	LYS
2	D	185	THR
2	D	192	ARG
2	D	237	LEU
2	D	268	VAL
2	D	285	LEU
2	D	289	MET
2	D	303	SER
2	D	387	ILE
2	D	388	ILE
2	D	390	ILE
2	D	472	LYS
2	E	10	THR
2	E	17	ILE
2	E	27	GLN
2	E	56	GLU
2	E	68	GLU
2	E	128	SER
2	E	132	GLU
2	E	136	THR
2	E	140	VAL

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Mol	Chain	Res	Type
2	E	152	LYS
2	E	164	THR
2	E	204	THR
2	E	210	GLU
2	E	221	GLN
2	E	224	GLU
2	E	232	VAL
2	E	263	GLN
2	E	275	ILE
2	E	292	LEU
2	E	337	ARG
2	E	352	ASP
2	E	366	GLU
2	E	378	LEU
2	E	386	ASP
2	E	388	ILE
2	E	390	ILE
2	E	391	LEU
2	E	399	GLN
2	E	403	THR
2	E	412	ARG
2	E	423	VAL
2	F	12	LYS
2	F	17	ILE
2	F	28	SER
2	F	30	LEU
2	F	43	GLN
2	F	68	GLU
2	F	77	LEU
2	F	128	SER
2	F	130	SER
2	F	133	ILE
2	F	140	VAL
2	F	167	ILE
2	F	168	GLN
2	F	176	LYS
2	F	191	THR
2	F	192	ARG
2	F	201	MET
2	F	206	VAL
2	F	208	ASN
2	F	215	VAL

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Mol	Chain	Res	Type
2	F	274	ARG
2	F	279	VAL
2	F	299	THR
2	F	306	SER
2	F	403	THR
2	F	422	GLU
2	F	423	VAL
2	F	472	LYS
3	G	3	LEU
3	G	4	LYS
3	G	7	GLU
3	G	22	THR
3	G	48	GLU
3	G	53	LYS
3	G	57	THR
3	G	102	GLN
3	G	118	LEU
3	G	133	ILE
3	G	136	ASP
3	G	143	SER
3	G	145	LEU
3	G	150	LEU
3	G	153	VAL
3	G	173	LEU
3	G	190	GLN
3	G	191	SER
3	G	202	ASP
3	G	204	ASN
3	G	207	ARG
3	G	231	SER
3	G	242	LYS
3	G	254	LEU
3	G	275	SER
4	H	20	THR
4	H	28	THR
4	H	35	LYS
4	H	42	LEU
4	H	46	VAL
4	H	48	THR
4	H	51	GLN
4	H	59	VAL
4	H	66	LYS

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Mol	Chain	Res	Type
4	H	70	ILE
4	H	112	VAL
5	I	14	LEU
5	I	28	GLU
5	I	29	LEU
5	I	35	LEU
5	I	37	ARG
5	I	38	SER
5	I	57	THR
1	J	27	LEU
1	J	54	LEU
1	J	58	SER
1	J	72	GLN
1	J	81	ASP
1	J	90	VAL
1	J	163	ARG
1	J	173	ARG
1	J	206	VAL
1	J	289	ARG
1	J	342	THR
1	J	369	VAL
1	J	375	ARG
1	J	394	LEU
1	J	407	GLN
1	J	419	THR
1	J	420	LEU
1	J	429	LEU
1	J	444	VAL
1	J	473	TYR
1	J	480	GLU
1	J	483	THR
1	J	509	THR
1	K	21	VAL
1	K	30	THR
1	K	52	GLU
1	K	59	SER
1	K	66	LEU
1	K	99	VAL
1	K	106	LEU
1	K	129	SER
1	K	178	THR
1	K	195	SER

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Mol	Chain	Res	Type
1	K	206	VAL
1	K	218	LEU
1	K	219	VAL
1	K	283	LEU
1	K	288	ARG
1	K	351	GLN
1	K	378	SER
1	K	401	GLU
1	K	407	GLN
1	K	458	ILE
1	L	54	LEU
1	L	66	LEU
1	L	72	GLN
1	L	89	LEU
1	L	99	VAL
1	L	105	LEU
1	L	139	LEU
1	L	173	ARG
1	L	214	THR
1	L	219	VAL
1	L	220	GLN
1	L	283	LEU
1	L	293	ARG
1	L	300	VAL
1	L	342	THR
1	L	351	GLN
1	L	358	LEU
1	L	394	LEU
1	L	433	ASN
1	L	477	ASN
1	L	479	ASN
1	L	487	GLU
1	L	507	VAL
2	M	17	ILE
2	M	26	GLU
2	M	113	LEU
2	M	133	ILE
2	M	165	VAL
2	M	206	VAL
2	M	215	VAL
2	M	247	GLU
2	M	249	GLN

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Mol	Chain	Res	Type
2	M	251	VAL
2	M	271	LEU
2	M	292	LEU
2	M	306	SER
2	M	342	LEU
2	M	344	ILE
2	M	366	GLU
2	M	377	THR
2	M	394	ASP
2	M	423	VAL
2	M	431	LEU
2	M	464	GLU
2	N	10	THR
2	N	21	VAL
2	N	35	ASN
2	N	41	THR
2	N	56	GLU
2	N	57	ASN
2	N	68	GLU
2	N	103	ILE
2	N	113	LEU
2	N	132	GLU
2	N	140	VAL
2	N	183	VAL
2	N	189	GLU
2	N	196	ASP
2	N	210	GLU
2	N	221	GLN
2	N	232	VAL
2	N	251	VAL
2	N	262	THR
2	N	263	GLN
2	N	275	ILE
2	N	298	THR
2	N	337	ARG
2	N	352	ASP
2	N	377	THR
2	N	405	GLU
2	N	423	VAL
2	N	436	ASP
2	N	437	THR
2	O	17	ILE

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Mol	Chain	Res	Type
2	O	40	LYS
2	O	68	GLU
2	O	74	GLU
2	O	111	SER
2	O	140	VAL
2	O	172	ASN
2	O	176	LYS
2	O	195	ASN
2	O	206	VAL
2	O	208	ASN
2	O	224	GLU
2	O	274	ARG
2	O	277	SER
2	O	279	VAL
2	O	289	MET
2	O	300	LYS
2	O	301	LYS
2	O	305	THR
2	O	359	ASP
2	O	377	THR
2	O	388	ILE
2	O	398	GLU
2	O	423	VAL
2	O	427	ILE
2	O	452	ILE
2	O	455	HIS
3	P	15	ASN
3	P	23	MET
3	P	29	THR
3	P	44	MET
3	P	78	THR
3	P	112	ASP
3	P	117	GLN
3	P	150	LEU
3	P	158	THR
3	P	186	LYS
3	P	190	GLN
3	P	202	ASP
3	P	204	ASN
3	P	248	ILE
3	P	254	LEU
3	P	266	GLU

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Mol	Chain	Res	Type
3	P	268	VAL
3	P	269	ASP
3	P	276	SER
4	Q	31	ASN
4	Q	51	GLN
4	Q	70	ILE
4	Q	76	THR
4	Q	85	VAL
4	Q	130	LEU
5	R	4	ARG
1	S	36	VAL
1	S	54	LEU
1	S	81	ASP
1	S	129	SER
1	S	153	LYS
1	S	206	VAL
1	S	221	THR
1	S	251	THR
1	S	288	ARG
1	S	289	ARG
1	S	318	GLU
1	S	363	ILE
1	S	364	ARG
1	S	378	SER
1	S	393	LYS
1	S	394	LEU
1	S	395	PHE
1	S	412	LEU
1	S	413	ASP
1	S	444	VAL
1	S	465	GLU
1	S	468	SER
1	S	495	LEU
1	S	509	THR
1	T	36	VAL
1	T	59	SER
1	T	62	LYS
1	T	91	LYS
1	T	99	VAL
1	T	159	VAL
1	T	206	VAL
1	T	214	THR

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Mol	Chain	Res	Type
1	T	283	LEU
1	T	289	ARG
1	T	316	GLU
1	T	317	LYS
1	T	323	LEU
1	T	351	GLN
1	T	369	VAL
1	T	394	LEU
1	T	400	ARG
1	T	402	VAL
1	T	412	LEU
1	T	419	THR
1	T	422	ARG
1	T	444	VAL
1	T	460	LEU
1	T	465	GLU
1	T	472	SER
1	T	481	LEU
1	T	484	GLU
1	T	501	SER
1	U	27	LEU
1	U	30	THR
1	U	54	LEU
1	U	56	GLU
1	U	61	VAL
1	U	72	GLN
1	U	97	VAL
1	U	99	VAL
1	U	129	SER
1	U	159	VAL
1	U	213	SER
1	U	220	GLN
1	U	254	SER
1	U	317	LYS
1	U	342	THR
1	U	346	SER
1	U	357	GLU
1	U	376	VAL
1	U	418	GLN
1	U	424	GLU
1	U	468	SER
1	U	472	SER

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Mol	Chain	Res	Type
1	U	495	LEU
2	V	9	ILE
2	V	17	ILE
2	V	87	VAL
2	V	99	ILE
2	V	167	ILE
2	V	192	ARG
2	V	204	THR
2	V	251	VAL
2	V	269	SER
2	V	285	LEU
2	V	301	LYS
2	V	332	THR
2	V	348	VAL
2	W	43	GLN
2	W	56	GLU
2	W	74	GLU
2	W	113	LEU
2	W	136	THR
2	W	140	VAL
2	W	204	THR
2	W	221	GLN
2	W	232	VAL
2	W	258	ILE
2	W	337	ARG
2	W	352	ASP
2	W	366	GLU
2	W	380	THR
2	W	403	THR
2	W	406	ARG
2	W	423	VAL
2	W	434	LEU
2	X	14	THR
2	X	68	GLU
2	X	140	VAL
2	X	153	ILE
2	X	167	ILE
2	X	201	MET
2	X	208	ASN
2	X	210	GLU
2	X	224	GLU
2	X	251	VAL

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Mol	Chain	Res	Type
2	X	279	VAL
2	X	285	LEU
2	X	300	LYS
2	X	383	SER
2	X	403	THR
2	X	420	VAL
2	X	452	ILE
3	Y	2	THR
3	Y	3	LEU
3	Y	16	ILE
3	Y	23	MET
3	Y	26	VAL
3	Y	219	LEU
3	Y	220	THR
3	Y	239	ASN
3	Y	254	LEU
3	Y	268	VAL
3	Y	275	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (122) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	GLN
1	A	188	GLN
1	A	217	GLN
1	A	220	GLN
1	A	351	GLN
1	A	418	GLN
1	A	479	ASN
1	B	26	ASN
1	B	50	GLN
1	B	95	ASN
1	B	115	ASN
1	B	193	ASN
1	B	332	GLN
1	B	381	GLN
1	C	28	ASN
1	C	48	ASN
1	C	50	GLN
1	C	95	ASN
1	C	174	GLN
1	C	188	GLN

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Mol	Chain	Res	Type
1	C	381	GLN
1	C	387	GLN
1	C	454	HIS
2	D	24	HIS
2	D	52	GLN
2	E	168	GLN
2	E	173	ASN
2	E	221	GLN
2	F	27	GLN
2	F	379	GLN
3	G	59	ASN
3	G	90	GLN
3	G	102	GLN
3	G	122	HIS
3	G	131	ASN
3	G	190	GLN
3	G	217	GLN
3	G	235	ASN
4	H	13	GLN
4	H	82	GLN
5	I	19	GLN
5	I	36	ASN
5	I	46	GLN
5	I	49	ASN
1	J	145	HIS
1	J	217	GLN
1	J	220	GLN
1	J	224	GLN
1	J	225	HIS
1	J	262	ASN
1	J	304	HIS
1	J	407	GLN
1	J	428	GLN
1	K	26	ASN
1	K	95	ASN
1	K	282	GLN
1	K	428	GLN
1	L	145	HIS
1	L	149	GLN
1	L	282	GLN
1	L	351	GLN
1	L	368	ASN

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Mol	Chain	Res	Type
1	L	387	GLN
1	L	418	GLN
2	M	24	HIS
2	M	52	GLN
2	M	57	ASN
2	M	97	ASN
2	M	178	HIS
2	M	195	ASN
2	M	249	GLN
2	N	24	HIS
2	N	127	GLN
2	N	263	GLN
2	N	411	GLN
2	O	24	HIS
2	O	35	ASN
2	O	97	ASN
2	O	118	HIS
2	O	178	HIS
2	O	208	ASN
3	P	125	ASN
3	P	216	ASN
4	Q	45	HIS
5	R	15	ASN
1	S	50	GLN
1	S	145	HIS
1	S	210	GLN
1	S	220	GLN
1	S	282	GLN
1	S	304	HIS
1	S	351	GLN
1	S	368	ASN
1	S	407	GLN
1	S	428	GLN
1	S	477	ASN
1	T	50	GLN
1	T	132	GLN
1	T	217	GLN
1	T	225	HIS
1	T	304	HIS
1	T	387	GLN
1	T	454	HIS
1	T	477	ASN

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Mol	Chain	Res	Type
1	U	50	GLN
1	U	282	GLN
1	U	332	GLN
1	U	418	GLN
2	V	52	GLN
2	V	57	ASN
2	V	249	GLN
2	W	168	GLN
2	W	172	ASN
2	W	263	GLN
2	W	367	HIS
2	X	35	ASN
2	X	52	GLN
2	X	208	ASN
2	X	293	GLN
2	X	367	HIS
2	X	379	GLN
2	X	385	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	D	600	7	33,33,33	1.97	9 (27%)	45,52,52	2.09	12 (26%)
6	ANP	F	600	7	33,33,33	2.06	12 (36%)	45,52,52	2.01	10 (22%)
6	ANP	X	600	7	33,33,33	1.86	11 (33%)	45,52,52	2.32	13 (28%)
6	ANP	J	600	7	33,33,33	1.96	12 (36%)	45,52,52	2.19	15 (33%)
6	ANP	V	600	7	33,33,33	2.33	10 (30%)	45,52,52	2.20	12 (26%)
6	ANP	T	600	7	33,33,33	2.06	12 (36%)	45,52,52	2.14	13 (28%)
6	ANP	U	600	7	33,33,33	2.07	11 (33%)	45,52,52	2.04	13 (28%)
6	ANP	M	600	7	33,33,33	1.97	11 (33%)	45,52,52	2.25	14 (31%)
6	ANP	O	600	7	33,33,33	2.06	12 (36%)	45,52,52	2.05	11 (24%)
6	ANP	B	600	7	33,33,33	2.07	12 (36%)	45,52,52	2.06	12 (26%)
6	ANP	L	600	7	33,33,33	1.94	10 (30%)	45,52,52	2.13	12 (26%)
6	ANP	A	600	7	33,33,33	1.90	10 (30%)	45,52,52	2.05	13 (28%)
6	ANP	C	600	7	33,33,33	1.99	10 (30%)	45,52,52	2.25	13 (28%)
6	ANP	S	600	7	33,33,33	2.02	10 (30%)	45,52,52	2.22	10 (22%)
6	ANP	K	600	7	33,33,33	2.05	9 (27%)	45,52,52	2.06	13 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ANP	D	600	7	-	4/18/38/38	0/3/3/3
6	ANP	F	600	7	-	6/18/38/38	0/3/3/3
6	ANP	X	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	V	600	7	-	6/18/38/38	0/3/3/3
6	ANP	T	600	7	-	6/18/38/38	0/3/3/3
6	ANP	U	600	7	-	4/18/38/38	0/3/3/3
6	ANP	M	600	7	-	2/18/38/38	0/3/3/3
6	ANP	O	600	7	-	3/18/38/38	0/3/3/3
6	ANP	B	600	7	-	5/18/38/38	0/3/3/3
6	ANP	L	600	7	-	3/18/38/38	0/3/3/3
6	ANP	A	600	7	-	3/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ANP	C	600	7	-	2/18/38/38	0/3/3/3
6	ANP	S	600	7	-	5/18/38/38	0/3/3/3
6	ANP	K	600	7	-	8/18/38/38	0/3/3/3

All (161) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	V	600	ANP	PG-N3B	5.51	1.77	1.63
6	V	600	ANP	PB-N3B	5.33	1.77	1.63
6	K	600	ANP	C5-C4	5.26	1.48	1.39
6	T	600	ANP	C5-C4	5.17	1.48	1.39
6	O	600	ANP	C5-C4	5.16	1.48	1.39
6	C	600	ANP	C5-C4	5.15	1.48	1.39
6	B	600	ANP	C5-C4	5.07	1.48	1.39
6	M	600	ANP	C5-C4	5.06	1.48	1.39
6	U	600	ANP	C5-C4	5.00	1.48	1.39
6	V	600	ANP	C5-C4	4.93	1.47	1.39
6	D	600	ANP	C5-C4	4.90	1.47	1.39
6	L	600	ANP	C5-C4	4.87	1.47	1.39
6	F	600	ANP	C5-C4	4.79	1.47	1.39
6	X	600	ANP	C5-C4	4.78	1.47	1.39
6	J	600	ANP	C5-C4	4.77	1.47	1.39
6	S	600	ANP	C5-C4	4.73	1.47	1.39
6	A	600	ANP	C5-C4	4.70	1.47	1.39
6	O	600	ANP	PB-N3B	4.68	1.75	1.63
6	S	600	ANP	PB-N3B	4.57	1.75	1.63
6	S	600	ANP	PG-N3B	4.43	1.74	1.63
6	F	600	ANP	PB-N3B	4.39	1.74	1.63
6	T	600	ANP	PB-N3B	4.38	1.74	1.63
6	F	600	ANP	PG-N3B	4.34	1.74	1.63
6	L	600	ANP	PG-N3B	4.29	1.74	1.63
6	U	600	ANP	PB-N3B	4.23	1.74	1.63
6	D	600	ANP	PB-N3B	4.23	1.74	1.63
6	B	600	ANP	PB-N3B	4.20	1.74	1.63
6	D	600	ANP	PG-N3B	4.19	1.74	1.63
6	O	600	ANP	PG-N3B	4.17	1.74	1.63
6	K	600	ANP	PB-N3B	4.12	1.74	1.63
6	T	600	ANP	PG-N3B	4.08	1.74	1.63
6	J	600	ANP	PB-N3B	4.07	1.74	1.63
6	M	600	ANP	PB-N3B	4.04	1.73	1.63
6	V	600	ANP	PA-O3A	4.01	1.63	1.59
6	K	600	ANP	PG-O1G	4.01	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	K	600	ANP	PG-N3B	4.00	1.73	1.63
6	B	600	ANP	PG-N3B	4.00	1.73	1.63
6	L	600	ANP	PB-N3B	3.97	1.73	1.63
6	U	600	ANP	PG-N3B	3.95	1.73	1.63
6	C	600	ANP	PG-N3B	3.93	1.73	1.63
6	C	600	ANP	PB-N3B	3.92	1.73	1.63
6	X	600	ANP	PG-N3B	3.85	1.73	1.63
6	M	600	ANP	PG-N3B	3.84	1.73	1.63
6	A	600	ANP	PB-N3B	3.79	1.73	1.63
6	V	600	ANP	PG-O1G	3.77	1.51	1.46
6	V	600	ANP	PB-O1B	3.77	1.51	1.46
6	X	600	ANP	PB-N3B	3.75	1.73	1.63
6	A	600	ANP	PG-N3B	3.73	1.73	1.63
6	J	600	ANP	PG-N3B	3.72	1.73	1.63
6	B	600	ANP	PG-O1G	3.65	1.51	1.46
6	D	600	ANP	PG-O1G	3.59	1.51	1.46
6	S	600	ANP	PB-O1B	3.57	1.51	1.46
6	T	600	ANP	PG-O1G	3.54	1.51	1.46
6	K	600	ANP	PB-O1B	3.53	1.51	1.46
6	C	600	ANP	PG-O1G	3.46	1.51	1.46
6	V	600	ANP	PB-O3A	3.46	1.63	1.59
6	C	600	ANP	PB-O1B	3.44	1.51	1.46
6	S	600	ANP	PG-O1G	3.42	1.51	1.46
6	A	600	ANP	PG-O1G	3.39	1.51	1.46
6	T	600	ANP	PB-O1B	3.39	1.51	1.46
6	J	600	ANP	PG-O1G	3.38	1.51	1.46
6	U	600	ANP	PG-O1G	3.34	1.51	1.46
6	F	600	ANP	PG-O1G	3.32	1.51	1.46
6	L	600	ANP	PG-O1G	3.32	1.51	1.46
6	F	600	ANP	PA-O3A	3.30	1.63	1.59
6	U	600	ANP	PB-O1B	3.24	1.51	1.46
6	M	600	ANP	PB-O1B	3.16	1.51	1.46
6	O	600	ANP	PG-O1G	3.15	1.51	1.46
6	O	600	ANP	PB-O1B	3.13	1.50	1.46
6	F	600	ANP	PB-O1B	3.13	1.50	1.46
6	C	600	ANP	C5-C6	3.11	1.49	1.41
6	L	600	ANP	PB-O1B	3.07	1.50	1.46
6	D	600	ANP	PB-O1B	3.07	1.50	1.46
6	B	600	ANP	PA-O3A	3.03	1.62	1.59
6	A	600	ANP	PB-O1B	3.03	1.50	1.46
6	U	600	ANP	PA-O3A	3.02	1.62	1.59
6	T	600	ANP	C5-C6	3.02	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	600	ANP	C5-C6	2.97	1.49	1.41
6	J	600	ANP	PB-O1B	2.95	1.50	1.46
6	O	600	ANP	C5-C6	2.94	1.49	1.41
6	M	600	ANP	PG-O1G	2.92	1.50	1.46
6	K	600	ANP	C5-C6	2.88	1.49	1.41
6	B	600	ANP	PB-O1B	2.82	1.50	1.46
6	D	600	ANP	C5-C6	2.81	1.48	1.41
6	F	600	ANP	PB-O3A	2.76	1.62	1.59
6	U	600	ANP	C5-N7	-2.72	1.34	1.39
6	X	600	ANP	C5-C6	2.71	1.48	1.41
6	B	600	ANP	C5-C6	2.71	1.48	1.41
6	L	600	ANP	C5-N7	-2.69	1.34	1.39
6	V	600	ANP	C5-N7	-2.69	1.34	1.39
6	S	600	ANP	C5-N7	-2.68	1.34	1.39
6	X	600	ANP	PG-O1G	2.68	1.50	1.46
6	A	600	ANP	C5-C6	2.67	1.48	1.41
6	J	600	ANP	C5-N7	-2.64	1.34	1.39
6	U	600	ANP	C5-C6	2.61	1.48	1.41
6	U	600	ANP	PB-O3A	2.59	1.62	1.59
6	F	600	ANP	C5-N7	-2.57	1.34	1.39
6	J	600	ANP	C5-C6	2.57	1.48	1.41
6	L	600	ANP	C8-N7	2.55	1.36	1.31
6	S	600	ANP	C5-C6	2.55	1.48	1.41
6	K	600	ANP	C8-N7	2.53	1.36	1.31
6	L	600	ANP	C5-C6	2.53	1.48	1.41
6	V	600	ANP	C5-C6	2.51	1.48	1.41
6	M	600	ANP	PG-O3G	-2.50	1.50	1.56
6	B	600	ANP	PB-O3A	2.50	1.62	1.59
6	B	600	ANP	C5-N7	-2.49	1.34	1.39
6	O	600	ANP	C8-N7	2.48	1.36	1.31
6	A	600	ANP	PG-O3G	-2.47	1.50	1.56
6	A	600	ANP	PG-O2G	-2.46	1.50	1.56
6	C	600	ANP	PG-O2G	-2.44	1.50	1.56
6	T	600	ANP	C8-N7	2.44	1.36	1.31
6	D	600	ANP	PG-O3G	-2.41	1.50	1.56
6	F	600	ANP	C5-C6	2.41	1.47	1.41
6	X	600	ANP	PB-O1B	2.40	1.49	1.46
6	O	600	ANP	PA-O3A	2.38	1.62	1.59
6	B	600	ANP	C8-N7	2.37	1.36	1.31
6	M	600	ANP	C5-N7	-2.36	1.34	1.39
6	X	600	ANP	C5-N7	-2.36	1.34	1.39
6	A	600	ANP	C5-N7	-2.34	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	600	ANP	C8-N7	2.34	1.36	1.31
6	X	600	ANP	PG-O2G	-2.32	1.50	1.56
6	D	600	ANP	C8-N7	2.29	1.36	1.31
6	J	600	ANP	PA-O3A	2.29	1.62	1.59
6	D	600	ANP	C5-N7	-2.29	1.34	1.39
6	X	600	ANP	C8-N7	2.27	1.36	1.31
6	V	600	ANP	C8-N7	2.26	1.36	1.31
6	B	600	ANP	PG-O2G	-2.25	1.50	1.56
6	C	600	ANP	C8-N7	2.24	1.36	1.31
6	U	600	ANP	C8-N7	2.22	1.35	1.31
6	O	600	ANP	PG-O3G	-2.21	1.50	1.56
6	A	600	ANP	C8-N7	2.18	1.35	1.31
6	O	600	ANP	PB-O3A	2.17	1.61	1.59
6	J	600	ANP	C8-N7	2.17	1.35	1.31
6	K	600	ANP	C5-N7	-2.17	1.35	1.39
6	O	600	ANP	PG-O2G	-2.16	1.51	1.56
6	T	600	ANP	C5-N7	-2.16	1.35	1.39
6	T	600	ANP	PB-O2B	-2.15	1.51	1.56
6	T	600	ANP	PG-O3G	-2.15	1.51	1.56
6	C	600	ANP	PG-O3G	-2.14	1.51	1.56
6	S	600	ANP	PG-O3G	-2.14	1.51	1.56
6	M	600	ANP	PA-O3A	2.14	1.61	1.59
6	M	600	ANP	PB-O3A	2.13	1.61	1.59
6	L	600	ANP	PB-O2B	-2.12	1.51	1.56
6	F	600	ANP	C8-N7	2.11	1.35	1.31
6	X	600	ANP	PG-O3G	-2.11	1.51	1.56
6	B	600	ANP	PG-O3G	-2.10	1.51	1.56
6	J	600	ANP	PG-O2G	-2.10	1.51	1.56
6	K	600	ANP	PB-O2B	-2.10	1.51	1.56
6	T	600	ANP	PB-O3A	2.09	1.61	1.59
6	F	600	ANP	PG-O3G	-2.08	1.51	1.56
6	F	600	ANP	PG-O2G	-2.07	1.51	1.56
6	C	600	ANP	C5-N7	-2.05	1.35	1.39
6	S	600	ANP	C8-N7	2.05	1.35	1.31
6	L	600	ANP	PG-O3G	-2.03	1.51	1.56
6	U	600	ANP	PB-O2B	-2.03	1.51	1.56
6	J	600	ANP	PG-O3G	-2.03	1.51	1.56
6	J	600	ANP	PB-O2B	-2.02	1.51	1.56
6	X	600	ANP	C4-N9	-2.02	1.33	1.37
6	T	600	ANP	PG-O2G	-2.02	1.51	1.56
6	O	600	ANP	C5-N7	-2.01	1.35	1.39
6	S	600	ANP	PG-O2G	-2.01	1.51	1.56

All (186) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	S	600	ANP	O1G-PG-N3B	-6.71	101.89	111.77
6	C	600	ANP	C5-C4-N3	-6.50	117.76	126.72
6	V	600	ANP	O1G-PG-N3B	-6.42	102.31	111.77
6	S	600	ANP	C5-C4-N3	-6.35	117.98	126.72
6	X	600	ANP	O1B-PB-N3B	-6.30	102.50	111.77
6	T	600	ANP	O1G-PG-N3B	-6.25	102.57	111.77
6	D	600	ANP	C5-C4-N3	-6.22	118.16	126.72
6	X	600	ANP	O1G-PG-N3B	-6.13	102.75	111.77
6	M	600	ANP	C5-C4-N3	-6.11	118.30	126.72
6	F	600	ANP	C5-C4-N3	-5.94	118.53	126.72
6	L	600	ANP	C5-C4-N3	-5.94	118.54	126.72
6	T	600	ANP	C5-C4-N3	-5.94	118.54	126.72
6	K	600	ANP	C5-C4-N3	-5.94	118.54	126.72
6	V	600	ANP	C5-C4-N3	-5.91	118.58	126.72
6	O	600	ANP	C5-C4-N3	-5.90	118.60	126.72
6	B	600	ANP	C5-C4-N3	-5.60	119.00	126.72
6	J	600	ANP	C5-C4-N3	-5.59	119.02	126.72
6	U	600	ANP	C5-C4-N3	-5.45	119.21	126.72
6	L	600	ANP	O2B-PB-O1B	5.42	121.49	109.87
6	X	600	ANP	O2B-PB-O1B	5.41	121.48	109.87
6	O	600	ANP	O1G-PG-N3B	-5.40	103.81	111.77
6	C	600	ANP	O2B-PB-O1B	5.32	121.29	109.87
6	S	600	ANP	N3-C4-N9	5.32	136.22	127.17
6	C	600	ANP	N3-C4-N9	5.29	136.17	127.17
6	A	600	ANP	C5-C4-N3	-5.27	119.47	126.72
6	X	600	ANP	C5-C4-N3	-5.11	119.68	126.72
6	L	600	ANP	O1G-PG-N3B	-5.07	104.31	111.77
6	V	600	ANP	N3-C4-N9	4.98	135.63	127.17
6	D	600	ANP	N3-C4-N9	4.96	135.60	127.17
6	M	600	ANP	O1B-PB-N3B	-4.94	104.49	111.77
6	A	600	ANP	O2B-PB-O1B	4.94	120.46	109.87
6	J	600	ANP	N3-C4-N9	4.86	135.44	127.17
6	F	600	ANP	N3-C4-N9	4.83	135.38	127.17
6	J	600	ANP	O2B-PB-O1B	4.80	120.16	109.87
6	K	600	ANP	O1G-PG-N3B	-4.78	104.73	111.77
6	M	600	ANP	O2B-PB-O1B	4.75	120.05	109.87
6	T	600	ANP	N3-C4-N9	4.74	135.23	127.17
6	C	600	ANP	O1G-PG-N3B	-4.69	104.86	111.77
6	O	600	ANP	N3-C4-N9	4.68	135.12	127.17
6	M	600	ANP	O1G-PG-N3B	-4.67	104.90	111.77
6	M	600	ANP	N3-C4-N9	4.63	135.04	127.17
6	B	600	ANP	O2B-PB-O1B	4.62	119.78	109.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	600	ANP	N3-C4-N9	4.61	135.01	127.17
6	U	600	ANP	N3-C4-N9	4.58	134.95	127.17
6	S	600	ANP	O2B-PB-O1B	4.57	119.68	109.87
6	J	600	ANP	O1G-PG-N3B	-4.57	105.04	111.77
6	L	600	ANP	N3-C4-N9	4.55	134.91	127.17
6	K	600	ANP	N3-C4-N9	4.50	134.82	127.17
6	B	600	ANP	O1G-PG-N3B	-4.50	105.15	111.77
6	D	600	ANP	O2B-PB-O1B	4.47	119.45	109.87
6	D	600	ANP	O1B-PB-N3B	-4.46	105.20	111.77
6	F	600	ANP	O1G-PG-N3B	-4.40	105.29	111.77
6	F	600	ANP	O2B-PB-O1B	4.35	119.20	109.87
6	B	600	ANP	O1B-PB-N3B	-4.33	105.39	111.77
6	K	600	ANP	O2B-PB-O1B	4.31	119.11	109.87
6	A	600	ANP	N3-C4-N9	4.30	134.48	127.17
6	V	600	ANP	O2B-PB-O1B	4.20	118.88	109.87
6	U	600	ANP	O1B-PB-N3B	-4.16	105.65	111.77
6	U	600	ANP	O1G-PG-N3B	-4.12	105.70	111.77
6	M	600	ANP	C2-N3-C4	4.00	121.61	111.83
6	X	600	ANP	N3-C4-N9	4.00	133.97	127.17
6	U	600	ANP	O2B-PB-O1B	4.00	118.45	109.87
6	C	600	ANP	C2-N3-C4	3.90	121.36	111.83
6	D	600	ANP	C2-N3-C4	3.89	121.34	111.83
6	M	600	ANP	C4-C5-N7	-3.85	106.18	110.58
6	S	600	ANP	C2-N3-C4	3.85	121.22	111.83
6	O	600	ANP	C2-N3-C4	3.80	121.12	111.83
6	T	600	ANP	O2B-PB-O1B	3.77	117.94	109.87
6	T	600	ANP	C2-N3-C4	3.76	121.01	111.83
6	T	600	ANP	C4-C5-N7	-3.75	106.30	110.58
6	M	600	ANP	N3-C2-N1	-3.73	122.93	128.58
6	J	600	ANP	O1B-PB-N3B	-3.73	106.28	111.77
6	J	600	ANP	N3-C2-N1	-3.70	122.98	128.58
6	K	600	ANP	C2-N3-C4	3.69	120.85	111.83
6	V	600	ANP	C2-N3-C4	3.67	120.80	111.83
6	J	600	ANP	C2-N3-C4	3.67	120.80	111.83
6	X	600	ANP	N3-C2-N1	-3.62	123.10	128.58
6	X	600	ANP	C2-N3-C4	3.62	120.68	111.83
6	A	600	ANP	O1G-PG-N3B	-3.62	106.44	111.77
6	B	600	ANP	C2-N3-C4	3.60	120.61	111.83
6	L	600	ANP	C2-N3-C4	3.59	120.60	111.83
6	A	600	ANP	O1B-PB-N3B	-3.58	106.50	111.77
6	C	600	ANP	C4-C5-N7	-3.56	106.51	110.58
6	F	600	ANP	C2-N3-C4	3.55	120.50	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	O	600	ANP	O2B-PB-O1B	3.54	117.45	109.87
6	A	600	ANP	N3-C2-N1	-3.52	123.25	128.58
6	U	600	ANP	C2-N3-C4	3.51	120.41	111.83
6	U	600	ANP	N3-C2-N1	-3.50	123.29	128.58
6	B	600	ANP	N3-C2-N1	-3.49	123.30	128.58
6	K	600	ANP	C4-C5-N7	-3.48	106.61	110.58
6	A	600	ANP	C2-N3-C4	3.46	120.28	111.83
6	T	600	ANP	N3-C2-N1	-3.38	123.47	128.58
6	V	600	ANP	N3-C2-N1	-3.34	123.52	128.58
6	O	600	ANP	N3-C2-N1	-3.34	123.53	128.58
6	A	600	ANP	C4-C5-N7	-3.31	106.79	110.58
6	L	600	ANP	O1B-PB-N3B	-3.31	106.90	111.77
6	L	600	ANP	C4-C5-N7	-3.29	106.81	110.58
6	D	600	ANP	C4-C5-N7	-3.28	106.83	110.58
6	K	600	ANP	N3-C2-N1	-3.25	123.66	128.58
6	D	600	ANP	N3-C2-N1	-3.23	123.70	128.58
6	D	600	ANP	O1G-PG-N3B	-3.20	107.06	111.77
6	S	600	ANP	N3-C2-N1	-3.19	123.75	128.58
6	V	600	ANP	O1B-PB-N3B	-3.13	107.16	111.77
6	C	600	ANP	O1B-PB-N3B	-3.12	107.18	111.77
6	O	600	ANP	C4-C5-N7	-3.11	107.02	110.58
6	J	600	ANP	C4-N9-C8	3.09	108.98	105.74
6	S	600	ANP	C4-C5-N7	-3.07	107.07	110.58
6	X	600	ANP	O2G-PG-O3G	3.07	115.83	107.59
6	F	600	ANP	N3-C2-N1	-3.05	123.96	128.58
6	C	600	ANP	N3-C2-N1	-3.02	124.01	128.58
6	X	600	ANP	C4-C5-N7	-3.00	107.15	110.58
6	L	600	ANP	N3-C2-N1	-3.00	124.04	128.58
6	J	600	ANP	C4-C5-N7	-3.00	107.16	110.58
6	U	600	ANP	C4-C5-N7	-2.99	107.16	110.58
6	U	600	ANP	O2G-PG-O3G	2.98	115.60	107.59
6	B	600	ANP	C4-C5-N7	-2.97	107.19	110.58
6	K	600	ANP	O1B-PB-N3B	-2.85	107.58	111.77
6	V	600	ANP	C4-C5-N7	-2.84	107.33	110.58
6	A	600	ANP	O2G-PG-O3G	2.79	115.10	107.59
6	M	600	ANP	O2G-PG-O3G	2.77	115.04	107.59
6	F	600	ANP	C4-C5-N7	-2.75	107.43	110.58
6	M	600	ANP	C5-N7-C8	2.74	107.76	103.45
6	T	600	ANP	C5-N7-C8	2.70	107.70	103.45
6	A	600	ANP	C4-N9-C8	2.70	108.57	105.74
6	T	600	ANP	C4-N9-C8	2.65	108.52	105.74
6	T	600	ANP	O1B-PB-N3B	-2.64	107.88	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	600	ANP	C2'-C1'-N9	-2.64	106.75	113.30
6	M	600	ANP	C2'-C1'-N9	-2.63	106.77	113.30
6	O	600	ANP	O1B-PB-N3B	-2.62	107.91	111.77
6	C	600	ANP	C5-N7-C8	2.61	107.55	103.45
6	S	600	ANP	C4-N9-C8	2.59	108.45	105.74
6	F	600	ANP	O1B-PB-N3B	-2.58	107.97	111.77
6	T	600	ANP	O2G-PG-O3G	2.57	114.49	107.59
6	C	600	ANP	O4'-C1'-N9	2.56	113.01	108.09
6	K	600	ANP	O2G-PG-O3G	2.53	114.38	107.59
6	U	600	ANP	C4-N9-C8	2.52	108.38	105.74
6	C	600	ANP	C4-N9-C8	2.49	108.35	105.74
6	L	600	ANP	O2G-PG-O3G	2.48	114.26	107.59
6	A	600	ANP	C2-N1-C6	2.47	122.79	118.73
6	A	600	ANP	C5-N7-C8	2.47	107.34	103.45
6	F	600	ANP	O2G-PG-O3G	2.46	114.19	107.59
6	D	600	ANP	C3'-C2'-C1'	2.44	106.09	101.46
6	O	600	ANP	O2G-PG-O3G	2.44	114.16	107.59
6	J	600	ANP	C5-N7-C8	2.44	107.28	103.45
6	S	600	ANP	C5-N7-C8	2.42	107.26	103.45
6	K	600	ANP	C5-N7-C8	2.42	107.25	103.45
6	D	600	ANP	C5-N7-C8	2.41	107.23	103.45
6	V	600	ANP	C3'-C2'-C1'	2.40	106.00	101.46
6	M	600	ANP	C6-C5-N7	2.39	136.69	132.09
6	L	600	ANP	C5-N7-C8	2.38	107.18	103.45
6	V	600	ANP	C2'-C1'-N9	-2.37	107.42	113.30
6	J	600	ANP	O2G-PG-O3G	2.35	113.92	107.59
6	B	600	ANP	C4-N9-C8	2.34	108.19	105.74
6	V	600	ANP	C5-N7-C8	2.33	107.11	103.45
6	U	600	ANP	C5-N7-C8	2.31	107.07	103.45
6	X	600	ANP	C2-N1-C6	2.29	122.49	118.73
6	B	600	ANP	O2G-PG-O3G	2.28	113.72	107.59
6	B	600	ANP	C2-N1-C6	2.27	122.46	118.73
6	K	600	ANP	O4'-C1'-N9	2.26	112.43	108.09
6	V	600	ANP	C4-N9-C8	2.25	108.10	105.74
6	D	600	ANP	O2G-PG-O3G	2.22	113.56	107.59
6	D	600	ANP	C4-N9-C8	2.22	108.07	105.74
6	L	600	ANP	C3'-C2'-C1'	2.21	105.64	101.46
6	X	600	ANP	C6-C5-N7	2.18	136.29	132.09
6	M	600	ANP	C2-N1-C6	2.16	122.28	118.73
6	C	600	ANP	O2G-PG-O3G	2.16	113.39	107.59
6	B	600	ANP	C5-N7-C8	2.15	106.84	103.45
6	J	600	ANP	C3'-C2'-C1'	2.15	105.54	101.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	600	ANP	C4-N9-C8	2.14	107.99	105.74
6	A	600	ANP	C6-C5-N7	2.14	136.22	132.09
6	X	600	ANP	C4-N9-C8	2.13	107.98	105.74
6	T	600	ANP	C6-C5-N7	2.13	136.20	132.09
6	O	600	ANP	C5-N7-C8	2.13	106.80	103.45
6	U	600	ANP	C3'-C2'-C1'	2.12	105.47	101.46
6	K	600	ANP	C6-C5-N7	2.09	136.11	132.09
6	S	600	ANP	N6-C6-N1	2.09	123.03	118.38
6	J	600	ANP	C2'-C1'-N9	-2.08	108.15	113.30
6	X	600	ANP	C5-N7-C8	2.06	106.69	103.45
6	J	600	ANP	C2-N1-C6	2.06	122.11	118.73
6	J	600	ANP	N9-C8-N7	-2.05	111.03	113.94
6	O	600	ANP	C4-N9-C8	2.04	107.88	105.74
6	K	600	ANP	C3'-C2'-C1'	2.04	105.32	101.46
6	T	600	ANP	C2-N1-C6	2.02	122.05	118.73
6	M	600	ANP	C4-N9-C8	2.01	107.85	105.74
6	U	600	ANP	C2-N1-C6	2.00	122.02	118.73
6	F	600	ANP	O2A-PA-O1A	2.00	121.75	112.44

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	600	ANP	PB-N3B-PG-O1G
6	A	600	ANP	PG-N3B-PB-O1B
6	B	600	ANP	PB-N3B-PG-O1G
6	B	600	ANP	PG-N3B-PB-O1B
6	C	600	ANP	PB-N3B-PG-O1G
6	C	600	ANP	PG-N3B-PB-O1B
6	D	600	ANP	PB-N3B-PG-O1G
6	D	600	ANP	PG-N3B-PB-O1B
6	D	600	ANP	PA-O3A-PB-O2B
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	C5'-O5'-PA-O1A
6	K	600	ANP	C5'-O5'-PA-O2A
6	K	600	ANP	C5'-O5'-PA-O3A

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

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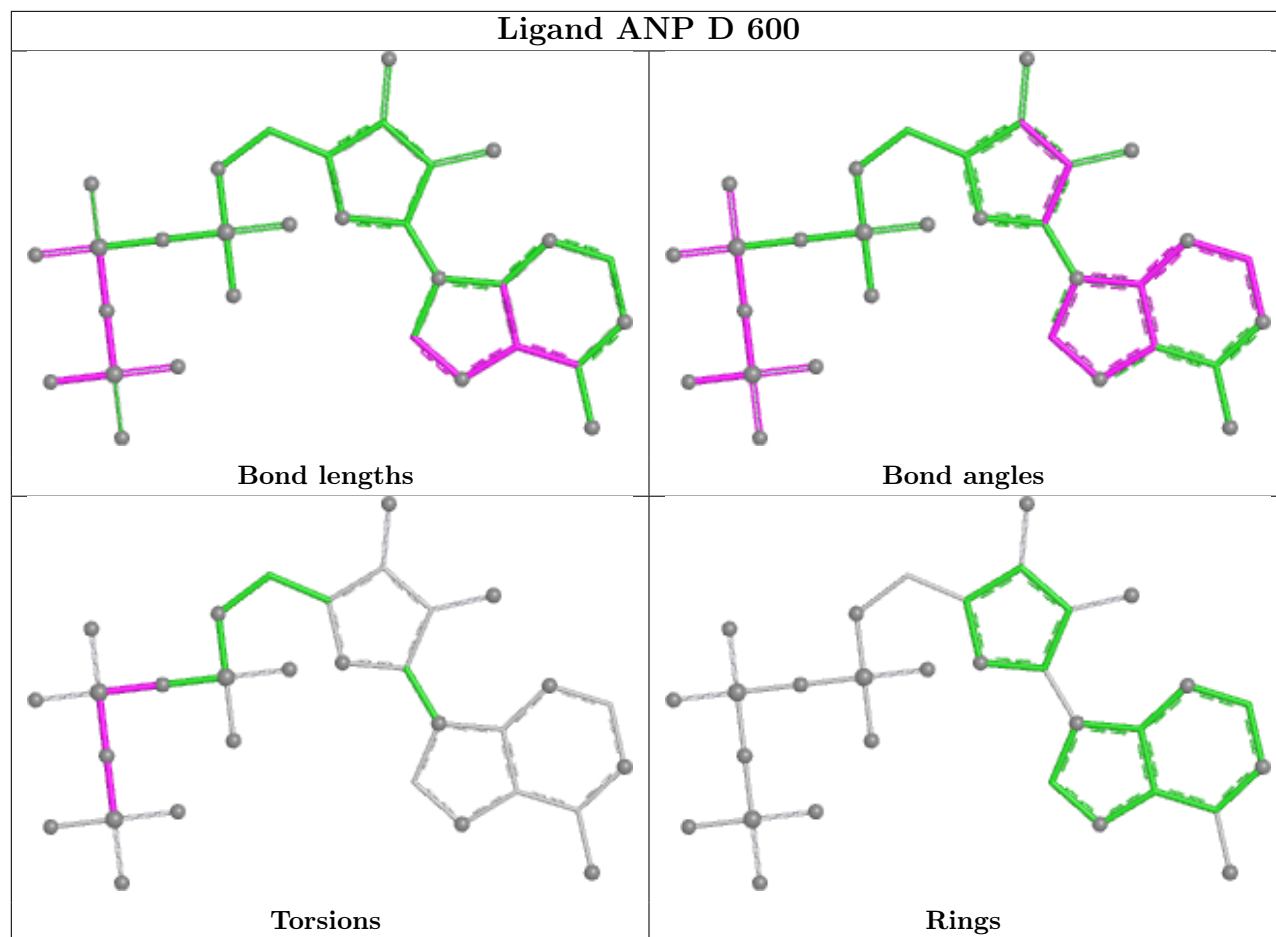
Mol	Chain	Res	Type	Atoms
6	F	600	ANP	O4'-C4'-C5'-O5'

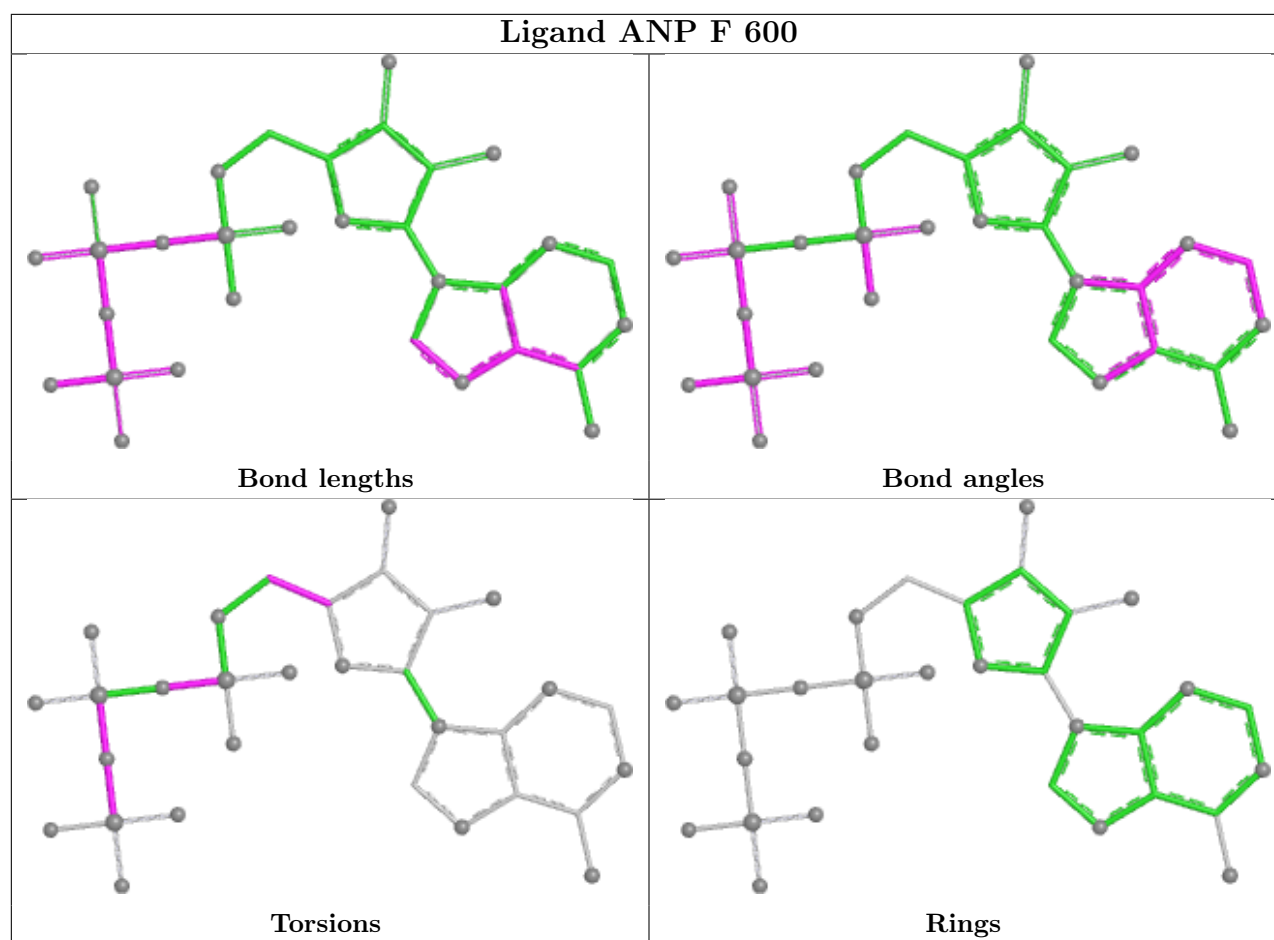
There are no ring outliers.

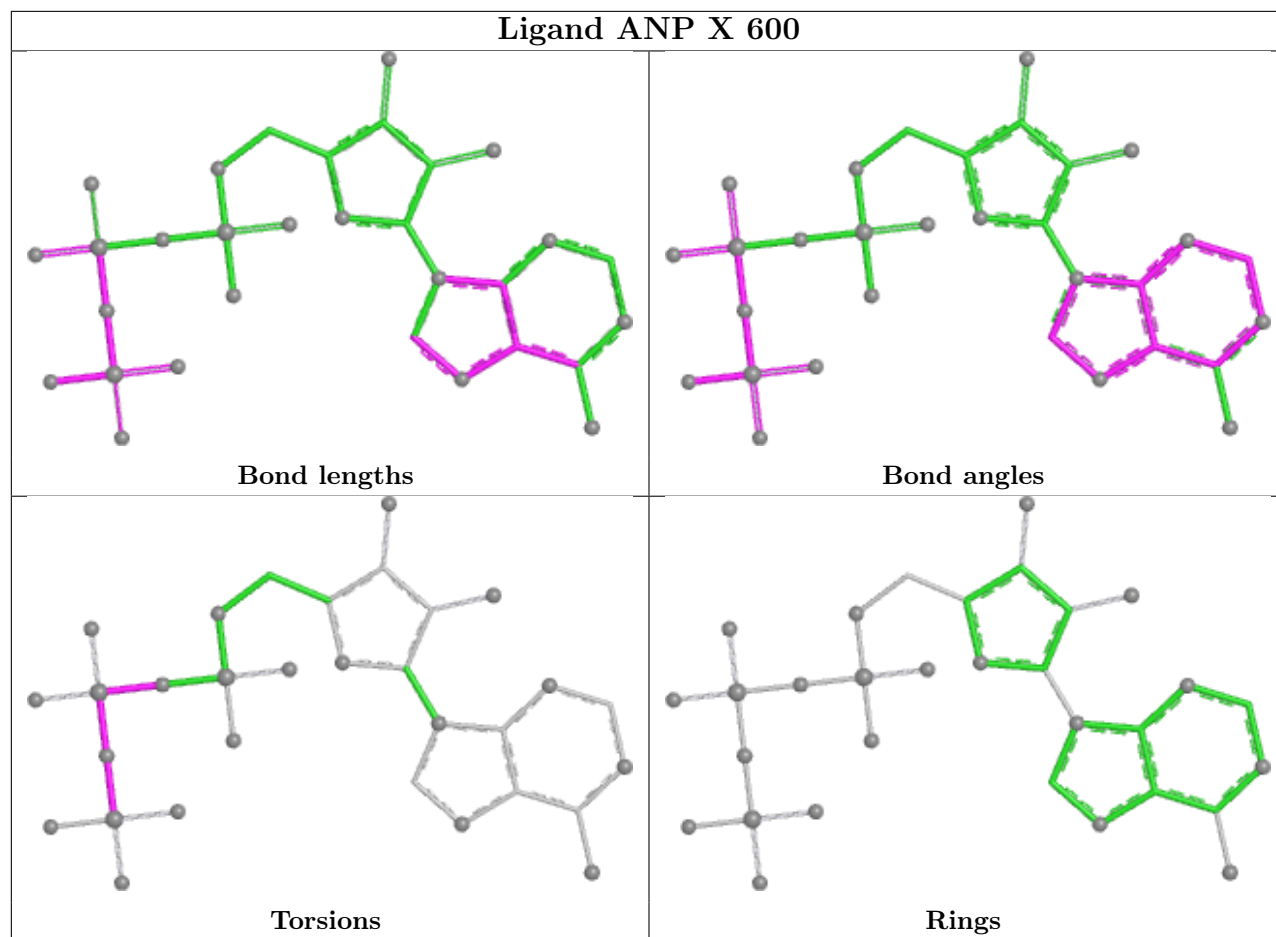
10 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	600	ANP	2	0
6	F	600	ANP	3	0
6	X	600	ANP	2	0
6	J	600	ANP	3	0
6	V	600	ANP	2	0
6	T	600	ANP	2	0
6	M	600	ANP	3	0
6	B	600	ANP	2	0
6	C	600	ANP	3	0
6	K	600	ANP	1	0

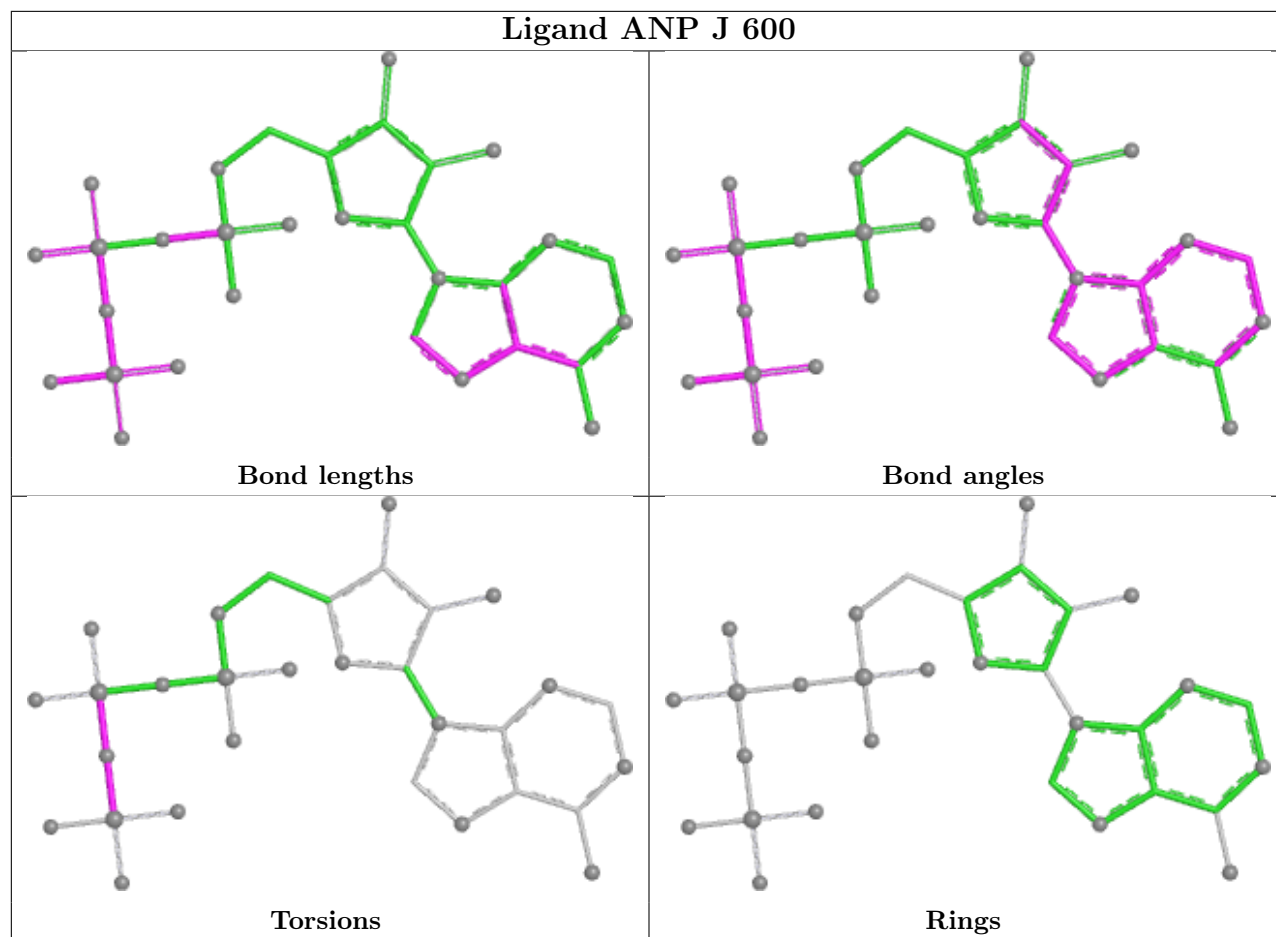
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

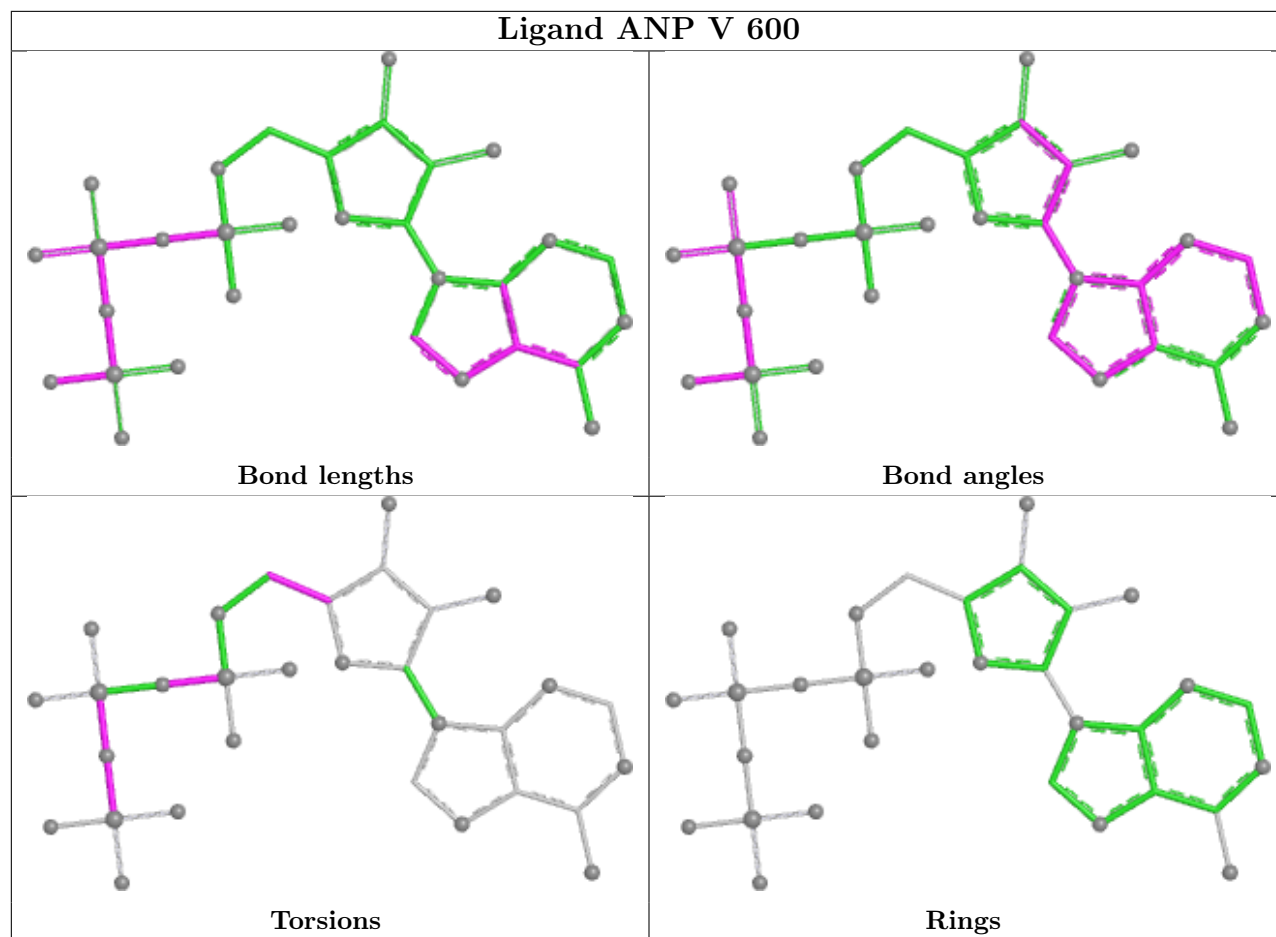


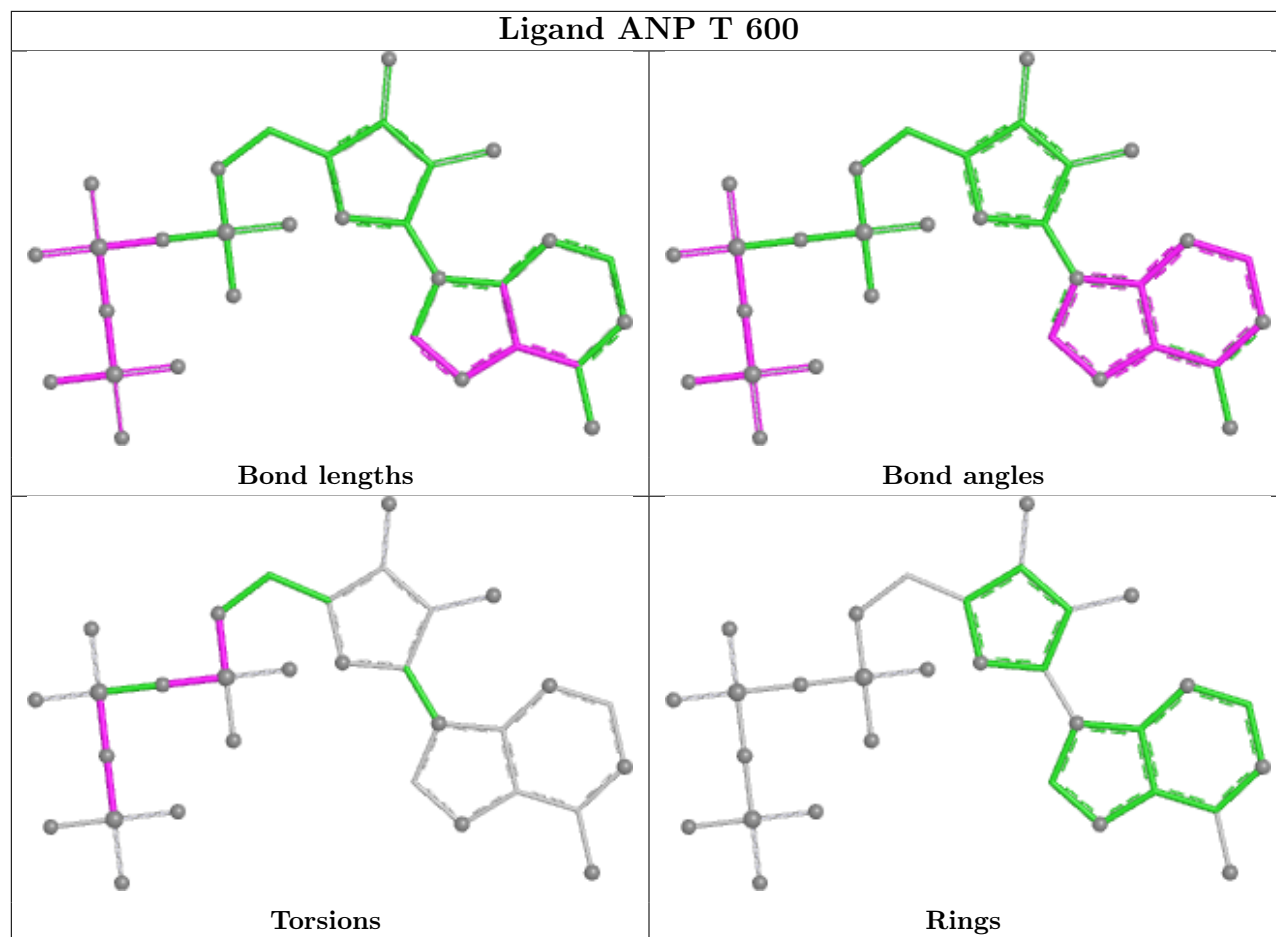


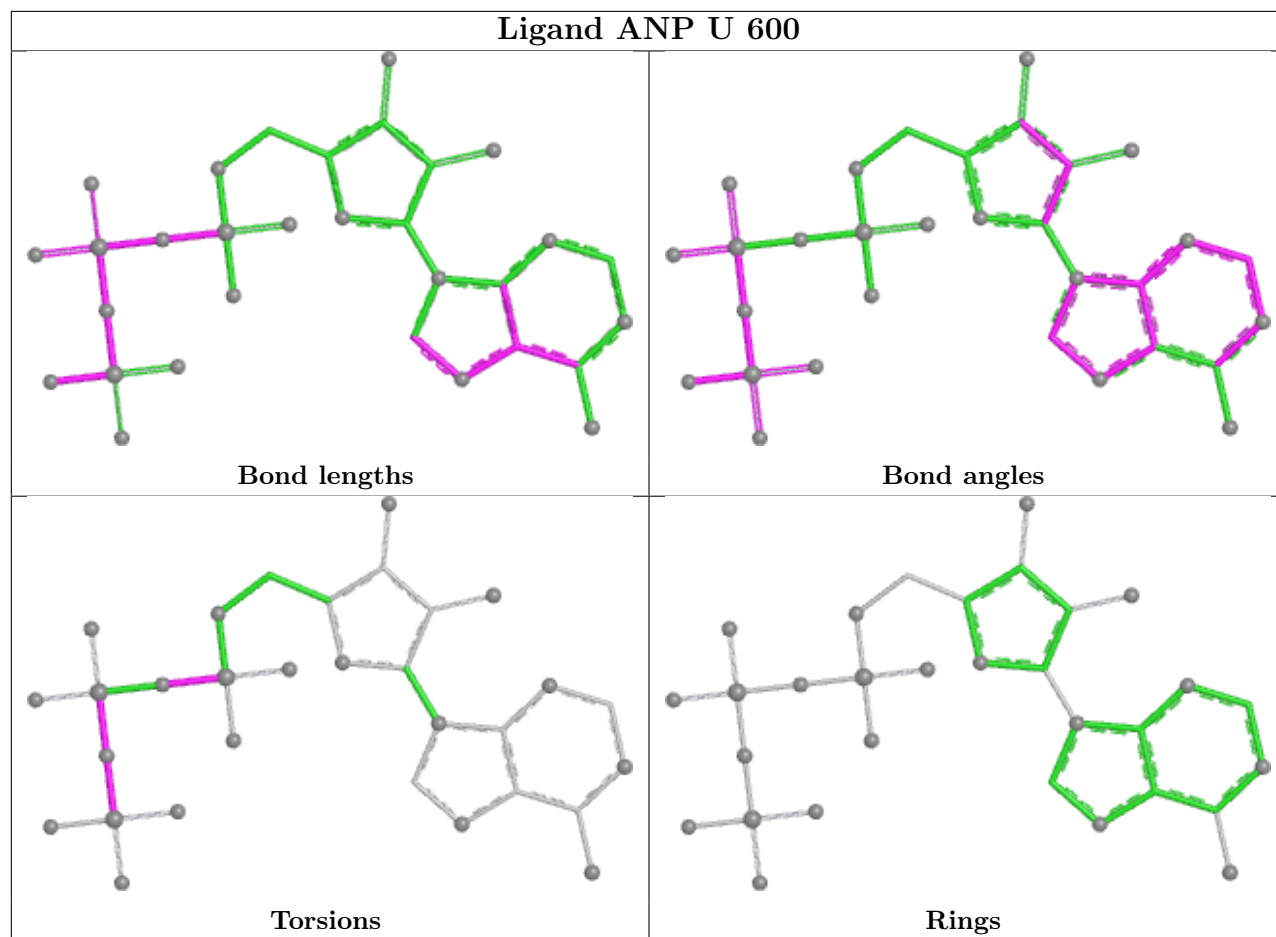


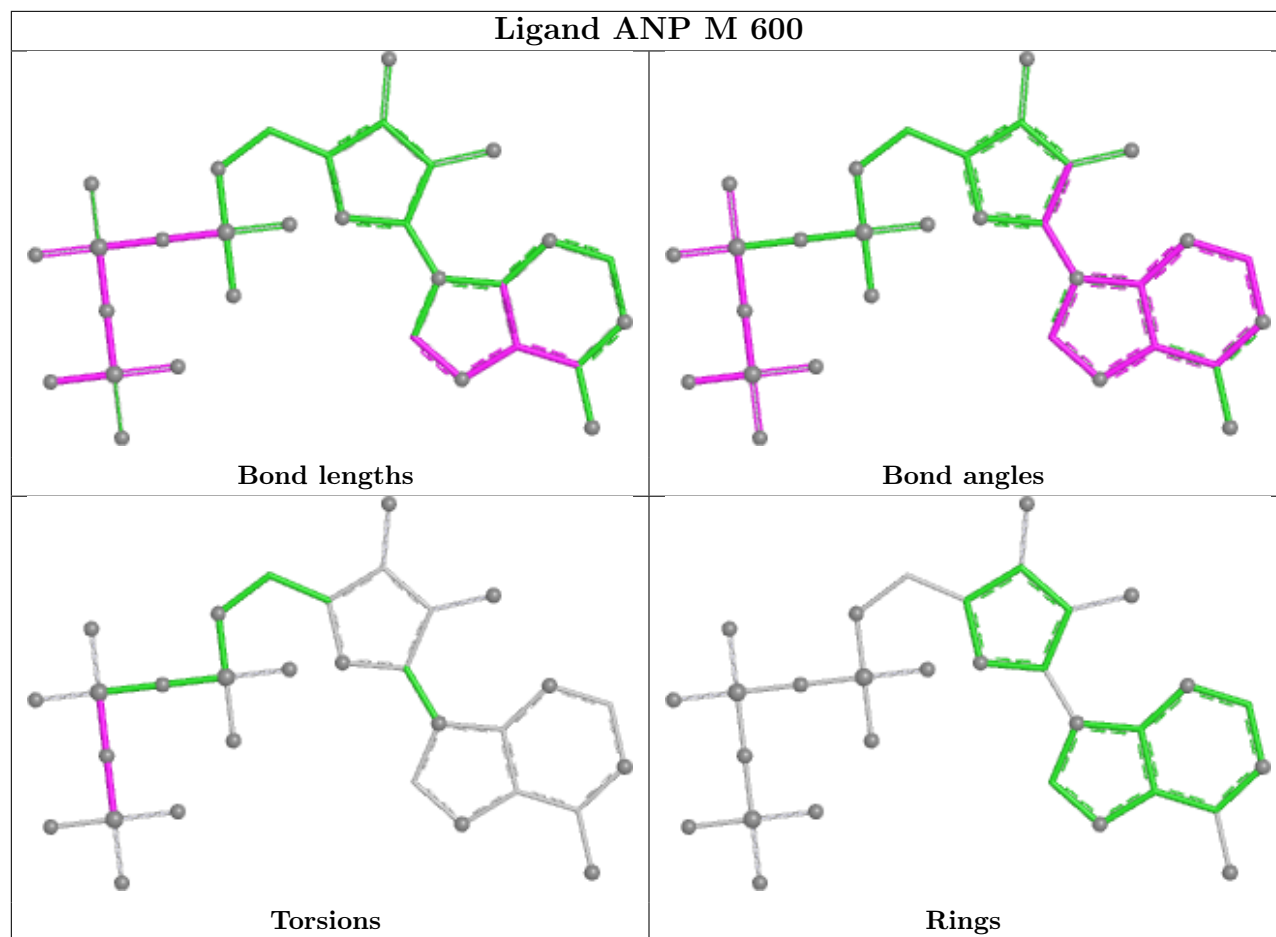
Ligand ANP J 600

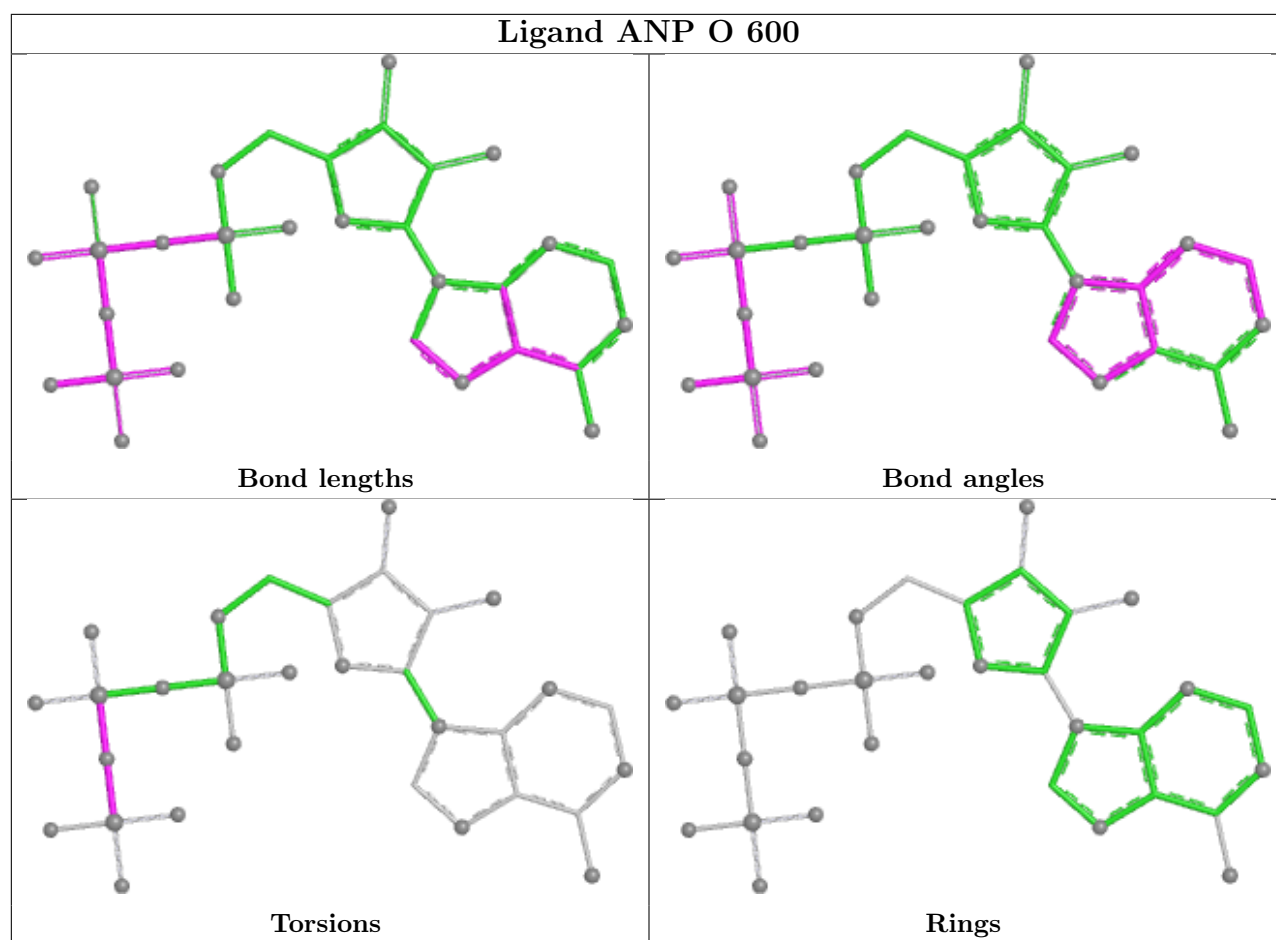


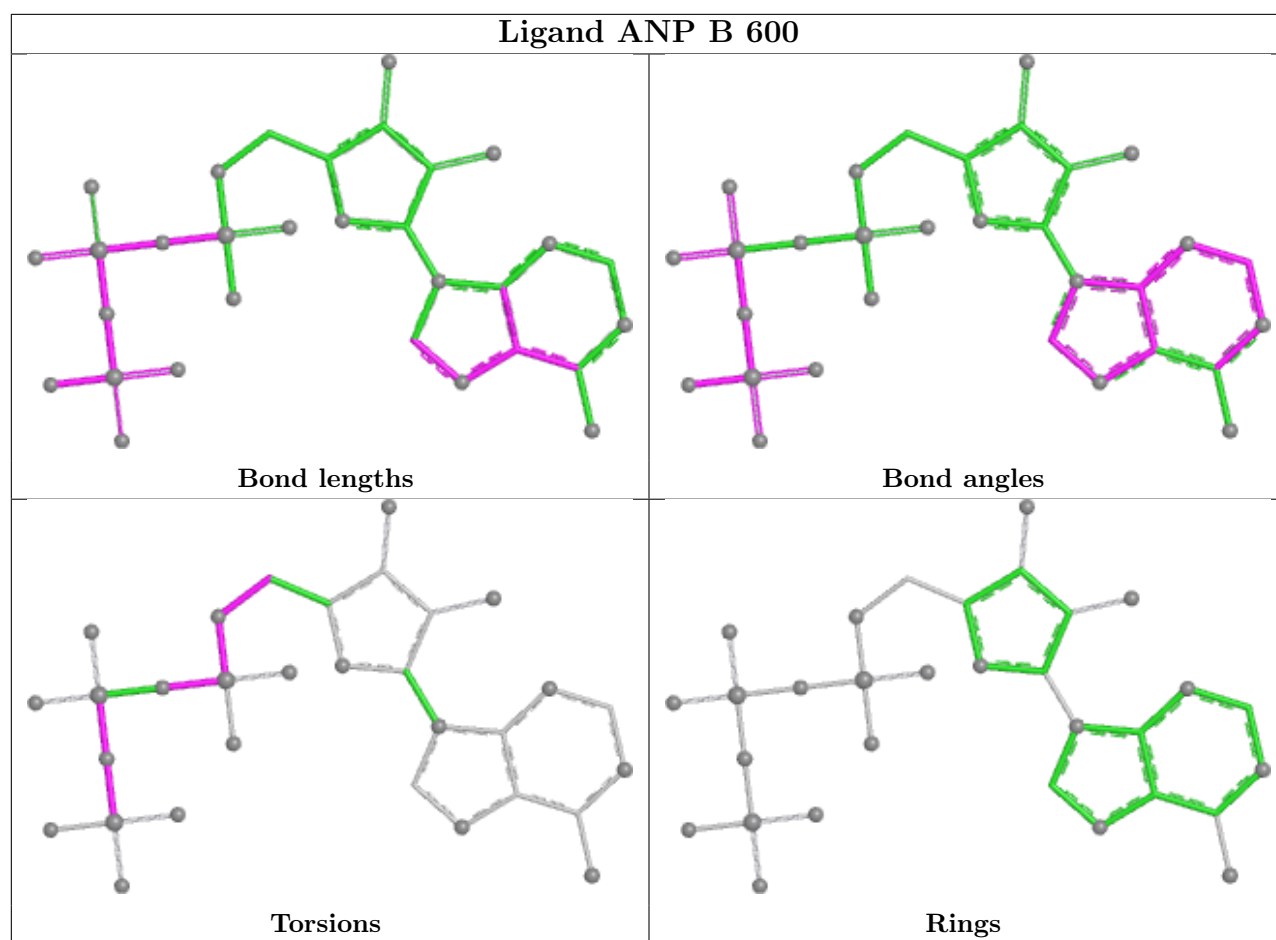


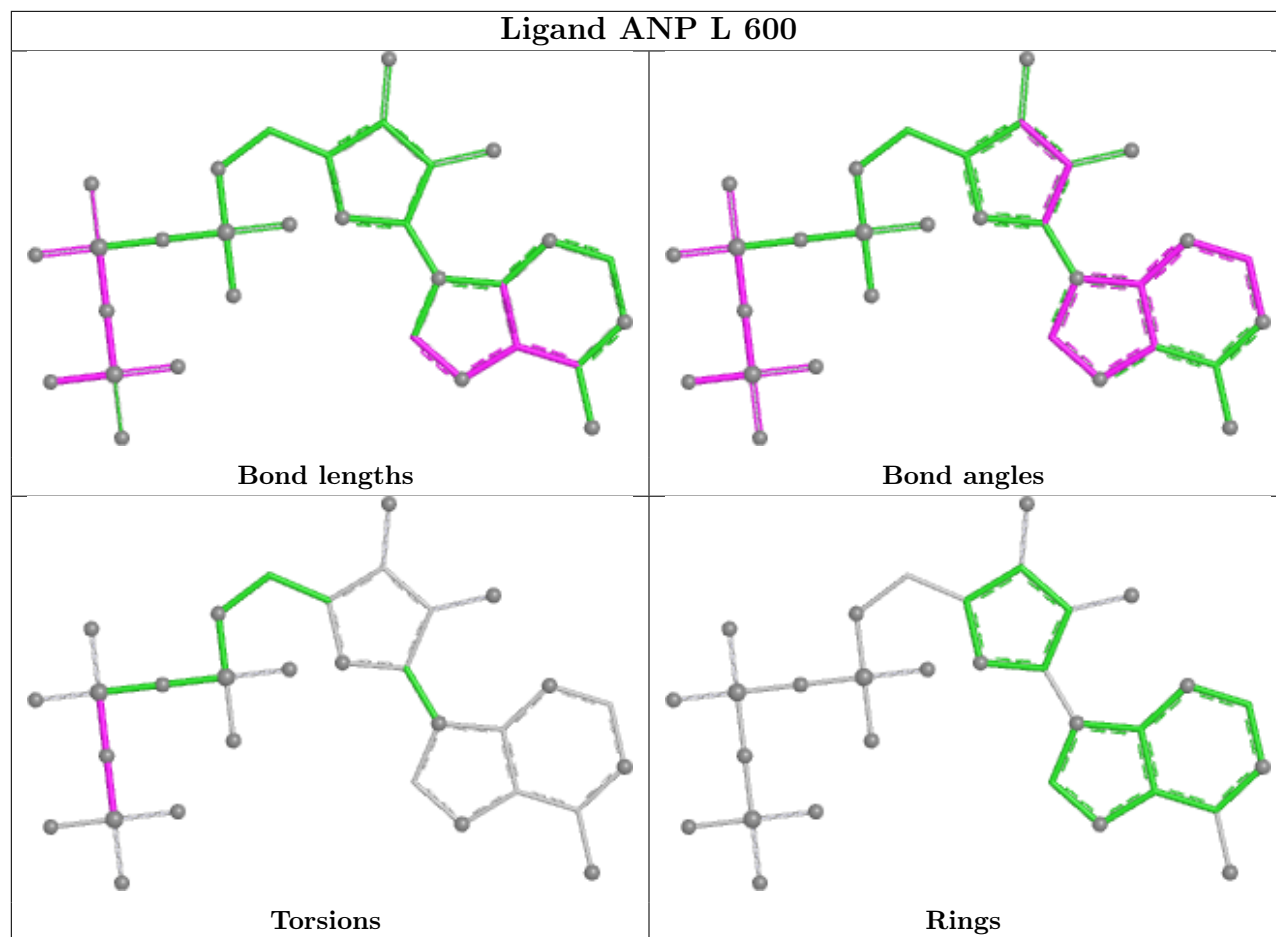


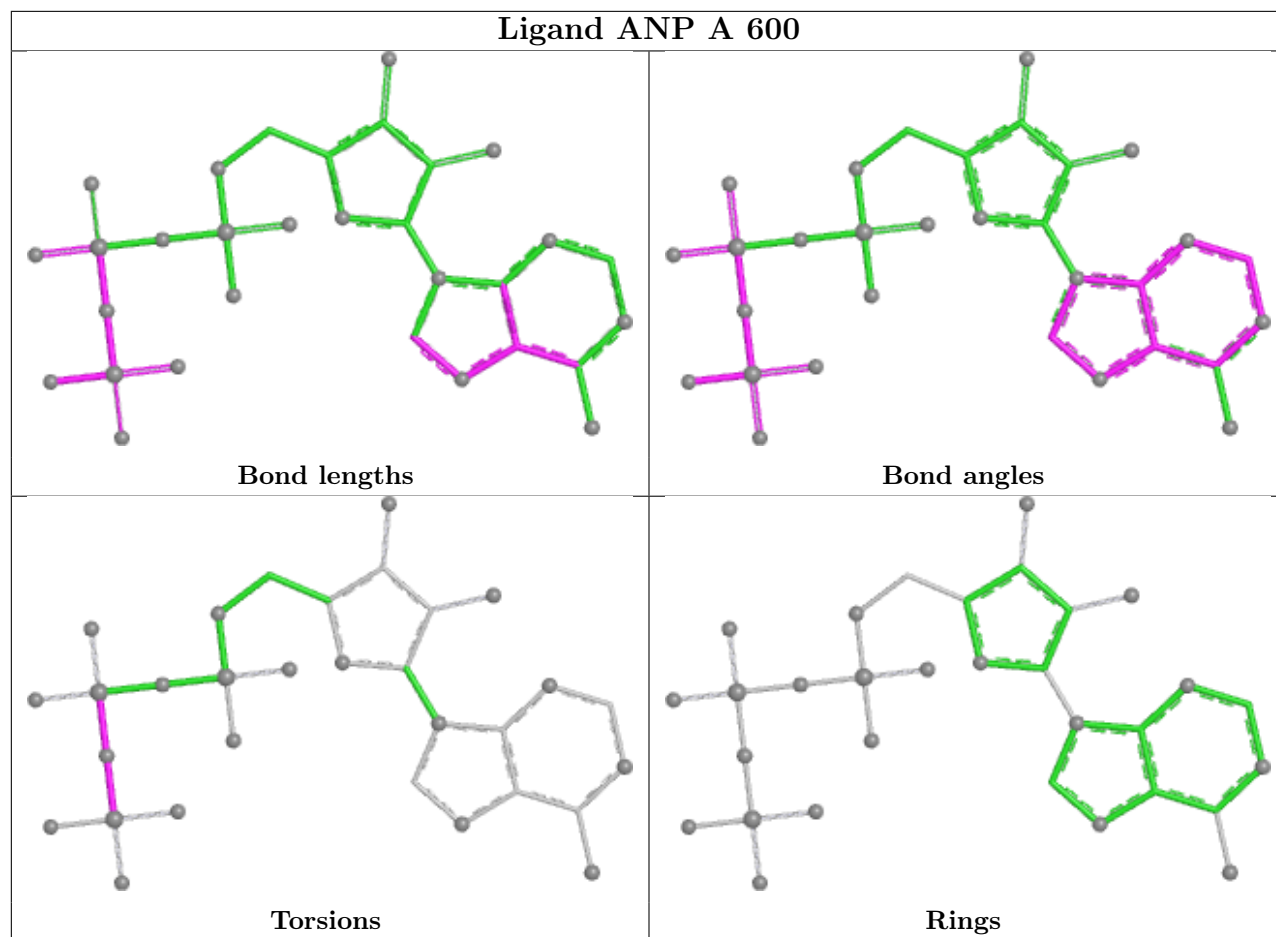


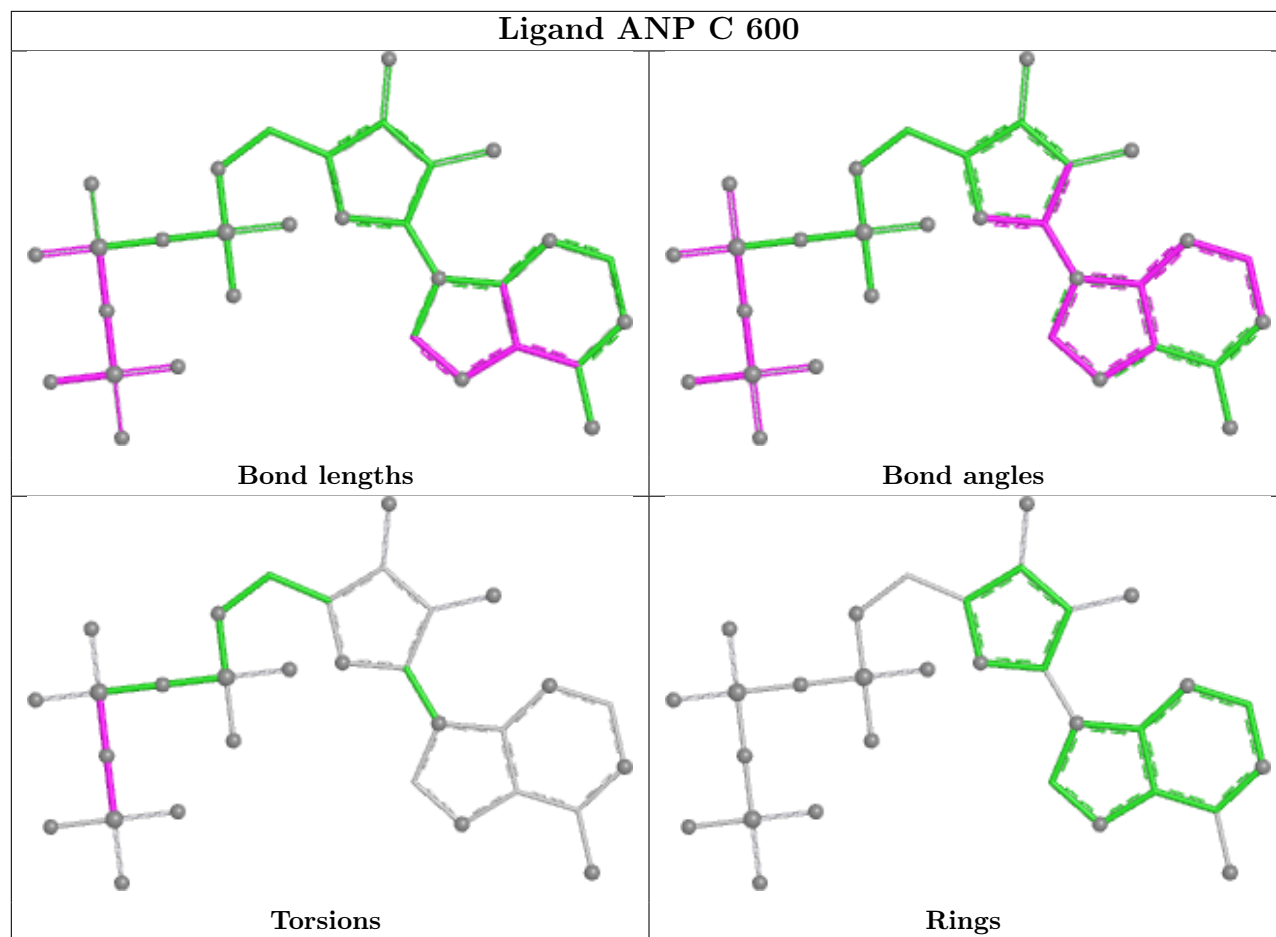




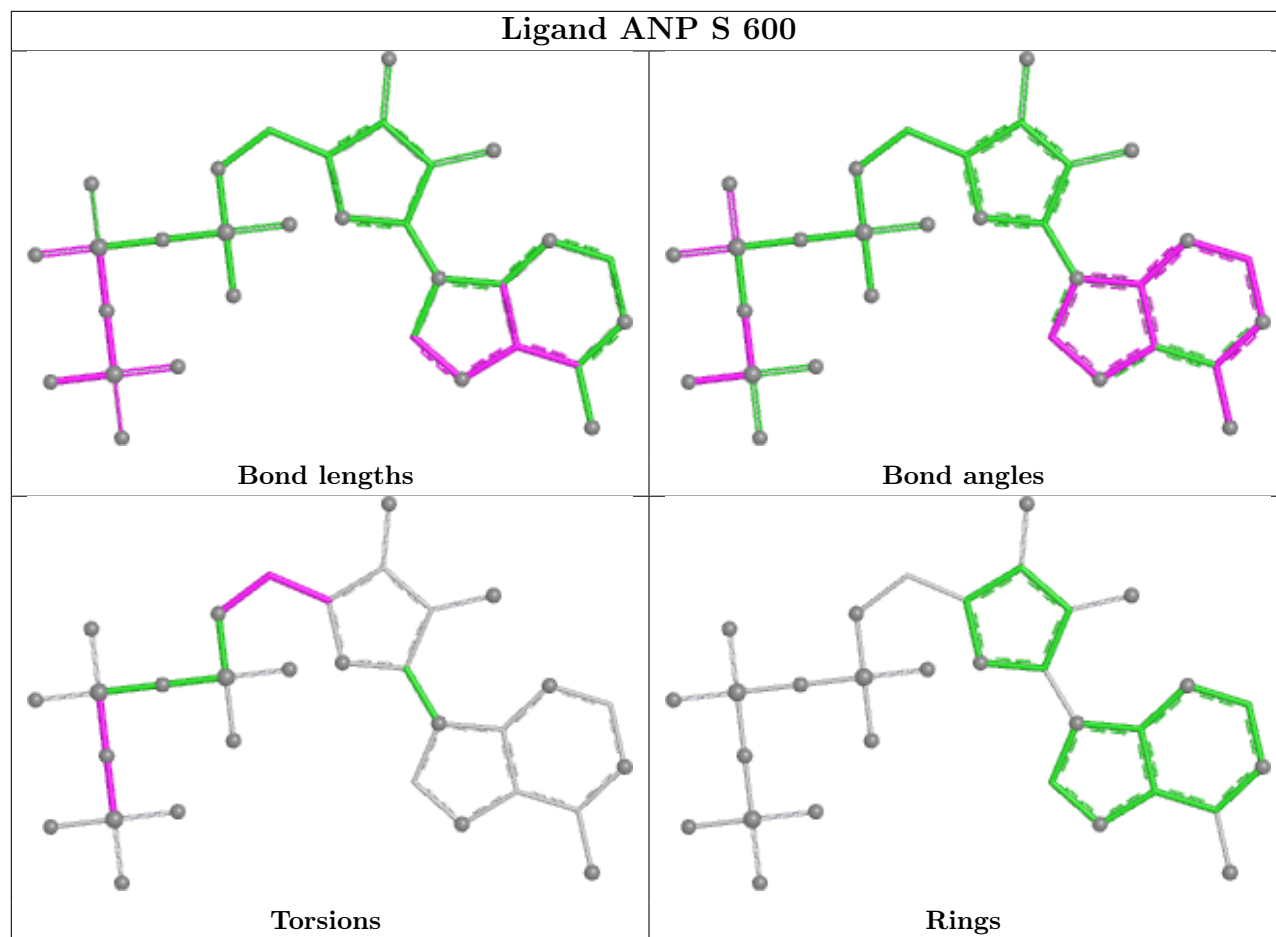


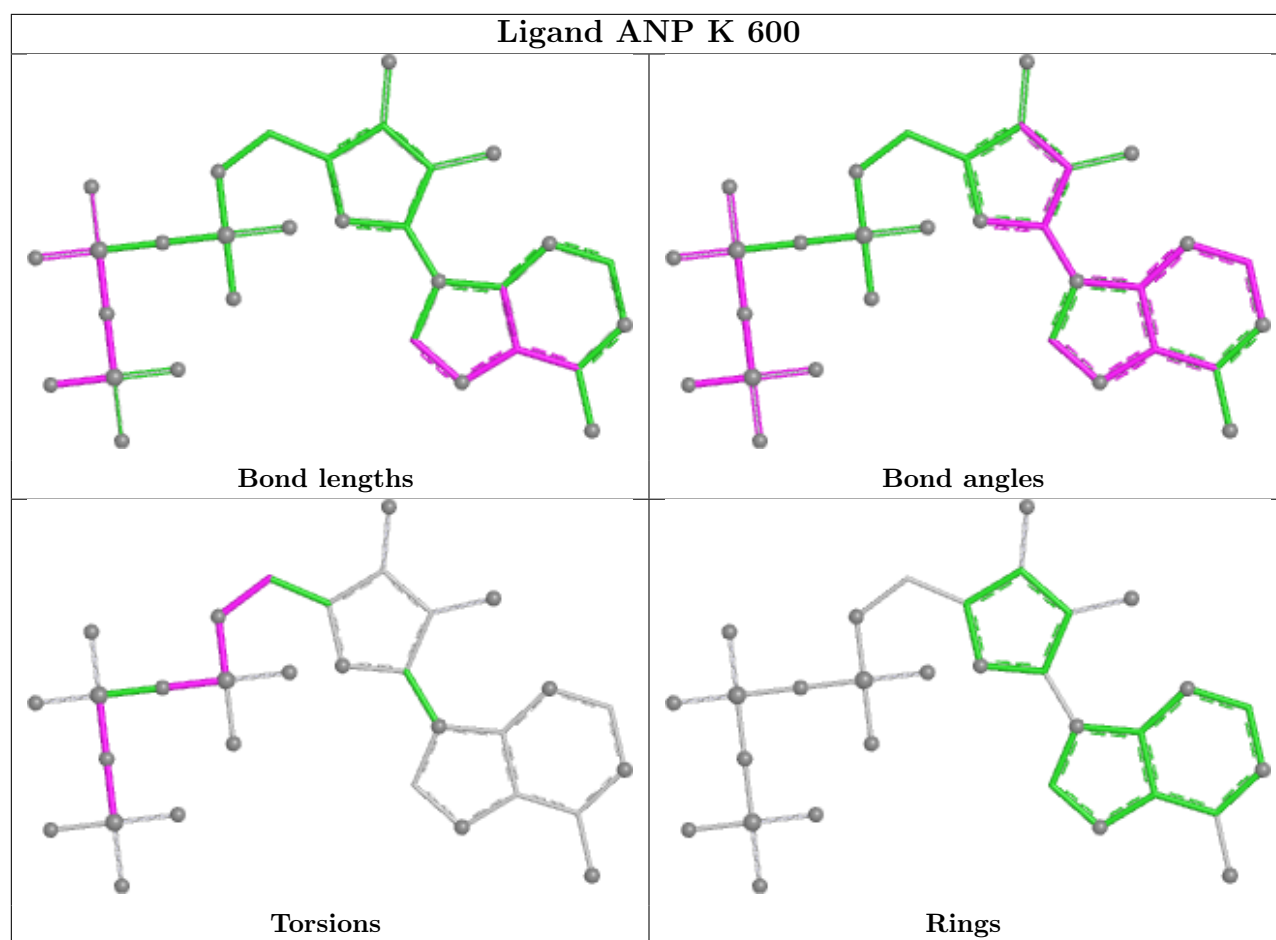






Ligand ANP S 600





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	485/510 (95%)	-0.55	0 100 100	49, 67, 102, 161	0
1	B	486/510 (95%)	-0.43	0 100 100	60, 94, 131, 172	0
1	C	484/510 (94%)	-0.46	1 (0%) 91 85	62, 83, 134, 166	0
1	J	482/510 (94%)	-0.36	1 (0%) 91 85	63, 91, 159, 179	0
1	K	483/510 (94%)	-0.16	1 (0%) 91 85	78, 118, 163, 170	0
1	L	479/510 (93%)	-0.33	0 100 100	63, 88, 145, 168	0
1	S	483/510 (94%)	-0.50	0 100 100	60, 84, 110, 171	0
1	T	484/510 (94%)	-0.59	0 100 100	59, 84, 108, 143	0
1	U	485/510 (95%)	-0.26	1 (0%) 91 85	81, 104, 132, 166	0
2	D	470/484 (97%)	-0.51	0 100 100	54, 80, 131, 155	0
2	E	469/484 (96%)	-0.47	0 100 100	56, 86, 126, 152	0
2	F	469/484 (96%)	-0.46	0 100 100	59, 89, 114, 134	0
2	M	460/484 (95%)	-0.29	5 (1%) 78 61	63, 87, 146, 171	0
2	N	463/484 (95%)	-0.20	1 (0%) 91 85	71, 115, 157, 166	0
2	O	469/484 (96%)	-0.18	3 (0%) 85 73	78, 110, 159, 167	0
2	V	360/484 (74%)	-0.00	9 (2%) 58 39	78, 109, 146, 178	0
2	W	468/484 (96%)	-0.62	1 (0%) 91 85	57, 72, 103, 143	0
2	X	469/484 (96%)	-0.42	0 100 100	65, 91, 113, 132	0
3	G	268/278 (96%)	-0.36	0 100 100	62, 92, 108, 115	0
3	P	268/278 (96%)	0.13	3 (1%) 78 61	82, 145, 165, 176	0
3	Y	115/278 (41%)	0.03	1 (0%) 81 64	73, 116, 148, 153	0
4	H	122/138 (88%)	0.19	2 (1%) 70 51	76, 97, 150, 167	0
4	Q	101/138 (73%)	0.62	12 (11%) 9 6	138, 152, 169, 175	0
5	I	55/61 (90%)	0.39	2 (3%) 46 28	90, 111, 134, 149	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
5	R	55/61 (90%)	0.31	1 (1%) 67 48	126, 146, 163, 167	0
All	All	9432/10178 (92%)	-0.34	44 (0%) 87 76	49, 93, 152, 179	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	85	VAL	3.7
2	M	432	VAL	3.6
2	M	404	VAL	3.3
2	W	474	ALA	3.3
2	V	143	LEU	3.3
2	O	404	VAL	3.2
2	V	167	ILE	3.2
3	Y	214	LEU	3.0
2	V	145	ALA	2.9
2	M	388	ILE	2.9
4	Q	101	ILE	2.8
5	I	61	LYS	2.7
4	Q	14	PHE	2.6
1	K	21	VAL	2.6
2	V	132	GLU	2.6
2	M	395	GLU	2.6
3	P	118	LEU	2.6
2	M	407	ALA	2.6
4	H	97	SER	2.6
4	Q	113	SER	2.6
2	O	445	LEU	2.5
4	Q	61	GLU	2.5
4	Q	54	PRO	2.5
2	N	159	ALA	2.5
2	V	359	ASP	2.4
2	V	147	TYR	2.3
2	V	346	PRO	2.3
4	Q	20	THR	2.3
4	Q	71	SER	2.3
2	V	170	LEU	2.2
4	Q	15	ALA	2.2
4	H	133	LEU	2.1
5	R	8	ILE	2.1
2	O	391	LEU	2.1
1	C	406	ALA	2.1
5	I	16	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
4	Q	75	ALA	2.1
2	V	172	ASN	2.1
1	J	481	LEU	2.1
1	U	490	GLU	2.1
3	P	95	VAL	2.0
4	Q	112	VAL	2.0
3	P	60	LEU	2.0
4	Q	72	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

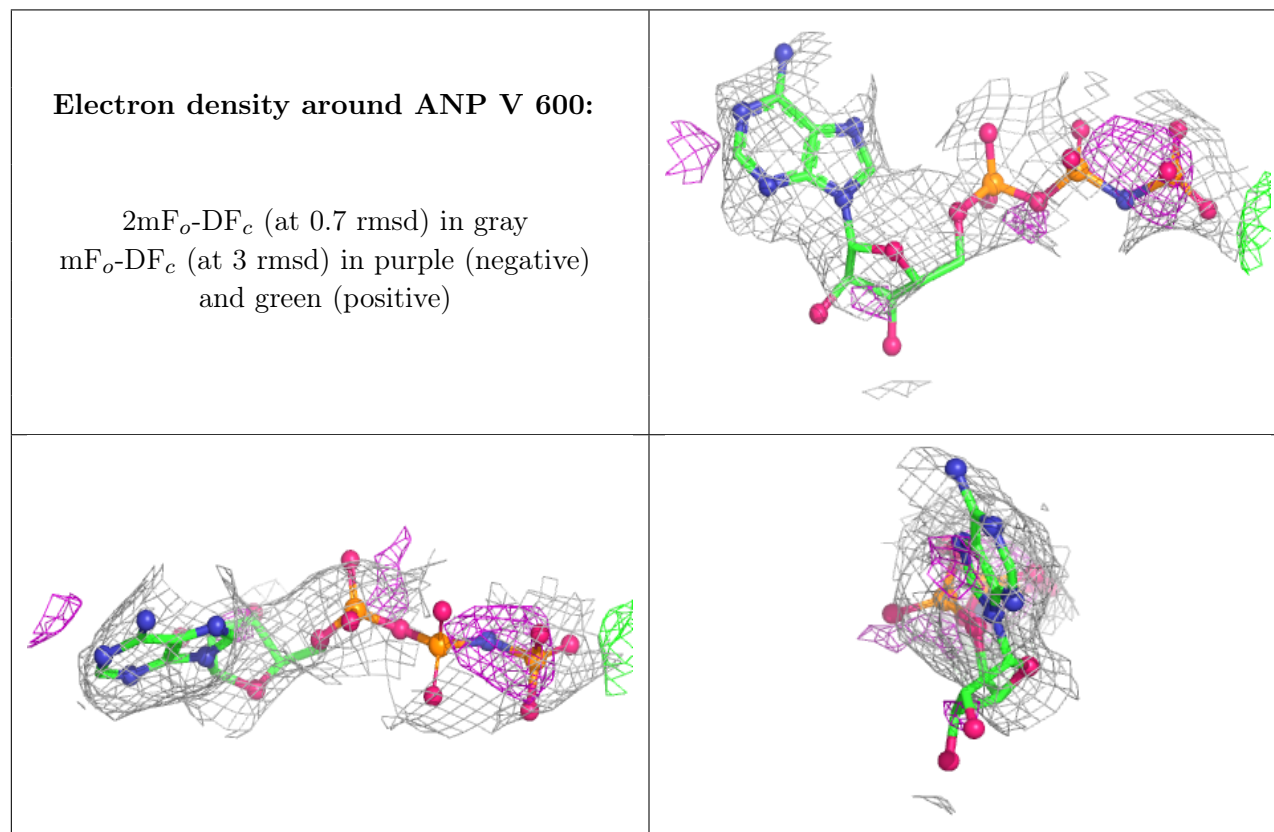
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	MG	D	700	1/1	0.52	0.33	83,83,83,83	0
7	MG	B	700	1/1	0.67	0.23	82,82,82,82	0
7	MG	M	700	1/1	0.74	0.26	80,80,80,80	0
7	MG	T	700	1/1	0.76	0.21	76,76,76,76	0
6	ANP	V	600	31/31	0.77	0.10	114,116,117,118	0
7	MG	K	700	1/1	0.79	0.18	102,102,102,102	0
7	MG	A	700	1/1	0.83	0.23	66,66,66,66	0
7	MG	F	700	1/1	0.84	0.20	83,83,83,83	0
7	MG	L	700	1/1	0.85	0.15	86,86,86,86	0
7	MG	O	700	1/1	0.88	0.14	91,91,91,91	0
7	MG	S	700	1/1	0.88	0.19	84,84,84,84	0
6	ANP	K	600	31/31	0.88	0.09	105,113,114,115	0
7	MG	U	700	1/1	0.88	0.17	83,83,83,83	0
7	MG	J	700	1/1	0.89	0.17	81,81,81,81	0
7	MG	X	700	1/1	0.89	0.17	80,80,80,80	0

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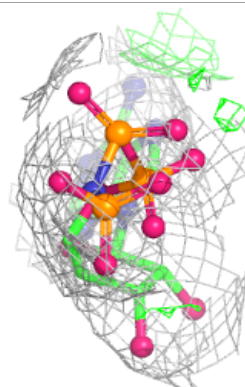
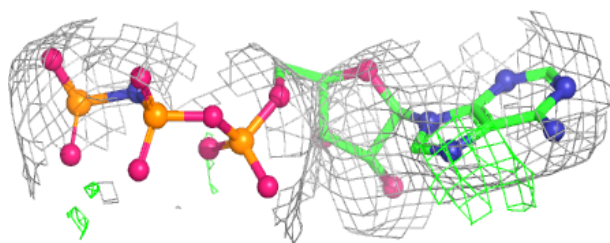
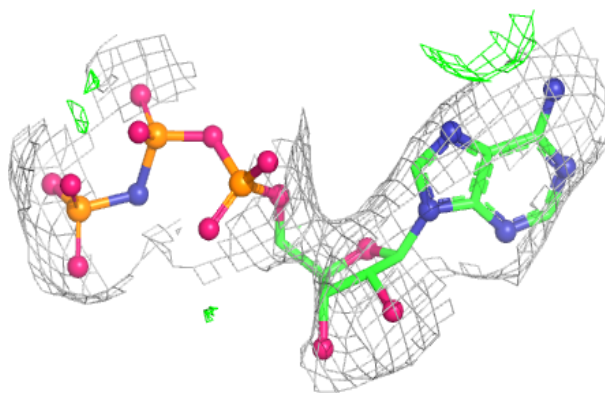
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	MG	C	700	1/1	0.90	0.22	78,78,78,78	0
6	ANP	S	600	31/31	0.92	0.07	83,85,86,86	0
6	ANP	D	600	31/31	0.92	0.08	82,89,91,91	0
7	MG	V	700	1/1	0.93	0.08	112,112,112,112	0
6	ANP	O	600	31/31	0.93	0.08	90,102,107,107	0
6	ANP	F	600	31/31	0.94	0.09	82,84,88,89	0
6	ANP	B	600	31/31	0.95	0.08	80,88,97,98	0
6	ANP	L	600	31/31	0.95	0.07	83,86,87,88	0
6	ANP	C	600	31/31	0.95	0.07	77,83,89,89	0
6	ANP	J	600	31/31	0.95	0.07	78,89,93,94	0
6	ANP	M	600	31/31	0.96	0.08	78,85,94,94	0
6	ANP	T	600	31/31	0.96	0.06	69,72,75,76	0
6	ANP	U	600	31/31	0.96	0.06	82,84,87,87	0
6	ANP	A	600	31/31	0.96	0.06	58,62,65,66	0
6	ANP	X	600	31/31	0.96	0.07	70,72,78,78	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.

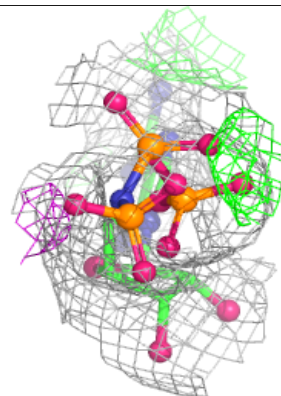
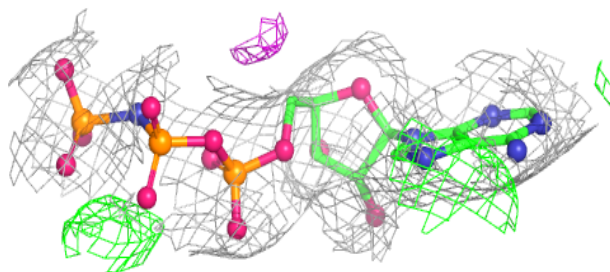
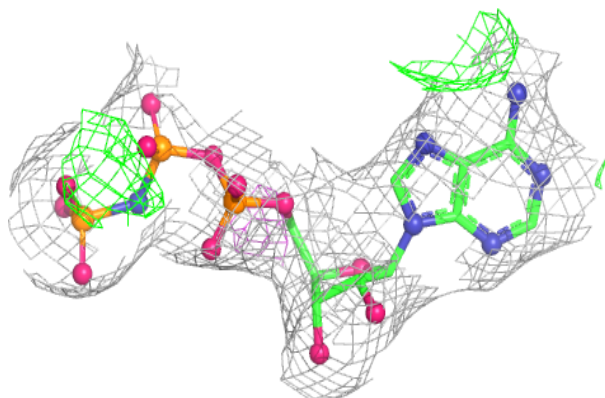


Electron density around ANP K 600:

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

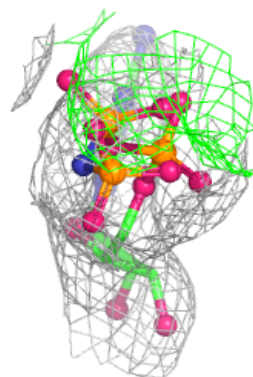
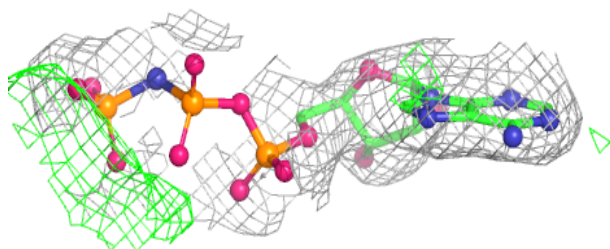
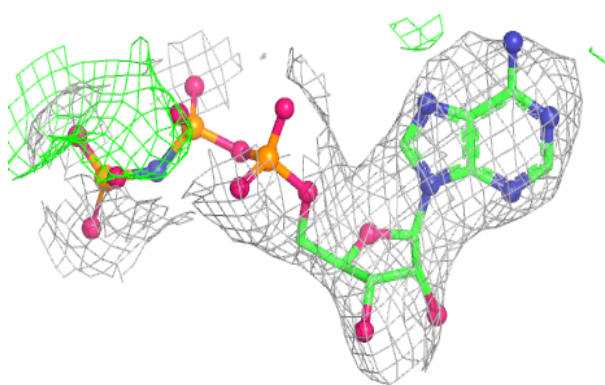
**Electron density around ANP S 600:**

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

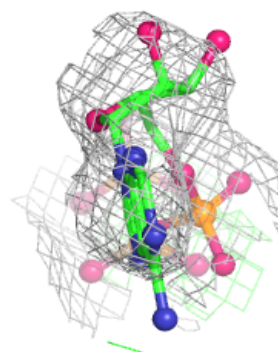
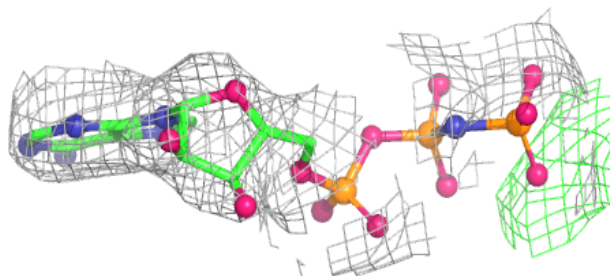
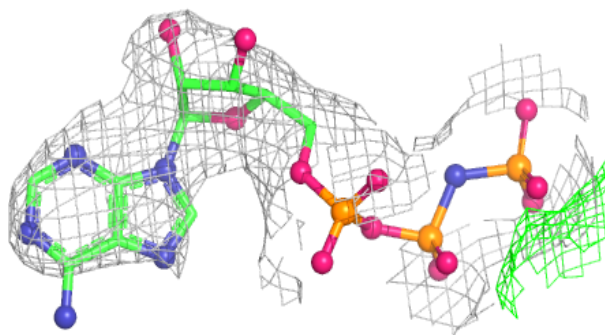


Electron density around ANP D 600:

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

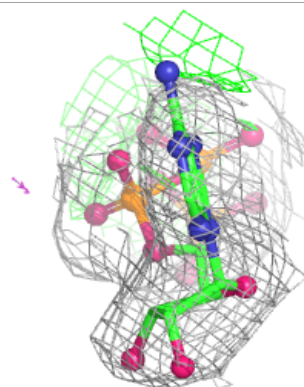
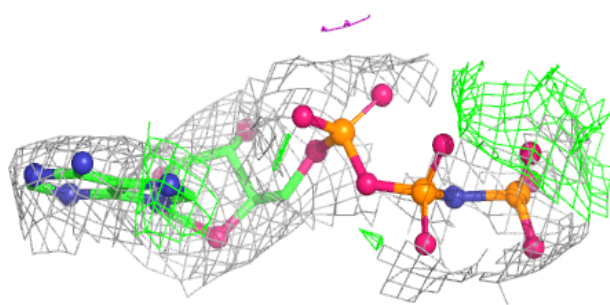
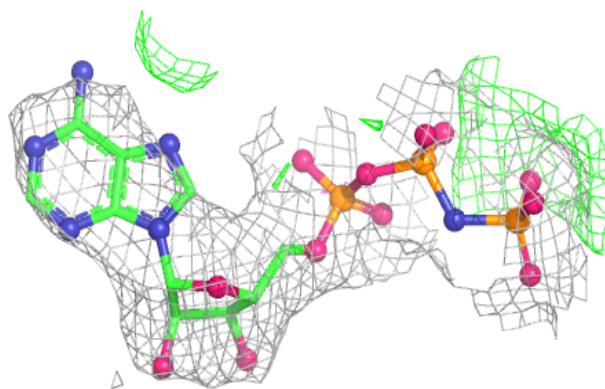
**Electron density around ANP O 600:**

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

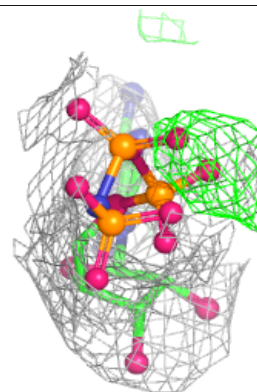
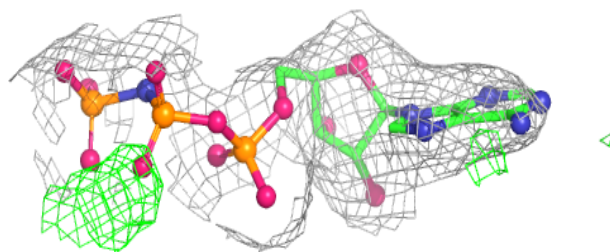
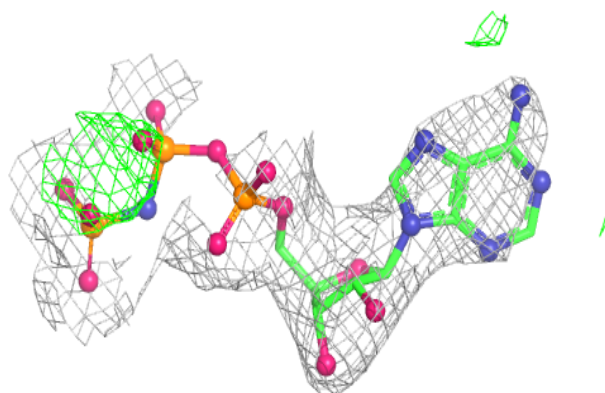


Electron density around ANP F 600:

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

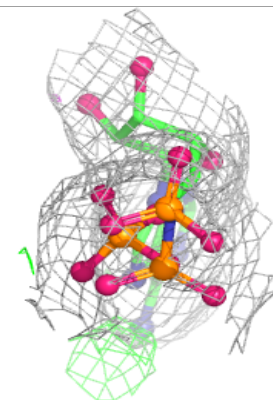
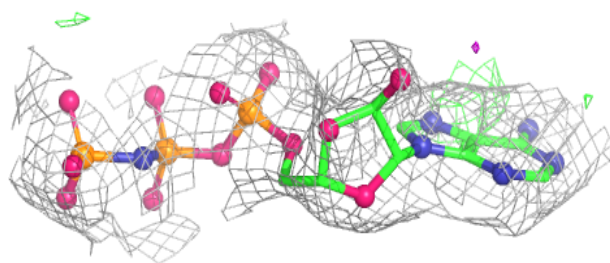
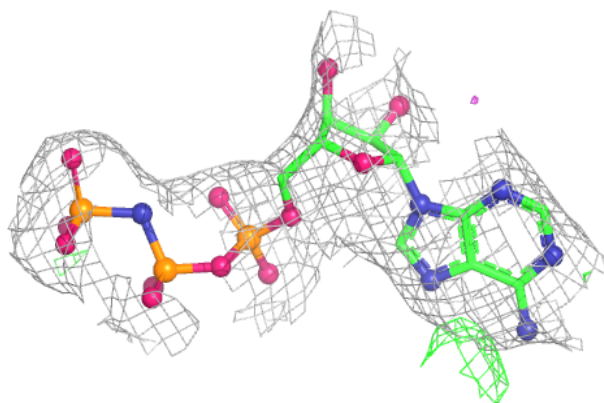
**Electron density around ANP B 600:**

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

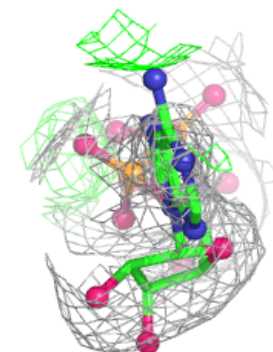
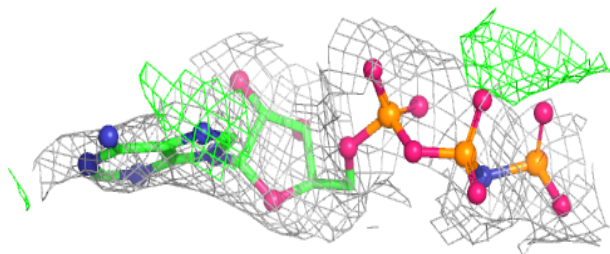
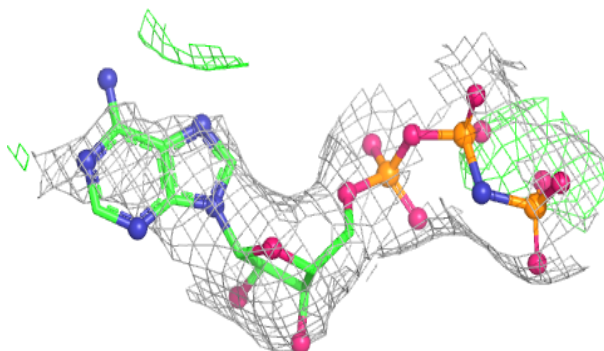


Electron density around ANP L 600:

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

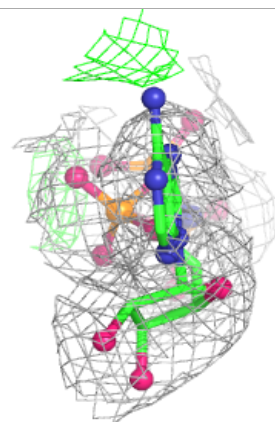
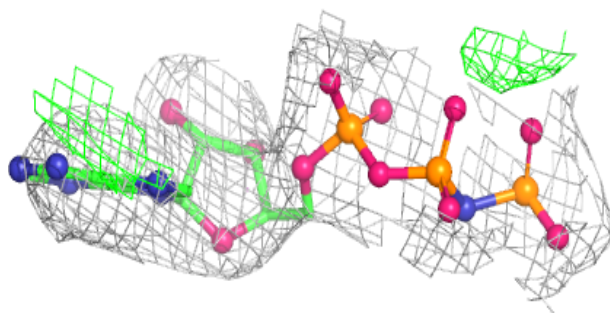
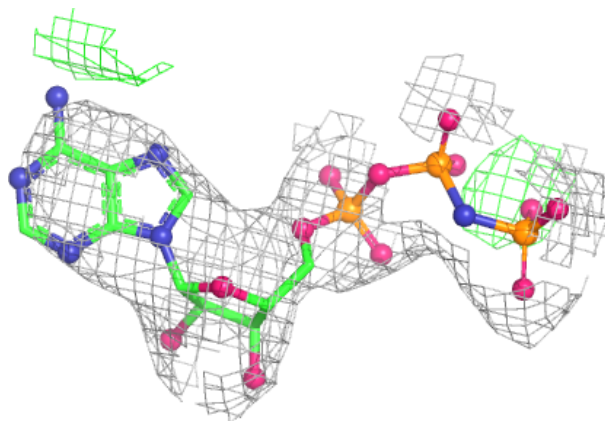
**Electron density around ANP C 600:**

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



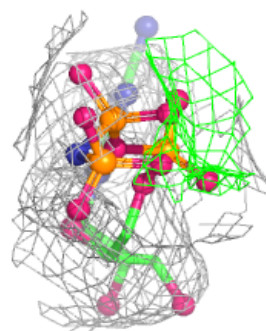
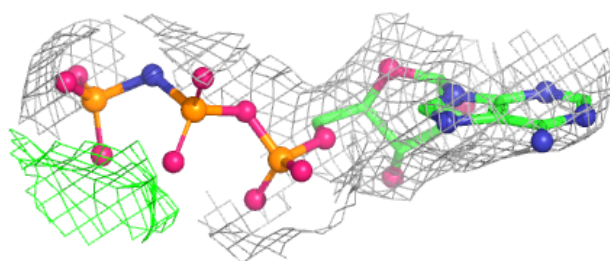
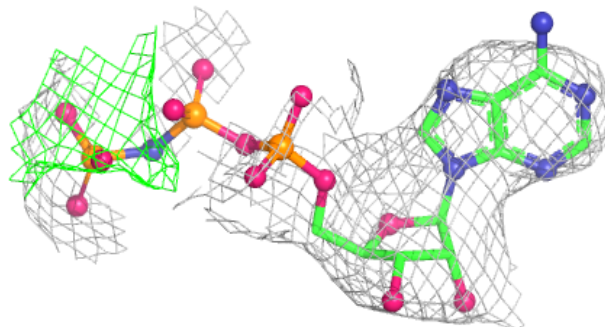
Electron density around ANP J 600:

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

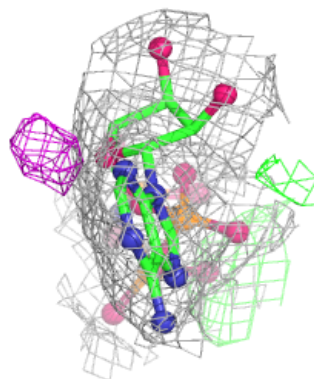
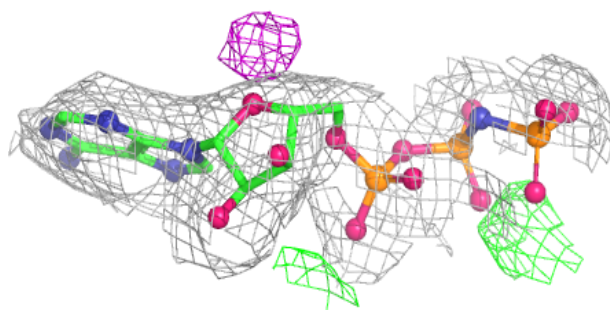
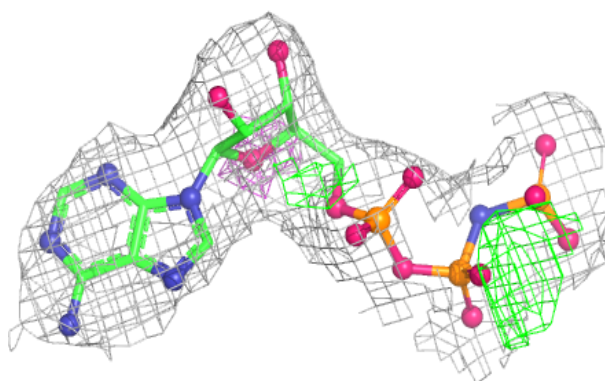


Electron density around ANP M 600:

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

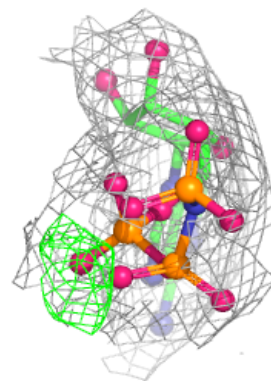
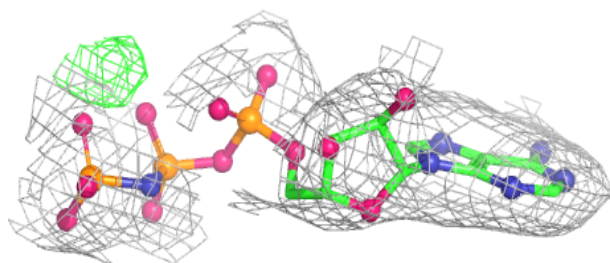
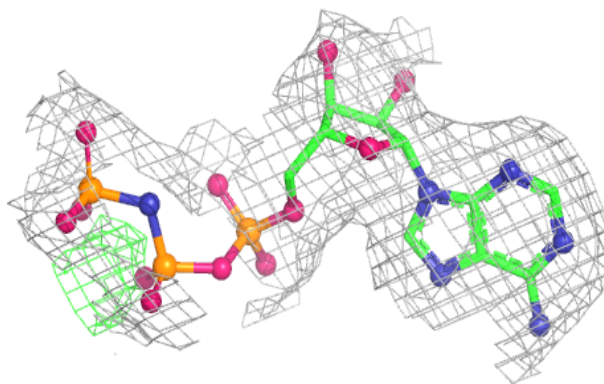
**Electron density around ANP T 600:**

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

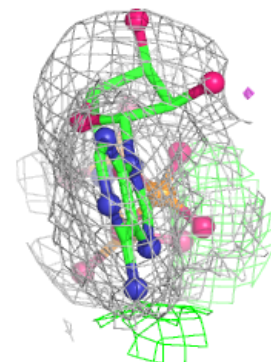
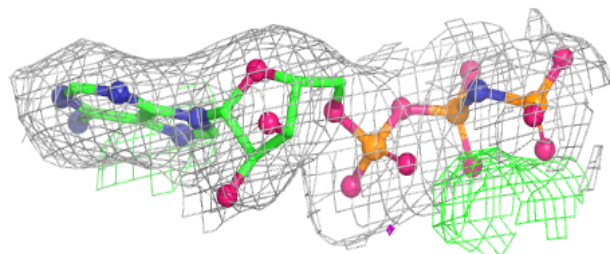
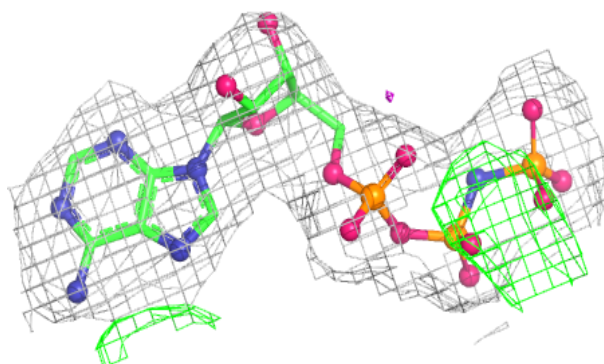


Electron density around ANP U 600:

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

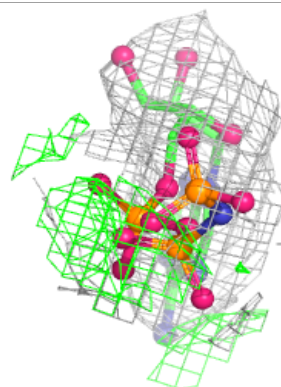
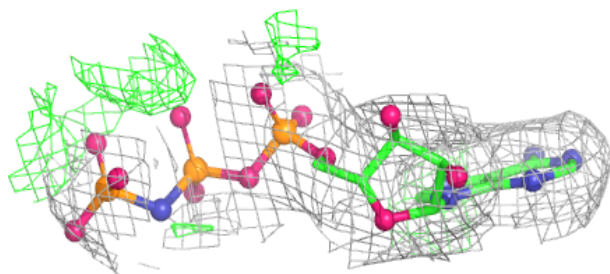
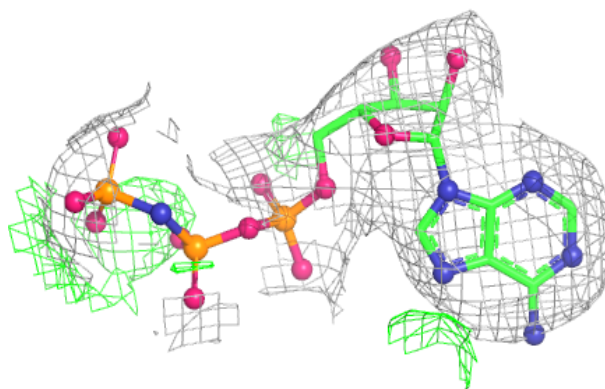
**Electron density around ANP A 600:**

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



Electron density around ANP X 600:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.