



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 10:15 PM UTC

PDB ID : 6KN7 / pdb_00006kn7
EMDB ID : EMD-0728
Title : Structure of human cardiac thin filament in the calcium free state
Authors : Fujii, T.; Yamada, Y.; Namba, K.
Deposited on : 2019-08-03
Resolution : 6.60 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:

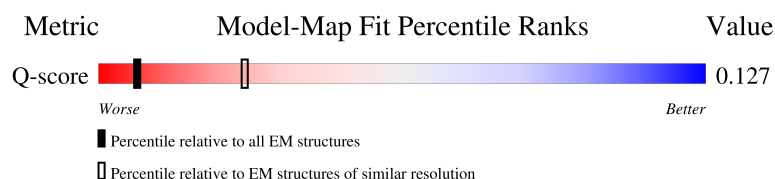
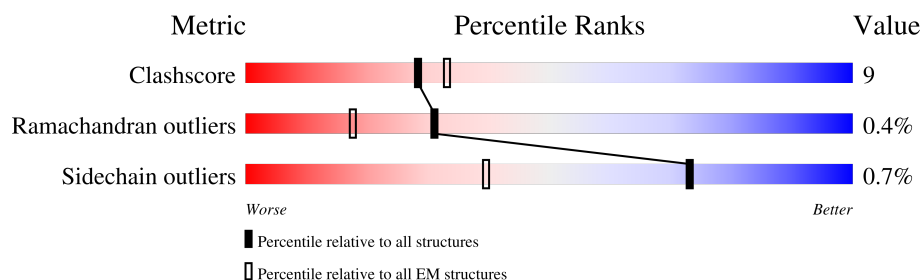
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 6.60 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.



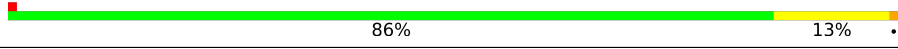
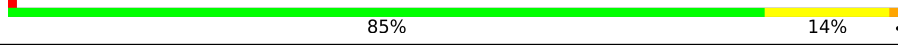
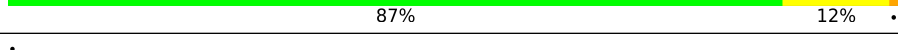
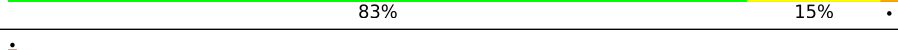
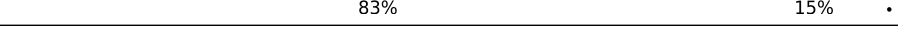
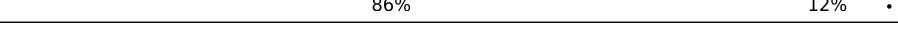
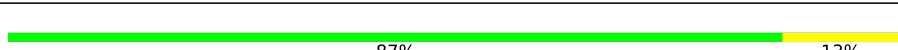
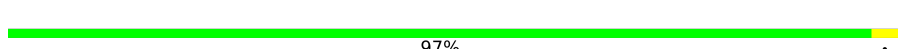
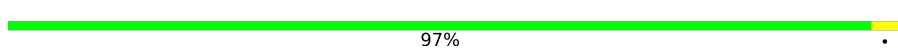
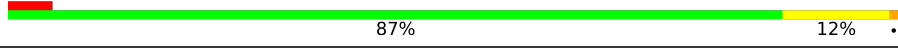
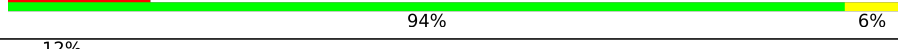
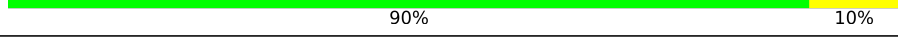
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	531 (6.10 - 7.10)

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	A	375	
1	B	375	
1	C	375	
1	D	375	

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Mol	Chain	Length	Quality of chain
1	E	375	
1	F	375	
1	G	375	
1	H	375	
1	I	375	
1	J	375	
1	K	375	
1	L	375	
1	M	375	
1	N	375	
1	O	375	
2	P	274	
2	Q	274	
2	W	274	
2	X	274	
3	R	31	
3	S	31	
3	Y	31	
3	Z	31	
4	T	186	
4	a	186	
5	U	170	
5	b	170	
6	V	160	
6	c	160	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 61916 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 Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	B	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	C	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	D	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	E	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	F	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	G	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	H	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	I	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	J	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	K	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	L	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	M	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	N	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	O	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		

- Molecule 2 is a protein called Tropomyosin alpha-1 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	274	Total	C	N	O	S	0	0
			2207	1347	376	480	4		
2	Q	274	Total	C	N	O	S	0	0
			2207	1347	376	480	4		
2	W	274	Total	C	N	O	S	0	0
			2207	1347	376	480	4		
2	X	274	Total	C	N	O	S	0	0
			2207	1347	376	480	4		

- Molecule 3 is a protein called Tropomyosin alpha-1 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	R	31	Total	C	N	O	S	0	0
			243	147	43	50	3		
3	S	31	Total	C	N	O	S	0	0
			243	147	43	50	3		
3	Y	31	Total	C	N	O	S	0	0
			243	147	43	50	3		
3	Z	31	Total	C	N	O	S	0	0
			243	147	43	50	3		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-1	ALA	-	expression tag	UNP P09493
R	0	SER	-	expression tag	UNP P09493
S	-1	ALA	-	expression tag	UNP P09493
S	0	SER	-	expression tag	UNP P09493
Y	-1	ALA	-	expression tag	UNP P09493
Y	0	SER	-	expression tag	UNP P09493
Z	-1	ALA	-	expression tag	UNP P09493
Z	0	SER	-	expression tag	UNP P09493

- Molecule 4 is a protein called Troponin T, cardiac muscle.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	T	138	Total	C	N	O	S	0	0
			1211	740	241	229	1		
4	a	138	Total	C	N	O	S	0	0
			1211	740	241	229	1		

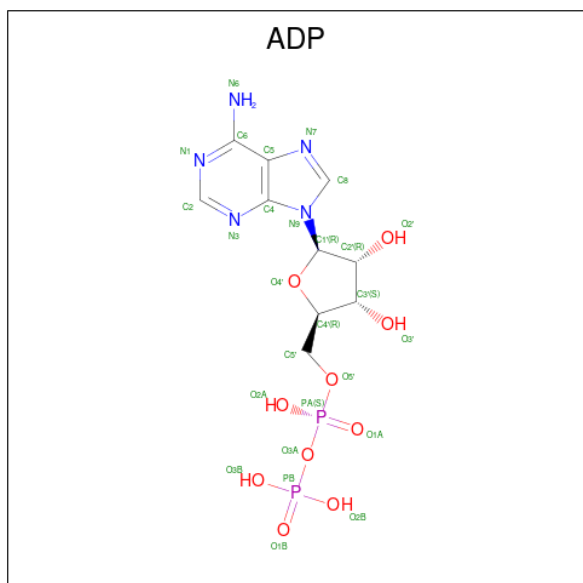
- Molecule 5 is a protein called Troponin I, cardiac muscle.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	U	170	Total 1374	C 848	N 263	O 258	S 5	0	0
5	b	170	Total 1374	C 848	N 263	O 258	S 5	0	0

- Molecule 6 is a protein called Troponin C, slow skeletal and cardiac muscles.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	V	160	Total 1273	C 788	N 195	O 278	S 12	0	0
6	c	160	Total 1273	C 788	N 195	O 278	S 12	0	0

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



Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total 27	C 10	N 5	O 10	P 2	0
7	B	1	Total 27	C 10	N 5	O 10	P 2	0
7	C	1	Total 27	C 10	N 5	O 10	P 2	0
7	D	1	Total 27	C 10	N 5	O 10	P 2	0
7	E	1	Total 27	C 10	N 5	O 10	P 2	0
7	F	1	Total 27	C 10	N 5	O 10	P 2	0

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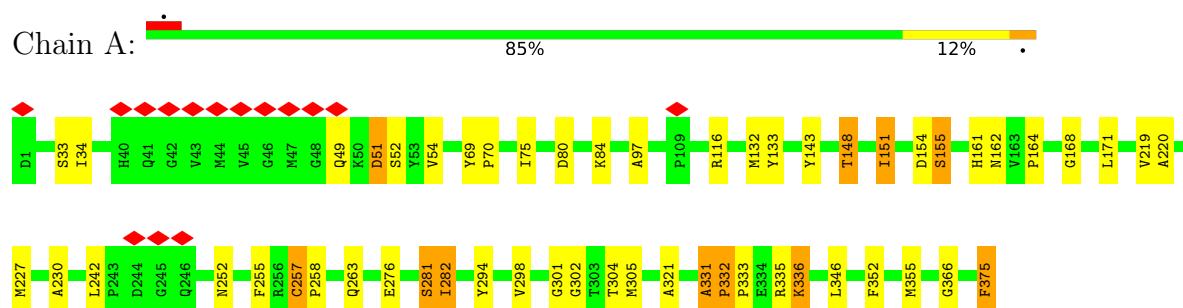
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Mol	Chain	Residues	Atoms					AltConf
7	G	1	Total 27	C 10	N 5	O 10	P 2	0
7	H	1	Total 27	C 10	N 5	O 10	P 2	0
7	I	1	Total 27	C 10	N 5	O 10	P 2	0
7	J	1	Total 27	C 10	N 5	O 10	P 2	0
7	K	1	Total 27	C 10	N 5	O 10	P 2	0
7	L	1	Total 27	C 10	N 5	O 10	P 2	0
7	M	1	Total 27	C 10	N 5	O 10	P 2	0
7	N	1	Total 27	C 10	N 5	O 10	P 2	0
7	O	1	Total 27	C 10	N 5	O 10	P 2	0

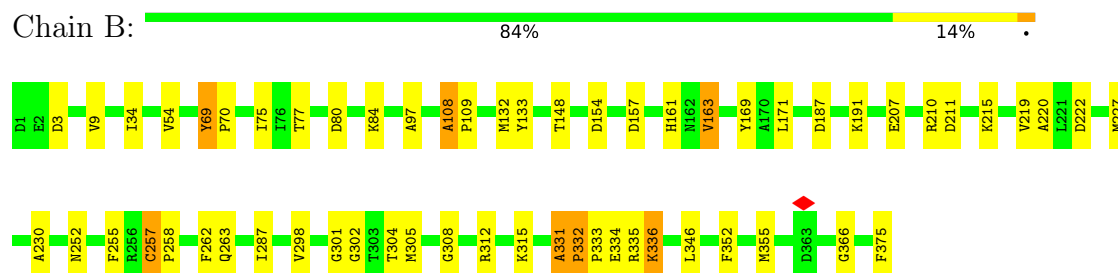
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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.

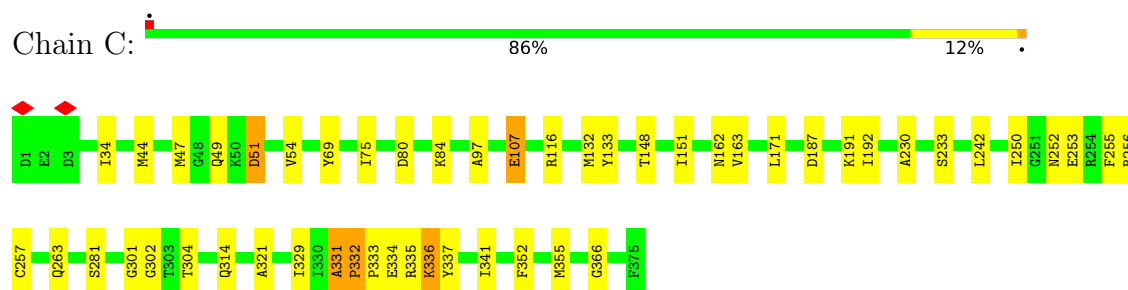
- Molecule 1: Actin, alpha skeletal muscle



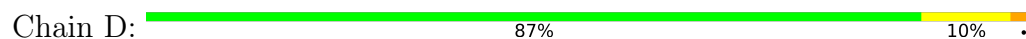
- Molecule 1: Actin, alpha skeletal muscle

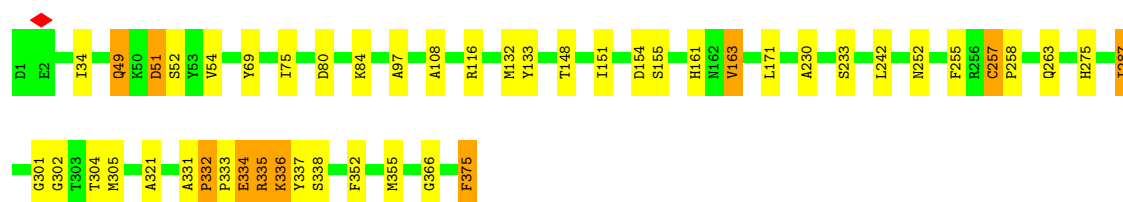


- Molecule 1: Actin, alpha skeletal muscle

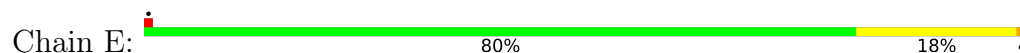


- Molecule 1: Actin, alpha skeletal muscle

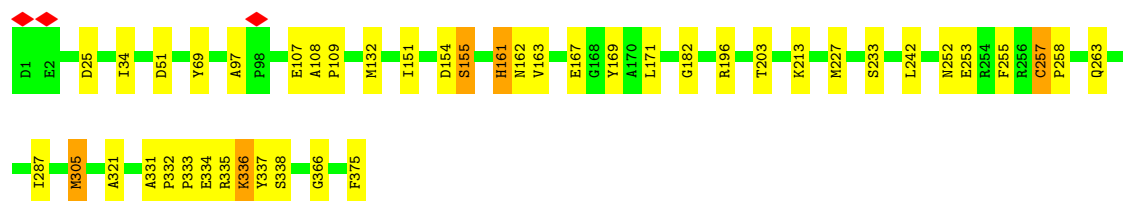
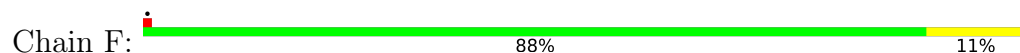




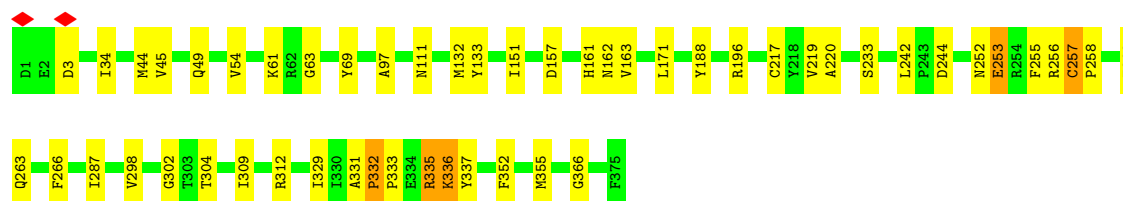
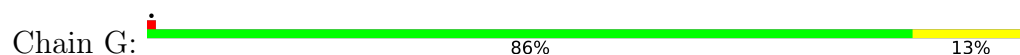
- Molecule 1: Actin, alpha skeletal muscle



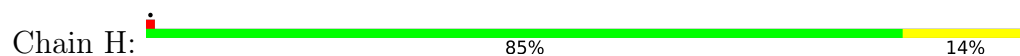
- Molecule 1: Actin, alpha skeletal muscle



- Molecule 1: Actin, alpha skeletal muscle



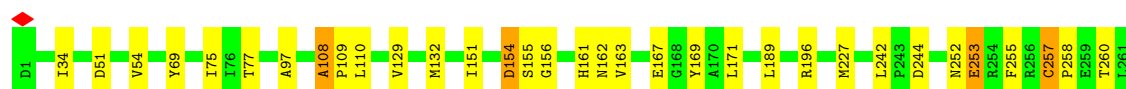
- Molecule 1: Actin, alpha skeletal muscle





- Molecule 1: Actin, alpha skeletal muscle

Chain I: 86% 13%



- Molecule 1: Actin, alpha skeletal muscle

Chain J: 86% 13%



- Molecule 1: Actin, alpha skeletal muscle

Chain K: 87% 12%



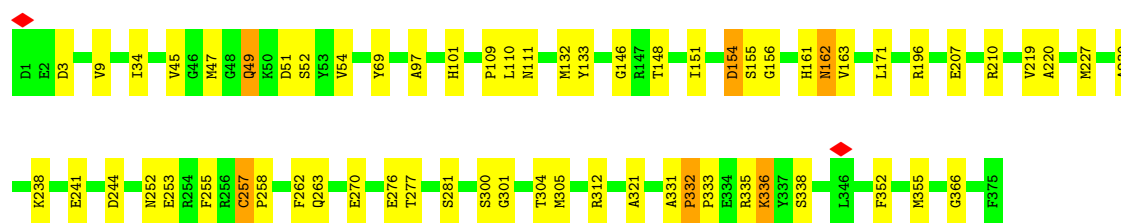
- Molecule 1: Actin, alpha skeletal muscle

Chain L: 83% 15%



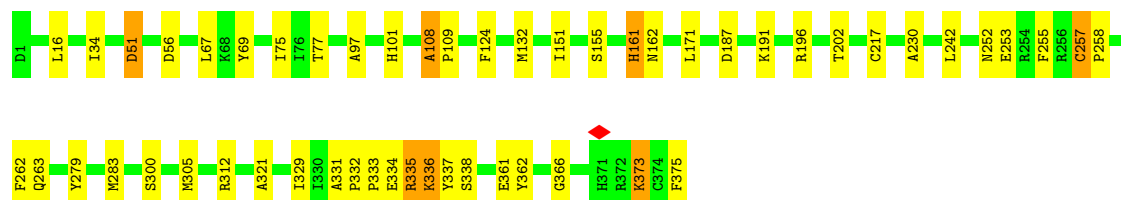
- Molecule 1: Actin, alpha skeletal muscle

Chain M: 83% 15%



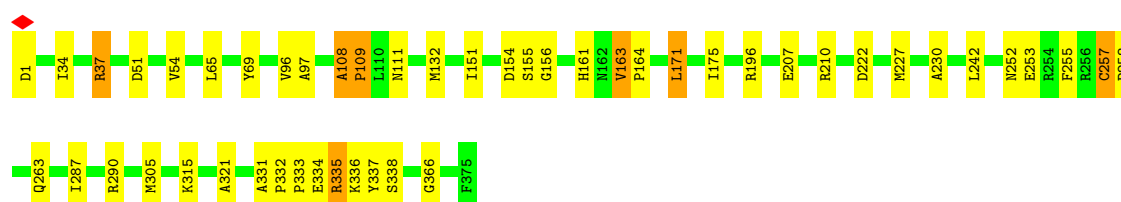
- Molecule 1: Actin, alpha skeletal muscle

Chain N: 86% 12% .



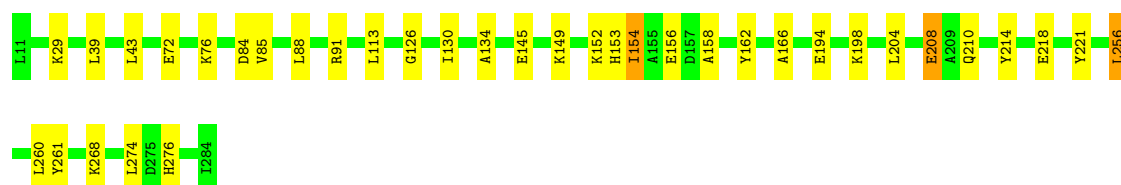
- Molecule 1: Actin, alpha skeletal muscle

Chain O: 87% 11% .



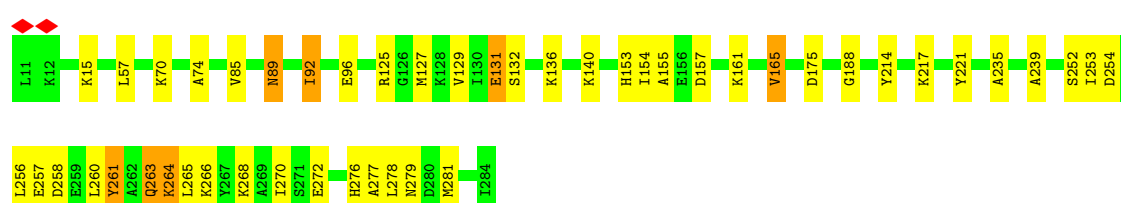
- Molecule 2: Tropomyosin alpha-1 chain

Chain P: 87% 12% .

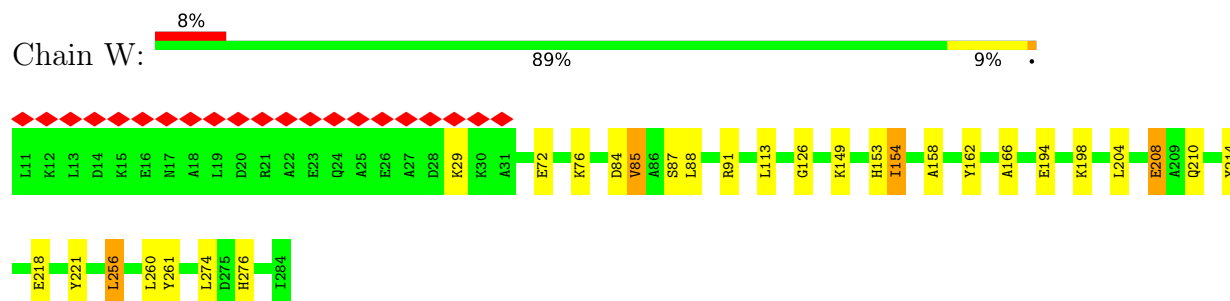


- Molecule 2: Tropomyosin alpha-1 chain

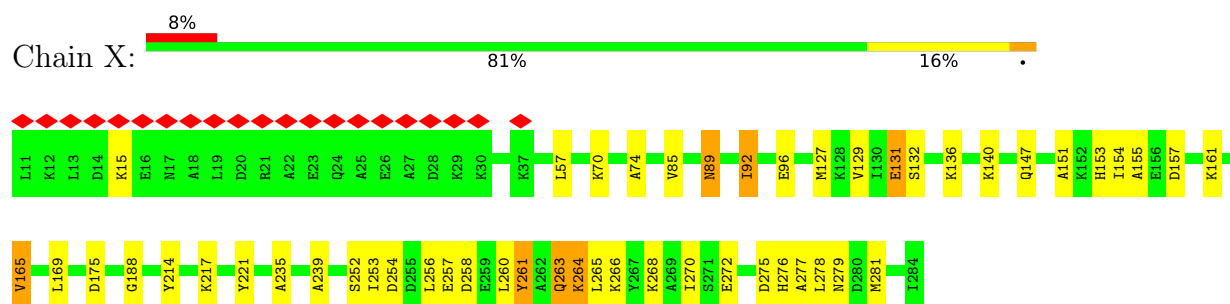
Chain Q: 82% 15% .



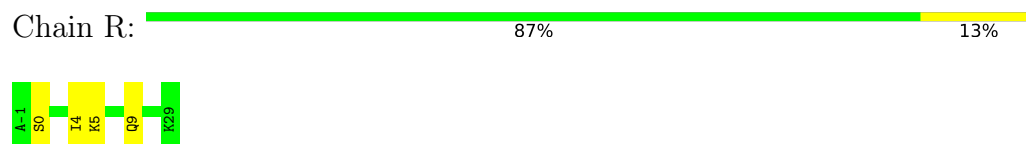
- Molecule 2: Tropomyosin alpha-1 chain



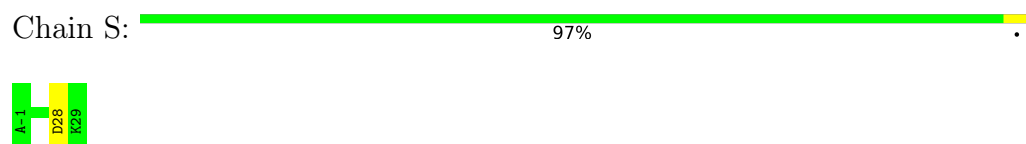
- Molecule 2: Tropomyosin alpha-1 chain



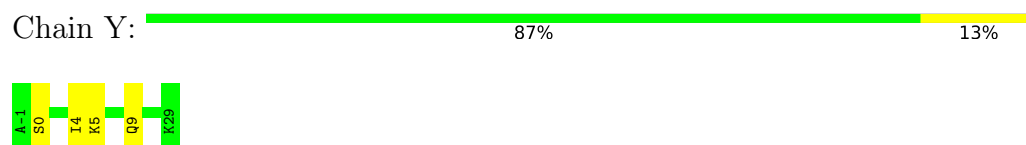
- Molecule 3: Tropomyosin alpha-1 chain



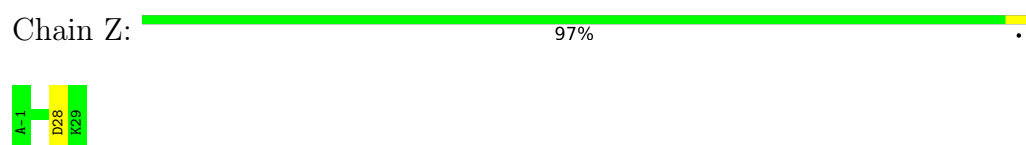
- Molecule 3: Tropomyosin alpha-1 chain



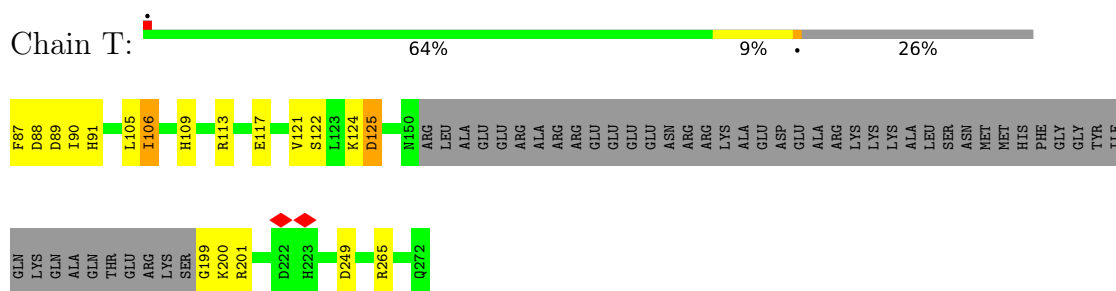
- Molecule 3: Tropomyosin alpha-1 chain



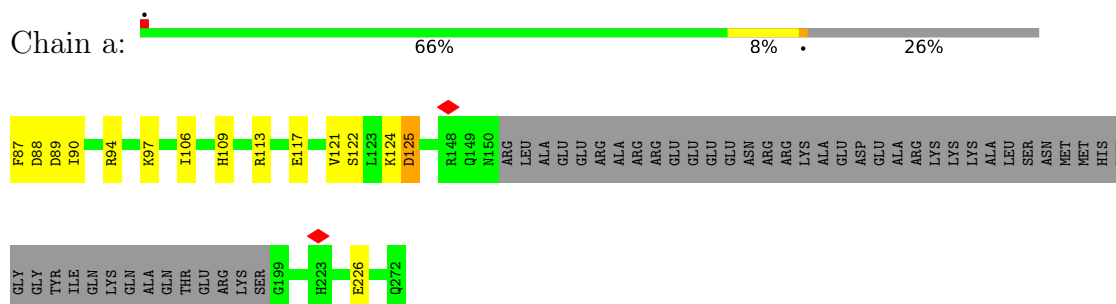
- Molecule 3: Tropomyosin alpha-1 chain



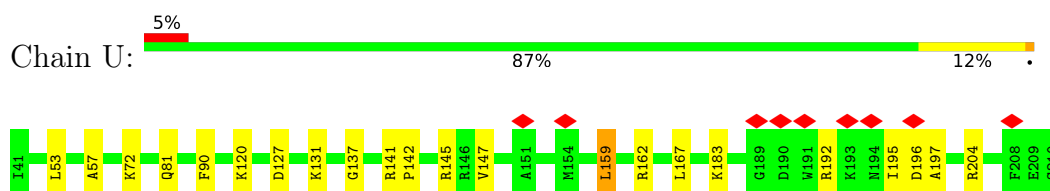
- Molecule 4: Troponin T, cardiac muscle



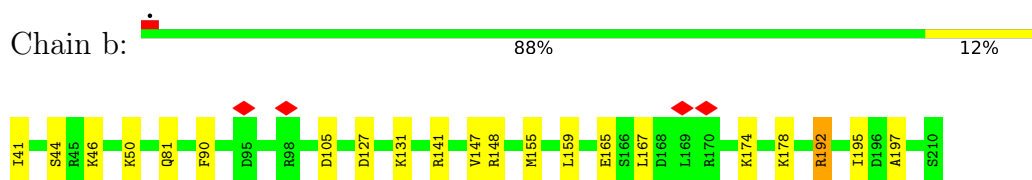
- Molecule 4: Troponin T, cardiac muscle



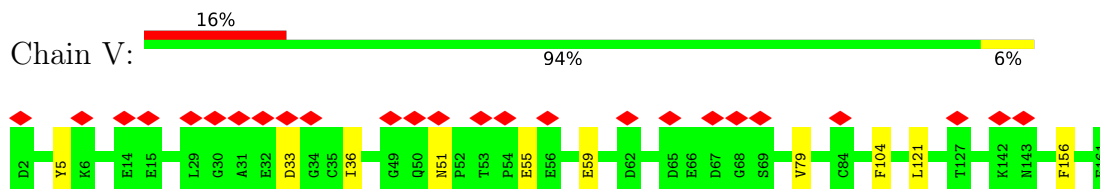
- Molecule 5: Troponin I, cardiac muscle



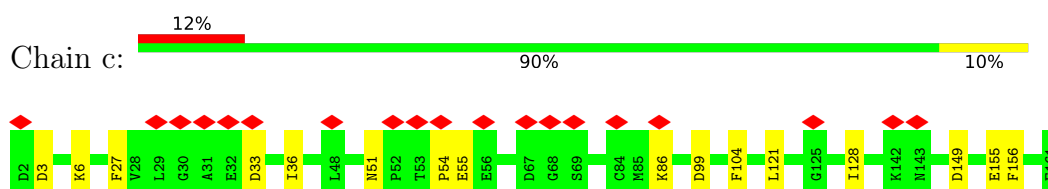
- Molecule 5: Troponin I, cardiac muscle



- Molecule 6: Troponin C, slow skeletal and cardiac muscles



- Molecule 6: Troponin C, slow skeletal and cardiac muscles



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	21588	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 200	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	65	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.226	Depositor
Minimum map value	-0.071	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.0376	Depositor
Map size (Å)	444.0, 444.0, 444.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.22, 2.22, 2.22	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.92	1/2996 (0.0%)	1.30	31/4058 (0.8%)
1	B	0.92	0/2996	1.33	30/4058 (0.7%)
1	C	0.93	0/2996	1.32	36/4058 (0.9%)
1	D	0.92	1/2996 (0.0%)	1.32	36/4058 (0.9%)
1	E	0.92	0/2996	1.33	34/4058 (0.8%)
1	F	0.89	0/2996	1.32	38/4058 (0.9%)
1	G	0.94	2/2996 (0.1%)	1.33	36/4058 (0.9%)
1	H	0.90	1/2996 (0.0%)	1.33	34/4058 (0.8%)
1	I	0.91	0/2996	1.31	34/4058 (0.8%)
1	J	0.90	0/2996	1.33	31/4058 (0.8%)
1	K	0.91	1/2996 (0.0%)	1.31	35/4058 (0.9%)
1	L	0.88	0/2996	1.31	34/4058 (0.8%)
1	M	0.90	0/2996	1.31	35/4058 (0.9%)
1	N	0.92	1/2996 (0.0%)	1.33	37/4058 (0.9%)
1	O	0.89	0/2996	1.31	32/4058 (0.8%)
2	P	1.30	1/2215 (0.0%)	1.27	7/2954 (0.2%)
2	Q	1.31	2/2215 (0.1%)	1.30	9/2954 (0.3%)
2	W	1.30	1/2215 (0.0%)	1.27	8/2954 (0.3%)
2	X	1.32	2/2215 (0.1%)	1.30	9/2954 (0.3%)
3	R	1.23	0/242	1.18	1/316 (0.3%)
3	S	1.17	0/242	1.16	1/316 (0.3%)
3	Y	1.23	0/242	1.18	1/316 (0.3%)
3	Z	1.18	0/242	1.16	1/316 (0.3%)
4	T	1.03	2/1220 (0.2%)	1.13	4/1613 (0.2%)
4	a	1.02	1/1220 (0.1%)	1.13	5/1613 (0.3%)
5	U	0.89	0/1384	1.15	7/1840 (0.4%)
5	b	0.93	0/1384	1.11	8/1840 (0.4%)
6	V	0.97	0/1286	1.20	4/1719 (0.2%)
6	c	0.95	0/1286	1.19	7/1719 (0.4%)
All	All	0.99	16/62548 (0.0%)	1.29	585/84294 (0.7%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	161	HIS	CB-CG	-5.99	1.41	1.50
2	W	256	LEU	CB-CG	-5.89	1.41	1.53
2	P	256	LEU	CB-CG	-5.89	1.41	1.53
1	K	161	HIS	CB-CG	-5.80	1.42	1.50
2	X	57	LEU	CG-CD2	-5.76	1.33	1.52
2	Q	57	LEU	CG-CD2	-5.75	1.33	1.52
1	D	161	HIS	CB-CG	-5.62	1.42	1.50
2	X	276	HIS	CB-CG	-5.46	1.42	1.50
2	Q	276	HIS	CB-CG	-5.39	1.42	1.50
1	G	161	HIS	CG-CD2	-5.30	1.30	1.35
1	N	67	LEU	CB-CG	5.23	1.64	1.53
1	G	256	ARG	NE-CZ	5.17	1.38	1.33
4	a	109	HIS	CB-CG	-5.17	1.43	1.50
4	T	265	ARG	NE-CZ	5.16	1.38	1.33
4	T	109	HIS	CB-CG	-5.12	1.43	1.50
1	A	161	HIS	CB-CG	-5.04	1.43	1.50

All (585) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	a	125	ASP	N-CA-C	-9.26	101.27	111.36
4	T	125	ASP	N-CA-C	-9.23	101.30	111.36
1	J	163	VAL	N-CA-C	9.03	116.49	107.55
1	K	163	VAL	N-CA-C	9.02	118.01	107.73
1	O	163	VAL	N-CA-C	8.72	117.13	109.02
1	C	163	VAL	N-CA-C	8.55	117.48	107.73
1	D	163	VAL	N-CA-C	8.52	117.44	107.73
1	N	263	GLN	CA-C-N	8.47	128.12	119.82
1	N	263	GLN	C-N-CA	8.47	128.12	119.82
1	O	263	GLN	CA-C-N	8.34	127.98	119.56
1	O	263	GLN	C-N-CA	8.34	127.98	119.56
1	F	69	TYR	CA-C-N	8.28	128.01	119.56
1	F	69	TYR	C-N-CA	8.28	128.01	119.56
5	U	147	VAL	N-CA-C	8.27	118.91	108.82
1	B	69	TYR	CA-C-N	8.26	127.90	119.56
1	B	69	TYR	C-N-CA	8.26	127.90	119.56
1	E	163	VAL	N-CA-C	8.22	116.85	107.89
6	V	51	ASN	CA-C-N	8.21	128.16	120.03
6	V	51	ASN	C-N-CA	8.21	128.16	120.03
1	H	263	GLN	CA-C-N	8.19	127.91	119.56
1	H	263	GLN	C-N-CA	8.19	127.91	119.56
1	K	111	ASN	CA-CB-CG	8.18	120.78	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	263	GLN	CA-C-N	8.16	127.88	119.56
1	K	263	GLN	C-N-CA	8.16	127.88	119.56
1	G	163	VAL	N-CA-C	8.09	117.24	107.61
1	A	263	GLN	CA-C-N	8.05	127.69	119.56
1	A	263	GLN	C-N-CA	8.05	127.69	119.56
1	O	69	TYR	CA-C-N	8.05	127.77	119.56
1	O	69	TYR	C-N-CA	8.05	127.77	119.56
1	B	366	GLY	CA-C-N	8.03	127.75	119.56
1	B	366	GLY	C-N-CA	8.03	127.75	119.56
1	L	163	VAL	N-CA-C	8.02	116.63	107.89
1	K	366	GLY	CA-C-N	8.01	127.73	119.56
1	K	366	GLY	C-N-CA	8.01	127.73	119.56
1	E	69	TYR	CA-C-N	7.99	127.71	119.56
1	E	69	TYR	C-N-CA	7.99	127.71	119.56
5	U	81	GLN	CA-C-N	7.93	127.88	120.03
5	U	81	GLN	C-N-CA	7.93	127.88	120.03
1	N	34	ILE	N-CA-C	7.88	120.21	108.46
5	b	81	GLN	CA-C-N	7.88	127.89	119.78
5	b	81	GLN	C-N-CA	7.88	127.89	119.78
1	J	366	GLY	CA-C-N	7.87	127.59	119.56
1	J	366	GLY	C-N-CA	7.87	127.59	119.56
1	F	263	GLN	CA-C-N	7.86	127.57	119.56
1	F	263	GLN	C-N-CA	7.86	127.57	119.56
1	E	263	GLN	CA-C-N	7.85	127.57	119.56
1	E	263	GLN	C-N-CA	7.85	127.57	119.56
1	H	366	GLY	CA-C-N	7.85	127.51	119.82
1	H	366	GLY	C-N-CA	7.85	127.51	119.82
1	N	69	TYR	CA-C-N	7.84	128.03	119.87
1	N	69	TYR	C-N-CA	7.84	128.03	119.87
1	K	69	TYR	CA-C-N	7.83	127.55	119.56
1	K	69	TYR	C-N-CA	7.83	127.55	119.56
6	c	104	PHE	CA-CB-CG	7.83	121.63	113.80
1	J	219	VAL	N-CA-C	7.78	118.58	110.72
6	c	27	PHE	CA-CB-CG	7.73	121.53	113.80
1	E	111	ASN	CA-CB-CG	7.69	120.29	112.60
1	M	69	TYR	CA-C-N	7.68	127.40	119.56
1	M	69	TYR	C-N-CA	7.68	127.40	119.56
1	D	263	GLN	CA-C-N	7.68	127.32	119.56
1	D	263	GLN	C-N-CA	7.68	127.32	119.56
1	J	263	GLN	CA-C-N	7.67	127.39	119.56
1	J	263	GLN	C-N-CA	7.67	127.39	119.56
1	G	366	GLY	CA-C-N	7.67	127.38	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	366	GLY	C-N-CA	7.67	127.38	119.56
1	E	366	GLY	CA-C-N	7.65	127.37	119.56
1	E	366	GLY	C-N-CA	7.65	127.37	119.56
1	A	69	TYR	CA-C-N	7.64	127.82	119.87
1	A	69	TYR	C-N-CA	7.64	127.82	119.87
1	C	69	TYR	CA-C-N	7.61	127.32	119.56
1	C	69	TYR	C-N-CA	7.61	127.32	119.56
1	G	69	TYR	CA-C-N	7.61	127.32	119.56
1	G	69	TYR	C-N-CA	7.61	127.32	119.56
1	H	69	TYR	CA-C-N	7.60	127.31	119.56
1	H	69	TYR	C-N-CA	7.60	127.31	119.56
1	L	69	TYR	CA-C-N	7.59	127.31	119.56
1	L	69	TYR	C-N-CA	7.59	127.31	119.56
1	J	69	TYR	CA-C-N	7.58	128.23	120.04
1	J	69	TYR	C-N-CA	7.58	128.23	120.04
1	L	366	GLY	CA-C-N	7.57	127.28	119.56
1	L	366	GLY	C-N-CA	7.57	127.28	119.56
6	V	156	PHE	CA-CB-CG	7.54	121.34	113.80
1	M	366	GLY	CA-C-N	7.47	127.18	119.56
1	M	366	GLY	C-N-CA	7.47	127.18	119.56
1	F	366	GLY	CA-C-N	7.47	128.13	119.47
1	F	366	GLY	C-N-CA	7.47	128.13	119.47
1	B	263	GLN	CA-C-N	7.46	127.09	119.56
1	B	263	GLN	C-N-CA	7.46	127.09	119.56
1	G	263	GLN	CA-C-N	7.45	127.08	119.56
1	G	263	GLN	C-N-CA	7.45	127.08	119.56
1	D	366	GLY	CA-C-N	7.43	127.14	119.56
1	D	366	GLY	C-N-CA	7.43	127.14	119.56
1	L	332	PRO	CA-C-N	7.38	127.09	119.56
1	L	332	PRO	C-N-CA	7.38	127.09	119.56
1	H	97	ALA	CA-C-N	7.38	127.09	119.56
1	H	97	ALA	C-N-CA	7.38	127.09	119.56
1	C	263	GLN	CA-C-N	7.37	127.07	119.56
1	C	263	GLN	C-N-CA	7.37	127.07	119.56
1	B	148	THR	N-CA-C	-7.34	104.85	114.31
1	L	263	GLN	CA-C-N	7.31	126.94	119.56
1	L	263	GLN	C-N-CA	7.31	126.94	119.56
1	F	331	ALA	CA-C-N	7.29	127.89	120.38
1	F	331	ALA	C-N-CA	7.29	127.89	120.38
1	L	171	LEU	CA-C-N	7.29	127.00	119.56
1	L	171	LEU	C-N-CA	7.29	127.00	119.56
1	D	34	ILE	N-CA-C	7.28	119.31	108.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	263	GLN	CA-C-N	7.23	126.86	119.56
1	M	263	GLN	C-N-CA	7.23	126.86	119.56
1	D	69	TYR	CA-C-N	7.22	127.83	120.04
1	D	69	TYR	C-N-CA	7.22	127.83	120.04
1	E	34	ILE	N-CA-C	7.21	119.20	108.46
1	J	97	ALA	CA-C-N	7.20	126.90	119.56
1	J	97	ALA	C-N-CA	7.20	126.90	119.56
1	B	331	ALA	CA-C-N	7.18	127.78	120.38
1	B	331	ALA	C-N-CA	7.18	127.78	120.38
1	L	34	ILE	N-CA-C	7.14	118.10	108.11
1	N	329	ILE	N-CA-C	7.14	118.16	108.17
1	O	151	ILE	CB-CA-C	-7.12	102.08	110.91
1	O	97	ALA	CA-C-N	7.12	126.82	119.56
1	O	97	ALA	C-N-CA	7.12	126.82	119.56
1	F	25	ASP	CA-CB-CG	7.11	119.71	112.60
1	C	366	GLY	CA-C-N	7.10	126.81	119.56
1	C	366	GLY	C-N-CA	7.10	126.81	119.56
6	c	51	ASN	CA-C-N	7.10	127.02	119.85
6	c	51	ASN	C-N-CA	7.10	127.02	119.85
1	O	171	LEU	CA-C-N	7.08	126.79	119.56
1	O	171	LEU	C-N-CA	7.08	126.79	119.56
1	I	263	GLN	CA-C-N	7.07	126.70	119.56
1	I	263	GLN	C-N-CA	7.07	126.70	119.56
1	O	366	GLY	CA-C-N	7.07	126.77	119.56
1	O	366	GLY	C-N-CA	7.07	126.77	119.56
1	I	171	LEU	CA-C-N	7.07	126.77	119.56
1	I	171	LEU	C-N-CA	7.07	126.77	119.56
1	A	366	GLY	CA-C-N	7.02	126.72	119.56
1	A	366	GLY	C-N-CA	7.02	126.72	119.56
1	J	321	ALA	CA-C-N	7.02	127.01	119.78
1	J	321	ALA	C-N-CA	7.02	127.01	119.78
1	D	97	ALA	CA-C-N	7.01	126.71	119.56
1	D	97	ALA	C-N-CA	7.01	126.71	119.56
1	A	97	ALA	CA-C-N	7.01	126.71	119.56
1	A	97	ALA	C-N-CA	7.01	126.71	119.56
1	H	171	LEU	CA-C-N	7.00	126.70	119.56
1	H	171	LEU	C-N-CA	7.00	126.70	119.56
1	J	148	THR	N-CA-C	-7.00	105.28	114.31
1	A	171	LEU	CA-C-N	6.99	126.69	119.56
1	A	171	LEU	C-N-CA	6.99	126.69	119.56
1	N	257	CYS	CA-C-N	6.96	127.55	119.47
1	N	257	CYS	C-N-CA	6.96	127.55	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	171	LEU	CA-C-N	6.96	126.66	119.56
1	C	171	LEU	C-N-CA	6.96	126.66	119.56
1	I	97	ALA	CA-C-N	6.96	126.66	119.56
1	I	97	ALA	C-N-CA	6.96	126.66	119.56
1	A	75	ILE	N-CA-C	6.92	117.86	108.17
1	E	161	HIS	N-CA-C	6.91	120.19	111.69
1	I	69	TYR	CA-C-N	6.91	126.60	119.56
1	I	69	TYR	C-N-CA	6.91	126.60	119.56
1	I	366	GLY	CA-C-N	6.90	126.59	119.56
1	I	366	GLY	C-N-CA	6.90	126.59	119.56
1	N	366	GLY	CA-C-N	6.89	126.59	119.56
1	N	366	GLY	C-N-CA	6.89	126.59	119.56
1	G	171	LEU	CA-C-N	6.87	126.57	119.56
1	G	171	LEU	C-N-CA	6.87	126.57	119.56
1	E	332	PRO	CA-C-N	6.82	126.52	119.56
1	E	332	PRO	C-N-CA	6.82	126.52	119.56
1	M	171	LEU	CA-C-N	6.82	126.51	119.56
1	M	171	LEU	C-N-CA	6.82	126.51	119.56
1	F	257	CYS	CA-C-N	6.81	127.37	119.47
1	F	257	CYS	C-N-CA	6.81	127.37	119.47
2	P	126	GLY	N-CA-C	-6.80	104.62	112.50
2	W	126	GLY	N-CA-C	-6.78	104.64	112.50
1	I	151	ILE	CA-C-N	-6.77	114.06	122.93
1	I	151	ILE	C-N-CA	-6.77	114.06	122.93
1	B	132	MET	N-CA-C	6.76	119.45	109.24
1	J	171	LEU	CA-C-N	6.76	126.45	119.56
1	J	171	LEU	C-N-CA	6.76	126.45	119.56
2	P	208	GLU	N-CA-C	-6.75	103.86	111.14
2	W	208	GLU	N-CA-C	-6.73	103.87	111.14
1	G	332	PRO	CA-C-N	6.72	126.42	119.56
1	G	332	PRO	C-N-CA	6.72	126.42	119.56
1	A	331	ALA	CA-C-N	6.72	127.30	120.38
1	A	331	ALA	C-N-CA	6.72	127.30	120.38
1	A	257	CYS	CA-C-N	6.71	127.25	119.47
1	A	257	CYS	C-N-CA	6.71	127.25	119.47
1	I	331	ALA	CA-C-N	6.71	127.29	120.38
1	I	331	ALA	C-N-CA	6.71	127.29	120.38
1	L	31	PHE	CA-C-N	6.71	126.67	119.76
1	L	31	PHE	C-N-CA	6.71	126.67	119.76
1	N	151	ILE	CA-C-N	-6.70	114.41	123.12
1	N	151	ILE	C-N-CA	-6.70	114.41	123.12
1	M	111	ASN	CA-CB-CG	6.68	119.28	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	171	LEU	CA-C-N	6.67	126.37	119.56
1	K	171	LEU	C-N-CA	6.67	126.37	119.56
1	N	331	ALA	CA-C-N	6.65	127.23	120.38
1	N	331	ALA	C-N-CA	6.65	127.23	120.38
1	E	257	CYS	CA-C-N	6.65	127.18	119.47
1	E	257	CYS	C-N-CA	6.65	127.18	119.47
1	F	171	LEU	CA-C-N	6.64	126.33	119.56
1	F	171	LEU	C-N-CA	6.64	126.33	119.56
1	B	171	LEU	CA-C-N	6.63	126.32	119.56
1	B	171	LEU	C-N-CA	6.63	126.32	119.56
2	X	263	GLN	N-CA-C	-6.61	103.76	110.97
4	a	109	HIS	CA-CB-CG	6.61	120.41	113.80
2	Q	263	GLN	N-CA-C	-6.60	103.77	110.97
4	T	109	HIS	CA-CB-CG	6.59	120.39	113.80
1	C	331	ALA	CA-C-N	6.59	127.16	120.38
1	C	331	ALA	C-N-CA	6.59	127.16	120.38
1	D	171	LEU	CA-C-N	6.58	126.27	119.56
1	D	171	LEU	C-N-CA	6.58	126.27	119.56
1	C	148	THR	N-CA-C	-6.56	105.85	114.31
1	O	321	ALA	CA-C-N	6.54	126.51	120.03
1	O	321	ALA	C-N-CA	6.54	126.51	120.03
1	N	97	ALA	CA-C-N	6.53	127.04	119.47
1	N	97	ALA	C-N-CA	6.53	127.04	119.47
1	C	329	ILE	N-CA-C	6.52	117.68	108.36
1	H	108	ALA	CA-C-N	6.50	126.19	119.82
1	H	108	ALA	C-N-CA	6.50	126.19	119.82
1	J	298	VAL	N-CA-C	6.48	117.18	108.11
1	I	257	CYS	CA-C-N	6.48	126.98	119.47
1	I	257	CYS	C-N-CA	6.48	126.98	119.47
1	C	34	ILE	N-CA-C	6.47	118.11	108.46
4	T	90	ILE	N-CA-C	-6.45	104.21	110.72
1	F	151	ILE	CA-C-N	-6.42	114.68	122.90
1	F	151	ILE	C-N-CA	-6.42	114.68	122.90
1	M	257	CYS	CA-C-N	6.42	126.92	119.47
1	M	257	CYS	C-N-CA	6.42	126.92	119.47
4	a	90	ILE	N-CA-C	-6.41	104.25	110.72
1	G	257	CYS	CA-C-N	6.41	126.90	119.47
1	G	257	CYS	C-N-CA	6.41	126.90	119.47
1	M	148	THR	N-CA-C	-6.41	105.22	114.12
3	R	0	SER	N-CA-C	-6.39	102.10	110.53
1	G	329	ILE	N-CA-C	6.38	117.11	108.17
3	Y	0	SER	N-CA-C	-6.38	102.11	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	171	LEU	CA-C-N	6.37	125.99	119.56
1	N	171	LEU	C-N-CA	6.37	125.99	119.56
1	B	34	ILE	N-CA-C	6.36	117.28	108.12
1	I	34	ILE	N-CA-C	6.36	117.93	108.46
1	K	332	PRO	CA-C-N	6.35	126.04	119.56
1	K	332	PRO	C-N-CA	6.35	126.04	119.56
1	J	108	ALA	CA-C-N	6.35	126.03	119.56
1	J	108	ALA	C-N-CA	6.35	126.03	119.56
1	K	151	ILE	CA-C-N	-6.34	114.78	122.90
1	K	151	ILE	C-N-CA	-6.34	114.78	122.90
1	O	108	ALA	CA-C-N	6.32	126.53	119.32
1	O	108	ALA	C-N-CA	6.32	126.53	119.32
1	H	148	THR	N-CA-C	-6.32	106.16	114.31
1	O	34	ILE	N-CA-C	6.30	117.85	108.46
1	L	217	CYS	N-CA-C	6.28	119.77	110.48
1	B	332	PRO	CA-C-N	6.28	126.75	119.47
1	B	332	PRO	C-N-CA	6.28	126.75	119.47
1	N	75	ILE	N-CA-C	6.28	116.95	108.17
1	F	132	MET	N-CA-C	6.27	118.95	109.23
1	K	34	ILE	N-CA-C	6.26	116.88	108.11
1	D	75	ILE	N-CA-C	6.24	116.91	108.17
1	O	257	CYS	CA-C-N	6.23	126.70	119.47
1	O	257	CYS	C-N-CA	6.23	126.70	119.47
1	I	163	VAL	N-CA-C	6.23	114.83	107.73
1	A	332	PRO	CA-C-N	6.21	125.89	119.56
1	A	332	PRO	C-N-CA	6.21	125.89	119.56
1	H	257	CYS	CA-C-N	6.20	126.66	119.47
1	H	257	CYS	C-N-CA	6.20	126.66	119.47
1	C	242	LEU	CA-C-N	6.19	125.88	119.56
1	C	242	LEU	C-N-CA	6.19	125.88	119.56
1	D	148	THR	N-CA-C	-6.18	106.33	114.31
1	F	332	PRO	CA-C-N	6.17	125.86	119.56
1	F	332	PRO	C-N-CA	6.17	125.86	119.56
5	b	105	ASP	CA-CB-CG	6.16	118.76	112.60
1	M	34	ILE	N-CA-C	6.16	116.99	108.12
1	M	163	VAL	N-CA-C	6.16	114.94	107.61
1	H	332	PRO	CA-C-N	6.16	125.78	119.56
1	H	332	PRO	C-N-CA	6.16	125.78	119.56
1	G	217	CYS	N-CA-C	6.14	118.84	110.55
1	J	332	PRO	CA-C-N	6.13	125.75	119.56
1	J	332	PRO	C-N-CA	6.13	125.75	119.56
1	D	332	PRO	CA-C-N	6.12	125.80	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	332	PRO	C-N-CA	6.12	125.80	119.56
1	M	151	ILE	CA-C-N	-6.09	115.10	122.90
1	M	151	ILE	C-N-CA	-6.09	115.10	122.90
1	E	151	ILE	CA-C-N	-6.08	114.96	122.93
1	E	151	ILE	C-N-CA	-6.08	114.96	122.93
1	K	97	ALA	CA-C-N	6.08	127.44	119.84
1	K	97	ALA	C-N-CA	6.08	127.44	119.84
1	H	132	MET	N-CA-C	6.08	118.66	109.23
1	E	331	ALA	CA-C-N	6.08	126.64	120.38
1	E	331	ALA	C-N-CA	6.08	126.64	120.38
1	C	332	PRO	CA-C-N	6.05	126.17	119.87
1	C	332	PRO	C-N-CA	6.05	126.17	119.87
1	F	97	ALA	CA-C-N	6.04	126.48	119.47
1	F	97	ALA	C-N-CA	6.04	126.48	119.47
2	Q	15	LYS	N-CA-C	-6.04	104.82	111.82
1	J	331	ALA	CA-C-N	6.03	126.59	120.38
1	J	331	ALA	C-N-CA	6.03	126.59	120.38
1	D	257	CYS	CA-C-N	6.03	126.46	119.47
1	D	257	CYS	C-N-CA	6.03	126.46	119.47
1	G	242	LEU	N-CA-C	-6.02	101.98	110.29
1	H	331	ALA	CA-C-N	6.02	126.58	120.38
1	H	331	ALA	C-N-CA	6.02	126.58	120.38
1	M	162	ASN	CA-C-N	-6.02	118.09	123.33
1	M	162	ASN	C-N-CA	-6.02	118.09	123.33
1	B	75	ILE	N-CA-C	6.02	116.60	108.17
1	A	148	THR	N-CA-C	-6.00	106.57	114.31
2	X	15	LYS	N-CA-C	-6.00	104.86	111.82
3	S	28	ASP	CA-CB-CG	5.98	118.58	112.60
1	F	163	VAL	N-CA-C	5.96	114.71	107.61
1	G	309	ILE	N-CA-C	5.96	116.74	110.72
3	Z	28	ASP	CA-CB-CG	5.96	118.56	112.60
1	I	154	ASP	N-CA-C	5.96	119.86	112.59
1	K	101	HIS	CA-C-N	5.94	127.27	119.84
1	K	101	HIS	C-N-CA	5.94	127.27	119.84
2	P	154	ILE	N-CA-C	-5.93	104.72	110.42
1	L	54	VAL	N-CA-C	5.92	117.01	108.48
1	M	154	ASP	CA-C-N	5.92	132.84	121.54
1	M	154	ASP	C-N-CA	5.92	132.84	121.54
1	K	154	ASP	CA-C-N	5.90	132.81	121.54
1	K	154	ASP	C-N-CA	5.90	132.81	121.54
1	O	51	ASP	CA-CB-CG	-5.90	106.70	112.60
1	A	34	ILE	N-CA-C	5.90	117.25	108.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	332	PRO	CA-C-N	5.89	126.31	119.47
1	N	332	PRO	C-N-CA	5.89	126.31	119.47
1	N	321	ALA	CA-C-N	5.89	125.87	120.21
1	N	321	ALA	C-N-CA	5.89	125.87	120.21
1	A	276	GLU	N-CA-C	-5.89	105.19	112.90
1	N	217	CYS	N-CA-C	5.89	119.23	110.52
1	O	151	ILE	N-CA-CB	5.88	117.13	110.72
2	W	154	ILE	N-CA-C	-5.88	104.78	110.42
6	c	149	ASP	CA-CB-CG	5.87	118.47	112.60
1	I	75	ILE	N-CA-C	5.87	116.92	108.48
1	B	257	CYS	CA-C-N	5.86	126.27	119.47
1	B	257	CYS	C-N-CA	5.86	126.27	119.47
1	D	331	ALA	CA-C-N	5.86	126.41	120.38
1	D	331	ALA	C-N-CA	5.86	126.41	120.38
1	A	298	VAL	N-CA-C	5.85	116.28	107.80
1	O	332	PRO	CA-C-N	5.84	126.25	119.47
1	O	332	PRO	C-N-CA	5.84	126.25	119.47
1	A	375	PHE	CA-CB-CG	5.83	119.63	113.80
1	N	162	ASN	N-CA-C	5.83	119.28	111.24
1	K	163	VAL	CA-C-N	5.82	126.28	119.99
1	K	163	VAL	C-N-CA	5.82	126.28	119.99
1	F	161	HIS	N-CA-C	5.82	118.85	111.69
1	D	375	PHE	CA-CB-CG	5.81	119.61	113.80
1	J	34	ILE	N-CA-C	5.81	116.49	108.12
1	M	101	HIS	CA-C-N	5.81	125.77	119.78
1	M	101	HIS	C-N-CA	5.81	125.77	119.78
4	a	106	ILE	N-CA-C	-5.80	104.85	110.42
1	N	161	HIS	N-CA-C	5.80	117.68	111.36
1	H	34	ILE	N-CA-C	5.80	117.10	108.46
1	K	242	LEU	CA-C-N	5.78	126.18	119.47
1	K	242	LEU	C-N-CA	5.78	126.18	119.47
4	T	106	ILE	N-CA-C	-5.78	104.87	110.42
1	O	132	MET	N-CA-C	5.78	118.63	109.50
1	L	148	THR	N-CA-C	-5.76	106.59	113.97
1	M	9	VAL	N-CA-C	5.76	116.18	108.11
1	N	242	LEU	CA-C-N	5.75	126.14	119.47
1	N	242	LEU	C-N-CA	5.75	126.14	119.47
1	C	54	VAL	N-CA-C	5.75	116.76	108.48
1	A	54	VAL	N-CA-C	5.75	116.16	108.11
1	G	132	MET	N-CA-C	5.73	118.11	109.23
5	b	147	VAL	N-CA-C	5.72	117.92	108.99
1	E	242	LEU	CA-C-N	5.72	126.11	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	242	LEU	C-N-CA	5.72	126.11	119.47
1	C	75	ILE	N-CA-C	5.72	116.18	108.17
1	H	329	ILE	N-CA-C	5.71	116.17	108.17
1	M	331	ALA	CA-C-N	5.70	126.25	120.38
1	M	331	ALA	C-N-CA	5.70	126.25	120.38
2	Q	89	ASN	N-CA-C	-5.70	105.15	111.36
1	C	321	ALA	CA-C-N	5.69	125.64	119.78
1	C	321	ALA	C-N-CA	5.69	125.64	119.78
1	L	298	VAL	N-CA-C	5.69	116.06	107.80
1	B	163	VAL	CA-C-N	5.69	126.17	120.14
1	B	163	VAL	C-N-CA	5.69	126.17	120.14
1	L	97	ALA	CA-C-N	5.69	126.07	119.47
1	L	97	ALA	C-N-CA	5.69	126.07	119.47
1	E	97	ALA	CA-C-N	5.69	125.36	119.56
1	E	97	ALA	C-N-CA	5.69	125.36	119.56
6	c	99	ASP	CA-CB-CG	5.69	118.29	112.60
1	G	54	VAL	N-CA-C	5.68	116.06	108.11
2	X	89	ASN	N-CA-C	-5.68	105.17	111.36
5	U	159	LEU	N-CA-C	-5.68	104.71	111.69
1	C	97	ALA	CA-C-N	5.67	126.04	119.47
1	C	97	ALA	C-N-CA	5.67	126.04	119.47
1	C	107	GLU	N-CA-C	5.66	117.12	108.52
1	A	242	LEU	CA-C-N	5.66	126.03	119.47
1	A	242	LEU	C-N-CA	5.66	126.03	119.47
1	B	157	ASP	CA-CB-CG	5.65	118.25	112.60
1	E	181	ALA	N-CA-C	5.64	116.53	108.74
1	C	151	ILE	CB-CA-C	-5.64	103.26	110.98
1	I	132	MET	N-CA-C	5.63	117.96	109.23
1	K	298	VAL	N-CA-C	5.63	115.97	107.80
1	E	321	ALA	CA-C-N	5.63	125.58	119.78
1	E	321	ALA	C-N-CA	5.63	125.58	119.78
1	M	132	MET	N-CA-C	5.63	117.96	109.23
1	M	54	VAL	N-CA-C	5.62	116.57	108.48
1	H	233	SER	N-CA-C	5.61	118.61	108.69
1	C	51	ASP	CA-CB-CG	-5.60	107.00	112.60
1	C	132	MET	N-CA-C	5.60	117.70	109.24
1	G	331	ALA	CA-C-N	5.59	126.14	120.38
1	G	331	ALA	C-N-CA	5.59	126.14	120.38
1	D	321	ALA	CA-C-N	5.58	125.53	119.78
1	D	321	ALA	C-N-CA	5.58	125.53	119.78
1	J	257	CYS	CA-C-N	5.58	125.25	119.56
1	J	257	CYS	C-N-CA	5.58	125.25	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	108	ALA	CA-C-N	5.58	125.94	119.47
1	F	108	ALA	C-N-CA	5.58	125.94	119.47
1	C	257	CYS	CA-C-N	5.57	125.24	119.56
1	C	257	CYS	C-N-CA	5.57	125.24	119.56
4	a	226	GLU	N-CA-C	5.56	117.34	111.28
1	H	321	ALA	CA-C-N	5.56	125.53	120.03
1	H	321	ALA	C-N-CA	5.56	125.53	120.03
2	P	154	ILE	N-CA-CB	5.56	117.05	110.55
2	W	154	ILE	N-CA-CB	5.55	117.05	110.55
1	N	108	ALA	CA-C-N	5.55	125.90	119.47
1	N	108	ALA	C-N-CA	5.55	125.90	119.47
1	G	151	ILE	CA-C-N	-5.54	115.91	123.12
1	G	151	ILE	C-N-CA	-5.54	115.91	123.12
1	D	54	VAL	N-CA-C	5.54	116.46	108.48
1	A	132	MET	N-CA-C	5.54	117.82	109.23
1	B	108	ALA	CA-C-N	5.54	125.89	119.47
1	B	108	ALA	C-N-CA	5.54	125.89	119.47
1	M	276	GLU	N-CA-C	-5.54	105.65	112.90
1	N	132	MET	N-CA-C	5.53	117.81	109.23
1	D	151	ILE	CA-C-N	-5.53	115.46	122.37
1	D	151	ILE	C-N-CA	-5.53	115.46	122.37
1	I	108	ALA	CA-C-N	5.52	125.88	119.47
1	I	108	ALA	C-N-CA	5.52	125.88	119.47
1	K	132	MET	N-CA-C	5.52	117.79	109.23
1	F	242	LEU	CA-C-N	5.51	125.86	119.47
1	F	242	LEU	C-N-CA	5.51	125.86	119.47
1	G	34	ILE	N-CA-C	5.50	116.66	108.46
1	B	77	THR	N-CA-C	-5.49	107.12	113.88
1	G	162	ASN	CA-C-N	-5.49	118.56	123.33
1	G	162	ASN	C-N-CA	-5.49	118.56	123.33
1	K	309	ILE	N-CA-C	5.48	116.26	110.72
1	E	171	LEU	CA-C-N	5.48	125.15	119.56
1	E	171	LEU	C-N-CA	5.48	125.15	119.56
5	b	141	ARG	CA-C-N	5.48	125.15	119.56
5	b	141	ARG	C-N-CA	5.48	125.15	119.56
1	D	108	ALA	CA-C-N	5.48	125.82	119.47
1	D	108	ALA	C-N-CA	5.48	125.82	119.47
1	F	162	ASN	CA-C-N	-5.47	118.57	123.33
1	F	162	ASN	C-N-CA	-5.47	118.57	123.33
1	J	132	MET	N-CA-C	5.46	117.70	109.23
1	H	80	ASP	N-CA-C	-5.45	104.99	111.69
1	G	97	ALA	CA-C-N	5.44	126.64	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	97	ALA	C-N-CA	5.44	126.64	119.84
1	K	331	ALA	CA-C-N	5.44	125.99	120.38
1	K	331	ALA	C-N-CA	5.44	125.99	120.38
1	L	242	LEU	CA-C-N	5.44	125.78	119.47
1	L	242	LEU	C-N-CA	5.44	125.78	119.47
1	I	77	THR	N-CA-C	-5.43	107.02	113.97
1	C	314	GLN	N-CA-C	-5.43	105.02	111.69
1	M	97	ALA	CA-C-N	5.42	126.62	119.84
1	M	97	ALA	C-N-CA	5.42	126.62	119.84
1	O	242	LEU	CA-C-N	5.42	125.76	119.47
1	O	242	LEU	C-N-CA	5.42	125.76	119.47
1	N	51	ASP	CA-CB-CG	-5.39	107.21	112.60
1	L	154	ASP	CA-C-N	5.39	131.84	121.54
1	L	154	ASP	C-N-CA	5.39	131.84	121.54
2	Q	276	HIS	CA-CB-CG	-5.39	108.41	113.80
1	B	97	ALA	CA-C-N	5.38	125.72	119.47
1	B	97	ALA	C-N-CA	5.38	125.72	119.47
2	X	276	HIS	CA-CB-CG	-5.38	108.42	113.80
1	O	111	ASN	CA-C-N	5.37	125.38	119.90
1	O	111	ASN	C-N-CA	5.37	125.38	119.90
1	N	373	LYS	N-CA-C	5.37	120.49	113.88
1	C	163	VAL	CA-C-N	5.37	125.79	119.99
1	C	163	VAL	C-N-CA	5.37	125.79	119.99
6	V	121	LEU	N-CA-C	5.37	117.21	111.36
1	G	233	SER	N-CA-C	5.36	117.41	108.99
1	K	108	ALA	CA-C-N	5.36	125.43	119.32
1	K	108	ALA	C-N-CA	5.36	125.43	119.32
2	X	131	GLU	N-CA-C	-5.36	105.52	111.36
1	K	321	ALA	CA-C-N	5.36	125.30	119.78
1	K	321	ALA	C-N-CA	5.36	125.30	119.78
2	X	188	GLY	N-CA-C	-5.36	106.28	112.50
1	I	54	VAL	N-CA-C	5.36	116.19	108.48
1	I	162	ASN	N-CA-C	5.36	118.63	111.24
1	J	222	ASP	CA-CB-CG	5.35	117.95	112.60
1	M	277	THR	N-CA-C	-5.35	105.34	111.07
2	Q	131	GLU	N-CA-C	-5.34	105.54	111.36
1	J	54	VAL	N-CA-C	5.33	116.41	108.46
1	G	244	ASP	N-CA-C	-5.33	106.27	114.16
1	E	54	VAL	N-CA-C	5.32	116.14	108.48
2	Q	188	GLY	N-CA-C	-5.32	106.33	112.50
5	U	90	PHE	CA-CB-CG	5.32	119.11	113.80
1	F	107	GLU	N-CA-C	5.31	117.25	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	242	LEU	CA-C-N	5.31	125.63	119.47
1	I	242	LEU	C-N-CA	5.31	125.63	119.47
1	K	233	SER	N-CA-C	5.30	117.32	108.99
1	B	298	VAL	N-CA-C	5.30	115.49	107.80
1	D	242	LEU	CA-C-N	5.30	124.96	119.56
1	D	242	LEU	C-N-CA	5.30	124.96	119.56
1	D	242	LEU	N-CA-C	-5.30	102.51	110.24
1	I	275	HIS	CA-CB-CG	-5.29	108.51	113.80
1	N	101	HIS	CA-CB-CG	5.29	119.09	113.80
2	W	113	LEU	N-CA-C	-5.29	105.60	111.36
1	F	34	ILE	N-CA-C	5.28	115.73	108.12
1	O	331	ALA	CA-C-N	5.28	125.82	120.38
1	O	331	ALA	C-N-CA	5.28	125.82	120.38
2	P	113	LEU	N-CA-C	-5.27	105.61	111.36
1	C	151	ILE	CA-C-N	-5.27	116.03	122.93
1	C	151	ILE	C-N-CA	-5.27	116.03	122.93
1	E	253	GLU	CA-C-N	5.26	127.86	120.28
1	E	253	GLU	C-N-CA	5.26	127.86	120.28
1	H	101	HIS	CA-C-N	5.26	125.20	119.78
1	H	101	HIS	C-N-CA	5.26	125.20	119.78
1	F	321	ALA	CA-C-N	5.25	125.19	119.78
1	F	321	ALA	C-N-CA	5.25	125.19	119.78
1	J	148	THR	CA-C-O	5.25	124.60	118.77
2	X	92	ILE	CB-CA-C	-5.25	105.25	111.97
1	N	16	LEU	N-CA-C	5.25	118.14	109.85
5	U	183	LYS	N-CA-C	5.25	117.08	111.36
1	D	233	SER	N-CA-C	5.24	117.22	108.99
1	B	9	VAL	N-CA-C	5.24	115.66	108.12
1	M	332	PRO	CA-C-N	5.23	125.53	119.47
1	M	332	PRO	C-N-CA	5.23	125.53	119.47
2	Q	92	ILE	CB-CA-C	-5.22	105.28	111.97
2	Q	175	ASP	CA-CB-CG	5.22	117.82	112.60
2	W	29	LYS	N-CA-C	-5.22	105.76	111.82
2	X	175	ASP	CA-CB-CG	5.22	117.82	112.60
1	B	375	PHE	CA-CB-CG	5.22	119.02	113.80
1	H	242	LEU	CA-C-N	5.22	125.52	119.47
1	H	242	LEU	C-N-CA	5.22	125.52	119.47
1	F	233	SER	N-CA-C	5.21	117.92	109.06
1	F	203	THR	N-CA-C	5.21	117.36	111.11
1	E	51	ASP	CA-CB-CG	-5.20	107.40	112.60
1	E	151	ILE	CB-CA-C	-5.19	103.87	110.98
2	P	29	LYS	N-CA-C	-5.19	105.80	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	163	VAL	CA-C-N	5.17	125.58	119.99
1	D	163	VAL	C-N-CA	5.17	125.58	119.99
1	H	161	HIS	CA-CB-CG	5.17	118.97	113.80
1	G	111	ASN	CA-C-N	5.17	125.17	119.90
1	G	111	ASN	C-N-CA	5.17	125.17	119.90
5	b	192	ARG	N-CA-C	5.16	116.91	111.28
1	E	162	ASN	N-CA-C	5.16	118.36	111.24
1	C	233	SER	N-CA-C	5.16	117.09	108.99
1	I	253	GLU	CA-C-N	5.16	127.70	120.28
1	I	253	GLU	C-N-CA	5.16	127.70	120.28
1	J	75	ILE	N-CA-C	5.16	116.79	108.85
1	N	77	THR	N-CA-C	-5.16	107.37	113.97
1	L	151	ILE	CA-C-N	-5.15	115.93	122.37
1	L	151	ILE	C-N-CA	-5.15	115.93	122.37
1	D	132	MET	N-CA-C	5.14	117.20	109.23
5	b	90	PHE	CA-CB-CG	5.14	118.94	113.80
1	L	321	ALA	CA-C-N	5.14	125.12	120.03
1	L	321	ALA	C-N-CA	5.14	125.12	120.03
1	L	51	ASP	CA-CB-CG	-5.13	107.47	112.60
1	G	157	ASP	N-CA-C	-5.13	106.18	112.90
1	L	233	SER	N-CA-C	5.12	117.03	108.99
1	A	321	ALA	CA-C-N	5.11	125.09	120.03
1	A	321	ALA	C-N-CA	5.11	125.09	120.03
1	F	163	VAL	CA-C-N	5.10	125.26	119.90
1	F	163	VAL	C-N-CA	5.10	125.26	119.90
1	O	109	PRO	N-CA-C	5.09	121.33	113.75
2	P	261	TYR	N-CA-C	-5.08	105.82	111.36
1	G	253	GLU	CA-C-N	5.08	127.59	120.28
1	G	253	GLU	C-N-CA	5.08	127.59	120.28
1	O	54	VAL	N-CA-C	5.08	115.79	108.48
1	D	51	ASP	CA-CB-CG	-5.07	107.53	112.60
1	F	151	ILE	CB-CA-C	-5.07	104.03	110.98
1	L	108	ALA	CA-C-N	5.07	125.35	119.47
1	L	108	ALA	C-N-CA	5.07	125.35	119.47
1	N	375	PHE	CA-CB-CG	5.07	118.87	113.80
1	A	151	ILE	CA-C-N	-5.07	116.29	122.93
1	A	151	ILE	C-N-CA	-5.07	116.29	122.93
1	H	77	THR	N-CA-C	-5.07	107.49	113.97
1	J	51	ASP	CA-CB-CG	-5.06	107.54	112.60
6	c	33	ASP	CA-CB-CG	-5.06	107.54	112.60
1	I	129	VAL	CA-C-N	5.06	124.67	119.56
1	I	129	VAL	C-N-CA	5.06	124.67	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	W	261	TYR	N-CA-C	-5.05	105.85	111.36
1	F	375	PHE	CA-CB-CG	5.05	118.85	113.80
1	G	298	VAL	N-CA-C	5.04	115.11	107.80
1	M	321	ALA	CA-C-N	5.04	124.97	119.78
1	M	321	ALA	C-N-CA	5.04	124.97	119.78
5	U	145	ARG	N-CA-C	5.04	115.80	108.14
1	L	257	CYS	CA-C-N	5.03	125.31	119.47
1	L	257	CYS	C-N-CA	5.03	125.31	119.47
2	W	85	VAL	N-CA-C	-5.03	105.49	110.62
1	H	111	ASN	CA-C-N	5.03	126.12	119.84
1	H	111	ASN	C-N-CA	5.03	126.12	119.84
2	Q	153	HIS	N-CA-C	-5.03	105.69	111.07
1	B	54	VAL	N-CA-C	5.02	115.13	108.11
2	X	153	HIS	N-CA-C	-5.01	105.70	111.07
1	A	51	ASP	CA-CB-CG	-5.01	107.59	112.60
1	E	132	MET	N-CA-C	5.01	117.00	109.23
1	I	151	ILE	CB-CA-C	-5.00	104.12	110.98

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2933	0	2894	72	0
1	B	2933	0	2894	61	0
1	C	2933	0	2894	58	0
1	D	2933	0	2894	41	0
1	E	2933	0	2894	77	0
1	F	2933	0	2894	42	0
1	G	2933	0	2894	36	0
1	H	2933	0	2894	74	0
1	I	2933	0	2894	55	0
1	J	2933	0	2894	36	0
1	K	2933	0	2894	63	0
1	L	2933	0	2894	78	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	M	2933	0	2894	92	0
1	N	2933	0	2894	57	0
1	O	2933	0	2894	39	0
2	P	2207	0	2200	92	0
2	Q	2207	0	2200	95	0
2	W	2207	0	2200	81	0
2	X	2207	0	2200	98	0
3	R	243	0	255	12	0
3	S	243	0	255	0	0
3	Y	243	0	255	3	0
3	Z	243	0	255	0	0
4	T	1211	0	1226	17	0
4	a	1211	0	1226	14	0
5	U	1374	0	1436	54	0
5	b	1374	0	1436	45	0
6	V	1273	0	1201	18	0
6	c	1273	0	1201	13	0
7	A	27	0	12	0	0
7	B	27	0	12	0	0
7	C	27	0	12	0	0
7	D	27	0	12	0	0
7	E	27	0	12	0	0
7	F	27	0	12	0	0
7	G	27	0	12	0	0
7	H	27	0	12	1	0
7	I	27	0	12	1	0
7	J	27	0	12	1	0
7	K	27	0	12	0	0
7	L	27	0	12	0	0
7	M	27	0	12	0	0
7	N	27	0	12	0	0
7	O	27	0	12	0	0
All	All	61916	0	61136	1166	0

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

All (1166) 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)
1:H:163:VAL:HG22	1:H:175:ILE:CG1	1.50	1.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:U:57:ALA:HB2	6:V:104:PHE:CZ	1.56	1.40
1:M:146:GLY:HA2	4:T:87:PHE:CZ	1.57	1.37
5:U:195:ILE:CD1	2:W:91:ARG:HB2	1.52	1.37
2:P:91:ARG:NH1	5:b:197:ALA:HB2	1.42	1.33
1:H:133:TYR:CD2	1:H:352:PHE:HZ	1.53	1.25
2:P:91:ARG:HH11	5:b:195:ILE:CD1	1.49	1.25
1:F:252:ASN:HB2	1:F:255:PHE:CZ	1.71	1.24
1:A:133:TYR:CD2	1:A:352:PHE:HZ	1.55	1.24
1:E:313:MET:SD	1:E:329:ILE:HD13	1.79	1.23
1:B:252:ASN:HA	1:B:255:PHE:CZ	1.73	1.23
2:P:153:HIS:ND1	6:c:55:GLU:HG3	1.53	1.23
5:U:195:ILE:HD12	2:W:91:ARG:CB	1.68	1.22
1:L:305:MET:CE	1:L:335:ARG:HB2	1.70	1.21
1:D:252:ASN:HA	1:D:255:PHE:CE2	1.73	1.21
1:J:306:TYR:O	1:J:309:ILE:HG22	1.31	1.21
1:B:332:PRO:O	1:B:335:ARG:HG3	1.36	1.21
1:A:332:PRO:O	1:A:335:ARG:HG3	1.38	1.20
1:E:313:MET:SD	1:E:329:ILE:CD1	2.30	1.19
1:H:163:VAL:HG22	1:H:175:ILE:CD1	1.73	1.19
1:I:305:MET:CE	1:I:335:ARG:HG3	1.72	1.19
1:H:133:TYR:CZ	1:H:352:PHE:CE1	2.31	1.17
1:B:252:ASN:HA	1:B:255:PHE:CE2	1.78	1.17
1:A:133:TYR:CE2	1:A:352:PHE:CZ	2.32	1.16
1:H:133:TYR:CZ	1:H:352:PHE:HE1	1.63	1.16
1:J:252:ASN:HA	1:J:255:PHE:CE2	1.78	1.16
1:K:252:ASN:HA	1:K:255:PHE:CE2	1.79	1.16
2:W:88:LEU:HD11	2:X:85:VAL:HG13	1.21	1.16
1:G:252:ASN:HA	1:G:255:PHE:CE2	1.80	1.15
1:M:333:PRO:HG3	3:R:9:GLN:CD	1.71	1.14
1:A:133:TYR:CD2	1:A:352:PHE:CZ	2.34	1.14
2:Q:140:LYS:HE3	5:b:159:LEU:HD23	1.18	1.14
5:U:195:ILE:HD12	2:W:91:ARG:CG	1.77	1.14
1:M:146:GLY:CA	4:T:87:PHE:HZ	1.61	1.14
1:N:252:ASN:HA	1:N:255:PHE:CE2	1.82	1.14
5:U:159:LEU:HG	2:X:140:LYS:CE	1.78	1.13
1:L:305:MET:HE2	1:L:335:ARG:HB2	1.30	1.13
1:H:133:TYR:CE2	1:H:352:PHE:CZ	2.37	1.13
5:U:197:ALA:O	2:W:84:ASP:HB2	1.48	1.12
1:L:257:CYS:HB3	1:L:258:PRO:HD3	1.14	1.12
2:P:91:ARG:HH21	2:Q:92:ILE:HG13	1.06	1.12
2:X:161:LYS:O	2:X:165:VAL:HG12	1.50	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:332:PRO:O	1:D:335:ARG:HG2	1.46	1.11
2:W:84:ASP:OD1	2:W:88:LEU:HG	1.50	1.11
2:W:91:ARG:HH21	2:X:92:ILE:HG13	1.07	1.11
1:A:148:THR:HB	1:C:47:MET:HE1	1.20	1.11
1:H:163:VAL:CG2	1:H:175:ILE:HD13	1.80	1.10
1:M:252:ASN:HA	1:M:255:PHE:CE2	1.86	1.10
1:C:252:ASN:HA	1:C:255:PHE:CE2	1.84	1.10
1:L:342:GLY:O	1:L:345:ILE:HG22	1.52	1.10
2:P:145:GLU:OE2	2:P:149:LYS:HE3	1.50	1.10
2:Q:161:LYS:O	2:Q:165:VAL:HG12	1.50	1.10
1:L:332:PRO:O	1:L:335:ARG:HG2	1.50	1.10
1:N:305:MET:SD	1:N:335:ARG:NE	2.24	1.10
1:B:133:TYR:CD2	1:B:352:PHE:HZ	1.70	1.09
1:C:332:PRO:O	1:C:335:ARG:HG3	1.52	1.09
1:C:192:ILE:CD1	1:C:256:ARG:HD3	1.83	1.08
1:F:305:MET:HE3	1:F:336:LYS:HD2	1.33	1.08
1:F:252:ASN:HA	1:F:255:PHE:CE2	1.88	1.07
1:H:133:TYR:CD2	1:H:352:PHE:CZ	2.42	1.07
1:M:333:PRO:HG2	3:R:9:GLN:HG3	1.15	1.06
1:A:148:THR:CB	1:C:47:MET:HE1	1.84	1.06
1:F:305:MET:HE3	1:F:336:LYS:CD	1.83	1.06
1:M:333:PRO:CG	3:R:9:GLN:HG3	1.84	1.05
2:P:91:ARG:NH1	5:b:195:ILE:HD13	1.70	1.05
5:U:57:ALA:CB	6:V:104:PHE:CZ	2.37	1.05
1:C:192:ILE:HD12	1:C:256:ARG:CD	1.87	1.05
1:H:163:VAL:HG22	1:H:175:ILE:HG12	1.09	1.05
5:U:195:ILE:HD12	2:W:91:ARG:HB2	1.13	1.05
2:P:91:ARG:HD2	5:b:195:ILE:HG12	1.39	1.05
1:N:109:PRO:HD2	1:N:161:HIS:NE2	1.70	1.04
1:A:143:TYR:CZ	1:C:44:MET:HE2	1.91	1.04
2:Q:140:LYS:HE3	5:b:159:LEU:CD2	1.87	1.03
1:A:143:TYR:CE2	1:C:44:MET:HE2	1.94	1.03
1:H:163:VAL:CG2	1:H:175:ILE:CD1	2.35	1.03
5:U:197:ALA:HB1	2:W:84:ASP:OD2	1.58	1.03
1:H:163:VAL:HG21	1:H:175:ILE:HD13	1.39	1.03
1:H:252:ASN:HA	1:H:255:PHE:CE2	1.94	1.03
1:N:252:ASN:HB2	1:N:255:PHE:CZ	1.93	1.02
1:E:289:ILE:HD11	1:G:63:GLY:O	1.58	1.02
2:P:91:ARG:HH11	5:b:195:ILE:HD13	0.87	1.02
2:P:91:ARG:NH2	2:Q:92:ILE:HG13	1.75	1.02
5:b:50:LYS:HE2	6:c:156:PHE:CE1	1.93	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:TYR:CG	1:A:352:PHE:HZ	1.78	1.02
2:P:91:ARG:NH1	5:b:195:ILE:CD1	2.20	1.02
2:W:91:ARG:NH2	2:X:92:ILE:HG13	1.75	1.02
1:A:148:THR:HB	1:C:47:MET:CE	1.91	1.01
2:P:91:ARG:HE	2:Q:92:ILE:CD1	1.74	1.01
1:I:305:MET:SD	1:I:335:ARG:NE	2.32	1.01
1:J:252:ASN:HB2	1:J:255:PHE:CZ	1.95	1.01
1:I:305:MET:HE2	1:I:335:ARG:CG	1.91	1.00
1:M:333:PRO:HG2	3:R:9:GLN:CG	1.91	1.00
2:W:91:ARG:HE	2:X:92:ILE:CD1	1.74	1.00
1:I:305:MET:HE2	1:I:335:ARG:HG3	1.00	1.00
1:M:333:PRO:CG	3:R:9:GLN:CD	2.35	1.00
1:K:305:MET:HG3	1:K:335:ARG:HD2	1.44	0.99
1:H:163:VAL:HG23	1:H:175:ILE:CG2	1.93	0.99
1:L:257:CYS:HB3	1:L:258:PRO:CD	1.91	0.99
1:K:133:TYR:CE1	1:K:352:PHE:HZ	1.81	0.99
5:U:195:ILE:CD1	2:W:91:ARG:CB	2.33	0.99
1:K:305:MET:CG	1:K:335:ARG:HD2	1.93	0.98
1:C:192:ILE:HD12	1:C:256:ARG:HD3	0.98	0.98
1:M:146:GLY:CA	4:T:87:PHE:CZ	2.41	0.98
1:D:305:MET:SD	1:D:335:ARG:HB2	2.02	0.98
1:N:305:MET:HE1	1:N:335:ARG:HH21	1.29	0.97
1:H:163:VAL:CG2	1:H:175:ILE:CG1	2.43	0.97
1:E:305:MET:HE3	1:E:336:LYS:HD2	1.44	0.97
1:E:313:MET:SD	1:E:329:ILE:HD11	2.05	0.97
1:K:252:ASN:HB2	1:K:255:PHE:CZ	2.00	0.96
1:I:305:MET:CE	1:I:335:ARG:CG	2.43	0.96
2:Q:140:LYS:CE	5:b:159:LEU:HB3	1.94	0.96
1:A:252:ASN:HA	1:A:255:PHE:CE2	2.00	0.96
1:L:305:MET:HE1	1:L:335:ARG:HB2	1.47	0.96
1:L:252:ASN:HA	1:L:255:PHE:CE2	2.01	0.96
2:P:256:LEU:CD1	2:Q:260:LEU:HD13	1.95	0.96
1:B:133:TYR:CD2	1:B:352:PHE:CZ	2.54	0.96
1:H:133:TYR:CG	1:H:352:PHE:HZ	1.84	0.95
5:U:195:ILE:HD12	2:W:91:ARG:CD	1.97	0.95
2:W:256:LEU:CD1	2:X:260:LEU:HD13	1.95	0.95
1:E:109:PRO:HD2	1:E:161:HIS:NE2	1.81	0.95
1:C:253:GLU:HA	1:C:256:ARG:CG	1.96	0.95
2:P:91:ARG:HH12	5:b:197:ALA:CB	1.80	0.94
1:H:133:TYR:CE2	1:H:352:PHE:HZ	1.82	0.94
1:A:252:ASN:HA	1:A:255:PHE:CZ	2.03	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:333:PRO:CG	3:R:9:GLN:CG	2.45	0.94
1:N:305:MET:CE	1:N:335:ARG:HH21	1.81	0.94
1:A:133:TYR:CZ	1:A:352:PHE:CE1	2.55	0.94
1:M:146:GLY:HA2	4:T:87:PHE:HZ	0.77	0.94
1:M:300:SER:HA	1:M:336:LYS:HA	1.46	0.94
5:U:57:ALA:HB2	6:V:104:PHE:CE1	2.03	0.94
1:H:163:VAL:HG23	1:H:175:ILE:HG23	1.48	0.93
5:U:159:LEU:HG	2:X:140:LYS:HE2	1.47	0.93
1:E:106:THR:HG22	1:E:135:ALA:HB3	1.50	0.93
1:C:253:GLU:HA	1:C:256:ARG:HG2	1.48	0.93
2:Q:140:LYS:HG3	5:b:159:LEU:HD22	1.48	0.93
5:U:197:ALA:HB1	2:W:84:ASP:CG	1.94	0.93
1:B:305:MET:CE	1:B:335:ARG:HB2	1.98	0.93
1:H:163:VAL:CG2	1:H:175:ILE:HG12	1.98	0.93
1:C:133:TYR:CD2	1:C:352:PHE:HZ	1.86	0.93
1:B:207:GLU:HA	1:B:210:ARG:HG2	1.50	0.92
1:O:252:ASN:HA	1:O:255:PHE:CE2	2.04	0.92
1:K:352:PHE:CD1	1:K:355:MET:HG3	2.05	0.92
5:U:204:ARG:HD2	2:W:76:LYS:NZ	1.84	0.92
1:N:109:PRO:HD2	1:N:161:HIS:CD2	2.04	0.91
1:N:109:PRO:CD	1:N:161:HIS:NE2	2.34	0.91
1:B:133:TYR:CE2	1:B:352:PHE:CE1	2.60	0.90
1:B:133:TYR:CZ	1:B:352:PHE:HE1	1.90	0.90
1:I:257:CYS:HB2	1:I:258:PRO:HD3	1.54	0.90
5:U:195:ILE:HD13	2:W:91:ARG:HB2	1.51	0.90
1:F:252:ASN:CB	1:F:255:PHE:CZ	2.55	0.90
1:C:133:TYR:CZ	1:C:352:PHE:HE1	1.90	0.90
1:A:148:THR:CG2	1:C:47:MET:HE1	2.02	0.89
1:F:252:ASN:HB2	1:F:255:PHE:HZ	1.37	0.89
5:U:195:ILE:HD12	2:W:91:ARG:HD3	1.53	0.89
1:B:252:ASN:CA	1:B:255:PHE:CZ	2.56	0.89
2:P:91:ARG:HH12	5:b:197:ALA:HB2	1.00	0.89
1:A:133:TYR:CE2	1:A:352:PHE:HZ	1.79	0.88
1:A:133:TYR:CZ	1:A:352:PHE:CZ	2.61	0.88
1:F:252:ASN:CA	1:F:255:PHE:CE2	2.57	0.88
1:I:257:CYS:CB	1:I:258:PRO:HD3	2.04	0.88
1:N:305:MET:CE	1:N:335:ARG:NH2	2.36	0.88
1:N:305:MET:HE1	1:N:335:ARG:NH2	1.89	0.88
1:L:207:GLU:HA	1:L:210:ARG:HG2	1.56	0.88
1:B:109:PRO:HD2	1:B:161:HIS:CD2	2.08	0.87
1:O:1:ASP:HA	1:O:96:VAL:HG22	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:U:192:ARG:NH2	2:X:96:GLU:HG3	1.89	0.87
1:E:283:MET:HA	1:E:290:ARG:HD3	1.54	0.87
2:P:91:ARG:HD2	5:b:195:ILE:CG1	2.05	0.87
1:E:133:TYR:CE1	1:E:355:MET:HB3	2.10	0.87
1:F:109:PRO:HG2	1:F:161:HIS:NE2	1.88	0.87
5:U:159:LEU:HG	2:X:140:LYS:HE3	1.53	0.87
1:M:230:ALA:HB3	1:M:255:PHE:HZ	1.39	0.86
1:L:342:GLY:O	1:L:345:ILE:CG2	2.22	0.86
1:M:252:ASN:HA	1:M:255:PHE:CZ	2.11	0.86
1:C:133:TYR:CD2	1:C:352:PHE:CZ	2.64	0.86
1:N:305:MET:HE1	1:N:335:ARG:HE	1.39	0.86
1:C:133:TYR:CE2	1:C:352:PHE:CE1	2.62	0.86
1:I:109:PRO:HD2	1:I:161:HIS:CD2	2.11	0.86
1:L:196:ARG:HD2	1:L:253:GLU:CD	2.01	0.86
1:B:262:PHE:CZ	1:B:312:ARG:HG2	2.12	0.85
1:K:252:ASN:CB	1:K:255:PHE:CZ	2.58	0.85
2:P:153:HIS:ND1	6:c:55:GLU:CG	2.37	0.85
1:B:230:ALA:HB3	1:B:255:PHE:HZ	1.40	0.85
1:L:133:TYR:CZ	1:L:352:PHE:HE1	1.92	0.85
1:M:333:PRO:HD3	3:R:9:GLN:OE1	1.76	0.85
2:P:91:ARG:HD3	5:b:195:ILE:HD13	1.58	0.85
1:H:133:TYR:CZ	1:H:352:PHE:CZ	2.62	0.85
1:J:252:ASN:HA	1:J:255:PHE:HE2	1.42	0.84
1:N:109:PRO:HD2	1:N:161:HIS:CE1	2.12	0.84
1:I:109:PRO:HD2	1:I:161:HIS:NE2	1.92	0.84
1:E:289:ILE:HD11	1:G:63:GLY:C	2.03	0.84
1:H:163:VAL:CG2	1:H:175:ILE:CG2	2.56	0.84
2:P:72:GLU:O	2:P:76:LYS:HG3	1.78	0.84
1:E:109:PRO:HG2	1:E:161:HIS:NE2	1.93	0.84
1:L:143:TYR:HB3	1:L:345:ILE:HG21	1.56	0.84
2:P:91:ARG:CD	5:b:195:ILE:HD13	2.08	0.84
2:P:256:LEU:HD11	2:Q:260:LEU:HD13	1.59	0.84
1:C:133:TYR:CE2	1:C:352:PHE:HE1	1.95	0.83
1:J:252:ASN:CA	1:J:255:PHE:CE2	2.61	0.83
1:D:252:ASN:HA	1:D:255:PHE:CZ	2.14	0.83
2:W:72:GLU:O	2:W:76:LYS:HG3	1.78	0.83
1:G:252:ASN:HB2	1:G:255:PHE:CZ	2.14	0.82
1:I:252:ASN:HA	1:I:255:PHE:CE2	2.14	0.82
2:P:145:GLU:OE2	2:P:149:LYS:CE	2.27	0.82
1:L:257:CYS:CB	1:L:258:PRO:HD3	2.04	0.82
2:W:256:LEU:HD11	2:X:260:LEU:HD13	1.59	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:133:TYR:CZ	1:K:352:PHE:HZ	1.97	0.82
1:D:252:ASN:HB2	1:D:255:PHE:CZ	2.13	0.82
1:B:133:TYR:CE2	1:B:352:PHE:CZ	2.68	0.81
1:L:332:PRO:O	1:L:335:ARG:CG	2.27	0.81
1:N:252:ASN:CB	1:N:255:PHE:CZ	2.62	0.81
5:U:204:ARG:HD2	2:W:76:LYS:HZ2	1.44	0.81
1:C:253:GLU:HA	1:C:256:ARG:CD	2.10	0.81
1:F:305:MET:HE3	1:F:336:LYS:HD3	1.62	0.81
2:P:91:ARG:HE	2:Q:92:ILE:HD12	1.44	0.81
1:H:133:TYR:CE1	1:H:352:PHE:CE1	2.68	0.81
2:P:145:GLU:CD	2:P:149:LYS:HE3	2.06	0.81
2:Q:140:LYS:HE2	5:b:159:LEU:HB3	1.61	0.81
1:N:305:MET:CE	1:N:335:ARG:HE	1.94	0.80
2:Q:140:LYS:HE3	5:b:159:LEU:HB3	1.62	0.80
1:E:282:ILE:O	1:E:290:ARG:HG2	1.81	0.80
2:P:91:ARG:NH1	5:b:197:ALA:CB	2.36	0.80
1:M:109:PRO:HD2	1:M:161:HIS:CD2	2.16	0.80
1:M:238:LYS:NZ	2:P:276:HIS:CE1	2.50	0.80
2:W:91:ARG:HE	2:X:92:ILE:HD12	1.44	0.80
1:E:109:PRO:CD	1:E:161:HIS:NE2	2.45	0.80
1:F:109:PRO:HD2	1:F:161:HIS:CD2	2.17	0.79
1:N:109:PRO:CG	1:N:161:HIS:NE2	2.45	0.79
2:Q:140:LYS:CE	5:b:159:LEU:HD23	2.09	0.79
1:E:289:ILE:CD1	1:G:63:GLY:O	2.30	0.79
1:G:262:PHE:CZ	1:G:312:ARG:HG2	2.17	0.79
1:B:133:TYR:CZ	1:B:352:PHE:CE1	2.71	0.79
1:M:238:LYS:NZ	2:P:276:HIS:NE2	2.31	0.79
5:U:197:ALA:O	2:W:84:ASP:CB	2.30	0.79
2:W:88:LEU:HD11	2:X:85:VAL:CG1	2.09	0.79
1:C:252:ASN:HA	1:C:255:PHE:CZ	2.17	0.79
1:H:133:TYR:CE2	1:H:352:PHE:CE1	2.68	0.79
1:K:133:TYR:CE1	1:K:352:PHE:CZ	2.69	0.79
1:M:238:LYS:HZ1	2:P:276:HIS:CE1	2.01	0.79
1:N:305:MET:HE1	1:N:335:ARG:NE	1.97	0.78
1:K:252:ASN:CA	1:K:255:PHE:CE2	2.66	0.78
1:D:133:TYR:CZ	1:D:352:PHE:HE1	2.02	0.78
1:G:252:ASN:HA	1:G:255:PHE:HE2	1.44	0.78
1:E:207:GLU:HA	1:E:210:ARG:HG2	1.65	0.78
1:D:252:ASN:CB	1:D:255:PHE:CZ	2.67	0.78
1:K:352:PHE:CE1	1:K:355:MET:HG3	2.18	0.78
1:M:301:GLY:O	1:M:336:LYS:HB2	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:252:ASN:CA	1:G:255:PHE:CE2	2.65	0.77
1:N:305:MET:CE	1:N:335:ARG:NE	2.47	0.77
1:L:342:GLY:C	1:L:345:ILE:HG22	2.08	0.77
1:I:169:TYR:OH	1:K:49:GLN:HG3	1.85	0.77
1:L:143:TYR:CB	1:L:345:ILE:HG21	2.15	0.77
1:H:133:TYR:CG	1:H:352:PHE:CZ	2.72	0.77
5:U:167:LEU:HD22	2:X:129:VAL:HG21	1.66	0.77
1:A:133:TYR:CG	1:A:352:PHE:CZ	2.67	0.76
6:V:5:TYR:CD2	6:V:79:VAL:HG21	2.19	0.76
1:B:230:ALA:HB3	1:B:255:PHE:CZ	2.20	0.76
1:M:146:GLY:HA3	4:T:91:HIS:HE1	1.50	0.76
1:D:133:TYR:CE2	1:D:352:PHE:HE1	2.04	0.76
1:E:252:ASN:HA	1:E:255:PHE:CE2	2.20	0.76
1:F:109:PRO:CG	1:F:161:HIS:NE2	2.49	0.76
1:J:252:ASN:CB	1:J:255:PHE:CZ	2.69	0.76
2:P:153:HIS:HE1	6:c:54:PRO:HB2	1.50	0.76
1:N:252:ASN:CA	1:N:255:PHE:CE2	2.64	0.76
1:B:305:MET:HE2	1:B:335:ARG:HB2	1.68	0.76
1:F:252:ASN:HA	1:F:255:PHE:HE2	1.45	0.76
1:M:230:ALA:HB3	1:M:255:PHE:CZ	2.21	0.76
1:M:207:GLU:HA	1:M:210:ARG:HG2	1.67	0.75
1:N:305:MET:SD	1:N:335:ARG:CZ	2.73	0.75
1:M:146:GLY:HA3	4:T:91:HIS:CE1	2.22	0.75
1:B:305:MET:HE2	1:B:335:ARG:CB	2.16	0.75
1:L:333:PRO:HG3	3:Y:9:GLN:HG3	1.69	0.75
2:Q:140:LYS:HG3	5:b:159:LEU:CD2	2.16	0.75
1:D:305:MET:SD	1:D:335:ARG:CB	2.75	0.75
2:P:145:GLU:CG	2:P:149:LYS:HE3	2.17	0.74
1:F:305:MET:CE	1:F:336:LYS:HD3	2.16	0.74
1:A:151:ILE:HD11	1:A:282:ILE:HG13	1.66	0.74
2:P:91:ARG:CD	5:b:195:ILE:CD1	2.65	0.74
2:P:149:LYS:O	2:P:153:HIS:CD2	2.41	0.74
2:X:260:LEU:O	2:X:260:LEU:HD23	1.88	0.74
5:U:57:ALA:CB	6:V:104:PHE:CE1	2.67	0.74
1:C:253:GLU:CA	1:C:256:ARG:HG2	2.18	0.73
1:L:196:ARG:HD2	1:L:253:GLU:OE2	1.89	0.73
1:A:282:ILE:HG21	1:A:294:TYR:CE2	2.23	0.73
1:E:109:PRO:CG	1:E:161:HIS:NE2	2.50	0.73
1:E:133:TYR:CE2	1:E:352:PHE:HE1	2.06	0.73
1:O:207:GLU:O	1:O:210:ARG:CG	2.37	0.73
1:A:133:TYR:CZ	1:A:352:PHE:HE1	2.05	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:260:LEU:HD23	2:Q:260:LEU:O	1.88	0.72
1:J:252:ASN:HB2	1:J:255:PHE:HZ	1.54	0.72
2:P:256:LEU:CD1	2:Q:257:GLU:HG2	2.19	0.72
1:C:133:TYR:CZ	1:C:352:PHE:CE1	2.76	0.72
1:L:133:TYR:CE2	1:L:352:PHE:HE1	2.08	0.72
1:N:252:ASN:HA	1:N:255:PHE:HE2	1.50	0.72
2:W:256:LEU:CD1	2:X:257:GLU:HG2	2.19	0.72
1:E:166:TYR:CD1	1:E:289:ILE:HG23	2.25	0.72
1:D:133:TYR:CE2	1:D:352:PHE:CE1	2.78	0.72
1:N:305:MET:HE1	1:N:335:ARG:CZ	2.20	0.71
1:K:305:MET:CG	1:K:335:ARG:CD	2.68	0.71
1:N:279:TYR:OH	1:N:283:MET:HE3	1.90	0.71
1:M:109:PRO:HD2	1:M:161:HIS:NE2	2.05	0.71
2:P:166:ALA:HA	2:Q:165:VAL:HG21	1.72	0.71
1:H:252:ASN:HA	1:H:255:PHE:HE2	1.50	0.71
1:E:106:THR:HG21	1:E:140:LEU:HD12	1.73	0.71
5:U:195:ILE:CD1	2:W:91:ARG:CG	2.64	0.71
1:A:230:ALA:HB3	1:A:255:PHE:HZ	1.56	0.71
1:M:304:THR:O	1:M:335:ARG:NE	2.24	0.71
1:M:305:MET:SD	1:M:335:ARG:CG	2.79	0.71
1:O:305:MET:HE1	1:O:335:ARG:HE	1.56	0.70
2:W:166:ALA:HA	2:X:165:VAL:HG21	1.72	0.70
1:I:189:LEU:HA	1:I:257:CYS:SG	2.30	0.70
6:V:59:GLU:OE2	2:W:153:HIS:NE2	2.24	0.70
1:A:143:TYR:CE2	1:C:44:MET:CE	2.73	0.70
1:K:352:PHE:CE1	1:K:355:MET:CB	2.74	0.70
1:B:133:TYR:CG	1:B:352:PHE:HZ	2.09	0.70
1:E:305:MET:CE	1:E:336:LYS:HD2	2.21	0.70
1:I:257:CYS:CB	1:I:258:PRO:CD	2.68	0.70
1:K:196:ARG:HD2	1:K:253:GLU:CD	2.17	0.70
2:P:91:ARG:HD2	5:b:195:ILE:CD1	2.22	0.70
1:E:104:LEU:HD12	1:E:133:TYR:O	1.90	0.70
1:I:109:PRO:CD	1:I:161:HIS:NE2	2.54	0.70
1:B:305:MET:HE1	1:B:335:ARG:HB2	1.72	0.69
1:E:106:THR:CG2	1:E:135:ALA:HB3	2.21	0.69
2:Q:260:LEU:HD23	2:Q:260:LEU:C	2.17	0.69
2:X:264:LYS:HE3	4:a:124:LYS:HB3	1.74	0.69
2:Q:264:LYS:HE3	4:T:124:LYS:HB3	1.74	0.69
5:U:159:LEU:CG	2:X:140:LYS:HE3	2.23	0.69
2:X:257:GLU:HA	2:X:260:LEU:HB3	1.75	0.69
5:U:204:ARG:HB3	2:W:76:LYS:HD3	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:252:ASN:CA	1:D:255:PHE:CZ	2.76	0.69
1:N:305:MET:CE	1:N:335:ARG:CZ	2.70	0.69
1:L:133:TYR:CE2	1:L:352:PHE:CE1	2.81	0.69
2:P:91:ARG:HE	2:Q:92:ILE:CG1	2.06	0.69
2:Q:96:GLU:OE2	5:b:192:ARG:NH2	2.25	0.69
1:B:133:TYR:CE2	1:B:352:PHE:HE1	2.05	0.69
1:M:305:MET:SD	1:M:335:ARG:HG3	2.33	0.69
1:L:334:GLU:O	1:L:338:SER:HB3	1.93	0.68
1:F:252:ASN:CB	1:F:255:PHE:CE2	2.76	0.68
2:Q:268:LYS:O	2:Q:272:GLU:HB2	1.93	0.68
5:U:204:ARG:HD2	2:W:76:LYS:HZ3	1.58	0.68
2:X:268:LYS:O	2:X:272:GLU:HB2	1.93	0.68
2:X:260:LEU:HD23	2:X:260:LEU:C	2.17	0.68
1:K:189:LEU:HB2	1:K:257:CYS:SG	2.33	0.68
2:P:91:ARG:NH1	5:b:195:ILE:HD11	2.07	0.68
1:D:252:ASN:CA	1:D:255:PHE:CE2	2.65	0.68
1:M:333:PRO:HG3	3:R:9:GLN:CG	2.17	0.68
1:I:257:CYS:HB2	1:I:258:PRO:CD	2.24	0.68
6:V:59:GLU:OE2	2:W:153:HIS:CE1	2.46	0.68
1:K:305:MET:HG2	1:K:335:ARG:CD	2.23	0.68
2:W:91:ARG:HE	2:X:92:ILE:CG1	2.06	0.68
2:Q:257:GLU:HA	2:Q:260:LEU:HB3	1.75	0.67
1:C:133:TYR:CE1	1:C:355:MET:HB3	2.29	0.67
2:W:256:LEU:HD21	2:X:256:LEU:HB3	1.75	0.67
1:K:133:TYR:CZ	1:K:352:PHE:CZ	2.80	0.67
1:M:332:PRO:O	1:M:335:ARG:HB3	1.95	0.67
1:N:262:PHE:CZ	1:N:312:ARG:HG2	2.30	0.67
1:L:207:GLU:O	1:L:210:ARG:HG3	1.94	0.67
1:M:333:PRO:CD	3:R:9:GLN:OE1	2.43	0.66
2:P:256:LEU:HD21	2:Q:256:LEU:HB3	1.75	0.66
1:H:163:VAL:HG23	1:H:175:ILE:HG21	1.74	0.66
1:J:335:ARG:C	1:J:337:TYR:H	2.03	0.66
1:N:109:PRO:HG2	1:N:161:HIS:NE2	2.09	0.66
2:P:91:ARG:NE	2:Q:92:ILE:HD12	2.11	0.66
5:U:141:ARG:HB3	5:U:142:PRO:HD3	1.77	0.66
1:M:241:GLU:OE2	2:P:268:LYS:CE	2.43	0.66
1:F:252:ASN:HB2	1:F:255:PHE:CE2	2.30	0.66
1:H:133:TYR:CE1	1:H:355:MET:HB3	2.30	0.66
1:O:207:GLU:O	1:O:210:ARG:HG2	1.96	0.66
1:E:108:ALA:HB1	1:E:161:HIS:CE1	2.31	0.66
2:P:145:GLU:HG3	2:P:149:LYS:HE3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:140:LYS:CG	5:b:159:LEU:HD22	2.23	0.66
1:M:109:PRO:CG	1:M:161:HIS:NE2	2.59	0.65
1:O:37:ARG:O	1:O:65:LEU:HA	1.96	0.65
2:Q:125:ARG:NH2	5:b:178:LYS:HZ1	1.94	0.65
1:E:133:TYR:CD2	1:E:352:PHE:CZ	2.84	0.65
1:J:169:TYR:OH	1:L:49:GLN:HB3	1.97	0.65
1:C:252:ASN:HB2	1:C:255:PHE:CZ	2.31	0.65
2:Q:261:TYR:CE1	2:Q:265:LEU:HD22	2.31	0.65
2:W:88:LEU:HD12	2:X:85:VAL:HA	1.78	0.65
1:E:143:TYR:OH	1:G:45:VAL:N	2.30	0.65
1:F:227:MET:HE3	1:F:255:PHE:HE1	1.60	0.65
1:C:133:TYR:CG	1:C:352:PHE:HZ	2.15	0.65
6:V:55:GLU:OE2	2:W:149:LYS:HD2	1.97	0.65
2:W:91:ARG:CZ	2:X:92:ILE:HG13	2.26	0.65
1:C:192:ILE:CD1	1:C:256:ARG:CD	2.61	0.65
1:A:133:TYR:CD1	1:A:352:PHE:HZ	2.14	0.65
1:E:106:THR:HG21	1:E:140:LEU:CD1	2.26	0.65
1:H:163:VAL:CG2	1:H:175:ILE:HG21	2.27	0.65
2:X:261:TYR:CE1	2:X:265:LEU:HD22	2.31	0.65
1:K:196:ARG:HD2	1:K:253:GLU:OE2	1.97	0.65
1:L:133:TYR:CE1	1:L:355:MET:HB3	2.32	0.65
1:D:333:PRO:C	1:D:335:ARG:H	2.02	0.65
2:P:91:ARG:CZ	2:Q:92:ILE:HG13	2.26	0.65
2:Q:261:TYR:CE1	2:Q:265:LEU:HB2	2.32	0.65
1:G:252:ASN:CB	1:G:255:PHE:CZ	2.80	0.64
2:P:91:ARG:HH21	2:Q:92:ILE:CG1	1.97	0.64
2:Q:261:TYR:HE1	2:Q:265:LEU:HD22	1.61	0.64
1:I:109:PRO:CG	1:I:161:HIS:NE2	2.60	0.64
1:O:207:GLU:O	1:O:210:ARG:HG3	1.96	0.64
2:W:91:ARG:HH21	2:X:92:ILE:CG1	1.97	0.64
1:I:305:MET:HE1	1:I:335:ARG:CG	2.26	0.64
1:L:144:ALA:O	4:a:94:ARG:NH1	2.31	0.64
1:A:252:ASN:CA	1:A:255:PHE:CZ	2.79	0.64
1:E:133:TYR:CD2	1:E:352:PHE:HZ	2.16	0.64
1:K:257:CYS:HB2	1:K:258:PRO:CD	2.27	0.64
2:X:261:TYR:CE1	2:X:265:LEU:HB2	2.32	0.64
2:X:261:TYR:HE1	2:X:265:LEU:HD22	1.61	0.64
1:B:252:ASN:CB	1:B:255:PHE:CZ	2.81	0.64
2:P:256:LEU:HD11	2:Q:257:GLU:HG2	1.80	0.64
2:W:88:LEU:CD1	2:X:85:VAL:HA	2.27	0.64
1:G:333:PRO:C	1:G:335:ARG:H	2.05	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:140:LYS:CE	5:b:159:LEU:CD2	2.71	0.64
5:U:195:ILE:HG22	5:U:196:ASP:N	2.11	0.64
2:W:91:ARG:NE	2:X:92:ILE:HD12	2.11	0.64
1:K:352:PHE:CD1	1:K:355:MET:CG	2.81	0.64
1:N:279:TYR:OH	1:N:283:MET:CE	2.45	0.64
1:O:305:MET:SD	1:O:335:ARG:NE	2.70	0.64
1:D:332:PRO:O	1:D:335:ARG:CG	2.35	0.64
1:E:133:TYR:CZ	1:E:352:PHE:HE1	2.14	0.64
5:U:192:ARG:NH2	2:X:96:GLU:CG	2.61	0.63
1:F:169:TYR:OH	1:H:49:GLN:HB3	1.97	0.63
1:D:133:TYR:CE1	1:D:355:MET:HB3	2.33	0.63
1:N:262:PHE:CE2	1:N:312:ARG:HG2	2.33	0.63
2:P:162:TYR:CD1	2:Q:165:VAL:HG11	2.34	0.63
1:E:133:TYR:CE2	1:E:352:PHE:CE1	2.86	0.63
1:M:336:LYS:C	1:M:338:SER:H	2.06	0.63
1:L:109:PRO:HD2	1:L:161:HIS:CD2	2.34	0.63
2:W:256:LEU:HD11	2:X:257:GLU:HG2	1.79	0.63
1:G:332:PRO:O	1:G:335:ARG:HG2	1.99	0.63
1:O:207:GLU:HA	1:O:210:ARG:HG2	1.80	0.63
5:U:195:ILE:CD1	2:W:91:ARG:HD3	2.28	0.63
1:H:133:TYR:CE1	1:H:352:PHE:HE1	2.08	0.62
2:P:88:LEU:HD13	2:P:91:ARG:NH2	2.14	0.62
1:B:207:GLU:CA	1:B:210:ARG:HG2	2.26	0.62
1:B:227:MET:HA	1:B:255:PHE:CE1	2.33	0.62
1:F:334:GLU:O	1:F:338:SER:HB3	1.99	0.62
1:O:109:PRO:CB	1:O:163:VAL:HG21	2.29	0.62
2:W:162:TYR:CD1	2:X:165:VAL:HG11	2.34	0.62
1:D:133:TYR:CD2	1:D:352:PHE:CZ	2.87	0.62
2:P:256:LEU:HG	2:Q:260:LEU:CD1	2.29	0.62
2:W:256:LEU:HG	2:X:260:LEU:CD1	2.29	0.62
1:L:207:GLU:CA	1:L:210:ARG:HG2	2.28	0.62
1:L:333:PRO:CG	3:Y:9:GLN:HG3	2.29	0.62
1:M:262:PHE:CZ	1:M:312:ARG:HG2	2.33	0.62
2:X:252:SER:O	2:X:256:LEU:HG	1.99	0.62
2:X:253:ILE:HA	2:X:256:LEU:HB2	1.82	0.62
5:U:57:ALA:HB2	6:V:104:PHE:CE2	2.30	0.62
1:H:252:ASN:CA	1:H:255:PHE:CE2	2.79	0.62
1:I:169:TYR:OH	1:K:49:GLN:CG	2.47	0.62
1:N:252:ASN:HB2	1:N:255:PHE:HZ	1.62	0.62
5:U:159:LEU:HD12	2:X:136:LYS:HB3	1.81	0.62
1:J:303:THR:O	1:J:306:TYR:CD1	2.53	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:333:PRO:C	1:N:335:ARG:H	2.08	0.62
1:O:196:ARG:HD2	1:O:253:GLU:CD	2.25	0.62
1:L:305:MET:HE1	1:L:335:ARG:CB	2.28	0.61
1:H:227:MET:HB3	1:H:255:PHE:CE1	2.35	0.61
1:N:334:GLU:O	1:N:338:SER:HB3	2.00	0.61
2:P:88:LEU:CD1	2:P:91:ARG:NH2	2.63	0.61
1:M:109:PRO:CD	1:M:161:HIS:NE2	2.63	0.61
1:M:196:ARG:HD2	1:M:253:GLU:CD	2.26	0.61
2:Q:252:SER:O	2:Q:256:LEU:HG	1.99	0.61
5:U:195:ILE:CG2	5:U:196:ASP:N	2.64	0.61
1:B:169:TYR:OH	1:D:49:GLN:HB3	2.00	0.61
1:H:133:TYR:CE1	1:H:352:PHE:CZ	2.89	0.61
2:P:256:LEU:CD1	2:Q:260:LEU:CD1	2.77	0.61
2:P:91:ARG:CD	5:b:195:ILE:CG1	2.77	0.61
1:B:332:PRO:O	1:B:335:ARG:CG	2.30	0.61
1:K:252:ASN:HA	1:K:255:PHE:CZ	2.34	0.61
1:L:305:MET:HE2	1:L:335:ARG:CB	2.19	0.61
2:W:256:LEU:CD1	2:X:260:LEU:CD1	2.77	0.61
1:J:219:VAL:HG11	1:J:312:ARG:HG2	1.83	0.60
1:M:305:MET:SD	1:M:335:ARG:NE	2.74	0.60
1:E:334:GLU:O	1:E:338:SER:HB3	2.01	0.60
1:I:262:PHE:CZ	1:I:312:ARG:HG2	2.35	0.60
1:A:227:MET:HA	1:A:255:PHE:CE1	2.37	0.60
1:E:133:TYR:HE1	1:E:355:MET:HB3	1.65	0.60
1:M:333:PRO:HG3	3:R:9:GLN:NE2	2.17	0.60
1:O:287:ILE:HD12	1:O:290:ARG:HD2	1.83	0.60
2:P:152:LYS:HE3	2:P:156:GLU:OE2	2.01	0.60
2:Q:253:ILE:HA	2:Q:256:LEU:HB2	1.82	0.60
1:I:301:GLY:O	1:I:336:LYS:CB	2.49	0.60
1:H:305:MET:SD	1:H:336:LYS:HD2	2.42	0.60
1:J:113:LYS:O	1:J:116:ARG:HG2	2.01	0.60
1:E:109:PRO:HD2	1:E:161:HIS:CE1	2.36	0.60
1:G:133:TYR:CE2	1:G:352:PHE:HE1	2.20	0.60
1:K:252:ASN:CA	1:K:255:PHE:CZ	2.85	0.60
1:B:207:GLU:O	1:B:210:ARG:HG3	2.02	0.59
2:Q:136:LYS:O	2:Q:140:LYS:HG2	2.00	0.59
2:W:256:LEU:HG	2:X:260:LEU:HD12	1.85	0.59
1:L:133:TYR:CD2	1:L:352:PHE:CZ	2.90	0.59
1:M:230:ALA:CB	1:M:255:PHE:CZ	2.84	0.59
1:A:133:TYR:CE1	1:A:352:PHE:CZ	2.90	0.59
1:H:160:THR:HG22	1:H:162:ASN:ND2	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:352:PHE:CE1	1:K:355:MET:CG	2.85	0.59
1:O:163:VAL:HG13	1:O:175:ILE:HG12	1.84	0.59
1:C:133:TYR:CE2	1:C:352:PHE:CZ	2.89	0.59
1:O:230:ALA:HB3	1:O:255:PHE:CZ	2.37	0.59
1:K:352:PHE:CD1	1:M:45:VAL:HG21	2.38	0.59
1:O:252:ASN:HA	1:O:255:PHE:CZ	2.36	0.59
1:M:252:ASN:CA	1:M:255:PHE:CZ	2.85	0.59
1:N:305:MET:SD	1:N:335:ARG:CD	2.91	0.59
1:D:301:GLY:O	1:D:336:LYS:HA	2.02	0.59
1:D:334:GLU:O	1:D:338:SER:HB3	2.03	0.59
1:E:283:MET:O	1:E:290:ARG:CZ	2.51	0.59
1:A:162:ASN:ND2	1:A:281:SER:OG	2.35	0.58
1:E:333:PRO:C	1:E:335:ARG:H	2.11	0.58
1:K:252:ASN:HA	1:K:255:PHE:HE2	1.59	0.58
1:K:257:CYS:CB	1:K:258:PRO:CD	2.81	0.58
1:L:25:ASP:OD2	4:a:97:LYS:NZ	2.35	0.58
1:L:109:PRO:HD2	1:L:161:HIS:NE2	2.17	0.58
1:J:306:TYR:HB2	1:J:309:ILE:HB	1.85	0.58
1:K:102:PRO:O	1:K:129:VAL:HG21	2.03	0.58
1:K:305:MET:SD	1:K:336:LYS:HD3	2.42	0.58
1:C:252:ASN:CB	1:C:255:PHE:CZ	2.86	0.58
1:C:304:THR:HB	1:C:335:ARG:HD2	1.86	0.58
1:K:169:TYR:OH	1:M:49:GLN:HB3	2.03	0.58
1:N:109:PRO:CD	1:N:161:HIS:CE1	2.81	0.58
1:A:133:TYR:CE1	1:A:352:PHE:CE1	2.92	0.58
1:A:133:TYR:HE2	1:A:346:LEU:HD21	1.68	0.58
1:L:230:ALA:HB3	1:L:255:PHE:HZ	1.68	0.58
2:X:261:TYR:CE1	2:X:265:LEU:CD2	2.87	0.58
1:B:331:ALA:O	1:B:335:ARG:NH1	2.36	0.58
1:E:109:PRO:HD2	1:E:161:HIS:CD2	2.39	0.58
1:L:207:GLU:HA	1:L:210:ARG:CG	2.32	0.58
2:P:91:ARG:HE	2:Q:92:ILE:HG13	1.69	0.57
5:U:192:ARG:HH21	2:X:96:GLU:HG3	1.63	0.57
1:A:133:TYR:CD1	1:A:352:PHE:CZ	2.92	0.57
1:F:109:PRO:HD2	1:F:161:HIS:NE2	2.19	0.57
1:G:133:TYR:CZ	1:G:352:PHE:HE1	2.22	0.57
1:L:109:PRO:CG	1:L:161:HIS:NE2	2.67	0.57
1:L:143:TYR:HB3	1:L:345:ILE:HD13	1.86	0.57
2:W:91:ARG:HE	2:X:92:ILE:HG13	1.69	0.57
2:P:256:LEU:HG	2:Q:260:LEU:HD12	1.85	0.57
2:P:256:LEU:HD23	2:Q:256:LEU:HD13	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:252:ASN:HA	1:D:255:PHE:HE2	1.60	0.57
1:E:305:MET:CE	1:E:336:LYS:CD	2.81	0.57
1:H:133:TYR:OH	1:H:352:PHE:HE1	1.87	0.57
6:c:3:ASP:OD1	6:c:6:LYS:NZ	2.31	0.57
1:F:257:CYS:HB3	1:F:258:PRO:HD3	1.87	0.57
1:H:133:TYR:CD1	1:H:352:PHE:CZ	2.92	0.57
2:P:256:LEU:HD12	2:Q:260:LEU:HD13	1.84	0.57
2:Q:261:TYR:CE1	2:Q:265:LEU:CD2	2.87	0.57
1:B:230:ALA:CB	1:B:255:PHE:CZ	2.87	0.57
1:K:230:ALA:HB3	1:K:255:PHE:HZ	1.69	0.57
1:M:109:PRO:HG2	1:M:161:HIS:NE2	2.20	0.57
2:W:162:TYR:CE1	2:X:165:VAL:HG11	2.39	0.57
1:C:252:ASN:CA	1:C:255:PHE:CZ	2.87	0.57
1:E:283:MET:HA	1:E:290:ARG:CD	2.30	0.57
1:O:305:MET:CE	1:O:335:ARG:HE	2.16	0.57
1:O:333:PRO:C	1:O:335:ARG:H	2.11	0.57
2:P:91:ARG:NE	2:Q:92:ILE:HG13	2.20	0.57
2:Q:132:SER:O	2:Q:136:LYS:HG2	2.04	0.57
2:W:256:LEU:HD23	2:X:256:LEU:HD13	1.85	0.57
1:J:305:MET:HE1	1:J:335:ARG:HE	1.69	0.57
2:X:132:SER:O	2:X:136:LYS:HG2	2.04	0.57
1:A:305:MET:SD	1:A:335:ARG:HB2	2.45	0.56
1:A:331:ALA:O	1:A:335:ARG:NH1	2.37	0.56
1:L:342:GLY:HA2	1:L:345:ILE:HG22	1.88	0.56
1:M:238:LYS:HZ3	2:P:276:HIS:CE1	2.23	0.56
1:N:305:MET:HE3	1:N:335:ARG:HH21	1.69	0.56
2:W:256:LEU:HD13	2:X:257:GLU:HG2	1.87	0.56
1:J:219:VAL:CG1	1:J:312:ARG:HG2	2.35	0.56
1:M:109:PRO:HD2	1:M:161:HIS:CE1	2.41	0.56
1:H:253:GLU:HA	1:H:256:ARG:HB2	1.86	0.56
1:J:80:ASP:OD2	1:J:84:LYS:NZ	2.39	0.56
1:L:252:ASN:HB2	1:L:255:PHE:CZ	2.40	0.56
2:P:153:HIS:CE1	6:c:54:PRO:HB2	2.36	0.56
1:B:207:GLU:HA	1:B:210:ARG:CG	2.32	0.56
1:M:333:PRO:CG	3:R:9:GLN:OE1	2.54	0.56
1:N:196:ARG:HD2	1:N:253:GLU:OE2	2.06	0.56
1:N:257:CYS:HB3	1:N:258:PRO:HD3	1.86	0.56
1:A:133:TYR:CE2	1:A:352:PHE:CE1	2.83	0.56
1:I:109:PRO:HD2	1:I:161:HIS:CE1	2.40	0.56
5:U:195:ILE:HB	2:W:91:ARG:HD3	1.87	0.56
2:W:91:ARG:NE	2:X:92:ILE:HG13	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:257:CYS:HB2	1:K:258:PRO:HD3	1.87	0.56
2:P:162:TYR:CE1	2:Q:165:VAL:HG11	2.40	0.56
1:B:305:MET:CE	1:B:335:ARG:CB	2.76	0.56
2:W:166:ALA:CA	2:X:165:VAL:HG21	2.35	0.56
1:I:189:LEU:CA	1:I:257:CYS:SG	2.93	0.55
1:J:334:GLU:O	1:J:338:SER:HB3	2.06	0.55
1:B:187:ASP:OD2	1:B:191:LYS:NZ	2.39	0.55
1:N:305:MET:HE3	1:N:335:ARG:NH2	2.21	0.55
1:J:222:ASP:OD1	1:J:315:LYS:NZ	2.40	0.55
1:E:282:ILE:O	1:E:290:ARG:CG	2.53	0.55
1:E:313:MET:CG	1:E:329:ILE:HD13	2.36	0.55
1:K:189:LEU:HD13	1:K:257:CYS:SG	2.45	0.55
1:L:333:PRO:C	1:L:335:ARG:H	2.15	0.55
1:L:342:GLY:CA	1:L:345:ILE:HG22	2.36	0.55
1:K:230:ALA:HB3	1:K:255:PHE:CZ	2.41	0.55
1:L:238:LYS:HE2	2:W:276:HIS:NE2	2.22	0.55
1:A:80:ASP:OD2	1:A:84:LYS:NZ	2.40	0.55
1:G:257:CYS:HB2	1:G:258:PRO:HD3	1.89	0.55
2:P:166:ALA:CA	2:Q:165:VAL:HG21	2.35	0.55
1:E:207:GLU:O	1:E:210:ARG:HG3	2.06	0.55
1:E:207:GLU:CA	1:E:210:ARG:HG2	2.37	0.55
1:B:109:PRO:CD	1:B:161:HIS:CD2	2.87	0.54
1:D:230:ALA:HB3	1:D:255:PHE:HZ	1.72	0.54
1:F:169:TYR:OH	1:H:49:GLN:CG	2.55	0.54
1:I:301:GLY:O	1:I:336:LYS:HB3	2.07	0.54
1:D:230:ALA:HB3	1:D:255:PHE:CZ	2.43	0.54
1:E:305:MET:HE3	1:E:336:LYS:CD	2.26	0.54
1:I:51:ASP:N	1:I:51:ASP:OD1	2.40	0.54
1:M:301:GLY:O	1:M:336:LYS:CB	2.54	0.54
1:F:333:PRO:C	1:F:335:ARG:H	2.14	0.54
1:D:133:TYR:CD2	1:D:352:PHE:HZ	2.25	0.54
1:H:333:PRO:C	1:H:335:ARG:H	2.15	0.54
6:V:5:TYR:CD2	6:V:79:VAL:CG2	2.91	0.54
1:G:61:LYS:NZ	5:b:165:GLU:OE2	2.41	0.54
2:Q:257:GLU:O	2:Q:261:TYR:N	2.38	0.54
1:A:301:GLY:C	1:A:336:LYS:HA	2.33	0.54
1:B:257:CYS:HB3	1:B:258:PRO:HD3	1.90	0.54
1:D:51:ASP:OD1	1:D:51:ASP:N	2.39	0.54
1:F:169:TYR:OH	1:H:49:GLN:CB	2.56	0.54
5:U:167:LEU:HD22	2:X:129:VAL:CG2	2.37	0.54
1:A:252:ASN:CB	1:A:255:PHE:CZ	2.91	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:PHE:CD1	1:A:355:MET:HG3	2.43	0.54
1:F:305:MET:CE	1:F:336:LYS:CD	2.67	0.54
2:X:261:TYR:OH	2:X:265:LEU:HD23	2.08	0.54
1:F:227:MET:HE3	1:F:255:PHE:CE1	2.42	0.53
1:H:227:MET:HB3	1:H:255:PHE:HE1	1.73	0.53
1:L:133:TYR:CD2	1:L:352:PHE:HZ	2.25	0.53
1:L:207:GLU:O	1:L:210:ARG:CG	2.56	0.53
1:M:257:CYS:HB3	1:M:258:PRO:HD3	1.89	0.53
1:O:164:PRO:HG2	1:O:171:LEU:HB2	1.90	0.53
2:P:256:LEU:HD13	2:Q:257:GLU:HG2	1.87	0.53
1:H:51:ASP:OD1	1:H:51:ASP:N	2.41	0.53
6:c:86:LYS:NZ	6:c:155:GLU:OE2	2.42	0.53
1:D:257:CYS:HB3	1:D:258:PRO:HD3	1.89	0.53
1:F:51:ASP:OD1	1:F:51:ASP:N	2.39	0.53
1:F:169:TYR:OH	1:H:49:GLN:HG3	2.07	0.53
1:H:154:ASP:O	1:H:156:GLY:N	2.41	0.53
1:K:51:ASP:OD1	1:K:51:ASP:N	2.40	0.53
1:L:222:ASP:OD1	1:L:315:LYS:NZ	2.41	0.53
1:N:335:ARG:C	1:N:337:TYR:H	2.15	0.53
2:Q:125:ARG:NH2	5:b:178:LYS:NZ	2.56	0.53
2:W:88:LEU:CD1	2:X:85:VAL:HG13	2.15	0.53
1:A:257:CYS:HB3	1:A:258:PRO:HD3	1.90	0.53
2:P:156:GLU:HG3	6:c:55:GLU:CD	2.32	0.53
1:E:335:ARG:C	1:E:337:TYR:H	2.16	0.53
1:J:51:ASP:OD1	1:J:51:ASP:N	2.39	0.53
1:O:227:MET:HA	1:O:255:PHE:CE1	2.44	0.53
2:Q:261:TYR:OH	2:Q:265:LEU:HD23	2.08	0.53
1:H:163:VAL:CG2	1:H:175:ILE:HG23	2.25	0.53
1:H:257:CYS:HB3	1:H:258:PRO:HD3	1.91	0.53
1:B:222:ASP:OD1	1:B:315:LYS:NZ	2.42	0.53
1:B:305:MET:HE2	1:B:335:ARG:C	2.34	0.53
1:E:313:MET:O	1:E:317:ILE:HD12	2.09	0.53
1:M:241:GLU:OE2	2:P:268:LYS:HE2	2.08	0.53
2:P:88:LEU:CD1	2:P:91:ARG:HH21	2.21	0.53
1:O:230:ALA:CB	1:O:255:PHE:CE2	2.92	0.53
1:G:133:TYR:CE2	1:G:352:PHE:CE1	2.97	0.53
1:G:133:TYR:CD2	1:G:352:PHE:CZ	2.97	0.52
1:O:257:CYS:HB3	1:O:258:PRO:HD3	1.91	0.52
1:K:113:LYS:O	1:K:116:ARG:HG2	2.08	0.52
1:M:241:GLU:OE2	2:P:268:LYS:NZ	2.41	0.52
2:X:257:GLU:O	2:X:261:TYR:N	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:196:ARG:HD2	1:H:253:GLU:OE2	2.10	0.52
1:J:305:MET:HE1	1:J:335:ARG:NE	2.24	0.52
1:B:227:MET:HA	1:B:255:PHE:HE1	1.75	0.52
1:E:283:MET:O	1:E:290:ARG:NE	2.43	0.52
1:G:196:ARG:HD2	1:G:253:GLU:CD	2.34	0.52
1:I:305:MET:HE1	1:I:335:ARG:HG2	1.90	0.52
1:M:301:GLY:N	1:M:336:LYS:HB2	2.24	0.52
1:N:187:ASP:OD2	1:N:191:LYS:NZ	2.42	0.52
2:X:253:ILE:O	2:X:257:GLU:N	2.43	0.52
6:V:59:GLU:HG2	2:W:153:HIS:HE1	1.74	0.52
1:L:252:ASN:CB	1:L:255:PHE:CZ	2.93	0.52
1:O:230:ALA:HB3	1:O:255:PHE:HZ	1.75	0.52
1:B:305:MET:HE2	1:B:335:ARG:O	2.10	0.52
1:C:133:TYR:CG	1:C:352:PHE:CZ	2.96	0.52
1:H:227:MET:HA	1:H:255:PHE:HZ	1.75	0.52
1:M:252:ASN:CB	1:M:255:PHE:CZ	2.92	0.52
4:a:88:ASP:N	4:a:88:ASP:OD1	2.43	0.52
1:A:51:ASP:OD1	1:A:51:ASP:N	2.39	0.52
1:E:257:CYS:HB2	1:E:258:PRO:HD3	1.92	0.52
1:G:335:ARG:C	1:G:337:TYR:H	2.18	0.52
1:G:335:ARG:CG	1:G:335:ARG:HH11	2.23	0.52
1:L:252:ASN:HA	1:L:255:PHE:CZ	2.43	0.52
1:N:257:CYS:CB	1:N:258:PRO:HD3	2.40	0.52
1:O:163:VAL:HG22	1:O:175:ILE:HG23	1.92	0.52
2:Q:265:LEU:HD12	2:Q:265:LEU:O	2.10	0.52
2:W:218:GLU:OE2	2:X:217:LYS:HB2	2.10	0.52
1:F:109:PRO:CD	1:F:161:HIS:NE2	2.72	0.51
1:K:305:MET:HG3	1:K:335:ARG:CD	2.28	0.51
4:T:88:ASP:N	4:T:88:ASP:OD1	2.43	0.51
1:B:154:ASP:OD2	1:B:161:HIS:HB2	2.09	0.51
1:A:332:PRO:O	1:A:335:ARG:CG	2.33	0.51
2:P:194:GLU:OE2	2:P:198:LYS:NZ	2.44	0.51
2:W:256:LEU:HD12	2:X:260:LEU:HD13	1.84	0.51
1:B:301:GLY:C	1:B:336:LYS:HA	2.35	0.51
6:V:5:TYR:HA	6:V:79:VAL:CG2	2.40	0.51
2:W:91:ARG:HG2	2:X:92:ILE:HD12	1.92	0.51
1:B:333:PRO:C	1:B:335:ARG:H	2.17	0.51
1:C:230:ALA:HB3	1:C:255:PHE:HZ	1.75	0.51
1:H:196:ARG:HD2	1:H:253:GLU:CD	2.36	0.51
1:J:333:PRO:C	1:J:335:ARG:H	2.18	0.51
1:L:25:ASP:CB	4:a:97:LYS:HE2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:109:PRO:CD	1:L:161:HIS:NE2	2.74	0.51
2:X:265:LEU:HD12	2:X:265:LEU:O	2.10	0.51
1:D:133:TYR:CD2	1:D:352:PHE:CE1	2.99	0.51
2:P:218:GLU:OE2	2:Q:217:LYS:HB2	2.10	0.51
1:A:252:ASN:HB2	1:A:255:PHE:CZ	2.46	0.51
1:H:216:LEU:O	1:H:254:ARG:HG2	2.10	0.51
1:L:51:ASP:OD1	1:L:51:ASP:N	2.44	0.51
1:N:252:ASN:CA	1:N:255:PHE:CZ	2.94	0.51
1:C:230:ALA:HB3	1:C:255:PHE:CZ	2.46	0.51
1:I:337:TYR:O	1:I:341:ILE:HD12	2.11	0.51
2:Q:70:LYS:O	2:Q:74:ALA:N	2.42	0.51
1:J:335:ARG:C	1:J:337:TYR:N	2.69	0.51
2:P:91:ARG:HG2	2:Q:92:ILE:HD12	1.92	0.51
2:W:194:GLU:OE2	2:W:198:LYS:NZ	2.44	0.51
1:C:107:GLU:OE2	1:C:116:ARG:NE	2.43	0.51
1:K:305:MET:HG2	1:K:335:ARG:NE	2.26	0.51
1:O:230:ALA:CB	1:O:255:PHE:HE2	2.23	0.51
1:O:334:GLU:O	1:O:338:SER:HB3	2.11	0.51
2:Q:235:ALA:O	2:Q:239:ALA:N	2.43	0.51
1:B:207:GLU:O	1:B:210:ARG:CG	2.59	0.50
2:Q:157:ASP:OD2	2:Q:161:LYS:NZ	2.41	0.50
2:X:264:LYS:HE3	4:a:124:LYS:CB	2.41	0.50
1:B:305:MET:CE	1:B:335:ARG:O	2.59	0.50
1:L:133:TYR:CG	1:L:352:PHE:HZ	2.30	0.50
1:M:133:TYR:CE1	1:M:352:PHE:HZ	2.29	0.50
1:O:222:ASP:OD1	1:O:315:LYS:NZ	2.44	0.50
3:R:4:ILE:O	3:R:5:LYS:C	2.53	0.50
1:E:207:GLU:O	1:E:210:ARG:CG	2.59	0.50
1:M:51:ASP:OD1	1:M:51:ASP:N	2.41	0.50
1:N:109:PRO:CD	1:N:161:HIS:CD2	2.87	0.50
1:C:331:ALA:O	1:C:335:ARG:NH1	2.44	0.50
1:F:335:ARG:C	1:F:337:TYR:H	2.19	0.50
5:U:141:ARG:HB3	5:U:142:PRO:CD	2.40	0.50
2:X:235:ALA:O	2:X:239:ALA:N	2.43	0.50
2:X:261:TYR:OH	2:X:265:LEU:CD2	2.60	0.50
1:L:262:PHE:CE2	1:L:312:ARG:HG3	2.47	0.50
1:A:168:GLY:CA	1:C:47:MET:HE2	2.42	0.50
1:A:352:PHE:CE1	1:A:355:MET:CB	2.94	0.50
1:F:154:ASP:OD2	1:F:161:HIS:HB3	2.11	0.50
1:I:167:GLU:O	1:I:169:TYR:CD1	2.65	0.50
2:W:84:ASP:OD1	2:W:84:ASP:O	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:252:ASN:HB2	1:H:255:PHE:CZ	2.46	0.50
1:L:109:PRO:HG2	1:L:161:HIS:NE2	2.27	0.50
1:C:162:ASN:ND2	1:C:281:SER:OG	2.45	0.50
1:I:109:PRO:HG2	1:I:161:HIS:NE2	2.25	0.50
1:K:129:VAL:CG2	1:K:130:PRO:HD2	2.42	0.50
6:V:33:ASP:OD1	6:V:33:ASP:N	2.44	0.50
2:X:278:LEU:O	2:X:279:ASN:C	2.54	0.50
1:O:227:MET:HA	1:O:255:PHE:CZ	2.47	0.50
2:X:252:SER:O	2:X:256:LEU:N	2.45	0.50
1:I:260:THR:HA	1:I:263:GLN:O	2.12	0.49
1:J:252:ASN:CA	1:J:255:PHE:CZ	2.95	0.49
1:L:189:LEU:HB2	1:L:257:CYS:SG	2.52	0.49
5:b:127:ASP:OD2	5:b:131:LYS:NZ	2.45	0.49
1:E:80:ASP:OD2	1:E:84:LYS:NZ	2.45	0.49
1:H:160:THR:HG22	1:H:162:ASN:CG	2.36	0.49
1:J:335:ARG:O	1:J:337:TYR:N	2.46	0.49
1:K:305:MET:SD	1:K:336:LYS:CD	3.00	0.49
1:K:333:PRO:C	1:K:335:ARG:H	2.18	0.49
1:K:352:PHE:HD1	1:M:45:VAL:HG21	1.74	0.49
1:M:133:TYR:CD1	1:M:352:PHE:HZ	2.30	0.49
2:Q:125:ARG:CZ	5:b:178:LYS:HZ1	2.26	0.49
1:M:207:GLU:O	1:M:210:ARG:CG	2.61	0.49
1:O:207:GLU:CA	1:O:210:ARG:HG2	2.42	0.49
2:P:145:GLU:O	2:P:149:LYS:HG3	2.11	0.49
1:A:133:TYR:CZ	1:A:352:PHE:HZ	2.17	0.49
1:A:333:PRO:C	1:A:335:ARG:H	2.20	0.49
1:C:80:ASP:OD2	1:C:84:LYS:NZ	2.46	0.49
1:M:257:CYS:CB	1:M:258:PRO:HD3	2.43	0.49
2:Q:253:ILE:O	2:Q:257:GLU:N	2.43	0.49
4:T:199:GLY:C	4:T:201:ARG:H	2.20	0.49
1:D:302:GLY:C	1:D:304:THR:H	2.21	0.49
1:E:133:TYR:CD2	1:E:352:PHE:CE1	3.01	0.49
2:Q:261:TYR:CE1	2:Q:265:LEU:CB	2.96	0.49
2:Q:261:TYR:OH	2:Q:265:LEU:CD2	2.60	0.49
5:U:159:LEU:CD1	2:X:140:LYS:HE3	2.42	0.49
1:J:306:TYR:C	1:J:308:GLY:H	2.19	0.49
1:L:133:TYR:CZ	1:L:352:PHE:CE1	2.85	0.49
2:Q:252:SER:O	2:Q:256:LEU:N	2.45	0.49
1:A:230:ALA:HB3	1:A:255:PHE:CZ	2.42	0.49
1:L:230:ALA:HB3	1:L:255:PHE:CZ	2.46	0.49
1:E:107:GLU:HG3	1:E:134:VAL:HG12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:334:GLU:O	1:H:338:SER:HB3	2.12	0.49
1:I:154:ASP:OD2	1:I:161:HIS:HB3	2.13	0.49
1:K:352:PHE:CE1	1:K:355:MET:HB3	2.48	0.49
1:M:352:PHE:CD1	1:M:355:MET:HG3	2.48	0.49
5:U:162:ARG:HE	2:X:136:LYS:HZ2	1.59	0.49
1:L:25:ASP:HB3	4:a:97:LYS:HE2	1.95	0.49
1:M:146:GLY:CA	4:T:87:PHE:CE2	2.95	0.49
1:C:107:GLU:OE1	1:C:116:ARG:HB3	2.13	0.49
1:C:187:ASP:OD2	1:C:191:LYS:NZ	2.46	0.49
1:L:345:ILE:HG23	1:L:346:LEU:N	2.28	0.49
2:Q:264:LYS:HE3	4:T:124:LYS:CB	2.41	0.49
1:D:305:MET:SD	1:D:335:ARG:NE	2.86	0.48
1:G:333:PRO:C	1:G:335:ARG:N	2.70	0.48
1:I:169:TYR:OH	1:K:49:GLN:CB	2.61	0.48
1:L:133:TYR:HE1	1:L:355:MET:HB3	1.78	0.48
3:Y:4:ILE:O	3:Y:5:LYS:C	2.52	0.48
1:B:211:ASP:OD1	1:B:215:LYS:NZ	2.46	0.48
1:C:252:ASN:O	1:C:256:ARG:HG2	2.13	0.48
1:H:352:PHE:CE1	1:H:355:MET:HB2	2.48	0.48
2:Q:260:LEU:C	2:Q:260:LEU:CD2	2.86	0.48
2:W:166:ALA:HA	2:X:165:VAL:CG2	2.42	0.48
2:X:261:TYR:CE1	2:X:265:LEU:CB	2.96	0.48
2:X:266:LYS:O	2:X:270:ILE:HG13	2.14	0.48
1:A:143:TYR:CD2	1:C:44:MET:CE	2.96	0.48
1:F:109:PRO:CD	1:F:161:HIS:CD2	2.95	0.48
1:J:187:ASP:OD2	1:J:191:LYS:NZ	2.45	0.48
1:N:230:ALA:HB3	1:N:255:PHE:CZ	2.49	0.48
1:O:109:PRO:HB2	1:O:163:VAL:HG21	1.94	0.48
1:F:257:CYS:CB	1:F:258:PRO:HD3	2.42	0.48
5:U:57:ALA:CB	6:V:104:PHE:HZ	2.19	0.48
5:U:127:ASP:OD2	5:U:131:LYS:NZ	2.46	0.48
1:A:302:GLY:C	1:A:304:THR:H	2.22	0.48
1:L:109:PRO:HB2	1:L:161:HIS:NE2	2.28	0.48
1:M:109:PRO:HB2	1:M:161:HIS:NE2	2.29	0.48
4:T:249:ASP:OD2	5:U:72:LYS:NZ	2.41	0.48
1:E:252:ASN:HA	1:E:255:PHE:HE2	1.76	0.48
1:E:289:ILE:O	1:E:293:LEU:HG	2.13	0.48
1:M:336:LYS:C	1:M:338:SER:N	2.72	0.48
5:b:50:LYS:HG3	6:c:156:PHE:CZ	2.48	0.48
1:B:302:GLY:C	1:B:304:THR:H	2.22	0.48
1:N:196:ARG:HD2	1:N:253:GLU:CD	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:153:HIS:ND1	6:c:55:GLU:CD	2.72	0.48
2:P:166:ALA:HA	2:Q:165:VAL:CG2	2.42	0.48
1:L:110:LEU:H	1:L:161:HIS:HE1	1.61	0.47
1:L:146:GLY:HA2	4:a:87:PHE:HZ	1.78	0.47
5:U:197:ALA:HA	2:W:87:SER:OG	2.13	0.47
1:E:133:TYR:CG	1:E:352:PHE:CZ	3.02	0.47
1:M:162:ASN:ND2	1:M:281:SER:OG	2.46	0.47
2:W:218:GLU:HG2	2:X:221:TYR:CE1	2.50	0.47
1:A:133:TYR:CE2	1:A:346:LEU:HD21	2.48	0.47
1:B:133:TYR:HE2	1:B:346:LEU:HD21	1.78	0.47
1:F:196:ARG:HD2	1:F:253:GLU:CD	2.39	0.47
6:c:121:LEU:HB3	6:c:128:ILE:HG13	1.96	0.47
2:Q:140:LYS:HE3	5:b:159:LEU:CB	2.39	0.47
1:B:308:GLY:O	1:B:312:ARG:HB3	2.14	0.47
1:G:188:TYR:CD2	1:G:257:CYS:HA	2.50	0.47
1:I:336:LYS:HE2	1:I:337:TYR:CE2	2.49	0.47
1:K:352:PHE:CE1	1:K:355:MET:HB2	2.50	0.47
1:M:133:TYR:CZ	1:M:352:PHE:HZ	2.33	0.47
1:O:207:GLU:C	1:O:210:ARG:HG2	2.39	0.47
2:P:218:GLU:OE2	2:Q:214:TYR:HA	2.14	0.47
1:A:227:MET:HA	1:A:255:PHE:HE1	1.78	0.47
1:B:333:PRO:HG2	2:W:72:GLU:OE1	2.14	0.47
1:C:333:PRO:C	1:C:335:ARG:H	2.23	0.47
1:C:335:ARG:C	1:C:337:TYR:H	2.22	0.47
1:D:154:ASP:O	1:D:155:SER:C	2.58	0.47
1:I:169:TYR:OH	1:K:49:GLN:HB3	2.15	0.47
2:P:218:GLU:HG2	2:Q:221:TYR:CE1	2.50	0.47
2:Q:266:LYS:O	2:Q:270:ILE:HG13	2.14	0.47
1:B:133:TYR:CE1	1:B:355:MET:HB3	2.50	0.47
1:E:106:THR:CG2	1:E:140:LEU:CD1	2.92	0.47
1:H:216:LEU:O	1:H:254:ARG:NE	2.36	0.47
5:U:195:ILE:HD12	2:W:91:ARG:HG3	1.84	0.47
1:A:133:TYR:HE2	1:A:346:LEU:CD2	2.28	0.47
1:A:352:PHE:CE1	1:A:355:MET:HB2	2.50	0.47
1:D:80:ASP:OD2	1:D:84:LYS:NZ	2.48	0.47
1:E:110:LEU:H	1:E:161:HIS:HE1	1.63	0.47
1:K:80:ASP:OD2	1:K:84:LYS:NZ	2.48	0.47
1:O:335:ARG:C	1:O:337:TYR:H	2.22	0.47
2:X:127:MET:O	2:X:131:GLU:N	2.45	0.47
1:A:230:ALA:CB	1:A:255:PHE:CZ	2.98	0.47
1:E:106:THR:CG2	1:E:140:LEU:HD11	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:133:TYR:CD2	1:G:352:PHE:CE1	3.02	0.47
1:N:300:SER:OG	1:N:338:SER:OG	2.31	0.47
2:X:157:ASP:OD2	2:X:161:LYS:NZ	2.41	0.47
1:A:164:PRO:HD3	1:A:281:SER:HB3	1.96	0.46
1:I:154:ASP:O	1:I:156:GLY:N	2.48	0.46
1:M:133:TYR:CG	1:M:352:PHE:HZ	2.33	0.46
1:M:207:GLU:O	1:M:210:ARG:HG3	2.15	0.46
2:P:256:LEU:CD2	2:Q:256:LEU:HB3	2.44	0.46
1:A:230:ALA:CB	1:A:255:PHE:HZ	2.27	0.46
1:L:109:PRO:HD2	1:L:161:HIS:CE1	2.51	0.46
2:P:91:ARG:CD	5:b:195:ILE:HG12	2.25	0.46
2:P:221:TYR:HB3	2:Q:221:TYR:HB3	1.96	0.46
2:X:260:LEU:C	2:X:260:LEU:CD2	2.86	0.46
1:I:257:CYS:HB3	1:I:258:PRO:HD3	1.94	0.46
1:K:129:VAL:HG22	1:K:130:PRO:HD2	1.98	0.46
1:L:133:TYR:HE2	1:L:346:LEU:HD21	1.81	0.46
2:P:91:ARG:NE	2:Q:92:ILE:CG1	2.77	0.46
1:E:108:ALA:HB1	1:E:161:HIS:ND1	2.30	0.46
1:E:301:GLY:C	1:E:336:LYS:HA	2.40	0.46
4:T:121:VAL:O	4:T:125:ASP:N	2.47	0.46
1:A:133:TYR:CE1	1:A:352:PHE:HZ	2.33	0.46
1:C:252:ASN:CA	1:C:255:PHE:CE2	2.77	0.46
1:M:133:TYR:CE1	1:M:352:PHE:CZ	3.03	0.46
2:P:88:LEU:HD13	2:P:91:ARG:HH21	1.79	0.46
2:Q:125:ARG:CZ	5:b:178:LYS:NZ	2.79	0.46
2:W:221:TYR:HB3	2:X:221:TYR:HB3	1.97	0.46
1:A:282:ILE:CG2	1:A:294:TYR:CZ	2.98	0.46
1:B:154:ASP:OD2	1:B:161:HIS:CB	2.63	0.46
1:H:282:ILE:O	1:H:290:ARG:HG2	2.15	0.46
1:H:352:PHE:CD1	1:H:355:MET:HG3	2.51	0.46
1:L:335:ARG:C	1:L:337:TYR:H	2.23	0.46
1:M:133:TYR:CZ	1:M:352:PHE:CZ	3.04	0.46
2:Q:125:ARG:HD3	5:b:174:LYS:HD2	1.97	0.46
5:U:53:LEU:O	6:V:104:PHE:CE2	2.68	0.46
1:B:80:ASP:OD2	1:B:84:LYS:NZ	2.49	0.46
1:N:56:ASP:OD1	1:N:56:ASP:N	2.49	0.46
2:W:218:GLU:OE2	2:X:214:TYR:HA	2.15	0.46
2:X:70:LYS:O	2:X:74:ALA:N	2.42	0.46
4:a:113:ARG:NH2	4:a:117:GLU:OE1	2.49	0.46
1:C:230:ALA:CB	1:C:255:PHE:CE2	2.99	0.46
2:Q:278:LEU:O	2:Q:279:ASN:C	2.54	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:333:PRO:C	1:D:335:ARG:N	2.70	0.46
1:E:133:TYR:CG	1:E:352:PHE:HZ	2.34	0.46
1:E:143:TYR:CE2	1:G:44:MET:HE2	2.51	0.46
1:H:257:CYS:CB	1:H:258:PRO:HD3	2.46	0.46
1:I:304:THR:OG1	1:I:335:ARG:HD2	2.16	0.46
1:J:113:LYS:O	1:J:116:ARG:CG	2.64	0.46
1:K:305:MET:HG2	1:K:335:ARG:HE	1.81	0.46
1:N:336:LYS:HG2	1:N:337:TYR:CD1	2.51	0.46
2:Q:261:TYR:HA	2:Q:264:LYS:HB3	1.98	0.46
4:T:113:ARG:NH2	4:T:117:GLU:OE1	2.49	0.46
1:C:250:ILE:HG23	1:C:253:GLU:HB2	1.98	0.45
1:M:227:MET:HA	1:M:255:PHE:CE1	2.51	0.45
6:V:59:GLU:CG	2:W:153:HIS:HE1	2.28	0.45
1:E:289:ILE:O	1:E:289:ILE:HG22	2.14	0.45
1:F:196:ARG:HD2	1:F:253:GLU:OE2	2.17	0.45
1:K:252:ASN:HB2	1:K:255:PHE:CE1	2.50	0.45
1:D:116:ARG:NH2	1:D:375:PHE:CE1	2.83	0.45
1:J:169:TYR:OH	1:L:49:GLN:CB	2.64	0.45
1:K:133:TYR:CD1	1:K:352:PHE:HZ	2.28	0.45
1:M:207:GLU:CA	1:M:210:ARG:HG2	2.42	0.45
5:U:159:LEU:HD13	2:X:136:LYS:HD2	1.97	0.45
1:J:302:GLY:C	1:J:304:THR:H	2.25	0.45
1:A:116:ARG:NH2	1:A:375:PHE:CE1	2.84	0.45
1:K:169:TYR:OH	1:M:49:GLN:CB	2.65	0.45
1:C:192:ILE:HD12	1:C:256:ARG:CG	2.47	0.45
1:H:352:PHE:CE1	1:H:355:MET:CB	2.99	0.45
1:J:162:ASN:HD21	1:J:278:THR:HA	1.82	0.45
1:O:154:ASP:O	1:O:156:GLY:N	2.49	0.45
1:B:262:PHE:CE2	1:B:312:ARG:HG2	2.49	0.45
5:U:159:LEU:CD1	2:X:136:LYS:HD2	2.47	0.45
2:X:261:TYR:HA	2:X:264:LYS:HB3	1.98	0.45
1:B:219:VAL:O	1:B:220:ALA:HB3	2.17	0.45
1:C:192:ILE:CD1	1:C:256:ARG:HG3	2.47	0.45
1:K:230:ALA:CB	1:K:255:PHE:CZ	2.99	0.45
1:L:133:TYR:CG	1:L:352:PHE:CZ	3.04	0.45
1:L:336:LYS:HB3	1:L:336:LYS:HE2	1.67	0.45
1:M:133:TYR:CE2	1:M:352:PHE:HZ	2.35	0.45
2:P:256:LEU:CG	2:Q:260:LEU:CD1	2.94	0.45
1:G:335:ARG:CG	1:G:335:ARG:NH1	2.80	0.45
1:K:252:ASN:CB	1:K:255:PHE:HZ	2.21	0.45
1:C:51:ASP:OD1	1:C:51:ASP:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:227:MET:HB3	1:E:255:PHE:CZ	2.53	0.44
2:P:154:ILE:O	2:P:158:ALA:N	2.42	0.44
1:B:108:ALA:HB1	1:B:161:HIS:CE1	2.52	0.44
1:N:252:ASN:CB	1:N:255:PHE:HZ	2.23	0.44
2:W:256:LEU:CG	2:X:260:LEU:CD1	2.94	0.44
1:N:108:ALA:HB1	1:N:161:HIS:ND1	2.32	0.44
1:C:334:GLU:HG2	1:C:341:ILE:HD13	2.00	0.44
1:E:282:ILE:O	1:E:290:ARG:CD	2.65	0.44
1:I:332:PRO:C	1:I:334:GLU:H	2.24	0.44
2:P:145:GLU:OE2	5:b:155:MET:SD	2.75	0.44
5:U:195:ILE:CG2	5:U:196:ASP:H	2.30	0.44
4:a:121:VAL:O	4:a:125:ASP:N	2.47	0.44
1:H:133:TYR:HE1	1:H:355:MET:HB3	1.81	0.44
1:L:260:THR:HA	1:L:263:GLN:O	2.18	0.44
1:D:252:ASN:CB	1:D:255:PHE:HZ	2.27	0.44
1:E:283:MET:O	1:E:290:ARG:NH2	2.50	0.44
1:E:302:GLY:C	1:E:304:THR:H	2.26	0.44
1:M:352:PHE:CD2	1:M:352:PHE:O	2.71	0.44
5:b:41:ILE:O	5:b:46:LYS:NZ	2.51	0.44
1:I:108:ALA:HB1	1:I:161:HIS:ND1	2.33	0.44
5:U:137:GLY:O	5:U:141:ARG:HB2	2.18	0.44
1:B:308:GLY:O	1:B:312:ARG:CB	2.66	0.44
1:B:331:ALA:HB1	1:B:335:ARG:HD3	2.00	0.44
1:H:99:GLU:OE1	5:U:120:LYS:NZ	2.51	0.44
1:H:352:PHE:O	1:H:352:PHE:CG	2.70	0.44
1:I:244:ASP:N	1:I:244:ASP:OD1	2.48	0.44
1:C:302:GLY:C	1:C:304:THR:H	2.26	0.43
1:H:352:PHE:CD1	1:H:355:MET:HB2	2.53	0.43
1:K:305:MET:HG2	1:K:335:ARG:HD2	1.77	0.43
1:M:110:LEU:H	1:M:161:HIS:HE1	1.66	0.43
2:X:261:TYR:CZ	2:X:265:LEU:HD23	2.53	0.43
1:O:163:VAL:HG22	1:O:175:ILE:CG2	2.48	0.43
2:P:204:LEU:O	2:P:208:GLU:N	2.49	0.43
2:Q:261:TYR:CZ	2:Q:265:LEU:HD23	2.53	0.43
1:F:109:PRO:HB2	1:F:161:HIS:CE1	2.53	0.43
1:G:252:ASN:CA	1:G:255:PHE:CZ	3.01	0.43
1:J:167:GLU:O	1:J:169:TYR:CD1	2.72	0.43
1:M:227:MET:HB2	1:M:255:PHE:HE1	1.83	0.43
1:G:133:TYR:CD2	1:G:352:PHE:HZ	2.37	0.43
1:M:133:TYR:CD2	1:M:352:PHE:HZ	2.36	0.43
2:P:84:ASP:O	2:P:85:VAL:C	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:THR:HG21	1:C:47:MET:HE1	1.96	0.43
1:G:302:GLY:C	1:G:304:THR:H	2.26	0.43
1:K:352:PHE:CG	1:K:352:PHE:O	2.71	0.43
1:L:154:ASP:O	1:L:156:GLY:N	2.51	0.43
2:W:256:LEU:CD2	2:X:256:LEU:HB3	2.44	0.43
1:I:304:THR:CB	1:I:335:ARG:HD2	2.48	0.43
2:P:153:HIS:CG	6:c:55:GLU:HG3	2.41	0.43
6:V:59:GLU:CG	2:W:153:HIS:CE1	3.02	0.43
2:X:154:ILE:O	2:X:155:ALA:C	2.59	0.43
1:A:133:TYR:CE1	1:A:352:PHE:HE1	2.35	0.43
1:E:154:ASP:O	1:E:156:GLY:N	2.52	0.43
1:I:301:GLY:O	1:I:336:LYS:HB2	2.19	0.43
4:T:89:ASP:OD1	4:T:89:ASP:N	2.51	0.43
2:W:204:LEU:O	2:W:208:GLU:N	2.49	0.43
1:E:285:CYS:O	1:E:290:ARG:NE	2.49	0.43
1:H:352:PHE:HB2	1:J:45:VAL:HG21	2.01	0.43
1:I:305:MET:HE3	1:I:337:TYR:CE1	2.54	0.43
1:J:303:THR:O	1:J:306:TYR:HD1	2.01	0.43
1:G:188:TYR:CE1	1:G:266:PHE:HB3	2.54	0.43
1:I:300:SER:OG	1:I:338:SER:OG	2.26	0.43
1:I:337:TYR:O	1:I:341:ILE:CD1	2.67	0.43
1:M:352:PHE:O	1:M:352:PHE:CG	2.72	0.43
1:O:305:MET:CE	1:O:335:ARG:HH21	2.31	0.43
5:U:195:ILE:HB	2:W:91:ARG:HH11	1.83	0.43
2:X:254:ASP:O	2:X:258:ASP:HB3	2.19	0.43
1:A:143:TYR:CE1	1:C:44:MET:HE2	2.49	0.42
1:A:151:ILE:HG13	1:A:282:ILE:CD1	2.49	0.42
1:A:305:MET:SD	1:A:335:ARG:CB	3.07	0.42
1:B:133:TYR:CG	1:B:352:PHE:CZ	2.96	0.42
1:B:334:GLU:OE1	1:B:334:GLU:N	2.51	0.42
1:G:262:PHE:CE2	1:G:312:ARG:HG2	2.53	0.42
1:M:109:PRO:CD	1:M:161:HIS:CD2	2.94	0.42
2:X:85:VAL:O	2:X:89:ASN:N	2.52	0.42
1:B:3:ASP:OD1	1:B:3:ASP:N	2.50	0.42
1:G:133:TYR:CE1	1:G:355:MET:HB3	2.54	0.42
1:M:109:PRO:CB	1:M:161:HIS:NE2	2.83	0.42
1:A:143:TYR:CZ	1:C:44:MET:CE	2.83	0.42
1:G:219:VAL:O	1:G:220:ALA:HB3	2.18	0.42
1:L:110:LEU:H	1:L:161:HIS:CE1	2.36	0.42
1:L:133:TYR:CD2	1:L:352:PHE:CE1	3.07	0.42
1:L:146:GLY:HA2	4:a:87:PHE:CZ	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:217:CYS:SG	1:H:254:ARG:O	2.77	0.42
1:I:283:MET:O	1:I:290:ARG:NE	2.52	0.42
1:N:51:ASP:OD1	1:N:51:ASP:N	2.44	0.42
1:N:361:GLU:OE2	1:N:373:LYS:NZ	2.52	0.42
2:W:84:ASP:OD1	2:W:88:LEU:CG	2.42	0.42
2:W:154:ILE:O	2:W:158:ALA:N	2.42	0.42
1:A:352:PHE:CD1	1:A:355:MET:HB2	2.54	0.42
1:J:162:ASN:ND2	1:J:277:THR:O	2.52	0.42
1:M:196:ARG:HD2	1:M:253:GLU:OE2	2.19	0.42
2:P:88:LEU:HD11	2:P:91:ARG:NH2	2.34	0.42
2:P:91:ARG:HD3	5:b:195:ILE:CD1	2.36	0.42
2:Q:261:TYR:O	2:Q:265:LEU:N	2.41	0.42
5:U:53:LEU:O	6:V:104:PHE:HE2	2.03	0.42
2:X:268:LYS:O	2:X:272:GLU:N	2.47	0.42
4:a:89:ASP:OD1	4:a:89:ASP:N	2.51	0.42
1:E:56:ASP:OD1	1:E:56:ASP:N	2.52	0.42
1:J:56:ASP:OD1	1:J:56:ASP:N	2.52	0.42
2:Q:254:ASP:O	2:Q:258:ASP:HB3	2.19	0.42
1:C:301:GLY:C	1:C:336:LYS:HA	2.45	0.42
1:D:230:ALA:CB	1:D:255:PHE:CE2	3.02	0.42
1:M:219:VAL:O	1:M:220:ALA:HB3	2.19	0.42
1:M:227:MET:HA	1:M:255:PHE:CZ	2.54	0.42
1:D:335:ARG:C	1:D:337:TYR:H	2.28	0.42
1:E:79:TRP:HZ3	1:E:83:GLU:OE1	2.02	0.42
1:G:133:TYR:CG	1:G:352:PHE:CZ	3.08	0.42
1:H:302:GLY:C	1:H:304:THR:H	2.27	0.42
1:K:230:ALA:CB	1:K:255:PHE:CE2	3.03	0.42
1:M:230:ALA:CB	1:M:255:PHE:CE2	3.03	0.42
5:U:195:ILE:CD1	2:W:91:ARG:HG3	2.46	0.42
5:b:44:SER:CB	6:c:3:ASP:H	2.32	0.42
1:A:154:ASP:O	1:A:155:SER:C	2.63	0.42
1:D:230:ALA:CB	1:D:255:PHE:CZ	3.03	0.42
1:F:154:ASP:O	1:F:155:SER:C	2.62	0.42
1:M:154:ASP:O	1:M:156:GLY:N	2.52	0.42
1:M:207:GLU:O	1:M:210:ARG:HG2	2.20	0.42
2:P:210:GLN:HB3	2:P:214:TYR:CE1	2.55	0.42
2:Q:127:MET:O	2:Q:131:GLU:N	2.45	0.42
2:Q:277:ALA:O	2:Q:281:MET:HG3	2.19	0.42
2:X:165:VAL:O	2:X:169:LEU:N	2.50	0.42
2:X:277:ALA:O	2:X:281:MET:HG3	2.19	0.42
1:E:219:VAL:O	1:E:220:ALA:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:51:ASP:CG	1:M:52:SER:N	2.78	0.42
1:O:196:ARG:HD2	1:O:253:GLU:OE2	2.19	0.42
2:W:210:GLN:HB3	2:W:214:TYR:CE1	2.55	0.42
1:A:352:PHE:O	1:A:352:PHE:CG	2.71	0.41
1:H:335:ARG:H	1:H:335:ARG:HG2	1.63	0.41
1:I:110:LEU:H	1:I:161:HIS:HE1	1.68	0.41
1:I:301:GLY:C	1:I:336:LYS:HB2	2.45	0.41
1:K:51:ASP:CG	1:K:52:SER:N	2.78	0.41
1:K:154:ASP:O	1:K:156:GLY:N	2.52	0.41
1:K:352:PHE:O	1:K:352:PHE:CD2	2.73	0.41
1:L:342:GLY:HA2	1:L:345:ILE:CG2	2.49	0.41
1:N:333:PRO:C	1:N:335:ARG:N	2.75	0.41
4:a:121:VAL:O	4:a:122:SER:C	2.63	0.41
1:E:282:ILE:O	1:E:290:ARG:HD3	2.21	0.41
1:F:275:HIS:ND1	1:F:275:HIS:N	2.64	0.41
1:H:164:PRO:HG2	1:H:171:LEU:HB2	2.02	0.41
1:H:227:MET:HA	1:H:255:PHE:CZ	2.54	0.41
1:M:110:LEU:H	1:M:161:HIS:CE1	2.39	0.41
1:N:230:ALA:HB3	1:N:255:PHE:HZ	1.85	0.41
1:N:279:TYR:CZ	1:N:283:MET:HE2	2.55	0.41
2:Q:253:ILE:CA	2:Q:256:LEU:HB2	2.50	0.41
4:T:105:LEU:O	4:T:106:ILE:C	2.62	0.41
1:B:69:TYR:HA	1:B:70:PRO:HD3	1.84	0.41
1:D:275:HIS:ND1	1:D:275:HIS:N	2.65	0.41
1:M:352:PHE:CE1	1:M:355:MET:CB	3.03	0.41
2:P:260:LEU:HD11	2:Q:263:GLN:OE1	2.20	0.41
2:X:275:ASP:OD2	4:a:113:ARG:NH1	2.53	0.41
1:D:133:TYR:CG	1:D:352:PHE:HZ	2.37	0.41
1:I:109:PRO:HB2	1:I:161:HIS:NE2	2.36	0.41
2:Q:85:VAL:O	2:Q:89:ASN:N	2.52	0.41
2:X:147:GLN:O	2:X:151:ALA:N	2.45	0.41
1:A:282:ILE:CG2	1:A:294:TYR:CE2	3.01	0.41
1:F:335:ARG:H	1:F:335:ARG:HG2	1.57	0.41
1:I:169:TYR:CZ	1:K:49:GLN:HG3	2.54	0.41
1:I:227:MET:HA	1:I:255:PHE:HZ	1.86	0.41
1:L:305:MET:CE	1:L:335:ARG:CB	2.65	0.41
2:Q:154:ILE:O	2:Q:155:ALA:C	2.59	0.41
1:E:335:ARG:C	1:E:337:TYR:N	2.79	0.41
1:F:167:GLU:O	1:F:169:TYR:CD1	2.74	0.41
1:L:336:LYS:HG2	1:L:337:TYR:CD1	2.56	0.41
1:O:108:ALA:HA	1:O:109:PRO:HD3	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:333:PRO:C	1:O:335:ARG:N	2.78	0.41
2:Q:129:VAL:CG2	5:b:167:LEU:HD13	2.50	0.41
1:A:51:ASP:CG	1:A:52:SER:N	2.79	0.41
1:H:219:VAL:O	1:H:220:ALA:HB3	2.21	0.41
1:H:256:ARG:HD2	1:H:256:ARG:HA	1.82	0.41
1:N:335:ARG:C	1:N:337:TYR:N	2.79	0.41
1:N:335:ARG:O	1:N:337:TYR:N	2.46	0.41
2:Q:125:ARG:HD3	5:b:174:LYS:CD	2.50	0.41
2:Q:252:SER:O	2:Q:256:LEU:CB	2.69	0.41
2:W:260:LEU:HD11	2:X:263:GLN:OE1	2.20	0.41
1:H:51:ASP:CG	1:H:52:SER:N	2.79	0.41
1:M:3:ASP:OD1	1:M:3:ASP:N	2.51	0.41
1:M:244:ASP:N	1:M:244:ASP:OD1	2.53	0.41
2:W:91:ARG:NE	2:X:92:ILE:CG1	2.77	0.41
1:D:133:TYR:CG	1:D:352:PHE:CZ	3.09	0.41
1:I:196:ARG:HD2	1:I:253:GLU:CD	2.46	0.41
1:O:161:HIS:HB3	1:O:163:VAL:HG23	2.03	0.41
2:P:260:LEU:CD1	2:Q:263:GLN:OE1	2.69	0.41
4:T:121:VAL:O	4:T:122:SER:C	2.63	0.41
2:W:260:LEU:CD1	2:X:263:GLN:OE1	2.69	0.41
1:D:51:ASP:CG	1:D:52:SER:N	2.79	0.41
1:F:169:TYR:HE1	1:H:49:GLN:CD	2.29	0.41
1:I:109:PRO:CD	1:I:161:HIS:CE1	3.04	0.41
1:O:230:ALA:HB3	1:O:255:PHE:CE2	2.56	0.41
2:P:91:ARG:NE	2:Q:92:ILE:CD1	2.58	0.41
2:P:156:GLU:OE1	5:b:148:ARG:NH1	2.54	0.41
2:X:252:SER:O	2:X:256:LEU:CB	2.69	0.41
1:B:333:PRO:C	1:B:335:ARG:N	2.79	0.40
1:E:50:LYS:NZ	1:E:57:GLU:OE2	2.54	0.40
1:E:227:MET:CB	1:E:255:PHE:HZ	2.34	0.40
1:G:335:ARG:C	1:G:337:TYR:N	2.79	0.40
1:K:189:LEU:CB	1:K:257:CYS:SG	3.07	0.40
2:X:266:LYS:O	2:X:270:ILE:CG1	2.69	0.40
1:A:219:VAL:O	1:A:220:ALA:HB3	2.21	0.40
1:N:124:PHE:CD1	1:N:362:TYR:CD1	3.09	0.40
2:P:39:LEU:O	2:P:43:LEU:N	2.48	0.40
2:Q:266:LYS:O	2:Q:270:ILE:CG1	2.69	0.40
2:X:253:ILE:O	2:X:256:LEU:HB2	2.21	0.40
1:C:192:ILE:CD1	1:C:256:ARG:CG	2.99	0.40
1:E:335:ARG:O	1:E:337:TYR:N	2.44	0.40
1:G:3:ASP:OD1	1:G:3:ASP:N	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:262:PHE:CE2	1:I:312:ARG:HG2	2.56	0.40
1:I:302:GLY:HA3	7:I:401:ADP:O4'	2.20	0.40
1:J:336:LYS:HE3	7:J:401:ADP:H8	1.85	0.40
1:L:219:VAL:O	1:L:220:ALA:HB3	2.21	0.40
2:W:84:ASP:O	2:W:85:VAL:C	2.60	0.40
1:A:33:SER:O	1:A:70:PRO:HD2	2.21	0.40
1:A:151:ILE:HG13	1:A:282:ILE:HD12	2.02	0.40
1:E:218:TYR:O	1:E:255:PHE:HA	2.22	0.40
1:F:182:GLY:O	1:F:213:LYS:NZ	2.52	0.40
1:I:305:MET:SD	1:I:335:ARG:CD	3.08	0.40
1:M:270:GLU:OE1	1:N:202:THR:HB	2.22	0.40
1:D:287:ILE:H	1:D:287:ILE:HD13	1.86	0.40
1:F:335:ARG:C	1:F:337:TYR:N	2.80	0.40
1:H:305:MET:SD	7:H:401:ADP:N7	2.94	0.40
2:P:130:ILE:O	2:P:134:ALA:N	2.47	0.40
2:X:253:ILE:CA	2:X:256:LEU:HB2	2.50	0.40
2:X:261:TYR:CZ	2:X:265:LEU:CD2	3.05	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	A	373/375 (100%)	362 (97%)	9 (2%)	2 (0%)	24	63
1	B	373/375 (100%)	360 (96%)	13 (4%)	0	100	100
1	C	373/375 (100%)	362 (97%)	10 (3%)	1 (0%)	36	72
1	D	373/375 (100%)	360 (96%)	11 (3%)	2 (0%)	24	63
1	E	373/375 (100%)	359 (96%)	13 (4%)	1 (0%)	36	72
1	F	373/375 (100%)	361 (97%)	11 (3%)	1 (0%)	36	72
1	G	373/375 (100%)	358 (96%)	13 (4%)	2 (0%)	24	63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	373/375 (100%)	360 (96%)	11 (3%)	2 (0%)	24	63
1	I	373/375 (100%)	362 (97%)	10 (3%)	1 (0%)	36	72
1	J	373/375 (100%)	360 (96%)	10 (3%)	3 (1%)	16	54
1	K	373/375 (100%)	358 (96%)	12 (3%)	3 (1%)	16	54
1	L	373/375 (100%)	359 (96%)	11 (3%)	3 (1%)	16	54
1	M	373/375 (100%)	358 (96%)	13 (4%)	2 (0%)	24	63
1	N	373/375 (100%)	362 (97%)	10 (3%)	1 (0%)	36	72
1	O	373/375 (100%)	358 (96%)	14 (4%)	1 (0%)	36	72
2	P	272/274 (99%)	272 (100%)	0	0	100	100
2	Q	272/274 (99%)	270 (99%)	2 (1%)	0	100	100
2	W	272/274 (99%)	272 (100%)	0	0	100	100
2	X	272/274 (99%)	270 (99%)	2 (1%)	0	100	100
3	R	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
3	S	29/31 (94%)	29 (100%)	0	0	100	100
3	Y	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
3	Z	29/31 (94%)	29 (100%)	0	0	100	100
4	T	134/186 (72%)	132 (98%)	1 (1%)	1 (1%)	18	56
4	a	134/186 (72%)	133 (99%)	1 (1%)	0	100	100
5	U	168/170 (99%)	166 (99%)	2 (1%)	0	100	100
5	b	168/170 (99%)	166 (99%)	2 (1%)	0	100	100
6	V	158/160 (99%)	151 (96%)	6 (4%)	1 (1%)	21	59
6	c	158/160 (99%)	153 (97%)	4 (2%)	1 (1%)	21	59
All	All	7719/7877 (98%)	7498 (97%)	193 (2%)	28 (0%)	31	67

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	155	SER
1	H	155	SER
1	I	155	SER
1	K	155	SER
1	L	155	SER
1	M	155	SER
1	O	155	SER

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Mol	Chain	Res	Type
1	A	155	SER
1	G	336	LYS
1	J	336	LYS
4	T	200	LYS
1	F	155	SER
1	J	220	ALA
1	N	155	SER
1	A	49	GLN
1	C	49	GLN
1	D	334	GLU
1	G	49	GLN
1	K	103	THR
1	L	336	LYS
1	M	49	GLN
1	D	49	GLN
1	H	49	GLN
1	J	49	GLN
1	K	49	GLN
1	L	49	GLN
6	V	36	ILE
6	c	36	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	A	318/318 (100%)	315 (99%)	3 (1%)	70	79
1	B	318/318 (100%)	315 (99%)	3 (1%)	70	79
1	C	318/318 (100%)	317 (100%)	1 (0%)	86	86
1	D	318/318 (100%)	314 (99%)	4 (1%)	61	74
1	E	318/318 (100%)	314 (99%)	4 (1%)	61	74
1	F	318/318 (100%)	315 (99%)	3 (1%)	70	79
1	G	318/318 (100%)	315 (99%)	3 (1%)	70	79
1	H	318/318 (100%)	315 (99%)	3 (1%)	70	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	318/318 (100%)	318 (100%)	0	100	100
1	J	318/318 (100%)	316 (99%)	2 (1%)	78	83
1	K	318/318 (100%)	316 (99%)	2 (1%)	78	83
1	L	318/318 (100%)	315 (99%)	3 (1%)	70	79
1	M	318/318 (100%)	316 (99%)	2 (1%)	78	83
1	N	318/318 (100%)	316 (99%)	2 (1%)	78	83
1	O	318/318 (100%)	315 (99%)	3 (1%)	70	79
2	P	236/236 (100%)	235 (100%)	1 (0%)	84	84
2	Q	236/236 (100%)	233 (99%)	3 (1%)	61	74
2	W	236/236 (100%)	235 (100%)	1 (0%)	84	84
2	X	236/236 (100%)	233 (99%)	3 (1%)	61	74
3	R	25/25 (100%)	25 (100%)	0	100	100
3	S	25/25 (100%)	25 (100%)	0	100	100
3	Y	25/25 (100%)	25 (100%)	0	100	100
3	Z	25/25 (100%)	25 (100%)	0	100	100
4	T	129/169 (76%)	129 (100%)	0	100	100
4	a	129/169 (76%)	129 (100%)	0	100	100
5	U	145/145 (100%)	145 (100%)	0	100	100
5	b	145/145 (100%)	145 (100%)	0	100	100
6	V	141/141 (100%)	141 (100%)	0	100	100
6	c	141/141 (100%)	141 (100%)	0	100	100
All	All	6644/6724 (99%)	6598 (99%)	46 (1%)	73	81

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	281	SER
1	A	282	ILE
1	A	336	LYS
1	B	163	VAL
1	B	287	ILE
1	B	336	LYS
1	C	336	LYS
1	D	163	VAL
1	D	287	ILE

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Mol	Chain	Res	Type
1	D	335	ARG
1	D	336	LYS
1	E	107	GLU
1	E	287	ILE
1	E	313	MET
1	E	336	LYS
1	F	287	ILE
1	F	305	MET
1	F	336	LYS
1	G	287	ILE
1	G	335	ARG
1	G	336	LYS
1	H	163	VAL
1	H	254	ARG
1	H	336	LYS
1	J	305	MET
1	J	336	LYS
1	K	163	VAL
1	K	336	LYS
1	L	177	ARG
1	L	287	ILE
1	L	335	ARG
1	M	47	MET
1	M	336	LYS
1	N	335	ARG
1	N	336	LYS
1	O	37	ARG
1	O	335	ARG
1	O	336	LYS
2	P	274	LEU
2	Q	165	VAL
2	Q	261	TYR
2	Q	264	LYS
2	W	274	LEU
2	X	165	VAL
2	X	261	TYR
2	X	264	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	ASN

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Mol	Chain	Res	Type
1	A	162	ASN
1	B	92	ASN
1	B	111	ASN
1	C	162	ASN
1	D	40	HIS
1	D	111	ASN
1	D	162	ASN
1	D	263	GLN
1	E	137	GLN
1	H	59	GLN
1	H	128	ASN
1	I	111	ASN
1	J	128	ASN
1	J	162	ASN
1	L	92	ASN
1	L	128	ASN
1	L	263	GLN
1	M	162	ASN
1	M	371	HIS
1	N	87	HIS
1	N	296	ASN
1	O	128	ASN
1	O	371	HIS
2	P	47	GLN
2	Q	153	HIS
2	Q	210	GLN
4	T	91	HIS
4	T	238	GLN
4	T	242	ASN
2	W	47	GLN
2	X	153	HIS
2	X	210	GLN
4	a	238	GLN
4	a	242	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

15 ligands are modelled in this entry.

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
7	ADP	I	401	-	28,29,29	1.72	5 (17%)	43,45,45	1.88	9 (20%)
7	ADP	B	401	-	28,29,29	1.66	4 (14%)	43,45,45	1.85	9 (20%)
7	ADP	H	401	-	28,29,29	1.88	9 (32%)	43,45,45	1.92	9 (20%)
7	ADP	E	401	-	28,29,29	1.78	7 (25%)	43,45,45	1.87	8 (18%)
7	ADP	G	401	-	28,29,29	1.79	8 (28%)	43,45,45	1.91	8 (18%)
7	ADP	L	401	-	28,29,29	1.96	9 (32%)	43,45,45	1.96	9 (20%)
7	ADP	N	401	-	28,29,29	1.77	6 (21%)	43,45,45	1.98	10 (23%)
7	ADP	A	401	-	28,29,29	1.95	10 (35%)	43,45,45	1.86	8 (18%)
7	ADP	D	401	-	28,29,29	1.84	8 (28%)	43,45,45	1.91	9 (20%)
7	ADP	M	401	-	28,29,29	1.83	7 (25%)	43,45,45	1.96	10 (23%)
7	ADP	J	401	-	28,29,29	1.82	8 (28%)	43,45,45	1.98	10 (23%)
7	ADP	O	401	-	28,29,29	1.82	8 (28%)	43,45,45	2.02	11 (25%)
7	ADP	K	401	-	28,29,29	1.78	7 (25%)	43,45,45	2.01	12 (27%)
7	ADP	C	401	-	28,29,29	1.78	6 (21%)	43,45,45	1.92	9 (20%)
7	ADP	F	401	-	28,29,29	1.88	11 (39%)	43,45,45	1.99	11 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	ADP	I	401	-	-	1/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	ADP	B	401	-	-	4/16/32/32	0/3/3/3
7	ADP	H	401	-	-	5/16/32/32	0/3/3/3
7	ADP	E	401	-	-	5/16/32/32	0/3/3/3
7	ADP	G	401	-	-	3/16/32/32	0/3/3/3
7	ADP	L	401	-	-	6/16/32/32	0/3/3/3
7	ADP	N	401	-	-	0/16/32/32	0/3/3/3
7	ADP	A	401	-	-	2/16/32/32	0/3/3/3
7	ADP	D	401	-	-	0/16/32/32	0/3/3/3
7	ADP	M	401	-	-	5/16/32/32	0/3/3/3
7	ADP	J	401	-	-	4/16/32/32	0/3/3/3
7	ADP	O	401	-	-	8/16/32/32	0/3/3/3
7	ADP	K	401	-	-	5/16/32/32	0/3/3/3
7	ADP	C	401	-	-	5/16/32/32	0/3/3/3
7	ADP	F	401	-	-	1/16/32/32	0/3/3/3

All (113) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	O	401	ADP	C5-C4	4.62	1.47	1.39
7	B	401	ADP	C5-C4	4.51	1.47	1.39
7	C	401	ADP	C5-C4	4.48	1.47	1.39
7	H	401	ADP	C5-C4	4.45	1.47	1.39
7	I	401	ADP	C5-C4	4.44	1.47	1.39
7	J	401	ADP	C5-C4	4.41	1.47	1.39
7	M	401	ADP	C5-C4	4.40	1.46	1.39
7	K	401	ADP	C5-C4	4.33	1.46	1.39
7	E	401	ADP	C5-C4	4.33	1.46	1.39
7	F	401	ADP	C5-C4	4.29	1.46	1.39
7	N	401	ADP	C5-C4	4.26	1.46	1.39
7	A	401	ADP	C5-C4	4.24	1.46	1.39
7	L	401	ADP	C5-C4	4.18	1.46	1.39
7	D	401	ADP	C5-C4	4.13	1.46	1.39
7	G	401	ADP	C5-C4	4.09	1.46	1.39
7	L	401	ADP	C4-N3	3.38	1.40	1.34
7	O	401	ADP	C5-C6	3.24	1.50	1.41
7	A	401	ADP	PA-O1A	3.23	1.62	1.50
7	C	401	ADP	C5-C6	3.21	1.49	1.41
7	K	401	ADP	C5-C6	3.17	1.49	1.41
7	E	401	ADP	PA-O1A	3.13	1.61	1.50
7	H	401	ADP	PA-O1A	3.08	1.61	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	401	ADP	C5-C6	3.04	1.49	1.41
7	D	401	ADP	PA-O1A	3.00	1.61	1.50
7	G	401	ADP	C4-N3	2.98	1.40	1.34
7	I	401	ADP	PA-O1A	2.97	1.61	1.50
7	B	401	ADP	PA-O1A	2.95	1.61	1.50
7	J	401	ADP	C5-C6	2.94	1.49	1.41
7	A	401	ADP	C5-C6	2.94	1.49	1.41
7	I	401	ADP	C5-C6	2.92	1.49	1.41
7	G	401	ADP	PA-O1A	2.90	1.60	1.50
7	F	401	ADP	PB-O1B	2.90	1.59	1.50
7	C	401	ADP	PA-O1A	2.88	1.60	1.50
7	A	401	ADP	C4-N3	2.87	1.39	1.34
7	N	401	ADP	PA-O1A	2.86	1.60	1.50
7	F	401	ADP	C5-C6	2.85	1.48	1.41
7	D	401	ADP	C4-N3	2.83	1.39	1.34
7	D	401	ADP	C5-C6	2.82	1.48	1.41
7	E	401	ADP	C5-C6	2.78	1.48	1.41
7	L	401	ADP	C2-N3	2.76	1.38	1.33
7	L	401	ADP	PA-O1A	2.73	1.60	1.50
7	C	401	ADP	C4-N3	2.73	1.39	1.34
7	M	401	ADP	C4-N3	2.73	1.39	1.34
7	J	401	ADP	PB-O1B	2.72	1.58	1.50
7	O	401	ADP	PA-O1A	2.70	1.60	1.50
7	J	401	ADP	C4-N3	2.70	1.39	1.34
7	N	401	ADP	C5-C6	2.70	1.48	1.41
7	N	401	ADP	C4-N3	2.69	1.39	1.34
7	B	401	ADP	C5-C6	2.68	1.48	1.41
7	M	401	ADP	PA-O1A	2.68	1.60	1.50
7	H	401	ADP	C5-C6	2.68	1.48	1.41
7	G	401	ADP	PB-O1B	2.64	1.58	1.50
7	L	401	ADP	PB-O1B	2.64	1.58	1.50
7	G	401	ADP	C2-N3	2.61	1.38	1.33
7	J	401	ADP	C3'-C4'	2.58	1.59	1.53
7	H	401	ADP	PB-O1B	2.57	1.58	1.50
7	F	401	ADP	C4-N3	2.55	1.39	1.34
7	H	401	ADP	C4-N3	2.54	1.39	1.34
7	B	401	ADP	C4-N3	2.51	1.39	1.34
7	I	401	ADP	C4-N3	2.50	1.39	1.34
7	A	401	ADP	PB-O1B	2.49	1.58	1.50
7	F	401	ADP	C3'-C4'	2.49	1.59	1.53
7	G	401	ADP	C2-N1	2.46	1.38	1.33
7	L	401	ADP	C2-N1	2.46	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	401	ADP	PA-O3A	2.45	1.62	1.59
7	J	401	ADP	O4'-C1'	2.44	1.47	1.42
7	F	401	ADP	PA-O3A	2.43	1.62	1.59
7	E	401	ADP	C4-N3	2.40	1.38	1.34
7	N	401	ADP	C2-N1	2.40	1.38	1.33
7	F	401	ADP	PB-O3B	-2.38	1.45	1.54
7	E	401	ADP	PA-O3A	2.38	1.62	1.59
7	L	401	ADP	C3'-C4'	2.35	1.59	1.53
7	K	401	ADP	PA-O1A	2.34	1.58	1.50
7	D	401	ADP	PB-O3B	-2.34	1.46	1.54
7	K	401	ADP	C3'-C4'	2.33	1.58	1.53
7	J	401	ADP	PB-O2B	-2.30	1.46	1.54
7	H	401	ADP	PB-O2B	-2.30	1.46	1.54
7	A	401	ADP	PB-O2B	-2.29	1.46	1.54
7	M	401	ADP	PB-O1B	2.29	1.57	1.50
7	F	401	ADP	C2-N1	2.27	1.38	1.33
7	O	401	ADP	C3'-C4'	2.27	1.58	1.53
7	K	401	ADP	PA-O3A	2.27	1.61	1.59
7	A	401	ADP	C1'-N9	2.27	1.52	1.46
7	G	401	ADP	PB-O2B	-2.27	1.46	1.54
7	I	401	ADP	C3'-C4'	2.26	1.58	1.53
7	D	401	ADP	PA-O3A	2.26	1.61	1.59
7	F	401	ADP	O4'-C1'	2.25	1.47	1.42
7	L	401	ADP	C5-C6	2.22	1.47	1.41
7	J	401	ADP	PA-O3A	2.22	1.61	1.59
7	O	401	ADP	PB-O1B	2.22	1.57	1.50
7	C	401	ADP	PA-O3A	2.21	1.61	1.59
7	H	401	ADP	C2-N1	2.20	1.37	1.33
7	K	401	ADP	C4-N3	2.20	1.38	1.34
7	O	401	ADP	C4-N3	2.19	1.38	1.34
7	M	401	ADP	C5'-C4'	2.19	1.58	1.51
7	N	401	ADP	PB-O2B	-2.15	1.46	1.54
7	E	401	ADP	C3'-C4'	2.13	1.58	1.53
7	D	401	ADP	PB-O1B	2.12	1.57	1.50
7	H	401	ADP	C3'-C4'	2.11	1.58	1.53
7	L	401	ADP	PA-O3A	2.11	1.61	1.59
7	G	401	ADP	C5-C6	2.10	1.46	1.41
7	C	401	ADP	C1'-N9	2.08	1.52	1.46
7	D	401	ADP	C2-N1	2.08	1.37	1.33
7	E	401	ADP	C1'-N9	2.07	1.52	1.46
7	A	401	ADP	C2-N1	2.06	1.37	1.33
7	H	401	ADP	PA-O3A	2.05	1.61	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	K	401	ADP	C1'-N9	2.04	1.52	1.46
7	F	401	ADP	C6-N6	2.04	1.39	1.34
7	F	401	ADP	C5'-C4'	2.04	1.57	1.51
7	A	401	ADP	C5'-C4'	2.03	1.57	1.51
7	O	401	ADP	C2-N1	2.02	1.37	1.33
7	O	401	ADP	C1'-N9	2.02	1.51	1.46
7	M	401	ADP	C1'-N9	2.02	1.51	1.46

All (142) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	401	ADP	C5-C4-N3	-5.80	118.73	126.72
7	E	401	ADP	C5-C4-N3	-5.58	119.04	126.72
7	G	401	ADP	C5-C4-N3	-5.56	119.06	126.72
7	M	401	ADP	C5-C4-N3	-5.53	119.11	126.72
7	A	401	ADP	C5-C4-N3	-5.51	119.13	126.72
7	F	401	ADP	C5-C4-N3	-5.49	119.16	126.72
7	C	401	ADP	C5-C4-N3	-5.44	119.23	126.72
7	D	401	ADP	C5-C4-N3	-5.41	119.27	126.72
7	B	401	ADP	C5-C4-N3	-5.40	119.28	126.72
7	J	401	ADP	C5-C4-N3	-5.34	119.37	126.72
7	N	401	ADP	C5-C4-N3	-5.32	119.40	126.72
7	I	401	ADP	C5-C4-N3	-5.25	119.49	126.72
7	H	401	ADP	C5-C4-N3	-5.25	119.49	126.72
7	K	401	ADP	C5-C4-N3	-5.23	119.52	126.72
7	O	401	ADP	C5-C4-N3	-5.16	119.62	126.72
7	L	401	ADP	N3-C4-N9	4.92	135.54	127.17
7	G	401	ADP	N3-C4-N9	4.90	135.50	127.17
7	M	401	ADP	C4-C5-N7	-4.70	105.21	110.58
7	E	401	ADP	N3-C2-N1	-4.67	121.51	128.58
7	K	401	ADP	O4'-C1'-C2'	-4.58	96.81	106.62
7	G	401	ADP	N3-C2-N1	-4.54	121.72	128.58
7	L	401	ADP	N3-C2-N1	-4.53	121.72	128.58
7	M	401	ADP	N3-C2-N1	-4.53	121.73	128.58
7	O	401	ADP	C4-C5-N7	-4.51	105.42	110.58
7	C	401	ADP	C4-C5-N7	-4.51	105.42	110.58
7	O	401	ADP	O4'-C1'-C2'	-4.49	97.00	106.62
7	F	401	ADP	N3-C2-N1	-4.37	121.96	128.58
7	D	401	ADP	C4-C5-N7	-4.24	105.74	110.58
7	F	401	ADP	C4-C5-N7	-4.20	105.78	110.58
7	J	401	ADP	O4'-C1'-C2'	-4.19	97.64	106.62
7	H	401	ADP	N3-C2-N1	-4.19	122.25	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	E	401	ADP	C2-N3-C4	4.15	121.96	111.83
7	N	401	ADP	N3-C2-N1	-4.10	122.38	128.58
7	K	401	ADP	N3-C2-N1	-4.08	122.40	128.58
7	D	401	ADP	C5-N7-C8	4.06	109.83	103.45
7	K	401	ADP	C4-C5-N7	-4.04	105.97	110.58
7	D	401	ADP	N3-C2-N1	-4.03	122.48	128.58
7	C	401	ADP	N3-C2-N1	-4.02	122.49	128.58
7	A	401	ADP	C4-C5-N7	-4.01	106.00	110.58
7	H	401	ADP	O4'-C1'-C2'	-4.00	98.06	106.62
7	O	401	ADP	N3-C2-N1	-3.99	122.55	128.58
7	M	401	ADP	C2-N3-C4	3.98	121.56	111.83
7	A	401	ADP	N3-C2-N1	-3.98	122.56	128.58
7	F	401	ADP	N3-C4-N9	3.96	133.91	127.17
7	N	401	ADP	N3-C4-N9	3.96	133.91	127.17
7	J	401	ADP	N3-C4-N9	3.96	133.90	127.17
7	I	401	ADP	O4'-C1'-C2'	-3.95	98.16	106.62
7	B	401	ADP	N3-C2-N1	-3.94	122.62	128.58
7	A	401	ADP	N3-C4-N9	3.93	133.84	127.17
7	N	401	ADP	C4-C5-N7	-3.90	106.12	110.58
7	F	401	ADP	C2-N3-C4	3.90	121.36	111.83
7	I	401	ADP	N3-C2-N1	-3.89	122.69	128.58
7	K	401	ADP	C2-N3-C4	3.88	121.32	111.83
7	F	401	ADP	C5-N7-C8	3.87	109.53	103.45
7	A	401	ADP	C5-N7-C8	3.86	109.52	103.45
7	J	401	ADP	N3-C2-N1	-3.83	122.78	128.58
7	E	401	ADP	C4-C5-N7	-3.83	106.20	110.58
7	M	401	ADP	N3-C4-N9	3.83	133.68	127.17
7	O	401	ADP	C2-N3-C4	3.82	121.17	111.83
7	J	401	ADP	O2B-PB-O3A	3.82	117.46	104.64
7	B	401	ADP	C4-C5-N7	-3.82	106.21	110.58
7	H	401	ADP	C4-C5-N7	-3.82	106.21	110.58
7	B	401	ADP	N3-C4-N9	3.82	133.66	127.17
7	C	401	ADP	C2-N3-C4	3.81	121.13	111.83
7	D	401	ADP	N3-C4-N9	3.80	133.63	127.17
7	L	401	ADP	C5-N7-C8	3.80	109.42	103.45
7	H	401	ADP	C2-N3-C4	3.79	121.08	111.83
7	M	401	ADP	C5-N7-C8	3.77	109.37	103.45
7	I	401	ADP	C4-C5-N7	-3.75	106.29	110.58
7	N	401	ADP	C5-N7-C8	3.74	109.33	103.45
7	L	401	ADP	C2-N3-C4	3.73	120.93	111.83
7	I	401	ADP	N3-C4-N9	3.72	133.50	127.17
7	D	401	ADP	C2-N3-C4	3.70	120.88	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N	401	ADP	C2-N3-C4	3.70	120.86	111.83
7	G	401	ADP	C2-N3-C4	3.69	120.85	111.83
7	A	401	ADP	C2-N3-C4	3.69	120.85	111.83
7	J	401	ADP	C2-N3-C4	3.68	120.81	111.83
7	B	401	ADP	C2-N3-C4	3.67	120.79	111.83
7	H	401	ADP	N3-C4-N9	3.66	133.40	127.17
7	G	401	ADP	C5-N7-C8	3.66	109.20	103.45
7	I	401	ADP	C2-N3-C4	3.66	120.76	111.83
7	E	401	ADP	N3-C4-N9	3.63	133.34	127.17
7	C	401	ADP	C5-N7-C8	3.60	109.11	103.45
7	F	401	ADP	O4'-C1'-C2'	-3.60	98.91	106.62
7	C	401	ADP	N3-C4-N9	3.55	133.21	127.17
7	B	401	ADP	O3B-PB-O3A	3.52	116.45	104.64
7	J	401	ADP	C4-C5-N7	-3.52	106.56	110.58
7	I	401	ADP	O3B-PB-O3A	3.51	116.39	104.64
7	O	401	ADP	C5-N7-C8	3.45	108.88	103.45
7	N	401	ADP	O4'-C1'-C2'	-3.39	99.35	106.62
7	G	401	ADP	O3B-PB-O3A	3.34	115.82	104.64
7	O	401	ADP	N3-C4-N9	3.31	132.80	127.17
7	K	401	ADP	N3-C4-N9	3.28	132.75	127.17
7	O	401	ADP	C6-C5-N7	3.26	138.38	132.09
7	B	401	ADP	C5-N7-C8	3.25	108.56	103.45
7	C	401	ADP	C6-C5-N7	3.21	138.28	132.09
7	L	401	ADP	O4'-C1'-C2'	-3.18	99.80	106.62
7	H	401	ADP	C5-N7-C8	3.13	108.38	103.45
7	L	401	ADP	C4-C5-N7	-3.12	107.01	110.58
7	E	401	ADP	C5-N7-C8	3.12	108.35	103.45
7	M	401	ADP	C6-C5-N7	3.09	138.04	132.09
7	G	401	ADP	C4-C5-N7	-3.03	107.11	110.58
7	K	401	ADP	C6-C5-N7	3.02	137.91	132.09
7	K	401	ADP	C5-N7-C8	3.00	108.17	103.45
7	N	401	ADP	O3B-PB-O3A	2.95	114.52	104.64
7	L	401	ADP	O3B-PB-O3A	2.89	114.31	104.64
7	I	401	ADP	C5-N7-C8	2.86	107.95	103.45
7	L	401	ADP	O2A-PA-O3A	2.83	114.93	107.27
7	O	401	ADP	O2B-PB-O3A	2.81	114.08	104.64
7	J	401	ADP	C5-N7-C8	2.79	107.83	103.45
7	E	401	ADP	C6-C5-N7	2.75	137.38	132.09
7	M	401	ADP	O3B-PB-O3A	2.74	113.82	104.64
7	D	401	ADP	C6-C5-N7	2.71	137.32	132.09
7	D	401	ADP	O2B-PB-O3A	2.71	113.72	104.64
7	H	401	ADP	C6-C5-N7	2.67	137.23	132.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	J	401	ADP	O4'-C1'-N9	2.64	113.16	108.09
7	F	401	ADP	O4'-C1'-N9	2.63	113.14	108.09
7	I	401	ADP	C6-C5-N7	2.62	137.14	132.09
7	B	401	ADP	C6-C5-N7	2.61	137.11	132.09
7	K	401	ADP	O3B-PB-O3A	2.60	113.36	104.64
7	C	401	ADP	O3B-PB-O3A	2.57	113.25	104.64
7	J	401	ADP	C6-C5-N7	2.56	137.03	132.09
7	N	401	ADP	C6-C5-N7	2.56	137.03	132.09
7	E	401	ADP	O3B-PB-O3A	2.55	113.19	104.64
7	F	401	ADP	C6-C5-N7	2.55	137.00	132.09
7	A	401	ADP	C6-C5-N7	2.48	136.87	132.09
7	K	401	ADP	O4'-C1'-N9	2.44	112.78	108.09
7	M	401	ADP	O2B-PB-O3A	2.44	112.83	104.64
7	F	401	ADP	O3B-PB-O3A	2.44	112.81	104.64
7	H	401	ADP	O2B-PB-O3A	2.42	112.77	104.64
7	F	401	ADP	O2B-PB-O3A	2.34	112.48	104.64
7	A	401	ADP	O2B-PB-O3A	2.29	112.32	104.64
7	K	401	ADP	N6-C6-N1	-2.23	113.40	118.38
7	N	401	ADP	O2B-PB-O1B	-2.23	102.16	110.83
7	B	401	ADP	C3'-C2'-C1'	2.21	105.65	101.46
7	C	401	ADP	N6-C6-N1	-2.20	113.47	118.38
7	O	401	ADP	O3B-PB-O3A	2.18	111.94	104.64
7	O	401	ADP	O4'-C1'-N9	2.14	112.19	108.09
7	D	401	ADP	O2A-PA-O3A	2.11	112.97	107.27
7	G	401	ADP	O2B-PB-O3A	2.08	111.61	104.64
7	K	401	ADP	O2A-PA-O1A	-2.06	102.88	112.44
7	M	401	ADP	C2-N1-C6	2.00	122.02	118.73

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	401	ADP	O4'-C4'-C5'-O5'
7	B	401	ADP	C5'-O5'-PA-O3A
7	C	401	ADP	C5'-O5'-PA-O1A
7	C	401	ADP	C5'-O5'-PA-O2A
7	C	401	ADP	C5'-O5'-PA-O3A
7	E	401	ADP	C5'-O5'-PA-O1A
7	E	401	ADP	C5'-O5'-PA-O2A
7	E	401	ADP	C5'-O5'-PA-O3A
7	H	401	ADP	C5'-O5'-PA-O1A
7	H	401	ADP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
7	J	401	ADP	PA-O3A-PB-O2B
7	K	401	ADP	C5'-O5'-PA-O1A
7	K	401	ADP	C5'-O5'-PA-O2A
7	K	401	ADP	C5'-O5'-PA-O3A
7	L	401	ADP	C5'-O5'-PA-O2A
7	L	401	ADP	C5'-O5'-PA-O3A
7	L	401	ADP	O4'-C4'-C5'-O5'
7	M	401	ADP	C5'-O5'-PA-O1A
7	M	401	ADP	C5'-O5'-PA-O2A
7	M	401	ADP	C5'-O5'-PA-O3A
7	O	401	ADP	C5'-O5'-PA-O1A
7	O	401	ADP	C5'-O5'-PA-O2A
7	O	401	ADP	C5'-O5'-PA-O3A
7	A	401	ADP	C3'-C4'-C5'-O5'
7	C	401	ADP	C3'-C4'-C5'-O5'
7	E	401	ADP	C3'-C4'-C5'-O5'
7	K	401	ADP	C3'-C4'-C5'-O5'
7	L	401	ADP	C3'-C4'-C5'-O5'
7	M	401	ADP	C3'-C4'-C5'-O5'
7	O	401	ADP	C3'-C4'-C5'-O5'
7	C	401	ADP	O4'-C4'-C5'-O5'
7	E	401	ADP	O4'-C4'-C5'-O5'
7	H	401	ADP	C3'-C4'-C5'-O5'
7	K	401	ADP	O4'-C4'-C5'-O5'
7	O	401	ADP	O4'-C4'-C5'-O5'
7	M	401	ADP	O4'-C4'-C5'-O5'
7	F	401	ADP	C4'-C5'-O5'-PA
7	J	401	ADP	C4'-C5'-O5'-PA
7	H	401	ADP	O4'-C4'-C5'-O5'
7	O	401	ADP	PA-O3A-PB-O2B
7	I	401	ADP	C3'-C4'-C5'-O5'
7	B	401	ADP	C5'-O5'-PA-O1A
7	G	401	ADP	C5'-O5'-PA-O1A
7	G	401	ADP	C5'-O5'-PA-O2A
7	G	401	ADP	C5'-O5'-PA-O3A
7	H	401	ADP	C5'-O5'-PA-O2A
7	J	401	ADP	C5'-O5'-PA-O1A
7	O	401	ADP	PA-O3A-PB-O1B
7	O	401	ADP	C4'-C5'-O5'-PA
7	J	401	ADP	PA-O3A-PB-O3B
7	B	401	ADP	O4'-C4'-C5'-O5'
7	B	401	ADP	C3'-C4'-C5'-O5'

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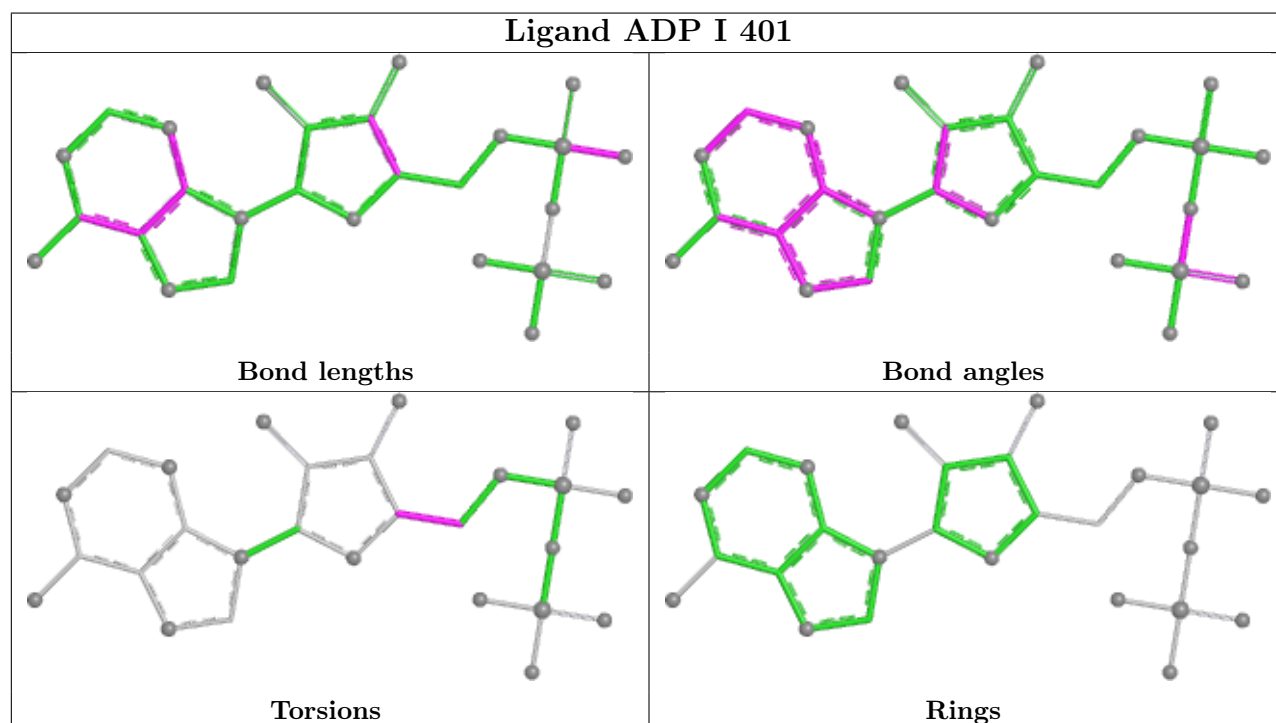
Mol	Chain	Res	Type	Atoms
7	L	401	ADP	C4'-C5'-O5'-PA
7	L	401	ADP	C2'-C1'-N9-C8

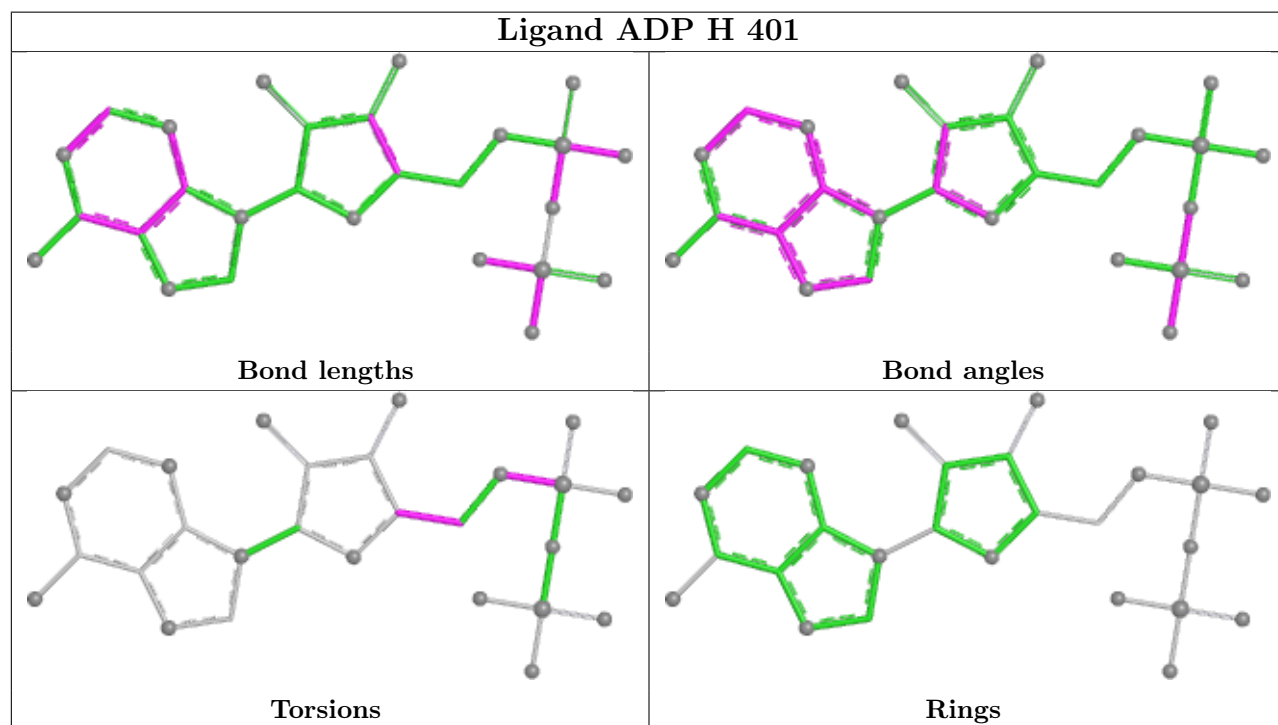
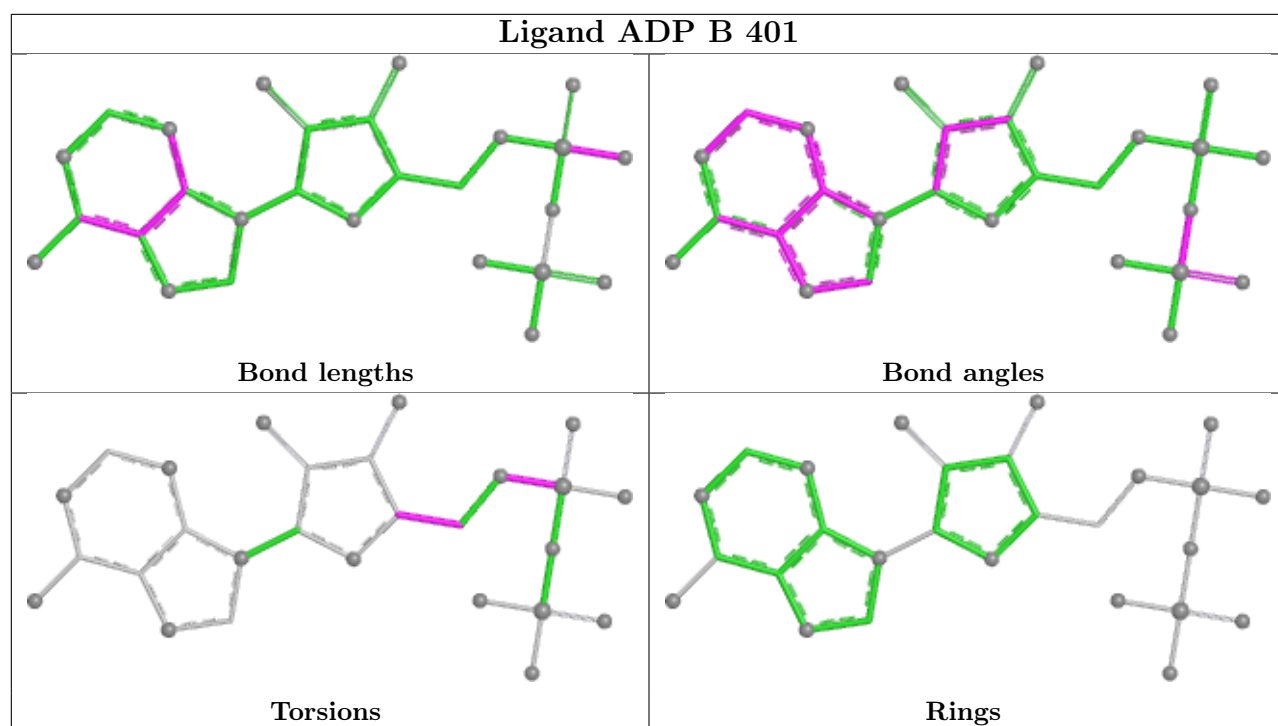
There are no ring outliers.

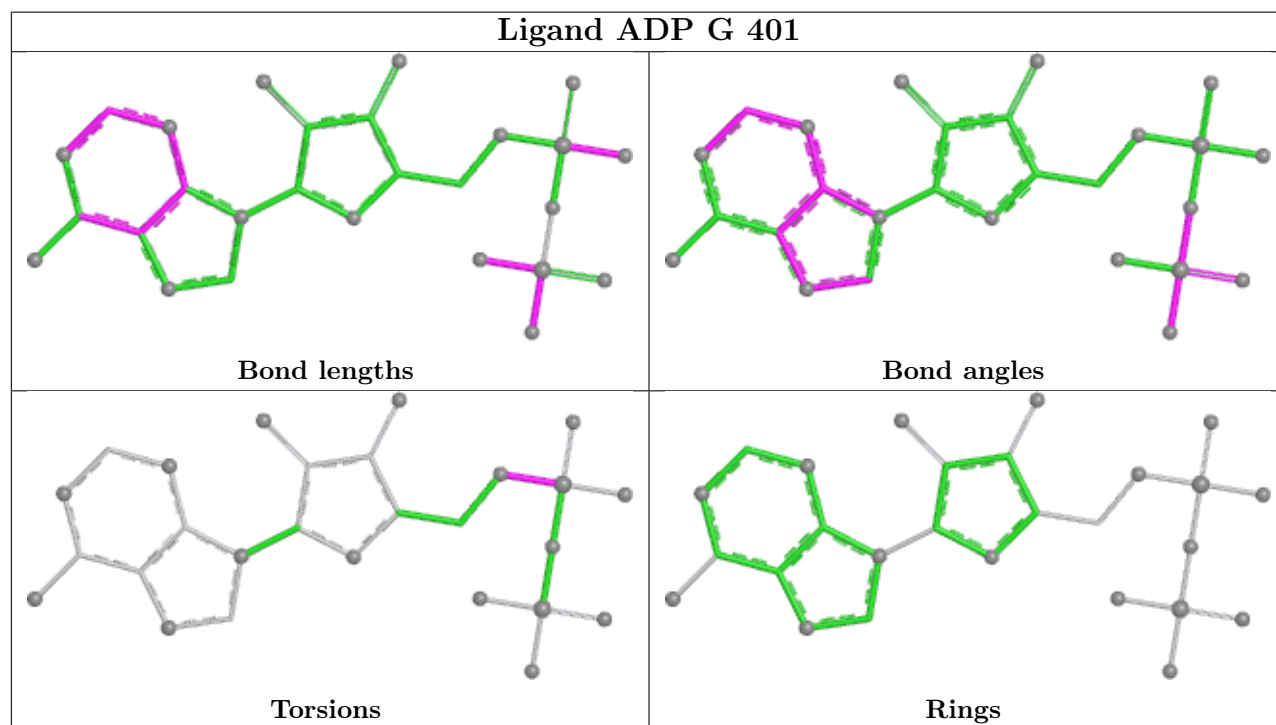
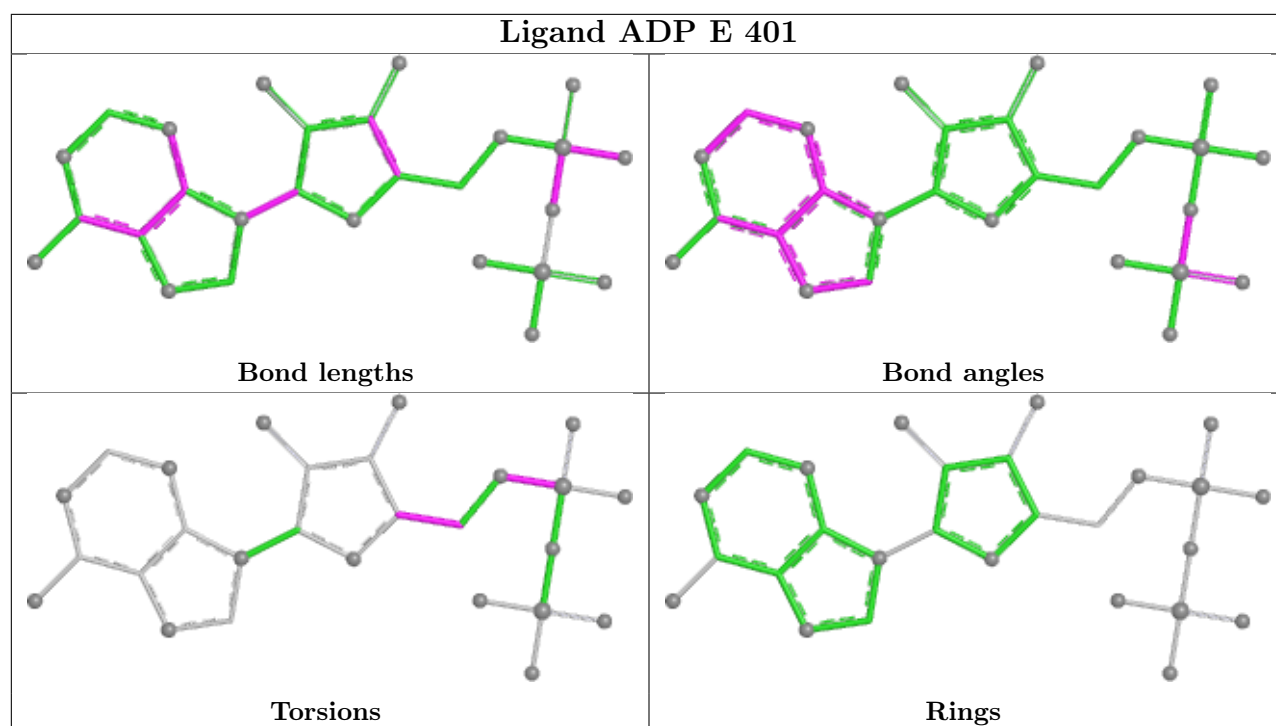
3 monomers are involved in 3 short contacts:

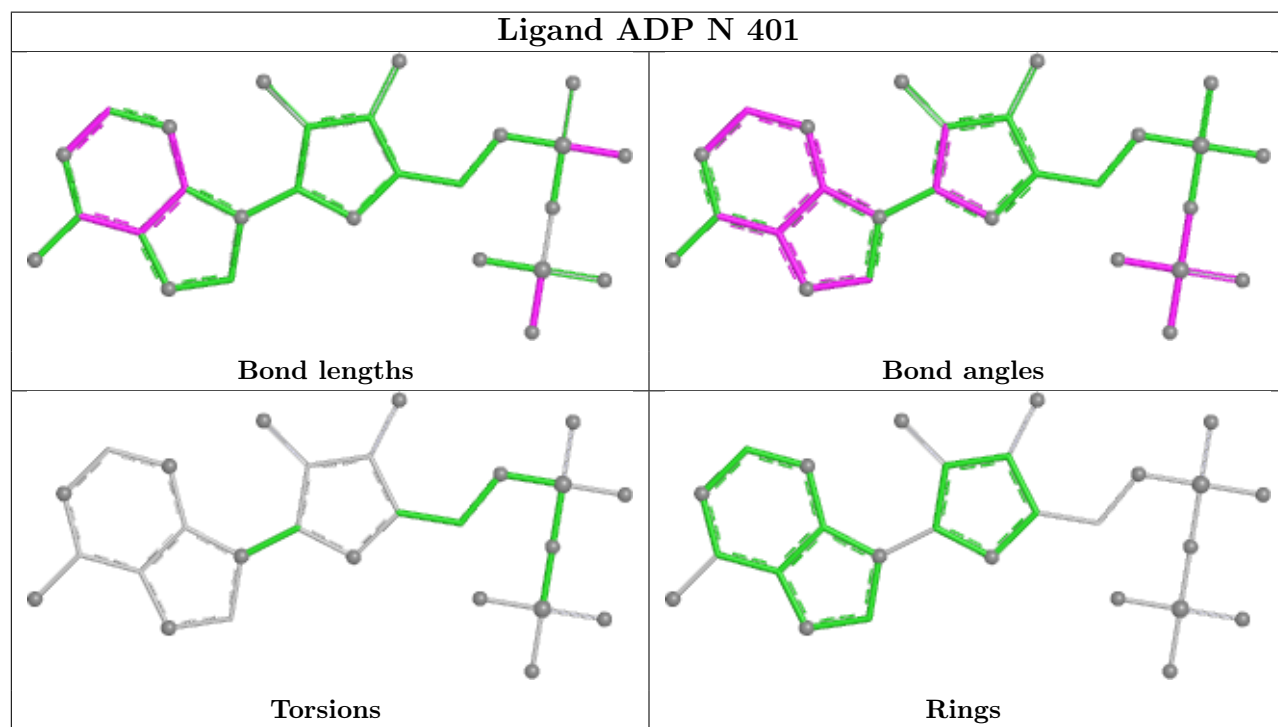
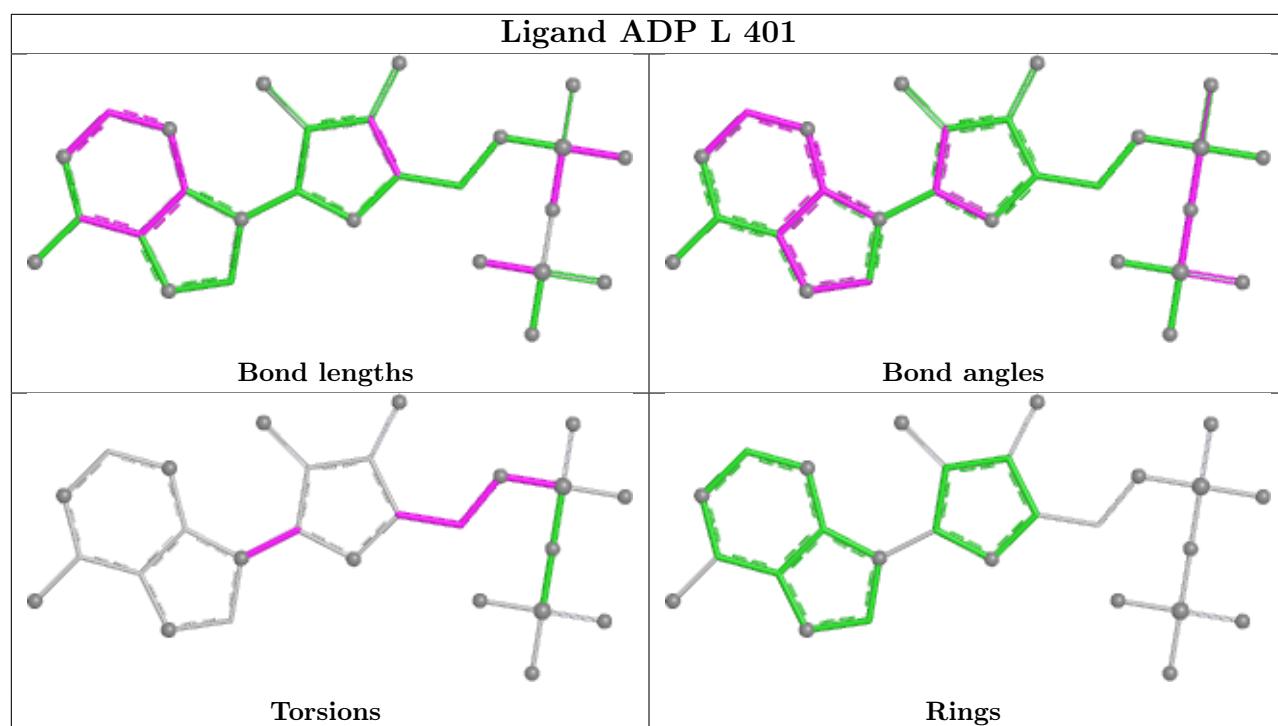
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	I	401	ADP	1	0
7	H	401	ADP	1	0
7	J	401	ADP	1	0

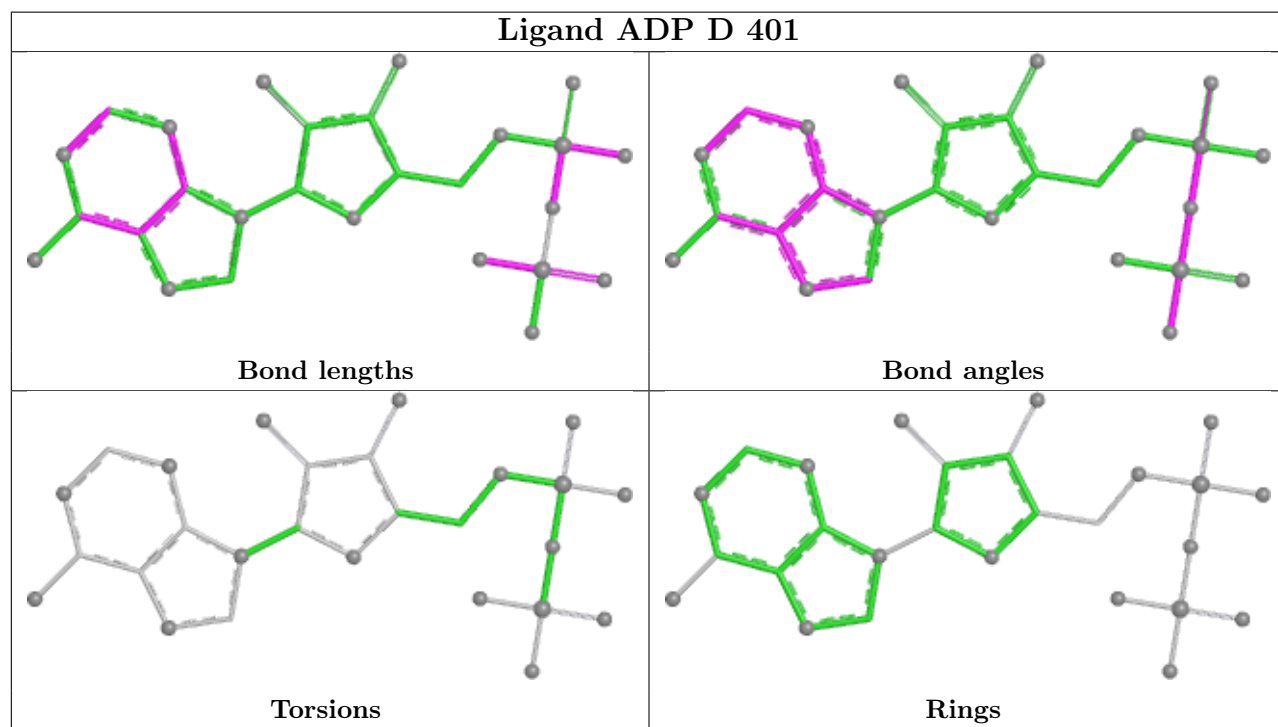
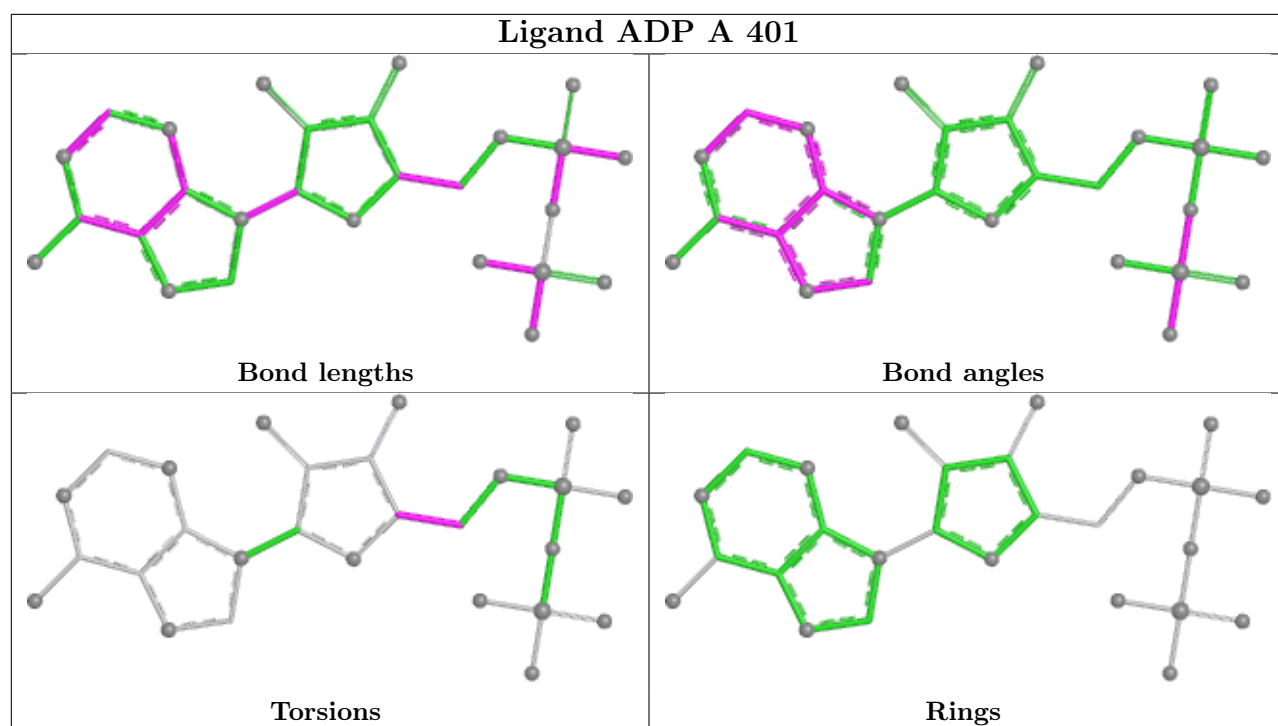
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

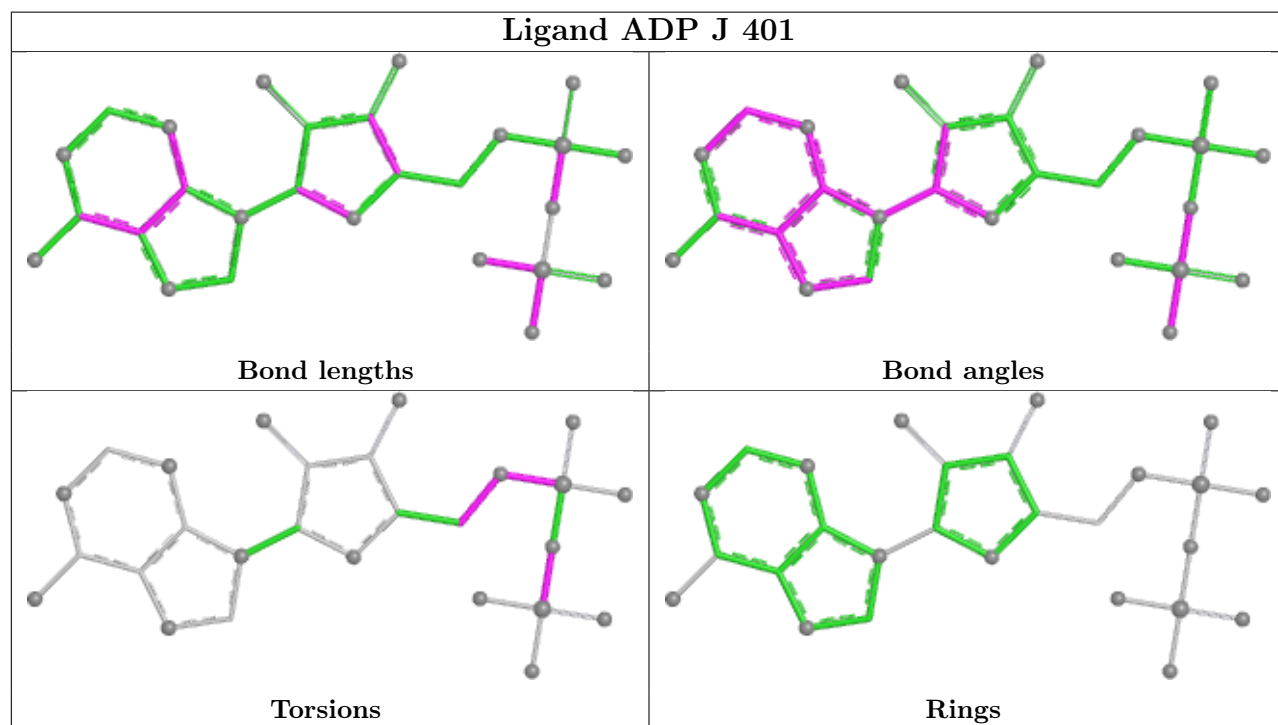
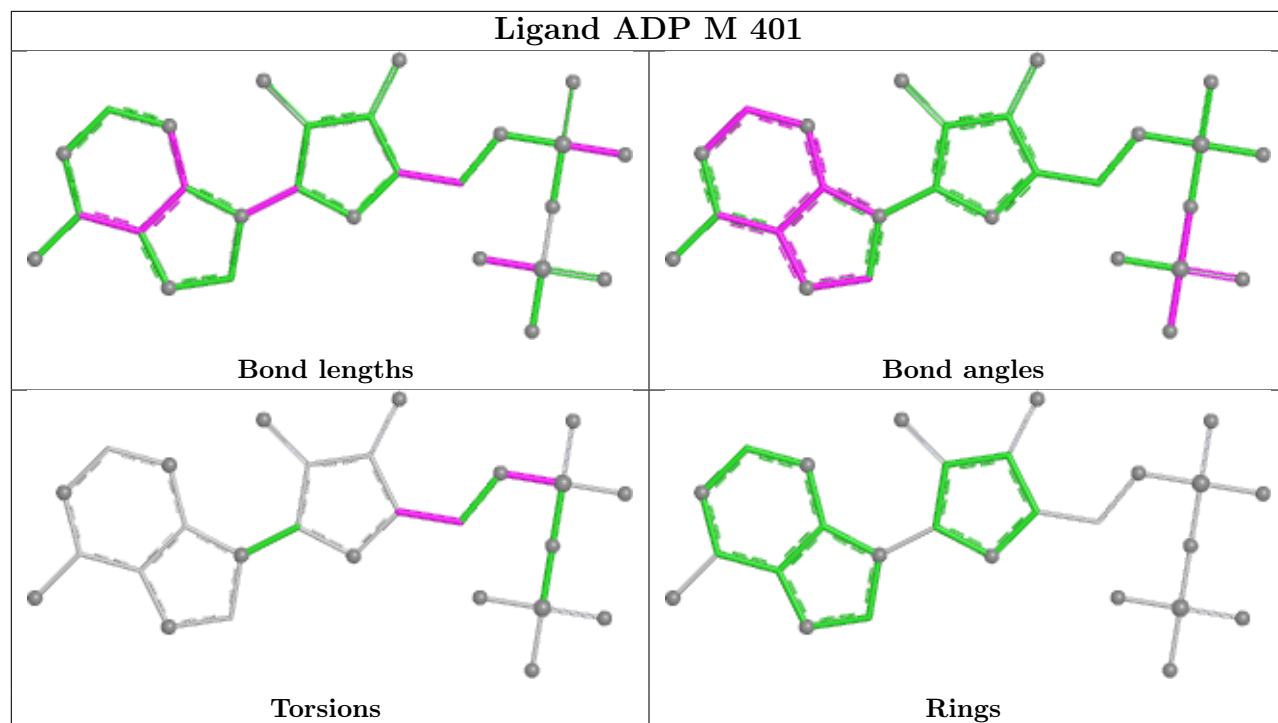


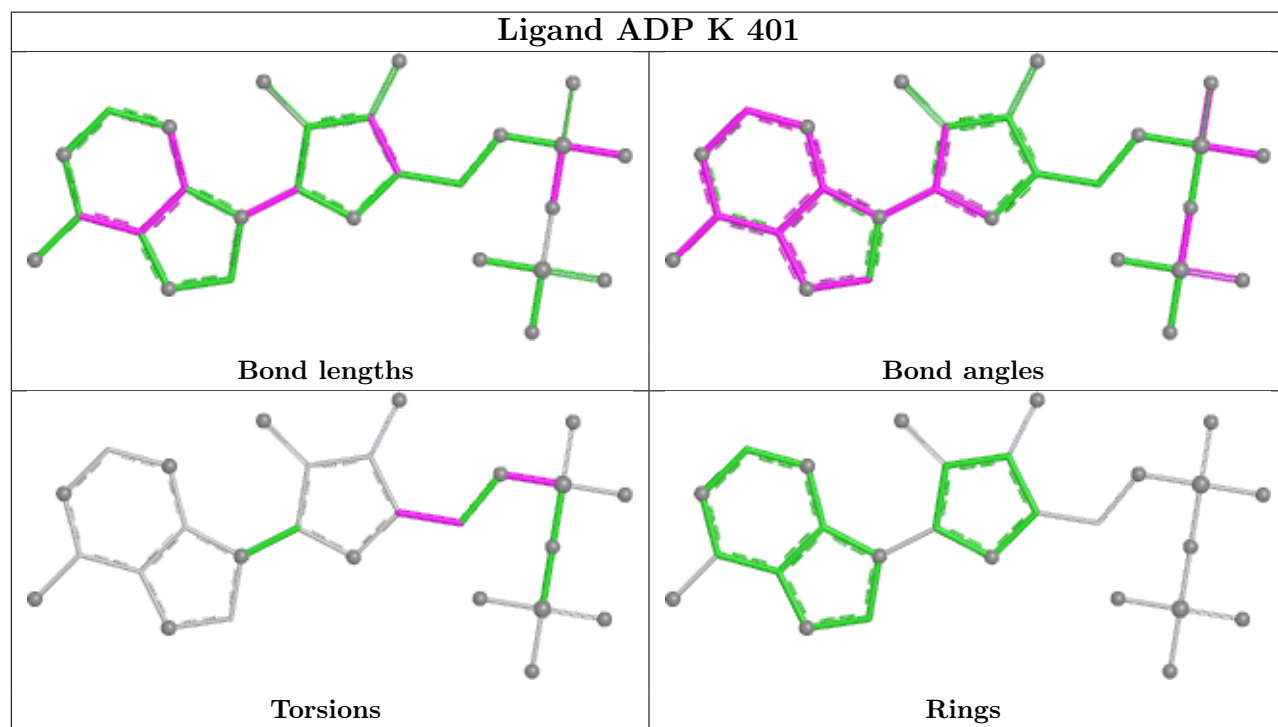
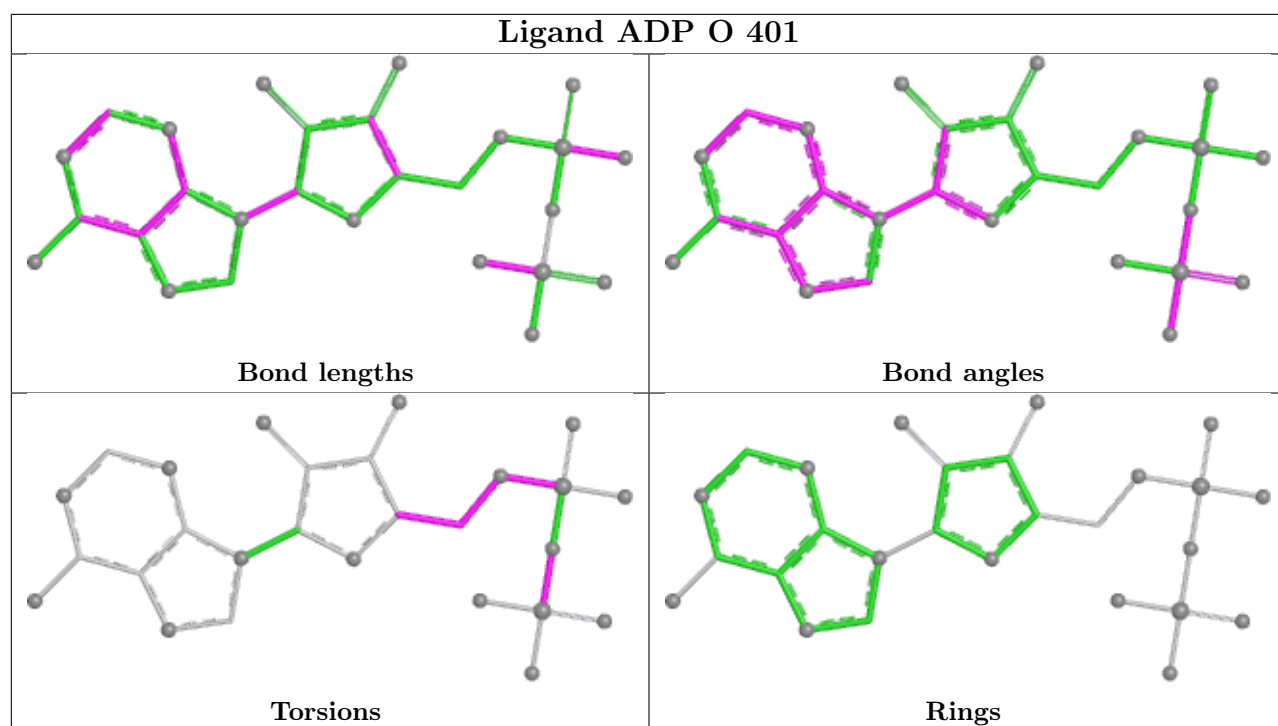


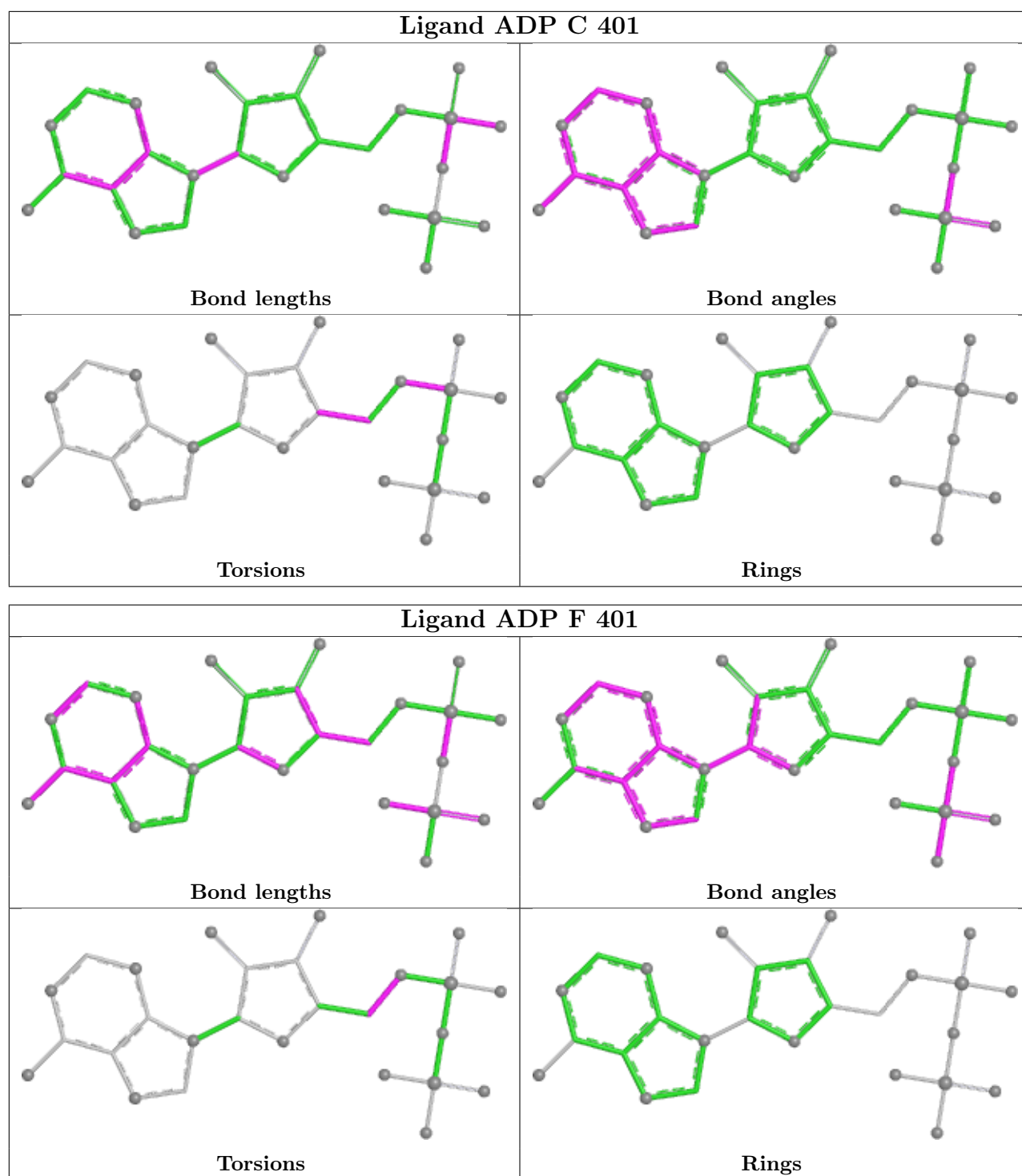












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

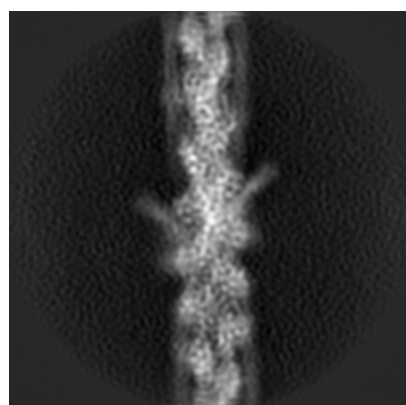
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0728. These allow visual inspection of the internal detail of the map and identification of artifacts.

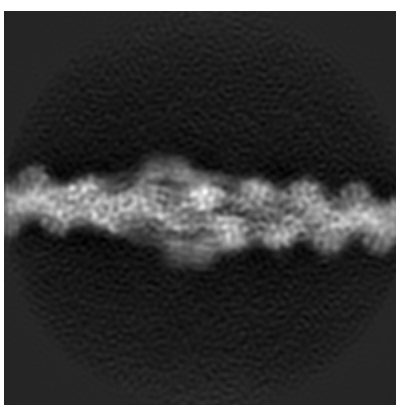
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

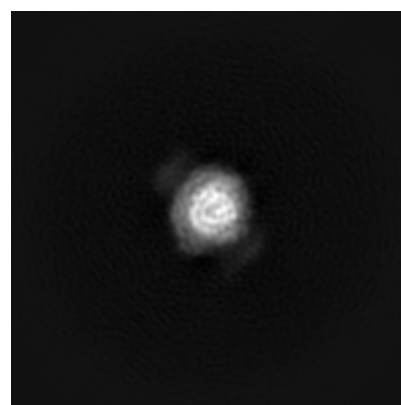
6.1.1 Primary map



X



Y

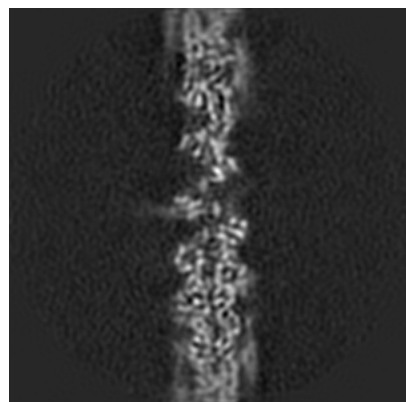


Z

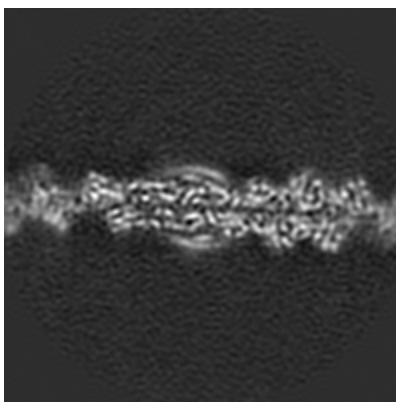
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

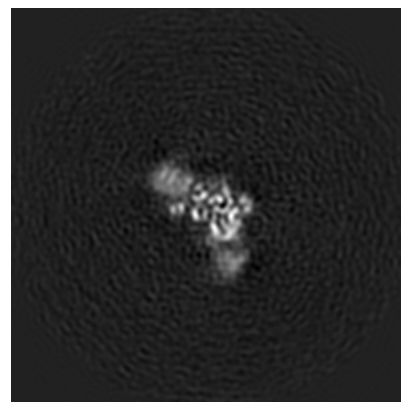
6.2.1 Primary map



X Index: 100



Y Index: 100

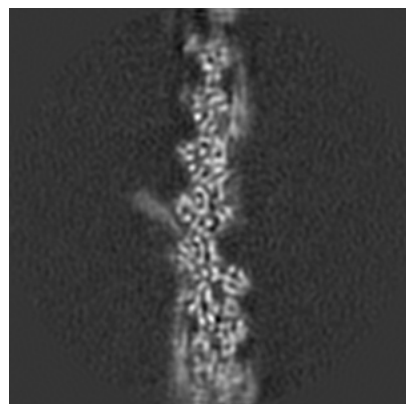


Z Index: 100

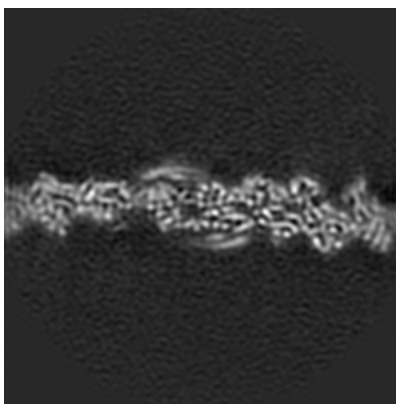
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

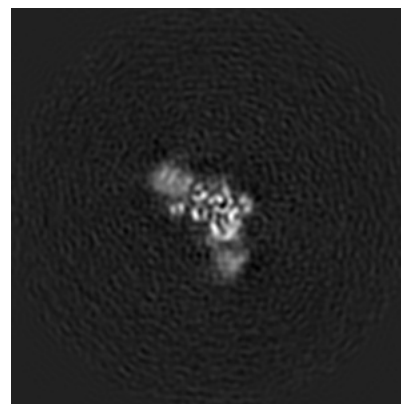
6.3.1 Primary map



X Index: 106



Y Index: 96

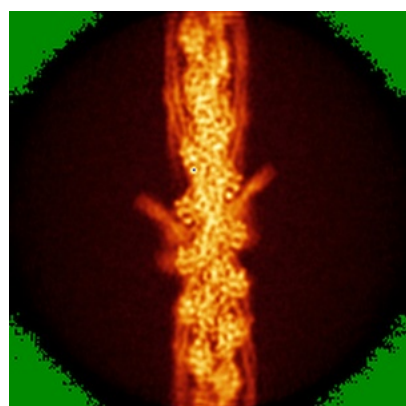


Z Index: 100

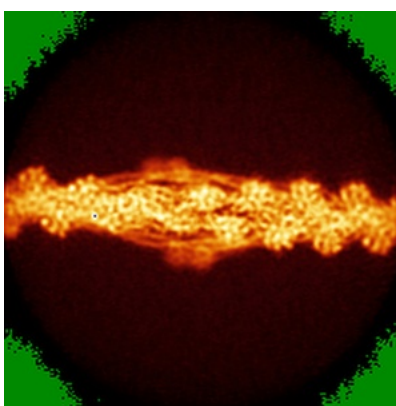
The images above show the largest variance slices of the map in three orthogonal directions.

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

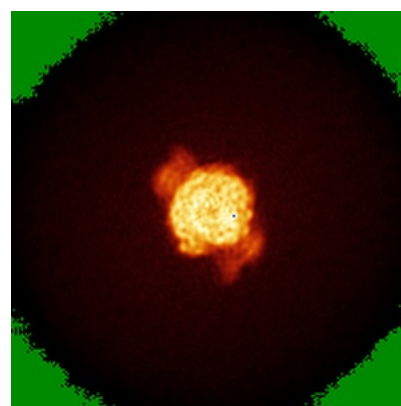
6.4.1 Primary map



X



Y



Z

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 0.0376. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

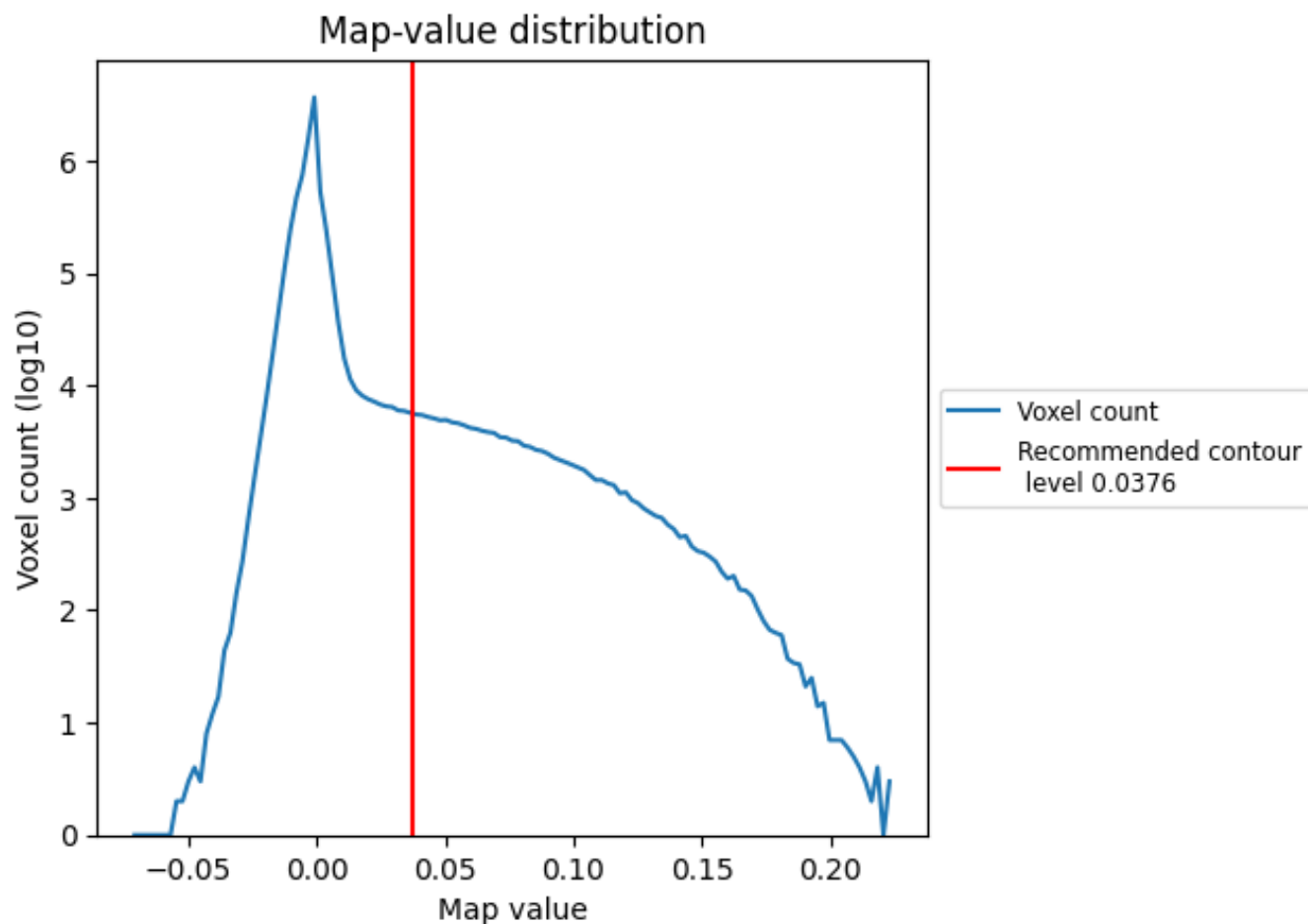
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

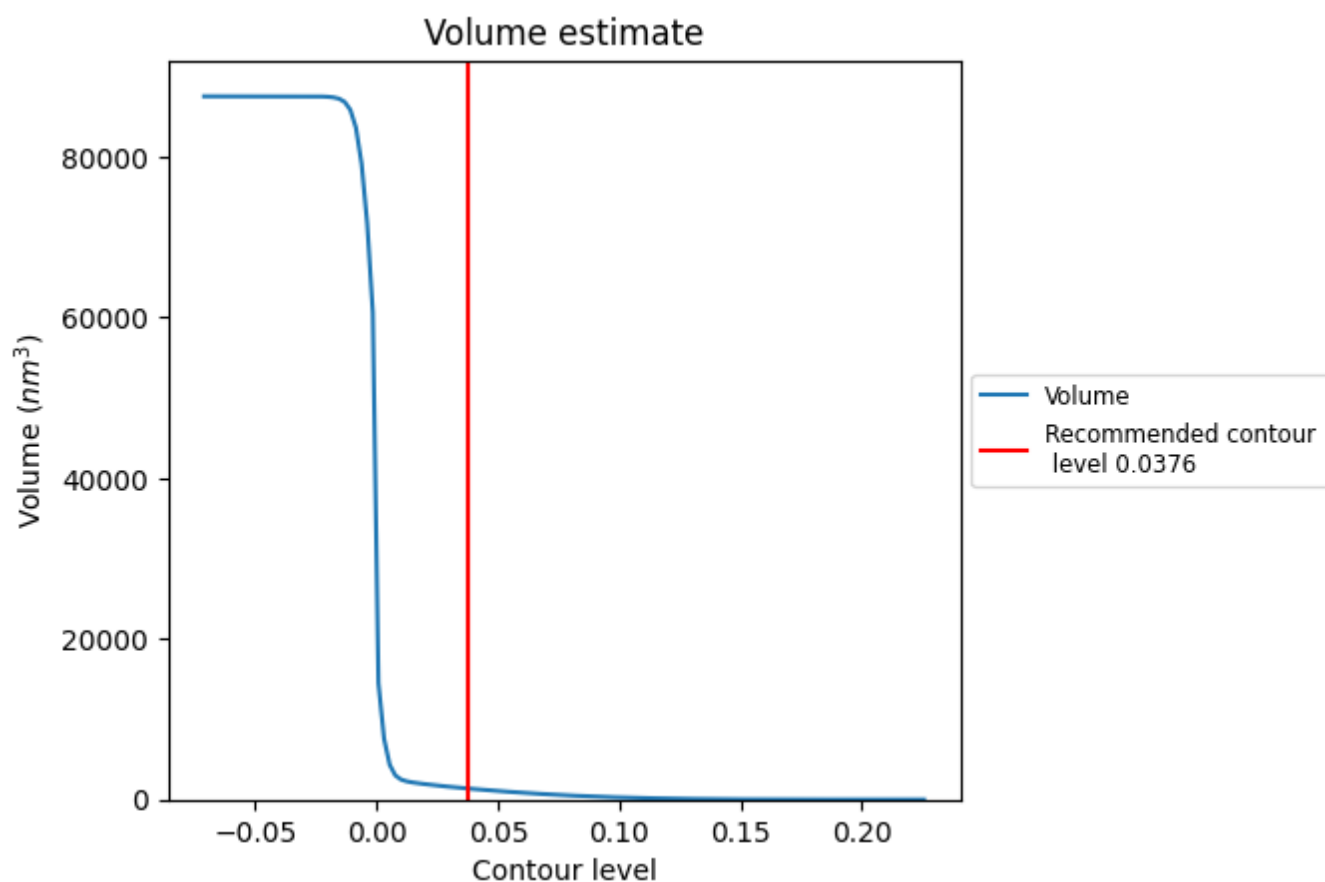
This section contains the results of statistical analysis of the map.

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.

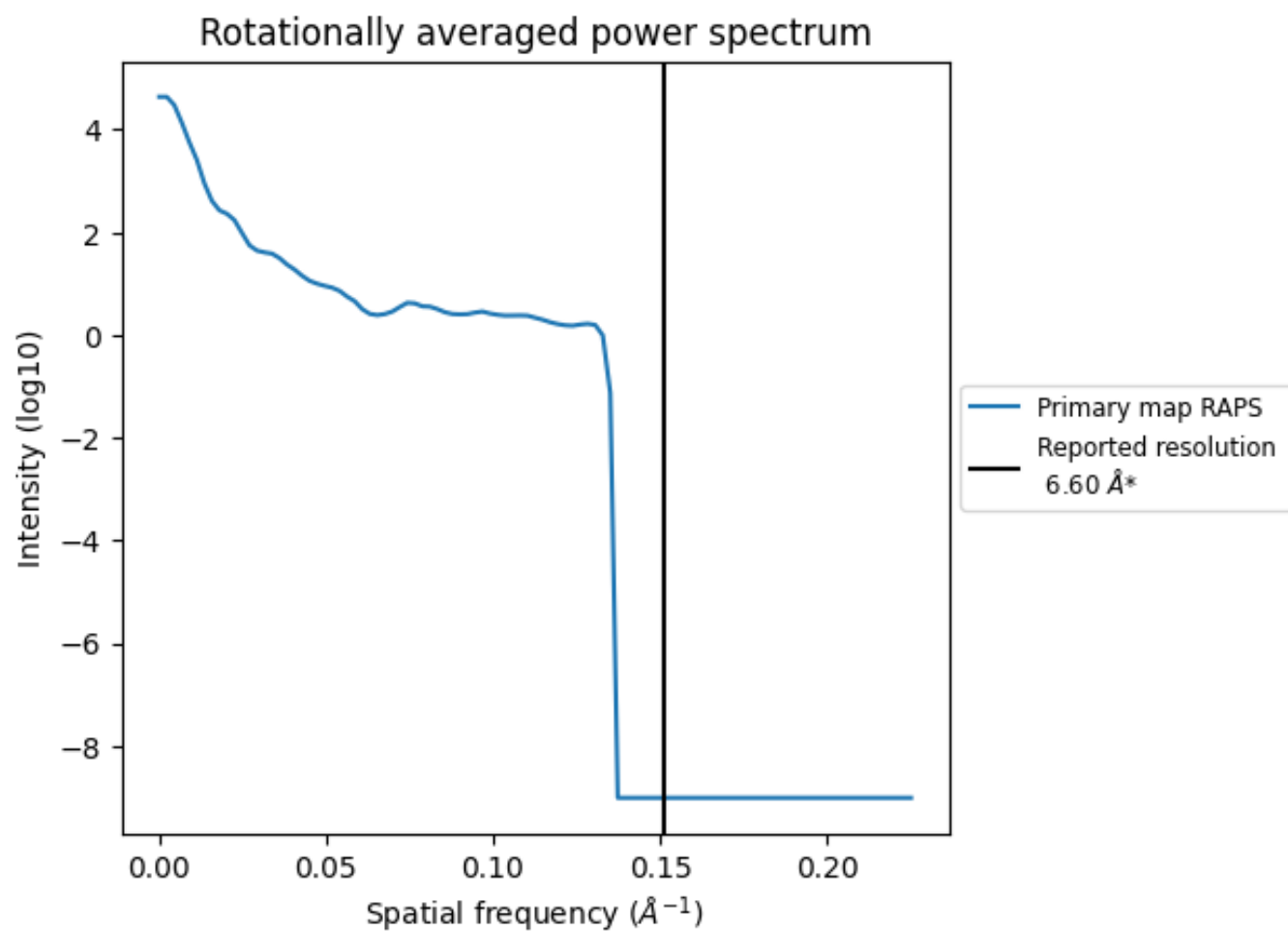
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1377 nm³; this corresponds to an approximate mass of 1244 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 ⓘ

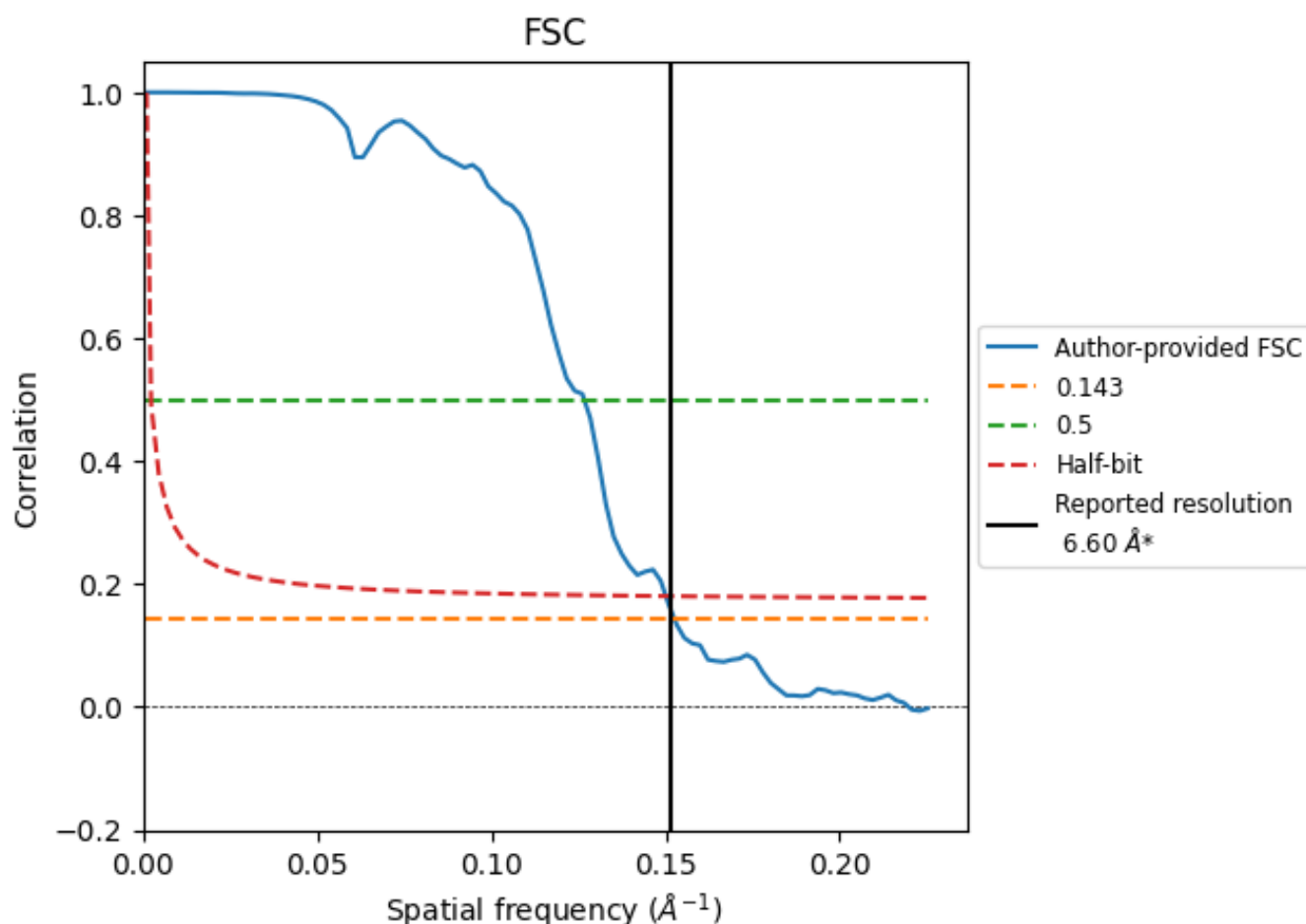


*Reported resolution corresponds to spatial frequency of 0.152 Å⁻¹

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 0.152 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

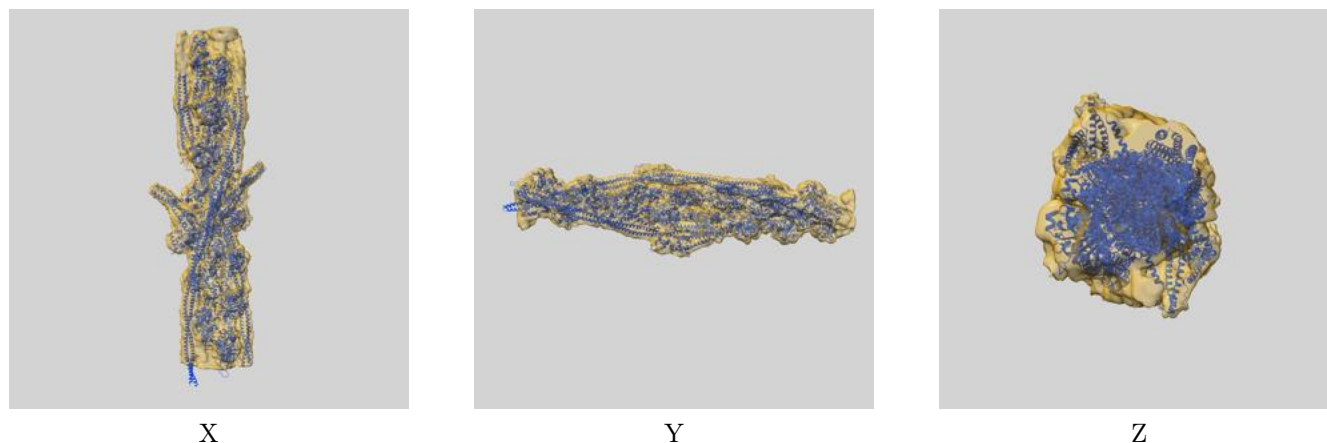
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.60	-	-
Author-provided FSC curve	6.56	7.89	6.66
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

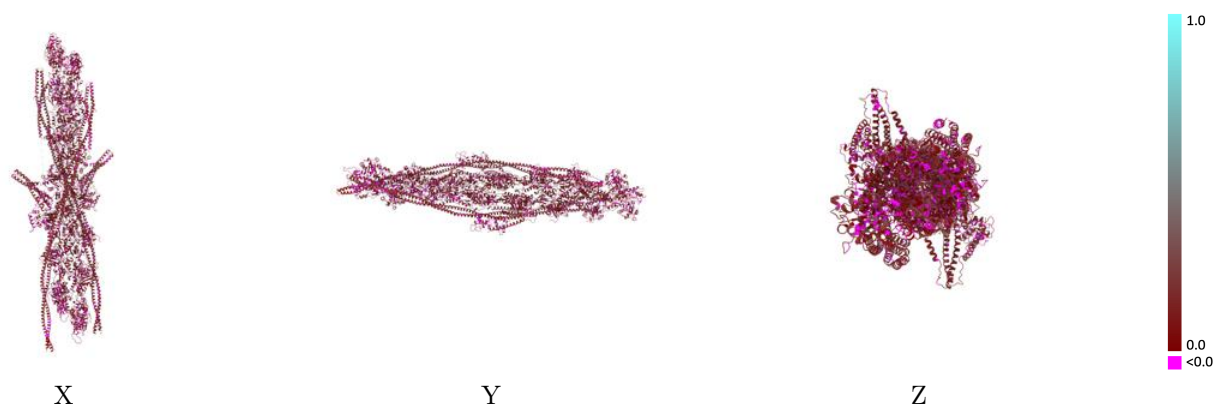
This section contains information regarding the fit between EMDB map EMD-0728 and PDB model 6KN7. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



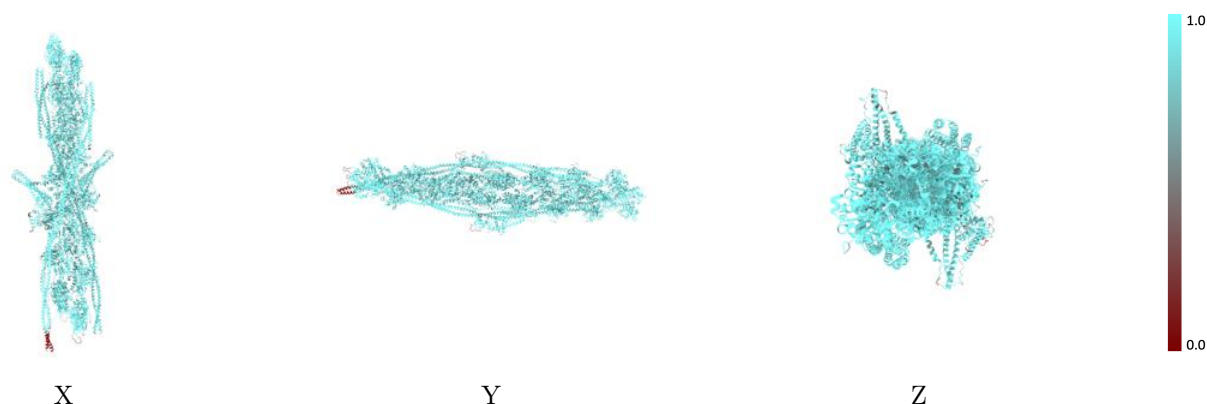
The images above show the 3D surface view of the map at the recommended contour level 0.0376 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



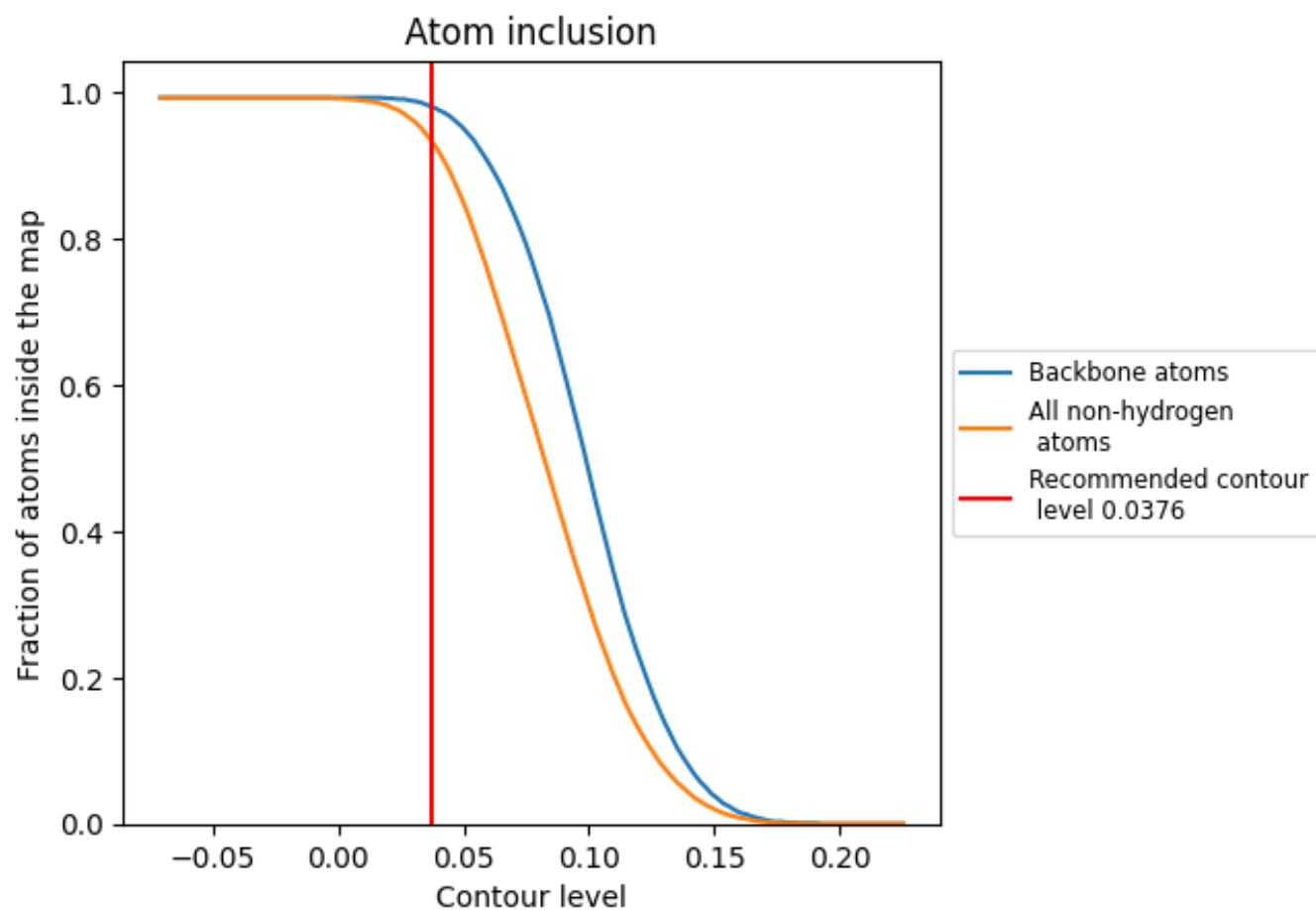
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0376).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 93% 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 (0.0376) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9320	 0.1270
A	 0.9490	 0.1060
B	 0.9570	 0.1060
C	 0.9400	 0.1280
D	 0.9510	 0.1240
E	 0.9430	 0.1350
F	 0.9310	 0.1380
G	 0.9360	 0.1320
H	 0.9450	 0.1410
I	 0.9410	 0.1380
J	 0.9470	 0.1330
K	 0.9360	 0.1320
L	 0.9320	 0.1220
M	 0.9540	 0.1260
N	 0.9430	 0.1100
O	 0.9800	 0.1160
P	 0.9500	 0.1630
Q	 0.9400	 0.1570
R	 0.9710	 0.1750
S	 0.9590	 0.1460
T	 0.9200	 0.1430
U	 0.8750	 0.1120
V	 0.8190	 0.0810
W	 0.8790	 0.1480
X	 0.8810	 0.1420
Y	 0.8880	 0.1320
Z	 0.9130	 0.0750
a	 0.8940	 0.1180
b	 0.9070	 0.1180
c	 0.8460	 0.0700

