



Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 04:43 AM UTC

PDB ID : 6B8H / pdb_00006b8h
EMDB ID : EMD-7067
Title : Mosaic model of yeast mitochondrial ATP synthase monomer
Authors : Guo, H.; Bueler, S.A.; Rubinstein, J.L.
Deposited on : 2017-10-07
Resolution : 3.60 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>

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:

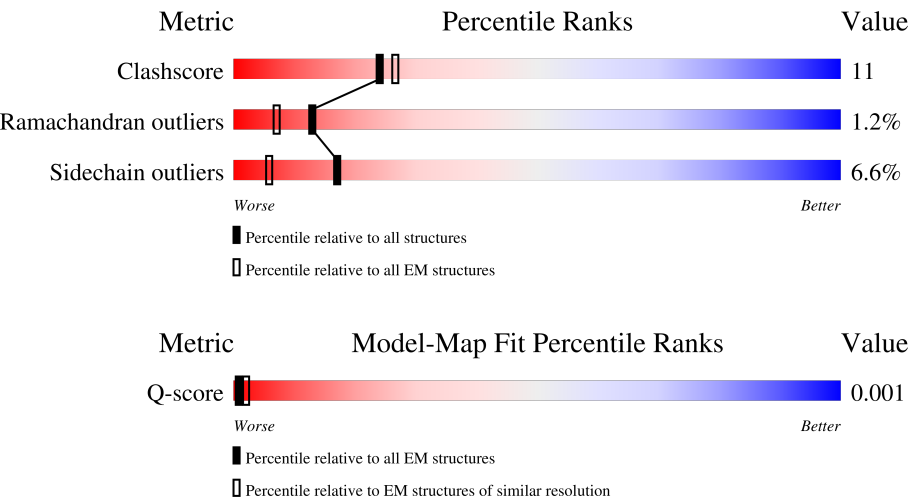
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
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:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	412 (6.90 - 7.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	76	36% 93% 5%
1	1	76	33% 92% 7%
1	2	76	30% 87% 12%
1	3	76	20% 92% 5%

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Mol	Chain	Length	Quality of chain
1	4	76	28% 92% 5% ..
1	5	76	29% 87% 11% ..
1	6	76	37% 88% 9% .
1	7	76	66% 87% 9% .
1	8	76	51% 93% 5% .
1	9	76	47% 92% 5% .
1	J	76	99% 93% 5% .
1	L	76	99% 92% 7% .
1	M	76	99% 86% 13% .
1	N	76	97% 91% 7% .
1	P	76	99% 91% 7% ..
1	Q	76	99% 87% 11% ..
1	R	76	97% 88% 9% .
1	S	76	96% 87% 9% .
1	T	76	99% 93% 5% .
1	U	76	97% 92% 5% .
2	A	48	100% 83% 17%
2	V	48	100% 83% 17%
3	a	249	60% 86% 14%
3	p	249	100% 87% 13%
4	b	209	96% 92% ...
4	q	209	96% 92% ...
5	d	173	87% 82% 8% . 9%
5	r	173	91% 82% 8% . 9%
6	e	49	100% 100%

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Mol	Chain	Length	Quality of chain
6	s	49	100%
7	f	95	88% 76% 12% 12%
7	t	95	88% 76% 12% 12%
8	g	106	100% 99%
8	u	106	100% 99%
9	i	59	100% 97%
9	w	59	100% 97%
10	k	68	16% 32% 65%
10	x	68	35% 32% 65%
11	B	510	96% 60% 32% 5%
11	C	510	98% 67% 29%
11	K	510	98% 68% 28%
11	W	510	96% 61% 31% 5%
11	X	510	98% 67% 28%
11	n	510	98% 68% 27%
12	D	478	98% 69% 27%
12	E	478	98% 65% 31%
12	F	478	98% 62% 33%
12	Y	478	98% 70% 26%
12	Z	478	98% 64% 32%
12	c	478	98% 64% 31%
13	G	278	54% 59% 29% 6% 5%
13	j	278	95% 59% 29% 6% 5%
14	H	138	17% 55% 23% 8% 14%
14	l	138	86% 55% 23% 8% 14%

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Mol	Chain	Length	Quality of chain
15	I	61	28% 39% 28% 10% • 21%
15	m	61	79% 39% 28% 10% • 21%
16	O	195	83% 76% 5% • 17%
16	o	195	83% 76% 5% • 17%
17	h	21	100% 76% 24%
17	v	21	100% 76% 24%

2 Entry composition [i](#)

There are 19 unique types of molecules in this entry. The entry contains 75614 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called ATP synthase subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	75	Total	C	N	O	S	0	0
			537	359	83	91	4		
1	2	75	Total	C	N	O	S	0	0
			537	359	83	91	4		
1	3	74	Total	C	N	O	S	0	0
			529	354	82	90	3		
1	4	75	Total	C	N	O	S	0	0
			537	359	83	91	4		
1	5	75	Total	C	N	O	S	0	0
			537	359	83	91	4		
1	6	74	Total	C	N	O	S	0	0
			529	354	82	90	3		
1	7	73	Total	C	N	O	S	0	0
			522	348	81	89	4		
1	8	75	Total	C	N	O	S	0	0
			537	359	83	91	4		
1	9	74	Total	C	N	O	S	0	0
			529	354	82	90	3		
1	0	75	Total	C	N	O	S	0	0
			537	359	83	91	4		
1	L	75	Total	C	N	O	S	0	0
			537	359	83	91	4		
1	M	75	Total	C	N	O	S	0	0
			537	359	83	91	4		
1	N	74	Total	C	N	O	S	0	0
			529	354	82	90	3		
1	P	75	Total	C	N	O	S	0	0
			537	359	83	91	4		
1	Q	75	Total	C	N	O	S	0	0
			537	359	83	91	4		
1	R	74	Total	C	N	O	S	0	0
			529	354	82	90	3		
1	S	73	Total	C	N	O	S	0	0
			522	348	81	89	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	T	75	Total	C	N	O	S	0	0
			537	359	83	91	4		
1	U	74	Total	C	N	O	S	0	0
			529	354	82	90	3		
1	J	75	Total	C	N	O	S	0	0
			537	359	83	91	4		

- Molecule 2 is a protein called ATP synthase protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	48	Total	C	N	O	S	0	0
			410	287	59	60	4		
2	V	48	Total	C	N	O	S	0	0
			410	287	59	60	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	a	249	Total	C	N	O	S	0	0
			1971	1338	296	326	11		
3	p	249	Total	C	N	O	S	0	0
			1971	1338	296	326	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	b	200	Total	C	N	O	S	0	0
			1153	715	210	227	1		
4	q	200	Total	C	N	O	S	0	0
			1153	715	210	227	1		

- Molecule 5 is a protein called ATP synthase subunit d, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	d	157	Total	C	N	O	S	0	0
			930	573	173	182	2		
5	r	157	Total	C	N	O	S	0	0
			930	573	173	182	2		

- Molecule 6 is a protein called ATP synthase subunit e, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	e	49	Total	C	N	O	0	0
			245	147	49	49		
6	s	49	Total	C	N	O	0	0
			245	147	49	49		

- Molecule 7 is a protein called ATP synthase subunit f, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	f	84	Total	C	N	O	S	0	0
			607	396	108	102	1		
7	t	84	Total	C	N	O	S	0	0
			607	396	108	102	1		

- Molecule 8 is a protein called AATP synthase subunit g.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	g	106	Total	C	N	O	0	0
			530	318	106	106		
8	u	106	Total	C	N	O	0	0
			530	318	106	106		

- Molecule 9 is a protein called ATP synthase subunit J, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	59	Total	C	N	O	S	0	0
			473	313	78	80	2		
9	w	59	Total	C	N	O	S	0	0
			473	313	78	80	2		

- Molecule 10 is a protein called ATP synthase subunit K, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	k	24	Total	C	N	O	S	0	0
			180	122	30	27	1		
10	x	24	Total	C	N	O	S	0	0
			180	122	30	27	1		

- Molecule 11 is a protein called ATP synthase subunit alpha, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	501	Total	C	N	O	S	0	0
			3745	2363	665	714	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
11	B	492	Total	C	N	O	S	0	0
			3700	2336	656	705	3		
11	C	500	Total	C	N	O	S	0	0
			3739	2359	664	713	3		
11	n	501	Total	C	N	O	S	0	0
			3745	2363	665	714	3		
11	W	492	Total	C	N	O	S	0	0
			3700	2336	656	705	3		
11	X	500	Total	C	N	O	S	0	0
			3739	2359	664	713	3		

- Molecule 12 is a protein called ATP synthase subunit beta, mitochondrial.

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

- Molecule 13 is a protein called ATP synthase subunit gamma, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	265	Total	C	N	O	S	0	0
			2030	1277	355	388	10		
13	j	265	Total	C	N	O	S	0	0
			2030	1277	355	388	10		

- Molecule 14 is a protein called ATP synthase subunit delta, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	H	119	Total	C	N	O	S	0	0
			751	470	133	146	2		
14	l	119	Total	C	N	O	S	0	0
			751	470	133	146	2		

- Molecule 15 is a protein called ATP synthase catalytic sector F1 epsilon subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	I	48	Total	C	N	O	0	0
			324	201	56	67		
15	m	48	Total	C	N	O	0	0
			324	201	56	67		

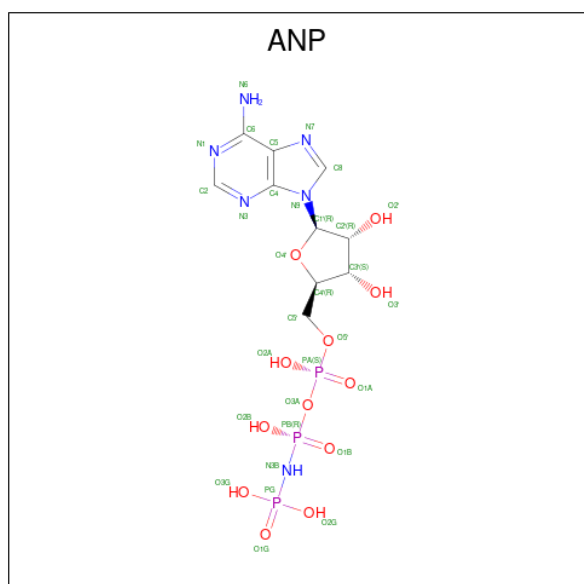
- Molecule 16 is a protein called ATP synthase subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	O	161	Total	C	N	O	0	0
			795	473	161	161		
16	o	161	Total	C	N	O	0	0
			795	473	161	161		

- Molecule 17 is a protein called ATP synthase subunit h.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	h	21	Total	C	N	O	0	0
			105	63	21	21		
17	v	21	Total	C	N	O	0	0
			105	63	21	21		

- Molecule 18 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms					AltConf
18	K	1	Total	C	N	O	P	0
			31	10	6	12	3	
18	B	1	Total	C	N	O	P	0
			31	10	6	12	3	
18	C	1	Total	C	N	O	P	0
			31	10	6	12	3	
18	D	1	Total	C	N	O	P	0
			31	10	6	12	3	
18	F	1	Total	C	N	O	P	0
			31	10	6	12	3	
18	n	1	Total	C	N	O	P	0
			31	10	6	12	3	
18	W	1	Total	C	N	O	P	0
			31	10	6	12	3	
18	X	1	Total	C	N	O	P	0
			31	10	6	12	3	
18	Y	1	Total	C	N	O	P	0
			31	10	6	12	3	
18	c	1	Total	C	N	O	P	0
			31	10	6	12	3	

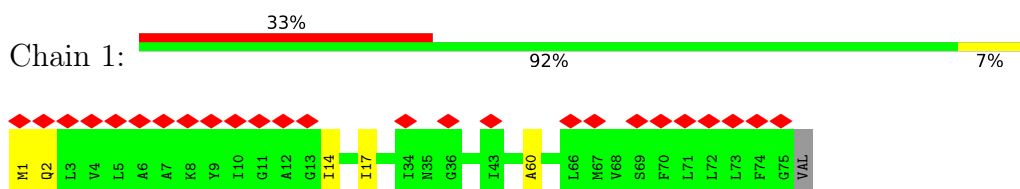
- Molecule 19 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
19	K	1	Total	Mg	0
			1	1	
19	B	1	Total	Mg	0
			1	1	
19	C	1	Total	Mg	0
			1	1	
19	D	1	Total	Mg	0
			1	1	
19	F	1	Total	Mg	0
			1	1	
19	n	1	Total	Mg	0
			1	1	
19	W	1	Total	Mg	0
			1	1	
19	X	1	Total	Mg	0
			1	1	
19	Y	1	Total	Mg	0
			1	1	
19	c	1	Total	Mg	0
			1	1	

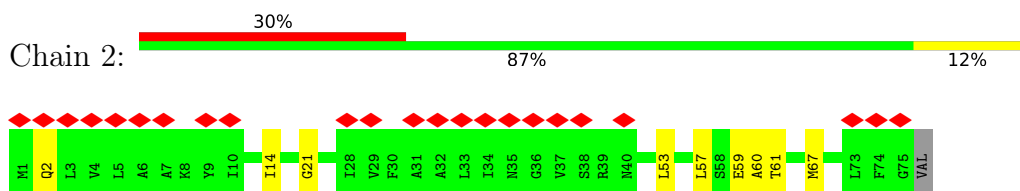
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

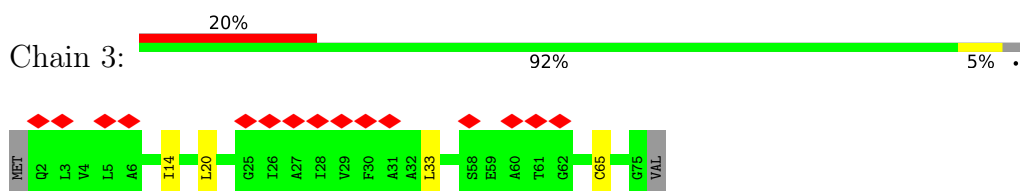
- Molecule 1: ATP synthase subunit 9, mitochondrial



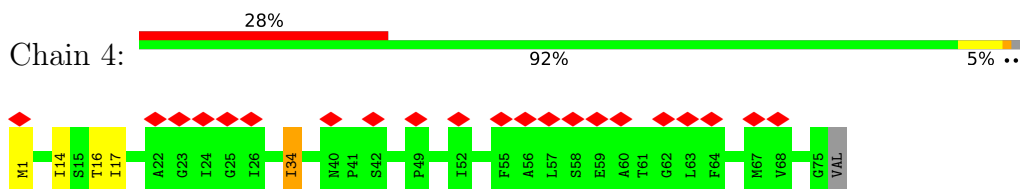
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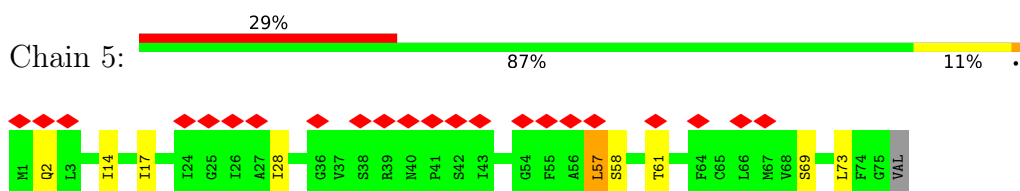
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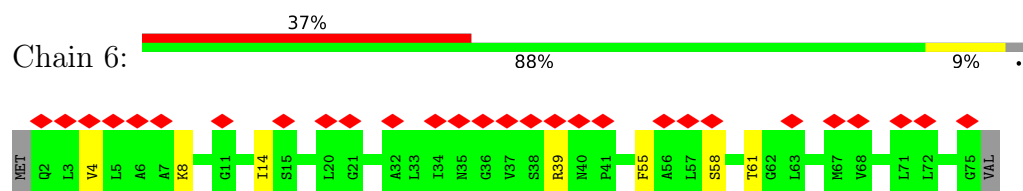
- Molecule 1: ATP synthase subunit 9, mitochondrial



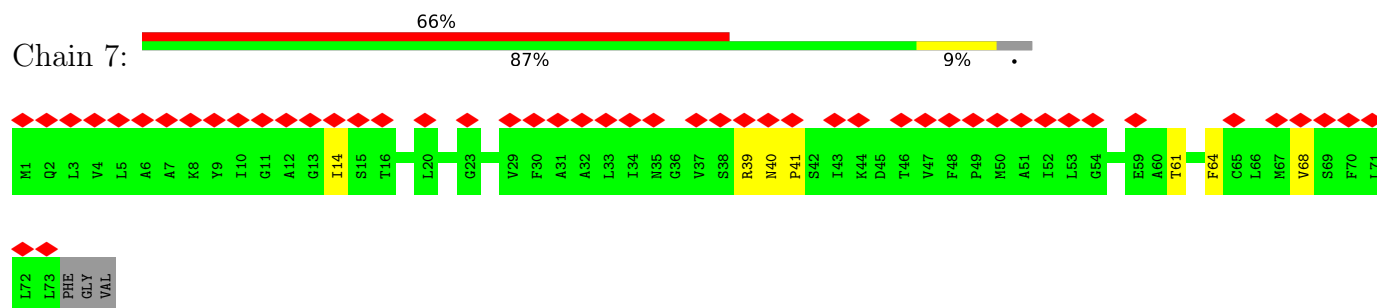
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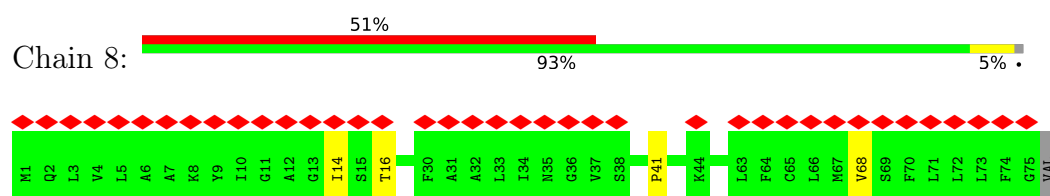
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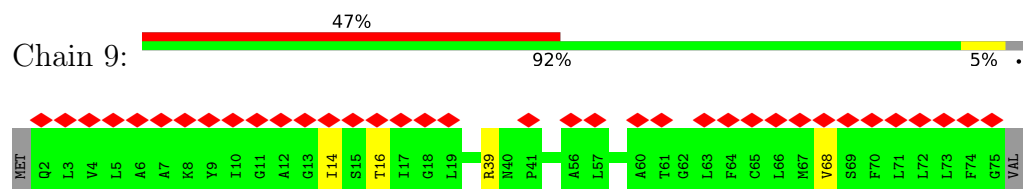
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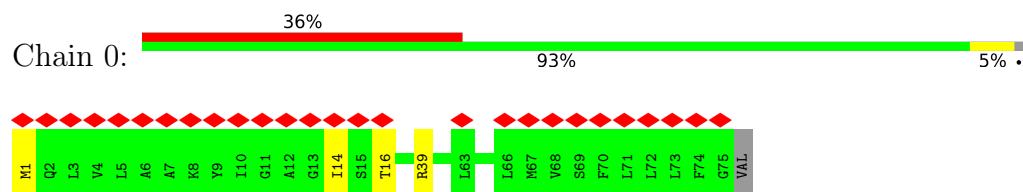
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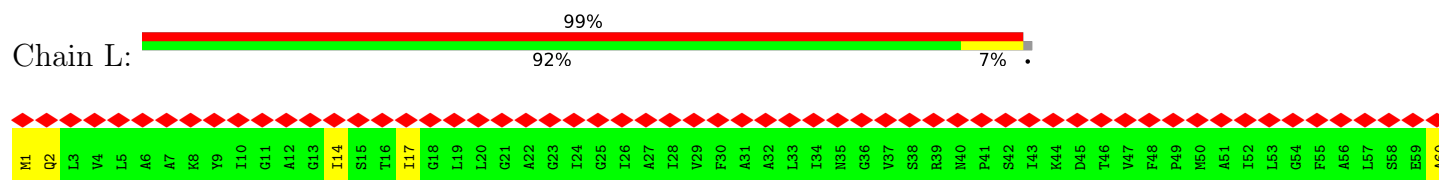
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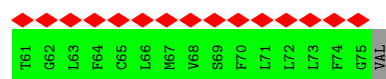


• Molecule 1: ATP synthase subunit 9, mitochondrial

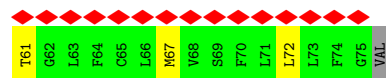
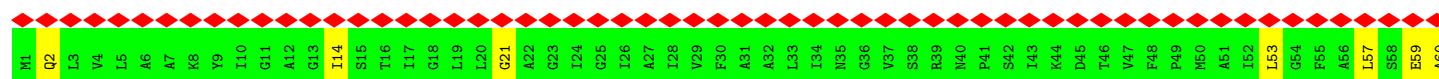
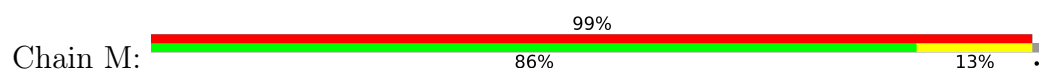


• Molecule 1: ATP synthase subunit 9, mitochondrial

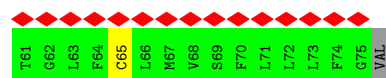
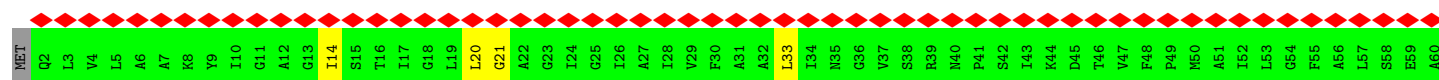
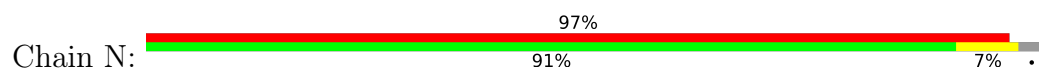




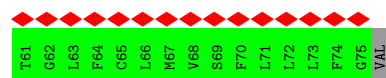
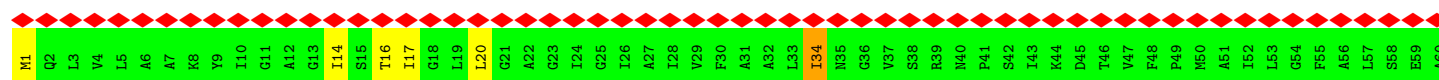
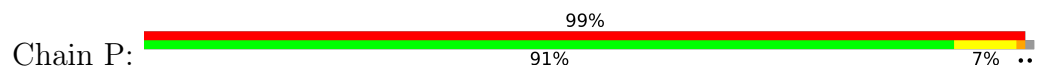
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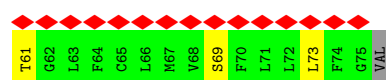
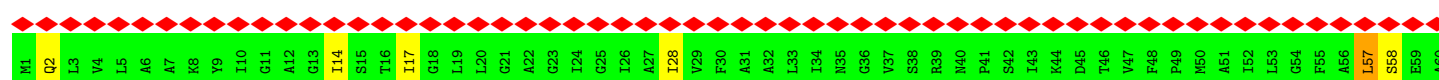
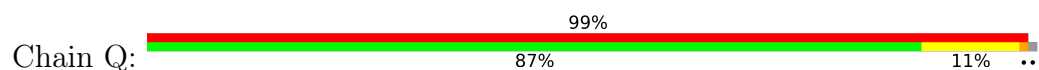
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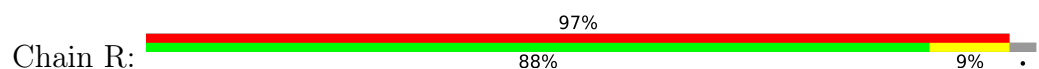
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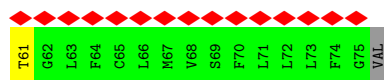
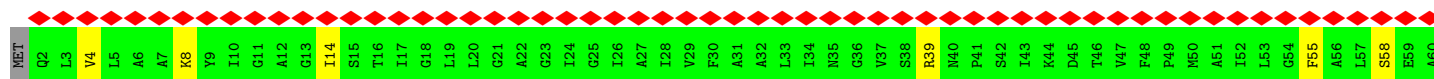


- Molecule 1: ATP synthase subunit 9, mitochondrial

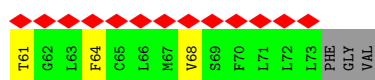
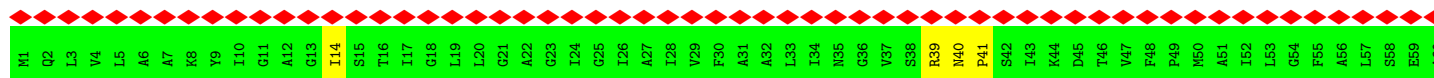
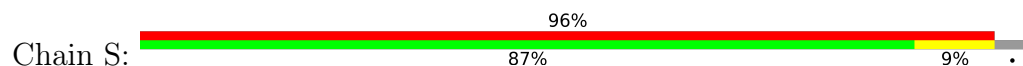


- Molecule 1: ATP synthase subunit 9, mitochondrial

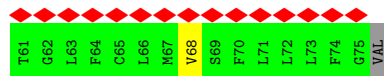
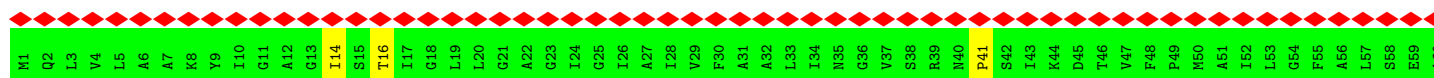




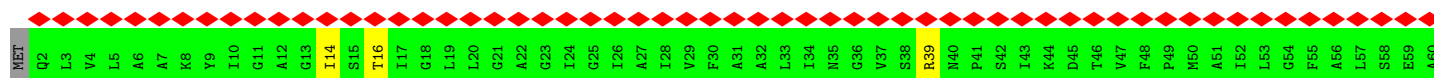
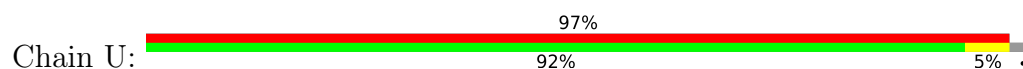
- Molecule 1: ATP synthase subunit 9, mitochondrial



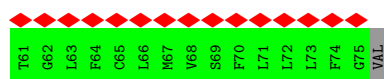
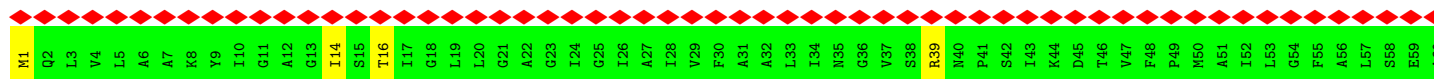
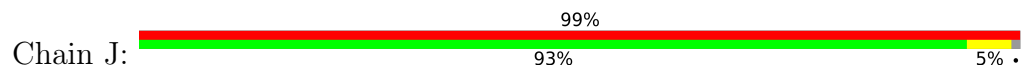
- Molecule 1: ATP synthase subunit 9, mitochondrial



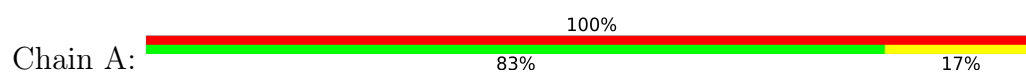
- Molecule 1: ATP synthase subunit 9, mitochondrial



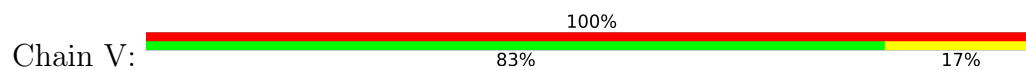
- Molecule 1: ATP synthase subunit 9, mitochondrial



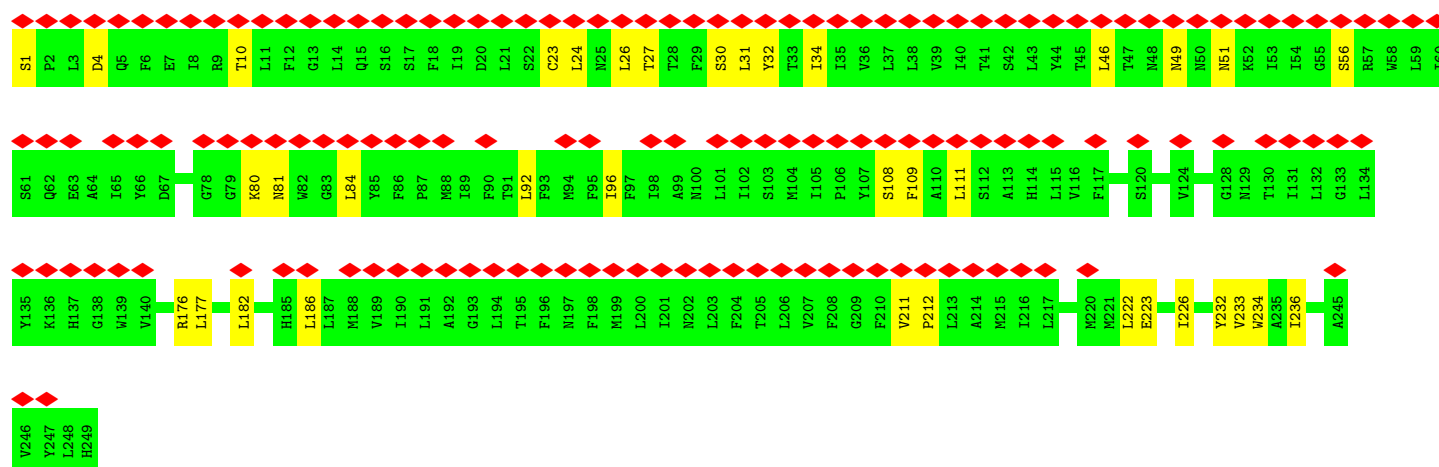
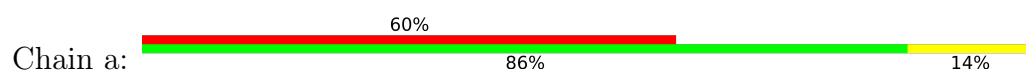
- Molecule 2: ATP synthase protein 8



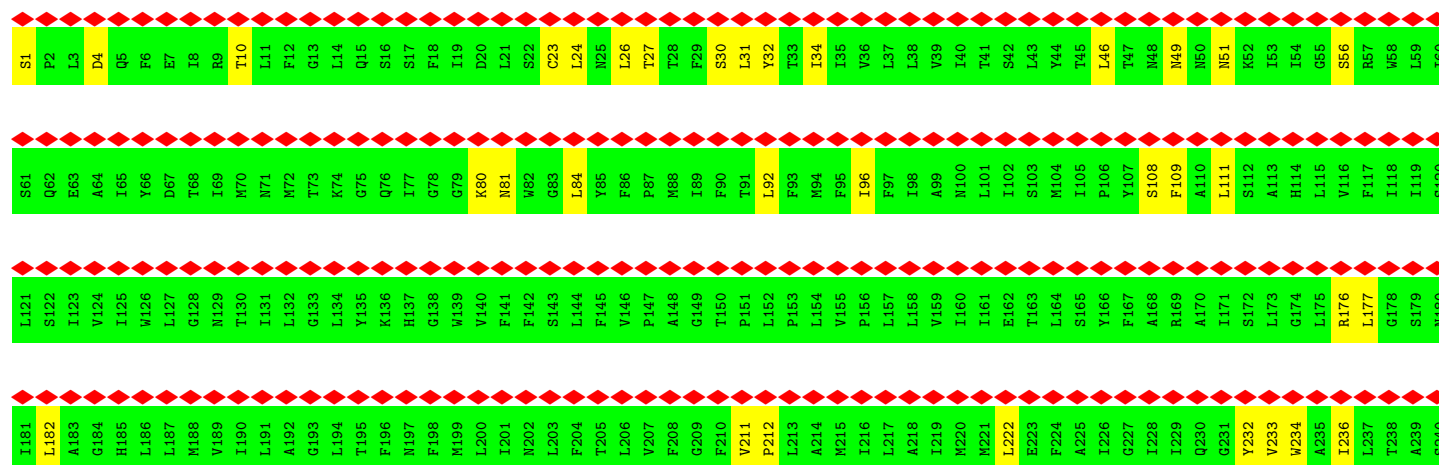
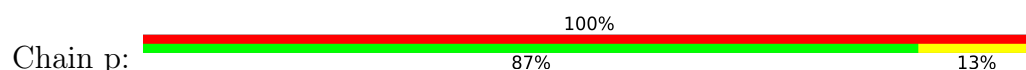
• Molecule 2: ATP synthase protein 8



• Molecule 3: ATP synthase subunit a

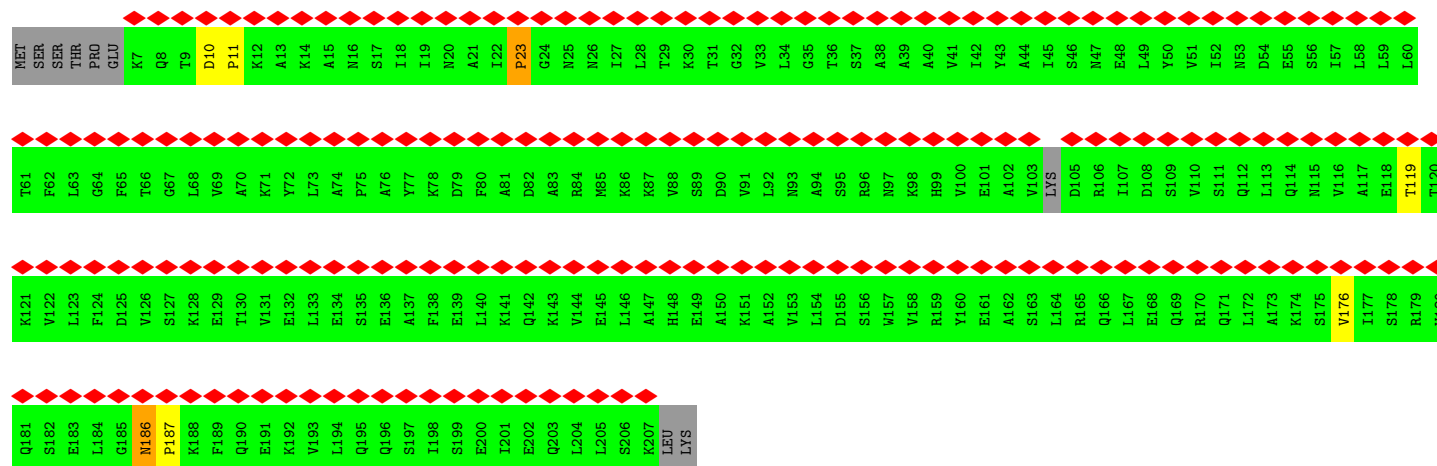
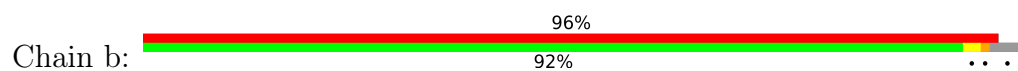


• Molecule 3: ATP synthase subunit a

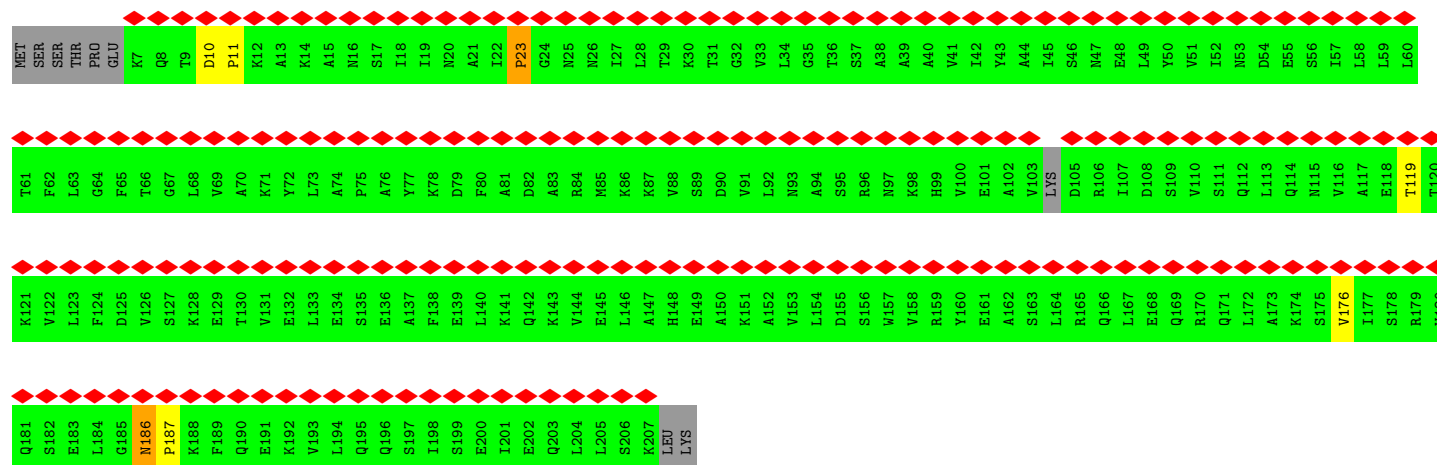
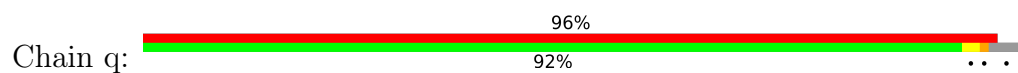




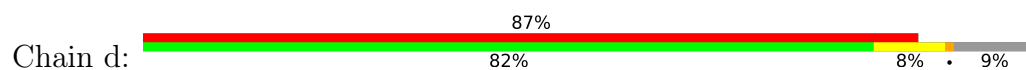
• Molecule 4: ATP synthase subunit 4, mitochondrial

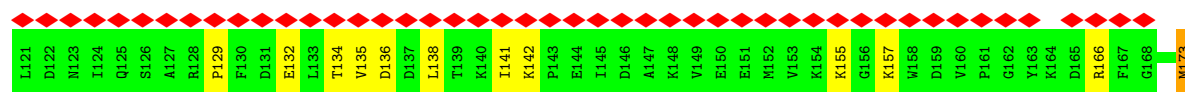


• Molecule 4: ATP synthase subunit 4, mitochondrial

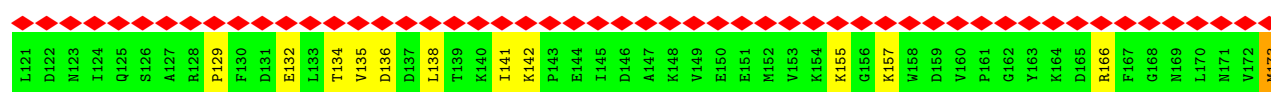
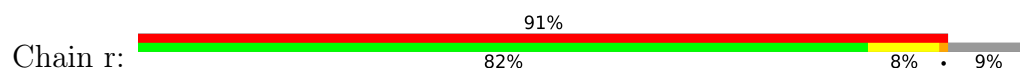


• Molecule 5: ATP synthase subunit d, mitochondrial

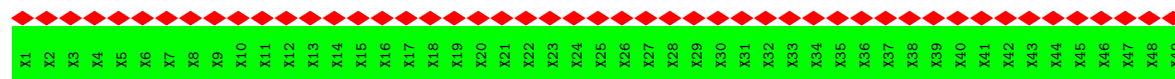




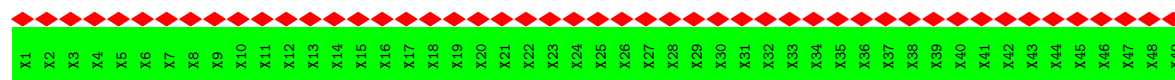
- Molecule 5: ATP synthase subunit d, mitochondrial



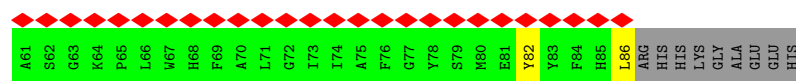
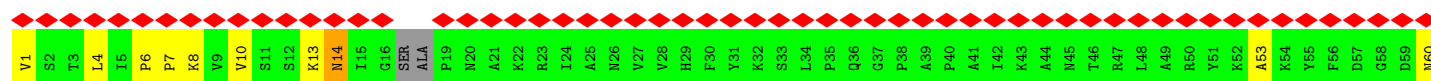
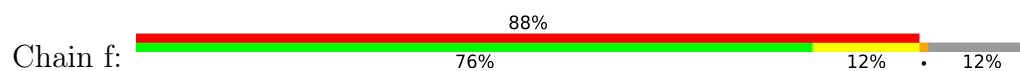
- Molecule 6: ATP synthase subunit e, mitochondrial



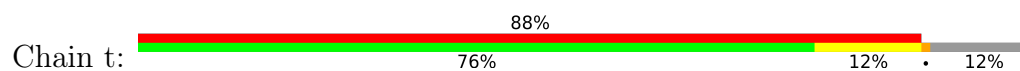
- Molecule 6: ATP synthase subunit e, mitochondrial

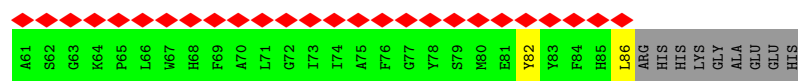


- Molecule 7: ATP synthase subunit f, mitochondrial

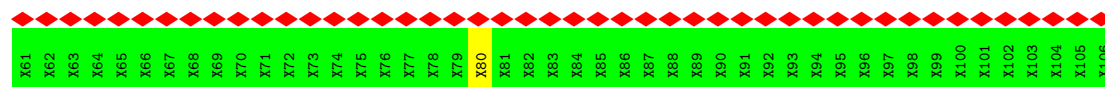
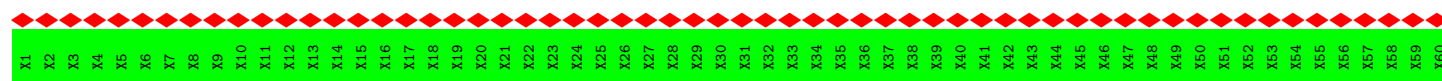


- Molecule 7: ATP synthase subunit f, mitochondrial

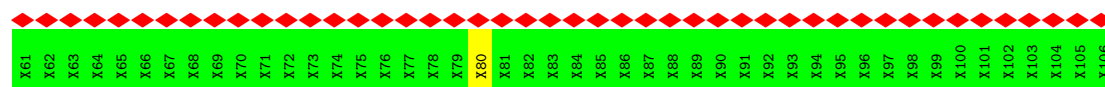
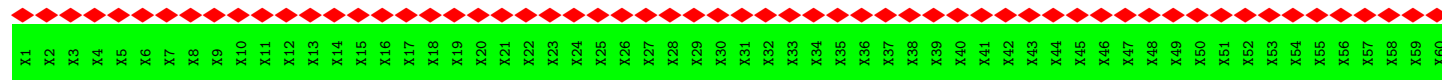




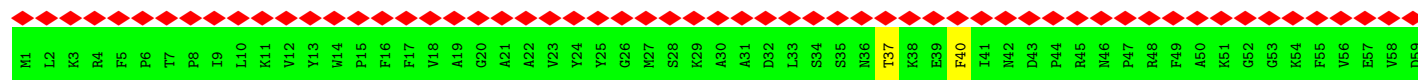
- Molecule 8: AATP synthase subunit g



- Molecule 8: AATP synthase subunit g



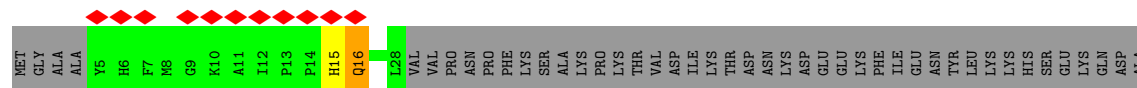
- Molecule 9: ATP synthase subunit J, mitochondrial



- Molecule 9: ATP synthase subunit J, mitochondrial

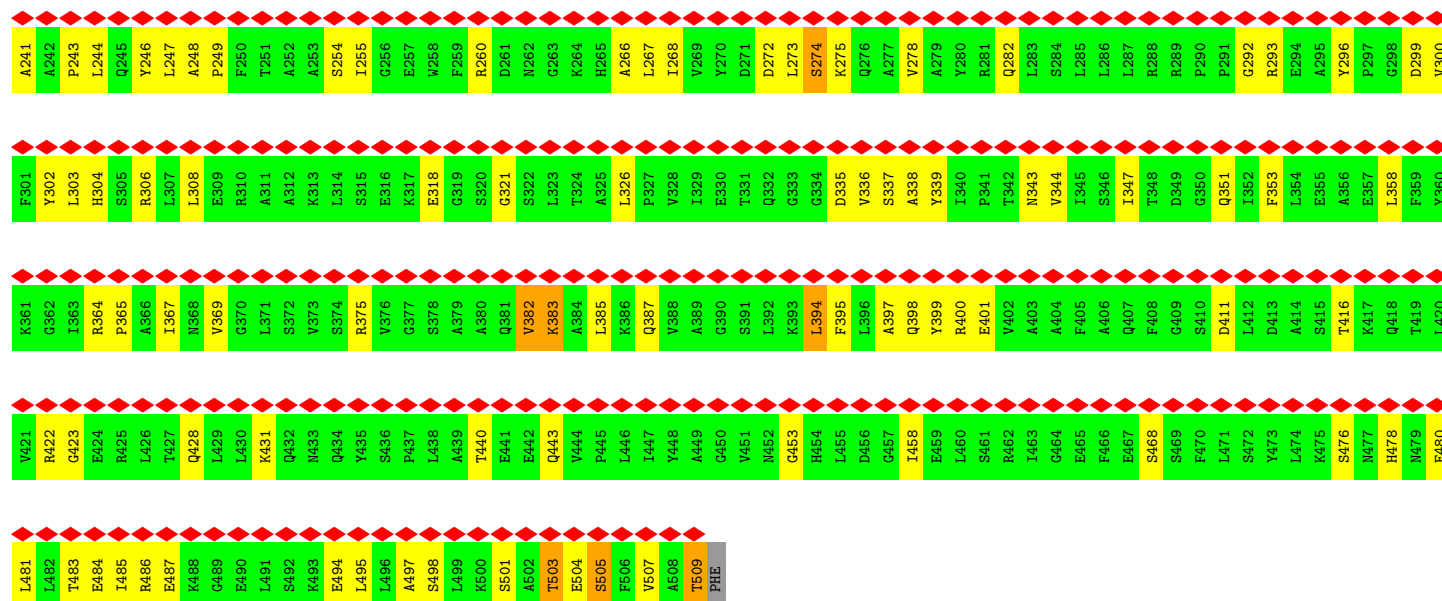


- Molecule 10: ATP synthase subunit K, mitochondrial

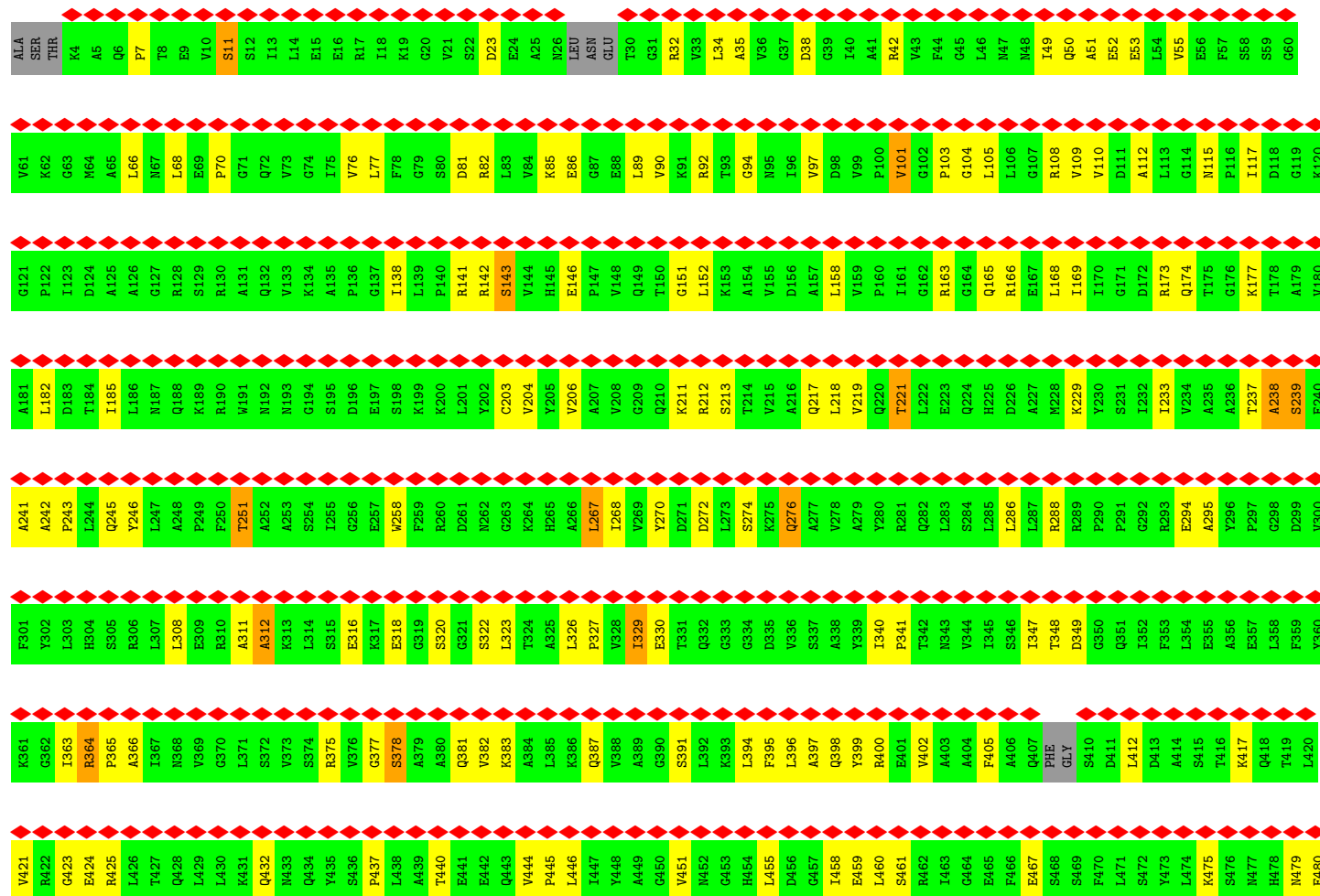


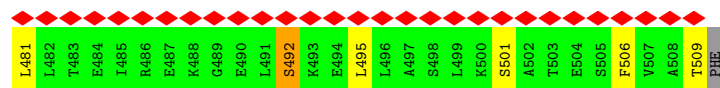
- Molecule 10: ATP synthase subunit K, mitochondrial



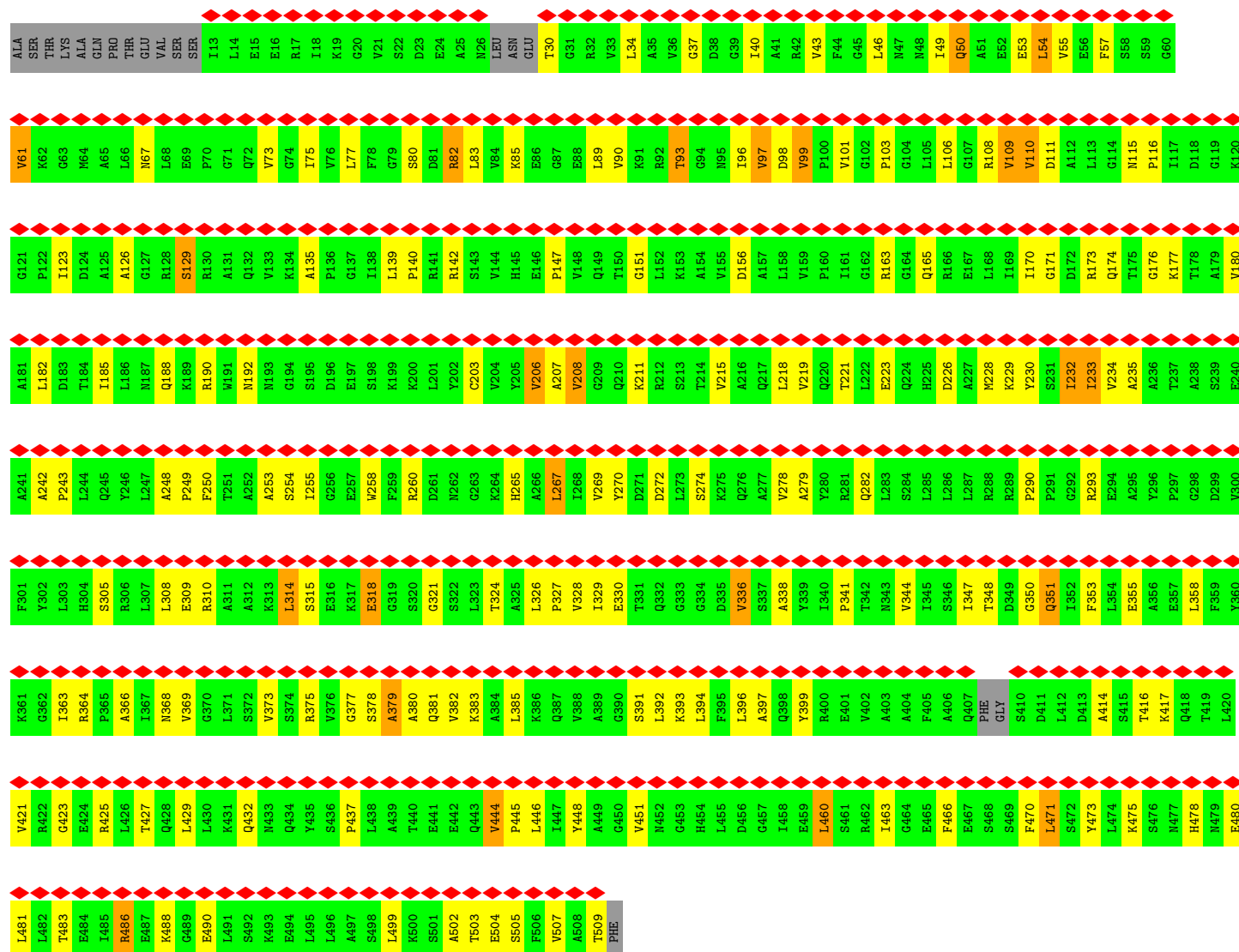


• Molecule 11: ATP synthase subunit alpha, mitochondrial

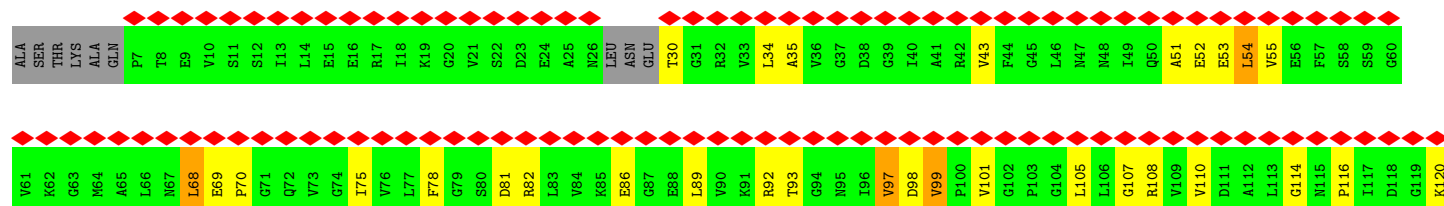




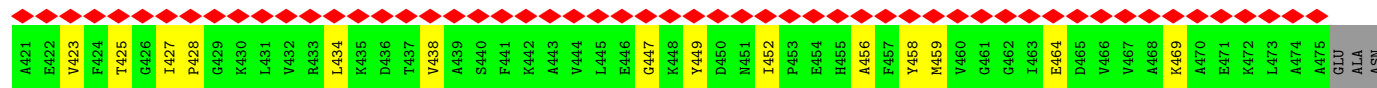
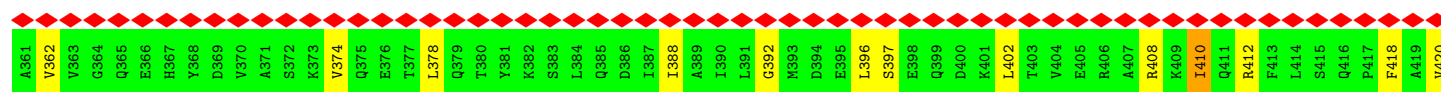
- Molecule 11: ATP synthase subunit alpha, mitochondrial



- Molecule 11: ATP synthase subunit alpha, mitochondrial

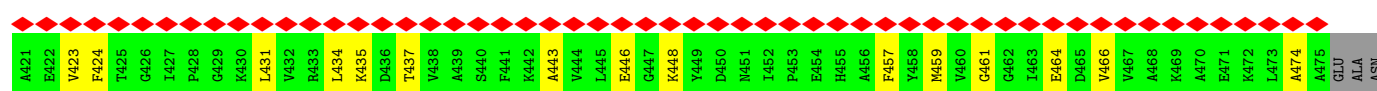
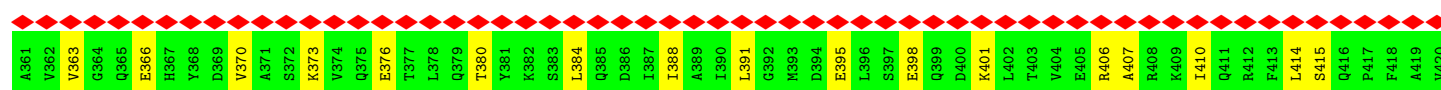
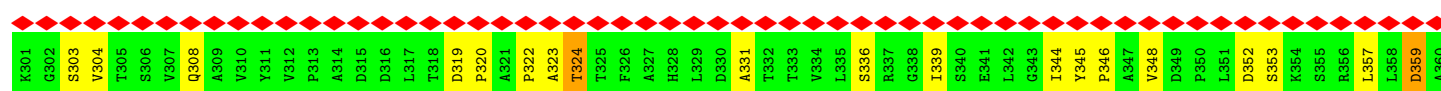
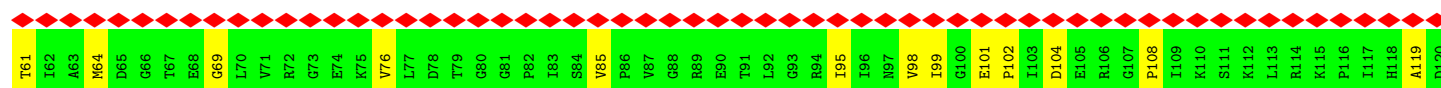






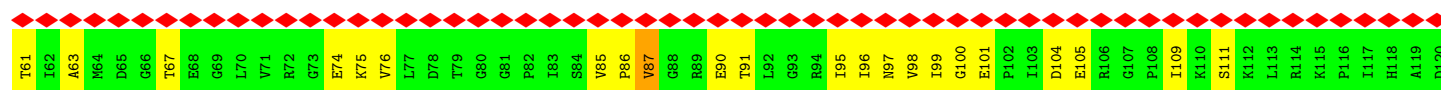
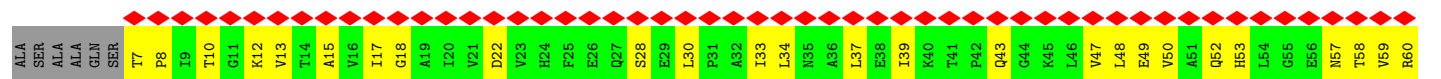
• Molecule 12: ATP synthase subunit beta, mitochondrial

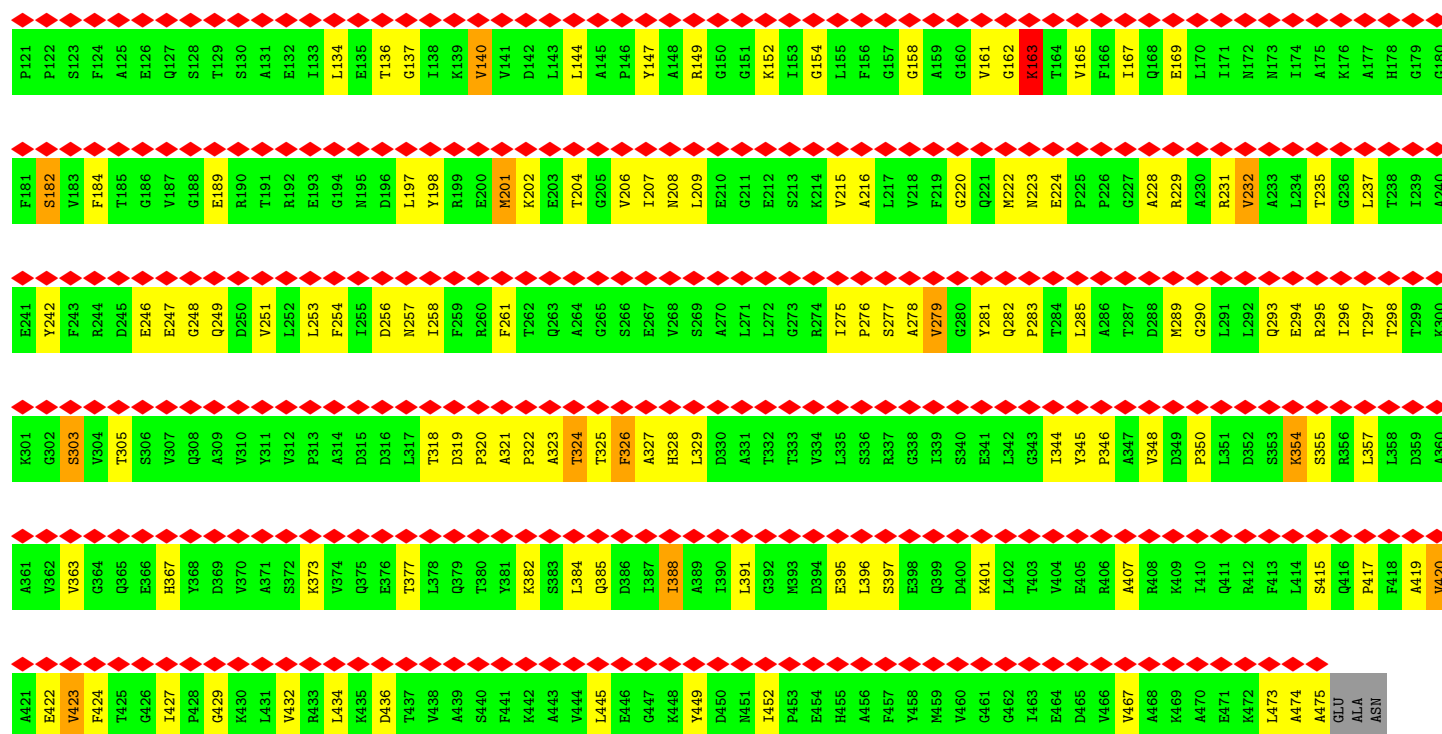
Chain E: 98% 65% 31%



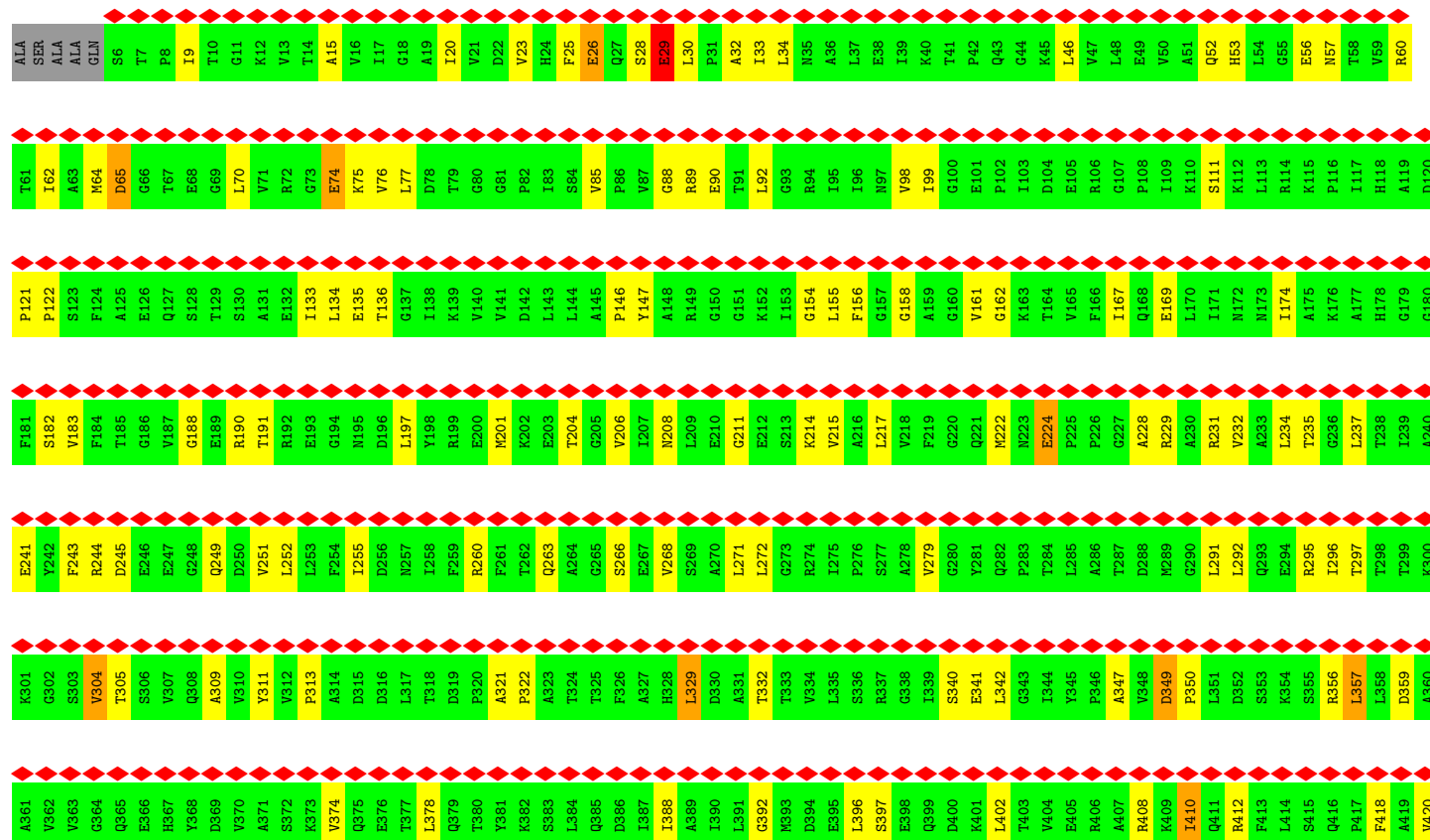
• Molecule 12: ATP synthase subunit beta, mitochondrial

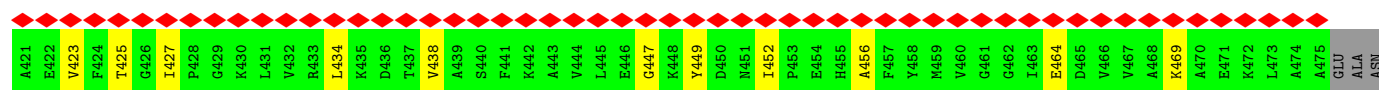
Chain F: 98% 62% 33%



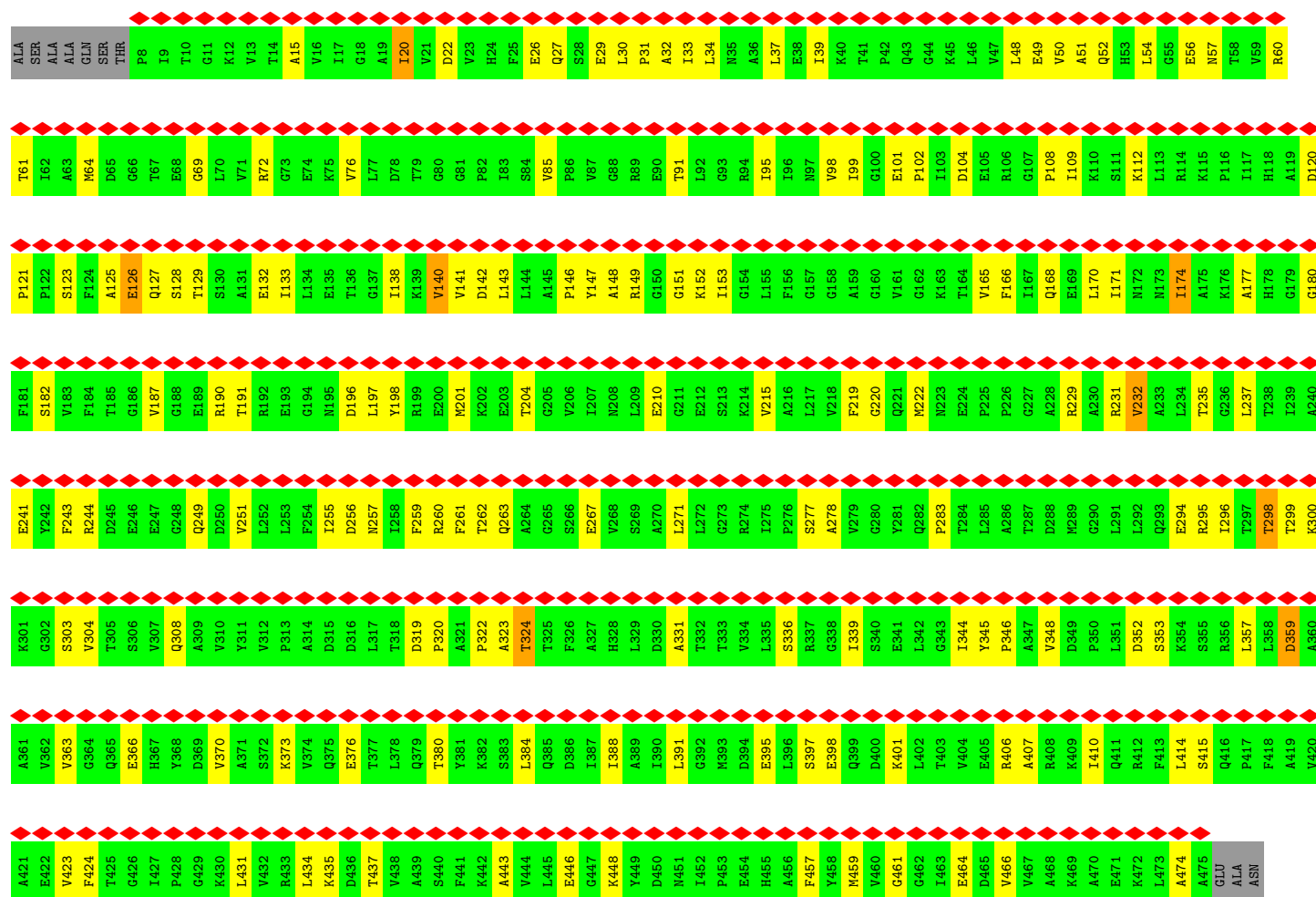


• Molecule 12: ATP synthase subunit beta, mitochondrial

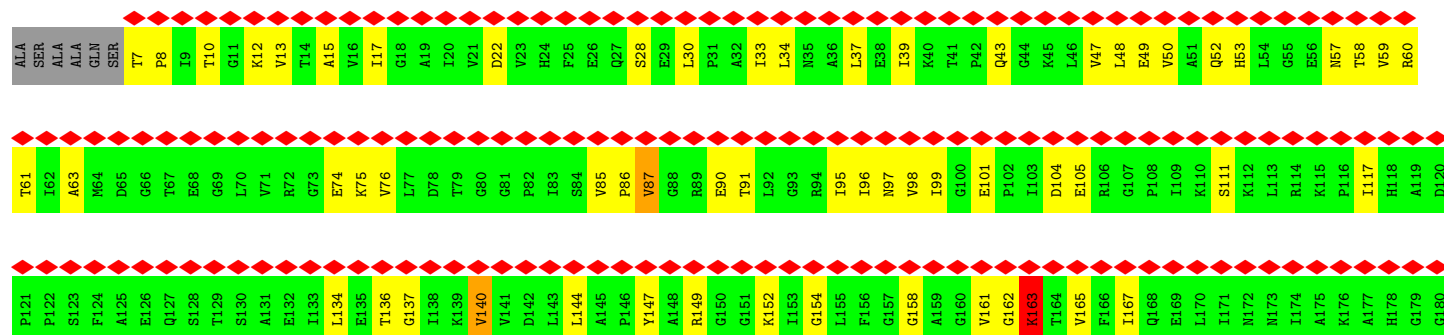


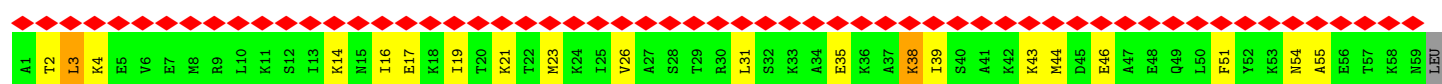


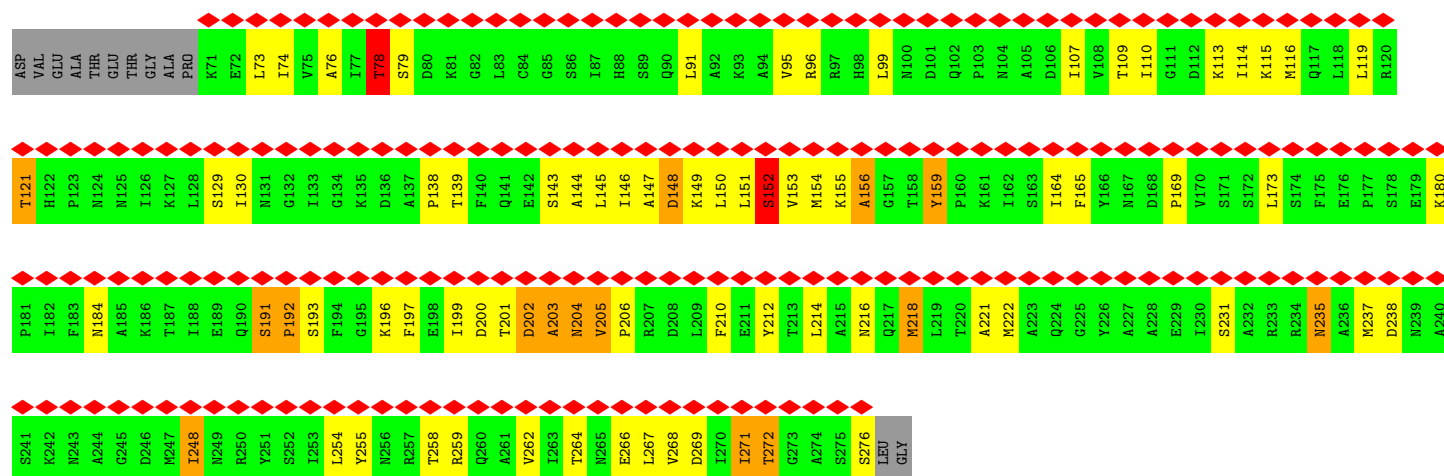
• Molecule 12: ATP synthase subunit beta, mitochondrial



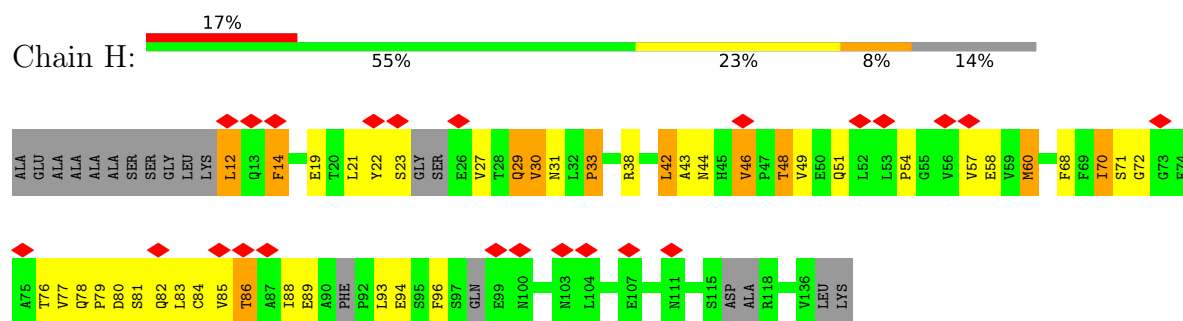
• Molecule 12: ATP synthase subunit beta, mitochondrial



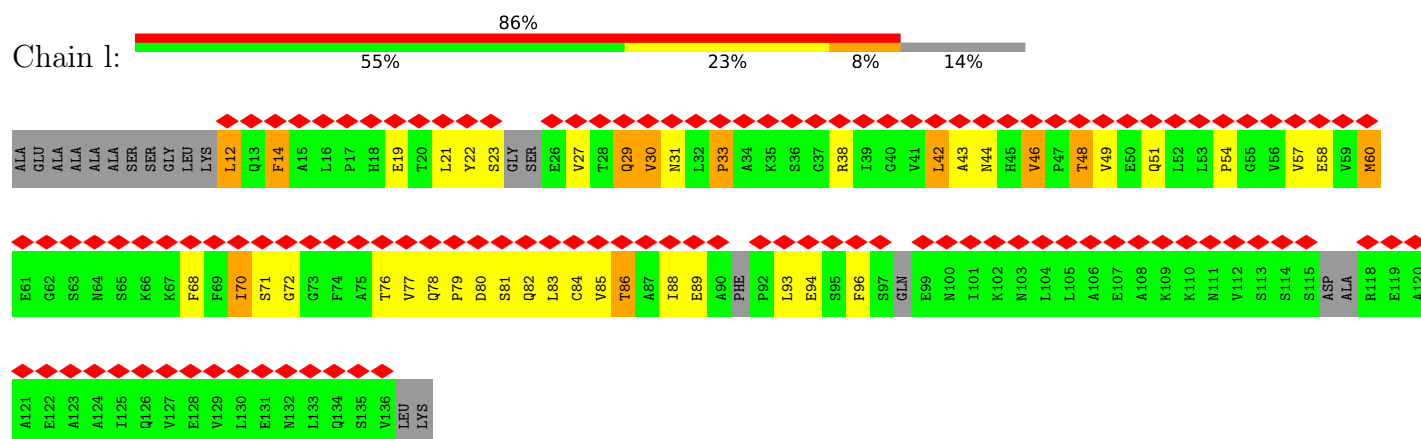




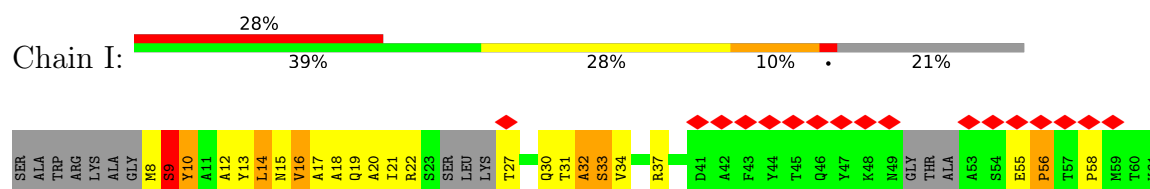
• Molecule 14: ATP synthase subunit delta, mitochondrial



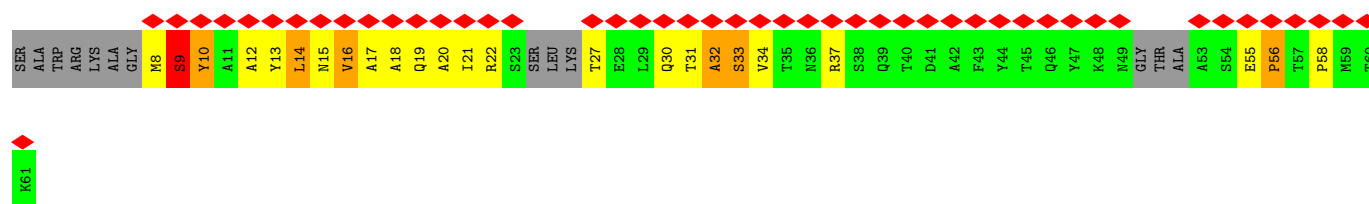
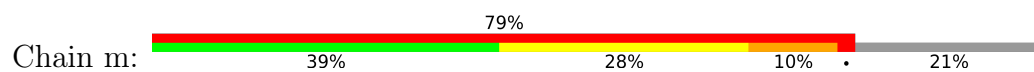
• Molecule 14: ATP synthase subunit delta, mitochondrial



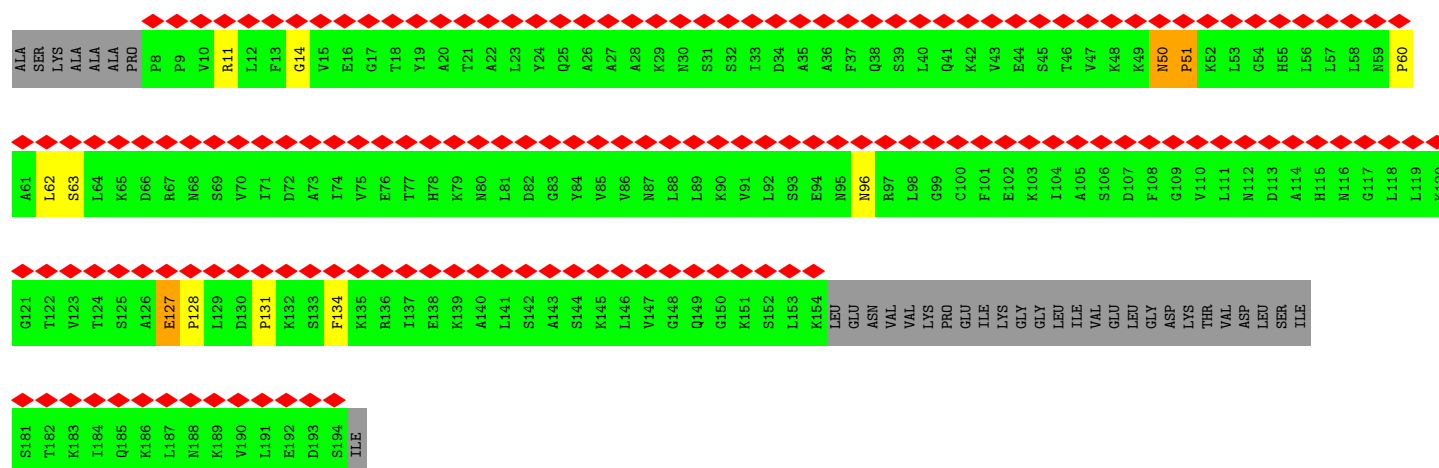
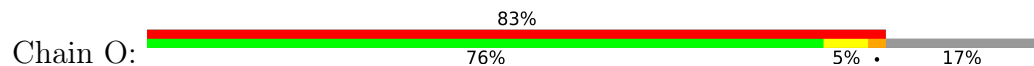
• Molecule 15: ATP synthase catalytic sector F1 epsilon subunit



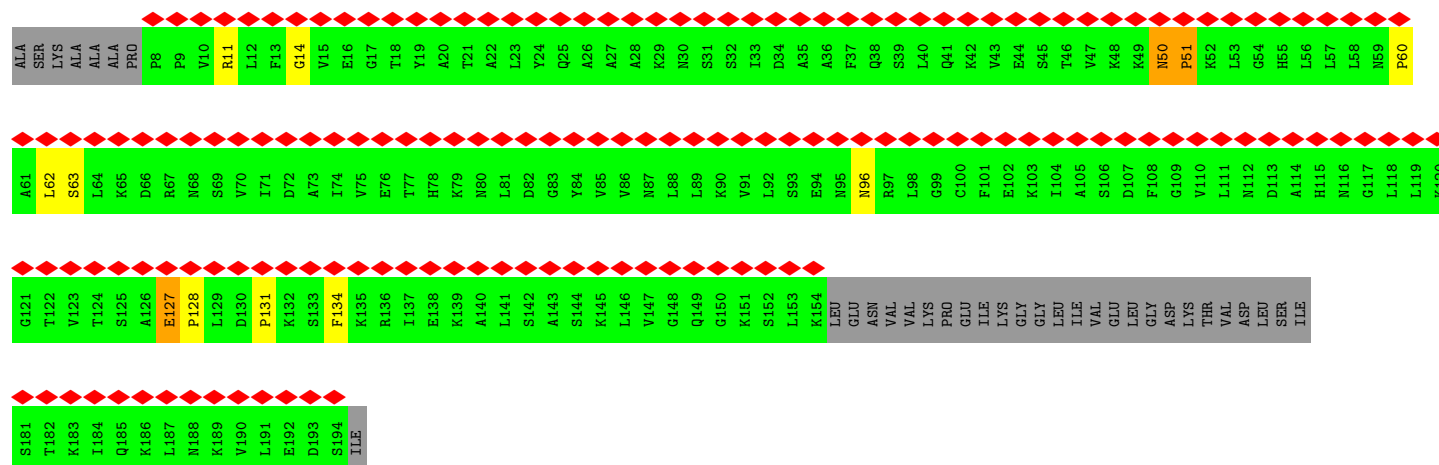
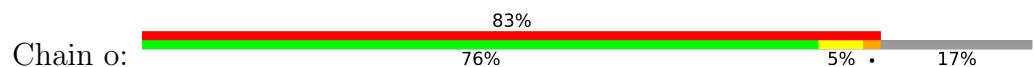
• Molecule 15: ATP synthase catalytic sector F1 epsilon subunit



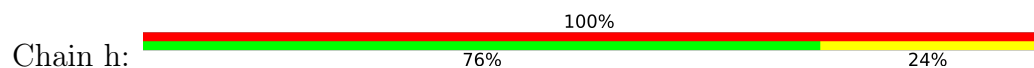
- Molecule 16: ATP synthase subunit 5, mitochondrial

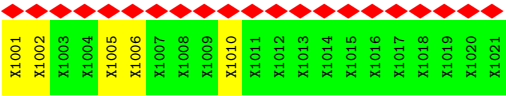


- Molecule 16: ATP synthase subunit 5, mitochondrial

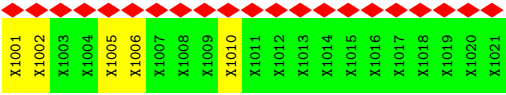
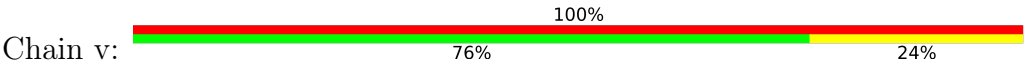


- Molecule 17: ATP synthase subunit h





● Molecule 17: ATP synthase subunit h



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	238848	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	71	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	1.103	Depositor
Minimum map value	-0.374	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.000	Depositor
Recommended contour level	0.156	Depositor
Map size ($\text{\AA}$)	464.0, 464.0, 464.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.45, 1.45, 1.45	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	0	0.29	0/545	0.63	0/737
1	1	0.32	0/545	0.61	0/737
1	2	0.37	0/545	0.67	0/737
1	3	0.35	0/537	0.64	0/727
1	4	0.28	0/545	0.57	0/737
1	5	0.27	0/545	0.58	0/737
1	6	0.27	0/537	0.58	0/727
1	7	0.25	0/529	0.55	0/716
1	8	0.27	0/545	0.55	0/737
1	9	0.28	0/537	0.52	0/727
1	J	0.29	0/545	0.63	0/737
1	L	0.32	0/545	0.61	0/737
1	M	0.37	0/545	0.66	0/737
1	N	0.35	0/537	0.64	0/727
1	P	0.28	0/545	0.57	0/737
1	Q	0.28	0/545	0.58	0/737
1	R	0.27	0/537	0.57	0/727
1	S	0.25	0/529	0.56	0/716
1	T	0.27	0/545	0.55	0/737
1	U	0.28	0/537	0.52	0/727
2	A	0.46	0/422	0.78	0/570
2	V	0.46	0/422	0.78	0/570
3	a	0.41	0/2023	0.76	0/2758
3	p	0.41	0/2023	0.76	0/2758
4	b	0.63	0/1159	1.13	3/1599 (0.2%)
4	q	0.63	0/1159	1.13	3/1599 (0.2%)
5	d	0.85	0/936	1.20	3/1286 (0.2%)
5	r	0.85	0/936	1.20	3/1286 (0.2%)
7	f	0.44	0/624	0.82	2/845 (0.2%)
7	t	0.44	0/624	0.82	2/845 (0.2%)
9	i	0.33	0/488	0.61	0/659
9	w	0.33	0/488	0.61	0/659

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
10	k	0.23	0/185	0.73	2/250 (0.8%)
10	x	0.23	0/185	0.73	2/250 (0.8%)
11	B	0.60	0/3753	0.93	5/5080 (0.1%)
11	C	0.71	0/3793	1.03	7/5137 (0.1%)
11	K	0.66	0/3798	0.95	3/5143 (0.1%)
11	W	0.60	0/3753	0.93	5/5080 (0.1%)
11	X	0.71	0/3793	1.03	7/5137 (0.1%)
11	n	0.66	0/3798	0.95	3/5143 (0.1%)
12	D	0.70	0/3605	1.03	9/4889 (0.2%)
12	E	0.57	0/3592	0.89	0/4870
12	F	0.67	1/3599 (0.0%)	1.00	4/4881 (0.1%)
12	Y	0.70	0/3605	1.03	9/4889 (0.2%)
12	Z	0.57	0/3592	0.89	0/4870
12	c	0.67	1/3599 (0.0%)	1.00	4/4881 (0.1%)
13	G	0.57	0/2055	0.96	5/2766 (0.2%)
13	j	0.56	0/2055	0.96	5/2766 (0.2%)
14	H	0.63	0/759	1.05	0/1040
14	l	0.63	0/759	1.04	0/1040
15	I	0.63	0/326	1.19	5/445 (1.1%)
15	m	0.63	0/326	1.19	5/445 (1.1%)
16	O	0.94	1/793 (0.1%)	1.45	6/1101 (0.5%)
16	o	0.95	1/793 (0.1%)	1.45	6/1101 (0.5%)
All	All	0.60	4/74640 (0.0%)	0.94	108/101276 (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
4	b	0	1
4	q	0	1
8	g	0	2
8	u	0	2
15	I	0	1
15	m	0	1
16	O	0	1
16	o	0	1
All	All	0	10

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	c	297	THR	CA-CB	5.85	1.63	1.53
12	F	297	THR	CA-CB	5.82	1.63	1.53
16	o	127	GLU	CA-C	5.46	1.59	1.52
16	O	127	GLU	CA-C	5.45	1.59	1.52

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	Y	224	GLU	CA-C-N	10.45	127.29	119.66
12	Y	224	GLU	C-N-CA	10.45	127.29	119.66
12	D	224	GLU	CA-C-N	10.38	127.24	119.66
12	D	224	GLU	C-N-CA	10.38	127.24	119.66
15	I	16	VAL	N-CA-C	-7.61	105.73	112.12
15	m	16	VAL	N-CA-C	-7.52	105.80	112.12
15	m	56	PRO	N-CA-CB	7.34	110.96	103.25
15	I	56	PRO	N-CA-CB	7.29	110.90	103.25
7	t	6	PRO	N-CA-CB	7.28	110.14	103.08
7	f	6	PRO	N-CA-CB	7.27	110.14	103.08
15	m	20	ALA	N-CA-C	-7.07	102.99	111.69
15	I	20	ALA	N-CA-C	-7.03	103.04	111.69
15	I	10	TYR	N-CA-C	-6.91	103.50	112.68
15	m	10	TYR	N-CA-C	-6.89	103.52	112.68
5	d	67	VAL	N-CA-CB	-6.80	106.06	111.64
5	r	67	VAL	N-CA-CB	-6.75	106.10	111.64
4	b	11	PRO	N-CA-CB	6.69	110.28	103.25
15	I	58	PRO	N-CA-CB	6.68	110.27	103.25
4	q	11	PRO	N-CA-CB	6.64	110.23	103.25
12	D	349	ASP	CA-C-N	6.62	126.31	119.56
12	D	349	ASP	C-N-CA	6.62	126.31	119.56
12	Y	349	ASP	CA-C-N	6.61	126.30	119.56
12	Y	349	ASP	C-N-CA	6.61	126.30	119.56
15	m	58	PRO	N-CA-CB	6.60	110.18	103.25
16	O	127	GLU	CA-C-N	6.55	128.02	119.84
16	O	127	GLU	C-N-CA	6.55	128.02	119.84
12	Y	215	VAL	N-CA-C	6.50	116.93	108.35
12	D	215	VAL	N-CA-C	6.49	116.92	108.35
16	o	127	GLU	CA-C-N	6.49	127.95	119.84
16	o	127	GLU	C-N-CA	6.49	127.95	119.84
4	b	23	PRO	N-CA-CB	6.48	110.05	103.25
4	q	23	PRO	N-CA-CB	6.41	109.98	103.25
13	j	191	SER	CA-C-N	6.35	127.78	119.84
13	j	191	SER	C-N-CA	6.35	127.78	119.84
13	G	191	SER	CA-C-N	6.31	127.73	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	G	191	SER	C-N-CA	6.31	127.73	119.84
7	f	7	PRO	N-CA-CB	6.15	110.09	103.33
13	j	159	TYR	CA-C-N	6.13	126.58	119.47
13	j	159	TYR	C-N-CA	6.13	126.58	119.47
7	t	7	PRO	N-CA-CB	6.09	110.03	103.33
13	G	159	TYR	CA-C-N	6.09	126.53	119.47
13	G	159	TYR	C-N-CA	6.09	126.53	119.47
11	K	312	ALA	N-CA-C	6.03	117.30	108.14
11	n	312	ALA	N-CA-C	5.99	117.25	108.14
16	o	127	GLU	CB-CA-C	5.92	121.84	110.17
16	o	134	PHE	CB-CA-C	-5.91	99.78	109.53
16	O	127	GLU	CB-CA-C	5.90	121.80	110.17
11	n	267	LEU	N-CA-C	-5.87	99.07	109.06
16	O	134	PHE	CB-CA-C	-5.87	99.85	109.53
11	K	267	LEU	N-CA-C	-5.84	99.13	109.06
5	d	67	VAL	CB-CA-C	-5.74	105.94	111.05
5	r	67	VAL	CB-CA-C	-5.74	105.94	111.05
16	O	51	PRO	N-CA-C	5.64	124.09	112.47
16	o	51	PRO	N-CA-C	5.63	124.08	112.47
12	c	163	LYS	N-CA-C	-5.57	104.71	112.45
12	F	163	LYS	N-CA-C	-5.57	104.71	112.45
11	X	121	GLY	CA-C-N	5.55	125.87	119.93
11	X	121	GLY	C-N-CA	5.55	125.87	119.93
11	C	121	GLY	CA-C-N	5.48	125.79	119.93
11	C	121	GLY	C-N-CA	5.48	125.79	119.93
11	W	98	ASP	N-CA-C	5.45	117.35	109.07
11	B	98	ASP	N-CA-C	5.42	117.31	109.07
11	B	110	VAL	N-CA-C	5.39	116.62	108.96
12	Y	65	ASP	N-CA-C	5.39	115.35	108.24
11	W	110	VAL	N-CA-C	5.37	116.59	108.96
11	C	268	ILE	N-CA-C	5.36	115.81	107.99
11	X	268	ILE	N-CA-C	5.34	115.79	107.99
12	D	65	ASP	N-CA-C	5.33	115.28	108.24
11	B	208	VAL	N-CA-C	5.33	116.03	107.98
12	c	275	ILE	N-CA-C	-5.32	103.74	108.95
12	c	282	GLN	CA-C-N	5.31	125.39	119.87
12	c	282	GLN	C-N-CA	5.31	125.39	119.87
11	W	208	VAL	N-CA-C	5.31	115.99	107.98
12	F	275	ILE	N-CA-C	-5.30	103.76	108.95
12	F	282	GLN	CA-C-N	5.28	125.36	119.87
12	F	282	GLN	C-N-CA	5.28	125.36	119.87
12	Y	452	ILE	CA-C-N	5.23	125.17	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	Y	452	ILE	C-N-CA	5.23	125.17	119.78
5	r	63	LYS	N-CA-C	5.19	116.74	111.14
5	d	63	LYS	N-CA-C	5.19	116.74	111.14
12	D	452	ILE	CA-C-N	5.18	125.11	119.78
12	D	452	ILE	C-N-CA	5.18	125.11	119.78
11	W	99	VAL	N-CA-C	5.17	114.66	108.45
11	X	139	LEU	CA-C-N	-5.17	116.43	121.65
11	X	139	LEU	C-N-CA	-5.17	116.43	121.65
4	q	119	THR	N-CA-CB	5.17	118.17	110.22
10	k	16	GLN	CA-C-N	5.16	131.40	121.54
10	k	16	GLN	C-N-CA	5.16	131.40	121.54
11	B	99	VAL	N-CA-C	5.16	114.64	108.45
10	x	16	GLN	CA-C-N	5.15	131.38	121.54
10	x	16	GLN	C-N-CA	5.15	131.38	121.54
11	C	139	LEU	CA-C-N	-5.15	116.45	121.65
11	C	139	LEU	C-N-CA	-5.15	116.45	121.65
4	b	119	THR	N-CA-CB	5.14	118.14	110.22
16	O	127	GLU	O-C-N	-5.09	115.47	121.32
11	X	135	ALA	CA-C-N	-5.08	114.68	119.76
11	X	135	ALA	C-N-CA	-5.08	114.68	119.76
11	K	104	GLY	N-CA-C	-5.08	109.01	115.31
11	C	135	ALA	CA-C-N	-5.07	114.69	119.76
11	C	135	ALA	C-N-CA	-5.07	114.69	119.76
13	G	156	ALA	N-CA-C	5.06	116.49	110.97
13	j	156	ALA	N-CA-C	5.06	116.49	110.97
12	D	297	THR	N-CA-C	5.05	116.74	108.55
12	Y	297	THR	N-CA-C	5.04	116.72	108.55
11	n	104	GLY	N-CA-C	-5.04	109.06	115.31
16	o	127	GLU	O-C-N	-5.03	115.54	121.32
11	W	379	ALA	N-CA-C	-5.00	106.33	114.09
11	B	379	ALA	N-CA-C	-5.00	106.34	114.09

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	I	9	SER	Peptide
16	O	50	ASN	Peptide
4	b	186	ASN	Peptide
8	g	80	UNK	Mainchain,Peptide
15	m	9	SER	Peptide
16	o	50	ASN	Peptide

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Mol	Chain	Res	Type	Group
4	q	186	ASN	Peptide
8	u	80	UNK	Mainchain,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	0	537	0	582	5	0
1	1	537	0	582	5	0
1	2	537	0	582	8	0
1	3	529	0	570	4	0
1	4	537	0	582	5	0
1	5	537	0	582	6	0
1	6	529	0	570	7	0
1	7	522	0	570	20	0
1	8	537	0	582	10	0
1	9	529	0	570	5	0
1	J	537	0	582	5	0
1	L	537	0	582	5	0
1	M	537	0	582	9	0
1	N	529	0	570	5	0
1	P	537	0	582	6	0
1	Q	537	0	582	6	0
1	R	529	0	570	7	0
1	S	522	0	570	20	0
1	T	537	0	582	10	0
1	U	529	0	570	5	0
2	A	410	0	444	5	0
2	V	410	0	444	5	0
3	a	1971	0	2071	39	0
3	p	1971	0	2071	37	0
4	b	1153	0	781	2	0
4	q	1153	0	781	2	0
5	d	930	0	618	15	0
5	r	930	0	618	16	0
6	e	245	0	51	0	0
6	s	245	0	51	0	0
7	f	607	0	527	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	t	607	0	527	30	0
8	g	530	0	108	0	0
8	u	530	0	108	0	0
9	i	473	0	476	1	0
9	w	473	0	476	1	0
10	k	180	0	192	1	0
10	x	180	0	192	1	0
11	B	3700	0	3749	125	0
11	C	3739	0	3767	94	0
11	K	3745	0	3769	95	0
11	W	3700	0	3749	124	0
11	X	3739	0	3767	93	0
11	n	3745	0	3769	99	0
12	D	3549	0	3620	81	0
12	E	3536	0	3610	101	0
12	F	3543	0	3615	112	0
12	Y	3549	0	3620	79	0
12	Z	3536	0	3610	108	0
12	c	3543	0	3615	109	0
13	G	2030	0	2081	57	0
13	j	2030	0	2081	57	0
14	H	751	0	598	58	0
14	l	751	0	598	56	0
15	I	324	0	249	23	0
15	m	324	0	249	21	0
16	O	795	0	367	12	0
16	o	795	0	367	12	0
17	h	105	0	23	4	0
17	v	105	0	23	4	0
18	B	31	0	13	1	0
18	C	31	0	13	3	0
18	D	31	0	13	3	0
18	F	31	0	13	7	0
18	K	31	0	13	1	0
18	W	31	0	13	1	0
18	X	31	0	13	3	0
18	Y	31	0	13	3	0
18	c	31	0	13	7	0
18	n	31	0	13	1	0
19	B	1	0	0	0	0
19	C	1	0	0	0	0
19	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	F	1	0	0	0	0
19	K	1	0	0	0	0
19	W	1	0	0	0	0
19	X	1	0	0	0	0
19	Y	1	0	0	0	0
19	c	1	0	0	0	0
19	n	1	0	0	0	0
All	All	75614	0	73106	1599	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 11.

All (1599) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:p:80:LYS:CG	7:t:1:VAL:CB	1.82	1.56
3:a:80:LYS:CG	7:f:1:VAL:CB	1.82	1.53
1:T:41:PRO:CG	14:l:42:LEU:HD11	1.46	1.45
3:p:80:LYS:HG3	7:t:1:VAL:CB	0.96	1.44
1:8:41:PRO:CG	14:H:42:LEU:HD11	1.46	1.42
3:a:80:LYS:HG3	7:f:1:VAL:CB	0.96	1.39
12:E:27:GLN:NE2	16:O:63:SER:CB	1.88	1.34
1:7:40:ASN:ND2	14:H:42:LEU:HB3	1.40	1.34
12:Z:27:GLN:NE2	16:o:63:SER:CB	1.89	1.33
1:S:40:ASN:ND2	14:l:42:LEU:HB3	1.40	1.33
3:p:80:LYS:HG3	7:t:1:VAL:CA	1.60	1.32
3:a:80:LYS:HG3	7:f:1:VAL:CA	1.60	1.29
12:Z:27:GLN:HE21	16:o:63:SER:CB	1.45	1.26
11:W:34:LEU:HD23	16:o:60:PRO:CB	1.65	1.25
11:B:34:LEU:HD23	16:O:60:PRO:CB	1.65	1.25
12:E:27:GLN:HE21	16:O:63:SER:CB	1.45	1.25
12:E:56:GLU:OE2	16:O:96:ASN:CB	1.87	1.21
12:Z:56:GLU:OE2	16:o:96:ASN:CB	1.87	1.20
3:a:80:LYS:HE2	7:f:1:VAL:N	1.57	1.17
1:S:41:PRO:HD2	14:l:44:ASN:HB2	1.27	1.17
3:p:80:LYS:HE2	7:t:1:VAL:N	1.57	1.16
1:T:41:PRO:CG	14:l:42:LEU:CD1	2.23	1.15
1:8:41:PRO:CG	14:H:42:LEU:CD1	2.23	1.14
1:7:41:PRO:HD2	14:H:44:ASN:HB2	1.27	1.12
1:S:40:ASN:ND2	14:l:42:LEU:CB	2.13	1.10
1:7:40:ASN:ND2	14:H:42:LEU:CB	2.13	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:7:41:PRO:CD	14:H:44:ASN:HB2	1.82	1.10
1:8:41:PRO:HG2	14:H:42:LEU:CD1	1.80	1.10
12:Z:27:GLN:HG2	16:o:62:LEU:O	1.52	1.10
3:p:80:LYS:CE	7:t:1:VAL:H3	1.65	1.09
12:E:27:GLN:HG2	16:O:62:LEU:O	1.52	1.08
1:S:41:PRO:CD	14:l:44:ASN:HB2	1.82	1.08
1:T:41:PRO:HG2	14:l:42:LEU:CD1	1.80	1.08
3:a:80:LYS:CE	7:f:1:VAL:H3	1.66	1.07
3:a:80:LYS:CE	7:f:1:VAL:N	2.19	1.05
1:S:40:ASN:HD21	14:l:42:LEU:HB3	0.93	1.03
12:c:7:THR:HB	12:c:8:PRO:HD2	1.41	1.03
1:7:40:ASN:HD21	14:H:42:LEU:HB3	0.93	1.02
3:p:80:LYS:CE	7:t:1:VAL:N	2.19	1.02
3:p:80:LYS:HE2	7:t:1:VAL:H3	0.85	1.02
3:a:80:LYS:HE2	7:f:1:VAL:H3	0.85	0.99
3:a:80:LYS:CD	7:f:1:VAL:H1	1.73	0.99
3:p:80:LYS:CD	7:t:1:VAL:H1	1.75	0.99
3:a:80:LYS:HD3	7:f:1:VAL:H1	1.27	0.99
1:8:41:PRO:HG3	14:H:42:LEU:CD1	1.92	0.98
3:p:80:LYS:CD	7:t:1:VAL:N	2.26	0.98
3:a:80:LYS:CD	7:f:1:VAL:N	2.26	0.98
3:p:80:LYS:HD3	7:t:1:VAL:H1	1.27	0.98
12:F:7:THR:HB	12:F:8:PRO:HD2	1.41	0.98
14:H:89:GLU:HG3	15:I:18:ALA:HB1	1.47	0.96
13:G:23:MET:HB3	13:G:237:MET:HG3	1.47	0.96
14:l:89:GLU:HG3	15:m:18:ALA:HB1	1.47	0.95
11:W:34:LEU:CD2	16:o:60:PRO:CB	2.45	0.95
11:B:34:LEU:CD2	16:O:60:PRO:CB	2.45	0.94
1:7:40:ASN:HD21	14:H:42:LEU:CB	1.76	0.94
1:T:41:PRO:HG3	14:l:42:LEU:CD1	1.92	0.94
1:S:40:ASN:HD21	14:l:42:LEU:CB	1.76	0.94
13:j:23:MET:HB3	13:j:237:MET:HG3	1.47	0.93
12:D:224:GLU:O	12:D:229:ARG:HD3	1.69	0.93
12:Z:148:ALA:HB3	12:Z:151:GLY:HA3	1.51	0.93
13:j:96:ARG:HE	13:j:121:THR:HG21	1.35	0.92
5:r:157:LYS:HE3	7:t:8:LYS:CB	1.99	0.92
12:Y:224:GLU:O	12:Y:229:ARG:HD3	1.69	0.92
15:I:9:SER:H	15:I:12:ALA:HB3	1.33	0.91
12:E:148:ALA:HB3	12:E:151:GLY:HA3	1.51	0.91
13:G:96:ARG:HE	13:G:121:THR:HG21	1.35	0.91
12:F:182:SER:HB3	12:F:215:VAL:HG23	1.52	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:d:157:LYS:HE3	7:f:8:LYS:CB	1.99	0.91
12:Z:27:GLN:HE21	16:o:63:SER:CA	1.83	0.90
15:m:9:SER:H	15:m:12:ALA:HB3	1.33	0.90
12:E:27:GLN:HE21	16:O:63:SER:CA	1.83	0.90
11:C:142:ARG:HG2	11:C:143:SER:N	1.88	0.89
12:c:182:SER:HB3	12:c:215:VAL:HG23	1.52	0.89
11:X:142:ARG:HG2	11:X:143:SER:N	1.88	0.88
7:f:10:VAL:O	7:f:14:ASN:N	2.07	0.88
3:a:80:LYS:CG	7:f:1:VAL:CA	2.35	0.88
12:Y:85:VAL:HG11	12:Y:235:THR:HG23	1.56	0.87
7:t:10:VAL:O	7:t:14:ASN:N	2.07	0.86
13:G:51:PHE:HA	14:H:78:GLN:HE22	1.40	0.86
15:I:10:TYR:HA	15:I:13:TYR:HB2	1.58	0.86
12:D:85:VAL:HG11	12:D:235:THR:HG23	1.56	0.86
3:p:80:LYS:CG	7:t:1:VAL:CA	2.35	0.86
13:j:51:PHE:HA	14:l:78:GLN:HE22	1.40	0.86
13:G:44:MET:HE2	14:H:86:THR:HG22	1.59	0.85
14:H:89:GLU:CG	15:I:18:ALA:HB1	2.06	0.84
12:Y:20:ILE:HG13	12:Y:271:LEU:HB3	1.59	0.84
14:l:89:GLU:CG	15:m:18:ALA:HB1	2.07	0.84
15:m:10:TYR:HA	15:m:13:TYR:HB2	1.58	0.84
1:S:41:PRO:CD	14:l:44:ASN:CB	2.56	0.84
1:T:41:PRO:HG2	14:l:42:LEU:HD11	0.84	0.83
14:l:88:ILE:HD12	15:m:14:LEU:HB2	1.59	0.83
13:j:44:MET:HE2	14:l:86:THR:HG22	1.58	0.83
11:W:385:LEU:HD23	11:W:444:VAL:HG13	1.58	0.83
11:B:385:LEU:HD23	11:B:444:VAL:HG13	1.58	0.83
12:Z:142:ASP:HB3	12:Z:434:LEU:HD13	1.59	0.82
12:E:142:ASP:HB3	12:E:434:LEU:HD13	1.59	0.82
14:H:88:ILE:HD12	15:I:14:LEU:HB2	1.59	0.82
1:7:41:PRO:CD	14:H:44:ASN:CB	2.56	0.82
12:D:20:ILE:HG13	12:D:271:LEU:HB3	1.59	0.82
11:X:375:ARG:HD3	18:Y:501:ANP:H5'2	1.62	0.81
1:8:41:PRO:HG2	14:H:42:LEU:HD11	0.84	0.81
11:K:11:SER:CB	12:D:56:GLU:OE1	2.28	0.81
11:C:375:ARG:HD3	18:D:501:ANP:H5'2	1.62	0.81
11:X:142:ARG:HG2	11:X:143:SER:H	1.45	0.81
11:C:142:ARG:HG2	11:C:143:SER:H	1.45	0.81
12:c:52:GLN:HE21	12:c:60:ARG:HD2	1.46	0.81
11:n:11:SER:CB	12:Y:56:GLU:OE1	2.28	0.81
12:F:52:GLN:HE21	12:F:60:ARG:HD2	1.46	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:G:96:ARG:NE	13:G:121:THR:HG21	1.96	0.80
13:j:96:ARG:NE	13:j:121:THR:HG21	1.96	0.79
3:p:80:LYS:CB	7:t:1:VAL:CB	2.60	0.79
11:B:444:VAL:HG23	11:B:445:PRO:HD3	1.64	0.79
3:a:80:LYS:CB	7:f:1:VAL:CB	2.60	0.79
12:F:158:GLY:O	12:F:161:VAL:HG22	1.84	0.78
12:Z:27:GLN:CD	16:o:63:SER:CB	2.56	0.78
11:W:444:VAL:HG23	11:W:445:PRO:HD3	1.64	0.78
12:c:158:GLY:O	12:c:161:VAL:HG22	1.84	0.78
11:W:425:ARG:HD3	11:W:460:LEU:HD13	1.67	0.77
12:Z:27:GLN:HE21	16:o:63:SER:N	1.83	0.77
11:B:425:ARG:HD3	11:B:460:LEU:HD13	1.67	0.77
12:E:27:GLN:CD	16:O:63:SER:CB	2.56	0.77
5:r:157:LYS:HE3	7:t:8:LYS:CA	2.15	0.77
5:d:157:LYS:HE3	7:f:8:LYS:CA	2.15	0.76
12:E:27:GLN:HE21	16:O:63:SER:N	1.83	0.76
12:F:388:ILE:HD12	12:F:396:LEU:HD11	1.67	0.76
11:B:109:VAL:HG22	11:B:233:ILE:HB	1.67	0.75
3:a:80:LYS:HG3	7:f:1:VAL:N	2.01	0.75
11:X:169:ILE:HD11	11:X:326:LEU:HD22	1.68	0.75
12:c:388:ILE:HD12	12:c:396:LEU:HD11	1.67	0.75
12:F:189:GLU:O	12:F:222:MET:HG2	1.86	0.75
12:c:189:GLU:O	12:c:222:MET:HG2	1.86	0.74
11:W:109:VAL:HG22	11:W:233:ILE:HB	1.67	0.74
11:C:169:ILE:HD11	11:C:326:LEU:HD22	1.68	0.74
3:p:80:LYS:HG3	7:t:1:VAL:N	2.01	0.74
3:a:80:LYS:HG2	7:f:1:VAL:CB	2.12	0.74
12:F:7:THR:HB	12:F:8:PRO:CD	2.17	0.73
12:c:7:THR:HB	12:c:8:PRO:CD	2.17	0.73
3:p:80:LYS:HG2	7:t:1:VAL:CB	2.12	0.73
11:C:282:GLN:HG3	12:F:283:PRO:O	1.89	0.73
14:H:31:ASN:HB3	14:H:38:ARG:HH21	1.55	0.72
14:H:76:THR:HG23	14:H:84:CYS:HB2	1.72	0.72
14:l:76:THR:HG23	14:l:84:CYS:HB2	1.72	0.72
11:n:185:ILE:HG12	11:n:203:CYS:SG	2.30	0.72
14:l:31:ASN:HB3	14:l:38:ARG:HH21	1.55	0.71
12:Z:384:LEU:O	12:Z:388:ILE:HG12	1.91	0.71
11:X:282:GLN:HG3	12:c:283:PRO:O	1.89	0.71
3:a:80:LYS:CG	7:f:1:VAL:N	2.52	0.71
1:S:40:ASN:HA	14:l:44:ASN:O	1.90	0.71
13:G:95:VAL:O	13:G:99:LEU:HB2	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:H:12:LEU:N	14:H:22:TYR:O	2.24	0.71
12:Y:29:GLU:O	12:Y:29:GLU:HG2	1.91	0.71
12:E:384:LEU:O	12:E:388:ILE:HG12	1.91	0.71
11:K:185:ILE:HG12	11:K:203:CYS:SG	2.30	0.71
12:F:162:GLY:HA2	18:F:501:ANP:O3A	1.91	0.71
1:7:41:PRO:HD2	14:H:44:ASN:CB	2.16	0.71
12:c:162:GLY:HA2	18:c:501:ANP:O3A	1.91	0.71
12:D:29:GLU:O	12:D:29:GLU:HG2	1.91	0.70
13:j:95:VAL:O	13:j:99:LEU:HB2	1.90	0.70
1:7:40:ASN:HA	14:H:44:ASN:O	1.90	0.70
3:p:80:LYS:CG	7:t:1:VAL:N	2.52	0.70
12:F:289:MET:HE1	12:F:324:THR:HB	1.73	0.70
14:l:12:LEU:N	14:l:22:TYR:O	2.24	0.70
11:C:116:PRO:HD3	11:C:123:ILE:HG12	1.74	0.69
11:C:365:PRO:HB2	11:C:367:ILE:HG13	1.75	0.69
12:F:391:LEU:HD22	12:F:395:GLU:HG3	1.74	0.69
15:I:9:SER:N	15:I:12:ALA:HB3	2.08	0.69
12:c:289:MET:HE1	12:c:324:THR:HB	1.73	0.69
12:c:391:LEU:HD22	12:c:395:GLU:HG3	1.74	0.69
12:F:97:ASN:HB2	12:F:101:GLU:H	1.58	0.68
11:X:69:GLU:HB3	11:X:70:PRO:CD	2.24	0.68
15:m:9:SER:N	15:m:12:ALA:HB3	2.08	0.68
1:T:41:PRO:HG3	14:l:42:LEU:HD13	1.75	0.68
11:X:116:PRO:HD3	11:X:123:ILE:HG12	1.74	0.68
7:f:13:LYS:O	7:f:14:ASN:CB	2.42	0.68
11:B:375:ARG:HG2	18:F:501:ANP:O3'	1.93	0.68
11:C:69:GLU:HB3	11:C:70:PRO:CD	2.24	0.68
11:X:365:PRO:HB2	11:X:367:ILE:HG13	1.75	0.68
11:W:375:ARG:HG2	18:c:501:ANP:O3'	1.93	0.68
13:G:113:LYS:HA	13:G:116:MET:HE3	1.76	0.67
11:B:272:ASP:HB2	11:B:328:VAL:O	1.95	0.67
11:X:299:ASP:OD1	11:X:299:ASP:N	2.28	0.67
13:j:113:LYS:HA	13:j:116:MET:HE3	1.76	0.67
12:Y:197:LEU:O	12:Y:201:MET:HG2	1.95	0.67
5:d:155:LYS:HD3	7:f:4:LEU:HA	1.77	0.67
11:W:272:ASP:HB2	11:W:328:VAL:O	1.95	0.67
12:Y:237:LEU:HD13	12:Y:296:ILE:HG12	1.76	0.67
5:d:157:LYS:CE	7:f:8:LYS:CB	2.73	0.66
12:D:237:LEU:HD13	12:D:296:ILE:HG12	1.76	0.66
7:t:13:LYS:O	7:t:14:ASN:CB	2.42	0.66
12:Z:20:ILE:HD11	12:Z:271:LEU:HB3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:c:97:ASN:HB2	12:c:101:GLU:H	1.58	0.66
12:c:322:PRO:O	12:c:323:ALA:C	2.38	0.66
5:r:155:LYS:HD3	7:t:4:LEU:HA	1.77	0.66
12:c:197:LEU:O	12:c:201:MET:HG2	1.96	0.66
12:E:20:ILE:HD11	12:E:271:LEU:HB3	1.78	0.66
12:D:197:LEU:O	12:D:201:MET:HG2	1.95	0.66
14:l:29:GLN:HB3	14:l:60:MET:HE2	1.78	0.66
1:S:41:PRO:HD2	14:l:44:ASN:CB	2.16	0.65
1:8:41:PRO:HG3	14:H:42:LEU:HD13	1.75	0.65
12:F:197:LEU:O	12:F:201:MET:HG2	1.96	0.65
11:K:506:PHE:HA	11:K:509:THR:HG22	1.78	0.65
5:r:157:LYS:CE	7:t:8:LYS:CB	2.73	0.65
11:n:349:ASP:HA	11:n:375:ARG:HD3	1.79	0.65
12:E:49:GLU:HB2	12:E:64:MET:HE3	1.79	0.65
14:H:29:GLN:HB3	14:H:60:MET:HE2	1.78	0.65
3:p:27:THR:H	3:p:30:SER:HB3	1.60	0.65
11:n:506:PHE:HA	11:n:509:THR:HG22	1.78	0.65
3:a:27:THR:H	3:a:30:SER:HB3	1.60	0.64
12:F:322:PRO:O	12:F:323:ALA:C	2.38	0.64
11:K:168:LEU:HB2	11:K:348:THR:HG21	1.80	0.64
12:c:53:HIS:CD2	12:c:59:VAL:HG12	2.33	0.64
11:K:349:ASP:HA	11:K:375:ARG:HD3	1.79	0.64
12:c:202:LYS:HE3	12:c:209:LEU:HD11	1.79	0.64
12:F:53:HIS:CD2	12:F:59:VAL:HG12	2.33	0.64
12:F:202:LYS:HE3	12:F:209:LEU:HD11	1.79	0.64
1:S:41:PRO:HD3	14:l:44:ASN:CB	2.28	0.64
11:n:168:LEU:HB2	11:n:348:THR:HG21	1.80	0.64
12:Z:49:GLU:HB2	12:Z:64:MET:HE3	1.79	0.64
11:B:171:GLY:H	11:B:177:LYS:HD3	1.62	0.64
11:W:171:GLY:H	11:W:177:LYS:HD3	1.62	0.64
11:X:43:VAL:HG21	11:X:75:ILE:HD12	1.80	0.64
12:Y:222:MET:HA	12:Y:229:ARG:HD2	1.80	0.64
12:D:222:MET:HA	12:D:229:ARG:HD2	1.79	0.63
11:W:106:LEU:HD23	11:W:230:TYR:HA	1.80	0.63
11:B:108:ARG:HH22	11:B:116:PRO:HB3	1.63	0.63
14:H:88:ILE:HG22	14:H:89:GLU:HG2	1.79	0.63
11:C:43:VAL:HG21	11:C:75:ILE:HD12	1.80	0.63
14:H:70:ILE:HG23	14:H:72:GLY:H	1.63	0.63
14:l:88:ILE:HG22	14:l:89:GLU:HG2	1.79	0.63
11:C:494:GLU:CD	11:C:494:GLU:H	2.07	0.63
11:W:108:ARG:HH22	11:W:116:PRO:HB3	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:7:41:PRO:HD3	14:H:44:ASN:CB	2.28	0.63
11:C:274:SER:O	11:C:278:VAL:HG23	1.99	0.63
11:B:106:LEU:HD23	11:B:230:TYR:HA	1.80	0.63
12:D:33:ILE:HG22	12:D:34:LEU:HG	1.81	0.63
12:Z:102:PRO:HG3	12:Z:108:PRO:HA	1.80	0.63
14:l:70:ILE:HG23	14:l:72:GLY:H	1.63	0.63
12:F:473:LEU:C	12:F:475:ALA:H	2.07	0.62
11:n:32:ARG:NH1	11:n:89:LEU:HB2	2.14	0.62
11:X:54:LEU:HD13	11:X:97:VAL:HG22	1.80	0.62
11:X:494:GLU:CD	11:X:494:GLU:H	2.07	0.62
13:G:115:LYS:O	13:G:119:LEU:HB2	1.99	0.62
1:R:39:ARG:HD3	14:l:46:VAL:HG11	1.81	0.62
12:Z:148:ALA:CB	12:Z:151:GLY:HA3	2.28	0.62
11:C:97:VAL:HG11	11:C:247:LEU:HD21	1.80	0.62
11:B:211:LYS:O	11:B:215:VAL:HG23	1.99	0.62
12:E:102:PRO:HG3	12:E:108:PRO:HA	1.80	0.62
13:G:35:GLU:O	13:G:39:ILE:HG12	2.00	0.62
11:X:375:ARG:NH1	18:Y:501:ANP:HNB1	1.97	0.62
12:Z:168:GLN:HA	12:Z:171:ILE:HD12	1.81	0.62
13:G:144:ALA:HB1	15:l:12:ALA:HB2	1.82	0.62
11:W:211:LYS:O	11:W:215:VAL:HG23	2.00	0.62
11:X:440:THR:HA	11:X:443:GLN:HE21	1.65	0.62
12:c:473:LEU:C	12:c:475:ALA:H	2.07	0.62
13:j:115:LYS:O	13:j:119:LEU:HB2	1.99	0.62
11:n:364:ARG:HA	11:n:365:PRO:C	2.25	0.62
12:E:15:ALA:HB3	12:E:22:ASP:HB2	1.82	0.62
11:W:329:ILE:HD11	11:W:344:VAL:HG21	1.82	0.62
12:Y:33:ILE:HG22	12:Y:34:LEU:HG	1.81	0.62
12:c:384:LEU:O	12:c:388:ILE:HG12	1.99	0.62
13:j:35:GLU:O	13:j:39:ILE:HG12	2.00	0.62
11:K:32:ARG:NH1	11:K:89:LEU:HB2	2.14	0.62
11:C:375:ARG:NH1	18:D:501:ANP:HNB1	1.97	0.62
12:D:263:GLN:O	12:D:266:SER:HB3	2.00	0.62
11:X:97:VAL:HG11	11:X:247:LEU:HD21	1.80	0.62
14:H:29:GLN:O	14:H:60:MET:HB2	2.00	0.61
12:Y:279:VAL:HG12	12:Y:279:VAL:O	2.00	0.61
14:l:29:GLN:O	14:l:60:MET:HB2	2.00	0.61
12:Y:263:GLN:O	12:Y:266:SER:HB3	2.00	0.61
11:C:241:ALA:HB3	11:C:244:LEU:HD12	1.83	0.61
13:G:200:ASP:C	13:G:202:ASP:H	2.07	0.61
11:n:316:GLU:HA	11:n:320:SER:OG	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:X:241:ALA:HB3	11:X:244:LEU:HD12	1.83	0.61
11:K:444:VAL:HG22	11:K:445:PRO:HD3	1.81	0.61
14:l:12:LEU:N	14:l:23:SER:HA	2.16	0.61
11:C:54:LEU:HD13	11:C:97:VAL:HG22	1.80	0.61
12:F:33:ILE:O	12:F:34:LEU:HB2	2.00	0.61
12:F:285:LEU:C	12:F:285:LEU:HD23	2.26	0.61
11:n:272:ASP:OD2	11:n:274:SER:HB2	2.00	0.61
11:K:364:ARG:HA	11:K:365:PRO:C	2.25	0.61
11:B:329:ILE:HD11	11:B:344:VAL:HG21	1.82	0.61
11:C:440:THR:HA	11:C:443:GLN:HE21	1.65	0.61
1:6:39:ARG:HD3	14:H:46:VAL:HG11	1.81	0.61
11:K:382:VAL:HG11	11:K:440:THR:HG21	1.83	0.61
11:C:483:THR:HG23	11:C:486:ARG:NH2	2.16	0.61
12:F:384:LEU:O	12:F:388:ILE:HG12	1.99	0.61
11:X:483:THR:HG23	11:X:486:ARG:NH2	2.16	0.61
12:c:285:LEU:HD23	12:c:285:LEU:C	2.26	0.61
4:b:176:VAL:CB	17:h:1010:UNK:HA	2.30	0.61
4:q:176:VAL:CB	17:v:1010:UNK:HA	2.30	0.61
12:Z:15:ALA:HB3	12:Z:22:ASP:HB2	1.82	0.61
12:c:162:GLY:HA2	18:c:501:ANP:PA	2.41	0.61
13:j:200:ASP:C	13:j:202:ASP:H	2.07	0.61
12:E:398:GLU:HA	12:E:401:LYS:HE2	1.83	0.61
12:c:33:ILE:O	12:c:34:LEU:HB2	2.00	0.61
3:a:80:LYS:HA	7:f:1:VAL:CB	2.31	0.60
12:E:168:GLN:HA	12:E:171:ILE:HD12	1.81	0.60
12:F:162:GLY:HA2	18:F:501:ANP:PA	2.41	0.60
11:n:182:LEU:HD13	11:n:218:LEU:HD11	1.83	0.60
11:X:274:SER:O	11:X:278:VAL:HG23	1.99	0.60
11:K:77:LEU:CD1	11:K:81:ASP:HB3	2.31	0.60
11:K:182:LEU:HD13	11:K:218:LEU:HD11	1.82	0.60
12:D:279:VAL:HG12	12:D:279:VAL:O	2.00	0.60
11:n:211:LYS:HE3	11:n:213:SER:OG	2.01	0.60
13:j:144:ALA:HB1	15:m:12:ALA:HB2	1.82	0.60
3:a:80:LYS:CE	7:f:1:VAL:H1	2.00	0.60
14:H:12:LEU:N	14:H:23:SER:HA	2.16	0.60
11:n:444:VAL:HG22	11:n:445:PRO:HD3	1.82	0.60
11:W:185:ILE:HG23	11:W:203:CYS:SG	2.42	0.60
11:X:222:LEU:HB3	11:X:228:MET:HG2	1.84	0.60
11:X:272:ASP:OD1	11:X:275:LYS:HD2	2.01	0.60
12:c:345:TYR:HA	12:c:346:PRO:C	2.26	0.60
13:j:3:LEU:CD2	13:j:255:TYR:CE1	2.85	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:272:ASP:OD2	11:K:274:SER:HB2	2.00	0.60
3:p:80:LYS:HA	7:t:1:VAL:CB	2.31	0.60
11:n:382:VAL:HG11	11:n:440:THR:HG21	1.83	0.60
11:C:187:ASN:OD1	11:C:190:ARG:NH1	2.34	0.60
12:E:243:PHE:HB2	12:E:251:VAL:HG21	1.83	0.60
3:a:80:LYS:CA	7:f:1:VAL:CB	2.80	0.60
11:K:211:LYS:HE3	11:K:213:SER:OG	2.01	0.60
11:K:212:ARG:HG2	11:K:237:THR:HG21	1.83	0.60
11:C:272:ASP:OD1	11:C:275:LYS:HD2	2.01	0.60
11:C:299:ASP:OD1	11:C:299:ASP:N	2.28	0.60
3:p:80:LYS:CA	7:t:1:VAL:CB	2.80	0.60
11:X:174:GLN:HA	18:X:601:ANP:HNB1	1.67	0.60
12:Y:252:LEU:HD23	12:Y:305:THR:HB	1.83	0.60
12:Z:398:GLU:HA	12:Z:401:LYS:HE2	1.83	0.60
11:C:55:VAL:HG21	11:C:75:ILE:HD13	1.84	0.60
11:X:187:ASN:OD1	11:X:190:ARG:NH1	2.34	0.60
12:D:252:LEU:HD23	12:D:305:THR:HB	1.83	0.60
13:G:3:LEU:CD2	13:G:255:TYR:CE1	2.85	0.60
11:n:77:LEU:CD1	11:n:81:ASP:HB3	2.31	0.60
12:Z:423:VAL:HG23	12:Z:424:PHE:HD1	1.67	0.60
12:E:148:ALA:CB	12:E:151:GLY:HA3	2.28	0.59
11:B:185:ILE:HG23	11:B:203:CYS:SG	2.41	0.59
12:F:345:TYR:HA	12:F:346:PRO:C	2.26	0.59
11:C:222:LEU:HB3	11:C:228:MET:HG2	1.84	0.59
12:E:423:VAL:HG23	12:E:424:PHE:HD1	1.67	0.59
12:F:201:MET:HA	12:F:201:MET:HE2	1.85	0.59
13:G:54:ASN:ND2	14:H:78:GLN:HE21	1.99	0.59
1:R:39:ARG:HD3	14:l:46:VAL:CG1	2.32	0.59
12:Z:243:PHE:HB2	12:Z:251:VAL:HG21	1.83	0.59
12:c:13:VAL:CG2	12:c:74:GLU:HB3	2.32	0.59
13:j:54:ASN:ND2	14:l:78:GLN:HE21	1.99	0.59
1:6:39:ARG:HD3	14:H:46:VAL:CG1	2.32	0.59
11:C:174:GLN:HA	18:C:601:ANP:HNB1	1.67	0.59
1:8:14:ILE:HG21	1:9:14:ILE:HD13	1.83	0.59
12:F:13:VAL:CG2	12:F:74:GLU:HB3	2.32	0.59
11:X:55:VAL:HG21	11:X:75:ILE:HD13	1.84	0.59
12:c:201:MET:HA	12:c:201:MET:HE2	1.85	0.59
11:K:316:GLU:HA	11:K:320:SER:OG	2.01	0.59
1:T:14:ILE:HG21	1:U:14:ILE:HD13	1.83	0.59
11:X:146:GLU:HB2	11:X:163:ARG:HB2	1.85	0.59
11:n:446:LEU:HD11	11:n:467:GLU:HG3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:126:GLU:HA	12:Z:300:LYS:HE3	1.85	0.59
11:n:38:ASP:O	11:n:286:LEU:HD13	2.03	0.58
12:Y:26:GLU:HA	12:Y:26:GLU:OE1	2.03	0.58
11:X:336:VAL:HG11	11:X:353:PHE:CE1	2.37	0.58
11:K:138:ILE:HD13	12:E:191:THR:HG23	1.85	0.58
11:C:336:VAL:HG11	11:C:353:PHE:CE1	2.37	0.58
11:W:182:LEU:HA	11:W:185:ILE:HD12	1.84	0.58
11:K:446:LEU:HD11	11:K:467:GLU:HG3	1.85	0.58
12:E:320:PRO:O	12:E:324:THR:OG1	2.20	0.58
11:K:38:ASP:O	11:K:286:LEU:HD13	2.03	0.58
12:D:46:LEU:CD1	12:D:65:ASP:HB3	2.33	0.58
12:Y:46:LEU:CD1	12:Y:65:ASP:HB3	2.33	0.58
11:K:151:GLY:HA3	11:K:437:PRO:HB2	1.86	0.58
12:D:26:GLU:OE1	12:D:26:GLU:HA	2.04	0.58
11:n:311:ALA:HA	11:n:323:LEU:HD23	1.85	0.58
11:W:206:VAL:HG23	11:W:269:VAL:O	2.04	0.58
12:Z:320:PRO:O	12:Z:324:THR:OG1	2.20	0.58
15:I:9:SER:HB3	15:I:12:ALA:H	1.69	0.58
11:n:212:ARG:HG2	11:n:237:THR:HG21	1.83	0.58
15:m:9:SER:HB3	15:m:12:ALA:H	1.69	0.58
11:C:146:GLU:HB2	11:C:163:ARG:HB2	1.85	0.58
11:n:138:ILE:HD13	12:Z:191:THR:HG23	1.85	0.58
11:B:182:LEU:HA	11:B:185:ILE:HD12	1.84	0.57
11:n:475:LYS:O	11:n:479:ASN:HB2	2.04	0.57
12:c:321:ALA:HB3	12:c:322:PRO:HD3	1.86	0.57
11:B:206:VAL:HG23	11:B:269:VAL:O	2.04	0.57
11:C:398:GLN:O	11:C:401:GLU:HB3	2.05	0.57
1:2:67:MET:HE1	3:a:182:LEU:HD23	1.86	0.57
12:D:20:ILE:CG1	12:D:271:LEU:HB3	2.34	0.57
13:G:149:LYS:HA	13:G:152:SER:HB2	1.86	0.57
12:Y:20:ILE:CG1	12:Y:271:LEU:HB3	2.34	0.57
12:Z:345:TYR:HB2	12:Z:459:MET:HE1	1.86	0.57
13:j:149:LYS:HA	13:j:152:SER:HB2	1.86	0.57
11:K:311:ALA:HA	11:K:323:LEU:HD23	1.85	0.57
12:E:345:TYR:HB2	12:E:459:MET:HE1	1.86	0.57
1:M:67:MET:HE1	3:p:182:LEU:HD23	1.86	0.57
11:K:475:LYS:O	11:K:479:ASN:HB2	2.04	0.57
12:F:321:ALA:HB3	12:F:322:PRO:HD3	1.86	0.57
17:h:1002:UNK:O	17:h:1006:UNK:N	2.38	0.57
11:W:142:ARG:HB2	11:W:315:SER:HA	1.85	0.57
12:Z:27:GLN:CG	16:o:63:SER:CB	2.82	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:c:320:PRO:O	12:c:324:THR:OG1	2.22	0.57
3:p:211:VAL:HG23	3:p:212:PRO:HD3	1.87	0.57
11:W:242:ALA:HB2	11:W:282:GLN:NE2	2.20	0.57
3:a:211:VAL:HG23	3:a:212:PRO:HD3	1.87	0.57
11:B:142:ARG:HB2	11:B:315:SER:HA	1.85	0.57
12:E:126:GLU:HA	12:E:300:LYS:HE3	1.85	0.57
12:E:140:VAL:HG13	12:E:414:LEU:HD22	1.87	0.57
11:X:344:VAL:HA	11:X:347:ILE:HD12	1.87	0.57
12:D:244:ARG:HD3	12:D:304:VAL:CG2	2.35	0.57
11:n:101:VAL:HG23	11:n:258:TRP:CD1	2.40	0.57
11:K:101:VAL:HG23	11:K:258:TRP:CD1	2.40	0.57
12:E:391:LEU:HB3	12:E:395:GLU:HG3	1.87	0.57
11:W:293:ARG:HH21	12:c:319:ASP:HB2	1.70	0.57
1:P:17:ILE:HB	1:Q:17:ILE:HG12	1.87	0.56
11:W:414:ALA:HA	11:W:417:LYS:HB3	1.87	0.56
11:C:260:ARG:O	11:C:321:GLY:HA3	2.05	0.56
11:n:347:ILE:HA	12:Z:222:MET:HE1	1.87	0.56
11:X:398:GLN:O	11:X:401:GLU:HB3	2.04	0.56
12:Y:85:VAL:CG1	12:Y:235:THR:HG23	2.32	0.56
12:E:132:GLU:HG3	12:E:149:ARG:HB3	1.87	0.56
12:F:85:VAL:HG11	12:F:235:THR:HG23	1.87	0.56
11:X:260:ARG:O	11:X:321:GLY:HA3	2.05	0.56
12:Z:259:PHE:CZ	12:Z:263:GLN:HG2	2.40	0.56
12:c:298:THR:HG23	12:c:303:SER:HA	1.88	0.56
13:j:76:ALA:HB3	13:j:109:THR:HG22	1.87	0.56
11:B:293:ARG:HH21	12:F:319:ASP:HB2	1.69	0.56
12:E:27:GLN:CG	16:O:63:SER:CB	2.82	0.56
12:E:229:ARG:HH22	12:E:267:GLU:CD	2.14	0.56
12:F:152:LYS:NZ	12:F:293:GLN:HG3	2.21	0.56
3:p:80:LYS:CE	7:t:1:VAL:H1	2.01	0.56
12:Z:132:GLU:HG3	12:Z:149:ARG:HB3	1.87	0.56
11:B:414:ALA:HA	11:B:417:LYS:HB3	1.87	0.56
12:E:220:GLY:HA3	12:E:232:VAL:HG11	1.88	0.56
11:n:151:GLY:HA3	11:n:437:PRO:HB2	1.86	0.56
12:c:152:LYS:NZ	12:c:293:GLN:HG3	2.21	0.56
11:n:66:LEU:HD12	11:n:76:VAL:HG11	1.86	0.56
12:Y:244:ARG:HD3	12:Y:304:VAL:CG2	2.35	0.56
12:Z:182:SER:O	12:Z:215:VAL:HA	2.06	0.56
12:c:85:VAL:HG11	12:c:235:THR:HG23	1.87	0.56
11:K:66:LEU:HD12	11:K:76:VAL:HG11	1.86	0.56
11:B:338:ALA:HB3	11:B:341:PRO:HG2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:C:344:VAL:HA	11:C:347:ILE:HD12	1.87	0.56
2:V:46:SER:OG	5:r:166:ARG:NH1	2.39	0.56
11:W:269:VAL:HG22	11:W:326:LEU:HB2	1.86	0.56
11:X:34:LEU:O	11:X:86:GLU:HG3	2.06	0.56
11:B:269:VAL:HG22	11:B:326:LEU:HB2	1.86	0.56
17:v:1002:UNK:O	17:v:1006:UNK:N	2.38	0.56
1:4:17:ILE:HB	1:5:17:ILE:HG12	1.87	0.56
11:B:163:ARG:HH11	11:B:265:HIS:CD2	2.24	0.56
12:E:98:VAL:HG13	12:E:99:ILE:HG23	1.88	0.56
12:E:259:PHE:CZ	12:E:263:GLN:HG2	2.40	0.56
12:F:298:THR:HG23	12:F:303:SER:HA	1.88	0.56
11:W:429:LEU:HD11	11:W:446:LEU:HB3	1.88	0.56
12:Z:140:VAL:HG13	12:Z:414:LEU:HD22	1.87	0.56
12:Z:391:LEU:HB3	12:Z:395:GLU:HG3	1.87	0.56
11:B:135:ALA:HB3	12:F:223:ASN:HD22	1.71	0.56
12:E:182:SER:O	12:E:215:VAL:HA	2.06	0.56
12:F:320:PRO:O	12:F:324:THR:OG1	2.22	0.56
12:D:98:VAL:HA	12:D:232:VAL:HG23	1.89	0.55
12:Z:98:VAL:HG13	12:Z:99:ILE:HG23	1.88	0.55
11:K:212:ARG:CG	11:K:237:THR:HG21	2.37	0.55
11:C:267:LEU:HD11	11:C:326:LEU:HD12	1.89	0.55
13:G:76:ALA:HB3	13:G:109:THR:HG22	1.87	0.55
14:H:78:GLN:HG3	14:H:79:PRO:HD2	1.89	0.55
11:n:165:GLN:HG2	11:n:166:ARG:N	2.22	0.55
12:Y:98:VAL:HA	12:Y:232:VAL:HG23	1.88	0.55
11:B:242:ALA:HB2	11:B:282:GLN:NE2	2.20	0.55
11:W:135:ALA:HB3	12:c:223:ASN:HD22	1.71	0.55
12:Z:229:ARG:HH22	12:Z:267:GLU:CD	2.14	0.55
12:c:53:HIS:HD2	12:c:59:VAL:HG12	1.71	0.55
5:d:134:THR:HG22	5:d:136:ASP:H	1.72	0.55
11:B:248:ALA:HB3	11:B:249:PRO:HD3	1.88	0.55
11:B:429:LEU:HD11	11:B:446:LEU:HB3	1.88	0.55
11:n:421:VAL:O	11:n:425:ARG:NH1	2.39	0.55
12:Z:220:GLY:HA3	12:Z:232:VAL:HG11	1.88	0.55
14:l:78:GLN:HG3	14:l:79:PRO:HD2	1.89	0.55
2:A:46:SER:OG	5:d:166:ARG:NH1	2.39	0.55
11:K:35:ALA:HB3	11:K:42:ARG:NH1	2.22	0.55
11:K:165:GLN:HG2	11:K:166:ARG:N	2.22	0.55
11:C:34:LEU:O	11:C:86:GLU:HG3	2.05	0.55
11:B:171:GLY:N	11:B:177:LYS:HD3	2.21	0.55
12:D:85:VAL:CG1	12:D:235:THR:HG23	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:F:53:HIS:HD2	12:F:59:VAL:HG12	1.71	0.55
5:r:134:THR:HG22	5:r:136:ASP:H	1.72	0.55
11:K:112:ALA:O	11:K:251:THR:HG21	2.06	0.55
11:K:347:ILE:HA	12:E:222:MET:HE1	1.88	0.55
12:F:137:GLY:HA2	12:F:432:VAL:O	2.07	0.55
11:n:35:ALA:HB3	11:n:42:ARG:NH1	2.22	0.55
12:Z:133:ILE:HD12	12:Z:146:PRO:HB2	1.89	0.55
11:C:397:ALA:HA	11:C:400:ARG:NH2	2.21	0.55
12:F:258:ILE:HD13	12:F:293:GLN:HE22	1.71	0.55
13:G:14:LYS:HA	13:G:248:ILE:HD11	1.89	0.55
15:I:12:ALA:O	15:I:15:ASN:N	2.33	0.55
11:W:248:ALA:HB3	11:W:249:PRO:HD3	1.88	0.55
11:W:338:ALA:HB3	11:W:341:PRO:HG2	1.88	0.55
13:G:268:VAL:O	13:G:272:THR:HG23	2.07	0.55
11:X:51:ALA:O	11:X:52:GLU:HB2	2.07	0.55
11:X:267:LEU:HD11	11:X:326:LEU:HD12	1.89	0.55
12:c:137:GLY:HA2	12:c:432:VAL:O	2.07	0.55
12:c:258:ILE:HD13	12:c:293:GLN:HE22	1.71	0.55
13:j:268:VAL:O	13:j:272:THR:HG23	2.07	0.55
1:1:14:ILE:HG21	1:2:14:ILE:HD13	1.89	0.54
11:C:51:ALA:O	11:C:52:GLU:HB2	2.07	0.54
1:L:14:ILE:HG21	1:M:14:ILE:HD13	1.89	0.54
12:Z:85:VAL:HG11	12:Z:235:THR:HG23	1.89	0.54
11:K:51:ALA:O	11:K:52:GLU:HB2	2.07	0.54
11:W:163:ARG:HH11	11:W:265:HIS:CD2	2.24	0.54
11:W:171:GLY:N	11:W:177:LYS:HD3	2.21	0.54
11:X:397:ALA:HA	11:X:400:ARG:NH2	2.21	0.54
12:Y:434:LEU:O	12:Y:438:VAL:HG23	2.08	0.54
12:c:242:TYR:CE1	12:c:246:GLU:HG3	2.43	0.54
11:K:103:PRO:C	11:K:105:LEU:H	2.15	0.54
12:E:85:VAL:HG11	12:E:235:THR:HG23	1.89	0.54
12:E:153:ILE:HD12	12:E:153:ILE:N	2.22	0.54
11:n:212:ARG:CG	11:n:237:THR:HG21	2.37	0.54
12:Z:166:PHE:HE1	12:Z:170:LEU:HD11	1.72	0.54
11:B:55:VAL:HG21	11:B:75:ILE:HD13	1.90	0.54
11:C:494:GLU:CD	11:C:494:GLU:N	2.66	0.54
11:n:112:ALA:O	11:n:251:THR:HG21	2.07	0.54
13:j:14:LYS:HA	13:j:248:ILE:HD11	1.89	0.54
12:E:259:PHE:O	12:E:262:THR:HB	2.08	0.54
12:c:50:VAL:HA	12:c:61:THR:HG22	1.88	0.54
11:B:293:ARG:NH2	12:F:319:ASP:HB2	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:D:98:VAL:HG13	12:D:99:ILE:HG23	1.89	0.54
11:C:174:GLN:HB3	12:F:354:LYS:HD2	1.89	0.54
12:D:434:LEU:O	12:D:438:VAL:HG23	2.08	0.54
11:W:50:GLN:OE1	11:W:96:ILE:HD11	2.08	0.54
11:W:101:VAL:HG12	11:W:255:ILE:HA	1.89	0.54
11:X:174:GLN:HB3	12:c:354:LYS:HD2	1.89	0.54
1:7:41:PRO:HD3	14:H:44:ASN:HB3	1.90	0.54
11:B:110:VAL:CG1	11:B:123:ILE:HD11	2.38	0.54
11:W:110:VAL:CG1	11:W:123:ILE:HD11	2.38	0.54
11:W:293:ARG:NH2	12:c:319:ASP:HB2	2.22	0.54
12:F:50:VAL:HA	12:F:61:THR:HG22	1.89	0.54
3:p:23:CYS:SG	3:p:24:LEU:N	2.81	0.54
12:Z:153:ILE:N	12:Z:153:ILE:HD12	2.22	0.54
12:c:363:VAL:HB	12:c:367:HIS:ND1	2.23	0.54
3:a:23:CYS:SG	3:a:24:LEU:N	2.81	0.53
12:F:242:TYR:CE1	12:F:246:GLU:HG3	2.42	0.53
11:B:50:GLN:OE1	11:B:96:ILE:HD11	2.08	0.53
12:E:166:PHE:HE1	12:E:170:LEU:HD11	1.72	0.53
12:F:95:ILE:HD11	12:F:198:TYR:CD1	2.42	0.53
11:n:174:GLN:HA	18:n:601:ANP:HNB1	1.73	0.53
12:Z:50:VAL:HA	12:Z:61:THR:HG22	1.90	0.53
12:c:95:ILE:HD11	12:c:198:TYR:CD1	2.42	0.53
12:c:325:THR:O	12:c:326:PHE:C	2.50	0.53
12:Y:98:VAL:HG13	12:Y:99:ILE:HG23	1.89	0.53
11:n:103:PRO:HD3	11:n:258:TRP:CZ2	2.43	0.53
11:X:69:GLU:HB3	11:X:70:PRO:HD3	1.91	0.53
12:F:363:VAL:HB	12:F:367:HIS:ND1	2.23	0.53
3:p:49:ASN:ND2	3:p:56:SER:OG	2.42	0.53
11:n:425:ARG:HG3	11:n:460:LEU:HD12	1.91	0.53
11:W:377:GLY:C	11:W:379:ALA:H	2.16	0.53
11:K:103:PRO:HD3	11:K:258:TRP:CZ2	2.43	0.53
11:B:101:VAL:HG12	11:B:255:ILE:HA	1.89	0.53
12:E:50:VAL:HA	12:E:61:THR:HG22	1.90	0.53
11:W:250:PHE:O	11:W:253:ALA:HB3	2.09	0.53
12:Z:30:LEU:HD21	12:Z:57:ASN:HA	1.91	0.53
3:a:49:ASN:ND2	3:a:56:SER:OG	2.42	0.53
11:K:174:GLN:HA	18:K:601:ANP:HNB1	1.73	0.53
12:E:133:ILE:HD12	12:E:146:PRO:HB2	1.89	0.53
1:S:41:PRO:HD3	14:l:44:ASN:HB3	1.89	0.53
11:W:385:LEU:HD23	11:W:444:VAL:CG1	2.34	0.53
11:B:250:PHE:O	11:B:253:ALA:HB3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:F:325:THR:O	12:F:326:PHE:C	2.50	0.53
12:c:48:LEU:HD23	12:c:63:ALA:HA	1.90	0.53
11:W:55:VAL:HG21	11:W:75:ILE:HD13	1.90	0.53
11:K:421:VAL:O	11:K:425:ARG:NH1	2.39	0.53
11:B:30:THR:HA	11:B:90:VAL:O	2.09	0.53
12:F:377:THR:HG22	12:F:407:ALA:HB2	1.91	0.53
15:I:8:MET:N	15:I:12:ALA:O	2.42	0.53
11:n:50:GLN:HB3	12:Z:69:GLY:HA2	1.91	0.53
11:n:417:LYS:O	11:n:421:VAL:HG23	2.09	0.53
11:W:30:THR:HA	11:W:90:VAL:O	2.09	0.53
11:W:46:LEU:HD13	11:W:49:ILE:HD12	1.91	0.53
11:X:494:GLU:CD	11:X:494:GLU:N	2.66	0.53
12:F:48:LEU:HD23	12:F:63:ALA:HA	1.90	0.52
13:G:23:MET:CB	13:G:237:MET:HG3	2.30	0.52
15:m:8:MET:N	15:m:12:ALA:O	2.42	0.52
11:K:425:ARG:HG3	11:K:460:LEU:HD12	1.90	0.52
11:B:385:LEU:HD23	11:B:444:VAL:CG1	2.34	0.52
14:H:78:GLN:HB2	14:H:82:GLN:O	2.09	0.52
3:p:32:TYR:HB3	3:p:111:LEU:HD11	1.91	0.52
12:Z:259:PHE:O	12:Z:262:THR:HB	2.08	0.52
11:K:32:ARG:HH12	11:K:89:LEU:HB2	1.74	0.52
11:B:267:LEU:HD12	11:B:324:THR:HB	1.91	0.52
13:G:31:LEU:O	13:G:35:GLU:HG2	2.09	0.52
11:X:132:GLN:OE1	11:X:306:ARG:NH1	2.43	0.52
12:D:26:GLU:OE1	12:D:26:GLU:CA	2.58	0.52
12:E:359:ASP:O	12:E:363:VAL:HG22	2.10	0.52
5:r:157:LYS:HE3	7:t:8:LYS:N	2.24	0.52
11:n:51:ALA:O	11:n:52:GLU:HB2	2.07	0.52
11:W:267:LEU:HD12	11:W:324:THR:HB	1.91	0.52
12:Y:244:ARG:NE	12:Y:245:ASP:OD1	2.40	0.52
13:j:31:LEU:O	13:j:35:GLU:HG2	2.09	0.52
11:B:471:LEU:O	11:B:475:LYS:HG3	2.10	0.52
12:D:156:PHE:CD1	12:D:156:PHE:N	2.77	0.52
11:n:103:PRO:C	11:n:105:LEU:H	2.15	0.52
12:c:348:VAL:O	12:c:350:PRO:HD3	2.10	0.52
12:c:377:THR:HG22	12:c:407:ALA:HB2	1.91	0.52
13:j:3:LEU:HD21	13:j:255:TYR:CE1	2.45	0.52
13:j:23:MET:CB	13:j:237:MET:HG3	2.30	0.52
11:B:377:GLY:C	11:B:379:ALA:H	2.16	0.52
11:W:478:HIS:CE1	11:W:502:ALA:HB2	2.44	0.52
3:a:32:TYR:HB3	3:a:111:LEU:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:B:478:HIS:CE1	11:B:502:ALA:HB2	2.44	0.52
11:C:132:GLN:OE1	11:C:306:ARG:NH1	2.43	0.52
11:K:105:LEU:O	11:K:108:ARG:HB2	2.10	0.52
11:K:417:LYS:O	11:K:421:VAL:HG23	2.09	0.52
11:B:505:SER:O	11:B:509:THR:HG22	2.10	0.52
12:E:201:MET:HA	12:E:204:THR:HG22	1.92	0.52
12:E:319:ASP:O	12:E:322:PRO:HD2	2.10	0.52
12:Z:166:PHE:CE1	12:Z:170:LEU:HD11	2.45	0.52
5:d:157:LYS:HE3	7:f:8:LYS:N	2.25	0.52
11:X:101:VAL:HG12	11:X:255:ILE:HA	1.91	0.52
1:4:1:MET:SD	1:5:2:GLN:NE2	2.83	0.52
11:W:471:LEU:O	11:W:475:LYS:HG3	2.10	0.52
12:c:281:TYR:CE2	12:c:320:PRO:HD2	2.45	0.52
11:K:50:GLN:HB3	12:E:69:GLY:HA2	1.91	0.51
12:E:177:ALA:HB2	12:E:431:LEU:HD11	1.92	0.51
12:F:281:TYR:CE2	12:F:320:PRO:HD2	2.45	0.51
12:F:397:SER:O	12:F:401:LYS:HB2	2.11	0.51
14:H:14:PHE:CD1	14:H:85:VAL:HG23	2.46	0.51
11:n:270:TYR:HB2	11:n:327:PRO:HA	1.93	0.51
12:Z:319:ASP:O	12:Z:322:PRO:HD2	2.10	0.51
11:C:140:PRO:HB2	11:C:318:GLU:HG3	1.93	0.51
13:G:262:VAL:O	13:G:266:GLU:HG3	2.10	0.51
11:W:151:GLY:O	11:W:432:GLN:NE2	2.40	0.51
11:B:46:LEU:HD13	11:B:49:ILE:HD12	1.91	0.51
11:C:82:ARG:HA	12:F:33:ILE:HB	1.92	0.51
12:E:26:GLU:HB2	12:E:29:GLU:OE1	2.10	0.51
13:G:3:LEU:HD21	13:G:255:TYR:CE1	2.45	0.51
1:S:68:VAL:HG11	1:T:16:THR:HG21	1.93	0.51
12:Z:255:ILE:HB	12:Z:308:GLN:HG2	1.93	0.51
14:l:78:GLN:HB2	14:l:82:GLN:O	2.09	0.51
12:E:30:LEU:HD21	12:E:57:ASN:HA	1.91	0.51
12:E:241:GLU:OE2	12:E:295:ARG:HB3	2.10	0.51
12:F:15:ALA:HB3	12:F:22:ASP:HB2	1.93	0.51
12:F:134:LEU:HB2	12:F:149:ARG:HG2	1.93	0.51
11:X:140:PRO:HB2	11:X:318:GLU:HG3	1.93	0.51
12:Z:345:TYR:HA	12:Z:346:PRO:C	2.36	0.51
12:E:277:SER:HB2	12:E:283:PRO:HA	1.93	0.51
1:Q:14:ILE:HG21	1:R:14:ILE:HD13	1.92	0.51
11:W:505:SER:O	11:W:509:THR:HG22	2.10	0.51
12:Y:378:LEU:HD21	12:Y:410:ILE:HG22	1.93	0.51
13:j:262:VAL:O	13:j:266:GLU:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:65:CYS:SG	1:4:16:THR:OG1	2.68	0.51
11:n:152:LEU:HD23	11:n:432:GLN:NE2	2.26	0.51
11:X:155:VAL:HG23	11:X:367:ILE:HD11	1.92	0.51
12:Z:359:ASP:O	12:Z:363:VAL:HG22	2.10	0.51
3:a:81:ASN:HB2	3:a:84:LEU:HD13	1.93	0.51
12:E:166:PHE:CE1	12:E:170:LEU:HD11	2.45	0.51
13:G:184:ASN:HA	13:G:210:PHE:CD1	2.46	0.51
12:Z:277:SER:HB2	12:Z:283:PRO:HA	1.93	0.51
12:c:397:SER:O	12:c:401:LYS:HB2	2.10	0.51
3:a:80:LYS:HD3	7:f:1:VAL:N	2.06	0.51
12:D:425:THR:C	12:D:427:ILE:H	2.19	0.51
13:G:73:LEU:CD1	13:G:154:MET:HE2	2.40	0.51
3:p:81:ASN:HB2	3:p:84:LEU:HD13	1.93	0.51
12:Z:26:GLU:HB2	12:Z:29:GLU:OE1	2.10	0.51
12:c:15:ALA:HB3	12:c:22:ASP:HB2	1.93	0.51
12:c:39:ILE:HG13	12:c:76:VAL:HG13	1.93	0.51
12:c:154:GLY:HA3	12:c:329:LEU:HD13	1.93	0.51
14:l:14:PHE:CD1	14:l:85:VAL:HG23	2.46	0.51
11:K:270:TYR:HB2	11:K:327:PRO:HA	1.93	0.51
11:K:444:VAL:CG2	11:K:445:PRO:HD3	2.40	0.51
11:n:444:VAL:CG2	11:n:445:PRO:HD3	2.40	0.51
13:j:73:LEU:CD1	13:j:154:MET:HE2	2.40	0.51
1:2:53:LEU:O	1:2:57:LEU:HB3	2.11	0.51
11:B:43:VAL:HG21	11:B:75:ILE:HD12	1.93	0.51
11:C:101:VAL:HG12	11:C:255:ILE:HA	1.91	0.51
12:Z:201:MET:HA	12:Z:204:THR:HG22	1.92	0.51
11:K:383:LYS:O	11:K:387:GLN:HG3	2.12	0.50
12:F:154:GLY:HA3	12:F:329:LEU:HD13	1.93	0.50
11:W:43:VAL:HG21	11:W:75:ILE:HD12	1.93	0.50
11:X:197:GLU:HA	11:X:200:LYS:HD2	1.93	0.50
12:c:290:GLY:O	12:c:294:GLU:HB2	2.11	0.50
1:5:14:ILE:HG21	1:6:14:ILE:HD13	1.92	0.50
3:a:92:LEU:HD22	3:a:234:TRP:HE1	1.76	0.50
12:D:447:GLY:C	12:D:449:TYR:H	2.20	0.50
1:P:1:MET:SD	1:Q:2:GLN:NE2	2.84	0.50
11:X:336:VAL:HG11	11:X:353:PHE:HE1	1.75	0.50
12:Y:26:GLU:OE1	12:Y:26:GLU:CA	2.58	0.50
12:Y:133:ILE:HD11	12:Y:146:PRO:HB2	1.92	0.50
12:Y:425:THR:C	12:Y:427:ILE:H	2.19	0.50
12:Z:241:GLU:OE2	12:Z:295:ARG:HB3	2.10	0.50
12:c:134:LEU:HB2	12:c:149:ARG:HG2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:j:184:ASN:HA	13:j:210:PHE:CD1	2.46	0.50
1:9:14:ILE:HG21	1:0:14:ILE:HD13	1.93	0.50
11:B:151:GLY:O	11:B:432:GLN:NE2	2.40	0.50
12:F:39:ILE:HG13	12:F:76:VAL:HG13	1.93	0.50
1:M:53:LEU:O	1:M:57:LEU:HB3	2.11	0.50
3:p:26:LEU:HD21	3:p:31:LEU:HD12	1.94	0.50
12:c:382:LYS:HA	12:c:385:GLN:HG2	1.93	0.50
11:K:77:LEU:HD13	11:K:81:ASP:HB3	1.93	0.50
12:F:220:GLY:N	12:F:232:VAL:HG21	2.27	0.50
12:Y:156:PHE:N	12:Y:156:PHE:CD1	2.78	0.50
3:a:26:LEU:HD21	3:a:31:LEU:HD12	1.94	0.50
11:B:111:ASP:OD2	11:B:115:ASN:HB2	2.12	0.50
11:C:155:VAL:HG23	11:C:367:ILE:HD11	1.92	0.50
12:D:133:ILE:HD11	12:D:146:PRO:HB2	1.92	0.50
12:F:348:VAL:O	12:F:350:PRO:HD3	2.10	0.50
11:n:105:LEU:O	11:n:108:ARG:HB2	2.10	0.50
11:W:358:LEU:HB2	11:W:366:ALA:HB1	1.94	0.50
11:K:424:GLU:HB3	11:K:460:LEU:HD21	1.94	0.50
12:F:290:GLY:O	12:F:294:GLU:HB2	2.11	0.50
1:U:14:ILE:HG21	1:J:14:ILE:HD13	1.93	0.50
3:p:233:VAL:HA	3:p:236:ILE:HG22	1.94	0.50
11:W:108:ARG:NH1	11:W:123:ILE:HD13	2.27	0.50
11:W:111:ASP:OD2	11:W:115:ASN:HB2	2.12	0.50
11:X:82:ARG:HA	12:c:33:ILE:HB	1.91	0.50
11:C:69:GLU:HB3	11:C:70:PRO:HD3	1.91	0.50
11:C:197:GLU:HA	11:C:200:LYS:HD2	1.93	0.50
12:E:345:TYR:HA	12:E:346:PRO:C	2.36	0.50
3:p:92:LEU:HD22	3:p:234:TRP:HE1	1.76	0.50
12:Z:177:ALA:HB2	12:Z:431:LEU:HD11	1.92	0.50
1:7:68:VAL:HG11	1:8:16:THR:HG21	1.93	0.50
12:E:255:ILE:HB	12:E:308:GLN:HG2	1.93	0.50
12:F:204:THR:OG1	12:F:206:VAL:HG23	2.12	0.50
14:H:29:GLN:HG2	14:H:60:MET:HG3	1.93	0.50
11:W:129:SER:HB3	11:W:254:SER:HB3	1.94	0.50
11:B:163:ARG:HH11	11:B:265:HIS:HD2	1.59	0.50
12:D:378:LEU:HD21	12:D:410:ILE:HG22	1.93	0.50
7:t:53:ALA:O	7:t:60:ASN:ND2	2.44	0.50
11:n:32:ARG:HH12	11:n:89:LEU:HB2	1.74	0.50
11:n:166:ARG:HD3	11:n:308:LEU:O	2.12	0.50
11:n:383:LYS:O	11:n:387:GLN:HG3	2.11	0.50
12:Y:447:GLY:C	12:Y:449:TYR:H	2.19	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:152:LEU:HD23	11:K:432:GLN:NE2	2.26	0.49
11:B:129:SER:HB3	11:B:254:SER:HB3	1.94	0.49
12:F:382:LYS:HA	12:F:385:GLN:HG2	1.93	0.49
11:n:424:GLU:HB3	11:n:460:LEU:HD21	1.94	0.49
11:X:395:PHE:CD1	11:X:395:PHE:C	2.89	0.49
11:X:422:ARG:HH12	11:X:453:GLY:CA	2.25	0.49
12:c:90:GLU:HG3	12:c:111:SER:HA	1.94	0.49
12:c:204:THR:OG1	12:c:206:VAL:HG23	2.12	0.49
12:c:237:LEU:HD13	12:c:296:ILE:HG12	1.94	0.49
14:l:29:GLN:HG2	14:l:60:MET:HG3	1.93	0.49
11:B:358:LEU:HB2	11:B:366:ALA:HB1	1.94	0.49
11:C:273:LEU:HD13	11:C:304:HIS:CD2	2.47	0.49
12:F:242:TYR:CD1	12:F:246:GLU:HG3	2.47	0.49
11:W:163:ARG:HH11	11:W:265:HIS:HD2	1.59	0.49
11:X:273:LEU:HD13	11:X:304:HIS:CD2	2.47	0.49
12:c:96:ILE:HG22	12:c:97:ASN:N	2.28	0.49
14:l:80:ASP:O	14:l:81:SER:HB3	2.12	0.49
11:B:108:ARG:NH1	11:B:123:ILE:HD13	2.27	0.49
11:B:208:VAL:HG21	11:B:249:PRO:HG3	1.94	0.49
11:C:336:VAL:HG11	11:C:353:PHE:HE1	1.75	0.49
11:W:82:ARG:NH1	12:Z:33:ILE:O	2.45	0.49
12:Y:190:ARG:O	12:Y:191:THR:C	2.55	0.49
11:K:166:ARG:HD3	11:K:308:LEU:O	2.12	0.49
11:B:82:ARG:NH1	12:E:33:ILE:O	2.45	0.49
12:E:85:VAL:CG1	12:E:235:THR:HG23	2.42	0.49
12:F:96:ILE:HG22	12:F:97:ASN:N	2.28	0.49
11:W:77:LEU:O	11:W:243:PRO:HG2	2.12	0.49
12:c:242:TYR:CD1	12:c:246:GLU:HG3	2.47	0.49
13:j:110:ILE:HD11	13:j:146:ILE:HG21	1.94	0.49
11:K:492:SER:HB2	11:K:495:LEU:H	1.78	0.49
12:D:89:ARG:HG2	12:D:92:LEU:HD12	1.95	0.49
11:W:43:VAL:CG2	11:W:75:ILE:HD12	2.43	0.49
11:K:391:SER:OG	11:K:451:VAL:HG11	2.13	0.49
11:K:459:GLU:OE1	11:K:461:SER:OG	2.31	0.49
11:n:492:SER:HB2	11:n:495:LEU:H	1.78	0.49
11:B:139:LEU:HD23	12:F:105:GLU:HG3	1.95	0.49
11:C:395:PHE:CD1	11:C:395:PHE:C	2.89	0.49
13:G:258:THR:O	13:G:259:ARG:C	2.55	0.49
11:n:103:PRO:HD3	11:n:258:TRP:CH2	2.48	0.49
12:Z:85:VAL:CG1	12:Z:235:THR:HG23	2.42	0.49
13:j:258:THR:O	13:j:259:ARG:C	2.55	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:7:40:ASN:CG	14:H:42:LEU:HB3	2.27	0.49
7:f:53:ALA:O	7:f:60:ASN:ND2	2.44	0.49
11:n:77:LEU:HD13	11:n:81:ASP:HB3	1.93	0.49
11:W:290:PRO:HB3	12:c:276:PRO:HG3	1.95	0.49
11:X:155:VAL:HG23	11:X:367:ILE:CD1	2.43	0.49
10:k:15:HIS:CD2	10:k:16:GLN:H	2.31	0.49
11:B:77:LEU:O	11:B:243:PRO:HG2	2.13	0.49
12:D:135:GLU:HG3	12:D:434:LEU:HB2	1.94	0.49
11:W:139:LEU:HD23	12:c:105:GLU:HG3	1.95	0.49
11:W:478:HIS:HB3	11:W:481:LEU:HG	1.94	0.49
12:Z:257:ASN:OD1	12:Z:259:PHE:HB3	2.12	0.49
12:c:49:GLU:CD	12:c:231:ARG:HE	2.21	0.49
12:c:140:VAL:O	12:c:144:LEU:HB2	2.13	0.49
11:B:478:HIS:HB3	11:B:481:LEU:HG	1.94	0.49
12:F:237:LEU:HD13	12:F:296:ILE:HG12	1.94	0.49
15:I:19:GLN:HA	15:I:22:ARG:CB	2.43	0.49
12:Y:208:ASN:ND2	12:Y:211:GLY:HA3	2.27	0.49
13:j:44:MET:CE	14:l:86:THR:HG22	2.39	0.49
13:j:205:VAL:HA	14:l:51:GLN:NE2	2.28	0.49
1:1:1:MET:HE2	1:2:2:GLN:HE21	1.78	0.48
1:7:14:ILE:HG21	1:8:14:ILE:HD13	1.95	0.48
11:B:305:SER:O	11:B:309:GLU:HG2	2.13	0.48
11:C:216:ALA:O	11:C:217:GLN:C	2.55	0.48
11:C:422:ARG:HH12	11:C:453:GLY:CA	2.25	0.48
12:D:208:ASN:ND2	12:D:211:GLY:HA3	2.27	0.48
12:E:257:ASN:OD1	12:E:259:PHE:HB3	2.12	0.48
11:n:459:GLU:OE1	11:n:461:SER:OG	2.31	0.48
3:a:233:VAL:HA	3:a:236:ILE:HG22	1.94	0.48
12:D:190:ARG:O	12:D:191:THR:C	2.55	0.48
13:G:205:VAL:HA	14:H:51:GLN:NE2	2.28	0.48
15:I:9:SER:OG	15:I:10:TYR:N	2.46	0.48
11:W:208:VAL:HG21	11:W:249:PRO:HG3	1.94	0.48
11:X:216:ALA:C	11:X:218:LEU:N	2.70	0.48
12:c:220:GLY:N	12:c:232:VAL:HG21	2.27	0.48
11:K:394:LEU:HG	11:K:398:GLN:NE2	2.29	0.48
11:C:383:LYS:O	11:C:387:GLN:HG3	2.13	0.48
12:F:344:ILE:HG23	12:F:415:SER:HB3	1.96	0.48
10:x:15:HIS:CD2	10:x:16:GLN:H	2.31	0.48
11:n:446:LEU:CD1	11:n:467:GLU:HG3	2.43	0.48
11:X:54:LEU:HD11	11:X:78:PHE:HE2	1.78	0.48
12:Y:408:ARG:O	12:Y:412:ARG:HD2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:c:152:LYS:HZ1	12:c:293:GLN:HG3	1.77	0.48
15:m:19:GLN:HA	15:m:22:ARG:CB	2.43	0.48
12:D:408:ARG:O	12:D:412:ARG:HD2	2.13	0.48
12:F:432:VAL:HG12	12:F:436:ASP:HB3	1.95	0.48
15:I:12:ALA:O	15:I:13:TYR:C	2.56	0.48
11:W:305:SER:O	11:W:309:GLU:HG2	2.13	0.48
11:W:399:TYR:CE1	11:W:423:GLY:HA3	2.48	0.48
11:B:473:TYR:HE2	11:B:502:ALA:O	1.97	0.48
11:X:216:ALA:O	11:X:217:GLN:C	2.55	0.48
11:X:399:TYR:CD1	11:X:423:GLY:HA3	2.48	0.48
15:m:12:ALA:O	15:m:15:ASN:N	2.33	0.48
3:a:108:SER:OG	3:a:109:PHE:N	2.46	0.48
12:D:23:VAL:CG1	12:D:76:VAL:HG21	2.44	0.48
12:F:90:GLU:HG3	12:F:111:SER:HA	1.94	0.48
12:F:152:LYS:HZ1	12:F:293:GLN:HG3	1.78	0.48
11:K:103:PRO:HD3	11:K:258:TRP:CH2	2.48	0.48
11:K:168:LEU:HD11	11:K:329:ILE:HB	1.95	0.48
11:C:292:GLY:N	11:C:296:TYR:O	2.36	0.48
12:D:244:ARG:NE	12:D:245:ASP:OD1	2.40	0.48
12:Y:89:ARG:HG2	12:Y:92:LEU:HD12	1.95	0.48
12:Y:188:GLY:O	12:Y:260:ARG:HD2	2.12	0.48
11:C:399:TYR:CD1	11:C:423:GLY:HA3	2.48	0.48
12:D:188:GLY:O	12:D:260:ARG:HD2	2.12	0.48
3:p:96:ILE:HG21	3:p:177:LEU:HD11	1.96	0.48
11:n:168:LEU:HD11	11:n:329:ILE:HB	1.95	0.48
11:W:466:PHE:CZ	11:W:470:PHE:HB2	2.48	0.48
11:W:473:TYR:HE2	11:W:502:ALA:O	1.97	0.48
11:X:248:ALA:HB3	11:X:249:PRO:HD3	1.96	0.48
11:K:85:LYS:HE2	12:D:32:ALA:HB2	1.96	0.48
11:B:85:LYS:HE2	12:E:32:ALA:HB2	1.96	0.48
11:B:290:PRO:HB3	12:F:276:PRO:HG3	1.95	0.48
12:F:140:VAL:O	12:F:144:LEU:HB2	2.13	0.48
12:F:384:LEU:HB3	12:F:388:ILE:HD11	1.96	0.48
13:G:271:ILE:HD13	13:G:271:ILE:N	2.29	0.48
1:M:60:ALA:HB2	3:p:176:ARG:HE	1.79	0.48
11:W:174:GLN:HA	18:W:601:ANP:HNB1	1.79	0.48
11:X:507:VAL:C	11:X:509:THR:H	2.22	0.48
12:Z:423:VAL:HG23	12:Z:424:PHE:CD1	2.49	0.48
12:c:432:VAL:HG12	12:c:436:ASP:HB3	1.95	0.48
13:j:271:ILE:HD13	13:j:271:ILE:N	2.29	0.48
1:S:14:ILE:HG21	1:T:14:ILE:HD13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:W:314:LEU:HD22	11:W:318:GLU:HB2	1.96	0.48
12:Y:62:ILE:HD11	12:Y:272:LEU:HD11	1.96	0.48
12:Y:135:GLU:HG3	12:Y:434:LEU:HB2	1.94	0.48
15:m:12:ALA:O	15:m:13:TYR:C	2.56	0.48
1:2:60:ALA:HB2	3:a:176:ARG:HE	1.79	0.47
11:C:155:VAL:HG23	11:C:367:ILE:CD1	2.43	0.47
12:E:277:SER:OG	12:E:278:ALA:N	2.47	0.47
13:G:110:ILE:HD11	13:G:146:ILE:HG21	1.94	0.47
11:n:394:LEU:HG	11:n:398:GLN:NE2	2.28	0.47
11:W:53:GLU:HA	11:W:96:ILE:HA	1.96	0.47
12:Y:23:VAL:CG1	12:Y:76:VAL:HG21	2.44	0.47
12:Y:311:TYR:CE2	12:Y:313:PRO:HA	2.49	0.47
2:A:26:LEU:O	2:A:30:PHE:HB2	2.15	0.47
11:K:158:LEU:HD11	11:K:396:LEU:HD12	1.95	0.47
11:K:446:LEU:CD1	11:K:467:GLU:HG3	2.43	0.47
11:B:399:TYR:CE1	11:B:423:GLY:HA3	2.48	0.47
12:D:388:ILE:HA	12:D:392:GLY:O	2.14	0.47
12:E:168:GLN:HE21	12:E:201:MET:HG3	1.79	0.47
12:F:253:LEU:HD23	12:F:296:ILE:HG23	1.95	0.47
12:F:281:TYR:HE2	12:F:320:PRO:HD2	1.79	0.47
11:X:382:VAL:HG11	11:X:440:THR:HG21	1.96	0.47
12:c:281:TYR:HE2	12:c:320:PRO:HD2	1.78	0.47
11:B:377:GLY:HA2	11:B:380:ALA:HB3	1.97	0.47
11:B:499:LEU:HD12	11:B:502:ALA:HB3	1.97	0.47
11:C:484:GLU:O	11:C:485:ILE:C	2.58	0.47
12:F:49:GLU:CD	12:F:231:ARG:HE	2.21	0.47
13:G:180:LYS:HE2	13:G:221:ALA:HB2	1.96	0.47
14:H:80:ASP:O	14:H:81:SER:HB3	2.12	0.47
1:L:1:MET:HE2	1:M:2:GLN:HE21	1.78	0.47
1:M:59:GLU:O	1:M:60:ALA:C	2.57	0.47
11:W:85:LYS:HE2	12:Z:32:ALA:HB2	1.96	0.47
12:Y:340:SER:HB3	12:Y:347:ALA:HB2	1.97	0.47
12:Z:197:LEU:HD23	12:Z:219:PHE:HZ	1.79	0.47
13:j:235:ASN:O	13:j:238:ASP:HB3	2.14	0.47
1:2:59:GLU:O	1:2:60:ALA:C	2.57	0.47
11:K:109:VAL:HG12	11:K:117:ILE:CG1	2.45	0.47
12:Y:425:THR:C	12:Y:427:ILE:N	2.73	0.47
3:a:96:ILE:HG21	3:a:177:LEU:HD11	1.96	0.47
11:B:43:VAL:CG2	11:B:75:ILE:HD12	2.43	0.47
12:D:62:ILE:HD11	12:D:272:LEU:HD11	1.96	0.47
11:W:188:GLN:HB3	11:W:192:ASN:ND2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:X:383:LYS:O	11:X:387:GLN:HG3	2.13	0.47
12:Z:168:GLN:HE21	12:Z:201:MET:HG3	1.79	0.47
12:c:37:LEU:HB2	12:c:48:LEU:HB2	1.96	0.47
12:c:253:LEU:HD23	12:c:296:ILE:HG23	1.95	0.47
11:n:158:LEU:HD11	11:n:396:LEU:HD12	1.95	0.47
11:n:391:SER:OG	11:n:451:VAL:HG11	2.13	0.47
11:W:226:ASP:O	11:W:229:LYS:HG2	2.15	0.47
3:a:51:ASN:HB3	5:d:135:VAL:HG22	1.96	0.47
5:d:155:LYS:HD3	7:f:4:LEU:CA	2.45	0.47
11:B:53:GLU:HA	11:B:96:ILE:HA	1.96	0.47
11:B:173:ARG:HG2	11:B:174:GLN:HG2	1.96	0.47
11:B:174:GLN:HA	18:B:601:ANP:HNB1	1.79	0.47
11:B:188:GLN:HB3	11:B:192:ASN:ND2	2.29	0.47
11:B:226:ASP:O	11:B:229:LYS:HG2	2.15	0.47
11:C:54:LEU:HD11	11:C:78:PHE:HE2	1.78	0.47
12:D:237:LEU:HD22	12:D:292:LEU:HD12	1.97	0.47
12:D:311:TYR:CE2	12:D:313:PRO:HA	2.49	0.47
12:E:256:ASP:HA	12:E:257:ASN:HA	1.69	0.47
12:F:37:LEU:HB2	12:F:48:LEU:HB2	1.96	0.47
3:p:51:ASN:HB3	5:r:135:VAL:HG22	1.96	0.47
5:r:155:LYS:HD3	7:t:4:LEU:CA	2.45	0.47
11:n:109:VAL:HG12	11:n:117:ILE:CG1	2.45	0.47
11:W:103:PRO:HD2	11:W:126:ALA:HB2	1.96	0.47
11:W:173:ARG:HG2	11:W:174:GLN:HG2	1.96	0.47
11:X:218:LEU:C	11:X:218:LEU:HD23	2.40	0.47
12:Y:23:VAL:HG13	12:Y:76:VAL:HG21	1.97	0.47
12:c:344:ILE:HG23	12:c:415:SER:HB3	1.95	0.47
11:B:109:VAL:HG23	11:B:228:MET:HE1	1.97	0.47
11:C:507:VAL:C	11:C:509:THR:H	2.22	0.47
11:n:85:LYS:HE2	12:Y:32:ALA:HB2	1.96	0.47
11:X:503:THR:O	11:X:507:VAL:HG23	2.15	0.47
12:Z:277:SER:OG	12:Z:278:ALA:N	2.47	0.47
12:c:384:LEU:HB3	12:c:388:ILE:HD11	1.96	0.47
5:d:155:LYS:HD3	7:f:4:LEU:CB	2.45	0.47
12:D:23:VAL:HG13	12:D:76:VAL:HG21	1.97	0.47
12:E:197:LEU:HD23	12:E:219:PHE:HZ	1.79	0.47
3:p:108:SER:OG	3:p:109:PHE:N	2.46	0.47
11:W:377:GLY:HA2	11:W:380:ALA:HB3	1.97	0.47
11:W:499:LEU:HD12	11:W:502:ALA:HB3	1.97	0.47
12:Z:322:PRO:O	12:Z:323:ALA:C	2.58	0.47
1:1:14:ILE:HD13	1:0:14:ILE:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:B:103:PRO:HD2	11:B:126:ALA:HB2	1.96	0.47
11:B:466:PHE:CZ	11:B:470:PHE:HB2	2.48	0.47
11:W:109:VAL:HG23	11:W:228:MET:HE1	1.97	0.47
13:j:74:ILE:O	13:j:107:ILE:HA	2.15	0.47
11:B:314:LEU:HD22	11:B:318:GLU:HB2	1.96	0.46
12:Y:388:ILE:HA	12:Y:392:GLY:O	2.14	0.46
13:j:200:ASP:C	13:j:202:ASP:N	2.72	0.46
9:i:37:THR:HG23	9:i:40:PHE:H	1.80	0.46
11:C:248:ALA:HB3	11:C:249:PRO:HD3	1.96	0.46
12:E:322:PRO:O	12:E:323:ALA:C	2.58	0.46
12:F:30:LEU:HD11	12:F:57:ASN:HA	1.97	0.46
13:G:235:ASN:O	13:G:238:ASP:HB3	2.14	0.46
2:V:26:LEU:O	2:V:30:PHE:HB2	2.15	0.46
11:W:67:ASN:HB2	12:c:17:ILE:HG12	1.97	0.46
11:K:169:ILE:HD11	11:K:326:LEU:HD13	1.96	0.46
11:B:67:ASN:HB2	12:F:17:ILE:HG12	1.97	0.46
11:B:396:LEU:HA	11:B:399:TYR:HB3	1.98	0.46
11:C:218:LEU:C	11:C:218:LEU:HD23	2.40	0.46
11:W:344:VAL:HA	11:W:347:ILE:HD12	1.97	0.46
11:X:35:ALA:HB1	12:c:53:HIS:O	2.16	0.46
12:Z:39:ILE:HG12	12:Z:76:VAL:HG22	1.98	0.46
12:c:13:VAL:HG23	12:c:74:GLU:HB3	1.97	0.46
11:C:503:THR:O	11:C:507:VAL:HG23	2.15	0.46
12:c:201:MET:HA	12:c:201:MET:CE	2.46	0.46
11:B:344:VAL:HA	11:B:347:ILE:HD12	1.97	0.46
11:C:216:ALA:O	11:C:218:LEU:N	2.48	0.46
11:C:478:HIS:HB3	11:C:481:LEU:HG	1.97	0.46
12:E:423:VAL:HG23	12:E:424:PHE:CD1	2.49	0.46
5:r:155:LYS:HD3	7:t:4:LEU:CB	2.45	0.46
12:Y:237:LEU:HD22	12:Y:292:LEU:HD12	1.97	0.46
15:m:9:SER:OG	15:m:10:TYR:N	2.47	0.46
9:w:37:THR:HG23	9:w:40:PHE:H	1.80	0.46
11:n:92:ARG:HH21	11:n:94:GLY:HA2	1.79	0.46
11:X:152:LEU:O	11:X:153:LYS:C	2.59	0.46
11:X:216:ALA:O	11:X:218:LEU:N	2.48	0.46
11:K:92:ARG:HH21	11:K:94:GLY:HA2	1.80	0.46
11:C:382:VAL:HG11	11:C:440:THR:HG21	1.97	0.46
12:F:162:GLY:CA	18:F:501:ANP:O3A	2.61	0.46
14:H:70:ILE:HG23	14:H:71:SER:N	2.31	0.46
12:Z:457:PHE:CE1	12:Z:466:VAL:HG11	2.51	0.46
12:c:162:GLY:CA	18:c:501:ANP:O3A	2.61	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:B:73:VAL:HG12	11:B:75:ILE:HG13	1.98	0.46
12:E:31:PRO:HG3	12:E:37:LEU:HD21	1.98	0.46
11:n:169:ILE:HD11	11:n:326:LEU:HD13	1.97	0.46
11:W:73:VAL:HG12	11:W:75:ILE:HG13	1.98	0.46
12:D:90:GLU:HA	12:D:90:GLU:OE1	2.15	0.46
12:D:340:SER:HB3	12:D:347:ALA:HB2	1.97	0.46
12:E:407:ALA:HA	12:E:410:ILE:HD12	1.98	0.46
13:G:74:ILE:O	13:G:107:ILE:HA	2.15	0.46
11:n:399:TYR:CD1	11:n:423:GLY:HA3	2.51	0.46
11:X:484:GLU:O	11:X:485:ILE:C	2.58	0.46
12:c:30:LEU:HD11	12:c:57:ASN:HA	1.97	0.46
1:6:14:ILE:HG21	1:7:14:ILE:HD13	1.98	0.46
1:Q:69:SER:O	1:Q:73:LEU:HB2	2.15	0.46
12:Y:90:GLU:HA	12:Y:90:GLU:OE1	2.14	0.46
12:Z:346:PRO:HB2	12:Z:348:VAL:HG23	1.98	0.46
11:C:35:ALA:HB1	12:F:53:HIS:O	2.16	0.45
11:C:216:ALA:C	11:C:218:LEU:N	2.70	0.45
12:D:136:THR:HG21	12:D:147:TYR:CD2	2.51	0.45
11:n:391:SER:O	11:n:394:LEU:HB3	2.16	0.45
11:W:260:ARG:HG2	11:W:314:LEU:HD12	1.97	0.45
11:X:478:HIS:HB3	11:X:481:LEU:HG	1.97	0.45
12:Z:336:SER:HB3	12:Z:339:ILE:HG12	1.99	0.45
11:K:391:SER:O	11:K:394:LEU:HB3	2.16	0.45
11:B:190:ARG:HH12	11:B:437:PRO:HB2	1.82	0.45
11:C:152:LEU:O	11:C:153:LYS:C	2.59	0.45
12:D:425:THR:C	12:D:427:ILE:N	2.73	0.45
12:E:152:LYS:HE3	12:E:296:ILE:O	2.17	0.45
12:E:180:GLY:HA2	12:E:249:GLN:OE1	2.16	0.45
12:E:457:PHE:CE1	12:E:466:VAL:HG11	2.51	0.45
12:F:13:VAL:HG23	12:F:74:GLU:HB3	1.97	0.45
13:G:205:VAL:HB	14:H:51:GLN:HE22	1.81	0.45
11:n:363:ILE:O	11:n:366:ALA:HA	2.16	0.45
11:W:173:ARG:O	11:W:174:GLN:HB2	2.17	0.45
12:Z:31:PRO:HG3	12:Z:37:LEU:HD21	1.98	0.45
1:7:39:ARG:O	14:H:44:ASN:O	2.34	0.45
11:C:98:ASP:HB2	11:C:129:SER:O	2.17	0.45
13:G:200:ASP:C	13:G:202:ASP:N	2.72	0.45
1:S:39:ARG:O	14:I:44:ASN:O	2.35	0.45
11:W:156:ASP:O	11:W:381:GLN:NE2	2.49	0.45
11:W:176:GLY:O	11:W:180:VAL:HG23	2.16	0.45
12:Z:407:ALA:HA	12:Z:410:ILE:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:399:TYR:CD1	11:K:423:GLY:HA3	2.51	0.45
14:H:57:VAL:HG12	14:H:58:GLU:N	2.32	0.45
1:L:14:ILE:HD13	1:J:14:ILE:HG21	1.97	0.45
11:n:70:PRO:HD3	12:Z:15:ALA:HB2	1.99	0.45
11:W:190:ARG:HH12	11:W:437:PRO:HB2	1.81	0.45
11:X:343:ASN:O	11:X:347:ILE:HG13	2.16	0.45
12:Z:180:GLY:HA2	12:Z:249:GLN:OE1	2.16	0.45
12:c:473:LEU:C	12:c:475:ALA:N	2.74	0.45
13:j:180:LYS:HE2	13:j:221:ALA:HB2	1.96	0.45
17:v:1001:UNK:O	17:v:1005:UNK:N	2.49	0.45
11:W:110:VAL:O	11:W:234:VAL:HA	2.17	0.45
12:Y:456:ALA:HA	12:Y:469:LYS:HD3	1.98	0.45
2:A:36:LEU:HA	2:A:39:TYR:HD2	1.81	0.45
11:B:363:ILE:C	11:B:364:ARG:HG2	2.41	0.45
12:F:256:ASP:HA	12:F:257:ASN:HA	1.73	0.45
17:h:1001:UNK:O	17:h:1005:UNK:N	2.49	0.45
2:V:36:LEU:HA	2:V:39:TYR:HD2	1.81	0.45
11:n:272:ASP:OD2	11:n:274:SER:CB	2.65	0.45
11:W:139:LEU:N	11:W:140:PRO:CD	2.80	0.45
11:X:98:ASP:HB2	11:X:129:SER:O	2.17	0.45
12:Y:342:LEU:HD23	12:Y:342:LEU:HA	1.77	0.45
12:Z:95:ILE:HB	12:Z:104:ASP:HB3	1.99	0.45
14:l:57:VAL:HG12	14:l:58:GLU:N	2.32	0.45
1:8:68:VAL:HG11	1:9:16:THR:HG21	1.98	0.45
11:K:241:ALA:HB1	11:K:243:PRO:HD2	1.99	0.45
11:B:139:LEU:N	11:B:140:PRO:CD	2.80	0.45
11:B:176:GLY:O	11:B:180:VAL:HG23	2.16	0.45
12:F:163:LYS:H	18:F:501:ANP:PB	2.40	0.45
12:Y:136:THR:HG21	12:Y:147:TYR:CD2	2.51	0.45
12:Z:152:LYS:HE3	12:Z:296:ILE:O	2.17	0.45
12:c:163:LYS:H	18:c:501:ANP:PB	2.40	0.45
1:5:69:SER:O	1:5:73:LEU:HB2	2.15	0.45
2:A:45:ILE:HD11	5:d:138:LEU:HD11	1.99	0.45
11:B:391:SER:O	11:B:393:LYS:N	2.50	0.45
11:B:444:VAL:CG2	11:B:445:PRO:HD3	2.42	0.45
11:C:343:ASN:O	11:C:347:ILE:HG13	2.17	0.45
12:F:134:LEU:HB2	12:F:149:ARG:CG	2.47	0.45
2:V:45:ILE:HD11	5:r:138:LEU:HD11	1.99	0.45
11:B:108:ARG:NH2	11:B:116:PRO:HB3	2.32	0.45
11:C:108:ARG:NH2	11:C:120:LYS:HB2	2.32	0.45
11:C:158:LEU:CD1	11:C:369:VAL:HG22	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:E:39:ILE:HG12	12:E:76:VAL:HG22	1.98	0.45
13:G:205:VAL:HG13	13:G:206:PRO:HD3	1.99	0.45
11:n:103:PRO:C	11:n:105:LEU:N	2.74	0.45
11:W:396:LEU:HA	11:W:399:TYR:HB3	1.98	0.45
11:X:158:LEU:CD1	11:X:369:VAL:HG22	2.46	0.45
12:Z:33:ILE:O	12:Z:34:LEU:HB2	2.17	0.45
12:Z:391:LEU:CB	12:Z:395:GLU:HG3	2.47	0.45
12:c:201:MET:CB	12:c:207:ILE:HD12	2.47	0.45
11:B:173:ARG:O	11:B:174:GLN:HB2	2.17	0.45
11:B:260:ARG:HG2	11:B:314:LEU:HD12	1.97	0.45
11:C:99:VAL:O	11:C:128:ARG:HA	2.17	0.45
12:D:456:ALA:HA	12:D:469:LYS:HD3	1.99	0.45
12:E:143:LEU:HB2	12:E:437:THR:HG22	1.99	0.45
12:E:336:SER:HB3	12:E:339:ILE:HG12	1.99	0.45
12:F:201:MET:HA	12:F:201:MET:CE	2.45	0.45
12:F:201:MET:CB	12:F:207:ILE:HD12	2.47	0.45
5:r:138:LEU:HA	5:r:141:ILE:HG22	1.99	0.45
12:Y:52:GLN:OE1	12:Y:60:ARG:HD2	2.17	0.45
14:l:70:ILE:HG23	14:l:71:SER:N	2.31	0.45
11:K:70:PRO:HD3	12:E:15:ALA:HB2	1.99	0.44
11:K:272:ASP:OD2	11:K:274:SER:CB	2.65	0.44
11:B:110:VAL:O	11:B:234:VAL:HA	2.16	0.44
11:B:270:TYR:O	11:B:272:ASP:HA	2.17	0.44
11:C:241:ALA:HB1	11:C:243:PRO:HD2	1.99	0.44
12:F:10:THR:HG21	12:F:75:LYS:HD3	1.99	0.44
14:H:33:PRO:HD3	14:H:57:VAL:HG22	1.99	0.44
11:W:165:GLN:O	11:W:324:THR:HG23	2.17	0.44
15:m:13:TYR:O	15:m:16:VAL:HG12	2.17	0.44
11:K:242:ALA:N	11:K:243:PRO:CD	2.81	0.44
11:B:147:PRO:HG3	11:B:380:ALA:O	2.17	0.44
11:B:156:ASP:O	11:B:381:GLN:NE2	2.49	0.44
12:E:33:ILE:O	12:E:34:LEU:HB2	2.17	0.44
1:S:40:ASN:ND2	14:l:42:LEU:HB2	2.20	0.44
11:X:108:ARG:NH2	11:X:120:LYS:HB2	2.32	0.44
11:X:504:GLU:O	11:X:505:SER:C	2.60	0.44
12:Y:349:ASP:HA	12:Y:350:PRO:HD2	1.83	0.44
12:Z:143:LEU:HB2	12:Z:437:THR:HG22	1.99	0.44
1:2:21:GLY:HA3	1:3:20:LEU:HA	1.99	0.44
1:5:58:SER:O	1:5:61:THR:OG1	2.29	0.44
11:K:363:ILE:O	11:K:366:ALA:HA	2.16	0.44
12:F:18:GLY:O	12:F:67:THR:OG1	2.28	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:G:214:LEU:O	13:G:218:MET:HB2	2.18	0.44
11:W:279:ALA:O	11:W:282:GLN:HB3	2.18	0.44
12:Y:30:LEU:HD11	12:Y:57:ASN:HA	2.00	0.44
12:c:136:THR:HG21	12:c:147:TYR:CD2	2.53	0.44
13:j:139:THR:HG21	15:m:37:ARG:HA	2.00	0.44
1:1:2:GLN:HE21	1:0:1:MET:HG2	1.82	0.44
1:7:61:THR:HA	1:7:64:PHE:HD2	1.83	0.44
12:D:182:SER:OG	12:D:252:LEU:HB2	2.18	0.44
13:G:154:MET:O	13:G:159:TYR:HE1	2.01	0.44
15:I:13:TYR:O	15:I:16:VAL:HG12	2.17	0.44
1:T:68:VAL:HG11	1:U:16:THR:HG21	1.98	0.44
11:W:270:TYR:O	11:W:272:ASP:HA	2.17	0.44
11:B:37:GLY:HA3	12:E:52:GLN:HG2	2.00	0.44
11:B:488:LYS:HD3	11:B:490:GLU:HB2	1.99	0.44
11:C:364:ARG:HA	11:C:365:PRO:C	2.43	0.44
1:S:40:ASN:CG	14:l:42:LEU:HB3	2.27	0.44
12:Z:138:ILE:HG22	12:Z:140:VAL:HG23	2.00	0.44
13:j:205:VAL:HB	14:l:51:GLN:HE22	1.81	0.44
13:j:214:LEU:O	13:j:218:MET:HB2	2.18	0.44
14:l:33:PRO:HD3	14:l:57:VAL:HG22	1.98	0.44
11:B:279:ALA:O	11:B:282:GLN:HB3	2.18	0.44
11:B:336:VAL:HG13	11:B:353:PHE:CE1	2.53	0.44
12:E:391:LEU:CB	12:E:395:GLU:HG3	2.47	0.44
15:I:32:ALA:O	15:I:33:SER:C	2.61	0.44
11:n:177:LYS:HB2	11:n:177:LYS:HE2	1.81	0.44
11:W:106:LEU:HA	11:W:232:ILE:HG12	1.99	0.44
11:W:336:VAL:HG13	11:W:353:PHE:CE1	2.53	0.44
13:j:78:THR:HB	13:j:79:SER:H	1.52	0.44
11:B:165:GLN:O	11:B:324:THR:HG23	2.17	0.44
12:E:344:ILE:HG23	12:E:415:SER:HB3	1.99	0.44
11:W:391:SER:O	11:W:393:LYS:N	2.50	0.44
11:W:488:LYS:HD3	11:W:490:GLU:HB2	1.99	0.44
12:c:12:LYS:HA	12:c:74:GLU:O	2.18	0.44
12:c:96:ILE:CG2	12:c:97:ASN:N	2.81	0.44
14:l:72:GLY:C	15:m:14:LEU:HD22	2.43	0.44
12:D:30:LEU:HD11	12:D:57:ASN:HA	2.00	0.44
12:D:52:GLN:OE1	12:D:60:ARG:HD2	2.18	0.44
12:D:169:GLU:HG2	12:D:418:PHE:CG	2.53	0.44
12:E:138:ILE:HG22	12:E:140:VAL:HG23	2.00	0.44
12:E:147:TYR:CZ	12:E:153:ILE:HG21	2.53	0.44
12:E:244:ARG:HG3	12:E:303:SER:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:F:237:LEU:HD21	12:F:295:ARG:HB2	1.99	0.44
14:H:48:THR:H	14:H:77:VAL:HB	1.83	0.44
11:n:241:ALA:HB1	11:n:243:PRO:HD2	1.99	0.44
11:W:363:ILE:C	11:W:364:ARG:HG2	2.41	0.44
11:W:421:VAL:O	11:W:425:ARG:HG2	2.18	0.44
11:X:99:VAL:O	11:X:128:ARG:HA	2.17	0.44
12:Y:169:GLU:HG2	12:Y:418:PHE:CG	2.53	0.44
12:Y:321:ALA:HB3	12:Y:322:PRO:CD	2.48	0.44
12:c:13:VAL:HG21	12:c:74:GLU:HB3	2.00	0.44
12:c:134:LEU:HB2	12:c:149:ARG:CG	2.47	0.44
13:j:148:ASP:HA	13:j:151:LEU:HD12	2.00	0.44
14:l:48:THR:H	14:l:77:VAL:HB	1.83	0.44
11:B:270:TYR:HB2	11:B:327:PRO:HA	1.99	0.44
11:C:504:GLU:O	11:C:505:SER:C	2.60	0.44
14:H:72:GLY:C	15:I:14:LEU:HD22	2.43	0.44
1:L:2:GLN:HE21	1:J:1:MET:HG2	1.82	0.44
1:R:14:ILE:HG21	1:S:14:ILE:HD13	1.99	0.44
11:W:270:TYR:HB2	11:W:327:PRO:HA	1.99	0.44
11:X:176:GLY:N	18:X:601:ANP:O3A	2.51	0.44
5:d:138:LEU:HA	5:d:141:ILE:HG22	1.99	0.43
11:B:394:LEU:HA	11:B:397:ALA:HB3	2.00	0.43
12:D:321:ALA:HB3	12:D:322:PRO:CD	2.48	0.43
12:E:346:PRO:HB2	12:E:348:VAL:HG23	1.98	0.43
12:F:326:PHE:C	12:F:328:HIS:H	2.26	0.43
11:X:241:ALA:HB1	11:X:243:PRO:HD2	1.99	0.43
12:Y:162:GLY:HA2	18:Y:501:ANP:H8	2.00	0.43
12:Z:166:PHE:CD1	12:Z:166:PHE:C	2.96	0.43
12:c:326:PHE:C	12:c:328:HIS:H	2.26	0.43
1:7:41:PRO:HG2	14:H:44:ASN:HD22	1.84	0.43
11:K:146:GLU:HB2	11:K:163:ARG:HD2	1.99	0.43
11:K:294:GLU:O	11:K:295:ALA:HB3	2.18	0.43
11:K:446:LEU:HD21	11:K:467:GLU:HA	1.99	0.43
11:B:139:LEU:HD22	12:F:104:ASP:HA	2.00	0.43
11:B:290:PRO:HA	11:B:291:PRO:HD3	1.81	0.43
12:E:95:ILE:HB	12:E:104:ASP:HB3	1.99	0.43
12:F:12:LYS:HA	12:F:74:GLU:O	2.17	0.43
11:n:294:GLU:O	11:n:295:ALA:HB3	2.18	0.43
11:W:488:LYS:HB3	11:W:490:GLU:H	1.83	0.43
12:Z:344:ILE:HG23	12:Z:415:SER:HB3	2.00	0.43
12:c:449:TYR:HD2	12:c:452:ILE:HD12	1.84	0.43
13:j:154:MET:O	13:j:159:TYR:HE1	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:l:30:VAL:HG21	14:l:83:LEU:HD23	2.00	0.43
11:K:217:GLN:HG2	12:D:356:ARG:NH2	2.33	0.43
11:B:139:LEU:N	11:B:140:PRO:HD2	2.33	0.43
11:B:140:PRO:O	11:B:314:LEU:HD23	2.19	0.43
11:C:336:VAL:CG1	11:C:353:PHE:HE1	2.32	0.43
13:G:91:LEU:HD23	13:G:114:ILE:HD13	2.01	0.43
11:n:68:LEU:O	12:Z:15:ALA:HA	2.18	0.43
11:W:139:LEU:N	11:W:140:PRO:HD2	2.33	0.43
12:Y:26:GLU:HB2	12:Y:29:GLU:OE1	2.18	0.43
12:c:10:THR:HG21	12:c:75:LYS:HD3	1.99	0.43
1:2:59:GLU:O	1:2:61:THR:N	2.52	0.43
12:D:26:GLU:HB2	12:D:29:GLU:OE1	2.18	0.43
12:D:162:GLY:HA2	18:D:501:ANP:H8	2.00	0.43
12:F:96:ILE:CG2	12:F:97:ASN:N	2.81	0.43
1:M:21:GLY:HA3	1:N:20:LEU:HA	1.99	0.43
11:n:242:ALA:N	11:n:243:PRO:CD	2.81	0.43
11:n:340:ILE:HB	11:n:341:PRO:HD3	1.99	0.43
11:W:147:PRO:HG3	11:W:380:ALA:O	2.17	0.43
12:Y:182:SER:OG	12:Y:252:LEU:HB2	2.18	0.43
12:Z:27:GLN:HG3	16:o:63:SER:CB	2.48	0.43
12:c:87:VAL:HG21	12:c:242:TYR:CD1	2.54	0.43
2:A:23:LEU:HD23	2:A:26:LEU:HD22	2.00	0.43
3:a:232:TYR:CZ	5:d:173:MET:HE1	2.53	0.43
5:d:129:PRO:HB2	5:d:132:GLU:HG2	2.01	0.43
11:K:34:LEU:O	11:K:86:GLU:HG3	2.19	0.43
11:C:176:GLY:N	18:C:601:ANP:O3A	2.51	0.43
12:E:125:ALA:C	12:E:127:GLN:H	2.26	0.43
12:F:136:THR:HG21	12:F:147:TYR:CD2	2.53	0.43
15:I:14:LEU:H	15:I:14:LEU:HG	1.36	0.43
1:R:58:SER:O	1:R:61:THR:OG1	2.34	0.43
11:W:139:LEU:HD22	12:c:104:ASP:HA	2.00	0.43
12:Z:244:ARG:HG3	12:Z:303:SER:N	2.33	0.43
12:c:34:LEU:HD23	12:c:34:LEU:HA	1.83	0.43
12:c:201:MET:HB2	12:c:207:ILE:HD12	2.00	0.43
12:c:373:LYS:HB3	12:c:445:LEU:HD13	2.01	0.43
3:a:1:SER:OG	3:a:4:ASP:OD2	2.33	0.43
11:K:340:ILE:HB	11:K:341:PRO:HD3	1.99	0.43
11:B:106:LEU:HA	11:B:232:ILE:HG12	1.99	0.43
11:B:421:VAL:O	11:B:425:ARG:HG2	2.18	0.43
12:D:121:PRO:HA	12:D:122:PRO:HD3	1.94	0.43
12:F:373:LYS:HB3	12:F:445:LEU:HD13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:23:LEU:HD23	2:V:26:LEU:HD22	2.00	0.43
11:n:146:GLU:HB2	11:n:163:ARG:HD2	1.99	0.43
11:n:152:LEU:HA	11:n:432:GLN:HE22	1.83	0.43
11:n:402:VAL:HG13	11:n:405:PHE:CD2	2.54	0.43
11:W:140:PRO:O	11:W:314:LEU:HD23	2.19	0.43
11:W:394:LEU:HA	11:W:397:ALA:HB3	2.00	0.43
12:Z:147:TYR:CZ	12:Z:153:ILE:HG21	2.53	0.43
15:m:32:ALA:O	15:m:33:SER:C	2.61	0.43
1:9:68:VAL:HG11	1:0:16:THR:HG21	2.01	0.43
11:K:103:PRO:C	11:K:105:LEU:N	2.74	0.43
11:C:208:VAL:O	11:C:275:LYS:HD3	2.19	0.43
13:G:78:THR:OG1	13:G:114:ILE:HB	2.19	0.43
11:W:37:GLY:HA3	12:Z:52:GLN:HG2	2.00	0.43
12:Z:125:ALA:C	12:Z:127:GLN:H	2.26	0.43
12:c:237:LEU:HD21	12:c:295:ARG:HB2	1.99	0.43
11:C:107:GLY:HA2	11:C:228:MET:O	2.19	0.43
12:E:54:LEU:HD11	12:E:60:ARG:HB2	2.01	0.43
12:F:87:VAL:HG21	12:F:242:TYR:CD1	2.54	0.43
11:n:34:LEU:O	11:n:86:GLU:HG3	2.19	0.43
11:W:54:LEU:HB3	11:W:93:THR:OG1	2.19	0.43
11:W:260:ARG:O	11:W:321:GLY:HA3	2.19	0.43
11:X:208:VAL:O	11:X:275:LYS:HD3	2.19	0.43
12:Y:134:LEU:HD11	12:Y:174:ILE:HD12	2.00	0.43
13:j:73:LEU:HD11	13:j:154:MET:HE2	1.99	0.43
12:F:449:TYR:HD2	12:F:452:ILE:HD12	1.84	0.43
1:S:41:PRO:HG2	14:l:44:ASN:HD22	1.84	0.43
11:n:382:VAL:O	11:n:383:LYS:C	2.62	0.43
11:X:336:VAL:CG1	11:X:353:PHE:HE1	2.31	0.43
12:Z:256:ASP:HA	12:Z:257:ASN:HA	1.69	0.43
3:a:10:THR:HA	3:a:27:THR:HG23	2.01	0.43
4:b:176:VAL:CB	17:h:1010:UNK:CA	2.97	0.43
11:K:49:ILE:HD11	11:K:55:VAL:CG1	2.49	0.43
11:K:68:LEU:O	12:E:15:ALA:HA	2.18	0.43
11:B:188:GLN:HB3	11:B:192:ASN:HD22	1.83	0.43
11:B:488:LYS:HB3	11:B:490:GLU:H	1.83	0.43
12:D:134:LEU:HD11	12:D:174:ILE:HD12	2.00	0.43
12:E:27:GLN:NE2	16:O:63:SER:N	2.61	0.43
12:E:166:PHE:CD1	12:E:166:PHE:C	2.96	0.43
12:F:201:MET:HB2	12:F:207:ILE:HD12	2.00	0.43
13:G:139:THR:HG21	15:I:37:ARG:HA	2.00	0.43
3:p:232:TYR:CZ	5:r:173:MET:HE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:n:237:THR:O	11:n:238:ALA:C	2.62	0.43
11:n:446:LEU:HD21	11:n:467:GLU:HA	2.00	0.43
11:W:108:ARG:NH2	11:W:116:PRO:HB3	2.32	0.43
11:W:444:VAL:CG2	11:W:445:PRO:HD3	2.42	0.43
11:X:166:ARG:NH1	11:X:347:ILE:O	2.52	0.43
1:5:57:LEU:HD13	1:6:55:PHE:HZ	1.83	0.42
11:B:103:PRO:HD3	11:B:258:TRP:CZ2	2.54	0.42
11:B:260:ARG:O	11:B:321:GLY:HA3	2.19	0.42
11:C:222:LEU:CB	11:C:228:MET:HG2	2.49	0.42
12:D:349:ASP:HA	12:D:350:PRO:HD2	1.84	0.42
13:G:54:ASN:CG	14:H:78:GLN:HE21	2.27	0.42
13:G:73:LEU:HD11	13:G:154:MET:HE2	1.99	0.42
13:G:212:TYR:OH	14:H:86:THR:HB	2.19	0.42
11:n:35:ALA:HB3	11:n:42:ARG:HH12	1.84	0.42
11:n:217:GLN:HG2	12:Y:356:ARG:NH2	2.33	0.42
11:n:397:ALA:HA	11:n:400:ARG:NH2	2.34	0.42
12:Y:88:GLY:O	12:Y:243:PHE:CZ	2.72	0.42
12:Z:39:ILE:HD11	12:Z:48:LEU:HD11	2.01	0.42
12:Z:237:LEU:HD21	12:Z:295:ARG:HB2	2.01	0.42
13:j:205:VAL:HG13	13:j:206:PRO:HD3	1.99	0.42
14:l:94:GLU:C	14:l:96:PHE:H	2.27	0.42
11:K:152:LEU:HA	11:K:432:GLN:HE22	1.83	0.42
11:K:471:LEU:HD23	11:K:471:LEU:HA	1.90	0.42
12:D:90:GLU:HB2	12:D:111:SER:HB3	2.02	0.42
12:E:260:ARG:HA	12:E:263:GLN:HB2	2.01	0.42
1:N:65:CYS:SG	1:P:16:THR:OG1	2.68	0.42
3:p:10:THR:HA	3:p:27:THR:HG23	2.01	0.42
11:W:57:PHE:HD1	11:W:61:VAL:O	2.02	0.42
12:Y:64:MET:HE1	12:Y:231:ARG:HB2	2.01	0.42
13:j:78:THR:OG1	13:j:114:ILE:HB	2.18	0.42
11:B:110:VAL:HG12	11:B:116:PRO:HA	2.01	0.42
12:E:244:ARG:HD3	12:E:304:VAL:HG23	2.02	0.42
13:G:147:ALA:O	13:G:151:LEU:HG	2.19	0.42
13:G:148:ASP:HA	13:G:151:LEU:HD12	2.00	0.42
15:I:17:ALA:O	15:I:21:ILE:CB	2.67	0.42
1:M:59:GLU:O	1:M:61:THR:N	2.51	0.42
5:r:129:PRO:HB2	5:r:132:GLU:HG2	2.01	0.42
11:X:107:GLY:HA2	11:X:228:MET:O	2.19	0.42
12:Z:260:ARG:HA	12:Z:263:GLN:HB2	2.01	0.42
12:c:47:VAL:HG21	12:c:99:ILE:HG21	2.01	0.42
1:1:60:ALA:HB2	3:a:222:LEU:HD21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:d:141:ILE:HG23	5:d:142:LYS:HG2	2.01	0.42
11:K:402:VAL:HG13	11:K:405:PHE:CD2	2.54	0.42
11:B:308:LEU:HD12	11:B:347:ILE:HG21	2.01	0.42
13:G:38:LYS:HD2	13:G:169:PRO:HG2	2.01	0.42
1:Q:57:LEU:HD13	1:R:55:PHE:HZ	1.83	0.42
1:S:61:THR:HA	1:S:64:PHE:HD2	1.83	0.42
3:p:1:SER:OG	3:p:4:ASP:OD2	2.33	0.42
7:t:82:TYR:HA	7:t:86:LEU:HB2	2.01	0.42
11:n:53:GLU:OE2	11:n:92:ARG:NE	2.44	0.42
11:n:81:ASP:OD1	11:n:81:ASP:N	2.52	0.42
11:W:425:ARG:HD2	11:W:463:ILE:HD11	2.02	0.42
11:X:166:ARG:HD3	11:X:308:LEU:O	2.20	0.42
11:X:302:TYR:CE1	11:X:306:ARG:HD3	2.54	0.42
11:X:364:ARG:HA	11:X:365:PRO:C	2.43	0.42
12:Y:201:MET:HE3	12:Y:217:LEU:HD21	2.01	0.42
12:Z:298:THR:HG23	12:Z:303:SER:HB3	2.01	0.42
1:7:40:ASN:ND2	14:H:42:LEU:HB2	2.20	0.42
11:K:11:SER:CB	12:D:56:GLU:CD	2.92	0.42
11:K:397:ALA:HA	11:K:400:ARG:NH2	2.34	0.42
11:B:54:LEU:HB3	11:B:93:THR:OG1	2.19	0.42
11:B:249:PRO:HB3	11:B:270:TYR:CD1	2.55	0.42
11:C:166:ARG:HD3	11:C:308:LEU:O	2.19	0.42
12:E:99:ILE:HG13	12:E:101:GLU:HG3	2.02	0.42
12:E:443:ALA:O	12:E:448:LYS:HB2	2.19	0.42
12:F:47:VAL:HG21	12:F:99:ILE:HG21	2.01	0.42
12:F:162:GLY:HA3	18:F:501:ANP:H8	2.02	0.42
13:G:74:ILE:HG23	13:G:165:PHE:HD2	1.85	0.42
13:G:115:LYS:HD3	13:G:129:SER:OG	2.20	0.42
13:G:150:LEU:HD22	13:G:218:MET:HE2	2.01	0.42
14:H:94:GLU:C	14:H:96:PHE:H	2.27	0.42
11:W:110:VAL:HG12	11:W:116:PRO:HA	2.01	0.42
11:W:223:GLU:HG3	11:W:228:MET:HB2	2.01	0.42
11:X:53:GLU:CD	11:X:92:ARG:HH21	2.28	0.42
12:Y:90:GLU:HB2	12:Y:111:SER:HB3	2.02	0.42
12:Z:54:LEU:HD11	12:Z:60:ARG:HB2	2.01	0.42
12:Z:196:ASP:O	12:Z:197:LEU:C	2.63	0.42
12:c:345:TYR:CD1	18:c:501:ANP:C5	3.03	0.42
11:K:391:SER:O	11:K:395:PHE:HD1	2.03	0.42
11:B:57:PHE:HD1	11:B:61:VAL:O	2.02	0.42
11:C:302:TYR:CE1	11:C:306:ARG:HD3	2.54	0.42
12:E:27:GLN:HG3	16:O:63:SER:CB	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:F:224:GLU:HB2	12:F:229:ARG:HG3	2.02	0.42
12:Y:64:MET:HE3	12:Y:228:ALA:HA	2.02	0.42
13:j:91:LEU:HD23	13:j:114:ILE:HD13	2.00	0.42
13:j:212:TYR:OH	14:l:86:THR:HB	2.19	0.42
11:B:223:GLU:HG3	11:B:228:MET:HB2	2.01	0.42
12:D:33:ILE:O	12:D:34:LEU:HB2	2.20	0.42
12:F:417:PRO:HB2	12:F:429:GLY:HA2	2.02	0.42
12:F:422:GLU:C	12:F:424:PHE:H	2.27	0.42
13:G:43:LYS:O	13:G:46:GLU:HB2	2.20	0.42
11:W:483:THR:HA	11:W:486:ARG:NH2	2.35	0.42
12:Z:49:GLU:CD	12:Z:231:ARG:HE	2.28	0.42
12:Z:99:ILE:HG13	12:Z:101:GLU:HG3	2.02	0.42
12:c:184:PHE:CD2	12:c:254:PHE:HB2	2.55	0.42
11:K:237:THR:O	11:K:238:ALA:C	2.62	0.42
12:D:158:GLY:O	12:D:161:VAL:HG22	2.20	0.42
12:E:237:LEU:HD21	12:E:295:ARG:HB2	2.01	0.42
11:n:11:SER:CB	12:Y:56:GLU:CD	2.92	0.42
11:X:54:LEU:O	11:X:93:THR:HB	2.20	0.42
12:c:224:GLU:HB2	12:c:229:ARG:HG3	2.02	0.42
12:c:417:PRO:HB2	12:c:429:GLY:HA2	2.02	0.42
13:j:38:LYS:HD2	13:j:169:PRO:HG2	2.01	0.42
13:j:138:PRO:HB3	13:j:222:MET:HE2	2.02	0.42
11:B:368:ASN:C	11:B:368:ASN:OD1	2.62	0.42
11:C:166:ARG:NH1	11:C:347:ILE:O	2.52	0.42
11:C:174:GLN:HA	18:C:601:ANP:N3B	2.34	0.42
12:D:64:MET:HE1	12:D:231:ARG:HB2	2.01	0.42
15:I:33:SER:HB3	15:I:37:ARG:NH2	2.35	0.42
11:W:308:LEU:HD12	11:W:347:ILE:HG21	2.01	0.42
12:Y:70:LEU:HD23	12:Y:70:LEU:HA	1.93	0.42
12:Z:153:ILE:HA	12:Z:331:ALA:O	2.19	0.42
12:Z:443:ALA:O	12:Z:448:LYS:HB2	2.19	0.42
1:3:14:ILE:HG21	1:4:14:ILE:HG12	2.02	0.42
11:K:382:VAL:O	11:K:383:LYS:C	2.62	0.42
11:B:308:LEU:C	11:B:310:ARG:H	2.27	0.42
11:B:425:ARG:HD2	11:B:463:ILE:HD11	2.02	0.42
11:C:394:LEU:O	11:C:398:GLN:HG3	2.19	0.42
12:D:201:MET:HE3	12:D:217:LEU:HD21	2.01	0.42
12:F:169:GLU:OE1	12:F:420:VAL:HB	2.20	0.42
12:F:184:PHE:CD2	12:F:254:PHE:HB2	2.55	0.42
13:G:191:SER:HA	13:G:192:PRO:HD2	1.73	0.42
1:R:4:VAL:O	1:R:8:LYS:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:41:PRO:CG	14:l:44:ASN:HB2	2.48	0.42
1:U:68:VAL:HG11	1:J:16:THR:HG21	2.01	0.42
11:n:49:ILE:HD11	11:n:55:VAL:CG1	2.49	0.42
11:W:103:PRO:HD3	11:W:258:TRP:CZ2	2.54	0.42
11:X:222:LEU:CB	11:X:228:MET:HG2	2.49	0.42
11:X:394:LEU:O	11:X:398:GLN:HG3	2.20	0.42
12:D:222:MET:C	12:D:224:GLU:H	2.28	0.41
12:E:366:GLU:O	12:E:370:VAL:HG23	2.20	0.41
1:L:60:ALA:HB2	3:p:222:LEU:HD21	2.02	0.41
11:W:188:GLN:HB3	11:W:192:ASN:HD22	1.83	0.41
11:X:292:GLY:N	11:X:296:TYR:O	2.36	0.41
12:Y:89:ARG:HG2	12:Y:92:LEU:CD1	2.50	0.41
12:c:422:GLU:C	12:c:424:PHE:H	2.27	0.41
13:j:74:ILE:HG23	13:j:165:PHE:HD2	1.85	0.41
13:j:147:ALA:O	13:j:151:LEU:HG	2.19	0.41
11:K:142:ARG:HG2	11:K:143:SER:H	1.85	0.41
11:B:242:ALA:HB3	11:B:243:PRO:HD3	2.03	0.41
11:B:350:GLY:C	11:B:351:GLN:HG3	2.45	0.41
11:B:483:THR:HA	11:B:486:ARG:NH2	2.35	0.41
11:C:202:TYR:O	11:C:266:ALA:HA	2.21	0.41
11:C:428:GLN:NE2	11:C:431:LYS:HD2	2.35	0.41
12:D:88:GLY:O	12:D:243:PHE:CZ	2.72	0.41
12:E:49:GLU:CD	12:E:231:ARG:HE	2.28	0.41
1:U:39:ARG:HH12	1:J:39:ARG:HE	1.68	0.41
11:X:428:GLN:NE2	11:X:431:LYS:HD2	2.35	0.41
15:m:10:TYR:C	15:m:12:ALA:N	2.78	0.41
11:K:66:LEU:HD12	11:K:76:VAL:CG1	2.50	0.41
11:B:57:PHE:HB2	11:B:61:VAL:HG13	2.03	0.41
11:B:170:ILE:HD11	11:B:341:PRO:HB3	2.02	0.41
11:B:177:LYS:NZ	11:B:330:GLU:HG3	2.36	0.41
11:C:54:LEU:O	11:C:93:THR:HB	2.20	0.41
11:C:81:ASP:O	11:C:82:ARG:C	2.63	0.41
12:D:427:ILE:HA	12:D:428:PRO:HD3	1.93	0.41
12:E:39:ILE:HD11	12:E:48:LEU:HD11	2.01	0.41
12:E:153:ILE:HA	12:E:331:ALA:O	2.19	0.41
14:H:30:VAL:HG21	14:H:83:LEU:HD23	2.00	0.41
12:c:388:ILE:CD1	12:c:396:LEU:HD11	2.45	0.41
13:j:115:LYS:HD3	13:j:129:SER:OG	2.20	0.41
15:m:33:SER:HB3	15:m:37:ARG:NH2	2.35	0.41
11:C:494:GLU:O	11:C:497:ALA:HB3	2.21	0.41
12:D:25:PHE:O	12:D:57:ASN:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:D:89:ARG:HG2	12:D:92:LEU:CD1	2.50	0.41
12:D:357:LEU:HD13	12:D:362:VAL:HG11	2.03	0.41
15:I:10:TYR:C	15:I:12:ALA:N	2.78	0.41
11:n:142:ARG:HG2	11:n:143:SER:H	1.86	0.41
11:n:455:LEU:HD22	11:n:458:ILE:HD12	2.02	0.41
12:Y:158:GLY:O	12:Y:161:VAL:HG22	2.20	0.41
13:j:150:LEU:HD22	13:j:218:MET:HE2	2.01	0.41
11:K:53:GLU:OE2	11:K:94:GLY:HA2	2.21	0.41
11:K:204:VAL:HB	11:K:268:ILE:HG13	2.02	0.41
11:B:381:GLN:HG2	11:B:382:VAL:N	2.36	0.41
11:B:503:THR:O	11:B:507:VAL:HG23	2.21	0.41
11:C:53:GLU:CD	11:C:92:ARG:HH21	2.28	0.41
11:C:202:TYR:O	11:C:267:LEU:N	2.53	0.41
15:I:8:MET:N	15:I:16:VAL:HB	2.35	0.41
11:W:177:LYS:NZ	11:W:330:GLU:HG3	2.36	0.41
11:W:308:LEU:C	11:W:310:ARG:H	2.27	0.41
11:W:350:GLY:C	11:W:351:GLN:HG3	2.45	0.41
11:W:368:ASN:OD1	11:W:368:ASN:C	2.62	0.41
12:Y:25:PHE:O	12:Y:57:ASN:HB3	2.20	0.41
12:Y:33:ILE:O	12:Y:34:LEU:HB2	2.20	0.41
12:c:224:GLU:HB3	12:c:228:ALA:HB3	2.02	0.41
12:c:282:GLN:HA	12:c:283:PRO:HD3	1.78	0.41
13:j:54:ASN:CG	14:l:78:GLN:HE21	2.27	0.41
15:m:17:ALA:O	15:m:21:ILE:CB	2.67	0.41
11:K:110:VAL:HA	11:K:115:ASN:O	2.21	0.41
11:K:381:GLN:O	11:K:382:VAL:C	2.64	0.41
11:K:455:LEU:HD22	11:K:458:ILE:HD12	2.02	0.41
11:B:207:ALA:HB3	11:B:235:ALA:CB	2.51	0.41
11:C:223:GLU:C	11:C:225:HIS:N	2.78	0.41
12:E:196:ASP:O	12:E:197:LEU:C	2.63	0.41
12:E:298:THR:HG23	12:E:303:SER:HB3	2.01	0.41
12:F:345:TYR:CD1	18:F:501:ANP:C5	3.03	0.41
14:H:70:ILE:HG23	14:H:72:GLY:N	2.34	0.41
1:N:21:GLY:HA3	1:P:20:LEU:HB2	2.02	0.41
1:N:33:LEU:HA	1:P:34:ILE:HG21	2.03	0.41
4:q:176:VAL:CB	17:v:1010:UNK:CA	2.97	0.41
11:n:204:VAL:HB	11:n:268:ILE:HG13	2.03	0.41
11:n:329:ILE:HD13	11:n:329:ILE:HA	1.98	0.41
11:W:96:ILE:O	11:W:97:VAL:C	2.64	0.41
11:W:381:GLN:HG2	11:W:382:VAL:N	2.36	0.41
11:X:212:ARG:HG3	11:X:237:THR:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Y:241:GLU:OE2	12:Y:295:ARG:HB3	2.21	0.41
13:j:55:ALA:HA	13:j:193:SER:HB2	2.03	0.41
14:l:22:TYR:HE2	14:l:68:PHE:CZ	2.39	0.41
1:3:33:LEU:HA	1:4:34:ILE:HG21	2.02	0.41
12:F:224:GLU:HB3	12:F:228:ALA:HB3	2.02	0.41
1:Q:58:SER:O	1:Q:61:THR:OG1	2.29	0.41
11:n:391:SER:O	11:n:395:PHE:HD1	2.03	0.41
11:W:242:ALA:HB3	11:W:243:PRO:HD3	2.03	0.41
12:c:86:PRO:O	12:c:91:THR:HG21	2.21	0.41
13:j:43:LYS:O	13:j:46:GLU:HB2	2.20	0.41
1:6:4:VAL:O	1:6:8:LYS:HB2	2.20	0.41
7:f:82:TYR:HA	7:f:86:LEU:HB2	2.01	0.41
11:B:64:MET:HG2	11:B:65:ALA:N	2.36	0.41
11:C:300:VAL:O	11:C:303:LEU:HB3	2.21	0.41
12:F:85:VAL:HG12	12:F:100:GLY:HA3	2.03	0.41
11:X:68:LEU:O	12:Y:15:ALA:HA	2.21	0.41
12:Z:26:GLU:O	12:Z:29:GLU:HB2	2.21	0.41
12:Z:187:VAL:HG11	12:Z:261:PHE:HB2	2.03	0.41
12:c:162:GLY:HA3	18:c:501:ANP:H8	2.02	0.41
12:c:419:ALA:O	12:c:422:GLU:HB2	2.21	0.41
13:j:150:LEU:O	13:j:156:ALA:HB2	2.20	0.41
13:j:152:SER:HB3	13:j:153:VAL:H	1.70	0.41
11:K:35:ALA:HB3	11:K:42:ARG:HH12	1.84	0.41
11:K:82:ARG:HG3	12:D:33:ILE:O	2.21	0.41
11:C:335:ASP:OD2	11:C:338:ALA:HB2	2.21	0.41
11:C:358:LEU:HD23	11:C:358:LEU:HA	1.93	0.41
12:D:98:VAL:HG23	12:D:232:VAL:HA	2.03	0.41
12:D:154:GLY:HA3	12:D:329:LEU:HD13	2.02	0.41
12:D:241:GLU:OE2	12:D:295:ARG:HB3	2.21	0.41
12:D:356:ARG:CG	12:D:357:LEU:HD23	2.51	0.41
12:D:458:TYR:CZ	12:D:459:MET:HE2	2.56	0.41
12:E:187:VAL:HG11	12:E:261:PHE:HB2	2.03	0.41
12:E:237:LEU:HD21	12:E:295:ARG:HD3	2.03	0.41
12:F:13:VAL:HG21	12:F:74:GLU:HB3	2.00	0.41
13:G:43:LYS:HA	13:G:46:GLU:HG2	2.03	0.41
13:G:55:ALA:HA	13:G:193:SER:HB2	2.03	0.41
13:G:150:LEU:O	13:G:156:ALA:HB2	2.20	0.41
13:G:197:PHE:C	13:G:199:ILE:H	2.29	0.41
14:H:22:TYR:HE2	14:H:68:PHE:CZ	2.39	0.41
1:M:72:LEU:HD23	1:M:72:LEU:HA	1.94	0.41
11:n:377:GLY:O	11:n:378:SER:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:W:57:PHE:HB2	11:W:61:VAL:HG13	2.03	0.41
11:W:249:PRO:HB3	11:W:270:TYR:CD1	2.55	0.41
11:X:81:ASP:O	11:X:82:ARG:C	2.63	0.41
11:X:174:GLN:HA	18:X:601:ANP:N3B	2.34	0.41
12:Y:222:MET:C	12:Y:224:GLU:H	2.28	0.41
12:Z:91:THR:HG22	12:Z:109:ILE:HG21	2.03	0.41
12:Z:244:ARG:HD3	12:Z:304:VAL:HG23	2.02	0.41
12:c:277:SER:HB3	12:c:281:TYR:O	2.21	0.41
13:j:191:SER:HA	13:j:192:PRO:HD2	1.73	0.41
11:K:109:VAL:HG22	11:K:233:ILE:HG13	2.02	0.41
11:B:96:ILE:O	11:B:97:VAL:C	2.64	0.41
11:B:383:LYS:HD2	11:B:490:GLU:HG2	2.03	0.41
11:C:212:ARG:HG3	11:C:237:THR:HG21	2.03	0.41
12:E:95:ILE:HD11	12:E:198:TYR:CD1	2.56	0.41
12:E:119:ALA:HB3	12:E:295:ARG:HH21	1.86	0.41
12:F:86:PRO:O	12:F:91:THR:HG21	2.21	0.41
12:F:247:GLU:O	12:F:249:GLN:NE2	2.41	0.41
12:F:277:SER:OG	12:F:278:ALA:N	2.52	0.41
12:F:382:LYS:O	12:F:385:GLN:HG2	2.21	0.41
12:F:449:TYR:HD2	12:F:452:ILE:CD1	2.34	0.41
13:G:44:MET:CE	14:H:86:THR:HG22	2.39	0.41
13:G:78:THR:HB	13:G:79:SER:H	1.52	0.41
13:G:138:PRO:HB3	13:G:222:MET:HE2	2.02	0.41
11:n:53:GLU:OE2	11:n:94:GLY:HA2	2.20	0.41
11:n:381:GLN:O	11:n:382:VAL:C	2.64	0.41
11:W:503:THR:O	11:W:507:VAL:HG23	2.21	0.41
11:X:202:TYR:O	11:X:266:ALA:HA	2.21	0.41
12:Z:366:GLU:O	12:Z:370:VAL:HG23	2.20	0.41
13:j:197:PHE:C	13:j:199:ILE:H	2.29	0.41
1:7:41:PRO:CG	14:H:44:ASN:HB2	2.48	0.40
11:K:141:ARG:NH1	11:K:312:ALA:HB2	2.36	0.40
12:D:155:LEU:HB2	12:D:309:ALA:HA	2.03	0.40
13:G:203:ALA:O	13:G:204:ASN:C	2.64	0.40
15:I:10:TYR:CA	15:I:13:TYR:HB2	2.41	0.40
1:N:14:ILE:HG21	1:P:14:ILE:HG12	2.03	0.40
3:p:32:TYR:HD1	3:p:32:TYR:HA	1.80	0.40
5:r:141:ILE:HG23	5:r:142:LYS:HG2	2.01	0.40
11:n:109:VAL:HG22	11:n:233:ILE:HG13	2.02	0.40
11:n:110:VAL:HA	11:n:115:ASN:O	2.21	0.40
11:X:110:VAL:HB	11:X:114:GLY:HA2	2.03	0.40
11:X:300:VAL:O	11:X:303:LEU:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:X:411:ASP:OD1	11:X:411:ASP:N	2.54	0.40
12:Y:154:GLY:HA3	12:Y:329:LEU:HD13	2.02	0.40
12:Y:155:LEU:HB2	12:Y:309:ALA:HA	2.03	0.40
12:Y:244:ARG:HD3	12:Y:304:VAL:HG23	2.03	0.40
12:Z:120:ASP:HA	12:Z:121:PRO:HD2	1.88	0.40
1:6:58:SER:O	1:6:61:THR:OG1	2.34	0.40
11:K:52:GLU:HG2	11:K:64:MET:HE2	2.04	0.40
12:E:26:GLU:O	12:E:29:GLU:HB2	2.21	0.40
12:F:277:SER:HB3	12:F:281:TYR:O	2.21	0.40
11:n:141:ARG:NH1	11:n:312:ALA:HB2	2.36	0.40
11:W:355:GLU:HB3	11:W:358:LEU:HD12	2.03	0.40
12:Z:51:ALA:O	12:Z:52:GLN:HG3	2.21	0.40
12:Z:174:ILE:HD13	12:Z:174:ILE:HA	1.78	0.40
11:K:35:ALA:HB1	12:D:53:HIS:O	2.21	0.40
12:D:90:GLU:HG3	12:D:110:LYS:O	2.21	0.40
12:D:257:ASN:OD1	12:D:259:PHE:HB3	2.22	0.40
12:F:419:ALA:O	12:F:422:GLU:HB2	2.21	0.40
14:H:14:PHE:HD1	14:H:85:VAL:O	2.05	0.40
11:n:82:ARG:HG3	12:Y:33:ILE:O	2.21	0.40
11:n:246:TYR:O	11:n:276:GLN:NE2	2.51	0.40
11:W:207:ALA:HB3	11:W:235:ALA:CB	2.51	0.40
11:X:202:TYR:O	11:X:267:LEU:N	2.53	0.40
11:X:494:GLU:O	11:X:497:ALA:HB3	2.21	0.40
12:Y:74:GLU:HG3	12:Y:75:LYS:N	2.36	0.40
12:Z:95:ILE:HD11	12:Z:198:TYR:CD1	2.56	0.40
12:c:277:SER:OG	12:c:278:ALA:N	2.52	0.40
1:9:39:ARG:HH12	1:0:39:ARG:HE	1.68	0.40
11:C:68:LEU:O	12:D:15:ALA:HA	2.21	0.40
12:D:64:MET:HE3	12:D:228:ALA:HA	2.02	0.40
12:D:244:ARG:HD3	12:D:304:VAL:HG23	2.03	0.40
12:F:91:THR:HG22	12:F:109:ILE:HG21	2.03	0.40
12:Y:98:VAL:HG23	12:Y:232:VAL:HA	2.03	0.40
12:Y:121:PRO:HA	12:Y:122:PRO:HD3	1.94	0.40
12:Y:356:ARG:CG	12:Y:357:LEU:HD23	2.51	0.40
12:Z:112:LYS:HE2	12:Z:112:LYS:HB3	1.94	0.40
12:c:117:ILE:HG22	12:c:235:THR:HA	2.03	0.40
13:j:203:ALA:O	13:j:204:ASN:C	2.64	0.40
3:a:186:LEU:HD12	3:a:186:LEU:HA	1.95	0.40
3:a:223:GLU:HA	3:a:226:ILE:HG22	2.04	0.40
11:K:355:GLU:HB2	11:K:358:LEU:HD12	2.04	0.40
11:C:411:ASP:N	11:C:411:ASP:OD1	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:F:215:VAL:HG22	12:F:216:ALA:H	1.86	0.40
5:r:157:LYS:CD	7:t:8:LYS:CB	3.00	0.40
11:n:35:ALA:HB1	12:Y:53:HIS:O	2.21	0.40
11:n:182:LEU:HD21	11:n:221:THR:HG21	2.04	0.40
11:n:237:THR:O	11:n:239:SER:N	2.55	0.40
11:W:170:ILE:HD11	11:W:341:PRO:HB3	2.02	0.40
11:W:383:LYS:HD2	11:W:490:GLU:HG2	2.04	0.40
11:X:197:GLU:OE2	11:X:202:TYR:OH	2.35	0.40
12:Z:27:GLN:NE2	16:o:63:SER:N	2.61	0.40
12:Z:72:ARG:HE	12:Z:72:ARG:HB2	1.69	0.40
12:Z:102:PRO:HD3	12:Z:109:ILE:HD12	2.04	0.40
12:Z:168:GLN:HE21	12:Z:201:MET:CG	2.35	0.40
12:Z:397:SER:O	12:Z:401:LYS:HG2	2.22	0.40
12:c:449:TYR:HD2	12:c:452:ILE:CD1	2.34	0.40
15:m:8:MET:N	15:m:16:VAL:HB	2.35	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 PDB entries followed by that with respect to all EM entries.

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	0	73/76 (96%)	73 (100%)	0	0	100	100
1	1	73/76 (96%)	71 (97%)	2 (3%)	0	100	100
1	2	73/76 (96%)	71 (97%)	2 (3%)	0	100	100
1	3	72/76 (95%)	72 (100%)	0	0	100	100
1	4	73/76 (96%)	73 (100%)	0	0	100	100
1	5	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
1	6	72/76 (95%)	72 (100%)	0	0	100	100
1	7	71/76 (93%)	71 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	8	73/76 (96%)	73 (100%)	0	0	100	100
1	9	72/76 (95%)	70 (97%)	2 (3%)	0	100	100
1	J	73/76 (96%)	73 (100%)	0	0	100	100
1	L	73/76 (96%)	71 (97%)	2 (3%)	0	100	100
1	M	73/76 (96%)	71 (97%)	2 (3%)	0	100	100
1	N	72/76 (95%)	72 (100%)	0	0	100	100
1	P	73/76 (96%)	73 (100%)	0	0	100	100
1	Q	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
1	R	72/76 (95%)	72 (100%)	0	0	100	100
1	S	71/76 (93%)	71 (100%)	0	0	100	100
1	T	73/76 (96%)	73 (100%)	0	0	100	100
1	U	72/76 (95%)	70 (97%)	2 (3%)	0	100	100
2	A	46/48 (96%)	43 (94%)	2 (4%)	1 (2%)	5	30
2	V	46/48 (96%)	43 (94%)	2 (4%)	1 (2%)	5	30
3	a	247/249 (99%)	228 (92%)	19 (8%)	0	100	100
3	p	247/249 (99%)	228 (92%)	19 (8%)	0	100	100
4	b	196/209 (94%)	186 (95%)	6 (3%)	4 (2%)	6	32
4	q	196/209 (94%)	186 (95%)	6 (3%)	4 (2%)	6	32
5	d	153/173 (88%)	145 (95%)	7 (5%)	1 (1%)	18	51
5	r	153/173 (88%)	145 (95%)	7 (5%)	1 (1%)	18	51
7	f	80/95 (84%)	70 (88%)	9 (11%)	1 (1%)	9	39
7	t	80/95 (84%)	70 (88%)	9 (11%)	1 (1%)	9	39
9	i	57/59 (97%)	50 (88%)	7 (12%)	0	100	100
9	w	57/59 (97%)	50 (88%)	7 (12%)	0	100	100
10	k	22/68 (32%)	19 (86%)	3 (14%)	0	100	100
10	x	22/68 (32%)	19 (86%)	3 (14%)	0	100	100
11	B	486/510 (95%)	439 (90%)	45 (9%)	2 (0%)	30	61
11	C	496/510 (97%)	449 (90%)	44 (9%)	3 (1%)	21	54
11	K	495/510 (97%)	434 (88%)	56 (11%)	5 (1%)	12	45
11	W	486/510 (95%)	439 (90%)	45 (9%)	2 (0%)	30	61
11	X	496/510 (97%)	449 (90%)	44 (9%)	3 (1%)	21	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	n	495/510 (97%)	434 (88%)	56 (11%)	5 (1%)	12	45
12	D	468/478 (98%)	429 (92%)	37 (8%)	2 (0%)	30	61
12	E	466/478 (98%)	424 (91%)	36 (8%)	6 (1%)	9	39
12	F	467/478 (98%)	417 (89%)	42 (9%)	8 (2%)	7	35
12	Y	468/478 (98%)	429 (92%)	37 (8%)	2 (0%)	30	61
12	Z	466/478 (98%)	424 (91%)	36 (8%)	6 (1%)	9	39
12	c	467/478 (98%)	417 (89%)	42 (9%)	8 (2%)	7	35
13	G	261/278 (94%)	229 (88%)	25 (10%)	7 (3%)	4	27
13	j	261/278 (94%)	230 (88%)	24 (9%)	7 (3%)	4	27
14	H	109/138 (79%)	89 (82%)	15 (14%)	5 (5%)	2	17
14	l	109/138 (79%)	89 (82%)	15 (14%)	5 (5%)	2	17
15	I	42/61 (69%)	27 (64%)	9 (21%)	6 (14%)	0	3
15	m	42/61 (69%)	27 (64%)	9 (21%)	6 (14%)	0	3
16	O	157/195 (80%)	126 (80%)	24 (15%)	7 (4%)	2	17
16	o	157/195 (80%)	126 (80%)	24 (15%)	7 (4%)	2	17
All	All	9946/10594 (94%)	9045 (91%)	785 (8%)	116 (1%)	13	41

All (116) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	b	187	PRO
7	f	14	ASN
12	D	29	GLU
12	F	28	SER
13	G	152	SER
13	G	202	ASP
13	G	204	ASN
15	I	9	SER
15	I	33	SER
15	I	55	GLU
15	I	56	PRO
16	O	51	PRO
16	O	127	GLU
4	q	187	PRO
7	t	14	ASN
12	Y	29	GLU
12	Z	474	ALA

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Mol	Chain	Res	Type
12	c	28	SER
13	j	152	SER
13	j	202	ASP
13	j	204	ASN
15	m	9	SER
15	m	33	SER
15	m	55	GLU
15	m	56	PRO
16	o	51	PRO
16	o	127	GLU
5	d	50	PRO
11	K	7	PRO
11	C	238	ALA
12	E	123	SER
12	E	474	ALA
12	F	43	GLN
12	F	423	VAL
13	G	203	ALA
14	H	14	PHE
15	I	32	ALA
16	O	131	PRO
5	r	50	PRO
11	n	7	PRO
11	X	238	ALA
12	Z	123	SER
12	c	43	GLN
12	c	423	VAL
13	j	203	ALA
14	l	14	PHE
15	m	32	ALA
16	o	131	PRO
11	K	11	SER
11	K	23	ASP
11	B	392	LEU
12	D	28	SER
12	E	353	SER
14	H	43	ALA
14	H	93	LEU
16	O	14	GLY
11	n	11	SER
11	n	23	ASP
11	W	392	LEU

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Mol	Chain	Res	Type
12	Y	28	SER
12	Z	353	SER
14	l	43	ALA
14	l	93	LEU
16	o	14	GLY
11	K	238	ALA
12	E	126	GLU
12	F	279	VAL
12	F	327	ALA
13	G	192	PRO
13	G	201	THR
16	O	11	ARG
16	O	128	PRO
11	n	229	LYS
11	n	238	ALA
12	Z	126	GLU
12	c	279	VAL
12	c	327	ALA
13	j	192	PRO
13	j	201	THR
16	o	11	ARG
16	o	128	PRO
11	K	229	LYS
11	B	448	TYR
11	C	505	SER
12	F	474	ALA
13	G	78	THR
16	O	50	ASN
11	W	448	TYR
11	X	505	SER
12	c	326	PHE
12	c	474	ALA
13	j	78	THR
16	o	50	ASN
11	C	339	TYR
12	F	326	PHE
14	H	33	PRO
15	I	30	GLN
11	X	339	TYR
14	l	33	PRO
15	m	30	GLN
12	E	461	GLY

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Mol	Chain	Res	Type
12	Z	461	GLY
4	b	186	ASN
4	q	186	ASN
4	b	10	ASP
4	q	10	ASP
2	A	6	PRO
4	b	23	PRO
12	E	141	VAL
12	F	248	GLY
14	H	54	PRO
2	V	6	PRO
4	q	23	PRO
12	Z	141	VAL
12	c	248	GLY
14	l	54	PRO

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 PDB entries followed by that with respect to all EM entries.

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	0	55/56 (98%)	55 (100%)	0	100	100
1	1	55/56 (98%)	54 (98%)	1 (2%)	51	68
1	2	55/56 (98%)	55 (100%)	0	100	100
1	3	54/56 (96%)	54 (100%)	0	100	100
1	4	55/56 (98%)	54 (98%)	1 (2%)	51	68
1	5	55/56 (98%)	53 (96%)	2 (4%)	31	56
1	6	54/56 (96%)	54 (100%)	0	100	100
1	7	54/56 (96%)	54 (100%)	0	100	100
1	8	55/56 (98%)	55 (100%)	0	100	100
1	9	54/56 (96%)	54 (100%)	0	100	100
1	J	55/56 (98%)	55 (100%)	0	100	100
1	L	55/56 (98%)	54 (98%)	1 (2%)	51	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	55/56 (98%)	55 (100%)	0	100	100
1	N	54/56 (96%)	54 (100%)	0	100	100
1	P	55/56 (98%)	54 (98%)	1 (2%)	51	68
1	Q	55/56 (98%)	53 (96%)	2 (4%)	31	56
1	R	54/56 (96%)	54 (100%)	0	100	100
1	S	54/56 (96%)	54 (100%)	0	100	100
1	T	55/56 (98%)	55 (100%)	0	100	100
1	U	54/56 (96%)	54 (100%)	0	100	100
2	A	47/47 (100%)	47 (100%)	0	100	100
2	V	47/47 (100%)	47 (100%)	0	100	100
3	a	217/217 (100%)	215 (99%)	2 (1%)	70	76
3	p	217/217 (100%)	215 (99%)	2 (1%)	70	76
4	b	48/182 (26%)	48 (100%)	0	100	100
4	q	48/182 (26%)	48 (100%)	0	100	100
5	d	42/158 (27%)	41 (98%)	1 (2%)	43	63
5	r	42/158 (27%)	41 (98%)	1 (2%)	43	63
7	f	46/76 (60%)	46 (100%)	0	100	100
7	t	46/76 (60%)	46 (100%)	0	100	100
9	i	49/49 (100%)	49 (100%)	0	100	100
9	w	49/49 (100%)	49 (100%)	0	100	100
10	k	18/57 (32%)	18 (100%)	0	100	100
10	x	18/57 (32%)	18 (100%)	0	100	100
11	B	384/412 (93%)	345 (90%)	39 (10%)	7	30
11	C	384/412 (93%)	349 (91%)	35 (9%)	9	33
11	K	384/412 (93%)	359 (94%)	25 (6%)	15	43
11	W	384/412 (93%)	345 (90%)	39 (10%)	7	30
11	X	384/412 (93%)	349 (91%)	35 (9%)	9	33
11	n	384/412 (93%)	359 (94%)	25 (6%)	15	43
12	D	380/384 (99%)	350 (92%)	30 (8%)	11	37
12	E	378/384 (98%)	355 (94%)	23 (6%)	17	45
12	F	379/384 (99%)	352 (93%)	27 (7%)	13	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	Y	380/384 (99%)	350 (92%)	30 (8%)	11	37
12	Z	378/384 (98%)	355 (94%)	23 (6%)	17	45
12	c	379/384 (99%)	352 (93%)	27 (7%)	13	40
13	G	218/236 (92%)	185 (85%)	33 (15%)	3	17
13	j	218/236 (92%)	185 (85%)	33 (15%)	3	17
14	H	54/112 (48%)	41 (76%)	13 (24%)	1	5
14	l	54/112 (48%)	41 (76%)	13 (24%)	1	5
15	I	23/48 (48%)	19 (83%)	4 (17%)	2	12
15	m	23/48 (48%)	19 (83%)	4 (17%)	2	12
All	All	7194/8260 (87%)	6722 (93%)	472 (7%)	17	43

All (472) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	17	ILE
1	4	34	ILE
1	5	28	ILE
1	5	57	LEU
3	a	34	ILE
3	a	46	LEU
5	d	173	MET
11	K	90	VAL
11	K	97	VAL
11	K	101	VAL
11	K	143	SER
11	K	173	ARG
11	K	206	VAL
11	K	219	VAL
11	K	221	THR
11	K	239	SER
11	K	245	GLN
11	K	251	THR
11	K	267	LEU
11	K	276	GLN
11	K	288	ARG
11	K	318	GLU
11	K	322	SER
11	K	329	ILE
11	K	330	GLU

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Mol	Chain	Res	Type
11	K	364	ARG
11	K	378	SER
11	K	412	LEU
11	K	480	GLU
11	K	481	LEU
11	K	492	SER
11	K	501	SER
11	B	40	ILE
11	B	50	GLN
11	B	54	LEU
11	B	61	VAL
11	B	80	SER
11	B	82	ARG
11	B	83	LEU
11	B	89	LEU
11	B	93	THR
11	B	97	VAL
11	B	99	VAL
11	B	109	VAL
11	B	129	SER
11	B	206	VAL
11	B	218	LEU
11	B	219	VAL
11	B	221	THR
11	B	232	ILE
11	B	233	ILE
11	B	267	LEU
11	B	274	SER
11	B	278	VAL
11	B	314	LEU
11	B	318	GLU
11	B	336	VAL
11	B	348	THR
11	B	351	GLN
11	B	369	VAL
11	B	373	VAL
11	B	378	SER
11	B	416	THR
11	B	427	THR
11	B	444	VAL
11	B	451	VAL
11	B	460	LEU

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Mol	Chain	Res	Type
11	B	471	LEU
11	B	480	GLU
11	B	486	ARG
11	B	504	GLU
11	C	30	THR
11	C	54	LEU
11	C	68	LEU
11	C	89	LEU
11	C	97	VAL
11	C	99	VAL
11	C	105	LEU
11	C	133	VAL
11	C	138	ILE
11	C	142	ARG
11	C	159	VAL
11	C	165	GLN
11	C	210	GLN
11	C	221	THR
11	C	246	TYR
11	C	254	SER
11	C	274	SER
11	C	293	ARG
11	C	337	SER
11	C	351	GLN
11	C	382	VAL
11	C	383	LYS
11	C	385	LEU
11	C	394	LEU
11	C	416	THR
11	C	458	ILE
11	C	468	SER
11	C	476	SER
11	C	480	GLU
11	C	487	GLU
11	C	495	LEU
11	C	498	SER
11	C	501	SER
11	C	503	THR
11	C	509	THR
12	D	9	ILE
12	D	26	GLU
12	D	29	GLU

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Mol	Chain	Res	Type
12	D	74	GLU
12	D	77	LEU
12	D	167	ILE
12	D	183	VAL
12	D	204	THR
12	D	206	VAL
12	D	214	LYS
12	D	234	LEU
12	D	249	GLN
12	D	251	VAL
12	D	255	ILE
12	D	268	VAL
12	D	291	LEU
12	D	304	VAL
12	D	329	LEU
12	D	332	THR
12	D	341	GLU
12	D	357	LEU
12	D	359	ASP
12	D	374	VAL
12	D	396	LEU
12	D	397	SER
12	D	402	LEU
12	D	410	ILE
12	D	420	VAL
12	D	423	VAL
12	D	464	GLU
12	E	20	ILE
12	E	128	SER
12	E	129	THR
12	E	140	VAL
12	E	165	VAL
12	E	174	ILE
12	E	190	ARG
12	E	210	GLU
12	E	232	VAL
12	E	294	GLU
12	E	298	THR
12	E	299	THR
12	E	324	THR
12	E	352	ASP
12	E	357	LEU

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Mol	Chain	Res	Type
12	E	359	ASP
12	E	373	LYS
12	E	376	GLU
12	E	380	THR
12	E	406	ARG
12	E	435	LYS
12	E	446	GLU
12	E	464	GLU
12	F	58	THR
12	F	87	VAL
12	F	98	VAL
12	F	140	VAL
12	F	163	LYS
12	F	165	VAL
12	F	167	ILE
12	F	182	SER
12	F	201	MET
12	F	208	ASN
12	F	232	VAL
12	F	251	VAL
12	F	261	PHE
12	F	279	VAL
12	F	303	SER
12	F	305	THR
12	F	318	THR
12	F	324	THR
12	F	354	LYS
12	F	355	SER
12	F	357	LEU
12	F	388	ILE
12	F	420	VAL
12	F	423	VAL
12	F	427	ILE
12	F	434	LEU
12	F	467	VAL
13	G	2	THR
13	G	3	LEU
13	G	4	LYS
13	G	16	ILE
13	G	17	GLU
13	G	19	ILE
13	G	21	LYS

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Mol	Chain	Res	Type
13	G	26	VAL
13	G	38	LYS
13	G	78	THR
13	G	121	THR
13	G	130	ILE
13	G	143	SER
13	G	145	LEU
13	G	148	ASP
13	G	152	SER
13	G	155	LYS
13	G	164	ILE
13	G	173	LEU
13	G	196	LYS
13	G	205	VAL
13	G	216	ASN
13	G	218	MET
13	G	231	SER
13	G	235	ASN
13	G	248	ILE
13	G	254	LEU
13	G	264	THR
13	G	267	LEU
13	G	269	ASP
13	G	271	ILE
13	G	272	THR
13	G	276	SER
14	H	12	LEU
14	H	19	GLU
14	H	21	LEU
14	H	27	VAL
14	H	29	GLN
14	H	30	VAL
14	H	42	LEU
14	H	46	VAL
14	H	48	THR
14	H	49	VAL
14	H	60	MET
14	H	70	ILE
14	H	86	THR
15	I	14	LEU
15	I	27	THR
15	I	31	THR

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Mol	Chain	Res	Type
15	I	34	VAL
1	L	17	ILE
1	P	34	ILE
1	Q	28	ILE
1	Q	57	LEU
3	p	34	ILE
3	p	46	LEU
5	r	173	MET
11	n	90	VAL
11	n	97	VAL
11	n	101	VAL
11	n	143	SER
11	n	173	ARG
11	n	206	VAL
11	n	219	VAL
11	n	221	THR
11	n	239	SER
11	n	245	GLN
11	n	251	THR
11	n	267	LEU
11	n	276	GLN
11	n	288	ARG
11	n	318	GLU
11	n	322	SER
11	n	329	ILE
11	n	330	GLU
11	n	364	ARG
11	n	378	SER
11	n	412	LEU
11	n	480	GLU
11	n	481	LEU
11	n	492	SER
11	n	501	SER
11	W	40	ILE
11	W	50	GLN
11	W	54	LEU
11	W	61	VAL
11	W	80	SER
11	W	82	ARG
11	W	83	LEU
11	W	89	LEU
11	W	93	THR

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Mol	Chain	Res	Type
11	W	97	VAL
11	W	99	VAL
11	W	109	VAL
11	W	129	SER
11	W	206	VAL
11	W	218	LEU
11	W	219	VAL
11	W	221	THR
11	W	232	ILE
11	W	233	ILE
11	W	267	LEU
11	W	274	SER
11	W	278	VAL
11	W	314	LEU
11	W	318	GLU
11	W	336	VAL
11	W	348	THR
11	W	351	GLN
11	W	369	VAL
11	W	373	VAL
11	W	378	SER
11	W	416	THR
11	W	427	THR
11	W	444	VAL
11	W	451	VAL
11	W	460	LEU
11	W	471	LEU
11	W	480	GLU
11	W	486	ARG
11	W	504	GLU
11	X	30	THR
11	X	54	LEU
11	X	68	LEU
11	X	89	LEU
11	X	97	VAL
11	X	99	VAL
11	X	105	LEU
11	X	133	VAL
11	X	138	ILE
11	X	142	ARG
11	X	159	VAL
11	X	165	GLN

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Mol	Chain	Res	Type
11	X	210	GLN
11	X	221	THR
11	X	246	TYR
11	X	254	SER
11	X	274	SER
11	X	293	ARG
11	X	337	SER
11	X	351	GLN
11	X	382	VAL
11	X	383	LYS
11	X	385	LEU
11	X	394	LEU
11	X	416	THR
11	X	458	ILE
11	X	468	SER
11	X	476	SER
11	X	480	GLU
11	X	487	GLU
11	X	495	LEU
11	X	498	SER
11	X	501	SER
11	X	503	THR
11	X	509	THR
12	Y	9	ILE
12	Y	26	GLU
12	Y	29	GLU
12	Y	74	GLU
12	Y	77	LEU
12	Y	167	ILE
12	Y	183	VAL
12	Y	204	THR
12	Y	206	VAL
12	Y	214	LYS
12	Y	234	LEU
12	Y	249	GLN
12	Y	251	VAL
12	Y	255	ILE
12	Y	268	VAL
12	Y	291	LEU
12	Y	304	VAL
12	Y	329	LEU
12	Y	332	THR

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Mol	Chain	Res	Type
12	Y	341	GLU
12	Y	357	LEU
12	Y	359	ASP
12	Y	374	VAL
12	Y	396	LEU
12	Y	397	SER
12	Y	402	LEU
12	Y	410	ILE
12	Y	420	VAL
12	Y	423	VAL
12	Y	464	GLU
12	Z	20	ILE
12	Z	128	SER
12	Z	129	THR
12	Z	140	VAL
12	Z	165	VAL
12	Z	174	ILE
12	Z	190	ARG
12	Z	210	GLU
12	Z	232	VAL
12	Z	294	GLU
12	Z	298	THR
12	Z	299	THR
12	Z	324	THR
12	Z	352	ASP
12	Z	357	LEU
12	Z	359	ASP
12	Z	373	LYS
12	Z	376	GLU
12	Z	380	THR
12	Z	406	ARG
12	Z	435	LYS
12	Z	446	GLU
12	Z	464	GLU
12	c	58	THR
12	c	87	VAL
12	c	98	VAL
12	c	140	VAL
12	c	163	LYS
12	c	165	VAL
12	c	167	ILE
12	c	182	SER

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Mol	Chain	Res	Type
12	c	201	MET
12	c	208	ASN
12	c	232	VAL
12	c	251	VAL
12	c	261	PHE
12	c	279	VAL
12	c	303	SER
12	c	305	THR
12	c	318	THR
12	c	324	THR
12	c	354	LYS
12	c	355	SER
12	c	357	LEU
12	c	388	ILE
12	c	420	VAL
12	c	423	VAL
12	c	427	ILE
12	c	434	LEU
12	c	467	VAL
13	j	2	THR
13	j	3	LEU
13	j	4	LYS
13	j	16	ILE
13	j	17	GLU
13	j	19	ILE
13	j	21	LYS
13	j	26	VAL
13	j	38	LYS
13	j	78	THR
13	j	121	THR
13	j	130	ILE
13	j	143	SER
13	j	145	LEU
13	j	148	ASP
13	j	152	SER
13	j	155	LYS
13	j	164	ILE
13	j	173	LEU
13	j	196	LYS
13	j	205	VAL
13	j	216	ASN
13	j	218	MET

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Mol	Chain	Res	Type
13	j	231	SER
13	j	235	ASN
13	j	248	ILE
13	j	254	LEU
13	j	264	THR
13	j	267	LEU
13	j	269	ASP
13	j	271	ILE
13	j	272	THR
13	j	276	SER
14	l	12	LEU
14	l	19	GLU
14	l	21	LEU
14	l	27	VAL
14	l	29	GLN
14	l	30	VAL
14	l	42	LEU
14	l	46	VAL
14	l	48	THR
14	l	49	VAL
14	l	60	MET
14	l	70	ILE
14	l	86	THR
15	m	14	LEU
15	m	27	THR
15	m	31	THR
15	m	34	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (96) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	2	GLN
1	2	2	GLN
1	7	40	ASN
3	a	48	ASN
3	a	62	GLN
3	a	76	GLN
3	a	230	GLN
11	K	72	GLN
11	K	145	HIS
11	K	398	GLN
11	K	407	GLN

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Mol	Chain	Res	Type
11	K	454	HIS
11	B	47	ASN
11	B	67	ASN
11	B	149	GLN
11	B	192	ASN
11	B	245	GLN
11	B	265	HIS
11	B	398	GLN
11	B	428	GLN
11	B	454	HIS
11	B	477	ASN
11	C	210	GLN
11	C	217	GLN
11	C	304	HIS
12	D	365	GLN
12	E	27	GLN
12	E	43	GLN
12	E	52	GLN
12	E	168	GLN
12	E	221	GLN
12	E	328	HIS
12	E	379	GLN
12	F	24	HIS
12	F	52	GLN
12	F	127	GLN
12	F	208	ASN
12	F	308	GLN
12	F	328	HIS
13	G	54	ASN
13	G	124	ASN
13	G	216	ASN
13	G	224	GLN
14	H	13	GLN
14	H	44	ASN
14	H	78	GLN
15	I	30	GLN
1	L	2	GLN
1	M	2	GLN
1	S	40	ASN
2	V	3	GLN
3	p	48	ASN
3	p	76	GLN

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Mol	Chain	Res	Type
11	n	145	HIS
11	n	304	HIS
11	n	398	GLN
11	n	407	GLN
11	n	454	HIS
11	W	47	ASN
11	W	67	ASN
11	W	149	GLN
11	W	192	ASN
11	W	245	GLN
11	W	265	HIS
11	W	282	GLN
11	W	343	ASN
11	W	398	GLN
11	W	428	GLN
11	W	454	HIS
11	W	477	ASN
11	X	210	GLN
11	X	217	GLN
11	X	304	HIS
12	Y	365	GLN
12	Z	27	GLN
12	Z	43	GLN
12	Z	52	GLN
12	Z	168	GLN
12	Z	221	GLN
12	Z	328	HIS
12	Z	379	GLN
12	Z	385	GLN
12	c	24	HIS
12	c	52	GLN
12	c	127	GLN
12	c	208	ASN
12	c	308	GLN
12	c	328	HIS
13	j	54	ASN
13	j	124	ASN
13	j	216	ASN
13	j	224	GLN
14	l	13	GLN
14	l	44	ASN
14	l	78	GLN

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Mol	Chain	Res	Type
15	m	30	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 10 are monoatomic - leaving 10 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$
18	ANP	c	501	19	33,33,33	2.88	11 (33%)	45,52,52	2.08	15 (33%)
18	ANP	n	601	19	33,33,33	2.89	11 (33%)	45,52,52	1.90	12 (26%)
18	ANP	K	601	19	33,33,33	2.88	11 (33%)	45,52,52	1.90	12 (26%)
18	ANP	D	501	19	33,33,33	2.95	11 (33%)	45,52,52	2.15	16 (35%)
18	ANP	C	601	19	33,33,33	2.80	12 (36%)	45,52,52	2.24	14 (31%)
18	ANP	W	601	19	33,33,33	2.90	10 (30%)	45,52,52	1.85	11 (24%)
18	ANP	Y	501	19	33,33,33	2.96	11 (33%)	45,52,52	2.14	17 (37%)
18	ANP	X	601	19	33,33,33	2.81	12 (36%)	45,52,52	2.23	14 (31%)
18	ANP	F	501	19	33,33,33	2.88	11 (33%)	45,52,52	2.08	15 (33%)
18	ANP	B	601	19	33,33,33	2.90	11 (33%)	45,52,52	1.86	11 (24%)

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
18	ANP	c	501	19	-	1/18/38/38	0/3/3/3
18	ANP	n	601	19	-	1/18/38/38	0/3/3/3
18	ANP	K	601	19	-	1/18/38/38	0/3/3/3
18	ANP	D	501	19	-	3/18/38/38	0/3/3/3
18	ANP	C	601	19	-	3/18/38/38	0/3/3/3
18	ANP	W	601	19	-	3/18/38/38	0/3/3/3
18	ANP	Y	501	19	-	3/18/38/38	0/3/3/3
18	ANP	X	601	19	-	3/18/38/38	0/3/3/3
18	ANP	F	501	19	-	1/18/38/38	0/3/3/3
18	ANP	B	601	19	-	3/18/38/38	0/3/3/3

All (111) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	n	601	ANP	PG-O1G	9.91	1.61	1.46
18	K	601	ANP	PG-O1G	9.86	1.61	1.46
18	Y	501	ANP	PG-O1G	9.25	1.60	1.46
18	D	501	ANP	PG-O1G	9.22	1.60	1.46
18	X	601	ANP	PG-O1G	9.18	1.60	1.46
18	C	601	ANP	PG-O1G	9.18	1.60	1.46
18	B	601	ANP	PG-O1G	9.07	1.59	1.46
18	W	601	ANP	PG-O1G	9.07	1.59	1.46
18	c	501	ANP	PG-O1G	9.05	1.59	1.46
18	F	501	ANP	PG-O1G	8.99	1.59	1.46
18	Y	501	ANP	PB-O1B	8.53	1.59	1.46
18	W	601	ANP	PB-O1B	8.53	1.59	1.46
18	B	601	ANP	PB-O1B	8.50	1.59	1.46
18	D	501	ANP	PB-O1B	8.48	1.59	1.46
18	n	601	ANP	PB-O1B	7.93	1.58	1.46
18	K	601	ANP	PB-O1B	7.91	1.58	1.46
18	c	501	ANP	PB-O1B	7.68	1.57	1.46
18	C	601	ANP	PB-O1B	7.67	1.57	1.46
18	X	601	ANP	PB-O1B	7.66	1.57	1.46
18	F	501	ANP	PB-O1B	7.65	1.57	1.46
18	F	501	ANP	C4-N3	5.93	1.45	1.34
18	c	501	ANP	C4-N3	5.91	1.45	1.34
18	D	501	ANP	C4-N3	5.84	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	Y	501	ANP	C4-N3	5.83	1.45	1.34
18	B	601	ANP	C4-N3	5.75	1.45	1.34
18	W	601	ANP	C4-N3	5.75	1.45	1.34
18	X	601	ANP	C4-N3	4.88	1.43	1.34
18	C	601	ANP	C4-N3	4.85	1.43	1.34
18	K	601	ANP	C4-N3	4.73	1.43	1.34
18	n	601	ANP	C4-N3	4.71	1.43	1.34
18	F	501	ANP	PB-N3B	4.30	1.74	1.63
18	c	501	ANP	PB-N3B	4.26	1.74	1.63
18	Y	501	ANP	PG-N3B	4.25	1.74	1.63
18	D	501	ANP	PG-N3B	4.21	1.74	1.63
18	c	501	ANP	PG-N3B	4.14	1.74	1.63
18	F	501	ANP	PG-N3B	4.11	1.74	1.63
18	B	601	ANP	PG-N3B	4.01	1.73	1.63
18	W	601	ANP	PG-N3B	4.01	1.73	1.63
18	B	601	ANP	C5-C4	3.98	1.46	1.39
18	Y	501	ANP	C5-C4	3.96	1.46	1.39
18	W	601	ANP	C5-C4	3.95	1.46	1.39
18	D	501	ANP	C5-C4	3.92	1.46	1.39
18	n	601	ANP	C8-N7	3.73	1.38	1.31
18	K	601	ANP	C8-N7	3.72	1.38	1.31
18	B	601	ANP	PB-N3B	3.70	1.73	1.63
18	W	601	ANP	PB-N3B	3.69	1.73	1.63
18	X	601	ANP	PG-N3B	3.64	1.72	1.63
18	C	601	ANP	PG-N3B	3.62	1.72	1.63
18	Y	501	ANP	C8-N7	3.58	1.38	1.31
18	X	601	ANP	C8-N7	3.58	1.38	1.31
18	D	501	ANP	C8-N7	3.57	1.38	1.31
18	K	601	ANP	PB-N3B	3.56	1.72	1.63
18	n	601	ANP	PB-N3B	3.53	1.72	1.63
18	X	601	ANP	PB-N3B	3.51	1.72	1.63
18	C	601	ANP	C8-N7	3.50	1.38	1.31
18	C	601	ANP	PB-N3B	3.50	1.72	1.63
18	c	501	ANP	C5-C4	3.49	1.45	1.39
18	F	501	ANP	C5-C4	3.45	1.45	1.39
18	n	601	ANP	PG-N3B	3.41	1.72	1.63
18	K	601	ANP	PG-N3B	3.41	1.72	1.63
18	B	601	ANP	C8-N7	3.36	1.38	1.31
18	W	601	ANP	C8-N7	3.36	1.38	1.31
18	n	601	ANP	C5-C4	3.27	1.44	1.39
18	K	601	ANP	C5-C4	3.25	1.44	1.39
18	C	601	ANP	C4-N9	-3.18	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	X	601	ANP	C4-N9	-3.18	1.31	1.37
18	Y	501	ANP	C5-C6	3.17	1.49	1.41
18	D	501	ANP	PB-N3B	3.14	1.71	1.63
18	D	501	ANP	C5-C6	3.14	1.49	1.41
18	F	501	ANP	C8-N7	3.13	1.37	1.31
18	c	501	ANP	C8-N7	3.12	1.37	1.31
18	Y	501	ANP	PB-N3B	3.12	1.71	1.63
18	C	601	ANP	C5-C4	3.00	1.44	1.39
18	B	601	ANP	C5-C6	2.97	1.49	1.41
18	W	601	ANP	C5-C6	2.96	1.49	1.41
18	X	601	ANP	C5-C4	2.90	1.44	1.39
18	K	601	ANP	C5-C6	2.86	1.48	1.41
18	n	601	ANP	C5-C6	2.85	1.48	1.41
18	F	501	ANP	PA-O1A	2.52	1.59	1.50
18	C	601	ANP	C5-N7	-2.50	1.34	1.39
18	c	501	ANP	PA-O1A	2.49	1.59	1.50
18	K	601	ANP	PA-O1A	2.47	1.59	1.50
18	n	601	ANP	PA-O1A	2.47	1.59	1.50
18	X	601	ANP	C5-N7	-2.46	1.34	1.39
18	D	501	ANP	PA-O1A	2.45	1.59	1.50
18	Y	501	ANP	PA-O1A	2.45	1.59	1.50
18	n	601	ANP	C4-N9	-2.43	1.32	1.37
18	X	601	ANP	PA-O1A	2.43	1.59	1.50
18	K	601	ANP	C4-N9	-2.42	1.32	1.37
18	C	601	ANP	PA-O1A	2.41	1.59	1.50
18	B	601	ANP	PA-O1A	2.40	1.59	1.50
18	W	601	ANP	PA-O1A	2.40	1.59	1.50
18	n	601	ANP	PA-O3A	2.38	1.62	1.59
18	c	501	ANP	PG-O3G	2.31	1.63	1.56
18	F	501	ANP	PG-O3G	2.30	1.62	1.56
18	F	501	ANP	C5-C6	2.30	1.47	1.41
18	c	501	ANP	C5-C6	2.27	1.47	1.41
18	K	601	ANP	PA-O3A	2.27	1.61	1.59
18	F	501	ANP	C4-N9	-2.21	1.33	1.37
18	C	601	ANP	PB-O3A	2.20	1.61	1.59
18	B	601	ANP	C5-N7	-2.19	1.35	1.39
18	X	601	ANP	PB-O3A	2.18	1.61	1.59
18	X	601	ANP	C5-C6	2.18	1.47	1.41
18	c	501	ANP	C4-N9	-2.17	1.33	1.37
18	C	601	ANP	C5-C6	2.16	1.47	1.41
18	W	601	ANP	C5-N7	-2.15	1.35	1.39
18	Y	501	ANP	C4-N9	-2.09	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	D	501	ANP	C4-N9	-2.08	1.33	1.37
18	D	501	ANP	PG-O2G	2.03	1.62	1.56
18	Y	501	ANP	PG-O2G	2.01	1.62	1.56
18	B	601	ANP	C4-N9	-2.00	1.33	1.37

All (137) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	X	601	ANP	O4'-C1'-N9	6.66	120.89	108.09
18	C	601	ANP	O4'-C1'-N9	6.64	120.83	108.09
18	c	501	ANP	O1B-PB-N3B	-5.49	103.68	111.77
18	F	501	ANP	O1B-PB-N3B	-5.47	103.71	111.77
18	C	601	ANP	O1G-PG-N3B	-5.20	104.11	111.77
18	X	601	ANP	O1G-PG-N3B	-5.19	104.12	111.77
18	D	501	ANP	C4-C5-N7	-4.79	105.10	110.58
18	Y	501	ANP	C4-C5-N7	-4.76	105.14	110.58
18	n	601	ANP	C4-C5-N7	-4.46	105.49	110.58
18	K	601	ANP	C4-C5-N7	-4.44	105.50	110.58
18	B	601	ANP	C4-C5-N7	-4.37	105.58	110.58
18	Y	501	ANP	C6-C5-N7	4.37	140.52	132.09
18	B	601	ANP	C5-C4-N3	-4.35	120.72	126.72
18	W	601	ANP	C4-C5-N7	-4.34	105.62	110.58
18	D	501	ANP	C6-C5-N7	4.32	140.43	132.09
18	W	601	ANP	C5-C4-N3	-4.32	120.77	126.72
18	n	601	ANP	C5-C4-N9	4.27	110.47	105.81
18	K	601	ANP	C5-C4-N9	4.25	110.44	105.81
18	C	601	ANP	C6-C5-N7	4.23	140.25	132.09
18	X	601	ANP	C6-C5-N7	4.17	140.13	132.09
18	X	601	ANP	C5-C4-N9	4.13	110.31	105.81
18	C	601	ANP	C5-C4-N9	4.11	110.29	105.81
18	B	601	ANP	C5-C4-N9	4.11	110.29	105.81
18	W	601	ANP	C5-C4-N9	4.11	110.29	105.81
18	C	601	ANP	C4-C5-N7	-4.11	105.89	110.58
18	K	601	ANP	C5-C4-N3	-4.09	121.08	126.72
18	n	601	ANP	C5-C4-N3	-4.09	121.09	126.72
18	K	601	ANP	C6-C5-N7	4.07	139.94	132.09
18	n	601	ANP	C6-C5-N7	4.06	139.93	132.09
18	X	601	ANP	C4-C5-N7	-4.04	105.96	110.58
18	B	601	ANP	N3-C2-N1	-3.97	122.58	128.58
18	W	601	ANP	N3-C2-N1	-3.96	122.59	128.58
18	B	601	ANP	C6-C5-N7	3.88	139.57	132.09
18	Y	501	ANP	C2'-C1'-N9	-3.88	103.67	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	F	501	ANP	N3-C2-N1	-3.88	122.71	128.58
18	D	501	ANP	C5-C4-N9	3.87	110.03	105.81
18	W	601	ANP	C6-C5-N7	3.87	139.55	132.09
18	D	501	ANP	C2'-C1'-N9	-3.87	103.69	113.30
18	c	501	ANP	N3-C2-N1	-3.86	122.74	128.58
18	Y	501	ANP	C5-C4-N9	3.81	109.96	105.81
18	C	601	ANP	N3-C2-N1	-3.73	122.94	128.58
18	X	601	ANP	N3-C2-N1	-3.69	122.99	128.58
18	c	501	ANP	C6-C5-N7	3.64	139.11	132.09
18	F	501	ANP	C6-C5-N7	3.61	139.06	132.09
18	D	501	ANP	C5-C4-N3	-3.60	121.76	126.72
18	Y	501	ANP	C5-C4-N3	-3.55	121.82	126.72
18	D	501	ANP	O2'-C2'-C1'	-3.52	98.00	110.10
18	Y	501	ANP	O2'-C2'-C1'	-3.51	98.02	110.10
18	D	501	ANP	O1G-PG-N3B	-3.51	106.61	111.77
18	Y	501	ANP	O1G-PG-N3B	-3.50	106.61	111.77
18	F	501	ANP	O3G-PG-O1G	-3.41	104.89	113.45
18	c	501	ANP	O3G-PG-O1G	-3.41	104.89	113.45
18	D	501	ANP	N3-C2-N1	-3.30	123.58	128.58
18	n	601	ANP	N3-C2-N1	-3.26	123.65	128.58
18	F	501	ANP	C2'-C1'-N9	-3.25	105.24	113.30
18	c	501	ANP	C2'-C1'-N9	-3.24	105.25	113.30
18	K	601	ANP	N3-C2-N1	-3.23	123.69	128.58
18	Y	501	ANP	N3-C2-N1	-3.22	123.70	128.58
18	c	501	ANP	C5-C6-N6	-3.11	115.58	123.29
18	F	501	ANP	C5-C6-N6	-3.11	115.59	123.29
18	Y	501	ANP	O2G-PG-O3G	3.04	115.75	107.59
18	D	501	ANP	O2G-PG-O3G	3.01	115.69	107.59
18	K	601	ANP	O1G-PG-N3B	-3.01	107.34	111.77
18	n	601	ANP	O1G-PG-N3B	-3.01	107.34	111.77
18	F	501	ANP	O2B-PB-O1B	2.98	116.27	109.87
18	c	501	ANP	O2B-PB-O1B	2.98	116.26	109.87
18	D	501	ANP	C2-N1-C6	2.96	123.60	118.73
18	Y	501	ANP	O2B-PB-O3A	2.94	114.45	104.64
18	D	501	ANP	O2B-PB-O3A	2.92	114.40	104.64
18	c	501	ANP	O2G-PG-O3G	2.89	115.37	107.59
18	B	601	ANP	C2-N3-C4	2.89	118.88	111.83
18	F	501	ANP	O2G-PG-O3G	2.88	115.34	107.59
18	Y	501	ANP	C2-N1-C6	2.88	123.45	118.73
18	W	601	ANP	C2-N3-C4	2.87	118.84	111.83
18	C	601	ANP	C2-N1-C6	2.86	123.43	118.73
18	X	601	ANP	C2-N1-C6	2.86	123.43	118.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	601	ANP	C2-N1-C6	2.81	123.34	118.73
18	W	601	ANP	C2-N1-C6	2.79	123.32	118.73
18	n	601	ANP	C2-N3-C4	2.79	118.64	111.83
18	K	601	ANP	C2-N3-C4	2.77	118.60	111.83
18	c	501	ANP	C6-C5-C4	-2.77	113.40	117.18
18	C	601	ANP	C5-C4-N3	-2.75	122.93	126.72
18	Y	501	ANP	O4'-C1'-N9	2.74	113.35	108.09
18	F	501	ANP	C6-C5-C4	-2.73	113.45	117.18
18	D	501	ANP	O4'-C1'-N9	2.72	113.31	108.09
18	c	501	ANP	C4-C5-N7	-2.71	107.48	110.58
18	F	501	ANP	C4-C5-N7	-2.71	107.49	110.58
18	X	601	ANP	C5-C4-N3	-2.70	122.99	126.72
18	F	501	ANP	C5-C4-N3	-2.68	123.03	126.72
18	c	501	ANP	C5-C4-N3	-2.67	123.03	126.72
18	W	601	ANP	O1G-PG-N3B	-2.63	107.90	111.77
18	B	601	ANP	O1G-PG-N3B	-2.62	107.91	111.77
18	c	501	ANP	O4'-C1'-C2'	2.62	112.23	106.62
18	F	501	ANP	O4'-C1'-C2'	2.61	112.21	106.62
18	F	501	ANP	C2-N1-C6	2.58	122.96	118.73
18	D	501	ANP	C3'-C2'-C1'	2.55	106.30	101.46
18	F	501	ANP	N6-C6-N1	2.52	123.99	118.38
18	Y	501	ANP	C3'-C2'-C1'	2.52	106.22	101.46
18	c	501	ANP	C2-N1-C6	2.51	122.85	118.73
18	Y	501	ANP	C5-N7-C8	2.49	107.37	103.45
18	c	501	ANP	N6-C6-N1	2.48	123.91	118.38
18	D	501	ANP	C5-N7-C8	2.46	107.32	103.45
18	C	601	ANP	C6-C5-C4	-2.43	113.85	117.18
18	K	601	ANP	O3'-C3'-C4'	-2.42	104.14	111.08
18	X	601	ANP	C6-C5-C4	-2.40	113.90	117.18
18	n	601	ANP	O3'-C3'-C4'	-2.40	104.19	111.08
18	B	601	ANP	C3'-C2'-C1'	2.39	105.98	101.46
18	W	601	ANP	C3'-C2'-C1'	2.36	105.92	101.46
18	C	601	ANP	C1'-N9-C8	2.33	132.26	127.09
18	c	501	ANP	C2-N3-C4	2.30	117.45	111.83
18	X	601	ANP	C1'-N9-C8	2.29	132.19	127.09
18	F	501	ANP	C2-N3-C4	2.29	117.42	111.83
18	D	501	ANP	C2-N3-C4	2.28	117.40	111.83
18	Y	501	ANP	C2-N3-C4	2.26	117.35	111.83
18	n	601	ANP	O2B-PB-O3A	2.24	112.13	104.64
18	X	601	ANP	C2'-C3'-C4'	2.24	106.94	102.61
18	K	601	ANP	O2B-PB-O3A	2.23	112.10	104.64
18	D	501	ANP	O3G-PG-O1G	-2.22	107.87	113.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	Y	501	ANP	O3G-PG-O1G	-2.22	107.89	113.45
18	C	601	ANP	C2'-C3'-C4'	2.21	106.88	102.61
18	n	601	ANP	C2'-C3'-C4'	2.15	106.76	102.61
18	C	601	ANP	C2-N3-C4	2.15	117.07	111.83
18	K	601	ANP	C2'-C3'-C4'	2.13	106.72	102.61
18	X	601	ANP	O1B-PB-N3B	-2.12	108.64	111.77
18	W	601	ANP	C2'-C3'-C4'	2.11	106.68	102.61
18	X	601	ANP	C2-N3-C4	2.11	116.98	111.83
18	B	601	ANP	C5'-C4'-C3'	-2.11	107.63	115.21
18	W	601	ANP	C5'-C4'-C3'	-2.11	107.63	115.21
18	C	601	ANP	O1B-PB-N3B	-2.10	108.67	111.77
18	B	601	ANP	C2'-C3'-C4'	2.09	106.64	102.61
18	Y	501	ANP	C6-C5-C4	-2.08	114.34	117.18
18	C	601	ANP	C4-N9-C1'	-2.07	121.79	126.63
18	X	601	ANP	C4-N9-C1'	-2.05	121.84	126.63
18	n	601	ANP	C3'-C2'-C1'	2.04	105.32	101.46
18	K	601	ANP	O3A-PB-N3B	-2.03	100.95	106.59
18	K	601	ANP	C3'-C2'-C1'	2.03	105.31	101.46
18	n	601	ANP	O3A-PB-N3B	-2.02	100.99	106.59

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	K	601	ANP	PG-N3B-PB-O1B
18	B	601	ANP	PG-N3B-PB-O1B
18	C	601	ANP	PB-N3B-PG-O1G
18	C	601	ANP	PG-N3B-PB-O1B
18	D	501	ANP	PB-N3B-PG-O1G
18	D	501	ANP	PG-N3B-PB-O1B
18	D	501	ANP	PG-N3B-PB-O3A
18	F	501	ANP	PG-N3B-PB-O1B
18	n	601	ANP	PG-N3B-PB-O1B
18	W	601	ANP	PG-N3B-PB-O1B
18	X	601	ANP	PB-N3B-PG-O1G
18	X	601	ANP	PG-N3B-PB-O1B
18	Y	501	ANP	PB-N3B-PG-O1G
18	Y	501	ANP	PG-N3B-PB-O1B
18	Y	501	ANP	PG-N3B-PB-O3A
18	c	501	ANP	PG-N3B-PB-O1B
18	W	601	ANP	C3'-C4'-C5'-O5'
18	B	601	ANP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
18	B	601	ANP	C3'-C4'-C5'-O5'
18	W	601	ANP	O4'-C4'-C5'-O5'
18	C	601	ANP	PB-O3A-PA-O1A
18	X	601	ANP	PB-O3A-PA-O1A

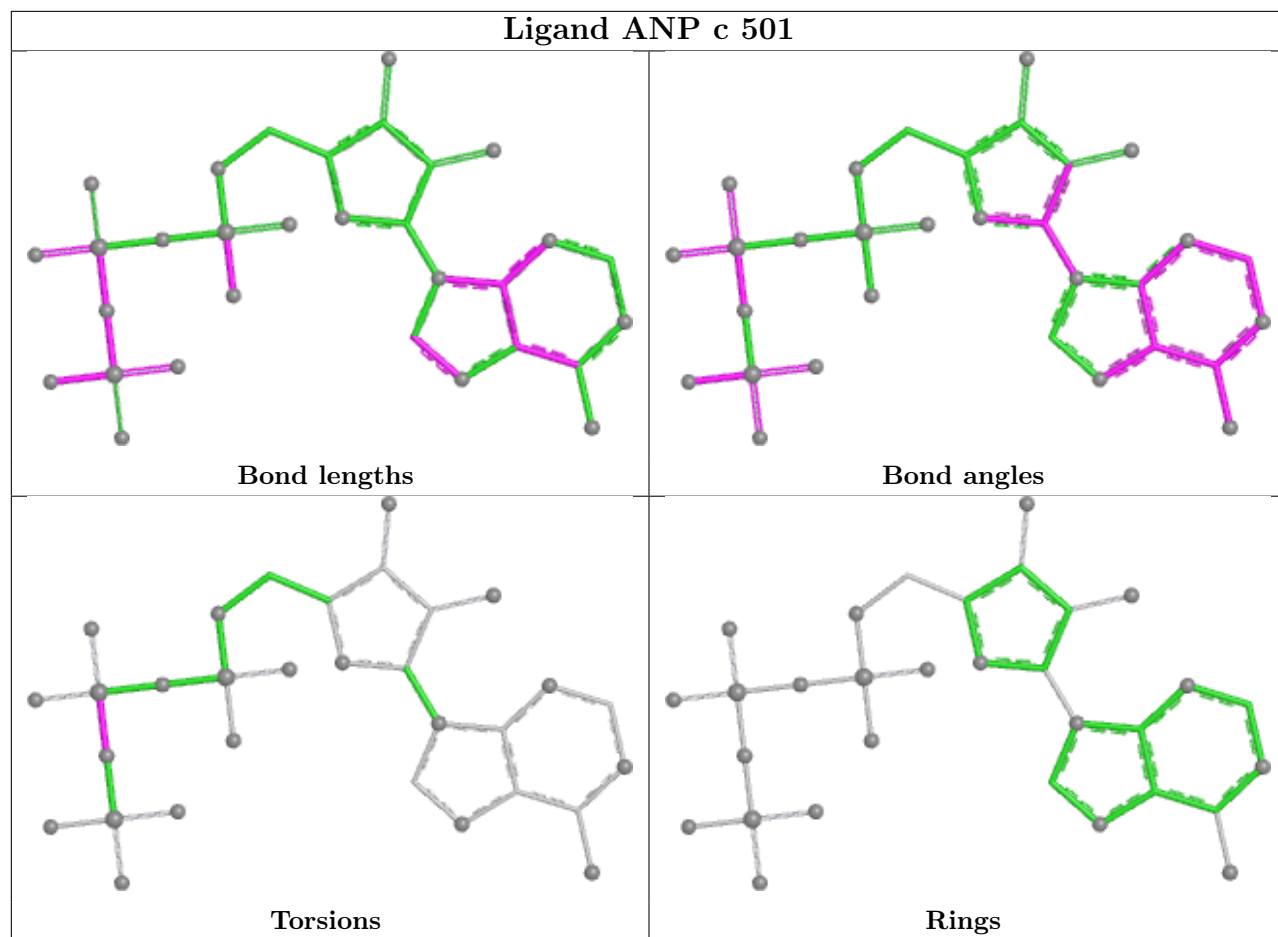
There are no ring outliers.

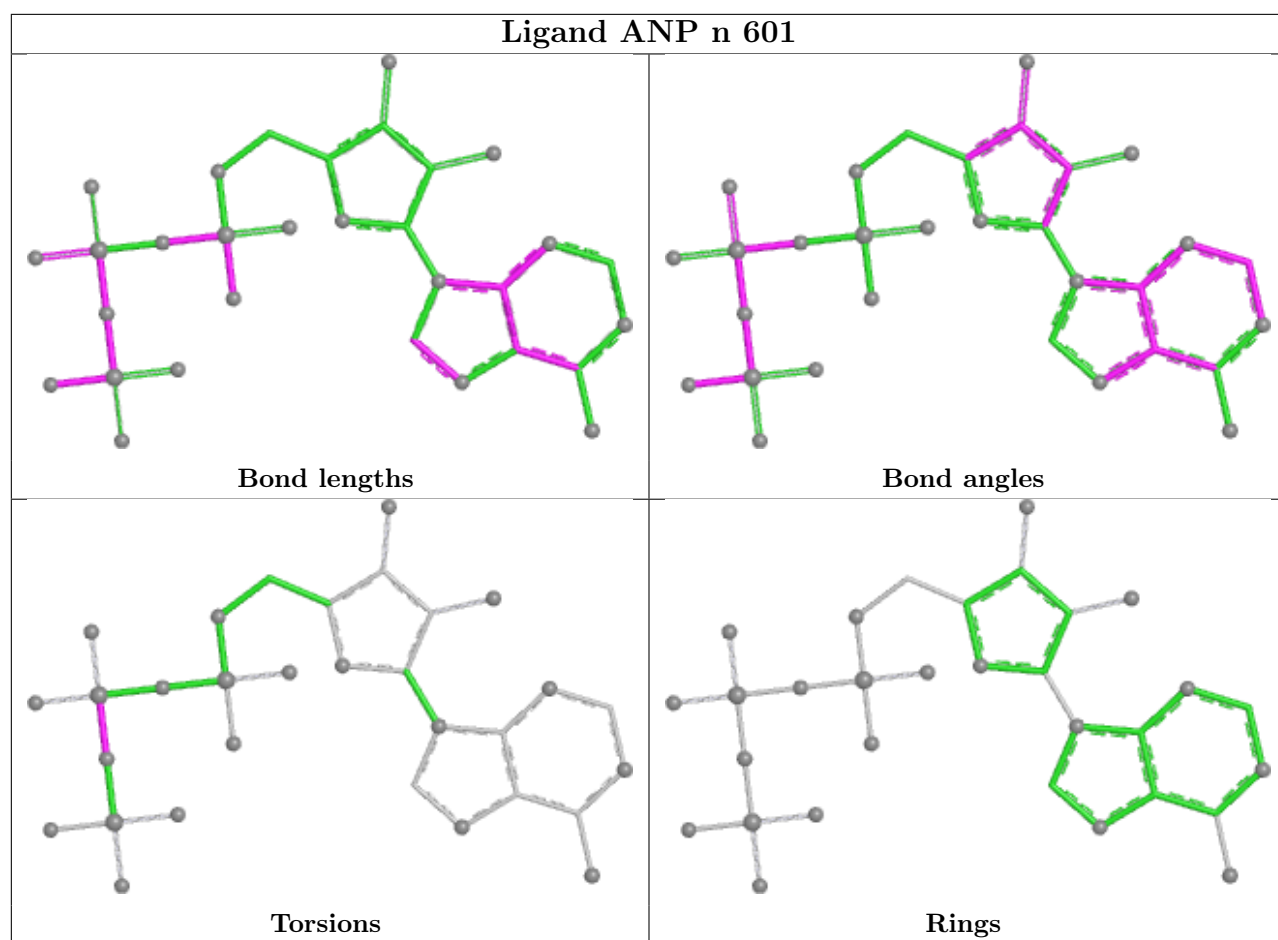
10 monomers are involved in 30 short contacts:

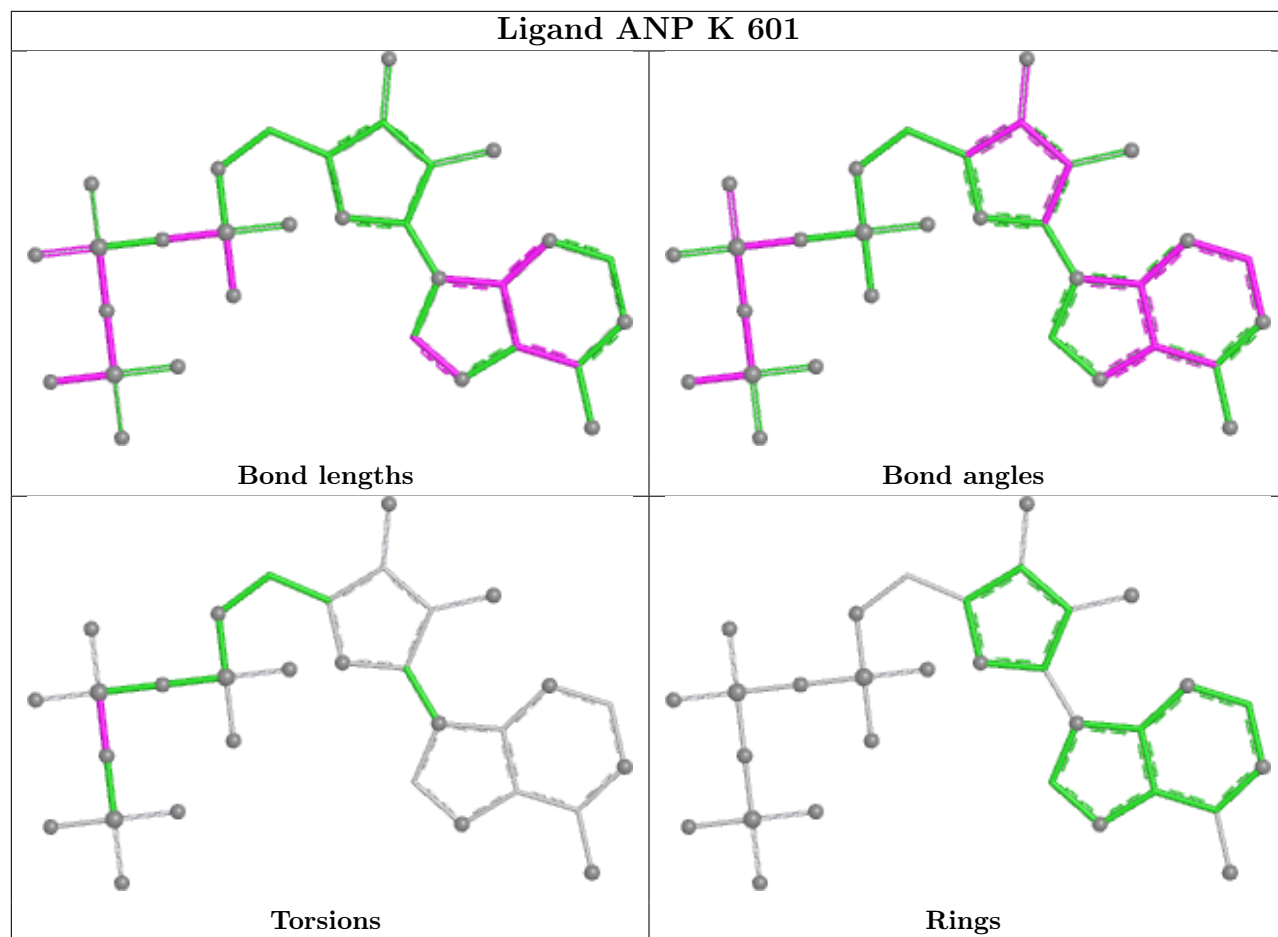
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	c	501	ANP	7	0
18	n	601	ANP	1	0
18	K	601	ANP	1	0
18	D	501	ANP	3	0
18	C	601	ANP	3	0
18	W	601	ANP	1	0
18	Y	501	ANP	3	0
18	X	601	ANP	3	0
18	F	501	ANP	7	0
18	B	601	ANP	1	0

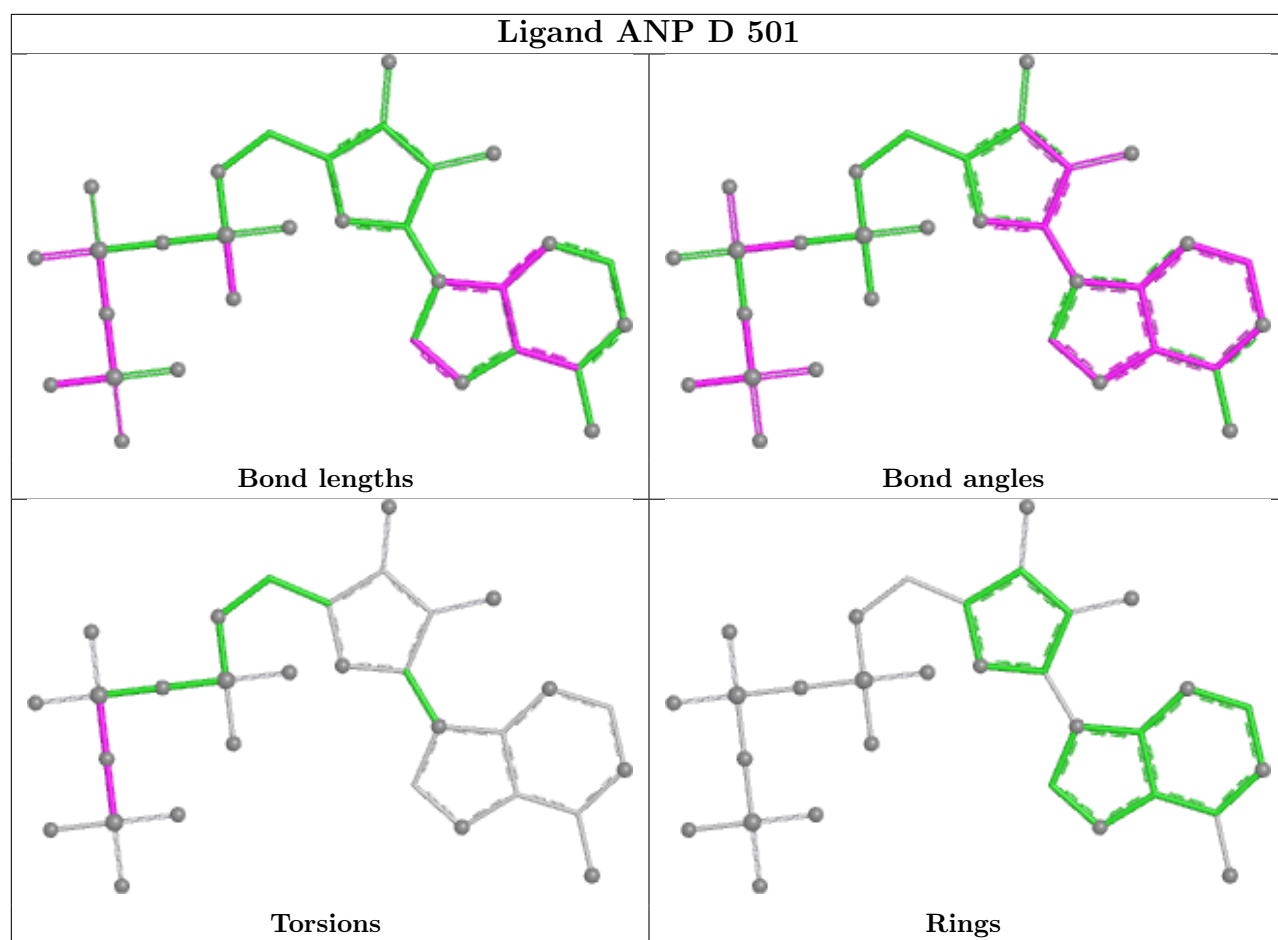
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

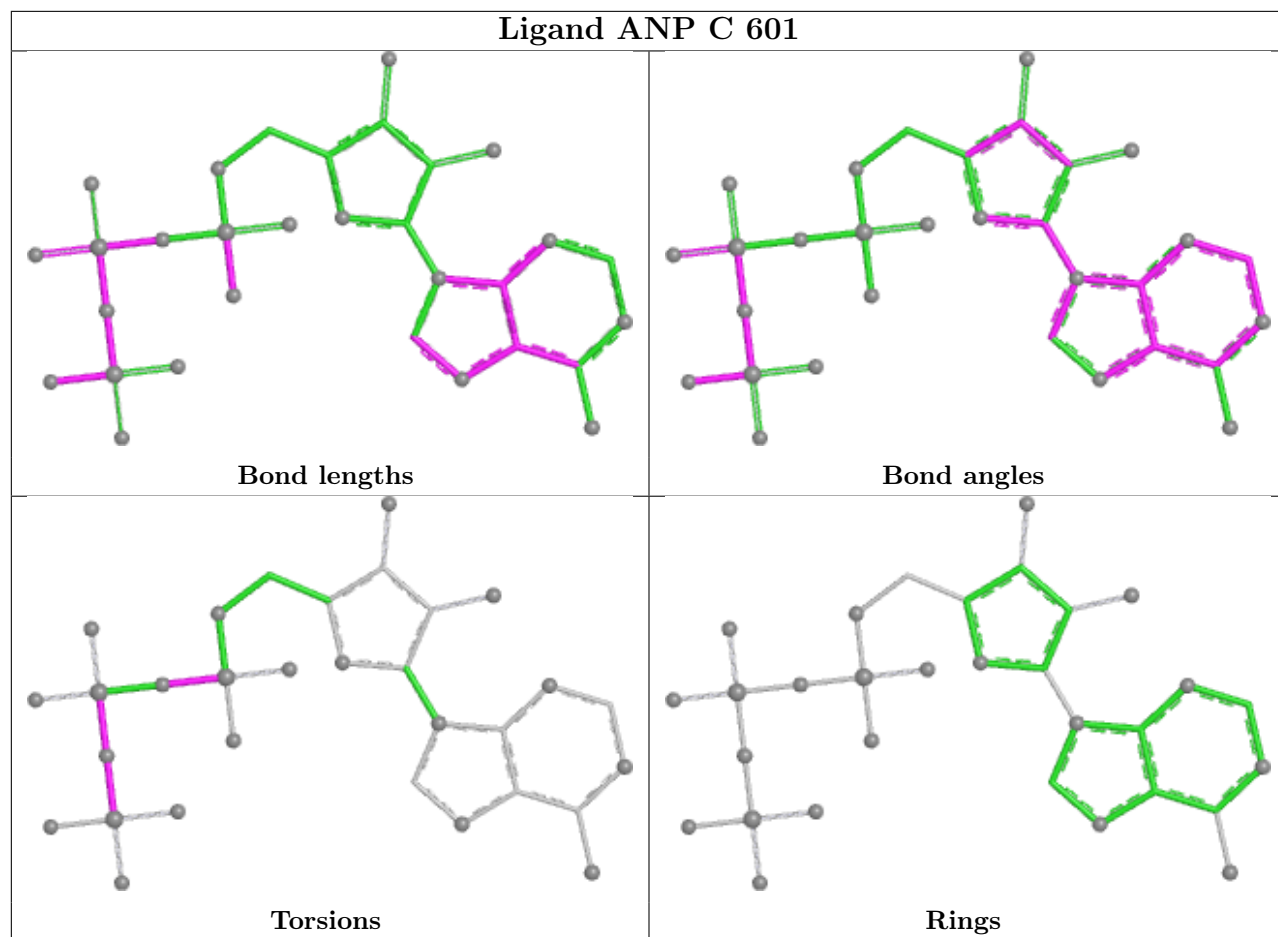
Ligand ANP c 501

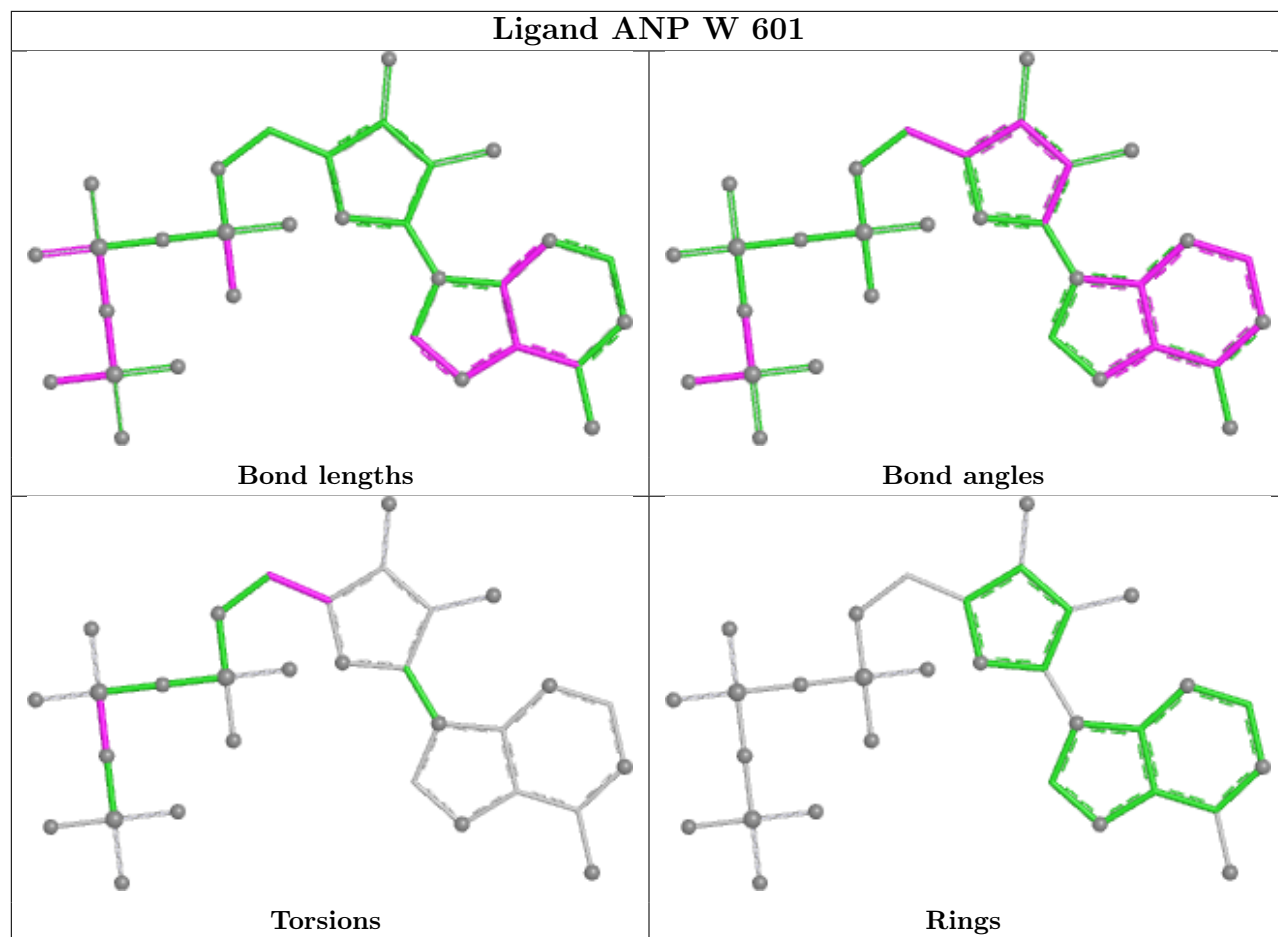


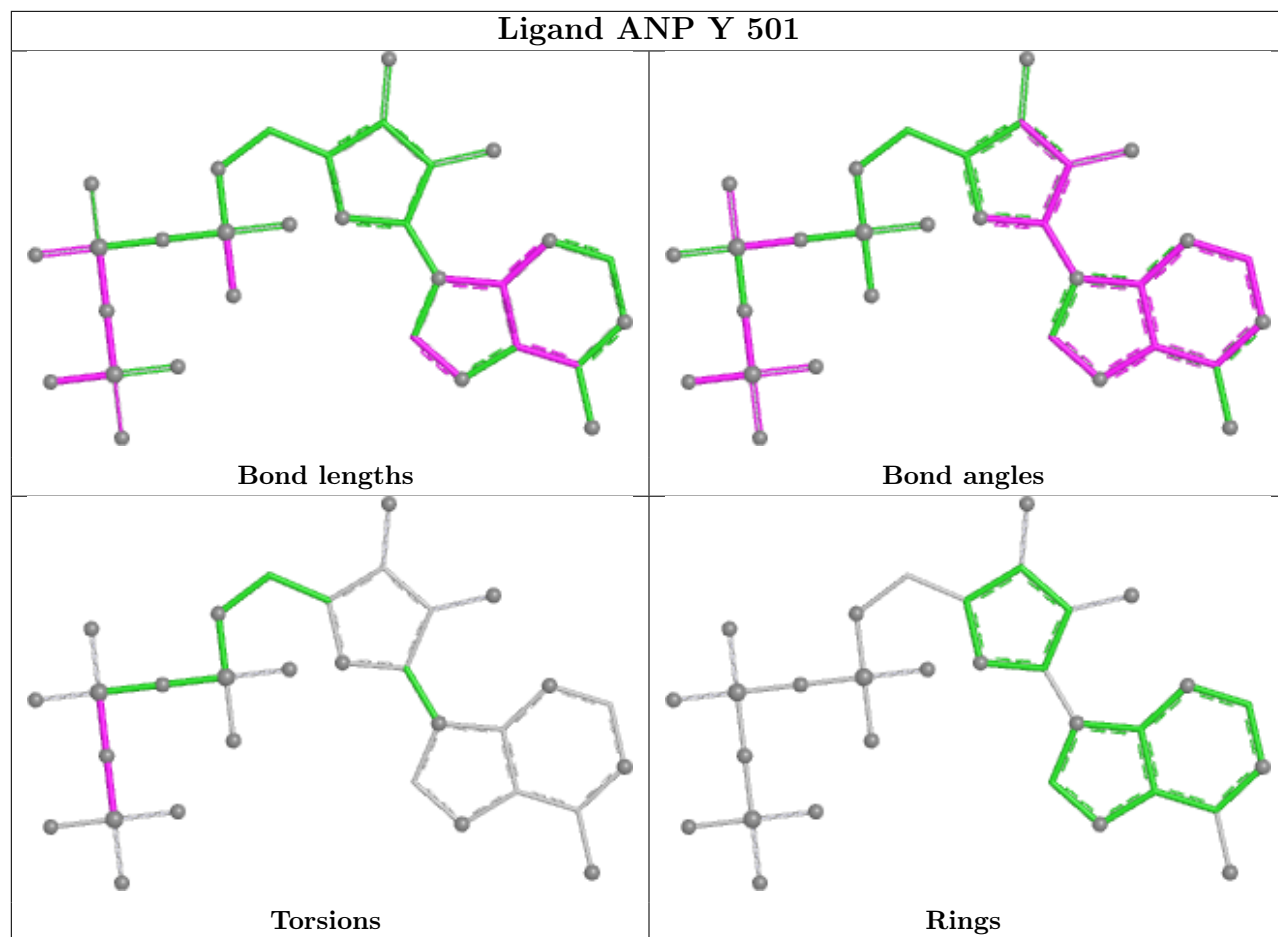


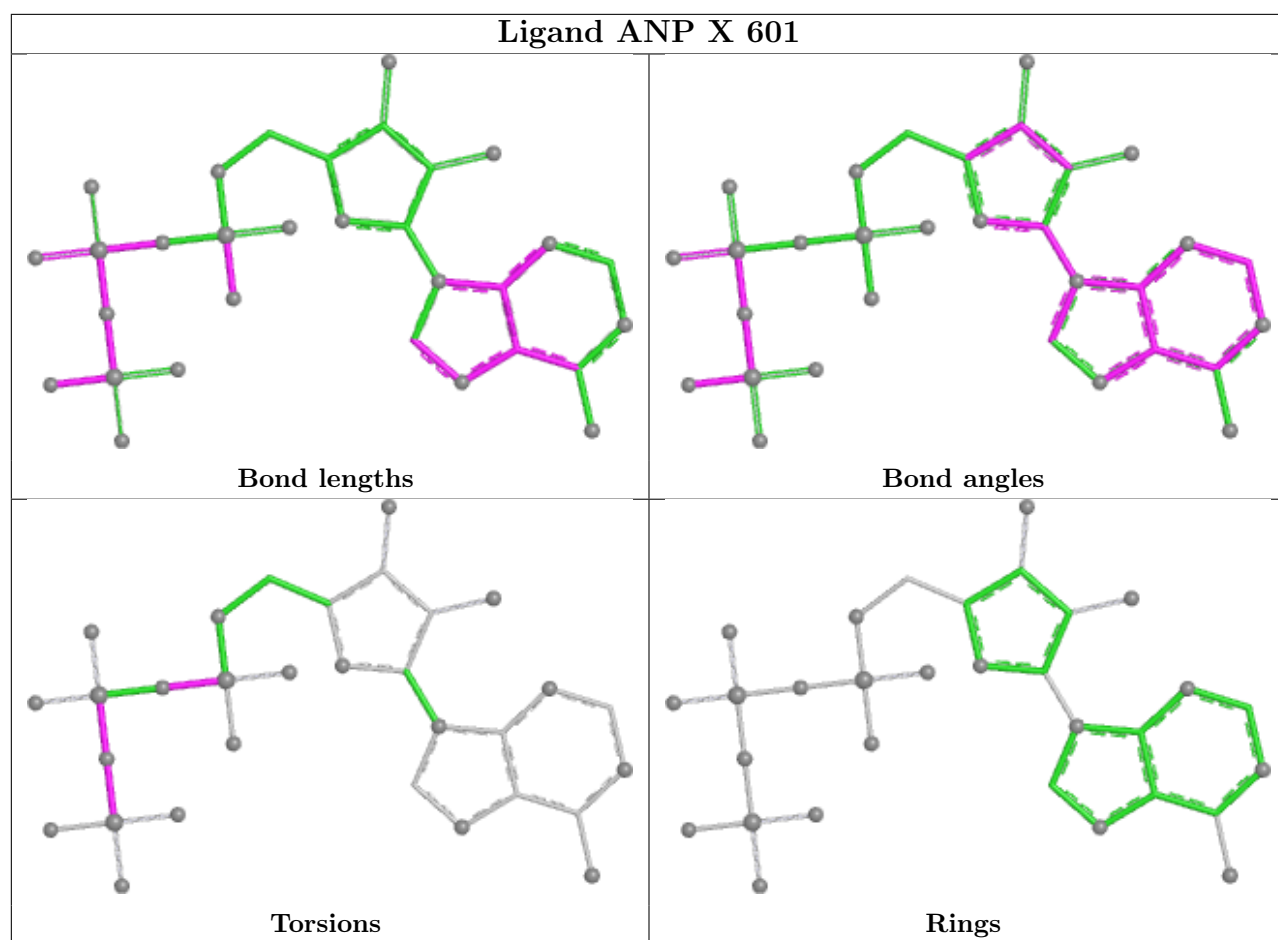


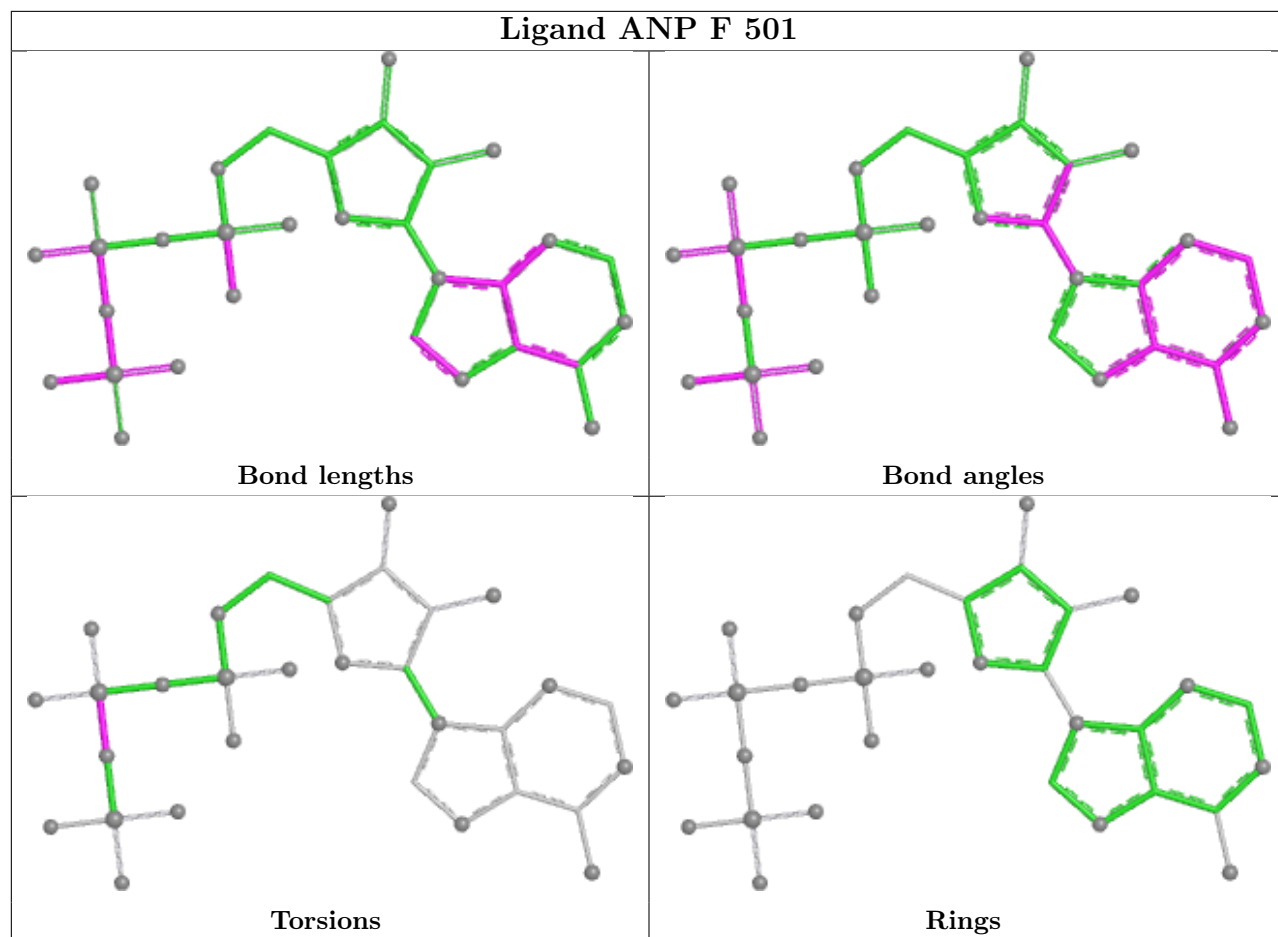


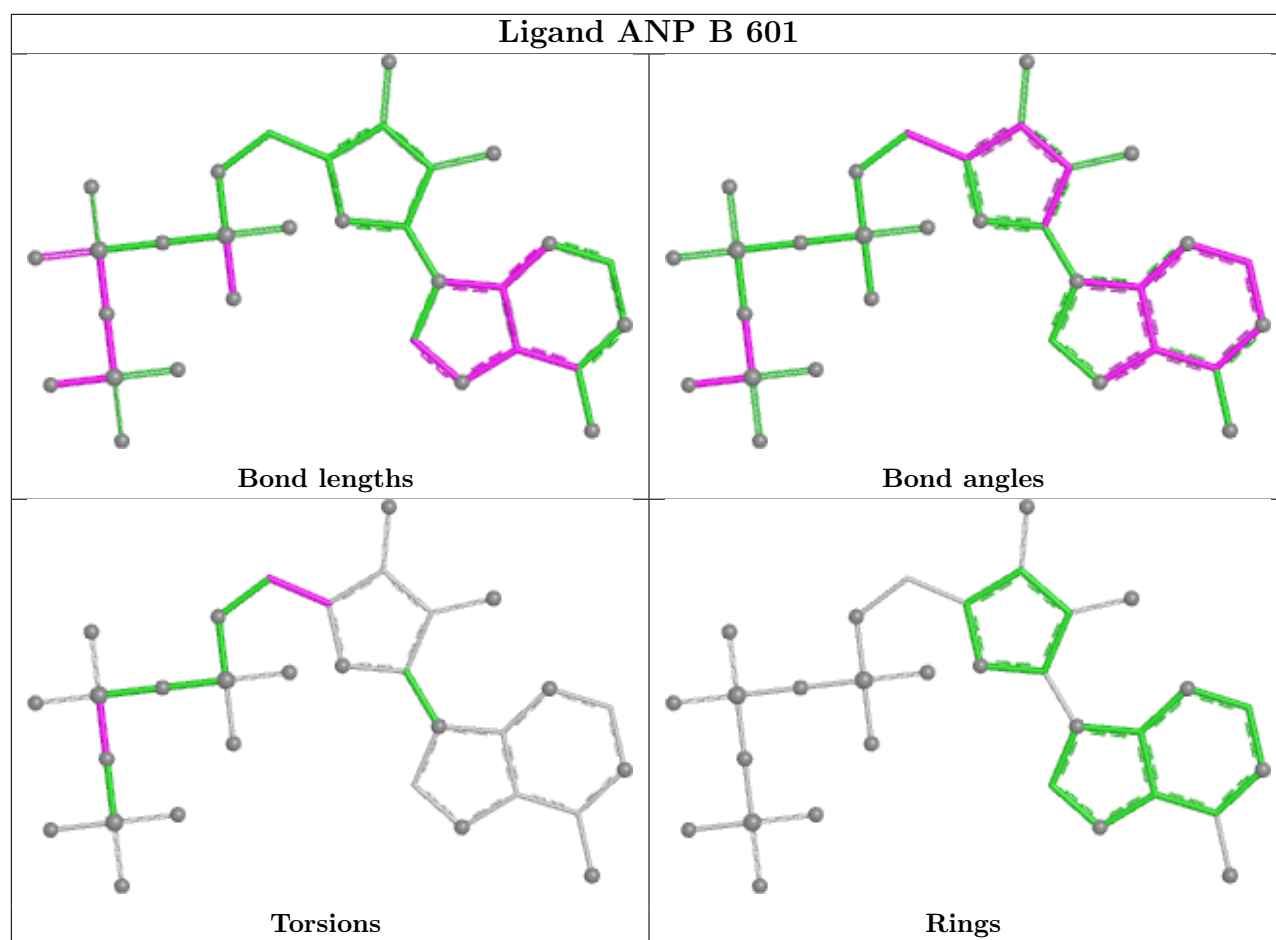












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

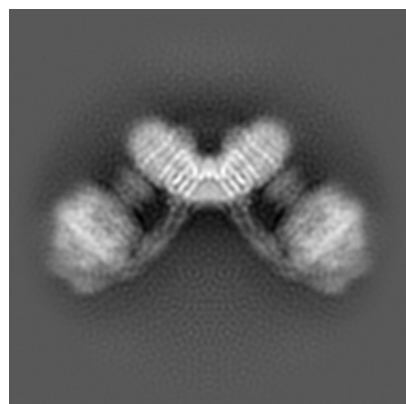
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7067. These allow visual inspection of the internal detail of the map and identification of artifacts.

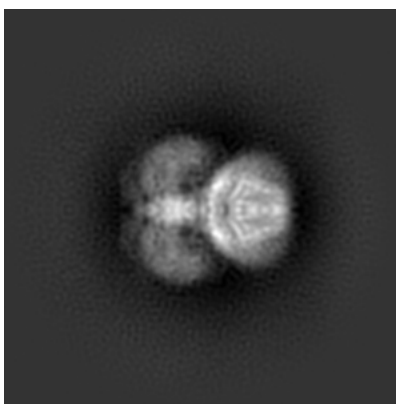
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

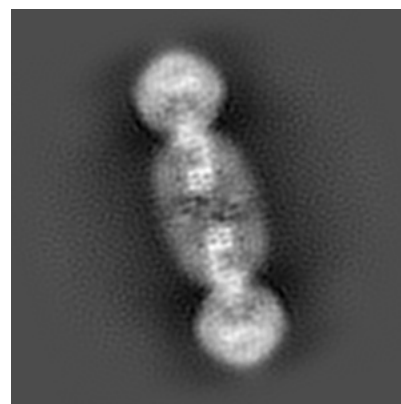
6.1.1 Primary map



X

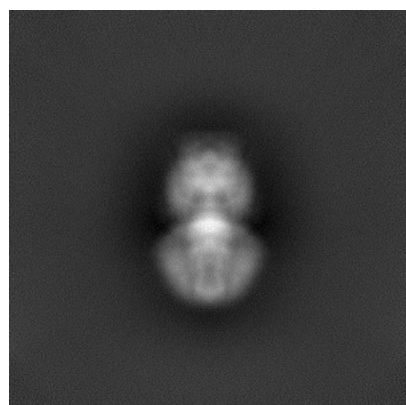


Y

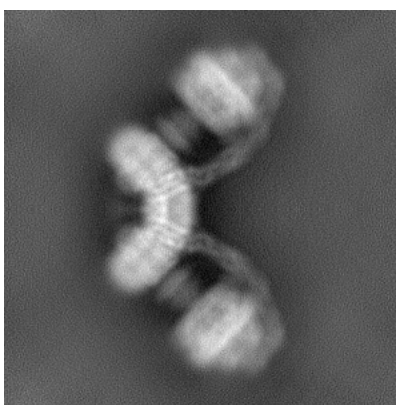


Z

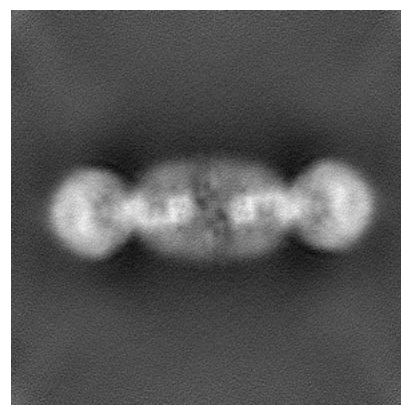
6.1.2 Raw map



X



Y

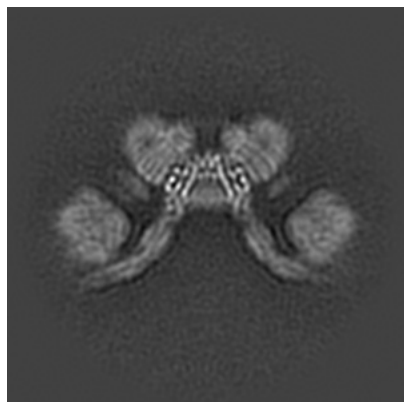


Z

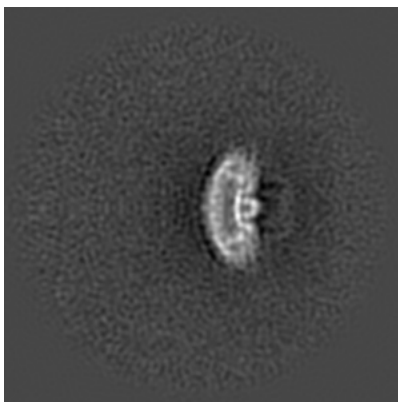
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

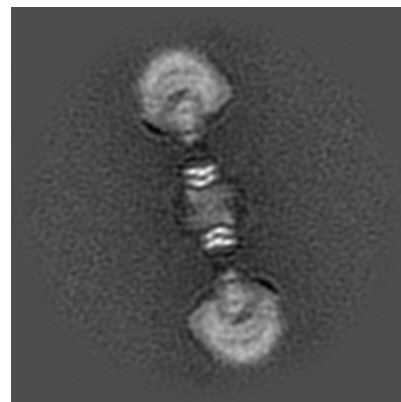
6.2.1 Primary map



X Index: 160

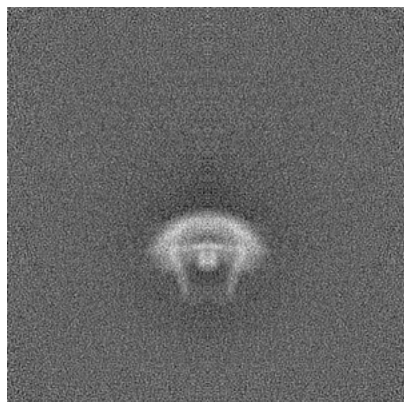


Y Index: 160

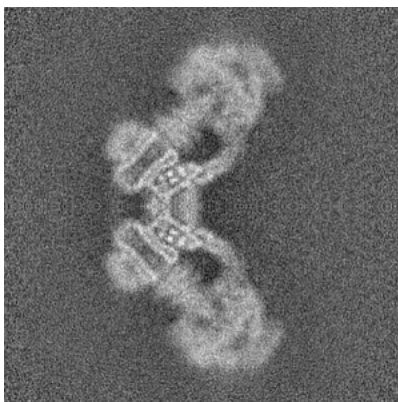


Z Index: 160

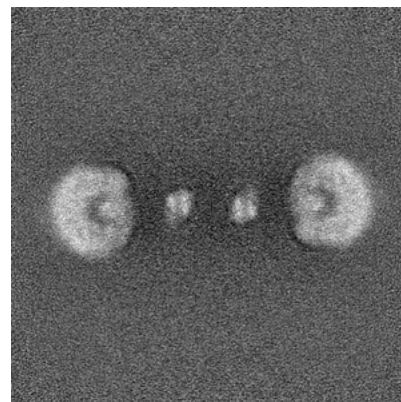
6.2.2 Raw map



X Index: 160



Y Index: 160

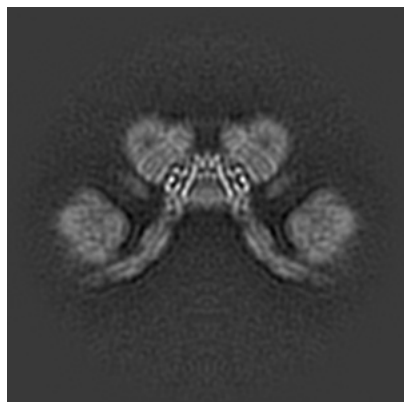


Z Index: 160

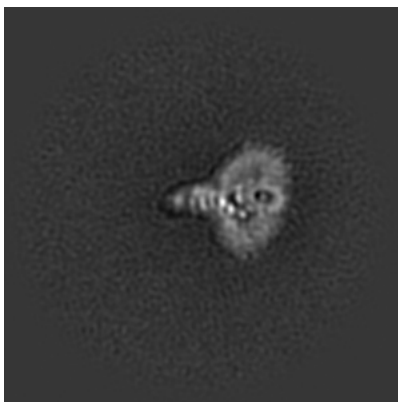
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

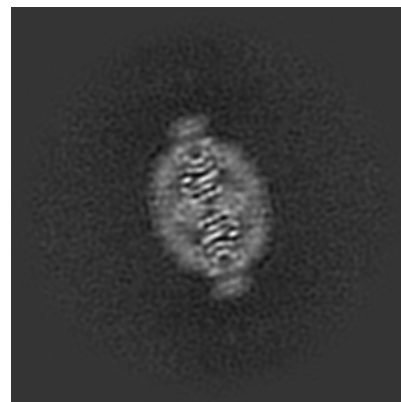
6.3.1 Primary map



X Index: 159

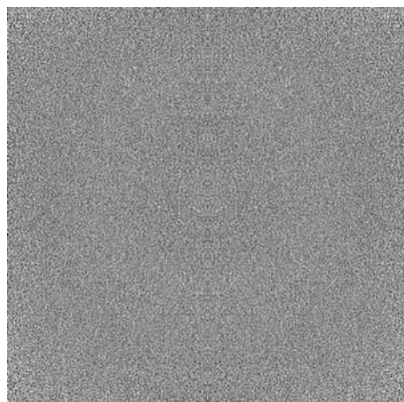


Y Index: 130

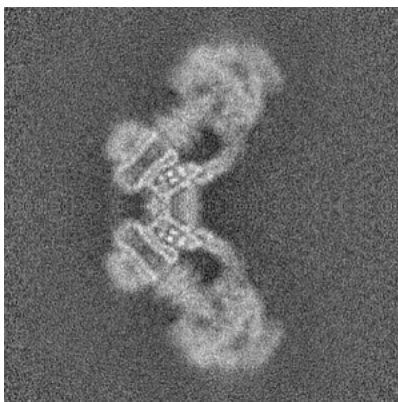


Z Index: 188

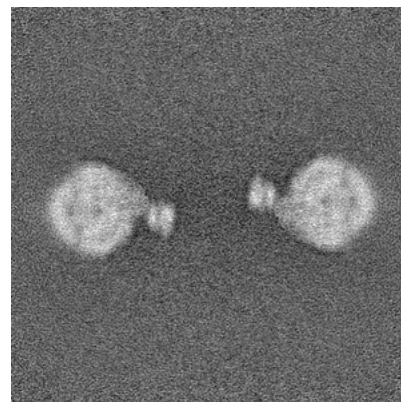
6.3.2 Raw map



X Index: 0



Y Index: 160

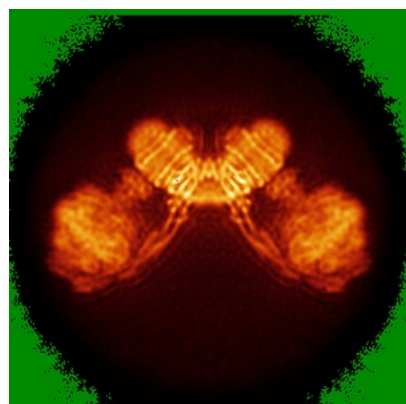


Z Index: 181

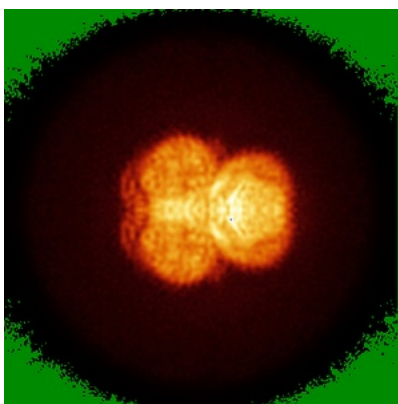
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

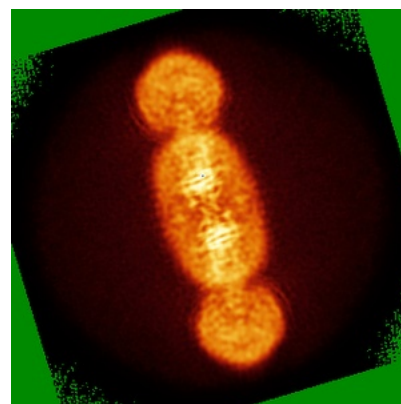
6.4.1 Primary map



X

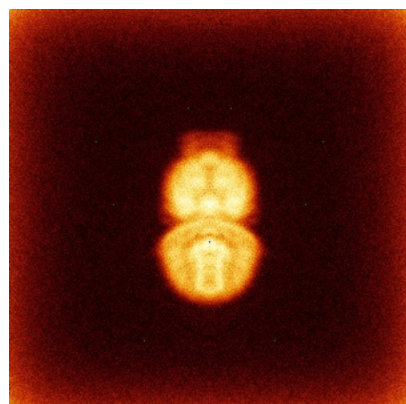


Y

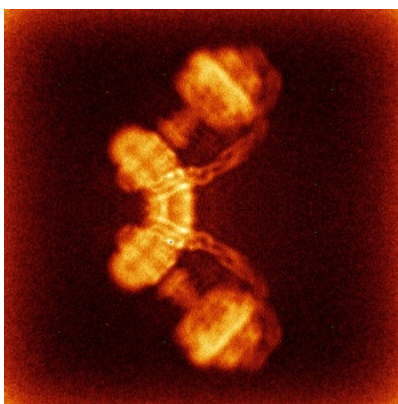


Z

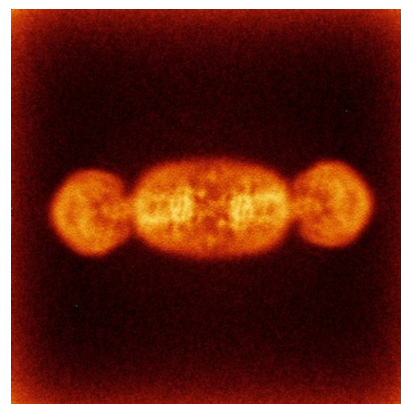
6.4.2 Raw map



X



Y

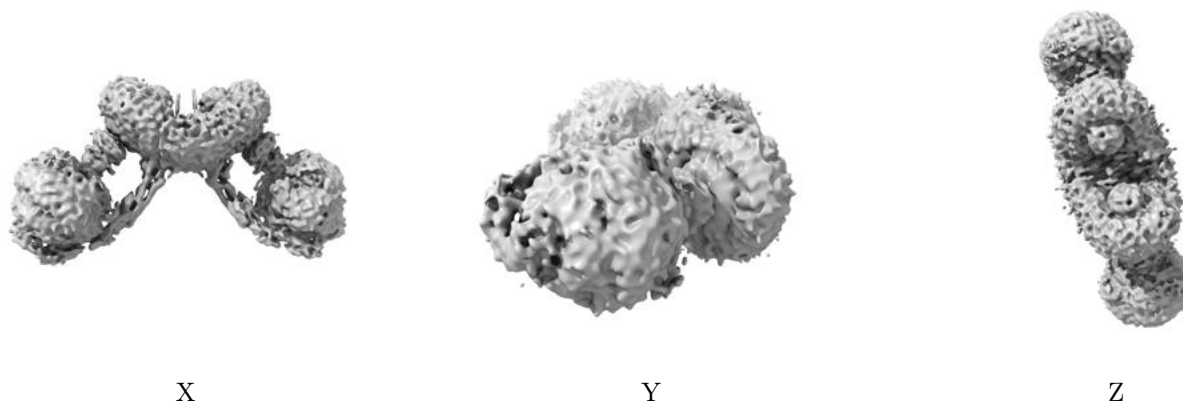


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

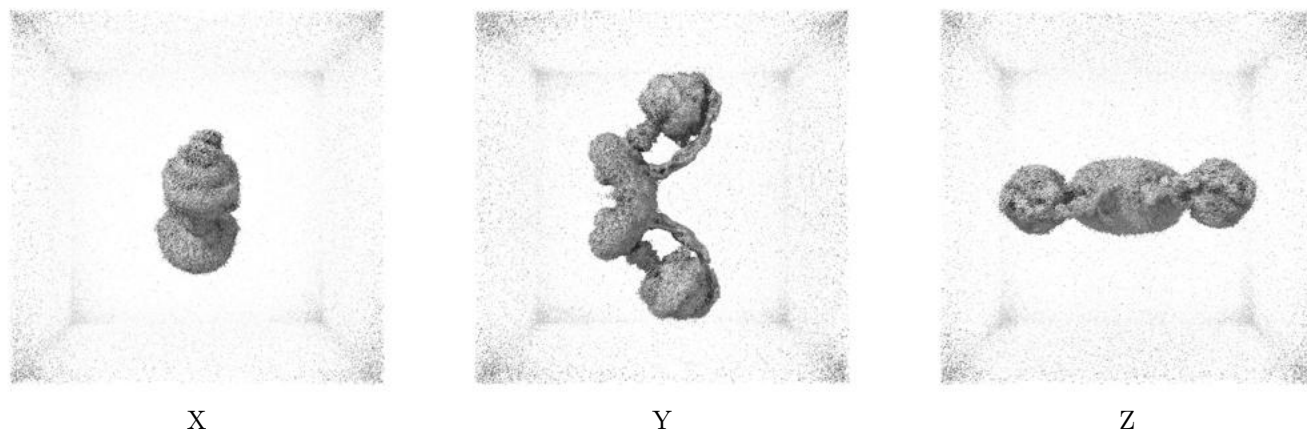
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.156. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

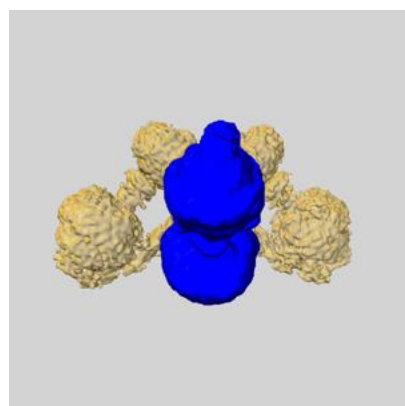
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

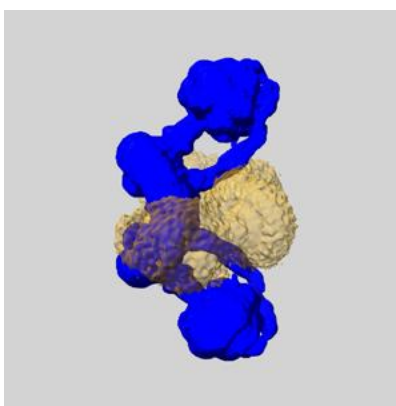
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

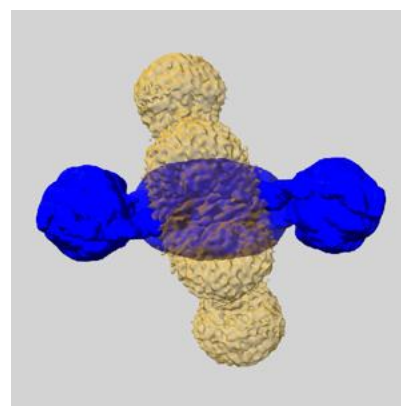
6.6.1 emd_7067_msk_1.map [i](#)



X



Y

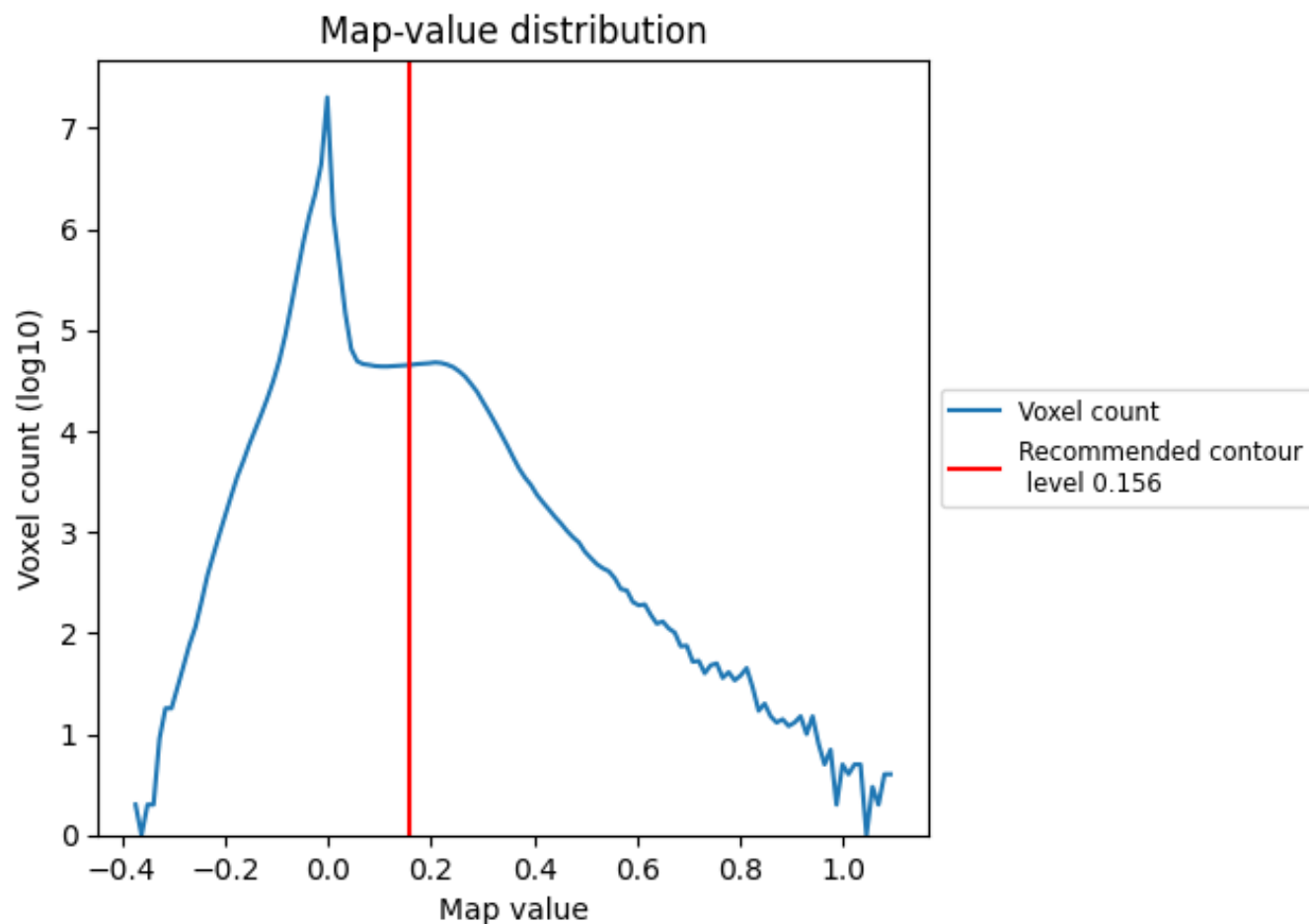


Z

7 Map analysis [i](#)

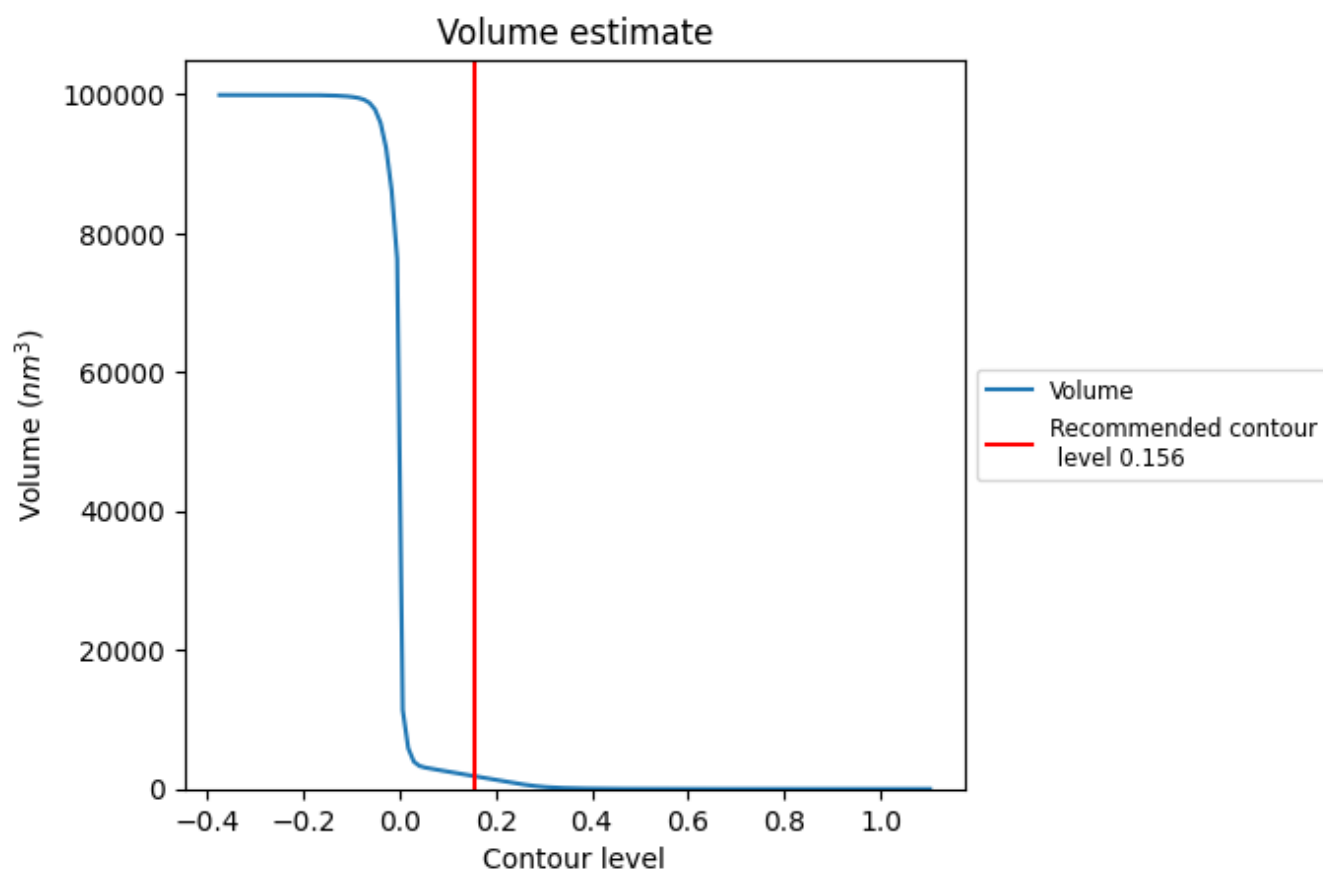
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

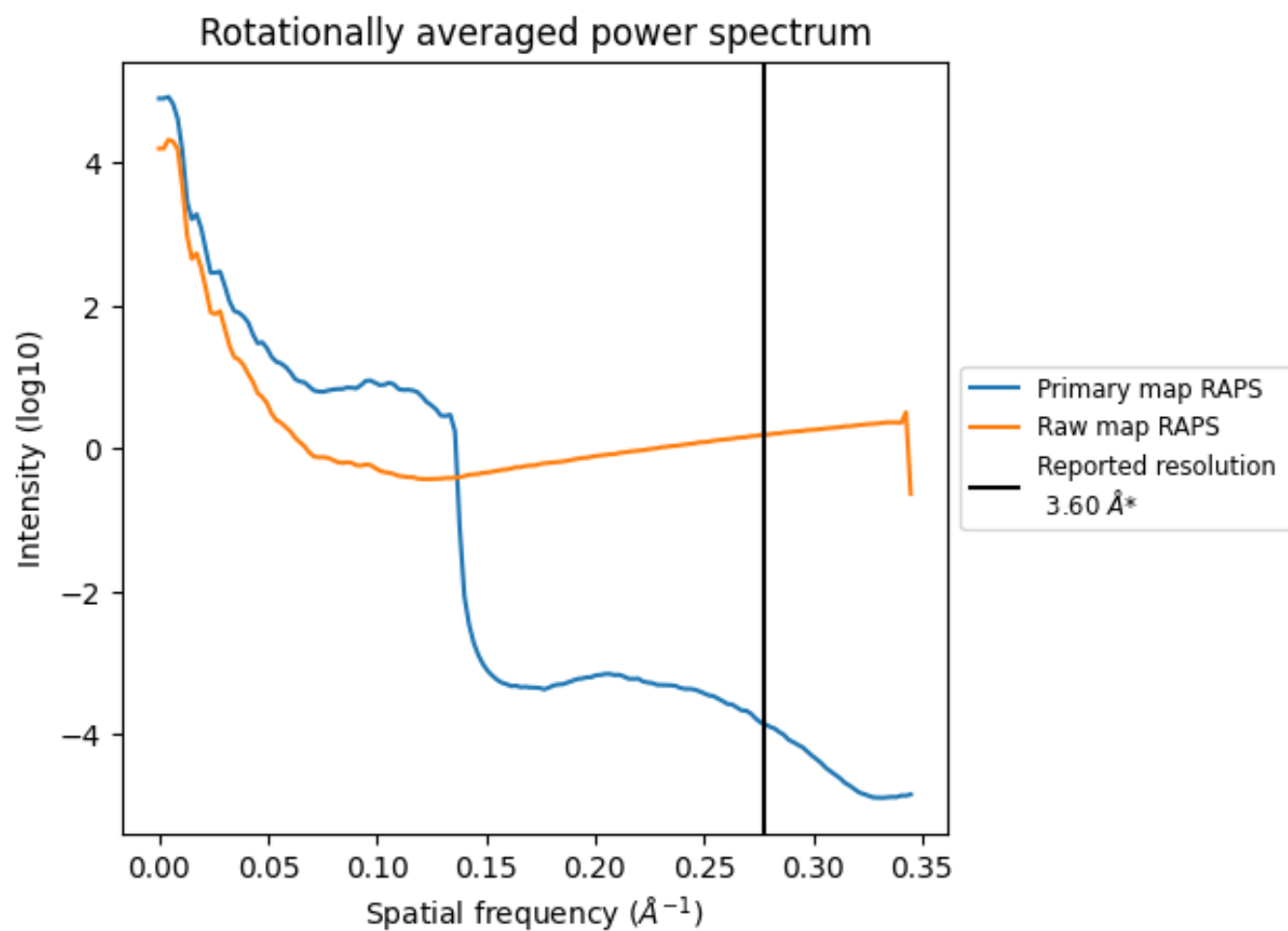
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1866 nm^3 ; this corresponds to an approximate mass of 1686 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

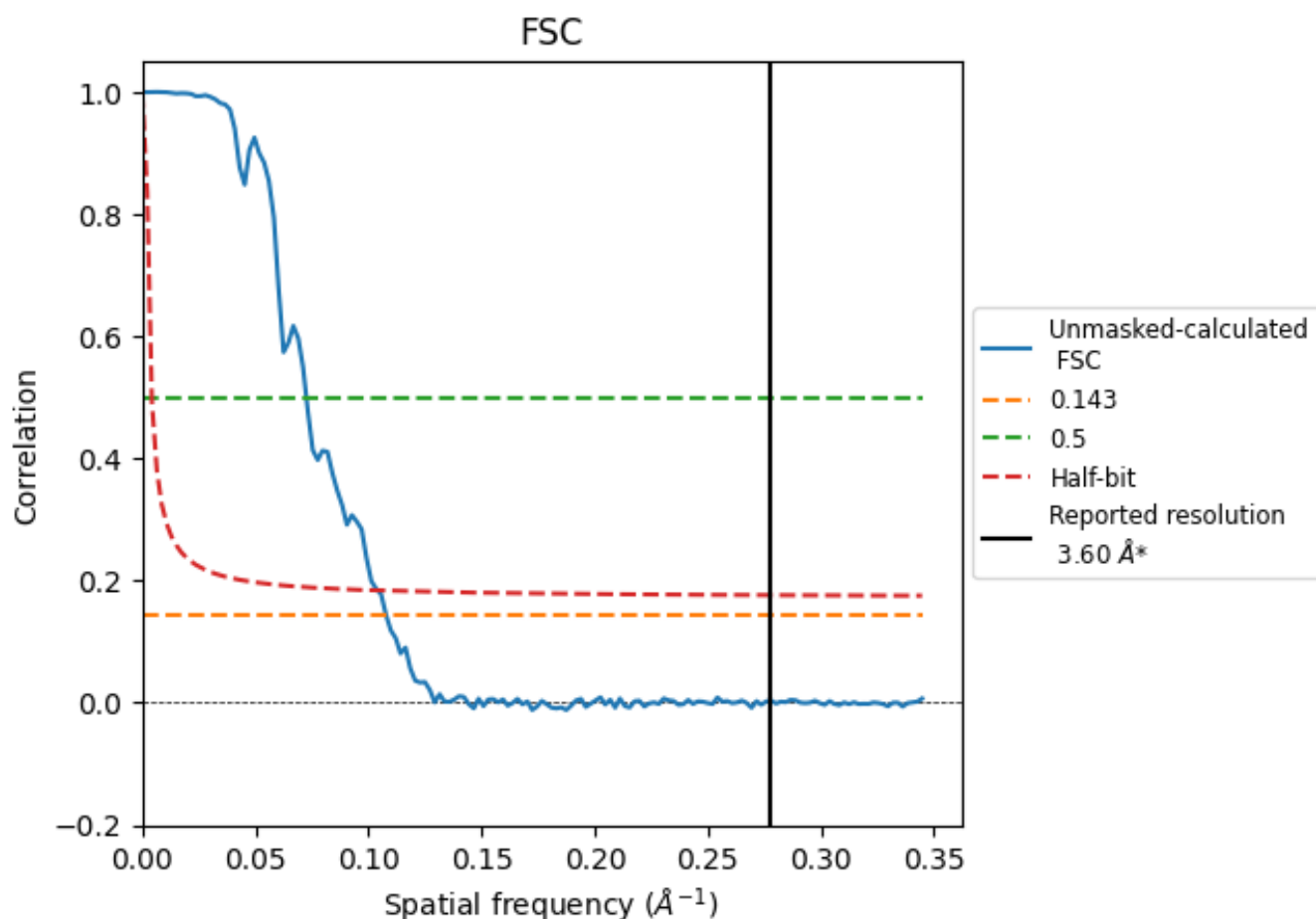


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.278 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

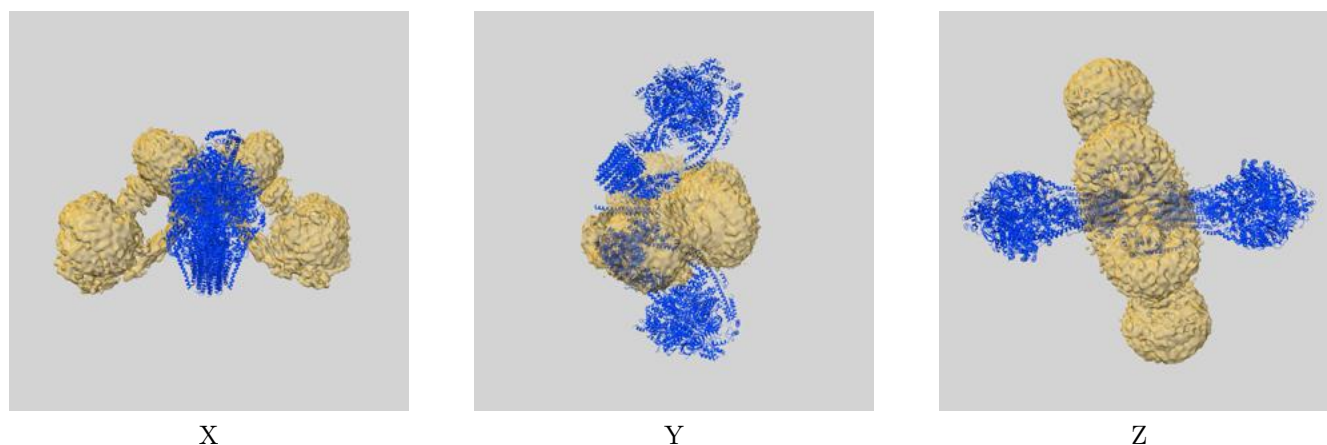
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	9.28	13.77	9.61

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 9.28 differs from the reported value 3.6 by more than 10 %

9 Map-model fit [i](#)

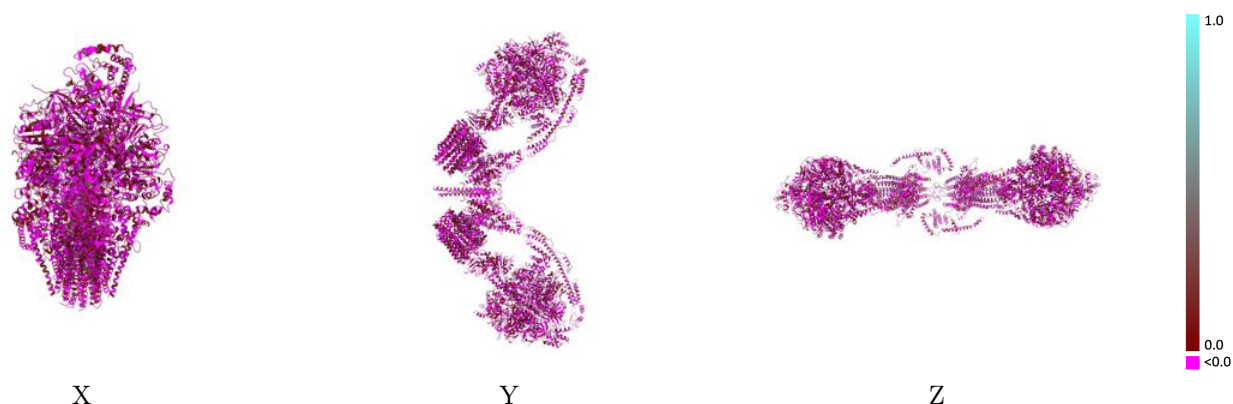
This section contains information regarding the fit between EMDB map EMD-7067 and PDB model 6B8H. Per-residue inclusion information can be found in section [3](#) on page [12](#).

9.1 Map-model overlay [i](#)



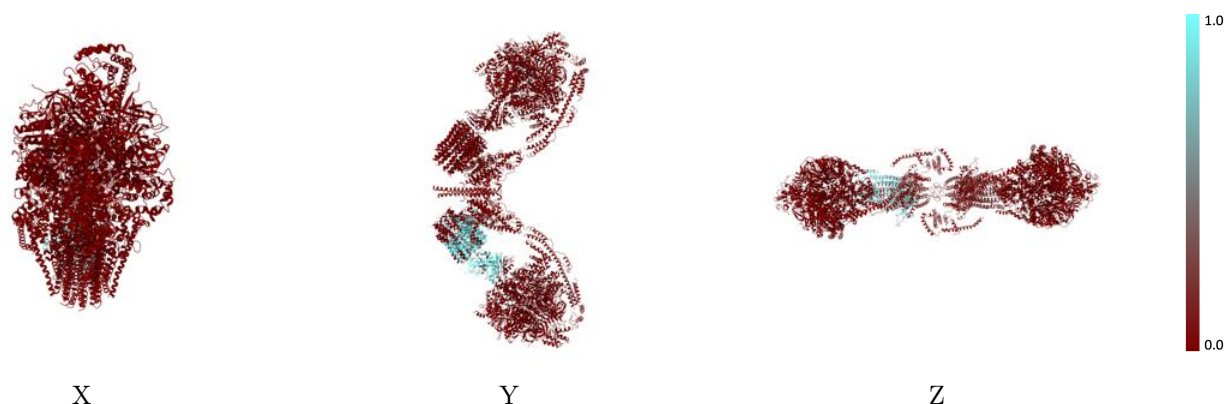
The images above show the 3D surface view of the map at the recommended contour level 0.156 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



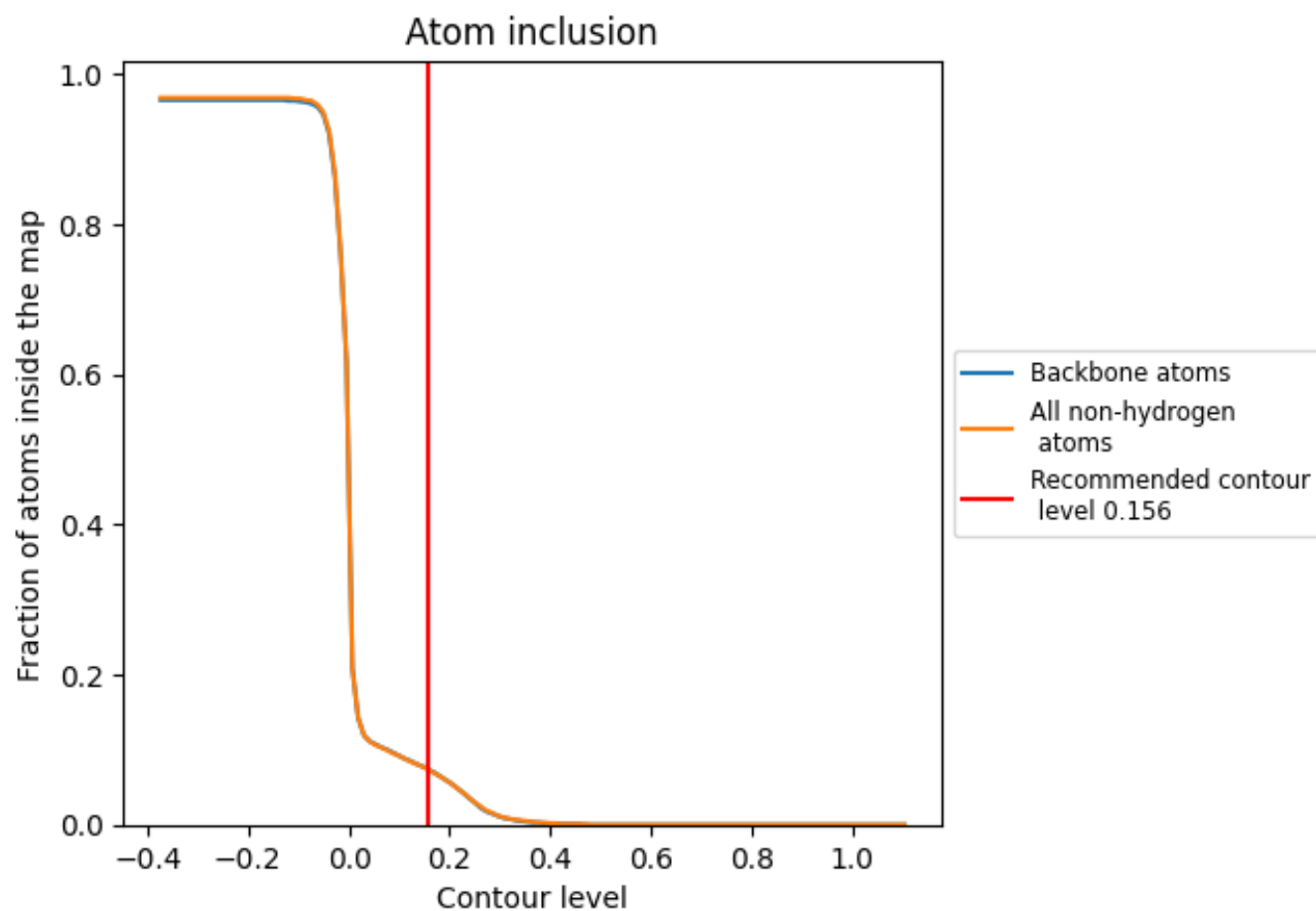
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.156).

9.4 Atom inclusion [i](#)



At the recommended contour level, 8% of all backbone atoms, 7% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.156) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.0740	 0.0010
0	 0.5750	 -0.0100
1	 0.6350	 0.0120
2	 0.6700	 0.0120
3	 0.7660	 -0.0290
4	 0.6780	 -0.0130
5	 0.6540	 -0.0530
6	 0.5630	 0.0120
7	 0.3080	 -0.0080
8	 0.4190	 0.0180
9	 0.4900	 -0.0090
A	 0.0100	 0.0150
B	 0.0000	 0.0050
C	 0.0000	 -0.0040
D	 0.0000	 -0.0040
E	 0.0010	 0.0140
F	 0.0000	 0.0020
G	 0.4170	 0.0020
H	 0.7950	 0.0290
I	 0.5910	 0.0070
J	 0.0000	 -0.0160
K	 0.0000	 -0.0030
L	 0.0000	 0.0190
M	 0.0000	 0.0340
N	 0.0000	 -0.0280
O	 0.0000	 0.0050
P	 0.0000	 0.0020
Q	 0.0000	 0.0060
R	 0.0000	 -0.0160
S	 0.0000	 0.0000
T	 0.0000	 0.0250
U	 0.0000	 -0.0190
V	 0.0000	 0.0110
W	 0.0000	 -0.0040
X	 0.0000	 -0.0050



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Chain	Atom inclusion	Q-score
Y	 0.0000	 0.0060
Z	 0.0000	 0.0020
a	 0.3590	 -0.0080
b	 0.0050	 0.0120
c	 0.0000	 0.0050
d	 0.0440	 0.0250
e	 0.0000	 0.0130
f	 0.0000	 0.0010
g	 0.0000	 -0.0100
h	 0.0000	 0.0980
i	 0.0000	 -0.0340
j	 0.0000	 0.0040
k	 0.4860	 0.0580
l	 0.0000	 0.0020
m	 0.0000	 -0.0070
n	 0.0000	 -0.0040
o	 0.0000	 0.0180
p	 0.0000	 -0.0150
q	 0.0000	 0.0040
r	 0.0000	 -0.0180
s	 0.0040	 0.0420
t	 0.0000	 -0.0100
u	 0.0000	 -0.0330
v	 0.0000	 0.0890
w	 0.0000	 0.0140
x	 0.0000	 -0.0200