



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 01:25 PM BST

PDB ID : 3OAA
Title : Structure of the E.coli F1-ATP synthase inhibited by subunit Epsilon
Authors : Cingolani, G.; Duncan, T.M.
Deposited on : 2010-08-05
Resolution : 3.26 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 following versions of software and data (see [references](#) ⓘ) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13

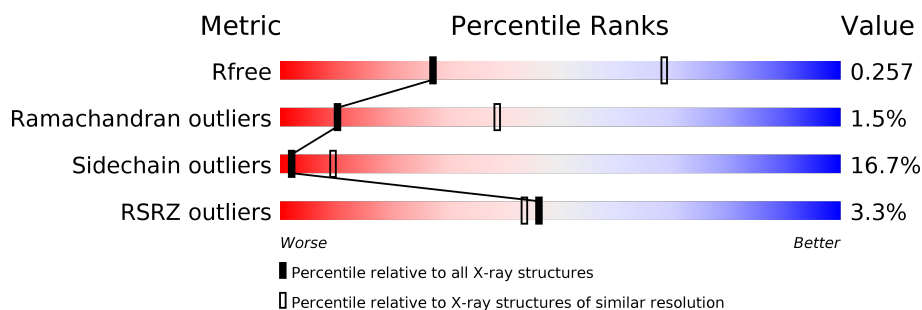
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.26 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1191 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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 on 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	513	<div> <div></div> <div>82%13%5%</div> </div>
1	B	513	<div> <div>2%</div> <div>79%16%5%</div> </div>
1	C	513	<div> <div>0%</div> <div>80%14%5%</div> </div>
1	I	513	<div> <div>2%</div> <div>82%12%5%</div> </div>
1	J	513	<div> <div>3%</div> <div>79%16%5%</div> </div>
1	K	513	<div> <div>2%</div> <div>81%13%5%</div> </div>
1	Q	513	<div> <div>2%</div> <div>83%12%5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	R	513	
1	S	513	
1	Y	513	
1	Z	513	
1	a	513	
2	D	459	
2	E	459	
2	F	459	
2	L	459	
2	M	459	
2	N	459	
2	T	459	
2	U	459	
2	V	459	
2	b	459	
2	c	459	
2	d	459	
3	G	286	
3	O	286	
3	W	286	
3	e	286	
4	H	138	
4	P	138	
4	X	138	
4	f	138	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 99573 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	488	Total	C	N	O	S	0	0	0
			3667	2301	648	705	13			
1	B	486	Total	C	N	O	S	0	0	0
			3627	2278	642	694	13			
1	C	487	Total	C	N	O	S	0	0	0
			3646	2288	646	699	13			
1	I	488	Total	C	N	O	S	0	0	0
			3667	2301	648	705	13			
1	J	486	Total	C	N	O	S	0	0	0
			3627	2278	642	694	13			
1	K	487	Total	C	N	O	S	0	0	0
			3646	2288	646	699	13			
1	Q	488	Total	C	N	O	S	0	0	0
			3667	2301	648	705	13			
1	R	486	Total	C	N	O	S	0	0	0
			3627	2278	642	694	13			
1	S	487	Total	C	N	O	S	0	0	0
			3646	2288	646	699	13			
1	Y	488	Total	C	N	O	S	0	0	0
			3667	2301	648	705	13			
1	Z	486	Total	C	N	O	S	0	0	0
			3627	2278	642	694	13			
1	a	487	Total	C	N	O	S	0	0	0
			3646	2288	646	699	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	458	Total	C	N	O	S	0	0	0
			3521	2218	601	687	15			
2	E	458	Total	C	N	O	S	0	0	0
			3521	2218	601	687	15			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	458	Total	C	N	O	S	0	0	0
			3521	2218	601	687	15			
2	L	458	Total	C	N	O	S	0	0	0
			3521	2218	601	687	15			
2	M	458	Total	C	N	O	S	0	0	0
			3521	2218	601	687	15			
2	N	458	Total	C	N	O	S	0	0	0
			3521	2218	601	687	15			
2	T	458	Total	C	N	O	S	0	0	0
			3521	2218	601	687	15			
2	U	458	Total	C	N	O	S	0	0	0
			3521	2218	601	687	15			
2	V	458	Total	C	N	O	S	0	0	0
			3521	2218	601	687	15			
2	b	458	Total	C	N	O	S	0	0	0
			3521	2218	601	687	15			
2	c	458	Total	C	N	O	S	0	0	0
			3521	2218	601	687	15			
2	d	458	Total	C	N	O	S	0	0	0
			3521	2218	601	687	15			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	81	GLU	LYS	ENGINEERED MUTATION	UNP C9QXA4
E	81	GLU	LYS	ENGINEERED MUTATION	UNP C9QXA4
F	81	GLU	LYS	ENGINEERED MUTATION	UNP C9QXA4
L	81	GLU	LYS	ENGINEERED MUTATION	UNP C9QXA4
M	81	GLU	LYS	ENGINEERED MUTATION	UNP C9QXA4
N	81	GLU	LYS	ENGINEERED MUTATION	UNP C9QXA4
T	81	GLU	LYS	ENGINEERED MUTATION	UNP C9QXA4
U	81	GLU	LYS	ENGINEERED MUTATION	UNP C9QXA4
V	81	GLU	LYS	ENGINEERED MUTATION	UNP C9QXA4
b	81	GLU	LYS	ENGINEERED MUTATION	UNP C9QXA4
c	81	GLU	LYS	ENGINEERED MUTATION	UNP C9QXA4
d	81	GLU	LYS	ENGINEERED MUTATION	UNP C9QXA4

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	284	Total	C	N	O	S	0	0	0
			2182	1369	382	417	14			

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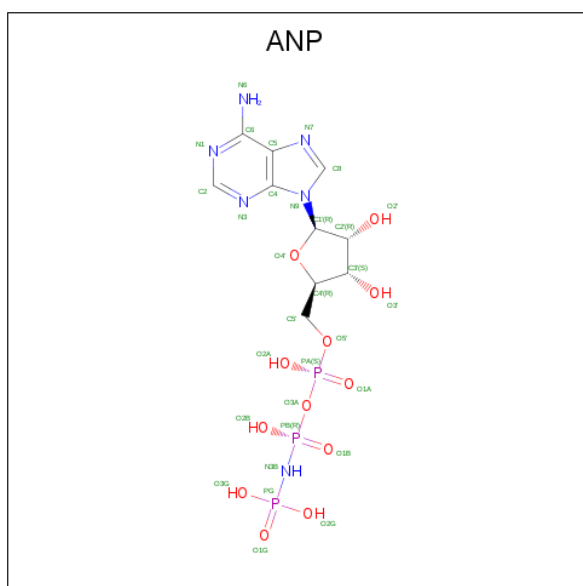
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	O	284	Total	C	N	O	S	0	0	0
			2182	1369	382	417	14			
3	W	284	Total	C	N	O	S	0	0	0
			2182	1369	382	417	14			
3	e	284	Total	C	N	O	S	0	0	0
			2182	1369	382	417	14			

- Molecule 4 is a protein called ATP synthase epsilon chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	138	Total	C	N	O	S	0	0	0
			1047	657	182	203	5			
4	P	138	Total	C	N	O	S	0	0	0
			1047	657	182	203	5			
4	X	138	Total	C	N	O	S	0	0	0
			1047	657	182	203	5			
4	f	138	Total	C	N	O	S	0	0	0
			1047	657	182	203	5			

- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	I	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	J	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	K	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	Q	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	R	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	S	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	Y	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	Z	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	a	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

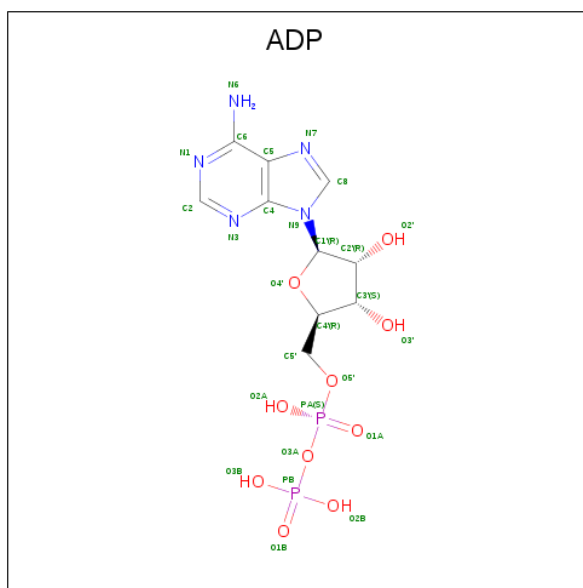
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	J	1	Total	Mg	0	0
			1	1		
6	Q	1	Total	Mg	0	0
			1	1		
6	D	1	Total	Mg	0	0
			1	1		
6	K	1	Total	Mg	0	0
			1	1		
6	b	1	Total	Mg	0	0
			1	1		
6	B	1	Total	Mg	0	0
			1	1		
6	I	1	Total	Mg	0	0
			1	1		
6	C	1	Total	Mg	0	0
			1	1		
6	a	1	Total	Mg	0	0
			1	1		

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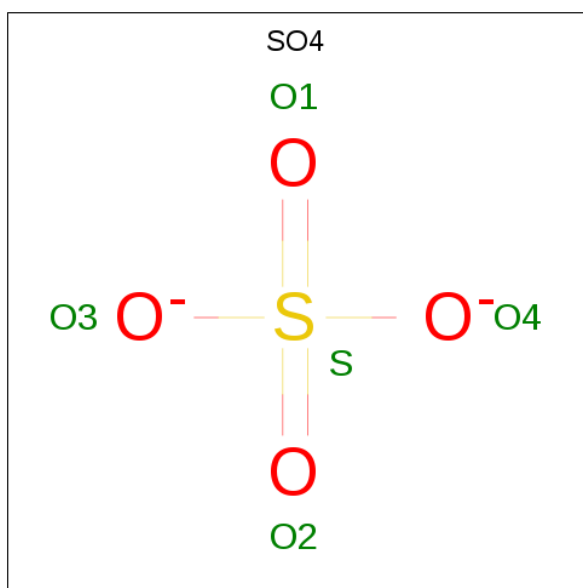
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	Z	1	Total	Mg	0	0
			1	1		
6	A	1	Total	Mg	0	0
			1	1		
6	T	1	Total	Mg	0	0
			1	1		
6	R	1	Total	Mg	0	0
			1	1		
6	Y	1	Total	Mg	0	0
			1	1		
6	L	1	Total	Mg	0	0
			1	1		
6	S	1	Total	Mg	0	0
			1	1		

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	L	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	T	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	b	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	D	1	Total	O	S	0	0
			5	4	1		
8	E	1	Total	O	S	0	0
			5	4	1		
8	F	1	Total	O	S	0	0
			5	4	1		
8	G	1	Total	O	S	0	0
			5	4	1		
8	H	1	Total	O	S	0	0
			5	4	1		
8	L	1	Total	O	S	0	0
			5	4	1		
8	M	1	Total	O	S	0	0
			5	4	1		
8	N	1	Total	O	S	0	0
			5	4	1		
8	O	1	Total	O	S	0	0
			5	4	1		
8	P	1	Total	O	S	0	0
			5	4	1		
8	T	1	Total	O	S	0	0
			5	4	1		
8	U	1	Total	O	S	0	0
			5	4	1		
8	V	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	W	1	Total	O	S	0	0
			5	4	1		
8	b	1	Total	O	S	0	0
			5	4	1		
8	c	1	Total	O	S	0	0
			5	4	1		
8	d	1	Total	O	S	0	0
			5	4	1		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	3	Total	O	0	0
			3	3		
9	B	2	Total	O	0	0
			2	2		
9	C	2	Total	O	0	0
			2	2		
9	D	8	Total	O	0	0
			8	8		
9	E	1	Total	O	0	0
			1	1		
9	F	5	Total	O	0	0
			5	5		
9	G	10	Total	O	0	0
			10	10		
9	H	4	Total	O	0	0
			4	4		
9	J	3	Total	O	0	0
			3	3		
9	L	6	Total	O	0	0
			6	6		
9	N	3	Total	O	0	0
			3	3		
9	O	5	Total	O	0	0
			5	5		
9	P	2	Total	O	0	0
			2	2		
9	Q	1	Total	O	0	0
			1	1		
9	R	1	Total	O	0	0
			1	1		

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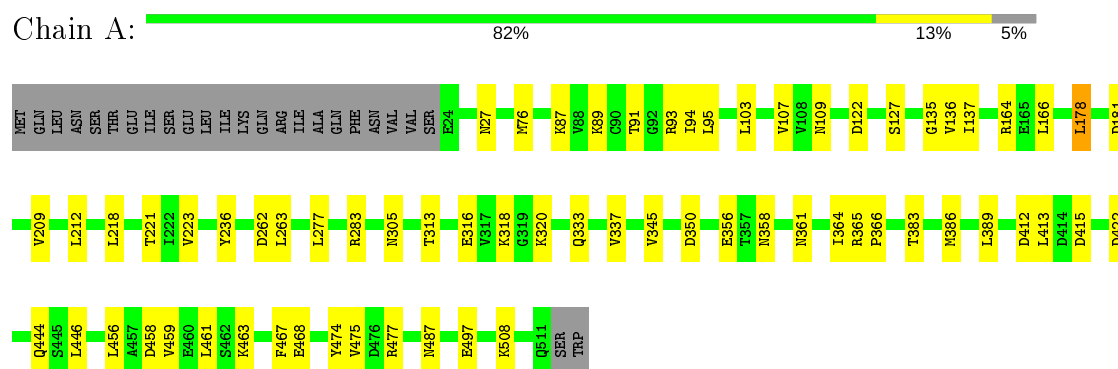
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	S	1	Total 1	O 1	0	0
9	V	2	Total 2	O 2	0	0
9	X	1	Total 1	O 1	0	0
9	a	1	Total 1	O 1	0	0
9	b	1	Total 1	O 1	0	0
9	d	2	Total 2	O 2	0	0

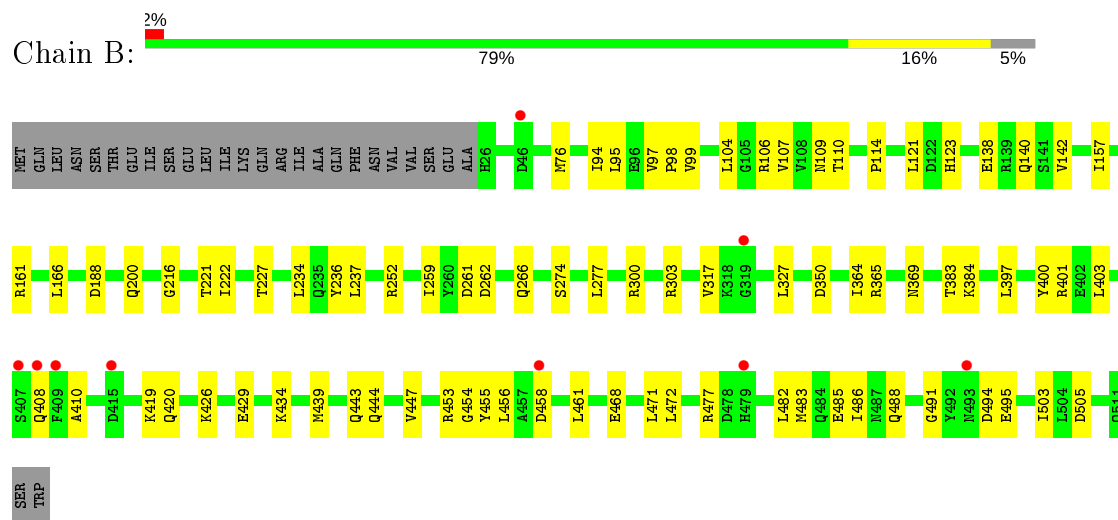
3 Residue-property plots [i](#)

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

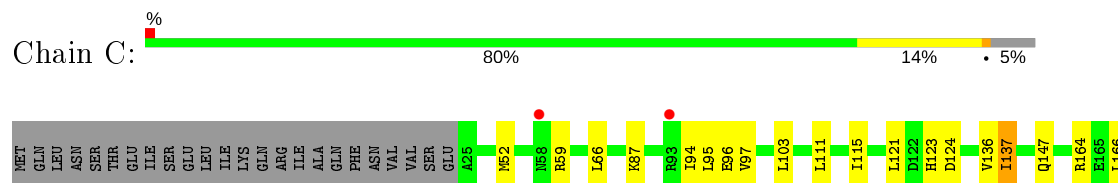
• Molecule 1: ATP synthase subunit alpha

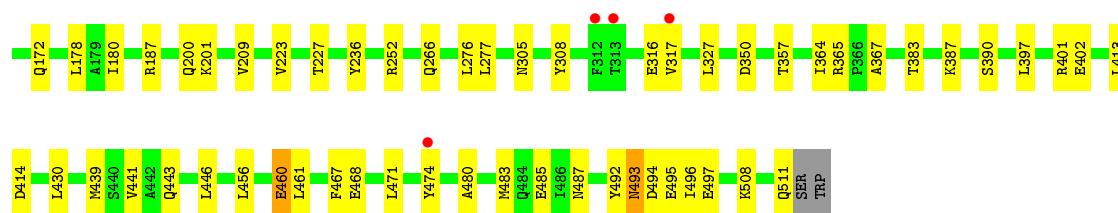


• Molecule 1: ATP synthase subunit alpha

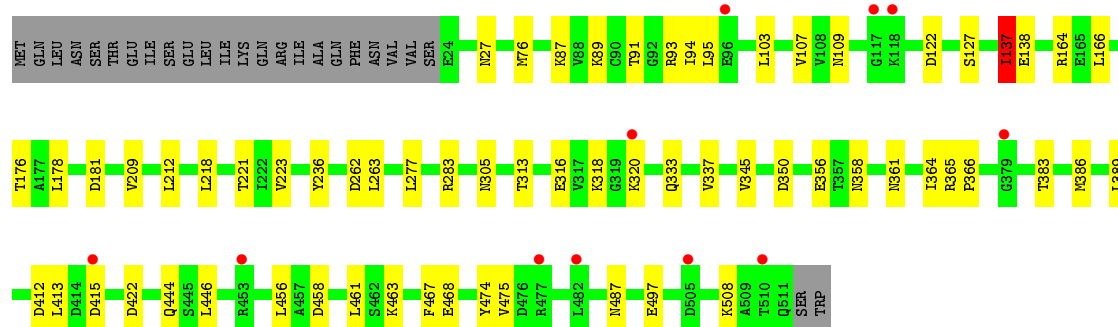
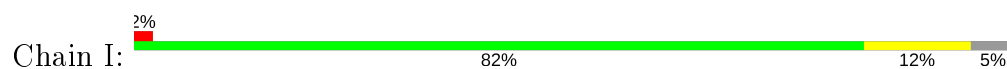


• Molecule 1: ATP synthase subunit alpha

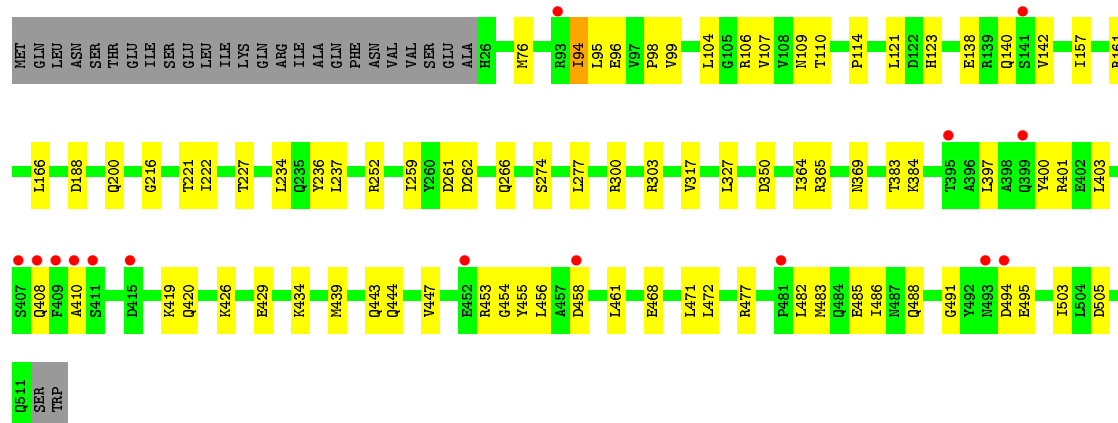
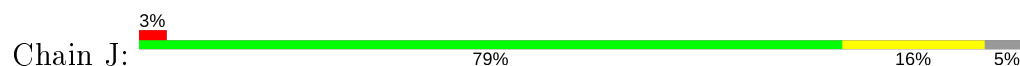




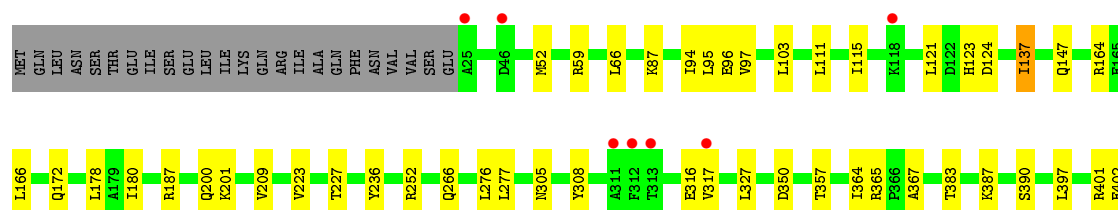
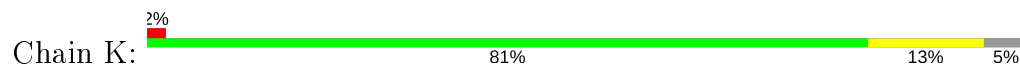
● Molecule 1: ATP synthase subunit alpha



● Molecule 1: ATP synthase subunit alpha

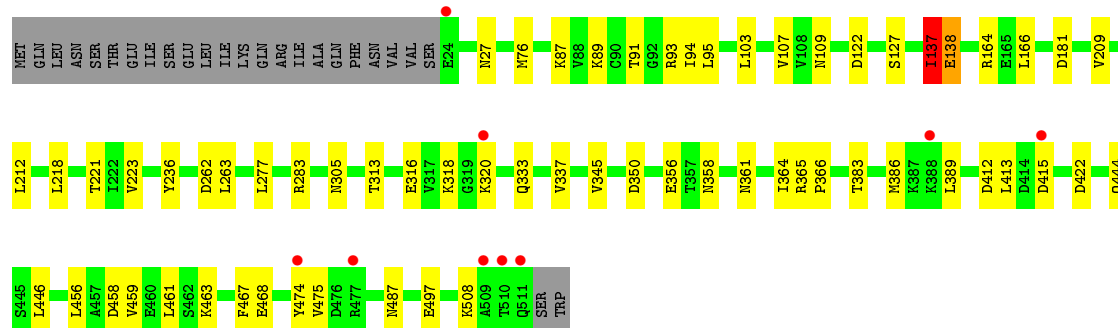
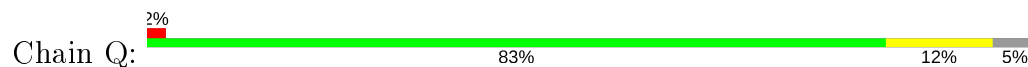


● Molecule 1: ATP synthase subunit alpha

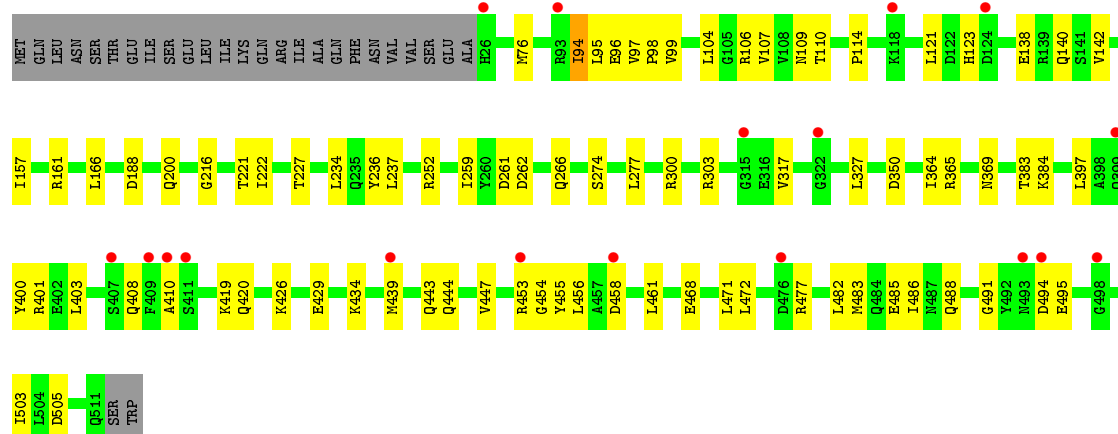
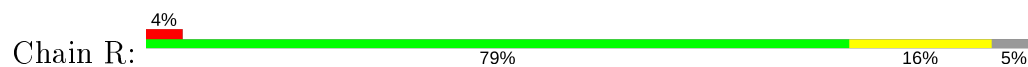




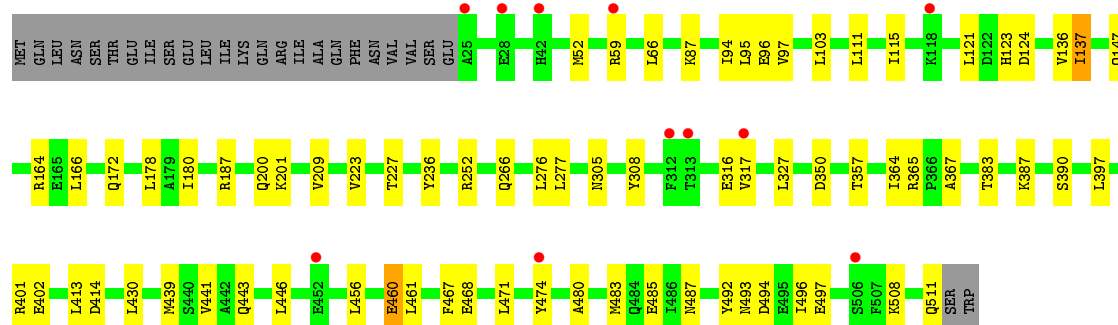
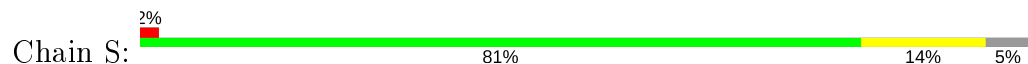
• Molecule 1: ATP synthase subunit alpha



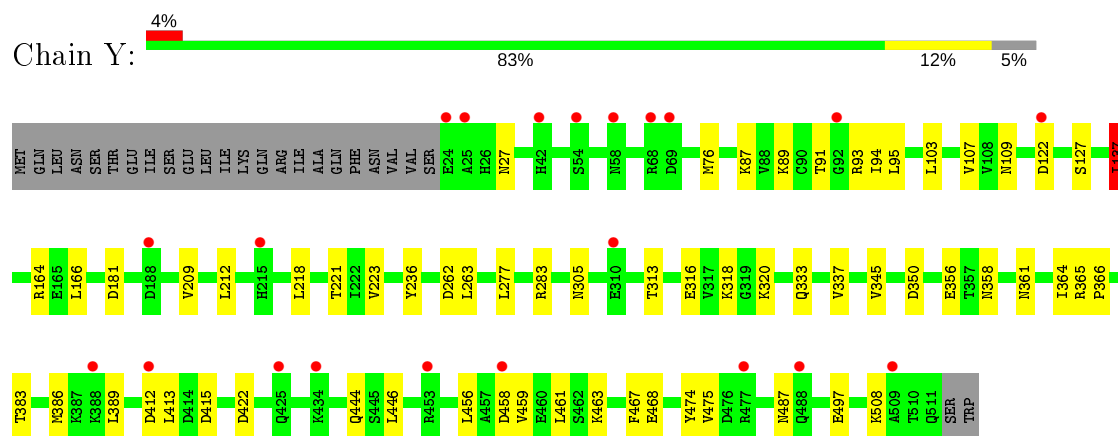
• Molecule 1: ATP synthase subunit alpha



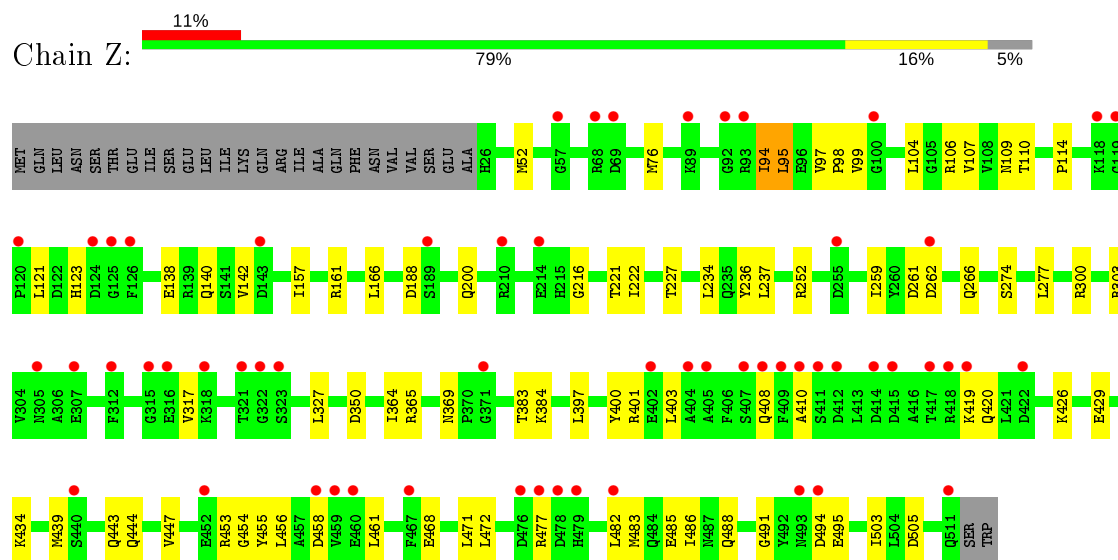
• Molecule 1: ATP synthase subunit alpha



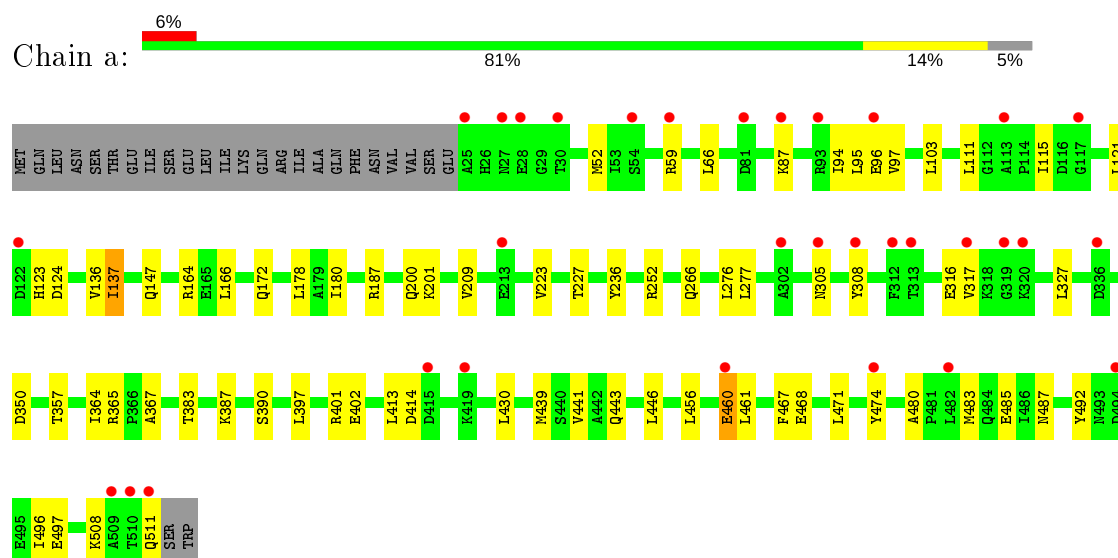
- Molecule 1: ATP synthase subunit alpha



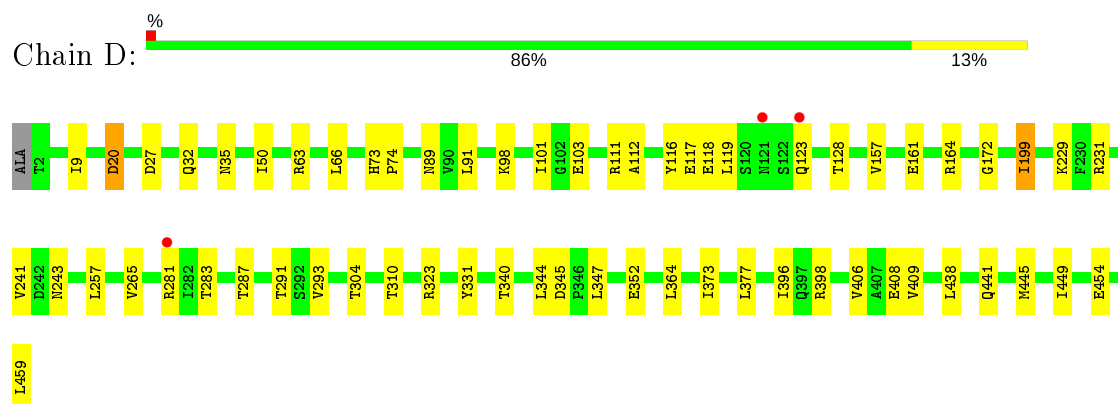
- Molecule 1: ATP synthase subunit alpha



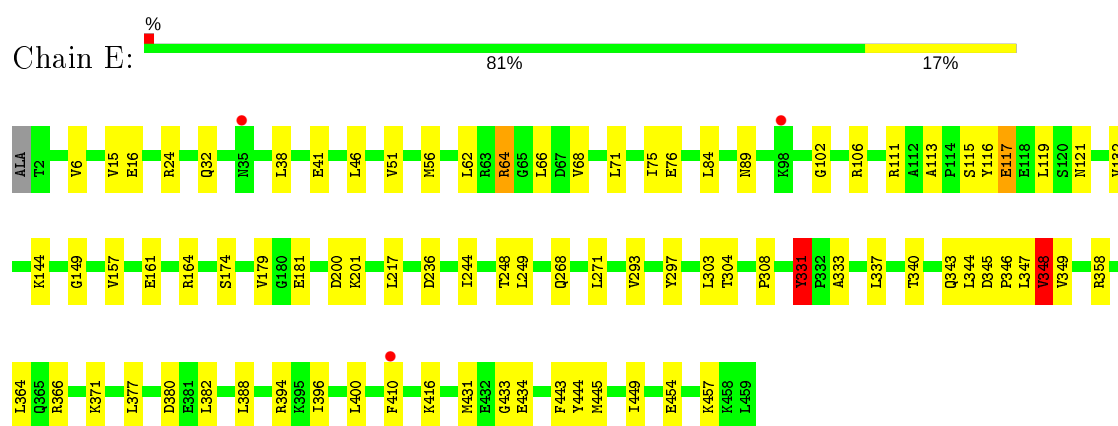
- Molecule 1: ATP synthase subunit alpha



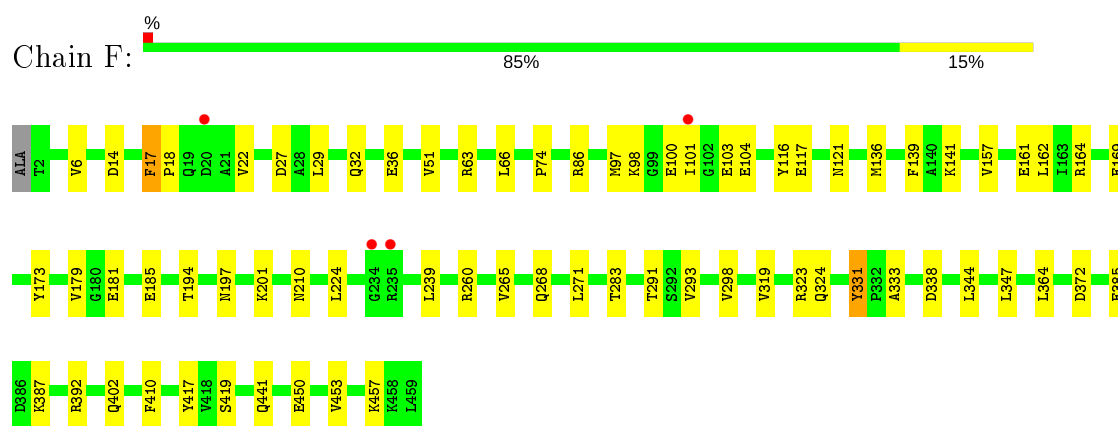
- Molecule 2: ATP synthase subunit beta



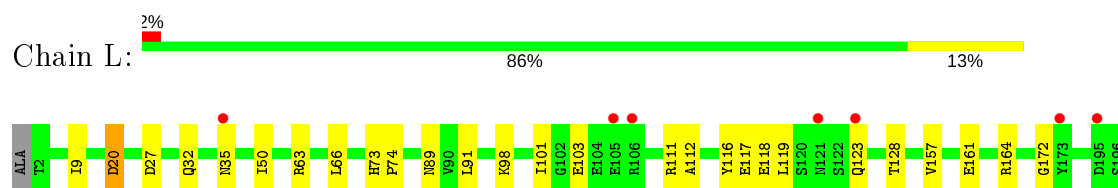
- Molecule 2: ATP synthase subunit beta

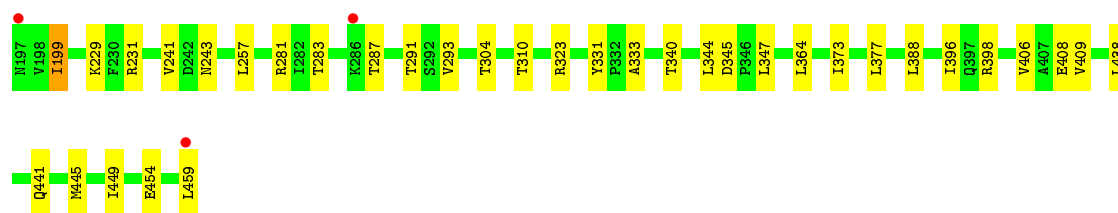


- Molecule 2: ATP synthase subunit beta

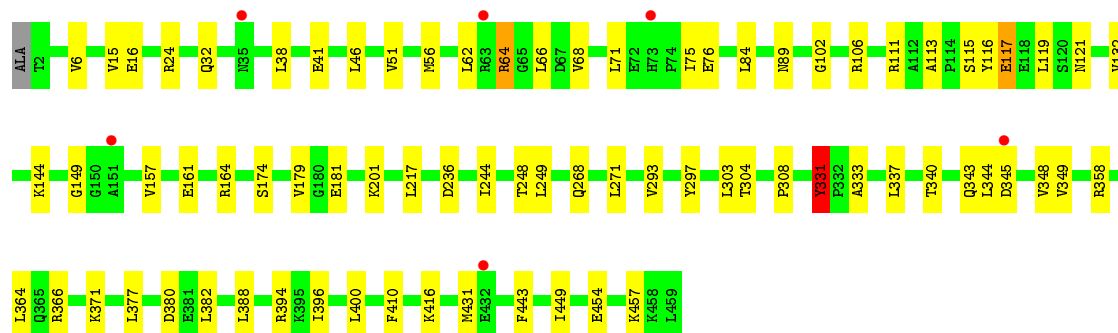
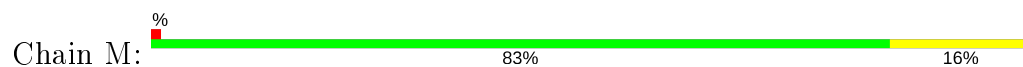


- Molecule 2: ATP synthase subunit beta

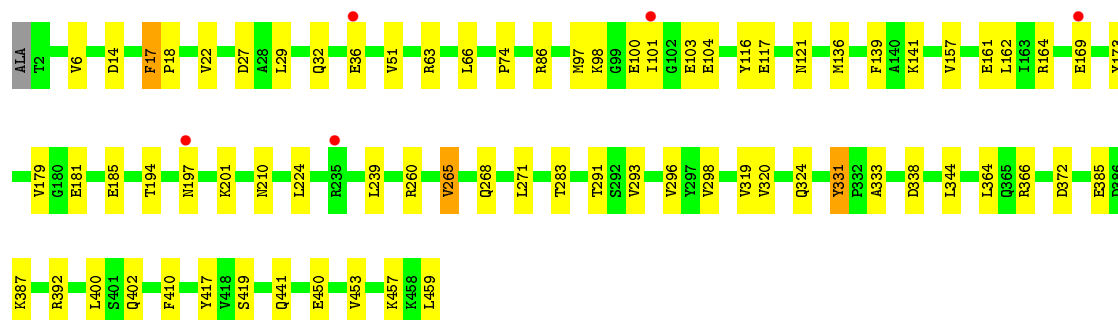
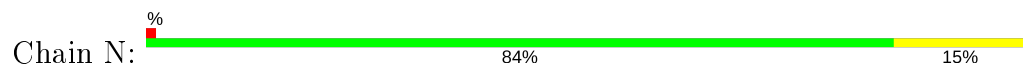




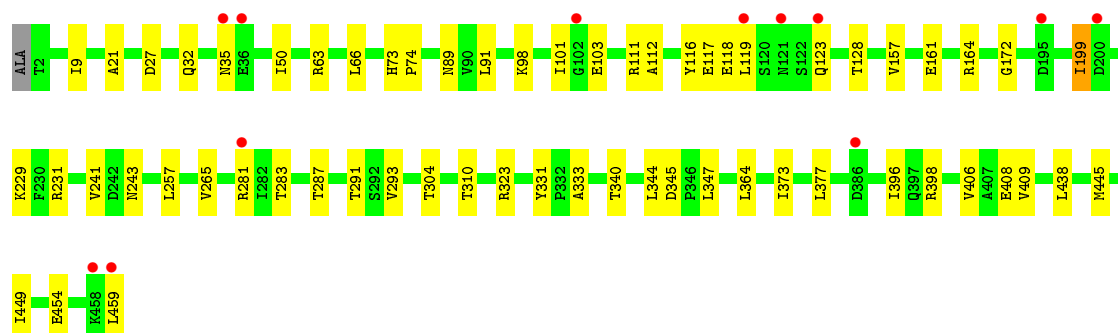
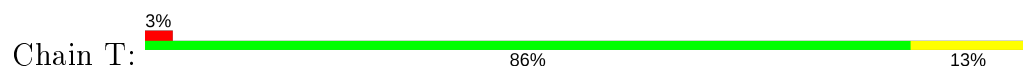
• Molecule 2: ATP synthase subunit beta



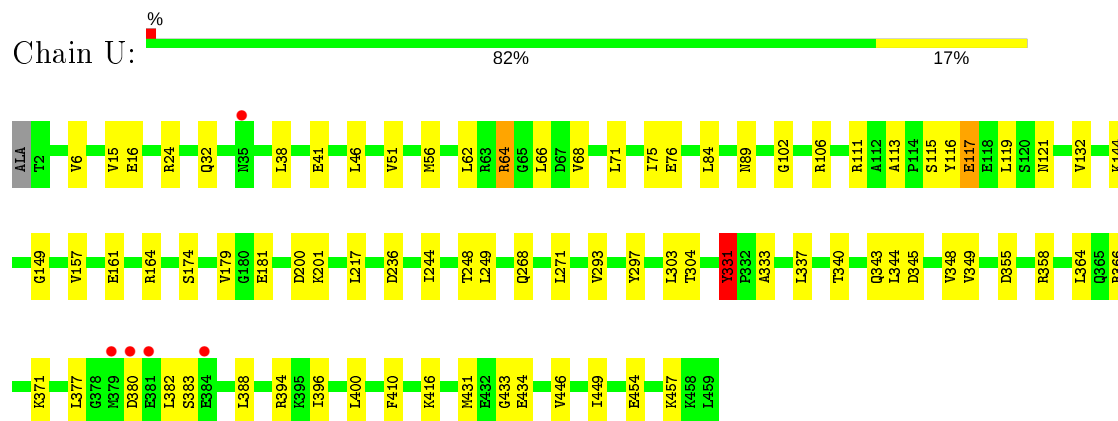
• Molecule 2: ATP synthase subunit beta



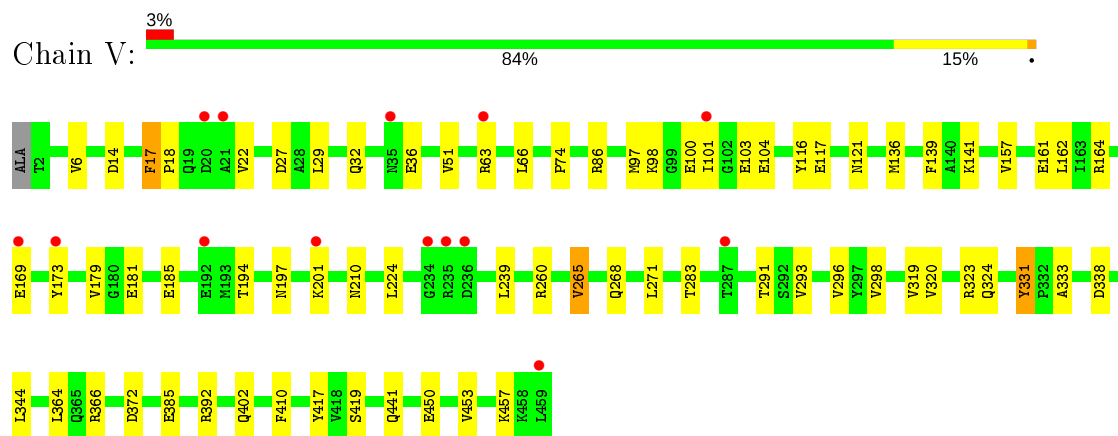
• Molecule 2: ATP synthase subunit beta



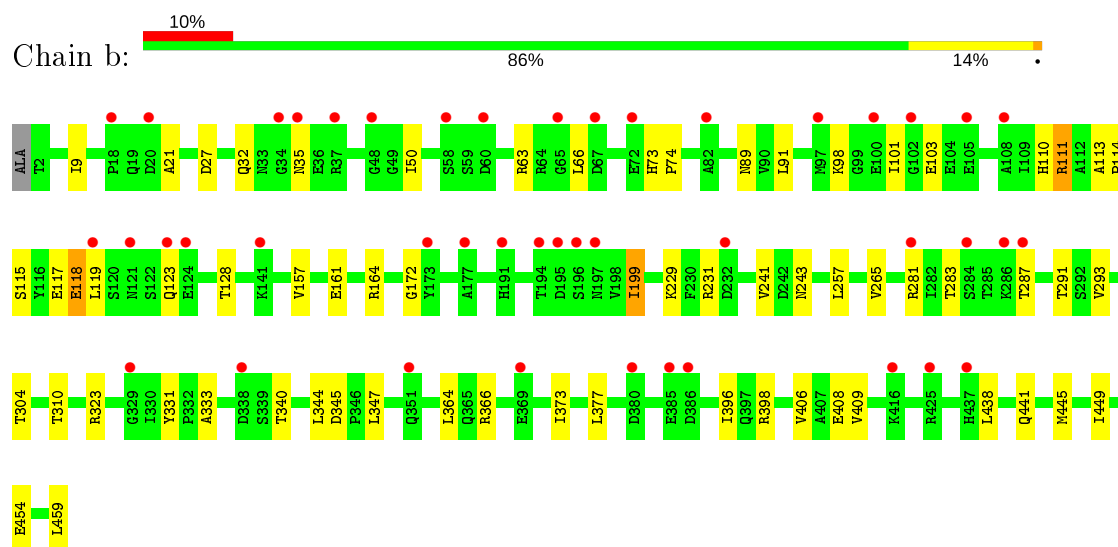
- Molecule 2: ATP synthase subunit beta



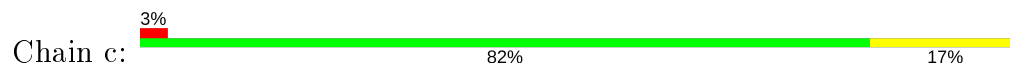
- Molecule 2: ATP synthase subunit beta

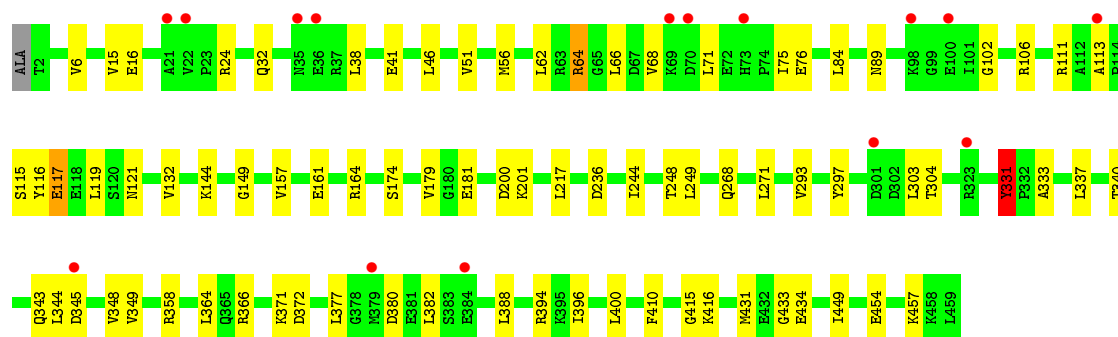


- Molecule 2: ATP synthase subunit beta

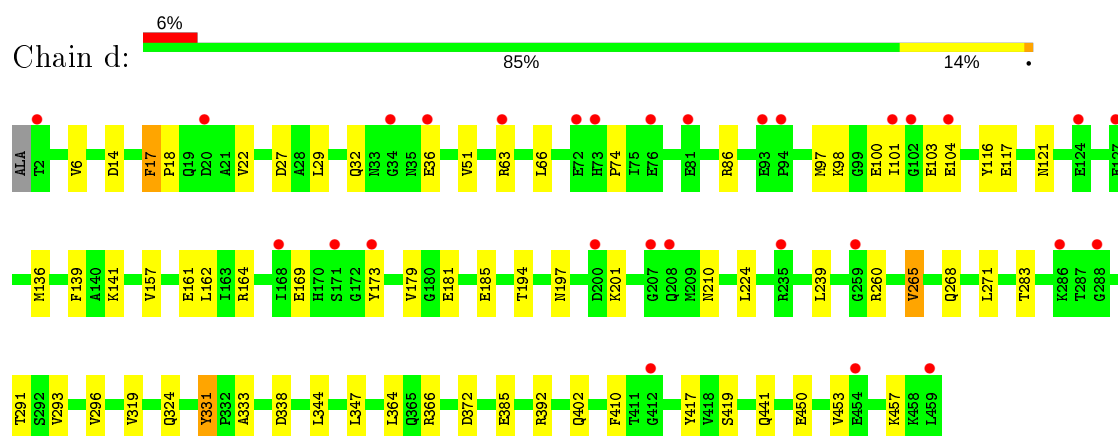


- Molecule 2: ATP synthase subunit beta

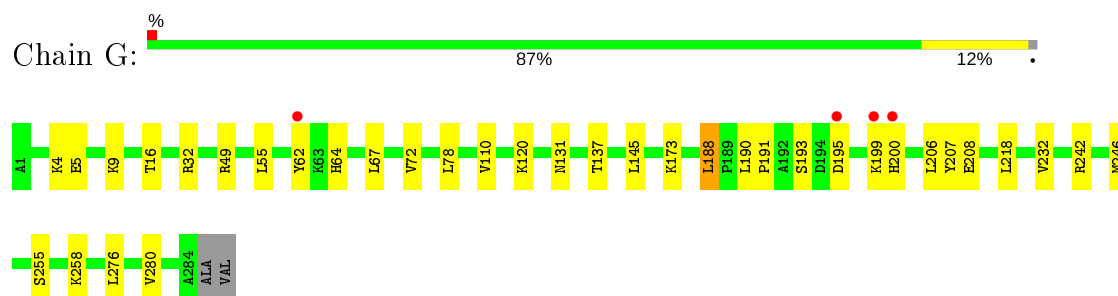




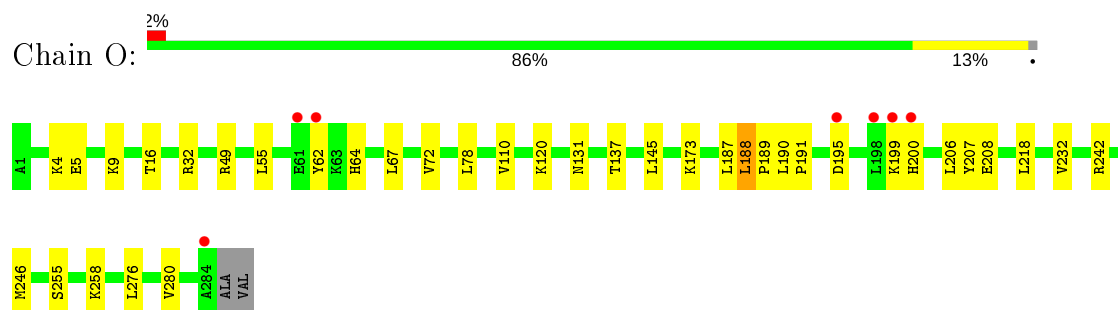
• Molecule 2: ATP synthase subunit beta



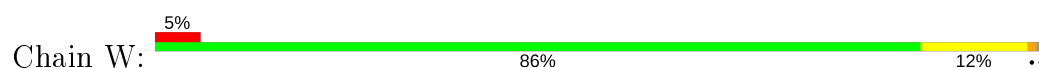
• Molecule 3: ATP synthase gamma chain

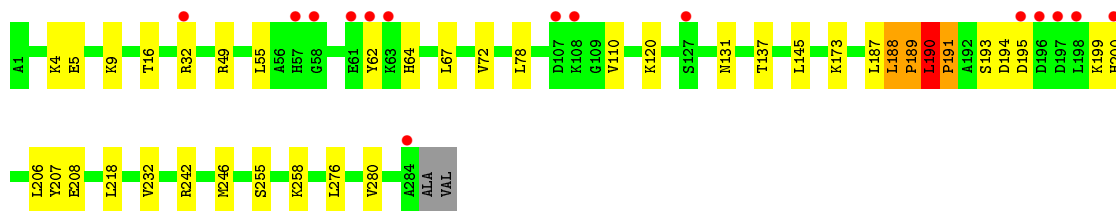


• Molecule 3: ATP synthase gamma chain

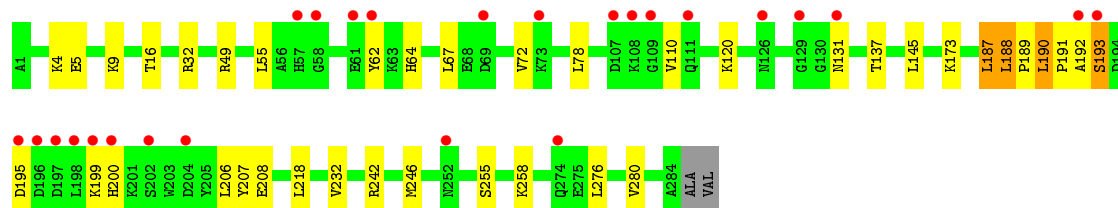
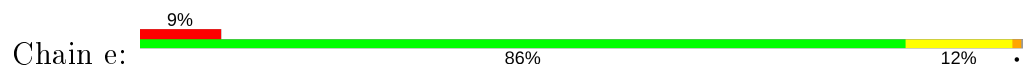


• Molecule 3: ATP synthase gamma chain

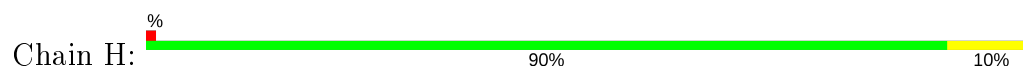




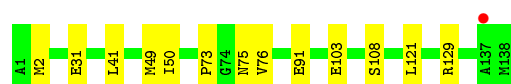
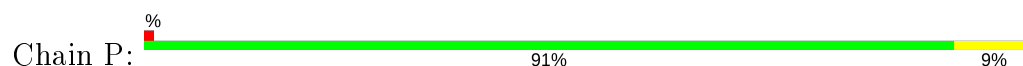
• Molecule 3: ATP synthase gamma chain



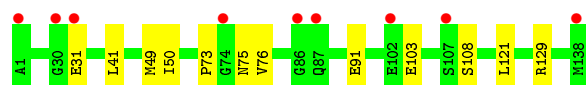
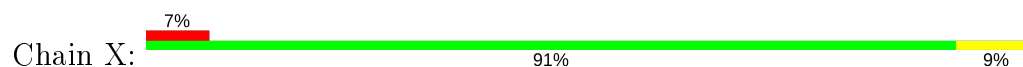
• Molecule 4: ATP synthase epsilon chain



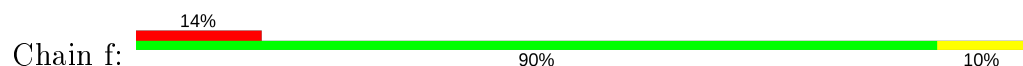
• Molecule 4: ATP synthase epsilon chain



• Molecule 4: ATP synthase epsilon chain



• Molecule 4: ATP synthase epsilon chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	435.97Å 183.00Å 225.39Å 90.00° 108.99° 90.00°	Depositor
Resolution (Å)	15.00 – 3.26 15.11 – 3.26	Depositor EDS
% Data completeness (in resolution range)	98.0 (15.00-3.26) 98.0 (15.11-3.26)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 3.26Å)	Xtriage
Refinement program	PHENIX 1.6.3 _473	Depositor
R, R_{free}	0.243 , 0.265 0.238 , 0.257	Depositor DCC
R_{free} test set	2000 reflections (0.79%)	wwPDB-VP
Wilson B-factor (Å ²)	79.5	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 65.8	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	0.91	EDS
Total number of atoms	99573	wwPDB-VP
Average B, all atoms (Å ²)	118.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% 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: MG, ANP, SO4, ADP

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	0.27	0/3720	0.45	1/5032 (0.0%)
1	B	0.25	0/3679	0.48	1/4979 (0.0%)
1	C	0.24	0/3699	0.46	0/5005
1	I	0.28	0/3720	0.48	2/5032 (0.0%)
1	J	0.25	0/3679	0.48	1/4979 (0.0%)
1	K	0.24	0/3699	0.46	0/5005
1	Q	0.25	0/3720	0.45	1/5032 (0.0%)
1	R	0.25	0/3679	0.48	1/4979 (0.0%)
1	S	0.23	0/3699	0.46	0/5005
1	Y	0.22	0/3720	0.53	2/5032 (0.0%)
1	Z	0.25	0/3679	0.48	1/4979 (0.0%)
1	a	0.23	0/3699	0.46	0/5005
2	D	0.25	0/3578	0.47	1/4843 (0.0%)
2	E	0.28	0/3578	0.48	0/4843
2	F	0.23	0/3578	0.47	0/4843
2	L	0.24	0/3578	0.48	2/4843 (0.0%)
2	M	0.26	0/3578	0.48	0/4843
2	N	0.24	0/3578	0.48	0/4843
2	T	0.23	0/3578	0.50	3/4843 (0.1%)
2	U	0.26	0/3578	0.48	0/4843
2	V	0.23	0/3578	0.47	0/4843
2	b	0.25	0/3578	0.47	1/4843 (0.0%)
2	c	0.25	0/3578	0.47	0/4843
2	d	0.23	0/3578	0.46	0/4843
3	G	0.30	0/2213	0.46	1/2984 (0.0%)
3	O	0.28	0/2213	0.46	1/2984 (0.0%)
3	W	0.25	0/2213	0.44	1/2984 (0.0%)
3	e	0.24	0/2213	0.52	1/2984 (0.0%)
4	H	0.22	0/1062	0.85	2/1432 (0.1%)
4	P	0.22	0/1062	0.40	0/1432
4	X	0.22	0/1062	0.40	0/1432
4	f	0.23	0/1062	0.86	2/1432 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.25	0/100428	0.48	25/135844 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	2
1	I	1	1
1	J	0	1
1	K	0	1
1	Q	0	1
1	R	0	1
1	S	0	2
1	Y	1	1
1	Z	0	2
1	a	0	1
2	D	0	2
2	E	0	4
2	F	0	1
2	L	0	2
2	M	0	1
2	N	0	1
2	T	0	1
2	U	0	1
2	V	0	1
2	b	0	5
2	c	0	1
2	d	0	1
3	G	0	2
3	O	0	2
3	W	0	4
3	e	0	4
All	All	2	47

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1	ALA	CB-CA-C	27.46	151.29	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	f	1	ALA	CB-CA-C	27.44	151.26	110.10
1	Y	137	ILE	C-N-CA	-16.64	80.11	121.70
3	e	190	LEU	C-N-CD	-15.49	86.52	120.60
1	Y	137	ILE	N-CA-C	11.89	143.09	111.00
2	T	112	ALA	CB-CA-C	10.66	126.10	110.10
2	L	112	ALA	CB-CA-C	7.97	122.06	110.10
4	H	1	ALA	N-CA-C	-7.69	90.24	111.00
4	f	1	ALA	N-CA-C	-7.67	90.28	111.00
1	R	408	GLN	N-CA-C	7.33	130.80	111.00
1	I	138	GLU	N-CA-C	6.79	129.34	111.00
2	T	112	ALA	N-CA-C	-6.45	93.58	111.00
3	W	190	LEU	C-N-CD	-6.42	106.47	120.60
1	Z	408	GLN	N-CA-C	6.13	127.55	111.00
1	B	408	GLN	N-CA-C	6.13	127.54	111.00
1	J	408	GLN	N-CA-C	6.12	127.52	111.00
2	L	112	ALA	N-CA-C	-5.56	95.98	111.00
1	Q	137	ILE	CB-CA-C	-5.45	100.69	111.60
1	I	137	ILE	C-N-CA	-5.35	108.32	121.70
2	D	112	ALA	CB-CA-C	5.31	118.07	110.10
3	G	188	LEU	C-N-CD	-5.29	108.97	120.60
2	b	21	ALA	N-CA-C	-5.28	96.75	111.00
2	T	21	ALA	N-CA-C	-5.26	96.79	111.00
1	A	178	LEU	N-CA-C	-5.24	96.85	111.00
3	O	188	LEU	C-N-CD	-5.09	109.39	120.60

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	I	138	GLU	CA
1	Y	137	ILE	CA

All (47) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	135	GLY	Peptide
1	C	460	GLU	Peptide
1	C	493	ASN	Peptide
2	D	119	LEU	Peptide
2	D	20	ASP	Peptide
2	E	331	TYR	Peptide
2	E	346	PRO	Peptide
2	E	348	VAL	Peptide

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Mol	Chain	Res	Type	Group
2	E	444	TYR	Peptide
2	F	331	TYR	Peptide
3	G	188	LEU	Peptide
3	G	191	PRO	Peptide
1	I	137	ILE	Peptide
1	J	94	ILE	Mainchain
1	K	460	GLU	Peptide
2	L	119	LEU	Peptide
2	L	20	ASP	Peptide
2	M	331	TYR	Peptide
2	N	331	TYR	Peptide
3	O	188	LEU	Peptide
3	O	191	PRO	Peptide
1	Q	138	GLU	Peptide
1	R	94	ILE	Peptide
1	S	460	GLU	Peptide
1	S	493	ASN	Peptide
2	T	119	LEU	Peptide
2	U	331	TYR	Peptide
2	V	331	TYR	Peptide
3	W	188	LEU	Peptide
3	W	189	PRO	Peptide
3	W	190	LEU	Peptide
3	W	191	PRO	Peptide
1	Y	137	ILE	Peptide
1	Z	94	ILE	Peptide
1	Z	95	LEU	Peptide
1	a	460	GLU	Peptide
2	b	110	HIS	Peptide
2	b	113	ALA	Peptide
2	b	115	SER	Peptide
2	b	118	GLU	Peptide
2	b	119	LEU	Peptide
2	c	331	TYR	Peptide
2	d	331	TYR	Peptide
3	e	187	LEU	Peptide
3	e	188	LEU	Peptide
3	e	191	PRO	Peptide
3	e	193	SER	Peptide

5.2 Too-close contacts ⓘ

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	486/513 (95%)	433 (89%)	48 (10%)	5 (1%)	15	47
1	B	484/513 (94%)	421 (87%)	54 (11%)	9 (2%)	8	34
1	C	485/513 (94%)	429 (88%)	48 (10%)	8 (2%)	9	37
1	I	486/513 (95%)	433 (89%)	49 (10%)	4 (1%)	19	52
1	J	484/513 (94%)	419 (87%)	56 (12%)	9 (2%)	8	34
1	K	485/513 (94%)	428 (88%)	49 (10%)	8 (2%)	9	37
1	Q	486/513 (95%)	433 (89%)	47 (10%)	6 (1%)	13	43
1	R	484/513 (94%)	417 (86%)	58 (12%)	9 (2%)	8	34
1	S	485/513 (94%)	429 (88%)	48 (10%)	8 (2%)	9	37
1	Y	486/513 (95%)	431 (89%)	49 (10%)	6 (1%)	13	43
1	Z	484/513 (94%)	418 (86%)	57 (12%)	9 (2%)	8	34
1	a	485/513 (94%)	427 (88%)	50 (10%)	8 (2%)	9	37
2	D	456/459 (99%)	397 (87%)	54 (12%)	5 (1%)	14	46
2	E	456/459 (99%)	406 (89%)	38 (8%)	12 (3%)	5	27
2	F	456/459 (99%)	411 (90%)	40 (9%)	5 (1%)	14	46
2	L	456/459 (99%)	398 (87%)	53 (12%)	5 (1%)	14	46
2	M	456/459 (99%)	405 (89%)	41 (9%)	10 (2%)	6	31
2	N	456/459 (99%)	413 (91%)	37 (8%)	6 (1%)	12	41
2	T	456/459 (99%)	402 (88%)	48 (10%)	6 (1%)	12	41
2	U	456/459 (99%)	406 (89%)	38 (8%)	12 (3%)	5	27
2	V	456/459 (99%)	410 (90%)	40 (9%)	6 (1%)	12	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	b	456/459 (99%)	398 (87%)	51 (11%)	7 (2%)	10	39
2	c	456/459 (99%)	406 (89%)	38 (8%)	12 (3%)	5	27
2	d	456/459 (99%)	411 (90%)	39 (9%)	6 (1%)	12	41
3	G	282/286 (99%)	265 (94%)	17 (6%)	0	100	100
3	O	282/286 (99%)	266 (94%)	15 (5%)	1 (0%)	34	67
3	W	282/286 (99%)	264 (94%)	16 (6%)	2 (1%)	22	56
3	e	282/286 (99%)	265 (94%)	15 (5%)	2 (1%)	22	56
4	H	136/138 (99%)	123 (90%)	11 (8%)	2 (2%)	10	39
4	P	136/138 (99%)	123 (90%)	11 (8%)	2 (2%)	10	39
4	X	136/138 (99%)	123 (90%)	11 (8%)	2 (2%)	10	39
4	f	136/138 (99%)	123 (90%)	11 (8%)	2 (2%)	10	39
All	All	12964/13360 (97%)	11533 (89%)	1237 (10%)	194 (2%)	10	39

All (194) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	455	TYR
1	B	491	GLY
1	C	137	ILE
2	E	333	ALA
2	E	348	VAL
2	F	18	PRO
1	I	137	ILE
1	J	455	TYR
1	J	491	GLY
1	K	137	ILE
2	M	348	VAL
2	N	18	PRO
1	Q	137	ILE
1	R	455	TYR
1	R	491	GLY
1	S	137	ILE
2	U	348	VAL
2	V	18	PRO
1	Y	137	ILE
1	Z	455	TYR
1	Z	491	GLY
1	a	137	ILE

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Mol	Chain	Res	Type
2	c	348	VAL
2	d	18	PRO
1	A	458	ASP
1	B	216	GLY
1	B	410	ALA
1	C	441	VAL
2	E	102	GLY
2	F	333	ALA
1	J	216	GLY
1	J	410	ALA
1	K	441	VAL
2	M	102	GLY
2	M	333	ALA
2	N	333	ALA
1	Q	458	ASP
1	R	216	GLY
1	R	410	ALA
1	S	441	VAL
2	U	102	GLY
2	U	333	ALA
2	V	333	ALA
1	Y	458	ASP
1	Z	216	GLY
1	Z	410	ALA
1	a	441	VAL
2	b	111	ARG
2	b	333	ALA
2	c	102	GLY
2	c	333	ALA
2	d	333	ALA
1	A	459	VAL
1	C	316	GLU
1	C	508	LYS
2	E	117	GLU
1	K	316	GLU
1	K	508	LYS
2	L	333	ALA
2	M	117	GLU
1	Q	459	VAL
1	S	316	GLU
1	S	508	LYS
2	T	333	ALA

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Mol	Chain	Res	Type
2	U	117	GLU
1	Y	459	VAL
1	a	316	GLU
1	a	508	LYS
2	c	117	GLU
2	c	434	GLU
1	A	316	GLU
1	B	98	PRO
1	B	114	PRO
1	C	367	ALA
2	D	116	TYR
2	D	199	ILE
2	E	64	ARG
1	I	316	GLU
1	J	98	PRO
1	J	114	PRO
1	K	367	ALA
2	L	116	TYR
2	L	199	ILE
2	M	64	ARG
1	Q	316	GLU
1	R	98	PRO
1	R	114	PRO
1	S	367	ALA
2	T	116	TYR
2	T	199	ILE
2	U	64	ARG
2	U	75	ILE
3	W	191	PRO
1	Y	316	GLU
1	Z	98	PRO
1	Z	114	PRO
1	a	367	ALA
2	b	199	ILE
2	c	64	ARG
2	D	172	GLY
2	E	75	ILE
2	E	434	GLU
2	F	17	PHE
4	H	31	GLU
2	L	172	GLY
2	M	75	ILE

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Mol	Chain	Res	Type
2	N	17	PHE
4	P	31	GLU
2	T	172	GLY
2	V	17	PHE
3	W	189	PRO
4	X	31	GLU
2	b	172	GLY
2	c	75	ILE
2	d	17	PHE
3	e	192	ALA
4	f	31	GLU
2	E	149	GLY
2	M	149	GLY
2	U	149	GLY
2	U	383	SER
2	U	434	GLU
2	c	149	GLY
1	B	364	ILE
1	B	454	GLY
1	J	364	ILE
1	J	454	GLY
1	R	364	ILE
1	R	454	GLY
1	Z	364	ILE
1	Z	454	GLY
2	b	114	PRO
2	c	433	GLY
3	e	189	PRO
1	A	364	ILE
2	D	74	PRO
2	D	265	VAL
2	F	74	PRO
2	F	331	TYR
1	I	364	ILE
2	L	74	PRO
2	N	74	PRO
3	O	189	PRO
1	Q	364	ILE
2	T	74	PRO
2	V	74	PRO
1	Y	364	ILE
2	b	74	PRO

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Mol	Chain	Res	Type
2	b	265	VAL
2	d	74	PRO
2	d	331	TYR
2	E	113	ALA
2	E	308	PRO
2	M	113	ALA
2	N	331	TYR
2	T	265	VAL
2	U	113	ALA
2	U	433	GLY
2	V	265	VAL
2	V	331	TYR
2	c	113	ALA
2	c	331	TYR
1	A	366	PRO
1	B	99	VAL
2	E	331	TYR
4	H	73	PRO
1	I	366	PRO
1	J	99	VAL
1	K	317	VAL
2	M	308	PRO
2	M	331	TYR
4	P	73	PRO
1	Q	366	PRO
1	R	99	VAL
2	U	331	TYR
4	X	73	PRO
1	Y	366	PRO
1	Z	99	VAL
2	c	415	GLY
2	d	265	VAL
4	f	73	PRO
1	C	317	VAL
1	C	364	ILE
1	C	480	ALA
2	E	433	GLY
1	K	364	ILE
1	K	480	ALA
2	N	265	VAL
1	S	317	VAL
1	S	364	ILE

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Mol	Chain	Res	Type
1	S	480	ALA
1	a	317	VAL
1	a	364	ILE
1	a	480	ALA

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	380/407 (93%)	319 (84%)	61 (16%)	2	10
1	B	371/407 (91%)	300 (81%)	71 (19%)	1	6
1	C	375/407 (92%)	307 (82%)	68 (18%)	1	7
1	I	380/407 (93%)	319 (84%)	61 (16%)	2	10
1	J	371/407 (91%)	300 (81%)	71 (19%)	1	6
1	K	375/407 (92%)	311 (83%)	64 (17%)	2	9
1	Q	380/407 (93%)	321 (84%)	59 (16%)	2	11
1	R	371/407 (91%)	299 (81%)	72 (19%)	1	5
1	S	375/407 (92%)	309 (82%)	66 (18%)	2	8
1	Y	380/407 (93%)	322 (85%)	58 (15%)	2	12
1	Z	371/407 (91%)	299 (81%)	72 (19%)	1	5
1	a	375/407 (92%)	310 (83%)	65 (17%)	2	8
2	D	380/380 (100%)	324 (85%)	56 (15%)	3	13
2	E	380/380 (100%)	306 (80%)	74 (20%)	1	5
2	F	380/380 (100%)	314 (83%)	66 (17%)	2	8
2	L	380/380 (100%)	324 (85%)	56 (15%)	3	13
2	M	380/380 (100%)	310 (82%)	70 (18%)	1	7
2	N	380/380 (100%)	311 (82%)	69 (18%)	1	7
2	T	380/380 (100%)	327 (86%)	53 (14%)	3	15
2	U	380/380 (100%)	308 (81%)	72 (19%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	V	380/380 (100%)	313 (82%)	67 (18%)	2	8
2	b	380/380 (100%)	325 (86%)	55 (14%)	3	14
2	c	380/380 (100%)	309 (81%)	71 (19%)	1	6
2	d	380/380 (100%)	315 (83%)	65 (17%)	2	9
3	G	236/239 (99%)	202 (86%)	34 (14%)	3	14
3	O	236/239 (99%)	202 (86%)	34 (14%)	3	14
3	W	236/239 (99%)	199 (84%)	37 (16%)	2	11
3	e	236/239 (99%)	200 (85%)	36 (15%)	2	12
4	H	109/109 (100%)	98 (90%)	11 (10%)	7	27
4	P	109/109 (100%)	98 (90%)	11 (10%)	7	27
4	X	109/109 (100%)	99 (91%)	10 (9%)	9	31
4	f	109/109 (100%)	98 (90%)	11 (10%)	7	27
All	All	10444/10836 (96%)	8698 (83%)	1746 (17%)	2	9

All (1746) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	76	MET
1	A	87	LYS
1	A	89	LYS
1	A	91	THR
1	A	93	ARG
1	A	94	ILE
1	A	95	LEU
1	A	103	LEU
1	A	107	VAL
1	A	109	ASN
1	A	122	ASP
1	A	127	SER
1	A	136	VAL
1	A	137	ILE
1	A	164	ARG
1	A	166	LEU
1	A	178	LEU
1	A	181	ASP
1	A	209	VAL
1	A	212	LEU

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Mol	Chain	Res	Type
1	A	218	LEU
1	A	221	THR
1	A	223	VAL
1	A	236	TYR
1	A	262	ASP
1	A	263	LEU
1	A	277	LEU
1	A	283	ARG
1	A	305	ASN
1	A	313	THR
1	A	318	LYS
1	A	320	LYS
1	A	333	GLN
1	A	337	VAL
1	A	345	VAL
1	A	350	ASP
1	A	356	GLU
1	A	358	ASN
1	A	361	ASN
1	A	365	ARG
1	A	383	THR
1	A	386	MET
1	A	389	LEU
1	A	412	ASP
1	A	413	LEU
1	A	415	ASP
1	A	422	ASP
1	A	444	GLN
1	A	446	LEU
1	A	456	LEU
1	A	461	LEU
1	A	463	LYS
1	A	467	PHE
1	A	468	GLU
1	A	474	TYR
1	A	475	VAL
1	A	477	ARG
1	A	487	ASN
1	A	497	GLU
1	A	508	LYS
1	B	76	MET
1	B	94	ILE

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Mol	Chain	Res	Type
1	B	95	LEU
1	B	97	VAL
1	B	104	LEU
1	B	106	ARG
1	B	107	VAL
1	B	109	ASN
1	B	110	THR
1	B	121	LEU
1	B	123	HIS
1	B	138	GLU
1	B	140	GLN
1	B	142	VAL
1	B	157	ILE
1	B	161	ARG
1	B	166	LEU
1	B	188	ASP
1	B	200	GLN
1	B	221	THR
1	B	222	ILE
1	B	227	THR
1	B	234	LEU
1	B	236	TYR
1	B	237	LEU
1	B	252	ARG
1	B	259	ILE
1	B	261	ASP
1	B	262	ASP
1	B	266	GLN
1	B	274	SER
1	B	277	LEU
1	B	300	ARG
1	B	303	ARG
1	B	317	VAL
1	B	327	LEU
1	B	350	ASP
1	B	365	ARG
1	B	369	ASN
1	B	383	THR
1	B	384	LYS
1	B	397	LEU
1	B	400	TYR
1	B	401	ARG

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Mol	Chain	Res	Type
1	B	403	LEU
1	B	419	LYS
1	B	420	GLN
1	B	426	LYS
1	B	429	GLU
1	B	434	LYS
1	B	439	MET
1	B	443	GLN
1	B	444	GLN
1	B	447	VAL
1	B	453	ARG
1	B	456	LEU
1	B	458	ASP
1	B	461	LEU
1	B	468	GLU
1	B	471	LEU
1	B	472	LEU
1	B	477	ARG
1	B	482	LEU
1	B	483	MET
1	B	485	GLU
1	B	486	ILE
1	B	488	GLN
1	B	494	ASP
1	B	495	GLU
1	B	503	ILE
1	B	505	ASP
1	C	52	MET
1	C	59	ARG
1	C	66	LEU
1	C	87	LYS
1	C	94	ILE
1	C	95	LEU
1	C	96	GLU
1	C	97	VAL
1	C	103	LEU
1	C	111	LEU
1	C	115	ILE
1	C	121	LEU
1	C	123	HIS
1	C	124	ASP
1	C	136	VAL

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Mol	Chain	Res	Type
1	C	137	ILE
1	C	147	GLN
1	C	164	ARG
1	C	166	LEU
1	C	172	GLN
1	C	178	LEU
1	C	180	ILE
1	C	187	ARG
1	C	200	GLN
1	C	201	LYS
1	C	209	VAL
1	C	223	VAL
1	C	227	THR
1	C	236	TYR
1	C	252	ARG
1	C	266	GLN
1	C	276	LEU
1	C	277	LEU
1	C	305	ASN
1	C	308	TYR
1	C	327	LEU
1	C	350	ASP
1	C	357	THR
1	C	365	ARG
1	C	383	THR
1	C	387	LYS
1	C	390	SER
1	C	397	LEU
1	C	401	ARG
1	C	402	GLU
1	C	413	LEU
1	C	414	ASP
1	C	430	LEU
1	C	439	MET
1	C	443	GLN
1	C	446	LEU
1	C	456	LEU
1	C	460	GLU
1	C	461	LEU
1	C	467	PHE
1	C	468	GLU
1	C	471	LEU

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Mol	Chain	Res	Type
1	C	474	TYR
1	C	483	MET
1	C	485	GLU
1	C	487	ASN
1	C	492	TYR
1	C	493	ASN
1	C	494	ASP
1	C	495	GLU
1	C	496	ILE
1	C	497	GLU
1	C	511	GLN
2	D	9	ILE
2	D	20	ASP
2	D	27	ASP
2	D	32	GLN
2	D	35	ASN
2	D	50	ILE
2	D	63	ARG
2	D	66	LEU
2	D	73	HIS
2	D	89	ASN
2	D	91	LEU
2	D	98	LYS
2	D	101	ILE
2	D	103	GLU
2	D	111	ARG
2	D	117	GLU
2	D	118	GLU
2	D	123	GLN
2	D	128	THR
2	D	157	VAL
2	D	161	GLU
2	D	164	ARG
2	D	199	ILE
2	D	229	LYS
2	D	231	ARG
2	D	241	VAL
2	D	243	ASN
2	D	257	LEU
2	D	281	ARG
2	D	283	THR
2	D	287	THR

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Mol	Chain	Res	Type
2	D	291	THR
2	D	293	VAL
2	D	304	THR
2	D	310	THR
2	D	323	ARG
2	D	331	TYR
2	D	340	THR
2	D	344	LEU
2	D	345	ASP
2	D	347	LEU
2	D	352	GLU
2	D	364	LEU
2	D	373	ILE
2	D	377	LEU
2	D	396	ILE
2	D	398	ARG
2	D	406	VAL
2	D	408	GLU
2	D	409	VAL
2	D	438	LEU
2	D	441	GLN
2	D	445	MET
2	D	449	ILE
2	D	454	GLU
2	D	459	LEU
2	E	6	VAL
2	E	15	VAL
2	E	16	GLU
2	E	24	ARG
2	E	32	GLN
2	E	38	LEU
2	E	41	GLU
2	E	46	LEU
2	E	51	VAL
2	E	56	MET
2	E	62	LEU
2	E	64	ARG
2	E	66	LEU
2	E	68	VAL
2	E	71	LEU
2	E	76	GLU
2	E	84	LEU

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Mol	Chain	Res	Type
2	E	89	ASN
2	E	106	ARG
2	E	111	ARG
2	E	115	SER
2	E	116	TYR
2	E	117	GLU
2	E	119	LEU
2	E	121	ASN
2	E	132	VAL
2	E	144	LYS
2	E	157	VAL
2	E	161	GLU
2	E	164	ARG
2	E	174	SER
2	E	179	VAL
2	E	181	GLU
2	E	200	ASP
2	E	201	LYS
2	E	217	LEU
2	E	236	ASP
2	E	244	ILE
2	E	248	THR
2	E	249	LEU
2	E	268	GLN
2	E	271	LEU
2	E	293	VAL
2	E	297	TYR
2	E	303	LEU
2	E	304	THR
2	E	331	TYR
2	E	337	LEU
2	E	340	THR
2	E	343	GLN
2	E	344	LEU
2	E	345	ASP
2	E	347	LEU
2	E	348	VAL
2	E	349	VAL
2	E	358	ARG
2	E	364	LEU
2	E	366	ARG
2	E	371	LYS

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Mol	Chain	Res	Type
2	E	377	LEU
2	E	380	ASP
2	E	382	LEU
2	E	388	LEU
2	E	394	ARG
2	E	396	ILE
2	E	400	LEU
2	E	410	PHE
2	E	416	LYS
2	E	431	MET
2	E	443	PHE
2	E	445	MET
2	E	449	ILE
2	E	454	GLU
2	E	457	LYS
2	F	6	VAL
2	F	14	ASP
2	F	17	PHE
2	F	22	VAL
2	F	27	ASP
2	F	29	LEU
2	F	32	GLN
2	F	36	GLU
2	F	51	VAL
2	F	63	ARG
2	F	66	LEU
2	F	86	ARG
2	F	97	MET
2	F	98	LYS
2	F	100	GLU
2	F	101	ILE
2	F	103	GLU
2	F	104	GLU
2	F	116	TYR
2	F	117	GLU
2	F	121	ASN
2	F	136	MET
2	F	139	PHE
2	F	141	LYS
2	F	157	VAL
2	F	161	GLU
2	F	162	LEU

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Mol	Chain	Res	Type
2	F	164	ARG
2	F	169	GLU
2	F	173	TYR
2	F	179	VAL
2	F	181	GLU
2	F	185	GLU
2	F	194	THR
2	F	197	ASN
2	F	201	LYS
2	F	210	ASN
2	F	224	LEU
2	F	239	LEU
2	F	260	ARG
2	F	265	VAL
2	F	268	GLN
2	F	271	LEU
2	F	283	THR
2	F	291	THR
2	F	293	VAL
2	F	298	VAL
2	F	319	VAL
2	F	323	ARG
2	F	324	GLN
2	F	338	ASP
2	F	344	LEU
2	F	347	LEU
2	F	364	LEU
2	F	372	ASP
2	F	385	GLU
2	F	387	LYS
2	F	392	ARG
2	F	402	GLN
2	F	410	PHE
2	F	417	TYR
2	F	419	SER
2	F	441	GLN
2	F	450	GLU
2	F	453	VAL
2	F	457	LYS
3	G	4	LYS
3	G	5	GLU
3	G	9	LYS

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Mol	Chain	Res	Type
3	G	16	THR
3	G	32	ARG
3	G	49	ARG
3	G	55	LEU
3	G	62	TYR
3	G	64	HIS
3	G	67	LEU
3	G	72	VAL
3	G	78	LEU
3	G	110	VAL
3	G	120	LYS
3	G	131	ASN
3	G	137	THR
3	G	145	LEU
3	G	173	LYS
3	G	190	LEU
3	G	193	SER
3	G	195	ASP
3	G	199	LYS
3	G	200	HIS
3	G	206	LEU
3	G	207	TYR
3	G	208	GLU
3	G	218	LEU
3	G	232	VAL
3	G	242	ARG
3	G	246	MET
3	G	255	SER
3	G	258	LYS
3	G	276	LEU
3	G	280	VAL
4	H	2	MET
4	H	41	LEU
4	H	49	MET
4	H	50	ILE
4	H	75	ASN
4	H	76	VAL
4	H	91	GLU
4	H	103	GLU
4	H	108	SER
4	H	121	LEU
4	H	129	ARG

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Mol	Chain	Res	Type
1	I	27	ASN
1	I	76	MET
1	I	87	LYS
1	I	89	LYS
1	I	91	THR
1	I	93	ARG
1	I	94	ILE
1	I	95	LEU
1	I	103	LEU
1	I	107	VAL
1	I	109	ASN
1	I	122	ASP
1	I	127	SER
1	I	137	ILE
1	I	164	ARG
1	I	166	LEU
1	I	176	THR
1	I	178	LEU
1	I	181	ASP
1	I	209	VAL
1	I	212	LEU
1	I	218	LEU
1	I	221	THR
1	I	223	VAL
1	I	236	TYR
1	I	262	ASP
1	I	263	LEU
1	I	277	LEU
1	I	283	ARG
1	I	305	ASN
1	I	313	THR
1	I	318	LYS
1	I	320	LYS
1	I	333	GLN
1	I	337	VAL
1	I	345	VAL
1	I	350	ASP
1	I	356	GLU
1	I	358	ASN
1	I	361	ASN
1	I	365	ARG
1	I	383	THR

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Mol	Chain	Res	Type
1	I	386	MET
1	I	389	LEU
1	I	412	ASP
1	I	413	LEU
1	I	415	ASP
1	I	422	ASP
1	I	444	GLN
1	I	446	LEU
1	I	456	LEU
1	I	458	ASP
1	I	461	LEU
1	I	463	LYS
1	I	467	PHE
1	I	468	GLU
1	I	474	TYR
1	I	475	VAL
1	I	487	ASN
1	I	497	GLU
1	I	508	LYS
1	J	76	MET
1	J	94	ILE
1	J	95	LEU
1	J	96	GLU
1	J	104	LEU
1	J	106	ARG
1	J	107	VAL
1	J	109	ASN
1	J	110	THR
1	J	121	LEU
1	J	123	HIS
1	J	138	GLU
1	J	140	GLN
1	J	142	VAL
1	J	157	ILE
1	J	161	ARG
1	J	166	LEU
1	J	188	ASP
1	J	200	GLN
1	J	221	THR
1	J	222	ILE
1	J	227	THR
1	J	234	LEU

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Mol	Chain	Res	Type
1	J	236	TYR
1	J	237	LEU
1	J	252	ARG
1	J	259	ILE
1	J	261	ASP
1	J	262	ASP
1	J	266	GLN
1	J	274	SER
1	J	277	LEU
1	J	300	ARG
1	J	303	ARG
1	J	317	VAL
1	J	327	LEU
1	J	350	ASP
1	J	365	ARG
1	J	369	ASN
1	J	383	THR
1	J	384	LYS
1	J	397	LEU
1	J	400	TYR
1	J	401	ARG
1	J	403	LEU
1	J	419	LYS
1	J	420	GLN
1	J	426	LYS
1	J	429	GLU
1	J	434	LYS
1	J	439	MET
1	J	443	GLN
1	J	444	GLN
1	J	447	VAL
1	J	453	ARG
1	J	456	LEU
1	J	458	ASP
1	J	461	LEU
1	J	468	GLU
1	J	471	LEU
1	J	472	LEU
1	J	477	ARG
1	J	482	LEU
1	J	483	MET
1	J	485	GLU

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Mol	Chain	Res	Type
1	J	486	ILE
1	J	488	GLN
1	J	494	ASP
1	J	495	GLU
1	J	503	ILE
1	J	505	ASP
1	K	52	MET
1	K	59	ARG
1	K	66	LEU
1	K	87	LYS
1	K	94	ILE
1	K	95	LEU
1	K	96	GLU
1	K	97	VAL
1	K	103	LEU
1	K	111	LEU
1	K	115	ILE
1	K	121	LEU
1	K	123	HIS
1	K	124	ASP
1	K	137	ILE
1	K	147	GLN
1	K	164	ARG
1	K	166	LEU
1	K	172	GLN
1	K	178	LEU
1	K	180	ILE
1	K	187	ARG
1	K	200	GLN
1	K	201	LYS
1	K	209	VAL
1	K	223	VAL
1	K	227	THR
1	K	236	TYR
1	K	252	ARG
1	K	266	GLN
1	K	276	LEU
1	K	277	LEU
1	K	305	ASN
1	K	308	TYR
1	K	327	LEU
1	K	350	ASP

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Mol	Chain	Res	Type
1	K	357	THR
1	K	365	ARG
1	K	383	THR
1	K	387	LYS
1	K	390	SER
1	K	397	LEU
1	K	401	ARG
1	K	402	GLU
1	K	413	LEU
1	K	414	ASP
1	K	430	LEU
1	K	439	MET
1	K	443	GLN
1	K	446	LEU
1	K	456	LEU
1	K	460	GLU
1	K	461	LEU
1	K	467	PHE
1	K	468	GLU
1	K	471	LEU
1	K	474	TYR
1	K	483	MET
1	K	485	GLU
1	K	487	ASN
1	K	492	TYR
1	K	496	ILE
1	K	497	GLU
1	K	511	GLN
2	L	9	ILE
2	L	20	ASP
2	L	27	ASP
2	L	32	GLN
2	L	35	ASN
2	L	50	ILE
2	L	63	ARG
2	L	66	LEU
2	L	73	HIS
2	L	89	ASN
2	L	91	LEU
2	L	98	LYS
2	L	101	ILE
2	L	103	GLU

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Mol	Chain	Res	Type
2	L	111	ARG
2	L	117	GLU
2	L	118	GLU
2	L	123	GLN
2	L	128	THR
2	L	157	VAL
2	L	161	GLU
2	L	164	ARG
2	L	199	ILE
2	L	229	LYS
2	L	231	ARG
2	L	241	VAL
2	L	243	ASN
2	L	257	LEU
2	L	281	ARG
2	L	283	THR
2	L	287	THR
2	L	291	THR
2	L	293	VAL
2	L	304	THR
2	L	310	THR
2	L	323	ARG
2	L	331	TYR
2	L	340	THR
2	L	344	LEU
2	L	345	ASP
2	L	347	LEU
2	L	364	LEU
2	L	373	ILE
2	L	377	LEU
2	L	388	LEU
2	L	396	ILE
2	L	398	ARG
2	L	406	VAL
2	L	408	GLU
2	L	409	VAL
2	L	438	LEU
2	L	441	GLN
2	L	445	MET
2	L	449	ILE
2	L	454	GLU
2	L	459	LEU

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Mol	Chain	Res	Type
2	M	6	VAL
2	M	15	VAL
2	M	16	GLU
2	M	24	ARG
2	M	32	GLN
2	M	38	LEU
2	M	41	GLU
2	M	46	LEU
2	M	51	VAL
2	M	56	MET
2	M	62	LEU
2	M	64	ARG
2	M	66	LEU
2	M	68	VAL
2	M	71	LEU
2	M	76	GLU
2	M	84	LEU
2	M	89	ASN
2	M	106	ARG
2	M	111	ARG
2	M	115	SER
2	M	116	TYR
2	M	117	GLU
2	M	119	LEU
2	M	121	ASN
2	M	132	VAL
2	M	144	LYS
2	M	157	VAL
2	M	161	GLU
2	M	164	ARG
2	M	174	SER
2	M	179	VAL
2	M	181	GLU
2	M	201	LYS
2	M	217	LEU
2	M	236	ASP
2	M	244	ILE
2	M	248	THR
2	M	249	LEU
2	M	268	GLN
2	M	271	LEU
2	M	293	VAL

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Mol	Chain	Res	Type
2	M	297	TYR
2	M	303	LEU
2	M	304	THR
2	M	331	TYR
2	M	337	LEU
2	M	340	THR
2	M	343	GLN
2	M	344	LEU
2	M	345	ASP
2	M	349	VAL
2	M	358	ARG
2	M	364	LEU
2	M	366	ARG
2	M	371	LYS
2	M	377	LEU
2	M	380	ASP
2	M	382	LEU
2	M	388	LEU
2	M	394	ARG
2	M	396	ILE
2	M	400	LEU
2	M	410	PHE
2	M	416	LYS
2	M	431	MET
2	M	443	PHE
2	M	449	ILE
2	M	454	GLU
2	M	457	LYS
2	N	6	VAL
2	N	14	ASP
2	N	17	PHE
2	N	22	VAL
2	N	27	ASP
2	N	29	LEU
2	N	32	GLN
2	N	36	GLU
2	N	51	VAL
2	N	63	ARG
2	N	66	LEU
2	N	86	ARG
2	N	97	MET
2	N	98	LYS

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Mol	Chain	Res	Type
2	N	100	GLU
2	N	101	ILE
2	N	103	GLU
2	N	104	GLU
2	N	116	TYR
2	N	117	GLU
2	N	121	ASN
2	N	136	MET
2	N	139	PHE
2	N	141	LYS
2	N	157	VAL
2	N	161	GLU
2	N	162	LEU
2	N	164	ARG
2	N	169	GLU
2	N	173	TYR
2	N	179	VAL
2	N	181	GLU
2	N	185	GLU
2	N	194	THR
2	N	197	ASN
2	N	201	LYS
2	N	210	ASN
2	N	224	LEU
2	N	239	LEU
2	N	260	ARG
2	N	265	VAL
2	N	268	GLN
2	N	271	LEU
2	N	283	THR
2	N	291	THR
2	N	293	VAL
2	N	296	VAL
2	N	298	VAL
2	N	319	VAL
2	N	320	VAL
2	N	324	GLN
2	N	338	ASP
2	N	344	LEU
2	N	364	LEU
2	N	366	ARG
2	N	372	ASP

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Mol	Chain	Res	Type
2	N	385	GLU
2	N	387	LYS
2	N	392	ARG
2	N	400	LEU
2	N	402	GLN
2	N	410	PHE
2	N	417	TYR
2	N	419	SER
2	N	441	GLN
2	N	450	GLU
2	N	453	VAL
2	N	457	LYS
2	N	459	LEU
3	O	4	LYS
3	O	5	GLU
3	O	9	LYS
3	O	16	THR
3	O	32	ARG
3	O	49	ARG
3	O	55	LEU
3	O	62	TYR
3	O	64	HIS
3	O	67	LEU
3	O	72	VAL
3	O	78	LEU
3	O	110	VAL
3	O	120	LYS
3	O	131	ASN
3	O	137	THR
3	O	145	LEU
3	O	173	LYS
3	O	187	LEU
3	O	190	LEU
3	O	195	ASP
3	O	199	LYS
3	O	200	HIS
3	O	206	LEU
3	O	207	TYR
3	O	208	GLU
3	O	218	LEU
3	O	232	VAL
3	O	242	ARG

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Mol	Chain	Res	Type
3	O	246	MET
3	O	255	SER
3	O	258	LYS
3	O	276	LEU
3	O	280	VAL
4	P	2	MET
4	P	41	LEU
4	P	49	MET
4	P	50	ILE
4	P	75	ASN
4	P	76	VAL
4	P	91	GLU
4	P	103	GLU
4	P	108	SER
4	P	121	LEU
4	P	129	ARG
1	Q	27	ASN
1	Q	76	MET
1	Q	87	LYS
1	Q	89	LYS
1	Q	91	THR
1	Q	93	ARG
1	Q	94	ILE
1	Q	95	LEU
1	Q	103	LEU
1	Q	107	VAL
1	Q	109	ASN
1	Q	122	ASP
1	Q	127	SER
1	Q	137	ILE
1	Q	138	GLU
1	Q	164	ARG
1	Q	166	LEU
1	Q	181	ASP
1	Q	209	VAL
1	Q	212	LEU
1	Q	218	LEU
1	Q	221	THR
1	Q	223	VAL
1	Q	236	TYR
1	Q	262	ASP
1	Q	263	LEU

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Mol	Chain	Res	Type
1	Q	277	LEU
1	Q	283	ARG
1	Q	305	ASN
1	Q	313	THR
1	Q	318	LYS
1	Q	320	LYS
1	Q	333	GLN
1	Q	337	VAL
1	Q	345	VAL
1	Q	350	ASP
1	Q	356	GLU
1	Q	358	ASN
1	Q	361	ASN
1	Q	365	ARG
1	Q	383	THR
1	Q	386	MET
1	Q	389	LEU
1	Q	412	ASP
1	Q	413	LEU
1	Q	415	ASP
1	Q	422	ASP
1	Q	444	GLN
1	Q	446	LEU
1	Q	456	LEU
1	Q	461	LEU
1	Q	463	LYS
1	Q	467	PHE
1	Q	468	GLU
1	Q	474	TYR
1	Q	475	VAL
1	Q	487	ASN
1	Q	497	GLU
1	Q	508	LYS
1	R	76	MET
1	R	94	ILE
1	R	95	LEU
1	R	96	GLU
1	R	97	VAL
1	R	104	LEU
1	R	106	ARG
1	R	107	VAL
1	R	109	ASN

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Mol	Chain	Res	Type
1	R	110	THR
1	R	121	LEU
1	R	123	HIS
1	R	138	GLU
1	R	140	GLN
1	R	142	VAL
1	R	157	ILE
1	R	161	ARG
1	R	166	LEU
1	R	188	ASP
1	R	200	GLN
1	R	221	THR
1	R	222	ILE
1	R	227	THR
1	R	234	LEU
1	R	236	TYR
1	R	237	LEU
1	R	252	ARG
1	R	259	ILE
1	R	261	ASP
1	R	262	ASP
1	R	266	GLN
1	R	274	SER
1	R	277	LEU
1	R	300	ARG
1	R	303	ARG
1	R	317	VAL
1	R	327	LEU
1	R	350	ASP
1	R	365	ARG
1	R	369	ASN
1	R	383	THR
1	R	384	LYS
1	R	397	LEU
1	R	400	TYR
1	R	401	ARG
1	R	403	LEU
1	R	419	LYS
1	R	420	GLN
1	R	426	LYS
1	R	429	GLU
1	R	434	LYS

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Mol	Chain	Res	Type
1	R	439	MET
1	R	443	GLN
1	R	444	GLN
1	R	447	VAL
1	R	453	ARG
1	R	456	LEU
1	R	458	ASP
1	R	461	LEU
1	R	468	GLU
1	R	471	LEU
1	R	472	LEU
1	R	477	ARG
1	R	482	LEU
1	R	483	MET
1	R	485	GLU
1	R	486	ILE
1	R	488	GLN
1	R	494	ASP
1	R	495	GLU
1	R	503	ILE
1	R	505	ASP
1	S	52	MET
1	S	59	ARG
1	S	66	LEU
1	S	87	LYS
1	S	94	ILE
1	S	95	LEU
1	S	96	GLU
1	S	97	VAL
1	S	103	LEU
1	S	111	LEU
1	S	115	ILE
1	S	121	LEU
1	S	123	HIS
1	S	124	ASP
1	S	136	VAL
1	S	137	ILE
1	S	147	GLN
1	S	164	ARG
1	S	166	LEU
1	S	172	GLN
1	S	178	LEU

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Mol	Chain	Res	Type
1	S	180	ILE
1	S	187	ARG
1	S	200	GLN
1	S	201	LYS
1	S	209	VAL
1	S	223	VAL
1	S	227	THR
1	S	236	TYR
1	S	252	ARG
1	S	266	GLN
1	S	276	LEU
1	S	277	LEU
1	S	305	ASN
1	S	308	TYR
1	S	327	LEU
1	S	350	ASP
1	S	357	THR
1	S	365	ARG
1	S	383	THR
1	S	387	LYS
1	S	390	SER
1	S	397	LEU
1	S	401	ARG
1	S	402	GLU
1	S	413	LEU
1	S	414	ASP
1	S	430	LEU
1	S	439	MET
1	S	443	GLN
1	S	446	LEU
1	S	456	LEU
1	S	460	GLU
1	S	461	LEU
1	S	467	PHE
1	S	468	GLU
1	S	471	LEU
1	S	474	TYR
1	S	483	MET
1	S	485	GLU
1	S	487	ASN
1	S	492	TYR
1	S	494	ASP

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Mol	Chain	Res	Type
1	S	496	ILE
1	S	497	GLU
1	S	511	GLN
2	T	9	ILE
2	T	27	ASP
2	T	32	GLN
2	T	35	ASN
2	T	50	ILE
2	T	63	ARG
2	T	66	LEU
2	T	73	HIS
2	T	89	ASN
2	T	91	LEU
2	T	98	LYS
2	T	101	ILE
2	T	103	GLU
2	T	111	ARG
2	T	117	GLU
2	T	118	GLU
2	T	123	GLN
2	T	128	THR
2	T	157	VAL
2	T	161	GLU
2	T	164	ARG
2	T	199	ILE
2	T	229	LYS
2	T	231	ARG
2	T	241	VAL
2	T	243	ASN
2	T	257	LEU
2	T	281	ARG
2	T	283	THR
2	T	287	THR
2	T	291	THR
2	T	293	VAL
2	T	304	THR
2	T	310	THR
2	T	323	ARG
2	T	331	TYR
2	T	340	THR
2	T	344	LEU
2	T	345	ASP

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Mol	Chain	Res	Type
2	T	347	LEU
2	T	364	LEU
2	T	373	ILE
2	T	377	LEU
2	T	396	ILE
2	T	398	ARG
2	T	406	VAL
2	T	408	GLU
2	T	409	VAL
2	T	438	LEU
2	T	445	MET
2	T	449	ILE
2	T	454	GLU
2	T	459	LEU
2	U	6	VAL
2	U	15	VAL
2	U	16	GLU
2	U	24	ARG
2	U	32	GLN
2	U	38	LEU
2	U	41	GLU
2	U	46	LEU
2	U	51	VAL
2	U	56	MET
2	U	62	LEU
2	U	64	ARG
2	U	66	LEU
2	U	68	VAL
2	U	71	LEU
2	U	76	GLU
2	U	84	LEU
2	U	89	ASN
2	U	106	ARG
2	U	111	ARG
2	U	115	SER
2	U	116	TYR
2	U	117	GLU
2	U	119	LEU
2	U	121	ASN
2	U	132	VAL
2	U	144	LYS
2	U	157	VAL

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Mol	Chain	Res	Type
2	U	161	GLU
2	U	164	ARG
2	U	174	SER
2	U	179	VAL
2	U	181	GLU
2	U	200	ASP
2	U	201	LYS
2	U	217	LEU
2	U	236	ASP
2	U	244	ILE
2	U	248	THR
2	U	249	LEU
2	U	268	GLN
2	U	271	LEU
2	U	293	VAL
2	U	297	TYR
2	U	303	LEU
2	U	304	THR
2	U	331	TYR
2	U	337	LEU
2	U	340	THR
2	U	343	GLN
2	U	344	LEU
2	U	345	ASP
2	U	349	VAL
2	U	355	ASP
2	U	358	ARG
2	U	364	LEU
2	U	366	ARG
2	U	371	LYS
2	U	377	LEU
2	U	380	ASP
2	U	382	LEU
2	U	388	LEU
2	U	394	ARG
2	U	396	ILE
2	U	400	LEU
2	U	410	PHE
2	U	416	LYS
2	U	431	MET
2	U	446	VAL
2	U	449	ILE

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Mol	Chain	Res	Type
2	U	454	GLU
2	U	457	LYS
2	V	6	VAL
2	V	14	ASP
2	V	17	PHE
2	V	22	VAL
2	V	27	ASP
2	V	29	LEU
2	V	32	GLN
2	V	36	GLU
2	V	51	VAL
2	V	63	ARG
2	V	66	LEU
2	V	86	ARG
2	V	97	MET
2	V	98	LYS
2	V	100	GLU
2	V	101	ILE
2	V	103	GLU
2	V	104	GLU
2	V	116	TYR
2	V	117	GLU
2	V	121	ASN
2	V	136	MET
2	V	139	PHE
2	V	141	LYS
2	V	157	VAL
2	V	161	GLU
2	V	162	LEU
2	V	164	ARG
2	V	169	GLU
2	V	173	TYR
2	V	179	VAL
2	V	181	GLU
2	V	185	GLU
2	V	194	THR
2	V	197	ASN
2	V	201	LYS
2	V	210	ASN
2	V	224	LEU
2	V	239	LEU
2	V	260	ARG

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Mol	Chain	Res	Type
2	V	265	VAL
2	V	268	GLN
2	V	271	LEU
2	V	283	THR
2	V	291	THR
2	V	293	VAL
2	V	296	VAL
2	V	298	VAL
2	V	319	VAL
2	V	320	VAL
2	V	323	ARG
2	V	324	GLN
2	V	338	ASP
2	V	344	LEU
2	V	364	LEU
2	V	366	ARG
2	V	372	ASP
2	V	385	GLU
2	V	392	ARG
2	V	402	GLN
2	V	410	PHE
2	V	417	TYR
2	V	419	SER
2	V	441	GLN
2	V	450	GLU
2	V	453	VAL
2	V	457	LYS
3	W	4	LYS
3	W	5	GLU
3	W	9	LYS
3	W	16	THR
3	W	32	ARG
3	W	49	ARG
3	W	55	LEU
3	W	62	TYR
3	W	64	HIS
3	W	67	LEU
3	W	72	VAL
3	W	78	LEU
3	W	110	VAL
3	W	120	LYS
3	W	131	ASN

Continued on next page...

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Mol	Chain	Res	Type
3	W	137	THR
3	W	145	LEU
3	W	173	LYS
3	W	187	LEU
3	W	188	LEU
3	W	190	LEU
3	W	193	SER
3	W	194	ASP
3	W	195	ASP
3	W	199	LYS
3	W	200	HIS
3	W	206	LEU
3	W	207	TYR
3	W	208	GLU
3	W	218	LEU
3	W	232	VAL
3	W	242	ARG
3	W	246	MET
3	W	255	SER
3	W	258	LYS
3	W	276	LEU
3	W	280	VAL
4	X	41	LEU
4	X	49	MET
4	X	50	ILE
4	X	75	ASN
4	X	76	VAL
4	X	91	GLU
4	X	103	GLU
4	X	108	SER
4	X	121	LEU
4	X	129	ARG
1	Y	27	ASN
1	Y	76	MET
1	Y	87	LYS
1	Y	89	LYS
1	Y	91	THR
1	Y	93	ARG
1	Y	94	ILE
1	Y	95	LEU
1	Y	103	LEU
1	Y	107	VAL

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Mol	Chain	Res	Type
1	Y	109	ASN
1	Y	122	ASP
1	Y	127	SER
1	Y	137	ILE
1	Y	164	ARG
1	Y	166	LEU
1	Y	181	ASP
1	Y	209	VAL
1	Y	212	LEU
1	Y	218	LEU
1	Y	221	THR
1	Y	223	VAL
1	Y	236	TYR
1	Y	262	ASP
1	Y	263	LEU
1	Y	277	LEU
1	Y	283	ARG
1	Y	305	ASN
1	Y	313	THR
1	Y	318	LYS
1	Y	320	LYS
1	Y	333	GLN
1	Y	337	VAL
1	Y	345	VAL
1	Y	350	ASP
1	Y	356	GLU
1	Y	358	ASN
1	Y	361	ASN
1	Y	365	ARG
1	Y	383	THR
1	Y	386	MET
1	Y	389	LEU
1	Y	412	ASP
1	Y	413	LEU
1	Y	415	ASP
1	Y	422	ASP
1	Y	444	GLN
1	Y	446	LEU
1	Y	456	LEU
1	Y	461	LEU
1	Y	463	LYS
1	Y	467	PHE

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Mol	Chain	Res	Type
1	Y	468	GLU
1	Y	474	TYR
1	Y	475	VAL
1	Y	487	ASN
1	Y	497	GLU
1	Y	508	LYS
1	Z	52	MET
1	Z	76	MET
1	Z	94	ILE
1	Z	95	LEU
1	Z	97	VAL
1	Z	104	LEU
1	Z	106	ARG
1	Z	107	VAL
1	Z	109	ASN
1	Z	110	THR
1	Z	121	LEU
1	Z	123	HIS
1	Z	138	GLU
1	Z	140	GLN
1	Z	142	VAL
1	Z	157	ILE
1	Z	161	ARG
1	Z	166	LEU
1	Z	188	ASP
1	Z	200	GLN
1	Z	221	THR
1	Z	222	ILE
1	Z	227	THR
1	Z	234	LEU
1	Z	236	TYR
1	Z	237	LEU
1	Z	252	ARG
1	Z	259	ILE
1	Z	261	ASP
1	Z	262	ASP
1	Z	266	GLN
1	Z	274	SER
1	Z	277	LEU
1	Z	300	ARG
1	Z	303	ARG
1	Z	317	VAL

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Mol	Chain	Res	Type
1	Z	327	LEU
1	Z	350	ASP
1	Z	365	ARG
1	Z	369	ASN
1	Z	383	THR
1	Z	384	LYS
1	Z	397	LEU
1	Z	400	TYR
1	Z	401	ARG
1	Z	403	LEU
1	Z	419	LYS
1	Z	420	GLN
1	Z	426	LYS
1	Z	429	GLU
1	Z	434	LYS
1	Z	439	MET
1	Z	443	GLN
1	Z	444	GLN
1	Z	447	VAL
1	Z	453	ARG
1	Z	456	LEU
1	Z	458	ASP
1	Z	461	LEU
1	Z	468	GLU
1	Z	471	LEU
1	Z	472	LEU
1	Z	477	ARG
1	Z	482	LEU
1	Z	483	MET
1	Z	485	GLU
1	Z	486	ILE
1	Z	488	GLN
1	Z	494	ASP
1	Z	495	GLU
1	Z	503	ILE
1	Z	505	ASP
1	a	52	MET
1	a	59	ARG
1	a	66	LEU
1	a	87	LYS
1	a	94	ILE
1	a	95	LEU

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Mol	Chain	Res	Type
1	a	96	GLU
1	a	97	VAL
1	a	103	LEU
1	a	111	LEU
1	a	115	ILE
1	a	121	LEU
1	a	123	HIS
1	a	124	ASP
1	a	136	VAL
1	a	137	ILE
1	a	147	GLN
1	a	164	ARG
1	a	166	LEU
1	a	172	GLN
1	a	178	LEU
1	a	180	ILE
1	a	187	ARG
1	a	200	GLN
1	a	201	LYS
1	a	209	VAL
1	a	223	VAL
1	a	227	THR
1	a	236	TYR
1	a	252	ARG
1	a	266	GLN
1	a	276	LEU
1	a	277	LEU
1	a	305	ASN
1	a	308	TYR
1	a	327	LEU
1	a	350	ASP
1	a	357	THR
1	a	365	ARG
1	a	383	THR
1	a	387	LYS
1	a	390	SER
1	a	397	LEU
1	a	401	ARG
1	a	402	GLU
1	a	413	LEU
1	a	414	ASP
1	a	430	LEU

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Mol	Chain	Res	Type
1	a	439	MET
1	a	443	GLN
1	a	446	LEU
1	a	456	LEU
1	a	460	GLU
1	a	461	LEU
1	a	467	PHE
1	a	468	GLU
1	a	471	LEU
1	a	474	TYR
1	a	483	MET
1	a	485	GLU
1	a	487	ASN
1	a	492	TYR
1	a	496	ILE
1	a	497	GLU
1	a	511	GLN
2	b	9	ILE
2	b	27	ASP
2	b	32	GLN
2	b	35	ASN
2	b	50	ILE
2	b	63	ARG
2	b	66	LEU
2	b	73	HIS
2	b	89	ASN
2	b	91	LEU
2	b	98	LYS
2	b	101	ILE
2	b	103	GLU
2	b	111	ARG
2	b	117	GLU
2	b	118	GLU
2	b	123	GLN
2	b	128	THR
2	b	157	VAL
2	b	161	GLU
2	b	164	ARG
2	b	199	ILE
2	b	229	LYS
2	b	231	ARG
2	b	241	VAL

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Mol	Chain	Res	Type
2	b	243	ASN
2	b	257	LEU
2	b	281	ARG
2	b	283	THR
2	b	287	THR
2	b	291	THR
2	b	293	VAL
2	b	304	THR
2	b	310	THR
2	b	323	ARG
2	b	331	TYR
2	b	340	THR
2	b	344	LEU
2	b	345	ASP
2	b	347	LEU
2	b	364	LEU
2	b	366	ARG
2	b	373	ILE
2	b	377	LEU
2	b	396	ILE
2	b	398	ARG
2	b	406	VAL
2	b	408	GLU
2	b	409	VAL
2	b	438	LEU
2	b	441	GLN
2	b	445	MET
2	b	449	ILE
2	b	454	GLU
2	b	459	LEU
2	c	6	VAL
2	c	15	VAL
2	c	16	GLU
2	c	24	ARG
2	c	32	GLN
2	c	38	LEU
2	c	41	GLU
2	c	46	LEU
2	c	51	VAL
2	c	56	MET
2	c	62	LEU
2	c	64	ARG

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Mol	Chain	Res	Type
2	c	66	LEU
2	c	68	VAL
2	c	71	LEU
2	c	76	GLU
2	c	84	LEU
2	c	89	ASN
2	c	106	ARG
2	c	111	ARG
2	c	115	SER
2	c	116	TYR
2	c	117	GLU
2	c	119	LEU
2	c	121	ASN
2	c	132	VAL
2	c	144	LYS
2	c	157	VAL
2	c	161	GLU
2	c	164	ARG
2	c	174	SER
2	c	179	VAL
2	c	181	GLU
2	c	200	ASP
2	c	201	LYS
2	c	217	LEU
2	c	236	ASP
2	c	244	ILE
2	c	248	THR
2	c	249	LEU
2	c	268	GLN
2	c	271	LEU
2	c	293	VAL
2	c	297	TYR
2	c	303	LEU
2	c	304	THR
2	c	331	TYR
2	c	337	LEU
2	c	340	THR
2	c	343	GLN
2	c	344	LEU
2	c	345	ASP
2	c	349	VAL
2	c	358	ARG

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Mol	Chain	Res	Type
2	c	364	LEU
2	c	366	ARG
2	c	371	LYS
2	c	372	ASP
2	c	377	LEU
2	c	380	ASP
2	c	382	LEU
2	c	388	LEU
2	c	394	ARG
2	c	396	ILE
2	c	400	LEU
2	c	410	PHE
2	c	416	LYS
2	c	431	MET
2	c	449	ILE
2	c	454	GLU
2	c	457	LYS
2	d	6	VAL
2	d	14	ASP
2	d	17	PHE
2	d	22	VAL
2	d	27	ASP
2	d	29	LEU
2	d	32	GLN
2	d	36	GLU
2	d	51	VAL
2	d	63	ARG
2	d	66	LEU
2	d	86	ARG
2	d	97	MET
2	d	98	LYS
2	d	100	GLU
2	d	101	ILE
2	d	103	GLU
2	d	104	GLU
2	d	116	TYR
2	d	117	GLU
2	d	121	ASN
2	d	136	MET
2	d	139	PHE
2	d	141	LYS
2	d	157	VAL

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Mol	Chain	Res	Type
2	d	161	GLU
2	d	162	LEU
2	d	164	ARG
2	d	169	GLU
2	d	173	TYR
2	d	179	VAL
2	d	181	GLU
2	d	185	GLU
2	d	194	THR
2	d	197	ASN
2	d	201	LYS
2	d	210	ASN
2	d	224	LEU
2	d	239	LEU
2	d	260	ARG
2	d	265	VAL
2	d	268	GLN
2	d	271	LEU
2	d	283	THR
2	d	291	THR
2	d	293	VAL
2	d	296	VAL
2	d	319	VAL
2	d	324	GLN
2	d	338	ASP
2	d	344	LEU
2	d	347	LEU
2	d	364	LEU
2	d	366	ARG
2	d	372	ASP
2	d	385	GLU
2	d	392	ARG
2	d	402	GLN
2	d	410	PHE
2	d	417	TYR
2	d	419	SER
2	d	441	GLN
2	d	450	GLU
2	d	453	VAL
2	d	457	LYS
3	e	4	LYS
3	e	5	GLU

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Mol	Chain	Res	Type
3	e	9	LYS
3	e	16	THR
3	e	32	ARG
3	e	49	ARG
3	e	55	LEU
3	e	62	TYR
3	e	64	HIS
3	e	67	LEU
3	e	72	VAL
3	e	78	LEU
3	e	110	VAL
3	e	120	LYS
3	e	131	ASN
3	e	137	THR
3	e	145	LEU
3	e	173	LYS
3	e	187	LEU
3	e	188	LEU
3	e	190	LEU
3	e	193	SER
3	e	195	ASP
3	e	199	LYS
3	e	200	HIS
3	e	206	LEU
3	e	207	TYR
3	e	208	GLU
3	e	218	LEU
3	e	232	VAL
3	e	242	ARG
3	e	246	MET
3	e	255	SER
3	e	258	LYS
3	e	276	LEU
3	e	280	VAL
4	f	2	MET
4	f	41	LEU
4	f	49	MET
4	f	50	ILE
4	f	75	ASN
4	f	76	VAL
4	f	91	GLU
4	f	103	GLU

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Mol	Chain	Res	Type
4	f	108	SER
4	f	121	LEU
4	f	129	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (326) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	ASN
1	A	144	GLN
1	A	172	GLN
1	A	185	ASN
1	A	186	GLN
1	A	215	HIS
1	A	266	GLN
1	A	272	GLN
1	A	344	ASN
1	A	361	ASN
1	A	382	GLN
1	B	27	ASN
1	B	140	GLN
1	B	185	ASN
1	B	186	GLN
1	B	200	GLN
1	B	215	HIS
1	B	266	GLN
1	B	272	GLN
1	B	294	HIS
1	B	344	ASN
1	B	369	ASN
1	B	420	GLN
1	B	423	HIS
1	B	443	GLN
1	B	444	GLN
1	B	511	GLN
1	C	26	HIS
1	C	144	GLN
1	C	172	GLN
1	C	186	GLN
1	C	200	GLN
1	C	272	GLN
1	C	333	GLN
1	C	344	ASN

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Mol	Chain	Res	Type
1	C	382	GLN
1	C	443	GLN
2	D	35	ASN
2	D	89	ASN
2	D	158	ASN
2	D	170	HIS
2	D	208	GLN
2	D	279	GLN
2	D	324	GLN
2	D	397	GLN
2	E	32	GLN
2	E	89	ASN
2	E	121	ASN
2	E	158	ASN
2	E	268	GLN
2	E	314	HIS
2	E	343	GLN
2	E	351	GLN
2	E	353	HIS
2	E	368	GLN
2	E	397	GLN
2	E	402	GLN
2	F	7	GLN
2	F	19	GLN
2	F	32	GLN
2	F	73	HIS
2	F	123	GLN
2	F	210	ASN
2	F	243	ASN
2	F	268	GLN
2	F	279	GLN
2	F	361	GLN
2	F	368	GLN
2	F	402	GLN
3	G	54	HIS
3	G	59	ASN
3	G	111	GLN
3	G	157	GLN
3	G	265	ASN
4	H	24	GLN
4	H	55	GLN
4	H	56	HIS

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Mol	Chain	Res	Type
4	H	75	ASN
4	H	87	GLN
4	H	116	GLN
1	I	109	ASN
1	I	144	GLN
1	I	172	GLN
1	I	185	ASN
1	I	186	GLN
1	I	215	HIS
1	I	266	GLN
1	I	272	GLN
1	I	344	ASN
1	I	361	ASN
1	I	382	GLN
1	I	435	GLN
1	J	27	ASN
1	J	140	GLN
1	J	185	ASN
1	J	186	GLN
1	J	200	GLN
1	J	215	HIS
1	J	266	GLN
1	J	272	GLN
1	J	294	HIS
1	J	344	ASN
1	J	369	ASN
1	J	420	GLN
1	J	423	HIS
1	J	443	GLN
1	J	444	GLN
1	J	511	GLN
1	K	26	HIS
1	K	144	GLN
1	K	172	GLN
1	K	186	GLN
1	K	200	GLN
1	K	333	GLN
1	K	344	ASN
1	K	382	GLN
1	K	443	GLN
1	K	493	ASN
2	L	35	ASN

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Mol	Chain	Res	Type
2	L	89	ASN
2	L	158	ASN
2	L	170	HIS
2	L	208	GLN
2	L	279	GLN
2	L	324	GLN
2	L	397	GLN
2	M	32	GLN
2	M	89	ASN
2	M	121	ASN
2	M	158	ASN
2	M	268	GLN
2	M	343	GLN
2	M	351	GLN
2	M	368	GLN
2	M	397	GLN
2	M	402	GLN
2	N	7	GLN
2	N	19	GLN
2	N	32	GLN
2	N	73	HIS
2	N	123	GLN
2	N	243	ASN
2	N	268	GLN
2	N	279	GLN
2	N	351	GLN
2	N	361	GLN
2	N	402	GLN
2	N	437	HIS
3	O	54	HIS
3	O	59	ASN
3	O	111	GLN
3	O	157	GLN
4	P	24	GLN
4	P	55	GLN
4	P	56	HIS
4	P	75	ASN
4	P	116	GLN
1	Q	109	ASN
1	Q	144	GLN
1	Q	172	GLN
1	Q	185	ASN

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Mol	Chain	Res	Type
1	Q	186	GLN
1	Q	215	HIS
1	Q	266	GLN
1	Q	272	GLN
1	Q	344	ASN
1	Q	361	ASN
1	Q	382	GLN
1	R	27	ASN
1	R	140	GLN
1	R	185	ASN
1	R	186	GLN
1	R	200	GLN
1	R	215	HIS
1	R	266	GLN
1	R	272	GLN
1	R	294	HIS
1	R	344	ASN
1	R	369	ASN
1	R	420	GLN
1	R	423	HIS
1	R	443	GLN
1	R	444	GLN
1	R	511	GLN
1	S	26	HIS
1	S	144	GLN
1	S	172	GLN
1	S	186	GLN
1	S	200	GLN
1	S	272	GLN
1	S	333	GLN
1	S	344	ASN
1	S	443	GLN
1	S	493	ASN
2	T	35	ASN
2	T	89	ASN
2	T	158	ASN
2	T	170	HIS
2	T	208	GLN
2	T	279	GLN
2	T	324	GLN
2	T	397	GLN
2	U	32	GLN

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Mol	Chain	Res	Type
2	U	89	ASN
2	U	121	ASN
2	U	158	ASN
2	U	268	GLN
2	U	343	GLN
2	U	351	GLN
2	U	353	HIS
2	U	361	GLN
2	U	368	GLN
2	U	397	GLN
2	U	402	GLN
2	V	7	GLN
2	V	19	GLN
2	V	32	GLN
2	V	73	HIS
2	V	123	GLN
2	V	243	ASN
2	V	268	GLN
2	V	279	GLN
2	V	353	HIS
2	V	361	GLN
2	V	368	GLN
2	V	402	GLN
3	W	54	HIS
3	W	59	ASN
3	W	111	GLN
3	W	126	ASN
3	W	131	ASN
3	W	135	GLN
3	W	157	GLN
3	W	265	ASN
4	X	24	GLN
4	X	55	GLN
4	X	56	HIS
4	X	87	GLN
4	X	116	GLN
1	Y	109	ASN
1	Y	144	GLN
1	Y	172	GLN
1	Y	185	ASN
1	Y	186	GLN
1	Y	215	HIS

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Mol	Chain	Res	Type
1	Y	266	GLN
1	Y	272	GLN
1	Y	344	ASN
1	Y	361	ASN
1	Y	382	GLN
1	Y	435	GLN
1	Z	27	ASN
1	Z	140	GLN
1	Z	185	ASN
1	Z	186	GLN
1	Z	200	GLN
1	Z	215	HIS
1	Z	266	GLN
1	Z	272	GLN
1	Z	294	HIS
1	Z	344	ASN
1	Z	369	ASN
1	Z	420	GLN
1	Z	423	HIS
1	Z	443	GLN
1	Z	444	GLN
1	Z	511	GLN
1	a	26	HIS
1	a	144	GLN
1	a	172	GLN
1	a	186	GLN
1	a	200	GLN
1	a	272	GLN
1	a	333	GLN
1	a	344	ASN
1	a	382	GLN
1	a	443	GLN
1	a	493	ASN
2	b	35	ASN
2	b	89	ASN
2	b	158	ASN
2	b	170	HIS
2	b	208	GLN
2	b	279	GLN
2	b	324	GLN
2	b	397	GLN
2	c	32	GLN

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Mol	Chain	Res	Type
2	c	45	GLN
2	c	89	ASN
2	c	121	ASN
2	c	158	ASN
2	c	187	ASN
2	c	191	HIS
2	c	268	GLN
2	c	343	GLN
2	c	351	GLN
2	c	368	GLN
2	c	397	GLN
2	c	402	GLN
2	d	7	GLN
2	d	19	GLN
2	d	32	GLN
2	d	73	HIS
2	d	123	GLN
2	d	243	ASN
2	d	268	GLN
2	d	279	GLN
2	d	353	HIS
2	d	361	GLN
2	d	368	GLN
2	d	402	GLN
2	d	437	HIS
3	e	54	HIS
3	e	59	ASN
3	e	111	GLN
3	e	126	ASN
3	e	131	ASN
3	e	135	GLN
3	e	157	GLN
3	e	186	GLN
4	f	24	GLN
4	f	55	GLN
4	f	56	HIS
4	f	75	ASN
4	f	87	GLN
4	f	116	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 49 ligands modelled in this entry, 16 are monoatomic - leaving 33 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	$\# Z > 2$
5	ANP	I	600	6	29,33,33	2.87	10 (34%)	31,52,52	2.92	9 (29%)
8	SO4	b	630	6	4,4,4	0.15	0	6,6,6	0.07	0
8	SO4	V	530	-	4,4,4	0.13	0	6,6,6	0.11	0
8	SO4	c	530	-	4,4,4	0.12	0	6,6,6	0.08	0
8	SO4	D	630	6	4,4,4	0.14	0	6,6,6	0.10	0
5	ANP	a	600	6	29,33,33	2.89	10 (34%)	31,52,52	2.89	8 (25%)
8	SO4	U	530	-	4,4,4	0.13	0	6,6,6	0.06	0
5	ANP	K	600	6	29,33,33	2.87	10 (34%)	31,52,52	2.94	9 (29%)
5	ANP	Q	600	6	29,33,33	2.87	10 (34%)	31,52,52	2.92	9 (29%)
5	ANP	S	600	6	29,33,33	2.88	10 (34%)	31,52,52	2.91	8 (25%)
5	ANP	Y	600	6	29,33,33	2.88	10 (34%)	31,52,52	2.92	9 (29%)
8	SO4	O	300	-	4,4,4	0.48	0	6,6,6	0.63	0
8	SO4	M	530	-	4,4,4	0.12	0	6,6,6	0.07	0
8	SO4	F	530	-	4,4,4	0.14	0	6,6,6	0.09	0
7	ADP	D	600	6	24,29,29	1.78	8 (33%)	29,45,45	1.62	6 (20%)
7	ADP	T	600	6	24,29,29	1.78	8 (33%)	29,45,45	1.61	6 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	SO4	T	630	6	4,4,4	0.13	0	6,6,6	0.11	0
8	SO4	d	530	-	4,4,4	0.13	0	6,6,6	0.10	0
5	ANP	Z	600	6	29,33,33	2.56	9 (31%)	31,52,52	3.00	11 (35%)
8	SO4	W	300	-	4,4,4	0.21	0	6,6,6	0.25	0
8	SO4	E	530	-	4,4,4	0.12	0	6,6,6	0.07	0
8	SO4	P	200	-	4,4,4	0.40	0	6,6,6	0.46	0
5	ANP	J	600	6	29,33,33	2.54	9 (31%)	31,52,52	2.97	11 (35%)
8	SO4	G	300	-	4,4,4	0.52	0	6,6,6	0.49	0
8	SO4	L	630	6	4,4,4	0.15	0	6,6,6	0.09	0
5	ANP	R	600	6	29,33,33	2.55	10 (34%)	31,52,52	2.97	11 (35%)
8	SO4	H	200	-	4,4,4	0.45	0	6,6,6	0.37	0
5	ANP	B	600	6	29,33,33	2.57	10 (34%)	31,52,52	2.96	11 (35%)
8	SO4	N	530	-	4,4,4	0.17	0	6,6,6	0.09	0
7	ADP	b	600	6	24,29,29	1.76	8 (33%)	29,45,45	1.62	6 (20%)
5	ANP	A	600	6	29,33,33	2.87	10 (34%)	31,52,52	2.92	9 (29%)
5	ANP	C	600	6	29,33,33	2.87	10 (34%)	31,52,52	2.92	9 (29%)
7	ADP	L	600	6	24,29,29	1.79	8 (33%)	29,45,45	1.62	6 (20%)

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
5	ANP	I	600	6	-	2/14/38/38	0/3/3/3
5	ANP	K	600	6	-	2/14/38/38	0/3/3/3
7	ADP	T	600	6	-	5/12/32/32	0/3/3/3
7	ADP	D	600	6	-	5/12/32/32	0/3/3/3
5	ANP	Q	600	6	-	2/14/38/38	0/3/3/3
5	ANP	S	600	6	-	2/14/38/38	0/3/3/3
5	ANP	Z	600	6	-	6/14/38/38	0/3/3/3
5	ANP	a	600	6	-	2/14/38/38	0/3/3/3
5	ANP	R	600	6	-	6/14/38/38	0/3/3/3
5	ANP	Y	600	6	-	2/14/38/38	0/3/3/3
5	ANP	J	600	6	-	6/14/38/38	0/3/3/3
5	ANP	B	600	6	-	6/14/38/38	0/3/3/3
7	ADP	b	600	6	-	5/12/32/32	0/3/3/3
5	ANP	A	600	6	-	2/14/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ANP	C	600	6	-	2/14/38/38	0/3/3/3
7	ADP	L	600	6	-	5/12/32/32	0/3/3/3

All (150) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	a	600	ANP	PB-O1B	8.71	1.60	1.46
5	S	600	ANP	PB-O1B	8.55	1.59	1.46
5	A	600	ANP	PB-O1B	8.54	1.59	1.46
5	C	600	ANP	PB-O1B	8.54	1.59	1.46
5	Y	600	ANP	PB-O1B	8.54	1.59	1.46
5	Q	600	ANP	PB-O1B	8.54	1.59	1.46
5	I	600	ANP	PB-O1B	8.53	1.59	1.46
5	K	600	ANP	PB-O1B	8.49	1.59	1.46
5	B	600	ANP	PB-O1B	7.42	1.57	1.46
5	Z	600	ANP	PB-O1B	7.32	1.57	1.46
5	R	600	ANP	PB-O1B	7.21	1.57	1.46
5	J	600	ANP	PB-O1B	7.16	1.57	1.46
5	C	600	ANP	PG-O1G	6.33	1.56	1.46
5	Y	600	ANP	PG-O1G	6.31	1.56	1.46
5	a	600	ANP	PG-O1G	6.30	1.56	1.46
5	A	600	ANP	PG-O1G	6.30	1.56	1.46
5	S	600	ANP	PG-O1G	6.28	1.56	1.46
5	Q	600	ANP	PG-O1G	6.28	1.56	1.46
5	K	600	ANP	PG-O1G	6.26	1.56	1.46
5	I	600	ANP	PG-O1G	6.23	1.56	1.46
5	Q	600	ANP	O2'-C2'	-5.14	1.30	1.43
5	K	600	ANP	O2'-C2'	-5.14	1.30	1.43
5	Y	600	ANP	O2'-C2'	-5.14	1.30	1.43
5	A	600	ANP	O2'-C2'	-5.11	1.30	1.43
5	I	600	ANP	O2'-C2'	-5.10	1.31	1.43
5	C	600	ANP	O2'-C2'	-5.08	1.31	1.43
5	S	600	ANP	O2'-C2'	-5.08	1.31	1.43
5	Z	600	ANP	PB-N3B	5.02	1.76	1.63
5	a	600	ANP	O2'-C2'	-5.00	1.31	1.43
5	J	600	ANP	PB-N3B	4.93	1.76	1.63
5	B	600	ANP	PB-N3B	4.93	1.76	1.63
5	R	600	ANP	PB-N3B	4.91	1.76	1.63
5	J	600	ANP	O2'-C2'	-4.75	1.31	1.43
5	R	600	ANP	O2'-C2'	-4.75	1.31	1.43
5	B	600	ANP	O2'-C2'	-4.75	1.31	1.43
5	S	600	ANP	PB-N3B	4.69	1.75	1.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	S	600	ANP	C5'-C4'	-4.68	1.37	1.51
5	Z	600	ANP	O2'-C2'	-4.67	1.32	1.43
5	a	600	ANP	C5'-C4'	-4.66	1.37	1.51
5	I	600	ANP	C5'-C4'	-4.61	1.37	1.51
5	K	600	ANP	PB-N3B	4.61	1.75	1.63
5	a	600	ANP	PB-N3B	4.61	1.75	1.63
5	A	600	ANP	C5'-C4'	-4.60	1.37	1.51
5	C	600	ANP	C5'-C4'	-4.60	1.37	1.51
5	Y	600	ANP	C5'-C4'	-4.60	1.37	1.51
5	Q	600	ANP	C5'-C4'	-4.60	1.37	1.51
5	K	600	ANP	C5'-C4'	-4.57	1.37	1.51
5	A	600	ANP	PB-N3B	4.54	1.75	1.63
5	Y	600	ANP	PB-N3B	4.53	1.75	1.63
5	C	600	ANP	PB-N3B	4.53	1.75	1.63
5	I	600	ANP	PB-N3B	4.53	1.75	1.63
5	R	600	ANP	PG-O1G	4.52	1.53	1.46
5	Q	600	ANP	PB-N3B	4.51	1.75	1.63
7	D	600	ADP	C6-N6	4.46	1.50	1.34
7	L	600	ADP	C6-N6	4.46	1.50	1.34
7	T	600	ADP	C6-N6	4.45	1.50	1.34
7	b	600	ADP	C6-N6	4.45	1.50	1.34
5	Z	600	ANP	PG-O1G	4.38	1.53	1.46
5	B	600	ANP	PG-O1G	4.31	1.53	1.46
5	J	600	ANP	PG-O1G	4.27	1.52	1.46
5	J	600	ANP	C5'-C4'	-4.23	1.38	1.51
5	B	600	ANP	C5'-C4'	-4.22	1.38	1.51
5	Z	600	ANP	C5'-C4'	-4.21	1.38	1.51
5	Z	600	ANP	PG-N3B	4.21	1.74	1.63
5	R	600	ANP	C5'-C4'	-4.18	1.38	1.51
5	K	600	ANP	PG-N3B	4.13	1.74	1.63
5	R	600	ANP	PG-N3B	4.10	1.74	1.63
5	S	600	ANP	PG-N3B	4.09	1.74	1.63
5	J	600	ANP	PG-N3B	4.08	1.74	1.63
5	B	600	ANP	PG-N3B	4.06	1.74	1.63
5	Q	600	ANP	PG-N3B	4.06	1.74	1.63
5	I	600	ANP	PG-N3B	4.05	1.74	1.63
5	Y	600	ANP	PG-N3B	4.05	1.73	1.63
5	A	600	ANP	PG-N3B	4.04	1.73	1.63
5	C	600	ANP	PG-N3B	4.02	1.73	1.63
5	a	600	ANP	PG-N3B	3.96	1.73	1.63
5	S	600	ANP	C6-N6	3.07	1.45	1.34
5	a	600	ANP	C6-N6	3.05	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	K	600	ANP	C6-N6	3.05	1.45	1.34
5	I	600	ANP	C6-N6	3.03	1.45	1.34
5	Q	600	ANP	C6-N6	3.03	1.45	1.34
7	D	600	ADP	C2'-C1'	-3.03	1.49	1.53
5	A	600	ANP	C6-N6	3.02	1.45	1.34
5	C	600	ANP	C6-N6	3.02	1.45	1.34
5	Y	600	ANP	C6-N6	3.01	1.45	1.34
7	T	600	ADP	C2'-C1'	-3.01	1.49	1.53
7	b	600	ADP	O2'-C2'	-3.00	1.35	1.43
7	T	600	ADP	O2'-C2'	-2.97	1.36	1.43
7	L	600	ADP	C2'-C1'	-2.96	1.49	1.53
7	L	600	ADP	O2'-C2'	-2.96	1.36	1.43
7	D	600	ADP	O2'-C2'	-2.94	1.36	1.43
7	b	600	ADP	C2'-C1'	-2.88	1.49	1.53
5	R	600	ANP	C6-N6	2.50	1.43	1.34
7	L	600	ADP	O3'-C3'	-2.48	1.37	1.43
7	T	600	ADP	O3'-C3'	-2.48	1.37	1.43
5	Z	600	ANP	C6-N6	2.48	1.43	1.34
5	J	600	ANP	C6-N6	2.45	1.43	1.34
5	B	600	ANP	C6-N6	2.44	1.42	1.34
5	C	600	ANP	C2'-C1'	-2.41	1.50	1.53
5	Q	600	ANP	C2'-C1'	-2.40	1.50	1.53
7	D	600	ADP	O3'-C3'	-2.39	1.37	1.43
5	I	600	ANP	C3'-C4'	-2.39	1.46	1.53
5	Y	600	ANP	C2'-C1'	-2.39	1.50	1.53
5	A	600	ANP	C2'-C1'	-2.38	1.50	1.53
7	D	600	ADP	C5'-C4'	-2.38	1.44	1.51
5	Y	600	ANP	C3'-C4'	-2.37	1.46	1.53
5	A	600	ANP	C3'-C4'	-2.37	1.46	1.53
7	b	600	ADP	O3'-C3'	-2.37	1.37	1.43
5	C	600	ANP	C3'-C4'	-2.36	1.46	1.53
7	L	600	ADP	C5'-C4'	-2.36	1.44	1.51
7	b	600	ADP	C5'-C4'	-2.35	1.44	1.51
5	Q	600	ANP	C3'-C4'	-2.35	1.47	1.53
5	a	600	ANP	C3'-C4'	-2.35	1.47	1.53
7	T	600	ADP	C5'-C4'	-2.35	1.44	1.51
5	K	600	ANP	C2'-C1'	-2.34	1.50	1.53
5	I	600	ANP	C2'-C1'	-2.33	1.50	1.53
5	S	600	ANP	C3'-C4'	-2.30	1.47	1.53
5	K	600	ANP	C3'-C4'	-2.30	1.47	1.53
5	K	600	ANP	O3'-C3'	-2.30	1.37	1.43
5	a	600	ANP	O3'-C3'	-2.30	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	S	600	ANP	C2'-C1'	-2.29	1.50	1.53
5	Y	600	ANP	O3'-C3'	-2.28	1.37	1.43
5	a	600	ANP	C2'-C1'	-2.28	1.50	1.53
5	A	600	ANP	O3'-C3'	-2.28	1.37	1.43
5	Q	600	ANP	O3'-C3'	-2.26	1.37	1.43
5	C	600	ANP	O3'-C3'	-2.26	1.37	1.43
5	I	600	ANP	O3'-C3'	-2.25	1.37	1.43
7	L	600	ADP	C2'-C3'	-2.25	1.47	1.53
7	T	600	ADP	C2'-C3'	-2.24	1.47	1.53
5	S	600	ANP	O3'-C3'	-2.21	1.37	1.43
7	L	600	ADP	C2-N3	2.20	1.35	1.32
7	D	600	ADP	C3'-C4'	-2.20	1.47	1.53
7	b	600	ADP	C2-N3	2.20	1.35	1.32
7	D	600	ADP	C2'-C3'	-2.19	1.47	1.53
5	B	600	ANP	C3'-C4'	-2.18	1.47	1.53
7	L	600	ADP	C3'-C4'	-2.18	1.47	1.53
5	Z	600	ANP	C3'-C4'	-2.16	1.47	1.53
7	T	600	ADP	C2-N3	2.16	1.35	1.32
5	J	600	ANP	C3'-C4'	-2.16	1.47	1.53
7	D	600	ADP	C2-N3	2.15	1.35	1.32
7	T	600	ADP	C3'-C4'	-2.15	1.47	1.53
7	b	600	ADP	C2'-C3'	-2.14	1.47	1.53
7	b	600	ADP	C3'-C4'	-2.11	1.47	1.53
5	R	600	ANP	C3'-C4'	-2.09	1.47	1.53
5	R	600	ANP	C2'-C3'	-2.07	1.47	1.53
5	B	600	ANP	C2'-C3'	-2.07	1.47	1.53
5	J	600	ANP	C2'-C3'	-2.06	1.47	1.53
5	Z	600	ANP	C2'-C3'	-2.04	1.47	1.53
5	B	600	ANP	O3'-C3'	-2.04	1.38	1.43
5	R	600	ANP	O3'-C3'	-2.01	1.38	1.43

All (138) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	600	ANP	O1B-PB-N3B	-11.49	94.85	111.77
5	C	600	ANP	O1B-PB-N3B	-11.38	95.02	111.77
5	I	600	ANP	O1B-PB-N3B	-11.37	95.03	111.77
5	A	600	ANP	O1B-PB-N3B	-11.36	95.05	111.77
5	Q	600	ANP	O1B-PB-N3B	-11.35	95.05	111.77
5	Y	600	ANP	O1B-PB-N3B	-11.35	95.05	111.77
5	S	600	ANP	O1B-PB-N3B	-11.28	95.17	111.77
5	a	600	ANP	O1B-PB-N3B	-11.27	95.18	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Z	600	ANP	O1B-PB-N3B	-11.03	95.52	111.77
5	R	600	ANP	O1B-PB-N3B	-10.79	95.88	111.77
5	J	600	ANP	O1B-PB-N3B	-10.77	95.91	111.77
5	B	600	ANP	O1B-PB-N3B	-10.71	96.00	111.77
5	Z	600	ANP	O3A-PB-N3B	-5.22	92.12	106.59
5	B	600	ANP	O3A-PB-N3B	-5.21	92.15	106.59
5	Z	600	ANP	O2B-PB-O1B	5.17	120.77	109.92
5	J	600	ANP	O3A-PB-N3B	-5.17	92.25	106.59
5	R	600	ANP	O3A-PB-N3B	-5.15	92.30	106.59
5	R	600	ANP	O2B-PB-O1B	5.12	120.66	109.92
5	J	600	ANP	O2B-PB-O1B	5.11	120.63	109.92
5	B	600	ANP	O2B-PB-O1B	5.07	120.56	109.92
5	K	600	ANP	N3-C2-N1	-5.03	120.81	128.68
5	S	600	ANP	N3-C2-N1	-4.99	120.88	128.68
5	Y	600	ANP	N3-C2-N1	-4.97	120.90	128.68
5	Q	600	ANP	N3-C2-N1	-4.97	120.91	128.68
5	I	600	ANP	N3-C2-N1	-4.96	120.93	128.68
5	A	600	ANP	N3-C2-N1	-4.96	120.93	128.68
5	C	600	ANP	N3-C2-N1	-4.95	120.94	128.68
5	a	600	ANP	N3-C2-N1	-4.94	120.96	128.68
5	I	600	ANP	O2B-PB-O3A	4.83	120.75	104.64
5	A	600	ANP	O2B-PB-O3A	4.82	120.73	104.64
5	Y	600	ANP	O2B-PB-O3A	4.82	120.72	104.64
5	C	600	ANP	O2B-PB-O3A	4.82	120.72	104.64
5	Q	600	ANP	O2B-PB-O3A	4.82	120.72	104.64
5	K	600	ANP	O2B-PB-O3A	4.79	120.62	104.64
5	S	600	ANP	O2B-PB-O3A	4.78	120.59	104.64
5	a	600	ANP	O2B-PB-O3A	4.75	120.49	104.64
5	R	600	ANP	O2B-PB-O3A	4.66	120.19	104.64
5	Z	600	ANP	O2B-PB-O3A	4.63	120.10	104.64
5	J	600	ANP	O2B-PB-O3A	4.62	120.05	104.64
5	B	600	ANP	O2B-PB-O3A	4.61	120.04	104.64
7	D	600	ADP	N3-C2-N1	-4.60	121.49	128.68
7	L	600	ADP	N3-C2-N1	-4.60	121.49	128.68
7	b	600	ADP	N3-C2-N1	-4.56	121.55	128.68
7	T	600	ADP	N3-C2-N1	-4.50	121.64	128.68
5	K	600	ANP	O3A-PB-N3B	-4.44	94.28	106.59
5	J	600	ANP	N3-C2-N1	-4.41	121.78	128.68
5	Y	600	ANP	O3A-PB-N3B	-4.41	94.36	106.59
5	A	600	ANP	O3A-PB-N3B	-4.41	94.37	106.59
5	I	600	ANP	O3A-PB-N3B	-4.40	94.38	106.59
5	Q	600	ANP	O3A-PB-N3B	-4.40	94.38	106.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	600	ANP	O3A-PB-N3B	-4.40	94.38	106.59
5	B	600	ANP	N3-C2-N1	-4.34	121.89	128.68
5	S	600	ANP	O3A-PB-N3B	-4.32	94.61	106.59
5	Z	600	ANP	N3-C2-N1	-4.30	121.96	128.68
5	R	600	ANP	N3-C2-N1	-4.28	121.99	128.68
5	a	600	ANP	O3A-PB-N3B	-4.26	94.78	106.59
5	a	600	ANP	PA-O3A-PB	-4.09	118.20	132.62
5	A	600	ANP	PA-O3A-PB	-4.08	118.26	132.62
5	Y	600	ANP	PA-O3A-PB	-4.08	118.26	132.62
5	I	600	ANP	PA-O3A-PB	-4.07	118.27	132.62
5	Q	600	ANP	PA-O3A-PB	-4.07	118.27	132.62
5	C	600	ANP	PA-O3A-PB	-4.07	118.28	132.62
5	S	600	ANP	PA-O3A-PB	-4.07	118.29	132.62
5	K	600	ANP	O2B-PB-O1B	4.02	118.35	109.92
5	K	600	ANP	PA-O3A-PB	-4.02	118.46	132.62
7	D	600	ADP	PA-O3A-PB	-3.92	119.36	132.83
5	S	600	ANP	O2B-PB-O1B	3.92	118.14	109.92
5	Y	600	ANP	O2B-PB-O1B	3.89	118.08	109.92
7	b	600	ADP	PA-O3A-PB	-3.89	119.48	132.83
5	C	600	ANP	O2B-PB-O1B	3.89	118.07	109.92
5	A	600	ANP	O2B-PB-O1B	3.88	118.05	109.92
5	B	600	ANP	PA-O3A-PB	-3.87	118.97	132.62
5	J	600	ANP	PA-O3A-PB	-3.87	119.00	132.62
5	a	600	ANP	O2B-PB-O1B	3.86	118.02	109.92
5	R	600	ANP	PA-O3A-PB	-3.86	119.01	132.62
5	Q	600	ANP	O2B-PB-O1B	3.86	118.02	109.92
7	L	600	ADP	PA-O3A-PB	-3.86	119.58	132.83
7	T	600	ADP	PA-O3A-PB	-3.86	119.59	132.83
5	I	600	ANP	O2B-PB-O1B	3.85	118.00	109.92
5	Z	600	ANP	PA-O3A-PB	-3.84	119.10	132.62
7	T	600	ADP	C3'-C2'-C1'	3.30	105.95	100.98
5	Z	600	ANP	C3'-C2'-C1'	3.30	105.95	100.98
7	L	600	ADP	C3'-C2'-C1'	3.30	105.94	100.98
5	J	600	ANP	C3'-C2'-C1'	3.25	105.86	100.98
5	B	600	ANP	C3'-C2'-C1'	3.24	105.86	100.98
7	D	600	ADP	C3'-C2'-C1'	3.24	105.86	100.98
5	R	600	ANP	C3'-C2'-C1'	3.23	105.84	100.98
7	b	600	ADP	C3'-C2'-C1'	3.20	105.79	100.98
5	Z	600	ANP	O1G-PG-N3B	-3.01	107.33	111.77
5	J	600	ANP	O1G-PG-N3B	-2.91	107.48	111.77
5	B	600	ANP	O1G-PG-N3B	-2.77	107.69	111.77
5	R	600	ANP	O1G-PG-N3B	-2.74	107.73	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	b	600	ADP	C4-C5-N7	-2.56	106.73	109.40
5	B	600	ANP	O2G-PG-O1G	-2.52	107.11	113.45
5	J	600	ANP	O2G-PG-O1G	-2.52	107.13	113.45
5	R	600	ANP	O2G-PG-O1G	-2.49	107.19	113.45
7	L	600	ADP	C4-C5-N7	-2.49	106.80	109.40
7	T	600	ADP	C4-C5-N7	-2.47	106.83	109.40
5	Z	600	ANP	O2G-PG-O1G	-2.44	107.33	113.45
7	D	600	ADP	C4-C5-N7	-2.41	106.88	109.40
5	C	600	ANP	O2G-PG-O1G	-2.38	107.48	113.45
5	S	600	ANP	O2G-PG-O1G	-2.37	107.49	113.45
5	A	600	ANP	O2G-PG-O1G	-2.37	107.51	113.45
5	I	600	ANP	O2G-PG-O1G	-2.36	107.52	113.45
5	K	600	ANP	O2G-PG-O1G	-2.36	107.52	113.45
7	T	600	ADP	O5'-C5'-C4'	2.36	117.11	108.99
7	D	600	ADP	O5'-C5'-C4'	2.36	117.10	108.99
5	Q	600	ANP	O2G-PG-O1G	-2.35	107.53	113.45
5	Y	600	ANP	O2G-PG-O1G	-2.35	107.55	113.45
5	a	600	ANP	O2G-PG-O1G	-2.34	107.57	113.45
7	b	600	ADP	O5'-C5'-C4'	2.33	117.03	108.99
7	L	600	ADP	O5'-C5'-C4'	2.31	116.95	108.99
7	L	600	ADP	O3B-PB-O3A	2.28	112.29	104.64
7	D	600	ADP	O3B-PB-O3A	2.27	112.26	104.64
7	b	600	ADP	O3B-PB-O3A	2.26	112.22	104.64
5	B	600	ANP	C2'-C3'-C4'	2.23	106.97	102.64
5	R	600	ANP	C2'-C3'-C4'	2.22	106.96	102.64
7	T	600	ADP	O3B-PB-O3A	2.22	112.07	104.64
5	R	600	ANP	O5'-C5'-C4'	2.17	116.47	108.99
5	C	600	ANP	C3'-C2'-C1'	2.15	104.22	100.98
5	Y	600	ANP	C3'-C2'-C1'	2.15	104.21	100.98
5	J	600	ANP	C2'-C3'-C4'	2.14	106.80	102.64
5	A	600	ANP	C3'-C2'-C1'	2.13	104.18	100.98
5	I	600	ANP	C3'-C2'-C1'	2.13	104.18	100.98
5	Q	600	ANP	C3'-C2'-C1'	2.13	104.18	100.98
5	S	600	ANP	C3'-C2'-C1'	2.12	104.17	100.98
5	K	600	ANP	C3'-C2'-C1'	2.12	104.16	100.98
5	J	600	ANP	O5'-C5'-C4'	2.11	116.26	108.99
5	Z	600	ANP	C2'-C3'-C4'	2.10	106.73	102.64
5	a	600	ANP	C3'-C2'-C1'	2.08	104.11	100.98
5	B	600	ANP	O5'-C5'-C4'	2.07	116.11	108.99
5	Y	600	ANP	O1G-PG-N3B	-2.05	108.75	111.77
5	K	600	ANP	O1G-PG-N3B	-2.05	108.76	111.77
5	Q	600	ANP	O1G-PG-N3B	-2.04	108.77	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	600	ANP	O1G-PG-N3B	-2.04	108.77	111.77
5	Z	600	ANP	O5'-C5'-C4'	2.04	116.00	108.99
5	A	600	ANP	O1G-PG-N3B	-2.03	108.78	111.77
5	C	600	ANP	O1G-PG-N3B	-2.02	108.79	111.77

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	I	600	ANP	PB-N3B-PG-O1G
5	I	600	ANP	PG-N3B-PB-O1B
5	S	600	ANP	PB-N3B-PG-O1G
5	S	600	ANP	PG-N3B-PB-O1B
5	a	600	ANP	PB-N3B-PG-O1G
5	a	600	ANP	PG-N3B-PB-O1B
5	K	600	ANP	PB-N3B-PG-O1G
5	K	600	ANP	PG-N3B-PB-O1B
5	Q	600	ANP	PB-N3B-PG-O1G
5	Q	600	ANP	PG-N3B-PB-O1B
5	Y	600	ANP	PB-N3B-PG-O1G
5	Y	600	ANP	PG-N3B-PB-O1B
7	T	600	ADP	C5'-O5'-PA-O3A
5	Z	600	ANP	PG-N3B-PB-O1B
5	Z	600	ANP	C5'-O5'-PA-O1A
5	Z	600	ANP	O4'-C4'-C5'-O5'
5	J	600	ANP	PG-N3B-PB-O1B
5	J	600	ANP	C5'-O5'-PA-O1A
5	J	600	ANP	O4'-C4'-C5'-O5'
5	R	600	ANP	PG-N3B-PB-O1B
5	R	600	ANP	C5'-O5'-PA-O1A
5	R	600	ANP	O4'-C4'-C5'-O5'
7	D	600	ADP	C5'-O5'-PA-O3A
5	B	600	ANP	PG-N3B-PB-O1B
5	B	600	ANP	C5'-O5'-PA-O1A
5	B	600	ANP	O4'-C4'-C5'-O5'
7	b	600	ADP	C5'-O5'-PA-O3A
5	A	600	ANP	PB-N3B-PG-O1G
5	A	600	ANP	PG-N3B-PB-O1B
5	C	600	ANP	PB-N3B-PG-O1G
5	C	600	ANP	PG-N3B-PB-O1B
7	L	600	ADP	C5'-O5'-PA-O3A
7	T	600	ADP	O4'-C4'-C5'-O5'

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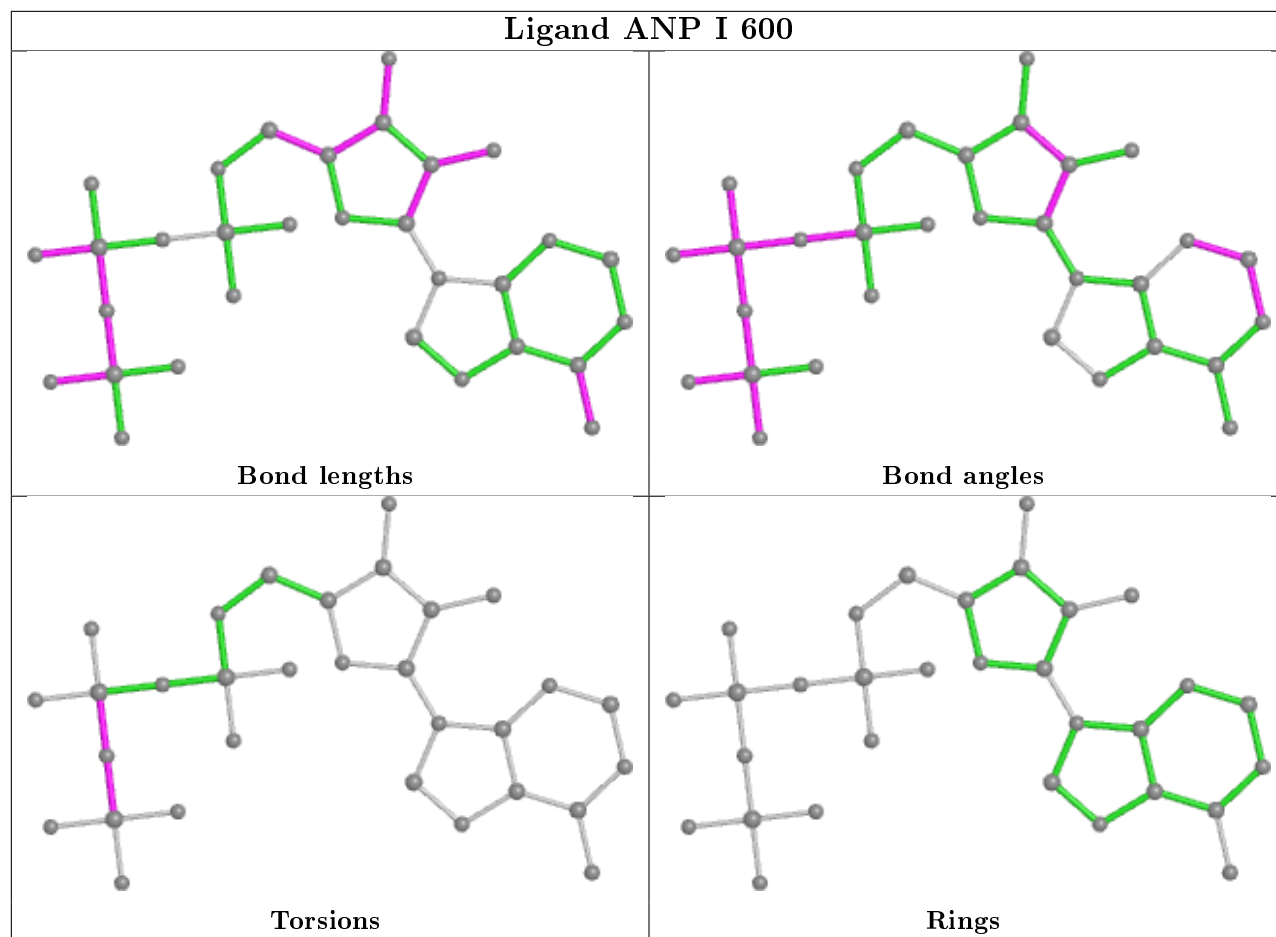
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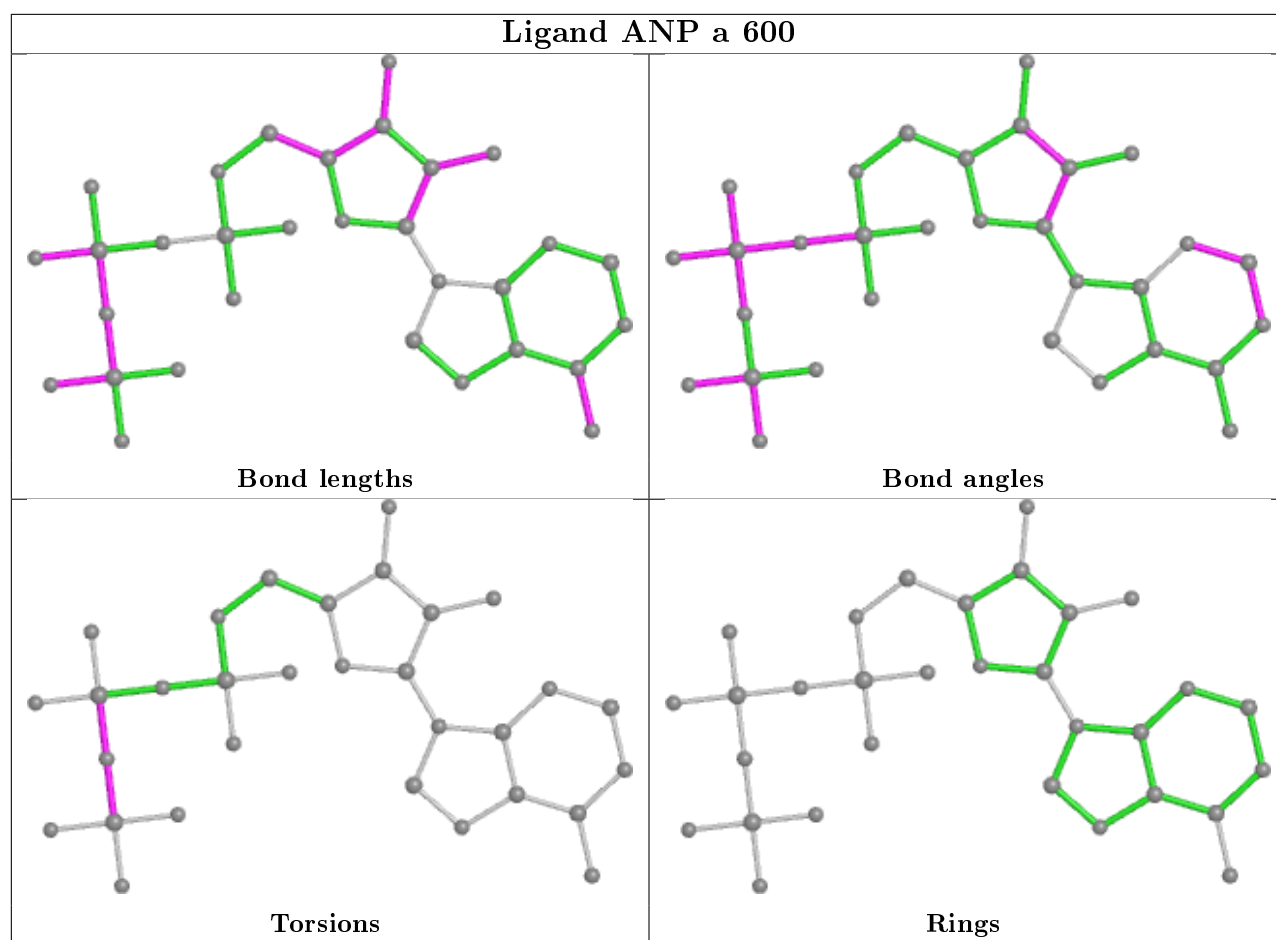
Mol	Chain	Res	Type	Atoms
5	Z	600	ANP	C3'-C4'-C5'-O5'
5	J	600	ANP	C3'-C4'-C5'-O5'
5	R	600	ANP	C3'-C4'-C5'-O5'
7	D	600	ADP	O4'-C4'-C5'-O5'
5	B	600	ANP	C3'-C4'-C5'-O5'
7	b	600	ADP	O4'-C4'-C5'-O5'
7	L	600	ADP	O4'-C4'-C5'-O5'
7	T	600	ADP	C3'-C4'-C5'-O5'
7	D	600	ADP	C3'-C4'-C5'-O5'
7	b	600	ADP	C3'-C4'-C5'-O5'
7	L	600	ADP	C3'-C4'-C5'-O5'
5	Z	600	ANP	C5'-O5'-PA-O3A
5	J	600	ANP	C5'-O5'-PA-O3A
5	R	600	ANP	C5'-O5'-PA-O3A
5	B	600	ANP	C5'-O5'-PA-O3A
7	T	600	ADP	C5'-O5'-PA-O2A
5	Z	600	ANP	C5'-O5'-PA-O2A
5	J	600	ANP	C5'-O5'-PA-O2A
5	R	600	ANP	C5'-O5'-PA-O2A
7	D	600	ADP	C5'-O5'-PA-O2A
5	B	600	ANP	C5'-O5'-PA-O2A
7	b	600	ADP	C5'-O5'-PA-O2A
7	L	600	ADP	C5'-O5'-PA-O2A
7	T	600	ADP	C5'-O5'-PA-O1A
7	D	600	ADP	C5'-O5'-PA-O1A
7	b	600	ADP	C5'-O5'-PA-O1A
7	L	600	ADP	C5'-O5'-PA-O1A

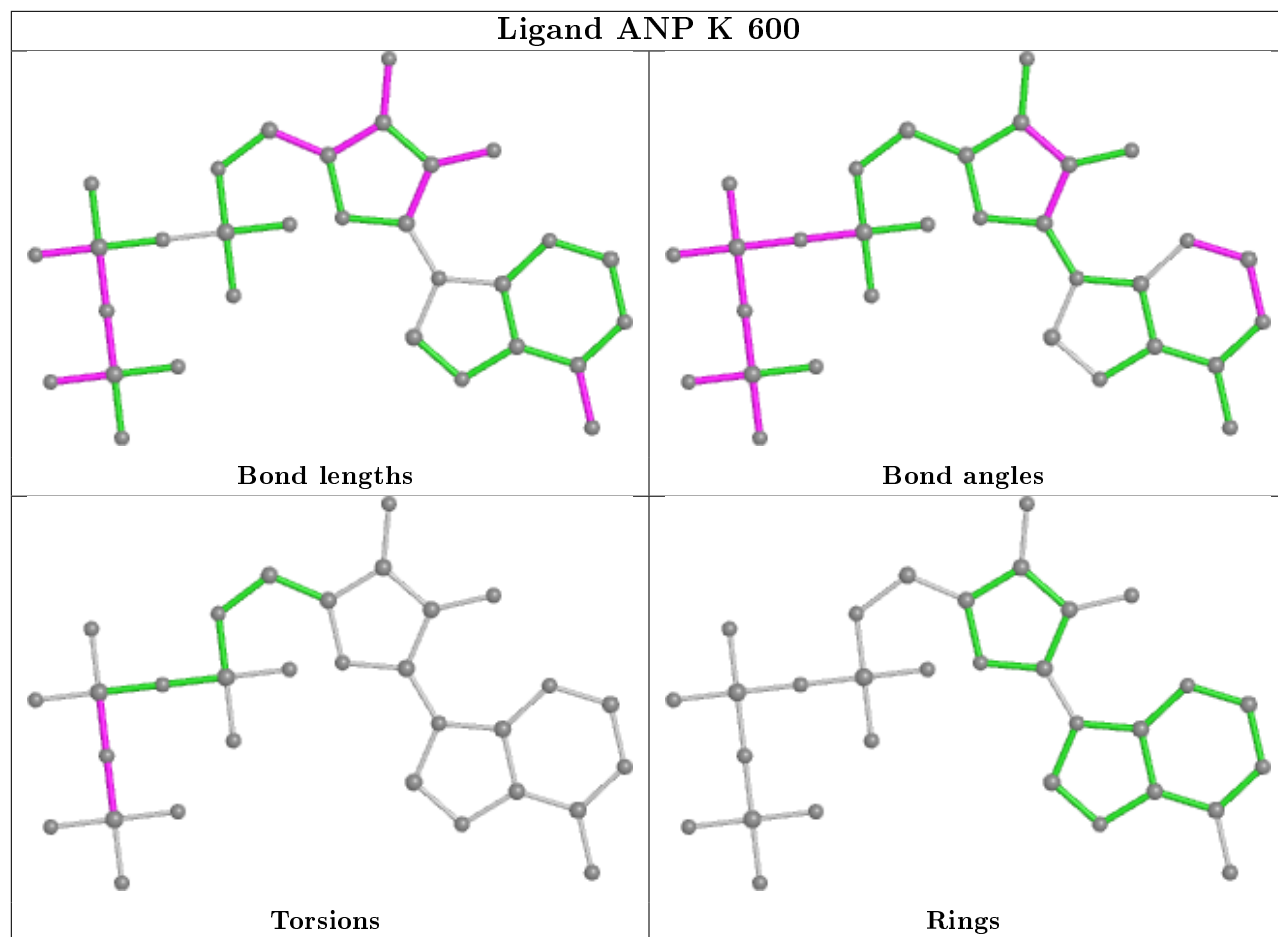
There are no ring outliers.

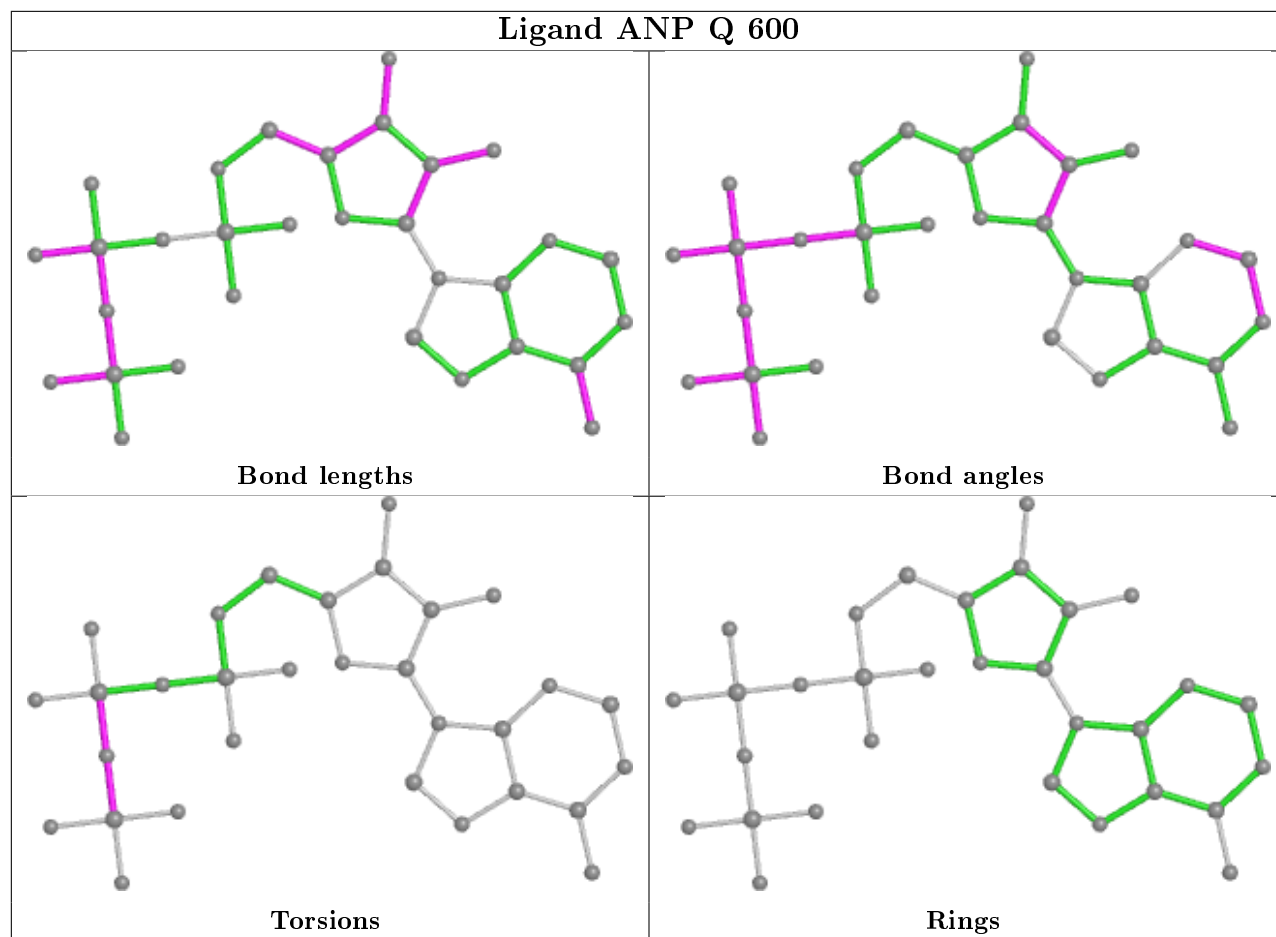
No monomer is involved in short contacts.

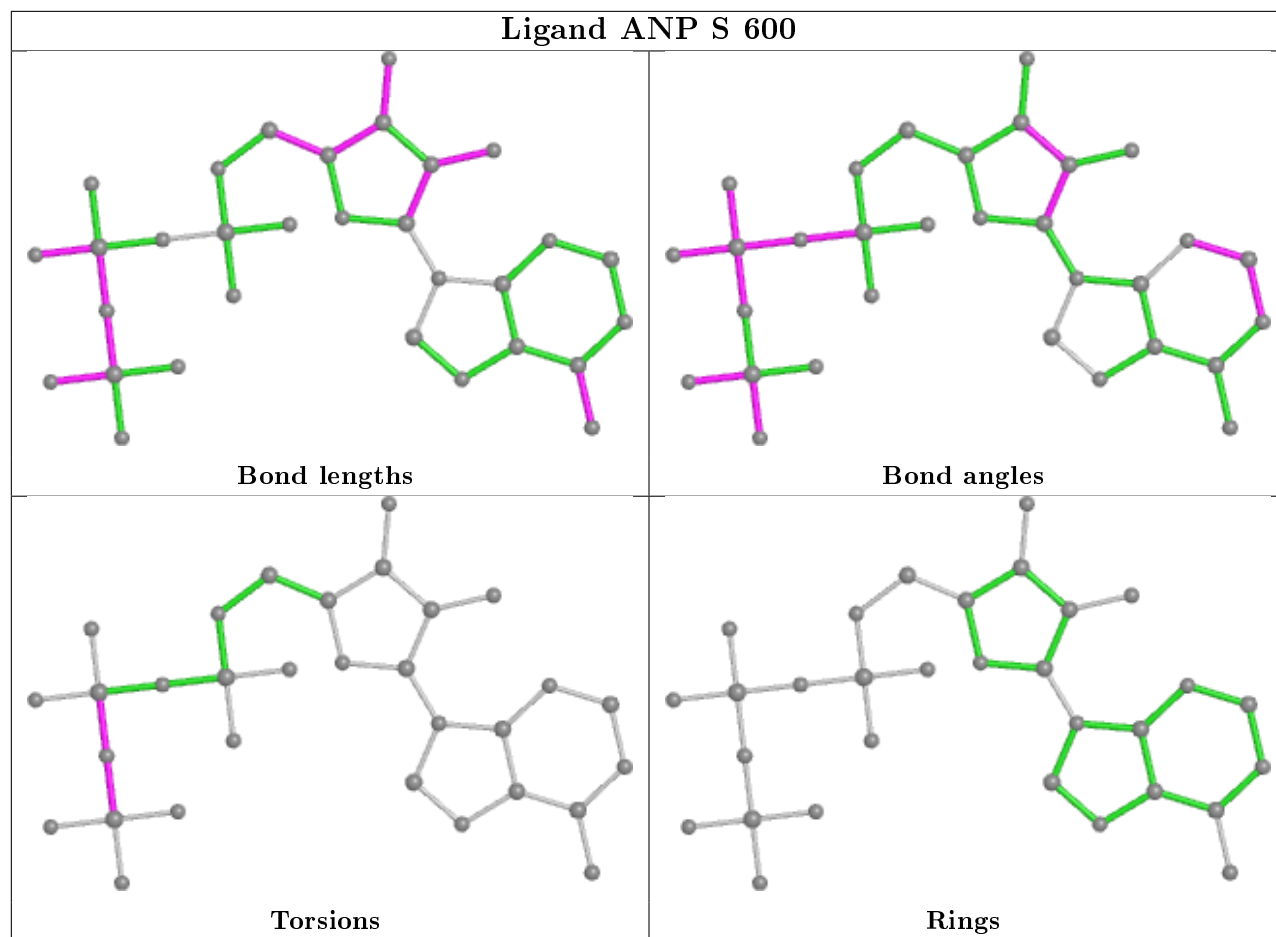
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

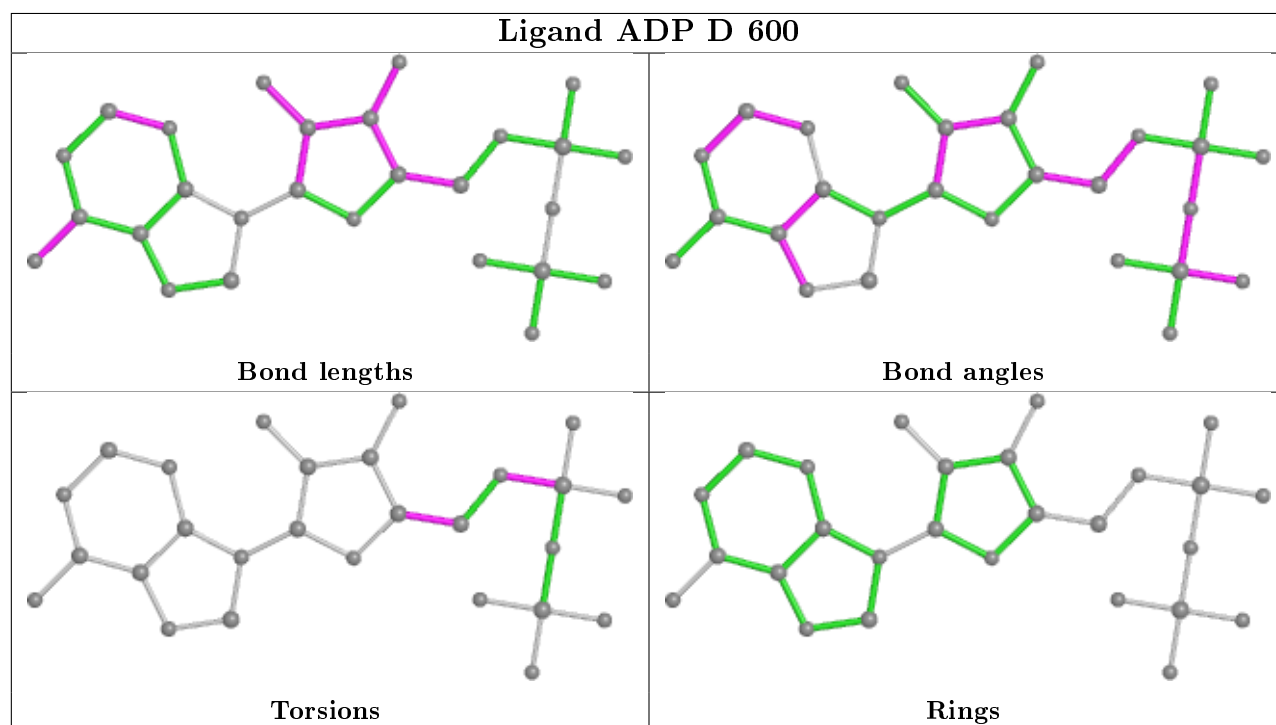
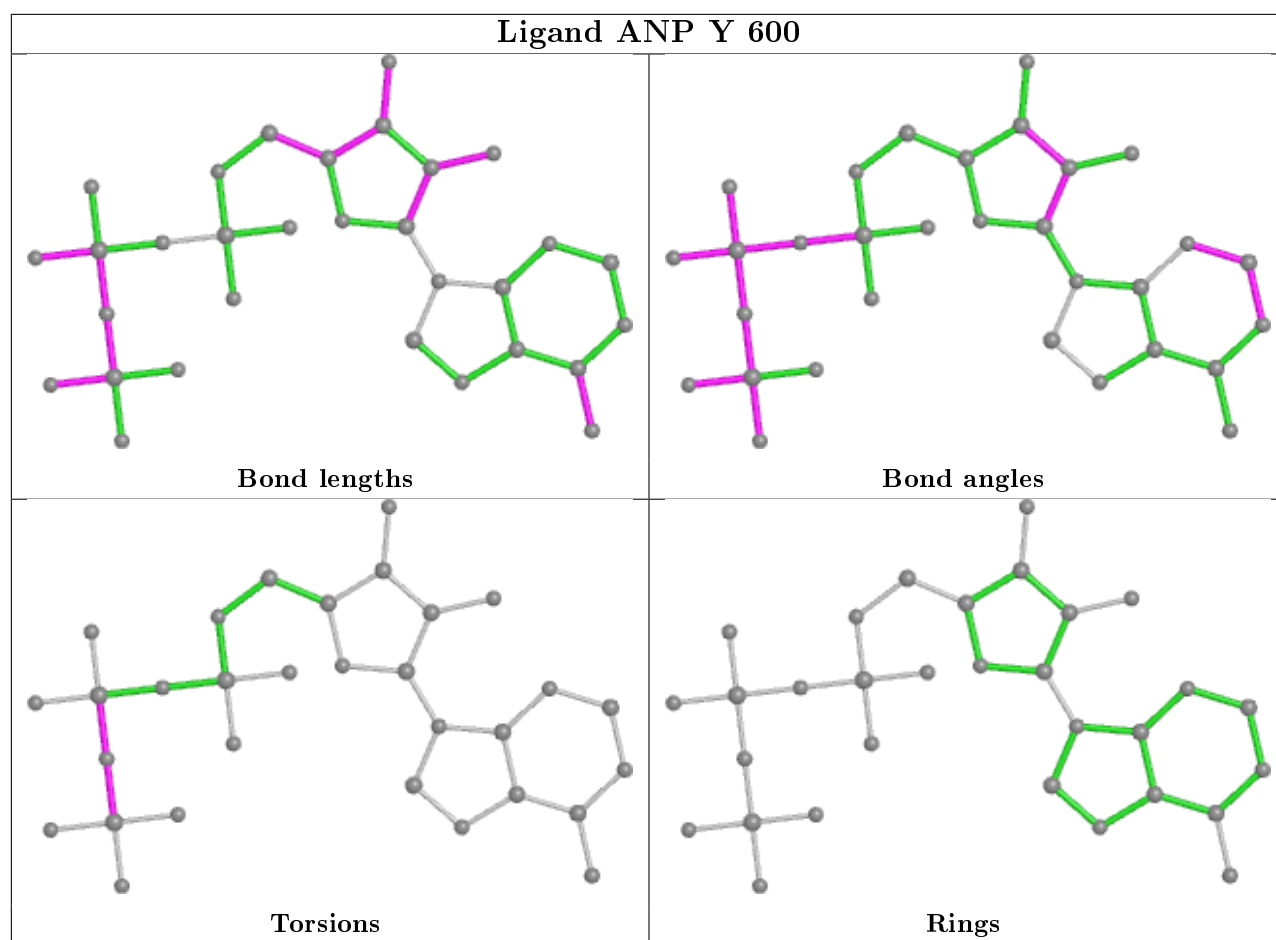


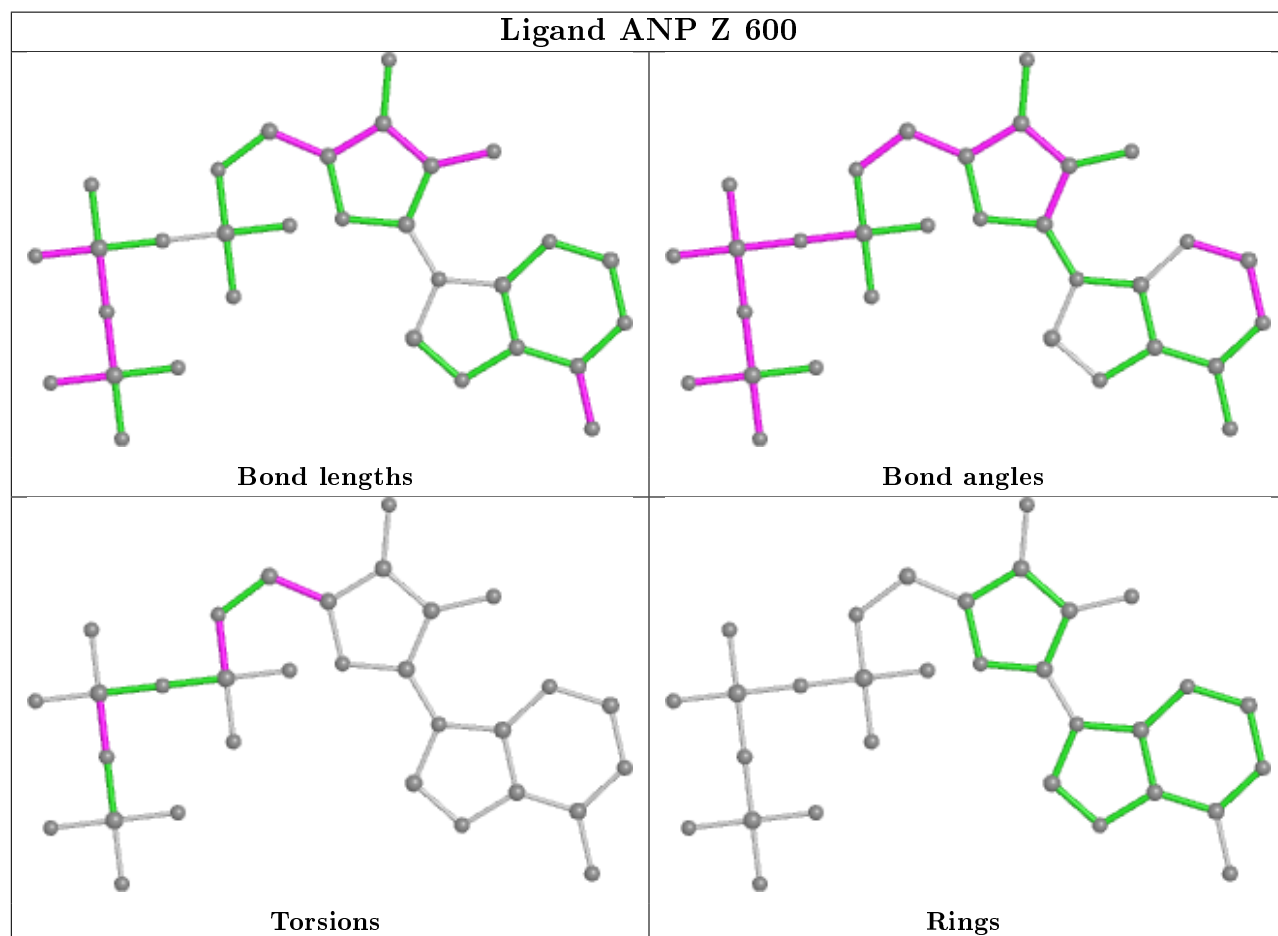
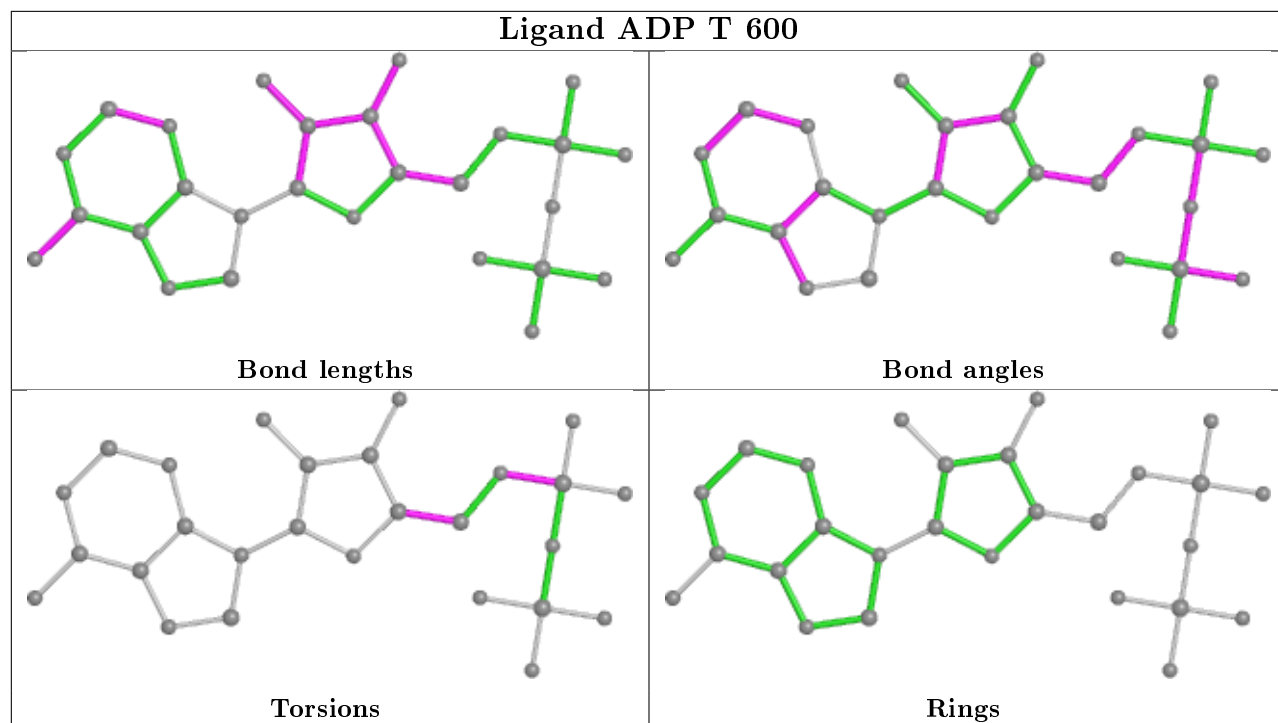




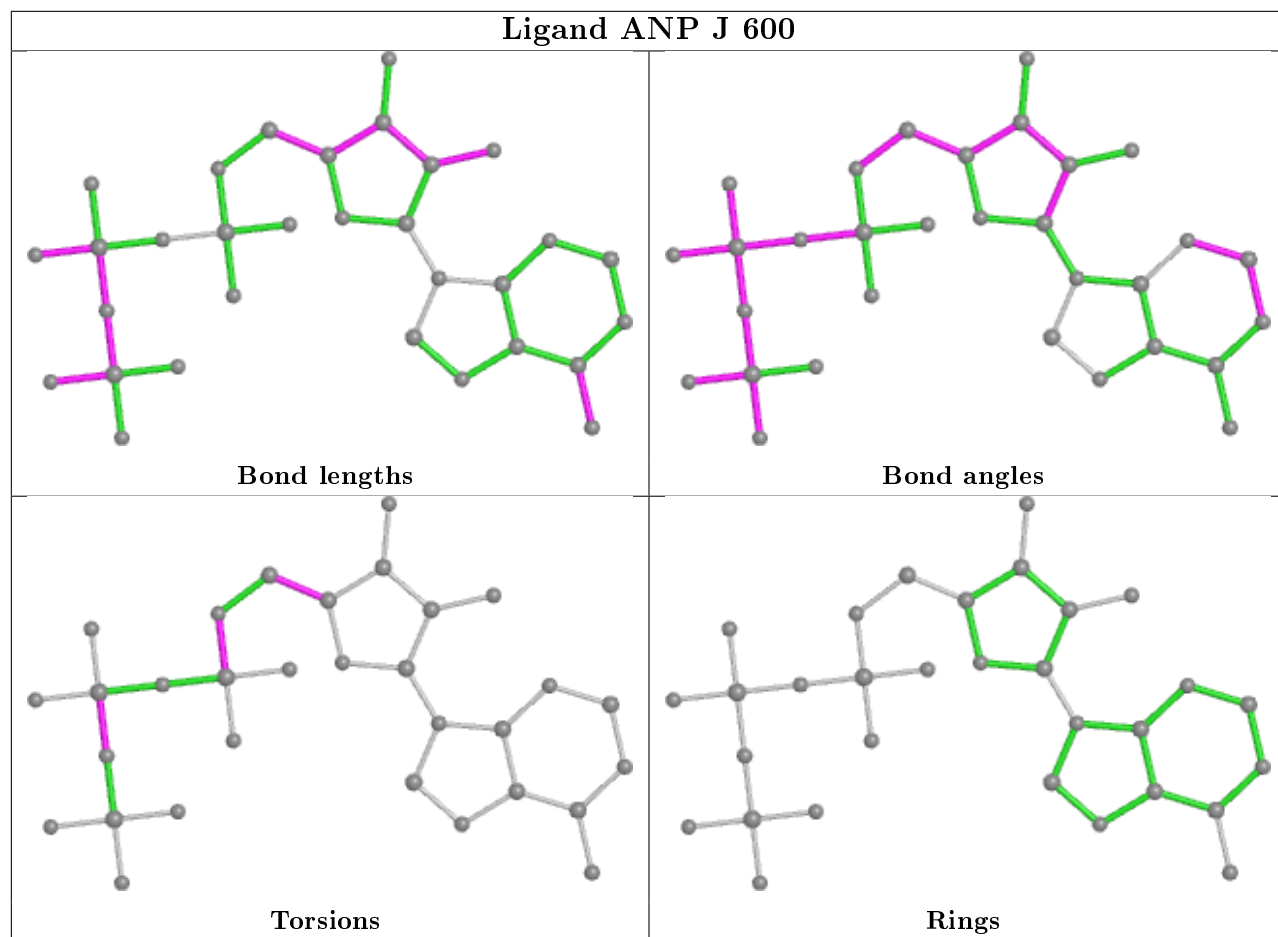


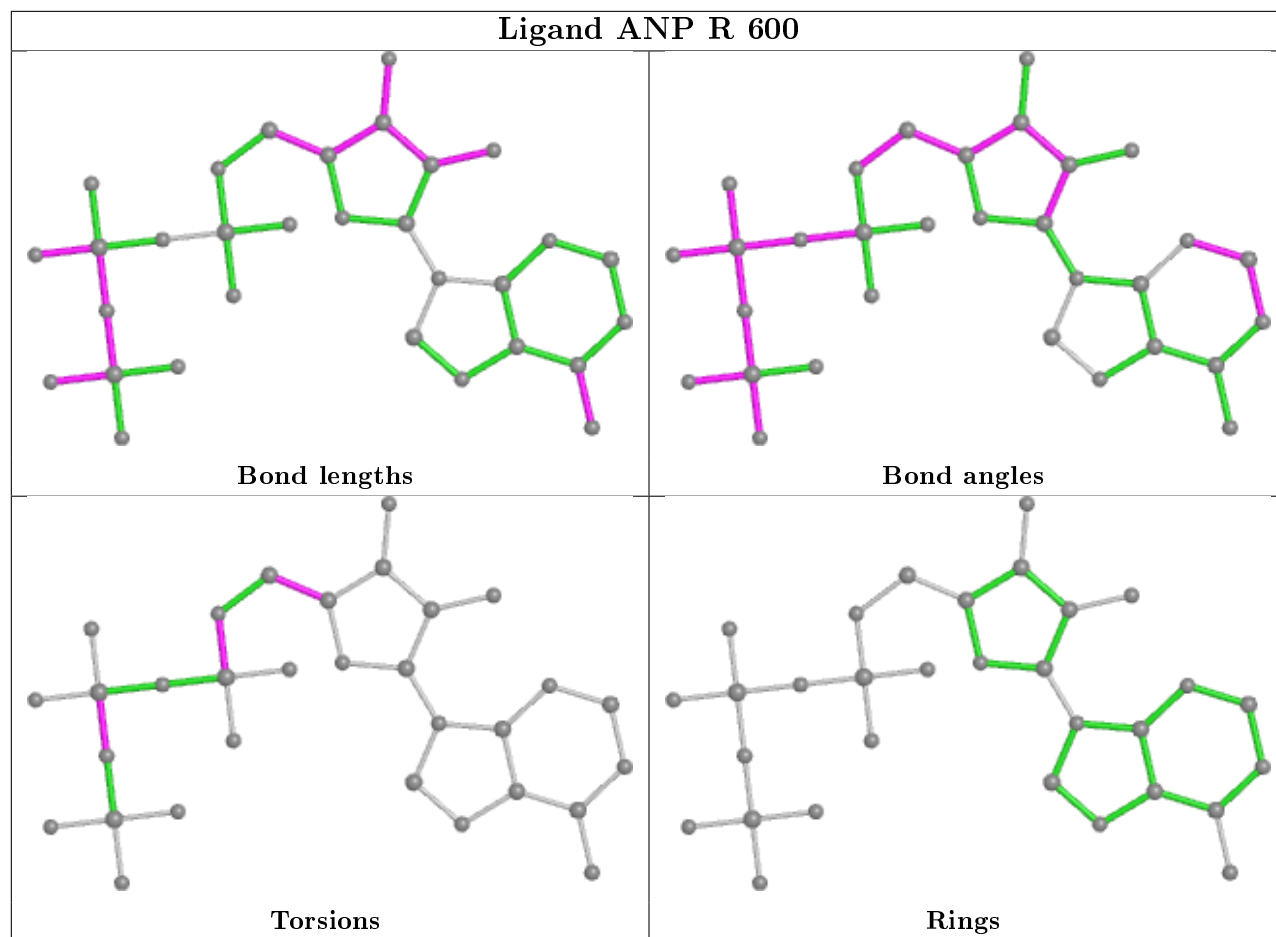


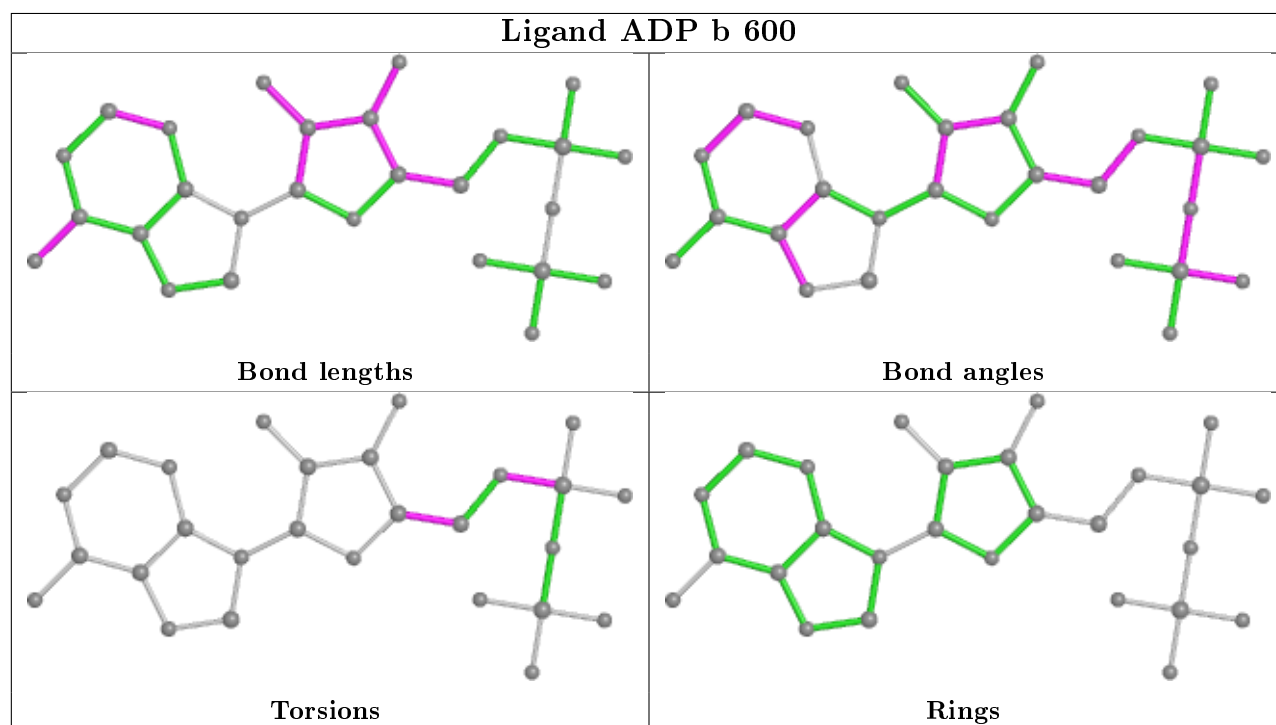
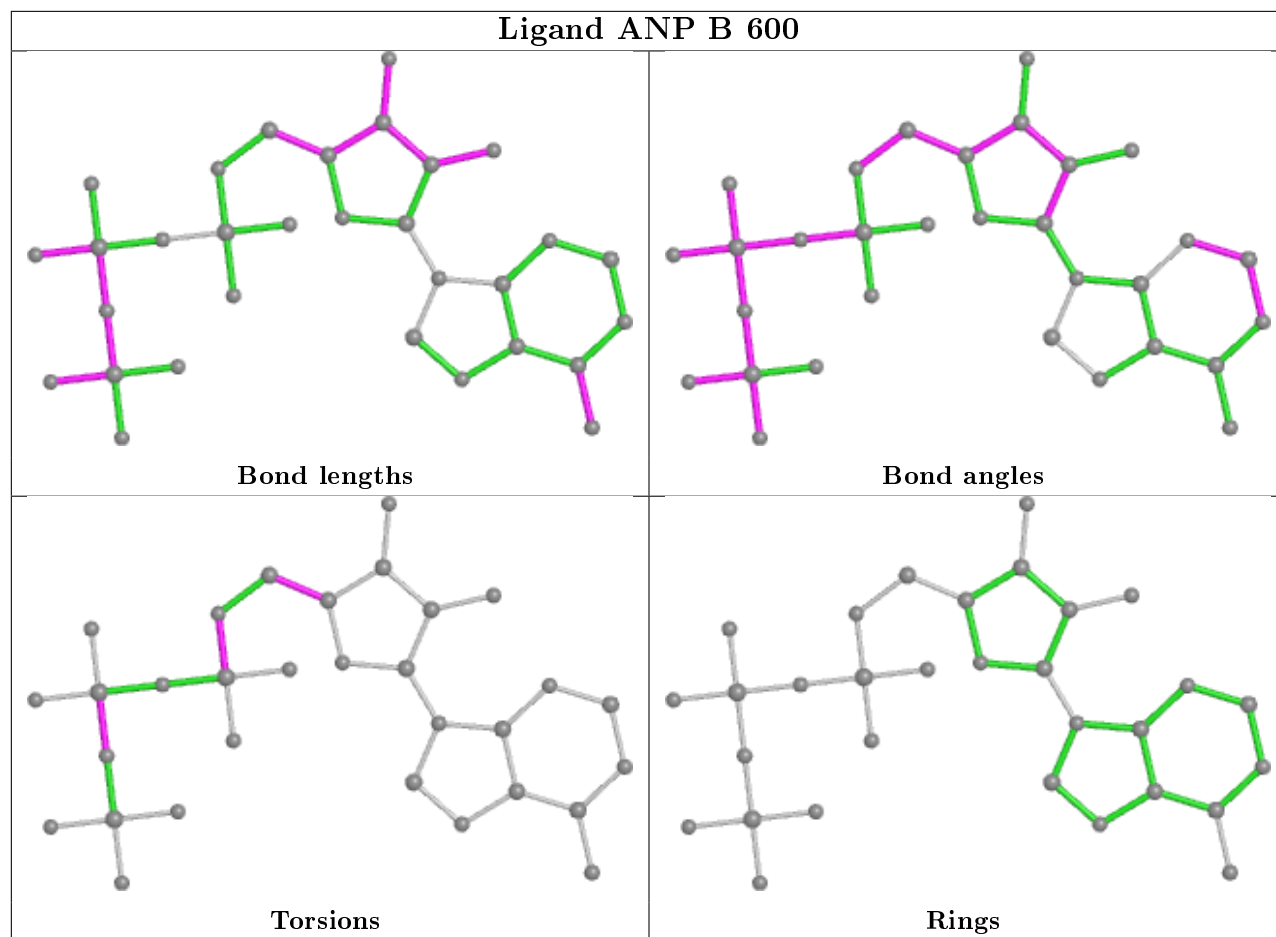


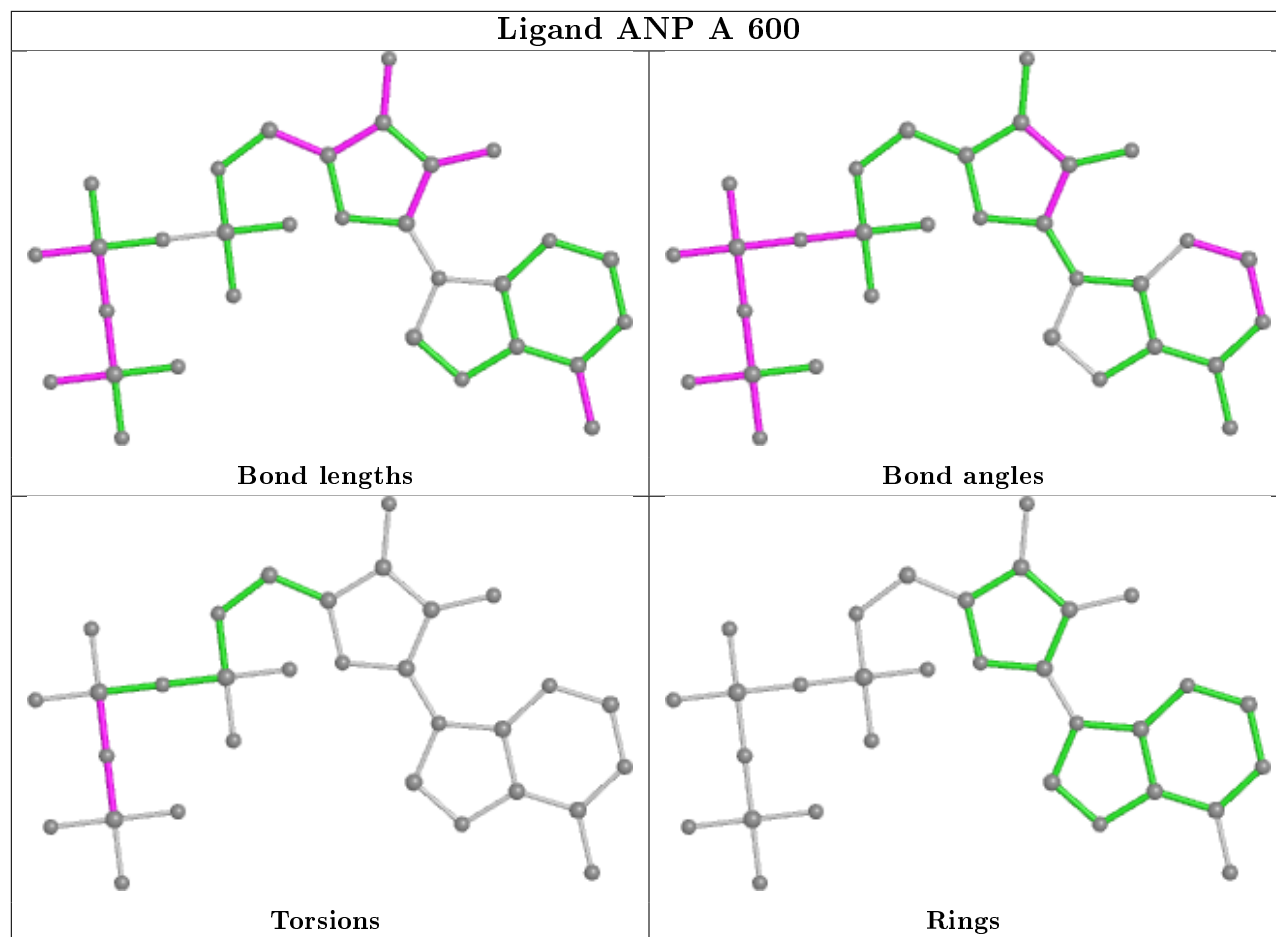


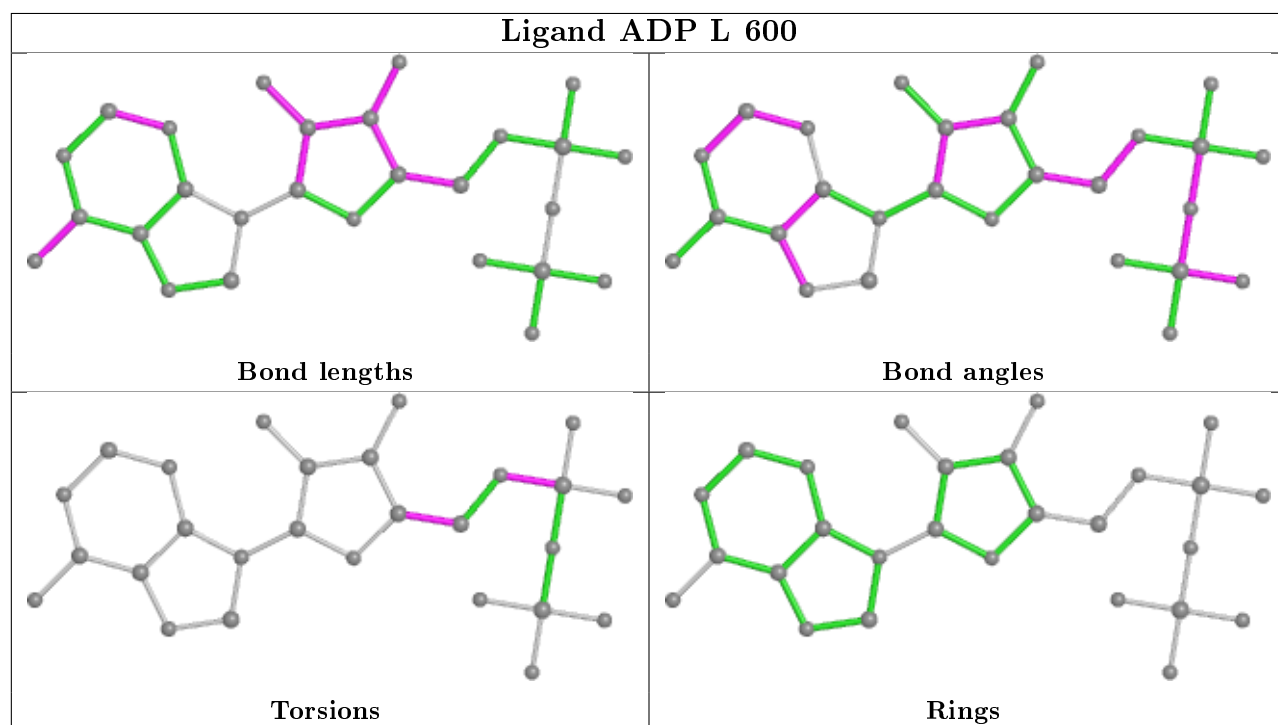
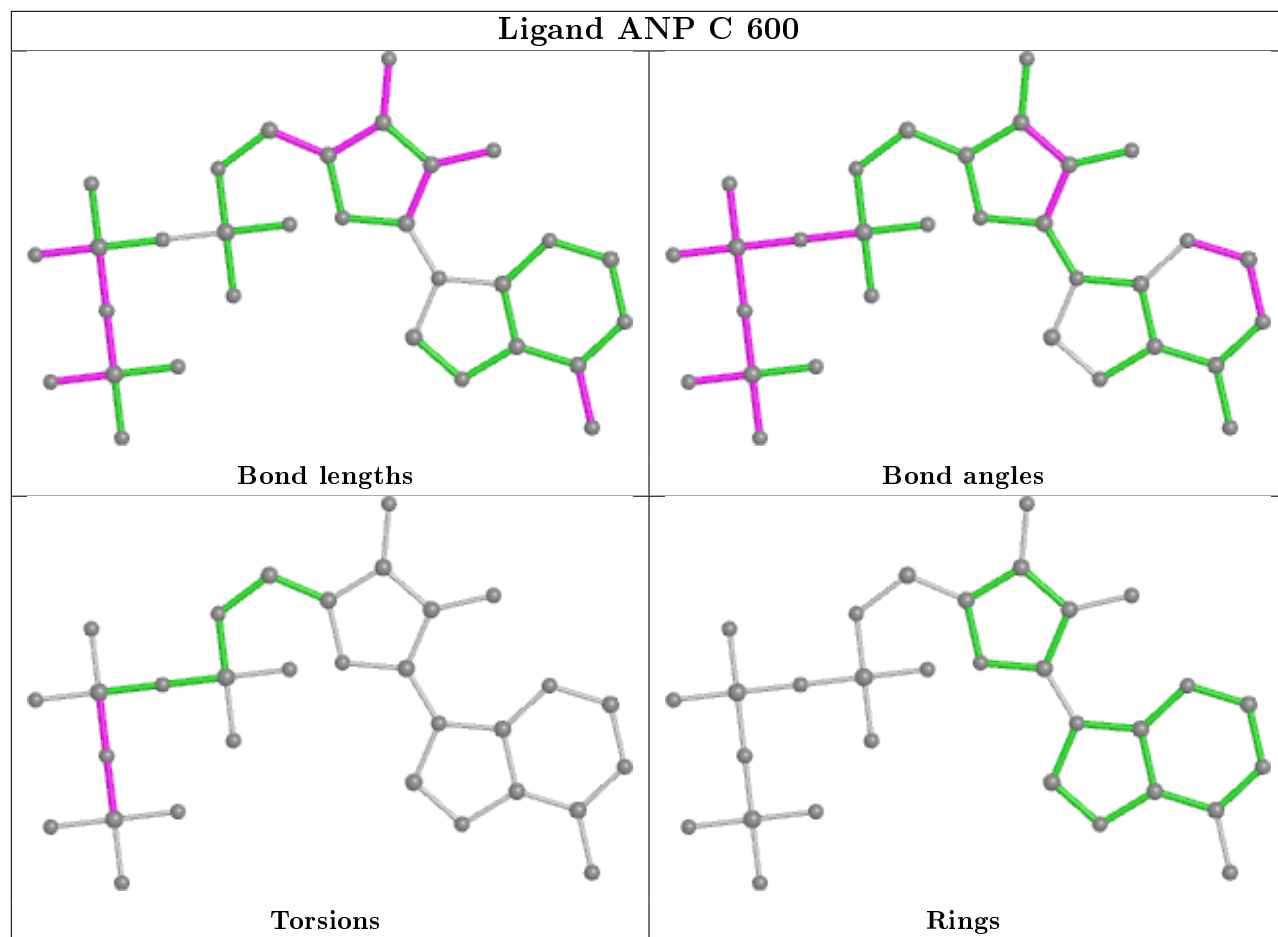
Ligand ANP J 600











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	488/513 (95%)	-0.36	0 100 100	49, 93, 144, 177	0
1	B	486/513 (94%)	-0.23	9 (1%) 66 64	55, 116, 181, 216	0
1	C	487/513 (94%)	-0.31	6 (1%) 79 77	51, 102, 151, 231	0
1	I	488/513 (95%)	-0.15	11 (2%) 60 58	66, 120, 167, 205	0
1	J	486/513 (94%)	-0.17	15 (3%) 49 47	47, 103, 183, 223	0
1	K	487/513 (94%)	-0.32	10 (2%) 63 61	46, 91, 149, 211	0
1	Q	488/513 (95%)	-0.31	9 (1%) 68 65	50, 104, 153, 214	0
1	R	486/513 (94%)	0.08	18 (3%) 41 38	66, 123, 195, 227	0
1	S	487/513 (94%)	-0.07	11 (2%) 60 58	78, 131, 180, 226	0
1	Y	488/513 (95%)	0.11	21 (4%) 35 33	79, 142, 184, 224	0
1	Z	486/513 (94%)	0.55	58 (11%) 4 4	77, 152, 215, 254	0
1	a	487/513 (94%)	0.27	32 (6%) 18 17	89, 146, 200, 249	0
2	D	458/459 (99%)	-0.46	3 (0%) 87 88	44, 92, 142, 186	0
2	E	458/459 (99%)	-0.38	3 (0%) 87 88	53, 102, 152, 184	0
2	F	458/459 (99%)	-0.43	4 (0%) 84 84	41, 103, 158, 216	0
2	L	458/459 (99%)	-0.20	10 (2%) 62 59	46, 111, 167, 217	0
2	M	458/459 (99%)	-0.23	6 (1%) 77 75	55, 114, 161, 219	0
2	N	458/459 (99%)	-0.45	5 (1%) 80 80	33, 73, 131, 186	0
2	T	458/459 (99%)	-0.14	12 (2%) 56 52	73, 124, 181, 229	0
2	U	458/459 (99%)	-0.23	5 (1%) 80 80	54, 102, 170, 232	0
2	V	458/459 (99%)	-0.03	14 (3%) 49 47	67, 124, 180, 233	0
2	b	458/459 (99%)	0.43	44 (9%) 8 8	102, 158, 204, 240	0
2	c	458/459 (99%)	-0.03	15 (3%) 46 43	68, 119, 174, 213	0
2	d	458/459 (99%)	0.29	29 (6%) 20 19	92, 151, 200, 243	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
3	G	284/286 (99%)	-0.55	4 (1%) 75 74	29, 54, 137, 200	0
3	O	284/286 (99%)	-0.47	7 (2%) 57 53	26, 57, 140, 209	0
3	W	284/286 (99%)	0.01	15 (5%) 26 24	51, 116, 192, 232	0
3	e	284/286 (99%)	0.25	25 (8%) 10 10	84, 142, 205, 230	0
4	H	138/138 (100%)	-0.42	1 (0%) 87 88	35, 72, 120, 144	0
4	P	138/138 (100%)	-0.38	1 (0%) 87 88	43, 71, 129, 156	0
4	X	138/138 (100%)	0.20	9 (6%) 18 18	77, 136, 175, 227	0
4	f	138/138 (100%)	0.48	19 (13%) 2 2	94, 151, 198, 217	0
All	All	13028/13360 (97%)	-0.12	431 (3%) 46 43	26, 116, 183, 254	0

All (431) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	a	312	PHE	7.2
1	C	312	PHE	6.8
2	b	48	GLY	6.6
1	K	313	THR	6.4
1	R	410	ALA	5.8
1	Z	407	SER	5.8
1	Z	482	LEU	5.3
1	a	113	ALA	5.3
3	e	195	ASP	5.3
1	S	312	PHE	5.3
2	d	235	ARG	5.2
3	e	57	HIS	5.2
1	K	312	PHE	5.2
2	d	459	LEU	5.0
2	b	121	ASN	5.0
1	Z	411	SER	4.9
1	Z	318	LYS	4.9
1	Z	410	ALA	4.9
2	d	101	ILE	4.9
2	b	284	SER	4.8
1	R	411	SER	4.8
2	V	21	ALA	4.8
1	Z	415	ASP	4.8
1	Z	119	GLY	4.8
1	J	408	GLN	4.7
3	W	196	ASP	4.7

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Mol	Chain	Res	Type	RSRZ
3	W	62	TYR	4.6
2	d	2	THR	4.6
1	Z	458	ASP	4.6
3	W	197	ASP	4.5
4	f	30	GLY	4.4
2	L	121	ASN	4.4
1	S	313	THR	4.4
2	U	381	GLU	4.4
2	c	36	GLU	4.4
1	R	409	PHE	4.4
1	Z	89	LYS	4.4
1	Z	315	GLY	4.4
1	Y	122	ASP	4.4
2	V	235	ARG	4.3
2	d	173	TYR	4.3
1	Z	143	ASP	4.3
3	e	200	HIS	4.3
2	T	121	ASN	4.3
2	b	34	GLY	4.2
2	d	200	ASP	4.2
4	X	102	GLU	4.2
1	a	81	ASP	4.2
2	V	101	ILE	4.2
1	Z	493	ASN	4.2
1	I	477	ARG	4.2
2	b	123	GLN	4.2
1	K	25	ALA	4.2
2	N	101	ILE	4.1
2	b	20	ASP	4.1
2	V	234	GLY	4.1
2	b	35	ASN	4.1
1	a	313	THR	4.1
1	Z	408	GLN	4.0
1	a	474	TYR	4.0
3	e	62	TYR	4.0
1	Y	477	ARG	4.0
2	T	35	ASN	4.0
3	e	69	ASP	4.0
4	f	106	SER	4.0
1	Q	474	TYR	4.0
1	J	409	PHE	4.0
1	B	493	ASN	4.0

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Mol	Chain	Res	Type	RSRZ
1	a	117	GLY	3.9
2	M	35	ASN	3.9
1	Z	126	PHE	3.8
1	C	313	THR	3.8
1	J	407	SER	3.8
1	R	494	ASP	3.8
1	Y	69	ASP	3.7
1	R	493	ASN	3.7
2	b	67	ASP	3.7
3	e	196	ASP	3.7
1	B	458	ASP	3.7
1	I	118	LYS	3.7
1	a	460	GLU	3.7
1	a	317	VAL	3.7
1	J	93	ARG	3.7
3	e	73	LYS	3.6
1	Z	125	GLY	3.6
1	R	315	GLY	3.6
1	B	46	ASP	3.6
4	f	31	GLU	3.6
2	b	197	ASN	3.6
2	b	329	GLY	3.6
2	b	232	ASP	3.6
2	M	345	ASP	3.6
3	G	62	TYR	3.6
1	Z	120	PRO	3.5
4	X	31	GLU	3.5
1	Z	511	GLN	3.5
1	Z	305	ASN	3.5
1	Z	417	THR	3.5
1	J	411	SER	3.5
2	T	102	GLY	3.5
1	Z	69	ASP	3.4
1	R	118	LYS	3.4
1	a	25	ALA	3.4
1	Z	412	ASP	3.4
3	O	62	TYR	3.4
2	V	20	ASP	3.4
2	d	94	PRO	3.4
2	b	287	THR	3.4
1	Z	478	ASP	3.4
2	D	121	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
1	a	30	THR	3.4
2	b	281	ARG	3.4
1	a	511	GLN	3.4
1	a	510	THR	3.4
1	S	452	GLU	3.3
1	B	409	PHE	3.3
2	d	93	GLU	3.3
1	Z	307	GLU	3.3
4	f	127	GLN	3.3
4	X	1	ALA	3.3
1	Z	414	ASP	3.3
2	T	36	GLU	3.3
2	d	412	GLY	3.3
3	e	131	ASN	3.2
3	e	197	ASP	3.2
2	d	127	GLU	3.2
1	a	509	ALA	3.2
2	b	65	GLY	3.2
1	J	395	THR	3.2
2	U	380	ASP	3.2
2	b	97	MET	3.2
2	M	151	ALA	3.2
4	X	87	GLN	3.2
4	f	58	HIS	3.2
2	c	384	GLU	3.2
2	c	35	ASN	3.2
2	d	102	GLY	3.2
1	R	399	GLN	3.2
1	a	213	GLU	3.2
2	b	18	PRO	3.2
1	B	408	GLN	3.2
2	V	173	TYR	3.2
2	L	106	ARG	3.1
1	S	474	TYR	3.1
1	R	458	ASP	3.1
2	T	458	LYS	3.1
2	b	119	LEU	3.1
3	O	61	GLU	3.1
1	Z	452	GLU	3.1
3	W	61	GLU	3.1
4	f	137	ALA	3.1
3	e	108	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
4	f	95	MET	3.1
4	f	91	GLU	3.1
2	b	195	ASP	3.1
3	O	284	ALA	3.1
1	Z	124	ASP	3.1
1	Y	412	ASP	3.1
2	F	234	GLY	3.1
2	d	207	GLY	3.0
1	Z	402	GLU	3.0
2	V	287	THR	3.0
4	f	86	GLY	3.0
2	L	195	ASP	3.0
1	Z	323	SER	3.0
2	U	384	GLU	3.0
2	c	379	MET	3.0
3	e	198	LEU	2.9
4	f	136	LYS	2.9
1	S	59	ARG	2.9
1	R	407	SER	2.9
1	Z	440	SER	2.9
2	V	169	GLU	2.9
1	Z	409	PHE	2.9
1	Y	434	LYS	2.9
3	e	58	GLY	2.9
2	T	459	LEU	2.9
1	J	410	ALA	2.9
1	S	25	ALA	2.9
1	I	320	LYS	2.9
1	S	42	HIS	2.9
1	Z	322	GLY	2.9
1	K	311	ALA	2.8
1	S	506	SER	2.8
1	Z	92	GLY	2.8
2	N	36	GLU	2.8
1	I	379	GLY	2.8
1	I	482	LEU	2.8
2	L	286	LYS	2.8
2	F	20	ASP	2.8
3	O	200	HIS	2.8
1	Q	510	THR	2.8
1	S	28	GLU	2.8
2	d	20	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
2	b	177	ALA	2.8
4	H	1	ALA	2.8
1	R	453	ARG	2.8
2	c	21	ALA	2.8
2	d	104	GLU	2.8
3	e	193	SER	2.8
1	Q	509	ALA	2.8
2	L	173	TYR	2.8
2	T	195	ASP	2.8
2	V	236	ASP	2.7
3	e	274	GLN	2.7
1	J	458	ASP	2.7
3	W	107	ASP	2.7
2	b	380	ASP	2.7
1	Z	419	LYS	2.7
2	L	105	GLU	2.7
2	V	35	ASN	2.7
3	W	108	LYS	2.7
1	B	415	ASP	2.7
1	a	320	LYS	2.7
1	C	317	VAL	2.7
1	Z	494	ASP	2.7
1	Z	459	VAL	2.7
3	O	199	LYS	2.7
1	a	87	LYS	2.6
2	c	69	LYS	2.6
2	M	73	HIS	2.6
1	B	407	SER	2.6
1	R	476	ASP	2.6
1	Z	422	ASP	2.6
4	f	26	THR	2.6
4	f	102	GLU	2.6
1	C	474	TYR	2.6
2	L	123	GLN	2.6
3	W	195	ASP	2.6
2	U	379	MET	2.6
1	a	96	GLU	2.6
1	Z	57	GLY	2.6
2	b	82	ALA	2.6
2	b	173	TYR	2.6
2	c	70	ASP	2.6
4	f	1	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	Y	58	ASN	2.6
2	N	197	ASN	2.6
2	E	98	LYS	2.6
1	J	494	ASP	2.6
1	J	493	ASN	2.6
1	K	317	VAL	2.6
1	Z	100	GLY	2.6
1	Z	118	LYS	2.6
2	b	385	GLU	2.6
2	b	386	ASP	2.6
2	d	63	ARG	2.6
3	W	200	HIS	2.6
1	Z	316	GLU	2.6
4	X	30	GLY	2.6
2	N	235	ARG	2.5
1	R	124	ASP	2.5
1	I	117	GLY	2.5
2	b	58	SER	2.5
1	Y	509	ALA	2.5
1	C	93	ARG	2.5
2	F	101	ILE	2.5
2	M	63	ARG	2.5
1	I	505	ASP	2.5
1	R	26	HIS	2.5
2	c	301	ASP	2.5
3	W	32	ARG	2.5
1	Z	189	SER	2.5
2	d	288	GLY	2.5
1	Q	24	GLU	2.5
2	U	35	ASN	2.5
2	d	72	GLU	2.5
1	Z	312	PHE	2.5
1	a	494	ASP	2.5
2	b	105	GLU	2.5
2	d	81	GLU	2.4
1	B	479	HIS	2.4
1	Y	54	SER	2.4
1	Z	371	GLY	2.4
1	Z	418	ARG	2.4
3	e	126	ASN	2.4
2	c	73	HIS	2.4
1	Q	477	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
3	e	61	GLU	2.4
1	B	319	GLY	2.4
1	Y	458	ASP	2.4
3	e	204	ASP	2.4
4	X	74	GLY	2.4
1	a	415	ASP	2.4
2	b	338	ASP	2.4
1	R	322	GLY	2.4
3	G	195	ASP	2.4
1	Z	404	ALA	2.4
1	I	510	THR	2.4
1	Q	320	LYS	2.4
3	W	58	GLY	2.4
1	I	415	ASP	2.4
3	W	198	LEU	2.4
1	Y	92	GLY	2.4
1	a	27	ASN	2.4
2	b	425	ARG	2.4
1	Q	511	GLN	2.4
3	W	127	SER	2.4
1	Y	68	ARG	2.4
2	D	123	GLN	2.4
1	I	96	GLU	2.4
3	W	284	ALA	2.4
2	b	37	ARG	2.4
1	Y	453	ARG	2.3
2	T	281	ARG	2.3
2	b	416	LYS	2.3
1	S	317	VAL	2.3
1	a	305	ASN	2.3
2	d	171	SER	2.3
1	Z	477	ARG	2.3
1	Y	42	HIS	2.3
1	Y	488	GLN	2.3
1	a	122	ASP	2.3
2	M	432	GLU	2.3
2	b	124	GLU	2.3
1	Z	321	THR	2.3
1	a	93	ARG	2.3
3	e	252	ASN	2.3
2	d	73	HIS	2.3
4	X	138	MET	2.3

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Mol	Chain	Res	Type	RSRZ
3	O	198	LEU	2.3
1	R	498	GLY	2.3
2	D	281	ARG	2.3
2	F	235	ARG	2.3
1	K	511	GLN	2.3
3	G	200	HIS	2.3
2	b	60	ASP	2.3
2	d	208	GLN	2.3
2	V	63	ARG	2.3
2	L	35	ASN	2.3
2	T	119	LEU	2.3
1	Z	93	ARG	2.3
2	d	286	LYS	2.3
2	L	197	ASN	2.3
1	Z	467	PHE	2.3
1	a	28	GLU	2.2
1	a	319	GLY	2.2
3	W	57	HIS	2.3
2	b	72	GLU	2.2
2	c	100	GLU	2.2
1	J	415	ASP	2.2
4	f	49	MET	2.2
1	a	302	ALA	2.2
2	b	196	SER	2.2
1	a	482	LEU	2.2
1	Z	262	ASP	2.2
3	e	107	ASP	2.2
2	c	113	ALA	2.2
2	d	34	GLY	2.2
1	J	481	PRO	2.2
1	R	93	ARG	2.2
1	Z	255	ASP	2.2
1	K	460	GLU	2.2
2	T	123	GLN	2.2
3	e	109	GLY	2.2
3	e	192	ALA	2.2
2	T	386	ASP	2.2
2	b	369	GLU	2.2
2	d	76	GLU	2.2
1	K	46	ASP	2.2
1	a	59	ARG	2.2
1	K	474	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
3	O	195	ASP	2.2
2	b	437	HIS	2.2
2	d	124	GLU	2.2
2	d	168	ILE	2.2
2	V	459	LEU	2.2
1	Z	476	ASP	2.2
1	Y	24	GLU	2.2
2	b	194	THR	2.2
3	W	63	LYS	2.2
1	J	141	SER	2.2
1	Y	188	ASP	2.2
2	N	169	GLU	2.2
2	c	345	ASP	2.2
1	Y	388	LYS	2.2
2	b	102	GLY	2.2
2	b	191	HIS	2.2
1	a	308	TYR	2.1
1	Y	425	GLN	2.1
2	d	36	GLU	2.1
2	b	286	LYS	2.1
3	e	129	GLY	2.1
1	C	58	ASN	2.1
1	Y	310	GLU	2.1
2	b	351	GLN	2.1
1	Z	405	ALA	2.1
2	E	35	ASN	2.1
1	J	399	GLN	2.1
1	Y	25	ALA	2.1
2	V	201	LYS	2.1
2	d	454	GLU	2.1
4	f	60	GLU	2.1
1	Z	460	GLU	2.1
2	L	459	LEU	2.1
4	X	86	GLY	2.1
2	T	200	ASP	2.1
1	Z	479	HIS	2.1
3	e	199	LYS	2.1
2	b	100	GLU	2.1
1	Q	415	ASP	2.1
1	I	453	ARG	2.1
2	c	22	VAL	2.1
4	X	107	SER	2.1

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Mol	Chain	Res	Type	RSRZ
2	b	108	ALA	2.1
1	Q	388	LYS	2.0
4	f	87	GLN	2.0
1	J	452	GLU	2.0
1	Z	210	ARG	2.0
4	f	59	GLU	2.0
1	S	118	LYS	2.0
3	G	199	LYS	2.0
1	Z	68	ARG	2.0
4	P	137	ALA	2.0
4	f	105	ILE	2.0
2	d	259	GLY	2.0
1	Y	215	HIS	2.0
1	a	54	SER	2.0
2	V	192	GLU	2.0
1	K	118	LYS	2.0
1	a	419	LYS	2.0
2	b	141	LYS	2.0
3	e	202	SER	2.0
2	c	98	LYS	2.0
1	Z	214	GLU	2.0
4	f	2	MET	2.0
1	a	336	ASP	2.0
2	E	410	PHE	2.0
1	R	439	MET	2.0
3	e	111	GLN	2.0
2	c	323	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 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.

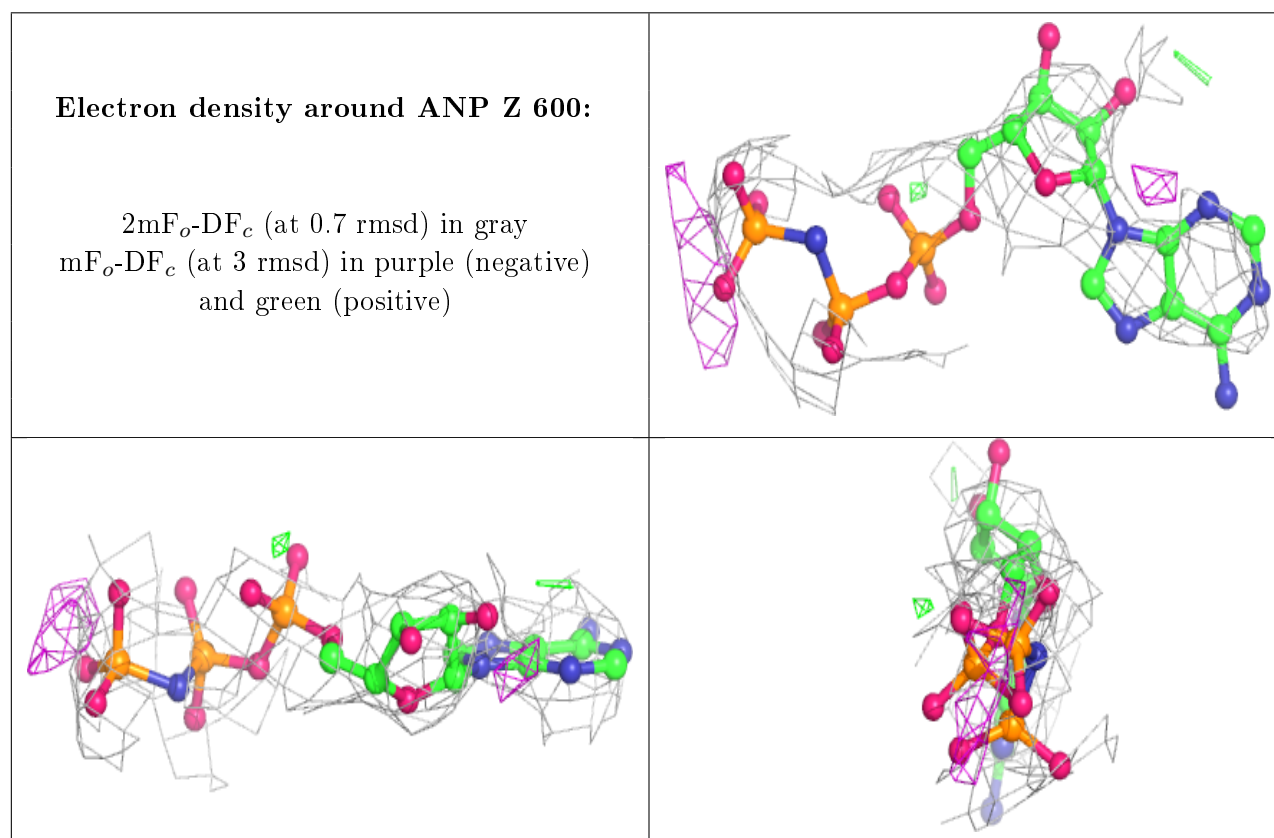
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	SO4	W	300	5/5	0.80	0.37	207,210,212,214	0
6	MG	Q	601	1/1	0.82	0.26	64,64,64,64	0
8	SO4	c	530	5/5	0.83	0.29	113,113,115,116	0
6	MG	a	601	1/1	0.83	0.18	83,83,83,83	0
8	SO4	M	530	5/5	0.85	0.28	117,118,119,119	0
6	MG	T	601	1/1	0.87	0.14	80,80,80,80	0
5	ANP	Z	600	31/31	0.88	0.24	147,151,153,154	0
5	ANP	A	600	31/31	0.88	0.21	87,93,109,129	0
6	MG	A	601	1/1	0.89	0.22	64,64,64,64	0
8	SO4	G	300	5/5	0.90	0.26	95,101,102,103	0
6	MG	Z	601	1/1	0.90	0.09	147,147,147,147	0
5	ANP	Y	600	31/31	0.90	0.23	87,93,109,129	0
5	ANP	a	600	31/31	0.91	0.20	123,126,130,136	0
7	ADP	b	600	27/27	0.91	0.18	136,139,142,143	0
5	ANP	Q	600	31/31	0.91	0.18	87,93,109,129	0
5	ANP	R	600	31/31	0.92	0.20	91,101,110,112	0
5	ANP	S	600	31/31	0.92	0.18	109,114,121,135	0
5	ANP	I	600	31/31	0.92	0.17	87,93,109,129	0
6	MG	I	601	1/1	0.92	0.16	64,64,64,64	0
6	MG	B	601	1/1	0.93	0.16	125,125,125,125	0
8	SO4	b	630	5/5	0.93	0.12	98,99,100,101	0
6	MG	Y	601	1/1	0.93	0.17	64,64,64,64	0
8	SO4	P	200	5/5	0.93	0.36	120,120,123,124	0
8	SO4	O	300	5/5	0.93	0.26	109,115,118,119	0
8	SO4	E	530	5/5	0.94	0.28	109,109,109,110	0
6	MG	S	601	1/1	0.94	0.12	60,60,60,60	0
6	MG	R	601	1/1	0.94	0.09	118,118,118,118	0
5	ANP	B	600	31/31	0.94	0.16	96,107,111,112	0
6	MG	K	601	1/1	0.94	0.09	44,44,44,44	0
8	SO4	U	530	5/5	0.94	0.23	106,106,107,107	0
5	ANP	C	600	31/31	0.94	0.16	87,93,109,129	0
7	ADP	T	600	27/27	0.95	0.12	114,118,121,123	0
6	MG	J	601	1/1	0.95	0.14	122,122,122,122	0
5	ANP	J	600	31/31	0.95	0.16	83,96,100,103	0
6	MG	C	601	1/1	0.95	0.10	64,64,64,64	0
7	ADP	L	600	27/27	0.95	0.13	77,86,95,98	0
6	MG	b	601	1/1	0.95	0.20	127,127,127,127	0
5	ANP	K	600	31/31	0.96	0.15	63,81,109,131	0
6	MG	L	601	1/1	0.96	0.07	66,66,66,66	0
8	SO4	H	200	5/5	0.96	0.23	114,115,117,119	0
7	ADP	D	600	27/27	0.96	0.12	75,81,87,90	0

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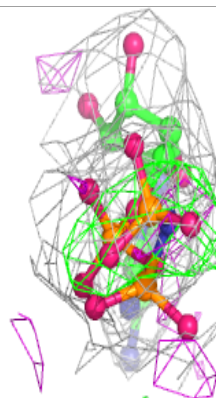
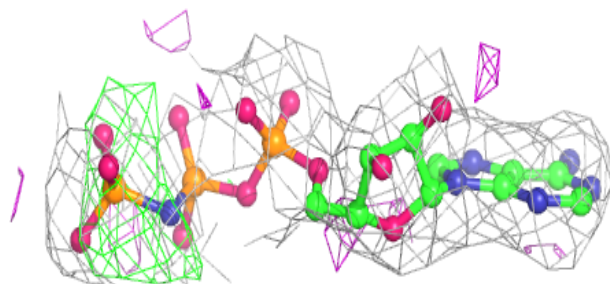
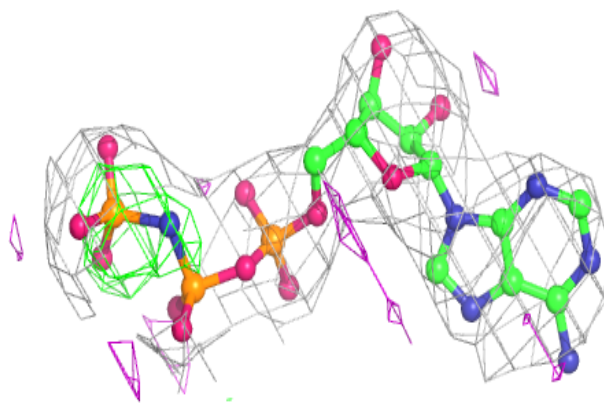
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	SO4	N	530	5/5	0.97	0.09	64,64,67,67	0
8	SO4	T	630	5/5	0.97	0.09	85,88,88,89	0
8	SO4	d	530	5/5	0.97	0.18	107,108,108,109	0
8	SO4	V	530	5/5	0.98	0.08	82,83,85,87	0
8	SO4	F	530	5/5	0.98	0.10	79,81,82,82	0
6	MG	D	601	1/1	0.98	0.12	51,51,51,51	0
8	SO4	D	630	5/5	0.98	0.10	72,74,75,77	0
8	SO4	L	630	5/5	0.99	0.07	81,83,84,85	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.

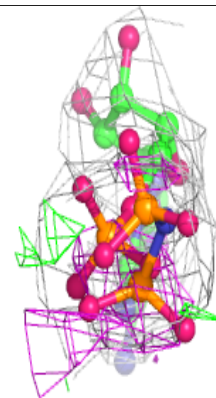
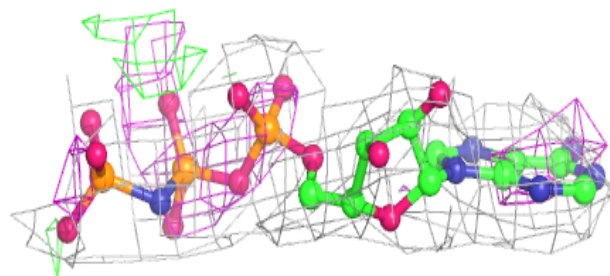
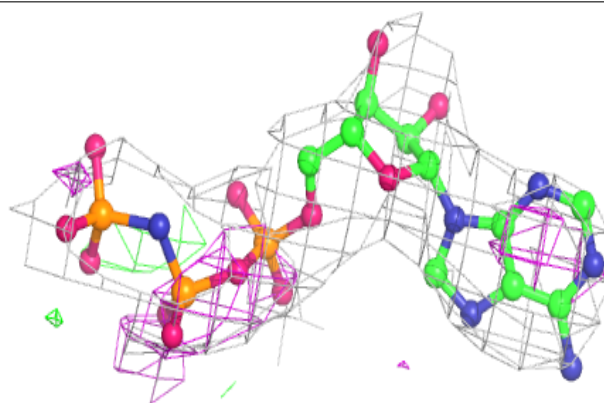


Electron density around ANP A 600:

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

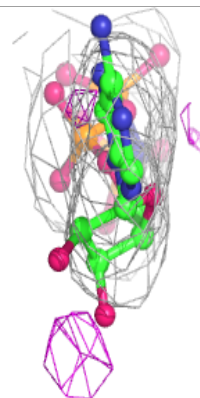
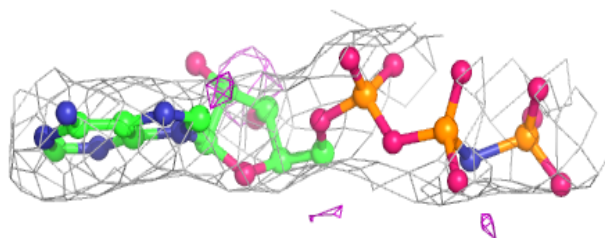
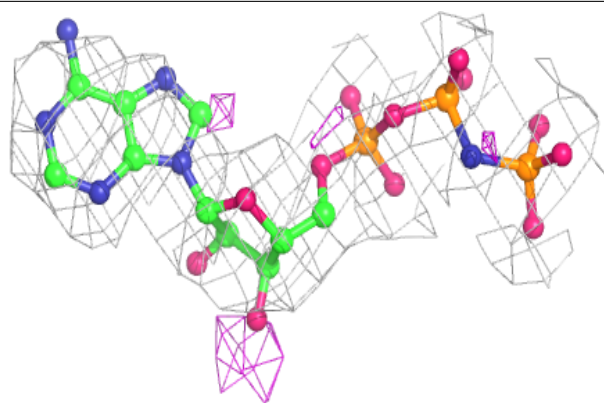
**Electron density around ANP Y 600:**

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

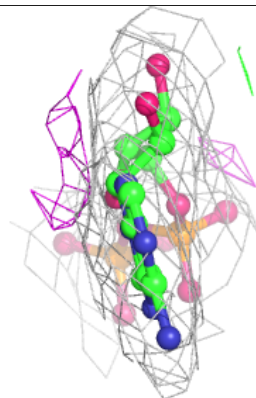
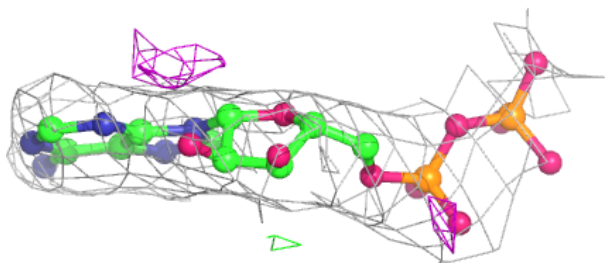
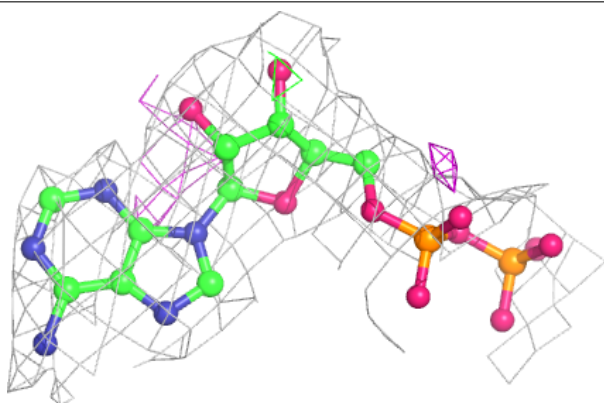


Electron density around ANP a 600:

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

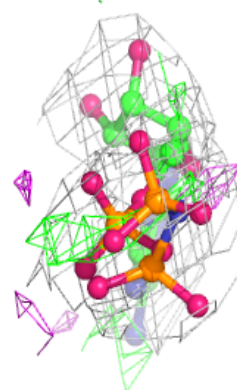
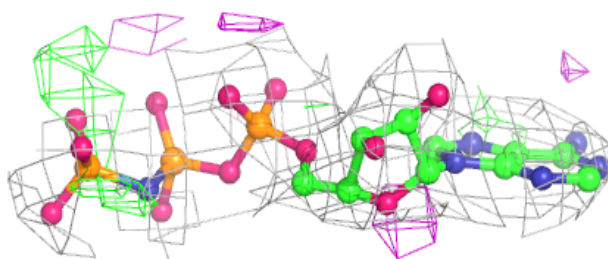
**Electron density around ADP b 600:**

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

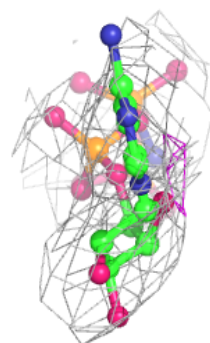
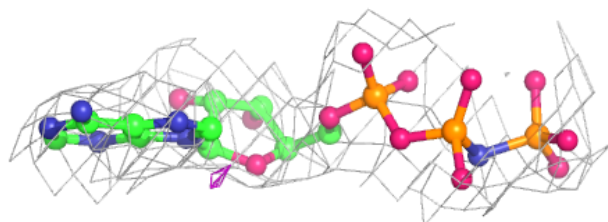
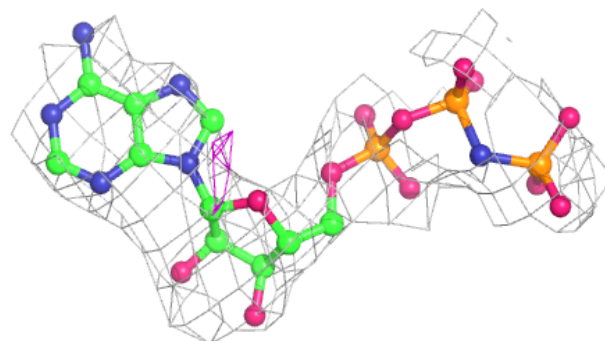


Electron density around ANP Q 600:

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

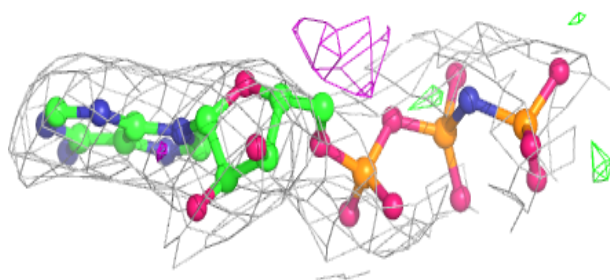
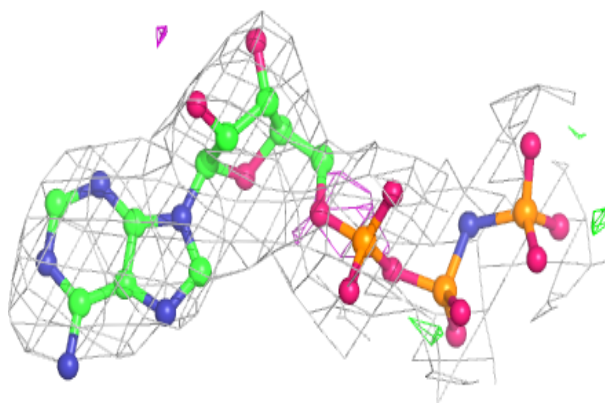
**Electron density around ANP R 600:**

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

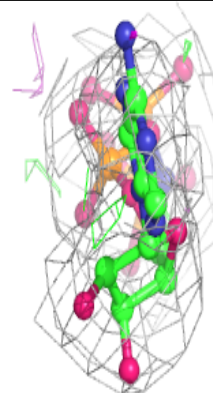
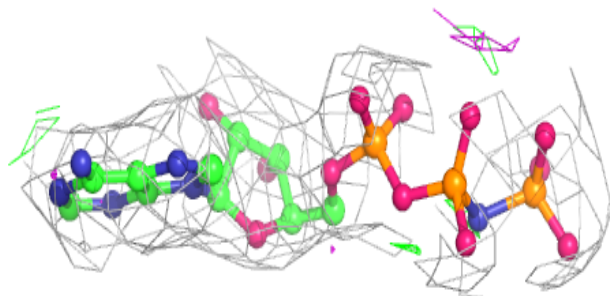
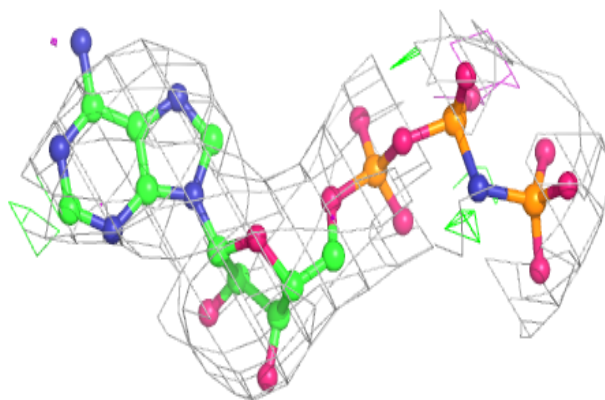


Electron density around ANP S 600:

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

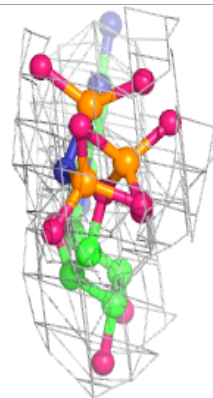
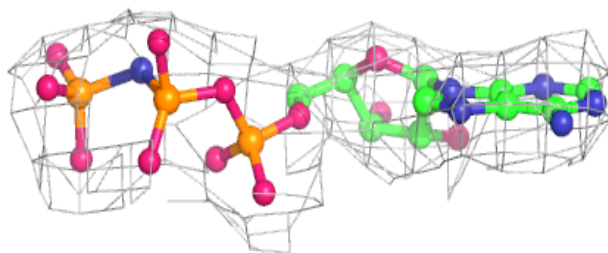
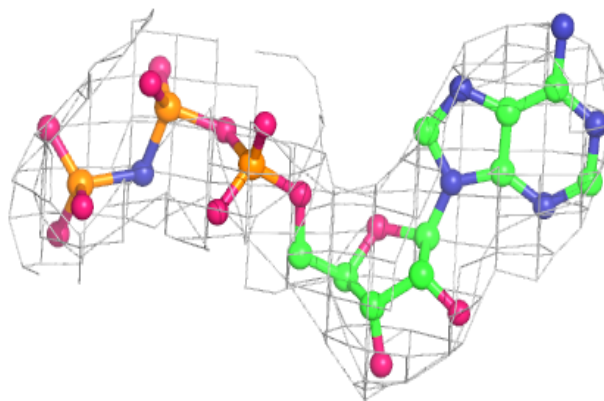
**Electron density around ANP I 600:**

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

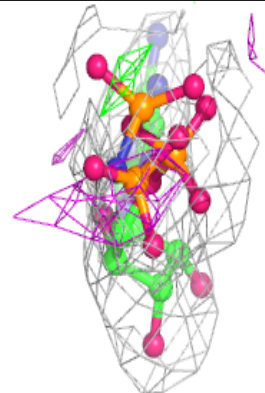
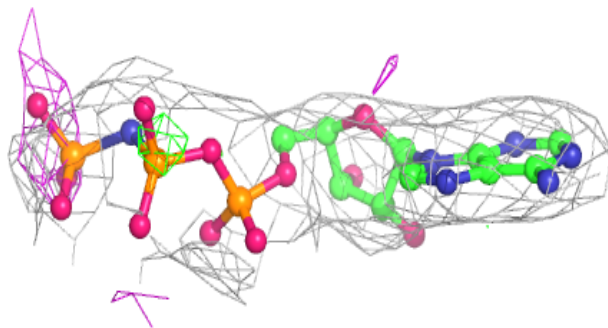
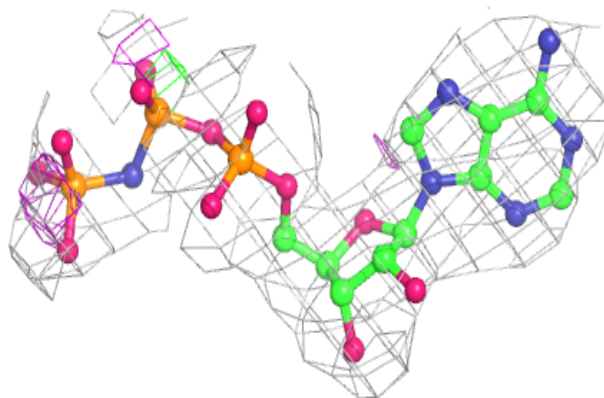


Electron density around ANP B 600:

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

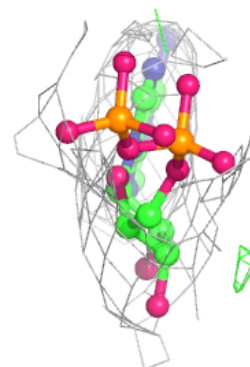
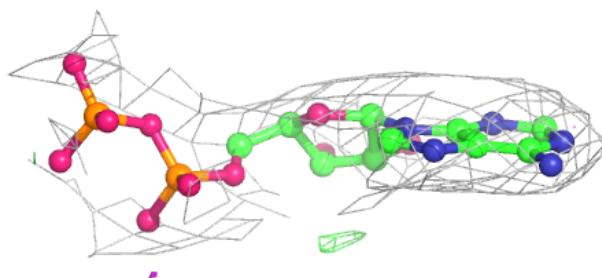
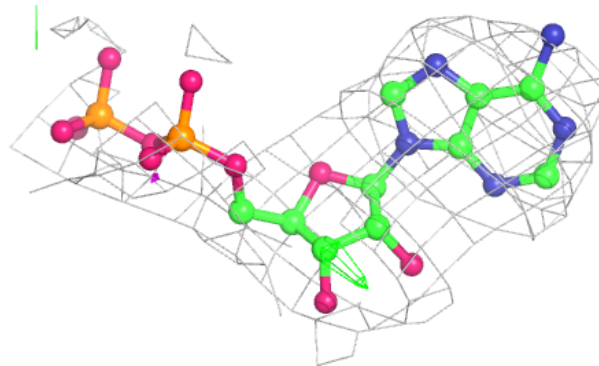
**Electron density around ANP C 600:**

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

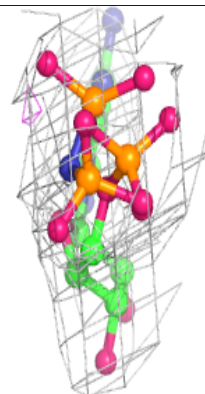
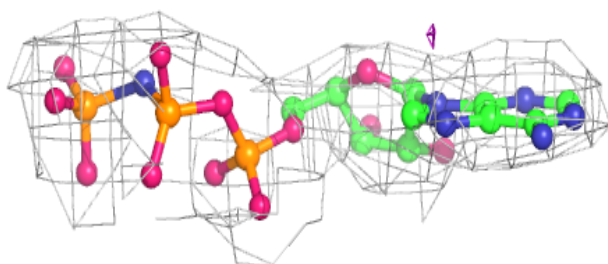
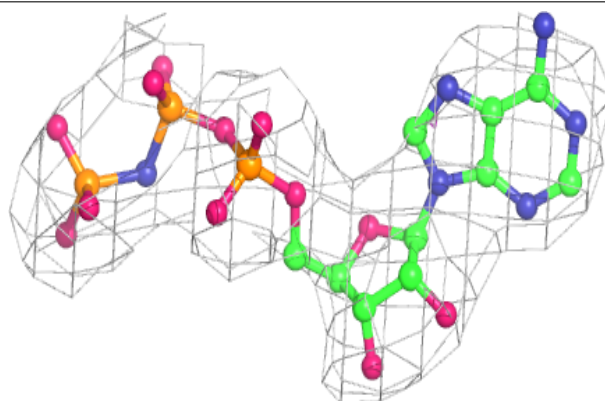


Electron density around ADP T 600:

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

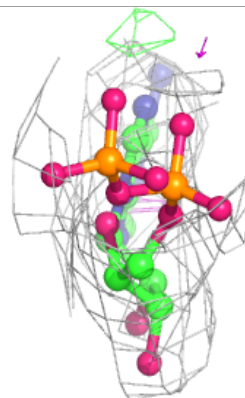
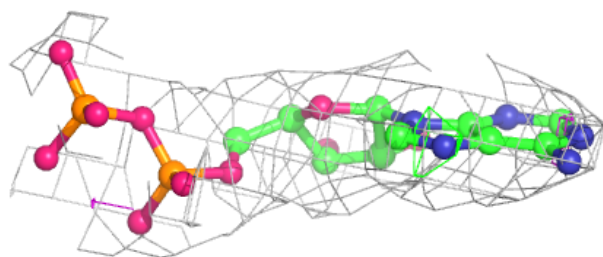
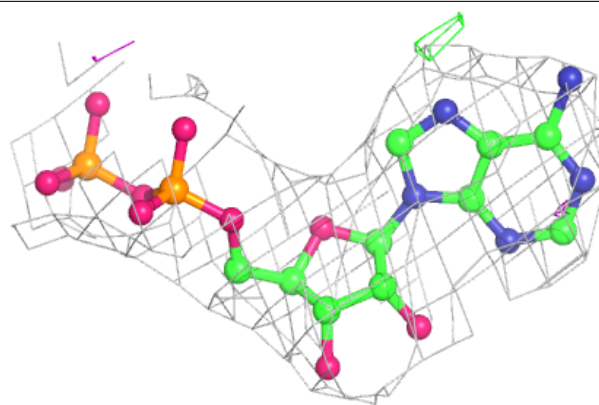
**Electron density around ANP J 600:**

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

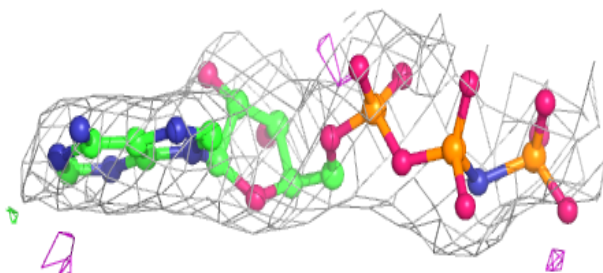
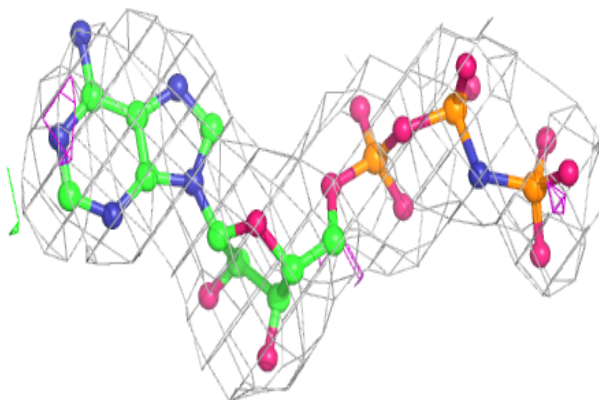


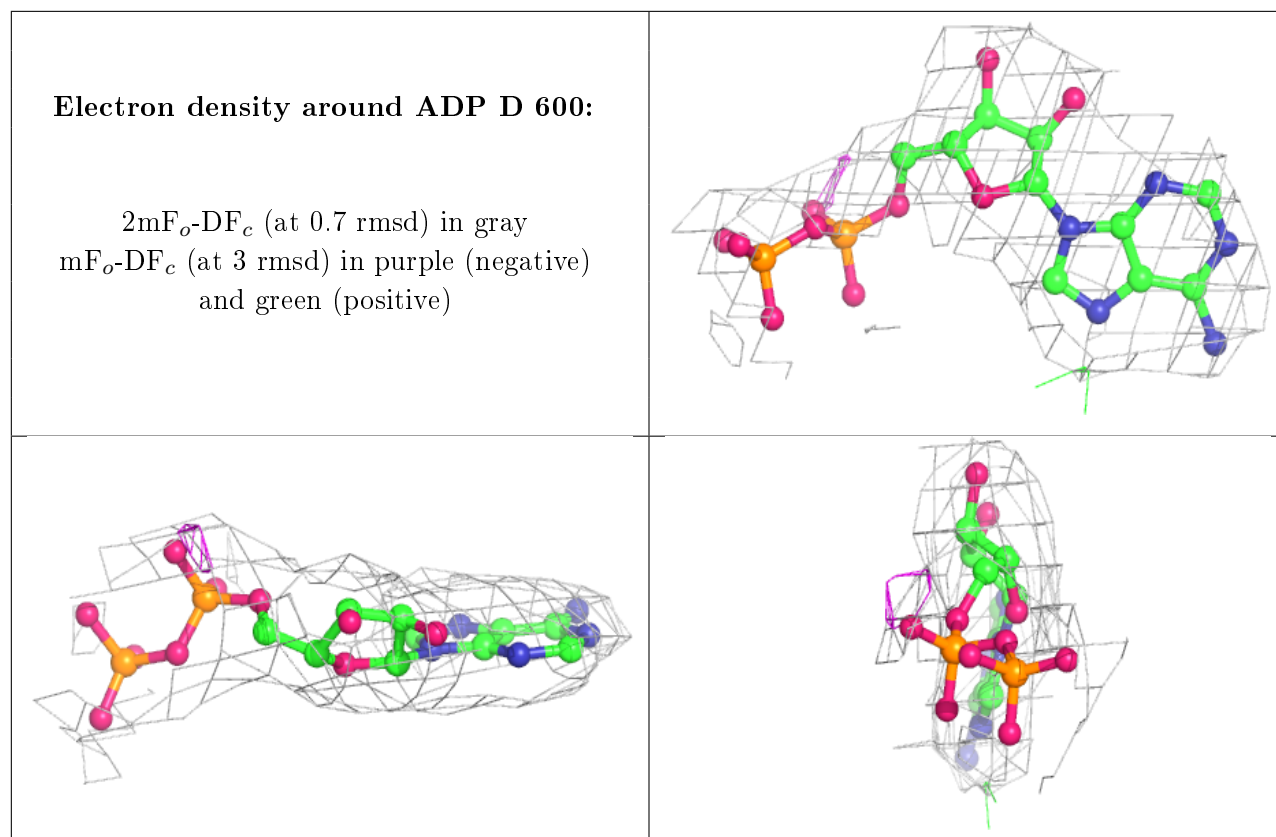
Electron density around ADP L 600:

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

**Electron density around ANP 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.