



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 30, 2026 – 10:28 AM UTC

PDB ID : 3OE7 / pdb_00003oe7
Title : Structure of four mutant forms of yeast f1 ATPase: gamma-I270T
Authors : Arsenieva, D.; Symersky, J.; Wang, Y.; Pagadala, V.; Mueller, D.M.
Deposited on : 2010-08-12
Resolution : 3.19 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

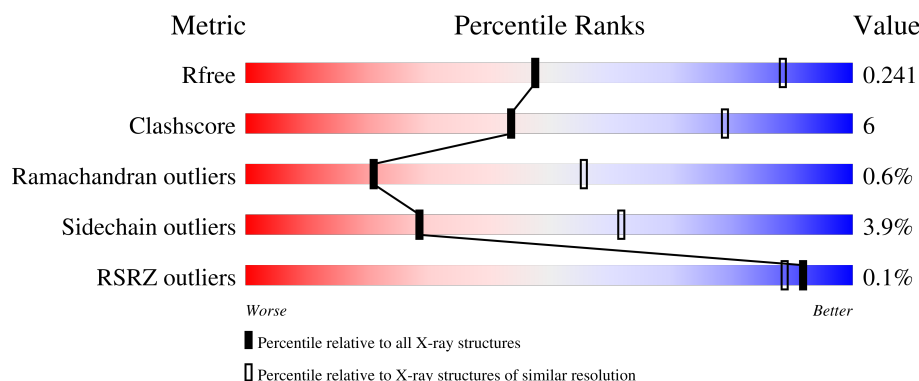
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.19 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



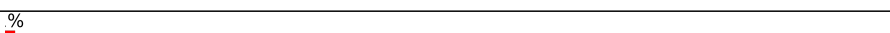
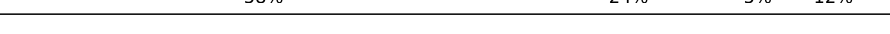
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	510	 76% 16% • 5%
1	B	510	 79% 14% • 5%
1	C	510	 82% 12% • 5%
1	J	510	 78% 15% • 6%
1	K	510	 78% 16% • 5%

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Mol	Chain	Length	Quality of chain
1	L	510	
1	S	510	
1	T	510	
1	U	510	
2	D	484	
2	E	484	
2	F	484	
2	M	484	
2	N	484	
2	O	484	
2	V	484	
2	W	484	
2	X	484	
3	G	278	
3	P	278	
3	Y	278	
4	H	137	
4	Q	137	
4	Z	137	
5	1	61	
5	I	61	
5	R	61	

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 72533 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ATP synthase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	482	Total	C	N	O	S	0	0	0
			3664	2314	648	699	3			
1	B	483	Total	C	N	O	S	0	0	0
			3669	2317	649	700	3			
1	C	484	Total	C	N	O	S	0	0	0
			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
			3694	2331	652	708	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 subunit beta.

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			

There are 72 discrepancies between the modelled and reference sequences:

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	265	Total	C	N	O	S	0	0	0
			2042	1282	356	394	10			
3	P	244	Total	C	N	O	S	0	0	0
			1847	1159	322	357	9			
3	Y	198	Total	C	N	O	S	0	0	0
			1356	827	250	272	7			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	270	THR	ILE	engineered mutation	UNP P38077
P	270	THR	ILE	engineered mutation	UNP P38077
Y	270	THR	ILE	engineered mutation	UNP P38077

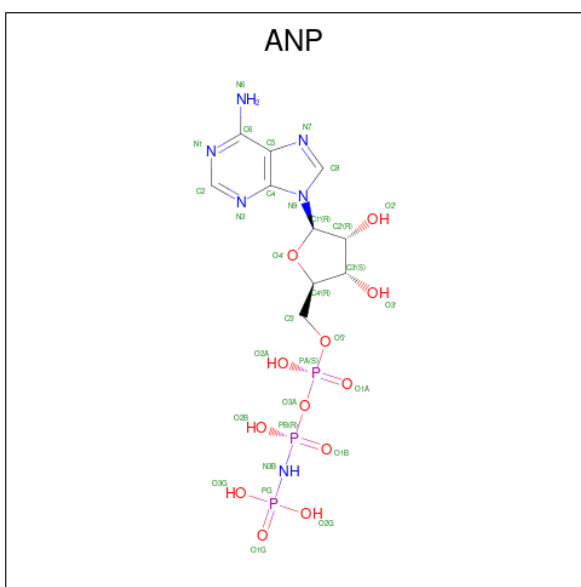
- Molecule 4 is a protein called ATP synthase subunit delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	120	Total	C	N	O	S	0	0	0
			775	484	135	154	2			
4	Q	84	Total	C	N	O		0	0	0
			449	271	88	90				
4	Z	15	Total	C	N	O		0	0	0
			75	45	15	15				

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	48	Total	C	N	O	0	0	0
			330	204	59	67			
5	R	31	Total	C	N	O	0	0	0
			173	107	32	34			
5	1	25	Total	C	N	O	0	0	0
			125	75	25	25			

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



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

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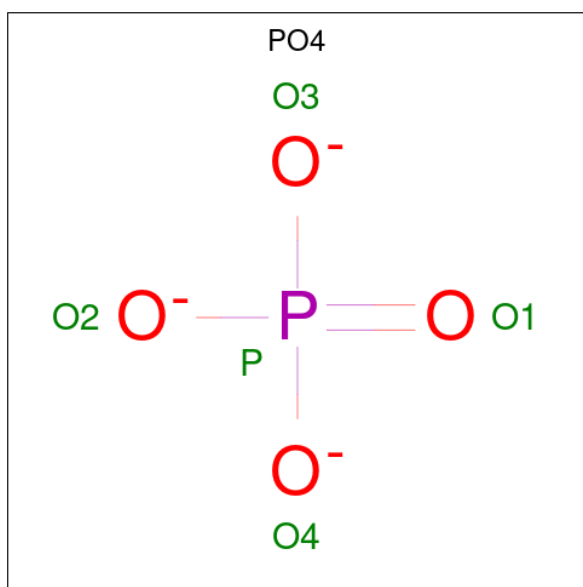
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	X	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

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

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

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

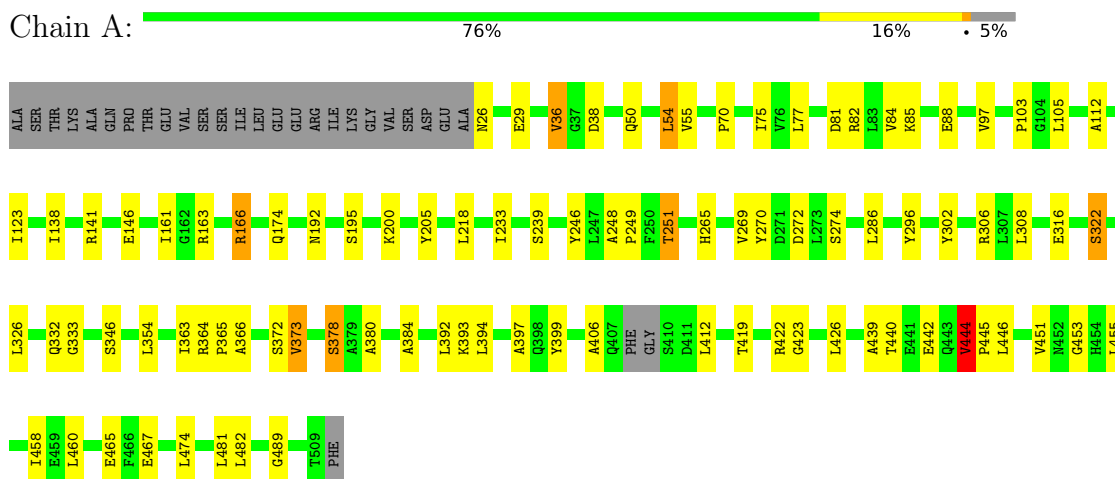


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	N	1	Total	O	P	0	0
			5	4	1		

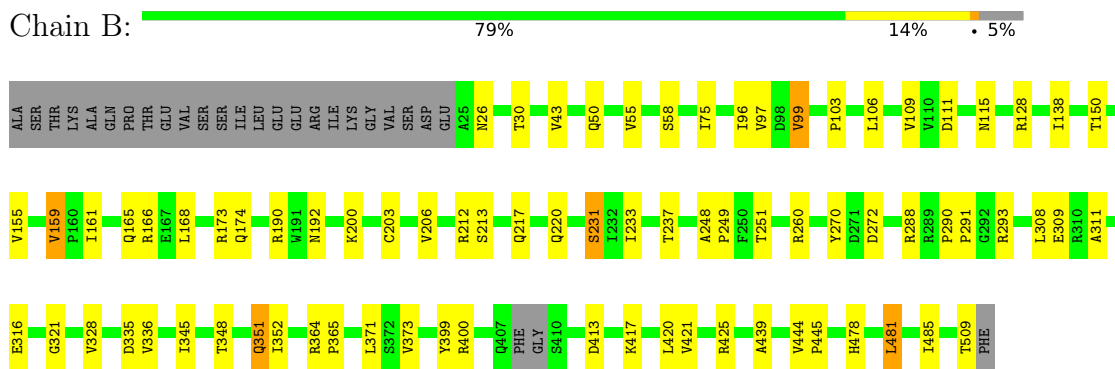
3 Residue-property plots

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

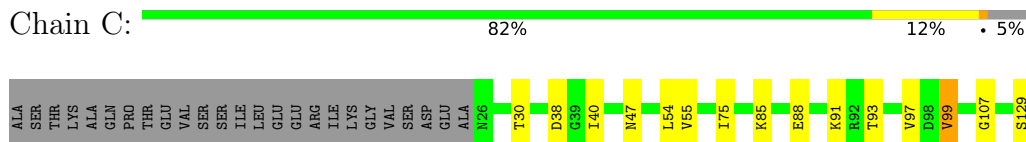
- Molecule 1: ATP synthase subunit alpha

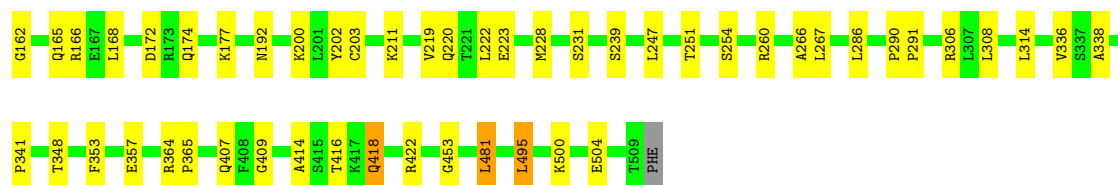


- Molecule 1: ATP synthase subunit alpha



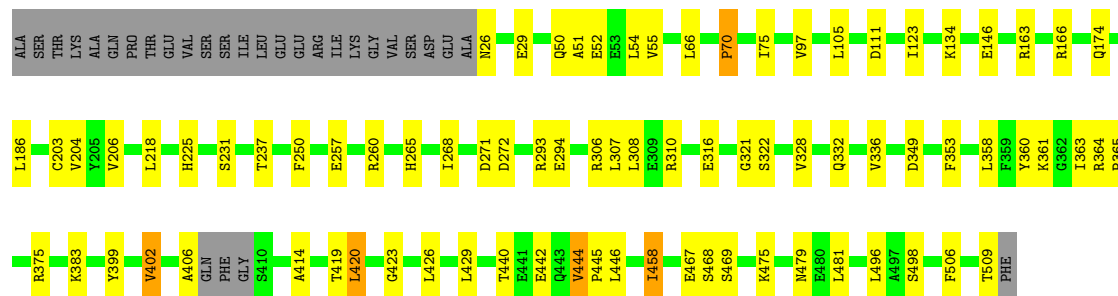
- Molecule 1: ATP synthase subunit alpha





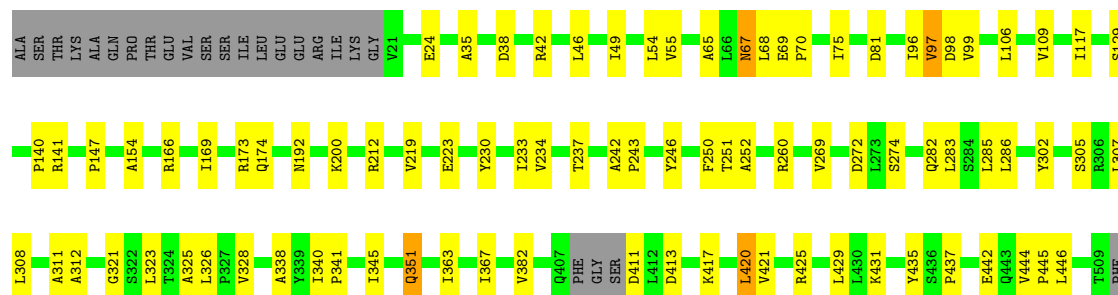
• Molecule 1: ATP synthase subunit alpha

Chain J:



• Molecule 1: ATP synthase subunit alpha

Chain K:



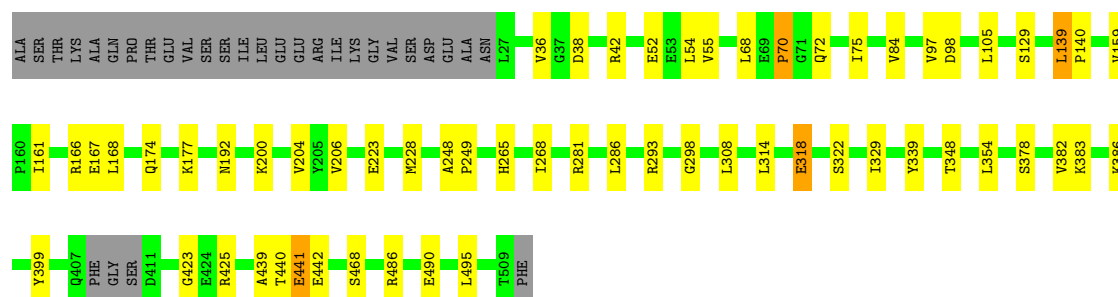
• Molecule 1: ATP synthase subunit alpha

Chain L:



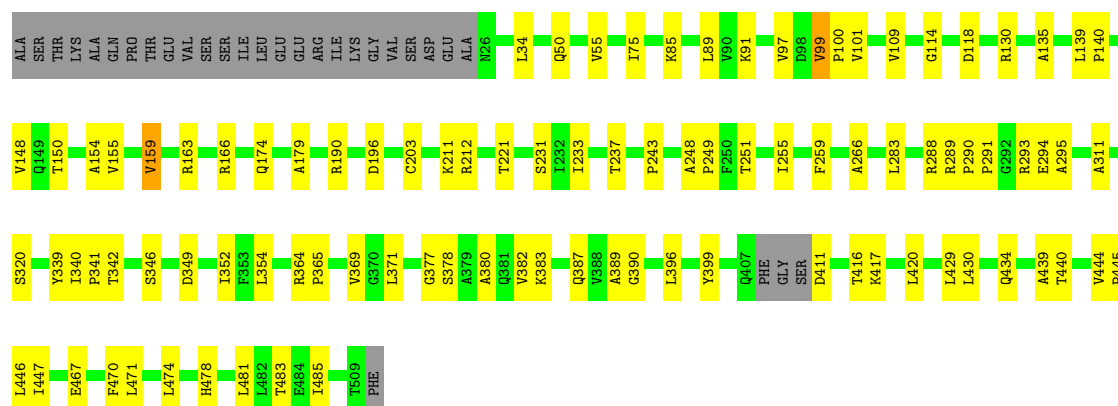
• Molecule 1: ATP synthase subunit alpha

Chain S:  82% 11% • 6%



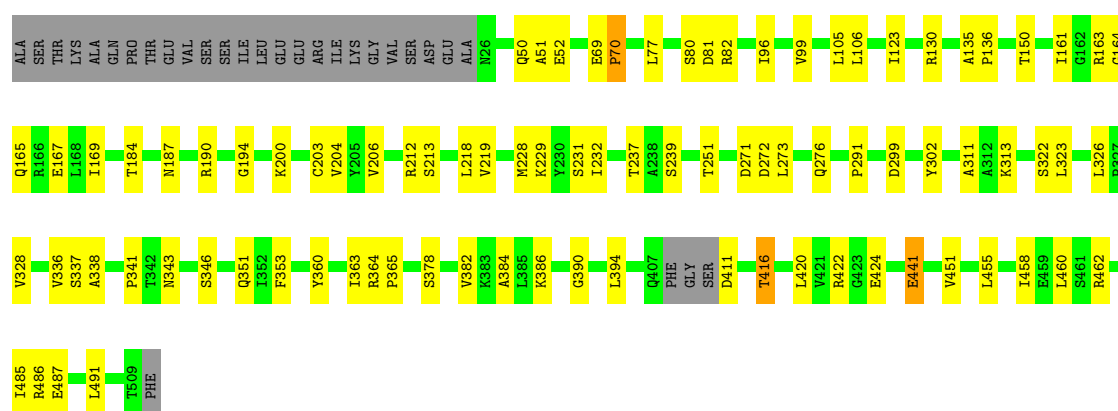
- Molecule 1: ATP synthase subunit alpha

Chain T:  75% 18% 6%



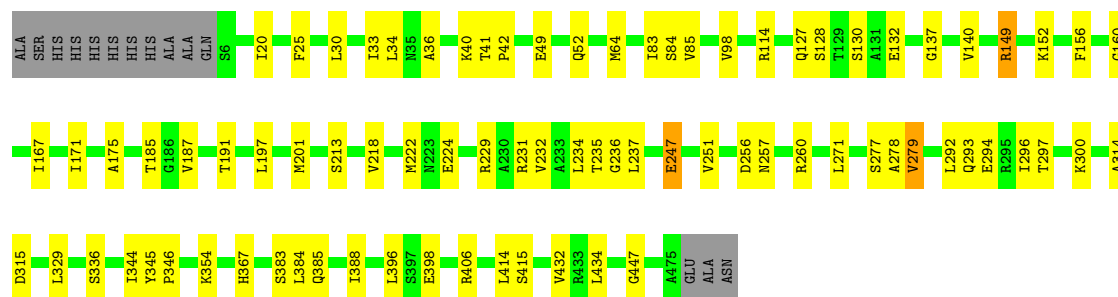
- Molecule 1: ATP synthase subunit alpha

Chain U:  77% 17% • 6%



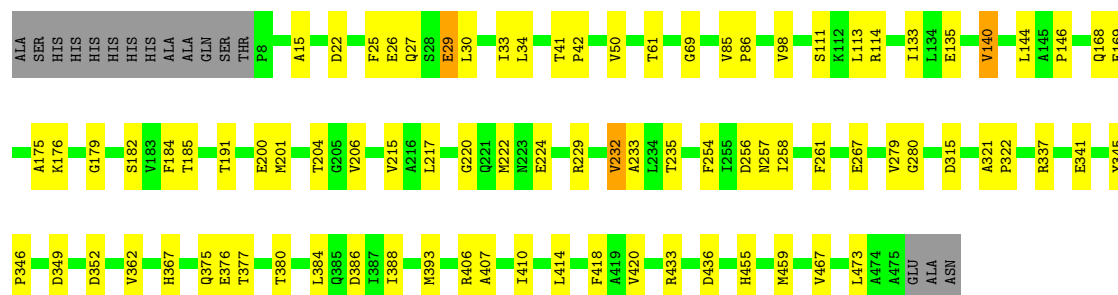
- Molecule 2: ATP synthase subunit beta

Chain D:  80% 16% • •



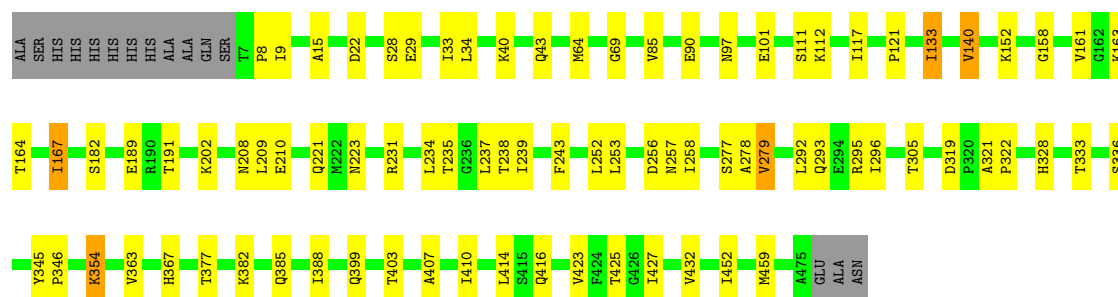
• Molecule 2: ATP synthase subunit beta

Chain E: 79% 17% ..



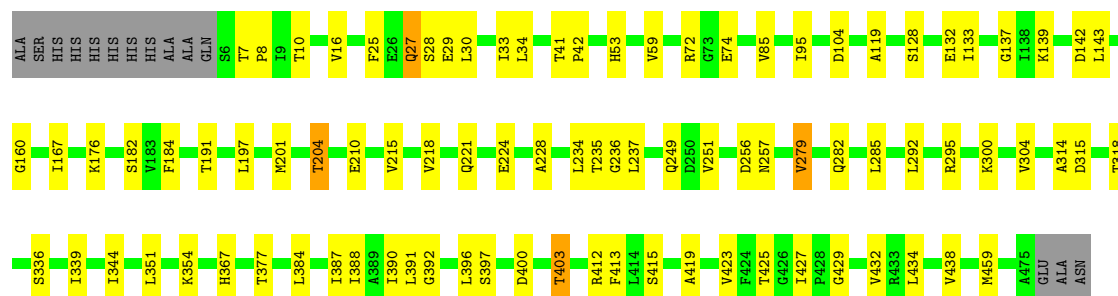
• Molecule 2: ATP synthase subunit beta

Chain F: 80% 16% ..



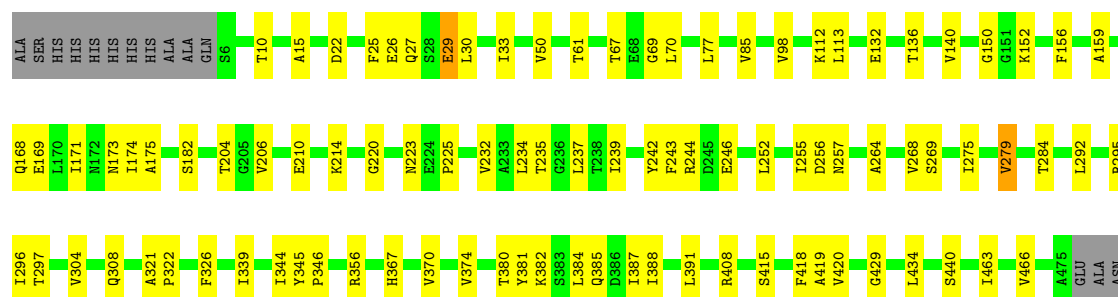
• Molecule 2: ATP synthase subunit beta

Chain M: 79% 18% ..



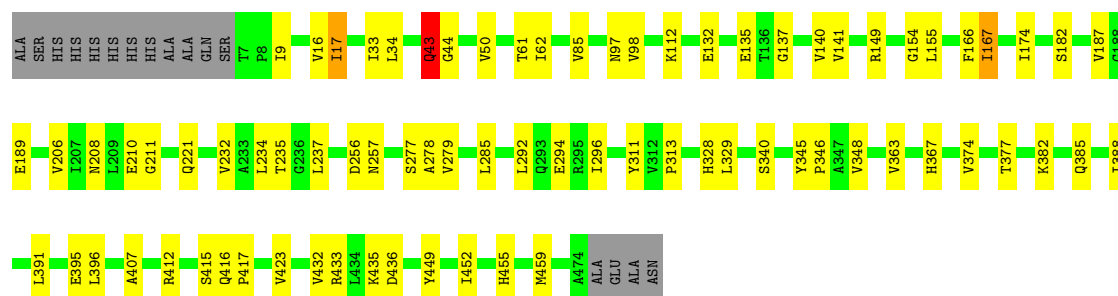
• Molecule 2: ATP synthase subunit beta

Chain N:  78% 19%



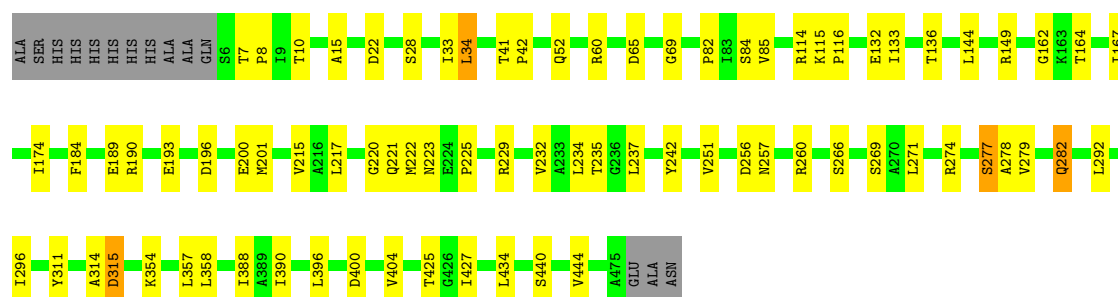
• Molecule 2: ATP synthase subunit beta

Chain O:  81% 15%



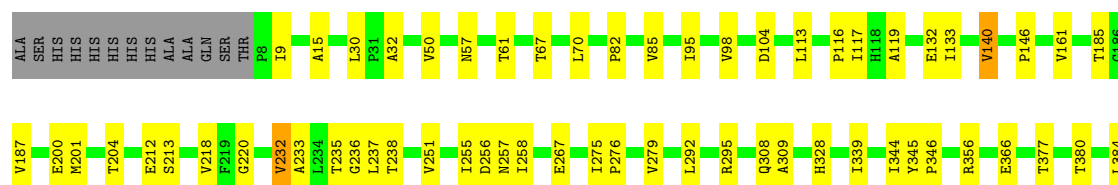
• Molecule 2: ATP synthase subunit beta

Chain V:  81% 15%



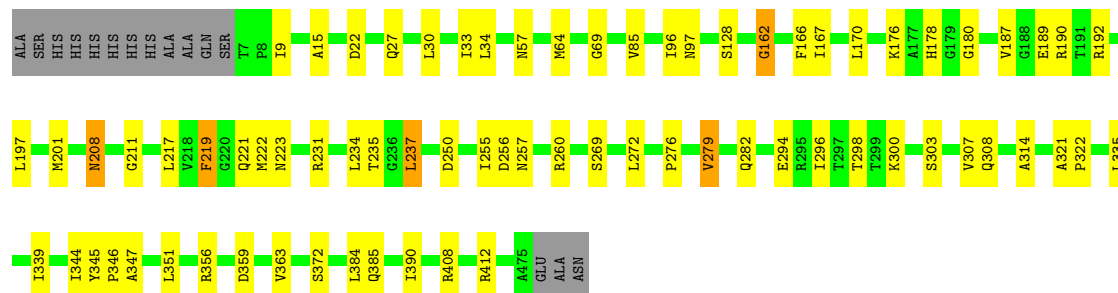
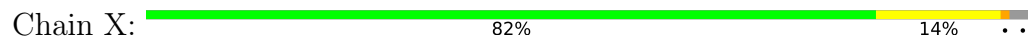
• Molecule 2: ATP synthase subunit beta

Chain W:  81% 15%

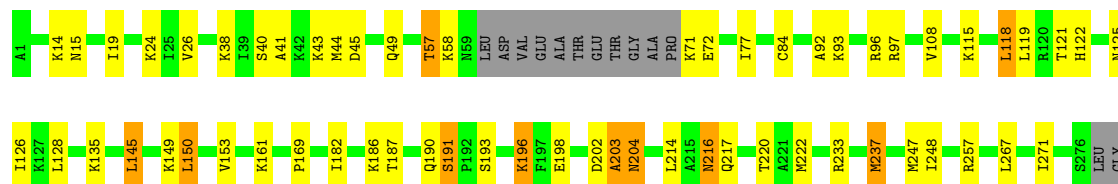




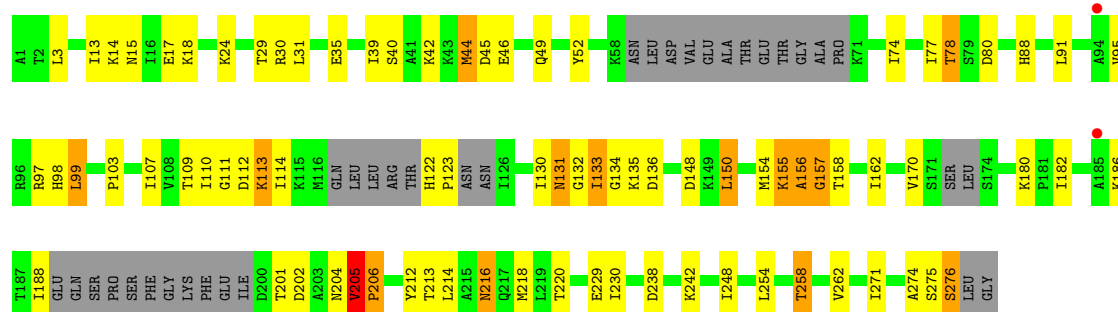
• Molecule 2: ATP synthase subunit beta



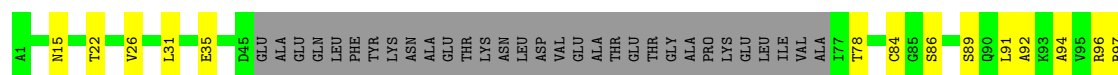
• Molecule 3: ATP synthase subunit gamma

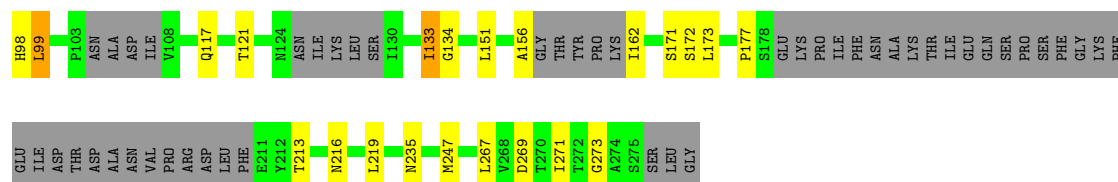


• Molecule 3: ATP synthase subunit gamma

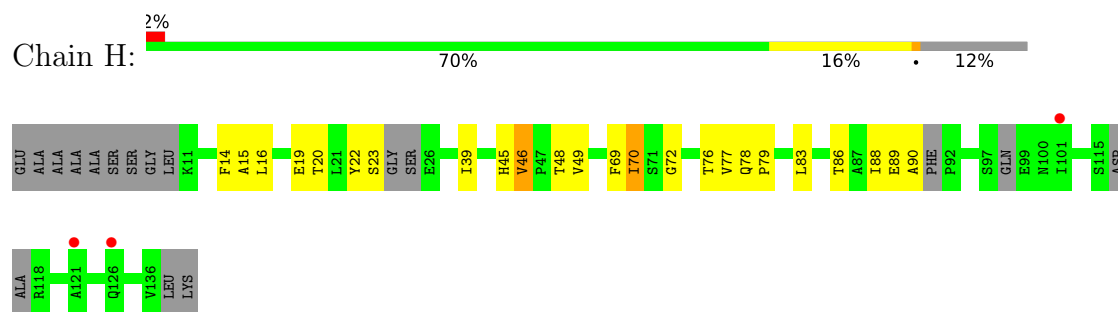


• Molecule 3: ATP synthase subunit gamma

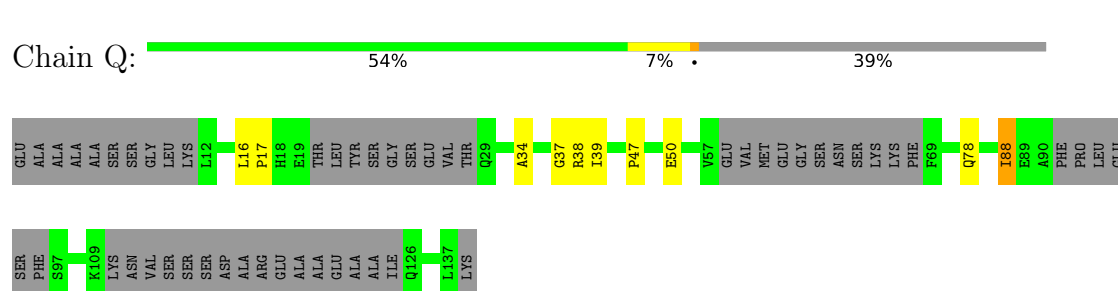




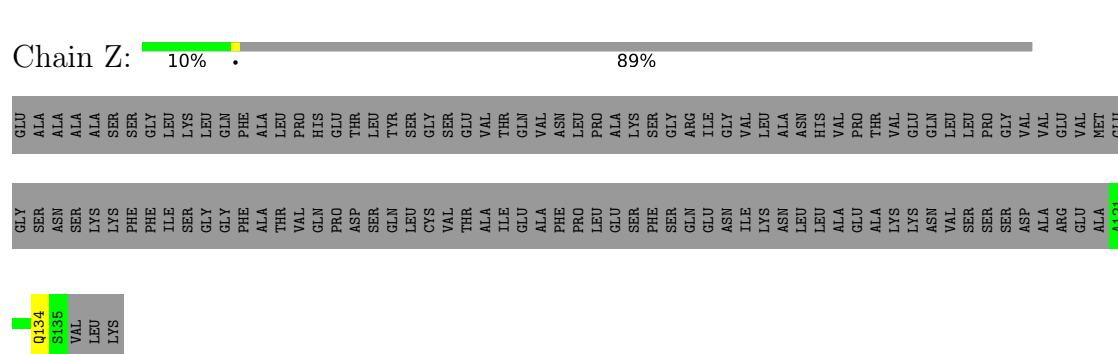
• Molecule 4: ATP synthase subunit delta



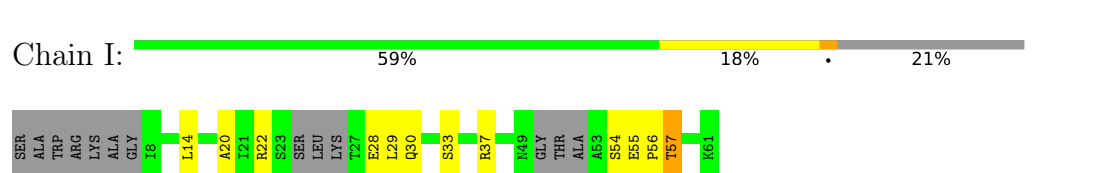
• Molecule 4: ATP synthase subunit delta



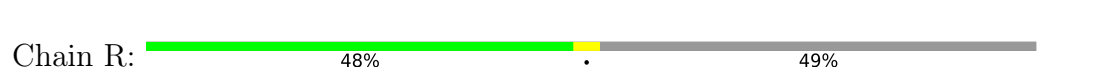
• Molecule 4: ATP synthase subunit delta



• Molecule 5: ATP synthase subunit epsilon

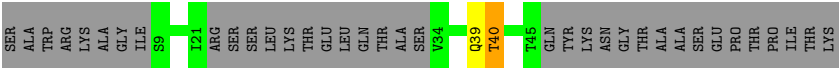


• Molecule 5: ATP synthase subunit epsilon





● Molecule 5: ATP synthase subunit epsilon



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	111.03Å 292.21Å 189.05Å 90.00° 101.82° 90.00°	Depositor
Resolution (Å)	20.00 – 3.19 20.00 – 3.19	Depositor EDS
% Data completeness (in resolution range)	95.4 (20.00-3.19) 95.0 (20.00-3.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.189 , 0.245 0.188 , 0.241	Depositor DCC
R_{free} test set	9702 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	84.9	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 62.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	72533	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, ANP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.56	1/3718 (0.0%)	0.91	5/5032 (0.1%)
1	B	0.51	0/3723	0.86	0/5039
1	C	0.51	0/3729	0.86	1/5048 (0.0%)
1	J	0.48	0/3709	0.84	0/5020
1	K	0.51	0/3748	0.85	1/5073 (0.0%)
1	L	0.54	0/3718	0.87	3/5032 (0.1%)
1	S	0.50	0/3705	0.86	0/5014
1	T	0.50	0/3713	0.83	2/5025 (0.0%)
1	U	0.50	0/3713	0.84	0/5025
2	D	0.54	0/3605	0.87	3/4889 (0.1%)
2	E	0.52	0/3592	0.83	1/4870 (0.0%)
2	F	0.51	0/3599	0.87	3/4881 (0.1%)
2	M	0.53	0/3605	0.87	1/4889 (0.0%)
2	N	0.51	0/3605	0.84	3/4889 (0.1%)
2	O	0.49	0/3594	0.84	0/4874
2	V	0.51	0/3605	0.85	2/4889 (0.0%)
2	W	0.50	0/3587	0.82	0/4863
2	X	0.51	0/3599	0.84	1/4881 (0.0%)
3	G	0.51	0/2067	0.88	4/2782 (0.1%)
3	P	0.51	0/1865	0.87	0/2508
3	Y	0.49	0/1361	0.86	0/1843
4	H	0.58	0/783	0.86	0/1072
4	Q	0.53	0/448	1.08	2/614 (0.3%)
4	Z	0.45	0/74	0.87	0/102
5	I	0.50	0/123	0.89	0/169
5	I	0.54	0/332	1.30	5/452 (1.1%)
5	R	0.54	0/173	0.92	0/238
All	All	0.51	1/73093 (0.0%)	0.86	37/99013 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	444	VAL	CA-CB	5.88	1.57	1.53

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	57	THR	CA-C-N	10.48	132.95	119.84
5	I	57	THR	C-N-CA	10.48	132.95	119.84
4	Q	78	GLN	CA-C-N	9.45	129.07	119.24
4	Q	78	GLN	C-N-CA	9.45	129.07	119.24
5	I	55	GLU	N-CA-C	7.74	114.95	108.07
5	I	55	GLU	CA-C-N	7.66	129.41	119.84
5	I	55	GLU	C-N-CA	7.66	129.41	119.84
1	A	444	VAL	N-CA-CB	7.17	115.02	110.50
2	D	247	GLU	N-CA-C	-6.60	104.46	113.30
2	N	225	PRO	CA-C-N	6.37	126.58	119.32
2	N	225	PRO	C-N-CA	6.37	126.58	119.32
3	G	191	SER	CA-C-N	6.26	127.66	119.84
3	G	191	SER	C-N-CA	6.26	127.66	119.84
2	E	29	GLU	N-CA-C	-6.22	104.33	112.41
1	C	93	THR	N-CA-C	-6.10	106.37	113.88
2	N	29	GLU	N-CA-C	-6.06	103.33	111.87
2	X	219	PHE	N-CA-C	5.88	117.99	108.34
1	A	296	TYR	CA-C-N	5.39	125.68	119.92
1	A	296	TYR	C-N-CA	5.39	125.68	119.92
1	K	67	ASN	N-CA-C	5.24	116.97	108.26
2	D	224	GLU	CA-C-N	5.23	125.77	120.38
2	D	224	GLU	C-N-CA	5.23	125.77	120.38
2	F	28	SER	N-CA-C	5.22	119.13	112.34
3	G	216	ASN	N-CA-C	5.20	117.35	111.11
2	F	121	PRO	CA-C-N	5.18	125.19	119.90
2	F	121	PRO	C-N-CA	5.18	125.19	119.90
1	T	99	VAL	N-CA-C	5.18	113.44	109.19
1	T	233	ILE	N-CA-C	5.17	114.19	106.85
2	M	392	GLY	N-CA-C	5.17	116.86	111.95
1	L	93	THR	N-CA-C	-5.16	107.06	113.55
3	G	196	LYS	N-CA-C	-5.09	107.24	113.50
1	A	460	LEU	N-CA-C	5.08	116.81	111.28
2	V	7	THR	CA-C-N	5.03	126.13	119.84
2	V	7	THR	C-N-CA	5.03	126.13	119.84
1	A	274	SER	N-CA-C	-5.02	105.72	111.14
1	L	235	ALA	N-CA-C	5.01	116.56	108.34
1	L	340	ILE	N-CA-CB	5.00	113.65	110.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3664	0	3747	49	0
1	B	3669	0	3752	43	0
1	C	3674	0	3756	34	0
1	J	3655	0	3739	46	0
1	K	3694	0	3774	52	0
1	L	3664	0	3747	46	0
1	S	3651	0	3739	35	0
1	T	3659	0	3745	51	0
1	U	3659	0	3745	49	0
2	D	3549	0	3620	45	0
2	E	3536	0	3610	45	0
2	F	3543	0	3616	47	0
2	M	3549	0	3620	58	0
2	N	3549	0	3621	55	0
2	O	3538	0	3610	40	0
2	V	3549	0	3620	48	0
2	W	3531	0	3605	43	0
2	X	3543	0	3616	44	0
3	G	2042	0	2102	35	0
3	P	1847	0	1873	45	0
3	Y	1356	0	1262	16	0
4	H	775	0	640	20	0
4	Q	449	0	240	5	0
4	Z	75	0	38	0	0
5	1	125	0	66	1	0
5	I	330	0	260	8	0
5	R	173	0	101	0	0
6	A	31	0	13	1	0
6	B	31	0	13	1	0
6	C	31	0	13	1	0
6	D	31	0	13	4	0
6	F	31	0	13	0	0
6	J	31	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	K	31	0	13	0	0
6	L	31	0	13	1	0
6	M	31	0	13	2	0
6	O	31	0	13	0	0
6	S	31	0	13	0	0
6	T	31	0	13	2	0
6	U	31	0	13	0	0
6	V	31	0	13	1	0
6	X	31	0	13	2	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
7	F	1	0	0	0	0
7	J	1	0	0	0	0
7	K	1	0	0	0	0
7	L	1	0	0	0	0
7	M	1	0	0	0	0
7	O	1	0	0	0	0
7	S	1	0	0	0	0
7	T	1	0	0	0	0
7	U	1	0	0	0	0
7	V	1	0	0	0	0
7	X	1	0	0	0	0
8	N	5	0	0	0	0
All	All	72533	0	73059	890	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 6.

All (890) 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)
3:G:96:ARG:HE	3:G:121:THR:HG21	1.25	0.98
2:E:85:VAL:HG11	2:E:235:THR:HG23	1.47	0.96
1:K:99:VAL:HG11	1:K:251:THR:HB	1.48	0.94
2:F:85:VAL:HG11	2:F:235:THR:HG23	1.51	0.92
2:M:85:VAL:HG11	2:M:235:THR:HG23	1.52	0.92
2:M:160:GLY:H	6:M:600:ANP:HNB1	1.08	0.91
3:P:180:LYS:HZ3	3:P:220:THR:HB	1.34	0.91
1:L:99:VAL:HG11	1:L:251:THR:HB	1.54	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:85:VAL:HG11	2:D:235:THR:HG23	1.54	0.87
4:H:14:PHE:HZ	4:H:70:ILE:HD11	1.45	0.82
3:P:95:VAL:O	3:P:99:LEU:HB2	1.79	0.81
1:J:481:LEU:HD13	1:J:498:SER:HB3	1.63	0.79
1:A:239:SER:HB3	2:D:294:GLU:HG3	1.64	0.78
4:H:16:LEU:HD11	4:H:90:ALA:HB3	1.66	0.78
1:U:212:ARG:HG3	1:U:237:THR:HG21	1.67	0.77
5:I:33:SER:O	5:I:37:ARG:HG3	1.85	0.77
3:P:45:ASP:O	3:P:49:GLN:HB2	1.85	0.76
1:S:441:GLU:HG2	1:S:486:ARG:HB2	1.66	0.76
1:A:55:VAL:HG21	1:A:75:ILE:HD13	1.66	0.76
2:E:135:GLU:OE2	2:E:433:ARG:HD3	1.85	0.76
1:L:398:GLN:HE22	2:M:412:ARG:HE	1.33	0.76
2:W:85:VAL:HG11	2:W:235:THR:HG23	1.65	0.76
3:G:45:ASP:O	3:G:49:GLN:HB2	1.85	0.76
2:V:65:ASP:HA	2:V:225:PRO:HG3	1.68	0.75
1:L:219:VAL:HG13	1:L:228:MET:HE3	1.69	0.75
3:P:31:LEU:O	3:P:35:GLU:HG2	1.87	0.75
1:S:223:GLU:HG3	1:S:228:MET:HG3	1.69	0.74
2:O:85:VAL:HG11	2:O:235:THR:HG23	1.68	0.74
1:J:70:PRO:HD3	2:N:15:ALA:HB2	1.70	0.74
1:B:444:VAL:HG23	1:B:445:PRO:HD3	1.70	0.73
1:B:413:ASP:O	1:B:417:LYS:HB2	1.90	0.72
3:P:180:LYS:NZ	3:P:220:THR:HB	2.02	0.72
1:S:425:ARG:HH11	1:S:425:ARG:HG2	1.55	0.72
2:M:388:ILE:HG12	2:M:396:LEU:HD21	1.73	0.71
1:B:26:ASN:O	1:B:30:THR:HB	1.90	0.71
3:Y:133:ILE:HD12	3:Y:134:GLY:H	1.55	0.70
3:G:72:GLU:HG3	3:G:161:LYS:HB3	1.73	0.70
2:D:41:THR:HB	2:D:42:PRO:HD2	1.73	0.70
1:B:212:ARG:HG2	1:B:237:THR:HG21	1.73	0.70
1:T:85:LYS:HE2	2:W:32:ALA:HB2	1.74	0.70
2:X:208:ASN:HD22	2:X:211:GLY:H	1.36	0.70
3:G:193:SER:HB3	3:G:196:LYS:HG3	1.73	0.70
3:G:43:LYS:HB2	4:H:20:THR:HG21	1.74	0.70
2:W:50:VAL:HA	2:W:61:THR:HG22	1.72	0.70
1:S:265:HIS:ND1	1:S:322:SER:HB2	2.07	0.69
4:H:45:HIS:HB3	4:H:77:VAL:HG11	1.74	0.69
4:H:14:PHE:CZ	4:H:70:ILE:HD11	2.28	0.69
1:J:469:SER:HB3	1:J:506:PHE:HZ	1.56	0.69
2:M:160:GLY:N	6:M:600:ANP:HNB1	1.87	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:234:LEU:CD2	2:D:292:LEU:HD13	2.23	0.68
2:D:218:VAL:HG21	2:D:236:GLY:HA2	1.74	0.68
1:U:77:LEU:HD13	1:U:81:ASP:HB3	1.76	0.68
1:K:212:ARG:HG2	1:K:237:THR:HG21	1.76	0.68
2:M:234:LEU:HD23	2:M:292:LEU:HD13	1.76	0.67
2:N:85:VAL:HG11	2:N:235:THR:HG23	1.77	0.67
2:N:419:ALA:HA	2:N:429:GLY:HA3	1.76	0.67
2:E:15:ALA:HB3	2:E:22:ASP:HB2	1.75	0.67
1:A:77:LEU:HD12	1:A:81:ASP:HB3	1.75	0.67
1:S:192:ASN:HA	1:S:200:LYS:HG2	1.76	0.66
2:V:33:ILE:O	2:V:34:LEU:HB2	1.94	0.66
3:G:93:LYS:HE3	3:G:97:ARG:HH12	1.60	0.66
2:M:384:LEU:HA	2:M:387:ILE:HD13	1.75	0.66
2:O:391:LEU:HB3	2:O:395:GLU:HG3	1.76	0.66
2:X:197:LEU:O	2:X:201:MET:HG2	1.96	0.66
1:K:444:VAL:HG23	1:K:445:PRO:HD3	1.76	0.65
1:L:55:VAL:HG21	1:L:75:ILE:HD13	1.77	0.65
1:J:336:VAL:HG11	1:J:353:PHE:HE1	1.61	0.65
1:K:54:LEU:HG	1:K:97:VAL:HG22	1.77	0.65
2:N:85:VAL:CG1	2:N:235:THR:HG23	2.26	0.65
2:V:41:THR:HB	2:V:42:PRO:HD2	1.77	0.65
1:J:265:HIS:ND1	1:J:322:SER:HB3	2.11	0.65
2:E:280:GLY:HA2	3:G:267:LEU:CD2	2.27	0.64
1:U:336:VAL:HG11	1:U:353:PHE:HE1	1.61	0.64
1:K:166:ARG:HD3	1:K:308:LEU:O	1.97	0.64
1:T:174:GLN:HA	6:T:600:ANP:HNB1	1.62	0.64
1:A:70:PRO:HD3	2:E:15:ALA:HB2	1.80	0.64
1:A:166:ARG:HD2	1:A:308:LEU:O	1.97	0.64
1:A:455:LEU:HA	1:A:458:ILE:HD12	1.79	0.64
1:L:383:LYS:HG2	1:L:490:GLU:HG3	1.79	0.64
1:T:99:VAL:HG11	1:T:251:THR:HB	1.79	0.63
2:D:171:ILE:O	2:D:175:ALA:HB3	1.98	0.63
3:P:78:THR:HG23	3:P:91:LEU:HD22	1.81	0.63
3:P:110:ILE:HG22	3:P:133:ILE:HD13	1.81	0.63
2:F:133:ILE:HD12	2:F:133:ILE:H	1.63	0.62
1:U:441:GLU:HG2	1:U:486:ARG:HB2	1.79	0.62
3:P:44:MET:HE3	4:Q:17:PRO:HD3	1.81	0.62
1:B:166:ARG:HD3	1:B:308:LEU:O	1.99	0.62
2:D:149:ARG:HH11	2:D:149:ARG:CG	2.12	0.62
2:M:387:ILE:HA	2:M:391:LEU:HD12	1.82	0.62
4:H:89:GLU:OE2	5:I:37:ARG:NH2	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:132:GLU:HB3	2:O:149:ARG:HB2	1.82	0.62
1:U:360:TYR:CE2	2:X:351:LEU:O	2.53	0.62
2:F:152:LYS:NZ	2:F:293:GLN:HG3	2.14	0.62
1:B:50:GLN:HB3	2:F:69:GLY:HA2	1.81	0.62
2:D:185:THR:HG23	2:D:218:VAL:HB	1.81	0.62
1:S:168:LEU:HB2	1:S:348:THR:HG21	1.82	0.62
1:L:68:LEU:HB3	2:M:72:ARG:HD3	1.81	0.61
2:W:133:ILE:HD12	2:W:146:PRO:HB2	1.81	0.61
2:D:160:GLY:HA2	6:D:600:ANP:HNB1	1.64	0.61
2:D:187:VAL:HG12	2:D:260:ARG:HB2	1.83	0.61
1:J:444:VAL:HG22	1:J:445:PRO:HD3	1.82	0.61
2:D:84:SER:HB3	2:D:114:ARG:HE	1.66	0.61
2:F:382:LYS:HA	2:F:385:GLN:HG2	1.83	0.61
1:U:336:VAL:HG11	1:U:353:PHE:CE1	2.36	0.61
2:V:84:SER:HB3	2:V:114:ARG:HE	1.66	0.61
1:A:439:ALA:HB3	1:A:442:GLU:HG3	1.83	0.61
1:L:492:SER:H	1:L:495:LEU:HD12	1.65	0.61
2:N:26:GLU:O	2:N:29:GLU:HB3	2.01	0.61
1:B:272:ASP:HB2	1:B:328:VAL:O	2.00	0.60
2:E:133:ILE:HD12	2:E:146:PRO:HB2	1.82	0.60
2:V:314:ALA:O	2:V:315:ASP:HB2	2.00	0.60
1:J:469:SER:HB3	1:J:506:PHE:CZ	2.35	0.60
1:K:81:ASP:HB3	2:N:33:ILE:HD12	1.83	0.60
2:E:345:TYR:HB2	2:E:459:MET:HE1	1.84	0.60
1:S:55:VAL:HG21	1:S:75:ILE:HD13	1.83	0.60
3:Y:91:LEU:HD12	3:Y:177:PRO:HB3	1.82	0.60
1:K:38:ASP:HB3	1:K:286:LEU:HD22	1.84	0.60
2:N:244:ARG:HD3	2:N:304:VAL:HG23	1.84	0.60
1:T:243:PRO:HG3	1:T:283:LEU:HD21	1.84	0.60
2:X:64:MET:HE1	2:X:231:ARG:HG3	1.84	0.60
1:U:69:GLU:HB3	1:U:70:PRO:HD2	1.84	0.59
1:B:111:ASP:OD2	1:B:115:ASN:HB2	2.02	0.59
1:J:250:PHE:CE1	1:J:307:LEU:HB2	2.38	0.59
1:A:192:ASN:HA	1:A:200:LYS:HG2	1.85	0.59
1:J:26:ASN:ND2	1:J:29:GLU:H	2.00	0.59
4:H:16:LEU:HD21	4:H:90:ALA:HB2	1.85	0.59
1:S:70:PRO:HD3	2:W:15:ALA:HB2	1.83	0.59
1:A:265:HIS:ND1	1:A:322:SER:HB3	2.17	0.59
1:K:169:ILE:O	1:K:328:VAL:HA	2.03	0.59
1:K:174:GLN:NE2	2:N:356:ARG:HD3	2.17	0.59
2:O:234:LEU:HD23	2:O:292:LEU:HD13	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:266:SER:HA	2:V:282:GLN:HG3	1.84	0.59
2:X:85:VAL:HG11	2:X:235:THR:HG23	1.85	0.59
1:A:174:GLN:HA	6:A:600:ANP:HNB1	1.67	0.58
2:E:220:GLY:HA3	2:E:232:VAL:HG11	1.86	0.58
3:P:30:ARG:HD2	3:P:230:ILE:HG12	1.84	0.58
1:T:248:ALA:HB3	1:T:249:PRO:HD3	1.84	0.58
1:K:69:GLU:HB2	1:K:70:PRO:HD2	1.83	0.58
1:C:97:VAL:HG11	1:C:247:LEU:HD21	1.86	0.58
2:V:85:VAL:HG11	2:V:235:THR:HG23	1.85	0.58
2:N:50:VAL:HA	2:N:61:THR:HG22	1.84	0.58
3:P:13:ILE:HG22	3:P:248:ILE:HG13	1.86	0.58
1:U:302:TYR:CE1	2:V:225:PRO:HA	2.39	0.58
1:B:260:ARG:O	1:B:321:GLY:HA3	2.03	0.57
3:P:91:LEU:O	3:P:95:VAL:HG23	2.04	0.57
1:S:425:ARG:HH11	1:S:425:ARG:CG	2.17	0.57
1:L:364:ARG:HA	1:L:365:PRO:C	2.29	0.57
1:T:89:LEU:HD21	1:T:91:LYS:HE3	1.87	0.57
1:A:270:TYR:O	1:A:272:ASP:HA	2.04	0.57
2:O:382:LYS:HA	2:O:385:GLN:HG2	1.85	0.57
2:D:33:ILE:O	2:D:34:LEU:HB2	2.03	0.57
2:O:33:ILE:O	2:O:34:LEU:HB2	2.05	0.57
2:N:255:ILE:HB	2:N:308:GLN:HG2	1.86	0.57
2:O:137:GLY:HA2	2:O:432:VAL:O	2.05	0.57
1:T:139:LEU:N	1:T:140:PRO:HD2	2.19	0.57
1:C:174:GLN:HA	6:C:600:ANP:HNB1	1.69	0.57
3:G:15:ASN:O	3:G:19:ILE:HG12	2.04	0.56
3:Y:78:THR:HG23	3:Y:91:LEU:HD22	1.86	0.56
1:S:248:ALA:HB3	1:S:249:PRO:HD3	1.86	0.56
2:W:388:ILE:HD12	2:W:393:MET:HG2	1.87	0.56
1:C:54:LEU:HD13	1:C:97:VAL:HG22	1.86	0.56
1:J:54:LEU:HD11	1:J:97:VAL:HG22	1.88	0.56
1:K:109:VAL:HG13	1:K:233:ILE:HB	1.87	0.56
2:O:363:VAL:HB	2:O:367:HIS:ND1	2.20	0.56
3:P:42:LYS:O	3:P:46:GLU:HG2	2.05	0.56
3:P:258:THR:O	3:P:262:VAL:HG23	2.06	0.56
1:U:337:SER:HB3	2:V:314:ALA:HB1	1.87	0.56
1:B:364:ARG:HA	1:B:365:PRO:C	2.29	0.56
1:K:413:ASP:O	1:K:417:LYS:HB2	2.05	0.56
2:F:33:ILE:O	2:F:34:LEU:HB2	2.05	0.56
2:F:97:ASN:HB2	2:F:101:GLU:H	1.70	0.56
3:Y:94:ALA:HA	3:Y:97:ARG:HD3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:TYR:CD1	1:A:423:GLY:HA3	2.40	0.56
1:S:36:VAL:HG21	1:S:84:VAL:HB	1.88	0.56
3:G:44:MET:HE2	4:H:86:THR:HB	1.87	0.56
2:N:156:PHE:HZ	2:N:326:PHE:HZ	1.53	0.55
1:U:346:SER:HB2	2:V:260:ARG:HH22	1.71	0.55
3:P:155:LYS:O	3:P:157:GLY:N	2.38	0.55
1:S:166:ARG:HD3	1:S:308:LEU:O	2.05	0.55
3:Y:31:LEU:O	3:Y:35:GLU:HG2	2.07	0.55
2:F:152:LYS:HZ3	2:F:293:GLN:HG3	1.70	0.55
2:F:252:LEU:HD23	2:F:305:THR:HB	1.89	0.55
1:L:242:ALA:HB3	1:L:243:PRO:HD3	1.89	0.55
1:C:364:ARG:HA	1:C:365:PRO:C	2.32	0.55
1:K:141:ARG:NH1	1:K:312:ALA:HB2	2.22	0.55
1:K:363:ILE:HA	1:K:431:LYS:HE2	1.87	0.55
2:O:135:GLU:OE1	2:O:433:ARG:NH2	2.40	0.55
2:O:311:TYR:CE2	2:O:313:PRO:HA	2.42	0.55
1:U:299:ASP:HB2	1:U:302:TYR:HB3	1.89	0.55
1:B:166:ARG:HG2	1:B:311:ALA:HB3	1.88	0.55
2:D:160:GLY:H	6:D:600:ANP:HNB1	1.54	0.55
3:P:40:SER:O	3:P:44:MET:HB2	2.06	0.55
1:U:336:VAL:CG1	1:U:353:PHE:HE1	2.20	0.55
1:A:392:LEU:HD13	1:A:426:LEU:HD22	1.88	0.55
2:F:234:LEU:HD23	2:F:292:LEU:HD13	1.89	0.55
1:L:342:THR:HG21	2:M:314:ALA:HA	1.88	0.55
3:P:274:ALA:O	3:P:276:SER:N	2.40	0.55
2:V:196:ASP:O	2:V:200:GLU:HG2	2.07	0.54
2:D:160:GLY:CA	6:D:600:ANP:HNB1	2.20	0.54
5:I:20:ALA:C	5:I:22:ARG:H	2.16	0.54
3:G:182:ILE:HD11	3:G:217:GLN:HB2	1.90	0.54
2:M:221:GLN:OE1	2:M:221:GLN:HA	2.08	0.54
1:B:444:VAL:HG21	1:B:485:ILE:HG21	1.90	0.54
1:T:109:VAL:HB	1:T:118:ASP:HB3	1.89	0.54
5:I:28:GLU:O	5:I:29:LEU:HB2	2.07	0.54
2:N:242:TYR:CE1	2:N:246:GLU:HG3	2.43	0.54
1:U:51:ALA:O	1:U:52:GLU:HB2	2.08	0.54
2:W:220:GLY:CA	2:W:232:VAL:HG11	2.38	0.54
1:A:54:LEU:CD1	1:A:97:VAL:HG22	2.37	0.54
2:D:234:LEU:HD23	2:D:292:LEU:HD13	1.89	0.54
2:M:387:ILE:HD12	2:M:387:ILE:H	1.73	0.54
1:T:291:PRO:HB2	1:T:295:ALA:HA	1.89	0.54
2:X:9:ILE:HG23	2:X:27:GLN:HE21	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:280:GLY:HA2	3:G:267:LEU:HD21	1.90	0.54
2:M:128:SER:HB2	2:M:300:LYS:HG2	1.90	0.54
2:F:90:GLU:HG3	2:F:111:SER:HA	1.90	0.54
1:J:260:ARG:O	1:J:321:GLY:HA3	2.08	0.54
1:J:360:TYR:OH	2:M:354:LYS:HE2	2.08	0.54
2:M:397:SER:HB3	2:M:400:ASP:OD2	2.08	0.54
2:N:156:PHE:HZ	2:N:326:PHE:CZ	2.25	0.54
3:P:186:LYS:C	3:P:188:ILE:H	2.16	0.54
4:Q:17:PRO:HD2	4:Q:88:ILE:O	2.08	0.54
1:B:168:LEU:HB2	1:B:348:THR:HG21	1.90	0.53
1:A:302:TYR:O	1:A:306:ARG:HB2	2.07	0.53
1:J:257:GLU:CD	1:J:310:ARG:HH21	2.16	0.53
3:P:109:THR:HB	3:P:114:ILE:HG23	1.89	0.53
1:S:382:VAL:HG11	1:S:440:THR:HG21	1.91	0.53
1:B:248:ALA:HB3	1:B:249:PRO:HD3	1.90	0.53
1:T:55:VAL:HG21	1:T:75:ILE:HD13	1.90	0.53
2:V:237:LEU:HD13	2:V:296:ILE:HG12	1.89	0.53
1:S:298:GLY:O	2:W:267:GLU:HG2	2.08	0.53
3:P:77:ILE:HG23	3:P:110:ILE:HB	1.90	0.53
2:E:204:THR:OG1	2:E:420:VAL:HB	2.08	0.53
1:K:166:ARG:HG2	1:K:325:ALA:HB3	1.90	0.53
1:L:192:ASN:HA	1:L:200:LYS:HG2	1.90	0.53
1:A:205:TYR:HB3	1:A:233:ILE:HD13	1.91	0.53
1:T:444:VAL:HG21	1:T:485:ILE:HG21	1.91	0.53
1:U:194:GLY:O	1:U:200:LYS:HE3	2.09	0.53
1:A:354:LEU:HA	1:A:366:ALA:O	2.09	0.53
1:C:166:ARG:HD2	1:C:308:LEU:O	2.09	0.53
2:E:204:THR:HG23	2:E:206:VAL:HG13	1.91	0.53
1:L:394:LEU:HD13	2:M:459:MET:HE3	1.89	0.53
3:P:40:SER:HB3	4:Q:17:PRO:O	2.08	0.53
2:E:50:VAL:HA	2:E:61:THR:HG22	1.91	0.53
1:B:399:TYR:HE1	1:B:420:LEU:HD12	1.72	0.52
2:D:98:VAL:HG23	2:D:232:VAL:HA	1.91	0.52
2:F:237:LEU:HD21	2:F:295:ARG:HB2	1.92	0.52
1:J:406:ALA:HB2	1:J:420:LEU:HD21	1.92	0.52
1:J:426:LEU:HD23	1:J:429:LEU:HD12	1.91	0.52
2:W:255:ILE:HB	2:W:308:GLN:HG2	1.91	0.52
2:X:255:ILE:HD12	2:X:308:GLN:HG2	1.91	0.52
2:D:314:ALA:O	2:D:315:ASP:HB2	2.08	0.52
2:M:25:PHE:HB2	2:M:30:LEU:HD23	1.90	0.52
1:T:174:GLN:HA	6:T:600:ANP:N3B	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:429:LEU:HD11	1:T:446:LEU:HB3	1.91	0.52
2:W:30:LEU:HD21	2:W:57:ASN:HA	1.90	0.52
2:V:133:ILE:HD11	2:V:434:LEU:HD13	1.90	0.52
2:D:160:GLY:N	6:D:600:ANP:HNB1	2.07	0.52
1:K:234:VAL:HG21	1:K:252:ALA:HB2	1.91	0.52
1:U:150:THR:HA	1:U:184:THR:HG23	1.91	0.52
2:X:269:SER:HB2	2:X:282:GLN:HB3	1.90	0.52
3:Y:96:ARG:HA	3:Y:99:LEU:HB2	1.91	0.52
2:O:237:LEU:HD13	2:O:296:ILE:HG12	1.91	0.52
1:A:50:GLN:HB3	2:E:69:GLY:HA2	1.92	0.52
3:G:122:HIS:HB3	3:G:125:ASN:HD22	1.75	0.52
1:K:444:VAL:CG2	1:K:445:PRO:HD3	2.39	0.52
2:V:133:ILE:HD11	2:V:434:LEU:CD1	2.39	0.52
1:A:82:ARG:HG3	2:D:33:ILE:O	2.09	0.52
2:X:231:ARG:HD3	2:X:234:LEU:CD1	2.39	0.52
2:F:117:ILE:HA	2:F:238:THR:OG1	2.10	0.52
2:N:344:ILE:HG23	2:N:415:SER:HB3	1.92	0.52
1:T:203:CYS:HB2	1:T:231:SER:HB3	1.92	0.52
2:W:276:PRO:HD2	3:Y:271:ILE:HG12	1.92	0.52
1:B:103:PRO:O	1:B:106:LEU:HD13	2.10	0.52
2:E:168:GLN:HE21	2:E:201:MET:CG	2.23	0.52
2:E:168:GLN:HE22	2:E:200:GLU:HG2	1.74	0.52
1:U:422:ARG:NH1	1:U:451:VAL:O	2.42	0.52
2:X:30:LEU:HD21	2:X:57:ASN:HA	1.92	0.52
2:D:156:PHE:HE1	2:D:329:LEU:CD1	2.22	0.51
2:D:197:LEU:O	2:D:201:MET:HG2	2.10	0.51
2:E:321:ALA:HB3	2:E:322:PRO:CD	2.40	0.51
1:K:345:ILE:HG12	1:K:351:GLN:HG2	1.90	0.51
2:N:169:GLU:HG2	2:N:418:PHE:CD1	2.45	0.51
3:P:155:LYS:HE3	3:P:155:LYS:HA	1.92	0.51
2:W:377:THR:HG22	2:W:407:ALA:HB2	1.92	0.51
5:I:28:GLU:CD	5:I:29:LEU:H	2.19	0.51
1:C:174:GLN:HB3	2:F:354:LYS:HE2	1.92	0.51
3:G:38:LYS:HD2	3:G:169:PRO:HG2	1.92	0.51
2:O:388:ILE:HD11	2:O:396:LEU:HD11	1.93	0.51
1:C:222:LEU:HB2	1:C:228:MET:HE2	1.91	0.51
2:X:384:LEU:O	2:X:385:GLN:C	2.53	0.51
2:W:410:ILE:HG23	2:W:441:PHE:HE2	1.75	0.51
2:F:152:LYS:NZ	2:F:293:GLN:O	2.44	0.51
4:H:16:LEU:HB2	4:H:19:GLU:O	2.11	0.51
2:O:377:THR:HG22	2:O:407:ALA:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:135:ALA:HB3	2:X:223:ASN:HD22	1.76	0.51
1:A:36:VAL:HG21	1:A:84:VAL:HB	1.93	0.51
1:K:192:ASN:HA	1:K:200:LYS:HG2	1.92	0.51
3:P:99:LEU:HG	3:P:103:PRO:HA	1.93	0.51
2:V:279:VAL:HG12	2:V:279:VAL:O	2.11	0.51
1:A:364:ARG:HA	1:A:365:PRO:C	2.35	0.51
4:H:70:ILE:HG23	4:H:72:GLY:H	1.76	0.51
1:L:109:VAL:HG22	1:L:233:ILE:HB	1.93	0.51
2:N:25:PHE:HB2	2:N:30:LEU:HD23	1.92	0.51
2:N:171:ILE:HG23	2:N:182:SER:HB2	1.93	0.51
2:V:234:LEU:HD23	2:V:292:LEU:HD13	1.93	0.51
1:B:335:ASP:HB2	3:G:257:ARG:NH1	2.25	0.51
1:J:50:GLN:HB3	2:N:69:GLY:HA2	1.92	0.51
1:T:150:THR:HG21	1:T:155:VAL:HG11	1.92	0.51
1:T:364:ARG:HA	1:T:365:PRO:C	2.36	0.51
2:X:187:VAL:HG12	2:X:260:ARG:HB2	1.93	0.50
2:F:425:THR:HG22	2:F:459:MET:HE3	1.93	0.50
3:P:205:VAL:N	3:P:206:PRO:HD3	2.26	0.50
2:V:15:ALA:HB3	2:V:22:ASP:HB2	1.92	0.50
2:O:412:ARG:O	2:O:415:SER:OG	2.29	0.50
1:T:470:PHE:O	1:T:474:LEU:HG	2.11	0.50
1:B:43:VAL:HG21	1:B:75:ILE:HD12	1.93	0.50
1:B:270:TYR:O	1:B:272:ASP:HA	2.12	0.50
1:C:338:ALA:HB3	1:C:341:PRO:HG2	1.92	0.50
2:M:377:THR:HG23	2:M:403:THR:HG22	1.93	0.50
2:W:345:TYR:HA	2:W:346:PRO:C	2.36	0.50
1:A:248:ALA:HB3	1:A:249:PRO:HD3	1.93	0.50
2:N:15:ALA:HB3	2:N:22:ASP:HB2	1.92	0.50
2:F:363:VAL:HB	2:F:367:HIS:HD1	1.77	0.50
1:J:51:ALA:O	1:J:52:GLU:HB2	2.11	0.50
1:B:444:VAL:CG2	1:B:445:PRO:HD3	2.40	0.50
2:D:20:ILE:HG13	2:D:271:LEU:HB3	1.92	0.50
2:D:367:HIS:CD2	2:D:434:LEU:HD21	2.47	0.50
2:F:377:THR:HG22	2:F:407:ALA:HB2	1.93	0.50
3:G:115:LYS:O	3:G:119:LEU:HB2	2.12	0.50
3:G:119:LEU:HD13	3:G:126:ILE:HD12	1.94	0.50
2:X:335:LEU:HA	2:X:347:ALA:O	2.12	0.50
2:N:264:ALA:O	2:N:268:VAL:HG23	2.12	0.49
1:T:389:ALA:HB2	1:T:447:ILE:HG21	1.94	0.49
1:T:444:VAL:HG23	1:T:445:PRO:HD3	1.93	0.49
1:A:422:ARG:HE	1:A:453:GLY:HA2	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:ILE:HG12	1:B:351:GLN:HG2	1.95	0.49
1:T:444:VAL:CG2	1:T:445:PRO:HD3	2.42	0.49
2:X:128:SER:HB2	2:X:300:LYS:HG2	1.94	0.49
2:D:222:MET:HA	2:D:229:ARG:HD2	1.93	0.49
2:F:140:VAL:HG13	2:F:414:LEU:HB3	1.94	0.49
1:J:402:VAL:O	1:J:402:VAL:CG1	2.59	0.49
1:S:68:LEU:O	2:W:15:ALA:HA	2.12	0.49
2:D:64:MET:HE1	2:D:231:ARG:HB2	1.93	0.49
2:E:455:HIS:CD2	2:E:473:LEU:HD11	2.48	0.49
1:J:332:GLN:HB3	2:M:318:THR:HB	1.95	0.49
1:L:412:LEU:HB3	1:L:416:THR:CG2	2.42	0.49
1:B:421:VAL:O	1:B:425:ARG:HG2	2.12	0.49
1:C:168:LEU:HB2	1:C:348:THR:HG21	1.93	0.49
1:J:336:VAL:HG11	1:J:353:PHE:CE1	2.46	0.49
1:T:382:VAL:HG11	1:T:440:THR:HG21	1.95	0.49
1:A:138:ILE:HD13	2:E:191:THR:HG23	1.95	0.49
1:A:205:TYR:HB3	1:A:233:ILE:CD1	2.41	0.49
1:C:40:ILE:HG13	1:C:286:LEU:HB3	1.95	0.49
1:L:211:LYS:HE3	1:L:213:SER:OG	2.12	0.49
2:N:174:ILE:HG13	2:N:252:LEU:HD11	1.93	0.49
1:B:165:GLN:HG2	1:B:166:ARG:N	2.27	0.49
2:E:184:PHE:HA	2:E:254:PHE:HB2	1.94	0.49
4:H:88:ILE:HD11	5:I:14:LEU:HB3	1.93	0.49
1:K:154:ALA:HB1	1:K:367:ILE:HD12	1.94	0.49
1:K:65:ALA:HA	1:K:75:ILE:HG12	1.94	0.49
1:L:187:ASN:OD1	1:L:190:ARG:NH1	2.46	0.49
2:V:41:THR:HB	2:V:42:PRO:CD	2.43	0.49
2:W:406:ARG:NH1	2:W:447:GLY:HA2	2.28	0.49
1:A:105:LEU:HD21	1:A:123:ILE:HG21	1.95	0.48
1:B:99:VAL:O	1:B:128:ARG:HA	2.13	0.48
1:B:309:GLU:OE1	2:F:223:ASN:HB3	2.13	0.48
1:J:203:CYS:O	1:J:231:SER:HA	2.12	0.48
1:K:429:LEU:HD11	1:K:446:LEU:HB3	1.95	0.48
1:U:187:ASN:OD1	1:U:190:ARG:NH1	2.46	0.48
2:X:359:ASP:O	2:X:363:VAL:HG22	2.13	0.48
1:J:446:LEU:HD11	1:J:467:GLU:HG3	1.94	0.48
1:K:260:ARG:O	1:K:321:GLY:HA3	2.13	0.48
3:P:254:LEU:O	3:P:258:THR:OG1	2.30	0.48
1:C:192:ASN:HA	1:C:200:LYS:HG2	1.95	0.48
2:W:380:THR:O	2:W:384:LEU:HG	2.12	0.48
2:D:140:VAL:HG23	2:D:414:LEU:HD22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:58:LYS:O	3:G:187:THR:CG2	2.62	0.48
3:G:118:LEU:HA	3:G:121:THR:HG22	1.95	0.48
1:S:166:ARG:CD	1:S:308:LEU:O	2.61	0.48
2:V:65:ASP:CA	2:V:225:PRO:HG3	2.42	0.48
2:E:384:LEU:O	2:E:388:ILE:HG12	2.12	0.48
4:H:16:LEU:HD11	4:H:90:ALA:CB	2.41	0.48
2:W:201:MET:HA	2:W:204:THR:HG22	1.95	0.48
2:W:386:ASP:OD1	2:W:386:ASP:N	2.47	0.48
1:K:46:LEU:O	1:K:49:ILE:HG22	2.13	0.48
1:L:82:ARG:HG2	2:O:34:LEU:HD12	1.95	0.48
2:V:136:THR:HA	2:V:174:ILE:HD11	1.95	0.48
2:D:85:VAL:CG1	2:D:235:THR:HG23	2.35	0.48
4:H:45:HIS:HD2	4:H:46:VAL:O	1.97	0.48
4:H:77:VAL:HG22	4:H:83:LEU:HD13	1.95	0.48
2:M:224:GLU:HB3	2:M:228:ALA:HB3	1.94	0.48
2:D:137:GLY:HA2	2:D:432:VAL:O	2.14	0.48
1:K:269:VAL:HG22	1:K:326:LEU:HB2	1.94	0.48
2:O:155:LEU:HD12	2:O:167:ILE:HG13	1.96	0.48
1:T:369:VAL:HG11	1:T:396:LEU:HB2	1.95	0.48
1:U:80:SER:OG	1:U:82:ARG:HG3	2.13	0.48
2:W:201:MET:HA	2:W:204:THR:CG2	2.44	0.48
2:D:36:ALA:HB2	2:D:83:ILE:HG13	1.95	0.48
1:L:455:LEU:HA	1:L:458:ILE:HD12	1.95	0.48
4:Q:34:ALA:H	4:Q:38:ARG:HA	1.77	0.48
1:C:219:VAL:HB	1:C:228:MET:HE3	1.96	0.48
1:J:174:GLN:HB3	2:M:354:LYS:HE3	1.96	0.48
1:J:375:ARG:HG2	2:N:159:ALA:CB	2.44	0.48
2:M:53:HIS:CD2	2:M:59:VAL:HG12	2.49	0.48
2:N:220:GLY:HA3	2:N:232:VAL:HG11	1.94	0.48
2:N:367:HIS:NE2	2:N:434:LEU:HD11	2.28	0.48
3:P:52:TYR:OH	3:P:213:THR:HG21	2.13	0.48
1:U:378:SER:HB2	1:U:386:LYS:HE2	1.95	0.48
2:M:53:HIS:HD2	2:M:59:VAL:HG12	1.79	0.47
2:E:41:THR:HB	2:E:42:PRO:HD2	1.95	0.47
2:E:258:ILE:O	2:E:261:PHE:HB3	2.14	0.47
1:S:52:GLU:O	1:S:97:VAL:HG23	2.14	0.47
1:T:416:THR:O	1:T:420:LEU:HB2	2.14	0.47
2:V:201:MET:SD	2:V:215:VAL:HG11	2.54	0.47
1:B:190:ARG:HE	1:B:439:ALA:HB2	1.80	0.47
2:N:152:LYS:HE3	2:N:296:ILE:HB	1.96	0.47
2:N:237:LEU:HD22	2:N:292:LEU:HD12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:281:ARG:NH1	2:V:278:ALA:HB2	2.28	0.47
1:K:243:PRO:HG3	1:K:283:LEU:HD21	1.96	0.47
2:M:427:ILE:CD1	2:M:459:MET:HG2	2.43	0.47
2:X:298:THR:HG23	2:X:303:SER:HA	1.97	0.47
1:U:135:ALA:HB3	2:V:223:ASN:HD22	1.79	0.47
1:U:291:PRO:HG2	3:Y:273:GLY:HA2	1.97	0.47
2:F:253:LEU:HD23	2:F:296:ILE:HG23	1.96	0.47
3:G:45:ASP:CG	3:G:220:THR:HG21	2.40	0.47
1:J:55:VAL:HG21	1:J:75:ILE:HD13	1.97	0.47
1:J:458:ILE:H	1:J:458:ILE:HG13	1.50	0.47
1:K:272:ASP:OD1	1:K:274:SER:HB2	2.14	0.47
2:N:237:LEU:HD21	2:N:295:ARG:HB2	1.95	0.47
3:P:154:MET:C	3:P:156:ALA:H	2.22	0.47
1:B:293:ARG:NH2	2:F:319:ASP:OD2	2.46	0.47
2:E:201:MET:SD	2:E:217:LEU:HD21	2.55	0.47
2:E:407:ALA:HA	2:E:410:ILE:HD12	1.95	0.47
1:K:272:ASP:HB2	1:K:328:VAL:O	2.15	0.47
1:L:187:ASN:O	1:L:190:ARG:HG3	2.14	0.47
2:O:208:ASN:HD22	2:O:211:GLY:H	1.63	0.47
2:W:220:GLY:HA3	2:W:232:VAL:HG11	1.96	0.47
2:X:321:ALA:HB3	2:X:322:PRO:CD	2.45	0.47
2:X:345:TYR:HA	2:X:346:PRO:C	2.40	0.47
2:O:345:TYR:HA	2:O:346:PRO:C	2.39	0.47
3:P:35:GLU:O	3:P:39:ILE:HG12	2.14	0.47
1:U:69:GLU:HB3	1:U:70:PRO:CD	2.45	0.47
2:E:169:GLU:HG2	2:E:418:PHE:CD1	2.50	0.47
2:O:388:ILE:CD1	2:O:396:LEU:HD11	2.45	0.47
2:D:344:ILE:HG23	2:D:415:SER:HB3	1.96	0.46
3:G:24:LYS:HB2	3:G:237:MET:HB3	1.97	0.46
1:K:96:ILE:O	1:K:97:VAL:C	2.58	0.46
1:K:338:ALA:HB3	1:K:341:PRO:HG2	1.97	0.46
3:P:205:VAL:N	3:P:206:PRO:CD	2.78	0.46
1:S:293:ARG:HG2	1:S:339:TYR:CD1	2.50	0.46
2:V:440:SER:O	2:V:444:VAL:HG23	2.15	0.46
1:C:481:LEU:HD13	1:C:495:LEU:HD23	1.97	0.46
1:A:161:ILE:HD13	1:A:326:LEU:HD21	1.98	0.46
2:F:237:LEU:HD13	2:F:296:ILE:HG12	1.97	0.46
1:J:364:ARG:HA	1:J:365:PRO:C	2.41	0.46
2:F:256:ASP:HA	2:F:257:ASN:HA	1.73	0.46
2:F:345:TYR:HA	2:F:346:PRO:C	2.40	0.46
1:T:467:GLU:O	1:T:471:LEU:HG	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:203:CYS:O	1:U:231:SER:HA	2.16	0.46
2:W:256:ASP:HA	2:W:257:ASN:HA	1.65	0.46
2:W:406:ARG:HH12	2:W:447:GLY:HA2	1.81	0.46
1:A:112:ALA:O	1:A:251:THR:HG21	2.15	0.46
1:B:203:CYS:HB2	1:B:231:SER:HB3	1.97	0.46
5:I:28:GLU:C	5:I:30:GLN:H	2.22	0.46
2:M:7:THR:HA	2:M:8:PRO:HD3	1.80	0.46
2:O:449:TYR:HB3	2:O:452:ILE:HD12	1.98	0.46
1:T:211:LYS:HD2	2:W:328:HIS:HA	1.98	0.46
1:U:106:LEU:HB3	1:U:229:LYS:O	2.16	0.46
1:A:54:LEU:HD12	1:A:97:VAL:HG22	1.97	0.46
1:L:40:ILE:HD12	1:L:76:VAL:HG12	1.98	0.46
1:T:154:ALA:HB2	1:T:430:LEU:HB3	1.98	0.46
1:T:349:ASP:OD1	2:X:192:ARG:NE	2.49	0.46
1:B:174:GLN:HA	6:B:600:ANP:HNB1	1.81	0.46
3:P:80:ASP:HA	3:P:112:ASP:HB2	1.98	0.46
1:S:204:VAL:O	1:S:268:ILE:HA	2.16	0.46
1:U:105:LEU:HG	1:U:123:ILE:HG21	1.97	0.46
2:W:67:THR:HB	2:W:70:LEU:HD12	1.98	0.46
2:X:231:ARG:HA	2:X:234:LEU:HD12	1.97	0.46
2:E:220:GLY:CA	2:E:232:VAL:HG11	2.46	0.46
2:F:416:GLN:NE2	2:F:432:VAL:HG23	2.31	0.46
1:J:399:TYR:CD1	1:J:423:GLY:HA3	2.51	0.46
1:L:429:LEU:HD11	1:L:446:LEU:HD22	1.98	0.46
2:M:285:LEU:HD23	2:M:285:LEU:C	2.41	0.46
2:N:67:THR:HB	2:N:70:LEU:HD12	1.98	0.46
2:O:16:VAL:C	2:O:17:ILE:HG13	2.41	0.46
2:W:140:VAL:HG13	2:W:414:LEU:HB3	1.97	0.46
2:W:200:GLU:O	2:W:204:THR:HG22	2.15	0.46
1:A:302:TYR:CE1	1:A:306:ARG:HG3	2.51	0.46
2:E:229:ARG:NH2	2:E:267:GLU:OE1	2.47	0.46
3:G:108:VAL:HG11	3:G:150:LEU:HD11	1.98	0.46
1:K:35:ALA:HB3	1:K:42:ARG:NH1	2.31	0.46
2:M:137:GLY:HA2	2:M:432:VAL:O	2.16	0.46
2:W:98:VAL:HB	2:W:232:VAL:HG13	1.98	0.46
2:X:190:ARG:NH1	6:X:600:ANP:O3G	2.48	0.46
2:X:237:LEU:HD13	2:X:296:ILE:CG1	2.46	0.46
3:Y:213:THR:HA	3:Y:216:ASN:HB3	1.98	0.46
1:A:378:SER:C	1:A:380:ALA:H	2.23	0.46
2:E:345:TYR:HA	2:E:346:PRO:C	2.40	0.46
5:I:20:ALA:C	5:I:22:ARG:N	2.72	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:41:THR:HB	2:M:42:PRO:HD2	1.96	0.46
1:S:383:LYS:HG2	1:S:490:GLU:HG2	1.97	0.46
1:S:425:ARG:CG	1:S:425:ARG:NH1	2.78	0.46
2:D:152:LYS:HZ1	2:D:293:GLN:HB3	1.81	0.45
2:F:377:THR:HG23	2:F:403:THR:HG22	1.98	0.45
2:V:425:THR:HB	2:V:427:ILE:HD12	1.97	0.45
2:W:218:VAL:HG21	2:W:236:GLY:HA2	1.98	0.45
2:X:178:HIS:CD2	2:X:180:GLY:H	2.33	0.45
2:F:293:GLN:HG2	2:F:328:HIS:HB3	1.98	0.45
3:G:14:LYS:HA	3:G:248:ILE:HD11	1.98	0.45
1:L:480:GLU:H	1:L:480:GLU:HG3	1.53	0.45
2:M:339:ILE:HG22	2:M:344:ILE:HB	1.98	0.45
2:M:434:LEU:O	2:M:438:VAL:HG23	2.16	0.45
1:U:164:GLY:HA3	1:U:313:LYS:HB2	1.99	0.45
1:U:455:LEU:HD23	1:U:458:ILE:HD12	1.97	0.45
2:W:119:ALA:O	2:W:295:ARG:HD2	2.16	0.45
1:C:203:CYS:O	1:C:231:SER:HA	2.17	0.45
4:H:14:PHE:HD1	4:H:15:ALA:N	2.14	0.45
1:L:484:GLU:HB3	1:L:495:LEU:HD21	1.97	0.45
2:M:182:SER:O	2:M:215:VAL:HA	2.16	0.45
2:N:239:ILE:O	2:N:243:PHE:HD2	1.99	0.45
1:C:407:GLN:C	1:C:409:GLY:H	2.25	0.45
2:N:29:GLU:O	2:N:29:GLU:HG2	2.16	0.45
2:N:234:LEU:HD23	2:N:292:LEU:HD13	1.98	0.45
1:B:111:ASP:CG	1:B:115:ASN:HB2	2.41	0.45
1:C:222:LEU:CB	1:C:228:MET:HE2	2.47	0.45
2:E:140:VAL:HG13	2:E:414:LEU:HD22	1.97	0.45
1:J:446:LEU:CD1	1:J:467:GLU:HG3	2.46	0.45
2:M:27:GLN:C	2:M:29:GLU:H	2.24	0.45
2:M:387:ILE:O	2:M:391:LEU:HB2	2.16	0.45
3:P:150:LEU:O	3:P:154:MET:HB2	2.17	0.45
2:V:222:MET:HA	2:V:229:ARG:HD2	1.97	0.45
4:H:22:TYR:O	4:H:23:SER:C	2.58	0.45
1:K:421:VAL:O	1:K:425:ARG:HG2	2.17	0.45
2:O:154:GLY:HA3	2:O:329:LEU:HD13	1.99	0.45
1:T:100:PRO:HD2	1:T:114:GLY:HA3	1.97	0.45
1:A:444:VAL:HG22	1:A:445:PRO:HD3	1.98	0.45
1:B:192:ASN:HA	1:B:200:LYS:HG2	1.97	0.45
1:C:129:SER:HB2	1:C:254:SER:HB3	1.98	0.45
2:E:349:ASP:HB3	2:E:352:ASP:HB2	1.99	0.45
1:L:109:VAL:HG12	1:L:117:ILE:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:24:LYS:HD2	3:P:238:ASP:OD1	2.16	0.45
1:T:179:ALA:CB	1:T:434:GLN:HE21	2.29	0.45
1:C:202:TYR:O	1:C:266:ALA:HA	2.17	0.45
3:G:108:VAL:HG22	3:G:128:LEU:HB3	1.99	0.45
1:K:219:VAL:O	1:K:223:GLU:HG3	2.17	0.45
2:N:98:VAL:HB	2:N:232:VAL:CG1	2.47	0.45
2:V:266:SER:HA	2:V:282:GLN:CG	2.47	0.45
1:C:260:ARG:HG2	1:C:314:LEU:HD12	1.98	0.45
2:E:168:GLN:HE21	2:E:201:MET:HG2	1.81	0.45
2:F:189:GLU:O	2:F:221:GLN:HB3	2.17	0.45
2:F:293:GLN:HG2	2:F:328:HIS:CG	2.52	0.45
1:J:204:VAL:O	1:J:268:ILE:HA	2.17	0.45
1:K:302:TYR:HA	1:K:305:SER:OG	2.17	0.45
2:M:95:ILE:HD12	2:M:104:ASP:HB3	1.99	0.45
1:S:168:LEU:HD11	1:S:329:ILE:HB	1.99	0.45
1:T:212:ARG:HG3	1:T:237:THR:HG21	1.98	0.45
2:V:269:SER:O	2:V:274:ARG:HB2	2.16	0.45
2:X:170:LEU:HD13	2:X:307:VAL:HG11	1.98	0.45
2:F:363:VAL:HB	2:F:367:HIS:ND1	2.32	0.45
3:G:145:LEU:O	3:G:149:LYS:HG2	2.17	0.45
1:J:146:GLU:HB2	1:J:163:ARG:HG3	1.99	0.45
2:M:176:LYS:HE2	2:M:204:THR:HG21	1.98	0.45
2:M:419:ALA:HA	2:M:429:GLY:HA3	1.98	0.45
1:T:293:ARG:HD2	1:T:339:TYR:CD1	2.52	0.45
2:V:220:GLY:HA3	2:V:232:VAL:HG21	1.98	0.45
2:E:86:PRO:HD3	2:E:114:ARG:NH1	2.32	0.44
2:M:139:LYS:NZ	2:M:413:PHE:O	2.47	0.44
2:M:427:ILE:HD13	2:M:459:MET:HG2	1.97	0.44
2:N:279:VAL:HG12	2:N:279:VAL:O	2.17	0.44
2:O:140:VAL:HG21	2:O:348:VAL:HG21	2.00	0.44
1:T:190:ARG:HE	1:T:439:ALA:HB2	1.81	0.44
1:U:343:ASN:O	1:U:346:SER:OG	2.31	0.44
2:W:82:PRO:HG2	2:W:116:PRO:HB3	1.99	0.44
1:A:384:ALA:HB2	1:A:489:GLY:O	2.17	0.44
1:A:446:LEU:HD11	1:A:467:GLU:HG3	1.99	0.44
1:B:96:ILE:O	1:B:97:VAL:C	2.60	0.44
2:M:237:LEU:HD21	2:M:295:ARG:HB2	1.99	0.44
3:P:162:ILE:HB	3:P:182:ILE:HB	1.98	0.44
1:T:139:LEU:N	1:T:140:PRO:CD	2.80	0.44
2:X:190:ARG:O	2:X:221:GLN:NE2	2.50	0.44
1:A:372:SER:O	1:A:373:VAL:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:33:ILE:O	2:E:34:LEU:HB2	2.17	0.44
2:F:164:THR:O	2:F:167:ILE:HG22	2.18	0.44
2:V:132:GLU:HB3	2:V:149:ARG:HB3	2.00	0.44
2:V:189:GLU:O	2:V:221:GLN:HB3	2.17	0.44
2:D:25:PHE:HB2	2:D:30:LEU:HD23	2.00	0.44
1:L:417:LYS:O	1:L:421:VAL:HG23	2.17	0.44
1:S:38:ASP:O	1:S:286:LEU:HD13	2.17	0.44
1:T:101:VAL:HG12	1:T:255:ILE:HA	2.00	0.44
1:C:336:VAL:HG11	1:C:353:PHE:CE1	2.52	0.44
1:C:414:ALA:O	1:C:418:GLN:HB3	2.18	0.44
2:E:25:PHE:HB2	2:E:30:LEU:HD23	1.97	0.44
2:E:367:HIS:HD1	2:E:367:HIS:C	2.26	0.44
1:L:40:ILE:CD1	1:L:76:VAL:HG12	2.48	0.44
2:M:143:LEU:O	2:M:367:HIS:HE1	2.01	0.44
2:M:279:VAL:O	2:M:279:VAL:HG12	2.17	0.44
1:C:107:GLY:HA2	1:C:228:MET:O	2.17	0.44
2:D:128:SER:HB2	2:D:300:LYS:HG2	1.99	0.44
2:E:175:ALA:O	2:E:179:GLY:HA2	2.18	0.44
2:M:142:ASP:HB3	2:M:434:LEU:HD12	2.00	0.44
3:P:14:LYS:HA	3:P:248:ILE:HD11	1.99	0.44
1:U:219:VAL:HB	1:U:228:MET:HE3	1.98	0.44
2:V:33:ILE:O	2:V:34:LEU:CB	2.64	0.44
2:W:339:ILE:HG22	2:W:344:ILE:HB	1.99	0.44
1:J:293:ARG:HG2	1:J:294:GLU:HG3	2.00	0.44
1:K:147:PRO:HG3	1:K:382:VAL:HG23	1.99	0.44
1:L:68:LEU:HB2	2:M:16:VAL:H	1.82	0.44
2:N:384:LEU:O	2:N:388:ILE:HG12	2.18	0.44
2:O:50:VAL:HA	2:O:61:THR:HG22	2.00	0.44
3:P:156:ALA:C	3:P:158:THR:H	2.25	0.44
2:V:184:PHE:HB3	2:V:217:LEU:HD23	2.00	0.44
2:V:257:ASN:HD21	2:V:311:TYR:N	2.16	0.44
2:W:237:LEU:HD22	2:W:292:LEU:HD12	1.99	0.44
1:U:364:ARG:HA	1:U:365:PRO:C	2.42	0.44
3:Y:151:LEU:HA	3:Y:156:ALA:HB3	1.99	0.44
1:A:346:SER:O	2:E:222:MET:HE1	2.17	0.44
2:F:191:THR:HA	2:F:221:GLN:HG3	1.99	0.44
1:K:169:ILE:HB	1:K:328:VAL:HG22	2.00	0.44
1:U:273:LEU:HD22	1:U:276:GLN:OE1	2.18	0.44
2:X:408:ARG:O	2:X:412:ARG:HG3	2.18	0.44
2:F:256:ASP:OD1	2:F:257:ASN:HB2	2.18	0.43
3:G:77:ILE:HG21	3:G:222:MET:HG2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:242:ALA:HB3	1:K:243:PRO:HD3	1.99	0.43
2:W:258:ILE:HG22	2:W:309:ALA:O	2.18	0.43
2:X:33:ILE:O	2:X:34:LEU:HB2	2.18	0.43
1:A:174:GLN:HB3	2:D:354:LYS:HD2	2.00	0.43
1:L:376:VAL:HG11	1:L:380:ALA:HB2	2.00	0.43
2:N:275:ILE:HG23	3:P:271:ILE:HD13	1.99	0.43
1:S:281:ARG:HH12	2:V:278:ALA:HB2	1.81	0.43
5:1:39:GLN:O	5:1:40:THR:CB	2.67	0.43
1:C:165:GLN:CG	1:C:166:ARG:N	2.81	0.43
2:E:377:THR:HG22	2:E:407:ALA:HB2	2.01	0.43
2:N:204:THR:OG1	2:N:420:VAL:HB	2.18	0.43
2:W:117:ILE:HG22	2:W:235:THR:HA	2.00	0.43
2:X:390:ILE:HD11	3:Y:247:MET:SD	2.58	0.43
2:D:406:ARG:HH21	2:D:447:GLY:HA3	1.82	0.43
1:L:455:LEU:HD13	1:L:463:ILE:HD12	1.99	0.43
2:N:156:PHE:CZ	2:N:326:PHE:HZ	2.35	0.43
1:T:342:THR:HG21	2:X:314:ALA:HA	2.00	0.43
1:U:239:SER:HB3	2:X:294:GLU:HG3	2.01	0.43
1:U:311:ALA:HA	1:U:323:LEU:HB3	2.00	0.43
1:A:85:LYS:O	1:A:88:GLU:HB2	2.19	0.43
1:A:440:THR:O	1:A:444:VAL:HG13	2.19	0.43
1:C:162:GLY:O	1:C:165:GLN:HB3	2.19	0.43
2:E:144:LEU:HD22	2:E:375:GLN:HG3	2.00	0.43
2:F:321:ALA:HB3	2:F:322:PRO:CD	2.49	0.43
3:G:182:ILE:HG21	3:G:214:LEU:HD13	2.00	0.43
2:M:218:VAL:HG21	2:M:236:GLY:HA2	2.00	0.43
3:P:74:ILE:HD11	3:P:98:HIS:HD2	1.83	0.43
1:T:346:SER:HA	6:X:600:ANP:O1G	2.19	0.43
2:W:187:VAL:HG21	2:W:233:ALA:HB2	2.01	0.43
2:X:256:ASP:HA	2:X:257:ASN:HA	1.81	0.43
3:Y:171:SER:C	3:Y:173:LEU:H	2.27	0.43
1:B:55:VAL:HG21	1:B:75:ILE:HD13	2.00	0.43
2:D:277:SER:OG	2:D:278:ALA:N	2.51	0.43
2:M:191:THR:HA	2:M:221:GLN:HG3	2.00	0.43
2:M:344:ILE:HG23	2:M:415:SER:HB3	2.00	0.43
2:N:419:ALA:CA	2:N:429:GLY:HA3	2.46	0.43
2:O:155:LEU:HD13	2:O:166:PHE:HB3	2.00	0.43
1:U:169:ILE:HB	1:U:328:VAL:HG22	2.01	0.43
1:A:332:GLN:O	1:A:333:GLY:C	2.62	0.43
1:C:165:GLN:HG3	1:C:166:ARG:N	2.34	0.43
1:L:56:GLU:OE2	1:L:62:LYS:HE3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:345:ILE:HG12	1:L:351:GLN:HG2	2.01	0.43
1:L:452:ASN:HB2	1:L:454:HIS:CE1	2.54	0.43
3:P:212:TYR:O	3:P:216:ASN:HB2	2.18	0.43
1:S:42:ARG:HE	1:S:72:GLN:HE22	1.67	0.43
1:T:383:LYS:HG2	1:T:387:GLN:HE21	1.84	0.43
1:U:50:GLN:HB3	2:V:69:GLY:HA2	2.00	0.43
3:Y:22:THR:HG22	3:Y:26:VAL:HG23	2.01	0.43
1:B:99:VAL:HG11	1:B:251:THR:HB	1.99	0.43
1:K:340:ILE:HB	1:K:341:PRO:HD3	2.01	0.43
1:L:52:GLU:HG2	1:L:64:MET:HE2	2.00	0.43
2:O:140:VAL:HG23	2:O:141:VAL:H	1.84	0.43
1:B:290:PRO:HA	1:B:291:PRO:HD2	1.93	0.43
4:H:49:VAL:HG22	4:H:76:THR:HG22	2.01	0.43
1:J:166:ARG:HH21	1:J:349:ASP:CG	2.27	0.43
1:L:238:ALA:HB1	2:O:328:HIS:HE1	1.84	0.43
2:N:150:GLY:O	2:N:297:THR:HA	2.19	0.43
2:N:345:TYR:HA	2:N:346:PRO:C	2.44	0.43
1:S:98:ASP:HB2	1:S:129:SER:O	2.19	0.43
1:T:478:HIS:HB3	1:T:481:LEU:HG	2.01	0.43
1:U:313:LYS:HD2	1:U:322:SER:HB3	1.99	0.43
1:A:394:LEU:O	1:A:397:ALA:N	2.52	0.42
2:E:256:ASP:HA	2:E:257:ASN:HA	1.75	0.42
3:G:271:ILE:HD13	3:G:271:ILE:HA	1.92	0.42
4:H:78:GLN:HB3	4:H:79:PRO:HD2	2.01	0.42
2:M:197:LEU:O	2:M:201:MET:HG2	2.19	0.42
1:S:174:GLN:HB3	2:V:354:LYS:HD3	2.01	0.42
1:S:378:SER:HB3	1:S:386:LYS:HE3	2.00	0.42
1:U:167:GLU:O	1:U:326:LEU:HA	2.19	0.42
2:V:190:ARG:HB2	2:V:193:GLU:HG3	2.01	0.42
2:X:237:LEU:HD13	2:X:296:ILE:HG12	2.01	0.42
1:B:478:HIS:HB3	1:B:481:LEU:HG	2.00	0.42
3:G:84:CYS:HA	3:G:233:ARG:HA	2.01	0.42
1:J:166:ARG:CD	1:J:308:LEU:O	2.67	0.42
2:M:256:ASP:HA	2:M:257:ASN:HA	1.85	0.42
1:U:161:ILE:HD13	1:U:326:LEU:HD21	2.01	0.42
2:V:256:ASP:HA	2:V:257:ASN:HA	1.70	0.42
1:A:146:GLU:O	1:A:163:ARG:HG3	2.19	0.42
1:K:67:ASN:HB3	2:O:17:ILE:HG23	2.00	0.42
1:L:103:PRO:HD3	1:L:258:TRP:CZ2	2.54	0.42
2:N:339:ILE:HG22	2:N:344:ILE:HB	2.01	0.42
1:S:161:ILE:HD11	1:S:167:GLU:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:290:PRO:HB3	2:X:276:PRO:HG3	2.01	0.42
1:T:378:SER:C	1:T:380:ALA:H	2.27	0.42
1:U:485:ILE:HG12	1:U:491:LEU:HD21	2.02	0.42
1:B:190:ARG:NE	1:B:439:ALA:HB2	2.34	0.42
1:K:311:ALA:HA	1:K:323:LEU:HB3	2.01	0.42
1:L:425:ARG:HD3	1:L:456:ASP:HA	2.00	0.42
2:M:251:VAL:HB	2:M:304:VAL:HG22	2.00	0.42
2:W:345:TYR:HB2	2:W:459:MET:HE1	2.01	0.42
2:X:339:ILE:CG2	2:X:344:ILE:HB	2.49	0.42
2:D:49:GLU:OE1	2:D:231:ARG:NE	2.44	0.42
2:F:158:GLY:O	2:F:163:LYS:NZ	2.53	0.42
2:F:202:LYS:HE3	2:F:209:LEU:HD11	2.02	0.42
2:F:239:ILE:O	2:F:243:PHE:HD2	2.02	0.42
1:K:250:PHE:CE1	1:K:307:LEU:HB2	2.55	0.42
2:O:311:TYR:HE2	2:O:313:PRO:HA	1.83	0.42
1:A:26:ASN:HD21	1:A:29:GLU:HB2	1.84	0.42
1:A:103:PRO:C	1:A:105:LEU:H	2.28	0.42
2:D:345:TYR:HA	2:D:346:PRO:C	2.44	0.42
2:E:98:VAL:HB	2:E:232:VAL:HG13	2.00	0.42
2:F:293:GLN:HG2	2:F:328:HIS:CB	2.50	0.42
3:G:186:LYS:HE3	3:G:190:GLN:HE22	1.85	0.42
1:J:272:ASP:HB2	1:J:328:VAL:O	2.20	0.42
1:J:475:LYS:O	1:J:479:ASN:HB2	2.19	0.42
1:K:98:ASP:HB2	1:K:129:SER:O	2.19	0.42
1:K:417:LYS:HA	1:K:420:LEU:HD22	2.01	0.42
1:S:139:LEU:N	1:S:140:PRO:HD2	2.34	0.42
1:U:204:VAL:HG22	1:U:232:ILE:HD12	2.01	0.42
1:U:271:ASP:HA	1:U:272:ASP:HA	1.79	0.42
1:C:422:ARG:NH1	1:C:453:GLY:HA2	2.35	0.42
3:G:203:ALA:O	3:G:204:ASN:C	2.61	0.42
3:P:78:THR:HG23	3:P:91:LEU:CD2	2.47	0.42
1:S:314:LEU:HB3	1:S:318:GLU:HB3	2.01	0.42
2:V:115:LYS:HE2	2:V:242:TYR:HD1	1.84	0.42
2:X:15:ALA:HB3	2:X:22:ASP:HB2	2.01	0.42
1:B:150:THR:HG21	1:B:155:VAL:HG11	2.01	0.42
1:B:217:GLN:O	1:B:220:GLN:HB3	2.20	0.42
2:F:258:ILE:HD13	2:F:293:GLN:HE22	1.85	0.42
2:F:410:ILE:O	2:F:414:LEU:HG	2.20	0.42
3:G:92:ALA:O	3:G:96:ARG:HG3	2.20	0.42
3:G:198:GLU:O	4:H:48:THR:HG23	2.20	0.42
1:J:105:LEU:HD23	1:J:123:ILE:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:141:ARG:NH1	1:K:312:ALA:CB	2.83	0.42
1:K:173:ARG:HG2	1:K:174:GLN:HG2	2.01	0.42
1:K:285:LEU:HD22	2:N:275:ILE:HG22	2.02	0.42
2:N:440:SER:OG	2:N:463:ILE:HB	2.19	0.42
2:V:388:ILE:HD13	2:V:396:LEU:HD21	2.01	0.42
2:V:400:ASP:O	2:V:404:VAL:HG23	2.20	0.42
3:Y:92:ALA:HB2	3:Y:117:GLN:HB3	2.02	0.42
1:C:30:THR:HG22	1:C:91:LYS:HA	2.02	0.42
1:C:99:VAL:HG11	1:C:251:THR:HB	2.02	0.42
4:H:69:PHE:O	4:H:90:ALA:HA	2.20	0.42
1:L:336:VAL:HG13	1:L:353:PHE:CE1	2.55	0.42
2:M:33:ILE:O	2:M:34:LEU:HB2	2.20	0.42
2:O:416:GLN:HA	2:O:417:PRO:HD3	1.94	0.42
1:T:340:ILE:HB	1:T:341:PRO:HD3	2.02	0.42
3:Y:86:SER:HB2	3:Y:89:SER:OG	2.20	0.42
2:D:279:VAL:HG12	2:D:279:VAL:O	2.20	0.42
2:M:425:THR:HB	2:M:427:ILE:HD12	2.01	0.42
2:X:189:GLU:O	2:X:222:MET:HG2	2.20	0.42
2:D:149:ARG:CG	2:D:149:ARG:NH1	2.75	0.41
2:O:417:PRO:HG3	2:O:459:MET:HG3	2.01	0.41
2:W:117:ILE:HA	2:W:238:THR:OG1	2.20	0.41
1:A:269:VAL:HG22	1:A:326:LEU:HB2	2.02	0.41
1:B:159:VAL:HG21	1:B:352:ILE:HG12	2.02	0.41
2:D:149:ARG:NH1	2:D:149:ARG:HG3	2.33	0.41
1:K:442:GLU:O	1:K:445:PRO:HD2	2.19	0.41
1:L:311:ALA:HA	1:L:323:LEU:HD23	2.00	0.41
2:M:27:GLN:O	2:M:29:GLU:N	2.53	0.41
4:Q:16:LEU:CB	4:Q:17:PRO:HD2	2.50	0.41
1:T:396:LEU:HA	1:T:399:TYR:HB3	2.02	0.41
2:W:276:PRO:HB2	3:Y:267:LEU:HD21	2.02	0.41
2:X:162:GLY:O	2:X:166:PHE:HB2	2.20	0.41
1:C:500:LYS:HG2	1:C:504:GLU:OE2	2.20	0.41
3:G:41:ALA:O	3:G:45:ASP:HB2	2.20	0.41
1:J:306:ARG:HA	2:N:223:ASN:HB2	2.01	0.41
2:N:321:ALA:HB3	2:N:322:PRO:CD	2.50	0.41
2:O:43:GLN:HB2	2:O:44:GLY:H	1.63	0.41
1:B:109:VAL:HG22	1:B:233:ILE:HB	2.02	0.41
2:E:185:THR:HG21	2:E:233:ALA:HA	2.02	0.41
2:F:182:SER:HA	2:F:252:LEU:O	2.21	0.41
2:N:381:TYR:O	2:N:385:GLN:HG2	2.21	0.41
2:O:189:GLU:O	2:O:221:GLN:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:277:SER:OG	2:O:278:ALA:N	2.53	0.41
1:T:166:ARG:HG2	1:T:311:ALA:HB3	2.02	0.41
1:T:289:ARG:HA	1:T:290:PRO:HD3	1.93	0.41
1:U:96:ILE:HB	1:U:130:ARG:HD3	2.03	0.41
1:U:165:GLN:NE2	1:U:167:GLU:OE1	2.53	0.41
1:U:416:THR:O	1:U:420:LEU:HB2	2.20	0.41
2:V:82:PRO:HB2	2:V:116:PRO:HB3	2.02	0.41
1:C:211:LYS:HD3	2:F:328:HIS:HA	2.02	0.41
2:E:26:GLU:O	2:E:29:GLU:HB3	2.21	0.41
2:F:158:GLY:O	2:F:161:VAL:HG22	2.20	0.41
1:J:358:LEU:HD22	1:J:363:ILE:HD12	2.03	0.41
1:J:360:TYR:CE2	2:M:351:LEU:O	2.74	0.41
2:N:387:ILE:HB	2:N:391:LEU:HD12	2.02	0.41
2:O:285:LEU:HD23	2:O:285:LEU:C	2.45	0.41
1:T:259:PHE:HB2	1:T:266:ALA:HB2	2.03	0.41
2:X:279:VAL:HG12	2:X:279:VAL:O	2.21	0.41
1:A:141:ARG:HH11	1:A:141:ARG:HD3	1.75	0.41
2:O:97:ASN:OD1	2:O:97:ASN:C	2.63	0.41
1:B:111:ASP:OD1	1:B:111:ASP:C	2.63	0.41
2:E:337:ARG:HG2	2:E:341:GLU:OE2	2.21	0.41
1:J:271:ASP:HA	1:J:272:ASP:HA	1.72	0.41
1:J:481:LEU:CD1	1:J:498:SER:HB3	2.42	0.41
1:K:55:VAL:HG21	1:K:75:ILE:HD13	2.02	0.41
1:L:243:PRO:HA	1:L:283:LEU:HD11	2.02	0.41
1:L:249:PRO:HB3	1:L:270:TYR:CD1	2.55	0.41
3:P:133:ILE:O	3:P:135:LYS:N	2.53	0.41
1:S:177:LYS:HG2	1:S:354:LEU:HD12	2.02	0.41
1:T:159:VAL:HG21	1:T:352:ILE:HG12	2.02	0.41
2:V:144:LEU:O	2:V:358:LEU:HD22	2.19	0.41
1:K:109:VAL:HG12	1:K:117:ILE:HD11	2.02	0.41
2:N:175:ALA:HB3	2:N:214:LYS:HD3	2.03	0.41
3:P:77:ILE:HG12	3:P:110:ILE:HD12	2.01	0.41
3:P:122:HIS:N	3:P:123:PRO:HD3	2.36	0.41
1:C:55:VAL:HG21	1:C:75:ILE:HD13	2.01	0.41
1:C:290:PRO:HA	1:C:291:PRO:HD3	1.96	0.41
2:E:182:SER:HB2	2:E:215:VAL:HG23	2.03	0.41
3:G:57:THR:HG23	3:G:191:SER:HB3	2.03	0.41
1:K:435:TYR:C	1:K:437:PRO:HD3	2.46	0.41
1:L:49:ILE:HD11	1:L:55:VAL:CG1	2.51	0.41
1:L:69:GLU:O	2:M:72:ARG:NH1	2.53	0.41
1:L:168:LEU:HB2	1:L:348:THR:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:184:PHE:CD1	2:M:184:PHE:C	2.99	0.41
2:N:136:THR:O	2:N:173:ASN:HB3	2.20	0.41
2:O:187:VAL:HG22	2:O:232:VAL:HG13	2.03	0.41
2:O:256:ASP:HA	2:O:257:ASN:HA	1.65	0.41
3:P:111:GLY:HA2	3:P:133:ILE:HD11	2.01	0.41
1:S:399:TYR:CD1	1:S:423:GLY:HA3	2.56	0.41
1:T:50:GLN:HB3	2:X:69:GLY:HA2	2.02	0.41
1:U:99:VAL:HG21	1:U:251:THR:HB	2.02	0.41
1:U:135:ALA:HA	1:U:136:PRO:HD2	1.84	0.41
2:V:162:GLY:HA2	6:V:600:ANP:H8	2.03	0.41
2:X:217:LEU:HB3	2:X:219:PHE:HE2	1.86	0.41
1:C:85:LYS:O	1:C:88:GLU:HB3	2.21	0.41
2:D:237:LEU:HD13	2:D:296:ILE:HG12	2.02	0.41
3:G:96:ARG:NE	3:G:121:THR:HG21	2.10	0.41
2:W:95:ILE:HD12	2:W:104:ASP:HB3	2.03	0.41
2:W:185:THR:OG1	2:W:236:GLY:HA3	2.21	0.41
2:X:231:ARG:HD3	2:X:234:LEU:HD12	2.02	0.41
2:X:339:ILE:HG23	2:X:344:ILE:HB	2.03	0.41
1:A:474:LEU:HD13	1:A:482:LEU:HD21	2.02	0.40
2:D:127:GLN:O	2:D:300:LYS:HE3	2.21	0.40
2:D:256:ASP:HA	2:D:257:ASN:HA	1.78	0.40
1:J:166:ARG:HD2	1:J:308:LEU:O	2.21	0.40
1:K:282:GLN:NE2	2:N:284:THR:HG22	2.36	0.40
1:L:174:GLN:HA	6:L:600:ANP:HNB1	1.86	0.40
2:N:168:GLN:NE2	2:N:204:THR:HG21	2.36	0.40
2:N:370:VAL:O	2:N:374:VAL:HG23	2.22	0.40
1:U:460:LEU:C	1:U:462:ARG:H	2.29	0.40
2:V:52:GLN:HB2	2:V:60:ARG:HB3	2.03	0.40
2:V:164:THR:HA	2:V:167:ILE:HG22	2.02	0.40
1:A:77:LEU:CD1	1:A:81:ASP:HB3	2.44	0.40
1:J:186:LEU:HD13	1:J:225:HIS:CD2	2.56	0.40
1:L:239:SER:HB3	2:O:294:GLU:HG3	2.03	0.40
2:O:43:GLN:H	2:O:43:GLN:HG2	1.65	0.40
3:P:133:ILE:H	3:P:133:ILE:HG13	1.76	0.40
1:S:439:ALA:HB3	1:S:442:GLU:HG3	2.02	0.40
1:U:338:ALA:HB3	1:U:341:PRO:HG2	2.03	0.40
1:A:38:ASP:HB3	1:A:286:LEU:HD13	2.02	0.40
1:B:161:ILE:HA	1:B:165:GLN:OE1	2.21	0.40
2:F:64:MET:HE1	2:F:231:ARG:HG3	2.03	0.40
2:F:277:SER:OG	2:F:278:ALA:N	2.54	0.40
2:M:314:ALA:O	2:M:315:ASP:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:336:SER:HB3	2:M:339:ILE:CG1	2.52	0.40
2:N:382:LYS:HA	2:N:385:GLN:HG3	2.02	0.40
1:U:382:VAL:HG12	1:U:384:ALA:H	1.86	0.40
1:C:172:ASP:O	1:C:177:LYS:NZ	2.54	0.40
2:F:15:ALA:HB3	2:F:22:ASP:HB2	2.03	0.40
1:J:111:ASP:OD1	1:J:111:ASP:C	2.64	0.40
1:J:442:GLU:C	1:J:445:PRO:HD2	2.47	0.40
2:N:204:THR:HG23	2:N:206:VAL:H	1.87	0.40
2:N:256:ASP:HA	2:N:257:ASN:HA	1.84	0.40
1:T:85:LYS:CE	2:W:32:ALA:HB2	2.49	0.40
1:T:148:VAL:HG22	1:T:163:ARG:HG2	2.03	0.40
2:W:393:MET:HE3	2:W:396:LEU:HD12	2.04	0.40
2:X:96:ILE:HG22	2:X:97:ASN:N	2.37	0.40
2:D:384:LEU:O	2:D:388:ILE:HG12	2.22	0.40
1:K:106:LEU:HD23	1:K:230:TYR:HA	2.03	0.40
1:L:349:ASP:HA	1:L:375:ARG:HD2	2.02	0.40
2:M:119:ALA:O	2:M:295:ARG:HD2	2.22	0.40
3:P:88:HIS:CD2	3:P:113:LYS:HB3	2.56	0.40
3:P:131:ASN:HB2	3:P:132:GLY:H	1.77	0.40
1:T:293:ARG:O	1:T:294:GLU:C	2.63	0.40
2:V:277:SER:OG	2:V:278:ALA:N	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	478/510 (94%)	456 (95%)	20 (4%)	2 (0%)	30	62
1	B	479/510 (94%)	457 (95%)	22 (5%)	0	100	100
1	C	482/510 (94%)	460 (95%)	21 (4%)	1 (0%)	43	73
1	J	477/510 (94%)	460 (96%)	15 (3%)	2 (0%)	30	62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	482/510 (94%)	458 (95%)	21 (4%)	3 (1%)	21	56
1	L	478/510 (94%)	454 (95%)	22 (5%)	2 (0%)	30	62
1	S	476/510 (93%)	454 (95%)	21 (4%)	1 (0%)	43	73
1	T	477/510 (94%)	452 (95%)	22 (5%)	3 (1%)	21	56
1	U	477/510 (94%)	447 (94%)	28 (6%)	2 (0%)	30	62
2	D	468/484 (97%)	444 (95%)	22 (5%)	2 (0%)	30	62
2	E	466/484 (96%)	437 (94%)	29 (6%)	0	100	100
2	F	467/484 (96%)	436 (93%)	29 (6%)	2 (0%)	30	62
2	M	468/484 (97%)	442 (94%)	23 (5%)	3 (1%)	21	56
2	N	468/484 (97%)	437 (93%)	29 (6%)	2 (0%)	30	62
2	O	466/484 (96%)	441 (95%)	23 (5%)	2 (0%)	30	62
2	V	468/484 (97%)	424 (91%)	40 (8%)	4 (1%)	14	47
2	W	465/484 (96%)	442 (95%)	23 (5%)	0	100	100
2	X	467/484 (96%)	439 (94%)	25 (5%)	3 (1%)	21	56
3	G	261/278 (94%)	244 (94%)	13 (5%)	4 (2%)	8	37
3	P	232/278 (84%)	202 (87%)	22 (10%)	8 (3%)	3	20
3	Y	186/278 (67%)	173 (93%)	12 (6%)	1 (0%)	24	59
4	H	110/137 (80%)	100 (91%)	10 (9%)	0	100	100
4	Q	74/137 (54%)	58 (78%)	11 (15%)	5 (7%)	1	7
4	Z	13/137 (10%)	10 (77%)	2 (15%)	1 (8%)	1	5
5	1	21/61 (34%)	18 (86%)	2 (10%)	1 (5%)	2	14
5	I	42/61 (69%)	32 (76%)	7 (17%)	3 (7%)	1	6
5	R	27/61 (44%)	22 (82%)	3 (11%)	2 (7%)	1	6
All	All	9475/10374 (91%)	8899 (94%)	517 (6%)	59 (1%)	21	56

All (59) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	202	ASP
1	J	414	ALA
2	M	28	SER
3	P	156	ALA
3	P	275	SER
4	Q	39	ILE

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Mol	Chain	Res	Type
5	R	32	ALA
5	1	40	THR
1	C	47	ASN
3	G	204	ASN
2	M	27	GLN
2	N	27	GLN
2	O	43	GLN
3	P	134	GLY
3	P	201	THR
3	P	204	ASN
4	Q	88	ILE
1	T	377	GLY
1	U	390	GLY
2	V	34	LEU
2	X	176	LYS
1	K	24	GLU
4	Q	47	PRO
1	A	406	ALA
3	G	135	LYS
3	G	203	ALA
1	L	508	ALA
2	V	8	PRO
2	V	277	SER
4	Z	134	GLN
2	D	398	GLU
5	I	54	SER
5	I	56	PRO
1	J	70	PRO
1	L	390	GLY
4	Q	50	GLU
5	R	31	THR
1	U	70	PRO
2	V	28	SER
3	Y	172	SER
2	D	279	VAL
2	N	279	VAL
3	P	205	VAL
4	Q	37	GLY
2	F	8	PRO
1	K	97	VAL
3	P	206	PRO
1	S	70	PRO

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Mol	Chain	Res	Type
1	T	97	VAL
2	F	279	VAL
5	I	57	THR
2	O	279	VAL
3	P	157	GLY
1	T	390	GLY
1	A	363	ILE
1	K	140	PRO
2	X	279	VAL
2	M	279	VAL
2	X	162	GLY

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%)	370 (95%)	18 (5%)	24	58
1	B	388/412 (94%)	371 (96%)	17 (4%)	25	59
1	C	389/412 (94%)	375 (96%)	14 (4%)	31	63
1	J	387/412 (94%)	370 (96%)	17 (4%)	25	59
1	K	392/412 (95%)	387 (99%)	5 (1%)	61	78
1	L	388/412 (94%)	368 (95%)	20 (5%)	21	54
1	S	387/412 (94%)	378 (98%)	9 (2%)	44	70
1	T	388/412 (94%)	376 (97%)	12 (3%)	35	66
1	U	388/412 (94%)	376 (97%)	12 (3%)	35	66
2	D	380/390 (97%)	365 (96%)	15 (4%)	28	62
2	E	378/390 (97%)	361 (96%)	17 (4%)	24	58
2	F	379/390 (97%)	360 (95%)	19 (5%)	22	55
2	M	380/390 (97%)	368 (97%)	12 (3%)	34	65
2	N	380/390 (97%)	369 (97%)	11 (3%)	37	67
2	O	379/390 (97%)	362 (96%)	17 (4%)	24	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	V	380/390 (97%)	373 (98%)	7 (2%)	51	74
2	W	378/390 (97%)	362 (96%)	16 (4%)	26	60
2	X	379/390 (97%)	372 (98%)	7 (2%)	51	74
3	G	223/236 (94%)	212 (95%)	11 (5%)	22	55
3	P	196/236 (83%)	168 (86%)	28 (14%)	3	16
3	Y	126/236 (53%)	116 (92%)	10 (8%)	11	40
4	H	62/112 (55%)	59 (95%)	3 (5%)	23	56
4	Q	9/112 (8%)	9 (100%)	0	100	100
5	I	24/48 (50%)	24 (100%)	0	100	100
5	R	3/48 (6%)	3 (100%)	0	100	100
All	All	7551/8246 (92%)	7254 (96%)	297 (4%)	28	62

All (297) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	VAL
1	A	54	LEU
1	A	166	ARG
1	A	195	SER
1	A	218	LEU
1	A	246	TYR
1	A	251	THR
1	A	316	GLU
1	A	322	SER
1	A	373	VAL
1	A	378	SER
1	A	393	LYS
1	A	412	LEU
1	A	419	THR
1	A	444	VAL
1	A	451	VAL
1	A	465	GLU
1	A	481	LEU
1	B	58	SER
1	B	99	VAL
1	B	138	ILE
1	B	159	VAL
1	B	173	ARG

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Mol	Chain	Res	Type
1	B	206	VAL
1	B	213	SER
1	B	231	SER
1	B	288	ARG
1	B	316	GLU
1	B	336	VAL
1	B	351	GLN
1	B	371	LEU
1	B	373	VAL
1	B	400	ARG
1	B	481	LEU
1	B	509	THR
1	C	38	ASP
1	C	99	VAL
1	C	139	LEU
1	C	143	SER
1	C	220	GLN
1	C	223	GLU
1	C	239	SER
1	C	267	LEU
1	C	306	ARG
1	C	357	GLU
1	C	416	THR
1	C	418	GLN
1	C	481	LEU
1	C	495	LEU
2	D	40	LYS
2	D	52	GLN
2	D	130	SER
2	D	132	GLU
2	D	149	ARG
2	D	167	ILE
2	D	191	THR
2	D	213	SER
2	D	247	GLU
2	D	251	VAL
2	D	297	THR
2	D	336	SER
2	D	383	SER
2	D	385	GLN
2	D	396	LEU
2	E	27	GLN

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Mol	Chain	Res	Type
2	E	111	SER
2	E	113	LEU
2	E	140	VAL
2	E	176	LYS
2	E	224	GLU
2	E	232	VAL
2	E	279	VAL
2	E	315	ASP
2	E	362	VAL
2	E	376	GLU
2	E	380	THR
2	E	386	ASP
2	E	393	MET
2	E	406	ARG
2	E	436	ASP
2	E	467	VAL
2	F	9	ILE
2	F	29	GLU
2	F	40	LYS
2	F	43	GLN
2	F	112	LYS
2	F	133	ILE
2	F	140	VAL
2	F	167	ILE
2	F	208	ASN
2	F	210	GLU
2	F	279	VAL
2	F	333	THR
2	F	336	SER
2	F	354	LYS
2	F	388	ILE
2	F	399	GLN
2	F	423	VAL
2	F	427	ILE
2	F	452	ILE
3	G	26	VAL
3	G	40	SER
3	G	57	THR
3	G	71	LYS
3	G	118	LEU
3	G	145	LEU
3	G	150	LEU

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Mol	Chain	Res	Type
3	G	153	VAL
3	G	216	ASN
3	G	237	MET
3	G	247	MET
4	H	39	ILE
4	H	46	VAL
4	H	70	ILE
1	J	66	LEU
1	J	134	LYS
1	J	206	VAL
1	J	218	LEU
1	J	237	THR
1	J	316	GLU
1	J	361	LYS
1	J	383	LYS
1	J	402	VAL
1	J	419	THR
1	J	420	LEU
1	J	440	THR
1	J	444	VAL
1	J	458	ILE
1	J	468	SER
1	J	496	LEU
1	J	509	THR
1	K	68	LEU
1	K	246	TYR
1	K	351	GLN
1	K	411	ASP
1	K	420	LEU
1	L	90	VAL
1	L	99	VAL
1	L	134	LYS
1	L	138	ILE
1	L	159	VAL
1	L	218	LEU
1	L	223	GLU
1	L	255	ILE
1	L	283	LEU
1	L	300	VAL
1	L	336	VAL
1	L	351	GLN
1	L	401	GLU

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Mol	Chain	Res	Type
1	L	416	THR
1	L	419	THR
1	L	420	LEU
1	L	468	SER
1	L	472	SER
1	L	480	GLU
1	L	481	LEU
2	M	10	THR
2	M	74	GLU
2	M	132	GLU
2	M	133	ILE
2	M	167	ILE
2	M	204	THR
2	M	210	GLU
2	M	249	GLN
2	M	282	GLN
2	M	390	ILE
2	M	403	THR
2	M	423	VAL
2	N	10	THR
2	N	77	LEU
2	N	112	LYS
2	N	113	LEU
2	N	132	GLU
2	N	140	VAL
2	N	210	GLU
2	N	269	SER
2	N	380	THR
2	N	408	ARG
2	N	466	VAL
2	O	9	ILE
2	O	17	ILE
2	O	43	GLN
2	O	62	ILE
2	O	98	VAL
2	O	112	LYS
2	O	167	ILE
2	O	174	ILE
2	O	182	SER
2	O	206	VAL
2	O	210	GLU
2	O	340	SER

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Mol	Chain	Res	Type
2	O	374	VAL
2	O	423	VAL
2	O	435	LYS
2	O	436	ASP
2	O	455	HIS
3	P	3	LEU
3	P	15	ASN
3	P	17	GLU
3	P	18	LYS
3	P	29	THR
3	P	44	MET
3	P	78	THR
3	P	97	ARG
3	P	99	LEU
3	P	107	ILE
3	P	113	LYS
3	P	130	ILE
3	P	131	ASN
3	P	133	ILE
3	P	136	ASP
3	P	148	ASP
3	P	150	LEU
3	P	155	LYS
3	P	170	VAL
3	P	202	ASP
3	P	205	VAL
3	P	214	LEU
3	P	216	ASN
3	P	218	MET
3	P	229	GLU
3	P	242	LYS
3	P	258	THR
3	P	276	SER
1	S	54	LEU
1	S	105	LEU
1	S	139	LEU
1	S	159	VAL
1	S	206	VAL
1	S	318	GLU
1	S	441	GLU
1	S	468	SER
1	S	495	LEU

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Mol	Chain	Res	Type
1	T	34	LEU
1	T	130	ARG
1	T	159	VAL
1	T	196	ASP
1	T	221	THR
1	T	288	ARG
1	T	320	SER
1	T	354	LEU
1	T	371	LEU
1	T	411	ASP
1	T	417	LYS
1	T	483	THR
1	U	163	ARG
1	U	206	VAL
1	U	213	SER
1	U	218	LEU
1	U	351	GLN
1	U	363	ILE
1	U	394	LEU
1	U	411	ASP
1	U	416	THR
1	U	424	GLU
1	U	441	GLU
1	U	487	GLU
2	V	10	THR
2	V	251	VAL
2	V	271	LEU
2	V	282	GLN
2	V	315	ASP
2	V	357	LEU
2	V	390	ILE
2	W	9	ILE
2	W	113	LEU
2	W	132	GLU
2	W	140	VAL
2	W	161	VAL
2	W	212	GLU
2	W	213	SER
2	W	232	VAL
2	W	251	VAL
2	W	275	ILE
2	W	279	VAL

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Mol	Chain	Res	Type
2	W	356	ARG
2	W	366	GLU
2	W	386	ASP
2	W	403	THR
2	W	434	LEU
2	X	167	ILE
2	X	208	ASN
2	X	237	LEU
2	X	250	ASP
2	X	272	LEU
2	X	356	ARG
2	X	372	SER
3	Y	15	ASN
3	Y	84	CYS
3	Y	98	HIS
3	Y	99	LEU
3	Y	121	THR
3	Y	133	ILE
3	Y	162	ILE
3	Y	219	LEU
3	Y	235	ASN
3	Y	269	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (108) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	145	HIS
1	A	210	GLN
1	A	217	GLN
1	A	332	GLN
1	A	351	GLN
1	A	454	HIS
1	B	145	HIS
1	B	225	HIS
1	B	262	ASN
1	B	282	GLN
1	B	428	GLN
1	C	95	ASN
1	C	145	HIS
1	C	224	GLN
1	C	418	GLN

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Mol	Chain	Res	Type
2	D	57	ASN
2	D	127	GLN
2	D	293	GLN
2	D	308	GLN
2	E	168	GLN
2	E	208	ASN
2	E	385	GLN
2	E	455	HIS
2	F	365	GLN
2	F	379	GLN
2	F	411	GLN
3	G	125	ASN
3	G	141	GLN
3	G	167	ASN
3	G	190	GLN
3	G	216	ASN
3	G	224	GLN
4	H	18	HIS
4	H	45	HIS
5	I	30	GLN
1	J	26	ASN
1	J	47	ASN
1	J	50	GLN
1	J	225	HIS
1	J	428	GLN
1	K	50	GLN
1	K	145	HIS
1	K	174	GLN
1	K	220	GLN
1	K	224	GLN
1	K	428	GLN
1	K	477	ASN
1	K	479	ASN
1	L	47	ASN
1	L	145	HIS
1	L	188	GLN
1	L	224	GLN
1	L	304	HIS
1	L	398	GLN
1	L	454	HIS
1	L	478	HIS
1	L	479	ASN

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Mol	Chain	Res	Type
2	M	263	GLN
2	M	379	GLN
2	N	57	ASN
2	N	97	ASN
2	N	127	GLN
2	N	168	GLN
2	N	195	ASN
2	N	379	GLN
2	O	52	GLN
2	O	118	HIS
2	O	208	ASN
2	O	293	GLN
2	O	308	GLN
2	O	328	HIS
2	O	379	GLN
3	P	54	ASN
3	P	88	HIS
3	P	90	GLN
3	P	122	HIS
3	P	216	ASN
1	S	50	GLN
1	S	332	GLN
1	S	454	HIS
1	T	26	ASN
1	T	28	ASN
1	T	67	ASN
1	T	387	GLN
1	T	434	GLN
1	U	50	GLN
1	U	217	GLN
1	U	332	GLN
1	U	398	GLN
1	U	479	ASN
2	V	52	GLN
2	V	118	HIS
2	V	172	ASN
2	W	172	ASN
2	W	195	ASN
2	W	328	HIS
2	W	365	GLN
2	W	379	GLN
2	X	27	GLN

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Mol	Chain	Res	Type
2	X	52	GLN
2	X	127	GLN
2	X	178	HIS
2	X	208	ASN
2	X	375	GLN
2	X	379	GLN
2	X	455	HIS
3	Y	15	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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$
6	ANP	A	600	7	33,33,33	2.14	12 (36%)	45,52,52	1.98	9 (20%)
6	ANP	D	600	7	33,33,33	1.98	9 (27%)	45,52,52	2.03	11 (24%)
6	ANP	S	600	7	33,33,33	2.00	9 (27%)	45,52,52	2.13	12 (26%)
6	ANP	J	600	7	33,33,33	1.99	10 (30%)	45,52,52	2.18	12 (26%)
6	ANP	M	600	7	33,33,33	1.95	10 (30%)	45,52,52	2.28	12 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	ANP	B	600	7	33,33,33	2.12	11 (33%)	45,52,52	2.18	12 (26%)
6	ANP	F	600	7	33,33,33	1.89	10 (30%)	45,52,52	2.02	13 (28%)
6	ANP	O	600	7	33,33,33	1.94	11 (33%)	45,52,52	2.08	14 (31%)
6	ANP	X	600	7	33,33,33	1.96	9 (27%)	45,52,52	2.21	11 (24%)
6	ANP	L	600	7	33,33,33	1.96	11 (33%)	45,52,52	2.11	13 (28%)
6	ANP	K	600	7	33,33,33	2.04	10 (30%)	45,52,52	2.14	12 (26%)
6	ANP	U	600	7	33,33,33	2.01	10 (30%)	45,52,52	2.19	12 (26%)
6	ANP	C	600	7	33,33,33	1.94	11 (33%)	45,52,52	2.05	11 (24%)
6	ANP	V	600	7	33,33,33	1.99	10 (30%)	45,52,52	2.17	14 (31%)
8	PO4	N	800	-	4,4,4	0.93	0	6,6,6	0.50	0
6	ANP	T	600	7	33,33,33	2.10	11 (33%)	45,52,52	2.07	14 (31%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ANP	A	600	7	-	2/18/38/38	0/3/3/3
6	ANP	D	600	7	-	4/18/38/38	0/3/3/3
6	ANP	S	600	7	-	3/18/38/38	0/3/3/3
6	ANP	J	600	7	-	3/18/38/38	0/3/3/3
6	ANP	M	600	7	-	4/18/38/38	0/3/3/3
6	ANP	B	600	7	-	6/18/38/38	0/3/3/3
6	ANP	F	600	7	-	6/18/38/38	0/3/3/3
6	ANP	O	600	7	-	3/18/38/38	0/3/3/3
6	ANP	X	600	7	-	9/18/38/38	0/3/3/3
6	ANP	L	600	7	-	3/18/38/38	0/3/3/3
6	ANP	K	600	7	-	5/18/38/38	0/3/3/3
6	ANP	U	600	7	-	5/18/38/38	0/3/3/3
6	ANP	C	600	7	-	3/18/38/38	0/3/3/3
6	ANP	V	600	7	-	5/18/38/38	0/3/3/3
6	ANP	T	600	7	-	2/18/38/38	0/3/3/3

All (154) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	U	600	ANP	C5-C4	5.21	1.48	1.39
6	T	600	ANP	C5-C4	5.19	1.48	1.39
6	B	600	ANP	C5-C4	5.16	1.48	1.39
6	O	600	ANP	C5-C4	5.00	1.48	1.39
6	K	600	ANP	C5-C4	4.95	1.47	1.39
6	D	600	ANP	C5-C4	4.91	1.47	1.39
6	S	600	ANP	C5-C4	4.89	1.47	1.39
6	J	600	ANP	C5-C4	4.87	1.47	1.39
6	X	600	ANP	C5-C4	4.87	1.47	1.39
6	F	600	ANP	C5-C4	4.83	1.47	1.39
6	A	600	ANP	C5-C4	4.83	1.47	1.39
6	V	600	ANP	C5-C4	4.71	1.47	1.39
6	A	600	ANP	PG-N3B	4.69	1.75	1.63
6	C	600	ANP	C5-C4	4.61	1.47	1.39
6	M	600	ANP	C5-C4	4.56	1.47	1.39
6	L	600	ANP	C5-C4	4.55	1.47	1.39
6	T	600	ANP	PB-N3B	4.54	1.75	1.63
6	S	600	ANP	PG-N3B	4.51	1.75	1.63
6	A	600	ANP	PB-N3B	4.50	1.75	1.63
6	V	600	ANP	PG-N3B	4.49	1.75	1.63
6	S	600	ANP	PB-N3B	4.46	1.75	1.63
6	T	600	ANP	PG-N3B	4.43	1.74	1.63
6	K	600	ANP	PB-N3B	4.42	1.74	1.63
6	B	600	ANP	PB-N3B	4.42	1.74	1.63
6	X	600	ANP	PB-N3B	4.40	1.74	1.63
6	M	600	ANP	PG-N3B	4.37	1.74	1.63
6	L	600	ANP	PG-N3B	4.33	1.74	1.63
6	L	600	ANP	PB-N3B	4.33	1.74	1.63
6	X	600	ANP	PG-N3B	4.29	1.74	1.63
6	V	600	ANP	PB-N3B	4.28	1.74	1.63
6	B	600	ANP	PG-N3B	4.25	1.74	1.63
6	J	600	ANP	PB-N3B	4.24	1.74	1.63
6	D	600	ANP	PG-N3B	4.22	1.74	1.63
6	K	600	ANP	PG-N3B	4.21	1.74	1.63
6	M	600	ANP	PB-N3B	4.11	1.74	1.63
6	D	600	ANP	PB-N3B	4.09	1.74	1.63
6	U	600	ANP	PG-N3B	4.07	1.74	1.63
6	J	600	ANP	PG-N3B	4.03	1.73	1.63
6	O	600	ANP	PB-N3B	3.93	1.73	1.63
6	T	600	ANP	PG-O1G	3.93	1.52	1.46
6	A	600	ANP	PG-O1G	3.92	1.52	1.46
6	U	600	ANP	PB-N3B	3.89	1.73	1.63
6	J	600	ANP	PG-O1G	3.86	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	600	ANP	PG-N3B	3.85	1.73	1.63
6	D	600	ANP	PG-O1G	3.80	1.51	1.46
6	O	600	ANP	PG-N3B	3.79	1.73	1.63
6	B	600	ANP	PB-O1B	3.78	1.51	1.46
6	C	600	ANP	PB-N3B	3.76	1.73	1.63
6	F	600	ANP	PG-N3B	3.74	1.73	1.63
6	F	600	ANP	PB-N3B	3.68	1.73	1.63
6	U	600	ANP	PG-O1G	3.65	1.51	1.46
6	K	600	ANP	PB-O1B	3.57	1.51	1.46
6	B	600	ANP	PG-O1G	3.49	1.51	1.46
6	M	600	ANP	PG-O1G	3.48	1.51	1.46
6	K	600	ANP	PG-O1G	3.48	1.51	1.46
6	A	600	ANP	PB-O1B	3.44	1.51	1.46
6	J	600	ANP	PB-O1B	3.43	1.51	1.46
6	T	600	ANP	PB-O1B	3.39	1.51	1.46
6	C	600	ANP	PG-O1G	3.39	1.51	1.46
6	V	600	ANP	PG-O1G	3.38	1.51	1.46
6	S	600	ANP	PB-O1B	3.34	1.51	1.46
6	C	600	ANP	PB-O1B	3.28	1.51	1.46
6	X	600	ANP	PB-O1B	3.24	1.51	1.46
6	F	600	ANP	PG-O1G	3.22	1.51	1.46
6	V	600	ANP	PB-O1B	3.09	1.50	1.46
6	O	600	ANP	PG-O1G	3.09	1.50	1.46
6	U	600	ANP	PB-O1B	3.09	1.50	1.46
6	L	600	ANP	PG-O1G	3.05	1.50	1.46
6	L	600	ANP	PB-O1B	3.04	1.50	1.46
6	O	600	ANP	PB-O1B	3.02	1.50	1.46
6	S	600	ANP	PG-O1G	2.99	1.50	1.46
6	M	600	ANP	PB-O1B	2.95	1.50	1.46
6	O	600	ANP	C5-C6	2.91	1.49	1.41
6	B	600	ANP	C5-C6	2.88	1.49	1.41
6	V	600	ANP	C5-C6	2.88	1.49	1.41
6	T	600	ANP	C5-C6	2.86	1.49	1.41
6	A	600	ANP	C5-N7	-2.86	1.33	1.39
6	K	600	ANP	C5-C6	2.86	1.49	1.41
6	U	600	ANP	C5-C6	2.82	1.48	1.41
6	X	600	ANP	PG-O1G	2.81	1.50	1.46
6	X	600	ANP	C5-C6	2.76	1.48	1.41
6	D	600	ANP	C5-C6	2.74	1.48	1.41
6	D	600	ANP	PB-O1B	2.74	1.50	1.46
6	B	600	ANP	PB-O3A	2.73	1.62	1.59
6	S	600	ANP	C5-C6	2.72	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	600	ANP	PB-O1B	2.72	1.50	1.46
6	F	600	ANP	C5-C6	2.70	1.48	1.41
6	L	600	ANP	C5-N7	-2.68	1.34	1.39
6	J	600	ANP	C5-C6	2.66	1.48	1.41
6	B	600	ANP	PA-O3A	2.65	1.62	1.59
6	M	600	ANP	C5-N7	-2.64	1.34	1.39
6	L	600	ANP	C5-C6	2.62	1.48	1.41
6	C	600	ANP	C5-N7	-2.59	1.34	1.39
6	A	600	ANP	PG-O2G	-2.58	1.50	1.56
6	S	600	ANP	PG-O3G	-2.57	1.50	1.56
6	X	600	ANP	C5-N7	-2.56	1.34	1.39
6	M	600	ANP	C5-C6	2.54	1.48	1.41
6	D	600	ANP	C8-N7	2.54	1.36	1.31
6	A	600	ANP	C5-C6	2.54	1.48	1.41
6	C	600	ANP	C5-C6	2.53	1.48	1.41
6	B	600	ANP	C5-N7	-2.52	1.34	1.39
6	S	600	ANP	C8-N7	2.52	1.36	1.31
6	J	600	ANP	PG-O2G	-2.52	1.50	1.56
6	O	600	ANP	C8-N7	2.52	1.36	1.31
6	J	600	ANP	C8-N7	2.50	1.36	1.31
6	A	600	ANP	PG-O3G	-2.49	1.50	1.56
6	A	600	ANP	PB-O3A	2.48	1.62	1.59
6	U	600	ANP	C5-N7	-2.48	1.34	1.39
6	F	600	ANP	C8-N7	2.46	1.36	1.31
6	F	600	ANP	C5-N7	-2.45	1.34	1.39
6	T	600	ANP	C8-N7	2.43	1.36	1.31
6	C	600	ANP	PB-O3A	2.42	1.62	1.59
6	T	600	ANP	PB-O3A	2.38	1.62	1.59
6	V	600	ANP	C8-N7	2.38	1.36	1.31
6	V	600	ANP	C5-N7	-2.36	1.34	1.39
6	U	600	ANP	C8-N7	2.36	1.36	1.31
6	K	600	ANP	C8-N7	2.34	1.36	1.31
6	C	600	ANP	C8-N7	2.32	1.36	1.31
6	B	600	ANP	C8-N7	2.32	1.36	1.31
6	X	600	ANP	C8-N7	2.32	1.36	1.31
6	D	600	ANP	C5-N7	-2.32	1.34	1.39
6	K	600	ANP	C5-N7	-2.32	1.34	1.39
6	S	600	ANP	C5-N7	-2.31	1.34	1.39
6	M	600	ANP	C8-N7	2.30	1.36	1.31
6	F	600	ANP	PB-O2B	-2.30	1.50	1.56
6	X	600	ANP	PG-O3G	-2.27	1.50	1.56
6	M	600	ANP	PG-O2G	-2.24	1.50	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	600	ANP	PG-O3G	-2.23	1.50	1.56
6	O	600	ANP	C5-N7	-2.21	1.35	1.39
6	T	600	ANP	C5-N7	-2.20	1.35	1.39
6	T	600	ANP	PA-O3A	2.19	1.61	1.59
6	A	600	ANP	C8-N7	2.16	1.35	1.31
6	O	600	ANP	PB-O3A	2.15	1.61	1.59
6	J	600	ANP	C5-N7	-2.14	1.35	1.39
6	D	600	ANP	PG-O3G	-2.14	1.51	1.56
6	J	600	ANP	PG-O3G	-2.13	1.51	1.56
6	U	600	ANP	PA-O3A	2.12	1.61	1.59
6	U	600	ANP	PB-O3A	2.12	1.61	1.59
6	O	600	ANP	PG-O3G	-2.12	1.51	1.56
6	C	600	ANP	PG-O3G	-2.11	1.51	1.56
6	L	600	ANP	C8-N9	-2.10	1.34	1.37
6	L	600	ANP	C8-N7	2.09	1.35	1.31
6	F	600	ANP	PG-O3G	-2.08	1.51	1.56
6	M	600	ANP	PG-O3G	-2.07	1.51	1.56
6	L	600	ANP	PB-O2B	-2.06	1.51	1.56
6	O	600	ANP	PB-O2B	-2.06	1.51	1.56
6	T	600	ANP	PG-O3G	-2.06	1.51	1.56
6	K	600	ANP	PG-O3G	-2.05	1.51	1.56
6	V	600	ANP	PG-O3G	-2.04	1.51	1.56
6	K	600	ANP	PB-O3A	2.02	1.61	1.59
6	V	600	ANP	PB-O2B	-2.01	1.51	1.56
6	A	600	ANP	PA-O3A	2.01	1.61	1.59
6	C	600	ANP	C4-N9	-2.01	1.33	1.37
6	B	600	ANP	PG-O2G	-2.01	1.51	1.56

All (182) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	X	600	ANP	C5-C4-N3	-6.44	117.85	126.72
6	A	600	ANP	C5-C4-N3	-6.38	117.94	126.72
6	M	600	ANP	C5-C4-N3	-6.35	117.97	126.72
6	D	600	ANP	C5-C4-N3	-6.33	118.00	126.72
6	X	600	ANP	O1G-PG-N3B	-6.32	102.46	111.77
6	K	600	ANP	C5-C4-N3	-6.09	118.33	126.72
6	S	600	ANP	C5-C4-N3	-6.06	118.38	126.72
6	U	600	ANP	C5-C4-N3	-6.04	118.40	126.72
6	J	600	ANP	O1G-PG-N3B	-6.02	102.90	111.77
6	B	600	ANP	C5-C4-N3	-6.01	118.44	126.72
6	B	600	ANP	O1G-PG-N3B	-6.00	102.94	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	V	600	ANP	O1G-PG-N3B	-5.95	103.00	111.77
6	V	600	ANP	C5-C4-N3	-5.93	118.55	126.72
6	T	600	ANP	C5-C4-N3	-5.85	118.66	126.72
6	F	600	ANP	C5-C4-N3	-5.83	118.68	126.72
6	J	600	ANP	C5-C4-N3	-5.81	118.72	126.72
6	M	600	ANP	O2B-PB-O1B	5.79	122.28	109.87
6	U	600	ANP	O1G-PG-N3B	-5.72	103.35	111.77
6	O	600	ANP	C5-C4-N3	-5.66	118.92	126.72
6	L	600	ANP	C5-C4-N3	-5.60	119.01	126.72
6	C	600	ANP	C5-C4-N3	-5.57	119.04	126.72
6	K	600	ANP	O1G-PG-N3B	-5.40	103.82	111.77
6	O	600	ANP	O1G-PG-N3B	-5.30	103.97	111.77
6	M	600	ANP	O1G-PG-N3B	-5.24	104.06	111.77
6	L	600	ANP	O2B-PB-O1B	5.16	120.93	109.87
6	B	600	ANP	O2B-PB-O1B	5.12	120.86	109.87
6	J	600	ANP	O2B-PB-O1B	5.06	120.72	109.87
6	L	600	ANP	O1G-PG-N3B	-5.03	104.36	111.77
6	A	600	ANP	N3-C4-N9	5.02	135.71	127.17
6	X	600	ANP	N3-C4-N9	4.98	135.63	127.17
6	U	600	ANP	N3-C4-N9	4.96	135.60	127.17
6	K	600	ANP	N3-C4-N9	4.83	135.39	127.17
6	S	600	ANP	N3-C4-N9	4.82	135.37	127.17
6	D	600	ANP	N3-C4-N9	4.81	135.35	127.17
6	M	600	ANP	N3-C4-N9	4.78	135.29	127.17
6	J	600	ANP	N3-C4-N9	4.76	135.26	127.17
6	C	600	ANP	O2B-PB-O1B	4.74	120.04	109.87
6	K	600	ANP	O2B-PB-O1B	4.71	119.97	109.87
6	S	600	ANP	O2B-PB-O1B	4.70	119.95	109.87
6	B	600	ANP	N3-C4-N9	4.69	135.14	127.17
6	C	600	ANP	O1G-PG-N3B	-4.67	104.89	111.77
6	T	600	ANP	N3-C4-N9	4.67	135.10	127.17
6	C	600	ANP	N3-C4-N9	4.65	135.07	127.17
6	L	600	ANP	N3-C4-N9	4.62	135.02	127.17
6	F	600	ANP	N3-C4-N9	4.58	134.96	127.17
6	V	600	ANP	O2B-PB-O1B	4.57	119.67	109.87
6	V	600	ANP	N3-C4-N9	4.56	134.92	127.17
6	D	600	ANP	O2B-PB-O1B	4.54	119.62	109.87
6	A	600	ANP	O2B-PB-O1B	4.47	119.45	109.87
6	D	600	ANP	O1G-PG-N3B	-4.42	105.27	111.77
6	F	600	ANP	O2B-PB-O1B	4.40	119.31	109.87
6	T	600	ANP	O1G-PG-N3B	-4.38	105.33	111.77
6	M	600	ANP	O1B-PB-N3B	-4.34	105.37	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	U	600	ANP	O2B-PB-O1B	4.32	119.14	109.87
6	O	600	ANP	N3-C4-N9	4.30	134.49	127.17
6	F	600	ANP	O1G-PG-N3B	-4.29	105.45	111.77
6	S	600	ANP	O1G-PG-N3B	-4.21	105.56	111.77
6	O	600	ANP	O2B-PB-O1B	4.17	118.81	109.87
6	T	600	ANP	O2B-PB-O1B	4.10	118.67	109.87
6	X	600	ANP	O2B-PB-O1B	4.05	118.56	109.87
6	X	600	ANP	C2-N3-C4	3.95	121.47	111.83
6	K	600	ANP	C2-N3-C4	3.94	121.46	111.83
6	S	600	ANP	C2-N3-C4	3.92	121.41	111.83
6	M	600	ANP	C2-N3-C4	3.86	121.25	111.83
6	U	600	ANP	C2-N3-C4	3.81	121.14	111.83
6	J	600	ANP	C2-N3-C4	3.79	121.08	111.83
6	F	600	ANP	C2-N3-C4	3.79	121.08	111.83
6	V	600	ANP	C4-C5-N7	-3.75	106.30	110.58
6	V	600	ANP	C2-N3-C4	3.74	120.96	111.83
6	T	600	ANP	C2-N3-C4	3.73	120.94	111.83
6	B	600	ANP	C2-N3-C4	3.72	120.93	111.83
6	D	600	ANP	C4-C5-N7	-3.69	106.36	110.58
6	A	600	ANP	C2-N3-C4	3.68	120.81	111.83
6	C	600	ANP	C2-N3-C4	3.66	120.76	111.83
6	K	600	ANP	N3-C2-N1	-3.65	123.06	128.58
6	S	600	ANP	N3-C2-N1	-3.65	123.06	128.58
6	O	600	ANP	C2-N3-C4	3.64	120.73	111.83
6	L	600	ANP	N3-C2-N1	-3.61	123.11	128.58
6	D	600	ANP	C2-N3-C4	3.61	120.65	111.83
6	M	600	ANP	C4-C5-N7	-3.59	106.47	110.58
6	O	600	ANP	C4-C5-N7	-3.59	106.47	110.58
6	A	600	ANP	O1G-PG-N3B	-3.58	106.50	111.77
6	T	600	ANP	O1B-PB-N3B	-3.56	106.53	111.77
6	L	600	ANP	C2-N3-C4	3.56	120.52	111.83
6	U	600	ANP	N3-C2-N1	-3.53	123.24	128.58
6	J	600	ANP	N3-C2-N1	-3.52	123.26	128.58
6	S	600	ANP	O1B-PB-N3B	-3.49	106.64	111.77
6	K	600	ANP	C4-C5-N7	-3.46	106.62	110.58
6	C	600	ANP	N3-C2-N1	-3.43	123.39	128.58
6	B	600	ANP	C4-C5-N7	-3.43	106.66	110.58
6	L	600	ANP	C4-C5-N7	-3.42	106.67	110.58
6	F	600	ANP	N3-C2-N1	-3.41	123.42	128.58
6	B	600	ANP	N3-C2-N1	-3.35	123.51	128.58
6	T	600	ANP	N3-C2-N1	-3.34	123.53	128.58
6	S	600	ANP	C4-C5-N7	-3.31	106.80	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	600	ANP	N3-C2-N1	-3.30	123.58	128.58
6	U	600	ANP	O1B-PB-N3B	-3.30	106.91	111.77
6	F	600	ANP	C4-C5-N7	-3.28	106.83	110.58
6	O	600	ANP	N3-C2-N1	-3.27	123.64	128.58
6	X	600	ANP	N3-C2-N1	-3.26	123.65	128.58
6	T	600	ANP	C4-C5-N7	-3.23	106.89	110.58
6	X	600	ANP	O1B-PB-N3B	-3.20	107.05	111.77
6	F	600	ANP	O2G-PG-O3G	3.17	116.11	107.59
6	X	600	ANP	C4-C5-N7	-3.14	107.00	110.58
6	V	600	ANP	N3-C2-N1	-3.12	123.86	128.58
6	U	600	ANP	C4-C5-N7	-3.11	107.03	110.58
6	J	600	ANP	C4-C5-N7	-3.08	107.06	110.58
6	C	600	ANP	O2G-PG-O3G	3.07	115.85	107.59
6	A	600	ANP	C4-C5-N7	-3.07	107.07	110.58
6	A	600	ANP	N3-C2-N1	-3.02	124.01	128.58
6	C	600	ANP	C4-C5-N7	-2.99	107.17	110.58
6	O	600	ANP	O2G-PG-O3G	2.93	115.46	107.59
6	D	600	ANP	O1B-PB-N3B	-2.91	107.49	111.77
6	L	600	ANP	C4-N9-C8	2.86	108.74	105.74
6	B	600	ANP	O2G-PG-O3G	2.78	115.07	107.59
6	C	600	ANP	C4-N9-C8	2.77	108.65	105.74
6	M	600	ANP	C2'-C1'-N9	-2.74	106.49	113.30
6	V	600	ANP	C5-N7-C8	2.71	107.71	103.45
6	T	600	ANP	O2G-PG-O3G	2.71	114.88	107.59
6	V	600	ANP	O1B-PB-N3B	-2.71	107.78	111.77
6	D	600	ANP	N3-C2-N1	-2.69	124.51	128.58
6	S	600	ANP	O2G-PG-O3G	2.64	114.69	107.59
6	L	600	ANP	O2G-PG-O3G	2.63	114.65	107.59
6	D	600	ANP	C5-N7-C8	2.60	107.54	103.45
6	L	600	ANP	O1B-PB-N3B	-2.60	107.94	111.77
6	V	600	ANP	C4-N9-C8	2.59	108.46	105.74
6	J	600	ANP	C4-N9-C8	2.58	108.45	105.74
6	K	600	ANP	O2G-PG-O3G	2.56	114.48	107.59
6	L	600	ANP	C5-N7-C8	2.55	107.45	103.45
6	M	600	ANP	C5-N7-C8	2.55	107.45	103.45
6	X	600	ANP	O2G-PG-O3G	2.54	114.42	107.59
6	O	600	ANP	C5-N7-C8	2.53	107.42	103.45
6	U	600	ANP	O2G-PG-O3G	2.53	114.38	107.59
6	C	600	ANP	O1B-PB-N3B	-2.52	108.05	111.77
6	K	600	ANP	C5-N7-C8	2.52	107.41	103.45
6	S	600	ANP	C5-N7-C8	2.49	107.37	103.45
6	K	600	ANP	O1B-PB-N3B	-2.46	108.15	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	600	ANP	C5-N7-C8	2.43	107.27	103.45
6	V	600	ANP	O2G-PG-O3G	2.43	114.11	107.59
6	T	600	ANP	C3'-C2'-C1'	2.42	106.04	101.46
6	A	600	ANP	O2G-PG-O3G	2.42	114.08	107.59
6	T	600	ANP	C5-N7-C8	2.38	107.18	103.45
6	B	600	ANP	C5-N7-C8	2.36	107.16	103.45
6	M	600	ANP	O2G-PG-O3G	2.33	113.86	107.59
6	F	600	ANP	C4-N9-C8	2.32	108.17	105.74
6	S	600	ANP	C4-N9-C8	2.30	108.15	105.74
6	L	600	ANP	C2-N1-C6	2.29	122.50	118.73
6	U	600	ANP	C5-N7-C8	2.28	107.03	103.45
6	J	600	ANP	C5-N7-C8	2.27	107.02	103.45
6	X	600	ANP	C3'-C2'-C1'	2.23	105.68	101.46
6	K	600	ANP	C4-N9-C8	2.22	108.07	105.74
6	V	600	ANP	C3'-C2'-C1'	2.22	105.66	101.46
6	B	600	ANP	O1B-PB-N3B	-2.22	108.51	111.77
6	C	600	ANP	C5-N7-C8	2.20	106.91	103.45
6	O	600	ANP	C4-N9-C8	2.20	108.05	105.74
6	V	600	ANP	C6-C5-N7	2.20	136.33	132.09
6	J	600	ANP	C3'-C2'-C1'	2.19	105.61	101.46
6	D	600	ANP	C4-N9-C8	2.17	108.01	105.74
6	X	600	ANP	C5-N7-C8	2.16	106.85	103.45
6	B	600	ANP	O4'-C1'-N9	2.16	112.25	108.09
6	O	600	ANP	C6-C5-N7	2.15	136.24	132.09
6	L	600	ANP	O2A-PA-O1A	2.15	122.45	112.44
6	K	600	ANP	C6-C5-N7	2.12	136.19	132.09
6	U	600	ANP	C4-N9-C8	2.12	107.96	105.74
6	O	600	ANP	O2B-PB-O3A	2.11	111.68	104.64
6	O	600	ANP	C2-N1-C6	2.10	122.17	118.73
6	D	600	ANP	O2G-PG-O3G	2.09	113.22	107.59
6	U	600	ANP	C3'-C2'-C1'	2.08	105.40	101.46
6	V	600	ANP	N9-C8-N7	-2.07	111.00	113.94
6	S	600	ANP	C6-C5-N7	2.07	136.07	132.09
6	T	600	ANP	C2-N1-C6	2.05	122.10	118.73
6	A	600	ANP	C5-N7-C8	2.05	106.67	103.45
6	O	600	ANP	O1B-PB-N3B	-2.05	108.75	111.77
6	B	600	ANP	C2-N1-C6	2.04	122.08	118.73
6	M	600	ANP	C4-N9-C8	2.04	107.88	105.74
6	J	600	ANP	C6-C5-N7	2.03	136.01	132.09
6	T	600	ANP	C4-N9-C8	2.02	107.86	105.74
6	F	600	ANP	O2B-PB-O3A	2.02	111.40	104.64
6	F	600	ANP	C6-C5-N7	2.02	135.99	132.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	600	ANP	C2-N1-C6	2.02	122.05	118.73
6	T	600	ANP	O4'-C1'-N9	2.02	111.96	108.09
6	F	600	ANP	O3A-PA-O1A	-2.01	104.66	110.70

There are no chirality outliers.

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	600	ANP	PB-N3B-PG-O1G
6	A	600	ANP	PG-N3B-PB-O1B
6	B	600	ANP	PB-N3B-PG-O1G
6	B	600	ANP	PG-N3B-PB-O1B
6	B	600	ANP	C5'-O5'-PA-O2A
6	C	600	ANP	PB-N3B-PG-O1G
6	C	600	ANP	PG-N3B-PB-O1B
6	D	600	ANP	PB-N3B-PG-O1G
6	D	600	ANP	PG-N3B-PB-O1B
6	D	600	ANP	PA-O3A-PB-O2B
6	F	600	ANP	PB-N3B-PG-O1G
6	F	600	ANP	PG-N3B-PB-O1B
6	F	600	ANP	C5'-O5'-PA-O2A
6	J	600	ANP	PB-N3B-PG-O1G
6	J	600	ANP	PG-N3B-PB-O1B
6	J	600	ANP	PG-N3B-PB-O3A
6	K	600	ANP	PB-N3B-PG-O1G
6	K	600	ANP	PG-N3B-PB-O1B
6	L	600	ANP	PB-N3B-PG-O1G
6	L	600	ANP	PG-N3B-PB-O1B
6	M	600	ANP	PB-N3B-PG-O1G
6	M	600	ANP	PG-N3B-PB-O1B
6	M	600	ANP	PA-O3A-PB-O2B
6	O	600	ANP	PB-N3B-PG-O1G
6	O	600	ANP	PG-N3B-PB-O1B
6	O	600	ANP	PG-N3B-PB-O3A
6	S	600	ANP	PB-N3B-PG-O1G
6	S	600	ANP	PG-N3B-PB-O1B
6	S	600	ANP	PG-N3B-PB-O3A
6	T	600	ANP	PB-N3B-PG-O1G
6	T	600	ANP	PG-N3B-PB-O1B
6	U	600	ANP	PB-N3B-PG-O1G
6	U	600	ANP	PG-N3B-PB-O1B
6	V	600	ANP	PB-N3B-PG-O1G

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Mol	Chain	Res	Type	Atoms
6	V	600	ANP	PG-N3B-PB-O1B
6	V	600	ANP	C5'-O5'-PA-O1A
6	V	600	ANP	C5'-O5'-PA-O2A
6	X	600	ANP	PB-N3B-PG-O1G
6	X	600	ANP	PG-N3B-PB-O1B
6	X	600	ANP	PA-O3A-PB-O1B
6	X	600	ANP	PA-O3A-PB-O2B
6	X	600	ANP	C5'-O5'-PA-O1A
6	X	600	ANP	C5'-O5'-PA-O2A
6	X	600	ANP	C5'-O5'-PA-O3A
6	X	600	ANP	O4'-C4'-C5'-O5'
6	X	600	ANP	C3'-C4'-C5'-O5'
6	K	600	ANP	O4'-C4'-C5'-O5'
6	F	600	ANP	O4'-C4'-C5'-O5'
6	K	600	ANP	C3'-C4'-C5'-O5'
6	L	600	ANP	PG-N3B-PB-O3A
6	B	600	ANP	C5'-O5'-PA-O3A
6	F	600	ANP	C5'-O5'-PA-O3A
6	V	600	ANP	C5'-O5'-PA-O3A
6	K	600	ANP	PB-O3A-PA-O1A
6	U	600	ANP	PB-O3A-PA-O2A
6	B	600	ANP	PB-O3A-PA-O1A
6	F	600	ANP	C3'-C4'-C5'-O5'
6	B	600	ANP	C2'-C1'-N9-C8
6	D	600	ANP	PA-O3A-PB-O1B
6	M	600	ANP	PA-O3A-PB-O1B
6	C	600	ANP	PG-N3B-PB-O3A
6	U	600	ANP	PG-N3B-PB-O3A
6	U	600	ANP	PB-O3A-PA-O1A

There are no ring outliers.

9 monomers are involved in 15 short contacts:

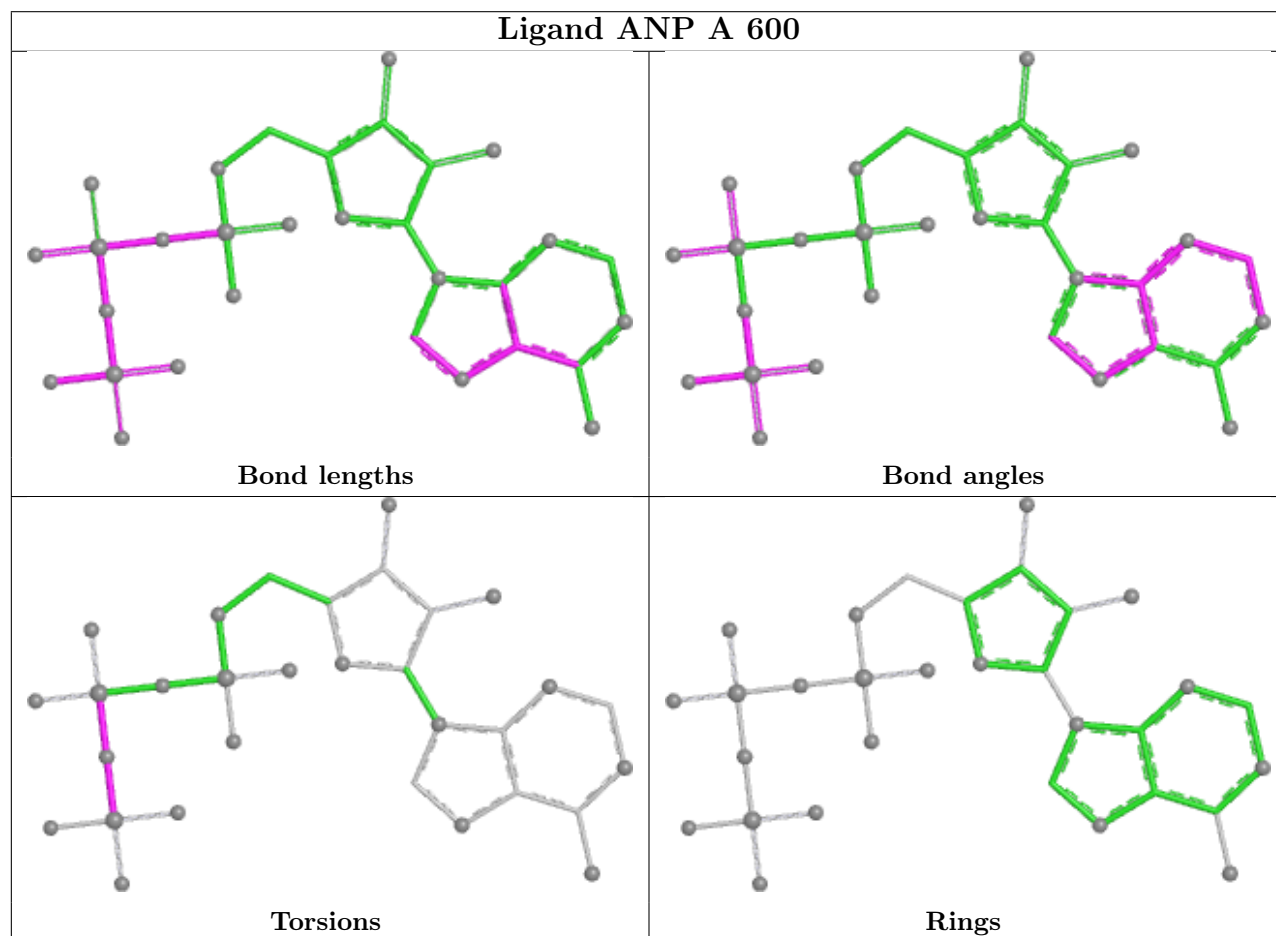
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	600	ANP	1	0
6	D	600	ANP	4	0
6	M	600	ANP	2	0
6	B	600	ANP	1	0
6	X	600	ANP	2	0
6	L	600	ANP	1	0
6	C	600	ANP	1	0
6	V	600	ANP	1	0

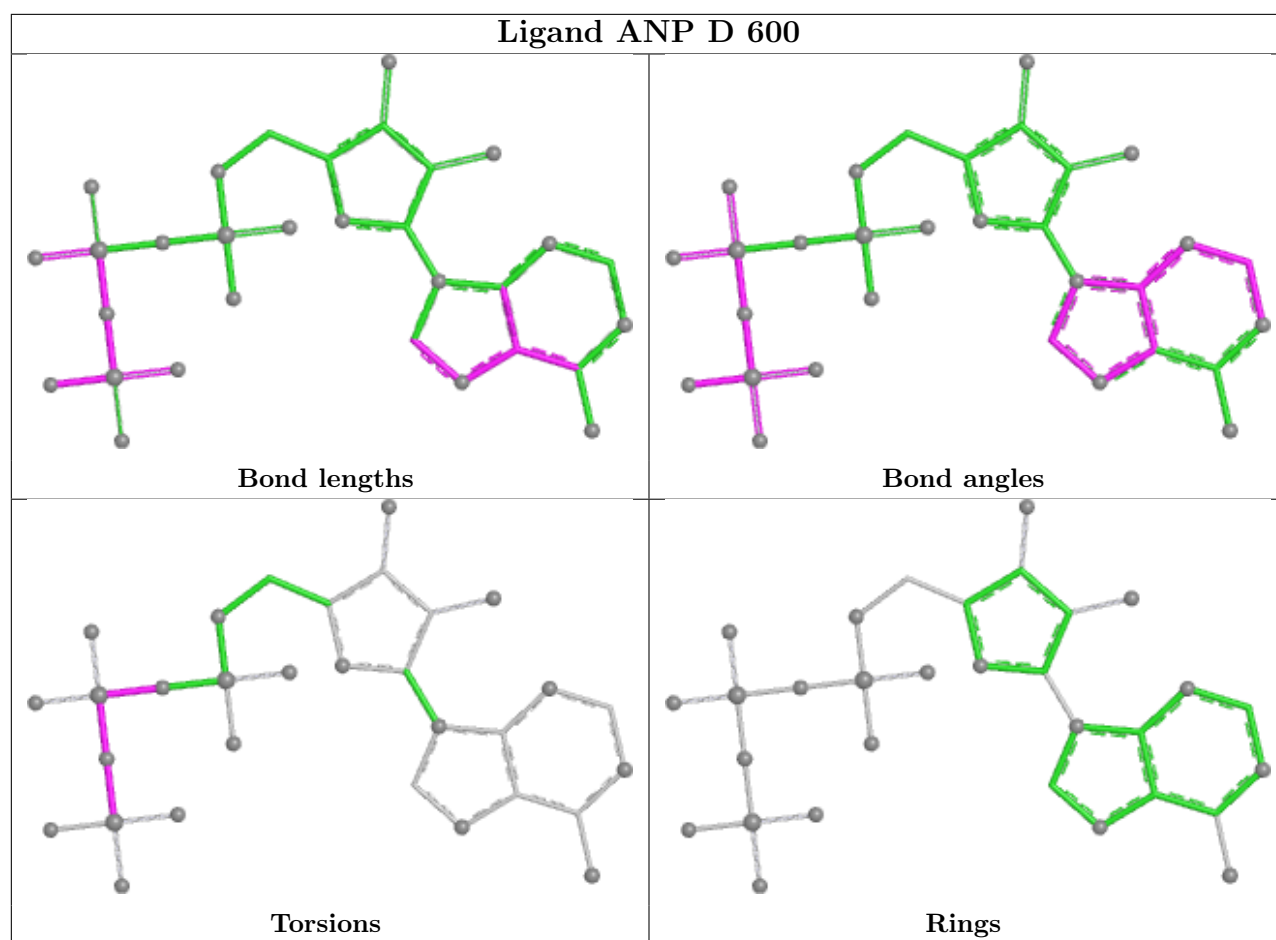
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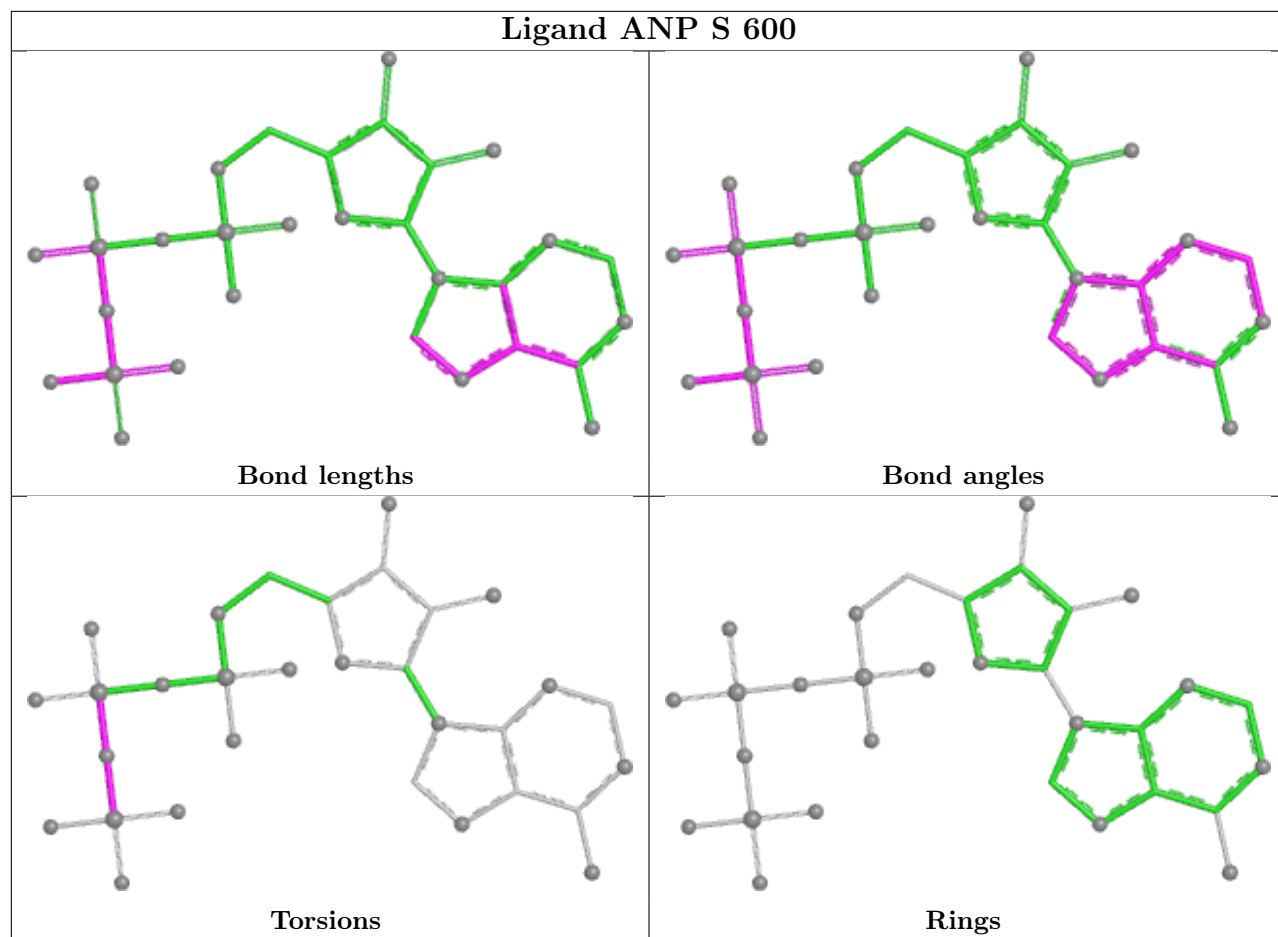
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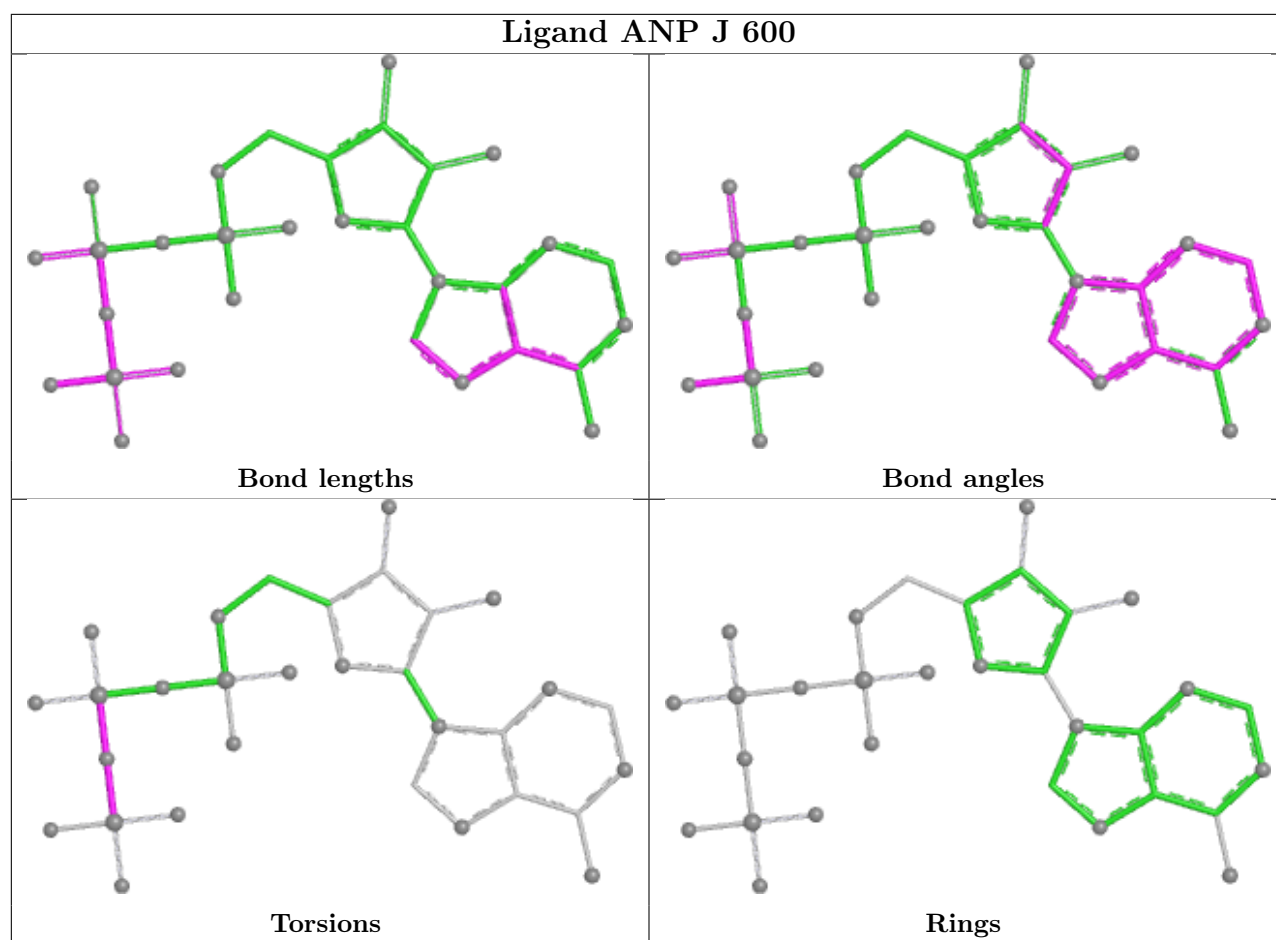
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	T	600	ANP	2	0

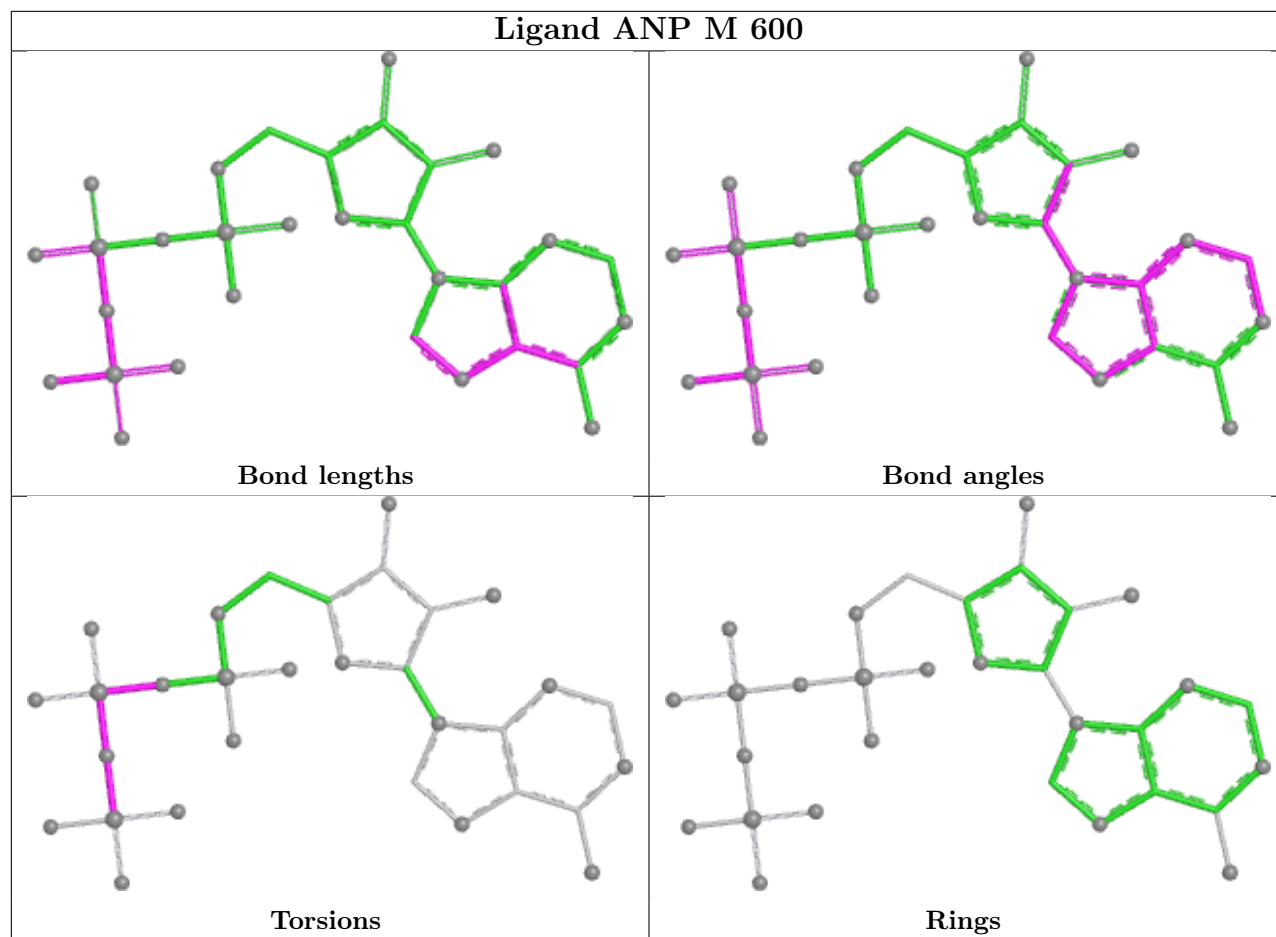
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

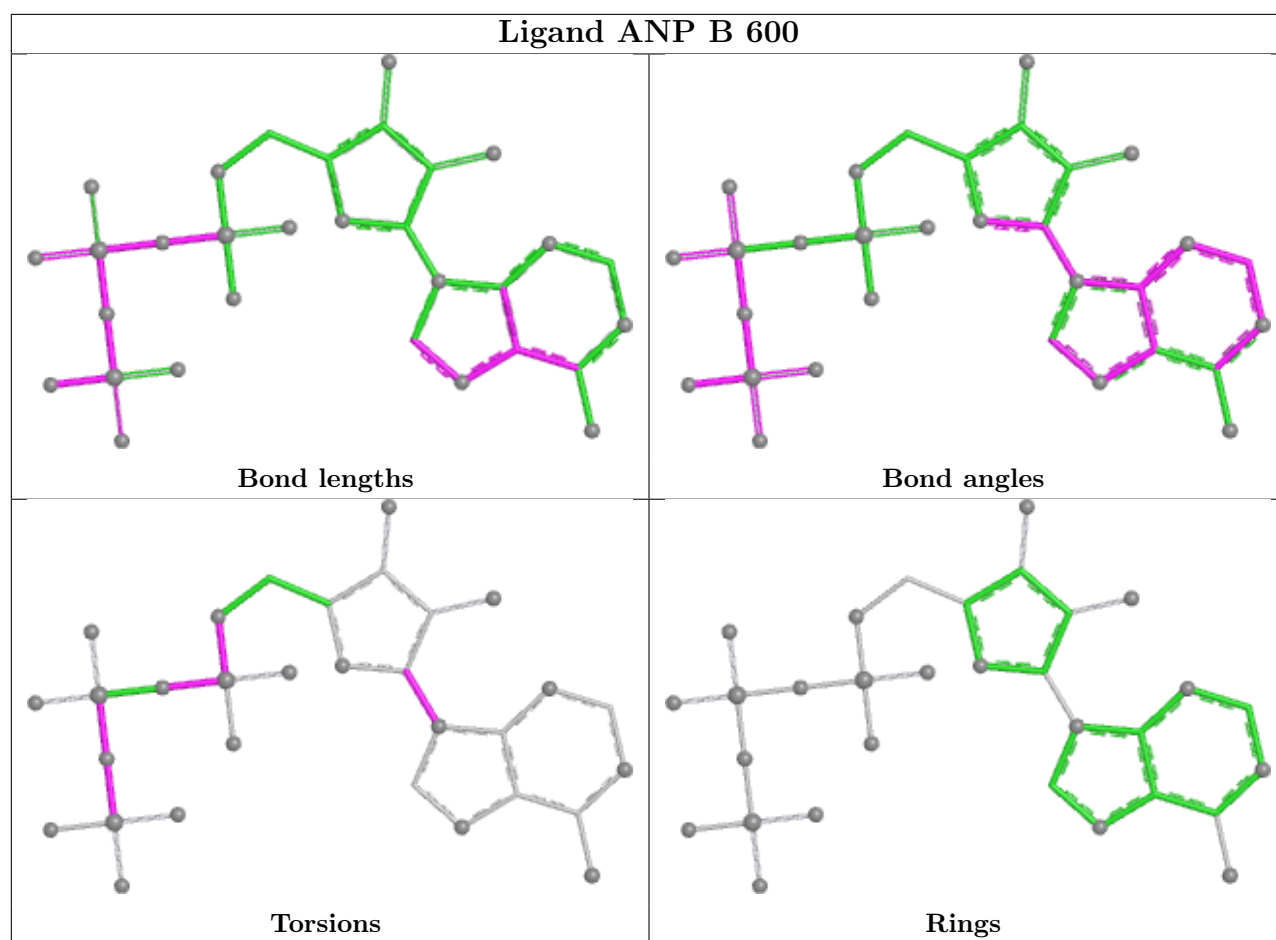


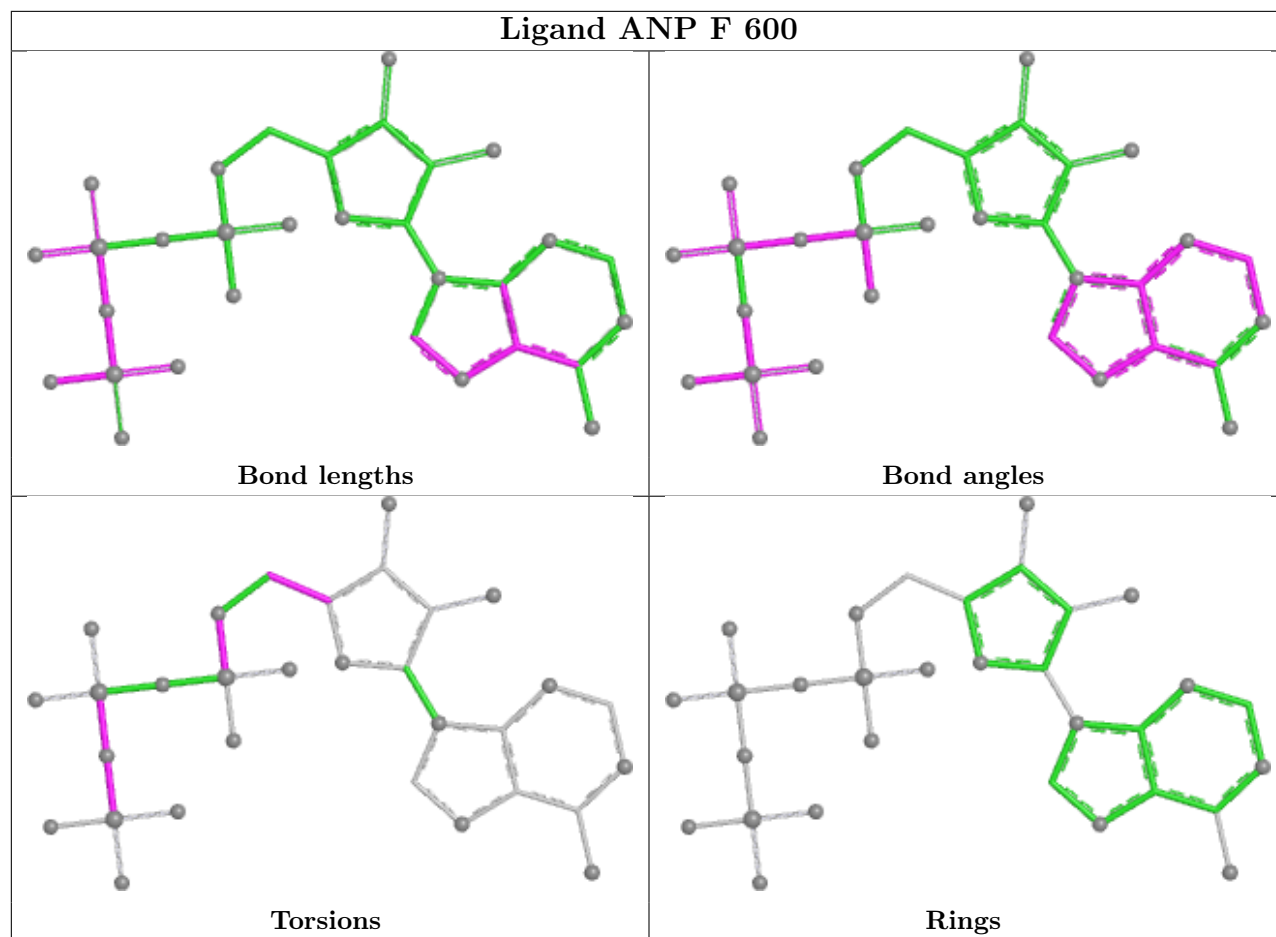


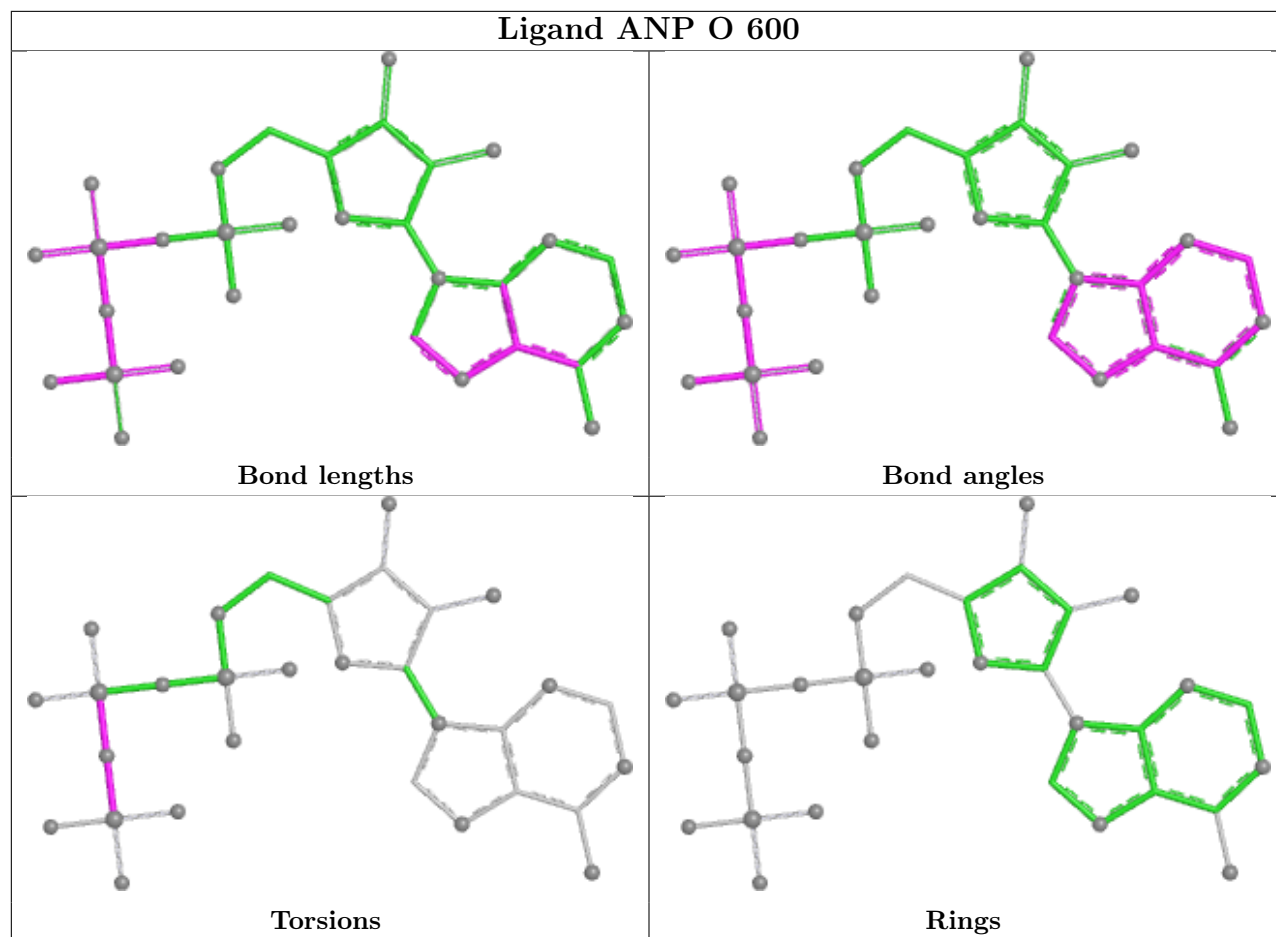


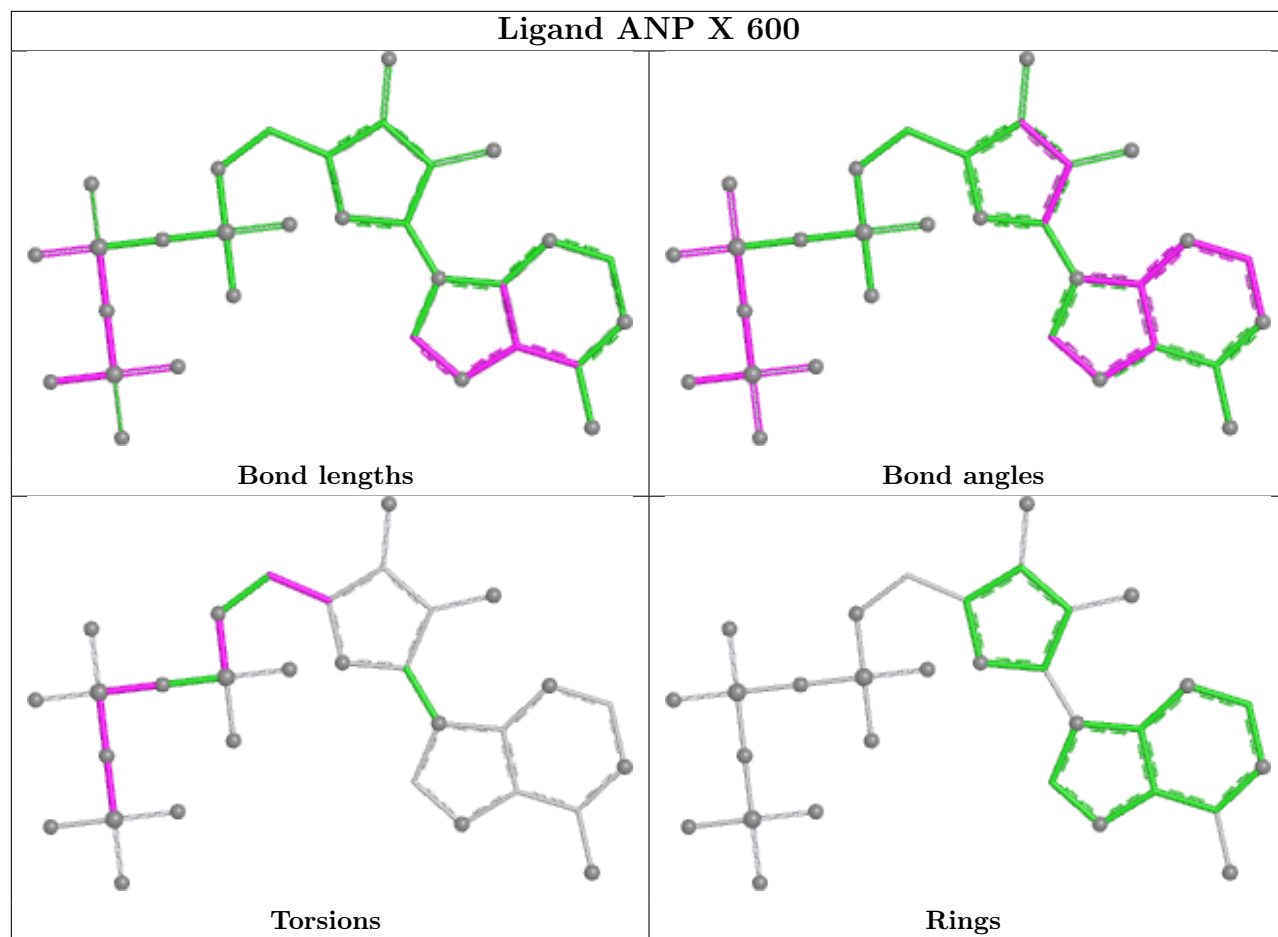


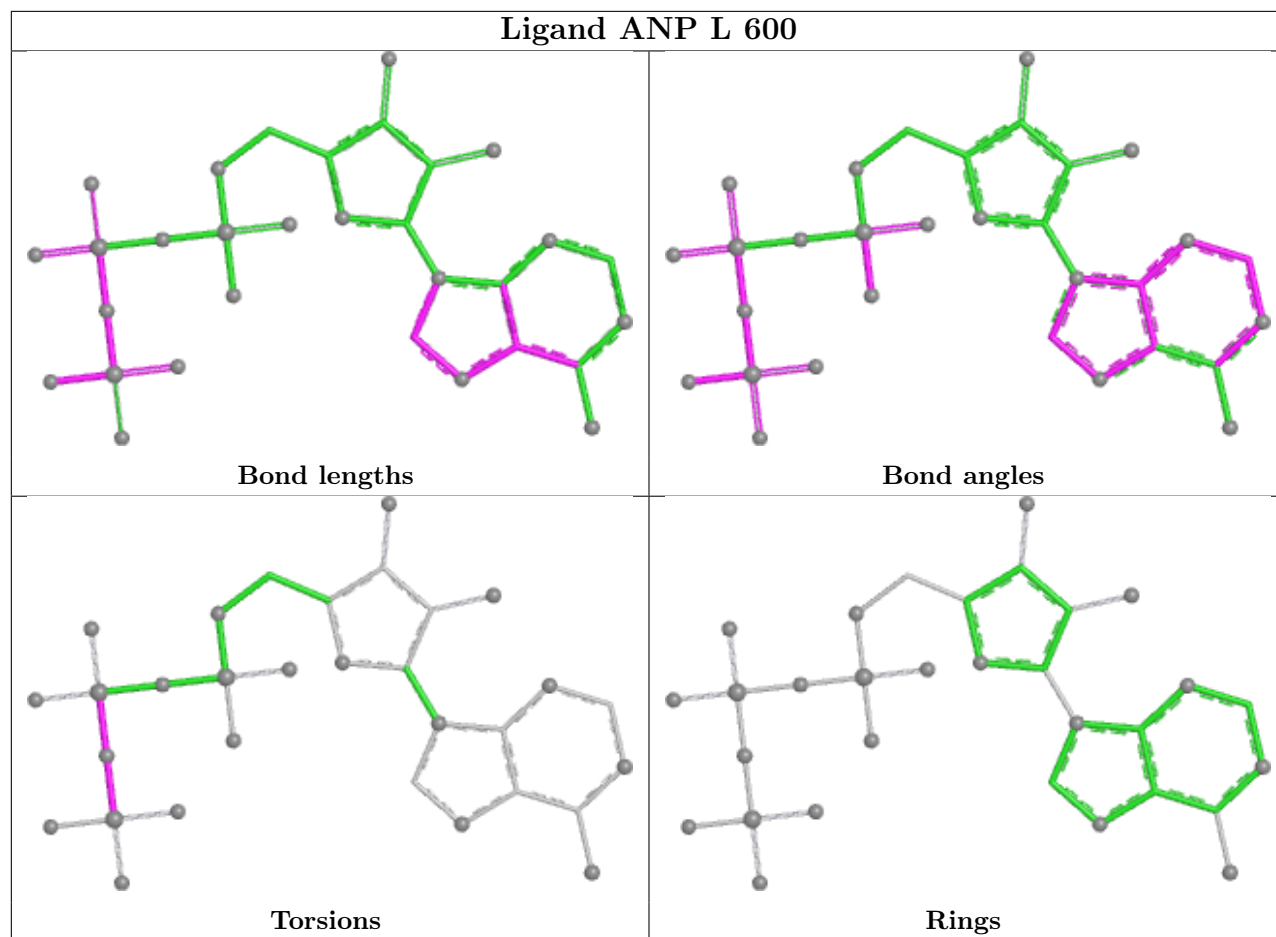


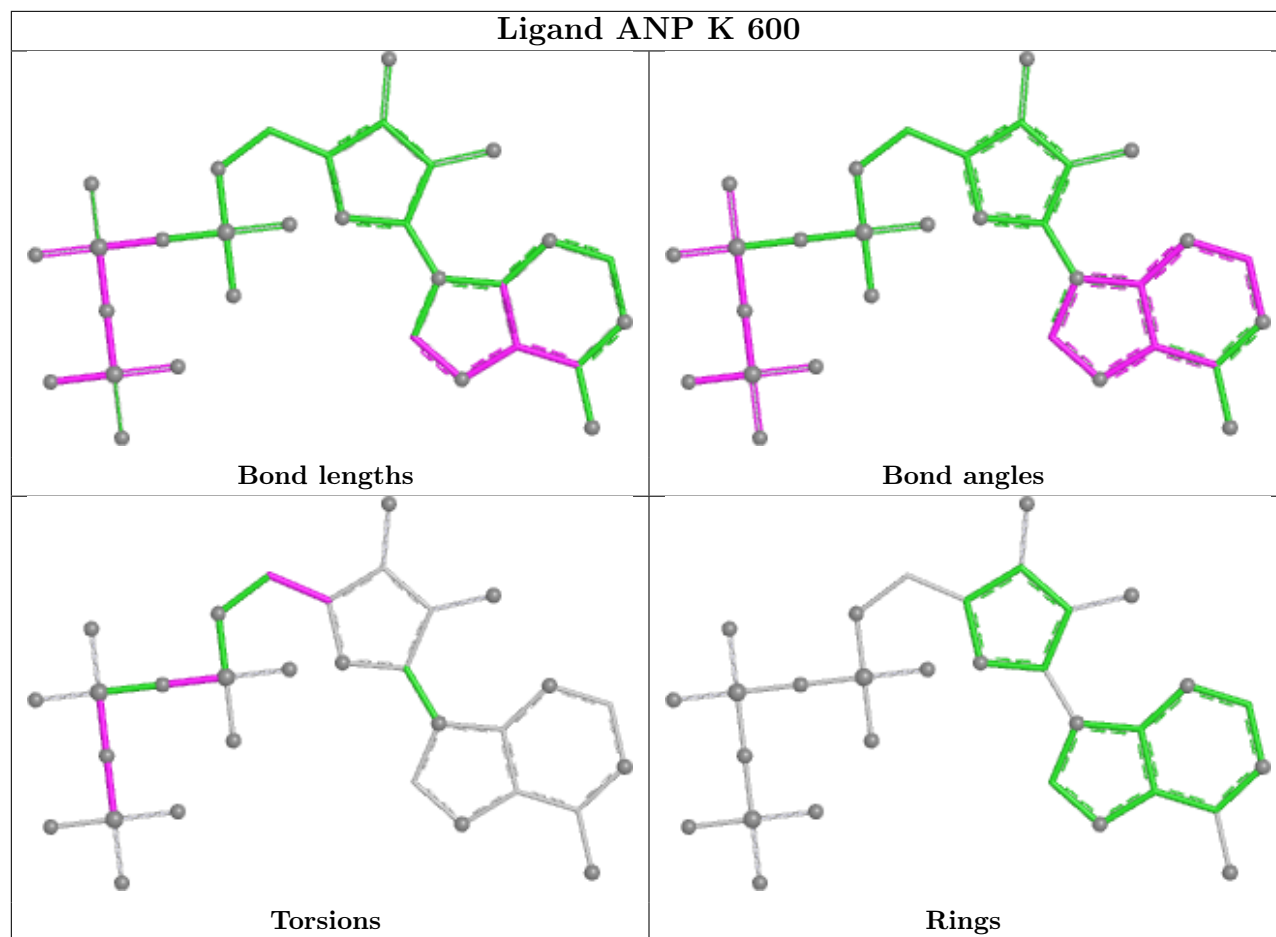


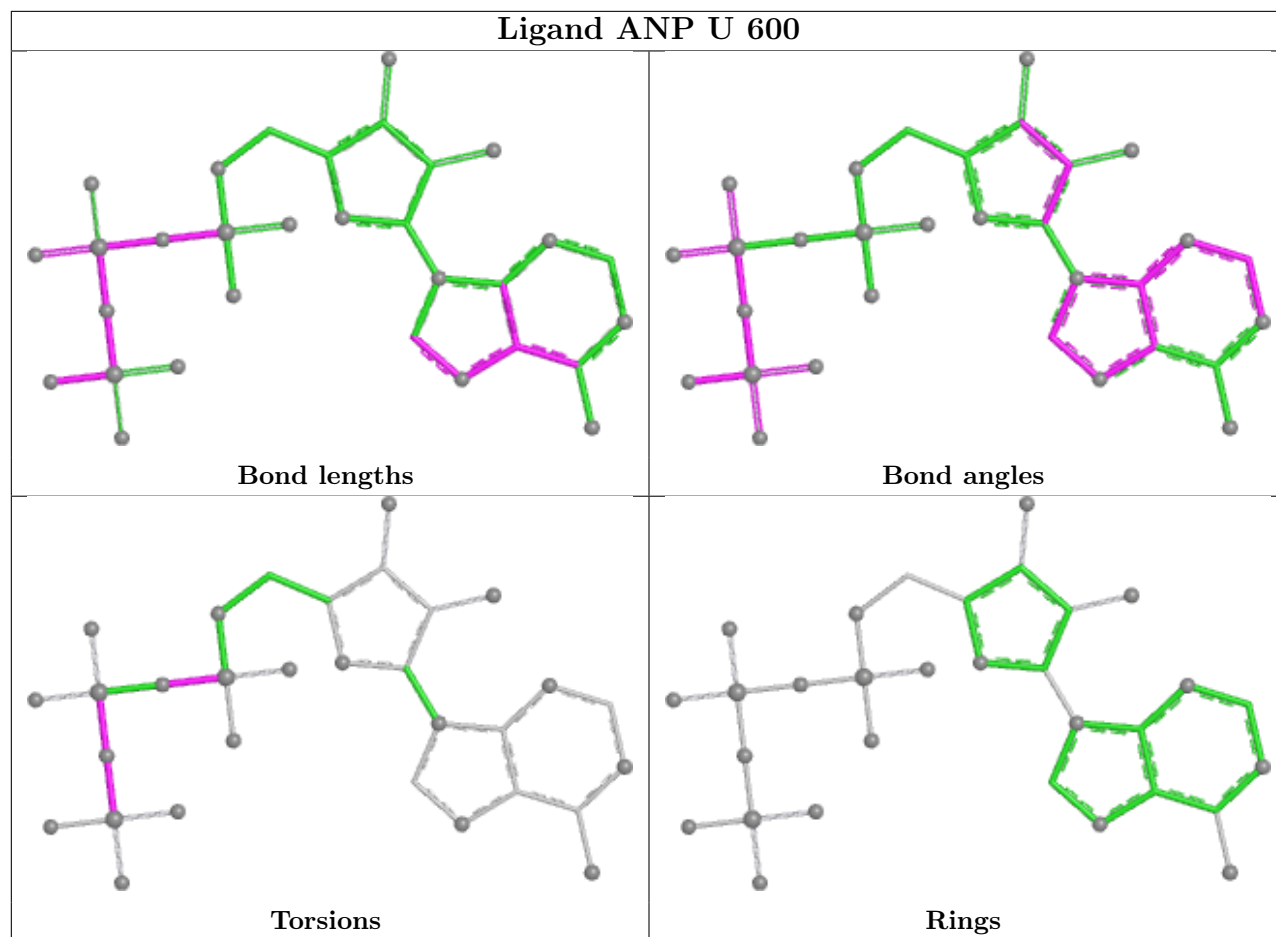


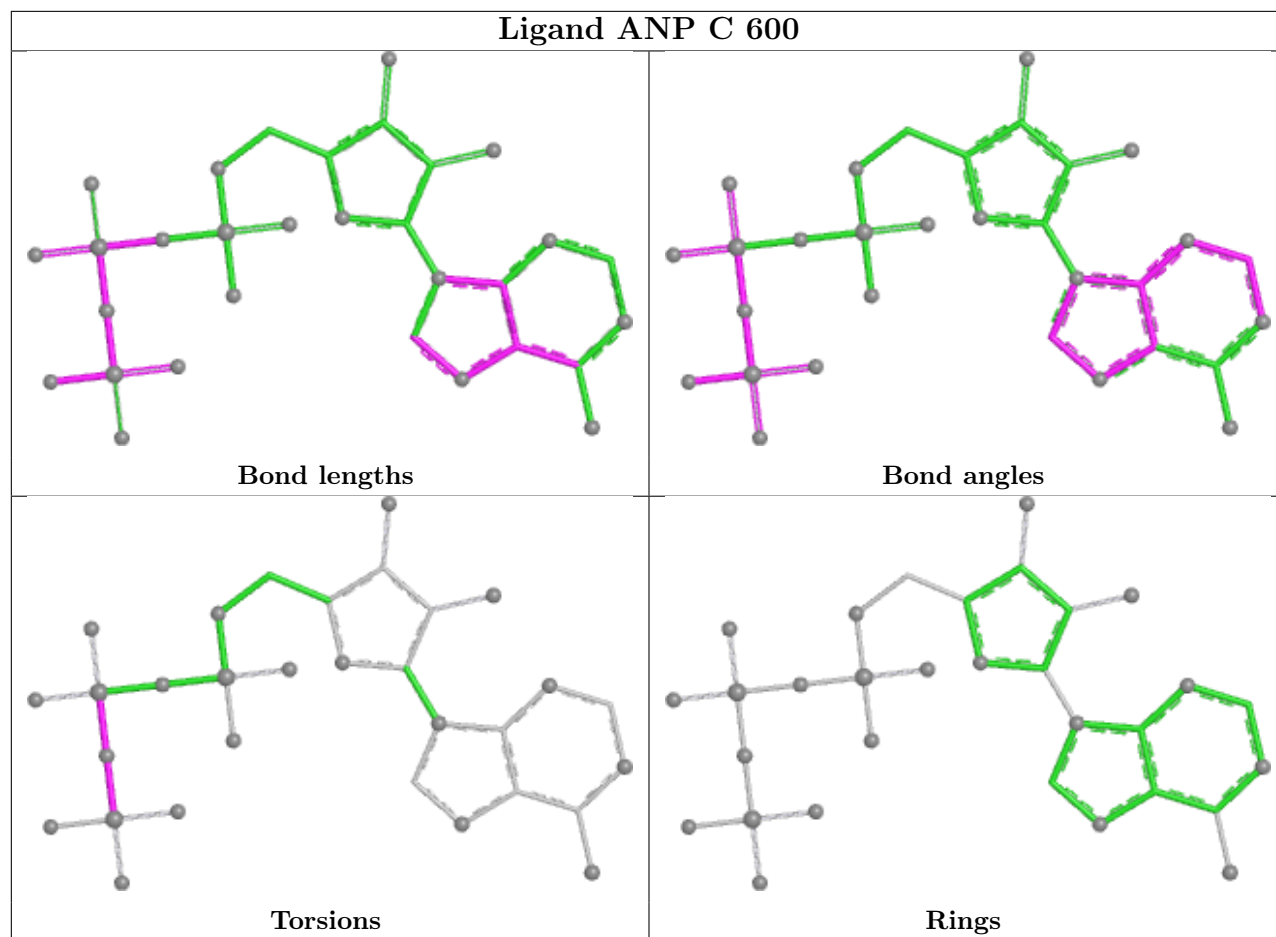


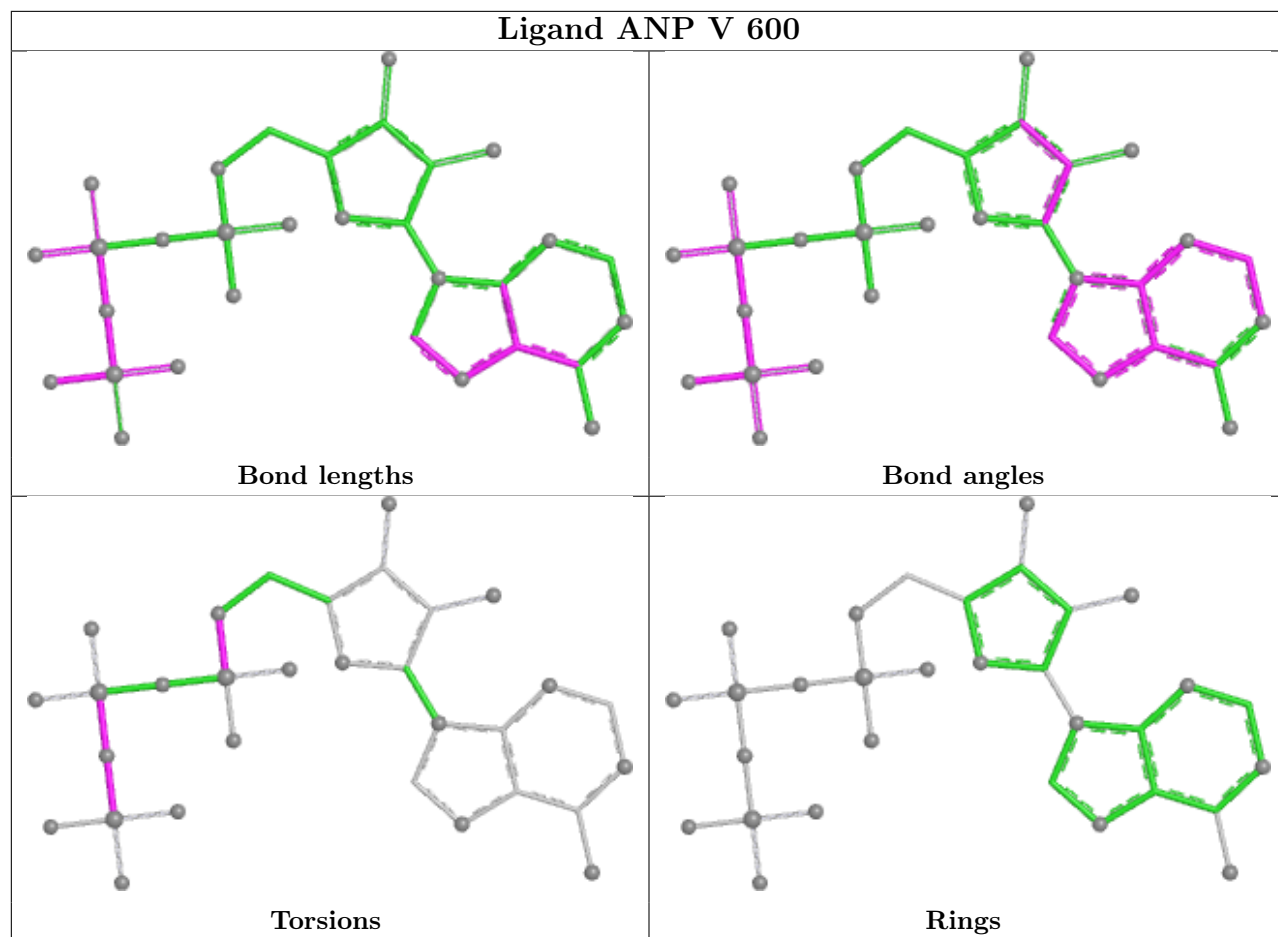


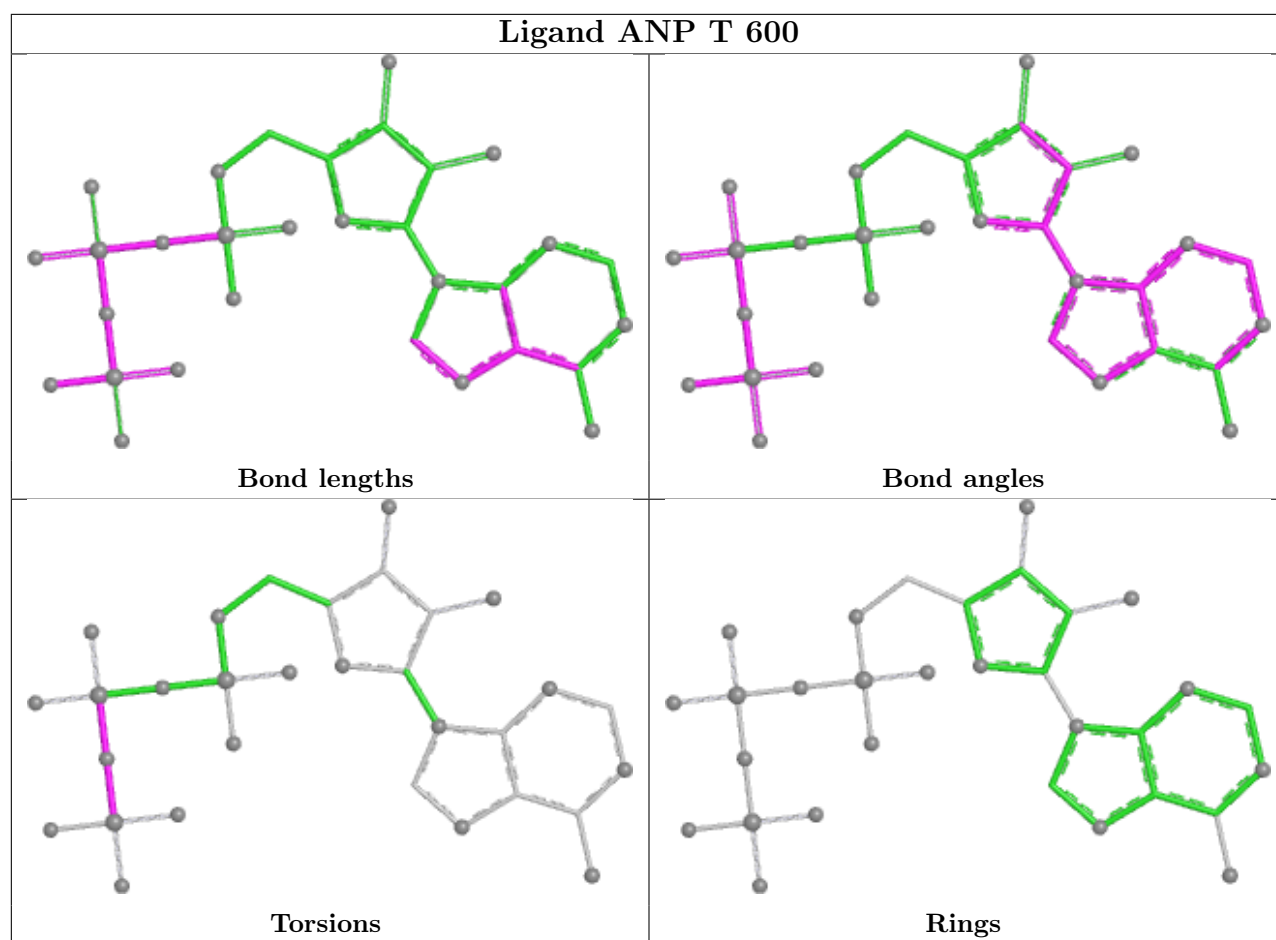












5.7 Other polymers [i](#)

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%)	-0.82	0 100 100	45, 64, 100, 166	0
1	B	483/510 (94%)	-0.70	0 100 100	48, 92, 165, 195	0
1	C	484/510 (94%)	-0.79	0 100 100	51, 75, 138, 181	0
1	J	481/510 (94%)	-0.72	0 100 100	59, 93, 137, 181	0
1	K	486/510 (95%)	-0.65	0 100 100	61, 107, 166, 182	0
1	L	482/510 (94%)	-0.82	0 100 100	47, 68, 123, 164	0
1	S	480/510 (94%)	-0.66	0 100 100	72, 106, 140, 186	0
1	T	481/510 (94%)	-0.54	0 100 100	91, 131, 153, 165	0
1	U	481/510 (94%)	-0.44	0 100 100	93, 133, 166, 194	0
2	D	470/484 (97%)	-0.82	0 100 100	46, 72, 121, 172	0
2	E	468/484 (96%)	-0.72	0 100 100	48, 85, 147, 186	0
2	F	469/484 (96%)	-0.76	0 100 100	48, 84, 117, 161	0
2	M	470/484 (97%)	-0.69	0 100 100	57, 84, 131, 172	0
2	N	470/484 (97%)	-0.63	0 100 100	64, 110, 165, 188	0
2	O	468/484 (96%)	-0.76	0 100 100	53, 92, 128, 153	0
2	V	470/484 (97%)	-0.45	0 100 100	93, 139, 171, 189	0
2	W	467/484 (96%)	-0.68	1 (0%) 91 85	76, 101, 137, 171	0
2	X	469/484 (96%)	-0.57	0 100 100	85, 121, 162, 187	0
3	G	265/278 (95%)	-0.59	0 100 100	56, 90, 117, 134	0
3	P	244/278 (87%)	-0.17	2 (0%) 82 67	64, 139, 185, 209	0
3	Y	198/278 (71%)	-0.19	0 100 100	98, 147, 190, 214	0
4	H	120/137 (87%)	-0.07	3 (2%) 58 39	86, 115, 166, 176	0
4	Q	84/137 (61%)	0.10	0 100 100	138, 163, 187, 198	0
4	Z	15/137 (10%)	0.06	0 100 100	192, 201, 222, 222	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
5	1	25/61 (40%)	0.23	0 100 100	176, 183, 194, 202	0
5	I	48/61 (78%)	-0.09	0 100 100	92, 112, 140, 157	0
5	R	31/61 (50%)	0.25	0 100 100	136, 153, 167, 178	0
All	All	9591/10374 (92%)	-0.63	6 (0%) 92 89	45, 100, 160, 222	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	121	ALA	2.6
4	H	101	ILE	2.1
4	H	126	GLN	2.1
3	P	185	ALA	2.1
2	W	474	ALA	2.1
3	P	94	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	MG	T	700	1/1	0.59	0.16	91,91,91,91	0
7	MG	X	700	1/1	0.65	0.19	96,96,96,96	0
7	MG	O	700	1/1	0.81	0.17	83,83,83,83	0
7	MG	S	700	1/1	0.84	0.19	77,77,77,77	0
7	MG	D	700	1/1	0.86	0.21	64,64,64,64	0
7	MG	J	700	1/1	0.86	0.17	67,67,67,67	0
8	PO4	N	800	5/5	0.87	0.09	131,131,131,132	0

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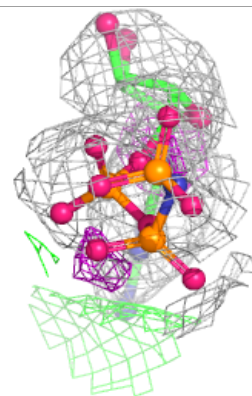
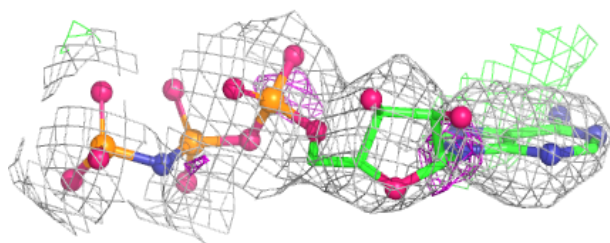
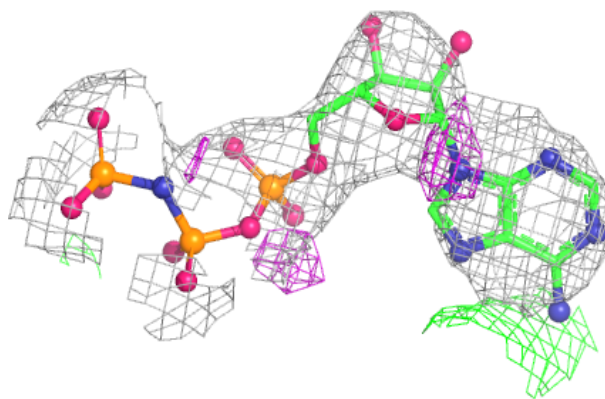
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	MG	V	700	1/1	0.88	0.13	107,107,107,107	0
7	MG	F	700	1/1	0.89	0.16	65,65,65,65	0
7	MG	A	700	1/1	0.89	0.16	48,48,48,48	0
6	ANP	T	600	31/31	0.90	0.08	91,101,106,106	0
7	MG	M	700	1/1	0.90	0.17	64,64,64,64	0
7	MG	B	700	1/1	0.91	0.17	72,72,72,72	0
6	ANP	V	600	31/31	0.92	0.09	102,106,109,109	0
7	MG	C	700	1/1	0.93	0.15	58,58,58,58	0
6	ANP	X	600	31/31	0.94	0.07	93,94,96,97	0
7	MG	K	700	1/1	0.94	0.12	90,90,90,90	0
6	ANP	U	600	31/31	0.94	0.07	84,89,90,91	0
6	ANP	S	600	31/31	0.95	0.06	76,82,83,85	0
7	MG	L	700	1/1	0.95	0.10	53,53,53,53	0
7	MG	U	700	1/1	0.95	0.10	88,88,88,88	0
6	ANP	D	600	31/31	0.96	0.07	62,65,68,69	0
6	ANP	F	600	31/31	0.96	0.07	66,70,78,78	0
6	ANP	K	600	31/31	0.96	0.05	90,97,99,100	0
6	ANP	B	600	31/31	0.96	0.06	71,82,85,85	0
6	ANP	L	600	31/31	0.97	0.05	53,59,62,62	0
6	ANP	M	600	31/31	0.97	0.07	64,68,70,71	0
6	ANP	O	600	31/31	0.97	0.06	84,88,92,92	0
6	ANP	C	600	31/31	0.97	0.05	58,64,68,70	0
6	ANP	J	600	31/31	0.97	0.06	67,73,80,81	0
6	ANP	A	600	31/31	0.97	0.06	48,58,61,62	0

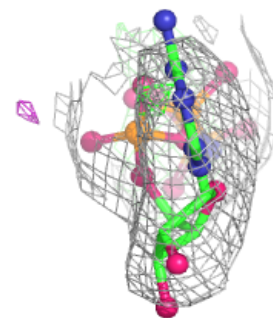
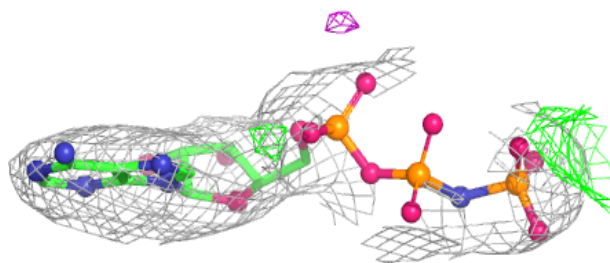
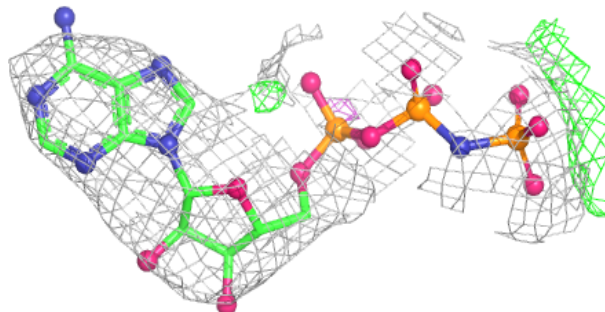
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ANP T 600:

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

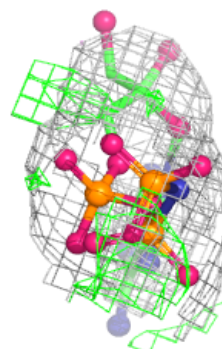
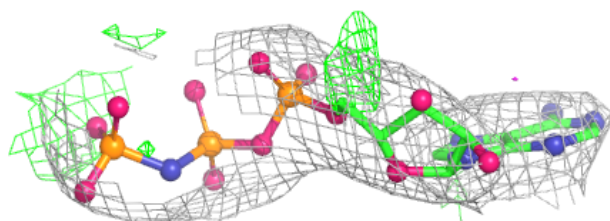
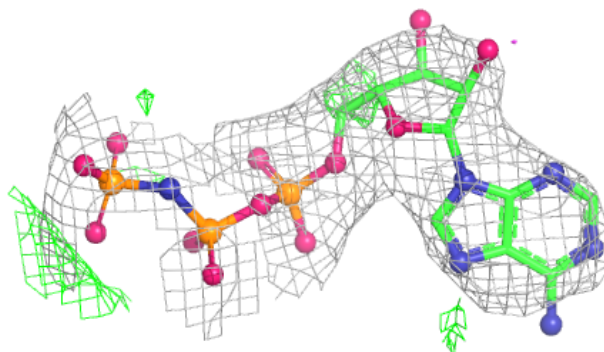
**Electron density around ANP V 600:**

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

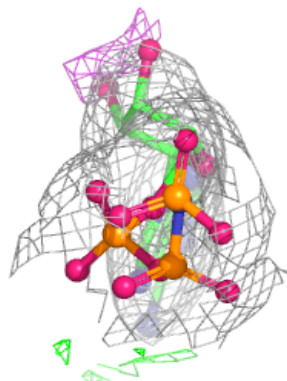
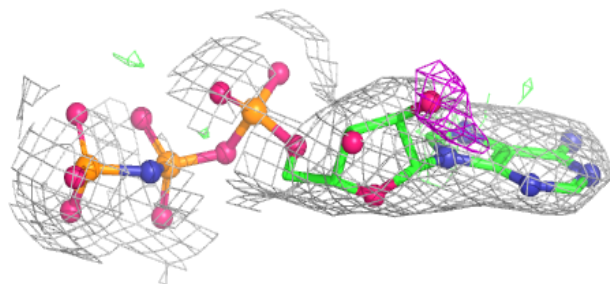
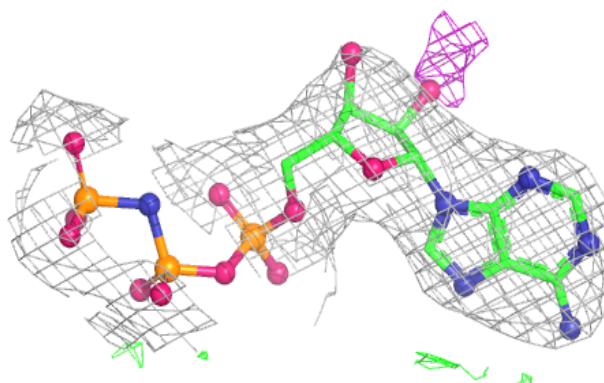


Electron density around ANP X 600:

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

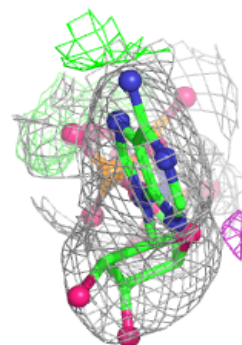
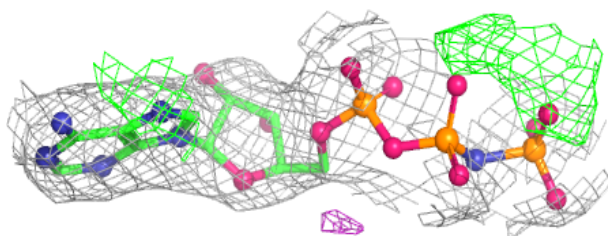
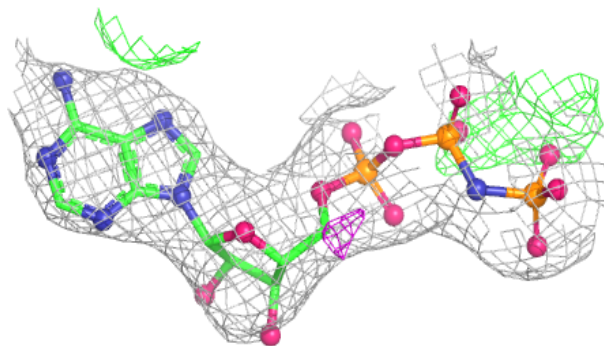
**Electron density around ANP U 600:**

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

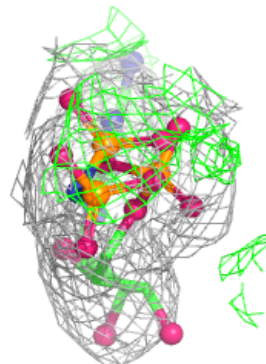
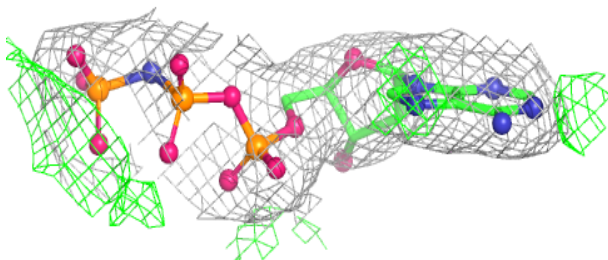
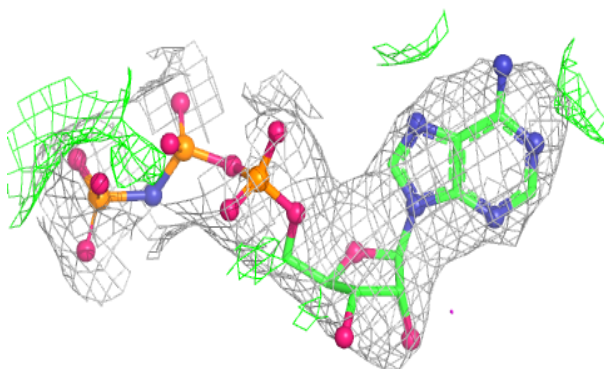


Electron density around ANP S 600:

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

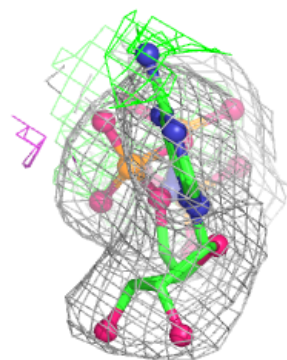
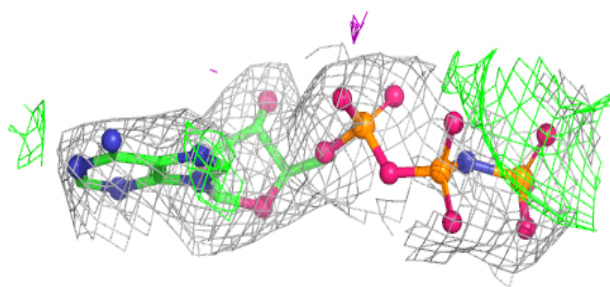
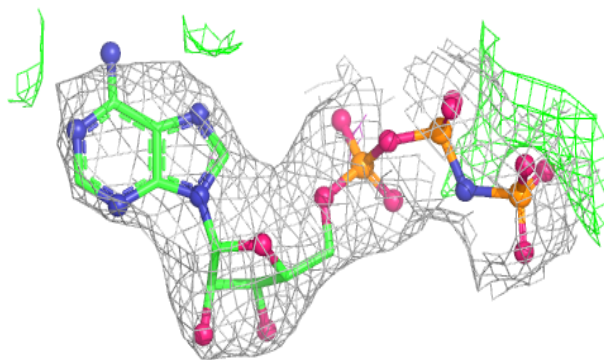
**Electron density around ANP D 600:**

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

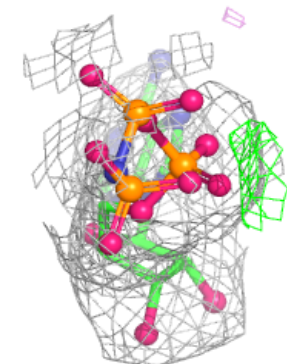
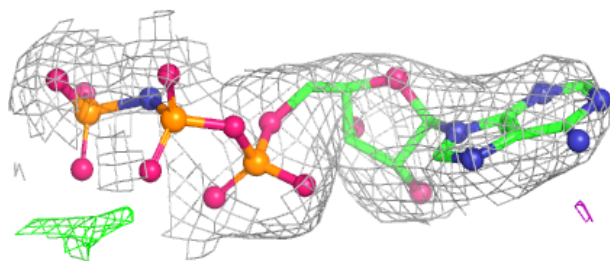
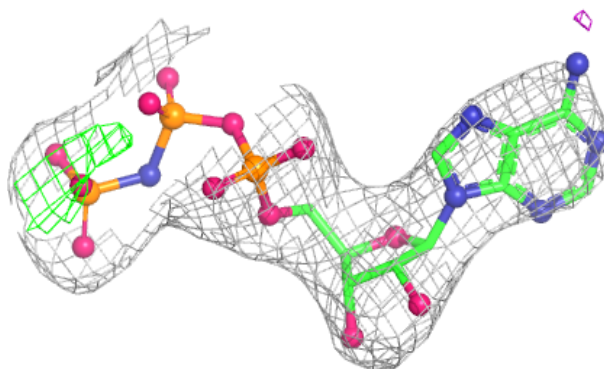


Electron density around ANP F 600:

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

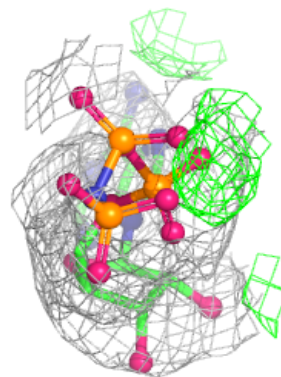
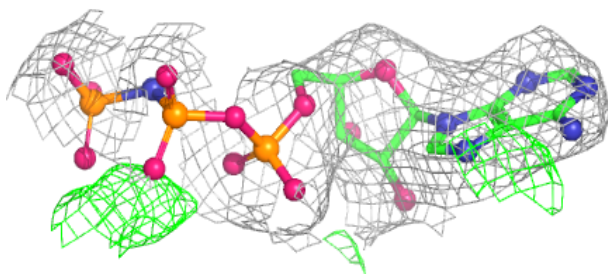
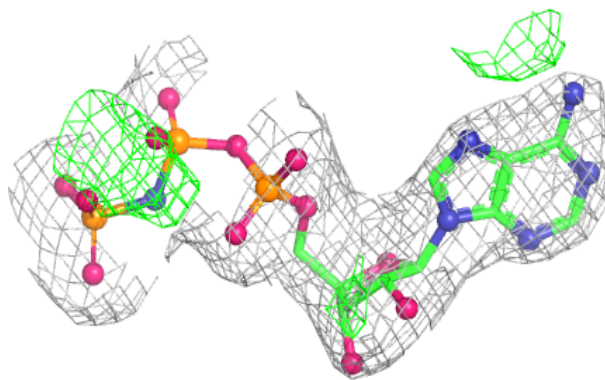
**Electron density around ANP K 600:**

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

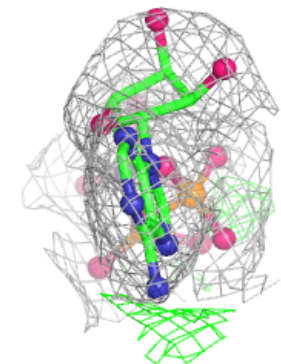
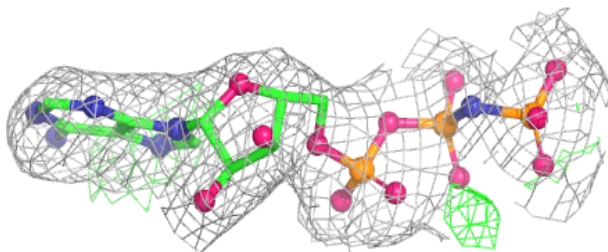
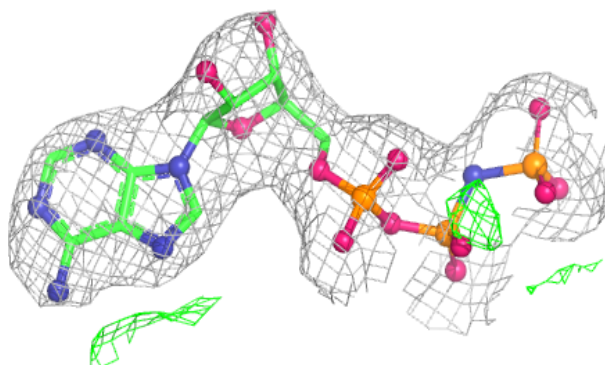


Electron density around ANP B 600:

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

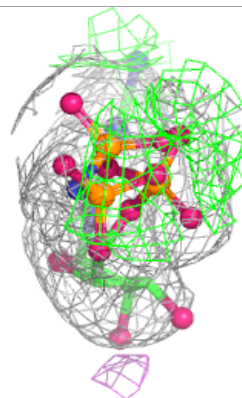
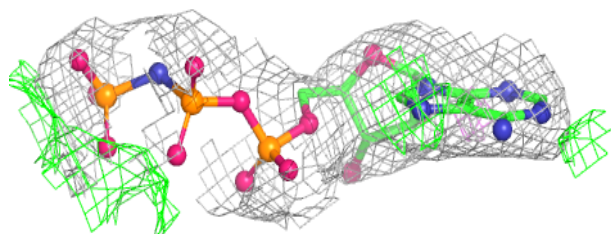
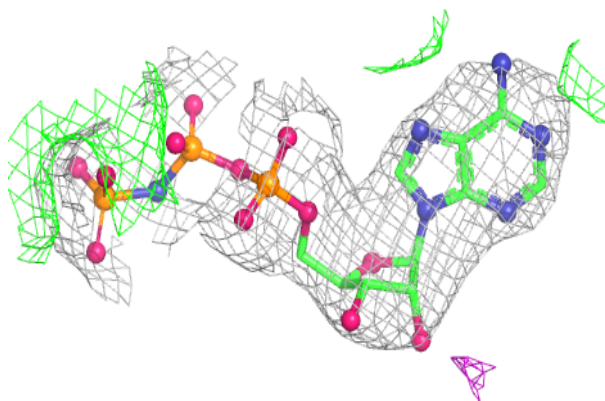
**Electron density around ANP L 600:**

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

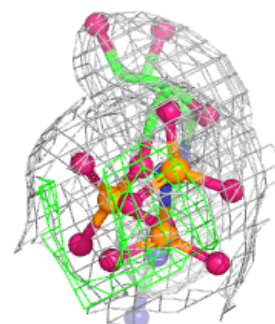
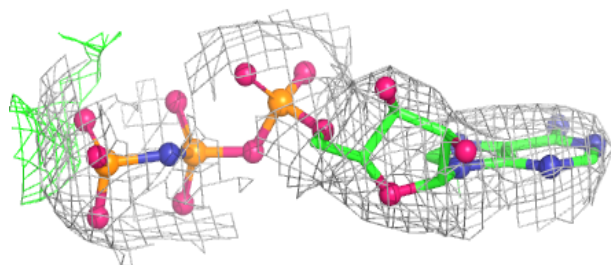
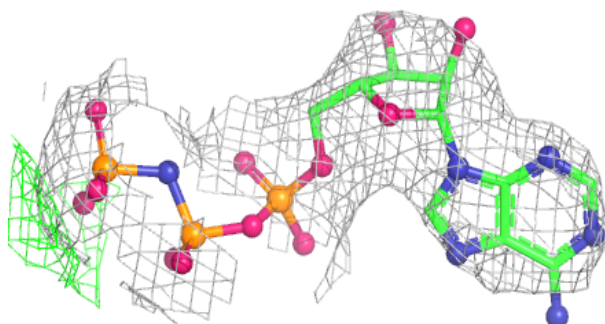


Electron density around ANP M 600:

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

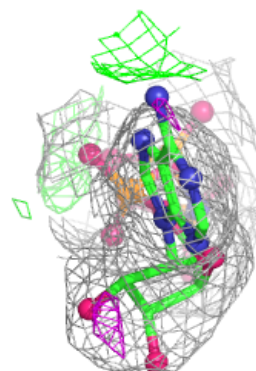
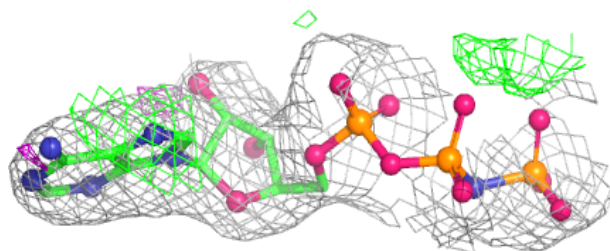
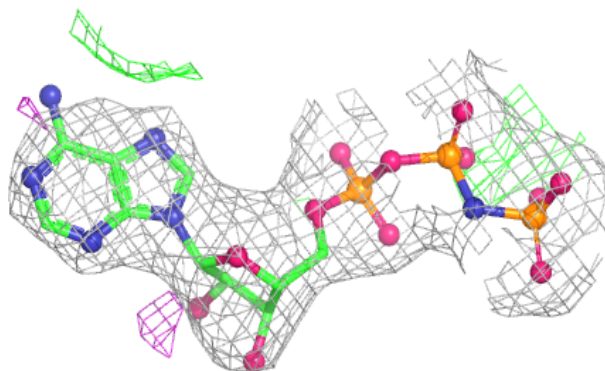
**Electron density around ANP O 600:**

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

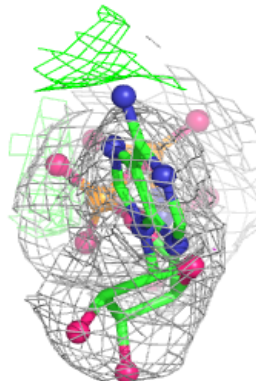
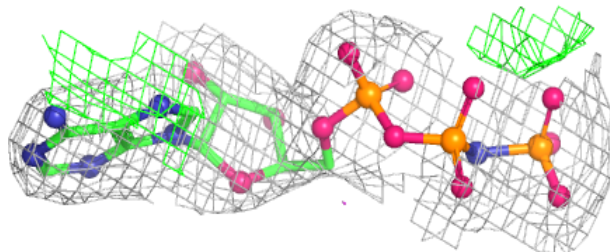
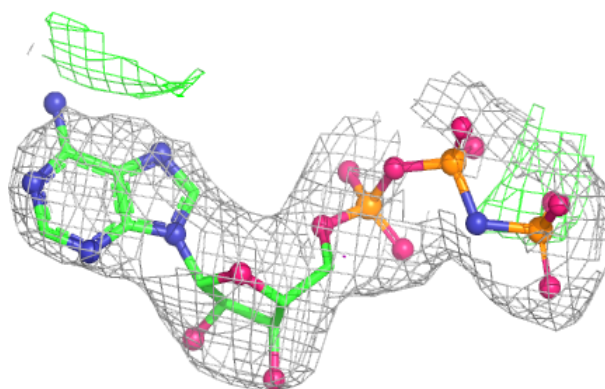


Electron density around ANP C 600:

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

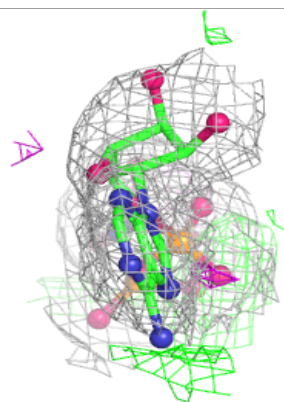
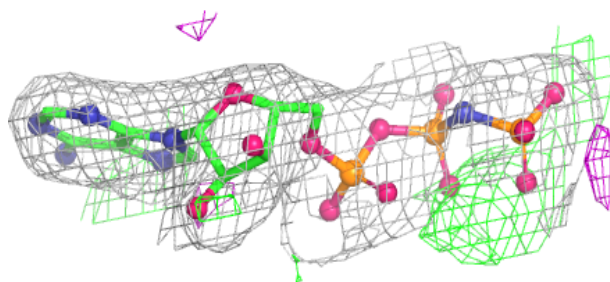
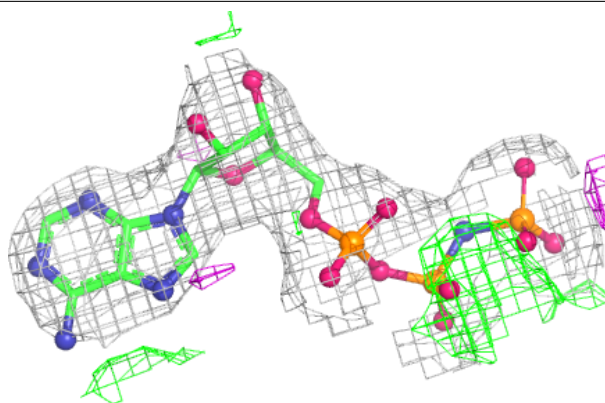
**Electron density around ANP J 600:**

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



Electron density around ANP A 600:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.