



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 09:31 AM UTC

PDB ID : 2C38 / pdb_00002c38
Title : RNase PH core of the archaeal exosome in complex with A5 RNA
Authors : Lorentzen, E.; Conti, E.
Deposited on : 2005-10-04
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

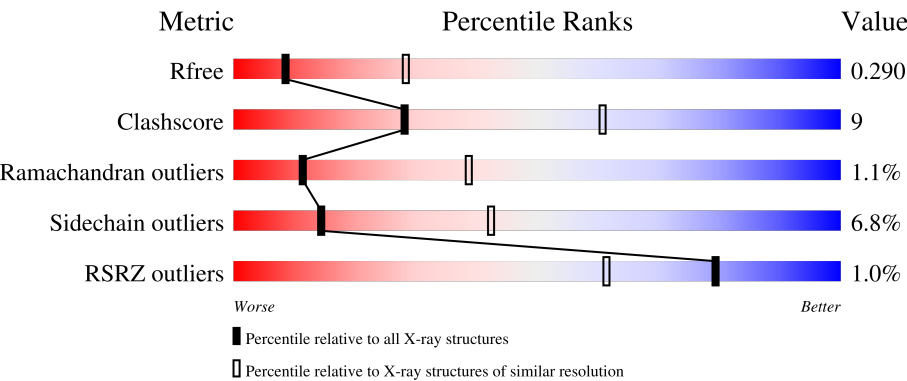
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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

Mol	Chain	Length	Quality of chain
1	A	275	% 80%18%..
1	C	275	% 75%21%..
1	E	275	% 78%17%..
1	G	275	% 75%22%..
1	I	275	% 74%22%..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	K	275	
1	M	275	
1	O	275	
1	Q	275	
1	S	275	
1	U	275	
1	W	275	
2	B	248	
2	D	248	
2	F	248	
2	H	248	
2	J	248	
2	L	248	
2	N	248	
2	P	248	
2	R	248	
2	T	248	
2	V	248	
2	X	248	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 47618 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 PROBABLE EXOSOME COMPLEX EXONUCLEASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	271	Total	C	N	O	S	0	0	0
			2032	1299	334	394	5			
1	C	271	Total	C	N	O	S	0	0	0
			2044	1306	336	397	5			
1	E	271	Total	C	N	O	S	0	0	0
			2042	1305	335	397	5			
1	G	271	Total	C	N	O	S	0	0	0
			2038	1303	335	395	5			
1	I	271	Total	C	N	O	S	0	0	0
			2034	1300	334	395	5			
1	K	271	Total	C	N	O	S	0	0	0
			2042	1305	335	397	5			
1	M	271	Total	C	N	O	S	0	0	0
			2046	1306	334	401	5			
1	O	271	Total	C	N	O	S	0	0	0
			2040	1304	335	396	5			
1	Q	271	Total	C	N	O	S	0	0	0
			2045	1307	335	398	5			
1	S	271	Total	C	N	O	S	0	0	0
			2049	1309	335	400	5			
1	U	270	Total	C	N	O	S	0	0	0
			2043	1304	335	399	5			
1	W	271	Total	C	N	O	S	0	0	0
			2044	1306	335	398	5			

- Molecule 2 is a protein called PROBABLE EXOSOME COMPLEX EXONUCLEASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	241	Total	C	N	O	S	0	0	0
			1855	1170	321	354	10			
2	D	247	Total	C	N	O	S	0	0	0
			1893	1195	328	359	11			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	241	Total	C	N	O	S	0	0	0
			1859	1172	321	356	10			
2	H	241	Total	C	N	O	S	0	0	0
			1859	1172	321	356	10			
2	J	241	Total	C	N	O	S	0	0	0
			1855	1170	321	354	10			
2	L	247	Total	C	N	O	S	0	0	0
			1901	1199	328	363	11			
2	N	241	Total	C	N	O	S	0	0	0
			1849	1166	317	356	10			
2	P	248	Total	C	N	O	S	0	0	0
			1909	1204	329	364	12			
2	R	247	Total	C	N	O	S	0	0	0
			1902	1198	331	363	10			
2	T	247	Total	C	N	O	S	0	0	0
			1901	1199	328	363	11			
2	V	239	Total	C	N	O	S	0	0	0
			1842	1162	319	351	10			
2	X	241	Total	C	N	O	S	0	0	0
			1859	1172	321	356	10			

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

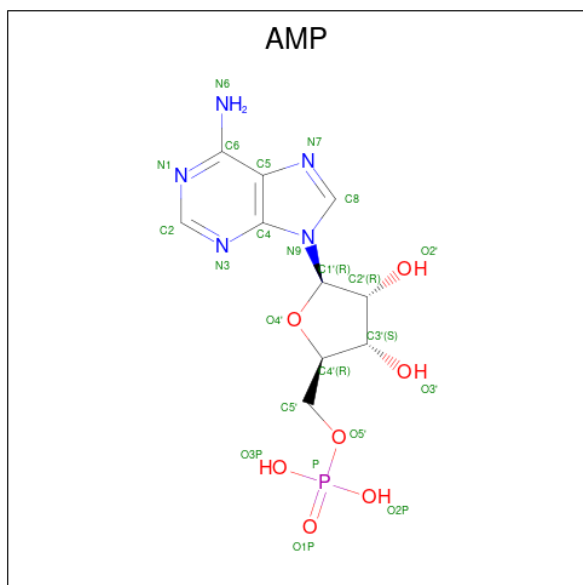
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		
3	D	1	Total	Cl	0	0
			1	1		
3	F	1	Total	Cl	0	0
			1	1		
3	H	1	Total	Cl	0	0
			1	1		
3	J	1	Total	Cl	0	0
			1	1		
3	L	1	Total	Cl	0	0
			1	1		
3	N	1	Total	Cl	0	0
			1	1		
3	P	1	Total	Cl	0	0
			1	1		
3	R	1	Total	Cl	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	T	1	Total	Cl	0	0
			1	1		
3	V	1	Total	Cl	0	0
			1	1		
3	X	1	Total	Cl	0	0
			1	1		

- Molecule 4 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	B	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
4	B	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
4	B	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
4	F	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	F	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
4	F	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
4	F	1	Total	C	N	O	P	0	0
			22	10	5	6	1		

Continued on next page...

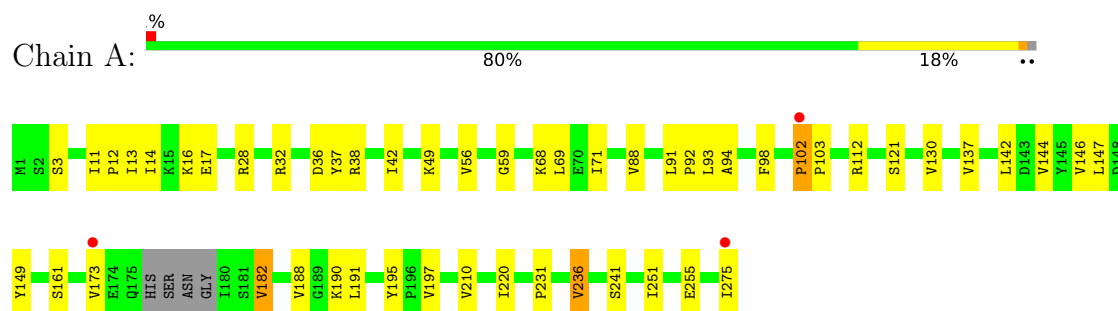
Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	H	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	H	1	Total 22	C 10	N 5	O 6	P 1	0	0
4	H	1	Total 22	C 10	N 5	O 6	P 1	0	0
4	H	1	Total 22	C 10	N 5	O 6	P 1	0	0
4	J	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	J	1	Total 22	C 10	N 5	O 6	P 1	0	0
4	J	1	Total 22	C 10	N 5	O 6	P 1	0	0
4	J	1	Total 22	C 10	N 5	O 6	P 1	0	0
4	N	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	N	1	Total 22	C 10	N 5	O 6	P 1	0	0
4	N	1	Total 22	C 10	N 5	O 6	P 1	0	0
4	N	1	Total 22	C 10	N 5	O 6	P 1	0	0
4	V	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	V	1	Total 22	C 10	N 5	O 6	P 1	0	0
4	V	1	Total 22	C 10	N 5	O 6	P 1	0	0
4	V	1	Total 22	C 10	N 5	O 6	P 1	0	0
4	X	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	X	1	Total 22	C 10	N 5	O 6	P 1	0	0
4	X	1	Total 22	C 10	N 5	O 6	P 1	0	0
4	X	1	Total 22	C 10	N 5	O 6	P 1	0	0

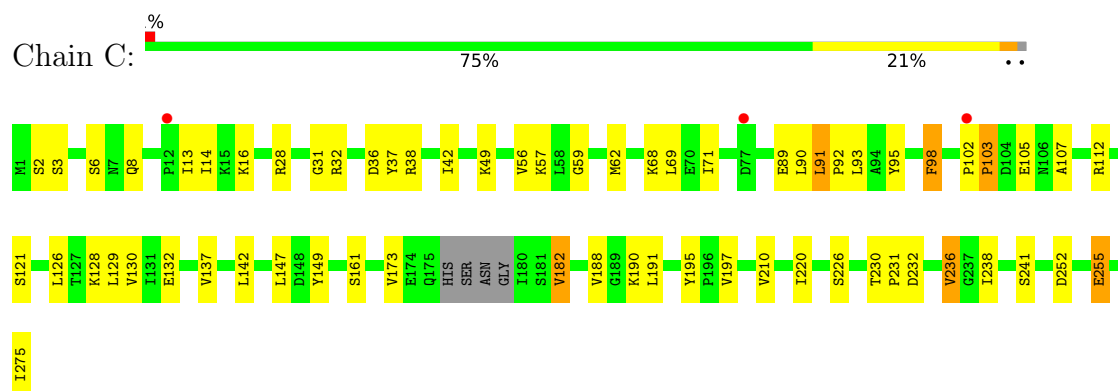
3 Residue-property plots

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

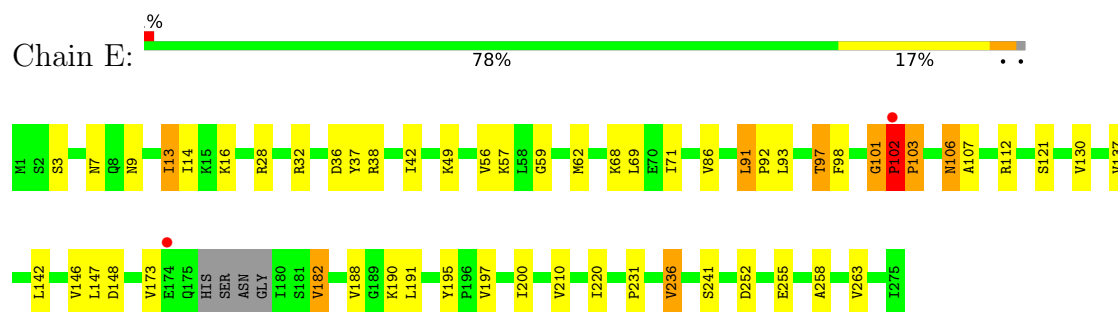
• Molecule 1: PROBABLE EXOSOME COMPLEX EXONUCLEASE 2



• Molecule 1: PROBABLE EXOSOME COMPLEX EXONUCLEASE 2

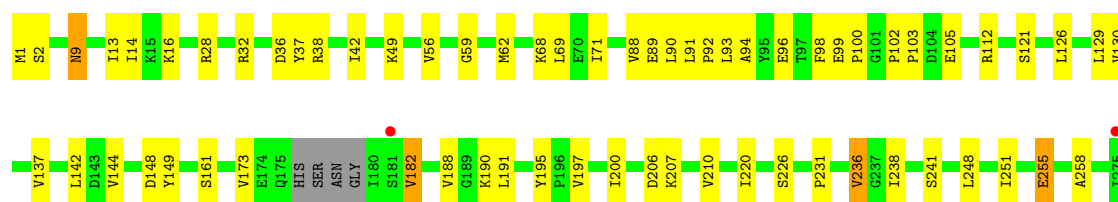


• Molecule 1: PROBABLE EXOSOME COMPLEX EXONUCLEASE 2

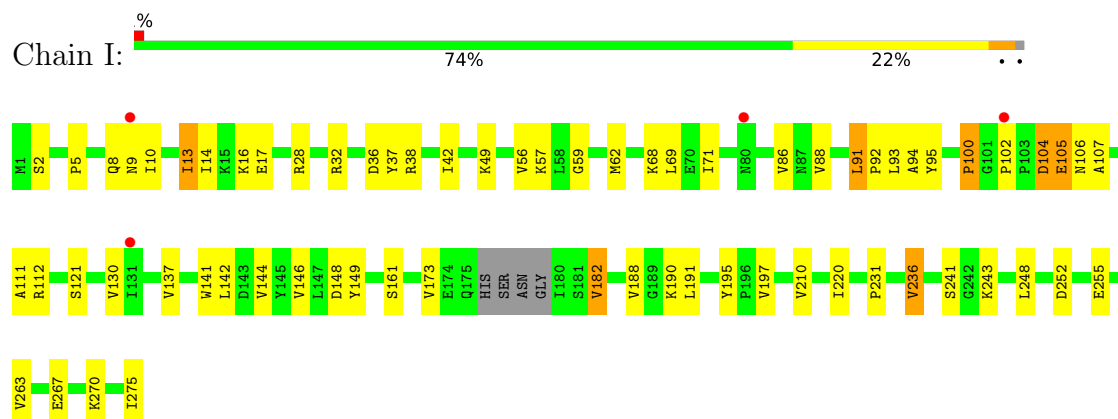


• Molecule 1: PROBABLE EXOSOME COMPLEX EXONUCLEASE 2

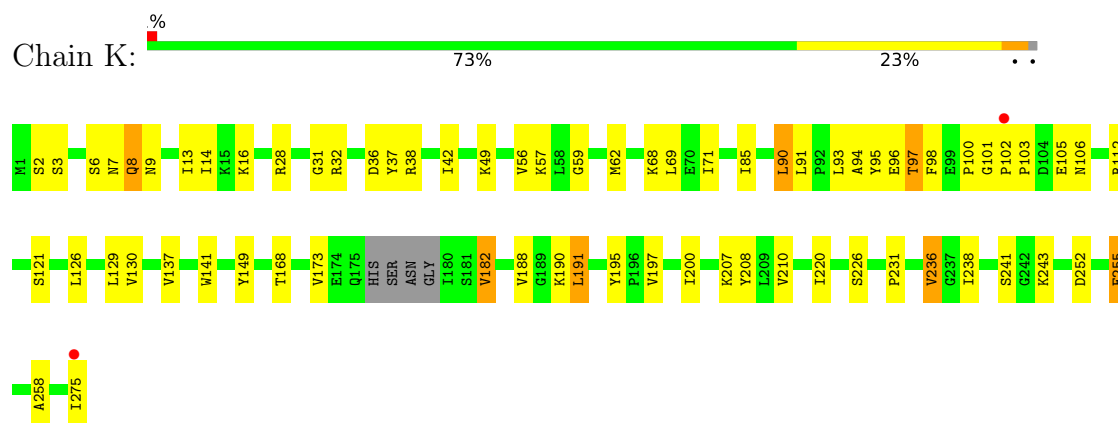




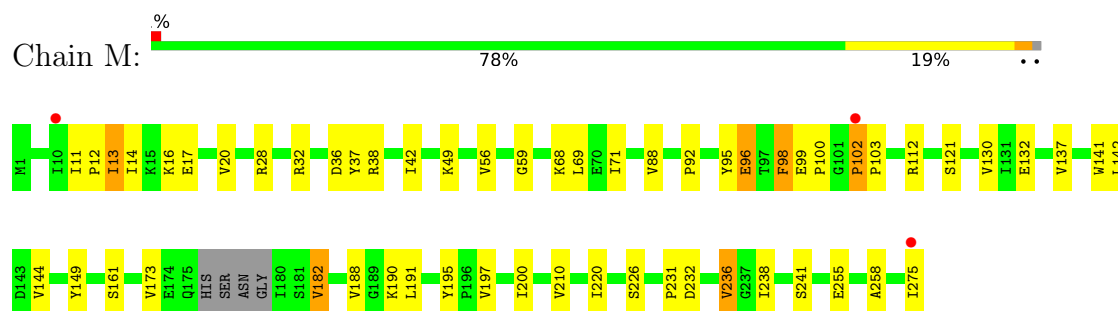
● Molecule 1: PROBABLE EXOSOME COMPLEX EXONUCLEASE 2



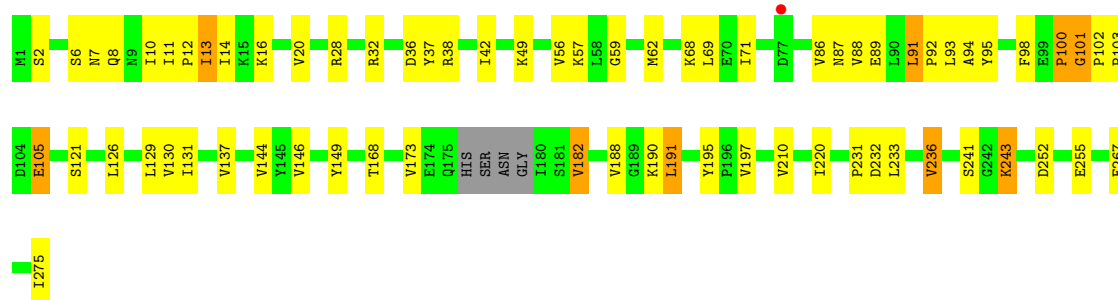
● Molecule 1: PROBABLE EXOSOME COMPLEX EXONUCLEASE 2



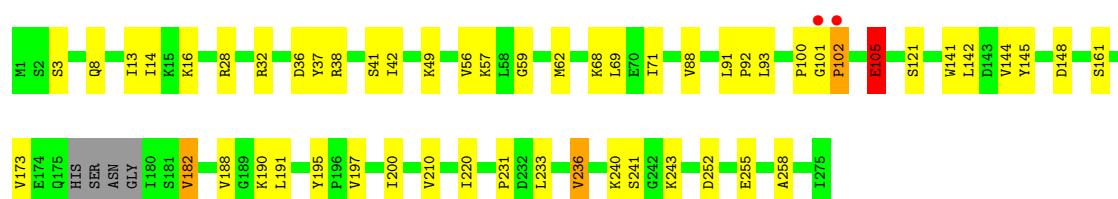
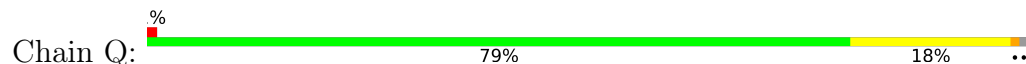
● Molecule 1: PROBABLE EXOSOME COMPLEX EXONUCLEASE 2



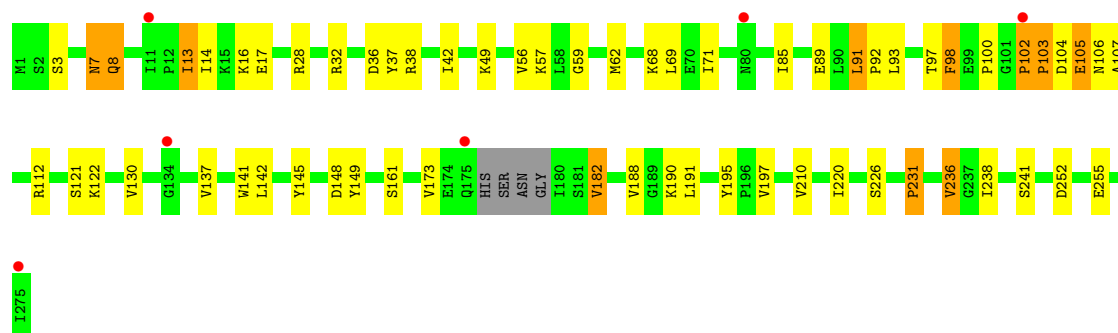
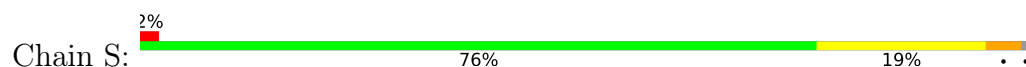
● Molecule 1: PROBABLE EXOSOME COMPLEX EXONUCLEASE 2



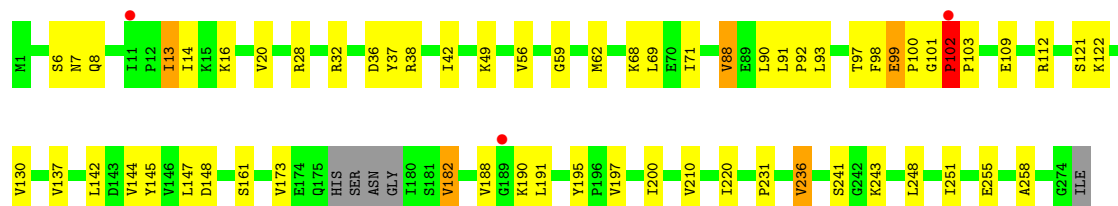
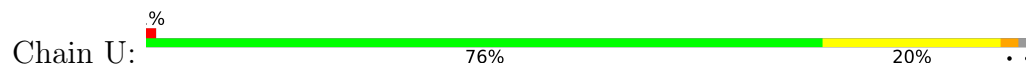
• Molecule 1: PROBABLE EXOSOME COMPLEX EXONUCLEASE 2



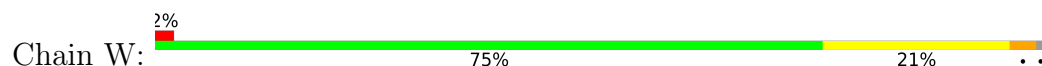
• Molecule 1: PROBABLE EXOSOME COMPLEX EXONUCLEASE 2

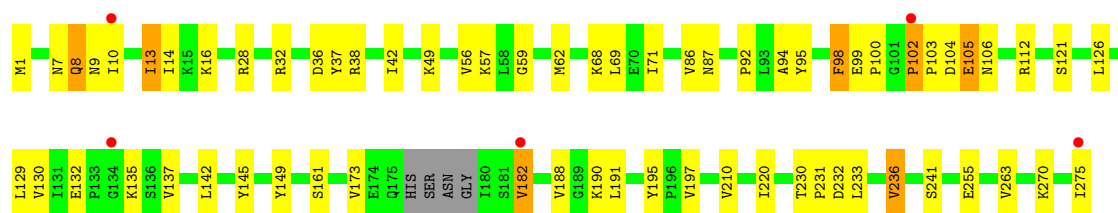


• Molecule 1: PROBABLE EXOSOME COMPLEX EXONUCLEASE 2



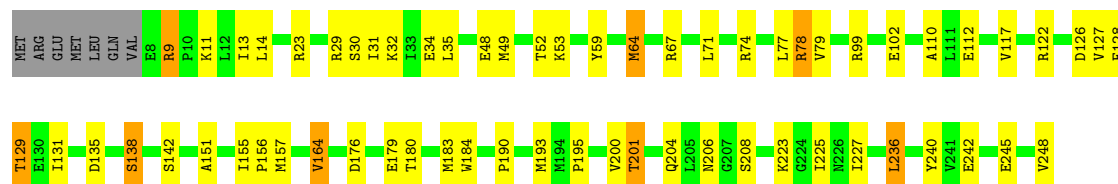
• Molecule 1: PROBABLE EXOSOME COMPLEX EXONUCLEASE 2





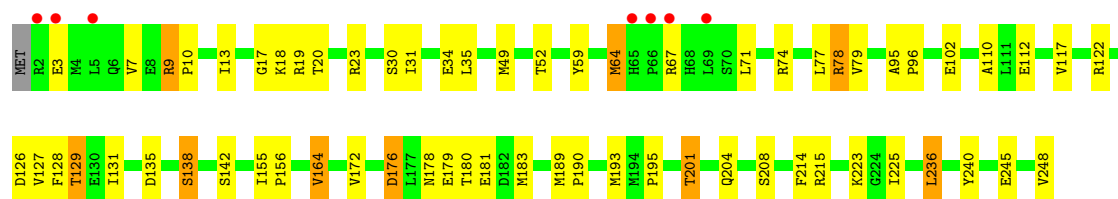
• Molecule 2: PROBABLE EXOSOME COMPLEX EXONUCLEASE 1

Chain B: 72% 22%



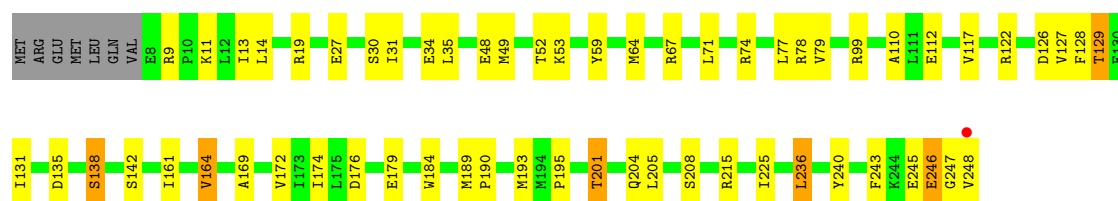
• Molecule 2: PROBABLE EXOSOME COMPLEX EXONUCLEASE 1

Chain D: 3% 74% 22%



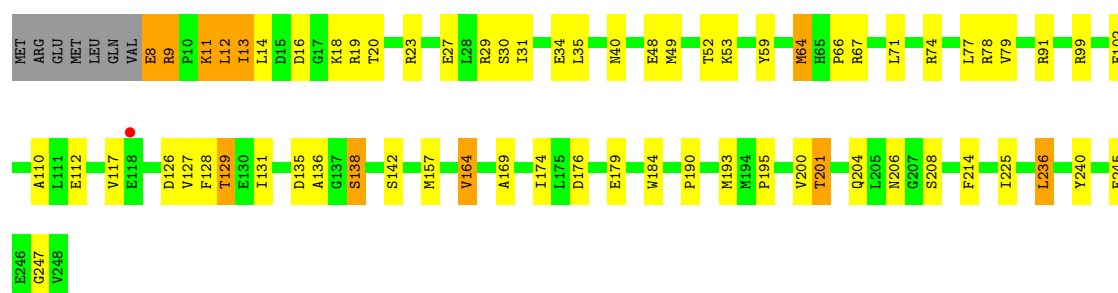
• Molecule 2: PROBABLE EXOSOME COMPLEX EXONUCLEASE 1

Chain F: 73% 22%



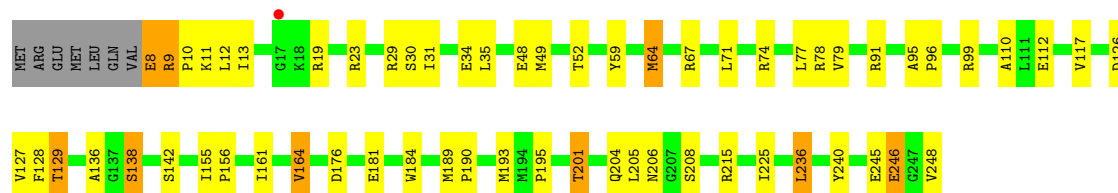
• Molecule 2: PROBABLE EXOSOME COMPLEX EXONUCLEASE 1

Chain H: 70% 23%



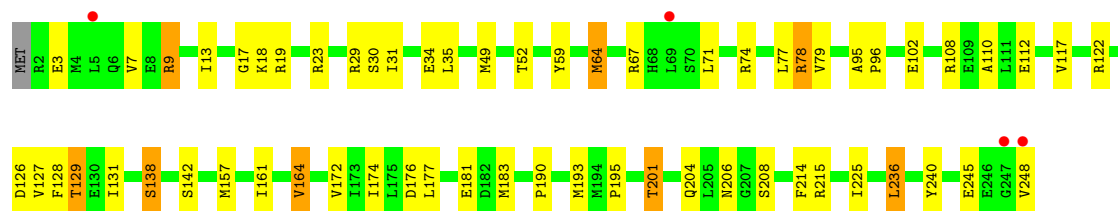
• Molecule 2: PROBABLE EXOSOME COMPLEX EXONUCLEASE 1

Chain J:  73% 21%



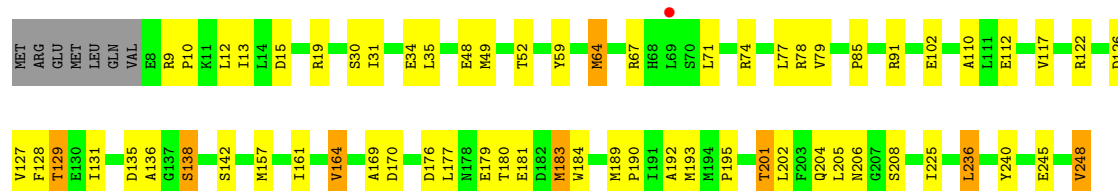
• Molecule 2: PROBABLE EXOSOME COMPLEX EXONUCLEASE 1

Chain L:  2% 75% 21%



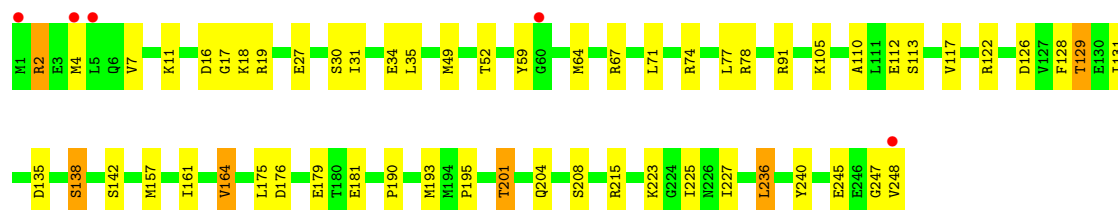
• Molecule 2: PROBABLE EXOSOME COMPLEX EXONUCLEASE 1

Chain N:  71% 23%



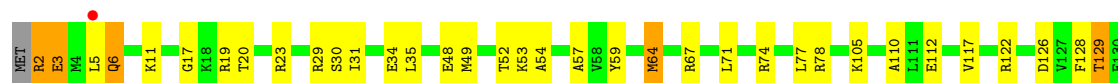
• Molecule 2: PROBABLE EXOSOME COMPLEX EXONUCLEASE 1

Chain P:  2% 77% 21%



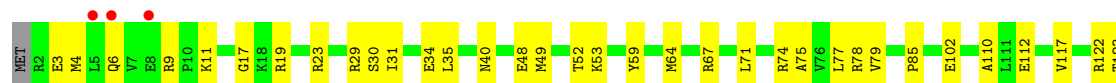
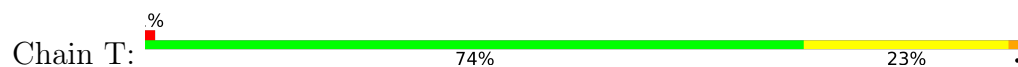
• Molecule 2: PROBABLE EXOSOME COMPLEX EXONUCLEASE 1

Chain R:  74% 22%





• Molecule 2: PROBABLE EXOSOME COMPLEX EXONUCLEASE 1



• Molecule 2: PROBABLE EXOSOME COMPLEX EXONUCLEASE 1



• Molecule 2: PROBABLE EXOSOME COMPLEX EXONUCLEASE 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	206.26Å 213.61Å 434.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	95.78 – 3.10 95.78 – 3.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (95.78-3.10) 98.5 (95.78-3.10)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 3.13Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.276 , 0.289 0.272 , 0.290	Depositor DCC
R_{free} test set	5102 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å ²)	65.4	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	0.100 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	47618	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.89 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.2640e-03.*

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: AMP, CL

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	0.61	0/2063	0.92	2/2809 (0.1%)
1	C	0.65	1/2075 (0.0%)	0.95	6/2823 (0.2%)
1	E	0.60	1/2073 (0.0%)	0.91	4/2821 (0.1%)
1	G	0.64	1/2069 (0.0%)	0.91	2/2816 (0.1%)
1	I	0.64	1/2065 (0.0%)	0.90	2/2810 (0.1%)
1	K	0.66	1/2073 (0.0%)	0.92	2/2821 (0.1%)
1	M	0.61	0/2077	0.93	4/2827 (0.1%)
1	O	0.64	1/2071 (0.0%)	0.90	3/2818 (0.1%)
1	Q	0.66	1/2076 (0.0%)	0.90	2/2824 (0.1%)
1	S	0.64	1/2080 (0.0%)	0.92	5/2831 (0.2%)
1	U	0.62	1/2074 (0.0%)	0.91	4/2822 (0.1%)
1	W	0.65	1/2075 (0.0%)	0.95	3/2823 (0.1%)
2	B	0.55	0/1883	0.90	2/2544 (0.1%)
2	D	0.61	0/1921	0.96	5/2596 (0.2%)
2	F	0.55	0/1887	0.90	2/2549 (0.1%)
2	H	0.55	0/1887	0.91	2/2549 (0.1%)
2	J	0.56	0/1883	0.92	4/2544 (0.2%)
2	L	0.62	0/1929	0.94	5/2606 (0.2%)
2	N	0.55	0/1877	0.92	2/2538 (0.1%)
2	P	0.61	0/1937	0.92	2/2616 (0.1%)
2	R	0.60	0/1930	0.92	2/2607 (0.1%)
2	T	0.65	0/1929	0.94	2/2606 (0.1%)
2	V	0.54	0/1870	0.91	2/2527 (0.1%)
2	X	0.55	0/1887	0.91	2/2549 (0.1%)
All	All	0.61	10/47691 (0.0%)	0.92	71/64676 (0.1%)

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	Q	0	1
2	D	0	1
2	L	0	1
2	P	0	1
2	R	0	1
2	T	0	1
All	All	0	6

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	W	102	PRO	CA-C	8.25	1.59	1.52
1	U	102	PRO	CA-C	7.43	1.59	1.52
1	I	102	PRO	CA-C	7.33	1.58	1.52
1	K	102	PRO	CA-C	7.24	1.58	1.52
1	Q	102	PRO	CA-C	6.91	1.58	1.52
1	C	102	PRO	CA-C	6.13	1.57	1.52
1	E	102	PRO	CA-C	6.12	1.57	1.52
1	S	102	PRO	CA-C	5.54	1.57	1.52
1	O	102	PRO	CA-C	5.43	1.57	1.52
1	G	102	PRO	CA-C	5.32	1.57	1.52

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	102	PRO	CA-C-N	11.68	134.44	119.84
1	C	102	PRO	C-N-CA	11.68	134.44	119.84
1	W	102	PRO	CA-C-N	10.92	133.49	119.84
1	W	102	PRO	C-N-CA	10.92	133.49	119.84
1	M	102	PRO	CA-C-N	9.63	131.88	119.84
1	M	102	PRO	C-N-CA	9.63	131.88	119.84
1	E	102	PRO	CA-C-N	8.98	131.07	119.84
1	E	102	PRO	C-N-CA	8.98	131.07	119.84
2	D	9	ARG	CA-C-N	8.94	128.97	119.76
2	D	9	ARG	C-N-CA	8.94	128.97	119.76
1	O	102	PRO	CA-C-N	8.86	130.91	119.84
1	O	102	PRO	C-N-CA	8.86	130.91	119.84
1	G	102	PRO	CA-C-N	8.72	130.74	119.84
1	G	102	PRO	C-N-CA	8.72	130.74	119.84
1	U	99	GLU	CA-C-N	8.26	130.17	119.84
1	U	99	GLU	C-N-CA	8.26	130.17	119.84
1	A	102	PRO	CA-C-N	8.06	129.92	119.84
1	A	102	PRO	C-N-CA	8.06	129.92	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	102	PRO	CA-C-N	8.01	129.86	119.84
1	K	102	PRO	C-N-CA	8.01	129.86	119.84
1	M	98	PHE	N-CA-C	7.86	119.94	108.86
1	O	86	VAL	CB-CA-C	-7.23	102.55	111.88
2	L	9	ARG	CA-C-N	6.94	126.97	119.89
2	L	9	ARG	C-N-CA	6.94	126.97	119.89
1	U	102	PRO	CA-C-N	6.86	128.42	119.84
1	U	102	PRO	C-N-CA	6.86	128.42	119.84
2	J	9	ARG	N-CA-C	6.66	119.27	110.08
1	E	102	PRO	N-CA-C	6.51	118.64	110.70
1	W	102	PRO	N-CA-C	6.33	118.42	110.70
1	C	102	PRO	N-CA-C	6.31	118.39	110.70
1	I	102	PRO	CA-C-N	6.15	127.53	119.84
1	I	102	PRO	C-N-CA	6.15	127.53	119.84
1	E	9	ASN	N-CA-C	6.11	118.58	109.59
1	S	231	PRO	CA-C-N	-5.96	113.65	122.83
1	S	231	PRO	C-N-CA	-5.96	113.65	122.83
2	L	71	LEU	CA-C-N	5.79	125.47	119.56
2	L	71	LEU	C-N-CA	5.79	125.47	119.56
1	S	102	PRO	CA-C-N	5.78	127.06	119.84
1	S	102	PRO	C-N-CA	5.78	127.06	119.84
2	V	71	LEU	CA-C-N	5.75	125.37	119.56
2	V	71	LEU	C-N-CA	5.75	125.37	119.56
1	C	6	SER	CA-C-N	5.72	128.22	120.38
1	C	6	SER	C-N-CA	5.72	128.22	120.38
2	D	71	LEU	CA-C-N	5.67	125.34	119.56
2	D	71	LEU	C-N-CA	5.67	125.34	119.56
2	X	71	LEU	CA-C-N	5.64	125.31	119.56
2	X	71	LEU	C-N-CA	5.64	125.31	119.56
2	B	71	LEU	CA-C-N	5.59	125.26	119.56
2	B	71	LEU	C-N-CA	5.59	125.26	119.56
2	L	18	LYS	N-CA-C	5.53	119.24	109.96
2	P	71	LEU	CA-C-N	5.52	125.19	119.56
2	P	71	LEU	C-N-CA	5.52	125.19	119.56
2	H	71	LEU	CA-C-N	5.51	125.18	119.56
2	H	71	LEU	C-N-CA	5.51	125.18	119.56
2	R	71	LEU	CA-C-N	5.47	125.08	119.56
2	R	71	LEU	C-N-CA	5.47	125.08	119.56
1	C	98	PHE	N-CA-C	5.44	118.42	109.72
2	D	18	LYS	N-CA-C	5.40	118.90	110.32
2	J	71	LEU	CA-C-N	5.39	125.01	119.56
2	J	71	LEU	C-N-CA	5.39	125.01	119.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	71	LEU	CA-C-N	5.32	124.98	119.56
2	T	71	LEU	C-N-CA	5.32	124.98	119.56
2	N	71	LEU	CA-C-N	5.29	124.95	119.56
2	N	71	LEU	C-N-CA	5.29	124.95	119.56
1	M	102	PRO	N-CA-C	5.28	117.14	110.70
2	J	246	GLU	N-CA-C	5.16	115.16	107.88
2	F	71	LEU	CA-C-N	5.13	124.74	119.56
2	F	71	LEU	C-N-CA	5.13	124.74	119.56
1	Q	102	PRO	CA-C-N	5.08	125.48	119.99
1	Q	102	PRO	C-N-CA	5.08	125.48	119.99
1	S	107	ALA	N-CA-C	-5.08	105.83	111.36

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	17	GLY	Peptide
2	L	17	GLY	Peptide
2	P	17	GLY	Peptide
1	Q	102	PRO	Peptide
2	R	17	GLY	Peptide
2	T	17	GLY	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2032	0	2057	26	0
1	C	2044	0	2078	36	0
1	E	2042	0	2077	38	0
1	G	2038	0	2073	39	0
1	I	2034	0	2059	41	0
1	K	2042	0	2077	44	0
1	M	2046	0	2074	27	0
1	O	2040	0	2072	34	0
1	Q	2045	0	2078	25	0
1	S	2049	0	2085	35	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	U	2043	0	2075	33	0
1	W	2044	0	2076	35	0
2	B	1855	0	1880	47	0
2	D	1893	0	1917	39	0
2	F	1859	0	1884	39	0
2	H	1859	0	1884	45	0
2	J	1855	0	1880	38	0
2	L	1901	0	1925	36	0
2	N	1849	0	1862	41	0
2	P	1909	0	1937	36	0
2	R	1902	0	1922	41	0
2	T	1901	0	1925	40	0
2	V	1842	0	1869	47	0
2	X	1859	0	1884	45	0
3	B	1	0	0	1	0
3	D	1	0	0	0	0
3	F	1	0	0	0	0
3	H	1	0	0	0	0
3	J	1	0	0	1	0
3	L	1	0	0	0	0
3	N	1	0	0	1	0
3	P	1	0	0	0	0
3	R	1	0	0	0	0
3	T	1	0	0	0	0
3	V	1	0	0	1	0
3	X	1	0	0	0	0
4	B	89	0	45	4	0
4	F	89	0	45	5	0
4	H	89	0	45	4	0
4	J	89	0	45	6	0
4	N	89	0	45	3	0
4	V	89	0	45	6	0
4	X	89	0	45	1	0
All	All	47618	0	47965	853	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (853) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:223:LYS:HB3	2:D:248:VAL:HG11	1.41	1.00
2:X:9:ARG:HG2	2:X:184:TRP:CE3	2.01	0.95
2:B:223:LYS:HB3	2:B:248:VAL:HG11	1.52	0.90
2:F:77:LEU:HD12	2:F:112:GLU:HG2	1.53	0.90
2:B:77:LEU:HD12	2:B:112:GLU:HG2	1.56	0.88
2:L:77:LEU:HD12	2:L:112:GLU:HG2	1.56	0.87
2:R:77:LEU:HD12	2:R:112:GLU:HG2	1.56	0.87
2:N:77:LEU:HD12	2:N:112:GLU:HG2	1.54	0.87
2:X:77:LEU:HD12	2:X:112:GLU:HG2	1.55	0.87
2:B:223:LYS:HB3	2:B:248:VAL:CG1	2.06	0.85
1:K:95:TYR:HD2	1:K:97:THR:HB	1.42	0.85
1:G:91:LEU:HB3	1:G:93:LEU:HD13	1.59	0.83
1:C:230:THR:OG1	1:C:232:ASP:OD1	1.97	0.83
2:H:77:LEU:HD12	2:H:112:GLU:HG2	1.61	0.83
2:T:77:LEU:HD12	2:T:112:GLU:HG2	1.60	0.82
2:D:77:LEU:HD12	2:D:112:GLU:HG2	1.61	0.82
2:J:77:LEU:HD12	2:J:112:GLU:HG2	1.62	0.81
2:P:77:LEU:HD12	2:P:112:GLU:HG2	1.62	0.81
2:V:13:ILE:HD11	2:V:169:ALA:HB3	1.63	0.81
2:B:99:ARG:NH1	4:B:404:AMP:O2P	2.14	0.80
2:V:77:LEU:HD12	2:V:112:GLU:HG2	1.65	0.79
2:H:8:GLU:OE2	2:H:8:GLU:HA	1.81	0.78
2:N:13:ILE:HD11	2:N:169:ALA:HB3	1.66	0.77
1:C:89:GLU:HG2	1:C:103:PRO:HG3	1.65	0.77
2:B:48:GLU:HG2	2:B:53:LYS:HG2	1.67	0.77
2:V:179:GLU:O	2:V:183:MET:HG3	1.83	0.77
2:V:48:GLU:HG2	2:V:53:LYS:HG2	1.68	0.76
2:V:99:ARG:NH1	4:V:404:AMP:O2P	2.19	0.75
2:T:48:GLU:HG2	2:T:53:LYS:HG2	1.69	0.74
1:U:112:ARG:NH2	4:V:403:AMP:O2P	2.20	0.74
2:P:223:LYS:HB3	2:P:248:VAL:CG1	2.17	0.73
2:H:99:ARG:NH1	4:H:404:AMP:O2P	2.21	0.73
1:E:103:PRO:HB3	1:E:107:ALA:CB	2.18	0.73
2:P:227:ILE:HD12	2:P:248:VAL:HG22	1.71	0.73
2:B:227:ILE:HD12	2:B:248:VAL:HG22	1.73	0.71
2:N:183:MET:HE3	2:N:184:TRP:NE1	2.05	0.71
1:A:91:LEU:HB3	1:A:93:LEU:HD13	1.73	0.71
1:A:112:ARG:NH2	4:B:403:AMP:O2P	2.24	0.70
1:C:91:LEU:HD23	1:C:91:LEU:H	1.57	0.69
3:N:301:CL:CL	4:N:404:AMP:H5'2	2.29	0.69
2:R:5:LEU:O	2:R:6:GLN:HB2	1.91	0.69
2:F:99:ARG:NH1	4:F:404:AMP:O2P	2.25	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:48:GLU:HG2	2:F:53:LYS:HG3	1.73	0.68
1:E:93:LEU:HD12	1:E:93:LEU:H	1.59	0.68
1:O:91:LEU:HD12	1:O:93:LEU:HB2	1.75	0.68
2:B:9:ARG:HB3	2:B:9:ARG:HH11	1.57	0.68
1:K:95:TYR:CD2	1:K:97:THR:HB	2.27	0.68
2:D:223:LYS:HB3	2:D:248:VAL:CG1	2.22	0.67
1:K:85:ILE:HG21	1:K:141:TRP:CE3	2.29	0.67
1:A:91:LEU:HD12	1:A:147:LEU:HD23	1.76	0.66
2:V:180:THR:HA	2:V:183:MET:HE2	1.78	0.66
1:E:92:PRO:HA	1:E:98:PHE:CB	2.25	0.66
2:D:180:THR:HA	2:D:183:MET:HE3	1.77	0.66
2:H:9:ARG:HH11	2:H:9:ARG:HB3	1.60	0.66
2:H:136:ALA:HA	4:H:404:AMP:H5'2	1.80	0.64
1:S:91:LEU:HD23	1:S:91:LEU:H	1.62	0.64
1:I:92:PRO:C	1:I:94:ALA:H	2.05	0.64
2:X:14:LEU:O	2:X:16:ASP:N	2.31	0.64
1:E:103:PRO:HB3	1:E:107:ALA:HB3	1.79	0.64
1:E:112:ARG:NH2	4:F:403:AMP:O2P	2.31	0.64
1:G:1:MET:CE	1:I:100:PRO:HG3	2.28	0.64
2:X:32:LYS:HG3	2:X:242:GLU:HG2	1.80	0.64
2:H:9:ARG:HB3	2:H:9:ARG:NH1	2.14	0.63
1:E:71:ILE:HD12	1:E:182:VAL:HG22	1.81	0.63
1:I:92:PRO:O	1:I:94:ALA:N	2.31	0.63
1:I:270:LYS:HD3	1:I:275:ILE:HG23	1.81	0.63
2:F:13:ILE:HD11	2:F:169:ALA:HB3	1.80	0.63
2:H:34:GLU:HB3	2:H:240:TYR:HD1	1.63	0.62
2:X:34:GLU:HB3	2:X:240:TYR:HD1	1.65	0.62
1:C:252:ASP:OD1	2:D:215:ARG:NH1	2.32	0.62
1:I:95:TYR:HB2	1:I:149:TYR:HB3	1.81	0.62
2:L:34:GLU:HB3	2:L:240:TYR:HD1	1.65	0.62
2:N:12:LEU:HD21	2:N:184:TRP:HB2	1.81	0.62
2:N:183:MET:HE3	2:N:184:TRP:CD1	2.34	0.62
2:J:34:GLU:HB3	2:J:240:TYR:HD1	1.64	0.62
2:B:48:GLU:CG	2:B:53:LYS:HG2	2.28	0.62
2:F:126:ASP:HB3	2:F:128:PHE:CE1	2.35	0.62
1:I:270:LYS:HB3	1:I:275:ILE:HA	1.82	0.62
2:T:34:GLU:HB3	2:T:240:TYR:HD1	1.64	0.62
1:A:93:LEU:O	2:D:59:TYR:OH	2.11	0.62
1:K:2:SER:HB2	1:K:105:GLU:OE2	1.99	0.62
1:A:92:PRO:HA	1:A:98:PHE:HB3	1.80	0.62
2:P:34:GLU:HB3	2:P:240:TYR:HD1	1.64	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:LEU:HD11	1:C:147:LEU:HD23	1.80	0.62
2:B:34:GLU:HB3	2:B:240:TYR:HD1	1.65	0.62
1:I:112:ARG:HH22	4:J:403:AMP:P	2.23	0.61
2:V:34:GLU:HB3	2:V:240:TYR:HD1	1.65	0.61
2:N:180:THR:HA	2:N:183:MET:HE2	1.81	0.61
1:S:14:ILE:HD12	1:S:14:ILE:H	1.65	0.61
1:E:91:LEU:HD23	1:E:91:LEU:H	1.64	0.61
4:J:403:AMP:O5'	4:J:403:AMP:H8	1.82	0.61
2:D:34:GLU:HB3	2:D:240:TYR:HD1	1.66	0.61
2:R:48:GLU:HG2	2:R:53:LYS:HG2	1.81	0.61
2:X:164:VAL:HG22	2:X:225:ILE:HG13	1.83	0.60
1:G:91:LEU:HB3	1:G:93:LEU:CD1	2.30	0.60
2:B:180:THR:HA	2:B:183:MET:HE2	1.83	0.60
1:I:14:ILE:HG22	2:V:116:LEU:HD22	1.82	0.60
2:N:34:GLU:HB3	2:N:240:TYR:HD1	1.65	0.60
1:S:71:ILE:HD12	1:S:182:VAL:HG22	1.84	0.60
1:C:95:TYR:HB2	1:C:149:TYR:CB	2.32	0.59
2:B:9:ARG:HG2	2:B:184:TRP:CE3	2.37	0.59
2:P:110:ALA:HB1	2:P:201:THR:CG2	2.33	0.59
1:E:106:ASN:H	1:E:106:ASN:ND2	2.00	0.59
2:R:34:GLU:HB3	2:R:240:TYR:HD1	1.67	0.59
1:S:98:PHE:HZ	1:S:149:TYR:CD1	2.20	0.59
1:O:2:SER:OG	1:O:105:GLU:OE2	2.21	0.59
2:F:129:THR:HG21	2:F:142:SER:OG	2.03	0.59
2:F:34:GLU:HB3	2:F:240:TYR:HD1	1.66	0.58
1:E:91:LEU:HD11	1:E:147:LEU:HD23	1.85	0.58
1:I:88:VAL:HG22	1:I:144:VAL:HB	1.85	0.58
2:X:126:ASP:HB3	2:X:128:PHE:CE1	2.38	0.58
1:G:94:ALA:HB1	1:G:149:TYR:HB2	1.85	0.58
1:Q:14:ILE:HD12	1:Q:14:ILE:H	1.68	0.58
1:W:71:ILE:HD12	1:W:182:VAL:HG22	1.84	0.58
2:B:190:PRO:HG2	2:B:204:GLN:HB2	1.85	0.58
1:C:2:SER:HB2	1:C:105:GLU:OE2	2.03	0.58
1:I:112:ARG:NH2	4:J:403:AMP:O2P	2.36	0.58
1:C:90:LEU:HD12	1:C:107:ALA:HB2	1.86	0.58
2:R:52:THR:HG21	2:R:138:SER:HA	1.84	0.58
1:C:95:TYR:HB2	1:C:149:TYR:HB3	1.85	0.58
2:D:164:VAL:HG22	2:D:225:ILE:HG13	1.85	0.58
2:F:110:ALA:HB1	2:F:201:THR:CG2	2.34	0.58
1:I:71:ILE:HD12	1:I:182:VAL:HG22	1.85	0.58
2:V:164:VAL:HG22	2:V:225:ILE:HG13	1.84	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:110:ALA:HB1	2:B:201:THR:CG2	2.34	0.58
1:K:31:GLY:HA2	2:R:233:ARG:CZ	2.34	0.58
1:Q:38:ARG:HD2	1:Q:59:GLY:HA3	1.86	0.58
1:W:94:ALA:HB1	1:W:149:TYR:HB2	1.85	0.58
2:L:126:ASP:HB3	2:L:128:PHE:CE1	2.39	0.57
1:S:42:ILE:HG12	1:S:56:VAL:HG22	1.86	0.57
2:V:129:THR:HG21	2:V:142:SER:OG	2.04	0.57
1:C:16:LYS:HG3	1:C:220:ILE:HB	1.85	0.57
1:M:42:ILE:HG12	1:M:56:VAL:HG22	1.86	0.57
1:E:112:ARG:HH22	4:F:403:AMP:P	2.27	0.57
1:Q:71:ILE:HD12	1:Q:182:VAL:HG22	1.86	0.57
1:C:71:ILE:HD12	1:C:182:VAL:HG22	1.86	0.57
1:I:38:ARG:HD2	1:I:59:GLY:HA3	1.86	0.57
1:M:14:ILE:H	1:M:14:ILE:HD12	1.68	0.57
2:V:74:ARG:HH21	2:V:117:VAL:HG21	1.70	0.57
2:H:48:GLU:HG2	2:H:53:LYS:HG2	1.85	0.57
2:L:164:VAL:HG22	2:L:225:ILE:HG13	1.86	0.57
1:G:248:LEU:HD21	2:H:193:MET:SD	2.45	0.57
1:W:38:ARG:HD2	1:W:59:GLY:HA3	1.85	0.57
1:A:38:ARG:HD2	1:A:59:GLY:HA3	1.87	0.57
2:H:126:ASP:HB3	2:H:128:PHE:CE1	2.40	0.57
1:U:38:ARG:HD2	1:U:59:GLY:HA3	1.87	0.57
1:W:42:ILE:HG12	1:W:56:VAL:HG22	1.86	0.57
2:X:223:LYS:HB3	2:X:248:VAL:CG1	2.35	0.57
2:J:8:GLU:HG3	2:J:9:ARG:N	2.20	0.57
1:K:91:LEU:HB3	1:K:93:LEU:HD13	1.86	0.57
1:O:38:ARG:HD2	1:O:59:GLY:HA3	1.87	0.57
1:A:91:LEU:HB2	1:A:146:VAL:O	2.05	0.56
2:B:9:ARG:HB3	2:B:9:ARG:NH1	2.21	0.56
2:F:52:THR:HG21	2:F:138:SER:HA	1.87	0.56
1:G:38:ARG:HD2	1:G:59:GLY:HA3	1.88	0.56
1:G:92:PRO:HA	1:G:98:PHE:HB2	1.87	0.56
1:S:93:LEU:CD1	2:V:128:PHE:HB3	2.35	0.56
2:T:110:ALA:HB1	2:T:201:THR:CG2	2.34	0.56
1:U:91:LEU:HD11	1:U:145:TYR:HD2	1.70	0.56
1:A:71:ILE:HD12	1:A:182:VAL:HG22	1.87	0.56
1:S:38:ARG:HD2	1:S:59:GLY:HA3	1.87	0.56
1:W:14:ILE:HD12	1:W:14:ILE:H	1.70	0.56
1:E:103:PRO:HB3	1:E:107:ALA:HB1	1.86	0.56
2:H:78:ARG:HD3	2:H:126:ASP:OD1	2.06	0.56
2:L:190:PRO:HG2	2:L:204:GLN:HB2	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:164:VAL:HG22	2:R:225:ILE:HG13	1.88	0.56
2:N:52:THR:HG21	2:N:138:SER:HA	1.88	0.56
2:B:126:ASP:HB3	2:B:128:PHE:CE1	2.41	0.56
1:G:71:ILE:HD12	1:G:182:VAL:HG22	1.85	0.56
1:C:14:ILE:H	1:C:14:ILE:HD12	1.71	0.56
2:H:52:THR:HG21	2:H:138:SER:HA	1.88	0.56
2:J:164:VAL:HG22	2:J:225:ILE:HG13	1.88	0.56
1:M:71:ILE:HD12	1:M:182:VAL:HG22	1.88	0.56
1:K:14:ILE:HD12	1:K:14:ILE:H	1.71	0.56
2:N:183:MET:HE3	2:N:184:TRP:HE1	1.70	0.56
2:V:9:ARG:HH21	2:V:184:TRP:HB3	1.70	0.56
2:X:110:ALA:HB1	2:X:201:THR:CG2	2.36	0.56
1:A:14:ILE:HD12	1:A:14:ILE:H	1.70	0.55
2:F:13:ILE:HD13	2:F:172:VAL:HB	1.88	0.55
2:J:52:THR:HG21	2:J:138:SER:HA	1.87	0.55
2:X:52:THR:HG21	2:X:138:SER:HA	1.87	0.55
2:D:52:THR:HG21	2:D:138:SER:HA	1.87	0.55
1:G:1:MET:HE2	1:I:100:PRO:HG3	1.87	0.55
1:M:38:ARG:HD2	1:M:59:GLY:HA3	1.87	0.55
2:F:78:ARG:HD3	2:F:126:ASP:OD1	2.07	0.55
2:F:164:VAL:HG22	2:F:225:ILE:HG13	1.87	0.55
2:B:129:THR:HG21	2:B:142:SER:OG	2.07	0.55
2:D:110:ALA:HB1	2:D:201:THR:CG2	2.37	0.55
1:E:14:ILE:HD12	1:E:14:ILE:H	1.72	0.55
2:L:52:THR:HG21	2:L:138:SER:HA	1.87	0.55
1:O:243:LYS:O	2:P:113:SER:HB3	2.06	0.55
2:P:164:VAL:HG22	2:P:225:ILE:HG13	1.87	0.55
2:L:110:ALA:HB1	2:L:201:THR:CG2	2.37	0.55
2:N:78:ARG:HD3	2:N:126:ASP:OD1	2.06	0.55
2:N:164:VAL:HG22	2:N:225:ILE:HG13	1.88	0.55
2:T:164:VAL:HG22	2:T:225:ILE:HG13	1.89	0.55
2:R:190:PRO:HG2	2:R:204:GLN:HB2	1.89	0.55
2:V:99:ARG:HH12	4:V:404:AMP:P	2.30	0.55
2:H:164:VAL:HG22	2:H:225:ILE:HG13	1.89	0.55
2:N:13:ILE:HD12	2:N:170:ASP:HB2	1.89	0.55
2:R:74:ARG:HH21	2:R:117:VAL:HG21	1.72	0.55
1:W:270:LYS:HB3	1:W:275:ILE:HA	1.87	0.55
2:D:126:ASP:HB3	2:D:128:PHE:CE1	2.42	0.55
1:O:71:ILE:HD12	1:O:182:VAL:HG22	1.89	0.55
2:T:190:PRO:HG2	2:T:204:GLN:HB2	1.89	0.54
2:V:126:ASP:HB3	2:V:128:PHE:CE1	2.43	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:ARG:NH1	2:B:102:GLU:OE1	2.41	0.54
1:E:16:LYS:HG3	1:E:220:ILE:HB	1.88	0.54
1:K:16:LYS:HG3	1:K:220:ILE:HB	1.89	0.54
1:K:71:ILE:HD12	1:K:182:VAL:HG22	1.89	0.54
1:U:71:ILE:HD12	1:U:182:VAL:HG22	1.90	0.54
2:V:78:ARG:HD3	2:V:126:ASP:OD1	2.07	0.54
2:D:129:THR:HG21	2:D:142:SER:OG	2.08	0.54
2:R:126:ASP:HB3	2:R:128:PHE:CE1	2.42	0.54
2:T:52:THR:HG21	2:T:138:SER:HA	1.89	0.54
2:X:129:THR:HG21	2:X:142:SER:OG	2.08	0.54
1:K:6:SER:C	1:K:8:GLN:H	2.15	0.54
1:W:95:TYR:HB3	1:W:98:PHE:HD1	1.71	0.54
2:X:78:ARG:HD3	2:X:126:ASP:OD1	2.08	0.54
2:H:110:ALA:HB1	2:H:201:THR:CG2	2.37	0.54
1:G:14:ILE:HD12	1:G:14:ILE:H	1.71	0.54
2:T:78:ARG:HD3	2:T:126:ASP:OD1	2.07	0.54
2:P:190:PRO:HG2	2:P:204:GLN:HB2	1.90	0.54
1:U:14:ILE:HD12	1:U:14:ILE:H	1.72	0.54
2:N:110:ALA:HB1	2:N:201:THR:CG2	2.38	0.54
2:B:52:THR:HG21	2:B:138:SER:HA	1.89	0.53
1:C:38:ARG:HD2	1:C:59:GLY:HA3	1.89	0.53
2:H:30:SER:N	2:H:245:GLU:HG2	2.23	0.53
2:X:9:ARG:HG2	2:X:184:TRP:HE3	1.62	0.53
2:X:99:ARG:HH12	4:X:404:AMP:P	2.31	0.53
2:B:164:VAL:HG22	2:B:225:ILE:HG13	1.89	0.53
1:E:97:THR:O	1:E:98:PHE:HD1	1.91	0.53
2:H:74:ARG:HH21	2:H:117:VAL:HG21	1.73	0.53
1:O:16:LYS:HG3	1:O:220:ILE:HB	1.91	0.53
2:D:223:LYS:CB	2:D:248:VAL:HG11	2.27	0.53
1:Q:252:ASP:OD1	2:R:215:ARG:NH1	2.41	0.53
1:K:98:PHE:CZ	1:K:149:TYR:CD1	2.97	0.53
2:T:248:VAL:OXT	2:T:248:VAL:HG13	2.07	0.53
2:V:110:ALA:HB1	2:V:201:THR:CG2	2.38	0.53
1:E:92:PRO:HA	1:E:98:PHE:HB3	1.91	0.53
2:P:126:ASP:HB3	2:P:128:PHE:CE1	2.43	0.53
1:Q:16:LYS:HG3	1:Q:220:ILE:HB	1.90	0.53
1:Q:42:ILE:HG12	1:Q:56:VAL:HG22	1.90	0.53
2:R:59:TYR:HB2	2:R:126:ASP:HB2	1.90	0.53
1:E:92:PRO:HA	1:E:98:PHE:HB2	1.89	0.53
1:I:16:LYS:HG3	1:I:220:ILE:HB	1.90	0.53
2:J:110:ALA:HB1	2:J:201:THR:CG2	2.39	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:31:ILE:HG12	2:N:49:MET:HG2	1.90	0.53
2:J:126:ASP:HB3	2:J:128:PHE:CE1	2.44	0.53
2:J:190:PRO:HG2	2:J:204:GLN:HB2	1.91	0.53
1:K:98:PHE:HZ	1:K:149:TYR:CD1	2.27	0.53
2:N:126:ASP:HB3	2:N:128:PHE:CE1	2.44	0.53
2:T:126:ASP:HB3	2:T:128:PHE:CE1	2.44	0.53
2:H:190:PRO:HG2	2:H:204:GLN:HB2	1.89	0.53
1:S:16:LYS:HG3	1:S:220:ILE:HB	1.91	0.53
2:V:190:PRO:HG2	2:V:204:GLN:HB2	1.91	0.53
1:E:38:ARG:HD2	1:E:59:GLY:HA3	1.91	0.52
1:O:14:ILE:H	1:O:14:ILE:HD12	1.74	0.52
2:V:52:THR:HG21	2:V:138:SER:HA	1.90	0.52
2:D:31:ILE:HG12	2:D:49:MET:HG2	1.91	0.52
1:I:14:ILE:HD12	1:I:14:ILE:H	1.73	0.52
2:N:190:PRO:HG2	2:N:204:GLN:HB2	1.90	0.52
2:B:32:LYS:HG3	2:B:242:GLU:HG3	1.92	0.52
1:K:252:ASP:OD1	2:L:215:ARG:NH1	2.40	0.52
1:M:16:LYS:HG3	1:M:220:ILE:HB	1.90	0.52
1:G:42:ILE:HG12	1:G:56:VAL:HG22	1.90	0.52
2:L:78:ARG:HD3	2:L:126:ASP:OD1	2.10	0.52
2:N:74:ARG:HH21	2:N:117:VAL:HG21	1.74	0.52
1:U:6:SER:C	1:U:8:GLN:H	2.18	0.52
2:D:74:ARG:HH21	2:D:117:VAL:HG21	1.75	0.52
1:K:32:ARG:HB2	1:K:36:ASP:HB2	1.92	0.52
2:P:78:ARG:HD3	2:P:126:ASP:OD1	2.09	0.52
1:K:42:ILE:HG12	1:K:56:VAL:HG22	1.92	0.52
1:Q:92:PRO:HD2	1:Q:93:LEU:HD12	1.92	0.52
1:A:42:ILE:HG12	1:A:56:VAL:HG22	1.91	0.52
2:N:85:PRO:HD3	1:Q:145:TYR:OH	2.10	0.52
1:S:49:LYS:O	1:S:68:LYS:HE2	2.10	0.52
2:X:190:PRO:HG2	2:X:204:GLN:HB2	1.90	0.52
2:X:223:LYS:HB3	2:X:248:VAL:HG13	1.91	0.52
2:P:59:TYR:HB2	2:P:126:ASP:HB2	1.92	0.51
2:V:30:SER:N	2:V:245:GLU:HG2	2.25	0.51
2:D:78:ARG:HD3	2:D:126:ASP:OD1	2.10	0.51
1:I:92:PRO:C	1:I:94:ALA:N	2.68	0.51
2:B:78:ARG:HD3	2:B:126:ASP:OD1	2.10	0.51
1:C:42:ILE:HG12	1:C:56:VAL:HG22	1.92	0.51
2:R:110:ALA:HB1	2:R:201:THR:CG2	2.40	0.51
2:V:180:THR:HA	2:V:183:MET:CE	2.40	0.51
2:B:30:SER:N	2:B:245:GLU:HG2	2.26	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:59:TYR:HB2	2:B:126:ASP:HB2	1.91	0.51
2:J:59:TYR:HB2	2:J:126:ASP:HB2	1.92	0.51
1:S:92:PRO:HA	1:S:98:PHE:HB3	1.92	0.51
2:P:52:THR:HG21	2:P:138:SER:HA	1.91	0.51
1:W:230:THR:OG1	1:W:232:ASP:OD1	2.26	0.51
2:X:30:SER:N	2:X:245:GLU:HG2	2.26	0.51
2:L:131:ILE:HD11	2:L:142:SER:HB2	1.93	0.51
2:D:190:PRO:HG2	2:D:204:GLN:HB2	1.93	0.51
1:G:94:ALA:HB3	1:G:98:PHE:CE1	2.46	0.51
2:D:59:TYR:HB2	2:D:126:ASP:HB2	1.92	0.51
2:F:74:ARG:HH21	2:F:117:VAL:HG21	1.76	0.51
2:P:74:ARG:HH21	2:P:117:VAL:HG21	1.76	0.51
1:O:42:ILE:HG12	1:O:56:VAL:HG22	1.93	0.50
2:X:74:ARG:HH21	2:X:117:VAL:HG21	1.75	0.50
1:C:28:ARG:CZ	1:C:210:VAL:HG13	2.41	0.50
2:F:31:ILE:HG12	2:F:49:MET:HG2	1.93	0.50
1:U:195:TYR:HB2	1:U:231:PRO:HG2	1.93	0.50
2:V:99:ARG:NH1	4:V:404:AMP:P	2.84	0.50
2:N:129:THR:HG21	2:N:142:SER:OG	2.11	0.50
1:Q:91:LEU:HD11	1:Q:145:TYR:CD2	2.46	0.50
1:W:16:LYS:HG3	1:W:220:ILE:HB	1.92	0.50
1:E:252:ASP:OD1	2:F:215:ARG:NH1	2.43	0.50
2:B:74:ARG:HH21	2:B:117:VAL:HG21	1.77	0.50
1:K:32:ARG:CZ	1:K:38:ARG:HG3	2.42	0.50
2:L:59:TYR:HB2	2:L:126:ASP:HB2	1.94	0.50
1:S:32:ARG:HB2	1:S:36:ASP:HB2	1.94	0.50
1:U:42:ILE:HG12	1:U:56:VAL:HG22	1.92	0.50
2:D:193:MET:HG3	2:D:225:ILE:HD13	1.94	0.50
2:F:13:ILE:CD1	2:F:169:ALA:HB3	2.41	0.50
1:W:28:ARG:CZ	1:W:210:VAL:HG13	2.42	0.50
1:E:195:TYR:HB2	1:E:231:PRO:HG2	1.93	0.50
2:B:193:MET:HE3	2:B:195:PRO:HA	1.94	0.50
1:M:32:ARG:HB2	1:M:36:ASP:HB2	1.93	0.50
2:T:48:GLU:CG	2:T:53:LYS:HG2	2.41	0.50
1:C:195:TYR:HB2	1:C:231:PRO:HG2	1.94	0.49
1:I:49:LYS:O	1:I:68:LYS:HE2	2.12	0.49
1:O:93:LEU:HG	2:R:57:ALA:HB3	1.93	0.49
1:G:112:ARG:NH1	2:H:102:GLU:OE1	2.45	0.49
1:Q:105:GLU:OE1	2:R:105:LYS:HG3	2.12	0.49
2:R:129:THR:HG21	2:R:142:SER:OG	2.13	0.49
2:B:193:MET:HG3	2:B:225:ILE:HD13	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:38:ARG:HD2	1:K:59:GLY:HA3	1.94	0.49
2:P:129:THR:HG21	2:P:142:SER:OG	2.13	0.49
1:O:195:TYR:HB2	1:O:231:PRO:HG2	1.94	0.49
2:R:48:GLU:CG	2:R:53:LYS:HG2	2.43	0.49
2:H:59:TYR:HB2	2:H:126:ASP:HB2	1.95	0.49
2:J:245:GLU:O	2:J:246:GLU:HB3	2.12	0.49
1:M:88:VAL:HG22	1:M:144:VAL:HB	1.95	0.49
1:U:28:ARG:CZ	1:U:210:VAL:HG13	2.43	0.49
1:S:252:ASP:OD1	2:T:215:ARG:NH1	2.42	0.49
1:A:16:LYS:HG3	1:A:220:ILE:HB	1.95	0.49
2:B:223:LYS:CB	2:B:248:VAL:HG11	2.33	0.49
2:H:99:ARG:HH12	4:H:404:AMP:P	2.36	0.49
2:L:31:ILE:HG12	2:L:49:MET:HG2	1.94	0.49
1:E:42:ILE:HG12	1:E:56:VAL:HG22	1.94	0.49
2:J:12:LEU:HD21	2:J:184:TRP:HB2	1.95	0.49
1:C:31:GLY:HA2	2:T:233:ARG:CZ	2.43	0.49
2:H:12:LEU:HD21	2:H:184:TRP:HB2	1.94	0.49
1:I:42:ILE:HG12	1:I:56:VAL:HG22	1.93	0.49
2:J:19:ARG:HD2	2:J:181:GLU:OE2	2.13	0.49
1:K:97:THR:HG22	1:K:98:PHE:HD1	1.76	0.48
1:Q:3:SER:HA	2:R:77:LEU:O	2.13	0.48
1:G:91:LEU:HD13	1:G:93:LEU:HD13	1.96	0.48
2:J:35:LEU:HD21	2:J:236:LEU:HD12	1.94	0.48
2:L:35:LEU:HD21	2:L:236:LEU:HD12	1.94	0.48
2:R:5:LEU:HG	2:R:6:GLN:H	1.78	0.48
2:T:30:SER:N	2:T:245:GLU:HG2	2.28	0.48
1:W:95:TYR:HB3	1:W:98:PHE:CD1	2.48	0.48
1:G:16:LYS:HG3	1:G:220:ILE:HB	1.95	0.48
1:I:252:ASP:OD1	2:J:215:ARG:NH1	2.45	0.48
2:N:59:TYR:HB2	2:N:126:ASP:HB2	1.95	0.48
2:V:31:ILE:HG12	2:V:49:MET:HG2	1.95	0.48
2:X:59:TYR:HB2	2:X:126:ASP:HB2	1.96	0.48
2:B:183:MET:HE3	2:B:184:TRP:HE1	1.77	0.48
1:K:28:ARG:CZ	1:K:210:VAL:HG13	2.44	0.48
1:M:195:TYR:HB2	1:M:231:PRO:HG2	1.94	0.48
1:S:121:SER:CB	1:S:236:VAL:HG21	2.43	0.48
2:B:31:ILE:HG12	2:B:49:MET:HG2	1.95	0.48
2:H:193:MET:HE3	2:H:195:PRO:HA	1.94	0.48
2:J:129:THR:HG21	2:J:142:SER:OG	2.13	0.48
1:G:195:TYR:HB2	1:G:231:PRO:HG2	1.95	0.48
2:J:193:MET:HE3	2:J:195:PRO:HA	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:88:VAL:HG22	1:O:144:VAL:HB	1.96	0.48
2:R:193:MET:HE3	2:R:195:PRO:HA	1.96	0.48
2:R:193:MET:HG3	2:R:225:ILE:HD13	1.95	0.48
2:V:35:LEU:HD21	2:V:236:LEU:HD12	1.96	0.48
1:A:32:ARG:HB2	1:A:36:ASP:HB2	1.96	0.48
2:J:99:ARG:NH1	4:J:404:AMP:O2P	2.46	0.48
2:N:91:ARG:HD2	1:Q:141:TRP:CG	2.49	0.48
1:O:32:ARG:HB2	1:O:36:ASP:HB2	1.96	0.48
2:X:31:ILE:HG12	2:X:49:MET:HG2	1.96	0.48
2:F:190:PRO:HG2	2:F:204:GLN:HB2	1.96	0.48
1:I:91:LEU:HG	1:I:146:VAL:O	2.13	0.48
2:L:74:ARG:HH21	2:L:117:VAL:HG21	1.79	0.48
2:N:13:ILE:CD1	2:N:170:ASP:H	2.27	0.48
1:Q:121:SER:CB	1:Q:236:VAL:HG21	2.44	0.48
2:R:48:GLU:OE1	2:R:53:LYS:HE2	2.14	0.48
1:U:49:LYS:O	1:U:68:LYS:HE2	2.14	0.48
1:W:195:TYR:HB2	1:W:231:PRO:HG2	1.96	0.48
2:H:91:ARG:HD2	1:I:141:TRP:CG	2.49	0.48
1:K:90:LEU:HD11	1:K:106:ASN:HB2	1.96	0.48
1:K:98:PHE:CD1	1:K:98:PHE:N	2.81	0.48
2:V:48:GLU:CG	2:V:53:LYS:HG2	2.40	0.48
2:V:59:TYR:HB2	2:V:126:ASP:HB2	1.94	0.48
2:B:9:ARG:HG2	2:B:184:TRP:CZ3	2.49	0.47
2:B:227:ILE:CD1	2:B:248:VAL:HG22	2.43	0.47
2:F:59:TYR:HB2	2:F:126:ASP:HB2	1.96	0.47
1:U:102:PRO:HB3	1:U:103:PRO:HD2	1.96	0.47
1:C:91:LEU:HD12	1:C:93:LEU:HD13	1.96	0.47
2:D:19:ARG:HD2	2:D:181:GLU:OE2	2.14	0.47
1:M:112:ARG:HH22	4:N:403:AMP:P	2.37	0.47
2:P:31:ILE:HG12	2:P:49:MET:HG2	1.96	0.47
2:X:35:LEU:HD21	2:X:236:LEU:HD12	1.96	0.47
1:C:32:ARG:HB2	1:C:36:ASP:HB2	1.95	0.47
2:F:9:ARG:HH21	2:F:184:TRP:HB3	1.79	0.47
2:X:193:MET:HG3	2:X:225:ILE:HD13	1.97	0.47
1:E:102:PRO:HA	1:E:103:PRO:HD3	1.81	0.47
2:T:31:ILE:HG12	2:T:49:MET:HG2	1.96	0.47
3:B:301:CL:CL	4:B:404:AMP:H5'2	2.51	0.47
2:D:193:MET:HE3	2:D:195:PRO:HA	1.97	0.47
1:E:32:ARG:HB2	1:E:36:ASP:HB2	1.96	0.47
1:E:91:LEU:HD12	1:E:93:LEU:HD13	1.96	0.47
2:P:30:SER:N	2:P:245:GLU:HG2	2.30	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:30:SER:N	2:R:245:GLU:HG2	2.30	0.47
2:R:78:ARG:HD3	2:R:126:ASP:OD1	2.14	0.47
1:U:13:ILE:H	1:U:13:ILE:HG13	1.34	0.47
1:K:85:ILE:HG21	1:K:141:TRP:CZ3	2.49	0.47
2:N:79:VAL:HG22	2:N:127:VAL:HB	1.96	0.47
2:V:12:LEU:HD11	2:V:184:TRP:HB2	1.97	0.47
1:C:89:GLU:HG2	1:C:103:PRO:CG	2.42	0.47
1:C:226:SER:O	1:C:238:ILE:HA	2.14	0.47
2:F:35:LEU:HD21	2:F:236:LEU:HD12	1.96	0.47
2:F:243:PHE:CZ	2:F:246:GLU:HB3	2.49	0.47
1:G:32:ARG:HB2	1:G:36:ASP:HB2	1.95	0.47
1:G:255:GLU:HG2	2:H:214:PHE:CE2	2.50	0.47
1:K:2:SER:CB	1:K:105:GLU:OE2	2.62	0.47
1:M:49:LYS:O	1:M:68:LYS:HE2	2.15	0.47
2:P:35:LEU:HD21	2:P:236:LEU:HD12	1.96	0.47
2:P:135:ASP:OD1	2:P:179:GLU:HB2	2.15	0.47
2:T:193:MET:HG3	2:T:225:ILE:HD13	1.97	0.47
1:U:97:THR:C	1:U:98:PHE:HD1	2.23	0.47
2:V:131:ILE:HD11	2:V:142:SER:HB2	1.96	0.47
1:W:32:ARG:HB2	1:W:36:ASP:HB2	1.96	0.47
1:W:104:ASP:O	1:W:106:ASN:N	2.48	0.47
1:C:32:ARG:CZ	1:C:38:ARG:HG3	2.45	0.47
1:E:49:LYS:O	1:E:68:LYS:HE2	2.15	0.47
1:U:88:VAL:HG22	1:U:144:VAL:HB	1.96	0.47
2:X:131:ILE:HD11	2:X:142:SER:HB2	1.96	0.47
2:H:31:ILE:HG12	2:H:49:MET:HG2	1.95	0.47
1:I:121:SER:CB	1:I:236:VAL:HG21	2.45	0.47
1:W:132:GLU:HG2	1:W:135:LYS:CB	2.45	0.47
1:A:195:TYR:HB2	1:A:231:PRO:HG2	1.96	0.47
1:E:86:VAL:HG22	1:E:142:LEU:HD23	1.97	0.47
1:I:5:PRO:HD2	1:I:243:LYS:HE2	1.97	0.47
2:J:78:ARG:HD3	2:J:126:ASP:OD1	2.14	0.47
2:L:157:MET:HE3	2:L:157:MET:HB2	1.85	0.47
2:R:64:MET:HE3	2:R:64:MET:HB2	1.71	0.47
1:U:91:LEU:C	1:U:93:LEU:N	2.72	0.47
1:W:57:LYS:HG2	1:W:62:MET:HG2	1.97	0.47
2:T:35:LEU:HD21	2:T:236:LEU:HD12	1.96	0.46
1:G:130:VAL:HA	1:G:137:VAL:HG12	1.95	0.46
2:N:131:ILE:HD11	2:N:142:SER:HB2	1.97	0.46
2:R:245:GLU:O	2:R:246:GLU:HB3	2.15	0.46
2:V:13:ILE:CD1	2:V:169:ALA:HB3	2.40	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:193:MET:HE3	2:F:195:PRO:HA	1.97	0.46
3:J:301:CL:CL	4:J:404:AMP:H5'2	2.52	0.46
2:P:19:ARG:HD2	2:P:181:GLU:OE2	2.15	0.46
1:S:93:LEU:HD12	2:V:128:PHE:HB3	1.97	0.46
1:S:98:PHE:CZ	1:S:149:TYR:CD1	3.02	0.46
1:E:3:SER:HA	2:F:77:LEU:O	2.16	0.46
2:F:131:ILE:HD11	2:F:142:SER:HB2	1.97	0.46
1:G:93:LEU:HG	2:L:128:PHE:HB2	1.97	0.46
1:S:7:ASN:O	1:S:8:GLN:C	2.58	0.46
1:A:142:LEU:HD21	1:A:161:SER:HB3	1.96	0.46
4:B:401:AMP:O3P	4:B:401:AMP:H8	1.98	0.46
2:F:193:MET:HG3	2:F:225:ILE:HD13	1.98	0.46
2:J:30:SER:N	2:J:245:GLU:HG2	2.30	0.46
1:M:95:TYR:HB2	1:M:149:TYR:HB3	1.96	0.46
2:D:79:VAL:HG22	2:D:127:VAL:HB	1.97	0.46
2:D:131:ILE:HD11	2:D:142:SER:HB2	1.97	0.46
2:L:79:VAL:HG22	2:L:127:VAL:HB	1.97	0.46
1:U:16:LYS:HG3	1:U:220:ILE:HB	1.97	0.46
1:U:32:ARG:HB2	1:U:36:ASP:HB2	1.98	0.46
1:U:130:VAL:HA	1:U:137:VAL:HG12	1.97	0.46
1:W:49:LYS:O	1:W:68:LYS:HE2	2.16	0.46
2:B:23:ARG:NH1	2:B:29:ARG:HG3	2.31	0.46
2:H:64:MET:HG2	2:H:66:PRO:HD2	1.98	0.46
2:N:30:SER:N	2:N:245:GLU:HG2	2.30	0.46
1:S:195:TYR:HB2	1:S:231:PRO:HG2	1.97	0.46
2:X:14:LEU:C	2:X:16:ASP:H	2.23	0.46
2:D:35:LEU:HD21	2:D:236:LEU:HD12	1.98	0.46
1:K:126:LEU:HA	1:K:129:LEU:HD12	1.98	0.46
2:L:23:ARG:NH1	2:L:29:ARG:HG3	2.30	0.46
2:L:129:THR:HG21	2:L:142:SER:OG	2.15	0.46
2:R:135:ASP:OD1	2:R:179:GLU:HB2	2.14	0.46
2:T:74:ARG:HH21	2:T:117:VAL:HG21	1.80	0.46
1:I:86:VAL:O	1:I:111:ALA:HB1	2.15	0.46
1:S:142:LEU:HD21	1:S:161:SER:HB3	1.98	0.46
2:T:59:TYR:HB2	2:T:126:ASP:HB2	1.98	0.46
2:B:11:LYS:HE3	2:B:14:LEU:HA	1.97	0.46
1:C:121:SER:CB	1:C:236:VAL:HG21	2.46	0.46
1:G:251:ILE:HD12	2:H:200:VAL:HG21	1.98	0.46
1:I:104:ASP:O	1:I:105:GLU:C	2.59	0.46
2:L:30:SER:N	2:L:245:GLU:HG2	2.30	0.46
1:U:91:LEU:C	1:U:93:LEU:H	2.24	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:16:ASP:C	2:H:18:LYS:H	2.24	0.45
2:N:35:LEU:HD21	2:N:236:LEU:HD12	1.98	0.45
2:D:64:MET:HE3	2:D:64:MET:HB2	1.74	0.45
1:I:130:VAL:HA	1:I:137:VAL:HG12	1.98	0.45
1:K:195:TYR:HB2	1:K:231:PRO:HG2	1.97	0.45
2:R:35:LEU:HD21	2:R:236:LEU:HD12	1.98	0.45
1:S:28:ARG:CZ	1:S:210:VAL:HG13	2.46	0.45
2:T:9:ARG:HG3	2:T:184:TRP:CE3	2.51	0.45
2:V:99:ARG:NH1	4:V:404:AMP:O5'	2.49	0.45
1:A:49:LYS:O	1:A:68:LYS:HE2	2.16	0.45
2:J:79:VAL:HG22	2:J:127:VAL:HB	1.98	0.45
2:N:64:MET:HE3	2:N:64:MET:HB2	1.71	0.45
1:S:130:VAL:HA	1:S:137:VAL:HG12	1.99	0.45
1:E:32:ARG:CZ	1:E:38:ARG:HG3	2.46	0.45
2:F:79:VAL:HG22	2:F:127:VAL:HB	1.98	0.45
2:F:99:ARG:HH12	4:F:404:AMP:P	2.39	0.45
1:G:28:ARG:CZ	1:G:210:VAL:HG13	2.46	0.45
1:I:28:ARG:CZ	1:I:210:VAL:HG13	2.47	0.45
2:L:19:ARG:HD2	2:L:181:GLU:OE2	2.16	0.45
2:N:248:VAL:OXT	2:N:248:VAL:HG13	2.15	0.45
1:Q:49:LYS:O	1:Q:68:LYS:HE2	2.17	0.45
2:R:122:ARG:HD3	2:R:122:ARG:HA	1.78	0.45
1:U:91:LEU:HD12	1:U:147:LEU:HD23	1.97	0.45
1:W:121:SER:CB	1:W:236:VAL:HG21	2.46	0.45
2:J:59:TYR:OH	1:K:93:LEU:O	2.33	0.45
1:O:49:LYS:O	1:O:68:LYS:HE2	2.15	0.45
1:A:88:VAL:HG22	1:A:144:VAL:HB	1.98	0.45
1:M:130:VAL:HA	1:M:137:VAL:HG12	1.99	0.45
2:P:223:LYS:HB3	2:P:248:VAL:HG11	1.97	0.45
2:R:31:ILE:HG12	2:R:49:MET:HG2	1.97	0.45
1:G:90:LEU:HD22	1:G:98:PHE:CZ	2.51	0.45
1:G:92:PRO:HA	1:G:98:PHE:CB	2.46	0.45
2:H:79:VAL:HG22	2:H:127:VAL:HB	1.99	0.45
1:K:255:GLU:HG2	2:L:214:PHE:CE2	2.52	0.45
1:M:28:ARG:CZ	1:M:210:VAL:HG13	2.47	0.45
1:O:32:ARG:CZ	1:O:38:ARG:HG3	2.46	0.45
1:O:94:ALA:HB1	1:O:149:TYR:HB2	1.99	0.45
1:O:105:GLU:HG2	2:P:105:LYS:HB2	1.98	0.45
1:C:49:LYS:O	1:C:68:LYS:HE2	2.16	0.45
1:C:92:PRO:HG2	2:F:128:PHE:CE2	2.52	0.45
2:D:30:SER:N	2:D:245:GLU:HG2	2.32	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:88:VAL:HG22	1:G:144:VAL:HB	1.99	0.45
1:O:28:ARG:CZ	1:O:210:VAL:HG13	2.47	0.45
1:Q:32:ARG:HB2	1:Q:36:ASP:HB2	1.99	0.45
1:A:130:VAL:HA	1:A:137:VAL:HG12	1.99	0.45
2:B:35:LEU:HD21	2:B:236:LEU:HD12	1.98	0.45
1:E:121:SER:CB	1:E:236:VAL:HG21	2.46	0.45
2:H:64:MET:HE3	2:H:64:MET:HB2	1.72	0.45
2:H:131:ILE:HD11	2:H:142:SER:HB2	1.99	0.45
1:I:32:ARG:HB2	1:I:36:ASP:HB2	1.99	0.45
2:J:31:ILE:HG12	2:J:49:MET:HG2	1.98	0.45
1:O:91:LEU:CD1	1:O:93:LEU:HD13	2.47	0.45
2:P:193:MET:HG3	2:P:225:ILE:HD13	1.98	0.45
1:S:3:SER:HA	2:T:77:LEU:O	2.17	0.45
1:W:92:PRO:HA	1:W:98:PHE:HB3	1.99	0.45
2:H:35:LEU:HD21	2:H:236:LEU:HD12	1.98	0.45
1:I:195:TYR:HB2	1:I:231:PRO:HG2	1.99	0.45
2:T:23:ARG:NH1	2:T:29:ARG:HG3	2.32	0.45
1:I:13:ILE:H	1:I:13:ILE:HG13	1.37	0.44
2:L:122:ARG:HA	2:L:122:ARG:HD3	1.79	0.44
2:P:157:MET:HE3	2:P:157:MET:HB2	1.89	0.44
2:T:129:THR:HG21	2:T:142:SER:OG	2.16	0.44
1:I:2:SER:HB2	1:I:105:GLU:OE2	2.17	0.44
2:J:23:ARG:CZ	2:J:29:ARG:HG3	2.48	0.44
2:L:64:MET:HE3	2:L:64:MET:HB2	1.73	0.44
1:M:92:PRO:HA	1:M:98:PHE:HB2	1.98	0.44
2:R:2:ARG:O	2:R:3:GLU:HB2	2.15	0.44
2:F:30:SER:N	2:F:245:GLU:HG2	2.32	0.44
1:O:121:SER:CB	1:O:236:VAL:HG21	2.46	0.44
2:T:53:LYS:HD2	2:T:133:GLN:CD	2.43	0.44
2:T:79:VAL:HG22	2:T:127:VAL:HB	1.99	0.44
1:A:121:SER:CB	1:A:236:VAL:HG21	2.48	0.44
2:B:135:ASP:OD1	2:B:179:GLU:HB2	2.18	0.44
1:G:121:SER:CB	1:G:236:VAL:HG21	2.47	0.44
2:J:64:MET:HE3	2:J:64:MET:HB2	1.73	0.44
1:M:99:GLU:HA	1:M:100:PRO:HD2	1.87	0.44
2:R:77:LEU:HD23	2:R:77:LEU:HA	1.85	0.44
2:X:23:ARG:NH1	2:X:29:ARG:HG3	2.33	0.44
2:B:131:ILE:HD11	2:B:142:SER:HB2	1.99	0.44
1:E:62:MET:HB2	1:E:148:ASP:HB2	1.99	0.44
1:K:91:LEU:C	1:K:93:LEU:H	2.25	0.44
1:K:112:ARG:NH1	2:L:102:GLU:OE1	2.49	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:40:ASN:HB2	1:W:94:ALA:O	2.17	0.44
1:E:91:LEU:HB2	1:E:93:LEU:HD13	2.00	0.44
2:H:8:GLU:OE2	2:H:8:GLU:CA	2.60	0.44
2:H:129:THR:HG21	2:H:142:SER:OG	2.18	0.44
2:H:157:MET:HE3	2:H:157:MET:HB2	1.84	0.44
1:I:142:LEU:HD21	1:I:161:SER:HB3	1.99	0.44
2:J:91:ARG:HD2	1:K:141:TRP:CG	2.52	0.44
2:L:193:MET:HG3	2:L:225:ILE:HD13	1.99	0.44
1:Q:195:TYR:HB2	1:Q:231:PRO:HG2	1.98	0.44
1:S:104:ASP:O	1:S:105:GLU:C	2.61	0.44
1:S:122:LYS:HB3	1:S:122:LYS:HE2	1.59	0.44
1:U:122:LYS:HD3	1:U:122:LYS:HA	1.81	0.44
2:V:155:ILE:HA	2:V:156:PRO:HD3	1.92	0.44
2:V:193:MET:HG3	2:V:225:ILE:HD13	2.00	0.44
1:M:13:ILE:H	1:M:13:ILE:HG13	1.38	0.44
1:S:89:GLU:HG2	1:S:103:PRO:HG3	2.00	0.44
2:T:122:ARG:HD3	2:T:122:ARG:HA	1.77	0.44
2:X:223:LYS:HB3	2:X:248:VAL:HG11	2.00	0.44
1:A:3:SER:HA	2:B:77:LEU:O	2.18	0.44
1:A:28:ARG:CZ	1:A:210:VAL:HG13	2.48	0.44
1:M:16:LYS:O	1:M:20:VAL:HG23	2.17	0.44
2:P:110:ALA:HB1	2:P:201:THR:HG22	1.99	0.44
1:U:121:SER:CB	1:U:236:VAL:HG21	2.48	0.44
2:V:193:MET:HE3	2:V:195:PRO:HA	2.00	0.44
1:W:32:ARG:CZ	1:W:38:ARG:HG3	2.48	0.44
2:H:48:GLU:CG	2:H:53:LYS:HG2	2.48	0.44
1:K:94:ALA:HB1	1:K:149:TYR:HB2	2.00	0.44
2:L:19:ARG:HD3	2:L:174:ILE:HG21	1.99	0.44
1:Q:32:ARG:CZ	1:Q:38:ARG:HG3	2.48	0.44
2:T:193:MET:HE3	2:T:195:PRO:HA	2.00	0.44
1:U:142:LEU:HD21	1:U:161:SER:HB3	2.00	0.44
2:X:122:ARG:HA	2:X:122:ARG:HD3	1.75	0.44
1:C:95:TYR:HB2	1:C:149:TYR:HB2	1.99	0.43
2:P:16:ASP:C	2:P:18:LYS:H	2.26	0.43
2:P:122:ARG:HA	2:P:122:ARG:HD3	1.80	0.43
1:Q:62:MET:HB2	1:Q:148:ASP:HB2	2.00	0.43
3:V:301:CL:CL	4:V:404:AMP:H5'2	2.55	0.43
2:F:13:ILE:CD1	2:F:172:VAL:HB	2.47	0.43
2:F:27:GLU:HG2	2:F:247:GLY:HA2	2.00	0.43
2:H:34:GLU:HB3	2:H:240:TYR:CD1	2.49	0.43
2:P:27:GLU:HG2	2:P:247:GLY:HA2	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:131:ILE:HD11	2:R:142:SER:HB2	2.00	0.43
1:S:91:LEU:HD12	1:S:93:LEU:HD13	2.01	0.43
2:V:122:ARG:HA	2:V:122:ARG:HD3	1.79	0.43
2:F:135:ASP:OD1	2:F:179:GLU:HB2	2.18	0.43
1:G:49:LYS:O	1:G:68:LYS:HE2	2.18	0.43
1:K:226:SER:O	1:K:238:ILE:HA	2.17	0.43
1:M:112:ARG:NH1	2:N:102:GLU:OE1	2.51	0.43
1:S:13:ILE:H	1:S:13:ILE:HG13	1.33	0.43
1:S:112:ARG:NH1	2:T:102:GLU:OE1	2.50	0.43
1:G:126:LEU:HA	1:G:129:LEU:HD12	2.00	0.43
1:K:6:SER:C	1:K:8:GLN:N	2.77	0.43
2:L:193:MET:HE3	2:L:195:PRO:HA	1.99	0.43
1:M:96:GLU:H	1:M:96:GLU:HG3	1.38	0.43
2:N:193:MET:HG3	2:N:225:ILE:HD13	2.00	0.43
1:O:243:LYS:HE3	1:O:243:LYS:HB3	1.90	0.43
1:Q:200:ILE:HG21	1:Q:258:ALA:HA	2.00	0.43
1:U:92:PRO:HB2	2:X:128:PHE:CD2	2.53	0.43
1:G:62:MET:HB2	1:G:148:ASP:HB2	2.00	0.43
2:P:161:ILE:HD13	2:P:201:THR:HG21	2.01	0.43
2:P:175:LEU:HD21	2:P:248:VAL:HG21	2.00	0.43
1:W:7:ASN:O	1:W:8:GLN:C	2.61	0.43
1:C:57:LYS:HG2	1:C:62:MET:HG2	1.99	0.43
2:D:9:ARG:HA	2:D:10:PRO:HD3	1.74	0.43
1:G:91:LEU:C	1:G:93:LEU:N	2.76	0.43
1:M:121:SER:CB	1:M:236:VAL:HG21	2.49	0.43
2:P:193:MET:HE3	2:P:195:PRO:HA	2.00	0.43
2:T:34:GLU:HB3	2:T:240:TYR:CD1	2.50	0.43
2:V:23:ARG:NH1	2:V:29:ARG:HG3	2.33	0.43
1:W:13:ILE:H	1:W:13:ILE:HG13	1.37	0.43
2:X:9:ARG:HH21	2:X:12:LEU:HG	1.84	0.43
2:L:95:ALA:HA	2:L:96:PRO:HD3	1.88	0.43
1:M:142:LEU:HD21	1:M:161:SER:HB3	2.01	0.43
1:O:92:PRO:HA	1:O:98:PHE:HB2	2.00	0.43
1:Q:142:LEU:HD21	1:Q:161:SER:HB3	2.00	0.43
1:W:32:ARG:HB2	1:W:36:ASP:CB	2.48	0.43
1:W:142:LEU:HD21	1:W:161:SER:HB3	2.01	0.43
2:X:19:ARG:HD2	2:X:181:GLU:OE2	2.19	0.43
2:B:64:MET:HE3	2:B:64:MET:HB2	1.79	0.43
1:G:142:LEU:HD21	1:G:161:SER:HB3	2.00	0.43
2:H:135:ASP:OD1	2:H:179:GLU:HB2	2.18	0.43
4:H:403:AMP:H5'2	4:H:404:AMP:O2P	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:155:ILE:HA	2:J:156:PRO:HD3	1.93	0.43
2:J:193:MET:HG3	2:J:225:ILE:HD13	2.01	0.43
1:M:141:TRP:CG	2:P:91:ARG:HD2	2.54	0.43
2:N:157:MET:HE3	2:N:157:MET:HB2	1.95	0.43
2:N:192:ALA:HB3	2:N:202:LEU:HB3	2.01	0.43
1:Q:28:ARG:CZ	1:Q:210:VAL:HG13	2.49	0.43
1:U:62:MET:HB2	1:U:148:ASP:HB2	2.00	0.43
1:U:100:PRO:HG2	1:W:1:MET:CE	2.49	0.43
1:E:28:ARG:CZ	1:E:210:VAL:HG13	2.48	0.43
2:J:11:LYS:HE2	2:J:11:LYS:HB3	1.79	0.43
1:M:200:ILE:HG21	1:M:258:ALA:HA	2.01	0.43
2:N:19:ARG:HD2	2:N:181:GLU:OE2	2.19	0.43
1:O:57:LYS:HG2	1:O:62:MET:HG2	2.01	0.43
1:Q:88:VAL:HG22	1:Q:144:VAL:HB	2.00	0.43
2:R:54:ALA:HB3	2:R:141:VAL:HG12	2.01	0.43
2:X:193:MET:HE3	2:X:195:PRO:HA	2.01	0.43
2:F:122:ARG:HD3	2:F:122:ARG:HA	1.80	0.43
1:S:32:ARG:CZ	1:S:38:ARG:HG3	2.48	0.43
1:S:226:SER:O	1:S:238:ILE:HA	2.19	0.43
2:B:79:VAL:HG22	2:B:127:VAL:HB	2.01	0.42
1:S:145:TYR:OH	2:V:85:PRO:HD3	2.19	0.42
1:U:99:GLU:HA	1:U:100:PRO:HD3	1.73	0.42
1:C:3:SER:HA	2:D:77:LEU:O	2.19	0.42
2:J:95:ALA:HA	2:J:96:PRO:HD3	1.84	0.42
1:O:232:ASP:O	1:O:233:LEU:HB2	2.17	0.42
1:E:57:LYS:HG2	1:E:62:MET:HG2	2.00	0.42
2:F:189:MET:HE3	2:F:205:LEU:HD13	1.99	0.42
1:O:126:LEU:HA	1:O:129:LEU:HD12	2.02	0.42
1:S:7:ASN:ND2	1:S:7:ASN:H	2.18	0.42
1:S:62:MET:HB2	1:S:148:ASP:HB2	2.00	0.42
2:T:75:ALA:HA	2:T:123:THR:O	2.20	0.42
1:W:86:VAL:HG12	1:W:87:ASN:H	1.84	0.42
1:C:130:VAL:HA	1:C:137:VAL:HG12	2.02	0.42
1:G:32:ARG:HB2	1:G:36:ASP:CB	2.50	0.42
2:H:40:ASN:HB2	1:I:94:ALA:O	2.19	0.42
2:X:77:LEU:HD23	2:X:77:LEU:HA	1.81	0.42
2:X:192:ALA:HB3	2:X:202:LEU:HB3	2.02	0.42
2:B:151:ALA:HB2	2:B:157:MET:HE1	2.01	0.42
1:C:142:LEU:HD21	1:C:161:SER:HB3	2.02	0.42
2:D:135:ASP:OD1	2:D:179:GLU:HB2	2.20	0.42
1:E:32:ARG:HB2	1:E:36:ASP:CB	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:79:VAL:HG22	2:V:127:VAL:HB	2.01	0.42
2:B:23:ARG:CZ	2:B:29:ARG:HG3	2.49	0.42
1:G:2:SER:OG	1:G:105:GLU:OE2	2.37	0.42
2:J:99:ARG:NH1	4:J:404:AMP:O5'	2.52	0.42
1:M:11:ILE:HA	1:M:12:PRO:HD3	1.95	0.42
1:M:232:ASP:OD1	1:M:232:ASP:N	2.49	0.42
2:N:193:MET:HE3	2:N:195:PRO:HA	2.02	0.42
2:T:131:ILE:HD11	2:T:142:SER:HB2	2.02	0.42
1:U:32:ARG:CZ	1:U:38:ARG:HG3	2.50	0.42
2:J:74:ARG:HH21	2:J:117:VAL:HG21	1.84	0.42
2:N:9:ARG:HA	2:N:10:PRO:HD3	1.92	0.42
1:O:13:ILE:H	1:O:13:ILE:HG13	1.39	0.42
1:O:91:LEU:HD12	1:O:93:LEU:HD13	2.02	0.42
2:R:223:LYS:HB3	2:R:248:VAL:HG11	2.01	0.42
2:T:77:LEU:HD23	2:T:77:LEU:HA	1.88	0.42
2:X:23:ARG:CZ	2:X:29:ARG:HG3	2.50	0.42
2:D:13:ILE:HG13	2:D:172:VAL:HB	2.01	0.42
2:D:122:ARG:HA	2:D:122:ARG:HD3	1.79	0.42
2:F:19:ARG:HD3	2:F:174:ILE:HG21	2.02	0.42
1:I:62:MET:HB2	1:I:148:ASP:HB2	2.01	0.42
2:J:34:GLU:HB3	2:J:240:TYR:CD1	2.50	0.42
2:N:161:ILE:HD13	2:N:201:THR:HG21	2.01	0.42
2:T:11:LYS:HB3	2:T:11:LYS:HE3	1.88	0.42
2:X:48:GLU:HG2	2:X:53:LYS:HG2	2.01	0.42
2:X:135:ASP:OD1	2:X:179:GLU:HB2	2.20	0.42
2:F:31:ILE:HA	2:F:48:GLU:O	2.20	0.42
1:G:1:MET:SD	1:I:100:PRO:HG3	2.59	0.42
2:H:27:GLU:HG2	2:H:247:GLY:HA2	2.02	0.42
1:K:32:ARG:HB2	1:K:36:ASP:CB	2.49	0.42
2:N:135:ASP:OD1	2:N:179:GLU:HB2	2.20	0.42
1:S:32:ARG:HB2	1:S:36:ASP:CB	2.50	0.42
2:D:95:ALA:HA	2:D:96:PRO:HD3	1.86	0.42
1:E:130:VAL:HA	1:E:137:VAL:HG12	2.02	0.42
1:G:99:GLU:HA	1:G:100:PRO:HD3	1.90	0.42
2:H:193:MET:HG3	2:H:225:ILE:HD13	2.01	0.42
2:J:161:ILE:HD13	2:J:201:THR:HG21	2.02	0.42
2:L:34:GLU:HB3	2:L:240:TYR:CD1	2.50	0.42
2:N:189:MET:HE3	2:N:205:LEU:HD13	2.01	0.42
1:O:6:SER:O	1:O:8:GLN:N	2.53	0.42
1:Q:91:LEU:HA	1:Q:92:PRO:HD3	1.80	0.42
1:U:248:LEU:HD21	2:V:193:MET:SD	2.59	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:157:MET:HE3	2:X:157:MET:HB2	1.86	0.42
2:B:34:GLU:HB3	2:B:240:TYR:CD1	2.51	0.41
2:B:183:MET:HE3	2:B:184:TRP:NE1	2.35	0.41
2:P:11:LYS:HE3	2:P:11:LYS:HB3	1.89	0.41
2:P:34:GLU:HB3	2:P:240:TYR:CD1	2.51	0.41
1:U:16:LYS:O	1:U:20:VAL:HG23	2.20	0.41
1:A:11:ILE:HA	1:A:12:PRO:HD3	1.92	0.41
1:E:91:LEU:HG	1:E:146:VAL:O	2.20	0.41
1:G:91:LEU:C	1:G:93:LEU:H	2.28	0.41
2:H:23:ARG:CZ	2:H:29:ARG:HG3	2.50	0.41
1:K:3:SER:HA	2:L:77:LEU:O	2.20	0.41
1:K:98:PHE:HD1	1:K:98:PHE:N	2.18	0.41
2:T:248:VAL:OXT	2:T:248:VAL:CG1	2.66	0.41
2:V:23:ARG:CZ	2:V:29:ARG:HG3	2.51	0.41
1:W:99:GLU:HA	1:W:100:PRO:HD3	1.94	0.41
1:C:126:LEU:HA	1:C:129:LEU:HD12	2.01	0.41
1:C:255:GLU:HG2	2:D:214:PHE:CE2	2.55	0.41
1:G:226:SER:O	1:G:238:ILE:HA	2.20	0.41
2:H:11:LYS:HB3	2:H:11:LYS:HE2	1.49	0.41
1:I:32:ARG:CZ	1:I:38:ARG:HG3	2.50	0.41
1:K:49:LYS:O	1:K:68:LYS:HE2	2.20	0.41
1:K:130:VAL:HA	1:K:137:VAL:HG12	2.02	0.41
2:L:77:LEU:HD23	2:L:77:LEU:HA	1.90	0.41
1:O:91:LEU:HG	1:O:146:VAL:O	2.20	0.41
2:V:192:ALA:HB3	2:V:202:LEU:HB3	2.02	0.41
2:X:19:ARG:HD3	2:X:174:ILE:HG21	2.01	0.41
1:E:13:ILE:H	1:E:13:ILE:HG13	1.37	0.41
2:F:161:ILE:HD13	2:F:201:THR:HG21	2.02	0.41
2:L:161:ILE:HD13	2:L:201:THR:HG21	2.02	0.41
1:M:32:ARG:HB2	1:M:36:ASP:CB	2.50	0.41
1:M:226:SER:O	1:M:238:ILE:HA	2.20	0.41
2:P:131:ILE:HD11	2:P:142:SER:HB2	2.03	0.41
2:R:2:ARG:O	2:R:3:GLU:CB	2.68	0.41
1:A:112:ARG:HD3	2:B:102:GLU:OE1	2.20	0.41
2:J:31:ILE:HA	2:J:48:GLU:O	2.20	0.41
1:O:252:ASP:OD1	2:P:215:ARG:NH1	2.50	0.41
2:T:31:ILE:HA	2:T:48:GLU:O	2.19	0.41
2:V:135:ASP:OD1	2:V:179:GLU:HB2	2.21	0.41
1:A:32:ARG:HB2	1:A:36:ASP:CB	2.50	0.41
1:A:251:ILE:HD12	2:B:200:VAL:HG21	2.02	0.41
2:D:155:ILE:HA	2:D:156:PRO:HD3	1.93	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:189:MET:HE1	2:D:214:PHE:HD1	1.86	0.41
1:I:248:LEU:HD21	2:J:193:MET:SD	2.60	0.41
2:J:189:MET:HE3	2:J:205:LEU:HD13	2.03	0.41
2:R:23:ARG:NH1	2:R:29:ARG:HG3	2.36	0.41
2:V:64:MET:HE3	2:V:64:MET:HB2	1.74	0.41
1:A:94:ALA:HB1	1:A:149:TYR:HB2	2.02	0.41
2:F:11:LYS:HE3	2:F:14:LEU:HA	2.01	0.41
2:P:2:ARG:HD3	2:P:2:ARG:N	2.35	0.41
2:R:19:ARG:HD2	2:R:181:GLU:OE2	2.21	0.41
2:T:135:ASP:OD1	2:T:179:GLU:HB2	2.21	0.41
2:V:19:ARG:HD2	2:V:181:GLU:OE2	2.21	0.41
2:J:8:GLU:CG	2:J:9:ARG:N	2.82	0.41
2:N:122:ARG:HD3	2:N:122:ARG:HA	1.76	0.41
2:X:75:ALA:HA	2:X:123:THR:O	2.21	0.41
2:X:243:PHE:CZ	2:X:246:GLU:HG2	2.55	0.41
1:C:32:ARG:HB2	1:C:36:ASP:CB	2.51	0.41
2:D:23:ARG:HH12	2:D:176:ASP:HB3	1.86	0.41
1:I:57:LYS:HG2	1:I:62:MET:HG2	2.02	0.41
1:K:121:SER:CB	1:K:236:VAL:HG21	2.51	0.41
1:K:168:THR:HB	1:K:191:LEU:HD22	2.03	0.41
2:N:136:ALA:HA	4:N:404:AMP:O3'	2.21	0.41
1:O:130:VAL:HA	1:O:137:VAL:HG12	2.02	0.41
1:Q:240:LYS:HB2	2:R:203:PHE:HB3	2.03	0.41
2:R:11:LYS:HE3	2:R:11:LYS:HB3	1.87	0.41
1:S:57:LYS:HG2	1:S:62:MET:HG2	2.03	0.41
1:S:85:ILE:HG21	1:S:141:TRP:CZ3	2.56	0.41
2:T:19:ARG:HD3	2:T:174:ILE:HG21	2.03	0.41
2:T:85:PRO:HD3	1:W:145:TYR:OH	2.20	0.41
1:W:104:ASP:O	1:W:105:GLU:C	2.64	0.41
1:W:112:ARG:NH1	2:X:102:GLU:OE1	2.54	0.41
1:W:130:VAL:HA	1:W:137:VAL:HG12	2.03	0.41
2:V:178:ASN:HD22	2:V:178:ASN:HA	1.69	0.41
2:X:54:ALA:HB3	2:X:141:VAL:HG12	2.02	0.41
2:B:122:ARG:HA	2:B:122:ARG:HD3	1.78	0.40
1:C:121:SER:HB3	1:C:236:VAL:HG21	2.02	0.40
2:D:178:ASN:HD22	2:D:178:ASN:HA	1.68	0.40
1:G:206:ASP:HB3	1:G:207:LYS:H	1.69	0.40
1:I:106:ASN:ND2	1:I:106:ASN:H	2.20	0.40
1:K:200:ILE:HG21	1:K:258:ALA:HA	2.02	0.40
2:L:13:ILE:HG13	2:L:172:VAL:HB	2.03	0.40
2:T:19:ARG:HD2	2:T:181:GLU:OE2	2.20	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:ARG:NH1	2:D:102:GLU:OE1	2.54	0.40
1:G:200:ILE:HG21	1:G:258:ALA:HA	2.03	0.40
2:H:19:ARG:HD3	2:H:174:ILE:HG21	2.02	0.40
2:J:23:ARG:NH1	2:J:29:ARG:HG3	2.36	0.40
2:L:23:ARG:CZ	2:L:29:ARG:HG3	2.51	0.40
1:O:11:ILE:HA	1:O:12:PRO:HD3	1.96	0.40
1:O:16:LYS:O	1:O:20:VAL:HG23	2.21	0.40
1:U:109:GLU:HG3	2:V:102:GLU:HG3	2.04	0.40
1:U:251:ILE:HD12	2:V:200:VAL:HG21	2.04	0.40
1:W:126:LEU:HA	1:W:129:LEU:HD12	2.02	0.40
2:X:64:MET:HB2	2:X:64:MET:HE3	1.75	0.40
2:X:95:ALA:HA	2:X:96:PRO:HD3	1.86	0.40
1:E:101:GLY:O	1:E:102:PRO:O	2.39	0.40
1:E:200:ILE:HG21	1:E:258:ALA:HA	2.03	0.40
2:R:151:ALA:HB2	2:R:157:MET:HE1	2.04	0.40
1:W:112:ARG:HD3	2:X:102:GLU:OE1	2.21	0.40
1:W:232:ASP:O	1:W:233:LEU:HB2	2.22	0.40
2:D:77:LEU:HD23	2:D:77:LEU:HA	1.88	0.40
2:F:99:ARG:NH1	4:F:404:AMP:P	2.94	0.40
2:H:13:ILE:CD1	2:H:169:ALA:HB3	2.51	0.40
1:I:88:VAL:O	1:I:107:ALA:HB1	2.22	0.40
1:I:121:SER:HB3	1:I:236:VAL:HG21	2.03	0.40
1:K:2:SER:OG	2:L:108:ARG:HD3	2.21	0.40
1:K:207:LYS:HE2	1:K:208:TYR:CZ	2.57	0.40
2:N:31:ILE:HA	2:N:48:GLU:O	2.21	0.40
1:O:100:PRO:HB2	1:O:101:GLY:H	1.75	0.40
1:Q:41:SER:HB2	1:Q:57:LYS:HB2	2.03	0.40
1:U:200:ILE:HG21	1:U:258:ALA:HA	2.03	0.40
2:B:155:ILE:HA	2:B:156:PRO:HD3	1.91	0.40
1:C:98:PHE:CZ	1:C:149:TYR:CD1	3.09	0.40
1:K:57:LYS:HG2	1:K:62:MET:HG2	2.03	0.40
1:O:168:THR:HB	1:O:191:LEU:HD22	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	267/275 (97%)	247 (92%)	18 (7%)	2 (1%)	18	49
1	C	267/275 (97%)	247 (92%)	19 (7%)	1 (0%)	30	61
1	E	267/275 (97%)	242 (91%)	22 (8%)	3 (1%)	11	39
1	G	267/275 (97%)	247 (92%)	17 (6%)	3 (1%)	11	39
1	I	267/275 (97%)	243 (91%)	18 (7%)	6 (2%)	5	24
1	K	267/275 (97%)	246 (92%)	15 (6%)	6 (2%)	5	24
1	M	267/275 (97%)	248 (93%)	17 (6%)	2 (1%)	18	49
1	O	267/275 (97%)	247 (92%)	13 (5%)	7 (3%)	4	21
1	Q	267/275 (97%)	249 (93%)	14 (5%)	4 (2%)	8	32
1	S	267/275 (97%)	244 (91%)	18 (7%)	5 (2%)	6	27
1	U	266/275 (97%)	248 (93%)	15 (6%)	3 (1%)	11	39
1	W	267/275 (97%)	242 (91%)	19 (7%)	6 (2%)	5	24
2	B	239/248 (96%)	224 (94%)	14 (6%)	1 (0%)	30	61
2	D	245/248 (99%)	230 (94%)	13 (5%)	2 (1%)	16	47
2	F	239/248 (96%)	226 (95%)	12 (5%)	1 (0%)	30	61
2	H	239/248 (96%)	226 (95%)	12 (5%)	1 (0%)	30	61
2	J	239/248 (96%)	221 (92%)	15 (6%)	3 (1%)	9	35
2	L	245/248 (99%)	227 (93%)	17 (7%)	1 (0%)	30	61
2	N	239/248 (96%)	226 (95%)	12 (5%)	1 (0%)	30	61
2	P	246/248 (99%)	228 (93%)	17 (7%)	1 (0%)	30	61
2	R	245/248 (99%)	227 (93%)	15 (6%)	3 (1%)	10	37
2	T	245/248 (99%)	229 (94%)	14 (6%)	2 (1%)	16	47
2	V	237/248 (96%)	223 (94%)	12 (5%)	2 (1%)	16	47
2	X	239/248 (96%)	225 (94%)	12 (5%)	2 (1%)	16	47
All	All	6100/6276 (97%)	5662 (93%)	370 (6%)	68 (1%)	11	39

All (68) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	103	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	102	PRO
1	I	10	ILE
1	I	93	LEU
1	I	105	GLU
1	Q	105	GLU
2	R	6	GLN
1	S	105	GLU
1	W	10	ILE
1	W	102	PRO
1	W	103	PRO
1	W	105	GLU
1	C	103	PRO
2	D	3	GLU
1	G	9	ASN
1	G	96	GLU
1	I	8	GLN
1	M	103	PRO
1	O	10	ILE
1	O	103	PRO
1	O	105	GLU
1	Q	100	PRO
2	R	3	GLU
1	S	8	GLN
1	W	9	ASN
2	X	15	ASP
1	E	103	PRO
1	G	103	PRO
1	I	9	ASN
1	K	7	ASN
1	K	8	GLN
1	O	7	ASN
1	O	100	PRO
1	A	102	PRO
2	B	176	ASP
2	F	176	ASP
1	K	9	ASN
1	K	100	PRO
1	O	101	GLY
2	P	176	ASP
2	T	176	ASP
1	U	102	PRO
1	W	8	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	X	176	ASP
2	D	176	ASP
1	E	101	GLY
2	H	176	ASP
2	J	10	PRO
2	J	136	ALA
2	J	176	ASP
2	L	176	ASP
1	M	102	PRO
2	N	176	ASP
1	Q	233	LEU
2	R	176	ASP
1	S	103	PRO
2	T	4	MET
1	U	7	ASN
2	V	176	ASP
1	K	101	GLY
1	S	100	PRO
1	I	100	PRO
1	Q	101	GLY
2	V	10	PRO
1	K	103	PRO
1	S	102	PRO
1	U	101	GLY
1	O	131	ILE

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	221/242 (91%)	207 (94%)	14 (6%)	16	45
1	C	224/242 (93%)	207 (92%)	17 (8%)	12	39
1	E	224/242 (93%)	206 (92%)	18 (8%)	11	37
1	G	223/242 (92%)	209 (94%)	14 (6%)	16	45
1	I	221/242 (91%)	204 (92%)	17 (8%)	12	38

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	224/242 (93%)	207 (92%)	17 (8%)	12	39
1	M	225/242 (93%)	209 (93%)	16 (7%)	13	41
1	O	223/242 (92%)	204 (92%)	19 (8%)	10	35
1	Q	224/242 (93%)	209 (93%)	15 (7%)	15	43
1	S	226/242 (93%)	208 (92%)	18 (8%)	11	37
1	U	225/242 (93%)	210 (93%)	15 (7%)	15	43
1	W	224/242 (93%)	210 (94%)	14 (6%)	16	45
2	B	197/208 (95%)	185 (94%)	12 (6%)	17	46
2	D	200/208 (96%)	189 (94%)	11 (6%)	19	50
2	F	198/208 (95%)	188 (95%)	10 (5%)	21	52
2	H	198/208 (95%)	182 (92%)	16 (8%)	11	36
2	J	197/208 (95%)	185 (94%)	12 (6%)	17	46
2	L	202/208 (97%)	186 (92%)	16 (8%)	11	37
2	N	196/208 (94%)	183 (93%)	13 (7%)	15	43
2	P	203/208 (98%)	192 (95%)	11 (5%)	20	50
2	R	201/208 (97%)	189 (94%)	12 (6%)	17	47
2	T	202/208 (97%)	190 (94%)	12 (6%)	18	48
2	V	196/208 (94%)	186 (95%)	10 (5%)	21	52
2	X	198/208 (95%)	184 (93%)	14 (7%)	13	41
All	All	5072/5400 (94%)	4729 (93%)	343 (7%)	14	42

All (343) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ILE
1	A	17	GLU
1	A	37	TYR
1	A	69	LEU
1	A	173	VAL
1	A	182	VAL
1	A	188	VAL
1	A	190	LYS
1	A	191	LEU
1	A	197	VAL
1	A	236	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	241	SER
1	A	255	GLU
1	A	275	ILE
2	B	9	ARG
2	B	13	ILE
2	B	64	MET
2	B	67	ARG
2	B	78	ARG
2	B	129	THR
2	B	138	SER
2	B	164	VAL
2	B	201	THR
2	B	206	ASN
2	B	208	SER
2	B	236	LEU
1	C	8	GLN
1	C	13	ILE
1	C	37	TYR
1	C	69	LEU
1	C	91	LEU
1	C	128	LYS
1	C	132	GLU
1	C	173	VAL
1	C	182	VAL
1	C	188	VAL
1	C	190	LYS
1	C	191	LEU
1	C	197	VAL
1	C	236	VAL
1	C	241	SER
1	C	255	GLU
1	C	275	ILE
2	D	7	VAL
2	D	20	THR
2	D	64	MET
2	D	67	ARG
2	D	78	ARG
2	D	129	THR
2	D	138	SER
2	D	164	VAL
2	D	201	THR
2	D	208	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	236	LEU
1	E	7	ASN
1	E	13	ILE
1	E	37	TYR
1	E	69	LEU
1	E	91	LEU
1	E	97	THR
1	E	102	PRO
1	E	106	ASN
1	E	173	VAL
1	E	182	VAL
1	E	188	VAL
1	E	190	LYS
1	E	191	LEU
1	E	197	VAL
1	E	236	VAL
1	E	241	SER
1	E	255	GLU
1	E	263	VAL
2	F	64	MET
2	F	67	ARG
2	F	129	THR
2	F	138	SER
2	F	164	VAL
2	F	201	THR
2	F	208	SER
2	F	236	LEU
2	F	246	GLU
2	F	248	VAL
1	G	9	ASN
1	G	13	ILE
1	G	37	TYR
1	G	69	LEU
1	G	89	GLU
1	G	173	VAL
1	G	182	VAL
1	G	188	VAL
1	G	190	LYS
1	G	191	LEU
1	G	197	VAL
1	G	236	VAL
1	G	241	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	255	GLU
2	H	8	GLU
2	H	9	ARG
2	H	11	LYS
2	H	12	LEU
2	H	13	ILE
2	H	14	LEU
2	H	20	THR
2	H	64	MET
2	H	67	ARG
2	H	129	THR
2	H	138	SER
2	H	164	VAL
2	H	201	THR
2	H	206	ASN
2	H	208	SER
2	H	236	LEU
1	I	13	ILE
1	I	17	GLU
1	I	37	TYR
1	I	69	LEU
1	I	91	LEU
1	I	104	ASP
1	I	173	VAL
1	I	182	VAL
1	I	188	VAL
1	I	190	LYS
1	I	191	LEU
1	I	197	VAL
1	I	236	VAL
1	I	241	SER
1	I	255	GLU
1	I	263	VAL
1	I	267	GLU
2	J	8	GLU
2	J	13	ILE
2	J	64	MET
2	J	67	ARG
2	J	129	THR
2	J	138	SER
2	J	164	VAL
2	J	201	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	J	206	ASN
2	J	208	SER
2	J	236	LEU
2	J	248	VAL
1	K	13	ILE
1	K	37	TYR
1	K	69	LEU
1	K	90	LEU
1	K	96	GLU
1	K	97	THR
1	K	173	VAL
1	K	182	VAL
1	K	188	VAL
1	K	190	LYS
1	K	191	LEU
1	K	197	VAL
1	K	236	VAL
1	K	241	SER
1	K	243	LYS
1	K	255	GLU
1	K	275	ILE
2	L	3	GLU
2	L	7	VAL
2	L	9	ARG
2	L	64	MET
2	L	67	ARG
2	L	78	ARG
2	L	129	THR
2	L	138	SER
2	L	164	VAL
2	L	177	LEU
2	L	183	MET
2	L	201	THR
2	L	206	ASN
2	L	208	SER
2	L	236	LEU
2	L	248	VAL
1	M	13	ILE
1	M	17	GLU
1	M	37	TYR
1	M	69	LEU
1	M	96	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	132	GLU
1	M	173	VAL
1	M	182	VAL
1	M	188	VAL
1	M	190	LYS
1	M	191	LEU
1	M	197	VAL
1	M	236	VAL
1	M	241	SER
1	M	255	GLU
1	M	275	ILE
2	N	15	ASP
2	N	64	MET
2	N	67	ARG
2	N	129	THR
2	N	138	SER
2	N	164	VAL
2	N	177	LEU
2	N	183	MET
2	N	201	THR
2	N	206	ASN
2	N	208	SER
2	N	236	LEU
2	N	248	VAL
1	O	13	ILE
1	O	37	TYR
1	O	69	LEU
1	O	87	ASN
1	O	89	GLU
1	O	91	LEU
1	O	95	TYR
1	O	173	VAL
1	O	182	VAL
1	O	188	VAL
1	O	190	LYS
1	O	191	LEU
1	O	197	VAL
1	O	236	VAL
1	O	241	SER
1	O	243	LYS
1	O	255	GLU
1	O	267	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	O	275	ILE
2	P	2	ARG
2	P	4	MET
2	P	7	VAL
2	P	64	MET
2	P	67	ARG
2	P	129	THR
2	P	138	SER
2	P	164	VAL
2	P	201	THR
2	P	208	SER
2	P	236	LEU
1	Q	8	GLN
1	Q	13	ILE
1	Q	37	TYR
1	Q	69	LEU
1	Q	105	GLU
1	Q	173	VAL
1	Q	182	VAL
1	Q	188	VAL
1	Q	190	LYS
1	Q	191	LEU
1	Q	197	VAL
1	Q	236	VAL
1	Q	241	SER
1	Q	243	LYS
1	Q	255	GLU
2	R	2	ARG
2	R	20	THR
2	R	64	MET
2	R	67	ARG
2	R	129	THR
2	R	138	SER
2	R	164	VAL
2	R	177	LEU
2	R	201	THR
2	R	206	ASN
2	R	208	SER
2	R	236	LEU
1	S	7	ASN
1	S	13	ILE
1	S	17	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	S	37	TYR
1	S	69	LEU
1	S	91	LEU
1	S	97	THR
1	S	98	PHE
1	S	106	ASN
1	S	173	VAL
1	S	182	VAL
1	S	188	VAL
1	S	190	LYS
1	S	191	LEU
1	S	197	VAL
1	S	236	VAL
1	S	241	SER
1	S	255	GLU
2	T	3	GLU
2	T	6	GLN
2	T	64	MET
2	T	67	ARG
2	T	129	THR
2	T	138	SER
2	T	164	VAL
2	T	177	LEU
2	T	201	THR
2	T	208	SER
2	T	236	LEU
2	T	248	VAL
1	U	13	ILE
1	U	37	TYR
1	U	69	LEU
1	U	88	VAL
1	U	90	LEU
1	U	173	VAL
1	U	182	VAL
1	U	188	VAL
1	U	190	LYS
1	U	191	LEU
1	U	197	VAL
1	U	236	VAL
1	U	241	SER
1	U	243	LYS
1	U	255	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	V	64	MET
2	V	67	ARG
2	V	78	ARG
2	V	129	THR
2	V	138	SER
2	V	164	VAL
2	V	177	LEU
2	V	201	THR
2	V	208	SER
2	V	236	LEU
1	W	13	ILE
1	W	37	TYR
1	W	69	LEU
1	W	98	PHE
1	W	173	VAL
1	W	182	VAL
1	W	188	VAL
1	W	190	LYS
1	W	191	LEU
1	W	197	VAL
1	W	236	VAL
1	W	241	SER
1	W	255	GLU
1	W	263	VAL
2	X	9	ARG
2	X	13	ILE
2	X	14	LEU
2	X	64	MET
2	X	67	ARG
2	X	78	ARG
2	X	129	THR
2	X	138	SER
2	X	164	VAL
2	X	177	LEU
2	X	201	THR
2	X	208	SER
2	X	236	LEU
2	X	248	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
2	B	68	HIS
2	B	178	ASN
2	B	198	ASN
2	B	206	ASN
2	B	216	GLN
1	C	83	ASN
2	D	40	ASN
2	D	68	HIS
2	D	178	ASN
2	D	198	ASN
2	D	206	ASN
1	E	106	ASN
2	F	68	HIS
2	F	178	ASN
2	F	206	ASN
2	F	216	GLN
2	H	68	HIS
2	H	178	ASN
2	H	206	ASN
2	H	216	GLN
1	I	7	ASN
1	I	83	ASN
1	I	87	ASN
1	I	106	ASN
2	J	68	HIS
2	J	178	ASN
2	J	206	ASN
2	J	216	GLN
1	K	7	ASN
1	K	9	ASN
1	K	83	ASN
2	L	68	HIS
2	L	178	ASN
2	L	198	ASN
2	L	206	ASN
2	L	216	GLN
1	M	87	ASN
2	N	68	HIS
2	N	178	ASN
2	N	206	ASN
2	N	216	GLN
1	O	7	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	O	87	ASN
2	P	40	ASN
2	P	68	HIS
2	P	178	ASN
2	P	198	ASN
2	P	206	ASN
2	P	216	GLN
1	Q	83	ASN
1	Q	106	ASN
2	R	68	HIS
2	R	178	ASN
2	R	198	ASN
2	R	206	ASN
2	R	216	GLN
1	S	7	ASN
1	S	9	ASN
1	S	83	ASN
1	S	87	ASN
2	T	68	HIS
2	T	178	ASN
2	T	198	ASN
1	U	7	ASN
1	U	9	ASN
2	V	68	HIS
2	V	178	ASN
2	V	198	ASN
2	V	206	ASN
2	V	216	GLN
1	W	9	ASN
1	W	83	ASN
1	W	272	HIS
2	X	68	HIS
2	X	178	ASN
2	X	206	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 40 ligands modelled in this entry, 12 are monoatomic - leaving 28 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$
4	AMP	B	404	4	21,24,25	0.38	0	30,35,38	0.86	2 (6%)
4	AMP	B	403	4	21,24,25	0.27	0	30,35,38	1.02	2 (6%)
4	AMP	B	402	4	21,24,25	0.32	0	30,35,38	0.72	1 (3%)
4	AMP	V	401	4	25,25,25	0.60	0	37,38,38	0.66	0
4	AMP	V	402	4	21,24,25	0.49	0	30,35,38	0.81	0
4	AMP	X	404	4,2	21,24,25	0.38	0	30,35,38	0.56	0
4	AMP	X	402	4	21,24,25	0.44	0	30,35,38	0.98	1 (3%)
4	AMP	H	404	4	21,24,25	0.44	0	30,35,38	0.84	2 (6%)
4	AMP	N	404	4	21,24,25	0.38	0	30,35,38	0.87	2 (6%)
4	AMP	V	403	4	21,24,25	0.27	0	30,35,38	0.71	1 (3%)
4	AMP	N	401	4	25,25,25	0.66	0	37,38,38	0.72	1 (2%)
4	AMP	H	402	4	21,24,25	0.49	0	30,35,38	0.57	0
4	AMP	N	402	4	21,24,25	0.43	0	30,35,38	0.48	0
4	AMP	H	403	4	21,24,25	0.34	0	30,35,38	0.59	0
4	AMP	F	401	4	25,25,25	0.57	0	37,38,38	0.99	3 (8%)
4	AMP	N	403	4	21,24,25	0.33	0	30,35,38	0.59	0
4	AMP	J	401	4	25,25,25	0.59	0	37,38,38	1.24	4 (10%)
4	AMP	F	403	4	21,24,25	0.40	0	30,35,38	0.44	0
4	AMP	B	401	4	25,25,25	0.60	0	37,38,38	1.03	3 (8%)
4	AMP	J	404	4	21,24,25	0.41	0	30,35,38	1.07	3 (10%)
4	AMP	X	401	4	25,25,25	0.56	0	37,38,38	0.77	2 (5%)
4	AMP	F	404	4	21,24,25	0.40	0	30,35,38	0.97	3 (10%)
4	AMP	F	402	4	21,24,25	0.43	0	30,35,38	0.78	0
4	AMP	J	403	4	21,24,25	0.36	0	30,35,38	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	AMP	V	404	4	21,24,25	0.42	0	30,35,38	0.83	1 (3%)
4	AMP	H	401	4	25,25,25	0.53	0	37,38,38	0.64	1 (2%)
4	AMP	X	403	4	21,24,25	0.38	0	30,35,38	0.56	0
4	AMP	J	402	4	21,24,25	0.35	0	30,35,38	0.68	0

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
4	AMP	B	404	4	-	2/7/25/26	0/3/3/3
4	AMP	B	403	4	-	0/7/25/26	0/3/3/3
4	AMP	B	402	4	-	0/7/25/26	0/3/3/3
4	AMP	V	401	4	-	0/10/26/26	0/3/3/3
4	AMP	V	402	4	-	0/7/25/26	0/3/3/3
4	AMP	X	404	4,2	-	2/7/25/26	0/3/3/3
4	AMP	X	402	4	-	0/7/25/26	0/3/3/3
4	AMP	H	404	4	-	0/7/25/26	0/3/3/3
4	AMP	N	404	4	-	2/7/25/26	0/3/3/3
4	AMP	V	403	4	-	0/7/25/26	0/3/3/3
4	AMP	N	401	4	-	3/10/26/26	0/3/3/3
4	AMP	H	402	4	-	0/7/25/26	0/3/3/3
4	AMP	N	402	4	-	0/7/25/26	0/3/3/3
4	AMP	H	403	4	-	2/7/25/26	0/3/3/3
4	AMP	F	401	4	-	5/10/26/26	0/3/3/3
4	AMP	N	403	4	-	2/7/25/26	0/3/3/3
4	AMP	J	401	4	-	2/10/26/26	0/3/3/3
4	AMP	F	403	4	-	0/7/25/26	0/3/3/3
4	AMP	B	401	4	-	1/10/26/26	0/3/3/3
4	AMP	J	404	4	-	3/7/25/26	0/3/3/3
4	AMP	X	401	4	-	1/10/26/26	0/3/3/3
4	AMP	F	404	4	-	1/7/25/26	0/3/3/3
4	AMP	F	402	4	-	2/7/25/26	0/3/3/3
4	AMP	J	403	4	-	2/7/25/26	0/3/3/3
4	AMP	V	404	4	-	2/7/25/26	0/3/3/3
4	AMP	H	401	4	-	0/10/26/26	0/3/3/3
4	AMP	X	403	4	-	1/7/25/26	0/3/3/3
4	AMP	J	402	4	-	0/7/25/26	0/3/3/3

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	401	AMP	C2'-C3'-C4'	-4.42	94.08	102.61
4	X	402	AMP	C3'-C2'-C1'	-3.44	94.96	101.46
4	B	401	AMP	C2'-C3'-C4'	-3.15	96.52	102.61
4	J	404	AMP	O4'-C1'-N9	3.15	114.13	108.09
4	J	404	AMP	C2'-C1'-N9	-3.12	105.56	113.30
4	B	401	AMP	O4'-C4'-C3'	-3.05	99.10	105.15
4	B	403	AMP	O4'-C1'-N9	3.02	113.89	108.09
4	F	404	AMP	C2'-C1'-N9	-2.93	106.02	113.30
4	F	401	AMP	C2'-C3'-C4'	-2.71	97.38	102.61
4	B	404	AMP	O4'-C1'-N9	2.69	113.27	108.09
4	H	401	AMP	O2P-P-O1P	2.64	121.12	110.83
4	J	401	AMP	O4'-C4'-C3'	-2.58	100.02	105.15
4	J	401	AMP	O4'-C1'-N9	2.53	112.95	108.09
4	F	404	AMP	C2'-C3'-C4'	-2.48	97.82	102.61
4	F	404	AMP	O4'-C1'-N9	2.46	112.81	108.09
4	F	401	AMP	O2P-P-O1P	2.42	120.27	110.83
4	B	404	AMP	C2'-C3'-C4'	-2.42	97.94	102.61
4	V	404	AMP	C2'-C3'-C4'	-2.41	97.95	102.61
4	X	401	AMP	O2P-P-O1P	2.40	120.17	110.83
4	X	401	AMP	C2'-C3'-C4'	-2.39	97.99	102.61
4	F	401	AMP	O4'-C1'-N9	2.38	112.66	108.09
4	V	403	AMP	C2'-C1'-N9	-2.33	107.50	113.30
4	N	401	AMP	O2P-P-O1P	2.33	119.90	110.83
4	J	404	AMP	C2'-C3'-C4'	-2.30	98.16	102.61
4	N	404	AMP	C2'-C1'-N9	-2.23	107.77	113.30
4	H	404	AMP	O4'-C1'-N9	2.20	112.32	108.09
4	N	404	AMP	C2'-C3'-C4'	-2.13	98.48	102.61
4	B	403	AMP	C2'-C1'-N9	-2.13	108.01	113.30
4	B	402	AMP	O4'-C1'-N9	2.09	112.10	108.09
4	J	401	AMP	C4'-O4'-C1'	-2.05	104.93	109.47
4	B	401	AMP	C5'-C4'-C3'	2.03	122.51	115.21
4	H	404	AMP	C2'-C1'-N9	-2.00	108.33	113.30

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	401	AMP	C5'-O5'-P-O3P
4	F	402	AMP	O4'-C4'-C5'-O5'
4	H	403	AMP	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	N	401	AMP	C4'-C5'-O5'-P
4	N	403	AMP	O4'-C4'-C5'-O5'
4	B	404	AMP	O4'-C4'-C5'-O5'
4	J	404	AMP	O4'-C4'-C5'-O5'
4	N	404	AMP	O4'-C4'-C5'-O5'
4	X	404	AMP	O4'-C4'-C5'-O5'
4	J	403	AMP	O4'-C4'-C5'-O5'
4	F	402	AMP	C3'-C4'-C5'-O5'
4	H	403	AMP	C3'-C4'-C5'-O5'
4	N	403	AMP	C3'-C4'-C5'-O5'
4	J	404	AMP	C3'-C4'-C5'-O5'
4	V	404	AMP	O4'-C4'-C5'-O5'
4	X	401	AMP	O4'-C4'-C5'-O5'
4	J	403	AMP	C3'-C4'-C5'-O5'
4	X	403	AMP	O4'-C4'-C5'-O5'
4	X	404	AMP	C3'-C4'-C5'-O5'
4	N	404	AMP	C3'-C4'-C5'-O5'
4	F	401	AMP	C5'-O5'-P-O2P
4	F	401	AMP	C3'-C4'-C5'-O5'
4	N	401	AMP	C3'-C4'-C5'-O5'
4	B	401	AMP	C4'-C5'-O5'-P
4	B	404	AMP	C3'-C4'-C5'-O5'
4	N	401	AMP	O4'-C4'-C5'-O5'
4	F	401	AMP	O4'-C4'-C5'-O5'
4	J	401	AMP	C4'-C5'-O5'-P
4	F	404	AMP	C4'-C5'-O5'-P
4	J	401	AMP	C3'-C4'-C5'-O5'
4	F	401	AMP	C5'-O5'-P-O1P
4	V	404	AMP	C3'-C4'-C5'-O5'
4	J	404	AMP	C4'-C5'-O5'-P

There are no ring outliers.

14 monomers are involved in 29 short contacts:

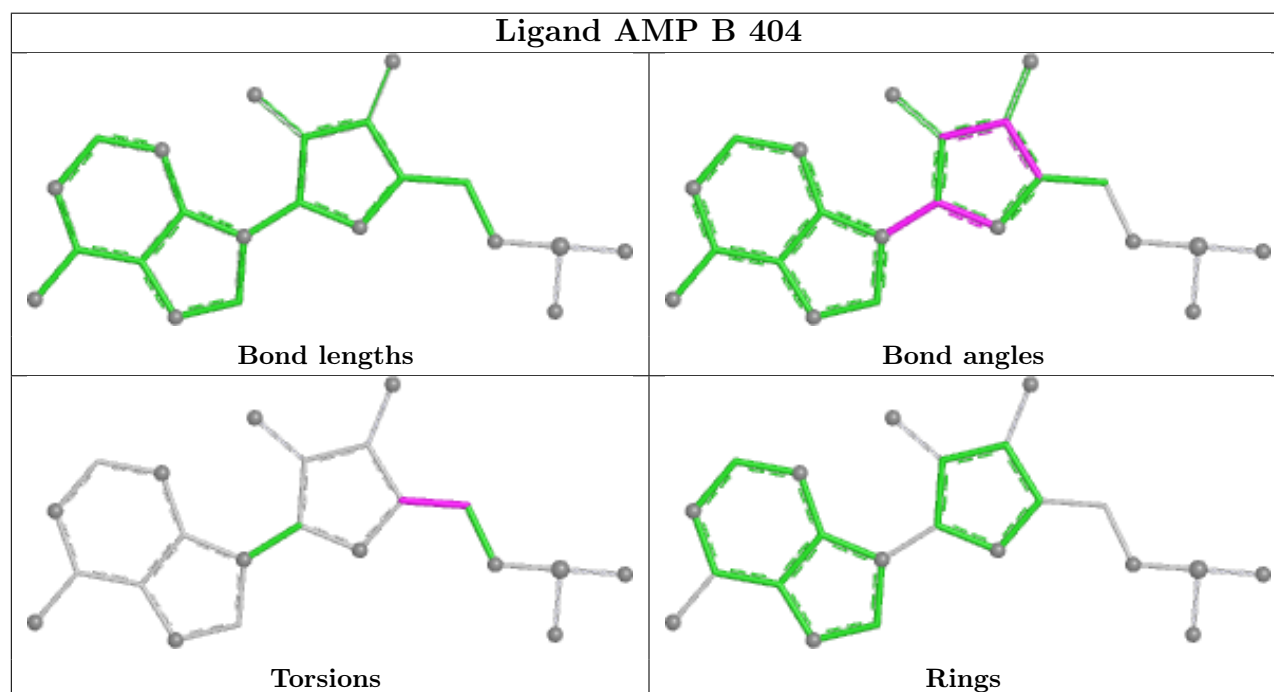
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	404	AMP	2	0
4	B	403	AMP	1	0
4	X	404	AMP	1	0
4	H	404	AMP	4	0
4	N	404	AMP	2	0
4	V	403	AMP	1	0
4	H	403	AMP	1	0

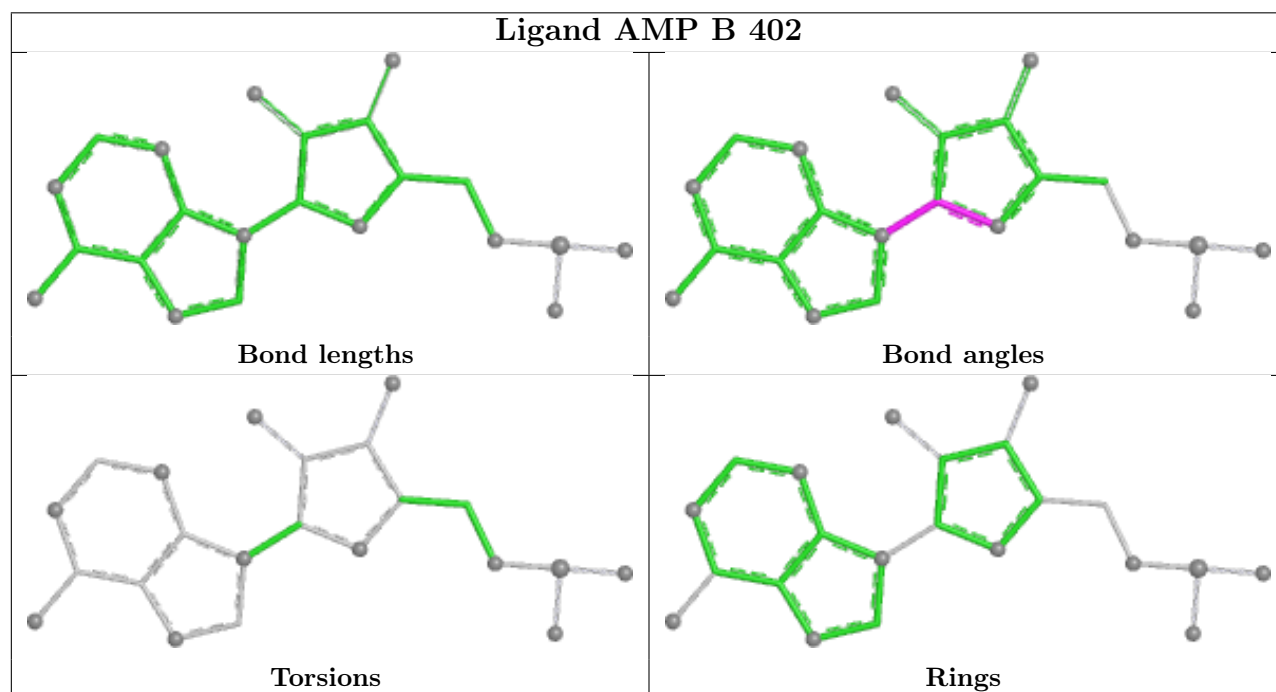
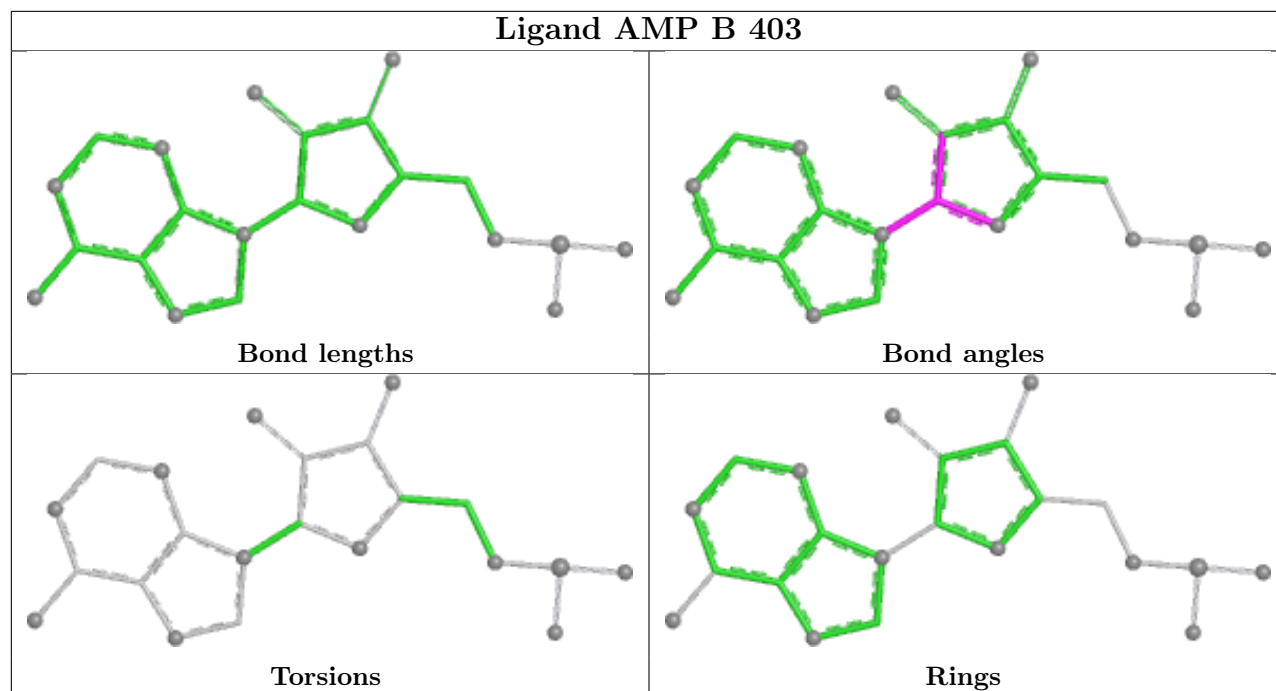
Continued on next page...

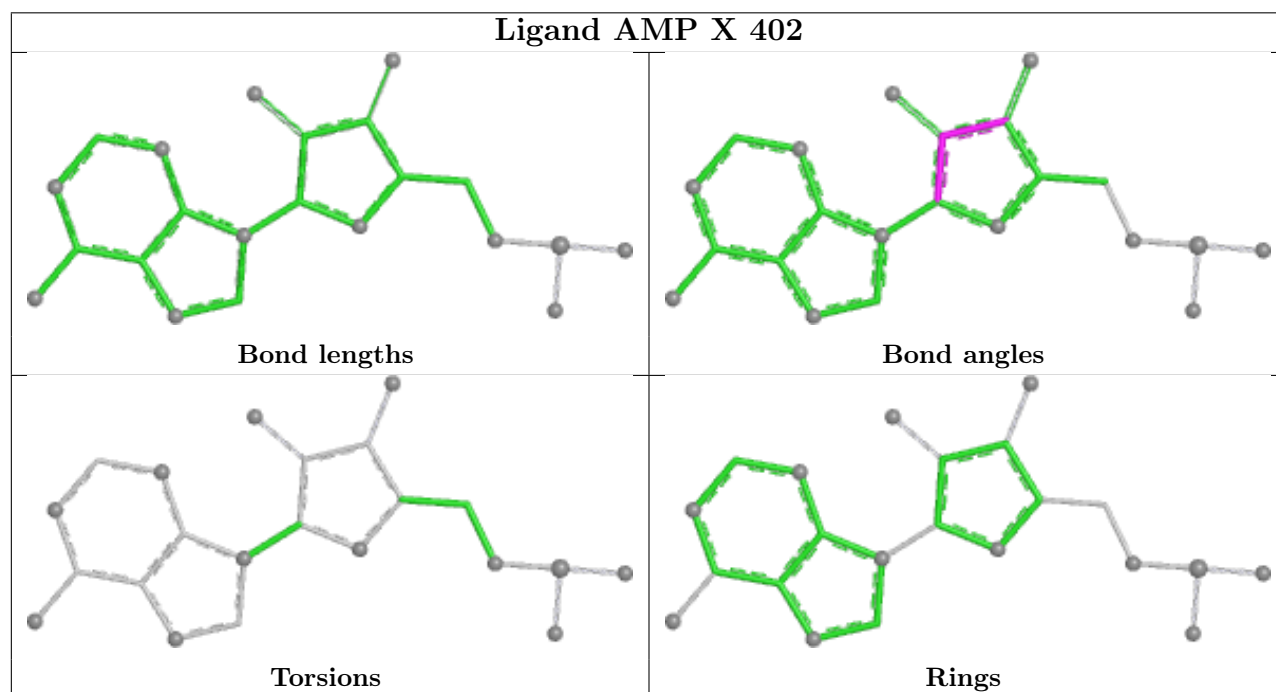
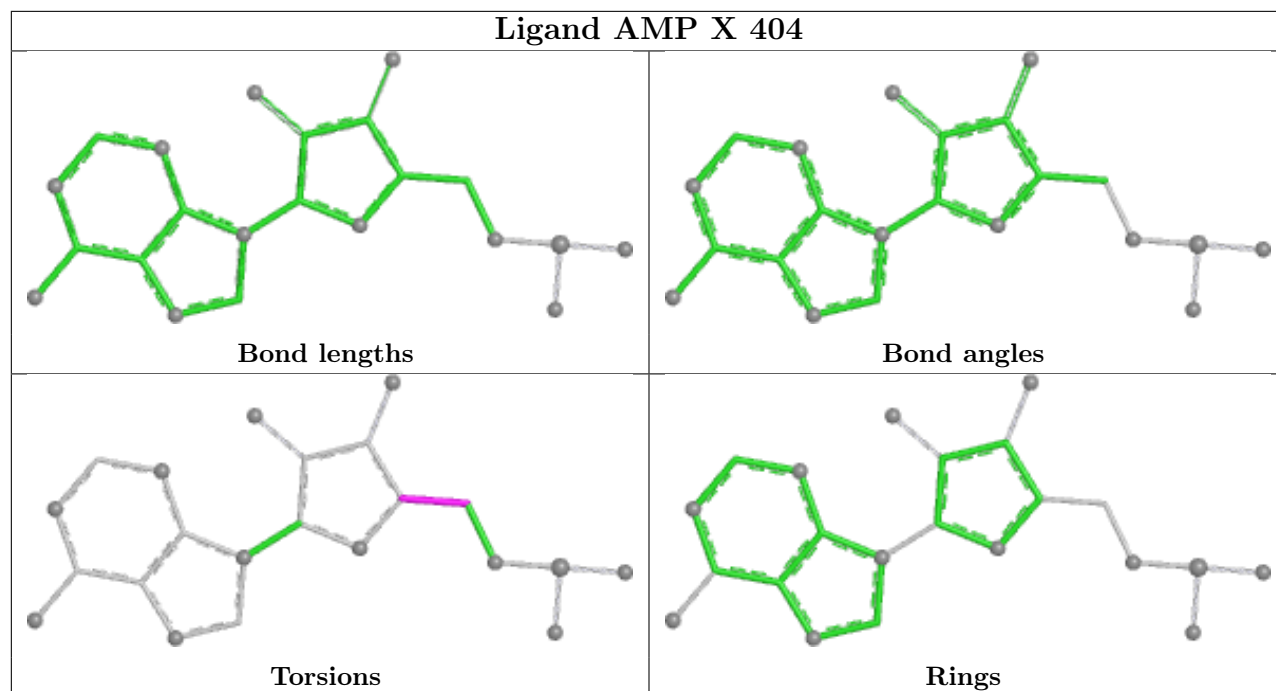
Continued from previous page...

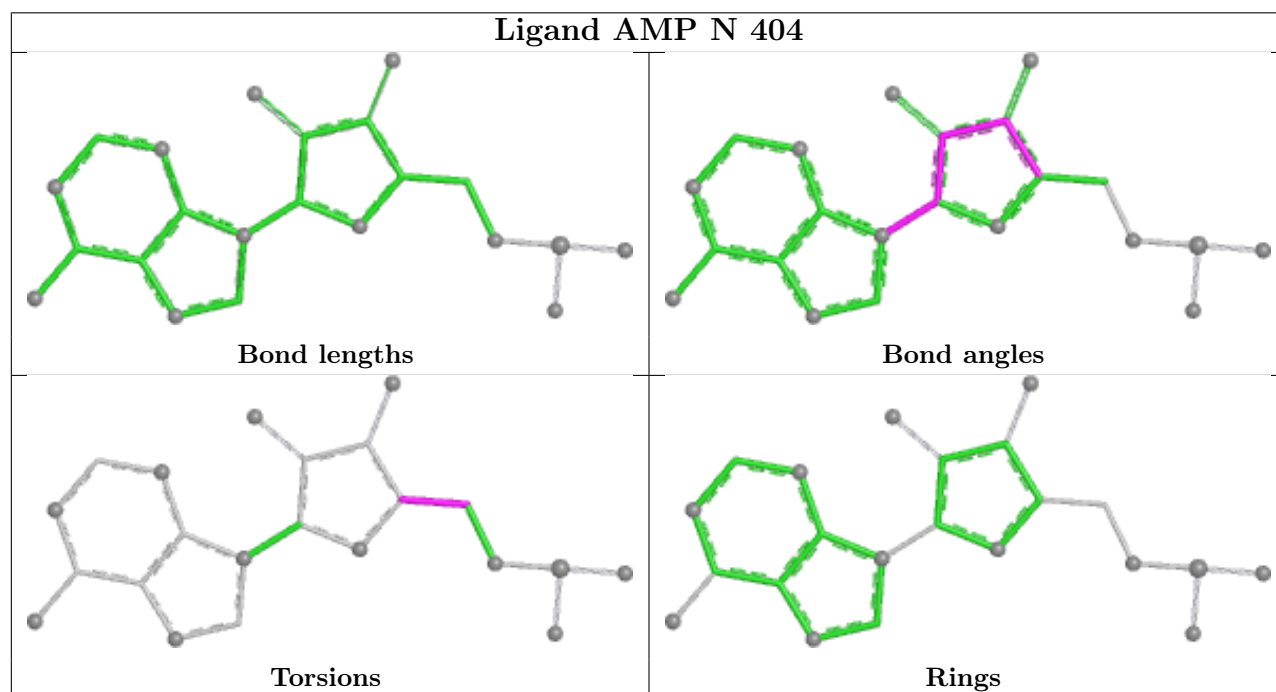
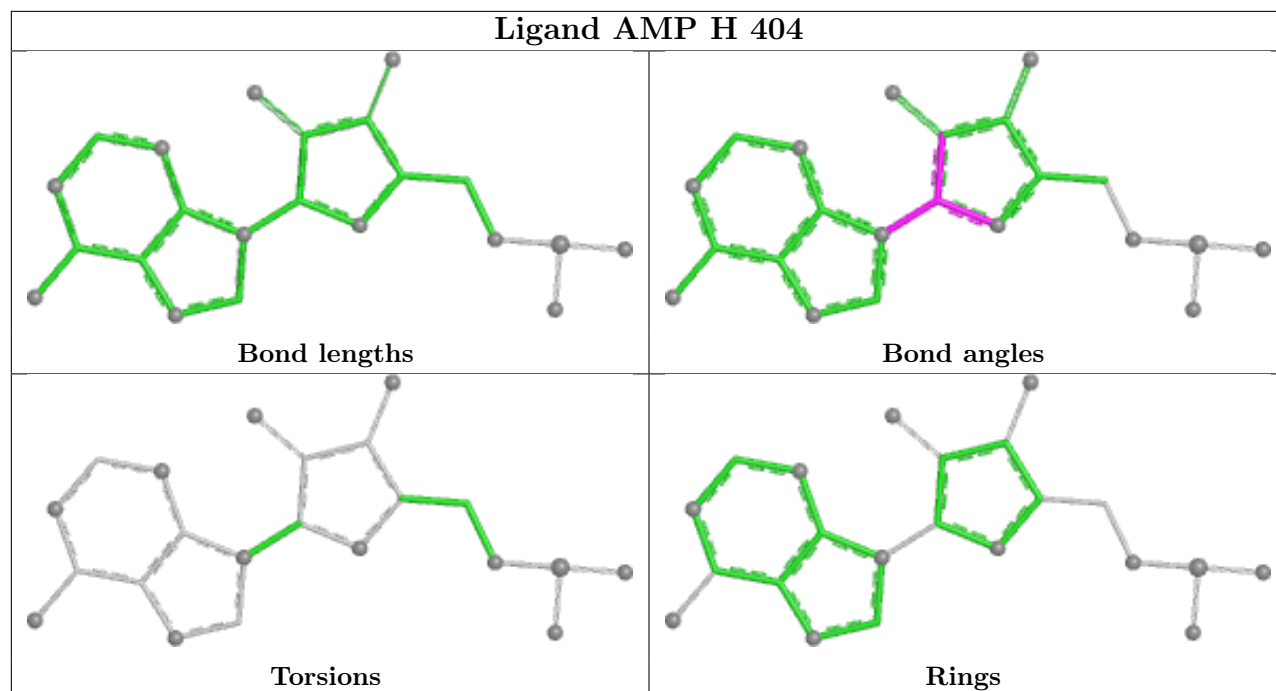
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	N	403	AMP	1	0
4	F	403	AMP	2	0
4	B	401	AMP	1	0
4	J	404	AMP	3	0
4	F	404	AMP	3	0
4	J	403	AMP	3	0
4	V	404	AMP	5	0

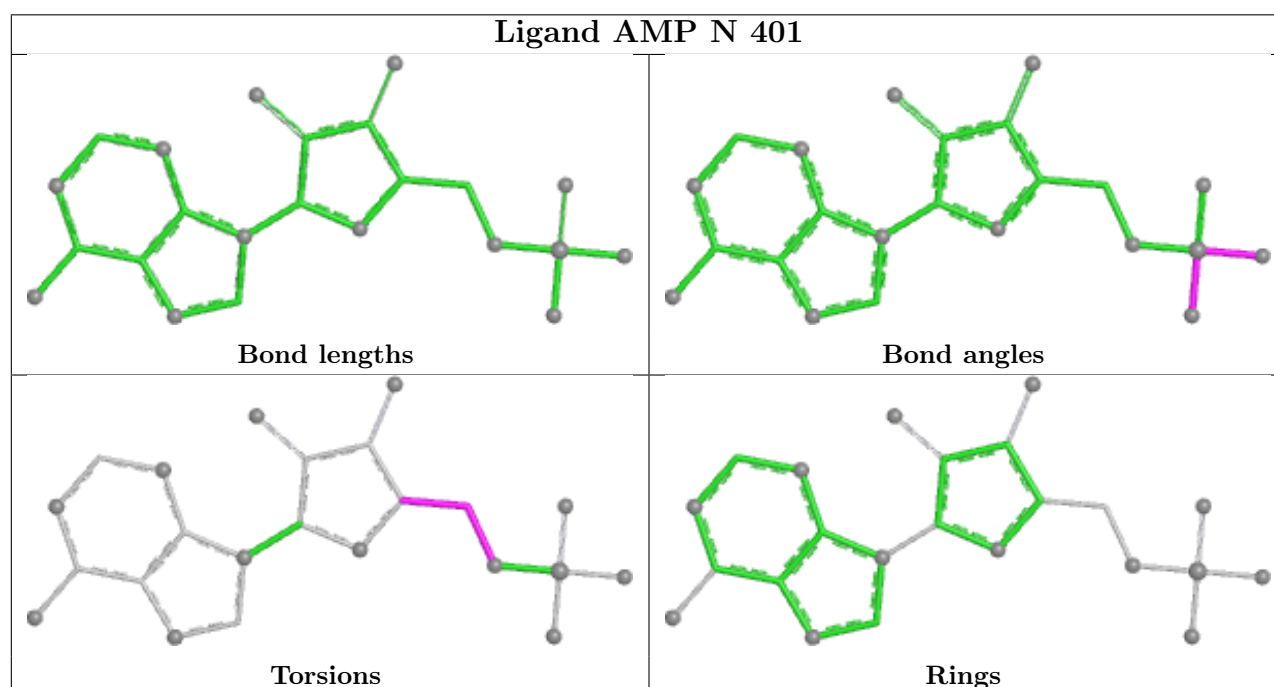
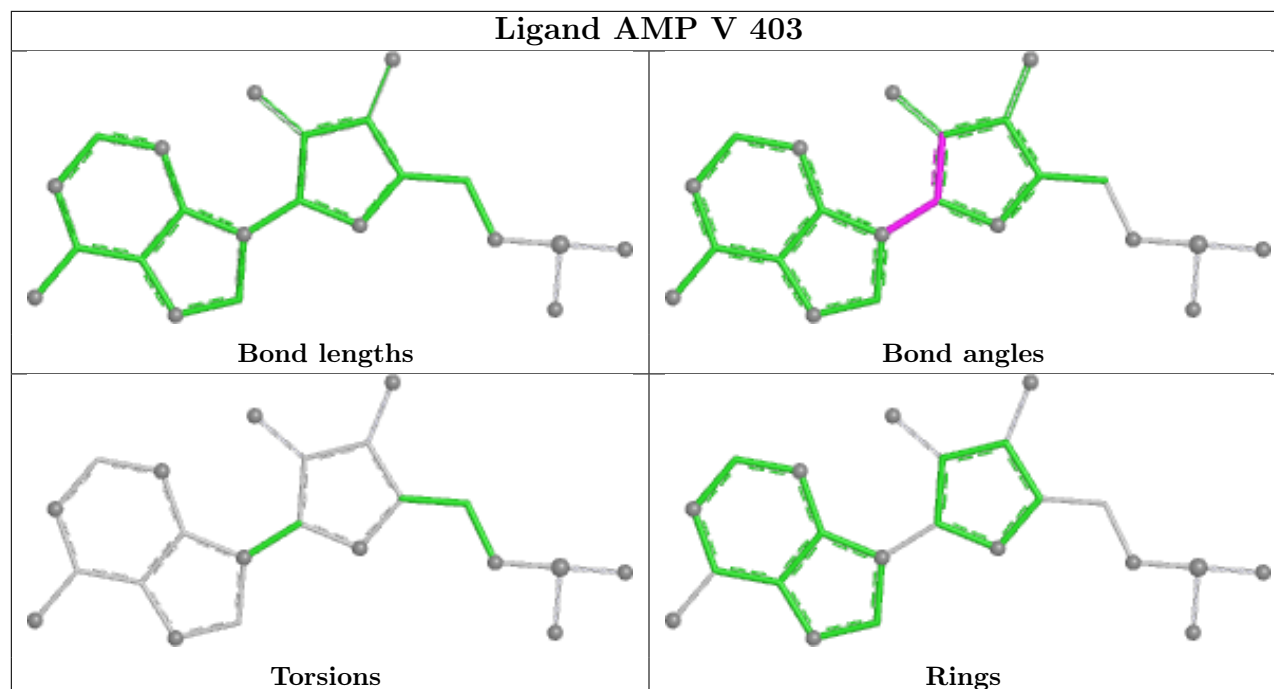
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

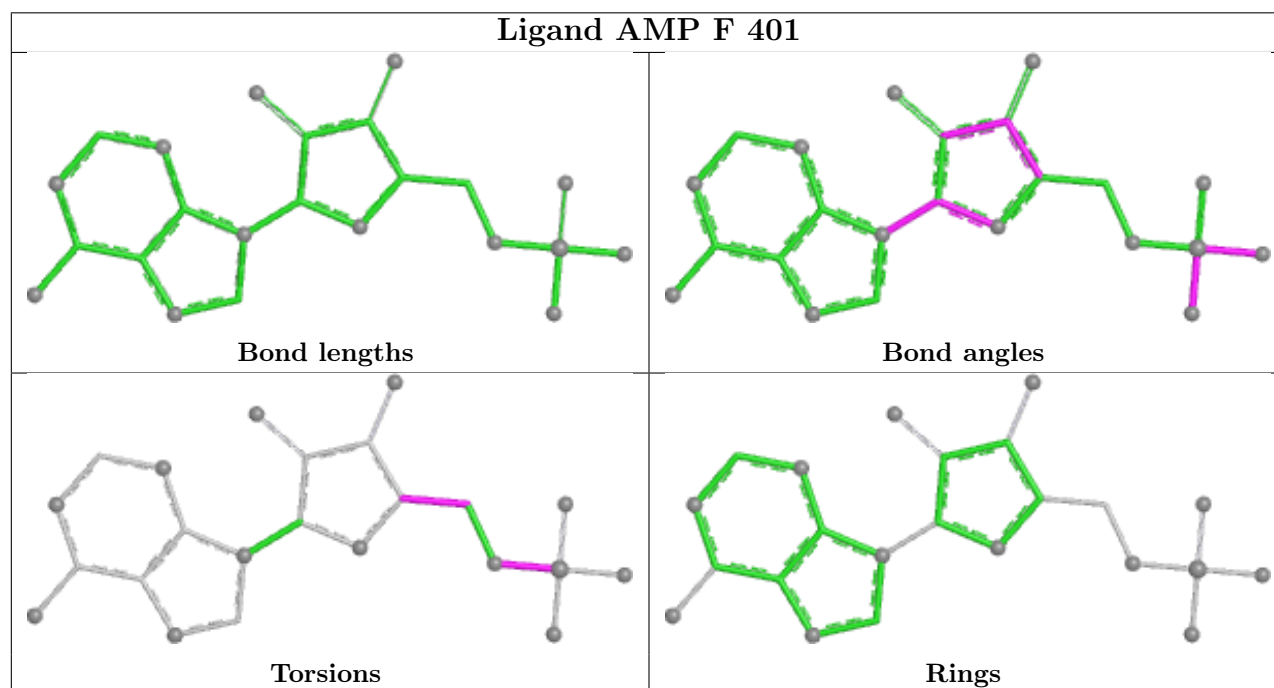
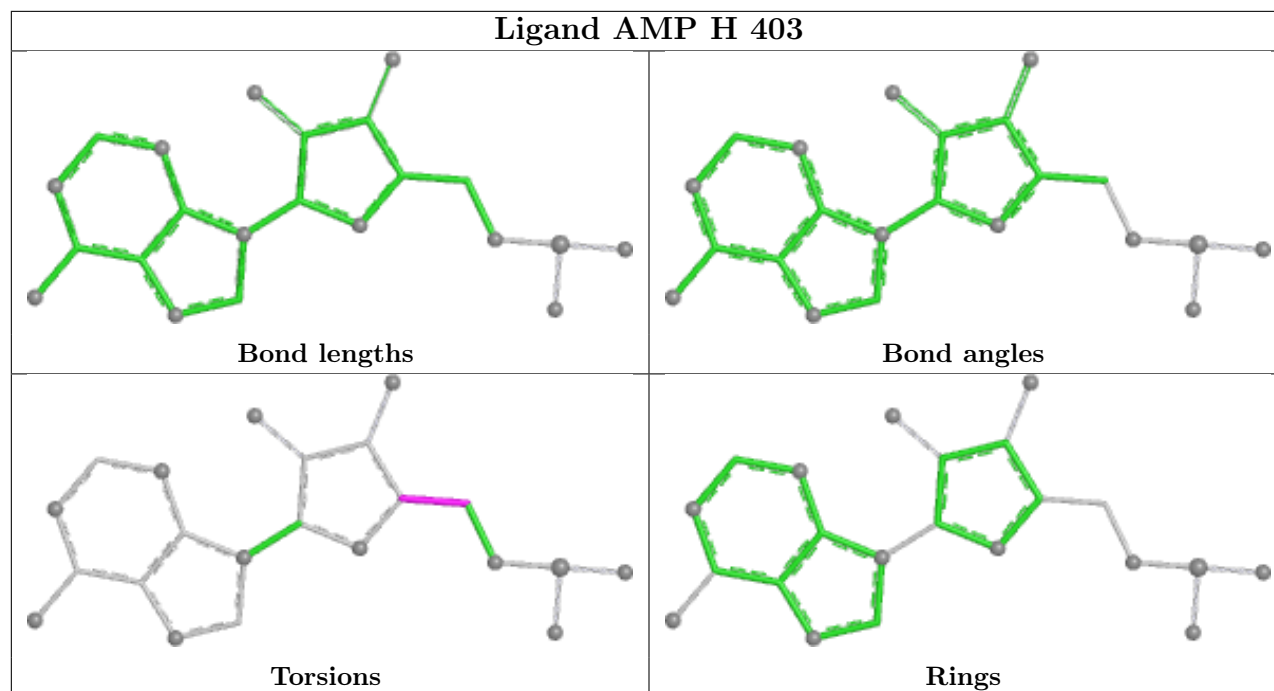




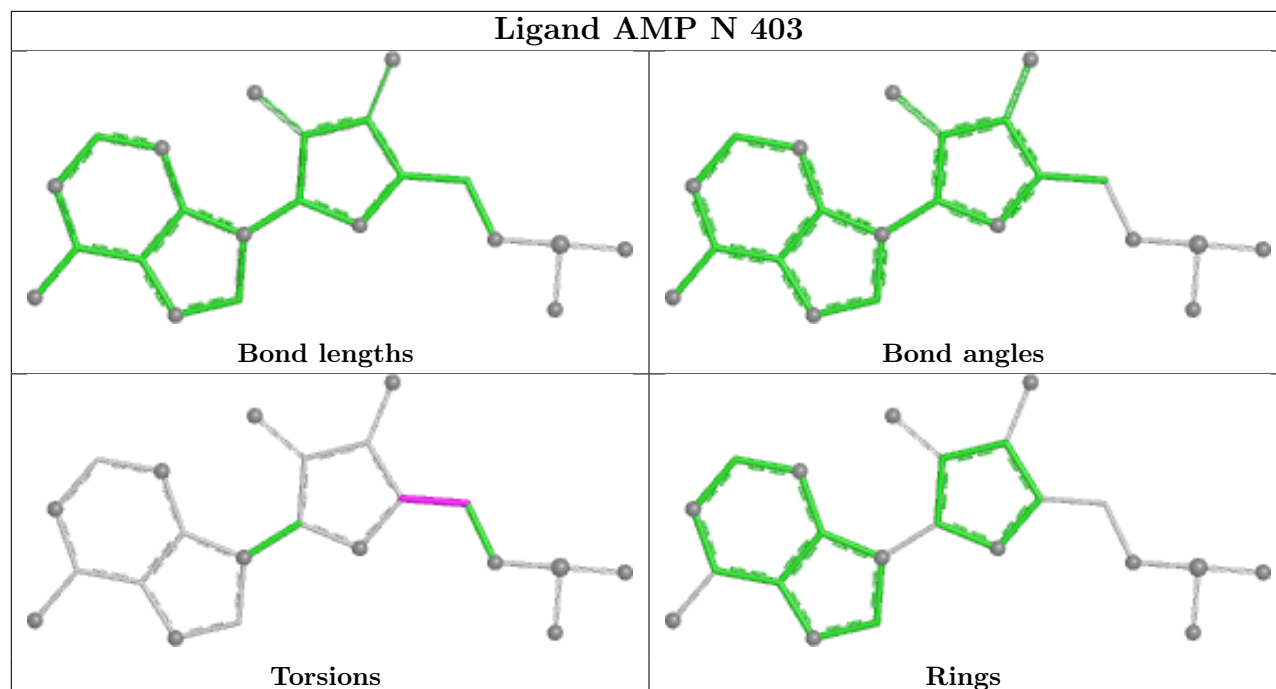




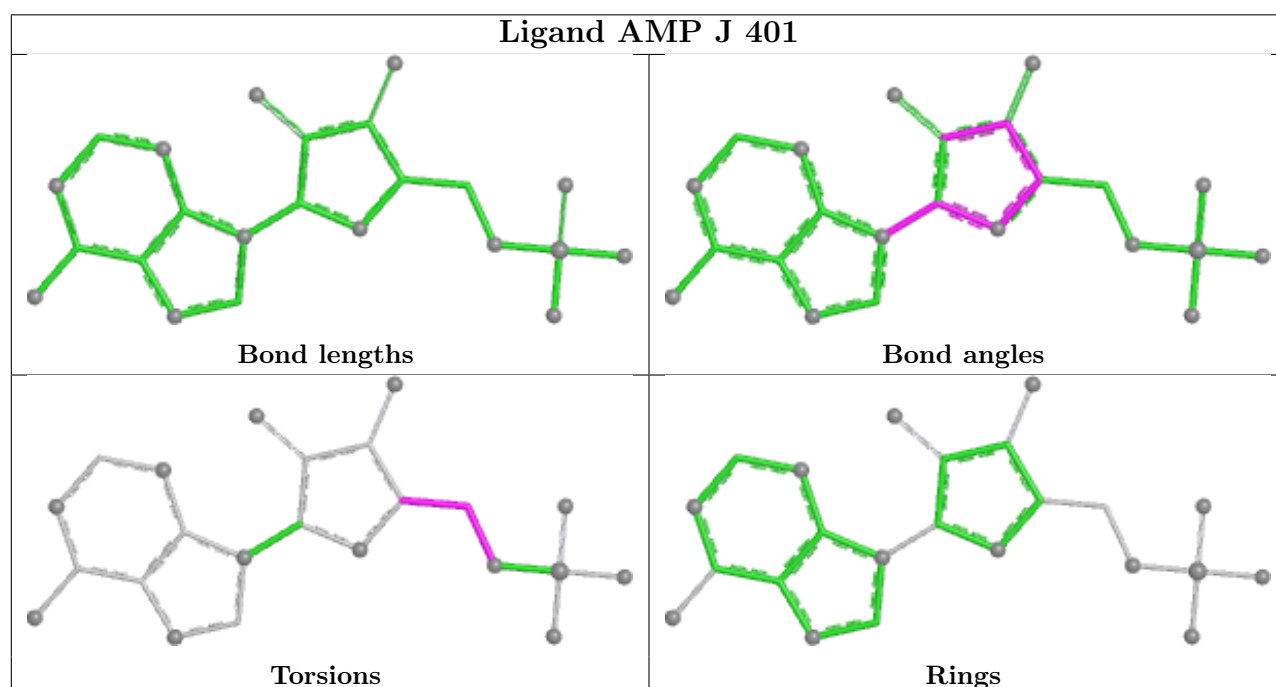


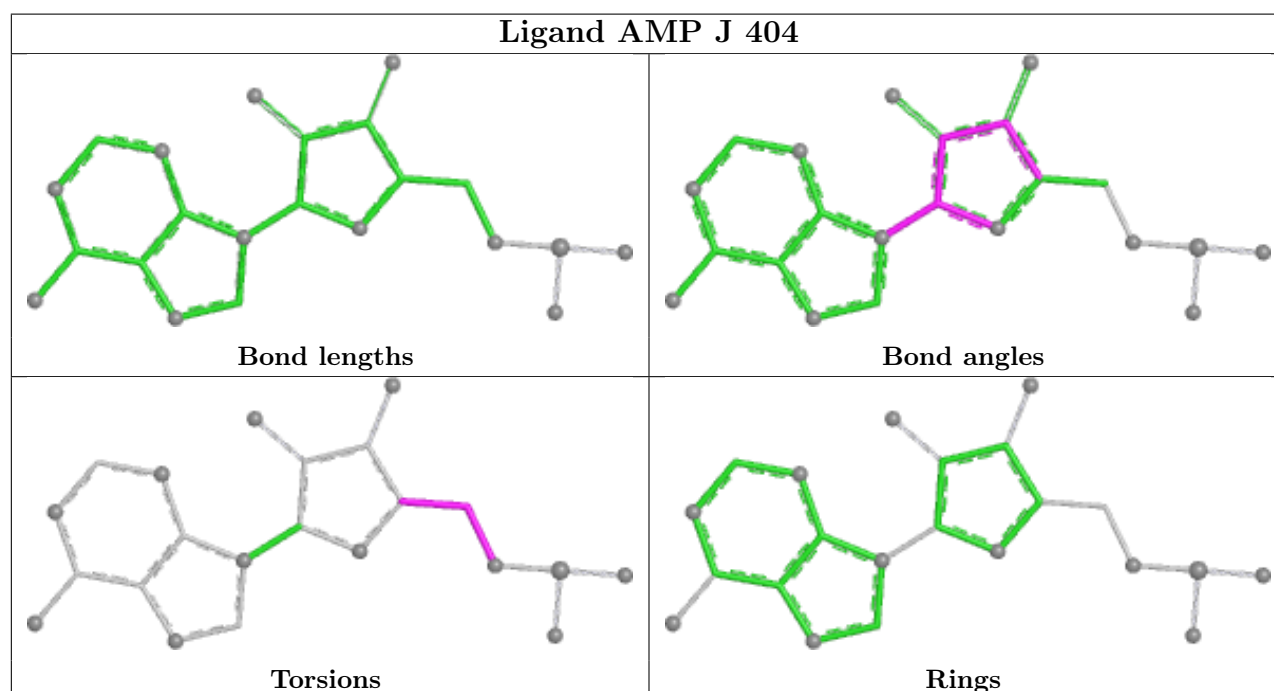
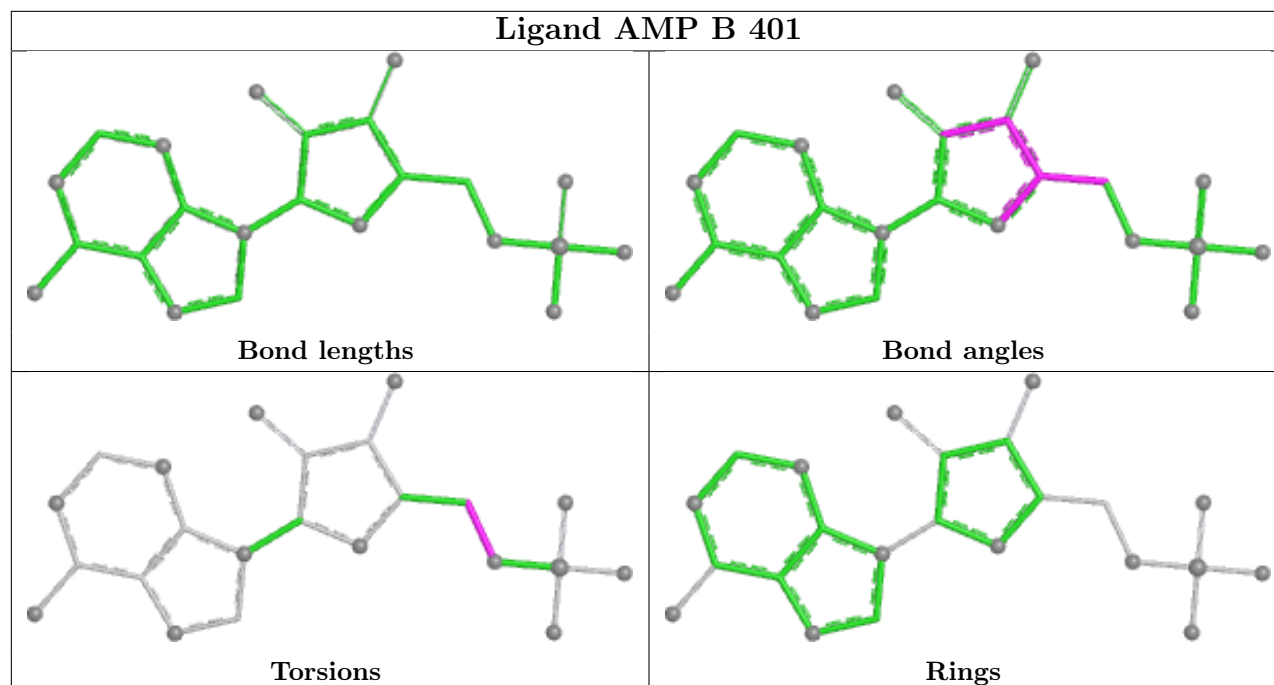


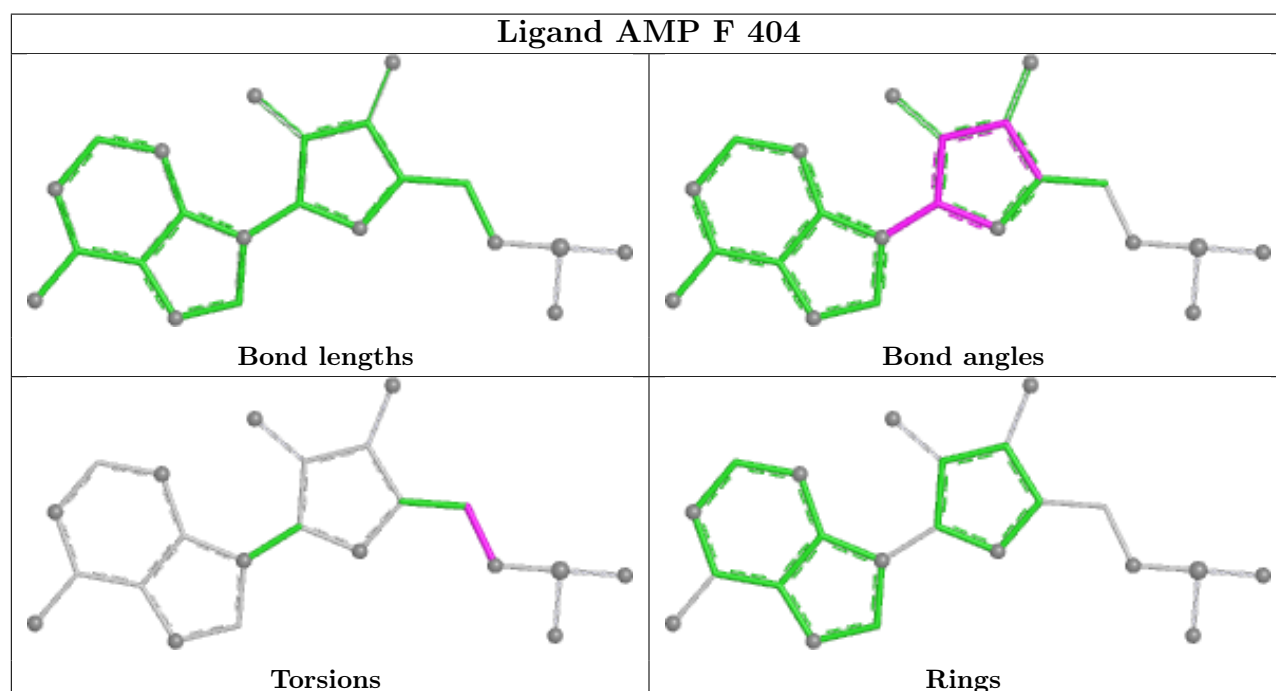
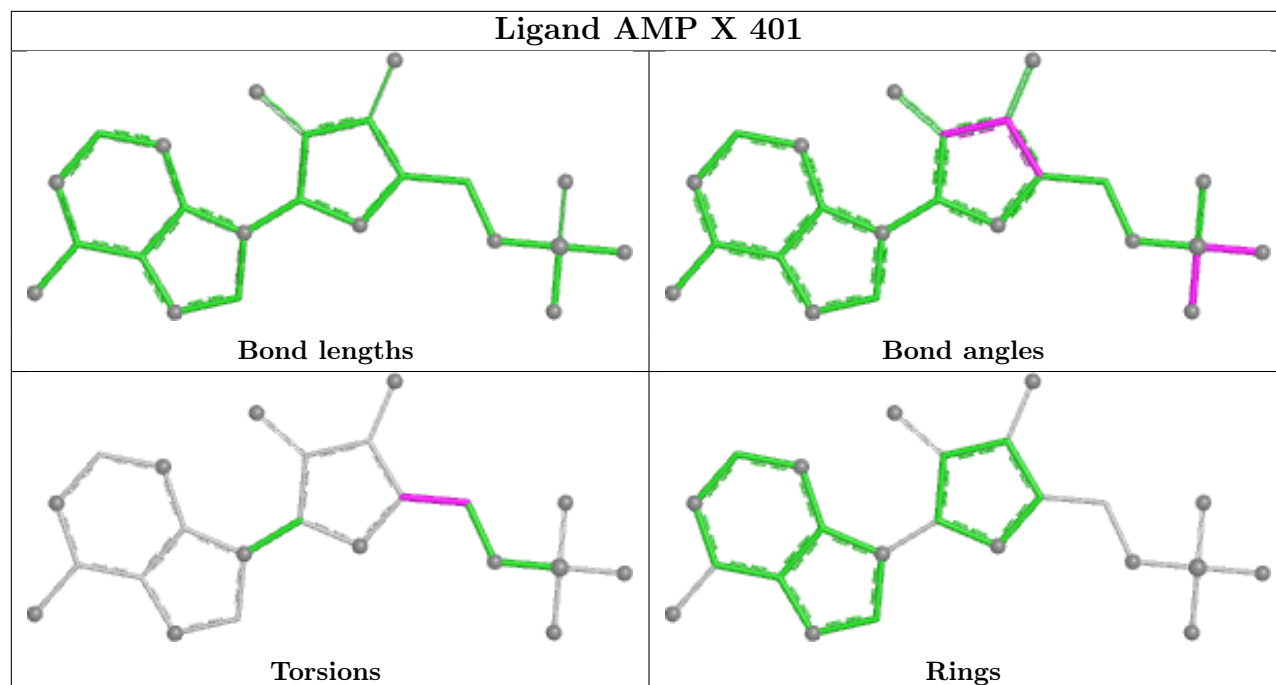
Ligand AMP N 403

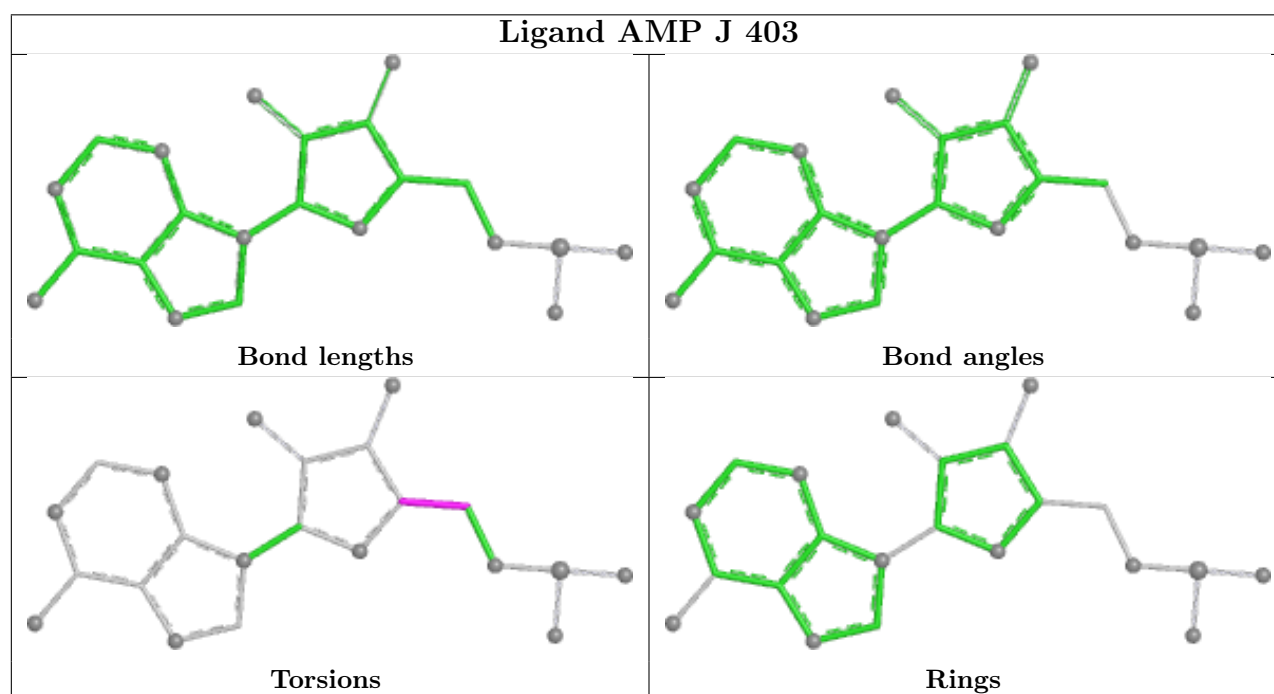
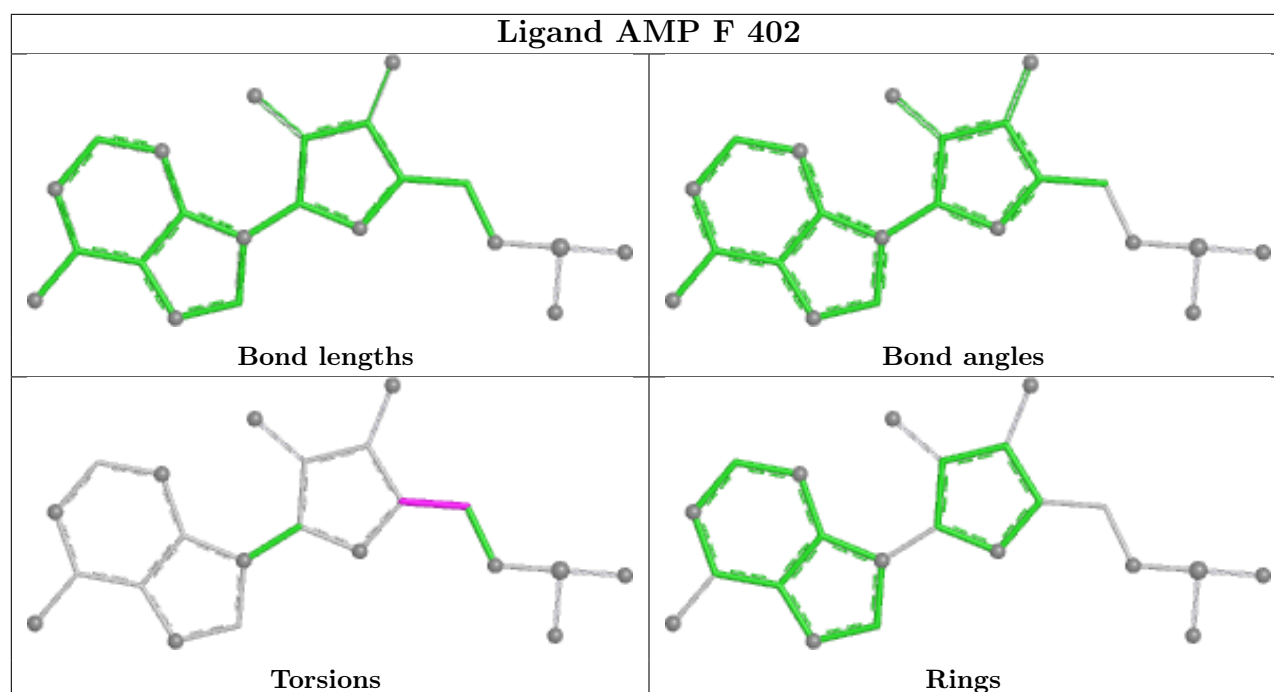


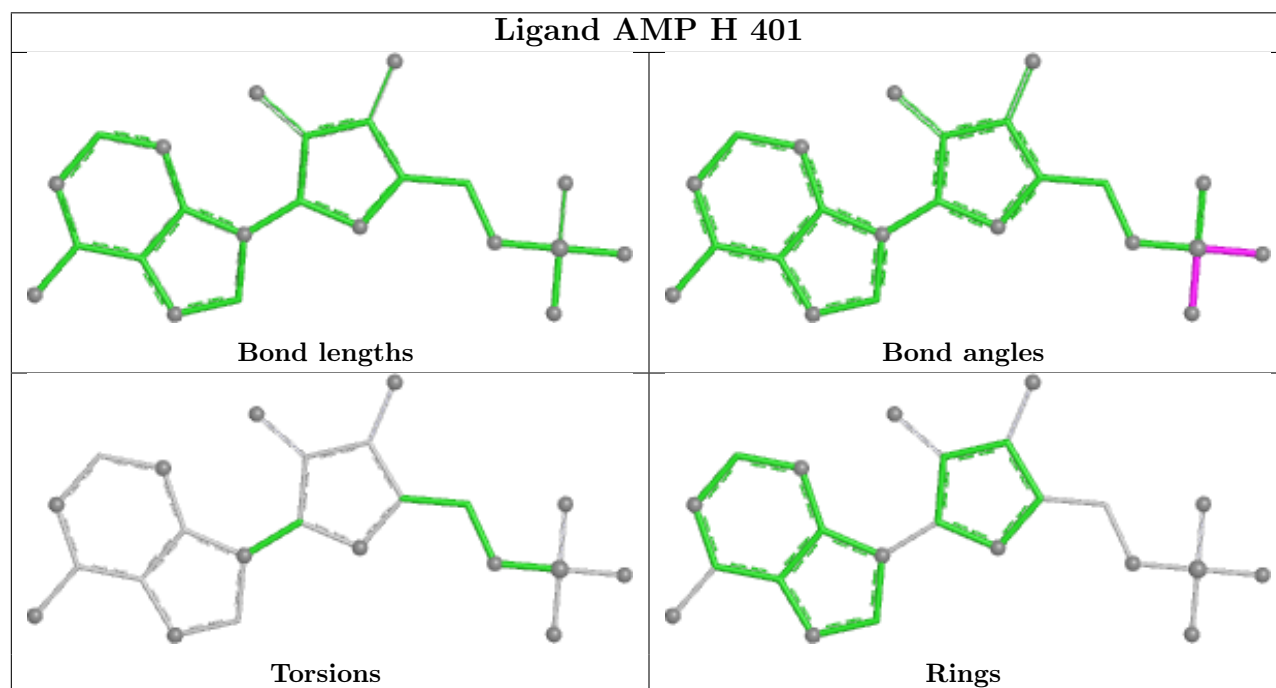
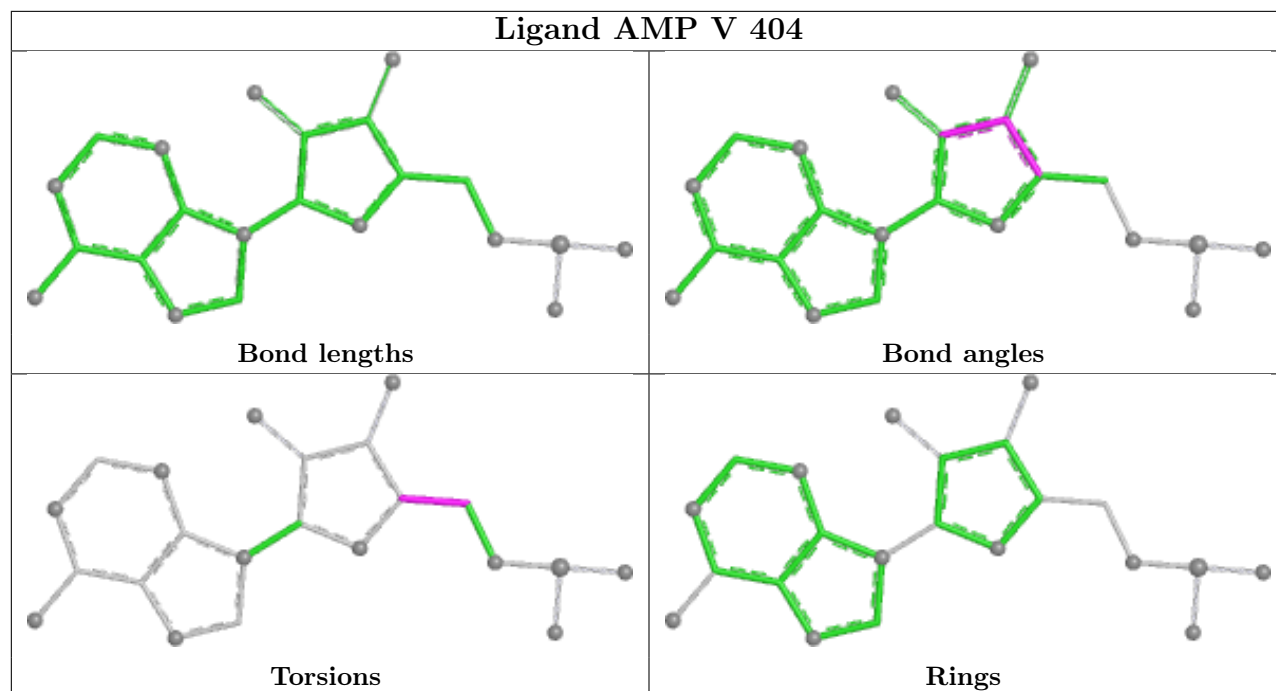
Ligand AMP J 401

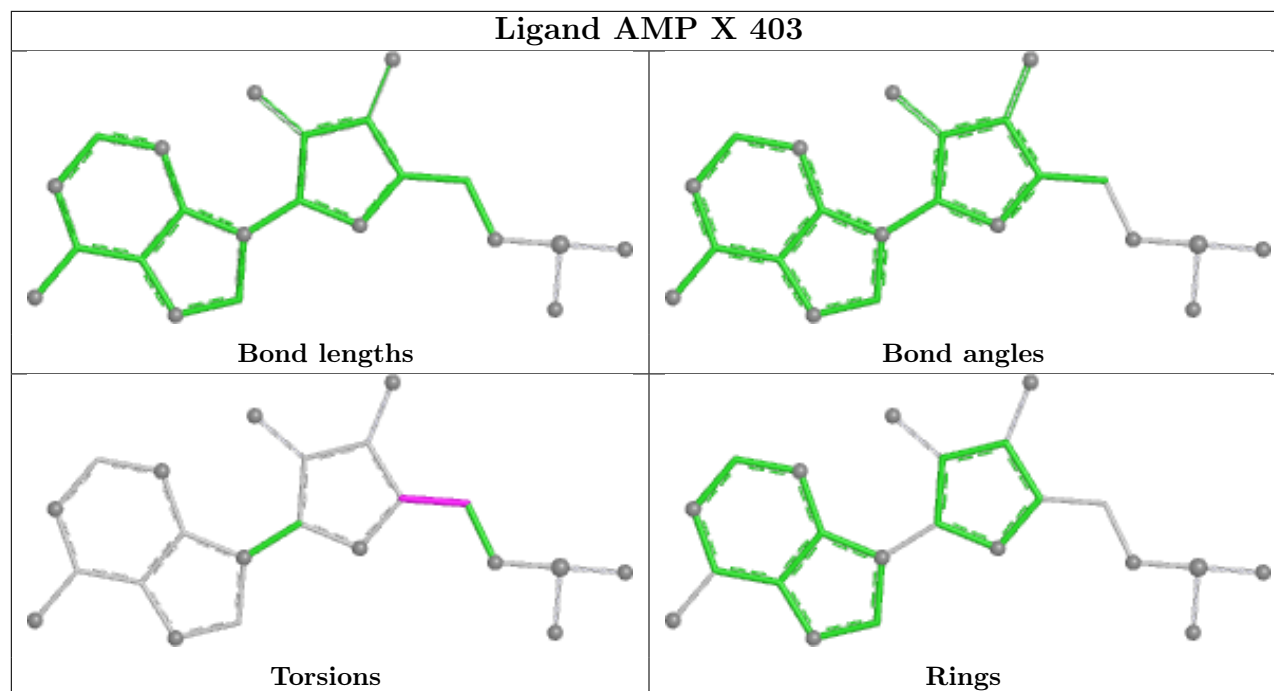












5.7 Other polymers [i](#)

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	271/275 (98%)	-0.04	3 (1%) 78 59	49, 56, 75, 83	0
1	C	271/275 (98%)	-0.04	3 (1%) 78 59	49, 56, 71, 78	0
1	E	271/275 (98%)	-0.11	2 (0%) 84 68	49, 56, 73, 80	0
1	G	271/275 (98%)	-0.04	2 (0%) 84 68	49, 56, 76, 88	0
1	I	271/275 (98%)	-0.05	4 (1%) 72 52	49, 56, 75, 82	0
1	K	271/275 (98%)	-0.08	2 (0%) 84 68	49, 56, 73, 79	0
1	M	271/275 (98%)	-0.12	3 (1%) 78 59	49, 56, 76, 83	0
1	O	271/275 (98%)	-0.01	1 (0%) 88 76	49, 56, 75, 85	0
1	Q	271/275 (98%)	-0.06	2 (0%) 84 68	49, 56, 74, 79	0
1	S	271/275 (98%)	-0.02	6 (2%) 62 41	49, 56, 76, 84	0
1	U	270/275 (98%)	0.03	3 (1%) 78 59	49, 56, 75, 79	0
1	W	271/275 (98%)	-0.00	5 (1%) 67 47	49, 56, 73, 78	0
2	B	241/248 (97%)	-0.09	0 100 100	49, 55, 71, 85	0
2	D	247/248 (99%)	0.06	7 (2%) 55 34	49, 55, 74, 93	0
2	F	241/248 (97%)	-0.18	1 (0%) 88 76	49, 55, 71, 86	0
2	H	241/248 (97%)	-0.14	1 (0%) 88 76	49, 55, 71, 85	0
2	J	241/248 (97%)	-0.07	1 (0%) 88 76	49, 55, 71, 86	0
2	L	247/248 (99%)	0.08	4 (1%) 70 49	49, 55, 74, 85	0
2	N	241/248 (97%)	-0.07	1 (0%) 88 76	49, 55, 71, 85	0
2	P	248/248 (100%)	0.02	5 (2%) 65 44	49, 55, 75, 84	0
2	R	247/248 (99%)	-0.03	1 (0%) 88 76	49, 55, 74, 85	0
2	T	247/248 (99%)	-0.10	3 (1%) 76 58	49, 55, 74, 89	0
2	V	239/248 (96%)	-0.14	0 100 100	49, 55, 71, 84	0
2	X	241/248 (97%)	-0.12	0 100 100	49, 55, 71, 84	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	6172/6276 (98%)	-0.05	60 (0%) 79 61	49, 56, 73, 93	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Q	102	PRO	4.1
2	D	65	HIS	3.7
1	I	102	PRO	3.6
2	T	5	LEU	3.6
1	S	80	ASN	3.3
2	L	247	GLY	3.2
1	I	80	ASN	3.1
1	E	102	PRO	3.1
1	K	275	ILE	3.1
1	S	102	PRO	3.0
2	P	4	MET	3.0
1	U	11	ILE	2.9
1	Q	101	GLY	2.9
2	D	66	PRO	2.8
1	I	131	ILE	2.8
1	O	77	ASP	2.7
2	P	5	LEU	2.7
2	L	69	LEU	2.7
2	D	69	LEU	2.6
1	M	10	ILE	2.6
1	C	12	PRO	2.6
1	I	9	ASN	2.6
1	M	102	PRO	2.6
1	U	102	PRO	2.6
2	P	1	MET	2.5
1	W	182	VAL	2.5
1	M	275	ILE	2.5
1	W	102	PRO	2.5
1	W	275	ILE	2.4
1	A	102	PRO	2.4
1	G	275	ILE	2.4
2	F	248	VAL	2.4
1	C	102	PRO	2.4
1	S	134	GLY	2.4
2	N	69	LEU	2.4
2	L	5	LEU	2.3
2	P	60	GLY	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	275	ILE	2.2
1	W	10	ILE	2.2
1	S	275	ILE	2.2
2	D	5	LEU	2.2
2	R	5	LEU	2.2
1	A	173	VAL	2.2
1	G	181	SER	2.2
2	T	8	GLU	2.2
1	S	11	ILE	2.1
1	E	174	GLU	2.1
1	U	189	GLY	2.1
2	P	248	VAL	2.1
1	S	175	GLN	2.1
2	D	67	ARG	2.1
1	K	102	PRO	2.1
1	W	134	GLY	2.1
2	D	2	ARG	2.1
2	L	248	VAL	2.1
1	C	77	ASP	2.1
2	J	17	GLY	2.0
2	H	118	GLU	2.0
2	T	6	GLN	2.0
2	D	3	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

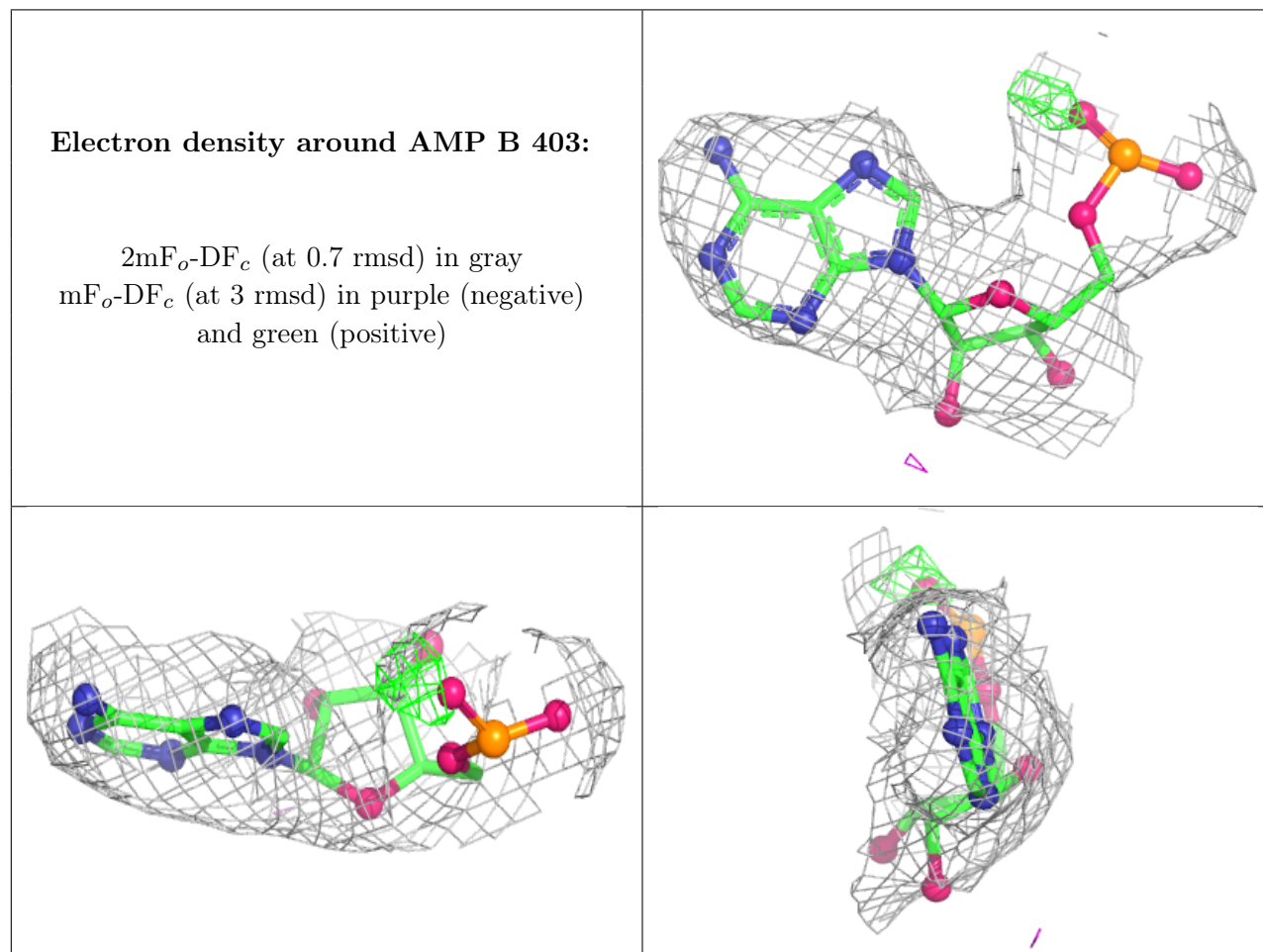
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Continued on next page...

Continued from previous page...

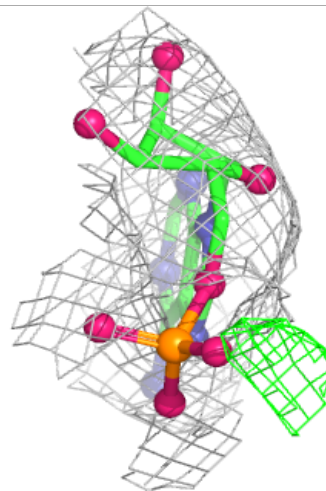
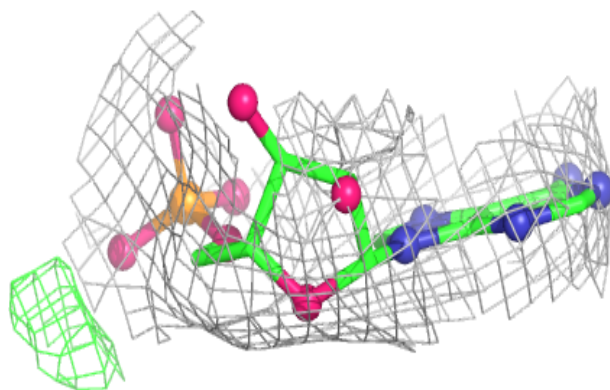
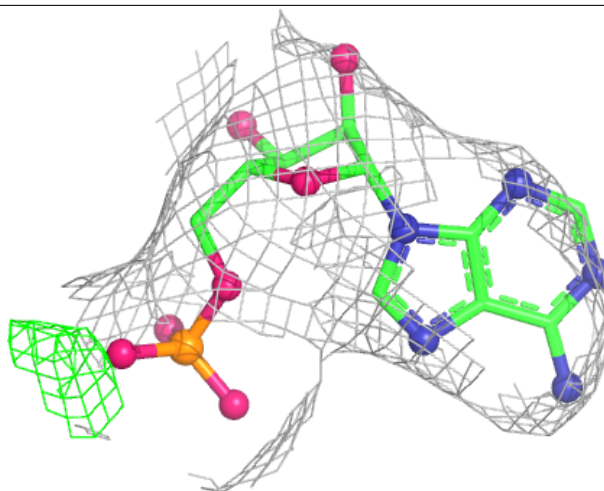
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	AMP	B	403	22/23	0.87	0.08	80,83,84,85	0
4	AMP	F	403	22/23	0.88	0.08	85,90,91,91	0
4	AMP	H	401	23/23	0.88	0.08	78,85,89,90	0
4	AMP	N	401	23/23	0.89	0.10	82,82,88,88	0
4	AMP	F	404	22/23	0.90	0.09	88,93,94,95	0
4	AMP	F	402	22/23	0.90	0.09	80,82,84,85	0
4	AMP	B	401	23/23	0.90	0.09	79,80,86,86	0
4	AMP	X	403	22/23	0.90	0.08	83,84,87,87	0
4	AMP	H	403	22/23	0.91	0.07	70,70,72,73	0
4	AMP	N	402	22/23	0.91	0.09	81,87,90,90	0
4	AMP	N	404	22/23	0.91	0.10	85,87,87,87	0
4	AMP	V	403	22/23	0.91	0.08	70,73,73,73	0
4	AMP	X	401	23/23	0.91	0.07	72,73,84,85	0
4	AMP	X	402	22/23	0.91	0.08	74,81,82,83	0
4	AMP	J	404	22/23	0.91	0.10	88,92,93,93	0
4	AMP	X	404	22/23	0.91	0.10	88,89,89,89	0
4	AMP	B	402	22/23	0.92	0.08	77,85,86,86	0
4	AMP	V	402	22/23	0.92	0.08	72,74,77,77	0
4	AMP	J	401	23/23	0.92	0.08	75,79,90,91	0
4	AMP	J	402	22/23	0.92	0.08	72,75,76,79	0
3	CL	D	301	1/1	0.92	0.05	20,20,20,20	0
4	AMP	B	404	22/23	0.92	0.09	86,91,93,93	0
4	AMP	F	401	23/23	0.92	0.09	81,85,90,91	0
4	AMP	V	401	23/23	0.93	0.08	73,75,79,79	0
4	AMP	H	404	22/23	0.93	0.08	74,78,80,80	0
4	AMP	J	403	22/23	0.93	0.07	80,88,89,89	0
4	AMP	V	404	22/23	0.93	0.09	68,69,72,73	0
4	AMP	N	403	22/23	0.94	0.07	84,84,86,87	0
4	AMP	H	402	22/23	0.94	0.08	72,75,78,78	0
3	CL	N	301	1/1	0.96	0.06	12,12,12,12	0
3	CL	L	301	1/1	0.97	0.03	44,44,44,44	0
3	CL	J	301	1/1	0.98	0.06	19,19,19,19	0
3	CL	R	301	1/1	0.98	0.03	22,22,22,22	0
3	CL	B	301	1/1	0.98	0.09	25,25,25,25	0
3	CL	V	301	1/1	0.99	0.04	13,13,13,13	0
3	CL	X	301	1/1	0.99	0.03	15,15,15,15	0
3	CL	P	301	1/1	0.99	0.05	28,28,28,28	0
3	CL	H	301	1/1	0.99	0.05	23,23,23,23	0
3	CL	T	301	1/1	0.99	0.03	10,10,10,10	0
3	CL	F	301	1/1	1.00	0.05	15,15,15,15	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.



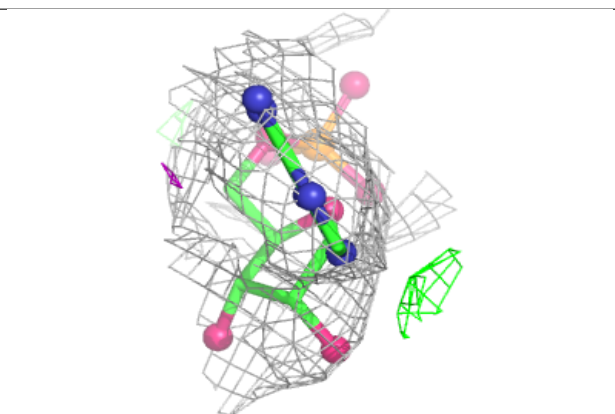
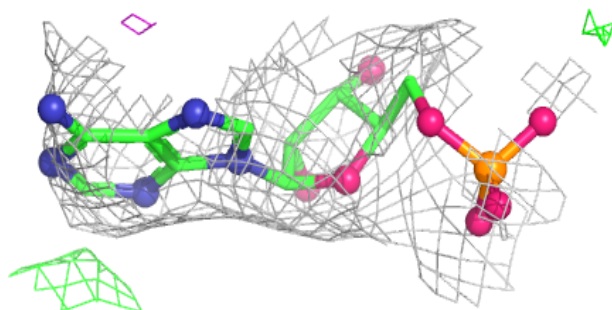
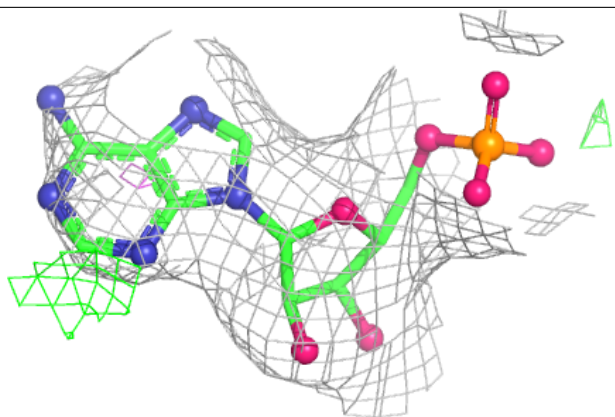
Electron density around AMP H 401:

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

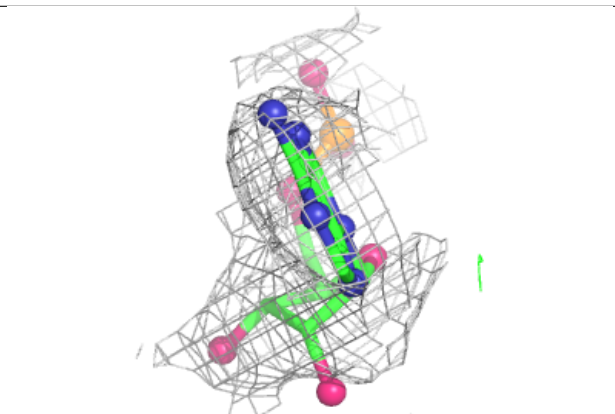
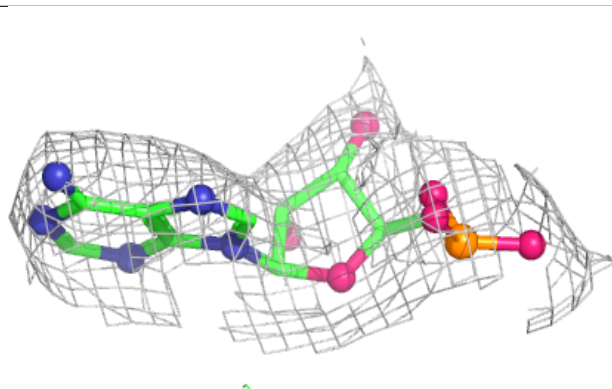


Electron density around AMP N 401:

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

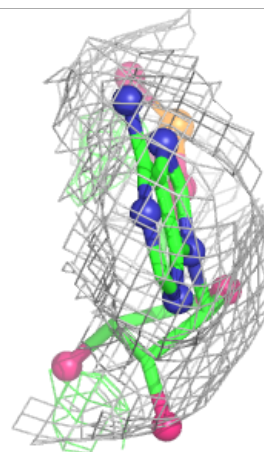
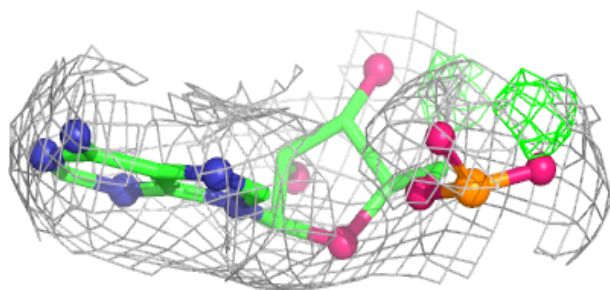
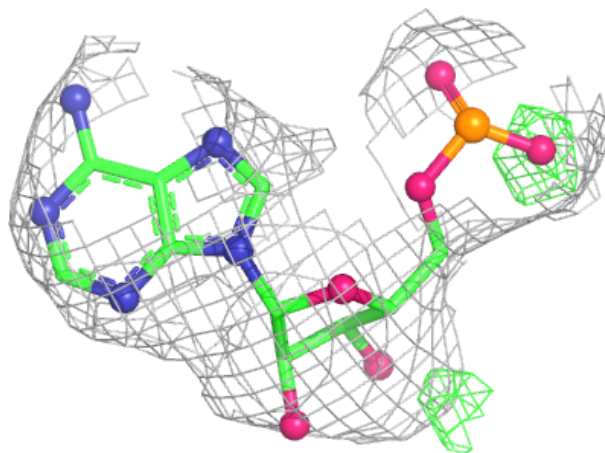
**Electron density around AMP F 404:**

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



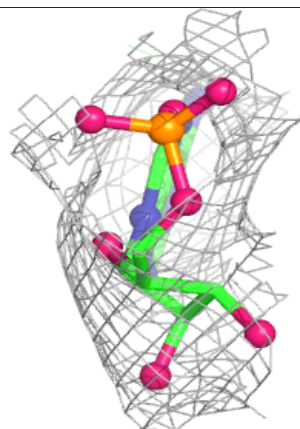
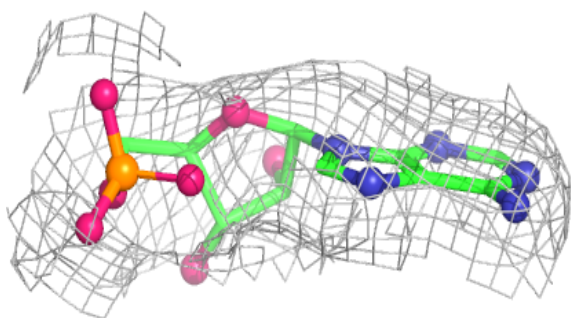
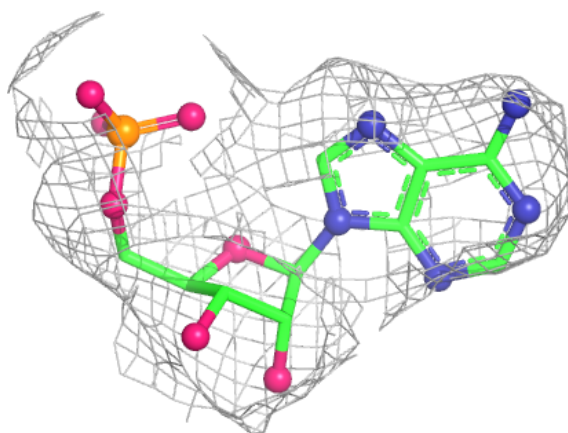
Electron density around AMP F 402:

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



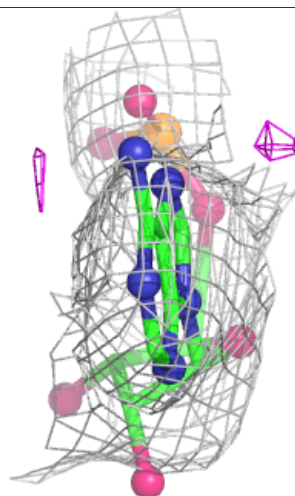
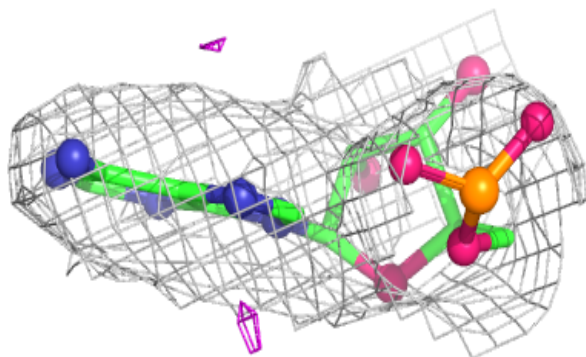
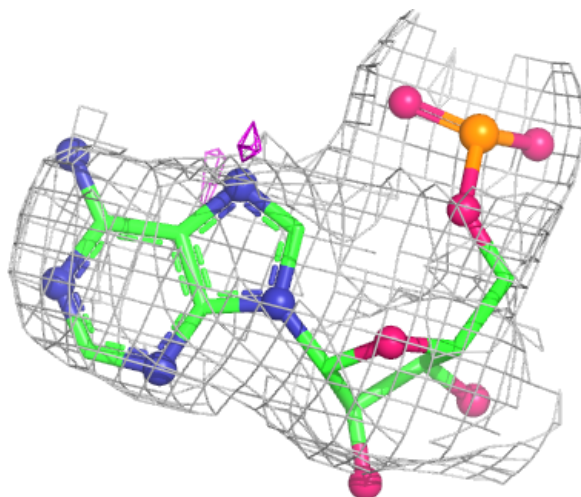
Electron density around AMP B 401:

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



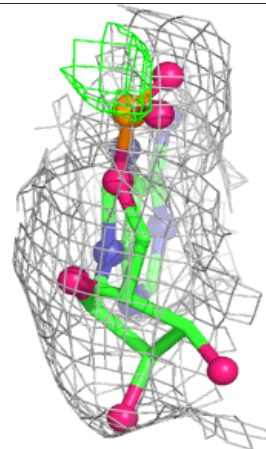
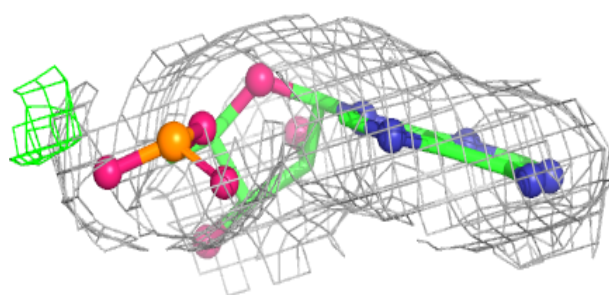
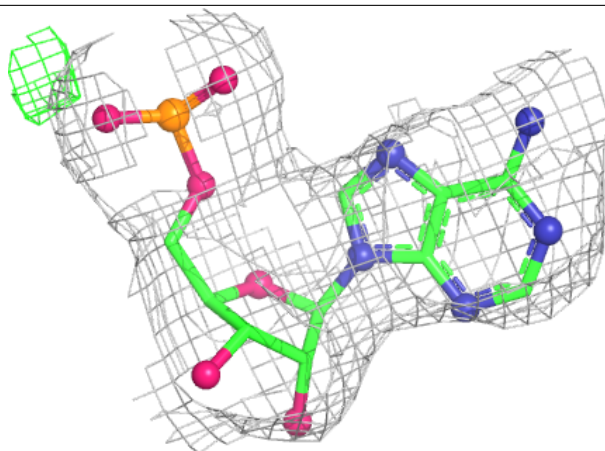
Electron density around AMP X 403:

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



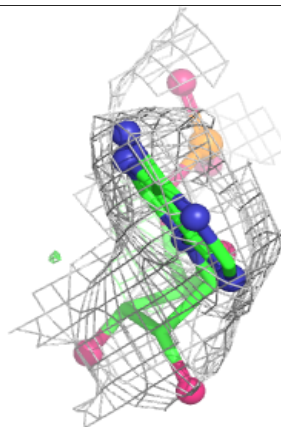
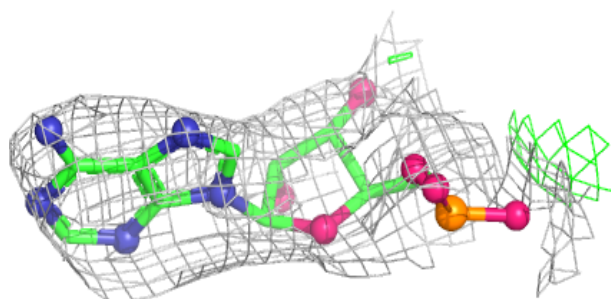
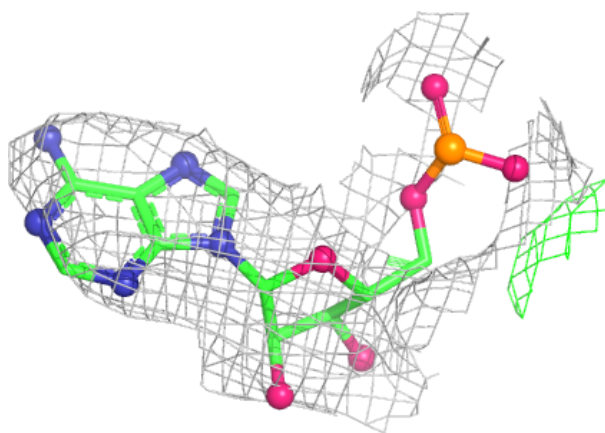
Electron density around AMP H 403:

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



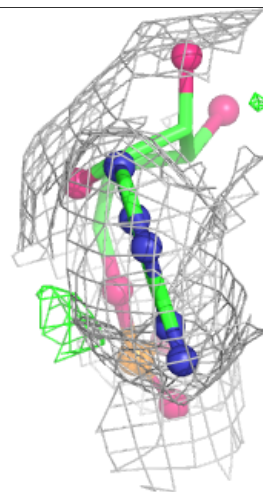
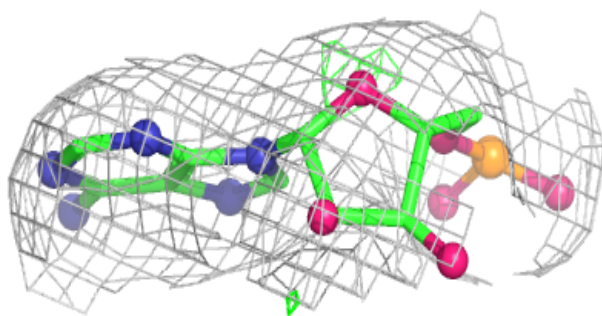
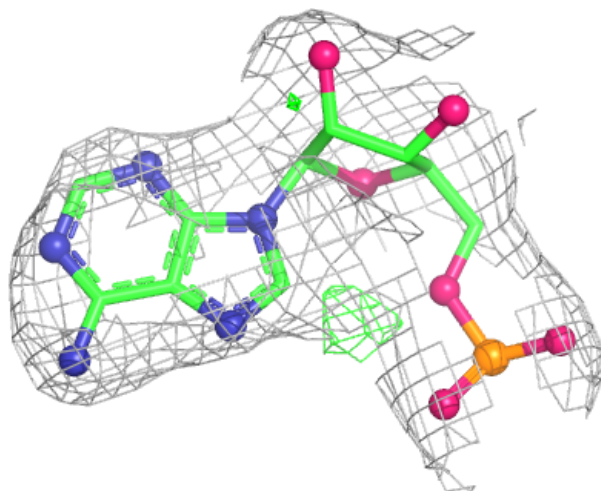
Electron density around AMP N 404:

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



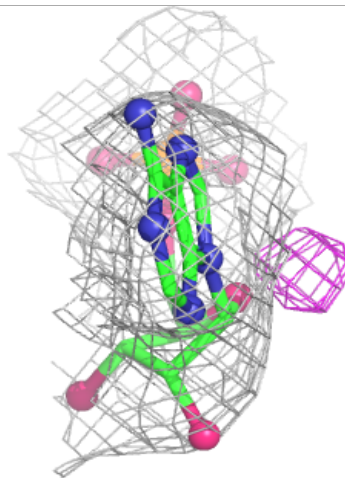
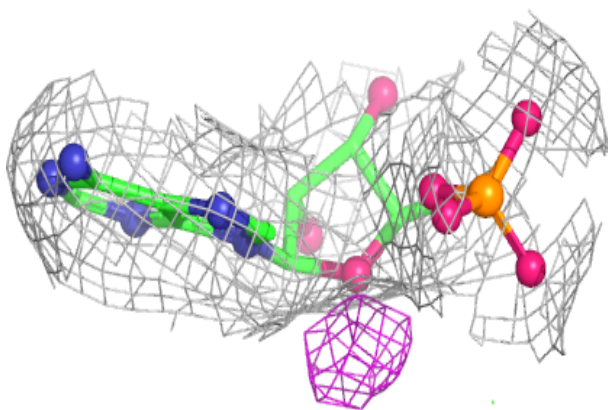
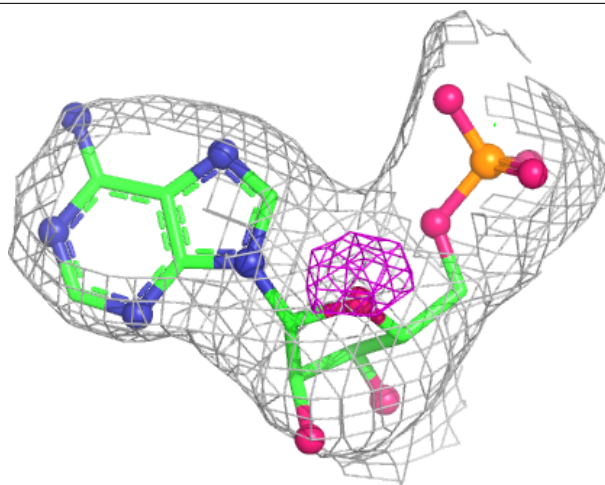
Electron density around AMP V 403:

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



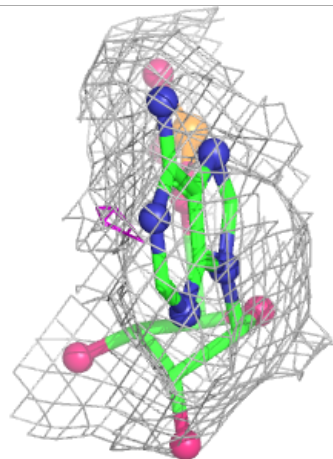
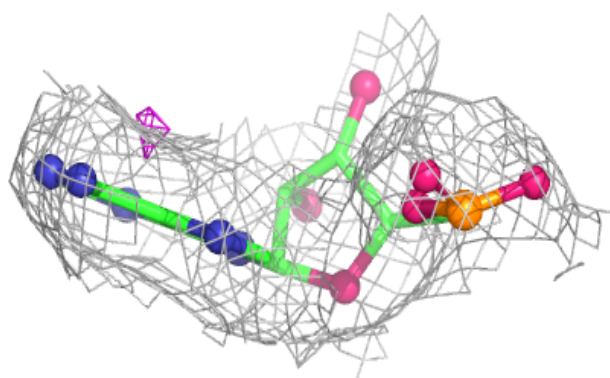
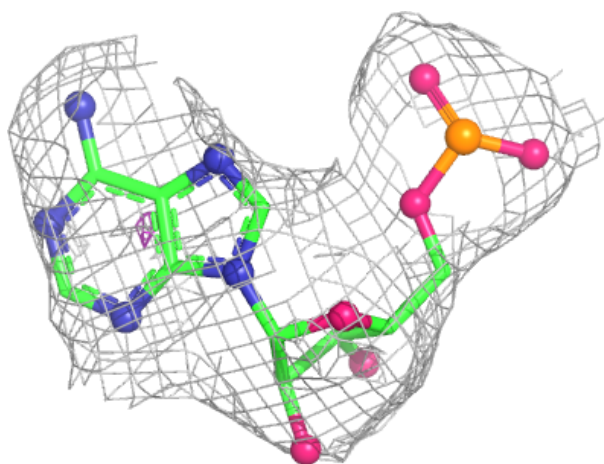
Electron density around AMP X 401:

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



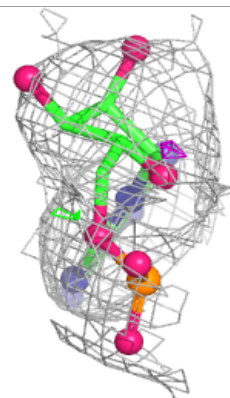
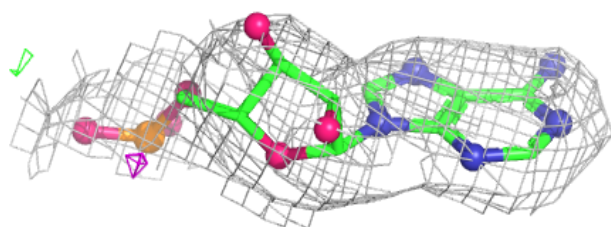
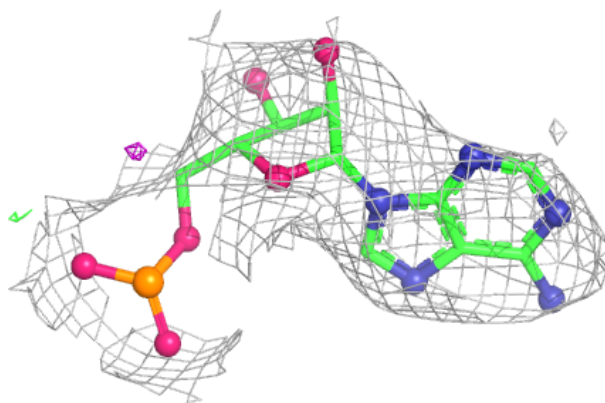
Electron density around AMP X 402:

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



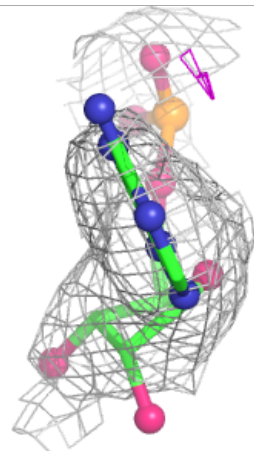
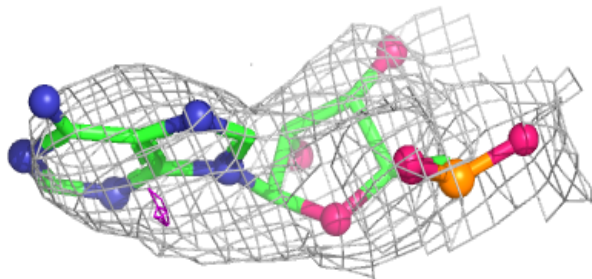
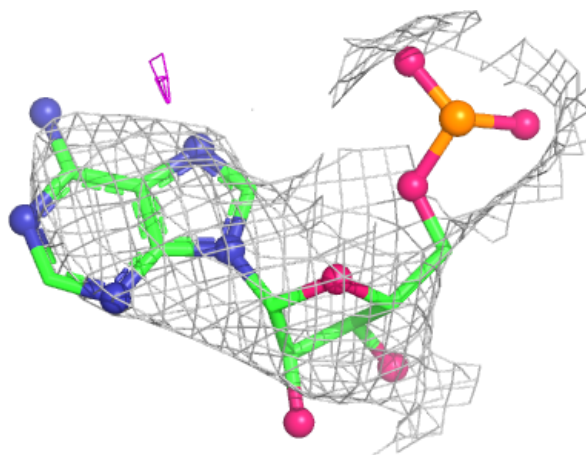
Electron density around AMP J 404:

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



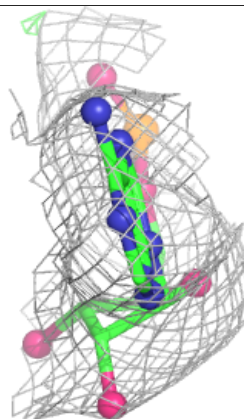
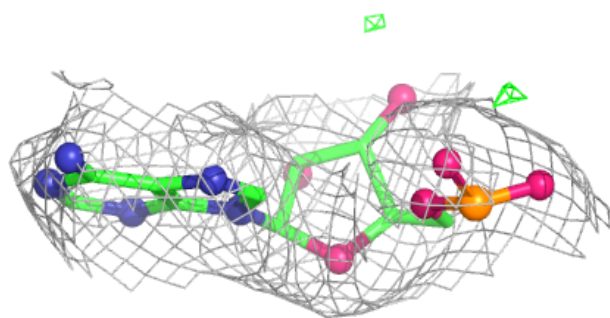
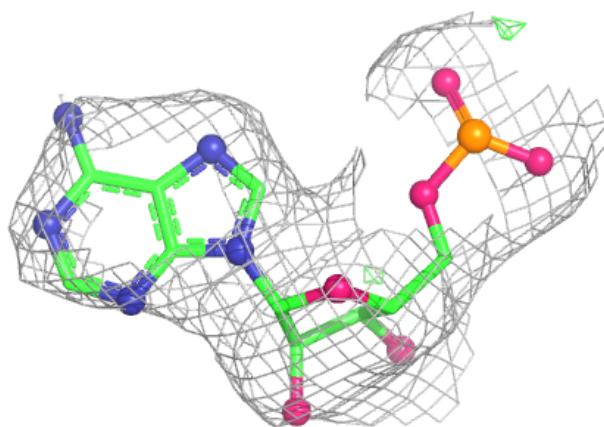
Electron density around AMP X 404:

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

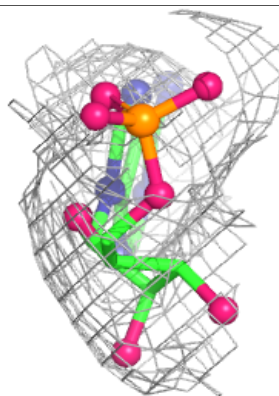
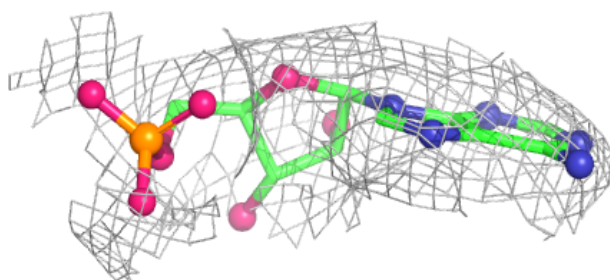
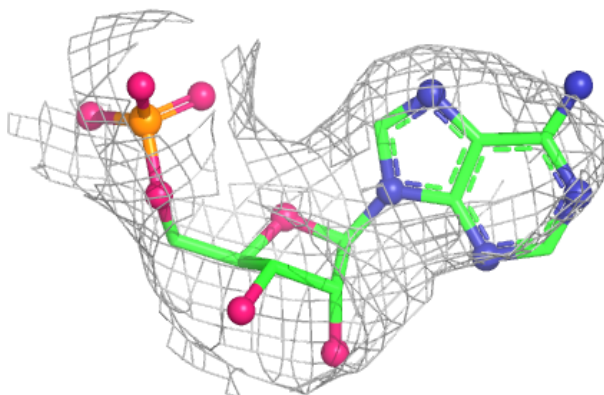


Electron density around AMP B 402:

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

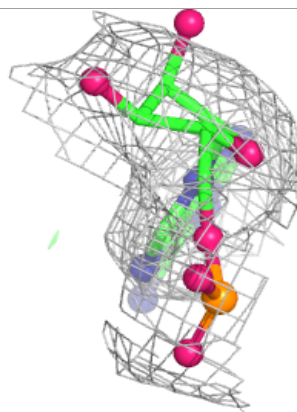
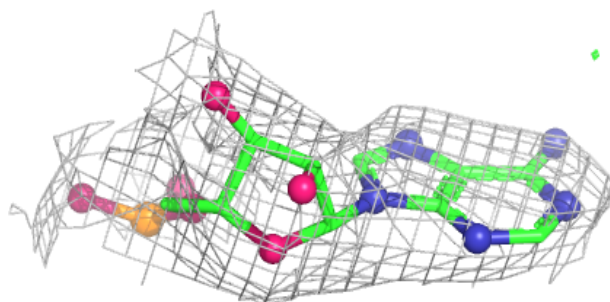
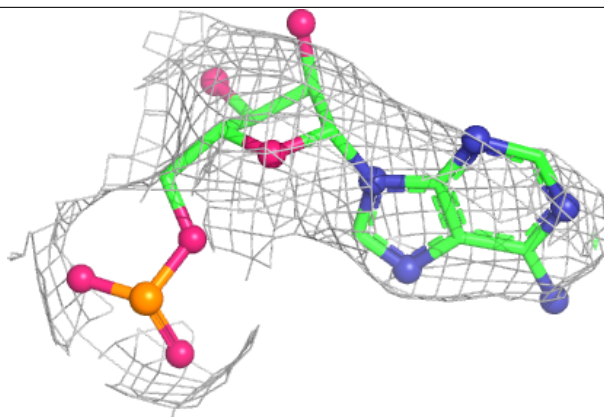
**Electron density around AMP J 401:**

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

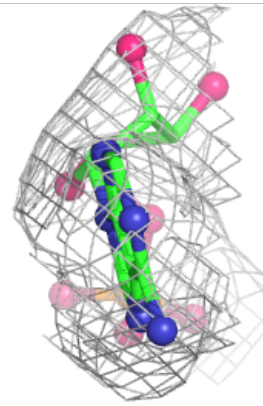
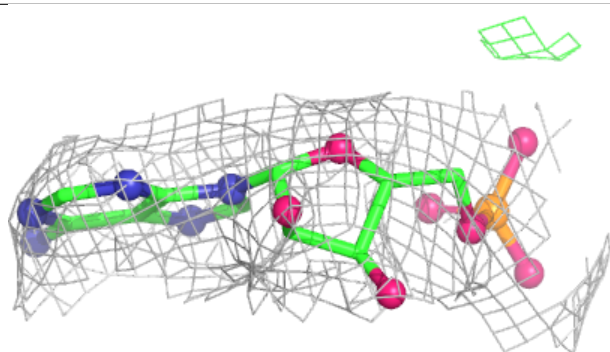
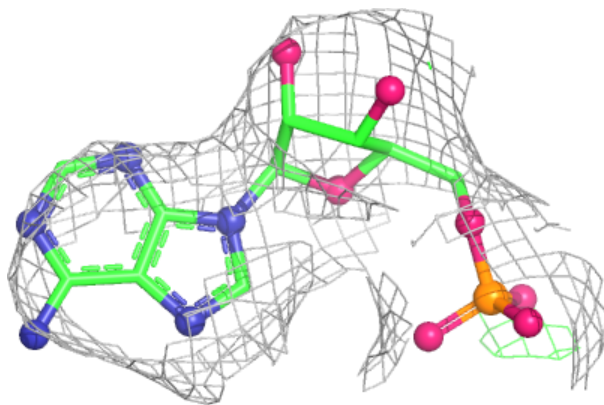


Electron density around AMP B 404:

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

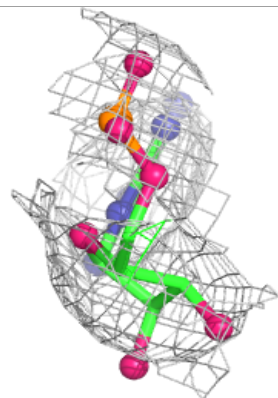
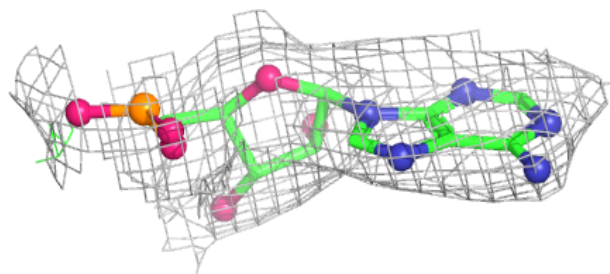
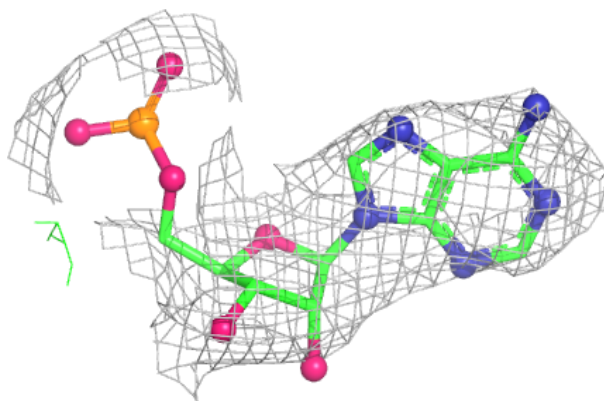
**Electron density around AMP F 401:**

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



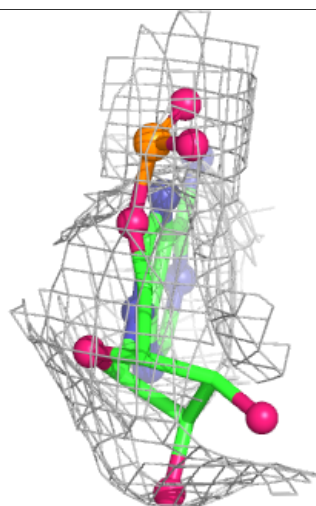
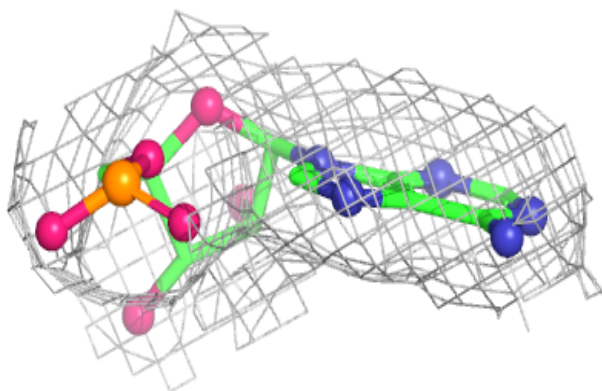
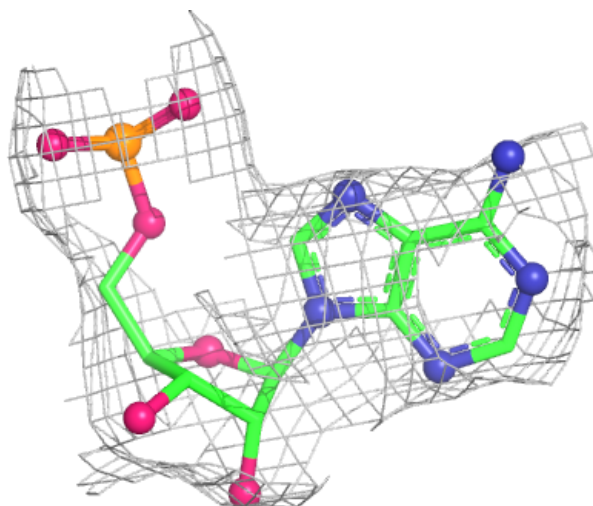
Electron density around AMP H 404:

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



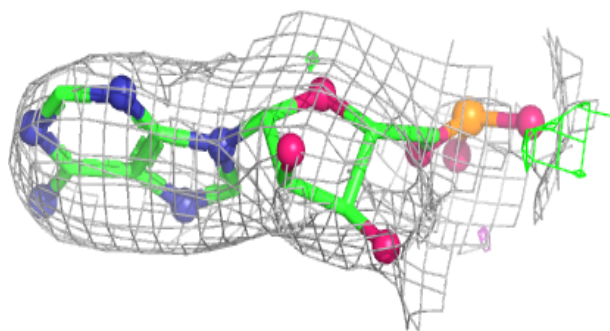
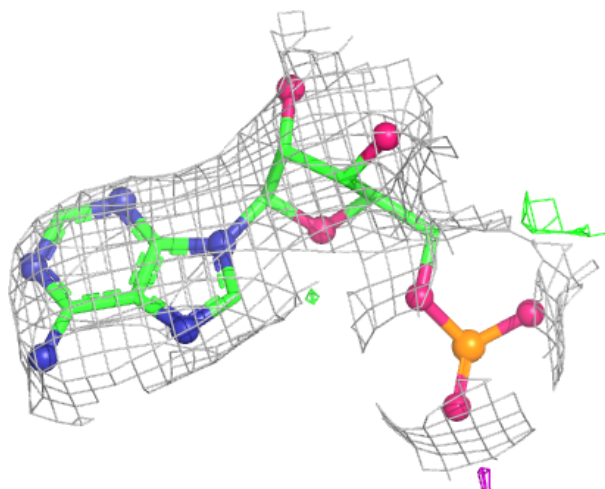
Electron density around AMP J 403:

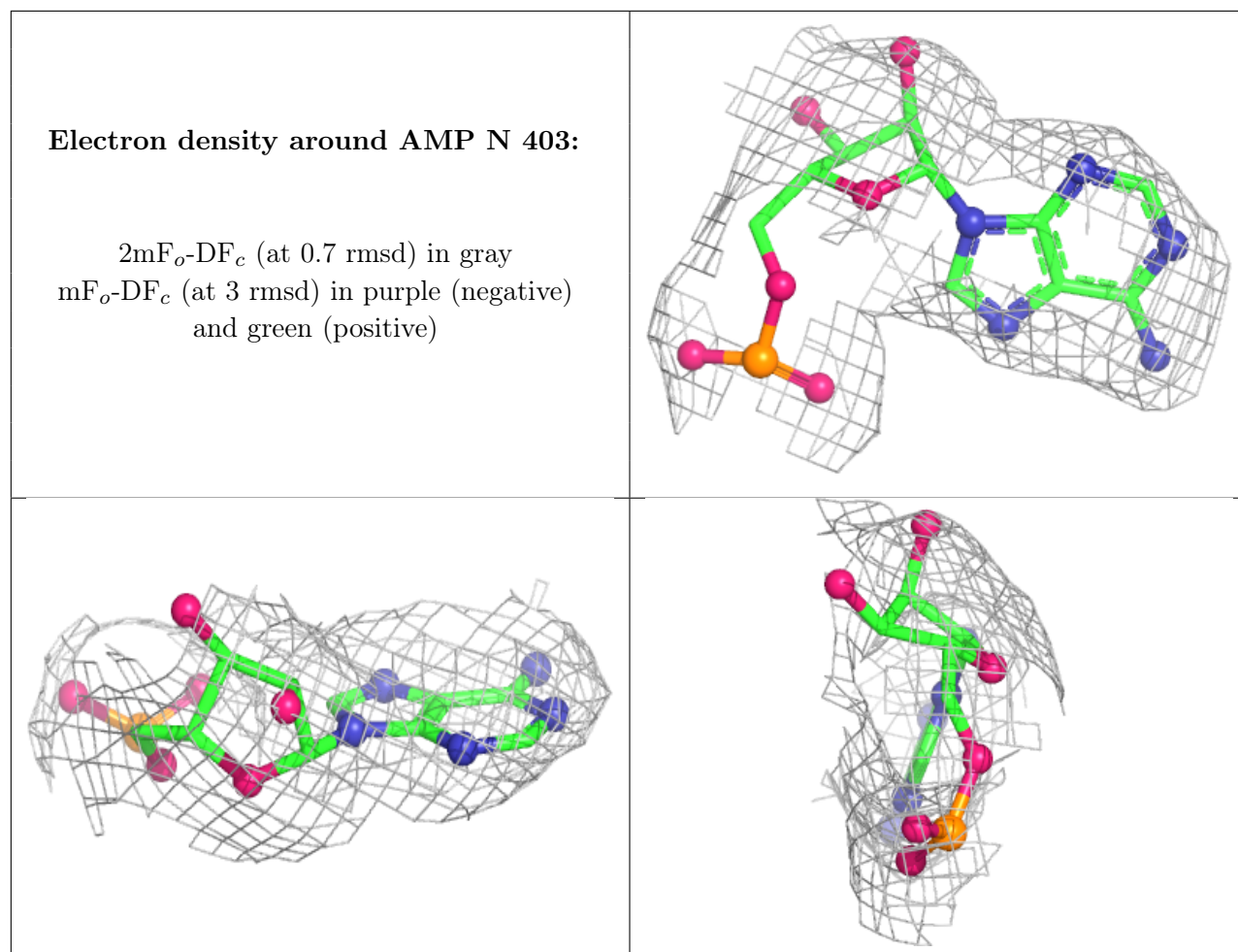
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around AMP V 404:

$2mF_o-DF_c$ (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.