



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 12:00 PM EDT

PDB ID : 2HLD / pdb_00002hld
Title : Crystal structure of yeast mitochondrial F1-ATPase
Authors : Kabaleeswaran, V.; Puri, N.; Walker, J.E.; Leslie, A.G.; Mueller, D.M.
Deposited on : 2006-07-06
Resolution : 2.80 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

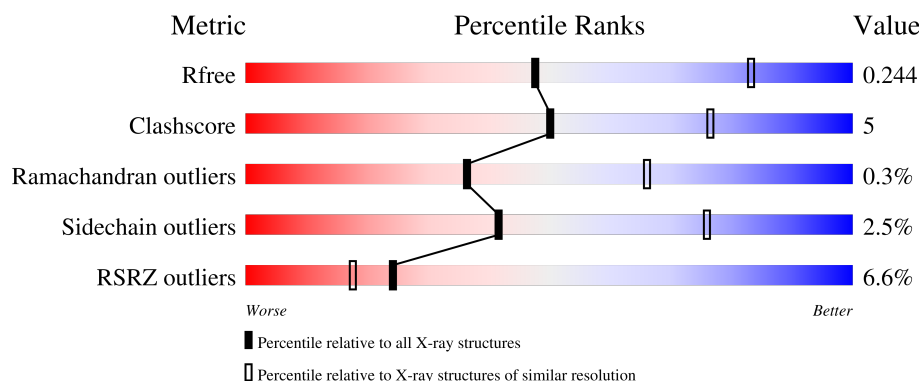
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	2% 84% 11% 5%
1	B	510	8% 82% 12% 5%
1	C	510	4% 83% 12% 5%
1	J	510	5% 84% 10% 6%
1	K	510	8% 81% 13% 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	478	
2	E	478	
2	F	478	
2	M	478	
2	N	478	
2	O	478	
2	V	478	
2	W	478	
2	X	478	
3	G	278	
3	P	278	
3	Y	278	
4	H	138	
4	Q	138	
4	Z	138	
5	1	61	
5	I	61	
5	R	61	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 72841 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 alpha chain, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	482	Total	C	N	O	S	0	0	0
			3664	2314	648	699	3			
1	B	483	Total	C	N	O	S	0	0	0
			3669	2317	649	700	3			
1	C	484	Total	C	N	O	S	0	0	0
			3674	2319	650	702	3			
1	J	481	Total	C	N	O	S	0	0	0
			3655	2309	646	697	3			
1	K	486	Total	C	N	O	S	0	0	0
			3684	2326	652	703	3			
1	L	482	Total	C	N	O	S	0	0	0
			3664	2314	648	699	3			
1	S	480	Total	C	N	O	S	0	0	0
			3651	2307	645	696	3			
1	T	481	Total	C	N	O	S	0	0	0
			3659	2311	647	698	3			
1	U	481	Total	C	N	O	S	0	0	0
			3659	2311	647	698	3			

- Molecule 2 is a protein called ATP synthase beta chain, mitochondrial.

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

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

- Molecule 3 is a protein called ATP synthase gamma chain, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	265	Total	C	N	O	S	0	0	0
			2031	1277	355	389	10			
3	P	243	Total	C	N	O	S	0	0	0
			1851	1165	322	355	9			
3	Y	200	Total	C	N	O	S	0	0	0
			1517	944	273	291	9			

- Molecule 4 is a protein called ATP synthase delta chain, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	120	Total	C	N	O	S	0	0	0
			758	475	134	147	2			
4	Q	84	Total	C	N	O		0	0	0
			436	262	87	87				
4	Z	17	Total	C	N	O		0	0	0
			85	51	17	17				

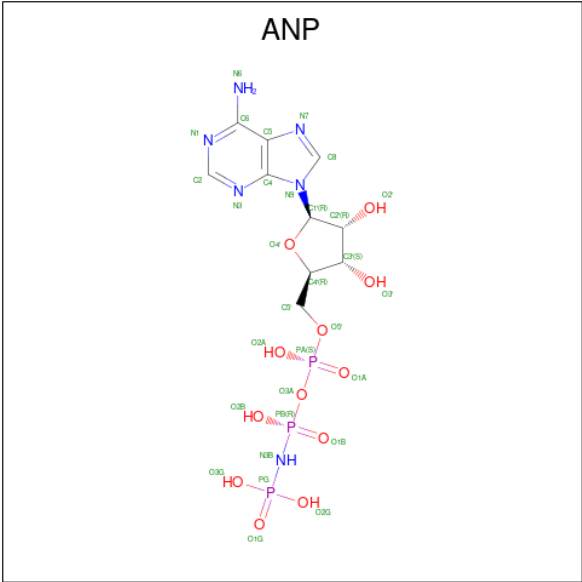
- Molecule 5 is a protein called ATP synthase epsilon chain, mitochondrial.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	48	Total	C	N	O	0	0	0
			324	201	56	67			
5	R	34	Total	C	N	O	0	0	0
			170	102	34	34			
5	1	27	Total	C	N	O	0	0	0
			135	81	27	27			

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 7 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



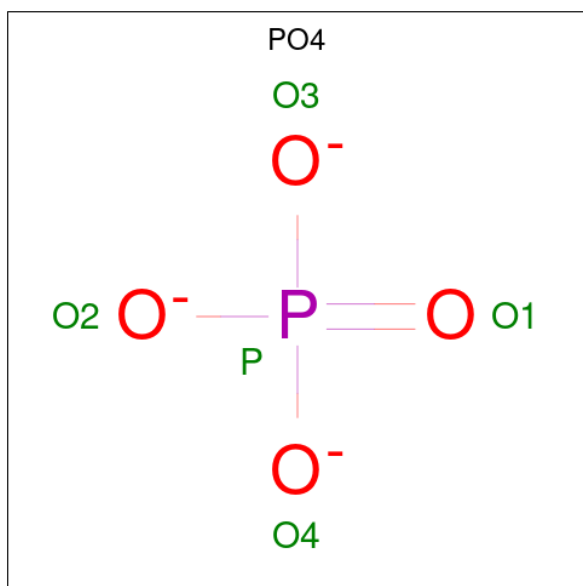
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
7	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
7	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
7	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
7	F	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
7	J	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
7	K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

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

- Molecule 8 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	26	Total	O	0	0
			26	26		
9	B	18	Total	O	0	0
			18	18		
9	C	13	Total	O	0	0
			13	13		
9	D	20	Total	O	0	0
			20	20		
9	E	13	Total	O	0	0
			13	13		
9	F	11	Total	O	0	0
			11	11		
9	G	3	Total	O	0	0
			3	3		

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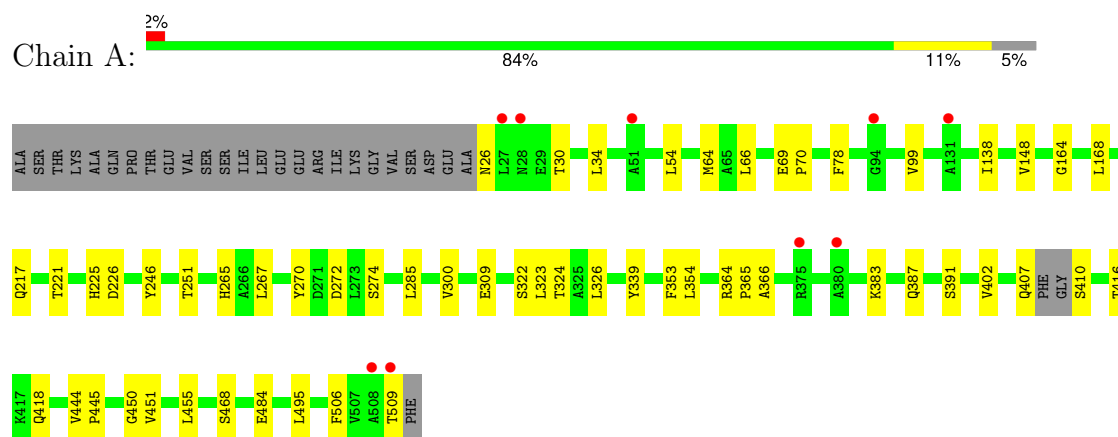
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	J	17	Total 17	O 17	0	0
9	K	4	Total 4	O 4	0	0
9	L	19	Total 19	O 19	0	0
9	M	9	Total 9	O 9	0	0
9	N	8	Total 8	O 8	0	0
9	O	7	Total 7	O 7	0	0
9	P	2	Total 2	O 2	0	0
9	Q	1	Total 1	O 1	0	0
9	S	6	Total 6	O 6	0	0
9	T	1	Total 1	O 1	0	0
9	U	3	Total 3	O 3	0	0
9	X	2	Total 2	O 2	0	0

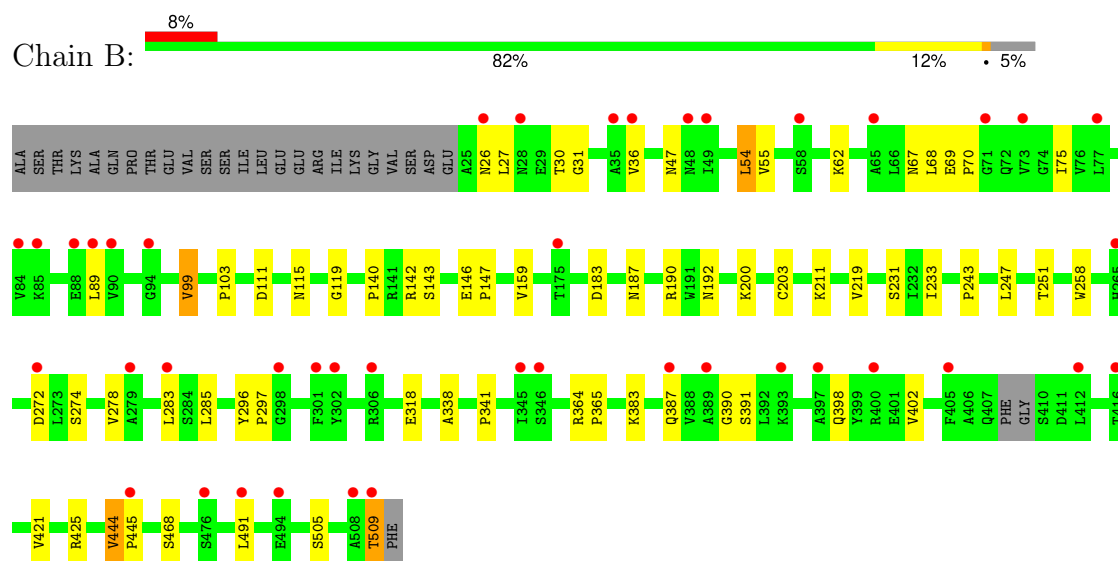
3 Residue-property plots [i](#)

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.

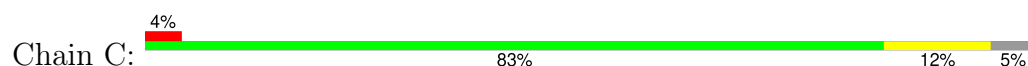
- Molecule 1: ATP synthase alpha chain, mitochondrial

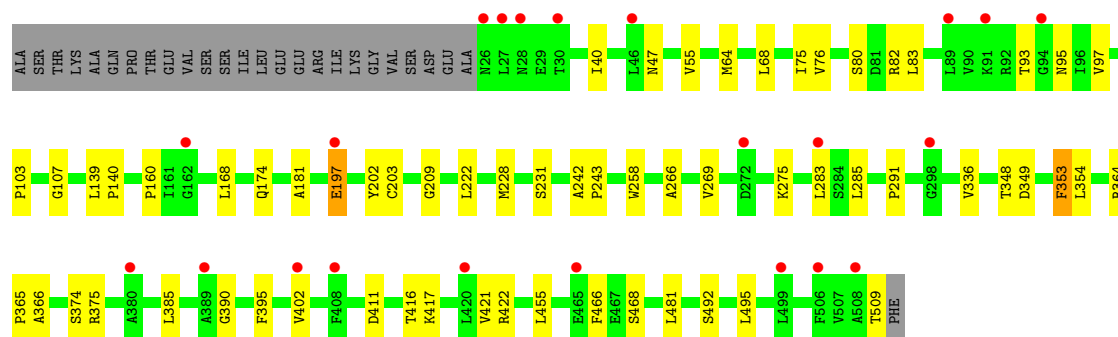


- Molecule 1: ATP synthase alpha chain, mitochondrial

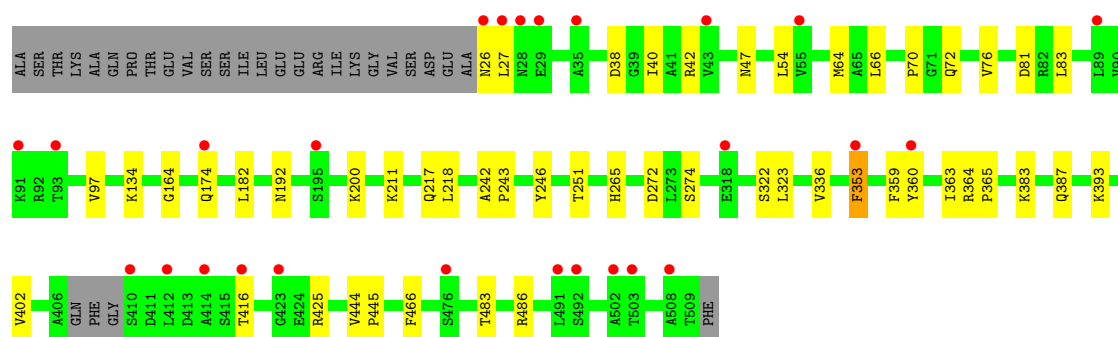
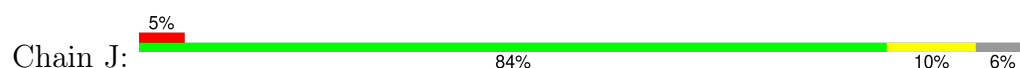


- Molecule 1: ATP synthase alpha chain, mitochondrial

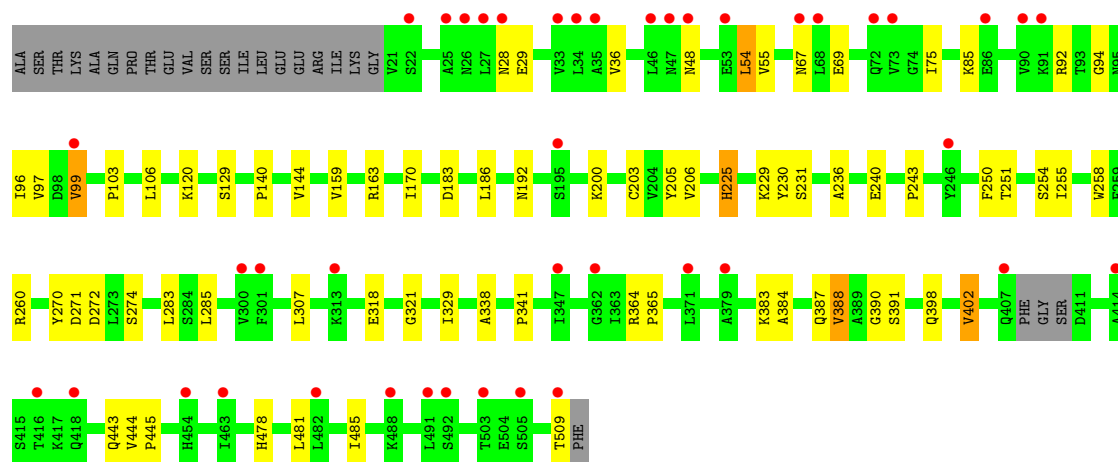
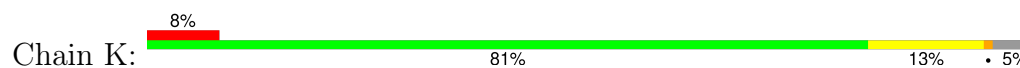




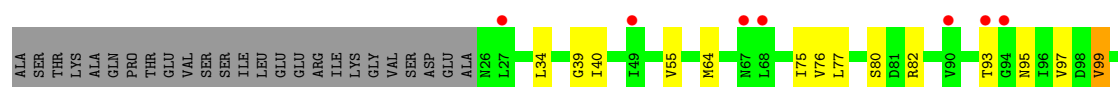
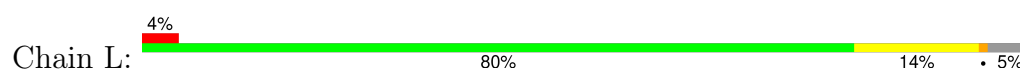
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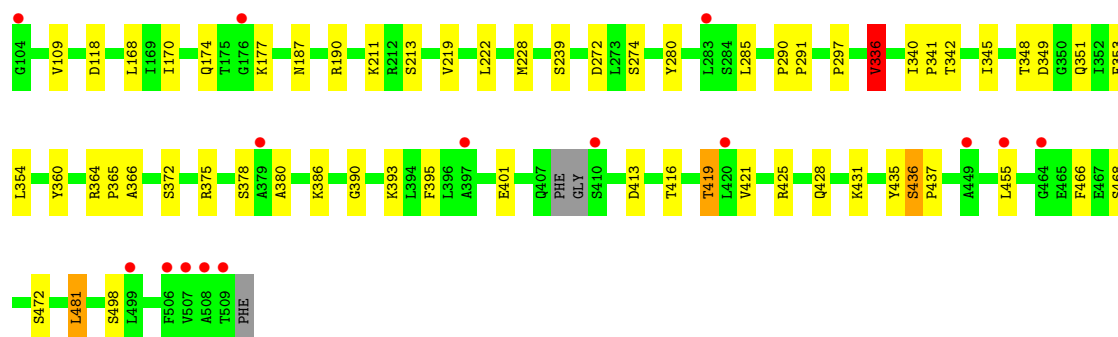


- Molecule 1: ATP synthase alpha chain, mitochondrial

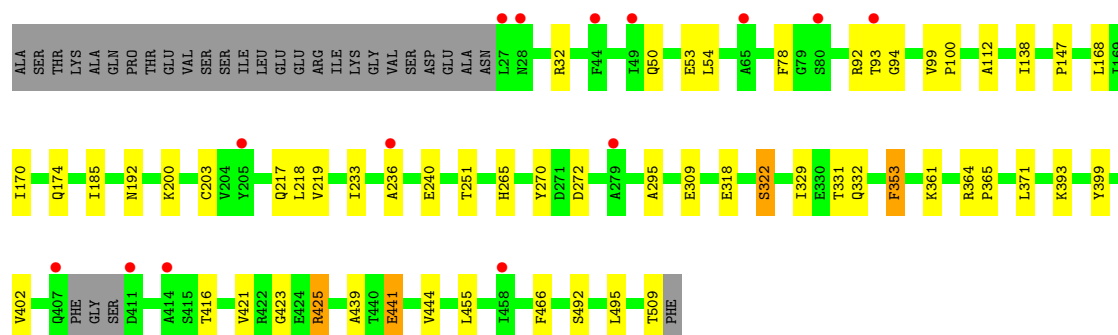
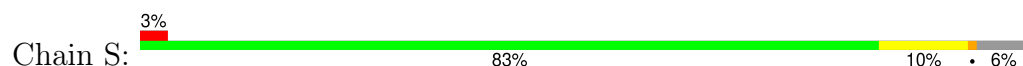


- Molecule 1: ATP synthase alpha chain, mitochondrial

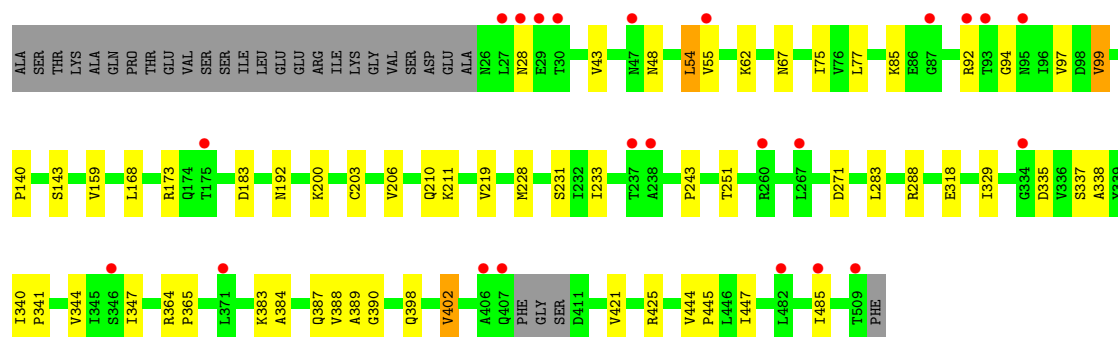
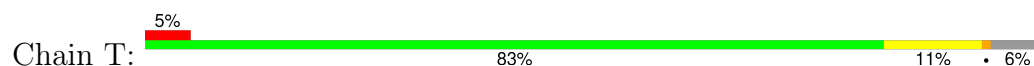




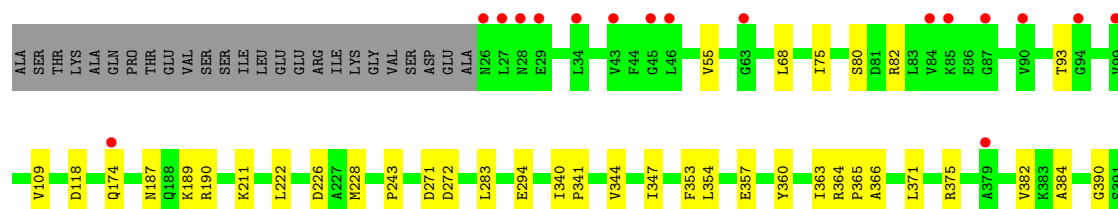
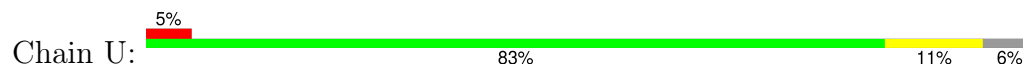
- Molecule 1: ATP synthase alpha chain, mitochondrial



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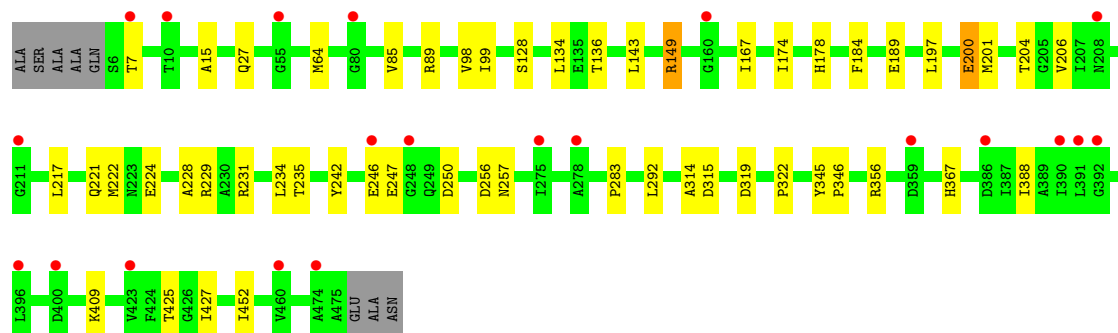
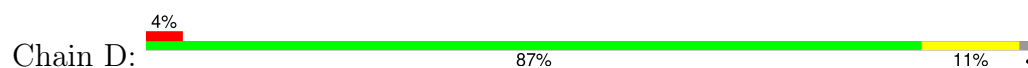


- Molecule 1: ATP synthase alpha chain, mitochondrial

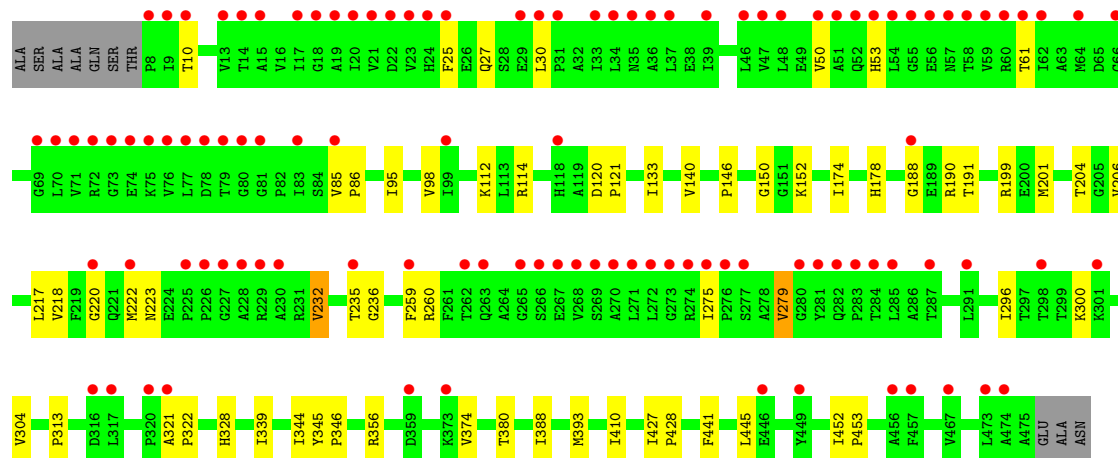
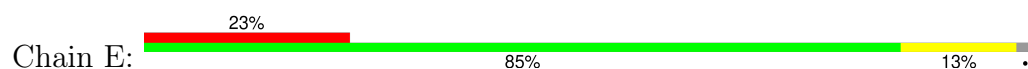




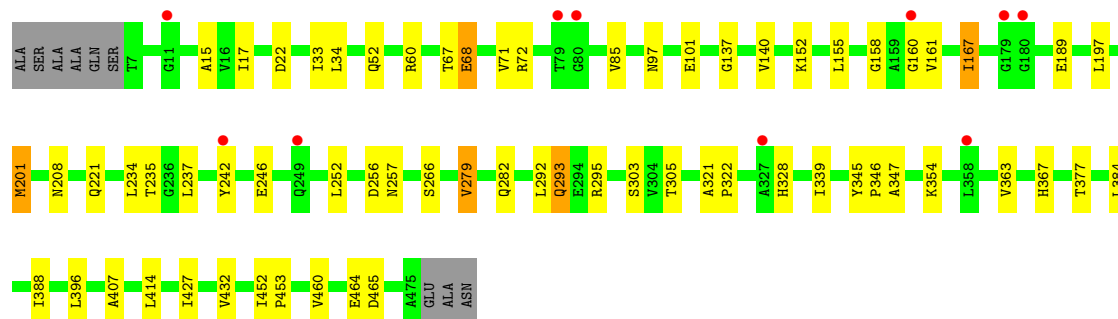
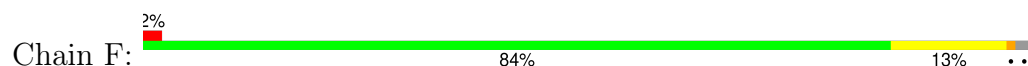
- Molecule 2: ATP synthase beta chain, mitochondrial



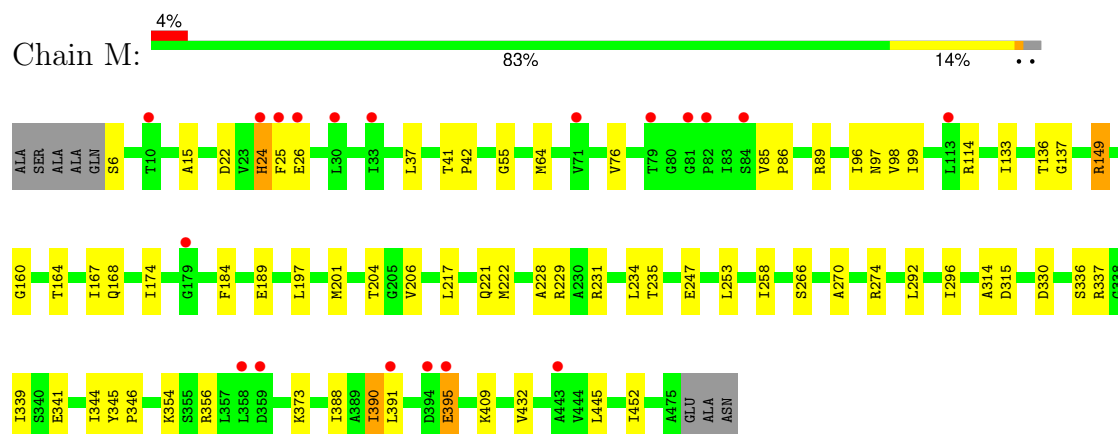
- Molecule 2: ATP synthase beta chain, mitochondrial



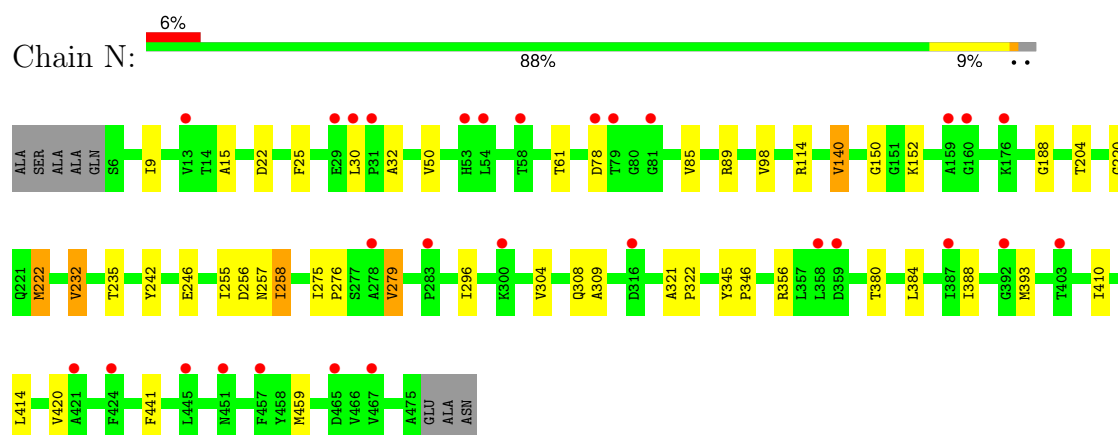
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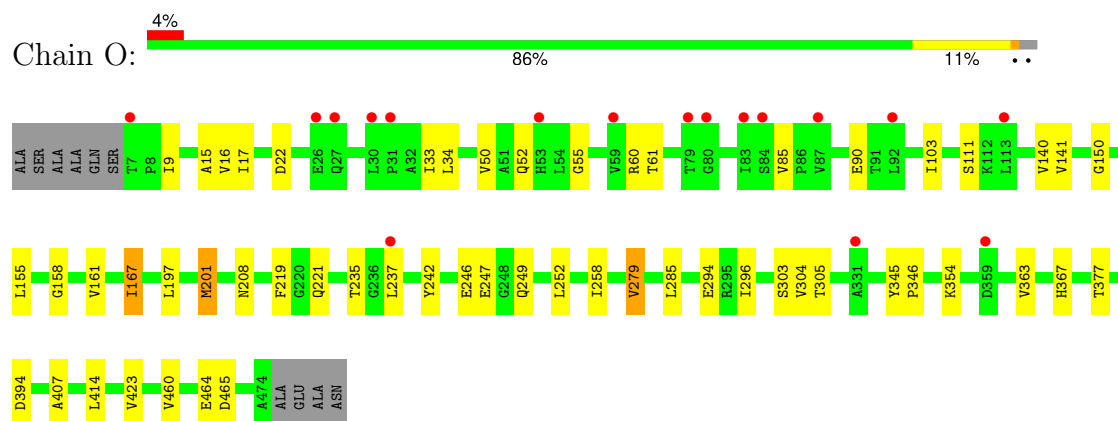
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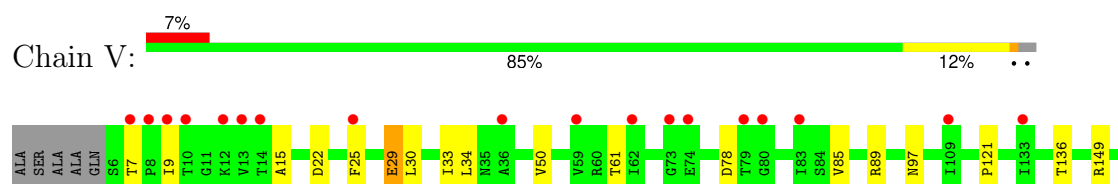
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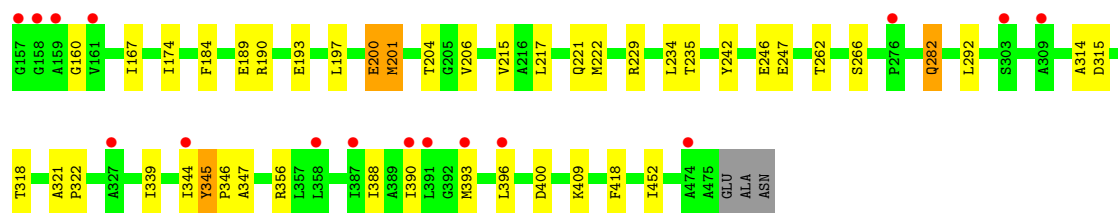


- Molecule 2: ATP synthase beta chain, mitochondrial

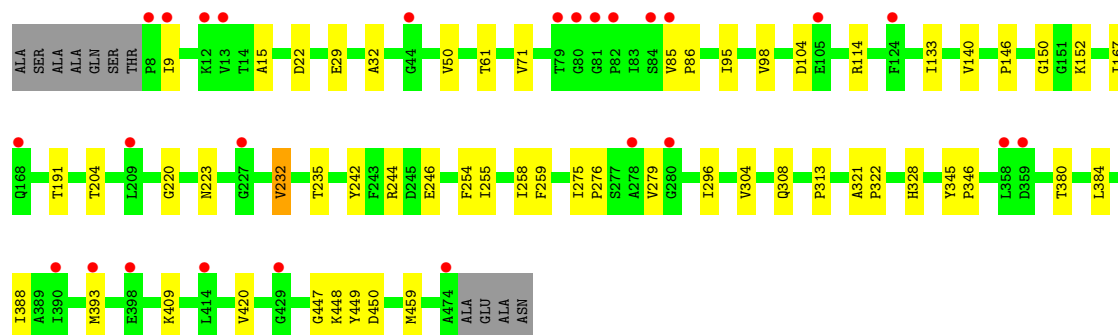
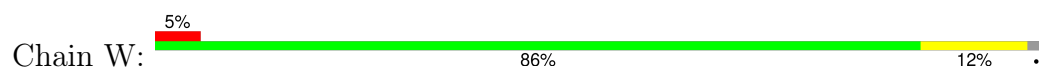


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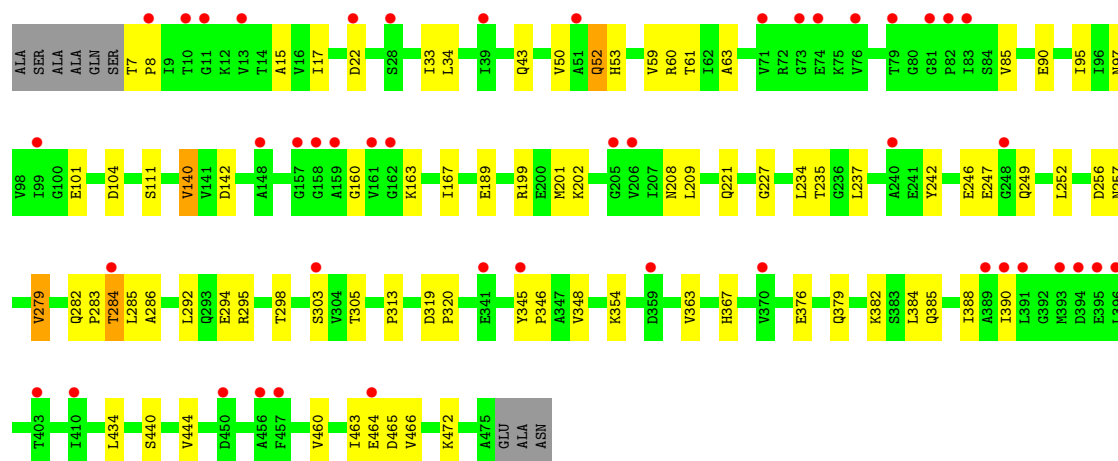
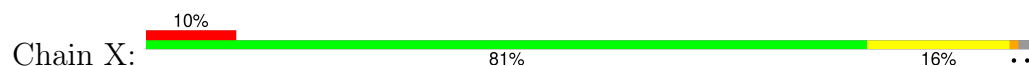




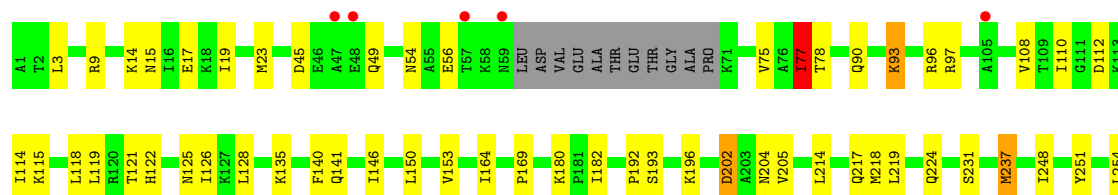
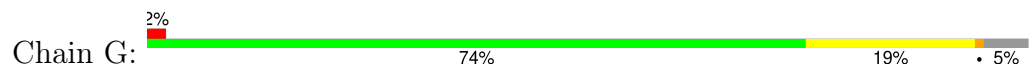
• Molecule 2: ATP synthase beta chain, mitochondrial



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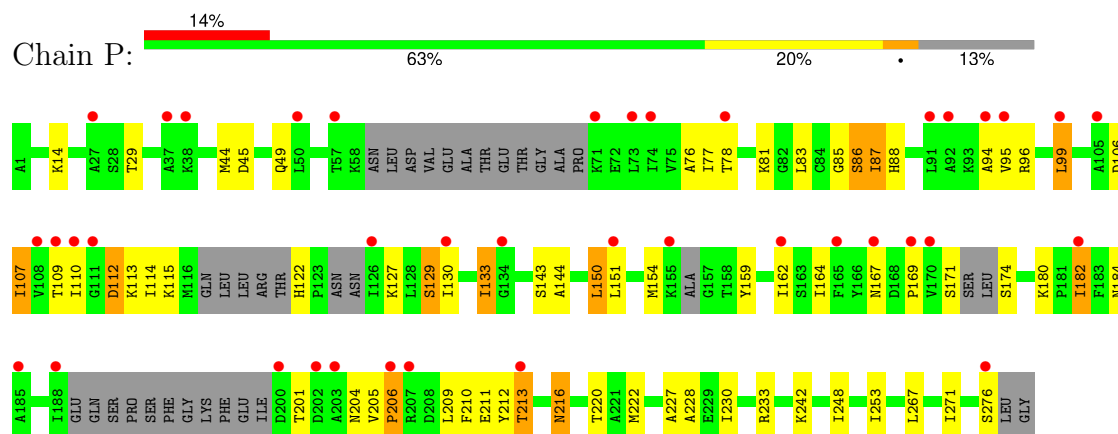


• Molecule 3: ATP synthase gamma chain, mitochondrial

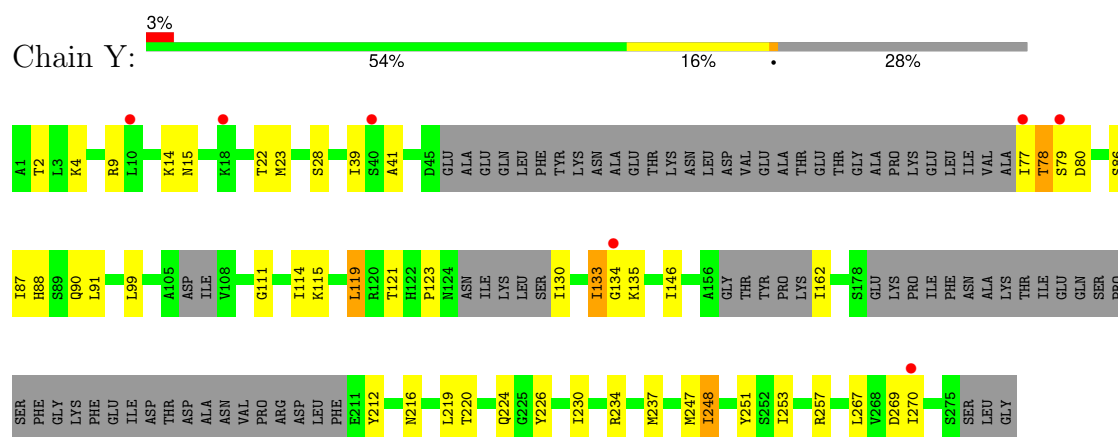




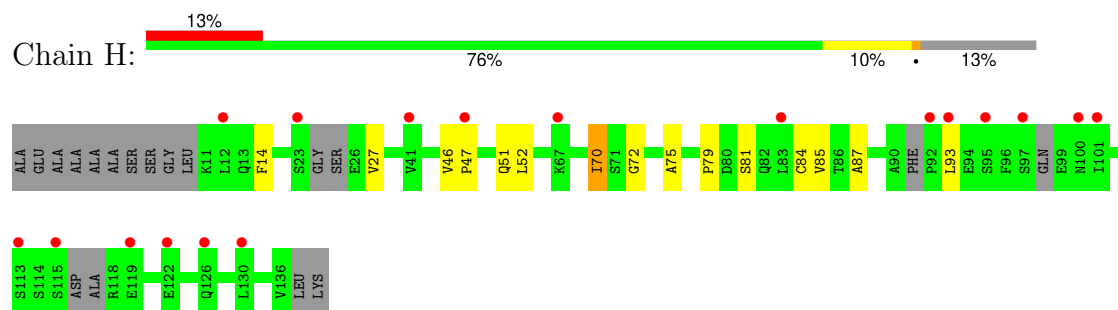
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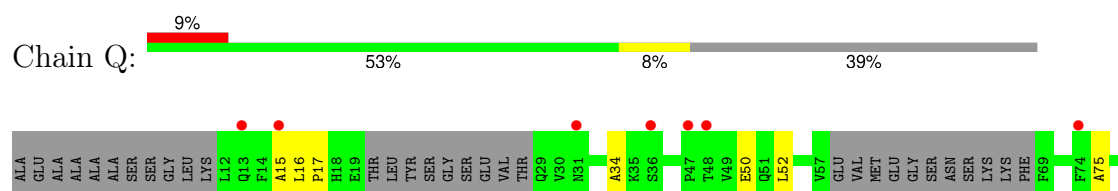
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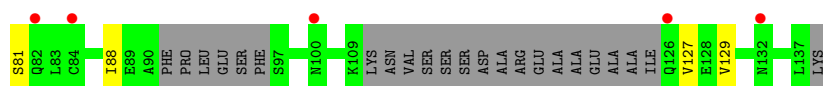


• Molecule 4: ATP synthase delta chain, mitochondrial

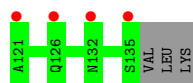
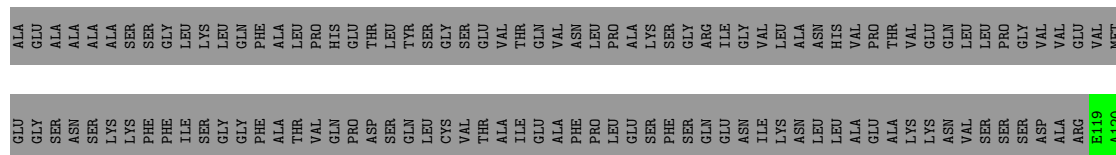


• Molecule 4: ATP synthase delta chain, mitochondrial

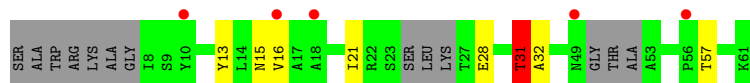




- Molecule 4: ATP synthase delta chain, mitochondrial



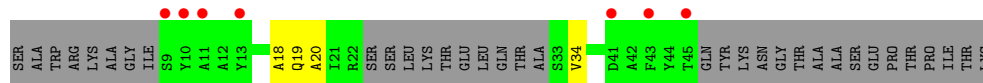
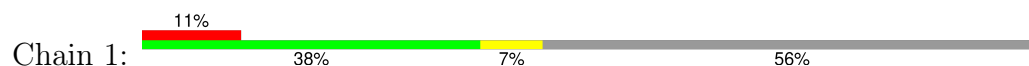
- Molecule 5: ATP synthase epsilon chain, mitochondrial



- Molecule 5: ATP synthase epsilon chain, mitochondrial



- Molecule 5: ATP synthase epsilon chain, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	111.52Å 294.13Å 190.43Å 90.00° 101.67° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 20.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-2.80) 99.6 (20.00-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 2.79Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.207 , 0.244 0.211 , 0.244	Depositor DCC
R_{free} test set	5938 reflections (2.03%)	wwPDB-VP
Wilson B-factor (Å ²)	72.1	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 86.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	72841	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.86% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ANP, PO4, 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	0.83	0/3718	1.01	0/5032
1	B	0.72	0/3723	0.97	2/5039 (0.0%)
1	C	0.73	0/3729	0.95	1/5048 (0.0%)
1	J	0.71	0/3709	0.95	1/5020 (0.0%)
1	K	0.59	1/3738 (0.0%)	0.89	2/5060 (0.0%)
1	L	0.78	0/3718	0.99	3/5032 (0.1%)
1	S	0.61	1/3705 (0.0%)	0.92	2/5014 (0.0%)
1	T	0.50	0/3713	0.86	0/5025
1	U	0.53	0/3713	0.88	1/5025 (0.0%)
2	D	0.74	0/3605	0.98	0/4889
2	E	0.72	0/3592	0.94	0/4870
2	F	0.70	0/3599	0.97	0/4881
2	M	0.72	0/3605	0.99	3/4889 (0.1%)
2	N	0.63	0/3605	0.89	0/4889
2	O	0.64	0/3594	0.95	2/4874 (0.0%)
2	V	0.56	0/3605	0.92	2/4889 (0.0%)
2	W	0.54	0/3587	0.89	0/4863
2	X	0.57	0/3599	0.88	0/4881
3	G	0.65	0/2056	0.94	2/2767 (0.1%)
3	P	0.61	0/1868	0.95	2/2508 (0.1%)
3	Y	0.51	0/1527	0.85	0/2048
4	H	0.67	0/766	0.98	0/1051
4	Q	0.65	0/434	1.10	2/595 (0.3%)
4	Z	0.62	0/84	1.17	0/116
5	I	0.62	0/133	0.85	0/183
5	I	0.68	0/326	1.07	2/445 (0.4%)
5	R	0.67	0/168	1.06	0/232
All	All	0.66	2/73219 (0.0%)	0.94	27/99165 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected

by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	S	0	1
2	D	0	1
2	V	0	1
2	W	0	1
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	225	HIS	CE1-NE2	5.89	1.38	1.32
1	S	444	VAL	CA-CB	5.69	1.57	1.54

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	345	TYR	C-N-CD	-8.22	91.28	125.00
3	P	253	ILE	N-CA-C	-7.48	103.05	110.30
1	S	444	VAL	N-CA-CB	7.08	115.97	110.45
1	L	336	VAL	CB-CA-C	-6.75	100.23	111.29
1	U	93	THR	N-CA-C	-6.51	106.29	114.56
2	V	121	PRO	O-C-N	6.42	124.17	121.15
1	J	47	ASN	N-CA-C	5.89	119.29	111.75
1	B	444	VAL	N-CA-CB	5.73	114.11	110.50
1	L	99	VAL	CB-CA-C	-5.62	103.82	109.33
4	Q	34	ALA	N-CA-C	5.57	117.09	110.19
3	G	112	ASP	N-CA-C	5.54	117.32	111.28
2	O	219	PHE	N-CA-C	5.41	117.89	108.76
1	L	99	VAL	N-CA-C	5.39	113.61	109.19
3	P	107	ILE	N-CA-C	5.38	115.64	108.11
4	Q	15	ALA	N-CA-C	5.30	117.93	110.14
2	M	55	GLY	N-CA-C	-5.24	106.42	112.29
2	O	221	GLN	N-CA-C	5.24	116.85	110.41
1	K	443	GLN	CA-C-N	5.22	123.53	120.24
1	K	443	GLN	C-N-CA	5.22	123.53	120.24
1	B	247	LEU	N-CA-C	5.21	117.03	111.36
5	I	57	THR	CA-C-N	5.16	125.15	119.89
5	I	57	THR	C-N-CA	5.16	125.15	119.89
1	C	47	ASN	N-CA-C	5.15	118.34	111.75
3	G	77	ILE	N-CA-C	5.12	115.42	107.28
1	S	93	THR	N-CA-C	-5.09	107.01	114.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	266	SER	N-CA-C	5.04	116.77	111.28
2	M	26	GLU	N-CA-C	5.03	117.02	110.53

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	7	THR	Peptide
1	S	147	PRO	Peptide
2	V	345	TYR	Peptide
2	W	447	GLY	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3664	0	3748	29	0
1	B	3669	0	3752	41	0
1	C	3674	0	3756	39	0
1	J	3655	0	3739	34	0
1	K	3684	0	3758	45	0
1	L	3664	0	3747	52	0
1	S	3651	0	3740	34	0
1	T	3659	0	3745	36	0
1	U	3659	0	3745	30	0
2	D	3549	0	3620	32	0
2	E	3536	0	3610	41	0
2	F	3543	0	3615	42	0
2	M	3549	0	3620	52	0
2	N	3549	0	3621	35	0
2	O	3538	0	3610	33	0
2	V	3549	0	3620	38	0
2	W	3531	0	3605	38	0
2	X	3543	0	3615	49	0
3	G	2031	0	2084	34	0
3	P	1851	0	1893	42	0
3	Y	1517	0	1561	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	758	0	602	9	0
4	Q	436	0	215	4	0
4	Z	85	0	45	0	0
5	1	135	0	70	1	0
5	I	324	0	249	2	0
5	R	170	0	87	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
6	J	1	0	0	0	0
6	K	1	0	0	0	0
6	L	1	0	0	0	0
6	M	1	0	0	0	0
6	O	1	0	0	0	0
6	S	1	0	0	0	0
6	T	1	0	0	0	0
6	U	1	0	0	0	0
6	V	1	0	0	0	0
6	X	1	0	0	0	0
7	A	31	0	13	0	0
7	B	31	0	13	0	0
7	C	31	0	13	1	0
7	D	31	0	13	0	0
7	F	31	0	13	2	0
7	J	31	0	13	0	0
7	K	31	0	13	1	0
7	L	31	0	13	1	0
7	M	31	0	13	6	0
7	O	31	0	13	0	0
7	S	31	0	13	1	0
7	T	31	0	13	0	0
7	U	31	0	13	0	0
7	V	31	0	13	3	0
7	X	31	0	13	4	0
8	N	5	0	0	0	0
9	A	26	0	0	2	0
9	B	18	0	0	0	0
9	C	13	0	0	0	0
9	D	20	0	0	0	0
9	E	13	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	F	11	0	0	0	0
9	G	3	0	0	0	0
9	J	17	0	0	0	0
9	K	4	0	0	0	0
9	L	19	0	0	0	0
9	M	9	0	0	0	0
9	N	8	0	0	0	0
9	O	7	0	0	0	0
9	P	2	0	0	0	0
9	Q	1	0	0	2	0
9	S	6	0	0	0	0
9	T	1	0	0	0	0
9	U	3	0	0	0	0
9	X	2	0	0	0	0
All	All	72841	0	73267	767	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 5.

All (767) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:85:VAL:HG11	2:V:235:THR:HG23	1.26	1.16
2:E:85:VAL:HG11	2:E:235:THR:HG23	1.27	1.12
2:N:85:VAL:HG11	2:N:235:THR:HG23	1.28	1.11
2:D:85:VAL:HG11	2:D:235:THR:HG23	1.25	1.11
3:G:96:ARG:HE	3:G:121:THR:HG21	1.10	1.09
2:M:85:VAL:HG11	2:M:235:THR:HG23	1.19	1.09
1:B:26:ASN:O	1:B:30:THR:HB	1.55	1.06
2:F:85:VAL:HG11	2:F:235:THR:HG23	1.38	1.02
2:W:85:VAL:HG11	2:W:235:THR:HG23	1.39	1.00
4:H:14:PHE:HZ	4:H:70:ILE:HD11	1.28	0.99
2:X:85:VAL:HG11	2:X:235:THR:HG23	1.45	0.98
1:C:336:VAL:HG11	1:C:353:PHE:CZ	1.99	0.97
2:O:85:VAL:HG11	2:O:235:THR:HG23	1.44	0.97
1:J:336:VAL:HG11	1:J:353:PHE:HZ	1.27	0.95
2:M:149:ARG:HG2	2:M:149:ARG:HH11	1.32	0.95
2:D:85:VAL:HG11	2:D:235:THR:CG2	1.99	0.93
2:M:160:GLY:H	7:M:600:ANP:HNB1	1.14	0.91
1:K:99:VAL:HG11	1:K:251:THR:HB	1.50	0.91
2:V:160:GLY:H	7:V:600:ANP:HNB1	1.10	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:88:HIS:HD2	3:P:113:LYS:HB2	1.34	0.90
3:P:88:HIS:CD2	3:P:113:LYS:HB2	2.09	0.88
1:C:336:VAL:HG11	1:C:353:PHE:CE1	2.09	0.87
1:J:336:VAL:HG11	1:J:353:PHE:CZ	2.10	0.87
3:Y:23:MET:HE2	3:Y:23:MET:HA	1.58	0.85
2:M:85:VAL:HG11	2:M:235:THR:CG2	2.05	0.84
3:P:112:ASP:O	3:P:115:LYS:HB3	1.77	0.84
1:C:242:ALA:HB3	1:C:243:PRO:HD3	1.58	0.83
2:D:85:VAL:CG1	2:D:235:THR:HG23	2.08	0.82
1:B:67:ASN:HB2	2:F:17:ILE:HG12	1.61	0.82
2:X:160:GLY:H	7:X:600:ANP:HNB1	1.28	0.82
2:F:52:GLN:HE21	2:F:60:ARG:HD2	1.44	0.81
2:N:242:TYR:CE1	2:N:246:GLU:HG3	2.16	0.81
3:G:96:ARG:NE	3:G:121:THR:HG21	1.95	0.81
2:M:149:ARG:HH11	2:M:149:ARG:CG	1.95	0.79
1:S:265:HIS:ND1	1:S:322:SER:HB2	1.98	0.78
1:U:68:LEU:O	2:V:15:ALA:HA	1.85	0.77
4:H:14:PHE:CZ	4:H:70:ILE:HD11	2.19	0.76
3:G:45:ASP:O	3:G:49:GLN:HB2	1.86	0.75
4:Q:75:ALA:HB2	9:Q:802:HOH:O	1.87	0.74
1:S:112:ALA:O	1:S:251:THR:HG21	1.87	0.74
1:K:67:ASN:HB2	2:O:17:ILE:HG12	1.67	0.74
1:K:236:ALA:HA	1:K:240:GLU:OE1	1.87	0.74
3:P:76:ALA:O	3:P:109:THR:HA	1.88	0.74
2:M:234:LEU:HD23	2:M:292:LEU:HD13	1.69	0.73
1:L:170:ILE:HG23	1:L:353:PHE:HD1	1.53	0.73
2:V:346:PRO:HG3	2:V:418:PHE:CZ	2.24	0.73
1:S:425:ARG:HH11	1:S:425:ARG:CG	2.01	0.73
1:C:336:VAL:HG11	1:C:353:PHE:HZ	1.51	0.72
2:W:220:GLY:HA3	2:W:232:VAL:HG11	1.71	0.72
3:Y:133:ILE:HD12	3:Y:134:GLY:H	1.54	0.72
1:B:243:PRO:HG3	1:B:283:LEU:HD21	1.72	0.72
3:G:122:HIS:HB3	3:G:125:ASN:HD22	1.56	0.71
2:M:189:GLU:O	2:M:221:GLN:HB3	1.91	0.71
1:L:174:GLN:HA	7:L:600:ANP:HNB1	1.56	0.70
2:W:242:TYR:CE1	2:W:246:GLU:HG3	2.27	0.70
1:T:99:VAL:HG11	1:T:251:THR:HB	1.73	0.70
2:E:85:VAL:HG11	2:E:235:THR:CG2	2.17	0.69
2:M:85:VAL:CG1	2:M:235:THR:HG23	2.10	0.69
1:K:106:LEU:HD23	1:K:230:TYR:HA	1.73	0.69
2:D:234:LEU:HD23	2:D:292:LEU:HD13	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:ASP:OD1	1:A:274:SER:HB2	1.93	0.68
3:P:205:VAL:N	3:P:206:PRO:HD3	2.08	0.68
9:A:825:HOH:O	2:E:260:ARG:HD3	1.94	0.68
1:J:336:VAL:CG1	1:J:353:PHE:HZ	2.04	0.68
1:L:372:SER:O	1:L:393:LYS:NZ	2.26	0.68
1:K:54:LEU:HD12	1:K:97:VAL:HA	1.76	0.68
3:G:96:ARG:HE	3:G:121:THR:CG2	1.99	0.67
2:V:346:PRO:O	2:V:347:ALA:HB3	1.93	0.67
4:H:14:PHE:HZ	4:H:70:ILE:CD1	2.04	0.67
1:S:425:ARG:HH11	1:S:425:ARG:HG3	1.58	0.67
1:A:506:PHE:O	1:A:509:THR:HG22	1.95	0.67
1:C:40:ILE:CD1	1:C:76:VAL:HG12	2.25	0.67
3:P:184:ASN:HA	3:P:210:PHE:CE1	2.30	0.67
3:P:88:HIS:HD2	3:P:113:LYS:CB	2.07	0.66
2:X:252:LEU:HD23	2:X:305:THR:HB	1.77	0.66
1:S:217:GLN:OE1	2:V:356:ARG:NH2	2.29	0.66
2:N:98:VAL:HB	2:N:232:VAL:HG13	1.76	0.66
1:J:265:HIS:ND1	1:J:322:SER:HB2	2.11	0.65
2:D:197:LEU:O	2:D:201:MET:HG2	1.95	0.65
1:A:265:HIS:ND1	1:A:322:SER:HB3	2.11	0.65
1:L:55:VAL:HG21	1:L:75:ILE:HD13	1.79	0.65
2:V:409:LYS:NZ	2:V:452:ILE:O	2.28	0.65
1:K:243:PRO:HG3	1:K:283:LEU:HD21	1.79	0.65
3:P:110:ILE:HG22	3:P:133:ILE:HD13	1.78	0.65
2:V:85:VAL:CG1	2:V:235:THR:HG23	2.17	0.65
3:Y:2:THR:HG22	3:Y:4:LYS:H	1.62	0.65
3:Y:14:LYS:HA	3:Y:248:ILE:HD11	1.79	0.64
2:M:89:ARG:NH1	2:M:247:GLU:OE2	2.30	0.64
1:B:285:LEU:HD22	2:E:275:ILE:HG22	1.80	0.64
1:T:28:ASN:HD22	1:T:48:ASN:CG	2.05	0.64
1:T:243:PRO:HG3	1:T:283:LEU:HD21	1.79	0.64
2:N:85:VAL:CG1	2:N:235:THR:HG23	2.17	0.64
1:C:174:GLN:HA	7:C:600:ANP:HNB1	1.62	0.64
2:M:160:GLY:N	7:M:600:ANP:HNB1	1.92	0.64
2:N:85:VAL:HG11	2:N:235:THR:CG2	2.17	0.64
1:B:99:VAL:HG11	1:B:251:THR:HB	1.80	0.64
3:P:45:ASP:O	3:P:49:GLN:HB2	1.97	0.64
2:D:409:LYS:NZ	2:D:452:ILE:O	2.31	0.63
1:U:55:VAL:HG21	1:U:75:ILE:HD13	1.78	0.63
1:J:425:ARG:HG3	1:J:425:ARG:HH11	1.63	0.63
1:S:455:LEU:HD21	1:S:466:PHE:CE2	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:390:GLY:O	1:K:391:SER:HB2	1.98	0.63
1:K:444:VAL:HG23	1:K:445:PRO:HD3	1.81	0.63
2:N:150:GLY:HA2	2:N:304:VAL:O	1.98	0.63
2:X:463:ILE:O	2:X:466:VAL:HB	1.99	0.63
2:W:50:VAL:HA	2:W:61:THR:HG22	1.81	0.62
2:X:52:GLN:HE21	2:X:60:ARG:HD2	1.63	0.62
1:K:186:LEU:HD13	1:K:225:HIS:HD2	1.63	0.62
2:E:85:VAL:CG1	2:E:235:THR:HG23	2.18	0.62
3:G:193:SER:HB3	3:G:196:LYS:HG3	1.81	0.62
2:W:388:ILE:HD12	2:W:393:MET:HG2	1.81	0.61
2:X:7:THR:HB	2:X:8:PRO:HD2	1.82	0.61
2:O:50:VAL:HA	2:O:61:THR:HG22	1.81	0.61
3:Y:77:ILE:N	3:Y:114:ILE:HG21	2.15	0.61
2:V:234:LEU:HD23	2:V:292:LEU:HD13	1.82	0.61
1:S:425:ARG:HG3	1:S:425:ARG:NH1	2.15	0.61
1:K:444:VAL:CG2	1:K:445:PRO:HD3	2.31	0.61
2:X:284:THR:O	2:X:285:LEU:C	2.44	0.61
1:S:364:ARG:HA	1:S:365:PRO:C	2.25	0.61
3:G:146:ILE:HG22	3:G:218:MET:HE1	1.81	0.60
1:U:80:SER:OG	1:U:82:ARG:HG3	2.01	0.60
3:G:205:VAL:HG22	4:H:51:GLN:HE22	1.66	0.60
1:B:67:ASN:HB2	2:F:17:ILE:CG1	2.30	0.60
3:Y:121:THR:O	3:Y:123:PRO:HD3	2.01	0.60
1:K:186:LEU:HD13	1:K:225:HIS:CD2	2.37	0.60
1:S:439:ALA:HB1	1:S:441:GLU:OE2	2.02	0.60
1:A:364:ARG:HA	1:A:365:PRO:C	2.27	0.60
1:B:55:VAL:HG21	1:B:75:ILE:HD13	1.84	0.60
1:B:140:PRO:HB3	1:B:318:GLU:HG3	1.83	0.60
2:N:388:ILE:HD12	2:N:393:MET:HG2	1.82	0.59
2:E:86:PRO:HD3	2:E:114:ARG:NH1	2.16	0.59
2:N:152:LYS:HE3	2:N:296:ILE:HB	1.84	0.59
3:P:205:VAL:N	3:P:206:PRO:CD	2.65	0.59
1:B:364:ARG:HA	1:B:365:PRO:C	2.27	0.59
1:L:80:SER:OG	1:L:82:ARG:HG3	2.02	0.59
1:L:170:ILE:HG23	1:L:353:PHE:CD1	2.37	0.59
1:A:164:GLY:HA2	1:A:323:LEU:O	2.03	0.59
2:F:252:LEU:HD23	2:F:305:THR:HB	1.84	0.59
1:C:364:ARG:HA	1:C:365:PRO:C	2.27	0.58
4:H:52:LEU:HD11	4:H:85:VAL:HG13	1.84	0.58
1:U:441:GLU:HG2	1:U:486:ARG:HB2	1.83	0.58
1:K:272:ASP:OD1	1:K:274:SER:HB2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:237:LEU:HD21	2:X:295:ARG:HB2	1.85	0.58
3:P:96:ARG:HA	3:P:122:HIS:HE1	1.68	0.58
2:W:86:PRO:HD3	2:W:114:ARG:NH1	2.17	0.58
1:U:397:ALA:HA	1:U:400:ARG:NH2	2.18	0.58
1:U:375:ARG:NH1	7:V:600:ANP:O3G	2.37	0.58
3:Y:133:ILE:HD12	3:Y:134:GLY:N	2.17	0.58
2:F:152:LYS:NZ	2:F:293:GLN:HG3	2.19	0.58
1:L:336:VAL:HG13	1:L:353:PHE:CZ	2.39	0.58
2:F:15:ALA:HB3	2:F:22:ASP:HB2	1.85	0.57
2:N:188:GLY:O	2:N:222:MET:HE3	2.03	0.57
1:S:170:ILE:HG23	1:S:353:PHE:CD1	2.38	0.57
2:N:50:VAL:HA	2:N:61:THR:HG22	1.85	0.57
3:P:167:ASN:HB2	3:P:228:ALA:CB	2.34	0.57
3:G:75:VAL:HB	3:G:164:ILE:HD13	1.86	0.57
2:W:220:GLY:CA	2:W:232:VAL:HG11	2.34	0.57
2:N:276:PRO:HD2	3:P:271:ILE:HD11	1.87	0.57
1:L:428:GLN:NE2	1:L:431:LYS:HD2	2.18	0.57
3:G:115:LYS:O	3:G:119:LEU:HB2	2.04	0.57
1:A:383:LYS:O	1:A:387:GLN:HG3	2.04	0.57
2:D:184:PHE:HB3	2:D:217:LEU:HD23	1.87	0.57
2:F:363:VAL:HB	2:F:367:HIS:ND1	2.19	0.57
2:F:388:ILE:HD11	2:F:396:LEU:HD21	1.87	0.57
1:K:364:ARG:HA	1:K:365:PRO:C	2.30	0.56
2:E:388:ILE:HD12	2:E:393:MET:HG2	1.87	0.56
1:L:336:VAL:CG1	1:L:353:PHE:CZ	2.88	0.56
1:L:336:VAL:CG1	1:L:353:PHE:CE1	2.88	0.56
1:J:192:ASN:HA	1:J:200:LYS:HG2	1.88	0.56
2:V:160:GLY:N	7:V:600:ANP:HNB1	1.91	0.56
1:L:219:VAL:HG13	1:L:228:MET:HE3	1.88	0.56
2:M:234:LEU:CD2	2:M:292:LEU:HD13	2.35	0.56
2:M:390:ILE:HG22	2:M:391:LEU:HG	1.87	0.55
2:D:204:THR:HB	2:D:206:VAL:HG23	1.88	0.55
2:E:86:PRO:HD3	2:E:114:ARG:HH12	1.72	0.55
1:J:265:HIS:ND1	1:J:322:SER:CB	2.70	0.55
1:K:192:ASN:HA	1:K:200:LYS:HG2	1.89	0.55
2:X:384:LEU:O	2:X:388:ILE:HG12	2.05	0.55
3:G:108:VAL:HG22	3:G:128:LEU:HB3	1.89	0.55
2:V:321:ALA:HB3	2:V:322:PRO:CD	2.37	0.55
1:T:55:VAL:HG21	1:T:75:ILE:HD13	1.88	0.55
1:J:364:ARG:HA	1:J:365:PRO:C	2.31	0.55
2:F:345:TYR:HA	2:F:346:PRO:C	2.31	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:197:LEU:O	2:V:201:MET:HG3	2.07	0.55
1:A:285:LEU:HD12	2:D:283:PRO:HB3	1.89	0.54
1:B:54:LEU:HD21	1:B:62:LYS:HD3	1.89	0.54
2:O:52:GLN:NE2	2:O:60:ARG:HD2	2.22	0.54
2:V:222:MET:HA	2:V:229:ARG:HD2	1.89	0.54
3:G:9:ARG:HG2	3:G:251:TYR:CE1	2.43	0.54
2:F:293:GLN:HG2	2:F:328:HIS:CG	2.43	0.54
2:V:346:PRO:O	2:V:347:ALA:CB	2.56	0.54
3:Y:79:SER:HB3	3:Y:88:HIS:HE1	1.73	0.54
2:E:152:LYS:HE3	2:E:296:ILE:HB	1.89	0.54
1:L:285:LEU:HD21	1:L:291:PRO:HB3	1.89	0.54
1:T:444:VAL:CG2	1:T:445:PRO:HD3	2.38	0.54
1:L:222:LEU:HB2	1:L:228:MET:HE2	1.89	0.54
1:T:67:ASN:HB2	2:X:17:ILE:HG12	1.90	0.54
1:T:364:ARG:HA	1:T:365:PRO:C	2.33	0.54
1:J:383:LYS:O	1:J:387:GLN:HG3	2.08	0.53
1:L:109:VAL:HB	1:L:118:ASP:HB3	1.90	0.53
2:O:252:LEU:HD23	2:O:305:THR:HB	1.89	0.53
1:U:294:GLU:N	3:Y:269:ASP:OD2	2.37	0.53
2:X:234:LEU:HD23	2:X:292:LEU:HD13	1.90	0.53
2:X:345:TYR:HA	2:X:346:PRO:C	2.33	0.53
2:F:97:ASN:HB2	2:F:101:GLU:H	1.73	0.53
1:K:29:GLU:HA	1:K:92:ARG:HD3	1.90	0.53
3:P:95:VAL:O	3:P:99:LEU:HB2	2.09	0.53
2:W:242:TYR:CZ	2:W:246:GLU:HG3	2.43	0.53
2:W:86:PRO:HD3	2:W:114:ARG:HH12	1.73	0.53
2:E:25:PHE:HB2	2:E:30:LEU:HD23	1.91	0.53
1:B:192:ASN:HA	1:B:200:LYS:HG2	1.91	0.52
2:E:98:VAL:HB	2:E:232:VAL:HG13	1.91	0.52
2:O:15:ALA:HB3	2:O:22:ASP:HB2	1.91	0.52
3:G:54:ASN:C	3:G:56:GLU:H	2.17	0.52
2:N:220:GLY:HA3	2:N:232:VAL:HG11	1.90	0.52
2:V:200:GLU:HA	2:V:200:GLU:OE1	2.09	0.52
1:A:54:LEU:HD11	1:A:78:PHE:HE2	1.73	0.52
1:T:288:ARG:HH12	2:W:275:ILE:HD11	1.74	0.52
2:V:204:THR:HB	2:V:206:VAL:HG23	1.92	0.52
2:E:50:VAL:HA	2:E:61:THR:HG22	1.92	0.52
2:F:152:LYS:HZ3	2:F:293:GLN:HG3	1.72	0.52
3:P:86:SER:O	3:P:87:ILE:C	2.51	0.52
1:A:402:VAL:O	1:A:402:VAL:HG12	2.09	0.52
2:V:25:PHE:HB2	2:V:30:LEU:HD23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:192:ASN:HA	1:T:200:LYS:HG2	1.91	0.52
1:B:111:ASP:OD2	1:B:115:ASN:HB2	2.09	0.52
3:P:106:ASP:HB3	3:P:127:LYS:HG3	1.91	0.52
1:U:441:GLU:CG	1:U:486:ARG:HB2	2.40	0.52
2:D:134:LEU:HD13	2:D:149:ARG:HH11	1.75	0.51
2:E:339:ILE:HG22	2:E:344:ILE:HB	1.92	0.51
1:J:272:ASP:OD1	1:J:274:SER:HB2	2.10	0.51
3:P:171:SER:HG	3:P:174:SER:N	2.08	0.51
2:E:300:LYS:HG3	9:E:814:HOH:O	2.10	0.51
2:O:279:VAL:HG12	2:O:279:VAL:O	2.10	0.51
2:X:7:THR:HB	2:X:8:PRO:CD	2.39	0.51
3:G:14:LYS:HA	3:G:248:ILE:HD11	1.92	0.51
2:M:391:LEU:HD22	3:P:83:LEU:HD13	1.92	0.51
2:O:242:TYR:CE1	2:O:246:GLU:HG3	2.45	0.51
2:X:460:VAL:HB	2:X:465:ASP:HB3	1.92	0.51
1:K:398:GLN:O	1:K:402:VAL:HG23	2.11	0.51
1:T:203:CYS:HB2	1:T:231:SER:HB3	1.92	0.51
1:C:68:LEU:O	2:D:15:ALA:HA	2.11	0.51
2:F:293:GLN:HG2	2:F:328:HIS:CB	2.41	0.51
1:K:144:VAL:HG12	1:K:163:ARG:O	2.11	0.51
2:M:86:PRO:HD3	2:M:114:ARG:NH1	2.26	0.51
1:S:399:TYR:CD1	1:S:423:GLY:HA3	2.45	0.51
2:V:266:SER:HB2	2:V:282:GLN:HE21	1.75	0.51
3:Y:226:TYR:O	3:Y:230:ILE:HG12	2.10	0.51
1:C:395:PHE:CZ	1:C:422:ARG:HB3	2.45	0.51
1:B:338:ALA:HB3	1:B:341:PRO:HG2	1.92	0.51
1:C:336:VAL:HG11	1:C:353:PHE:HE1	1.72	0.51
3:G:141:GLN:HG3	5:I:15:ASN:HD21	1.75	0.51
3:P:212:TYR:O	3:P:216:ASN:HB2	2.11	0.51
1:T:444:VAL:HG23	1:T:445:PRO:HD3	1.93	0.51
1:A:217:GLN:OE1	2:D:356:ARG:NH2	2.44	0.51
2:D:64:MET:HE1	2:D:231:ARG:HB2	1.92	0.51
4:H:75:ALA:HA	4:H:84:CYS:O	2.09	0.51
2:M:391:LEU:CD2	3:P:83:LEU:CD1	2.90	0.51
2:V:184:PHE:HB3	2:V:217:LEU:HD23	1.92	0.51
2:W:15:ALA:HB3	2:W:22:ASP:HB2	1.92	0.51
1:K:55:VAL:HG21	1:K:75:ILE:HD13	1.93	0.50
2:N:345:TYR:HA	2:N:346:PRO:C	2.36	0.50
1:T:389:ALA:HB2	1:T:447:ILE:HG21	1.92	0.50
1:B:187:ASN:OD1	1:B:190:ARG:NH1	2.43	0.50
1:B:272:ASP:OD1	1:B:274:SER:HB2	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:118:LEU:HB3	3:G:126:ILE:HD11	1.94	0.50
3:P:77:ILE:HG23	3:P:110:ILE:HB	1.93	0.50
1:A:444:VAL:HG22	1:A:445:PRO:HD3	1.92	0.50
3:G:15:ASN:O	3:G:19:ILE:HG12	2.10	0.50
3:P:81:LYS:HB3	3:P:233:ARG:NH2	2.26	0.50
1:S:92:ARG:HH21	1:S:94:GLY:HA2	1.76	0.50
2:X:284:THR:O	2:X:286:ALA:N	2.44	0.50
1:C:55:VAL:HG21	1:C:75:ILE:HD13	1.93	0.50
1:C:168:LEU:HB2	1:C:348:THR:HG21	1.93	0.50
2:X:390:ILE:HD11	3:Y:247:MET:SD	2.51	0.50
3:Y:79:SER:OG	3:Y:80:ASP:N	2.37	0.50
1:K:285:LEU:HD22	2:N:275:ILE:HG22	1.93	0.50
1:L:187:ASN:O	1:L:190:ARG:HG3	2.11	0.50
1:C:395:PHE:HZ	1:C:422:ARG:HB3	1.76	0.50
2:M:391:LEU:HD22	3:P:83:LEU:CD1	2.41	0.50
3:P:164:ILE:HD11	3:P:182:ILE:HG12	1.93	0.50
2:W:150:GLY:HA2	2:W:304:VAL:O	2.12	0.50
1:C:336:VAL:CG1	1:C:353:PHE:CZ	2.86	0.50
3:G:23:MET:HG3	3:G:237:MET:HG2	1.93	0.50
4:H:79:PRO:C	4:H:81:SER:H	2.20	0.50
2:M:314:ALA:O	2:M:315:ASP:HB2	2.12	0.50
2:X:15:ALA:HB3	2:X:22:ASP:HB2	1.94	0.50
3:Y:23:MET:HB3	3:Y:237:MET:HG3	1.93	0.50
1:B:30:THR:CG2	1:B:31:GLY:N	2.75	0.49
2:M:222:MET:HA	2:M:229:ARG:HD2	1.93	0.49
7:M:600:ANP:O5'	7:M:600:ANP:H8	2.11	0.49
2:D:64:MET:HE3	2:D:228:ALA:HA	1.94	0.49
2:D:345:TYR:HA	2:D:346:PRO:C	2.36	0.49
2:F:140:VAL:HG12	2:F:414:LEU:HB3	1.95	0.49
1:J:70:PRO:HD3	2:N:15:ALA:HB2	1.93	0.49
2:W:152:LYS:HE3	2:W:296:ILE:HB	1.93	0.49
2:X:63:ALA:O	2:X:227:GLY:HA3	2.12	0.49
3:G:182:ILE:HG21	3:G:214:LEU:HD13	1.93	0.49
2:W:255:ILE:HB	2:W:308:GLN:HG2	1.94	0.49
3:Y:115:LYS:O	3:Y:119:LEU:HB2	2.11	0.49
1:B:444:VAL:HG23	1:B:445:PRO:HD3	1.95	0.49
1:B:444:VAL:CG2	1:B:445:PRO:HD3	2.42	0.49
2:D:136:THR:HA	2:D:174:ILE:HD11	1.94	0.49
1:J:336:VAL:CG1	1:J:353:PHE:CZ	2.87	0.49
1:L:349:ASP:HA	1:L:375:ARG:HD2	1.94	0.49
2:O:140:VAL:HG12	2:O:414:LEU:HD22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:163:LYS:HG3	7:X:600:ANP:O1B	2.12	0.49
1:C:80:SER:OG	1:C:82:ARG:HG2	2.11	0.49
1:C:349:ASP:O	1:C:375:ARG:HB2	2.11	0.49
2:O:247:GLU:O	2:O:249:GLN:HG2	2.12	0.49
2:O:345:TYR:HA	2:O:346:PRO:C	2.38	0.49
3:Y:78:THR:HG23	3:Y:91:LEU:HD22	1.94	0.49
1:B:390:GLY:O	1:B:391:SER:HB2	2.11	0.49
3:G:78:THR:OG1	3:G:114:ILE:HB	2.12	0.49
2:M:336:SER:HB3	2:M:339:ILE:HG12	1.94	0.49
7:M:600:ANP:O2G	7:M:600:ANP:O2B	2.31	0.49
2:O:460:VAL:HB	2:O:465:ASP:HB3	1.93	0.49
2:W:98:VAL:HB	2:W:232:VAL:HG13	1.94	0.49
2:D:149:ARG:HH11	2:D:149:ARG:HG3	1.78	0.49
4:Q:16:LEU:CB	4:Q:17:PRO:HD2	2.43	0.49
2:D:197:LEU:HG	2:D:201:MET:HE2	1.94	0.49
2:D:319:ASP:O	2:D:322:PRO:HD2	2.13	0.49
1:J:164:GLY:HA2	1:J:323:LEU:O	2.13	0.49
1:J:425:ARG:HG3	1:J:425:ARG:NH1	2.28	0.49
3:P:150:LEU:O	3:P:154:MET:HB2	2.13	0.49
3:P:162:ILE:HB	3:P:182:ILE:O	2.12	0.49
2:F:33:ILE:O	2:F:34:LEU:HB2	2.12	0.49
3:P:109:THR:O	3:P:129:SER:HA	2.12	0.49
1:T:211:LYS:HD2	2:W:328:HIS:HA	1.95	0.49
2:V:15:ALA:HB3	2:V:22:ASP:HB2	1.94	0.49
1:B:387:GLN:OE1	1:B:491:LEU:HB2	2.12	0.49
1:C:203:CYS:O	1:C:231:SER:HA	2.13	0.49
2:F:137:GLY:HA2	2:F:432:VAL:O	2.13	0.49
2:M:345:TYR:HA	2:M:346:PRO:C	2.38	0.49
1:C:336:VAL:CG1	1:C:353:PHE:HZ	2.24	0.48
1:J:174:GLN:OE1	2:M:354:LYS:HD2	2.13	0.48
2:V:9:ILE:HB	2:V:78:ASP:HB3	1.95	0.48
1:L:375:ARG:NH1	7:M:600:ANP:O2A	2.46	0.48
2:M:149:ARG:HG2	2:M:149:ARG:NH1	2.10	0.48
2:O:9:ILE:H	2:O:9:ILE:HD12	1.78	0.48
3:P:94:ALA:C	3:P:96:ARG:N	2.71	0.48
2:W:204:THR:OG1	2:W:420:VAL:HB	2.14	0.48
2:X:298:THR:HG23	2:X:303:SER:HA	1.94	0.48
2:F:279:VAL:HG12	2:F:279:VAL:O	2.13	0.48
1:J:182:LEU:HD13	1:J:218:LEU:HD11	1.94	0.48
2:V:242:TYR:CE1	2:V:246:GLU:HG3	2.47	0.48
3:Y:121:THR:C	3:Y:123:PRO:HD3	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:383:LYS:O	1:K:387:GLN:HG3	2.13	0.48
3:P:115:LYS:HB2	3:P:129:SER:OG	2.14	0.48
1:A:484:GLU:HG2	1:A:495:LEU:HD11	1.94	0.48
1:B:119:GLY:O	2:N:89:ARG:NH2	2.47	0.48
2:E:133:ILE:HD12	2:E:146:PRO:HB2	1.96	0.48
2:F:377:THR:HG22	2:F:407:ALA:HB2	1.96	0.48
1:J:444:VAL:CG2	1:J:445:PRO:HD3	2.43	0.48
1:A:418:GLN:HG3	9:A:814:HOH:O	2.12	0.48
1:J:26:ASN:O	1:J:27:LEU:HB2	2.13	0.48
2:W:321:ALA:HB3	2:W:322:PRO:CD	2.44	0.48
2:D:242:TYR:CE1	2:D:246:GLU:HG3	2.48	0.48
1:J:217:GLN:OE1	2:M:356:ARG:NH2	2.47	0.48
2:V:89:ARG:NH1	2:V:247:GLU:OE2	2.46	0.48
1:J:359:PHE:CE1	1:J:364:ARG:NH2	2.82	0.48
2:O:150:GLY:HA2	2:O:304:VAL:O	2.14	0.48
1:T:54:LEU:HD21	1:T:62:LYS:HD3	1.96	0.48
1:T:219:VAL:HG22	1:T:233:ILE:HG13	1.95	0.48
2:W:345:TYR:HB2	2:W:459:MET:HE1	1.95	0.48
1:J:54:LEU:HD13	1:J:97:VAL:HG22	1.94	0.48
1:K:28:ASN:HB3	1:K:48:ASN:ND2	2.29	0.48
2:X:363:VAL:HB	2:X:367:HIS:ND1	2.28	0.48
1:S:138:ILE:HD13	2:W:191:THR:HG23	1.95	0.47
2:X:319:ASP:OD1	2:X:320:PRO:HD2	2.14	0.47
3:Y:130:ILE:HD13	3:Y:146:ILE:HG12	1.96	0.47
3:Y:220:THR:O	3:Y:224:GLN:HG3	2.13	0.47
1:C:103:PRO:HD3	1:C:258:TRP:CH2	2.49	0.47
1:L:413:ASP:O	1:L:416:THR:HG22	2.14	0.47
2:M:409:LYS:NZ	2:M:452:ILE:O	2.46	0.47
1:T:344:VAL:HA	1:T:347:ILE:HD12	1.95	0.47
3:G:93:LYS:HE2	3:G:97:ARG:HH22	1.79	0.47
1:U:395:PHE:CE2	1:U:422:ARG:HD2	2.50	0.47
1:L:39:GLY:HA2	1:L:77:LEU:HD12	1.96	0.47
1:L:345:ILE:HG12	1:L:351:GLN:HG2	1.97	0.47
1:L:378:SER:C	1:L:380:ALA:H	2.23	0.47
2:N:321:ALA:HB3	2:N:322:PRO:CD	2.45	0.47
2:X:97:ASN:HD22	2:X:101:GLU:HB2	1.79	0.47
1:C:64:MET:HG3	1:C:97:VAL:HG21	1.95	0.47
3:G:75:VAL:HB	3:G:164:ILE:CD1	2.44	0.47
1:B:398:GLN:O	1:B:402:VAL:HG23	2.15	0.47
1:A:354:LEU:HA	1:A:366:ALA:O	2.15	0.47
1:B:142:ARG:HG2	1:B:143:SER:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:314:ALA:O	2:D:315:ASP:HB2	2.15	0.47
2:F:293:GLN:HG2	2:F:328:HIS:HB3	1.96	0.47
3:G:169:PRO:HD3	3:G:224:GLN:O	2.14	0.47
1:K:92:ARG:HH21	1:K:94:GLY:HA2	1.78	0.47
1:L:290:PRO:HB2	2:M:270:ALA:HB1	1.97	0.47
2:N:255:ILE:HB	2:N:308:GLN:HG2	1.97	0.47
2:O:197:LEU:O	2:O:201:MET:HG2	2.15	0.47
2:W:345:TYR:HA	2:W:346:PRO:C	2.39	0.47
2:D:222:MET:HA	2:D:229:ARG:HD2	1.96	0.47
1:K:140:PRO:HB3	1:K:318:GLU:HG3	1.97	0.47
2:V:136:THR:HA	2:V:174:ILE:HD11	1.97	0.47
1:B:36:VAL:CG1	2:E:53:HIS:HB2	2.45	0.47
3:G:3:LEU:C	3:G:3:LEU:HD23	2.40	0.47
1:K:260:ARG:O	1:K:321:GLY:HA3	2.14	0.47
1:S:270:TYR:O	1:S:272:ASP:HA	2.14	0.47
5:1:18:ALA:C	5:1:20:ALA:H	2.23	0.47
2:D:189:GLU:O	2:D:221:GLN:HB3	2.15	0.47
2:M:136:THR:HA	2:M:174:ILE:HD11	1.97	0.47
2:M:391:LEU:CD2	3:P:83:LEU:HD13	2.45	0.47
2:N:15:ALA:HB3	2:N:22:ASP:HB2	1.97	0.47
2:N:220:GLY:CA	2:N:232:VAL:HG11	2.45	0.47
1:S:50:GLN:HG2	2:W:71:VAL:HG22	1.96	0.47
1:T:398:GLN:O	1:T:402:VAL:HG23	2.15	0.47
2:W:85:VAL:CG1	2:W:235:THR:HG23	2.28	0.47
1:C:222:LEU:HB2	1:C:228:MET:HE2	1.97	0.46
1:K:99:VAL:CG1	1:K:251:THR:HB	2.34	0.46
1:S:192:ASN:HA	1:S:200:LYS:HG2	1.97	0.46
2:E:201:MET:SD	2:E:217:LEU:HD21	2.55	0.46
1:K:384:ALA:O	1:K:388:VAL:HG13	2.15	0.46
3:P:180:LYS:NZ	3:P:220:THR:HB	2.29	0.46
1:S:353:PHE:HD2	1:S:371:LEU:HB3	1.80	0.46
1:J:64:MET:HE2	1:J:66:LEU:HD21	1.98	0.46
1:L:360:TYR:OH	2:O:354:LYS:NZ	2.23	0.46
1:U:364:ARG:HA	1:U:365:PRO:C	2.40	0.46
2:E:321:ALA:HB3	2:E:322:PRO:CD	2.46	0.46
2:E:374:VAL:HG23	2:E:445:LEU:HD11	1.97	0.46
2:F:460:VAL:HB	2:F:465:ASP:HB3	1.97	0.46
1:L:272:ASP:OD1	1:L:274:SER:HB2	2.16	0.46
1:L:481:LEU:HD21	1:L:498:SER:HB3	1.96	0.46
2:N:345:TYR:HB2	2:N:459:MET:HE1	1.97	0.46
2:E:112:LYS:HD2	1:K:120:LYS:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:211:LYS:NZ	2:M:330:ASP:OD1	2.44	0.46
2:M:197:LEU:O	2:M:201:MET:HG2	2.16	0.46
1:S:50:GLN:HB2	1:S:53:GLU:HB2	1.97	0.46
1:U:392:LEU:HD13	1:U:451:VAL:HG22	1.97	0.46
3:Y:9:ARG:HG2	3:Y:251:TYR:CE1	2.50	0.46
1:A:99:VAL:HG21	1:A:251:THR:HG23	1.98	0.46
1:C:209:GLY:HA3	1:C:275:LYS:HD3	1.97	0.46
2:E:410:ILE:HG23	2:E:441:PHE:HE2	1.81	0.46
1:K:106:LEU:HD23	1:K:229:LYS:O	2.15	0.46
3:P:14:LYS:HA	3:P:248:ILE:HD11	1.97	0.46
2:D:224:GLU:O	2:D:229:ARG:HD3	2.14	0.46
2:O:285:LEU:HD23	2:O:285:LEU:C	2.40	0.46
2:V:190:ARG:HD2	2:V:193:GLU:OE2	2.16	0.46
1:L:364:ARG:HA	1:L:365:PRO:C	2.40	0.46
1:A:270:TYR:O	1:A:272:ASP:HA	2.16	0.46
2:O:33:ILE:O	2:O:34:LEU:HB2	2.16	0.46
2:V:50:VAL:HA	2:V:61:THR:HG22	1.98	0.46
2:W:384:LEU:O	2:W:388:ILE:HG12	2.16	0.46
7:F:600:ANP:O5'	7:F:600:ANP:H8	2.15	0.46
1:J:360:TYR:HE1	2:M:354:LYS:HZ1	1.64	0.46
1:J:444:VAL:HG22	1:J:445:PRO:HD3	1.98	0.46
3:P:227:ALA:HA	3:P:230:ILE:HG22	1.98	0.46
1:T:421:VAL:O	1:T:425:ARG:HG2	2.16	0.46
2:V:339:ILE:HG22	2:V:344:ILE:HB	1.97	0.46
1:C:202:TYR:O	1:C:266:ALA:HA	2.16	0.45
2:D:200:GLU:OE1	2:D:200:GLU:HA	2.16	0.45
2:F:197:LEU:O	2:F:201:MET:HG2	2.16	0.45
2:F:242:TYR:CE1	2:F:246:GLU:HG3	2.51	0.45
2:O:377:THR:HG22	2:O:407:ALA:HB2	1.99	0.45
1:A:407:GLN:O	1:A:410:SER:N	2.49	0.45
1:C:417:LYS:O	1:C:421:VAL:HG23	2.15	0.45
2:F:155:LEU:HD12	2:F:167:ILE:HG13	1.99	0.45
2:O:363:VAL:HB	2:O:367:HIS:HD1	1.81	0.45
1:T:140:PRO:HB3	1:T:318:GLU:HG3	1.98	0.45
1:L:280:TYR:CD2	1:L:297:PRO:HG2	2.51	0.45
2:N:242:TYR:CZ	2:N:246:GLU:HG3	2.50	0.45
1:B:203:CYS:HB2	1:B:231:SER:HB3	1.98	0.45
2:E:220:GLY:HA3	2:E:232:VAL:HG11	1.98	0.45
1:J:402:VAL:HG12	1:J:402:VAL:O	2.14	0.45
1:T:54:LEU:HD12	1:T:97:VAL:HG22	1.98	0.45
1:B:36:VAL:HG13	2:E:53:HIS:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:LEU:HB3	2:F:72:ARG:HD3	1.98	0.45
2:D:89:ARG:NH1	2:D:247:GLU:OE2	2.49	0.45
2:E:259:PHE:CE1	2:E:313:PRO:HG3	2.51	0.45
5:I:31:THR:OG1	5:I:32:ALA:N	2.50	0.45
1:L:64:MET:HE3	1:L:97:VAL:CG2	2.47	0.45
1:T:92:ARG:HH21	1:T:94:GLY:HA2	1.81	0.45
3:G:77:ILE:HD13	3:G:110:ILE:HD12	1.99	0.45
1:T:77:LEU:O	1:T:243:PRO:HG2	2.16	0.45
1:T:338:ALA:HB3	1:T:341:PRO:HG2	1.99	0.45
3:Y:28:SER:OG	3:Y:234:ARG:HD2	2.17	0.45
1:A:391:SER:OG	1:A:451:VAL:HG11	2.17	0.45
1:K:444:VAL:HG21	1:K:485:ILE:HG21	1.97	0.45
2:M:339:ILE:HG22	2:M:344:ILE:HB	1.99	0.45
1:T:384:ALA:O	1:T:388:VAL:HG22	2.16	0.45
1:A:148:VAL:HG21	1:A:324:THR:HG21	1.98	0.45
1:K:203:CYS:HB2	1:K:231:SER:HB3	1.99	0.45
2:M:24:HIS:CE1	2:M:25:PHE:O	2.70	0.45
2:D:134:LEU:HD13	2:D:149:ARG:NH1	2.32	0.45
1:S:174:GLN:HA	7:S:600:ANP:HNB1	1.80	0.45
1:S:332:GLN:HB3	2:V:318:THR:HB	1.98	0.45
1:S:402:VAL:HG12	1:S:402:VAL:O	2.16	0.45
2:X:313:PRO:HG2	2:X:319:ASP:OD2	2.16	0.45
3:Y:237:MET:HA	3:Y:237:MET:HE2	1.98	0.45
1:K:250:PHE:CE1	1:K:307:LEU:HB2	2.52	0.45
4:Q:52:LEU:CB	9:Q:802:HOH:O	2.64	0.45
1:S:99:VAL:CG2	1:S:100:PRO:HD2	2.47	0.45
2:X:95:ILE:HD12	2:X:104:ASP:HB3	1.98	0.45
3:Y:253:ILE:CG2	3:Y:257:ARG:HH22	2.30	0.45
1:L:436:SER:N	1:L:437:PRO:HD3	2.31	0.44
2:N:321:ALA:N	2:N:322:PRO:HD2	2.32	0.44
3:P:88:HIS:CD2	3:P:113:LYS:CB	2.89	0.44
3:P:205:VAL:H	3:P:206:PRO:HD3	1.83	0.44
1:T:43:VAL:HG21	1:T:75:ILE:HD12	1.99	0.44
3:Y:23:MET:HA	3:Y:23:MET:CE	2.36	0.44
2:M:64:MET:HE3	2:M:228:ALA:HA	1.98	0.44
2:M:149:ARG:CG	2:M:149:ARG:NH1	2.65	0.44
2:M:395:GLU:OE1	2:M:395:GLU:HA	2.17	0.44
1:S:309:GLU:HG3	2:W:223:ASN:HB3	1.99	0.44
2:X:189:GLU:O	2:X:221:GLN:HB3	2.17	0.44
2:F:189:GLU:O	2:F:221:GLN:HB3	2.16	0.44
1:L:395:PHE:CD1	1:L:395:PHE:C	2.94	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:219:VAL:HG22	1:S:233:ILE:HG13	1.99	0.44
1:T:85:LYS:HE2	2:W:32:ALA:HB2	1.99	0.44
1:A:69:GLU:HB3	1:A:70:PRO:HD2	1.99	0.44
1:B:30:THR:HG21	1:B:89:LEU:HD11	2.00	0.44
1:C:103:PRO:HD3	1:C:258:TRP:CZ2	2.53	0.44
2:M:231:ARG:HA	2:M:231:ARG:HD3	1.81	0.44
2:N:25:PHE:HB2	2:N:30:LEU:HD23	1.99	0.44
2:W:167:ILE:HG23	2:W:254:PHE:CE2	2.53	0.44
2:W:244:ARG:HD3	2:W:304:VAL:HG23	2.00	0.44
1:B:103:PRO:HD3	1:B:258:TRP:CZ2	2.53	0.44
1:C:455:LEU:HD21	1:C:466:PHE:CE1	2.53	0.44
2:F:52:GLN:HG3	2:F:60:ARG:HB3	1.99	0.44
3:G:90:GLN:HA	3:G:93:LYS:HB2	1.99	0.44
1:L:455:LEU:HD21	1:L:466:PHE:CE1	2.53	0.44
3:P:143:SER:HA	3:P:222:MET:HE1	2.00	0.44
1:U:382:VAL:HG12	1:U:384:ALA:H	1.82	0.44
1:C:93:THR:HG22	1:C:95:ASN:OD1	2.17	0.44
1:J:40:ILE:CD1	1:J:76:VAL:HG12	2.46	0.44
1:L:222:LEU:HD12	1:L:228:MET:HE1	1.99	0.44
2:V:189:GLU:O	2:V:221:GLN:HB3	2.18	0.44
2:V:262:THR:O	2:V:282:GLN:NE2	2.50	0.44
2:V:396:LEU:HD12	2:V:400:ASP:HB3	2.00	0.44
1:B:444:VAL:N	1:B:445:PRO:CD	2.81	0.44
2:F:33:ILE:HG22	2:F:34:LEU:HG	1.99	0.44
2:F:160:GLY:HA2	7:F:600:ANP:HNB1	1.82	0.44
1:L:378:SER:HB2	1:L:386:LYS:HG3	2.00	0.44
2:V:29:GLU:HG3	2:V:29:GLU:O	2.18	0.44
2:W:409:LYS:NZ	2:W:450:ASP:O	2.50	0.44
2:X:160:GLY:N	7:X:600:ANP:HNB1	2.07	0.44
1:B:383:LYS:O	1:B:387:GLN:HG3	2.18	0.44
2:O:158:GLY:O	2:O:161:VAL:HG22	2.17	0.44
1:C:285:LEU:HD21	1:C:291:PRO:HB3	2.00	0.43
3:G:54:ASN:C	3:G:56:GLU:N	2.76	0.43
4:H:72:GLY:O	4:H:87:ALA:HA	2.17	0.43
1:K:251:THR:O	1:K:255:ILE:HG13	2.16	0.43
7:K:600:ANP:H5'1	7:K:600:ANP:H8	2.00	0.43
1:L:239:SER:HB3	2:O:294:GLU:HG3	1.99	0.43
1:L:416:THR:O	1:L:419:THR:HG22	2.17	0.43
2:M:184:PHE:HB3	2:M:217:LEU:HD23	1.99	0.43
2:O:90:GLU:HG3	2:O:111:SER:HA	2.00	0.43
1:S:509:THR:HG22	1:S:509:THR:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:448:LYS:O	2:W:449:TYR:HB2	2.18	0.43
1:B:27:LEU:O	1:B:47:ASN:ND2	2.51	0.43
2:E:174:ILE:HD12	2:E:178:HIS:HD2	1.82	0.43
2:N:384:LEU:O	2:N:388:ILE:HG12	2.17	0.43
1:U:416:THR:O	1:U:420:LEU:HB2	2.16	0.43
2:X:90:GLU:HG3	2:X:111:SER:HA	2.00	0.43
1:T:288:ARG:NH1	2:W:275:ILE:HD11	2.33	0.43
1:U:428:GLN:NE2	1:U:431:LYS:HD2	2.34	0.43
2:N:321:ALA:HB3	2:N:322:PRO:HD3	1.99	0.43
2:O:52:GLN:HE21	2:O:60:ARG:HD2	1.83	0.43
1:S:295:ALA:HB2	3:Y:270:ILE:HD13	2.01	0.43
1:B:421:VAL:O	1:B:425:ARG:HG2	2.19	0.43
1:C:354:LEU:HA	1:C:366:ALA:O	2.18	0.43
3:G:77:ILE:CD1	3:G:110:ILE:HD12	2.49	0.43
1:L:177:LYS:HB2	1:L:177:LYS:HE2	1.84	0.43
1:U:174:GLN:HB3	2:X:354:LYS:HD3	1.99	0.43
1:U:187:ASN:OD1	1:U:190:ARG:NH1	2.51	0.43
2:V:321:ALA:HB3	2:V:322:PRO:HD3	2.00	0.43
1:B:505:SER:O	1:B:509:THR:HG22	2.19	0.43
2:D:425:THR:HB	2:D:427:ILE:HD12	2.01	0.43
2:F:293:GLN:HA	2:F:293:GLN:OE1	2.19	0.43
1:K:478:HIS:HB3	1:K:481:LEU:HG	1.99	0.43
2:X:33:ILE:O	2:X:34:LEU:HB2	2.18	0.43
1:A:309:GLU:HG3	2:E:223:ASN:HB3	2.00	0.43
1:C:242:ALA:N	1:C:243:PRO:CD	2.81	0.43
1:K:270:TYR:O	1:K:272:ASP:HA	2.18	0.43
3:P:94:ALA:C	3:P:96:ARG:H	2.26	0.43
1:U:189:LYS:HE3	1:U:226:ASP:HB3	2.00	0.43
1:B:146:GLU:HA	1:B:147:PRO:HD3	1.88	0.43
3:G:118:LEU:HA	3:G:121:THR:HG22	2.00	0.43
1:L:211:LYS:HE3	1:L:213:SER:OG	2.18	0.43
2:N:256:ASP:HA	2:N:257:ASN:HA	1.77	0.43
2:O:363:VAL:HB	2:O:367:HIS:ND1	2.33	0.43
3:Y:133:ILE:O	3:Y:135:LYS:N	2.48	0.43
2:D:143:LEU:O	2:D:367:HIS:HE1	2.02	0.43
1:K:85:LYS:HE2	2:N:32:ALA:HB2	2.01	0.43
1:L:168:LEU:HB2	1:L:348:THR:HG21	2.01	0.43
1:T:383:LYS:O	1:T:387:GLN:HG3	2.18	0.43
1:U:353:PHE:CE2	1:U:371:LEU:O	2.72	0.43
1:U:478:HIS:O	1:U:481:LEU:HB2	2.19	0.43
2:V:33:ILE:O	2:V:34:LEU:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:202:LYS:HE3	2:X:209:LEU:HD11	2.01	0.43
2:X:440:SER:O	2:X:444:VAL:HG23	2.19	0.43
2:F:256:ASP:HA	2:F:257:ASN:HA	1.88	0.43
1:J:466:PHE:CD1	1:J:466:PHE:C	2.97	0.43
2:N:204:THR:OG1	2:N:420:VAL:HB	2.19	0.43
1:B:285:LEU:HD22	2:E:275:ILE:CG2	2.47	0.42
1:C:492:SER:H	1:C:495:LEU:HD12	1.83	0.42
2:M:204:THR:HB	2:M:206:VAL:HG23	2.01	0.42
1:S:168:LEU:HD11	1:S:329:ILE:HB	2.01	0.42
1:U:243:PRO:HA	1:U:283:LEU:HD11	2.01	0.42
2:X:50:VAL:HA	2:X:61:THR:HG22	2.00	0.42
2:X:345:TYR:HB3	7:X:600:ANP:C6	2.49	0.42
1:B:69:GLU:HB3	1:B:70:PRO:HD2	2.01	0.42
2:E:190:ARG:HG3	2:E:190:ARG:HH11	1.84	0.42
2:F:237:LEU:HD21	2:F:295:ARG:HB2	2.01	0.42
1:J:483:THR:HG23	1:J:486:ARG:NH2	2.34	0.42
2:V:314:ALA:O	2:V:315:ASP:HB2	2.19	0.42
3:Y:78:THR:HG23	3:Y:91:LEU:CD2	2.49	0.42
2:F:452:ILE:HA	2:F:453:PRO:HD3	1.90	0.42
2:O:155:LEU:HD12	2:O:167:ILE:HG13	2.00	0.42
2:O:237:LEU:HD13	2:O:296:ILE:HG12	2.01	0.42
2:V:201:MET:SD	2:V:215:VAL:HG11	2.59	0.42
2:W:9:ILE:HG23	2:W:29:GLU:HG2	2.01	0.42
1:A:26:ASN:HB3	1:A:30:THR:OG1	2.19	0.42
1:K:129:SER:HB2	1:K:254:SER:HB3	2.01	0.42
1:L:272:ASP:OD1	1:L:272:ASP:C	2.62	0.42
2:M:373:LYS:HB3	2:M:445:LEU:HD13	2.02	0.42
2:N:275:ILE:HA	2:N:276:PRO:HD3	1.81	0.42
1:S:185:ILE:HG23	1:S:203:CYS:SG	2.60	0.42
3:Y:80:ASP:OD2	3:Y:111:GLY:HA2	2.19	0.42
1:A:225:HIS:O	1:A:226:ASP:C	2.61	0.42
1:B:296:TYR:HB3	1:B:297:PRO:HD2	2.01	0.42
2:D:256:ASP:HA	2:D:257:ASN:HA	1.88	0.42
2:F:234:LEU:HD23	2:F:292:LEU:HD13	2.02	0.42
1:U:354:LEU:HA	1:U:366:ALA:O	2.19	0.42
1:J:38:ASP:OD1	2:M:274:ARG:NH2	2.47	0.42
1:L:34:LEU:O	2:O:55:GLY:HA2	2.20	0.42
2:E:150:GLY:HA2	2:E:304:VAL:O	2.20	0.42
1:K:96:ILE:O	1:K:97:VAL:C	2.62	0.42
1:L:378:SER:C	1:L:380:ALA:N	2.73	0.42
2:N:258:ILE:HG22	2:N:309:ALA:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:127:VAL:C	4:Q:129:VAL:H	2.26	0.42
1:T:340:ILE:HB	1:T:341:PRO:HD3	2.02	0.42
1:T:444:VAL:HG21	1:T:485:ILE:HG21	2.01	0.42
2:X:140:VAL:HG21	2:X:348:VAL:HB	2.01	0.42
2:X:464:GLU:O	2:X:464:GLU:HG3	2.20	0.42
1:C:242:ALA:HB3	1:C:243:PRO:CD	2.41	0.42
2:E:220:GLY:CA	2:E:232:VAL:HG11	2.49	0.42
1:L:93:THR:HG22	1:L:95:ASN:OD1	2.19	0.42
2:M:391:LEU:CD2	3:P:83:LEU:HD11	2.49	0.42
2:N:356:ARG:HB3	2:N:356:ARG:NH1	2.35	0.42
2:O:140:VAL:HG23	2:O:141:VAL:N	2.35	0.42
3:Y:39:ILE:C	3:Y:41:ALA:H	2.26	0.42
1:L:375:ARG:HA	7:M:600:ANP:O3'	2.20	0.42
1:U:271:ASP:HA	1:U:272:ASP:HA	1.80	0.42
2:X:282:GLN:HA	2:X:283:PRO:HD3	1.94	0.42
2:F:321:ALA:HB3	2:F:322:PRO:CD	2.49	0.42
3:G:140:PHE:HA	3:G:219:LEU:HD12	2.01	0.42
1:J:42:ARG:HE	1:J:72:GLN:HE22	1.66	0.42
1:T:228:MET:HE1	1:T:233:ILE:HG12	2.02	0.42
2:W:275:ILE:HA	2:W:276:PRO:HD3	1.88	0.42
1:B:219:VAL:HG22	1:B:233:ILE:HG13	2.02	0.41
2:E:452:ILE:HA	2:E:453:PRO:HD2	1.93	0.41
2:F:67:THR:O	2:F:68:GLU:C	2.64	0.41
2:F:71:VAL:HG12	2:F:72:ARG:O	2.20	0.41
3:G:146:ILE:CG2	3:G:218:MET:HE1	2.48	0.41
1:S:99:VAL:HG21	1:S:251:THR:CG2	2.49	0.41
2:V:282:GLN:H	2:V:282:GLN:HG3	1.50	0.41
2:N:140:VAL:HG13	2:N:414:LEU:HD22	2.02	0.41
1:U:357:GLU:HG3	2:X:379:GLN:NE2	2.35	0.41
1:B:111:ASP:OD1	1:B:111:ASP:C	2.62	0.41
1:C:139:LEU:N	1:C:140:PRO:HD2	2.35	0.41
2:E:95:ILE:HG12	2:E:217:LEU:HD12	2.02	0.41
1:L:211:LYS:HB2	2:O:294:GLU:OE2	2.20	0.41
2:M:64:MET:CE	2:M:228:ALA:HA	2.51	0.41
2:E:27:GLN:H	2:E:27:GLN:HG3	1.64	0.41
2:E:120:ASP:HA	2:E:121:PRO:HD3	1.90	0.41
2:E:345:TYR:HA	2:E:346:PRO:C	2.45	0.41
1:S:236:ALA:HA	1:S:240:GLU:OE1	2.19	0.41
1:S:425:ARG:HD3	1:S:455:LEU:O	2.20	0.41
1:T:335:ASP:OD1	1:T:337:SER:HB2	2.19	0.41
1:A:267:LEU:HD11	1:A:326:LEU:HG	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:PRO:O	1:C:374:SER:OG	2.26	0.41
2:D:98:VAL:HG13	2:D:99:ILE:HG23	2.03	0.41
3:P:106:ASP:OD2	3:P:159:TYR:OH	2.38	0.41
1:U:340:ILE:N	1:U:341:PRO:CD	2.83	0.41
1:C:83:LEU:HD23	1:C:83:LEU:HA	1.91	0.41
2:E:218:VAL:HG21	2:E:236:GLY:HA2	2.03	0.41
1:K:205:TYR:OH	1:K:271:ASP:OD2	2.34	0.41
1:L:435:TYR:C	1:L:437:PRO:HD3	2.45	0.41
2:M:15:ALA:HB3	2:M:22:ASP:HB2	2.03	0.41
2:X:247:GLU:O	2:X:249:GLN:HG2	2.21	0.41
3:Y:86:SER:O	3:Y:90:GLN:HB2	2.20	0.41
1:L:222:LEU:CB	1:L:228:MET:HE2	2.50	0.41
1:L:421:VAL:HG13	1:L:425:ARG:NH1	2.35	0.41
2:M:137:GLY:HA2	2:M:432:VAL:O	2.20	0.41
1:U:344:VAL:HA	1:U:347:ILE:HD12	2.01	0.41
1:A:450:GLY:HA2	1:A:455:LEU:HD12	2.03	0.41
1:C:181:ALA:HB1	1:C:269:VAL:HG21	2.02	0.41
1:C:197:GLU:OE1	1:C:202:TYR:OH	2.39	0.41
2:F:52:GLN:NE2	2:F:60:ARG:HD2	2.24	0.41
2:M:37:LEU:HB3	2:M:76:VAL:HG12	2.03	0.41
2:M:258:ILE:HD11	2:M:292:LEU:HD21	2.03	0.41
2:N:9:ILE:HB	2:N:78:ASP:HB3	2.03	0.41
1:S:421:VAL:HG13	1:S:425:ARG:NH2	2.36	0.41
1:U:222:LEU:HB2	1:U:228:MET:HE2	2.03	0.41
2:W:259:PHE:CE1	2:W:313:PRO:HG3	2.56	0.41
1:A:34:LEU:HD23	1:A:34:LEU:HA	1.89	0.41
1:A:64:MET:HE2	1:A:66:LEU:HD21	2.03	0.41
2:E:188:GLY:O	2:E:222:MET:HE3	2.20	0.41
3:G:202:ASP:OD1	3:G:202:ASP:N	2.50	0.41
1:J:134:LYS:HA	1:J:134:LYS:HD3	1.83	0.41
1:K:92:ARG:HE	1:K:92:ARG:HB3	1.74	0.41
1:K:338:ALA:HB3	1:K:341:PRO:HG2	2.03	0.41
1:L:280:TYR:CE2	1:L:297:PRO:HG2	2.56	0.41
2:M:98:VAL:HG13	2:M:99:ILE:HG23	2.03	0.41
2:M:164:THR:O	2:M:168:GLN:HG3	2.21	0.41
3:P:164:ILE:HG12	3:P:180:LYS:O	2.20	0.41
1:T:168:LEU:HD11	1:T:329:ILE:HB	2.03	0.41
1:T:210:GLN:NE2	1:T:271:ASP:O	2.51	0.41
1:T:444:VAL:N	1:T:445:PRO:CD	2.84	0.41
2:W:133:ILE:HD12	2:W:146:PRO:HB2	2.03	0.41
2:X:242:TYR:CE1	2:X:246:GLU:HG3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:256:ASP:HA	2:X:257:ASN:HA	1.85	0.41
1:A:138:ILE:HD13	2:E:191:THR:HG23	2.03	0.41
2:F:97:ASN:HD22	2:F:101:GLU:HB2	1.86	0.41
1:J:81:ASP:C	1:J:83:LEU:N	2.77	0.41
1:L:354:LEU:HA	1:L:366:ALA:O	2.21	0.41
1:L:378:SER:O	1:L:380:ALA:N	2.54	0.41
2:W:276:PRO:HG2	3:Y:267:LEU:HD21	2.03	0.41
2:X:97:ASN:HB2	2:X:101:GLU:H	1.86	0.41
2:X:142:ASP:HB3	2:X:434:LEU:HD12	2.02	0.41
1:C:243:PRO:HA	1:C:283:LEU:HD11	2.03	0.40
2:E:427:ILE:HA	2:E:428:PRO:HD2	1.94	0.40
3:G:180:LYS:HE3	3:G:217:GLN:HB3	2.03	0.40
1:K:444:VAL:HG23	1:K:445:PRO:CD	2.49	0.40
1:L:340:ILE:HB	1:L:341:PRO:HD3	2.03	0.40
2:M:96:ILE:HG22	2:M:97:ASN:O	2.21	0.40
1:U:211:LYS:HA	2:X:294:GLU:OE2	2.21	0.40
1:U:340:ILE:HB	1:U:341:PRO:HD3	2.03	0.40
2:V:97:ASN:OD1	2:V:97:ASN:C	2.64	0.40
2:X:382:LYS:O	2:X:385:GLN:HG2	2.20	0.40
2:E:204:THR:HG23	2:E:206:VAL:H	1.87	0.40
2:F:158:GLY:O	2:F:161:VAL:HG22	2.21	0.40
2:F:266:SER:HB3	2:F:282:GLN:OE1	2.21	0.40
1:K:103:PRO:HD3	1:K:258:TRP:CZ2	2.57	0.40
1:K:103:PRO:O	1:K:106:LEU:HD13	2.21	0.40
1:L:40:ILE:CD1	1:L:76:VAL:HG12	2.51	0.40
2:M:337:ARG:O	2:M:341:GLU:HG3	2.21	0.40
2:O:16:VAL:C	2:O:17:ILE:HG13	2.46	0.40
1:S:54:LEU:HD11	1:S:78:PHE:HE2	1.86	0.40
2:W:321:ALA:HB3	2:W:322:PRO:HD3	2.03	0.40
2:X:382:LYS:HA	2:X:385:GLN:HE21	1.87	0.40
1:B:211:LYS:HD2	2:E:328:HIS:HA	2.03	0.40
1:C:107:GLY:HA2	1:C:228:MET:O	2.20	0.40
2:F:384:LEU:O	2:F:388:ILE:HG12	2.20	0.40
1:J:242:ALA:N	1:J:243:PRO:CD	2.84	0.40
1:K:170:ILE:HG13	1:K:329:ILE:HG22	2.03	0.40
1:S:99:VAL:HG23	1:S:100:PRO:HD2	2.03	0.40
1:U:360:TYR:O	2:X:376:GLU:HA	2.20	0.40
1:A:300:VAL:CG1	1:A:339:TYR:HE2	2.35	0.40
2:D:178:HIS:NE2	2:D:250:ASP:HB3	2.37	0.40
3:G:205:VAL:HG22	4:H:51:GLN:NE2	2.34	0.40
2:M:41:THR:HB	2:M:42:PRO:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:253:LEU:HD23	2:M:296:ILE:HG23	2.03	0.40
2:N:410:ILE:HG23	2:N:441:PHE:HE2	1.85	0.40
1:T:143:SER:H	2:X:199:ARG:HH22	1.68	0.40
1:U:109:VAL:HB	1:U:118:ASP:HB3	2.03	0.40
2:W:95:ILE:HD12	2:W:104:ASP:HB3	2.04	0.40
1:K:67:ASN:HB2	2:O:17:ILE:CG1	2.44	0.40
2:O:394:ASP:CB	3:P:85:GLY:HA2	2.52	0.40
3:P:209:LEU:O	3:P:213:THR:OG1	2.39	0.40
2:X:53:HIS:CD2	2:X:59:VAL:HG12	2.57	0.40
3:Y:212:TYR:O	3:Y:216:ASN:HB2	2.21	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	478/510 (94%)	465 (97%)	13 (3%)	0	100	100
1	B	479/510 (94%)	462 (96%)	17 (4%)	0	100	100
1	C	482/510 (94%)	469 (97%)	12 (2%)	1 (0%)	43	72
1	J	477/510 (94%)	466 (98%)	11 (2%)	0	100	100
1	K	482/510 (94%)	469 (97%)	13 (3%)	0	100	100
1	L	478/510 (94%)	458 (96%)	19 (4%)	1 (0%)	43	72
1	S	476/510 (93%)	461 (97%)	15 (3%)	0	100	100
1	T	477/510 (94%)	466 (98%)	10 (2%)	1 (0%)	43	72
1	U	477/510 (94%)	462 (97%)	14 (3%)	1 (0%)	43	72
2	D	468/478 (98%)	452 (97%)	16 (3%)	0	100	100
2	E	466/478 (98%)	446 (96%)	19 (4%)	1 (0%)	43	72
2	F	467/478 (98%)	445 (95%)	19 (4%)	3 (1%)	21	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	M	468/478 (98%)	449 (96%)	19 (4%)	0	100	100
2	N	468/478 (98%)	454 (97%)	13 (3%)	1 (0%)	43	72
2	O	466/478 (98%)	446 (96%)	19 (4%)	1 (0%)	43	72
2	V	468/478 (98%)	448 (96%)	20 (4%)	0	100	100
2	W	465/478 (97%)	450 (97%)	14 (3%)	1 (0%)	43	72
2	X	467/478 (98%)	448 (96%)	18 (4%)	1 (0%)	43	72
3	G	261/278 (94%)	235 (90%)	23 (9%)	3 (1%)	11	36
3	P	229/278 (82%)	201 (88%)	21 (9%)	7 (3%)	3	12
3	Y	188/278 (68%)	172 (92%)	16 (8%)	0	100	100
4	H	110/138 (80%)	98 (89%)	10 (9%)	2 (2%)	6	23
4	Q	74/138 (54%)	59 (80%)	12 (16%)	3 (4%)	2	8
4	Z	15/138 (11%)	13 (87%)	2 (13%)	0	100	100
5	1	23/61 (38%)	20 (87%)	1 (4%)	2 (9%)	0	1
5	I	42/61 (69%)	35 (83%)	5 (12%)	2 (5%)	2	6
5	R	30/61 (49%)	23 (77%)	5 (17%)	2 (7%)	1	3
All	All	9481/10323 (92%)	9072 (96%)	376 (4%)	33 (0%)	36	66

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	135	LYS
5	I	31	THR
5	R	31	THR
5	R	32	ALA
3	G	204	ASN
4	H	93	LEU
1	L	390	GLY
3	P	204	ASN
3	P	211	GLU
4	Q	88	ILE
1	T	390	GLY
5	1	34	VAL
1	C	390	GLY
5	I	21	ILE
3	P	201	THR
3	P	206	PRO
2	F	68	GLU

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Mol	Chain	Res	Type
3	P	144	ALA
3	P	169	PRO
5	1	19	GLN
2	F	279	VAL
4	Q	50	GLU
2	F	347	ALA
3	G	192	PRO
4	Q	81	SER
1	U	390	GLY
2	E	279	VAL
2	N	279	VAL
4	H	47	PRO
2	O	279	VAL
3	P	87	ILE
2	W	279	VAL
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	388/412 (94%)	382 (98%)	6 (2%)	57	84
1	B	388/412 (94%)	381 (98%)	7 (2%)	51	82
1	C	389/412 (94%)	380 (98%)	9 (2%)	44	78
1	J	387/412 (94%)	381 (98%)	6 (2%)	55	83
1	K	388/412 (94%)	378 (97%)	10 (3%)	40	75
1	L	388/412 (94%)	379 (98%)	9 (2%)	44	78
1	S	387/412 (94%)	374 (97%)	13 (3%)	32	68
1	T	388/412 (94%)	381 (98%)	7 (2%)	51	82
1	U	388/412 (94%)	381 (98%)	7 (2%)	51	82
2	D	380/384 (99%)	374 (98%)	6 (2%)	55	83
2	E	378/384 (98%)	371 (98%)	7 (2%)	50	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	379/384 (99%)	370 (98%)	9 (2%)	43	77
2	M	380/384 (99%)	372 (98%)	8 (2%)	47	79
2	N	380/384 (99%)	373 (98%)	7 (2%)	51	82
2	O	379/384 (99%)	371 (98%)	8 (2%)	47	79
2	V	380/384 (99%)	370 (97%)	10 (3%)	40	75
2	W	378/384 (98%)	374 (99%)	4 (1%)	65	87
2	X	379/384 (99%)	370 (98%)	9 (2%)	43	77
3	G	219/236 (93%)	208 (95%)	11 (5%)	22	54
3	P	198/236 (84%)	179 (90%)	19 (10%)	8	26
3	Y	163/236 (69%)	153 (94%)	10 (6%)	17	46
4	H	54/112 (48%)	51 (94%)	3 (6%)	19	50
4	Q	5/112 (4%)	5 (100%)	0	100	100
5	I	23/48 (48%)	19 (83%)	4 (17%)	2	7
All	All	7566/8144 (93%)	7377 (98%)	189 (2%)	42	76

All (189) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	168	LEU
1	A	221	THR
1	A	246	TYR
1	A	353	PHE
1	A	416	THR
1	A	468	SER
1	B	54	LEU
1	B	99	VAL
1	B	159	VAL
1	B	183	ASP
1	B	278	VAL
1	B	468	SER
1	B	509	THR
1	C	197	GLU
1	C	353	PHE
1	C	385	LEU
1	C	402	VAL
1	C	411	ASP
1	C	416	THR

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Mol	Chain	Res	Type
1	C	468	SER
1	C	481	LEU
1	C	509	THR
2	D	27	GLN
2	D	128	SER
2	D	149	ARG
2	D	167	ILE
2	D	200	GLU
2	D	388	ILE
2	E	10	THR
2	E	140	VAL
2	E	199	ARG
2	E	232	VAL
2	E	279	VAL
2	E	356	ARG
2	E	380	THR
2	F	167	ILE
2	F	201	MET
2	F	208	ASN
2	F	293	GLN
2	F	303	SER
2	F	339	ILE
2	F	354	LYS
2	F	427	ILE
2	F	464	GLU
3	G	17	GLU
3	G	77	ILE
3	G	93	LYS
3	G	150	LEU
3	G	153	VAL
3	G	202	ASP
3	G	231	SER
3	G	237	MET
3	G	254	LEU
3	G	267	LEU
3	G	276	SER
4	H	27	VAL
4	H	46	VAL
4	H	70	ILE
5	I	13	TYR
5	I	16	VAL
5	I	28	GLU

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Mol	Chain	Res	Type
5	I	31	THR
1	J	246	TYR
1	J	251	THR
1	J	353	PHE
1	J	363	ILE
1	J	393	LYS
1	J	416	THR
1	K	36	VAL
1	K	54	LEU
1	K	69	GLU
1	K	99	VAL
1	K	159	VAL
1	K	183	ASP
1	K	206	VAL
1	K	388	VAL
1	K	402	VAL
1	K	509	THR
1	L	99	VAL
1	L	336	VAL
1	L	342	THR
1	L	401	GLU
1	L	419	THR
1	L	436	SER
1	L	468	SER
1	L	472	SER
1	L	481	LEU
2	M	6	SER
2	M	24	HIS
2	M	133	ILE
2	M	149	ARG
2	M	167	ILE
2	M	388	ILE
2	M	390	ILE
2	M	395	GLU
2	N	114	ARG
2	N	140	VAL
2	N	222	MET
2	N	232	VAL
2	N	258	ILE
2	N	279	VAL
2	N	380	THR
2	O	103	ILE

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Mol	Chain	Res	Type
2	O	167	ILE
2	O	201	MET
2	O	208	ASN
2	O	258	ILE
2	O	303	SER
2	O	423	VAL
2	O	464	GLU
3	P	29	THR
3	P	44	MET
3	P	78	THR
3	P	86	SER
3	P	99	LEU
3	P	107	ILE
3	P	112	ASP
3	P	114	ILE
3	P	129	SER
3	P	130	ILE
3	P	133	ILE
3	P	150	LEU
3	P	151	LEU
3	P	182	ILE
3	P	213	THR
3	P	216	ASN
3	P	242	LYS
3	P	267	LEU
3	P	276	SER
1	S	32	ARG
1	S	218	LEU
1	S	318	GLU
1	S	322	SER
1	S	331	THR
1	S	353	PHE
1	S	361	LYS
1	S	393	LYS
1	S	416	THR
1	S	425	ARG
1	S	441	GLU
1	S	492	SER
1	S	495	LEU
1	T	54	LEU
1	T	99	VAL
1	T	159	VAL

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Mol	Chain	Res	Type
1	T	173	ARG
1	T	183	ASP
1	T	206	VAL
1	T	402	VAL
1	U	363	ILE
1	U	394	LEU
1	U	412	LEU
1	U	413	ASP
1	U	441	GLU
1	U	481	LEU
1	U	509	THR
2	V	7	THR
2	V	29	GLU
2	V	149	ARG
2	V	167	ILE
2	V	200	GLU
2	V	201	MET
2	V	282	GLN
2	V	388	ILE
2	V	390	ILE
2	V	393	MET
2	W	140	VAL
2	W	232	VAL
2	W	258	ILE
2	W	380	THR
2	X	43	GLN
2	X	52	GLN
2	X	140	VAL
2	X	167	ILE
2	X	201	MET
2	X	208	ASN
2	X	279	VAL
2	X	284	THR
2	X	472	LYS
3	Y	15	ASN
3	Y	22	THR
3	Y	78	THR
3	Y	87	ILE
3	Y	99	LEU
3	Y	119	LEU
3	Y	133	ILE
3	Y	162	ILE

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Mol	Chain	Res	Type
3	Y	219	LEU
3	Y	248	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	GLN
1	A	145	HIS
1	A	332	GLN
1	B	67	ASN
1	B	332	GLN
1	B	477	ASN
1	C	174	GLN
1	C	188	GLN
1	C	224	GLN
1	C	282	GLN
1	C	434	GLN
2	D	52	GLN
2	D	195	ASN
2	E	328	HIS
2	E	379	GLN
2	F	52	GLN
2	F	118	HIS
2	F	455	HIS
3	G	90	GLN
3	G	125	ASN
3	G	190	GLN
4	H	13	GLN
4	H	18	HIS
4	H	45	HIS
5	I	15	ASN
1	J	145	HIS
1	J	225	HIS
1	J	332	GLN
1	J	454	HIS
1	K	26	ASN
1	K	48	ASN
1	K	282	GLN
1	K	407	GLN
1	K	454	HIS
1	L	174	GLN
1	L	188	GLN

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Mol	Chain	Res	Type
1	L	220	GLN
1	L	351	GLN
1	L	381	GLN
2	M	195	ASN
2	O	52	GLN
2	O	328	HIS
3	P	88	HIS
3	P	122	HIS
3	P	131	ASN
3	P	184	ASN
3	P	216	ASN
3	P	224	GLN
1	S	50	GLN
1	S	145	HIS
1	S	174	GLN
1	S	332	GLN
1	S	407	GLN
1	S	454	HIS
1	T	26	ASN
1	T	28	ASN
1	T	67	ASN
1	T	145	HIS
1	T	398	GLN
1	T	454	HIS
1	U	188	GLN
1	U	224	GLN
1	U	282	GLN
1	U	428	GLN
2	V	52	GLN
2	V	195	ASN
2	V	282	GLN
2	W	221	GLN
2	W	379	GLN
2	X	43	GLN
2	X	52	GLN
2	X	379	GLN
2	X	385	GLN
2	X	455	HIS
3	Y	15	ASN
3	Y	141	GLN
3	Y	216	ASN
3	Y	249	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	PO4	N	800	-	4,4,4	0.92	0	6,6,6	0.79	0
7	ANP	K	600	6	33,33,33	1.95	10 (30%)	45,52,52	2.19	14 (31%)
7	ANP	F	600	6	33,33,33	1.95	13 (39%)	45,52,52	2.05	11 (24%)
7	ANP	S	600	6	33,33,33	2.11	10 (30%)	45,52,52	2.21	19 (42%)
7	ANP	V	600	6	33,33,33	2.03	9 (27%)	45,52,52	2.09	12 (26%)
7	ANP	C	600	6	33,33,33	1.92	12 (36%)	45,52,52	2.24	13 (28%)
7	ANP	D	600	6	33,33,33	1.81	11 (33%)	45,52,52	2.11	14 (31%)
7	ANP	L	600	6	33,33,33	2.05	11 (33%)	45,52,52	2.14	12 (26%)
7	ANP	X	600	6	33,33,33	1.90	8 (24%)	45,52,52	2.22	13 (28%)
7	ANP	J	600	6	33,33,33	1.98	12 (36%)	45,52,52	2.41	13 (28%)
7	ANP	B	600	6	33,33,33	1.92	11 (33%)	45,52,52	2.28	14 (31%)
7	ANP	U	600	6	33,33,33	2.15	11 (33%)	45,52,52	2.10	12 (26%)
7	ANP	M	600	6	33,33,33	1.90	11 (33%)	45,52,52	2.38	13 (28%)
7	ANP	O	600	6	33,33,33	2.02	11 (33%)	45,52,52	2.03	12 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	ANP	T	600	6	33,33,33	2.09	10 (30%)	45,52,52	2.04	10 (22%)
7	ANP	A	600	6	33,33,33	2.18	12 (36%)	45,52,52	2.09	12 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	ANP	K	600	6	-	5/18/38/38	0/3/3/3
7	ANP	F	600	6	-	3/18/38/38	0/3/3/3
7	ANP	S	600	6	-	3/18/38/38	0/3/3/3
7	ANP	V	600	6	-	2/18/38/38	0/3/3/3
7	ANP	C	600	6	-	2/18/38/38	0/3/3/3
7	ANP	D	600	6	-	4/18/38/38	0/3/3/3
7	ANP	L	600	6	-	2/18/38/38	0/3/3/3
7	ANP	X	600	6	-	6/18/38/38	0/3/3/3
7	ANP	J	600	6	-	2/18/38/38	0/3/3/3
7	ANP	B	600	6	-	3/18/38/38	0/3/3/3
7	ANP	U	600	6	-	3/18/38/38	0/3/3/3
7	ANP	M	600	6	-	4/18/38/38	0/3/3/3
7	ANP	O	600	6	-	8/18/38/38	0/3/3/3
7	ANP	T	600	6	-	3/18/38/38	0/3/3/3
7	ANP	A	600	6	-	2/18/38/38	0/3/3/3

All (162) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	600	ANP	C5-C4	5.47	1.48	1.39
7	U	600	ANP	C5-C4	5.29	1.48	1.39
7	S	600	ANP	PG-O1G	5.20	1.54	1.46
7	X	600	ANP	C5-C4	5.07	1.48	1.39
7	T	600	ANP	C5-C4	5.04	1.48	1.39
7	S	600	ANP	C5-C4	5.01	1.48	1.39
7	K	600	ANP	C5-C4	4.98	1.48	1.39
7	V	600	ANP	C5-C4	4.87	1.47	1.39
7	O	600	ANP	C5-C4	4.87	1.47	1.39
7	A	600	ANP	C5-C4	4.84	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	S	600	ANP	PG-N3B	4.72	1.75	1.63
7	C	600	ANP	C5-C4	4.68	1.47	1.39
7	B	600	ANP	C5-C4	4.66	1.47	1.39
7	M	600	ANP	C5-C4	4.52	1.47	1.39
7	T	600	ANP	PB-N3B	4.49	1.75	1.63
7	O	600	ANP	PG-N3B	4.48	1.75	1.63
7	F	600	ANP	C5-C4	4.45	1.47	1.39
7	S	600	ANP	PB-N3B	4.42	1.74	1.63
7	U	600	ANP	PB-N3B	4.42	1.74	1.63
7	T	600	ANP	PG-N3B	4.41	1.74	1.63
7	V	600	ANP	PB-N3B	4.40	1.74	1.63
7	D	600	ANP	C5-C4	4.33	1.46	1.39
7	B	600	ANP	PB-O1B	4.30	1.52	1.46
7	A	600	ANP	PB-N3B	4.29	1.74	1.63
7	O	600	ANP	PB-N3B	4.28	1.74	1.63
7	K	600	ANP	PB-N3B	4.23	1.74	1.63
7	X	600	ANP	PB-N3B	4.22	1.74	1.63
7	K	600	ANP	PG-N3B	4.17	1.74	1.63
7	U	600	ANP	PA-O3A	4.16	1.64	1.59
7	T	600	ANP	PG-O1G	4.12	1.52	1.46
7	J	600	ANP	C5-C4	4.12	1.46	1.39
7	D	600	ANP	PB-N3B	4.09	1.74	1.63
7	F	600	ANP	PB-N3B	4.07	1.74	1.63
7	A	600	ANP	PG-N3B	4.02	1.73	1.63
7	A	600	ANP	PG-O1G	3.98	1.52	1.46
7	L	600	ANP	PB-O1B	3.97	1.52	1.46
7	D	600	ANP	PG-N3B	3.94	1.73	1.63
7	V	600	ANP	PG-O1G	3.91	1.52	1.46
7	X	600	ANP	PG-N3B	3.87	1.73	1.63
7	O	600	ANP	PG-O1G	3.82	1.52	1.46
7	A	600	ANP	PB-O1B	3.80	1.51	1.46
7	J	600	ANP	PG-N3B	3.79	1.73	1.63
7	F	600	ANP	PG-N3B	3.77	1.73	1.63
7	L	600	ANP	PG-N3B	3.76	1.73	1.63
7	V	600	ANP	PG-N3B	3.74	1.73	1.63
7	M	600	ANP	PB-N3B	3.72	1.73	1.63
7	T	600	ANP	PB-O1B	3.72	1.51	1.46
7	U	600	ANP	PG-N3B	3.64	1.72	1.63
7	C	600	ANP	PG-N3B	3.60	1.72	1.63
7	M	600	ANP	PG-O1G	3.58	1.51	1.46
7	L	600	ANP	PB-N3B	3.52	1.72	1.63
7	B	600	ANP	PG-N3B	3.51	1.72	1.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	600	ANP	PG-O1G	3.49	1.51	1.46
7	V	600	ANP	PB-O1B	3.43	1.51	1.46
7	J	600	ANP	PB-O3A	3.38	1.63	1.59
7	J	600	ANP	PG-O1G	3.35	1.51	1.46
7	J	600	ANP	PB-N3B	3.35	1.72	1.63
7	M	600	ANP	PB-O1B	3.28	1.51	1.46
7	B	600	ANP	PB-N3B	3.22	1.71	1.63
7	X	600	ANP	PB-O1B	3.15	1.51	1.46
7	F	600	ANP	PG-O1G	3.15	1.51	1.46
7	J	600	ANP	PA-O3A	3.14	1.62	1.59
7	A	600	ANP	PB-O2B	-3.12	1.48	1.56
7	U	600	ANP	PB-O1B	3.06	1.50	1.46
7	U	600	ANP	PB-O3A	3.04	1.62	1.59
7	S	600	ANP	C5-C6	3.03	1.49	1.41
7	C	600	ANP	PG-O2G	-3.01	1.48	1.56
7	J	600	ANP	PB-O1B	2.99	1.50	1.46
7	K	600	ANP	PG-O1G	2.99	1.50	1.46
7	C	600	ANP	PB-N3B	2.97	1.71	1.63
7	V	600	ANP	C5-C6	2.96	1.49	1.41
7	M	600	ANP	PG-N3B	2.95	1.71	1.63
7	T	600	ANP	C5-C6	2.95	1.49	1.41
7	X	600	ANP	PG-O1G	2.94	1.50	1.46
7	B	600	ANP	PG-O1G	2.90	1.50	1.46
7	A	600	ANP	C5-N7	-2.90	1.33	1.39
7	L	600	ANP	C5-N7	-2.89	1.33	1.39
7	F	600	ANP	C4-N9	-2.87	1.31	1.37
7	L	600	ANP	C8-N7	2.86	1.37	1.31
7	K	600	ANP	PB-O1B	2.85	1.50	1.46
7	A	600	ANP	PG-O2G	-2.85	1.49	1.56
7	U	600	ANP	C8-N7	2.83	1.37	1.31
7	A	600	ANP	C4-N9	-2.82	1.31	1.37
7	J	600	ANP	PG-O2G	-2.77	1.49	1.56
7	B	600	ANP	C5-C6	2.76	1.48	1.41
7	C	600	ANP	PA-O3A	2.74	1.62	1.59
7	U	600	ANP	PG-O1G	2.68	1.50	1.46
7	L	600	ANP	PG-O1G	2.67	1.50	1.46
7	C	600	ANP	PB-O1B	2.67	1.50	1.46
7	U	600	ANP	C5-C6	2.67	1.48	1.41
7	D	600	ANP	C5-N7	-2.67	1.34	1.39
7	J	600	ANP	C5-N7	-2.66	1.34	1.39
7	L	600	ANP	PB-O2B	-2.66	1.49	1.56
7	L	600	ANP	PG-O2G	-2.65	1.49	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	K	600	ANP	C5-C6	2.64	1.48	1.41
7	U	600	ANP	C5-N7	-2.63	1.34	1.39
7	F	600	ANP	PA-O3A	2.62	1.62	1.59
7	S	600	ANP	C8-N7	2.61	1.36	1.31
7	F	600	ANP	PB-O1B	2.60	1.50	1.46
7	O	600	ANP	PB-O2B	-2.60	1.49	1.56
7	F	600	ANP	C5-N7	-2.59	1.34	1.39
7	C	600	ANP	C5-C6	2.58	1.48	1.41
7	M	600	ANP	PB-O3A	2.57	1.62	1.59
7	X	600	ANP	C8-N7	2.56	1.36	1.31
7	M	600	ANP	C5-C6	2.56	1.48	1.41
7	V	600	ANP	C5-N7	-2.56	1.34	1.39
7	D	600	ANP	PG-O3G	-2.54	1.50	1.56
7	A	600	ANP	C5-C6	2.54	1.48	1.41
7	X	600	ANP	C5-C6	2.52	1.48	1.41
7	M	600	ANP	C8-N7	2.52	1.36	1.31
7	J	600	ANP	C5-C6	2.52	1.48	1.41
7	O	600	ANP	C5-C6	2.50	1.47	1.41
7	O	600	ANP	PA-O3A	2.48	1.62	1.59
7	A	600	ANP	PB-O3A	2.46	1.62	1.59
7	T	600	ANP	C8-N7	2.44	1.36	1.31
7	D	600	ANP	PG-O1G	2.41	1.49	1.46
7	F	600	ANP	C8-N7	2.41	1.36	1.31
7	D	600	ANP	C4-N9	-2.40	1.32	1.37
7	M	600	ANP	C5-N7	-2.40	1.34	1.39
7	F	600	ANP	PB-O2B	-2.40	1.50	1.56
7	B	600	ANP	C5-N7	-2.38	1.34	1.39
7	C	600	ANP	C8-N7	2.38	1.36	1.31
7	T	600	ANP	PG-O3G	-2.38	1.50	1.56
7	K	600	ANP	C5-N7	-2.38	1.34	1.39
7	S	600	ANP	PA-O3A	2.35	1.62	1.59
7	M	600	ANP	PG-O3G	-2.33	1.50	1.56
7	C	600	ANP	C4-N9	-2.33	1.32	1.37
7	V	600	ANP	PG-O3G	-2.31	1.50	1.56
7	T	600	ANP	C5-N7	-2.31	1.34	1.39
7	D	600	ANP	PB-O2B	-2.29	1.50	1.56
7	O	600	ANP	PG-O2G	-2.27	1.50	1.56
7	V	600	ANP	C8-N7	2.27	1.36	1.31
7	L	600	ANP	C5-C6	2.27	1.47	1.41
7	O	600	ANP	C8-N7	2.24	1.36	1.31
7	B	600	ANP	PA-O3A	2.24	1.61	1.59
7	K	600	ANP	C8-N7	2.24	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	600	ANP	PA-O3A	2.23	1.61	1.59
7	L	600	ANP	C4-N9	-2.22	1.33	1.37
7	B	600	ANP	C8-N7	2.21	1.35	1.31
7	D	600	ANP	PG-O2G	-2.20	1.51	1.56
7	D	600	ANP	PB-O1B	2.20	1.49	1.46
7	F	600	ANP	PG-O3G	-2.18	1.51	1.56
7	C	600	ANP	PB-O3A	2.17	1.61	1.59
7	O	600	ANP	C5-N7	-2.15	1.35	1.39
7	C	600	ANP	C5-N7	-2.15	1.35	1.39
7	X	600	ANP	C4-N9	-2.14	1.33	1.37
7	B	600	ANP	PG-O2G	-2.14	1.51	1.56
7	F	600	ANP	C5-C6	2.13	1.46	1.41
7	B	600	ANP	PB-O3A	2.12	1.61	1.59
7	S	600	ANP	PG-O2G	-2.12	1.51	1.56
7	S	600	ANP	PB-O2B	-2.12	1.51	1.56
7	T	600	ANP	PG-O2G	-2.11	1.51	1.56
7	O	600	ANP	PB-O1B	2.11	1.49	1.46
7	J	600	ANP	C8-N7	2.09	1.35	1.31
7	K	600	ANP	PG-O2G	-2.08	1.51	1.56
7	K	600	ANP	PB-O3A	2.05	1.61	1.59
7	M	600	ANP	PA-O3A	2.04	1.61	1.59
7	F	600	ANP	PG-O2G	-2.03	1.51	1.56
7	U	600	ANP	PG-O2G	-2.02	1.51	1.56
7	D	600	ANP	C5-C6	2.02	1.46	1.41
7	S	600	ANP	PB-O1B	2.02	1.49	1.46
7	J	600	ANP	C8-N9	-2.01	1.34	1.37

All (194) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	J	600	ANP	O1G-PG-N3B	-8.93	98.62	111.77
7	B	600	ANP	O1G-PG-N3B	-7.20	101.17	111.77
7	C	600	ANP	O1G-PG-N3B	-7.10	101.31	111.77
7	L	600	ANP	O1G-PG-N3B	-6.95	101.54	111.77
7	M	600	ANP	O1G-PG-N3B	-6.43	102.30	111.77
7	X	600	ANP	O1G-PG-N3B	-6.25	102.56	111.77
7	U	600	ANP	C5-C4-N3	-6.20	118.19	126.72
7	T	600	ANP	C5-C4-N3	-6.19	118.19	126.72
7	J	600	ANP	C5-C4-N3	-6.14	118.27	126.72
7	M	600	ANP	C5-C4-N3	-6.07	118.36	126.72
7	A	600	ANP	O1G-PG-N3B	-6.00	102.94	111.77
7	K	600	ANP	O1G-PG-N3B	-5.98	102.96	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	600	ANP	C5-C4-N3	-5.95	118.52	126.72
7	F	600	ANP	O1G-PG-N3B	-5.90	103.09	111.77
7	V	600	ANP	C5-C4-N3	-5.90	118.60	126.72
7	K	600	ANP	C5-C4-N3	-5.30	119.42	126.72
7	A	600	ANP	C5-C4-N3	-5.29	119.43	126.72
7	D	600	ANP	C5-C4-N3	-5.26	119.48	126.72
7	C	600	ANP	C5-C4-N3	-5.23	119.52	126.72
7	O	600	ANP	C5-C4-N3	-5.19	119.57	126.72
7	C	600	ANP	O2B-PB-O1B	5.15	120.92	109.87
7	X	600	ANP	O1B-PB-N3B	-5.06	104.32	111.77
7	M	600	ANP	O2B-PB-O1B	5.05	120.70	109.87
7	D	600	ANP	O1B-PB-N3B	-5.04	104.35	111.77
7	L	600	ANP	C5-C4-N3	-4.99	119.84	126.72
7	M	600	ANP	N3-C4-N9	4.93	135.55	127.17
7	J	600	ANP	N3-C4-N9	4.89	135.48	127.17
7	D	600	ANP	N3-C4-N9	4.80	135.34	127.17
7	T	600	ANP	O2B-PB-O1B	4.79	120.13	109.87
7	U	600	ANP	O1G-PG-N3B	-4.75	104.78	111.77
7	U	600	ANP	N3-C4-N9	4.73	135.21	127.17
7	F	600	ANP	N3-C2-N1	-4.68	121.50	128.58
7	T	600	ANP	N3-C4-N9	4.67	135.12	127.17
7	B	600	ANP	N3-C4-N9	4.62	135.02	127.17
7	S	600	ANP	C5-C4-N3	-4.58	120.41	126.72
7	A	600	ANP	N3-C4-N9	4.58	134.95	127.17
7	X	600	ANP	C5-C4-N3	-4.56	120.44	126.72
7	V	600	ANP	N3-C4-N9	4.53	134.87	127.17
7	T	600	ANP	O1G-PG-N3B	-4.52	105.11	111.77
7	K	600	ANP	N3-C4-N9	4.48	134.78	127.17
7	O	600	ANP	N3-C4-N9	4.48	134.78	127.17
7	V	600	ANP	O2B-PB-O1B	4.47	119.46	109.87
7	B	600	ANP	O2B-PB-O1B	4.39	119.28	109.87
7	F	600	ANP	C5-C4-N3	-4.36	120.71	126.72
7	V	600	ANP	O1B-PB-N3B	-4.36	105.35	111.77
7	X	600	ANP	N3-C2-N1	-4.31	122.05	128.58
7	C	600	ANP	N3-C4-N9	4.24	134.38	127.17
7	S	600	ANP	N3-C2-N1	-4.23	122.18	128.58
7	M	600	ANP	C2-N3-C4	4.23	122.15	111.83
7	L	600	ANP	O2B-PB-O1B	4.19	118.86	109.87
7	O	600	ANP	O1G-PG-N3B	-4.18	105.62	111.77
7	S	600	ANP	O1G-PG-N3B	-4.17	105.63	111.77
7	F	600	ANP	O2B-PB-O1B	4.16	118.78	109.87
7	J	600	ANP	C2-N3-C4	4.00	121.59	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	U	600	ANP	O2B-PB-O1B	3.98	118.41	109.87
7	M	600	ANP	N3-C2-N1	-3.98	122.56	128.58
7	L	600	ANP	N3-C4-N9	3.93	133.86	127.17
7	X	600	ANP	O2B-PB-O1B	3.92	118.28	109.87
7	K	600	ANP	N3-C2-N1	-3.92	122.65	128.58
7	D	600	ANP	O2G-PG-O3G	3.91	118.10	107.59
7	T	600	ANP	C2-N3-C4	3.87	121.28	111.83
7	O	600	ANP	O2B-PB-O1B	3.86	118.15	109.87
7	K	600	ANP	O2B-PB-O1B	3.84	118.10	109.87
7	B	600	ANP	C4-C5-N7	-3.80	106.24	110.58
7	J	600	ANP	O2B-PB-O1B	3.79	118.00	109.87
7	C	600	ANP	N3-C2-N1	-3.76	122.89	128.58
7	V	600	ANP	C4-C5-N7	-3.75	106.29	110.58
7	F	600	ANP	N3-C4-N9	3.75	133.55	127.17
7	X	600	ANP	N3-C4-N9	3.73	133.52	127.17
7	U	600	ANP	C4-C5-N7	-3.73	106.31	110.58
7	M	600	ANP	O1B-PB-N3B	-3.72	106.30	111.77
7	O	600	ANP	N3-C2-N1	-3.72	122.96	128.58
7	S	600	ANP	O4'-C1'-N9	3.71	115.22	108.09
7	K	600	ANP	C2-N3-C4	3.67	120.80	111.83
7	C	600	ANP	C2-N3-C4	3.65	120.75	111.83
7	J	600	ANP	N3-C2-N1	-3.64	123.07	128.58
7	T	600	ANP	C4-C5-N7	-3.64	106.42	110.58
7	K	600	ANP	O2G-PG-O3G	3.64	117.36	107.59
7	S	600	ANP	N3-C4-N9	3.63	133.34	127.17
7	S	600	ANP	C2-N3-C4	3.63	120.70	111.83
7	F	600	ANP	C2-N3-C4	3.62	120.67	111.83
7	V	600	ANP	C2-N3-C4	3.61	120.65	111.83
7	D	600	ANP	N3-C2-N1	-3.61	123.12	128.58
7	B	600	ANP	C2-N3-C4	3.57	120.55	111.83
7	L	600	ANP	N3-C2-N1	-3.56	123.19	128.58
7	M	600	ANP	C4-C5-N7	-3.56	106.51	110.58
7	A	600	ANP	O2G-PG-O3G	3.55	117.13	107.59
7	D	600	ANP	C4-N9-C8	3.51	109.43	105.74
7	X	600	ANP	C2-N3-C4	3.48	120.32	111.83
7	O	600	ANP	C2-N3-C4	3.45	120.26	111.83
7	U	600	ANP	C2-N3-C4	3.42	120.18	111.83
7	X	600	ANP	C2-N1-C6	3.37	124.27	118.73
7	J	600	ANP	C4-C5-N7	-3.37	106.73	110.58
7	O	600	ANP	O1B-PB-N3B	-3.36	106.82	111.77
7	S	600	ANP	O3G-PG-O1G	3.36	121.87	113.45
7	F	600	ANP	C2-N1-C6	3.35	124.23	118.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	600	ANP	C2-N3-C4	3.33	119.97	111.83
7	D	600	ANP	C2-N3-C4	3.33	119.97	111.83
7	C	600	ANP	O2B-PB-O3A	3.30	115.67	104.64
7	S	600	ANP	C4-C5-N7	-3.30	106.81	110.58
7	K	600	ANP	C4-C5-N7	-3.27	106.84	110.58
7	L	600	ANP	C2-N1-C6	3.27	124.10	118.73
7	L	600	ANP	O1B-PB-N3B	-3.27	106.96	111.77
7	A	600	ANP	N3-C2-N1	-3.25	123.67	128.58
7	T	600	ANP	N3-C2-N1	-3.25	123.67	128.58
7	M	600	ANP	C4-N9-C8	3.23	109.13	105.74
7	L	600	ANP	C2-N3-C4	3.22	119.69	111.83
7	A	600	ANP	O2B-PB-O3A	3.21	115.36	104.64
7	D	600	ANP	O1G-PG-N3B	-3.19	107.07	111.77
7	U	600	ANP	O2G-PG-O3G	3.15	116.06	107.59
7	U	600	ANP	O1B-PB-N3B	-3.09	107.22	111.77
7	C	600	ANP	C4-C5-N7	-3.07	107.07	110.58
7	M	600	ANP	C5-N7-C8	3.05	108.25	103.45
7	V	600	ANP	N3-C2-N1	-3.04	123.98	128.58
7	S	600	ANP	O2G-PG-O3G	3.04	115.75	107.59
7	S	600	ANP	C4-N9-C8	3.01	108.90	105.74
7	J	600	ANP	O3G-PG-O1G	3.01	120.99	113.45
7	X	600	ANP	O2G-PG-O3G	3.01	115.67	107.59
7	S	600	ANP	O2B-PB-O1B	3.00	116.30	109.87
7	C	600	ANP	C4-N9-C8	3.00	108.88	105.74
7	D	600	ANP	O2B-PB-O1B	2.99	116.27	109.87
7	S	600	ANP	C6-C5-N7	2.98	137.84	132.09
7	K	600	ANP	C4-N9-C8	2.94	108.82	105.74
7	O	600	ANP	C4-N9-C8	2.92	108.81	105.74
7	S	600	ANP	O2G-PG-O1G	-2.92	106.13	113.45
7	B	600	ANP	N3-C2-N1	-2.90	124.19	128.58
7	F	600	ANP	C4-N9-C8	2.86	108.74	105.74
7	B	600	ANP	C5-N7-C8	2.84	107.92	103.45
7	K	600	ANP	O2B-PB-O3A	2.84	114.14	104.64
7	O	600	ANP	C4-C5-N7	-2.83	107.34	110.58
7	V	600	ANP	C3'-C2'-C1'	2.80	106.76	101.46
7	S	600	ANP	C2-N1-C6	2.77	123.28	118.73
7	U	600	ANP	N3-C2-N1	-2.77	124.39	128.58
7	M	600	ANP	N9-C8-N7	-2.76	110.02	113.94
7	B	600	ANP	O3A-PA-O1A	-2.75	102.44	110.70
7	A	600	ANP	C4-N9-C8	2.74	108.61	105.74
7	M	600	ANP	C2'-C1'-N9	-2.72	106.54	113.30
7	X	600	ANP	C4-C5-N7	-2.71	107.49	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	600	ANP	C4-C5-N7	-2.69	107.51	110.58
7	A	600	ANP	O3G-PG-O1G	2.68	120.16	113.45
7	V	600	ANP	C5-N7-C8	2.67	107.65	103.45
7	T	600	ANP	C5-N7-C8	2.67	107.64	103.45
7	O	600	ANP	C2-N1-C6	2.67	123.11	118.73
7	C	600	ANP	C2-N1-C6	2.63	123.05	118.73
7	B	600	ANP	O3A-PB-N3B	-2.63	99.30	106.59
7	D	600	ANP	C4-C5-N7	-2.60	107.60	110.58
7	J	600	ANP	C5-N7-C8	2.58	107.51	103.45
7	U	600	ANP	C5-N7-C8	2.57	107.49	103.45
7	O	600	ANP	O2G-PG-O3G	2.57	114.50	107.59
7	X	600	ANP	C4-N9-C8	2.56	108.42	105.74
7	A	600	ANP	O3A-PB-N3B	-2.54	99.55	106.59
7	K	600	ANP	C5-N7-C8	2.52	107.41	103.45
7	D	600	ANP	O2B-PB-O3A	2.47	112.88	104.64
7	J	600	ANP	O2B-PB-O3A	2.46	112.84	104.64
7	X	600	ANP	C6-C5-N7	2.42	136.76	132.09
7	J	600	ANP	C4-N9-C8	2.42	108.28	105.74
7	U	600	ANP	C4-N9-C8	2.40	108.26	105.74
7	V	600	ANP	C4-N9-C8	2.38	108.23	105.74
7	K	600	ANP	C2-N1-C6	2.37	122.63	118.73
7	L	600	ANP	O2G-PG-O3G	2.37	113.96	107.59
7	D	600	ANP	C2-N1-C6	2.36	122.61	118.73
7	M	600	ANP	C6-C5-N7	2.35	136.62	132.09
7	F	600	ANP	O2G-PG-O3G	2.35	113.89	107.59
7	V	600	ANP	C2'-C1'-N9	-2.34	107.48	113.30
7	B	600	ANP	C4-N9-C8	2.34	108.19	105.74
7	S	600	ANP	C5-N7-C8	2.33	107.11	103.45
7	L	600	ANP	O2G-PG-O1G	2.32	119.28	113.45
7	C	600	ANP	O2G-PG-O3G	2.32	113.83	107.59
7	K	600	ANP	C6-C5-N7	2.30	136.53	132.09
7	L	600	ANP	C4-C5-N7	-2.29	107.97	110.58
7	B	600	ANP	C6-C5-N7	2.29	136.50	132.09
7	C	600	ANP	C6-C5-N7	2.27	136.46	132.09
7	L	600	ANP	O2A-PA-O1A	2.21	122.74	112.44
7	S	600	ANP	O2B-PB-O3A	2.20	112.00	104.64
7	D	600	ANP	C5-N7-C8	2.16	106.84	103.45
7	C	600	ANP	C5-N7-C8	2.15	106.84	103.45
7	T	600	ANP	C6-C5-N7	2.15	136.24	132.09
7	A	600	ANP	C2-N1-C6	2.15	122.26	118.73
7	S	600	ANP	C4-N9-C1'	-2.13	121.65	126.63
7	O	600	ANP	C5-N7-C8	2.13	106.80	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	U	600	ANP	O2A-PA-O1A	2.13	122.33	112.44
7	S	600	ANP	C2'-C1'-N9	-2.12	108.04	113.30
7	D	600	ANP	N9-C8-N7	-2.12	110.93	113.94
7	S	600	ANP	N9-C8-N7	-2.11	110.94	113.94
7	J	600	ANP	O4'-C1'-N9	2.11	112.15	108.09
7	F	600	ANP	C4-C5-N7	-2.08	108.20	110.58
7	K	600	ANP	O2A-PA-O1A	2.08	122.14	112.44
7	F	600	ANP	C6-C5-N7	2.08	136.10	132.09
7	T	600	ANP	O4'-C1'-N9	2.07	112.06	108.09
7	J	600	ANP	C6-C5-N7	2.06	136.06	132.09
7	B	600	ANP	O2G-PG-O3G	2.06	113.12	107.59
7	V	600	ANP	C6-C5-N7	2.05	136.05	132.09
7	X	600	ANP	O2A-PA-O1A	2.05	121.99	112.44
7	B	600	ANP	O2A-PA-O1A	2.04	121.93	112.44

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	600	ANP	PB-N3B-PG-O1G
7	A	600	ANP	PG-N3B-PB-O1B
7	B	600	ANP	PB-N3B-PG-O1G
7	B	600	ANP	PG-N3B-PB-O1B
7	C	600	ANP	PB-N3B-PG-O1G
7	C	600	ANP	PG-N3B-PB-O1B
7	D	600	ANP	PB-N3B-PG-O1G
7	D	600	ANP	PG-N3B-PB-O1B
7	D	600	ANP	PA-O3A-PB-O2B
7	F	600	ANP	PB-N3B-PG-O1G
7	F	600	ANP	PG-N3B-PB-O1B
7	F	600	ANP	PG-N3B-PB-O3A
7	J	600	ANP	PB-N3B-PG-O1G
7	J	600	ANP	PG-N3B-PB-O1B
7	K	600	ANP	PB-N3B-PG-O1G
7	K	600	ANP	PG-N3B-PB-O1B
7	L	600	ANP	PB-N3B-PG-O1G
7	L	600	ANP	PG-N3B-PB-O1B
7	M	600	ANP	PB-N3B-PG-O1G
7	M	600	ANP	PG-N3B-PB-O1B
7	M	600	ANP	PA-O3A-PB-O2B
7	O	600	ANP	PB-N3B-PG-O1G
7	O	600	ANP	PG-N3B-PB-O1B

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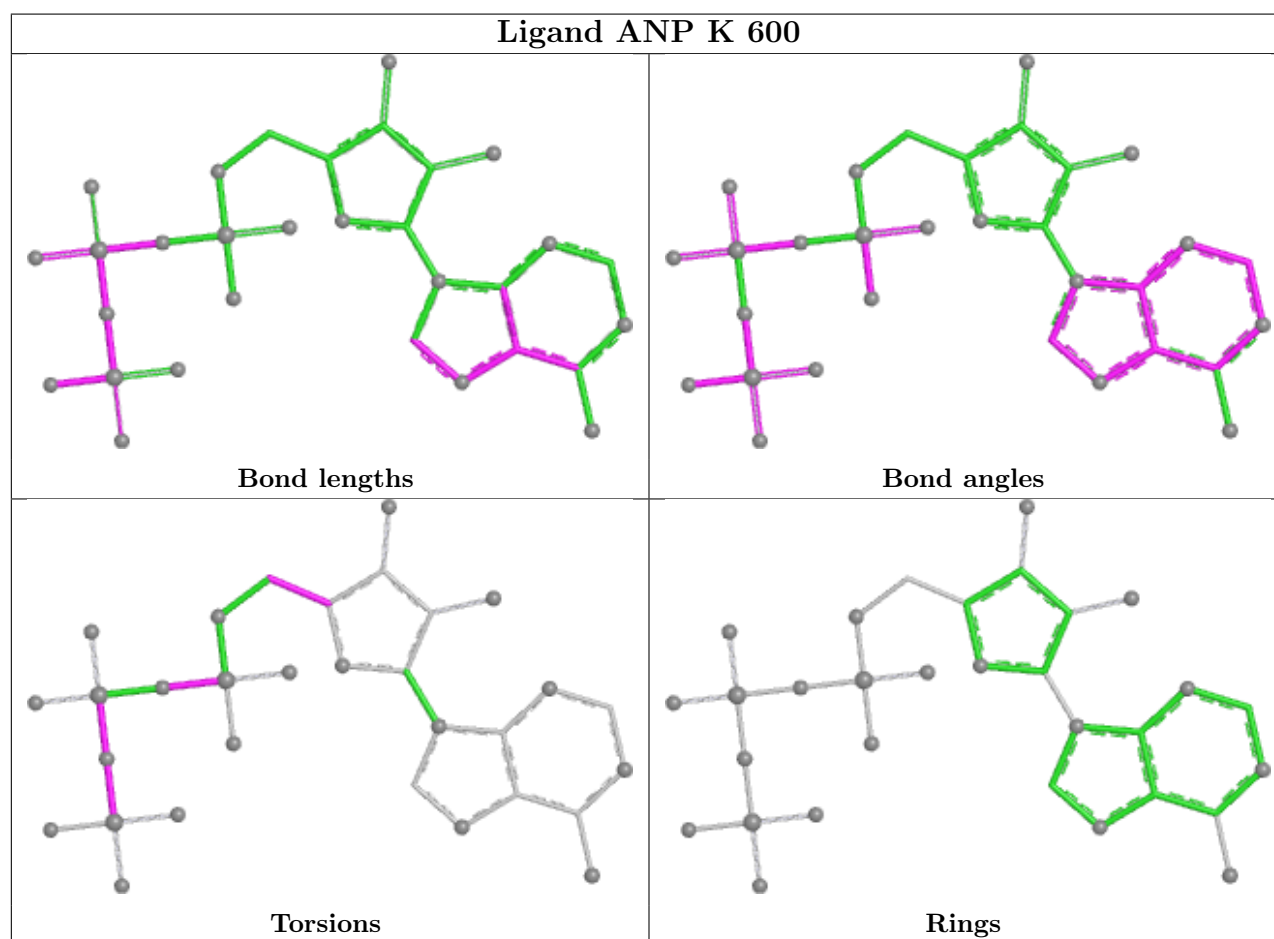
Mol	Chain	Res	Type	Atoms
7	O	600	ANP	PG-N3B-PB-O3A
7	O	600	ANP	C5'-O5'-PA-O2A
7	O	600	ANP	C5'-O5'-PA-O3A
7	S	600	ANP	PB-N3B-PG-O1G
7	S	600	ANP	PG-N3B-PB-O1B
7	S	600	ANP	PG-N3B-PB-O3A
7	T	600	ANP	PB-N3B-PG-O1G
7	T	600	ANP	PG-N3B-PB-O1B
7	U	600	ANP	PB-N3B-PG-O1G
7	U	600	ANP	PG-N3B-PB-O1B
7	U	600	ANP	PG-N3B-PB-O3A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

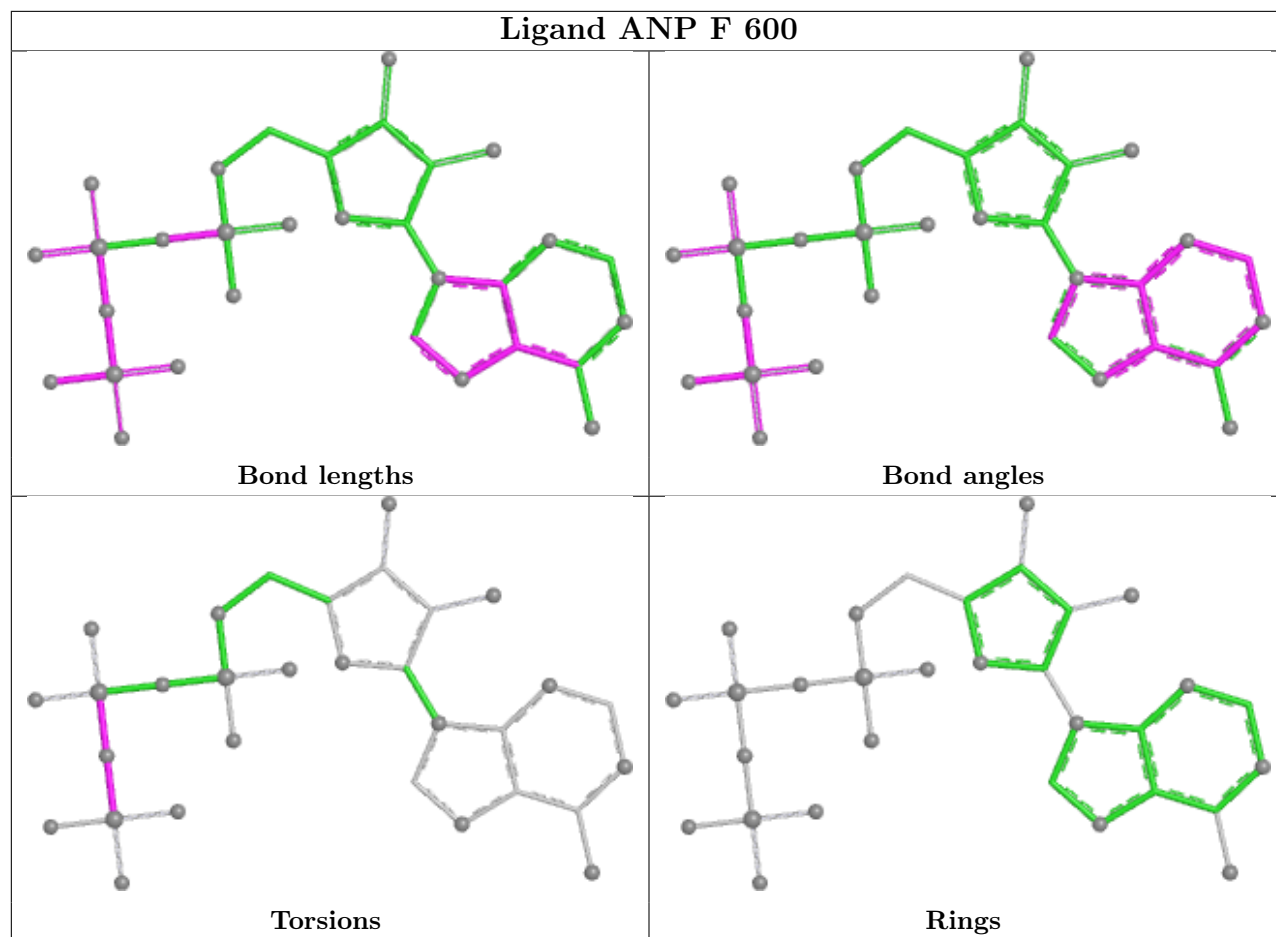
There are no ring outliers.

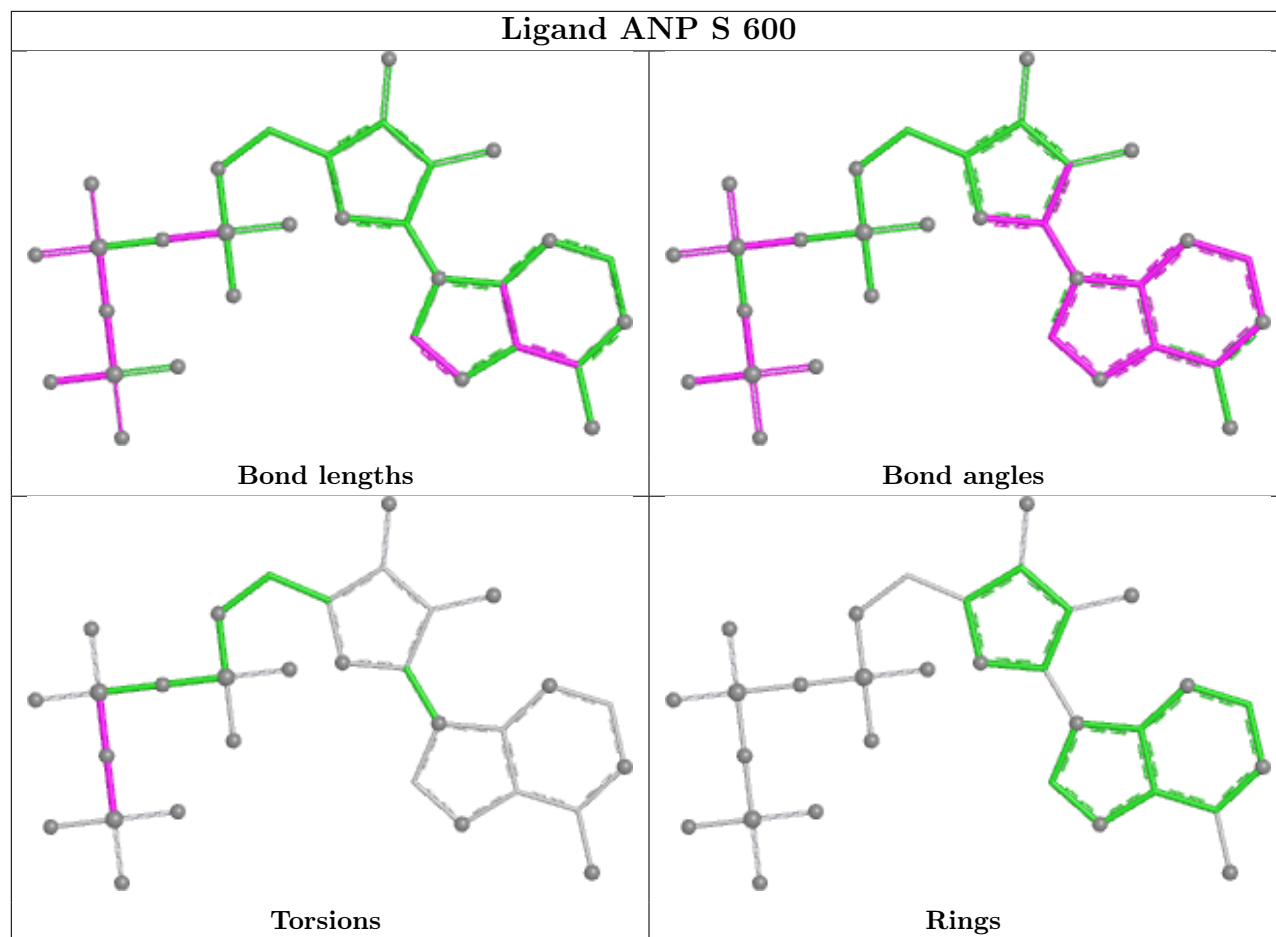
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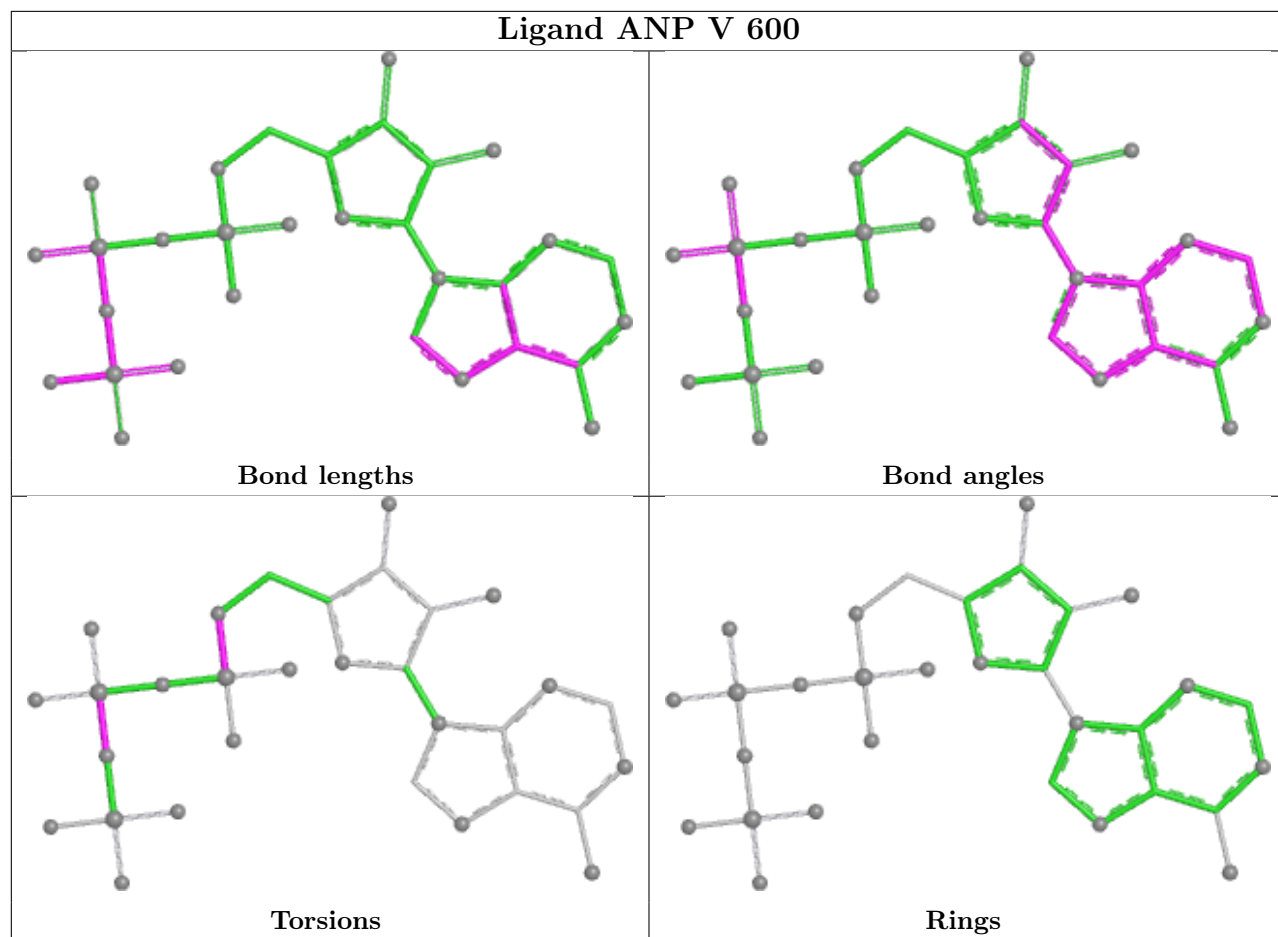
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	K	600	ANP	1	0
7	F	600	ANP	2	0
7	S	600	ANP	1	0
7	V	600	ANP	3	0
7	C	600	ANP	1	0
7	L	600	ANP	1	0
7	X	600	ANP	4	0
7	M	600	ANP	6	0

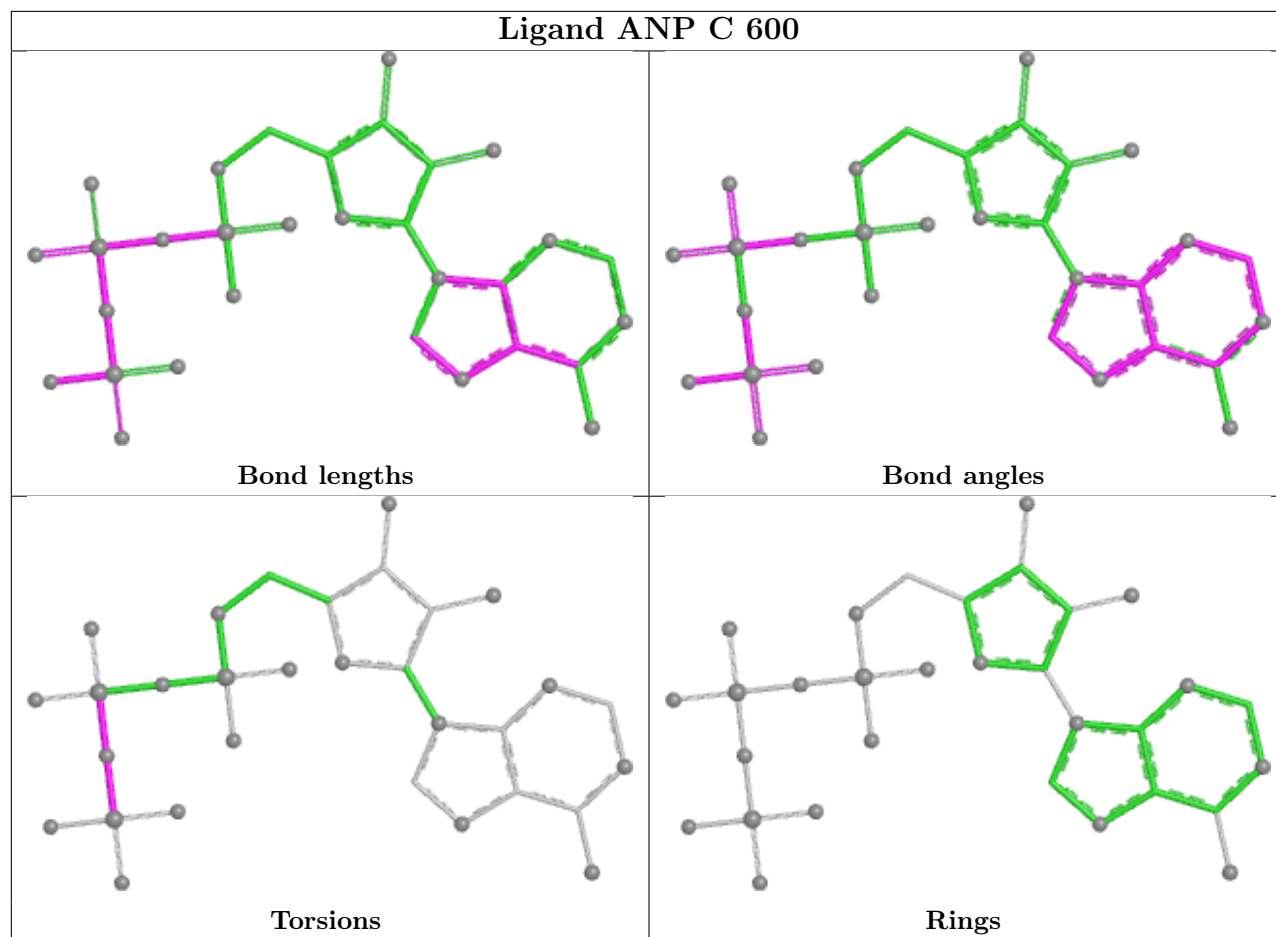
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

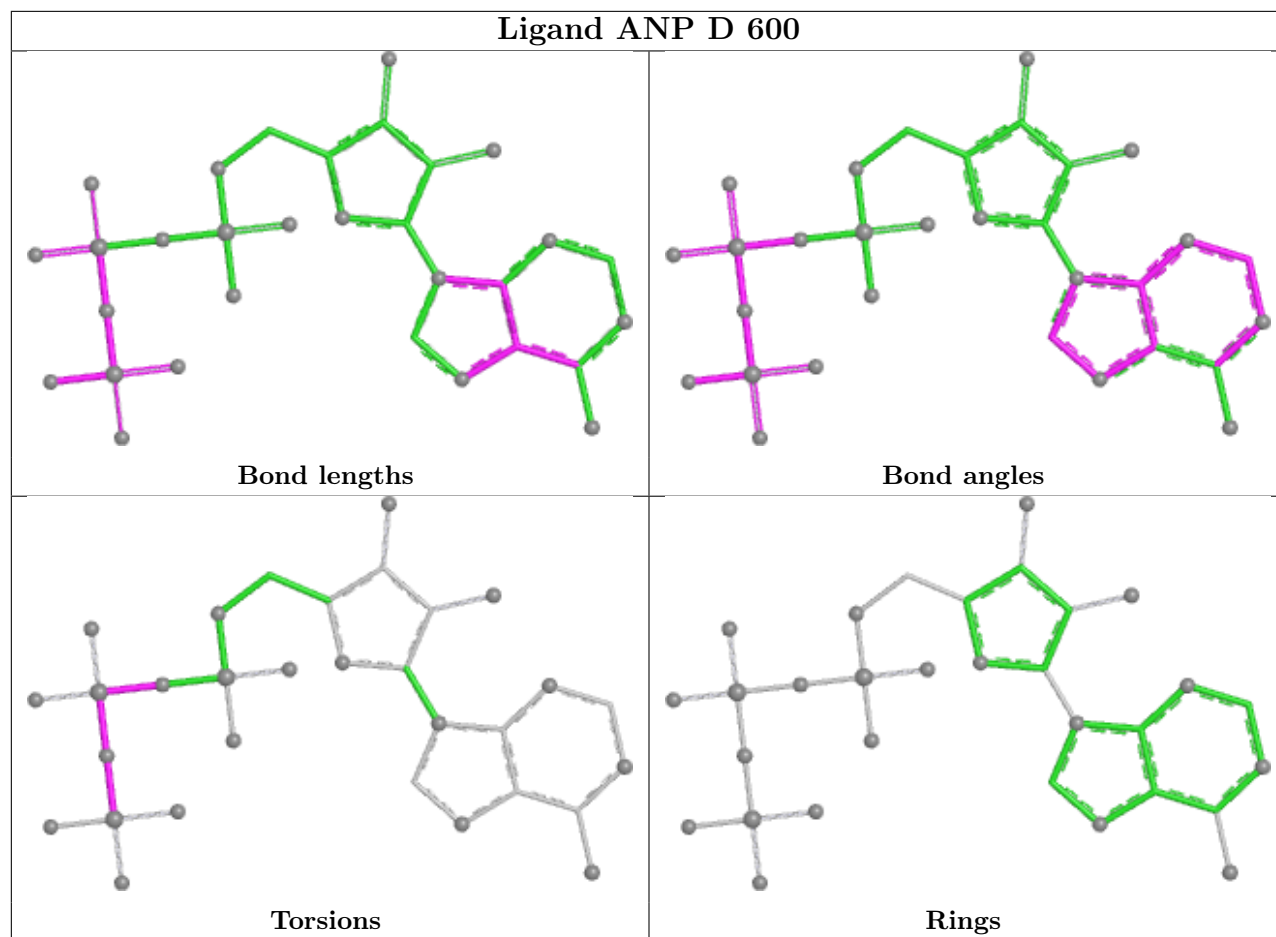


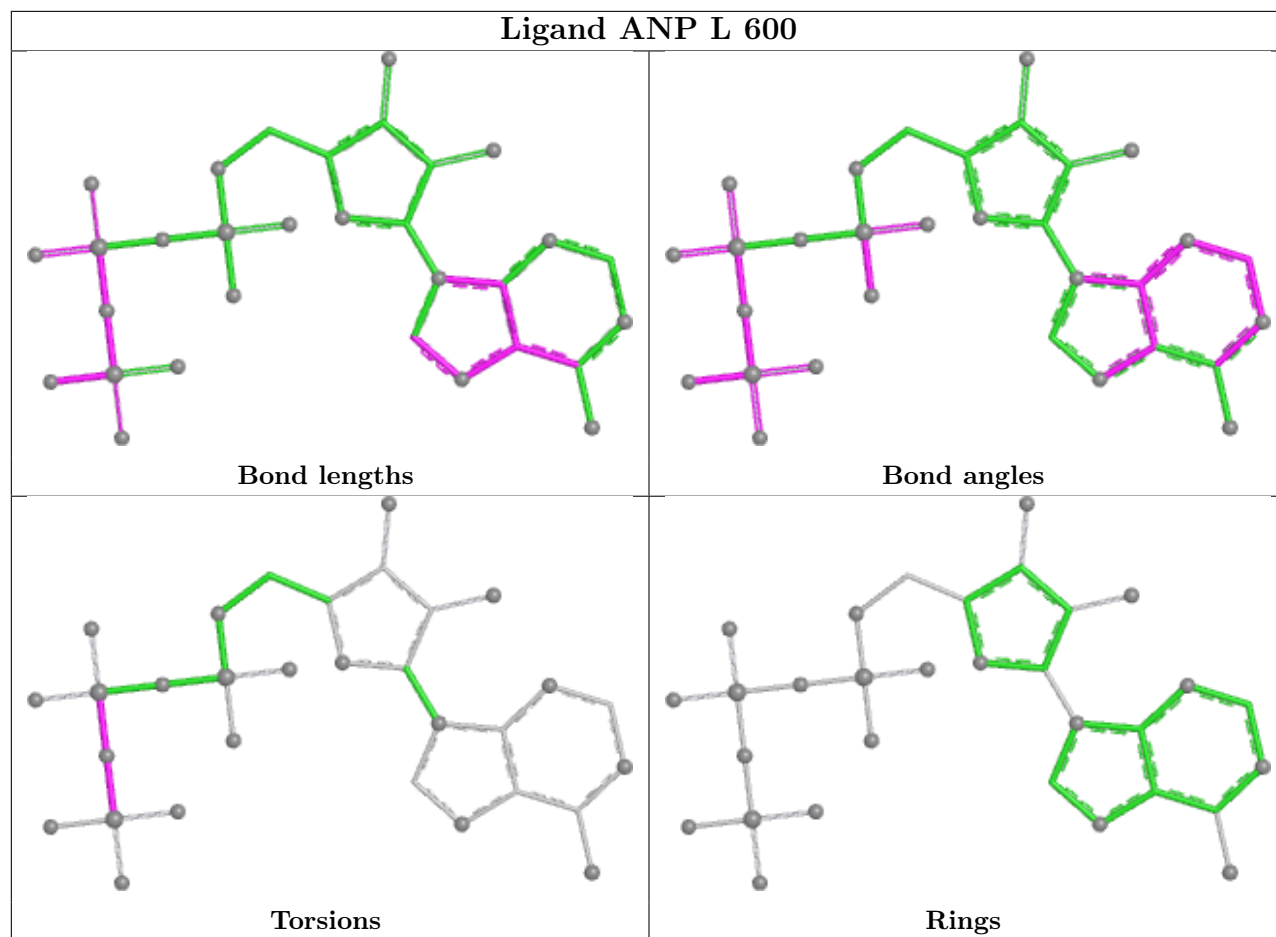


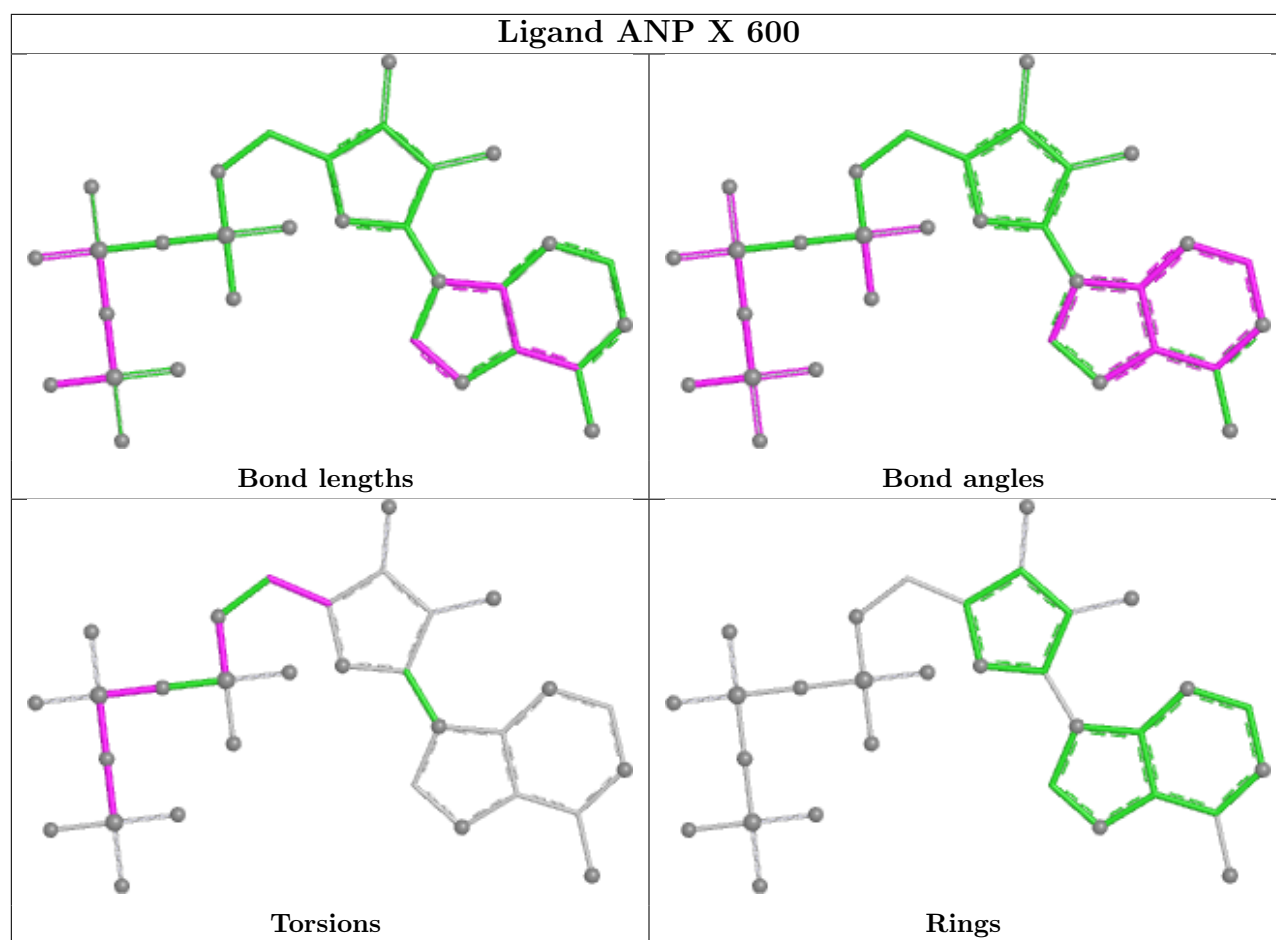


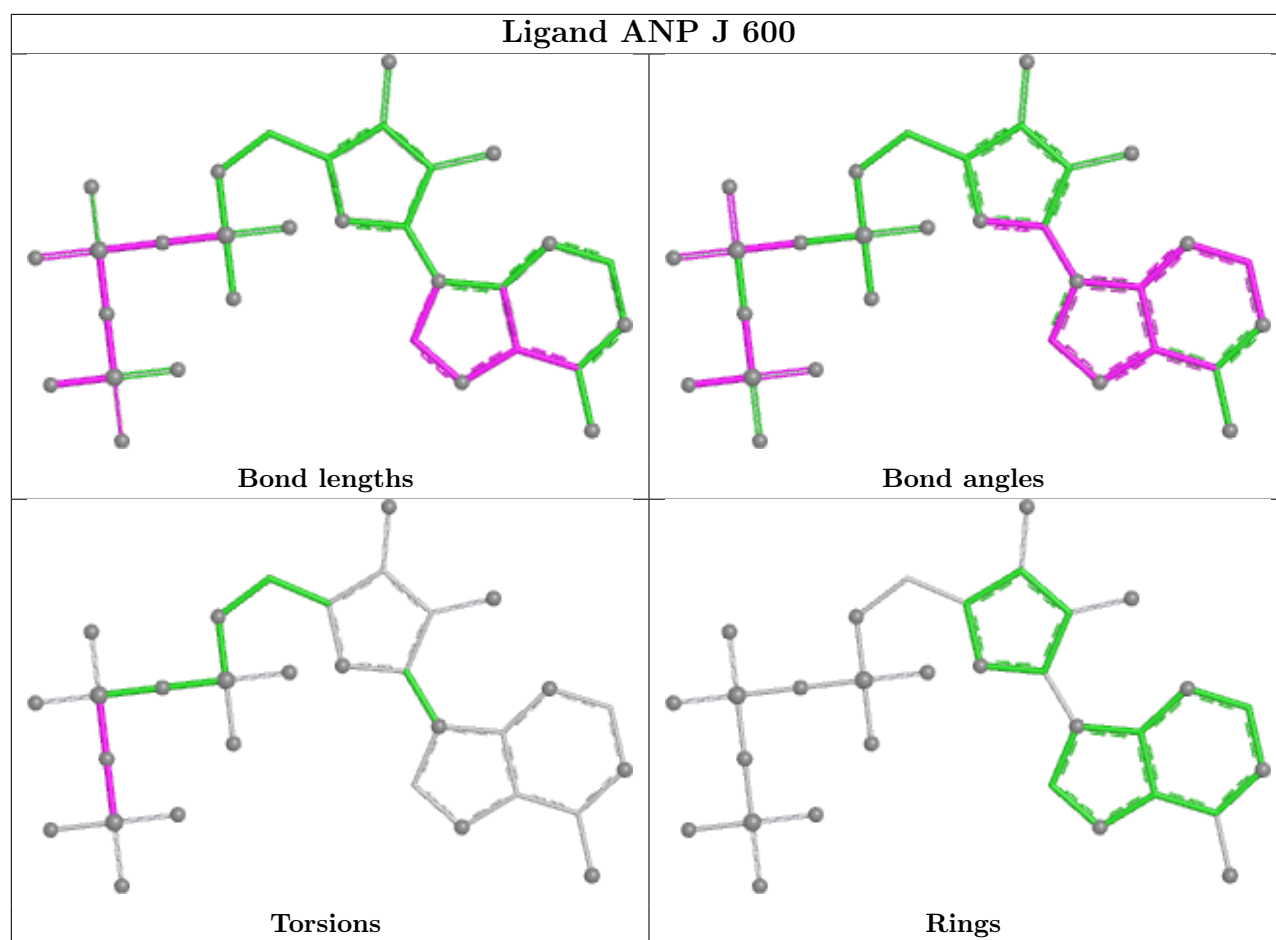


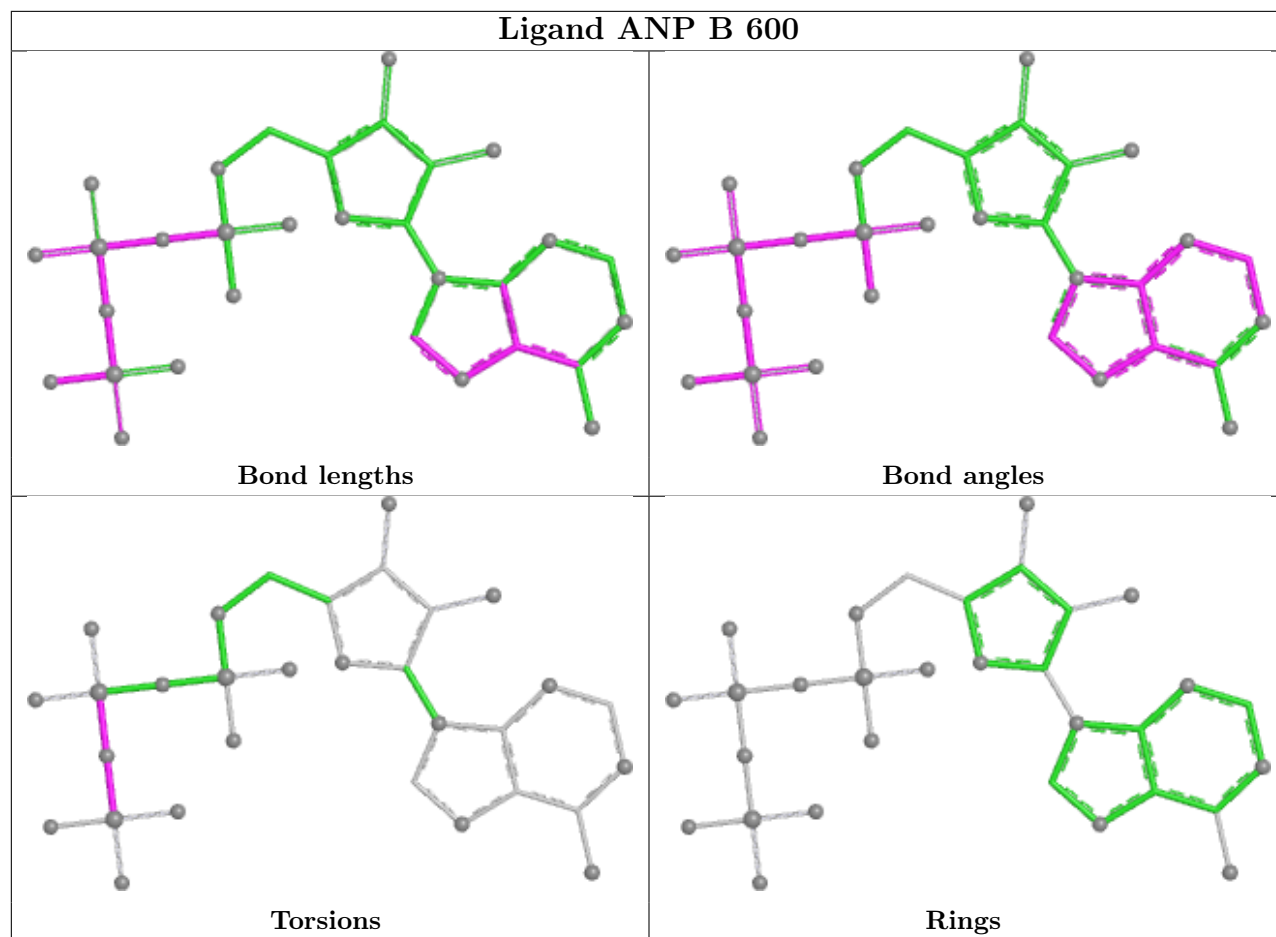


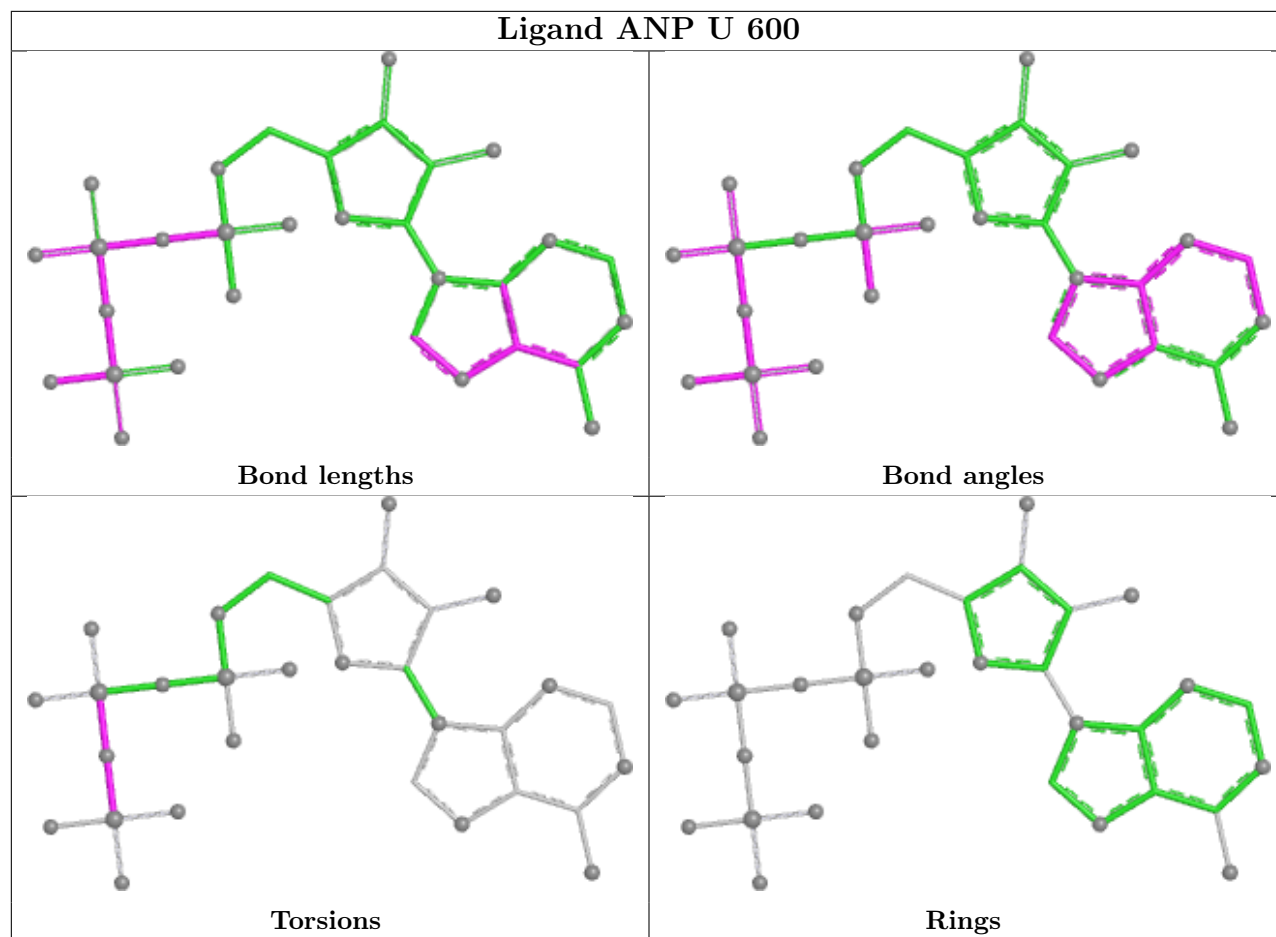


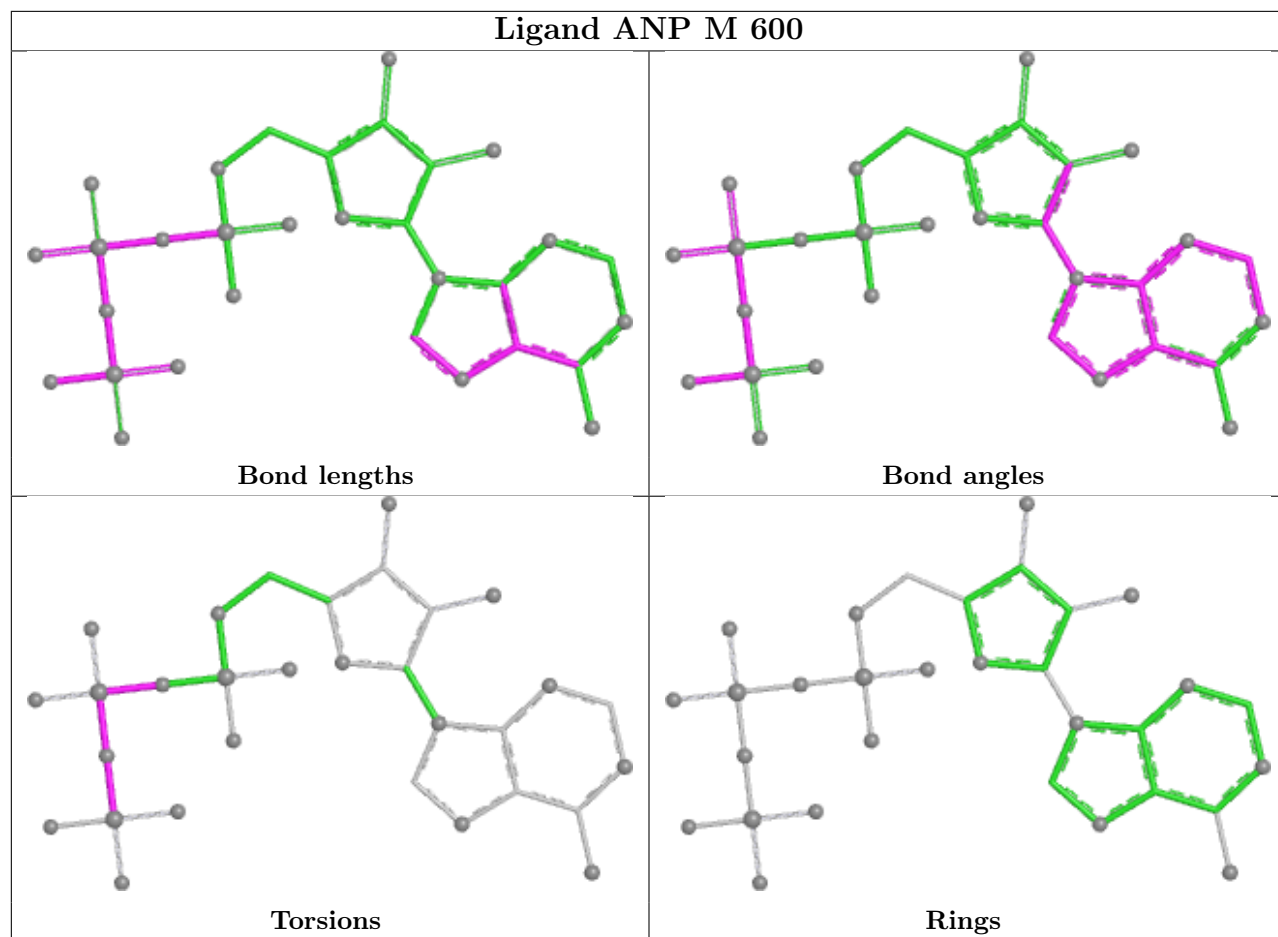


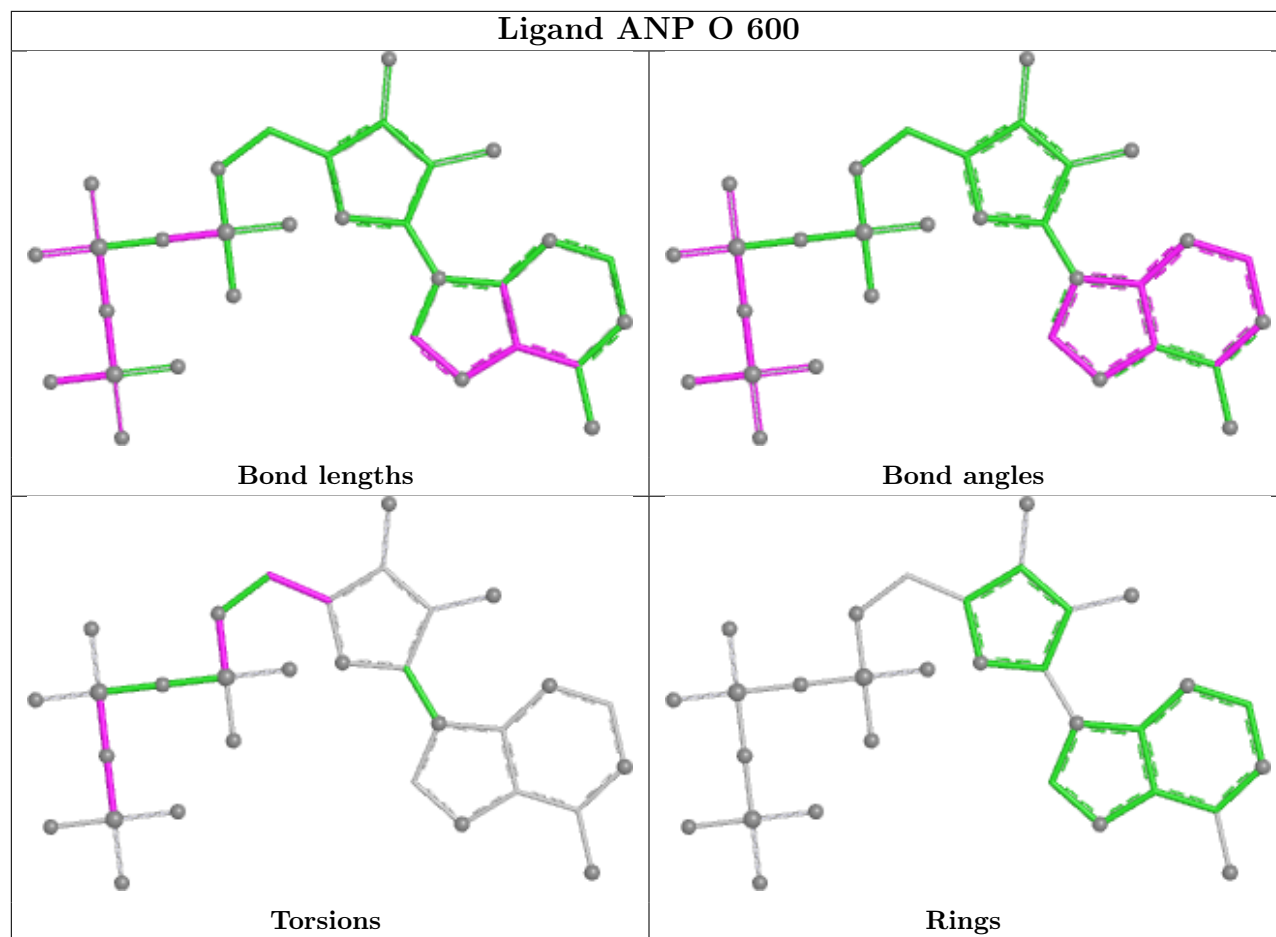


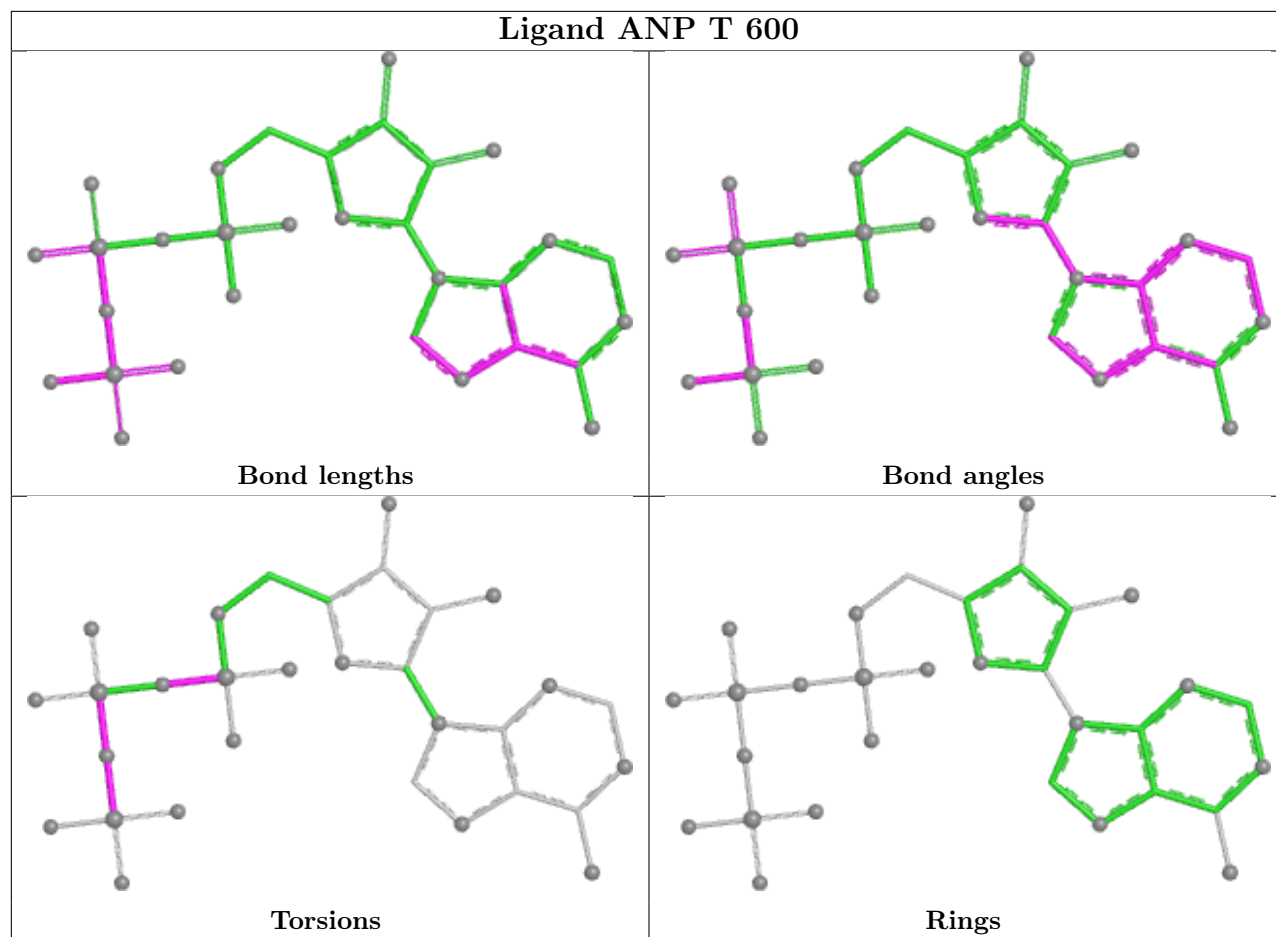


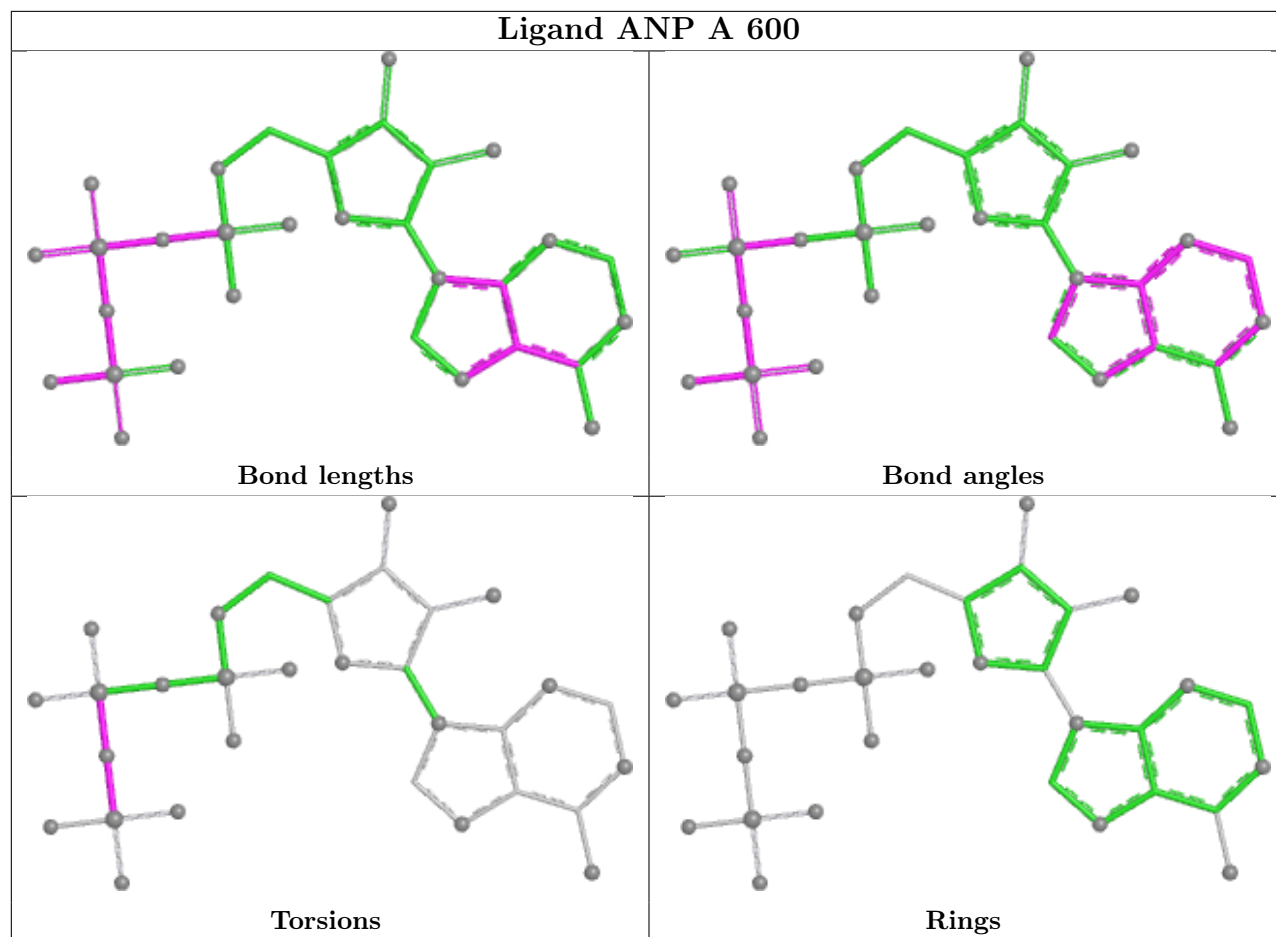












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	482/510 (94%)	0.51	9 (1%) 66 57	41, 64, 77, 93	0
1	B	483/510 (94%)	0.80	42 (8%) 16 11	49, 69, 89, 110	0
1	C	484/510 (94%)	0.63	22 (4%) 38 30	48, 66, 86, 108	0
1	J	481/510 (94%)	0.59	26 (5%) 31 24	50, 65, 82, 103	0
1	K	486/510 (95%)	0.81	42 (8%) 16 12	55, 72, 84, 107	0
1	L	482/510 (94%)	0.65	22 (4%) 37 29	49, 66, 82, 100	0
1	S	480/510 (94%)	0.51	14 (2%) 53 43	59, 71, 84, 99	0
1	T	481/510 (94%)	0.70	23 (4%) 35 28	54, 68, 84, 123	0
1	U	481/510 (94%)	0.65	25 (5%) 33 25	51, 67, 86, 111	0
2	D	470/478 (98%)	0.61	21 (4%) 38 30	45, 67, 93, 107	0
2	E	468/478 (97%)	1.18	108 (23%) 2 1	44, 68, 87, 100	0
2	F	469/478 (98%)	0.56	10 (2%) 63 54	51, 67, 83, 104	0
2	M	470/478 (98%)	0.64	19 (4%) 42 33	46, 66, 90, 112	0
2	N	470/478 (98%)	0.74	29 (6%) 26 20	53, 69, 88, 115	0
2	O	468/478 (97%)	0.61	17 (3%) 46 37	50, 68, 85, 102	0
2	V	470/478 (98%)	0.74	34 (7%) 21 16	57, 74, 94, 135	0
2	W	467/478 (97%)	0.56	26 (5%) 30 23	54, 67, 85, 108	0
2	X	469/478 (98%)	0.93	46 (9%) 13 9	54, 72, 90, 124	0
3	G	265/278 (95%)	0.79	5 (1%) 66 57	21, 64, 90, 97	0
3	P	243/278 (87%)	1.23	39 (16%) 5 4	28, 93, 121, 127	0
3	Y	200/278 (71%)	0.95	7 (3%) 47 38	64, 107, 127, 132	0
4	H	120/138 (86%)	1.38	18 (15%) 5 4	60, 91, 129, 131	0
4	Q	84/138 (60%)	1.30	12 (14%) 6 5	88, 107, 134, 137	0
4	Z	17/138 (12%)	1.52	4 (23%) 2 1	132, 134, 140, 140	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
5	1	27/61 (44%)	1.28	7 (25%) 1 1	107, 111, 115, 115	0
5	I	48/61 (78%)	1.18	5 (10%) 11 8	71, 84, 93, 94	0
5	R	34/61 (55%)	1.22	4 (11%) 9 7	95, 103, 112, 115	0
All	All	9599/10323 (92%)	0.73	636 (6%) 24 18	21, 69, 99, 140	0

All (636) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	U	94	GLY	5.5
2	M	395	GLU	5.2
1	K	379	ALA	5.0
1	B	26	ASN	4.9
2	X	76	VAL	4.7
2	W	358	LEU	4.5
2	E	30	LEU	4.5
1	J	416	THR	4.4
2	E	9	ILE	4.4
1	T	87	GLY	4.4
2	E	70	LEU	4.4
1	B	397	ALA	4.3
2	E	275	ILE	4.3
1	L	506	PHE	4.2
2	X	51	ALA	4.1
2	F	80	GLY	4.1
4	H	101	ILE	4.1
2	E	31	PRO	4.1
2	E	13	VAL	4.0
3	Y	134	GLY	4.0
1	T	29	GLU	4.0
2	E	54	LEU	3.9
2	O	30	LEU	3.9
2	E	473	LEU	3.9
2	V	474	ALA	3.9
2	E	14	THR	3.9
3	P	91	LEU	3.9
1	J	93	THR	3.8
1	K	22	SER	3.8
2	E	72	ARG	3.8
1	T	93	THR	3.8
2	E	58	THR	3.8
2	E	277	SER	3.7

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Mol	Chain	Res	Type	RSRZ
2	V	80	GLY	3.7
2	O	59	VAL	3.7
2	V	10	THR	3.7
4	Q	48	THR	3.7
1	K	27	LEU	3.7
1	J	503	THR	3.6
1	J	491	LEU	3.6
1	L	27	LEU	3.6
2	E	51	ALA	3.6
1	K	26	ASN	3.6
2	E	36	ALA	3.6
1	L	464	GLY	3.6
3	P	95	VAL	3.6
3	P	57	THR	3.6
2	O	92	LEU	3.6
2	E	55	GLY	3.6
2	E	53	HIS	3.5
1	B	94	GLY	3.5
2	E	56	GLU	3.5
2	E	15	ALA	3.5
1	K	407	GLN	3.5
2	X	8	PRO	3.5
2	D	208	ASN	3.5
5	I	49	ASN	3.5
3	P	151	LEU	3.4
1	J	29	GLU	3.4
2	E	276	PRO	3.4
1	T	47	ASN	3.4
2	W	84	SER	3.4
1	C	30	THR	3.4
2	E	71	VAL	3.4
3	P	130	ILE	3.4
2	E	25	PHE	3.4
2	X	248	GLY	3.4
1	T	346	SER	3.4
2	X	390	ILE	3.4
2	E	46	LEU	3.3
2	E	80	GLY	3.3
2	E	220	GLY	3.3
2	E	273	GLY	3.3
2	W	82	PRO	3.3
3	P	99	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
3	P	155	LYS	3.3
1	K	505	SER	3.3
1	U	379	ALA	3.2
2	E	270	ALA	3.2
2	M	25	PHE	3.2
3	P	165	PHE	3.2
2	D	391	LEU	3.2
2	M	358	LEU	3.2
2	E	284	THR	3.2
1	L	410	SER	3.2
3	P	188	ILE	3.2
2	V	59	VAL	3.2
2	W	12	LYS	3.2
1	A	94	GLY	3.2
2	X	393	MET	3.2
2	E	22	ASP	3.2
2	N	465	ASP	3.2
3	P	105	ALA	3.2
2	E	59	VAL	3.2
2	E	18	GLY	3.2
1	T	509	THR	3.2
2	M	10	THR	3.2
2	E	34	LEU	3.1
1	T	406	ALA	3.1
5	1	11	ALA	3.1
2	O	80	GLY	3.1
2	W	8	PRO	3.1
2	X	82	PRO	3.1
3	P	71	LYS	3.1
1	C	28	ASN	3.1
1	T	482	LEU	3.1
2	E	24	HIS	3.1
2	E	283	PRO	3.1
2	E	52	GLN	3.1
2	E	33	ILE	3.1
1	J	27	LEU	3.1
4	H	115	SER	3.0
2	E	60	ARG	3.0
3	P	207	ARG	3.0
1	C	499	LEU	3.0
2	O	31	PRO	3.0
1	C	272	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	U	411	ASP	3.0
1	L	455	LEU	3.0
2	V	327	ALA	3.0
2	E	457	PHE	3.0
1	B	400	ARG	3.0
1	U	28	ASN	3.0
2	E	76	VAL	3.0
2	E	62	ILE	3.0
2	E	263	GLN	3.0
4	H	95	SER	3.0
2	F	79	THR	3.0
2	X	240	ALA	3.0
1	L	90	VAL	3.0
2	E	48	LEU	2.9
2	E	66	GLY	2.9
1	T	28	ASN	2.9
2	E	35	ASN	2.9
1	B	508	ALA	2.9
2	E	17	ILE	2.9
2	E	73	GLY	2.9
2	N	31	PRO	2.9
4	Q	47	PRO	2.9
1	J	28	ASN	2.9
2	M	394	ASP	2.9
5	1	9	SER	2.9
1	B	36	VAL	2.9
1	K	33	VAL	2.9
3	P	37	ALA	2.9
1	J	89	LEU	2.9
2	F	11	GLY	2.9
2	E	282	GLN	2.9
2	E	268	VAL	2.9
4	H	97	SER	2.9
2	X	162	GLY	2.8
2	V	13	VAL	2.8
1	B	28	ASN	2.8
1	U	26	ASN	2.8
1	J	195	SER	2.8
1	K	72	GLN	2.8
2	X	74	GLU	2.8
1	K	28	ASN	2.8
4	Q	132	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
3	Y	40	SER	2.8
2	X	205	GLY	2.8
5	R	44	TYR	2.8
3	P	126	ILE	2.8
5	R	14	LEU	2.8
3	P	167	ASN	2.8
1	B	393	LYS	2.8
2	E	269	SER	2.8
2	F	179	GLY	2.8
2	V	8	PRO	2.8
4	H	122	GLU	2.7
4	Q	84	CYS	2.7
1	K	90	VAL	2.7
1	B	301	PHE	2.7
2	W	9	ILE	2.7
3	P	74	ILE	2.7
2	E	61	THR	2.7
2	E	19	ALA	2.7
2	V	9	ILE	2.7
2	D	359	ASP	2.7
1	J	410	SER	2.7
2	M	84	SER	2.7
1	U	174	GLN	2.7
1	U	29	GLU	2.7
1	B	283	LEU	2.7
1	K	68	LEU	2.7
2	E	285	LEU	2.7
2	N	30	LEU	2.7
2	E	281	TYR	2.7
4	H	100	ASN	2.7
1	B	298	GLY	2.7
4	H	126	GLN	2.7
2	X	13	VAL	2.7
1	T	371	LEU	2.7
3	P	111	GLY	2.7
2	N	359	ASP	2.7
3	P	27	ALA	2.6
2	W	80	GLY	2.6
1	K	48	ASN	2.6
1	L	507	VAL	2.6
2	E	272	LEU	2.6
2	V	390	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	506	PHE	2.6
2	E	266	SER	2.6
3	P	92	ALA	2.6
2	N	403	THR	2.6
2	V	79	THR	2.6
1	U	394	LEU	2.6
1	S	49	ILE	2.6
1	S	236	ALA	2.6
1	U	43	VAL	2.6
2	O	7	THR	2.6
2	D	246	GLU	2.6
2	E	222	MET	2.6
2	E	474	ALA	2.6
2	M	359	ASP	2.6
2	N	421	ALA	2.6
2	V	25	PHE	2.6
2	D	400	ASP	2.6
2	X	394	ASP	2.6
1	J	91	LYS	2.6
2	M	82	PRO	2.6
2	V	12	LYS	2.6
2	D	248	GLY	2.6
2	E	37	LEU	2.6
2	E	23	VAL	2.6
1	A	380	ALA	2.6
1	C	408	PHE	2.6
3	P	200	ASP	2.6
1	S	27	LEU	2.5
1	U	46	LEU	2.5
2	E	265	GLY	2.5
2	E	317	LEU	2.5
2	F	160	GLY	2.5
2	X	81	GLY	2.5
1	B	84	VAL	2.5
2	V	344	ILE	2.5
2	V	387	ILE	2.5
2	W	390	ILE	2.5
3	Y	77	ILE	2.5
2	N	79	THR	2.5
2	X	284	THR	2.5
3	G	48	GLU	2.5
1	B	265	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	272	ASP	2.5
1	S	411	ASP	2.5
3	P	202	ASP	2.5
2	E	301	LYS	2.5
2	E	226	PRO	2.5
2	E	280	GLY	2.5
2	F	180	GLY	2.5
2	N	81	GLY	2.5
2	N	160	GLY	2.5
2	N	392	GLY	2.5
2	W	81	GLY	2.5
1	U	507	VAL	2.5
2	W	13	VAL	2.5
2	W	79	THR	2.5
2	X	464	GLU	2.5
1	J	174	GLN	2.5
1	S	44	PHE	2.5
1	T	407	GLN	2.5
1	B	389	ALA	2.5
1	C	380	ALA	2.5
2	E	228	ALA	2.5
1	A	28	ASN	2.5
2	W	359	ASP	2.5
2	X	359	ASP	2.5
2	D	55	GLY	2.5
2	E	69	GLY	2.5
3	P	110	ILE	2.5
1	T	55	VAL	2.5
2	V	161	VAL	2.5
1	J	318	GLU	2.5
1	B	416	THR	2.5
1	J	502	ALA	2.5
1	S	93	THR	2.5
2	V	7	THR	2.5
3	P	185	ALA	2.5
3	P	203	ALA	2.5
4	Q	31	ASN	2.5
2	X	391	LEU	2.5
3	P	206	PRO	2.5
2	V	157	GLY	2.5
3	P	162	ILE	2.5
2	N	13	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	K	246	TYR	2.5
2	W	124	PHE	2.5
1	A	51	ALA	2.5
1	B	35	ALA	2.5
4	Q	15	ALA	2.5
2	V	391	LEU	2.4
4	H	12	LEU	2.4
1	K	195	SER	2.4
1	T	260	ARG	2.4
1	A	508	ALA	2.4
1	K	488	LYS	2.4
1	S	205	TYR	2.4
2	M	443	ALA	2.4
2	W	474	ALA	2.4
1	L	93	THR	2.4
2	E	10	THR	2.4
2	M	79	THR	2.4
2	E	64	MET	2.4
2	N	54	LEU	2.4
1	K	463	ILE	2.4
2	E	227	GLY	2.4
4	H	113	SER	2.4
1	K	53	GLU	2.4
2	N	29	GLU	2.4
2	N	457	PHE	2.4
3	P	38	LYS	2.4
1	U	407	GLN	2.4
2	X	148	ALA	2.4
1	T	175	THR	2.4
2	D	10	THR	2.4
2	X	79	THR	2.4
3	P	213	THR	2.4
1	J	412	LEU	2.4
2	N	451	ASN	2.4
4	H	47	PRO	2.4
2	X	395	GLU	2.4
1	A	131	ALA	2.4
2	E	456	ALA	2.4
2	E	449	TYR	2.4
2	M	24	HIS	2.4
1	B	77	LEU	2.4
1	U	34	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
2	E	271	LEU	2.4
2	M	30	LEU	2.4
2	V	358	LEU	2.4
3	Y	270	ILE	2.4
1	J	26	ASN	2.4
2	N	283	PRO	2.4
1	B	85	LYS	2.4
1	K	362	GLY	2.4
2	E	188	GLY	2.4
2	W	85	VAL	2.4
1	J	353	PHE	2.4
2	W	105	GLU	2.4
1	K	25	ALA	2.4
4	Z	126	GLN	2.4
1	B	302	TYR	2.4
1	U	509	THR	2.4
1	T	267	LEU	2.4
2	N	53	HIS	2.4
2	V	133	ILE	2.4
2	X	99	ILE	2.4
1	B	73	VAL	2.3
1	C	402	VAL	2.3
1	J	43	VAL	2.3
1	K	99	VAL	2.3
1	U	84	VAL	2.3
1	U	99	VAL	2.3
4	Z	132	ASN	2.3
1	T	238	ALA	2.3
2	E	74	GLU	2.3
2	X	389	ALA	2.3
1	A	27	LEU	2.3
1	K	503	THR	2.3
2	N	58	THR	2.3
3	P	50	LEU	2.3
4	H	83	LEU	2.3
2	N	387	ILE	2.3
2	E	50	VAL	2.3
2	E	467	VAL	2.3
2	M	71	VAL	2.3
2	N	467	VAL	2.3
1	C	26	ASN	2.3
1	C	162	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	L	104	GLY	2.3
1	T	334	GLY	2.3
2	E	81	GLY	2.3
3	G	59	ASN	2.3
2	N	424	PHE	2.3
1	J	35	ALA	2.3
2	M	26	GLU	2.3
2	W	398	GLU	2.3
2	W	393	MET	2.3
2	O	79	THR	2.3
2	V	14	THR	2.3
3	G	57	THR	2.3
2	D	423	VAL	2.3
2	X	370	VAL	2.3
1	C	197	GLU	2.3
1	K	35	ALA	2.3
1	K	414	ALA	2.3
1	L	508	ALA	2.3
2	E	78	ASP	2.3
2	E	359	ASP	2.3
1	K	371	LEU	2.3
1	K	418	GLN	2.3
2	M	391	LEU	2.3
4	H	130	LEU	2.3
4	Q	13	GLN	2.3
1	J	492	SER	2.3
1	S	80	SER	2.3
2	M	33	ILE	2.3
2	X	303	SER	2.3
1	U	90	VAL	2.3
2	X	71	VAL	2.3
3	P	169	PRO	2.3
1	J	423	GLY	2.3
2	M	81	GLY	2.3
1	K	47	ASN	2.3
2	E	259	PHE	2.3
5	1	43	PHE	2.3
1	L	449	ALA	2.3
1	S	279	ALA	2.3
2	X	341	GLU	2.3
5	I	18	ALA	2.3
1	B	491	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	K	482	LEU	2.3
1	L	420	LEU	2.3
2	E	77	LEU	2.3
2	N	176	LYS	2.3
1	B	345	ILE	2.3
1	T	485	ILE	2.3
2	E	39	ILE	2.3
2	O	53	HIS	2.3
1	A	509	THR	2.3
2	D	7	THR	2.3
1	K	73	VAL	2.3
1	C	94	GLY	2.3
2	M	179	GLY	2.3
2	X	457	PHE	2.2
1	J	414	ALA	2.2
1	U	508	ALA	2.2
2	D	474	ALA	2.2
4	H	119	GLU	2.2
2	V	396	LEU	2.2
3	P	73	LEU	2.2
1	K	91	LYS	2.2
5	I	41	ASP	2.2
1	B	445	PRO	2.2
3	P	109	THR	2.2
4	Q	36	SER	2.2
1	U	45	GLY	2.2
2	V	73	GLY	2.2
2	V	159	ALA	2.2
1	K	46	LEU	2.2
1	K	67	ASN	2.2
1	L	499	LEU	2.2
1	K	347	ILE	2.2
2	V	83	ILE	2.2
1	K	454	HIS	2.2
1	T	92	ARG	2.2
2	E	21	VAL	2.2
2	X	161	VAL	2.2
2	X	206	VAL	2.2
1	L	94	GLY	2.2
2	X	11	GLY	2.2
1	B	65	ALA	2.2
1	C	420	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	N	300	LYS	2.2
2	E	29	GLU	2.2
2	V	36	ALA	2.2
2	N	316	ASP	2.2
1	B	90	VAL	2.2
1	L	509	THR	2.2
1	T	237	THR	2.2
2	E	79	THR	2.2
2	D	211	GLY	2.2
2	X	157	GLY	2.2
3	P	134	GLY	2.2
1	B	405	PHE	2.2
4	Q	74	PHE	2.2
1	L	68	LEU	2.2
2	F	358	LEU	2.2
2	O	113	LEU	2.2
2	W	209	LEU	2.2
2	X	396	LEU	2.2
3	Y	10	LEU	2.2
1	K	86	GLU	2.2
2	E	446	GLU	2.2
2	X	456	ALA	2.2
1	B	49	ILE	2.2
1	B	387	GLN	2.2
2	O	27	GLN	2.2
1	J	55	VAL	2.2
1	K	300	VAL	2.2
2	N	78	ASP	2.2
2	V	276	PRO	2.2
3	P	170	VAL	2.2
1	K	416	THR	2.2
2	E	262	THR	2.2
1	L	176	GLY	2.2
2	D	80	GLY	2.2
2	V	158	GLY	2.2
2	X	158	GLY	2.2
5	1	13	TYR	2.2
1	K	492	SER	2.2
2	D	396	LEU	2.2
1	S	65	ALA	2.2
2	F	327	ALA	2.2
1	B	306	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
2	E	83	ILE	2.1
2	E	229	ARG	2.1
2	E	274	ARG	2.1
2	V	62	ILE	2.1
2	V	109	ILE	2.1
4	Q	126	GLN	2.1
2	E	225	PRO	2.1
2	E	320	PRO	2.1
5	I	56	PRO	2.1
2	E	316	ASP	2.1
2	E	75	LYS	2.1
2	W	227	GLY	2.1
1	U	495	LEU	2.1
5	I	10	TYR	2.1
1	C	389	ALA	2.1
1	J	508	ALA	2.1
1	L	397	ALA	2.1
1	S	414	ALA	2.1
2	N	159	ALA	2.1
3	G	47	ALA	2.1
2	X	83	ILE	2.1
2	E	47	VAL	2.1
2	O	87	VAL	2.1
4	H	41	VAL	2.1
2	V	393	MET	2.1
1	C	91	LYS	2.1
1	U	85	LYS	2.1
1	K	509	THR	2.1
2	E	235	THR	2.1
2	E	287	THR	2.1
2	W	429	GLY	2.1
1	C	46	LEU	2.1
2	X	159	ALA	2.1
2	X	345	TYR	2.1
1	B	476	SER	2.1
1	S	458	ILE	2.1
2	D	275	ILE	2.1
2	E	267	GLU	2.1
2	O	83	ILE	2.1
2	X	410	ILE	2.1
1	S	407	GLN	2.1
2	F	249	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
2	W	168	GLN	2.1
2	E	85	VAL	2.1
2	E	373	LYS	2.1
1	C	89	LEU	2.1
1	T	27	LEU	2.1
1	U	63	GLY	2.1
2	M	113	LEU	2.1
2	N	358	LEU	2.1
2	N	445	LEU	2.1
2	W	280	GLY	2.1
2	W	414	LEU	2.1
2	E	298	THR	2.1
5	1	45	THR	2.1
1	B	279	ALA	2.1
1	C	508	ALA	2.1
1	B	88	GLU	2.1
1	J	360	TYR	2.1
2	D	390	ILE	2.1
2	E	20	ILE	2.1
2	E	99	ILE	2.1
2	E	321	ALA	2.1
2	N	278	ALA	2.1
2	X	39	ILE	2.1
3	G	105	ALA	2.1
1	B	58	SER	2.1
2	E	118	HIS	2.1
3	P	108	VAL	2.1
5	I	16	VAL	2.1
2	E	8	PRO	2.1
1	L	67	ASN	2.1
2	E	57	ASN	2.1
1	B	89	LEU	2.1
1	C	27	LEU	2.1
1	C	283	LEU	2.1
1	K	491	LEU	2.1
1	U	27	LEU	2.1
2	E	291	LEU	2.1
4	H	93	LEU	2.1
1	U	87	GLY	2.1
2	D	160	GLY	2.1
2	W	44	GLY	2.1
2	X	73	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	375	ARG	2.1
1	T	30	THR	2.1
2	X	403	THR	2.1
2	X	450	ASP	2.1
5	R	22	ARG	2.1
1	L	49	ILE	2.1
1	L	379	ALA	2.1
2	V	309	ALA	2.1
3	P	94	ALA	2.1
4	Z	121	ALA	2.1
2	V	74	GLU	2.1
5	1	10	TYR	2.1
1	B	346	SER	2.0
1	J	476	SER	2.0
1	K	313	LYS	2.0
2	O	84	SER	2.0
2	V	303	SER	2.0
2	X	28	SER	2.0
3	Y	79	SER	2.0
4	H	67	LYS	2.0
4	Q	82	GLN	2.0
1	B	48	ASN	2.0
1	B	412	LEU	2.0
2	O	237	LEU	2.0
1	C	298	GLY	2.0
1	B	175	THR	2.0
1	B	509	THR	2.0
2	W	278	ALA	2.0
2	X	22	ASP	2.0
1	B	494	GLU	2.0
1	C	465	GLU	2.0
2	O	26	GLU	2.0
3	Y	18	LYS	2.0
3	P	276	SER	2.0
4	H	23	SER	2.0
4	Z	135	SER	2.0
4	H	92	PRO	2.0
1	K	34	LEU	2.0
1	L	283	LEU	2.0
1	S	28	ASN	2.0
1	T	95	ASN	2.0
4	Q	100	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	71	GLY	2.0
1	K	301	PHE	2.0
2	D	392	GLY	2.0
3	P	182	ILE	2.0
2	D	278	ALA	2.0
2	E	230	ALA	2.0
2	O	331	ALA	2.0
2	X	10	THR	2.0
3	P	78	THR	2.0
5	R	20	ALA	2.0
2	D	386	ASP	2.0
2	O	359	ASP	2.0
1	U	399	TYR	2.0
2	F	242	TYR	2.0
2	D	460	VAL	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
6	MG	T	700	1/1	0.81	0.08	70,70,70,70	0
6	MG	K	700	1/1	0.82	0.08	52,52,52,52	0
8	PO4	N	800	5/5	0.82	0.18	78,80,84,85	0
7	ANP	X	600	31/31	0.83	0.12	50,61,79,81	0
6	MG	S	700	1/1	0.83	0.11	40,40,40,40	0
7	ANP	U	600	31/31	0.85	0.12	42,57,69,70	0
6	MG	U	700	1/1	0.85	0.14	78,78,78,78	0
7	ANP	T	600	31/31	0.85	0.11	66,89,91,97	0

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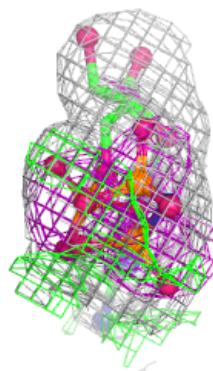
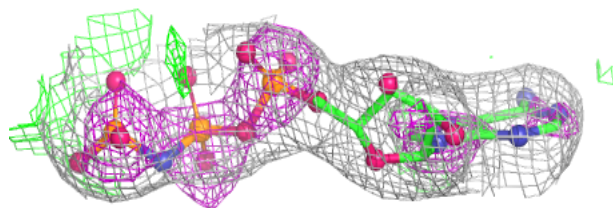
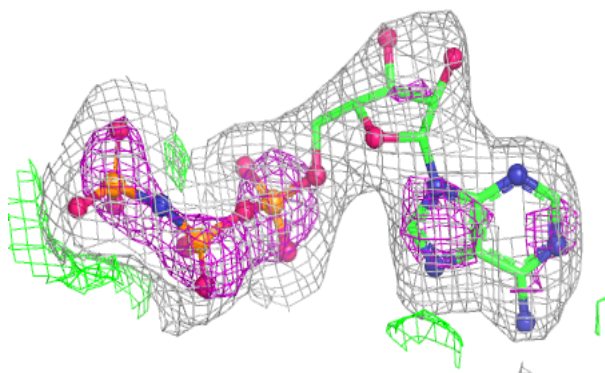
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	ANP	V	600	31/31	0.88	0.11	61,74,81,90	0
6	MG	O	700	1/1	0.89	0.14	48,48,48,48	0
7	ANP	S	600	31/31	0.90	0.12	37,52,58,63	0
6	MG	A	700	1/1	0.90	0.10	34,34,34,34	0
6	MG	B	700	1/1	0.91	0.07	43,43,43,43	0
6	MG	M	700	1/1	0.91	0.06	52,52,52,52	0
6	MG	X	700	1/1	0.91	0.07	67,67,67,67	0
6	MG	L	700	1/1	0.92	0.06	49,49,49,49	0
7	ANP	B	600	31/31	0.92	0.10	29,37,41,44	0
7	ANP	K	600	31/31	0.92	0.11	49,62,70,74	0
7	ANP	O	600	31/31	0.92	0.11	49,68,71,74	0
6	MG	D	700	1/1	0.92	0.07	46,46,46,46	0
7	ANP	F	600	31/31	0.93	0.10	36,52,60,61	0
7	ANP	A	600	31/31	0.94	0.10	14,35,42,43	0
7	ANP	J	600	31/31	0.94	0.10	23,46,52,53	0
6	MG	C	700	1/1	0.94	0.09	43,43,43,43	0
7	ANP	L	600	31/31	0.94	0.11	17,33,44,48	0
7	ANP	M	600	31/31	0.94	0.10	31,52,59,65	0
7	ANP	C	600	31/31	0.94	0.10	25,41,50,60	0
6	MG	F	700	1/1	0.95	0.06	44,44,44,44	0
6	MG	V	700	1/1	0.95	0.06	69,69,69,69	0
7	ANP	D	600	31/31	0.95	0.10	37,51,57,64	0
6	MG	J	700	1/1	0.96	0.06	30,30,30,30	0

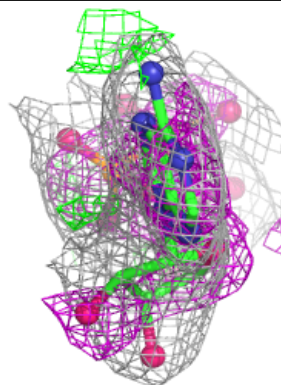
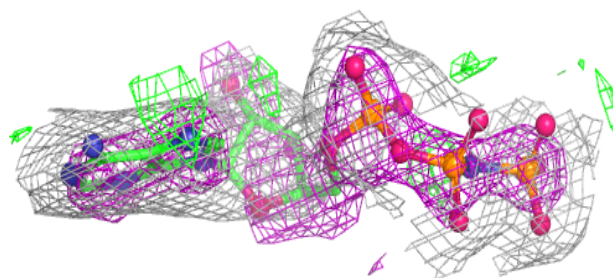
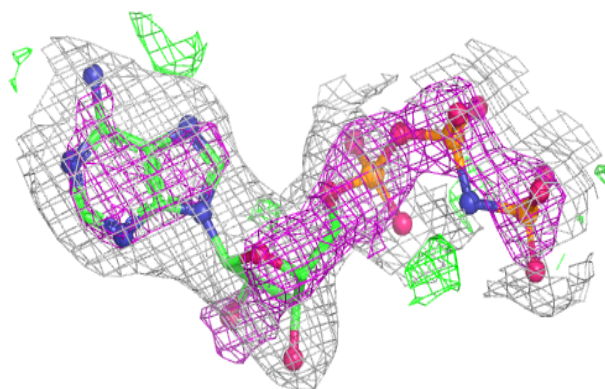
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ANP X 600:

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

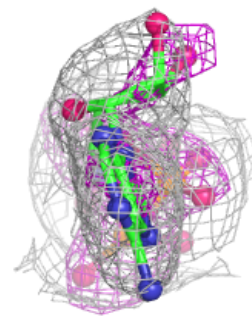
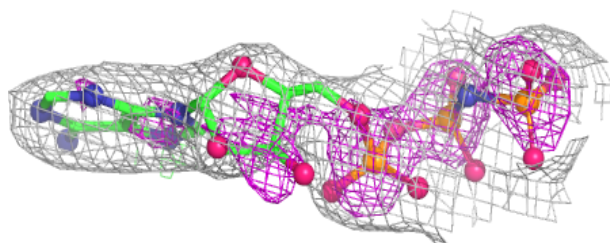
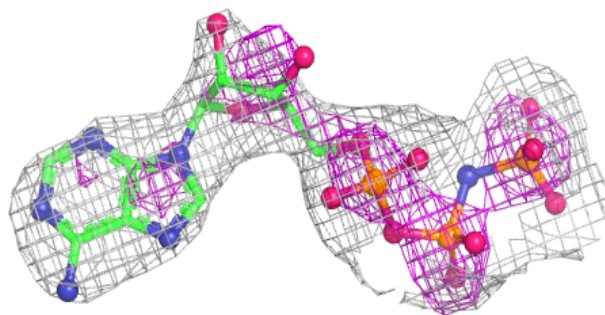
**Electron density around ANP U 600:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

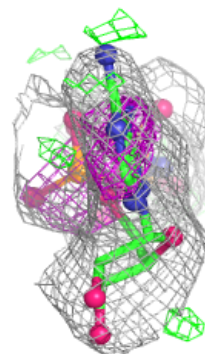
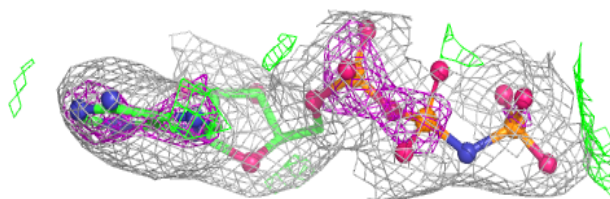
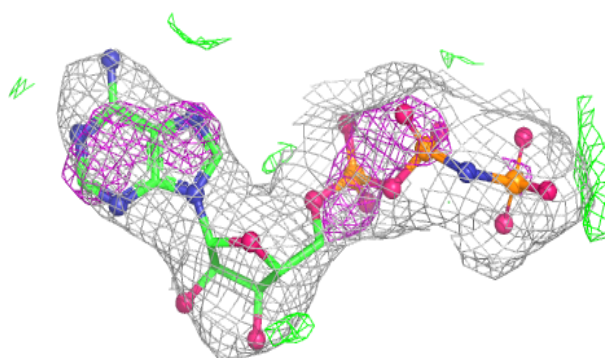


Electron density around ANP T 600:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

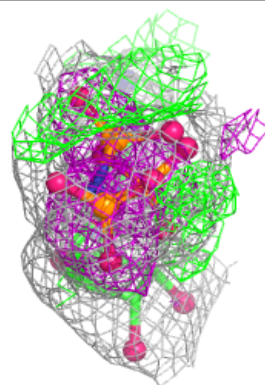
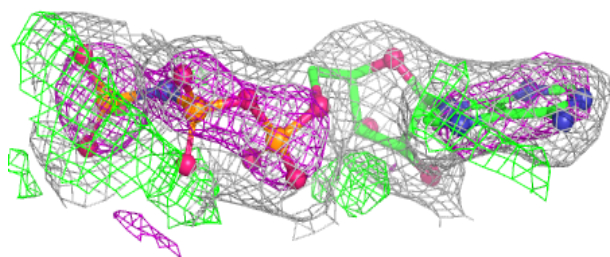
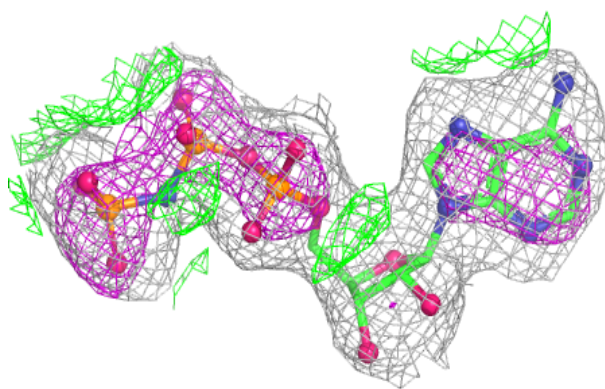
**Electron density around ANP V 600:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

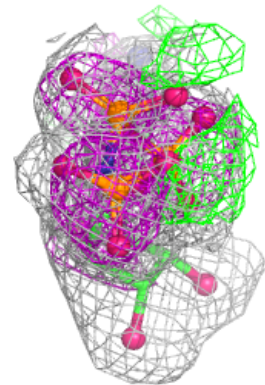
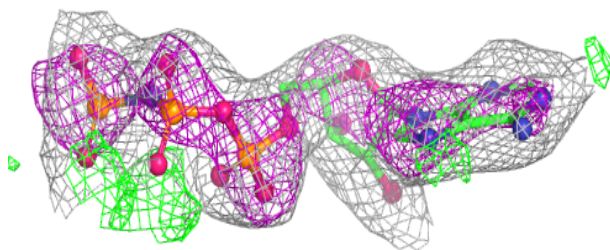
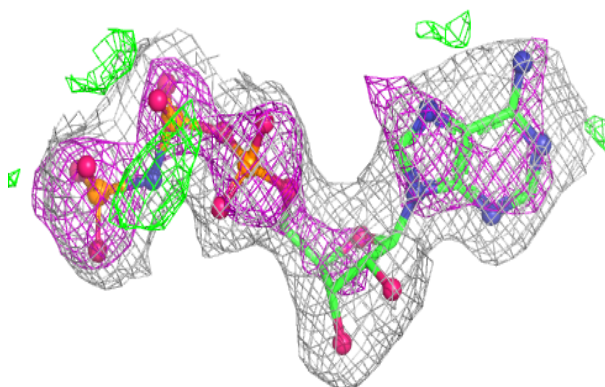


Electron density around ANP S 600:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

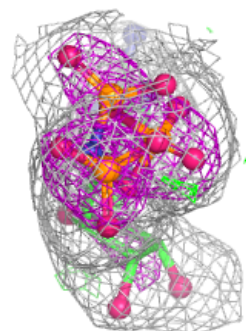
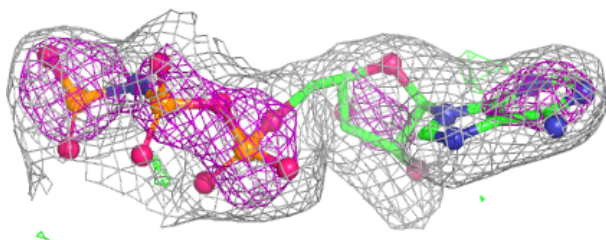
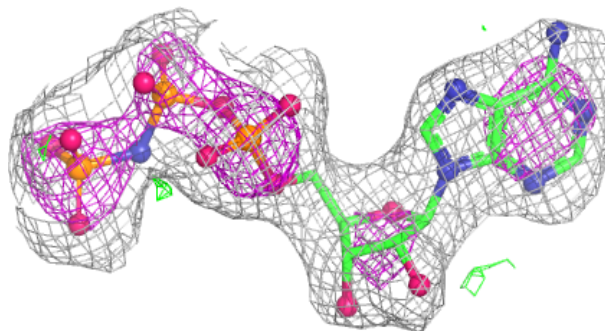
**Electron density around ANP B 600:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

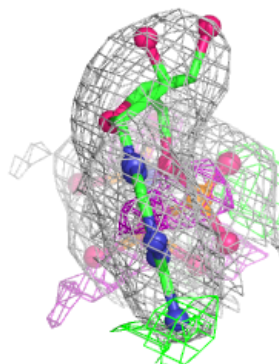
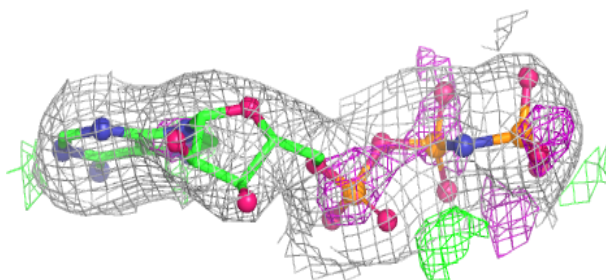
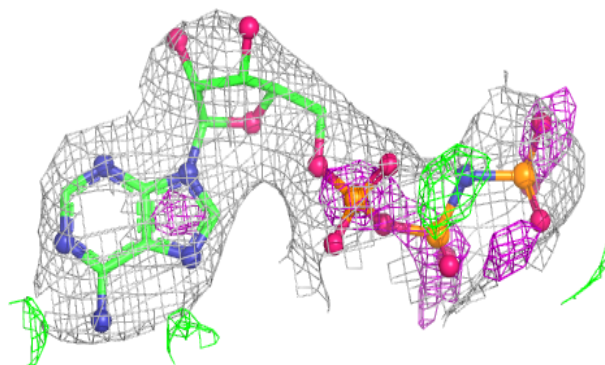


Electron density around ANP K 600:

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

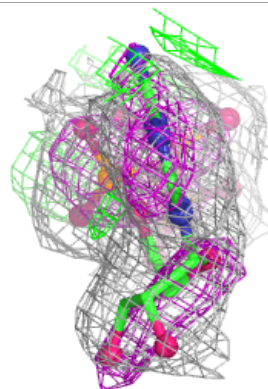
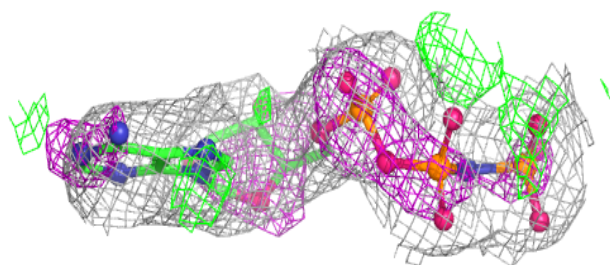
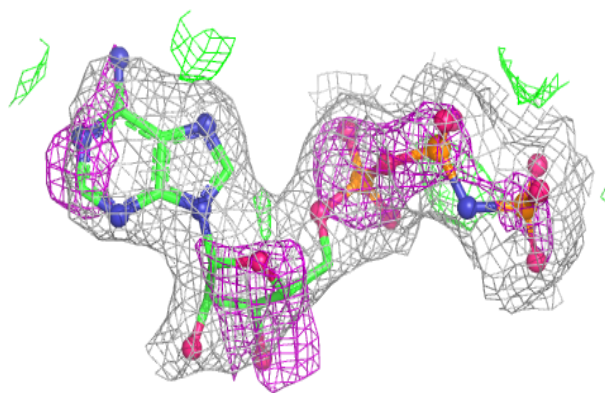
**Electron density around ANP O 600:**

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

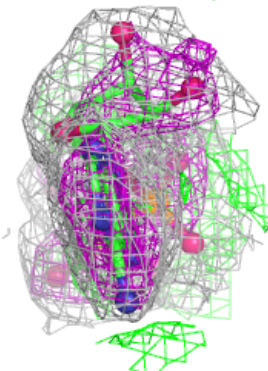
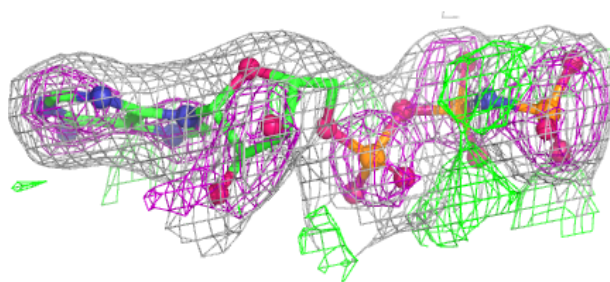
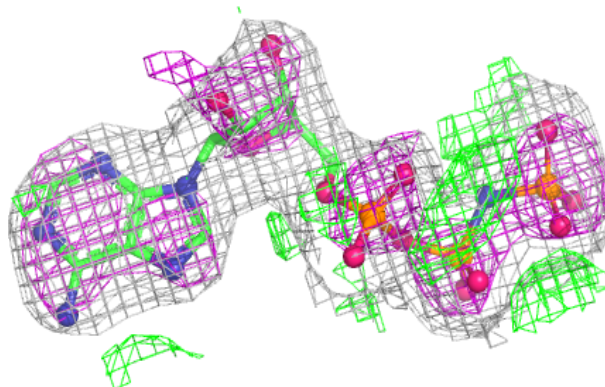


Electron density around ANP F 600:

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

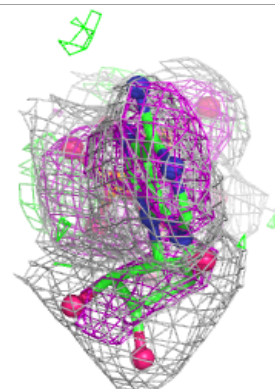
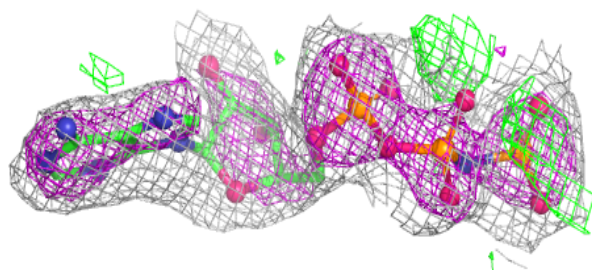
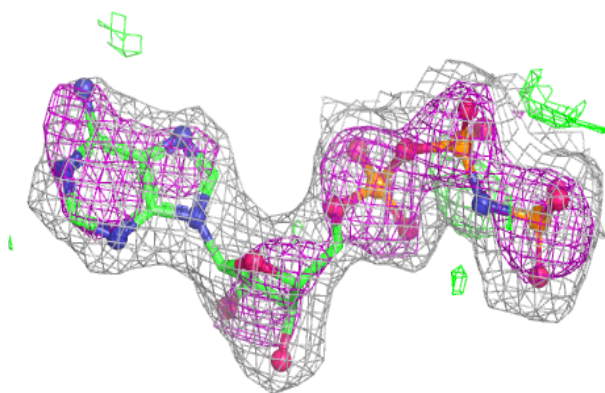
**Electron density around ANP A 600:**

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

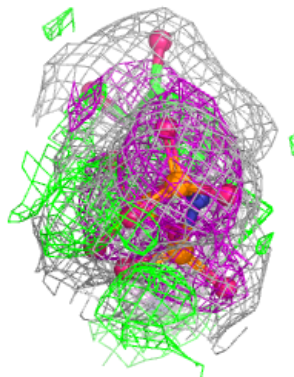
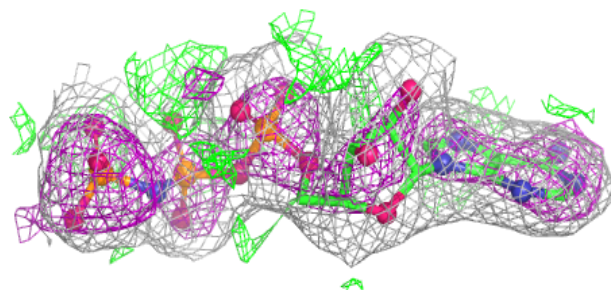
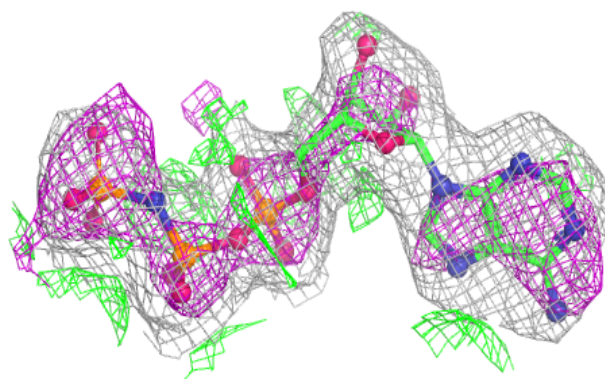


Electron density around ANP J 600:

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

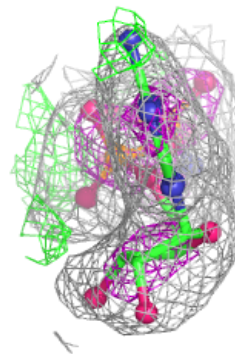
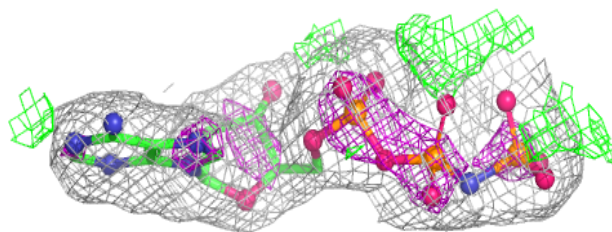
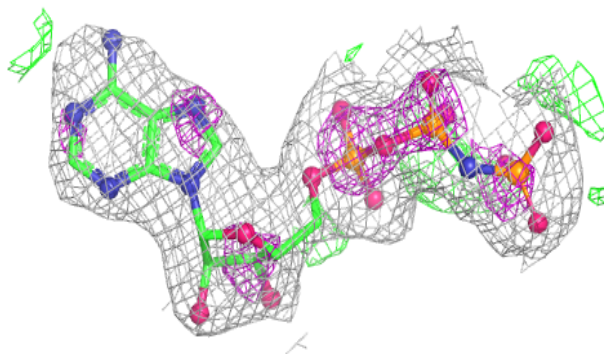
**Electron density around ANP L 600:**

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

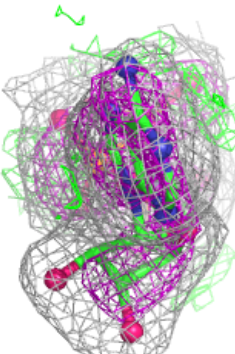
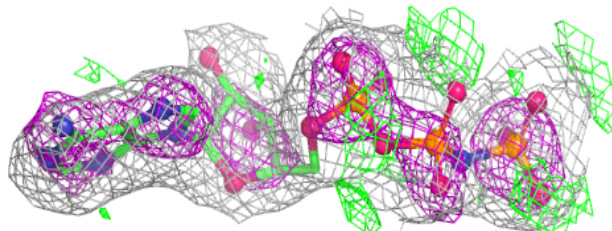
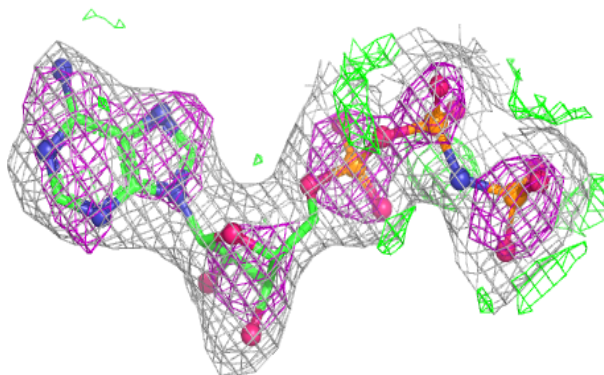


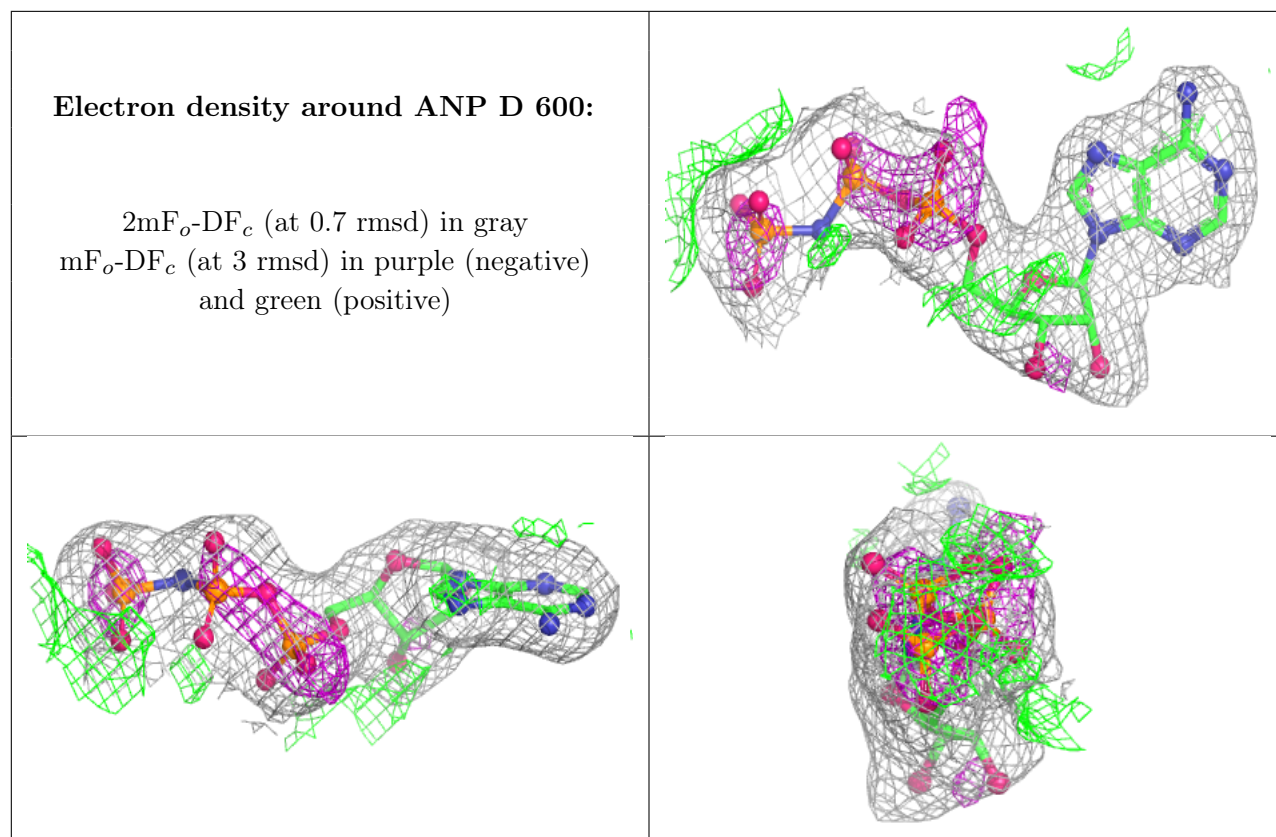
Electron density around ANP M 600:

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

**Electron density around ANP 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.