



Full wwPDB EM Validation Report ⓘ

Mar 17, 2026 – 11:29 PM UTC

PDB ID : 7UTL / pdb_00007utl
EMDB ID : EMD-0728
Title : ALTERNATIVE MODELING OF TROPOMYOSIN IN HUMAN CARDIAC
THIN FILAMENT IN THE CALCIUM FREE STATE
Authors : Rynkiewicz, M.J.; Pavadai, E.; Lehman, W.
Deposited on : 2022-04-27
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:

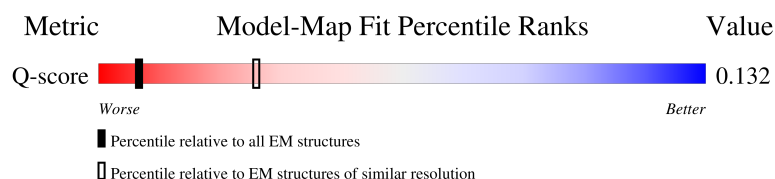
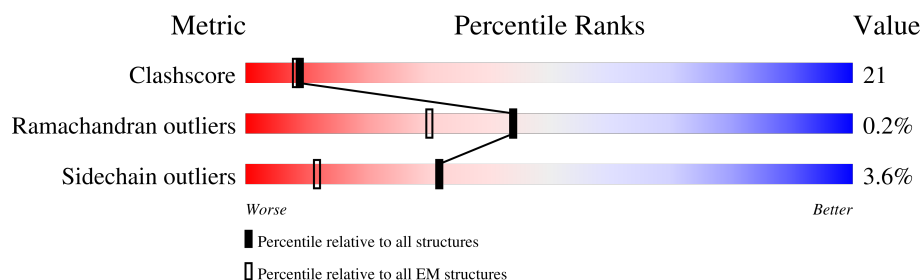
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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



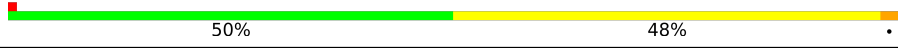
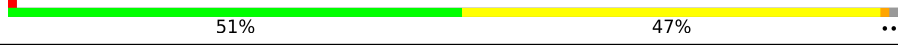
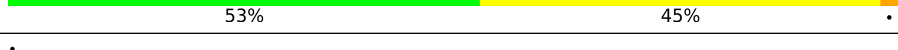
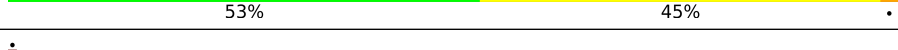
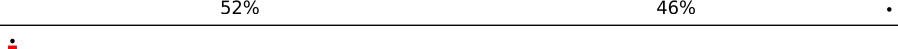
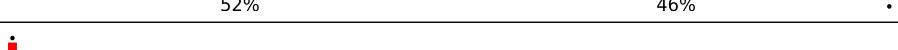
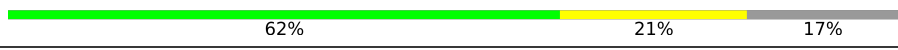
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	531 (6.10 - 7.10)

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	377	94% 50% 47% ..
1	B	377	43% 53% 44% ..
1	C	377	53% 45% ..
1	D	377	53% 45% ..

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Mol	Chain	Length	Quality of chain
1	E	377	
1	F	377	
1	G	377	
1	H	377	
1	I	377	
1	J	377	
1	K	377	
1	L	377	
1	M	377	
1	N	377	
1	O	377	
1	P	377	
1	Q	377	
1	R	377	
2	W	284	
2	Z	284	
2	a	284	
2	b	284	
2	g	284	
2	h	284	
2	i	284	
2	j	284	
3	X	288	
3	Y	288	
3	e	288	

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Mol	Chain	Length	Quality of chain
3	f	288	
4	V	210	
4	c	210	
5	U	161	
5	d	161	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 141796 atoms, of which 70424 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 5827	C 1855	H 2893	N 493	O 565	S 21	0	0
1	B	375	Total 5827	C 1855	H 2893	N 493	O 565	S 21	0	0
1	C	375	Total 5827	C 1855	H 2893	N 493	O 565	S 21	0	0
1	D	375	Total 5827	C 1855	H 2893	N 493	O 565	S 21	0	0
1	E	375	Total 5827	C 1855	H 2893	N 493	O 565	S 21	0	0
1	F	375	Total 5827	C 1855	H 2893	N 493	O 565	S 21	0	0
1	G	375	Total 5827	C 1855	H 2893	N 493	O 565	S 21	0	0
1	H	375	Total 5827	C 1855	H 2893	N 493	O 565	S 21	0	0
1	I	375	Total 5827	C 1855	H 2893	N 493	O 565	S 21	0	0
1	J	375	Total 5827	C 1855	H 2893	N 493	O 565	S 21	0	0
1	K	375	Total 5827	C 1855	H 2893	N 493	O 565	S 21	0	0
1	L	375	Total 5827	C 1855	H 2893	N 493	O 565	S 21	0	0
1	M	375	Total 5827	C 1855	H 2893	N 493	O 565	S 21	0	0
1	N	375	Total 5827	C 1855	H 2893	N 493	O 565	S 21	0	0
1	O	375	Total 5827	C 1855	H 2893	N 493	O 565	S 21	0	0
1	P	375	Total 5827	C 1855	H 2893	N 493	O 565	S 21	0	0
1	Q	375	Total 5827	C 1855	H 2893	N 493	O 565	S 21	0	0

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Mol	Chain	Residues	Atoms						AltConf	Trace
1	R	375	Total	C	H	N	O	S	0	0
			5827	1855	2893	493	565	21		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	a	257	Total	C	H	N	O	S	0	0
			4142	1267	2068	352	451	4		
2	b	257	Total	C	H	N	O	S	0	0
			4142	1267	2068	352	451	4		
2	W	65	Total	C	H	N	O	S	0	0
			1061	319	541	89	109	3		
2	Z	65	Total	C	H	N	O	S	0	0
			1061	319	541	89	109	3		
2	i	237	Total	C	H	N	O	S	0	0
			3822	1171	1908	324	415	4		
2	j	237	Total	C	H	N	O	S	0	0
			3822	1171	1908	324	415	4		
2	g	85	Total	C	H	N	O	S	0	0
			1358	410	687	113	145	3		
2	h	85	Total	C	H	N	O	S	0	0
			1358	410	687	113	145	3		

- Molecule 3 is a protein called Isoform 6 of Troponin T, cardiac muscle.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	X	63	Total	C	H	N	O	S	0	0
			1122	332	563	120	106	1		
3	Y	74	Total	C	H	N	O		0	0
			1306	401	663	123	119			
3	e	63	Total	C	H	N	O	S	0	0
			1122	332	563	120	106	1		
3	f	74	Total	C	H	N	O		0	0
			1306	401	663	123	119			

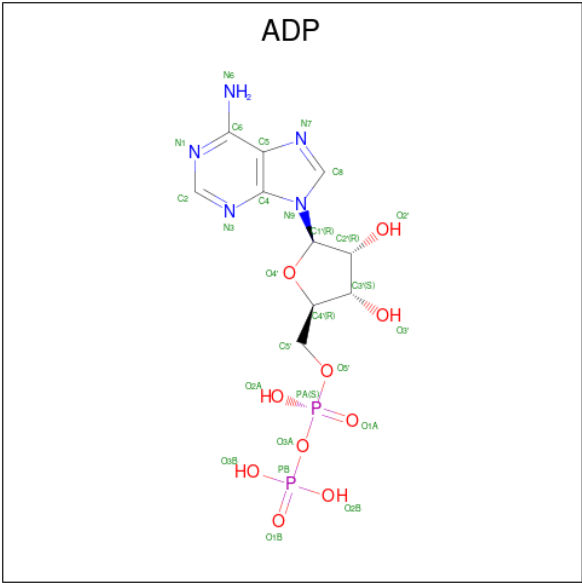
- Molecule 4 is a protein called Troponin I, cardiac muscle.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	V	170	Total	C	H	N	O	S	0	0
			2810	848	1436	263	258	5		
4	c	170	Total	C	H	N	O	S	0	0
			2810	848	1436	263	258	5		

- Molecule 5 is a protein called Troponin C, slow skeletal and cardiac muscles.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	U	160	Total	C	H	N	O	S	0	0
			2474	788	1201	195	278	12		
5	d	160	Total	C	H	N	O	S	0	0
			2474	788	1201	195	278	12		

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms						AltConf
6	A	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
6	B	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
6	C	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
6	D	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
6	E	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
6	F	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
6	G	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
6	H	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
6	I	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	

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Mol	Chain	Residues	Atoms						AltConf
6	J	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
6	K	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
6	L	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
6	M	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
6	N	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
6	O	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
6	P	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
6	Q	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
6	R	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	

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

Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total	Mg	0
			1	1	
7	B	1	Total	Mg	0
			1	1	
7	C	1	Total	Mg	0
			1	1	
7	D	1	Total	Mg	0
			1	1	
7	E	1	Total	Mg	0
			1	1	
7	F	1	Total	Mg	0
			1	1	
7	G	1	Total	Mg	0
			1	1	
7	H	1	Total	Mg	0
			1	1	
7	I	1	Total	Mg	0
			1	1	
7	J	1	Total	Mg	0
			1	1	

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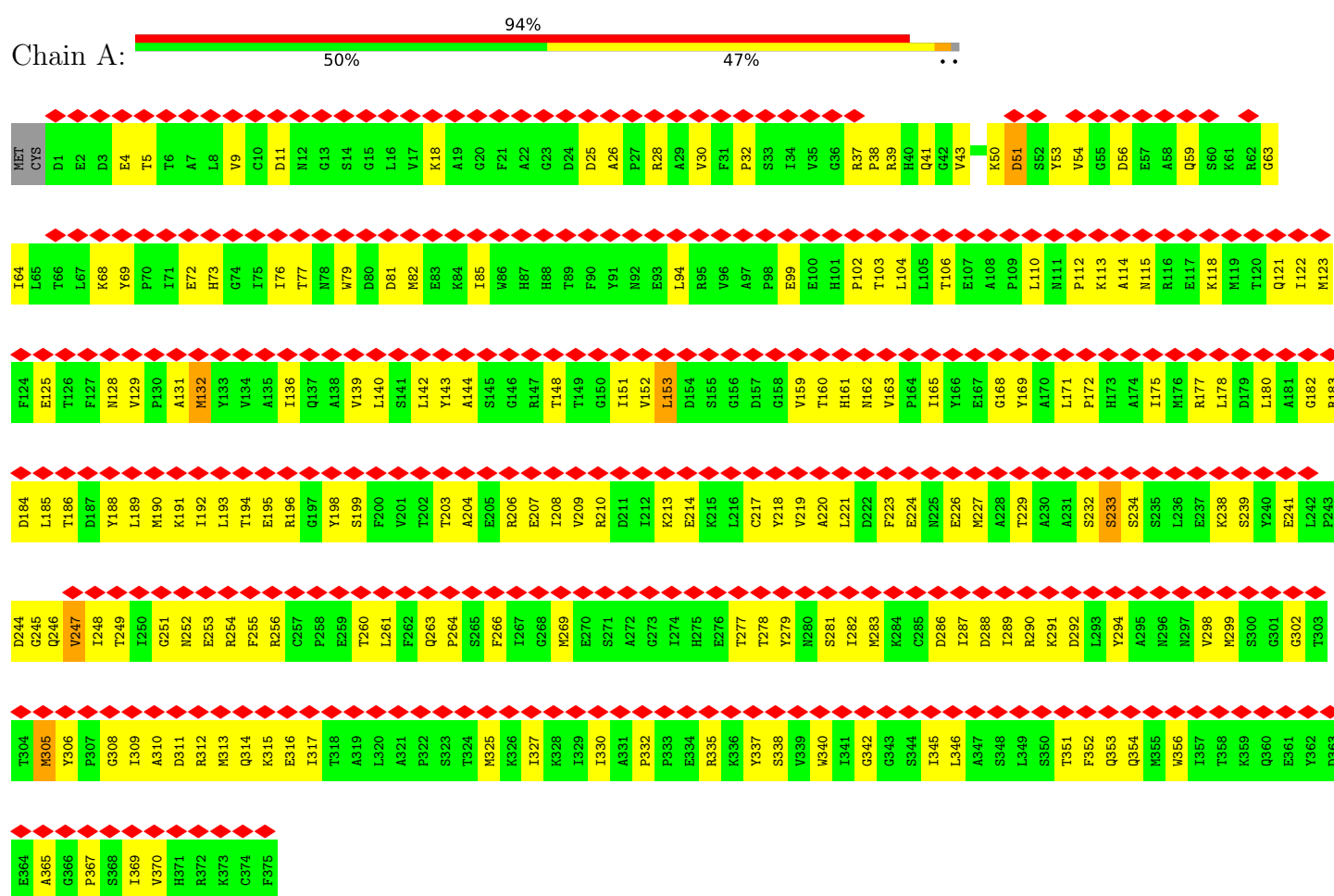
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Mol	Chain	Residues	Atoms		AltConf
7	K	1	Total 1	Mg 1	0
7	L	1	Total 1	Mg 1	0
7	M	1	Total 1	Mg 1	0
7	N	1	Total 1	Mg 1	0
7	O	1	Total 1	Mg 1	0
7	P	1	Total 1	Mg 1	0
7	Q	1	Total 1	Mg 1	0
7	R	1	Total 1	Mg 1	0

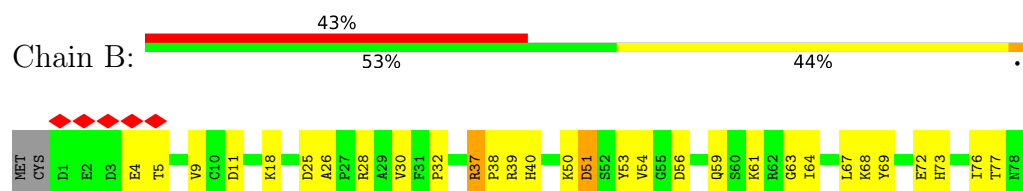
3 Residue-property plots

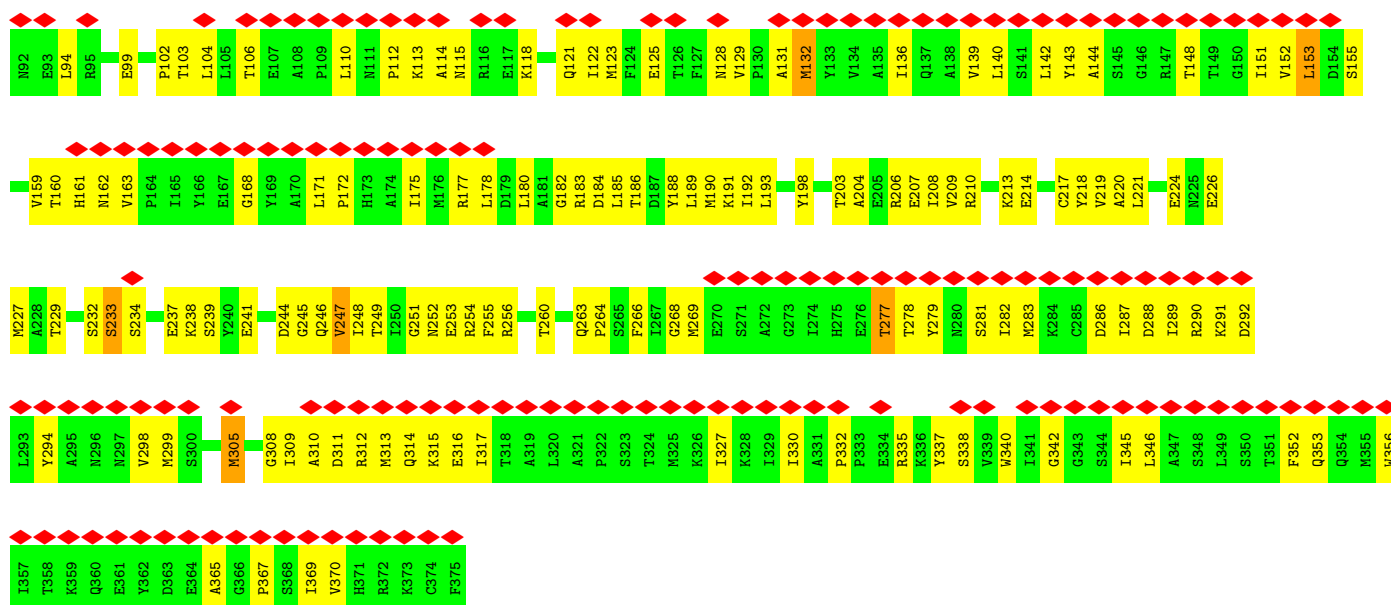
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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



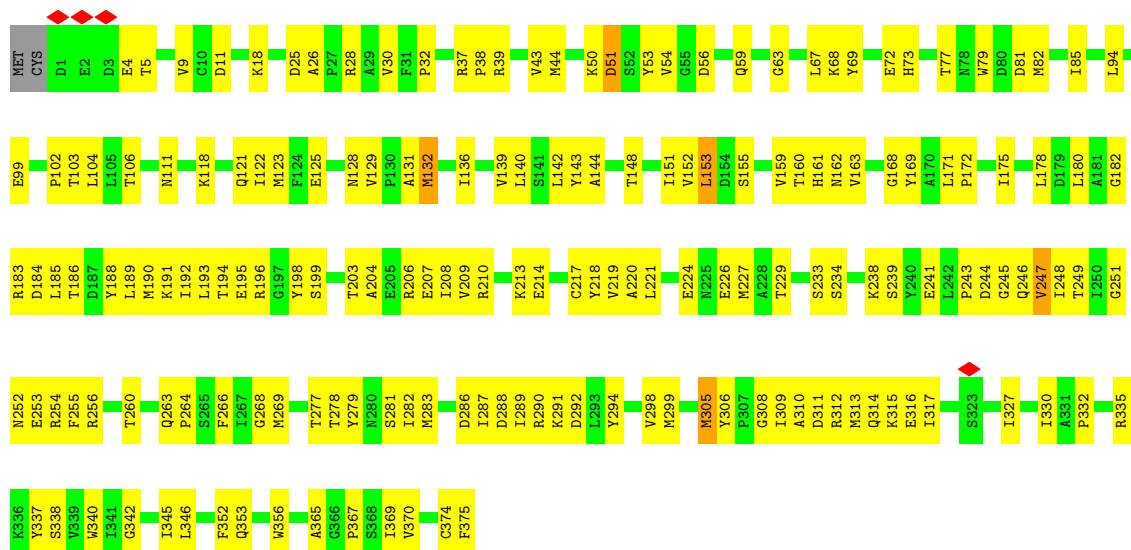
- Molecule 1: Actin, alpha skeletal muscle





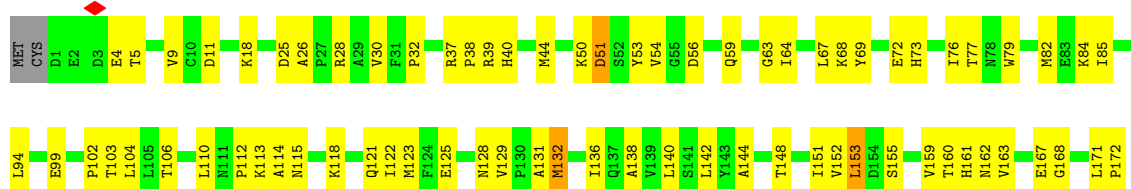
- Molecule 1: Actin, alpha skeletal muscle

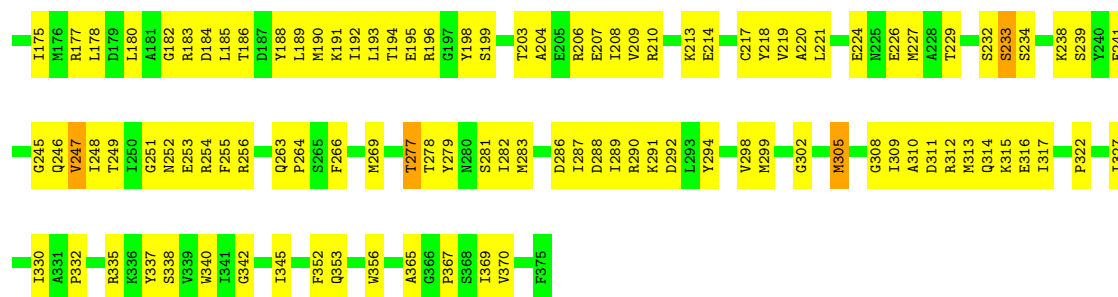
Chain C: 53% 45%



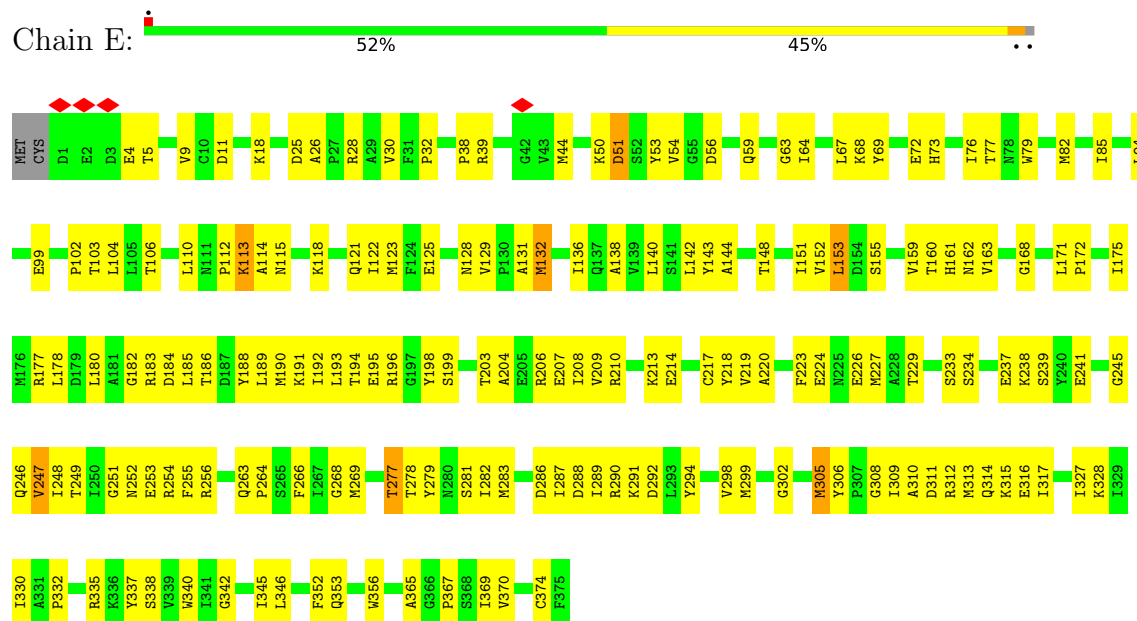
- Molecule 1: Actin, alpha skeletal muscle

Chain D: 53% 45%

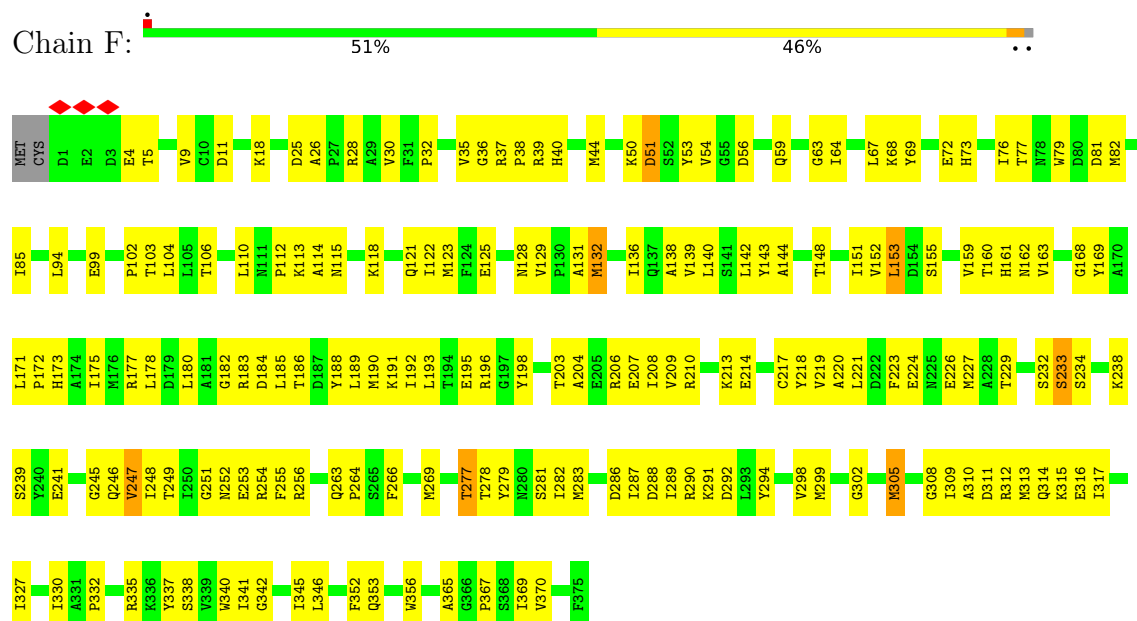




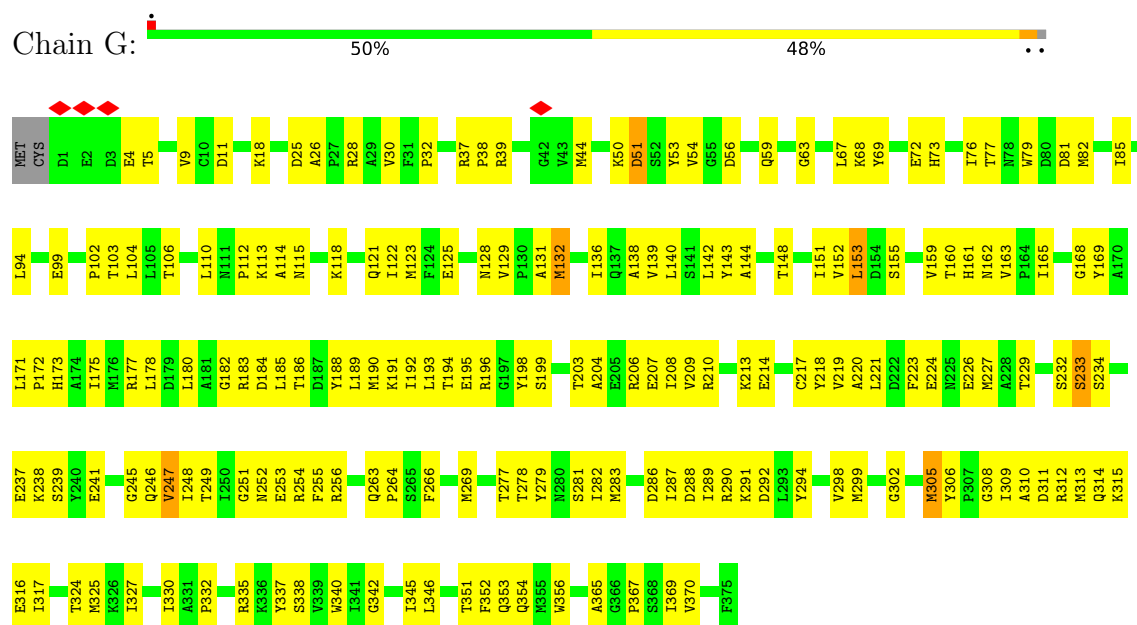
- Molecule 1: Actin, alpha skeletal muscle



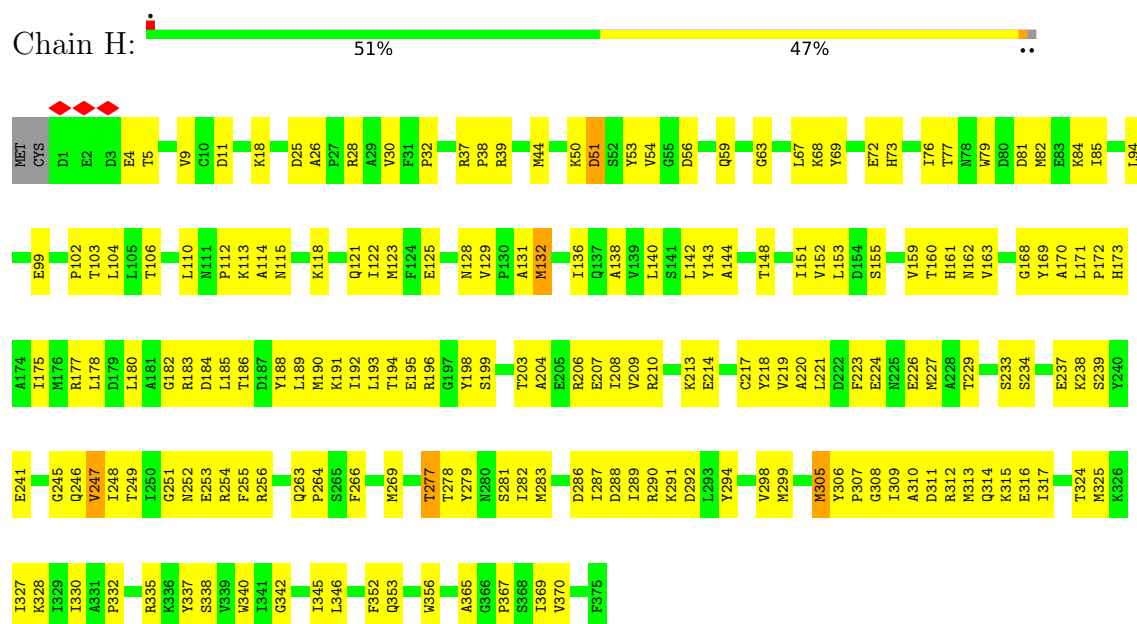
- Molecule 1: Actin, alpha skeletal muscle



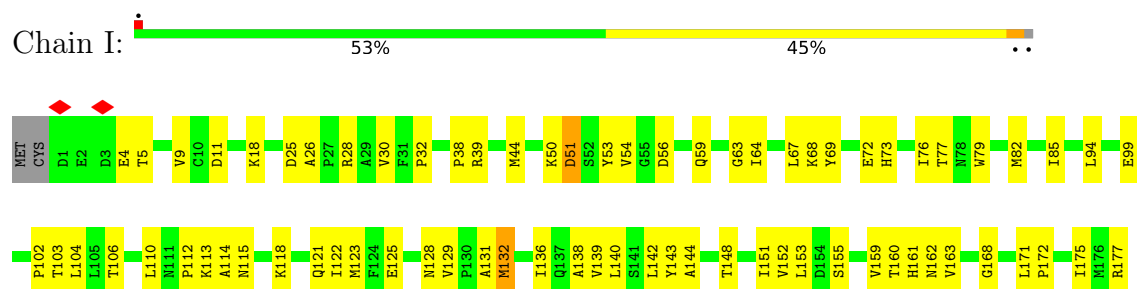
- Molecule 1: Actin, alpha skeletal muscle

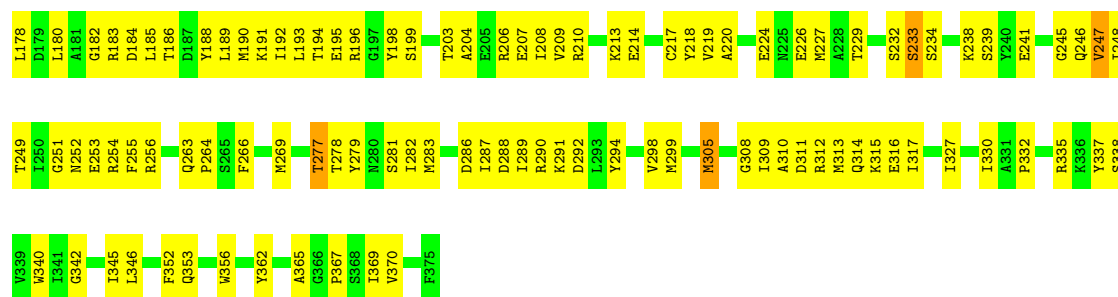


• Molecule 1: Actin, alpha skeletal muscle

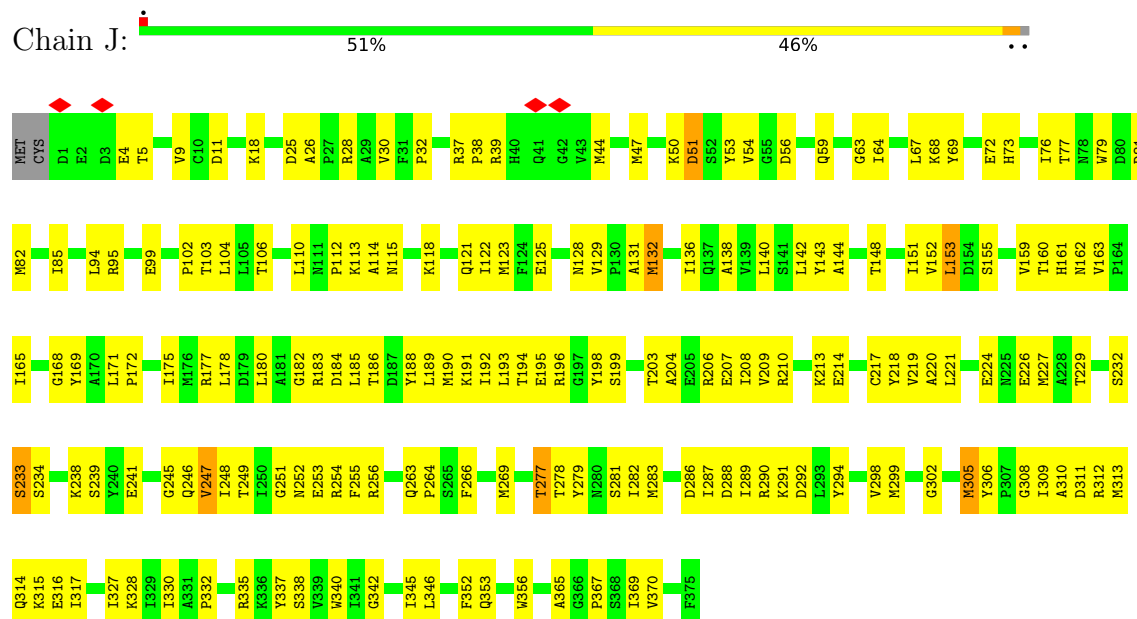


• Molecule 1: Actin, alpha skeletal muscle

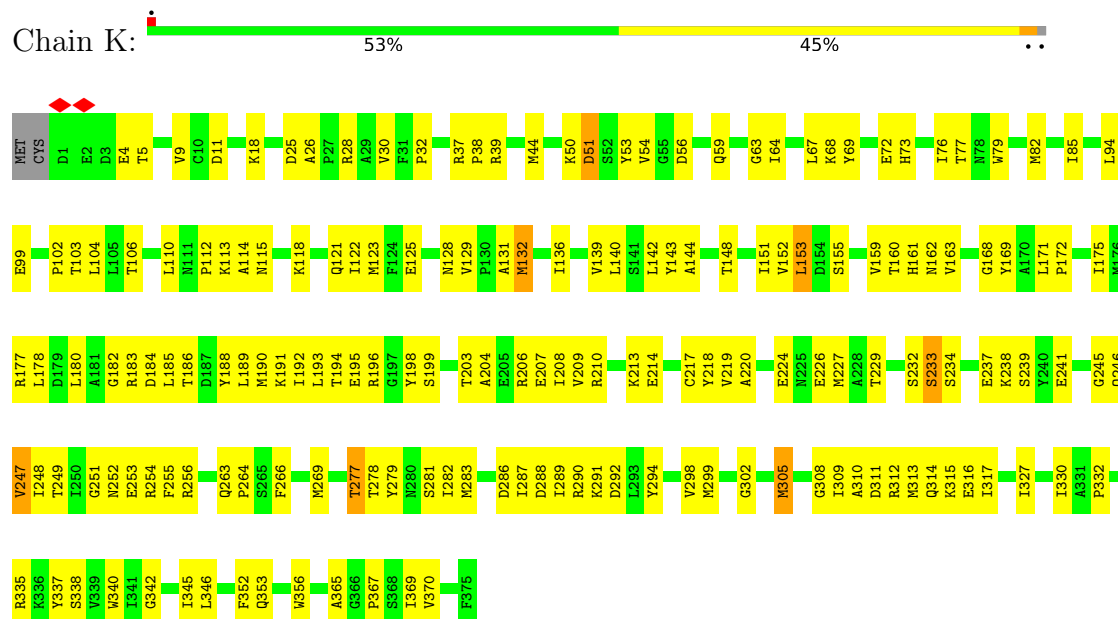




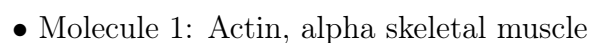
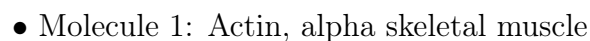
- Molecule 1: Actin, alpha skeletal muscle

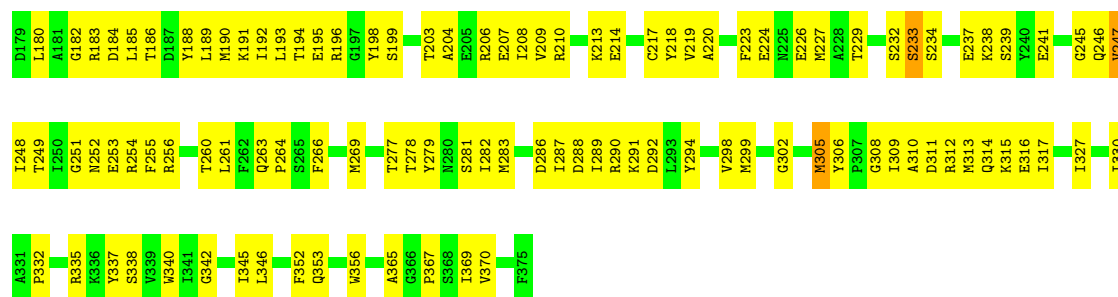


- Molecule 1: Actin, alpha skeletal muscle

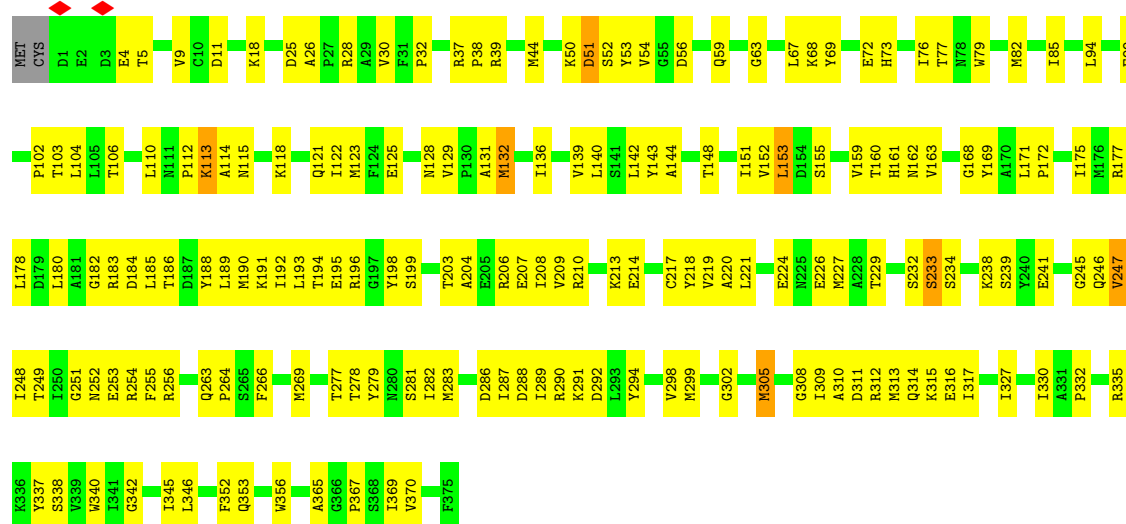


- Molecule 1: Actin, alpha skeletal muscle

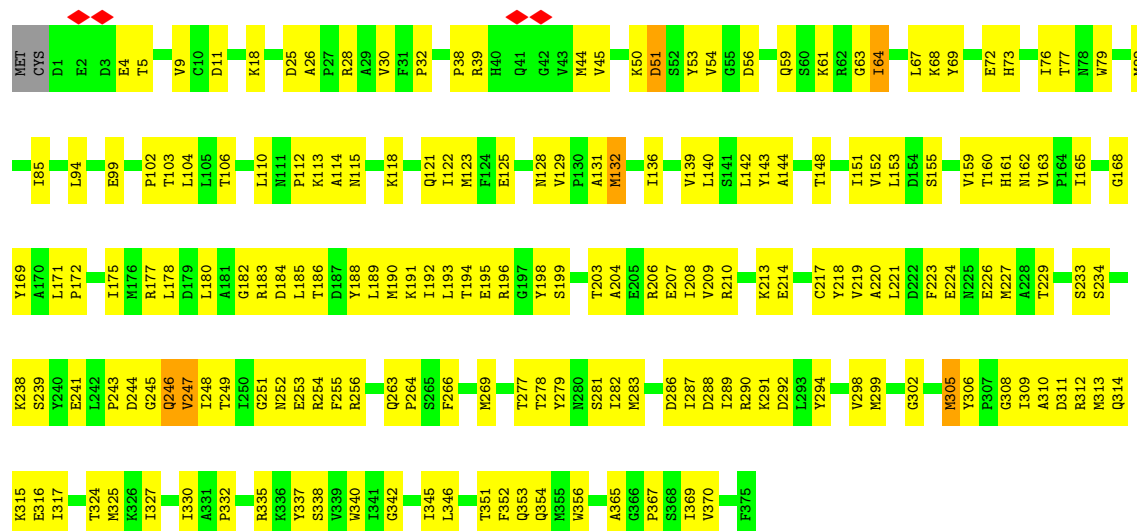




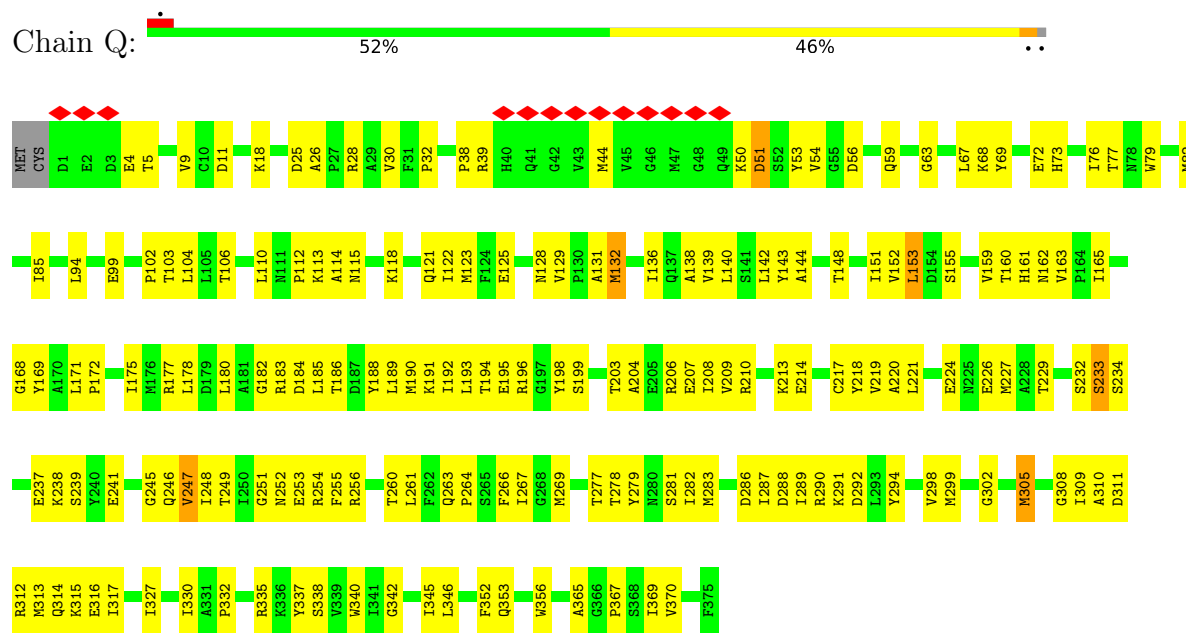
- Molecule 1: Actin, alpha skeletal muscle



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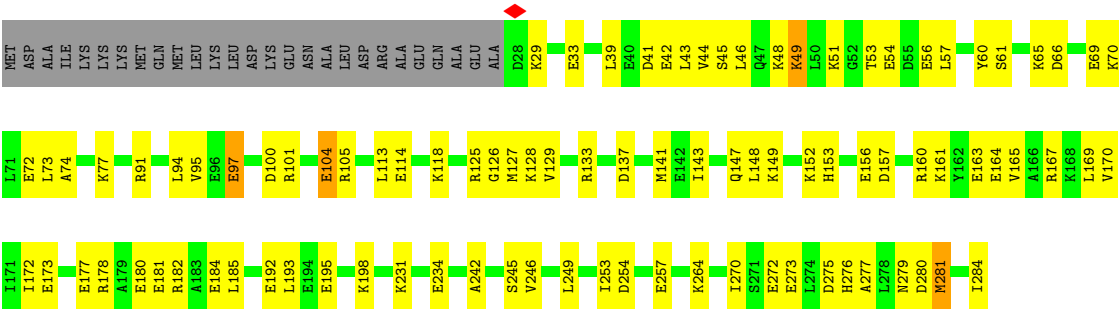


• Molecule 1: Actin, alpha skeletal muscle

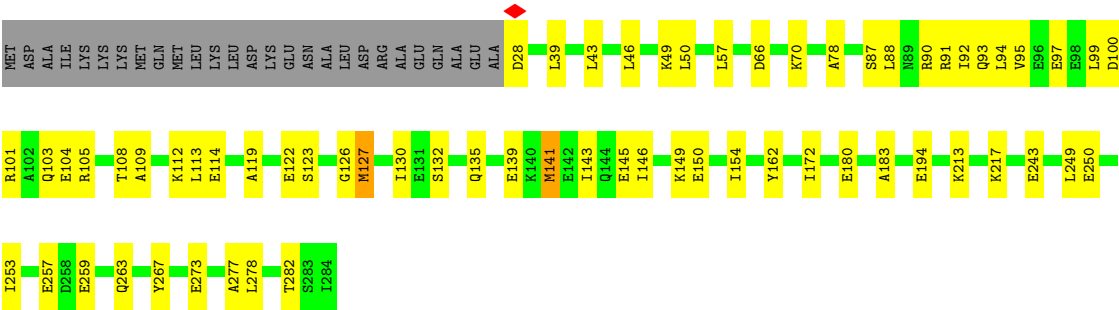


• Molecule 2: Tropomyosin alpha-1 chain

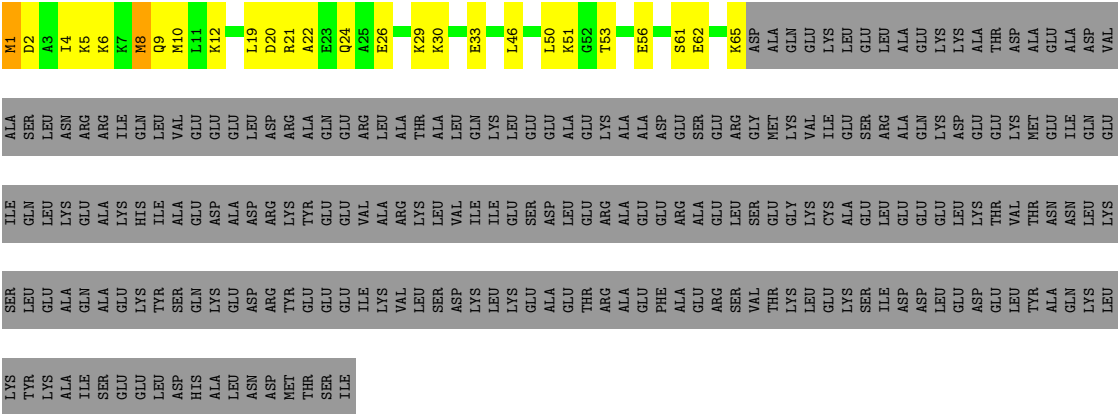




• Molecule 2: Tropomyosin alpha-1 chain



• Molecule 2: Tropomyosin alpha-1 chain



• Molecule 2: Tropomyosin alpha-1 chain



[illegible]

- Molecule 2: Tropomyosin alpha-1 chain



L270	S61	NET
S271	E62	ASP
E272	A63	ALA
E273	L64	ILE
	K65	LYS
H276	H66	LYS
A277		LYS
	E69	NET
	K70	GLN
M281	L71	NET
	E72	LEU
	L73	LYS
L284	A74	LEU
		ASP
	K77	LYS
	A78	GLU
		ASN
	L88	ALA
	H89	LEU
	R90	ASP
	R91	ARG
	I92	ALA
	A93	GLU
	L94	GLN
	R95	ALA
	E96	GLU
	E97	ALA
	E98	ASP
	L99	LYS
	D100	LYS
	R101	ALA
		ALA
	E104	GLU
	R105	ASP
	L106	ARG
		SER
	K112	LYS
	L113	GLN
	E114	LEU
		GLU
	K118	ASP
		GLU
		LEU
	S123	VAL
	E124	
	R125	SER
	G126	LEU
	M127	
	K128	
	V129	
	I130	
	E131	
	A132	K48
	R133	K49
		L50
		K51
		G52
		T53
	D137	E54
		D55
		E56
	M141	L57
	E142	D58
	I143	K59
		Y60

- Molecule 2: Tropomyosin alpha-1 chain



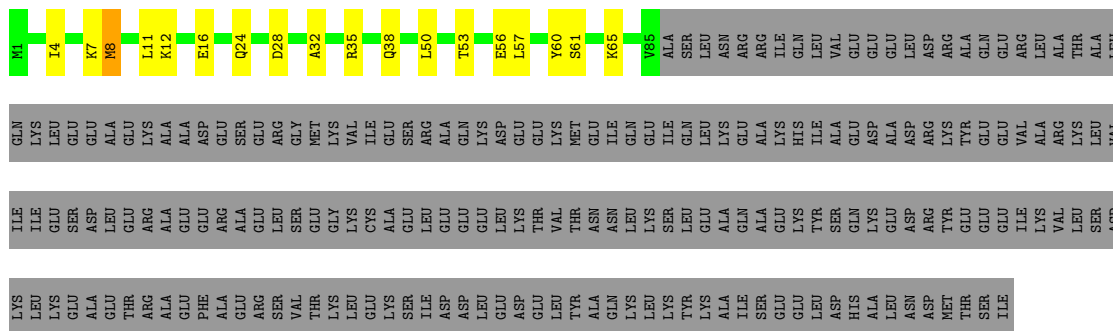
MET		ASP		ALA		ILE		LYS		LYS		MET		GLN		LEU		LYS		LEU		ASP		LYS		GLU		ASN		ALA		LEU		ASP		ALA		GLU		ALA		ASP		LYS		LYS		ALA		GLU		ASP		ARG		SER		LYS		GLN		LEU		GLU		ASP		GLU		LEU		VAL		SER		LEU		LEU		GLN		K43		K51		V60		S61		K65		D66		K70		A78																																							
K213		Y214		S215		Q216		K217		Y221		L225		F241		Y246		L249		L253		E259		L260		Y261		A262		Q263		Y267		L278		T282		S283		L284		V85		A86		S87		L88		N89		R90		R91		I92		Q93		L94		V95		E96		E97		E98		L99		D100		R101		A102		Q103		E104		R105		L106		A107		T108		A109		L110		Q111		K112		L113		A119		E122		S123		G126		M127		L130		E131		S132		Q135		M141		E145		I146		K149		E150		I154		I172		L193		L204	
MET		ASP		ALA		ILE		LYS		LYS		MET		GLN		LEU		LYS		LEU		ASP		LYS		GLU		ASN		ALA		LEU		ASP		ALA		GLU		ALA		ASP		LYS		LYS		ALA		GLU		ALA		GLU		ASP		ARG		SER		LYS		GLN		LEU		GLU		ASP		GLU		LEU		VAL		SER		LEU		LEU		GLN		K43		K51		V60		S61		K65		D66		K70		A78																																			

- Molecule 2: Tropomyosin alpha-1 chain

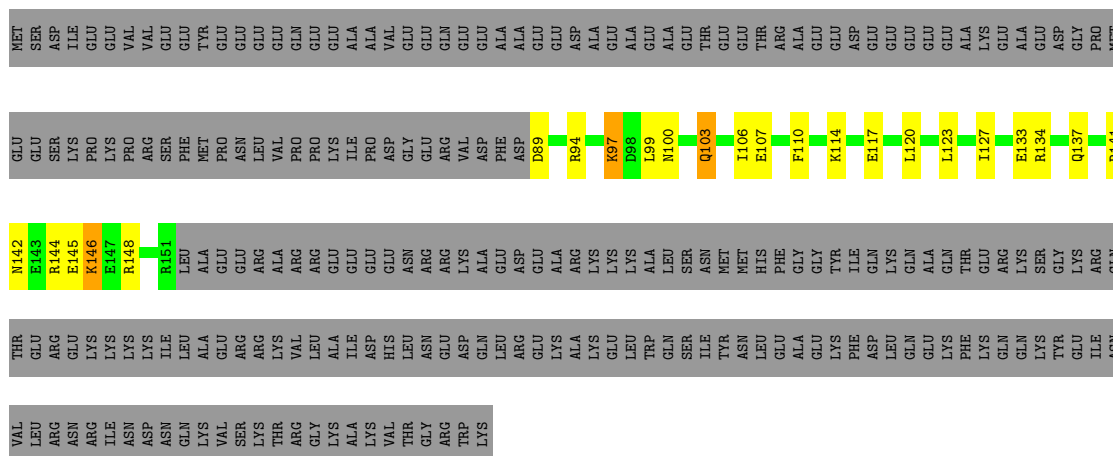


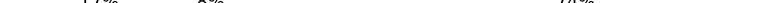
VAL	ARG	M1
ALA	LEU	D2
ARG	ALA	A3
LYS	THR	I4
LEU	ALA	K5
VAL	LEU	K6
ILE	GLN	K7
ILE	LYS	M8
GLU	LEU	Q9
SER	GLU	M10
ASP	GLU	L11
LEU	ALA	
GLU	GLU	L19
ARG	LYS	D20
ALA	ALA	R21
GLU	ALA	A22
GLU	ASP	E23
ARG	GLU	Q24
ALA	SER	A25
GLU	GLU	E26
LEU	ARG	
SER	GLY	K29
GLU	MET	K30
GLY	LYS	
LYS	VAL	E33
CYS	ILE	
ALA	GLU	L46
GLU	SER	
LEU	ARG	L50
GLU	ALA	
GLU	GLN	T53
GLU	LYS	
LEU	ASP	E56
LYS	GLU	L57
THR	GLY	
VAL	LYS	S61
THR	MET	E62
ASN	GLU	
ASN	ILE	K65
LEU	GLN	
LYS	GLU	V65
SER	ILE	
LEU	GLN	ALA
LEU	LEU	SER
ALA	LYS	LEU
GLN	GLU	ASN
ALA	GLU	ARG
ALA	ALA	ARG
GLU	LYS	ILE
LYS	HIS	GLN
TYR	ILE	LEU
SER	ALA	VAL
GLN	GLU	GLU
LYS	ASP	GLU
GLU	ALA	GLU
ASP	ASP	LEU
ARG	ARG	ASP
TYR	LYS	ARG
GLU	GLU	ALA
GLY	GLU	GLN
GLU	GLU	GLU

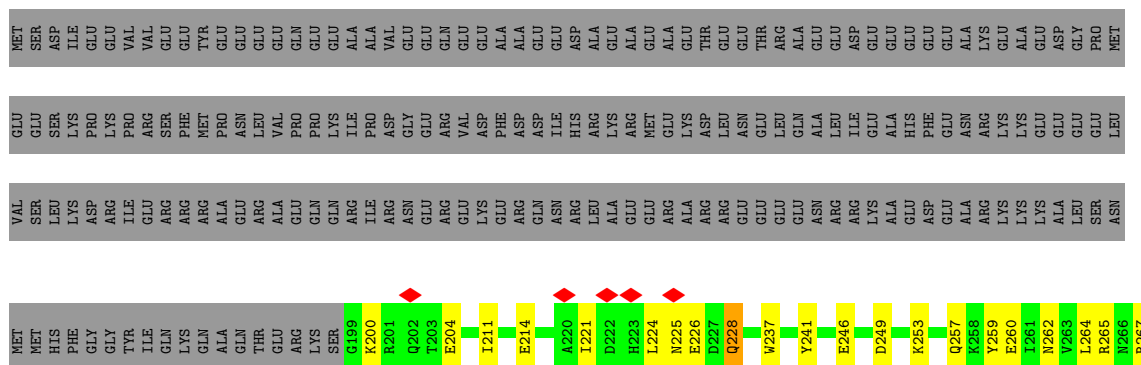
Chain h: 24% 6% 70%

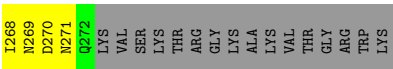


Chain X: 14% 7% 78%

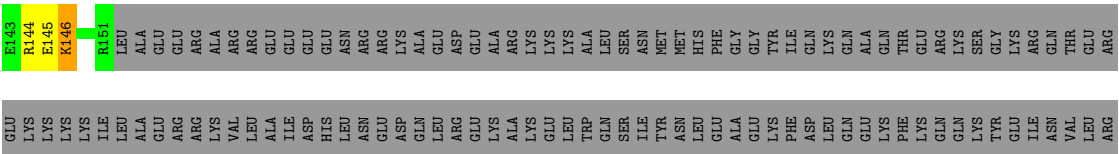
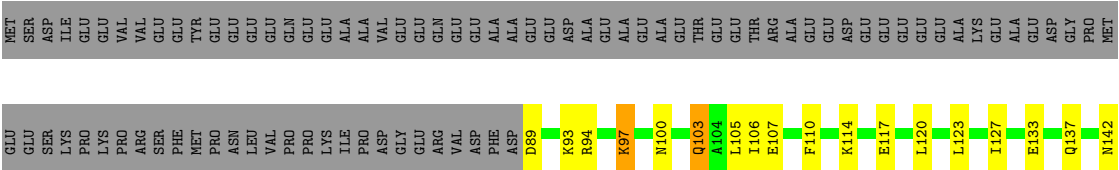


Chain Y:  17% 8% 74%

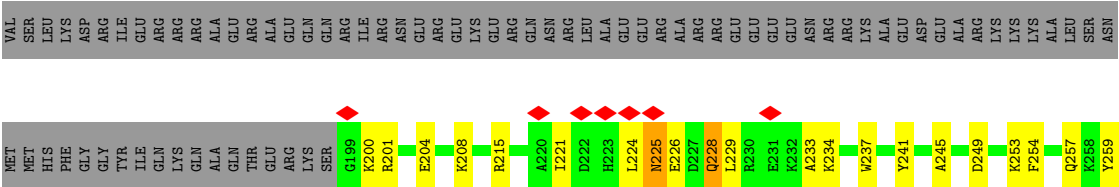
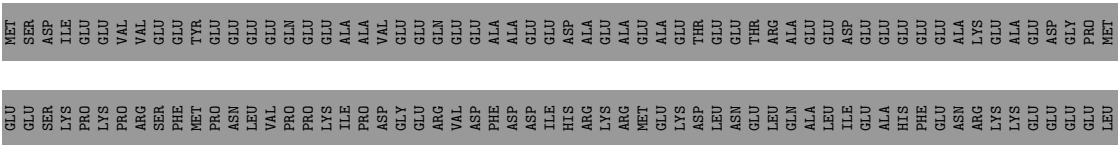




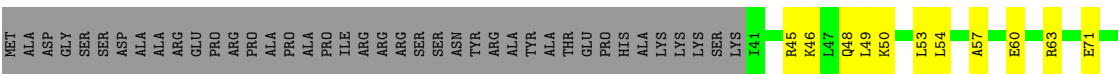
• Molecule 3: Isoform 6 of Troponin T, cardiac muscle



• Molecule 3: Isoform 6 of Troponin T, cardiac muscle



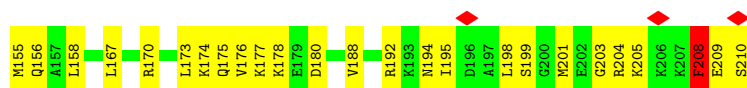
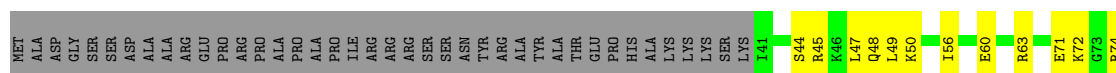
• Molecule 4: Troponin I, cardiac muscle





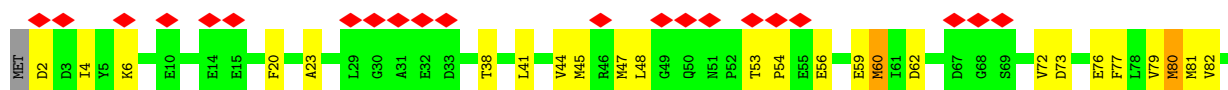
- Molecule 4: Troponin I, cardiac muscle

Chain c: 46% 35% 19%



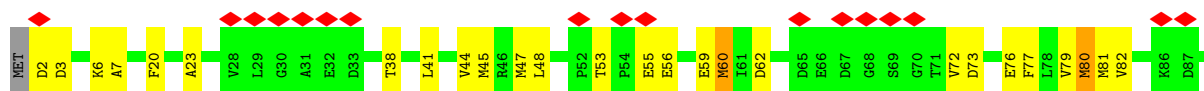
- Molecule 5: Troponin C, slow skeletal and cardiac muscles

Chain U: 17% 68% 30% ..



- Molecule 5: Troponin C, slow skeletal and cardiac muscles

Chain d: 11% 69% 29% ..



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)	700	Depositor
Maximum defocus (nm)	1800	Depositor
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: HIC, ADP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.25	0/2984	0.51	0/4040
1	B	0.28	1/2984 (0.0%)	0.55	0/4040
1	C	0.31	0/2984	0.59	1/4040 (0.0%)
1	D	0.25	1/2984 (0.0%)	0.51	0/4040
1	E	0.27	1/2984 (0.0%)	0.51	0/4040
1	F	0.25	1/2984 (0.0%)	0.51	0/4040
1	G	0.24	0/2984	0.51	0/4040
1	H	0.25	1/2984 (0.0%)	0.51	0/4040
1	I	0.26	1/2984 (0.0%)	0.51	0/4040
1	J	0.26	1/2984 (0.0%)	0.51	0/4040
1	K	0.26	1/2984 (0.0%)	0.51	0/4040
1	L	0.25	1/2984 (0.0%)	0.51	0/4040
1	M	0.25	0/2984	0.53	1/4040 (0.0%)
1	N	0.24	0/2984	0.51	0/4040
1	O	0.26	0/2984	0.52	0/4040
1	P	0.26	0/2984	0.52	0/4040
1	Q	0.25	0/2984	0.51	0/4040
1	R	0.24	0/2984	0.51	0/4040
2	W	0.25	0/520	0.67	0/686
2	Z	0.25	0/520	0.61	0/686
2	a	0.28	0/2082	0.59	1/2776 (0.0%)
2	b	0.21	0/2082	0.46	0/2776
2	g	0.23	0/671	0.61	0/889
2	h	0.23	0/671	0.55	1/889 (0.1%)
2	i	0.29	0/1922	0.61	2/2563 (0.1%)
2	j	0.21	0/1922	0.47	0/2563
3	X	0.36	0/561	0.73	0/739
3	Y	0.28	0/649	0.66	0/861
3	e	0.36	0/561	0.76	0/739
3	f	0.28	0/649	0.69	1/861 (0.1%)
4	V	0.26	0/1384	0.69	3/1840 (0.2%)
4	c	0.24	0/1384	0.68	3/1840 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
5	U	0.25	0/1286	0.59	0/1719
5	d	0.23	0/1286	0.58	0/1719
All	All	0.26	9/71862 (0.0%)	0.54	13/96866 (0.0%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	277	THR	C-O	-7.42	1.15	1.24
1	J	277	THR	C-O	-7.22	1.15	1.24
1	B	277	THR	C-O	-6.06	1.16	1.24
1	L	277	THR	C-O	-6.05	1.17	1.24
1	H	277	THR	C-O	-5.99	1.17	1.24
1	E	277	THR	C-O	-5.96	1.17	1.24
1	I	277	THR	C-O	-5.95	1.17	1.24
1	F	277	THR	C-O	-5.46	1.17	1.24
1	D	277	THR	C-O	-5.45	1.17	1.24

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	111	ASN	N-CA-C	-10.91	95.79	109.64
1	M	348	SER	CB-CA-C	-6.12	101.27	110.88
4	c	208	PHE	N-CA-CB	6.10	119.42	110.57
4	V	208	PHE	N-CA-CB	6.09	119.40	110.57
4	V	209	GLU	CA-C-N	5.98	132.47	121.70
4	V	209	GLU	C-N-CA	5.98	132.47	121.70
4	c	209	GLU	CA-C-N	5.98	132.46	121.70
4	c	209	GLU	C-N-CA	5.98	132.46	121.70
2	i	51	LYS	N-CA-CB	5.96	118.98	110.16
2	i	104	GLU	N-CA-CB	5.85	118.49	110.01
2	a	104	GLU	N-CA-CB	5.82	118.45	110.01
3	f	225	ASN	O-C-N	-5.11	117.03	122.85
2	h	8	MET	N-CA-C	-5.06	105.65	111.07

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2934	2893	2895	135	0
1	B	2934	2893	2895	139	0
1	C	2934	2893	2895	135	0
1	D	2934	2893	2895	148	0
1	E	2934	2893	2895	135	0
1	F	2934	2893	2895	143	0
1	G	2934	2893	2895	137	0
1	H	2934	2893	2895	138	0
1	I	2934	2893	2895	128	0
1	J	2934	2893	2895	138	0
1	K	2934	2893	2895	136	0
1	L	2934	2893	2895	131	0
1	M	2934	2893	2895	142	0
1	N	2934	2893	2895	130	0
1	O	2934	2893	2895	131	0
1	P	2934	2893	2895	138	0
1	Q	2934	2893	2895	136	0
1	R	2934	2893	2895	148	0
2	W	520	541	541	24	0
2	Z	520	541	541	25	0
2	a	2074	2068	2068	91	0
2	b	2074	2068	2068	63	0
2	g	671	687	687	23	0
2	h	671	687	687	27	0
2	i	1914	1908	1908	87	0
2	j	1914	1908	1908	71	0
3	X	559	563	563	20	0
3	Y	643	663	663	29	0
3	e	559	563	563	18	0
3	f	643	663	663	55	0
4	V	1374	1436	1436	80	0
4	c	1374	1436	1436	93	0
5	U	1273	1201	1201	45	0
5	d	1273	1201	1201	41	0
6	A	27	12	12	1	0
6	B	27	12	12	1	0
6	C	27	12	12	1	0
6	D	27	12	12	1	0
6	E	27	12	12	1	0
6	F	27	12	12	1	0
6	G	27	12	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	H	27	12	12	1	0
6	I	27	12	12	1	0
6	J	27	12	12	1	0
6	K	27	12	12	1	0
6	L	27	12	12	1	0
6	M	27	12	12	1	0
6	N	27	12	12	1	0
6	O	27	12	12	1	0
6	P	27	12	12	1	0
6	Q	27	12	12	1	0
6	R	27	12	12	1	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
7	E	1	0	0	0	0
7	F	1	0	0	0	0
7	G	1	0	0	0	0
7	H	1	0	0	0	0
7	I	1	0	0	0	0
7	J	1	0	0	0	0
7	K	1	0	0	0	0
7	L	1	0	0	0	0
7	M	1	0	0	0	0
7	N	1	0	0	0	0
7	O	1	0	0	0	0
7	P	1	0	0	0	0
7	Q	1	0	0	0	0
7	R	1	0	0	0	0
All	All	71372	70424	70460	2948	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 21.

All (2948) 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)
4:V:156:GLN:N	4:V:156:GLN:HE21	1.47	1.12
2:a:281:MET:HE1	2:Z:7:LYS:HG2	1.44	0.99
1:K:44:MET:HE3	1:M:168:GLY:O	1.64	0.98
1:A:43:VAL:HG23	1:C:374:CYS:O	1.65	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:GLY:HA3	1:D:322:PRO:HG2	1.50	0.94
1:N:195:GLU:HB3	1:O:113:LYS:HD2	1.49	0.94
1:G:129:VAL:HG11	1:G:132:MET:HE2	1.51	0.93
1:N:129:VAL:HG11	1:N:132:MET:HE2	1.51	0.93
2:a:280:ASP:HB3	2:W:8:MET:HE1	1.49	0.93
1:P:129:VAL:HG11	1:P:132:MET:HE2	1.51	0.93
1:B:129:VAL:HG11	1:B:132:MET:HE2	1.51	0.93
1:I:129:VAL:HG11	1:I:132:MET:HE2	1.51	0.93
1:L:129:VAL:HG11	1:L:132:MET:HE2	1.51	0.93
1:E:129:VAL:HG11	1:E:132:MET:HE2	1.51	0.93
1:Q:267:ILE:O	1:R:173:HIS:HB3	1.68	0.93
1:R:129:VAL:HG11	1:R:132:MET:HE2	1.51	0.93
1:C:129:VAL:HG11	1:C:132:MET:HE2	1.51	0.92
1:M:129:VAL:HG11	1:M:132:MET:HE2	1.51	0.92
1:K:129:VAL:HG11	1:K:132:MET:HE2	1.51	0.92
1:J:129:VAL:HG11	1:J:132:MET:HE2	1.51	0.92
1:A:129:VAL:HG11	1:A:132:MET:HE2	1.51	0.92
1:H:129:VAL:HG11	1:H:132:MET:HE2	1.51	0.92
1:F:129:VAL:HG11	1:F:132:MET:HE2	1.51	0.91
3:f:233:ALA:HB3	4:c:85:LEU:HD21	1.53	0.91
1:O:129:VAL:HG11	1:O:132:MET:HE2	1.51	0.91
1:D:129:VAL:HG11	1:D:132:MET:HE2	1.51	0.91
1:Q:129:VAL:HG11	1:Q:132:MET:HE2	1.51	0.90
2:i:281:MET:HE3	2:h:4:ILE:HD13	1.53	0.90
1:P:61:LYS:HG2	1:R:167:GLU:HG3	1.52	0.90
4:c:154:MET:HE3	4:c:156:GLN:HB2	1.54	0.89
1:B:244:ASP:O	1:D:322:PRO:HG2	1.74	0.87
4:V:154:MET:HE3	4:V:156:GLN:HB2	1.53	0.87
4:V:156:GLN:N	4:V:156:GLN:NE2	2.24	0.86
5:d:92:LYS:HE2	5:d:158:LYS:HA	1.58	0.85
5:U:92:LYS:HE2	5:U:158:LYS:HA	1.58	0.85
4:V:135:LEU:HA	4:V:138:LYS:HD3	1.58	0.84
4:c:135:LEU:HA	4:c:138:LYS:HD3	1.58	0.83
1:J:95:ARG:HG2	3:Y:265:ARG:HD2	1.61	0.83
1:Q:195:GLU:HA	1:R:112:PRO:HA	1.61	0.83
2:a:280:ASP:HB3	2:W:8:MET:CE	2.09	0.82
4:c:174:LYS:HG3	4:c:178:LYS:HZ3	1.42	0.82
2:b:145:GLU:HG2	2:b:149:LYS:HZ2	1.43	0.81
1:N:180:LEU:HD21	1:N:269:MET:HE3	1.63	0.81
1:Q:180:LEU:HD21	1:Q:269:MET:HE3	1.63	0.81
1:P:180:LEU:HD21	1:P:269:MET:HE3	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:180:LEU:HD21	1:O:269:MET:HE3	1.63	0.81
1:R:180:LEU:HD21	1:R:269:MET:HE3	1.63	0.81
1:C:180:LEU:HD21	1:C:269:MET:HE3	1.63	0.81
1:M:44:MET:HE3	1:O:168:GLY:O	1.79	0.81
1:M:180:LEU:HD21	1:M:269:MET:HE3	1.63	0.81
1:D:180:LEU:HD21	1:D:269:MET:HE3	1.63	0.81
1:E:180:LEU:HD21	1:E:269:MET:HE3	1.63	0.81
1:G:180:LEU:HD21	1:G:269:MET:HE3	1.63	0.81
1:H:180:LEU:HD21	1:H:269:MET:HE3	1.63	0.81
1:J:180:LEU:HD21	1:J:269:MET:HE3	1.63	0.81
1:A:180:LEU:HD21	1:A:269:MET:HE3	1.63	0.81
1:F:180:LEU:HD21	1:F:269:MET:HE3	1.63	0.81
1:I:180:LEU:HD21	1:I:269:MET:HE3	1.63	0.80
2:W:53:THR:HG21	2:Z:53:THR:HB	1.63	0.80
1:B:180:LEU:HD21	1:B:269:MET:HE3	1.63	0.80
1:K:180:LEU:HD21	1:K:269:MET:HE3	1.63	0.80
1:L:180:LEU:HD21	1:L:269:MET:HE3	1.63	0.80
2:h:7:LYS:HZ1	2:h:11:LEU:HD13	1.47	0.79
4:V:174:LYS:HG3	4:V:178:LYS:HZ3	1.46	0.79
2:i:113:LEU:HB2	2:j:112:LYS:HZ2	1.47	0.79
1:L:25:ASP:HA	4:V:145:ARG:HH22	1.46	0.79
2:i:130:ILE:HB	2:j:130:ILE:HD12	1.64	0.79
1:H:312:ARG:HA	1:H:315:LYS:HE2	1.65	0.79
1:J:312:ARG:HA	1:J:315:LYS:HE2	1.65	0.79
1:M:312:ARG:HA	1:M:315:LYS:HE2	1.65	0.78
1:K:312:ARG:HA	1:K:315:LYS:HE2	1.66	0.78
1:L:312:ARG:HA	1:L:315:LYS:HE2	1.65	0.78
1:O:283:MET:HA	1:O:290:ARG:HD3	1.65	0.78
1:A:283:MET:HA	1:A:290:ARG:HD3	1.65	0.78
1:M:283:MET:HA	1:M:290:ARG:HD3	1.65	0.78
1:O:312:ARG:HA	1:O:315:LYS:HE2	1.65	0.78
1:D:195:GLU:HB3	1:E:113:LYS:HD2	1.65	0.78
1:I:312:ARG:HA	1:I:315:LYS:HE2	1.65	0.78
1:N:312:ARG:HA	1:N:315:LYS:HE2	1.66	0.78
1:O:63:GLY:HA3	1:Q:286:ASP:OD2	1.82	0.78
1:K:283:MET:HA	1:K:290:ARG:HD3	1.65	0.78
1:Q:283:MET:HA	1:Q:290:ARG:HD3	1.65	0.78
1:F:312:ARG:HA	1:F:315:LYS:HE2	1.65	0.78
1:L:283:MET:HA	1:L:290:ARG:HD3	1.65	0.78
1:Q:312:ARG:HA	1:Q:315:LYS:HE2	1.66	0.78
1:R:312:ARG:HA	1:R:315:LYS:HE2	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:283:MET:HA	1:I:290:ARG:HD3	1.65	0.78
1:J:47:MET:CB	4:V:138:LYS:HE3	2.14	0.78
4:V:156:GLN:HE21	4:V:156:GLN:H	1.29	0.78
1:P:312:ARG:HA	1:P:315:LYS:HE2	1.65	0.78
1:R:283:MET:HA	1:R:290:ARG:HD3	1.65	0.78
1:R:326:LYS:HD3	2:j:65:LYS:HE2	1.66	0.78
1:C:312:ARG:HA	1:C:315:LYS:HE2	1.66	0.77
1:D:312:ARG:HA	1:D:315:LYS:HE2	1.65	0.77
1:G:312:ARG:HA	1:G:315:LYS:HE2	1.65	0.77
1:N:283:MET:HA	1:N:290:ARG:HD3	1.65	0.77
1:J:283:MET:HA	1:J:290:ARG:HD3	1.65	0.77
1:B:283:MET:HA	1:B:290:ARG:HD3	1.65	0.77
1:H:283:MET:HA	1:H:290:ARG:HD3	1.65	0.77
1:E:312:ARG:HA	1:E:315:LYS:HE2	1.66	0.77
1:A:312:ARG:HA	1:A:315:LYS:HE2	1.65	0.77
1:B:245:GLY:HA3	1:D:322:PRO:CG	2.14	0.77
3:Y:225:ASN:OD1	3:Y:226:GLU:N	2.18	0.77
1:B:312:ARG:HA	1:B:315:LYS:HE2	1.66	0.76
1:P:283:MET:HA	1:P:290:ARG:HD3	1.65	0.76
1:D:283:MET:HA	1:D:290:ARG:HD3	1.65	0.76
1:G:283:MET:HA	1:G:290:ARG:HD3	1.65	0.76
1:F:283:MET:HA	1:F:290:ARG:HD3	1.65	0.76
1:E:283:MET:HA	1:E:290:ARG:HD3	1.65	0.76
1:C:283:MET:HA	1:C:290:ARG:HD3	1.65	0.76
4:V:46:LYS:HD3	5:U:135:GLU:HB3	1.67	0.76
2:i:281:MET:CE	2:h:4:ILE:HD13	2.15	0.76
2:j:145:GLU:HG2	2:j:149:LYS:HZ2	1.51	0.75
3:f:229:LEU:HD12	4:c:90:PHE:CD1	2.21	0.75
4:c:205:LYS:HE2	4:c:210:SER:HB2	1.70	0.74
2:a:284:ILE:HD13	2:Z:7:LYS:HE2	1.68	0.74
2:Z:7:LYS:HZ1	2:Z:11:LEU:HD13	1.53	0.74
4:V:195:ILE:HD12	2:i:105:ARG:HH21	1.53	0.73
1:P:44:MET:HG2	1:R:139:VAL:HG21	1.70	0.72
1:O:218:TYR:HB3	1:O:255:PHE:HB3	1.72	0.72
1:Q:218:TYR:HB3	1:Q:255:PHE:HB3	1.72	0.72
2:i:71:LEU:HD22	2:j:70:LYS:NZ	2.05	0.72
4:V:205:LYS:HE2	4:V:210:SER:HB2	1.70	0.72
1:P:244:ASP:HA	1:R:291:LYS:HB3	1.72	0.71
1:R:218:TYR:HB3	1:R:255:PHE:HB3	1.72	0.71
1:M:218:TYR:HB3	1:M:255:PHE:HB3	1.72	0.71
1:N:218:TYR:HB3	1:N:255:PHE:HB3	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:218:TYR:HB3	1:P:255:PHE:HB3	1.72	0.71
1:B:64:ILE:HD13	1:D:171:LEU:HD21	1.71	0.71
1:E:218:TYR:HB3	1:E:255:PHE:HB3	1.72	0.71
1:B:218:TYR:HB3	1:B:255:PHE:HB3	1.72	0.71
1:K:218:TYR:HB3	1:K:255:PHE:HB3	1.72	0.70
1:L:218:TYR:HB3	1:L:255:PHE:HB3	1.72	0.70
2:b:139:GLU:HB3	4:c:167:LEU:HD11	1.73	0.70
2:j:123:SER:O	2:j:127:MET:HE2	1.92	0.70
2:b:123:SER:O	2:b:127:MET:HE2	1.92	0.70
1:C:218:TYR:HB3	1:C:255:PHE:HB3	1.72	0.70
1:G:218:TYR:HB3	1:G:255:PHE:HB3	1.72	0.70
1:J:218:TYR:HB3	1:J:255:PHE:HB3	1.72	0.70
1:I:218:TYR:HB3	1:I:255:PHE:HB3	1.72	0.70
1:A:365:ALA:HB3	1:A:369:ILE:HB	1.74	0.70
1:D:287:ILE:HD12	1:D:290:ARG:HH21	1.57	0.70
1:F:218:TYR:HB3	1:F:255:PHE:HB3	1.72	0.70
1:H:218:TYR:HB3	1:H:255:PHE:HB3	1.72	0.70
1:M:287:ILE:HD12	1:M:290:ARG:HH21	1.57	0.70
1:B:287:ILE:HD12	1:B:290:ARG:HH21	1.57	0.70
1:D:218:TYR:HB3	1:D:255:PHE:HB3	1.72	0.70
1:K:287:ILE:HD12	1:K:290:ARG:HH21	1.57	0.70
1:O:287:ILE:HD12	1:O:290:ARG:HH21	1.57	0.69
1:Q:287:ILE:HD12	1:Q:290:ARG:HH21	1.57	0.69
1:A:218:TYR:HB3	1:A:255:PHE:HB3	1.72	0.69
1:O:365:ALA:HB3	1:O:369:ILE:HB	1.74	0.69
1:Q:365:ALA:HB3	1:Q:369:ILE:HB	1.74	0.69
2:a:281:MET:HE1	2:Z:7:LYS:CG	2.21	0.69
1:J:287:ILE:HD12	1:J:290:ARG:HH21	1.57	0.69
1:R:365:ALA:HB3	1:R:369:ILE:HB	1.74	0.69
1:H:287:ILE:HD12	1:H:290:ARG:HH21	1.57	0.69
1:N:287:ILE:HD12	1:N:290:ARG:HH21	1.57	0.69
1:P:365:ALA:HB3	1:P:369:ILE:HB	1.74	0.69
3:Y:253:LYS:NZ	4:V:118:VAL:HG11	2.08	0.69
2:j:145:GLU:HG2	2:j:149:LYS:NZ	2.07	0.69
1:A:287:ILE:HD12	1:A:290:ARG:HH21	1.57	0.69
1:C:287:ILE:HD12	1:C:290:ARG:HH21	1.57	0.69
1:E:365:ALA:HB3	1:E:369:ILE:HB	1.74	0.69
1:F:287:ILE:HD12	1:F:290:ARG:HH21	1.57	0.69
1:L:287:ILE:HD12	1:L:290:ARG:HH21	1.57	0.69
2:b:145:GLU:HG2	2:b:149:LYS:NZ	2.07	0.69
1:I:287:ILE:HD12	1:I:290:ARG:HH21	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:365:ALA:HB3	1:N:369:ILE:HB	1.74	0.69
1:P:287:ILE:HD12	1:P:290:ARG:HH21	1.57	0.69
1:R:287:ILE:HD12	1:R:290:ARG:HH21	1.57	0.69
1:A:37:ARG:NH2	1:A:81:ASP:OD1	2.26	0.69
1:A:41:GLN:NE2	1:C:375:PHE:HB2	2.08	0.69
1:G:44:MET:HE3	1:I:168:GLY:O	1.92	0.69
1:L:365:ALA:HB3	1:L:369:ILE:HB	1.74	0.69
1:M:365:ALA:HB3	1:M:369:ILE:HB	1.74	0.69
4:c:175:GLN:HA	4:c:178:LYS:HE2	1.75	0.68
1:G:365:ALA:HB3	1:G:369:ILE:HB	1.74	0.68
2:i:71:LEU:HD22	2:j:70:LYS:HZ3	1.54	0.68
1:B:365:ALA:HB3	1:B:369:ILE:HB	1.74	0.68
1:M:195:GLU:HB3	1:N:113:LYS:HD2	1.73	0.68
2:a:105:ARG:HE	4:c:195:ILE:HD12	1.57	0.68
1:C:365:ALA:HB3	1:C:369:ILE:HB	1.74	0.68
1:D:365:ALA:HB3	1:D:369:ILE:HB	1.74	0.68
1:I:196:ARG:NH2	1:I:249:THR:O	2.27	0.68
1:J:365:ALA:HB3	1:J:369:ILE:HB	1.74	0.68
1:K:196:ARG:NH2	1:K:249:THR:O	2.27	0.68
1:O:196:ARG:NH2	1:O:249:THR:O	2.27	0.68
1:D:196:ARG:NH2	1:D:249:THR:O	2.27	0.68
1:L:196:ARG:NH2	1:L:249:THR:O	2.27	0.68
1:C:196:ARG:NH2	1:C:249:THR:O	2.27	0.68
1:E:287:ILE:HD12	1:E:290:ARG:HH21	1.57	0.68
1:R:196:ARG:NH2	1:R:249:THR:O	2.27	0.68
2:b:114:GLU:CD	4:c:192:ARG:HH12	2.02	0.68
1:E:196:ARG:NH2	1:E:249:THR:O	2.27	0.67
1:G:37:ARG:NH2	1:G:81:ASP:OD1	2.26	0.67
1:G:196:ARG:NH2	1:G:249:THR:O	2.27	0.67
1:G:287:ILE:HD12	1:G:290:ARG:HH21	1.57	0.67
1:K:365:ALA:HB3	1:K:369:ILE:HB	1.74	0.67
1:A:196:ARG:NH2	1:A:249:THR:O	2.27	0.67
1:F:365:ALA:HB3	1:F:369:ILE:HB	1.74	0.67
1:H:196:ARG:NH2	1:H:249:THR:O	2.27	0.67
1:I:365:ALA:HB3	1:I:369:ILE:HB	1.74	0.67
1:N:196:ARG:NH2	1:N:249:THR:O	2.27	0.67
1:P:196:ARG:NH2	1:P:249:THR:O	2.27	0.67
1:C:243:PRO:O	1:E:291:LYS:HD3	1.94	0.67
1:D:219:VAL:HB	1:D:308:GLY:HA3	1.77	0.67
1:M:196:ARG:NH2	1:M:249:THR:O	2.27	0.67
1:B:219:VAL:HB	1:B:308:GLY:HA3	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:VAL:HB	1:C:308:GLY:HA3	1.77	0.67
1:E:219:VAL:HB	1:E:308:GLY:HA3	1.77	0.67
1:H:365:ALA:HB3	1:H:369:ILE:HB	1.74	0.67
1:Q:196:ARG:NH2	1:Q:249:THR:O	2.27	0.67
2:a:272:GLU:O	2:a:276:HIS:ND1	2.28	0.67
1:F:219:VAL:HB	1:F:308:GLY:HA3	1.77	0.67
2:i:272:GLU:O	2:i:276:HIS:ND1	2.28	0.67
1:B:112:PRO:HB2	1:B:115:ASN:HB2	1.77	0.67
1:G:219:VAL:HB	1:G:308:GLY:HA3	1.77	0.67
1:I:112:PRO:HB2	1:I:115:ASN:HB2	1.77	0.67
1:F:44:MET:HE3	1:H:169:TYR:HA	1.76	0.67
1:F:196:ARG:NH2	1:F:249:THR:O	2.27	0.66
1:G:112:PRO:HB2	1:G:115:ASN:HB2	1.77	0.66
1:H:112:PRO:HB2	1:H:115:ASN:HB2	1.77	0.66
1:J:196:ARG:NH2	1:J:249:THR:O	2.27	0.66
1:O:37:ARG:NH1	1:O:52:SER:HA	2.09	0.66
2:a:152:LYS:HD2	4:c:156:GLN:HE21	1.60	0.66
1:O:219:VAL:HB	1:O:308:GLY:HA3	1.77	0.66
4:V:175:GLN:HA	4:V:178:LYS:HE2	1.75	0.66
1:I:219:VAL:HB	1:I:308:GLY:HA3	1.77	0.66
1:N:219:VAL:HB	1:N:308:GLY:HA3	1.77	0.66
1:K:219:VAL:HB	1:K:308:GLY:HA3	1.77	0.66
1:M:112:PRO:HB2	1:M:115:ASN:HB2	1.77	0.66
1:P:112:PRO:HB2	1:P:115:ASN:HB2	1.77	0.66
1:P:219:VAL:HB	1:P:308:GLY:HA3	1.77	0.66
1:R:219:VAL:HB	1:R:308:GLY:HA3	1.77	0.66
1:J:95:ARG:HD2	3:Y:265:ARG:NE	2.10	0.66
1:K:112:PRO:HB2	1:K:115:ASN:HB2	1.77	0.66
1:L:112:PRO:HB2	1:L:115:ASN:HB2	1.77	0.66
1:A:112:PRO:HB2	1:A:115:ASN:HB2	1.77	0.66
1:A:244:ASP:OD2	1:C:287:ILE:HG23	1.94	0.66
1:B:64:ILE:CD1	1:D:171:LEU:HD21	2.25	0.66
1:H:219:VAL:HB	1:H:308:GLY:HA3	1.77	0.66
1:Q:219:VAL:HB	1:Q:308:GLY:HA3	1.77	0.66
1:E:112:PRO:HB2	1:E:115:ASN:HB2	1.77	0.66
1:P:44:MET:CG	1:R:139:VAL:HG21	2.25	0.66
1:M:219:VAL:HB	1:M:308:GLY:HA3	1.77	0.65
2:a:41:ASP:O	2:a:44:VAL:HG22	1.96	0.65
1:J:219:VAL:HB	1:J:308:GLY:HA3	1.77	0.65
1:D:44:MET:HE3	1:F:169:TYR:HA	1.79	0.65
1:D:112:PRO:HB2	1:D:115:ASN:HB2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:112:PRO:HB2	1:O:115:ASN:HB2	1.77	0.65
1:R:112:PRO:HB2	1:R:115:ASN:HB2	1.77	0.65
2:b:99:LEU:O	2:b:103:GLN:HG3	1.97	0.65
4:c:147:VAL:O	5:d:53:THR:HG21	1.97	0.65
1:A:219:VAL:HB	1:A:308:GLY:HA3	1.77	0.65
1:N:112:PRO:HB2	1:N:115:ASN:HB2	1.77	0.65
1:R:162:ASN:ND2	1:R:281:SER:OG	2.30	0.65
1:E:162:ASN:ND2	1:E:281:SER:OG	2.30	0.65
1:N:69:TYR:OH	1:N:206:ARG:NH1	2.30	0.65
1:N:162:ASN:ND2	1:N:281:SER:OG	2.30	0.65
4:V:192:ARG:HD3	2:j:110:LEU:HD21	1.79	0.65
1:H:162:ASN:ND2	1:H:281:SER:OG	2.30	0.65
1:K:69:TYR:OH	1:K:206:ARG:NH1	2.30	0.65
1:L:219:VAL:HB	1:L:308:GLY:HA3	1.77	0.65
1:O:63:GLY:CA	1:Q:286:ASP:OD2	2.45	0.65
1:O:69:TYR:OH	1:O:206:ARG:NH1	2.30	0.65
1:Q:112:PRO:HB2	1:Q:115:ASN:HB2	1.77	0.65
1:Q:162:ASN:ND2	1:Q:281:SER:OG	2.30	0.65
1:F:69:TYR:OH	1:F:206:ARG:NH1	2.30	0.65
1:L:69:TYR:OH	1:L:206:ARG:NH1	2.30	0.65
2:j:99:LEU:O	2:j:103:GLN:HG3	1.97	0.65
1:F:112:PRO:HB2	1:F:115:ASN:HB2	1.77	0.65
1:G:69:TYR:OH	1:G:206:ARG:NH1	2.30	0.65
1:J:69:TYR:OH	1:J:206:ARG:NH1	2.30	0.65
4:c:129:THR:HA	4:c:132:ILE:HD12	1.77	0.65
1:A:69:TYR:OH	1:A:206:ARG:NH1	2.30	0.64
1:A:162:ASN:ND2	1:A:281:SER:OG	2.30	0.64
1:C:37:ARG:NH2	1:C:81:ASP:OD1	2.30	0.64
1:C:69:TYR:OH	1:C:206:ARG:NH1	2.30	0.64
1:M:162:ASN:ND2	1:M:281:SER:OG	2.30	0.64
1:O:162:ASN:ND2	1:O:281:SER:OG	2.30	0.64
1:R:69:TYR:OH	1:R:206:ARG:NH1	2.30	0.64
2:j:101:ARG:HG2	2:j:105:ARG:HE	1.62	0.64
1:D:69:TYR:OH	1:D:206:ARG:NH1	2.30	0.64
1:E:44:MET:HE3	1:G:168:GLY:O	1.97	0.64
1:J:112:PRO:HB2	1:J:115:ASN:HB2	1.77	0.64
2:b:101:ARG:HG2	2:b:105:ARG:HE	1.62	0.64
1:C:162:ASN:ND2	1:C:281:SER:OG	2.30	0.64
1:D:162:ASN:ND2	1:D:281:SER:OG	2.30	0.64
1:F:162:ASN:ND2	1:F:281:SER:OG	2.30	0.64
1:I:162:ASN:ND2	1:I:281:SER:OG	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:162:ASN:ND2	1:L:281:SER:OG	2.30	0.64
1:P:162:ASN:ND2	1:P:281:SER:OG	2.30	0.64
1:B:39:ARG:HD3	1:C:268:GLY:O	1.97	0.64
1:A:131:ALA:HB1	1:A:356:TRP:HB3	1.80	0.64
1:E:328:LYS:HZ3	2:W:20:ASP:HB3	1.62	0.64
1:L:131:ALA:HB1	1:L:356:TRP:HB3	1.80	0.64
1:Q:69:TYR:OH	1:Q:206:ARG:NH1	2.30	0.64
2:a:169:LEU:HD11	2:b:172:ILE:HD12	1.79	0.64
1:G:162:ASN:ND2	1:G:281:SER:OG	2.30	0.64
1:I:69:TYR:OH	1:I:206:ARG:NH1	2.30	0.64
1:J:162:ASN:ND2	1:J:281:SER:OG	2.30	0.64
3:f:215:ARG:HD3	4:c:111:ARG:NH2	2.13	0.64
1:B:69:TYR:OH	1:B:206:ARG:NH1	2.30	0.64
1:H:69:TYR:OH	1:H:206:ARG:NH1	2.30	0.64
1:M:69:TYR:OH	1:M:206:ARG:NH1	2.30	0.64
1:P:69:TYR:OH	1:P:206:ARG:NH1	2.30	0.64
1:P:131:ALA:HB1	1:P:356:TRP:HB3	1.80	0.64
3:f:271:ASN:HB3	4:c:135:LEU:HD22	1.78	0.64
1:A:244:ASP:OD2	1:C:287:ILE:CG2	2.46	0.64
1:K:162:ASN:ND2	1:K:281:SER:OG	2.30	0.64
1:A:64:ILE:HG12	1:C:169:TYR:CG	2.33	0.63
1:B:39:ARG:HD3	1:C:268:GLY:C	2.23	0.63
1:H:44:MET:HE3	1:J:168:GLY:O	1.98	0.63
1:H:131:ALA:HB1	1:H:356:TRP:HB3	1.80	0.63
5:d:104:PHE:HB3	5:d:112:ILE:HG12	1.80	0.63
1:E:69:TYR:OH	1:E:206:ARG:NH1	2.30	0.63
1:Q:131:ALA:HB1	1:Q:356:TRP:HB3	1.80	0.63
1:R:121:GLN:O	1:R:125:GLU:HG3	1.99	0.63
1:B:131:ALA:HB1	1:B:356:TRP:HB3	1.80	0.63
1:B:162:ASN:ND2	1:B:281:SER:OG	2.30	0.63
1:I:131:ALA:HB1	1:I:356:TRP:HB3	1.79	0.63
1:K:131:ALA:HB1	1:K:356:TRP:HB3	1.80	0.63
1:A:121:GLN:O	1:A:125:GLU:HG3	1.99	0.63
1:G:121:GLN:O	1:G:125:GLU:HG3	1.99	0.63
1:P:121:GLN:O	1:P:125:GLU:HG3	1.99	0.63
1:G:131:ALA:HB1	1:G:356:TRP:HB3	1.80	0.63
1:N:121:GLN:O	1:N:125:GLU:HG3	1.99	0.63
1:C:131:ALA:HB1	1:C:356:TRP:HB3	1.80	0.63
2:a:56:GLU:HB2	2:b:57:LEU:HD11	1.81	0.63
2:g:2:ASP:OD2	2:g:6:LYS:NZ	2.32	0.63
3:f:262:ASN:HA	3:f:265:ARG:NE	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:131:ALA:HB1	1:R:356:TRP:HB3	1.80	0.62
2:b:213:LYS:O	2:b:217:LYS:HG2	1.99	0.62
2:W:2:ASP:OD2	2:W:6:LYS:NZ	2.32	0.62
1:A:342:GLY:HA2	1:A:345:ILE:HD12	1.82	0.62
1:F:131:ALA:HB1	1:F:356:TRP:HB3	1.80	0.62
1:M:131:ALA:HB1	1:M:356:TRP:HB3	1.80	0.62
2:a:156:GLU:OE1	2:a:160:ARG:NH1	2.31	0.62
3:Y:270:ASP:OD1	5:U:147:ARG:NH2	2.31	0.62
4:V:103:ARG:HG2	4:V:106:LYS:HZ3	1.64	0.62
1:D:121:GLN:O	1:D:125:GLU:HG3	1.99	0.62
1:D:131:ALA:HB1	1:D:356:TRP:HB3	1.80	0.62
1:E:121:GLN:O	1:E:125:GLU:HG3	1.99	0.62
1:K:121:GLN:O	1:K:125:GLU:HG3	1.99	0.62
1:J:121:GLN:O	1:J:125:GLU:HG3	1.99	0.62
1:L:121:GLN:O	1:L:125:GLU:HG3	1.99	0.62
1:L:342:GLY:HA2	1:L:345:ILE:HD12	1.82	0.62
1:O:131:ALA:HB1	1:O:356:TRP:HB3	1.80	0.62
1:R:28:ARG:NH2	1:R:94:LEU:O	2.33	0.62
1:R:342:GLY:HA2	1:R:345:ILE:HD12	1.82	0.62
3:X:142:ASN:C	3:X:146:LYS:HZ3	2.07	0.62
2:i:112:LYS:HE2	2:j:113:LEU:HD13	1.81	0.62
1:C:121:GLN:O	1:C:125:GLU:HG3	1.99	0.62
1:E:131:ALA:HB1	1:E:356:TRP:HB3	1.80	0.62
1:J:37:ARG:NH2	1:J:81:ASP:OD1	2.32	0.62
1:J:342:GLY:HA2	1:J:345:ILE:HD12	1.82	0.62
1:L:28:ARG:NH2	1:L:94:LEU:O	2.33	0.62
5:U:104:PHE:HB3	5:U:112:ILE:HG12	1.80	0.62
1:E:28:ARG:NH2	1:E:94:LEU:O	2.33	0.62
1:J:28:ARG:NH2	1:J:94:LEU:O	2.33	0.62
1:N:342:GLY:HA2	1:N:345:ILE:HD12	1.81	0.62
2:i:113:LEU:HB2	2:j:112:LYS:NZ	2.14	0.62
2:i:156:GLU:OE1	2:i:160:ARG:NH1	2.31	0.62
1:B:245:GLY:CA	1:D:322:PRO:HG2	2.29	0.62
1:C:28:ARG:NH2	1:C:94:LEU:O	2.33	0.62
1:F:121:GLN:O	1:F:125:GLU:HG3	1.99	0.62
1:G:28:ARG:NH2	1:G:94:LEU:O	2.33	0.62
1:N:28:ARG:NH2	1:N:94:LEU:O	2.33	0.62
1:P:28:ARG:NH2	1:P:94:LEU:O	2.33	0.62
1:P:342:GLY:HA2	1:P:345:ILE:HD12	1.82	0.62
1:A:28:ARG:NH2	1:A:94:LEU:O	2.33	0.62
1:E:342:GLY:HA2	1:E:345:ILE:HD12	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:341:ILE:HD13	3:e:97:LYS:NZ	2.14	0.62
1:H:28:ARG:NH2	1:H:94:LEU:O	2.33	0.62
1:I:121:GLN:O	1:I:125:GLU:HG3	1.99	0.62
1:L:25:ASP:OD2	4:V:148:ARG:N	2.33	0.62
1:N:131:ALA:HB1	1:N:356:TRP:HB3	1.79	0.62
1:R:37:ARG:NH2	1:R:81:ASP:OD1	2.32	0.62
2:j:213:LYS:O	2:j:217:LYS:HG2	1.99	0.62
1:H:342:GLY:HA2	1:H:345:ILE:HD12	1.82	0.62
1:K:64:ILE:HG12	1:M:169:TYR:CE2	2.35	0.62
4:V:192:ARG:HD3	2:j:110:LEU:HD11	1.82	0.62
3:f:229:LEU:HD12	4:c:90:PHE:CE1	2.34	0.62
1:D:44:MET:HE1	1:F:169:TYR:HD1	1.63	0.62
1:I:28:ARG:NH2	1:I:94:LEU:O	2.33	0.62
2:a:281:MET:HA	2:a:284:ILE:HD12	1.82	0.62
1:H:121:GLN:O	1:H:125:GLU:HG3	1.99	0.61
3:Y:262:ASN:HA	3:Y:265:ARG:NE	2.14	0.61
1:A:64:ILE:HG12	1:C:169:TYR:CD2	2.35	0.61
1:Q:28:ARG:NH2	1:Q:94:LEU:O	2.33	0.61
1:M:44:MET:HE3	1:O:169:TYR:HA	1.82	0.61
1:G:342:GLY:HA2	1:G:345:ILE:HD12	1.82	0.61
1:K:28:ARG:NH2	1:K:94:LEU:O	2.33	0.61
1:M:121:GLN:O	1:M:125:GLU:HG3	1.99	0.61
1:O:121:GLN:O	1:O:125:GLU:HG3	1.99	0.61
4:V:129:THR:HG22	4:V:133:PHE:CE2	2.35	0.61
2:g:29:LYS:HZ3	2:h:32:ALA:HB2	1.64	0.61
1:J:131:ALA:HB1	1:J:356:TRP:HB3	1.80	0.61
4:c:78:THR:O	4:c:81:GLN:NE2	2.34	0.61
1:B:342:GLY:HA2	1:B:345:ILE:HD12	1.81	0.61
1:C:342:GLY:HA2	1:C:345:ILE:HD12	1.82	0.61
1:O:28:ARG:NH2	1:O:94:LEU:O	2.33	0.61
1:Q:121:GLN:O	1:Q:125:GLU:HG3	1.99	0.61
1:B:121:GLN:O	1:B:125:GLU:HG3	1.99	0.61
1:F:28:ARG:NH2	1:F:94:LEU:O	2.33	0.61
1:M:28:ARG:NH2	1:M:94:LEU:O	2.33	0.61
1:E:191:LYS:NZ	1:F:173:HIS:HA	2.15	0.61
4:V:78:THR:O	4:V:81:GLN:NE2	2.34	0.61
3:f:268:ILE:HD11	4:c:128:LEU:HB3	1.82	0.61
1:B:28:ARG:NH2	1:B:94:LEU:O	2.33	0.61
1:D:28:ARG:NH2	1:D:94:LEU:O	2.33	0.61
1:D:342:GLY:HA2	1:D:345:ILE:HD12	1.82	0.61
1:F:353:GLN:HA	1:F:356:TRP:CD1	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:44:MET:HE1	1:M:169:TYR:HD1	1.64	0.61
2:a:105:ARG:HB3	4:c:195:ILE:HD11	1.81	0.61
1:C:353:GLN:HA	1:C:356:TRP:CD1	2.36	0.60
1:H:353:GLN:HA	1:H:356:TRP:CD1	2.36	0.60
1:Q:353:GLN:HA	1:Q:356:TRP:CD1	2.37	0.60
2:a:46:LEU:HD21	2:b:46:LEU:HB3	1.84	0.60
2:b:143:ILE:HD11	4:c:167:LEU:HG	1.82	0.60
2:Z:7:LYS:NZ	2:Z:11:LEU:HB2	2.16	0.60
2:i:281:MET:HA	2:i:284:ILE:HD12	1.82	0.60
2:h:7:LYS:NZ	2:h:11:LEU:HB2	2.16	0.60
1:E:353:GLN:HA	1:E:356:TRP:CD1	2.37	0.60
1:F:151:ILE:HD13	1:F:278:THR:HG23	1.84	0.60
1:I:353:GLN:HA	1:I:356:TRP:CD1	2.36	0.60
1:Q:151:ILE:HD13	1:Q:278:THR:HG23	1.84	0.60
2:Z:4:ILE:O	2:Z:7:LYS:HB3	2.02	0.60
3:Y:253:LYS:O	3:Y:257:GLN:HG2	2.01	0.60
3:e:142:ASN:O	3:e:145:GLU:HG2	2.01	0.60
3:f:263:VAL:HG22	5:d:101:PHE:HE2	1.65	0.60
1:J:353:GLN:HA	1:J:356:TRP:CD1	2.36	0.60
1:O:353:GLN:HA	1:O:356:TRP:CD1	2.37	0.60
3:f:253:LYS:O	3:f:257:GLN:HG2	2.01	0.60
1:F:342:GLY:HA2	1:F:345:ILE:HD12	1.82	0.60
1:G:353:GLN:HA	1:G:356:TRP:CD1	2.37	0.60
1:O:342:GLY:HA2	1:O:345:ILE:HD12	1.82	0.60
1:P:353:GLN:HA	1:P:356:TRP:CD1	2.36	0.60
1:A:353:GLN:HA	1:A:356:TRP:CD1	2.37	0.60
1:D:353:GLN:HA	1:D:356:TRP:CD1	2.36	0.60
1:I:362:TYR:OH	3:f:201:ARG:NH2	2.34	0.60
1:L:353:GLN:HA	1:L:356:TRP:CD1	2.36	0.60
1:N:353:GLN:HA	1:N:356:TRP:CD1	2.36	0.60
2:a:29:LYS:HE3	2:a:33:GLU:HG3	1.84	0.60
4:c:156:GLN:OE1	4:c:156:GLN:N	2.35	0.60
1:L:151:ILE:HD13	1:L:278:THR:HG23	1.83	0.60
3:X:142:ASN:O	3:X:145:GLU:HG2	2.01	0.60
1:H:307:PRO:HG3	2:j:241:PHE:HE1	1.67	0.60
1:I:342:GLY:HA2	1:I:345:ILE:HD12	1.82	0.60
1:K:342:GLY:HA2	1:K:345:ILE:HD12	1.82	0.60
1:Q:342:GLY:HA2	1:Q:345:ILE:HD12	1.82	0.60
1:A:43:VAL:HG23	1:C:374:CYS:C	2.27	0.60
1:H:151:ILE:HD13	1:H:278:THR:HG23	1.84	0.60
2:b:126:GLY:O	2:b:130:ILE:HG12	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:i:88:LEU:HD21	2:j:89:ASN:ND2	2.17	0.60
2:i:176:LEU:HD22	2:j:172:ILE:HG23	1.82	0.60
2:h:4:ILE:O	2:h:7:LYS:HB3	2.02	0.60
1:D:151:ILE:HD13	1:D:278:THR:HG23	1.83	0.60
1:J:310:ALA:O	1:J:314:GLN:NE2	2.35	0.60
1:K:151:ILE:HD13	1:K:278:THR:HG23	1.84	0.60
1:Q:310:ALA:O	1:Q:314:GLN:NE2	2.35	0.60
3:f:263:VAL:HG22	5:d:101:PHE:CE2	2.35	0.60
1:H:310:ALA:O	1:H:314:GLN:NE2	2.35	0.60
1:I:310:ALA:O	1:I:314:GLN:NE2	2.35	0.60
1:K:310:ALA:O	1:K:314:GLN:NE2	2.35	0.60
1:K:353:GLN:HA	1:K:356:TRP:CD1	2.36	0.60
1:M:342:GLY:HA2	1:M:345:ILE:HD12	1.82	0.60
1:P:310:ALA:O	1:P:314:GLN:NE2	2.35	0.60
1:R:310:ALA:O	1:R:314:GLN:NE2	2.35	0.60
4:c:103:ARG:HA	4:c:106:LYS:HZ3	1.67	0.60
1:B:353:GLN:HA	1:B:356:TRP:CD1	2.36	0.59
1:M:37:ARG:NH2	1:M:52:SER:HA	2.17	0.59
1:M:353:GLN:HA	1:M:356:TRP:CD1	2.36	0.59
1:A:310:ALA:O	1:A:314:GLN:NE2	2.35	0.59
1:G:310:ALA:O	1:G:314:GLN:NE2	2.35	0.59
1:I:44:MET:CE	1:K:169:TYR:HD1	2.15	0.59
1:M:310:ALA:O	1:M:314:GLN:NE2	2.35	0.59
1:O:151:ILE:HD13	1:O:278:THR:HG23	1.84	0.59
1:E:310:ALA:O	1:E:314:GLN:NE2	2.35	0.59
1:F:310:ALA:O	1:F:314:GLN:NE2	2.35	0.59
1:L:310:ALA:O	1:L:314:GLN:NE2	2.35	0.59
1:R:151:ILE:HD13	1:R:278:THR:HG23	1.84	0.59
1:J:95:ARG:CG	3:Y:265:ARG:HD2	2.31	0.59
1:O:310:ALA:O	1:O:314:GLN:NE2	2.35	0.59
1:H:44:MET:HE1	1:J:169:TYR:CD1	2.37	0.59
1:M:151:ILE:HD13	1:M:278:THR:HG23	1.84	0.59
1:R:353:GLN:HA	1:R:356:TRP:CD1	2.36	0.59
1:J:151:ILE:HD13	1:J:278:THR:HG23	1.84	0.59
1:M:188:TYR:O	1:M:192:ILE:HG12	2.03	0.59
1:Q:142:LEU:HD21	1:Q:148:THR:HA	1.85	0.59
4:V:129:THR:HA	4:V:132:ILE:HD12	1.84	0.59
1:A:43:VAL:CG2	1:C:374:CYS:O	2.47	0.59
1:B:310:ALA:O	1:B:314:GLN:NE2	2.35	0.59
1:F:142:LEU:HD21	1:F:148:THR:HA	1.85	0.59
1:J:188:TYR:O	1:J:192:ILE:HG12	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:j:126:GLY:O	2:j:130:ILE:HG12	2.02	0.59
1:B:188:TYR:O	1:B:192:ILE:HG12	2.03	0.59
1:I:188:TYR:O	1:I:192:ILE:HG12	2.03	0.59
1:N:151:ILE:HD13	1:N:278:THR:HG23	1.83	0.59
1:O:188:TYR:O	1:O:192:ILE:HG12	2.03	0.59
1:Q:188:TYR:O	1:Q:192:ILE:HG12	2.03	0.59
2:a:94:LEU:HD22	4:c:203:GLY:CA	2.33	0.59
1:C:188:TYR:O	1:C:192:ILE:HG12	2.03	0.59
1:D:104:LEU:HD13	1:D:352:PHE:HZ	1.68	0.59
1:D:310:ALA:O	1:D:314:GLN:NE2	2.35	0.59
1:L:188:TYR:O	1:L:192:ILE:HG12	2.03	0.59
1:N:310:ALA:O	1:N:314:GLN:NE2	2.35	0.59
1:O:104:LEU:HD13	1:O:352:PHE:HZ	1.68	0.59
2:a:91:ARG:O	2:a:95:VAL:HG23	2.03	0.59
2:b:119:ALA:O	2:b:122:GLU:HG3	2.03	0.59
1:G:151:ILE:HD13	1:G:278:THR:HG23	1.84	0.59
1:A:104:LEU:HD13	1:A:352:PHE:HZ	1.68	0.58
1:C:151:ILE:HD13	1:C:278:THR:HG23	1.84	0.58
1:C:310:ALA:O	1:C:314:GLN:NE2	2.35	0.58
1:H:188:TYR:O	1:H:192:ILE:HG12	2.03	0.58
1:J:104:LEU:HD13	1:J:352:PHE:HZ	1.68	0.58
1:P:151:ILE:HD13	1:P:278:THR:HG23	1.84	0.58
2:i:91:ARG:O	2:i:95:VAL:HG23	2.03	0.58
5:d:77:PHE:CZ	5:d:81:MET:HE3	2.38	0.58
1:A:142:LEU:HD21	1:A:148:THR:HA	1.85	0.58
1:E:151:ILE:HD13	1:E:278:THR:HG23	1.84	0.58
1:G:188:TYR:O	1:G:192:ILE:HG12	2.03	0.58
1:H:142:LEU:HD21	1:H:148:THR:HA	1.85	0.58
1:I:151:ILE:HD13	1:I:278:THR:HG23	1.83	0.58
1:P:104:LEU:HD13	1:P:352:PHE:HZ	1.68	0.58
1:D:142:LEU:HD21	1:D:148:THR:HA	1.85	0.58
1:E:104:LEU:HD13	1:E:352:PHE:HZ	1.68	0.58
1:E:188:TYR:O	1:E:192:ILE:HG12	2.03	0.58
1:F:188:TYR:O	1:F:192:ILE:HG12	2.03	0.58
1:R:163:VAL:HA	1:R:175:ILE:HG12	1.86	0.58
1:A:151:ILE:HD13	1:A:278:THR:HG23	1.84	0.58
1:H:143:TYR:CE2	1:H:346:LEU:HD21	2.39	0.58
1:N:188:TYR:O	1:N:192:ILE:HG12	2.03	0.58
1:O:143:TYR:CE2	1:O:346:LEU:HD21	2.39	0.58
1:P:163:VAL:HA	1:P:175:ILE:HG12	1.86	0.58
1:Q:143:TYR:CE2	1:Q:346:LEU:HD21	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:188:TYR:O	1:R:192:ILE:HG12	2.03	0.58
2:W:29:LYS:HE2	2:Z:28:ASP:HB3	1.84	0.58
1:I:104:LEU:HD13	1:I:352:PHE:HZ	1.68	0.58
1:I:142:LEU:HD21	1:I:148:THR:HA	1.85	0.58
1:J:143:TYR:CE2	1:J:346:LEU:HD21	2.39	0.58
1:L:163:VAL:HA	1:L:175:ILE:HG12	1.86	0.58
1:M:143:TYR:CE2	1:M:346:LEU:HD21	2.39	0.58
1:N:163:VAL:HA	1:N:175:ILE:HG12	1.86	0.58
1:O:142:LEU:HD21	1:O:148:THR:HA	1.85	0.58
5:U:77:PHE:CZ	5:U:81:MET:HE3	2.38	0.58
1:B:142:LEU:HD21	1:B:148:THR:HA	1.85	0.58
1:B:151:ILE:HD13	1:B:278:THR:HG23	1.84	0.58
1:F:143:TYR:CE2	1:F:346:LEU:HD21	2.39	0.58
1:L:104:LEU:HD13	1:L:352:PHE:HZ	1.68	0.58
1:L:143:TYR:CE2	1:L:346:LEU:HD21	2.39	0.58
2:i:270:ILE:HG21	2:j:267:TYR:HE1	1.69	0.58
1:A:143:TYR:CE2	1:A:346:LEU:HD21	2.39	0.58
1:B:104:LEU:HD13	1:B:352:PHE:HZ	1.68	0.58
1:C:143:TYR:CE2	1:C:346:LEU:HD21	2.39	0.58
1:D:188:TYR:O	1:D:192:ILE:HG12	2.03	0.58
1:G:351:THR:HG22	1:G:354:GLN:HE22	1.69	0.58
1:K:142:LEU:HD21	1:K:148:THR:HA	1.85	0.58
2:h:7:LYS:HE3	2:h:11:LEU:HD22	1.86	0.58
1:A:188:TYR:O	1:A:192:ILE:HG12	2.03	0.58
1:E:143:TYR:CE2	1:E:346:LEU:HD21	2.39	0.58
1:F:37:ARG:NH2	1:F:81:ASP:OD1	2.36	0.58
1:J:142:LEU:HD21	1:J:148:THR:HA	1.85	0.58
1:J:163:VAL:HA	1:J:175:ILE:HG12	1.86	0.58
5:U:41:LEU:O	5:U:44:VAL:HG12	2.04	0.58
1:K:188:TYR:O	1:K:192:ILE:HG12	2.03	0.58
1:P:188:TYR:O	1:P:192:ILE:HG12	2.03	0.58
4:c:129:THR:HG22	4:c:133:PHE:CE2	2.39	0.58
1:A:163:VAL:HA	1:A:175:ILE:HG12	1.85	0.58
1:C:142:LEU:HD21	1:C:148:THR:HA	1.85	0.58
1:D:102:PRO:HB3	1:D:131:ALA:HB3	1.86	0.58
1:E:142:LEU:HD21	1:E:148:THR:HA	1.85	0.58
1:F:104:LEU:HD13	1:F:352:PHE:HZ	1.68	0.58
1:O:102:PRO:HB3	1:O:131:ALA:HB3	1.86	0.58
1:A:207:GLU:HA	1:A:210:ARG:HG2	1.86	0.57
1:K:104:LEU:HD13	1:K:352:PHE:HZ	1.68	0.57
1:M:104:LEU:HD13	1:M:352:PHE:HZ	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:351:THR:HG22	1:P:354:GLN:HE22	1.69	0.57
2:a:94:LEU:HA	2:a:97:GLU:OE2	2.04	0.57
2:i:94:LEU:HA	2:i:97:GLU:OE2	2.04	0.57
2:i:106:LEU:HA	2:j:106:LEU:HD21	1.86	0.57
1:B:63:GLY:CA	1:D:286:ASP:OD2	2.52	0.57
1:G:143:TYR:CE2	1:G:346:LEU:HD21	2.39	0.57
1:I:102:PRO:HB3	1:I:131:ALA:HB3	1.86	0.57
1:K:143:TYR:CE2	1:K:346:LEU:HD21	2.39	0.57
1:Q:195:GLU:CA	1:R:112:PRO:HA	2.31	0.57
1:A:351:THR:HG22	1:A:354:GLN:HE22	1.69	0.57
1:B:102:PRO:HB3	1:B:131:ALA:HB3	1.86	0.57
1:C:104:LEU:HD13	1:C:352:PHE:HZ	1.68	0.57
2:g:29:LYS:NZ	2:h:32:ALA:HB2	2.19	0.57
1:D:207:GLU:HA	1:D:210:ARG:HG2	1.86	0.57
1:F:102:PRO:HB3	1:F:131:ALA:HB3	1.86	0.57
1:M:142:LEU:HD21	1:M:148:THR:HA	1.85	0.57
1:N:104:LEU:HD13	1:N:352:PHE:HZ	1.68	0.57
1:N:143:TYR:CE2	1:N:346:LEU:HD21	2.39	0.57
1:R:104:LEU:HD13	1:R:352:PHE:HZ	1.68	0.57
1:G:142:LEU:HD21	1:G:148:THR:HA	1.85	0.57
1:H:104:LEU:HD13	1:H:352:PHE:HZ	1.68	0.57
1:O:207:GLU:HA	1:O:210:ARG:HG2	1.86	0.57
1:R:143:TYR:CE2	1:R:346:LEU:HD21	2.39	0.57
1:R:351:THR:HG22	1:R:354:GLN:HE22	1.69	0.57
5:U:93:SER:HB3	5:U:96:GLU:OE2	2.05	0.57
1:H:163:VAL:HA	1:H:175:ILE:HG12	1.86	0.57
1:J:102:PRO:HB3	1:J:131:ALA:HB3	1.86	0.57
1:M:102:PRO:HB3	1:M:131:ALA:HB3	1.86	0.57
1:P:207:GLU:HA	1:P:210:ARG:HG2	1.86	0.57
2:i:64:LEU:HD22	2:j:60:TYR:HD1	1.70	0.57
2:j:119:ALA:O	2:j:122:GLU:HG3	2.03	0.57
1:H:313:MET:O	1:H:317:ILE:HG12	2.05	0.57
1:N:142:LEU:HD21	1:N:148:THR:HA	1.85	0.57
1:R:207:GLU:HA	1:R:210:ARG:HG2	1.86	0.57
1:D:163:VAL:HA	1:D:175:ILE:HG12	1.86	0.57
1:E:207:GLU:HA	1:E:210:ARG:HG2	1.86	0.57
1:N:207:GLU:HA	1:N:210:ARG:HG2	1.86	0.57
1:P:143:TYR:CE2	1:P:346:LEU:HD21	2.39	0.57
1:B:143:TYR:CE2	1:B:346:LEU:HD21	2.39	0.57
1:E:313:MET:O	1:E:317:ILE:HG12	2.05	0.57
1:G:313:MET:O	1:G:317:ILE:HG12	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:243:PRO:CB	1:R:291:LYS:HD3	2.35	0.57
1:P:313:MET:O	1:P:317:ILE:HG12	2.05	0.57
1:Q:104:LEU:HD13	1:Q:352:PHE:HZ	1.68	0.57
1:Q:163:VAL:HA	1:Q:175:ILE:HG12	1.86	0.57
1:A:102:PRO:HB3	1:A:131:ALA:HB3	1.87	0.57
1:A:313:MET:O	1:A:317:ILE:HG12	2.05	0.57
1:C:102:PRO:HB3	1:C:131:ALA:HB3	1.87	0.57
1:E:163:VAL:HA	1:E:175:ILE:HG12	1.86	0.57
1:G:104:LEU:HD13	1:G:352:PHE:HZ	1.68	0.57
1:K:313:MET:O	1:K:317:ILE:HG12	2.05	0.57
1:L:142:LEU:HD21	1:L:148:THR:HA	1.85	0.57
1:L:313:MET:O	1:L:317:ILE:HG12	2.05	0.57
1:M:163:VAL:HA	1:M:175:ILE:HG12	1.85	0.57
1:Q:102:PRO:HB3	1:Q:131:ALA:HB3	1.86	0.57
2:a:101:ARG:HA	2:a:104:GLU:OE1	2.04	0.57
2:a:163:GLU:HB3	5:d:55:GLU:OE2	2.05	0.57
3:e:142:ASN:C	3:e:146:LYS:HZ3	2.13	0.57
1:I:143:TYR:CE2	1:I:346:LEU:HD21	2.39	0.56
1:O:163:VAL:HA	1:O:175:ILE:HG12	1.86	0.56
1:R:313:MET:O	1:R:317:ILE:HG12	2.05	0.56
2:b:94:LEU:O	2:b:97:GLU:HG2	2.05	0.56
2:j:94:LEU:O	2:j:97:GLU:HG2	2.05	0.56
4:c:208:PHE:C	4:c:210:SER:H	2.13	0.56
1:C:313:MET:O	1:C:317:ILE:HG12	2.05	0.56
1:G:163:VAL:HA	1:G:175:ILE:HG12	1.85	0.56
1:K:207:GLU:HA	1:K:210:ARG:HG2	1.86	0.56
1:M:313:MET:O	1:M:317:ILE:HG12	2.05	0.56
1:P:142:LEU:HD21	1:P:148:THR:HA	1.85	0.56
1:R:142:LEU:HD21	1:R:148:THR:HA	1.85	0.56
2:a:156:GLU:O	2:a:160:ARG:HD3	2.05	0.56
2:W:8:MET:SD	2:W:9:GLN:NE2	2.75	0.56
2:i:156:GLU:O	2:i:160:ARG:HD3	2.05	0.56
1:A:64:ILE:HG12	1:C:169:TYR:CB	2.35	0.56
1:A:190:MET:HE2	1:A:206:ARG:HG2	1.88	0.56
1:A:191:LYS:O	1:A:195:GLU:HG2	2.06	0.56
1:B:11:ASP:OD1	1:B:106:THR:OG1	2.24	0.56
1:B:163:VAL:HA	1:B:175:ILE:HG12	1.86	0.56
1:B:313:MET:O	1:B:317:ILE:HG12	2.05	0.56
1:C:163:VAL:HA	1:C:175:ILE:HG12	1.86	0.56
1:C:191:LYS:O	1:C:195:GLU:HG2	2.06	0.56
1:E:190:MET:HE2	1:E:206:ARG:HG2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:163:VAL:HA	1:F:175:ILE:HG12	1.86	0.56
1:F:313:MET:O	1:F:317:ILE:HG12	2.05	0.56
1:G:190:MET:HE2	1:G:206:ARG:HG2	1.88	0.56
1:H:102:PRO:HB3	1:H:131:ALA:HB3	1.86	0.56
1:H:207:GLU:HA	1:H:210:ARG:HG2	1.86	0.56
1:K:102:PRO:HB3	1:K:131:ALA:HB3	1.86	0.56
1:K:163:VAL:HA	1:K:175:ILE:HG12	1.86	0.56
1:L:207:GLU:HA	1:L:210:ARG:HG2	1.86	0.56
1:M:345:ILE:HG12	4:c:180:ASP:OD2	2.05	0.56
1:N:191:LYS:O	1:N:195:GLU:HG2	2.06	0.56
1:Q:313:MET:O	1:Q:317:ILE:HG12	2.05	0.56
1:R:191:LYS:O	1:R:195:GLU:HG2	2.06	0.56
2:Z:7:LYS:HE3	2:Z:11:LEU:HD22	1.86	0.56
2:i:101:ARG:HA	2:i:104:GLU:OE1	2.04	0.56
1:C:190:MET:HE2	1:C:206:ARG:HG2	1.88	0.56
1:D:313:MET:O	1:D:317:ILE:HG12	2.05	0.56
1:E:191:LYS:O	1:E:195:GLU:HG2	2.06	0.56
1:G:191:LYS:O	1:G:195:GLU:HG2	2.06	0.56
1:I:163:VAL:HA	1:I:175:ILE:HG12	1.86	0.56
1:I:190:MET:HE2	1:I:206:ARG:HG2	1.88	0.56
1:K:190:MET:HE2	1:K:206:ARG:HG2	1.88	0.56
1:L:11:ASP:OD1	1:L:106:THR:OG1	2.24	0.56
1:M:11:ASP:OD1	1:M:106:THR:OG1	2.24	0.56
1:N:313:MET:O	1:N:317:ILE:HG12	2.05	0.56
1:O:313:MET:O	1:O:317:ILE:HG12	2.05	0.56
3:f:225:ASN:OD1	3:f:226:GLU:N	2.37	0.56
5:d:93:SER:HB3	5:d:96:GLU:OE2	2.05	0.56
1:B:190:MET:HE2	1:B:206:ARG:HG2	1.88	0.56
1:G:11:ASP:OD1	1:G:106:THR:OG1	2.24	0.56
1:M:207:GLU:HA	1:M:210:ARG:HG2	1.86	0.56
1:N:102:PRO:HB3	1:N:131:ALA:HB3	1.87	0.56
1:P:190:MET:HE2	1:P:206:ARG:HG2	1.88	0.56
1:P:191:LYS:O	1:P:195:GLU:HG2	2.06	0.56
1:R:11:ASP:OD1	1:R:106:THR:OG1	2.24	0.56
1:R:190:MET:HE2	1:R:206:ARG:HG2	1.88	0.56
1:F:207:GLU:HA	1:F:210:ARG:HG2	1.86	0.56
1:G:102:PRO:HB3	1:G:131:ALA:HB3	1.86	0.56
1:J:207:GLU:HA	1:J:210:ARG:HG2	1.86	0.56
1:L:191:LYS:O	1:L:195:GLU:HG2	2.06	0.56
3:X:110:PHE:HB3	3:X:114:LYS:HZ3	1.71	0.56
2:i:61:SER:OG	2:i:65:LYS:NZ	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:i:88:LEU:HD11	2:j:85:VAL:HG13	1.88	0.56
5:d:41:LEU:O	5:d:44:VAL:HG12	2.04	0.56
1:F:341:ILE:HD13	3:e:97:LYS:HZ3	1.71	0.56
1:G:207:GLU:HA	1:G:210:ARG:HG2	1.86	0.56
1:I:191:LYS:O	1:I:195:GLU:HG2	2.06	0.56
1:I:207:GLU:HA	1:I:210:ARG:HG2	1.86	0.56
1:K:11:ASP:OD1	1:K:106:THR:OG1	2.24	0.56
1:M:191:LYS:O	1:M:195:GLU:HG2	2.06	0.56
1:O:11:ASP:OD1	1:O:106:THR:OG1	2.24	0.56
2:i:92:ILE:HG21	2:j:88:LEU:HD11	1.88	0.56
2:i:131:GLU:OE2	2:j:130:ILE:HG21	2.06	0.56
1:D:11:ASP:OD1	1:D:106:THR:OG1	2.24	0.56
1:E:102:PRO:HB3	1:E:131:ALA:HB3	1.86	0.56
1:J:191:LYS:O	1:J:195:GLU:HG2	2.06	0.56
1:K:191:LYS:O	1:K:195:GLU:HG2	2.06	0.56
2:a:77:LYS:NZ	2:b:78:ALA:HB3	2.21	0.56
2:Z:7:LYS:HZ1	2:Z:11:LEU:HB2	1.69	0.56
1:F:11:ASP:OD1	1:F:106:THR:OG1	2.24	0.56
1:J:11:ASP:OD1	1:J:106:THR:OG1	2.24	0.56
1:J:82:MET:HA	1:J:85:ILE:HG12	1.88	0.56
1:L:190:MET:HE2	1:L:206:ARG:HG2	1.88	0.56
1:M:37:ARG:CZ	1:M:52:SER:HA	2.36	0.56
1:N:82:MET:HA	1:N:85:ILE:HG12	1.88	0.56
1:N:190:MET:HE2	1:N:206:ARG:HG2	1.88	0.56
1:Q:207:GLU:HA	1:Q:210:ARG:HG2	1.86	0.56
2:b:109:ALA:O	2:b:112:LYS:HG3	2.06	0.56
1:A:203:THR:HA	1:A:206:ARG:HG3	1.88	0.56
1:C:11:ASP:OD1	1:C:106:THR:OG1	2.24	0.56
1:C:82:MET:HA	1:C:85:ILE:HG12	1.88	0.56
1:F:82:MET:HA	1:F:85:ILE:HG12	1.88	0.56
1:I:313:MET:O	1:I:317:ILE:HG12	2.05	0.56
1:M:190:MET:HE2	1:M:206:ARG:HG2	1.88	0.56
1:P:11:ASP:OD1	1:P:106:THR:OG1	2.24	0.56
4:V:90:PHE:HA	4:V:93:LEU:HD12	1.88	0.56
3:e:110:PHE:HB3	3:e:114:LYS:NZ	2.21	0.56
4:c:136:ARG:NH2	5:d:151:ASP:OD2	2.38	0.56
1:C:207:GLU:HA	1:C:210:ARG:HG2	1.86	0.55
1:D:190:MET:CE	1:D:206:ARG:HG2	2.37	0.55
1:L:44:MET:HE3	1:N:168:GLY:O	2.05	0.55
1:L:102:PRO:HB3	1:L:131:ALA:HB3	1.87	0.55
1:O:191:LYS:O	1:O:195:GLU:HG2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:102:PRO:HB3	1:P:131:ALA:HB3	1.86	0.55
1:A:286:ASP:OD1	1:A:289:ILE:HG12	2.07	0.55
1:D:82:MET:HA	1:D:85:ILE:HG12	1.88	0.55
1:E:11:ASP:OD1	1:E:106:THR:OG1	2.24	0.55
1:I:82:MET:HA	1:I:85:ILE:HG12	1.88	0.55
2:j:109:ALA:O	2:j:112:LYS:HG3	2.06	0.55
1:B:286:ASP:OD1	1:B:289:ILE:HG12	2.07	0.55
1:J:313:MET:O	1:J:317:ILE:HG12	2.05	0.55
1:M:286:ASP:OD1	1:M:289:ILE:HG12	2.07	0.55
1:N:11:ASP:OD1	1:N:106:THR:OG1	2.24	0.55
1:O:82:MET:HA	1:O:85:ILE:HG12	1.88	0.55
1:O:190:MET:HE2	1:O:206:ARG:HG2	1.88	0.55
1:Q:190:MET:CE	1:Q:206:ARG:HG2	2.37	0.55
3:Y:253:LYS:HZ3	4:V:118:VAL:HG11	1.70	0.55
1:B:207:GLU:HA	1:B:210:ARG:HG2	1.86	0.55
1:D:25:ASP:OD1	1:D:26:ALA:N	2.40	0.55
1:G:82:MET:HA	1:G:85:ILE:HG12	1.88	0.55
1:L:190:MET:CE	1:L:206:ARG:HG2	2.37	0.55
1:Q:82:MET:HA	1:Q:85:ILE:HG12	1.88	0.55
1:Q:191:LYS:O	1:Q:195:GLU:HG2	2.06	0.55
1:Q:286:ASP:OD1	1:Q:289:ILE:HG12	2.07	0.55
2:i:129:VAL:O	2:i:133:ARG:HG2	2.07	0.55
1:F:190:MET:CE	1:F:206:ARG:HG2	2.36	0.55
1:F:191:LYS:O	1:F:195:GLU:HG2	2.06	0.55
1:H:11:ASP:OD1	1:H:106:THR:OG1	2.24	0.55
1:I:32:PRO:HG2	1:I:59:GLN:NE2	2.22	0.55
1:J:190:MET:HE2	1:J:206:ARG:HG2	1.88	0.55
1:K:286:ASP:OD1	1:K:289:ILE:HG12	2.07	0.55
1:M:25:ASP:OD1	1:M:26:ALA:N	2.40	0.55
1:R:102:PRO:HB3	1:R:131:ALA:HB3	1.86	0.55
2:h:24:GLN:NE2	2:h:28:ASP:OD2	2.40	0.55
4:c:90:PHE:HA	4:c:93:LEU:HD12	1.88	0.55
1:G:286:ASP:OD1	1:G:289:ILE:HG12	2.07	0.55
1:H:190:MET:CE	1:H:206:ARG:HG2	2.37	0.55
1:I:11:ASP:OD1	1:I:106:THR:OG1	2.24	0.55
1:K:25:ASP:OD1	1:K:26:ALA:N	2.40	0.55
2:a:125:ARG:HA	2:a:128:LYS:HZ3	1.71	0.55
2:Z:24:GLN:NE2	2:Z:28:ASP:OD2	2.40	0.55
1:A:190:MET:CE	1:A:206:ARG:HG2	2.36	0.55
1:B:25:ASP:OD1	1:B:26:ALA:N	2.40	0.55
1:G:25:ASP:OD1	1:G:26:ALA:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:190:MET:CE	1:G:206:ARG:HG2	2.36	0.55
1:N:190:MET:CE	1:N:206:ARG:HG2	2.37	0.55
1:P:45:VAL:CG1	1:R:346:LEU:HD22	2.37	0.55
1:Q:32:PRO:HG2	1:Q:59:GLN:NE2	2.22	0.55
1:R:82:MET:HA	1:R:85:ILE:HG12	1.88	0.55
2:g:11:LEU:HB2	2:h:11:LEU:HD21	1.89	0.55
1:A:25:ASP:OD1	1:A:26:ALA:N	2.40	0.55
1:A:32:PRO:HG2	1:A:59:GLN:NE2	2.22	0.55
1:B:190:MET:CE	1:B:206:ARG:HG2	2.36	0.55
1:D:190:MET:HE2	1:D:206:ARG:HG2	1.88	0.55
1:E:25:ASP:OD1	1:E:26:ALA:N	2.40	0.55
1:E:82:MET:HA	1:E:85:ILE:HG12	1.88	0.55
1:E:190:MET:CE	1:E:206:ARG:HG2	2.37	0.55
1:I:190:MET:CE	1:I:206:ARG:HG2	2.36	0.55
1:L:163:VAL:HG12	1:L:175:ILE:HG23	1.89	0.55
1:N:311:ASP:OD1	1:N:312:ARG:N	2.40	0.55
1:O:25:ASP:OD1	1:O:26:ALA:N	2.40	0.55
1:P:185:LEU:HB3	1:P:213:LYS:HE3	1.89	0.55
1:R:190:MET:CE	1:R:206:ARG:HG2	2.36	0.55
2:a:61:SER:OG	2:a:65:LYS:NZ	2.39	0.55
2:a:129:VAL:O	2:a:133:ARG:HG2	2.07	0.55
2:b:46:LEU:HD12	2:b:49:LYS:HE3	1.89	0.55
3:Y:237:TRP:NE1	4:V:80:CYS:SG	2.79	0.55
1:A:163:VAL:HG12	1:A:175:ILE:HG23	1.89	0.55
1:C:190:MET:CE	1:C:206:ARG:HG2	2.37	0.55
1:F:190:MET:HE2	1:F:206:ARG:HG2	1.88	0.55
1:H:191:LYS:O	1:H:195:GLU:HG2	2.06	0.55
1:I:25:ASP:OD1	1:I:26:ALA:N	2.40	0.55
1:J:190:MET:CE	1:J:206:ARG:HG2	2.37	0.55
1:K:32:PRO:HG2	1:K:59:GLN:NE2	2.22	0.55
1:O:32:PRO:HG2	1:O:59:GLN:NE2	2.22	0.55
1:O:190:MET:CE	1:O:206:ARG:HG2	2.36	0.55
1:Q:11:ASP:OD1	1:Q:106:THR:OG1	2.24	0.55
1:Q:190:MET:HE2	1:Q:206:ARG:HG2	1.88	0.55
4:V:57:ALA:HB1	5:U:100:LEU:HD22	1.88	0.55
4:V:130:GLN:HA	4:V:133:PHE:HD2	1.72	0.55
1:A:311:ASP:OD1	1:A:312:ARG:N	2.40	0.55
1:B:82:MET:HA	1:B:85:ILE:HG12	1.88	0.55
1:F:163:VAL:HG12	1:F:175:ILE:HG23	1.89	0.55
1:H:82:MET:HA	1:H:85:ILE:HG12	1.88	0.55
1:H:163:VAL:HG12	1:H:175:ILE:HG23	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:311:ASP:OD1	1:H:312:ARG:N	2.40	0.55
1:I:311:ASP:OD1	1:I:312:ARG:N	2.40	0.55
1:L:185:LEU:HB3	1:L:213:LYS:HE3	1.89	0.55
1:N:185:LEU:HB3	1:N:213:LYS:HE3	1.89	0.55
1:O:286:ASP:OD1	1:O:289:ILE:HG12	2.07	0.55
1:R:32:PRO:HG2	1:R:59:GLN:NE2	2.22	0.55
2:b:250:GLU:HB3	3:X:141:ARG:HH11	1.71	0.55
1:B:32:PRO:HG2	1:B:59:GLN:NE2	2.22	0.54
1:B:63:GLY:HA3	1:D:286:ASP:CG	2.31	0.54
1:C:32:PRO:HG2	1:C:59:GLN:NE2	2.22	0.54
1:D:32:PRO:HG2	1:D:59:GLN:NE2	2.22	0.54
1:Q:25:ASP:OD1	1:Q:26:ALA:N	2.40	0.54
1:R:163:VAL:HG12	1:R:175:ILE:HG23	1.89	0.54
2:a:253:ILE:HG22	2:a:257:GLU:CD	2.33	0.54
2:a:264:LYS:HA	2:a:264:LYS:HE2	1.89	0.54
3:X:110:PHE:HB3	3:X:114:LYS:NZ	2.21	0.54
3:Y:264:LEU:HD22	4:V:132:ILE:HD11	1.88	0.54
4:V:208:PHE:C	4:V:210:SER:H	2.13	0.54
1:C:25:ASP:OD1	1:C:26:ALA:N	2.40	0.54
1:D:286:ASP:OD1	1:D:289:ILE:HG12	2.07	0.54
1:D:311:ASP:OD1	1:D:312:ARG:N	2.40	0.54
1:G:185:LEU:HB3	1:G:213:LYS:HE3	1.89	0.54
1:J:163:VAL:HG12	1:J:175:ILE:HG23	1.89	0.54
1:J:185:LEU:HB3	1:J:213:LYS:HE3	1.89	0.54
1:K:44:MET:CE	1:M:169:TYR:HD1	2.20	0.54
1:K:82:MET:HA	1:K:85:ILE:HG12	1.88	0.54
1:M:311:ASP:OD1	1:M:312:ARG:N	2.40	0.54
1:N:163:VAL:HG12	1:N:175:ILE:HG23	1.89	0.54
1:P:82:MET:HA	1:P:85:ILE:HG12	1.88	0.54
1:R:332:PRO:HB3	2:j:51:LYS:HE2	1.89	0.54
1:A:11:ASP:OD1	1:A:106:THR:OG1	2.24	0.54
1:B:311:ASP:OD1	1:B:312:ARG:N	2.40	0.54
1:C:311:ASP:OD1	1:C:312:ARG:N	2.40	0.54
1:D:163:VAL:HG12	1:D:175:ILE:HG23	1.89	0.54
1:E:163:VAL:HG12	1:E:175:ILE:HG23	1.89	0.54
1:E:185:LEU:HB3	1:E:213:LYS:HE3	1.89	0.54
1:E:286:ASP:OD1	1:E:289:ILE:HG12	2.07	0.54
1:F:25:ASP:OD1	1:F:26:ALA:N	2.40	0.54
1:F:286:ASP:OD1	1:F:289:ILE:HG12	2.07	0.54
1:H:286:ASP:OD1	1:H:289:ILE:HG12	2.07	0.54
1:J:25:ASP:OD1	1:J:26:ALA:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:182:GLY:O	1:J:186:THR:HG23	2.08	0.54
1:J:286:ASP:OD1	1:J:289:ILE:HG12	2.07	0.54
1:M:32:PRO:HG2	1:M:59:GLN:NE2	2.22	0.54
1:M:35:VAL:HG13	1:M:37:ARG:NH2	2.22	0.54
1:P:190:MET:CE	1:P:206:ARG:HG2	2.37	0.54
1:P:287:ILE:HD12	1:P:290:ARG:NH2	2.23	0.54
1:R:185:LEU:HB3	1:R:213:LYS:HE3	1.89	0.54
1:R:287:ILE:HD12	1:R:290:ARG:NH2	2.23	0.54
5:U:45:MET:HA	5:U:48:LEU:HD12	1.89	0.54
1:A:185:LEU:HB3	1:A:213:LYS:HE3	1.89	0.54
1:C:163:VAL:HG12	1:C:175:ILE:HG23	1.89	0.54
1:C:286:ASP:OD1	1:C:289:ILE:HG12	2.07	0.54
1:E:220:ALA:HB2	1:E:255:PHE:HB2	1.90	0.54
1:H:25:ASP:OD1	1:H:26:ALA:N	2.40	0.54
1:H:190:MET:HE2	1:H:206:ARG:HG2	1.88	0.54
1:M:82:MET:HA	1:M:85:ILE:HG12	1.88	0.54
1:O:311:ASP:OD1	1:O:312:ARG:N	2.40	0.54
1:P:25:ASP:OD1	1:P:26:ALA:N	2.40	0.54
1:P:163:VAL:HG12	1:P:175:ILE:HG23	1.89	0.54
1:P:286:ASP:OD1	1:P:289:ILE:HG12	2.07	0.54
1:A:182:GLY:O	1:A:186:THR:HG23	2.08	0.54
1:D:37:ARG:NH1	1:D:51:ASP:OD2	2.41	0.54
1:D:191:LYS:O	1:D:195:GLU:HG2	2.06	0.54
1:F:32:PRO:HG2	1:F:59:GLN:NE2	2.22	0.54
1:G:32:PRO:HG2	1:G:59:GLN:NE2	2.22	0.54
1:I:286:ASP:OD1	1:I:289:ILE:HG12	2.07	0.54
1:K:190:MET:CE	1:K:206:ARG:HG2	2.36	0.54
1:K:220:ALA:HB2	1:K:255:PHE:HB2	1.90	0.54
1:K:311:ASP:OD1	1:K:312:ARG:N	2.40	0.54
1:L:286:ASP:OD1	1:L:289:ILE:HG12	2.07	0.54
1:M:190:MET:CE	1:M:206:ARG:HG2	2.37	0.54
1:P:220:ALA:HB2	1:P:255:PHE:HB2	1.90	0.54
1:R:311:ASP:OD1	1:R:312:ARG:N	2.40	0.54
3:Y:241:TYR:CZ	4:V:76:LEU:HD13	2.43	0.54
4:c:130:GLN:HA	4:c:133:PHE:HD2	1.72	0.54
1:C:18:LYS:HG2	1:C:30:VAL:HG13	1.90	0.54
1:E:32:PRO:HG2	1:E:59:GLN:NE2	2.22	0.54
1:F:44:MET:HE3	1:H:168:GLY:O	2.07	0.54
1:G:163:VAL:HG12	1:G:175:ILE:HG23	1.89	0.54
1:H:32:PRO:HG2	1:H:59:GLN:NE2	2.22	0.54
1:H:185:LEU:HB3	1:H:213:LYS:HE3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:185:LEU:HB3	1:I:213:LYS:HE3	1.89	0.54
1:L:182:GLY:O	1:L:186:THR:HG23	2.08	0.54
1:L:311:ASP:OD1	1:L:312:ARG:N	2.40	0.54
1:P:18:LYS:HG2	1:P:30:VAL:HG13	1.90	0.54
1:Q:163:VAL:HG12	1:Q:175:ILE:HG23	1.89	0.54
1:A:287:ILE:HD12	1:A:290:ARG:NH2	2.23	0.54
1:B:40:HIS:CE1	1:C:268:GLY:HA3	2.42	0.54
1:B:182:GLY:O	1:B:186:THR:HG23	2.08	0.54
1:C:185:LEU:HB3	1:C:213:LYS:HE3	1.89	0.54
1:G:18:LYS:HG2	1:G:30:VAL:HG13	1.90	0.54
1:H:182:GLY:O	1:H:186:THR:HG23	2.08	0.54
1:L:82:MET:HA	1:L:85:ILE:HG12	1.88	0.54
1:N:25:ASP:OD1	1:N:26:ALA:N	2.40	0.54
1:R:25:ASP:OD1	1:R:26:ALA:N	2.40	0.54
2:a:245:SER:OG	3:X:144:ARG:NH1	2.41	0.54
1:A:18:LYS:HG2	1:A:30:VAL:HG13	1.90	0.54
1:A:82:MET:HA	1:A:85:ILE:HG12	1.88	0.54
1:F:56:ASP:N	1:F:56:ASP:OD1	2.41	0.54
1:J:56:ASP:OD1	1:J:56:ASP:N	2.41	0.54
1:O:264:PRO:HB3	1:O:269:MET:HE2	1.90	0.54
1:P:182:GLY:O	1:P:186:THR:HG23	2.08	0.54
2:i:164:GLU:OE2	2:i:167:ARG:NH2	2.41	0.54
5:d:45:MET:HA	5:d:48:LEU:HD12	1.89	0.54
1:A:56:ASP:OD1	1:A:56:ASP:N	2.41	0.54
1:B:185:LEU:HB3	1:B:213:LYS:HE3	1.89	0.54
1:D:264:PRO:HB3	1:D:269:MET:HE2	1.90	0.54
1:G:311:ASP:OD1	1:G:312:ARG:N	2.40	0.54
1:I:18:LYS:HG2	1:I:30:VAL:HG13	1.90	0.54
1:K:182:GLY:O	1:K:186:THR:HG23	2.08	0.54
1:L:32:PRO:HG2	1:L:59:GLN:NE2	2.22	0.54
1:M:163:VAL:HG12	1:M:175:ILE:HG23	1.89	0.54
1:N:32:PRO:HG2	1:N:59:GLN:NE2	2.22	0.54
1:O:163:VAL:HG12	1:O:175:ILE:HG23	1.89	0.54
1:R:286:ASP:OD1	1:R:289:ILE:HG12	2.07	0.54
2:b:278:LEU:O	2:b:282:THR:HG23	2.08	0.54
1:J:32:PRO:HG2	1:J:59:GLN:NE2	2.22	0.54
1:M:18:LYS:HG2	1:M:30:VAL:HG13	1.90	0.54
1:N:220:ALA:HB2	1:N:255:PHE:HB2	1.90	0.54
1:N:286:ASP:OD1	1:N:289:ILE:HG12	2.07	0.54
1:P:311:ASP:OD1	1:P:312:ARG:N	2.40	0.54
1:Q:56:ASP:N	1:Q:56:ASP:OD1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:182:GLY:O	1:R:186:THR:HG23	2.08	0.54
2:i:253:ILE:HG22	2:i:257:GLU:CD	2.32	0.54
5:d:23:ALA:HB1	5:d:47:MET:HE2	1.90	0.54
1:C:203:THR:HA	1:C:206:ARG:HG3	1.91	0.53
1:E:311:ASP:OD1	1:E:312:ARG:N	2.40	0.53
1:F:264:PRO:HB3	1:F:269:MET:HE2	1.90	0.53
1:F:311:ASP:OD1	1:F:312:ARG:N	2.40	0.53
1:G:203:THR:HA	1:G:206:ARG:HG3	1.90	0.53
1:G:287:ILE:HD12	1:G:290:ARG:NH2	2.23	0.53
1:J:18:LYS:HG2	1:J:30:VAL:HG13	1.90	0.53
1:J:148:THR:HB	1:J:168:GLY:N	2.23	0.53
1:J:220:ALA:HB2	1:J:255:PHE:HB2	1.90	0.53
1:J:311:ASP:OD1	1:J:312:ARG:N	2.40	0.53
1:L:25:ASP:OD1	1:L:26:ALA:N	2.40	0.53
1:M:264:PRO:HB3	1:M:269:MET:HE2	1.90	0.53
1:Q:264:PRO:HB3	1:Q:269:MET:HE2	1.90	0.53
1:Q:311:ASP:OD1	1:Q:312:ARG:N	2.40	0.53
1:R:56:ASP:OD1	1:R:56:ASP:N	2.41	0.53
2:i:207:LEU:HD21	2:j:204:LEU:HG	1.89	0.53
1:A:220:ALA:HB2	1:A:255:PHE:HB2	1.90	0.53
1:B:220:ALA:HB2	1:B:255:PHE:HB2	1.90	0.53
1:F:148:THR:HB	1:F:168:GLY:N	2.24	0.53
1:N:203:THR:HA	1:N:206:ARG:HG3	1.91	0.53
1:P:32:PRO:HG2	1:P:59:GLN:NE2	2.22	0.53
1:P:64:ILE:HD13	1:R:166:TYR:HB3	1.90	0.53
5:d:76:GLU:HA	5:d:79:VAL:HG22	1.90	0.53
1:B:203:THR:HA	1:B:206:ARG:HG3	1.91	0.53
1:G:220:ALA:HB2	1:G:255:PHE:HB2	1.90	0.53
1:H:148:THR:HB	1:H:168:GLY:N	2.24	0.53
1:I:203:THR:HA	1:I:206:ARG:HG3	1.91	0.53
1:K:163:VAL:HG12	1:K:175:ILE:HG23	1.89	0.53
1:K:203:THR:HA	1:K:206:ARG:HG3	1.91	0.53
1:L:18:LYS:HG2	1:L:30:VAL:HG13	1.90	0.53
1:N:18:LYS:HG2	1:N:30:VAL:HG13	1.90	0.53
1:O:182:GLY:O	1:O:186:THR:HG23	2.08	0.53
1:P:148:THR:HB	1:P:168:GLY:N	2.24	0.53
1:P:203:THR:HA	1:P:206:ARG:HG3	1.91	0.53
1:Q:267:ILE:O	1:R:173:HIS:CB	2.50	0.53
2:b:103:GLN:OE1	4:c:199:SER:HB2	2.08	0.53
3:Y:241:TYR:CE1	4:V:76:LEU:HD22	2.43	0.53
2:j:278:LEU:O	2:j:282:THR:HG23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:148:THR:HB	1:D:168:GLY:N	2.24	0.53
1:M:203:THR:HA	1:M:206:ARG:HG3	1.90	0.53
1:N:56:ASP:N	1:N:56:ASP:OD1	2.41	0.53
1:R:203:THR:HA	1:R:206:ARG:HG3	1.91	0.53
2:i:177:GLU:O	2:i:180:GLU:HG3	2.09	0.53
1:C:182:GLY:O	1:C:186:THR:HG23	2.08	0.53
1:D:37:ARG:HH12	1:D:84:LYS:HE3	1.74	0.53
1:F:185:LEU:HB3	1:F:213:LYS:HE3	1.89	0.53
1:M:220:ALA:HB2	1:M:255:PHE:HB2	1.90	0.53
1:N:148:THR:HB	1:N:168:GLY:N	2.24	0.53
1:N:182:GLY:O	1:N:186:THR:HG23	2.08	0.53
1:E:182:GLY:O	1:E:186:THR:HG23	2.08	0.53
1:E:203:THR:HA	1:E:206:ARG:HG3	1.91	0.53
1:G:182:GLY:O	1:G:186:THR:HG23	2.08	0.53
1:I:220:ALA:HB2	1:I:255:PHE:HB2	1.90	0.53
1:K:185:LEU:HB3	1:K:213:LYS:HE3	1.90	0.53
1:L:203:THR:HA	1:L:206:ARG:HG3	1.91	0.53
1:M:185:LEU:HB3	1:M:213:LYS:HE3	1.89	0.53
1:Q:220:ALA:HB2	1:Q:255:PHE:HB2	1.90	0.53
1:R:193:LEU:HG	1:R:198:TYR:HB2	1.91	0.53
5:U:76:GLU:HA	5:U:79:VAL:HG22	1.90	0.53
1:B:163:VAL:HG12	1:B:175:ILE:HG23	1.89	0.53
1:C:264:PRO:HB3	1:C:269:MET:HE2	1.90	0.53
1:H:307:PRO:HG3	2:j:241:PHE:CE1	2.44	0.53
1:K:18:LYS:HG2	1:K:30:VAL:HG13	1.90	0.53
1:K:148:THR:HB	1:K:168:GLY:N	2.24	0.53
1:L:220:ALA:HB2	1:L:255:PHE:HB2	1.90	0.53
1:R:220:ALA:HB2	1:R:255:PHE:HB2	1.90	0.53
2:i:125:ARG:HA	2:i:128:LYS:NZ	2.24	0.53
1:B:18:LYS:HG2	1:B:30:VAL:HG13	1.90	0.53
1:C:148:THR:HB	1:C:168:GLY:N	2.24	0.53
1:E:193:LEU:HG	1:E:198:TYR:HB2	1.91	0.53
1:E:287:ILE:HD12	1:E:290:ARG:NH2	2.23	0.53
1:F:182:GLY:O	1:F:186:THR:HG23	2.08	0.53
1:I:56:ASP:N	1:I:56:ASP:OD1	2.41	0.53
1:I:163:VAL:HG12	1:I:175:ILE:HG23	1.90	0.53
1:M:148:THR:HB	1:M:168:GLY:N	2.24	0.53
1:O:185:LEU:HB3	1:O:213:LYS:HE3	1.89	0.53
1:Q:18:LYS:HG2	1:Q:30:VAL:HG13	1.90	0.53
1:Q:185:LEU:HB3	1:Q:213:LYS:HE3	1.89	0.53
1:Q:203:THR:HA	1:Q:206:ARG:HG3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:125:ARG:HA	2:a:128:LYS:NZ	2.23	0.53
2:a:177:GLU:O	2:a:180:GLU:HG3	2.09	0.53
2:b:109:ALA:O	2:b:113:LEU:HG	2.09	0.53
2:g:53:THR:HG23	2:h:57:LEU:HD11	1.91	0.53
3:f:241:TYR:HD1	4:c:80:CYS:HB3	1.72	0.53
1:D:185:LEU:HB3	1:D:213:LYS:HE3	1.89	0.53
1:D:203:THR:HA	1:D:206:ARG:HG3	1.91	0.53
1:F:79:TRP:HZ2	1:F:118:LYS:HE2	1.74	0.53
1:H:203:THR:HA	1:H:206:ARG:HG3	1.91	0.53
1:I:148:THR:HB	1:I:168:GLY:N	2.24	0.53
1:J:203:THR:HA	1:J:206:ARG:HG3	1.91	0.53
1:N:193:LEU:HG	1:N:198:TYR:HB2	1.91	0.53
1:Q:79:TRP:HZ2	1:Q:118:LYS:HE2	1.74	0.53
1:Q:287:ILE:HD12	1:Q:290:ARG:NH2	2.23	0.53
1:R:18:LYS:HG2	1:R:30:VAL:HG13	1.90	0.53
2:b:257:GLU:HB2	3:X:134:ARG:HH21	1.74	0.53
1:D:182:GLY:O	1:D:186:THR:HG23	2.08	0.53
1:F:220:ALA:HB2	1:F:255:PHE:HB2	1.90	0.53
1:H:79:TRP:HZ2	1:H:118:LYS:HE2	1.74	0.53
1:K:264:PRO:HB3	1:K:269:MET:HE2	1.90	0.53
1:L:79:TRP:HZ2	1:L:118:LYS:HE2	1.74	0.53
1:L:148:THR:HB	1:L:168:GLY:N	2.24	0.53
1:L:193:LEU:HG	1:L:198:TYR:HB2	1.91	0.53
1:M:182:GLY:O	1:M:186:THR:HG23	2.08	0.53
1:N:287:ILE:HD12	1:N:290:ARG:NH2	2.23	0.53
1:O:203:THR:HA	1:O:206:ARG:HG3	1.91	0.53
2:a:277:ALA:HA	2:a:280:ASP:OD2	2.09	0.53
2:i:277:ALA:HA	2:i:280:ASP:OD2	2.09	0.53
1:B:56:ASP:OD1	1:B:56:ASP:N	2.41	0.52
1:C:220:ALA:HB2	1:C:255:PHE:HB2	1.90	0.52
1:D:18:LYS:HG2	1:D:30:VAL:HG13	1.90	0.52
1:E:79:TRP:HZ2	1:E:118:LYS:HE2	1.74	0.52
1:F:18:LYS:HG2	1:F:30:VAL:HG13	1.90	0.52
1:H:193:LEU:HG	1:H:198:TYR:HB2	1.91	0.52
1:J:79:TRP:HZ2	1:J:118:LYS:HE2	1.74	0.52
1:K:56:ASP:N	1:K:56:ASP:OD1	2.41	0.52
1:N:79:TRP:HZ2	1:N:118:LYS:HE2	1.74	0.52
1:P:79:TRP:HZ2	1:P:118:LYS:HE2	1.74	0.52
1:Q:182:GLY:O	1:Q:186:THR:HG23	2.08	0.52
1:D:287:ILE:HD12	1:D:290:ARG:NH2	2.23	0.52
1:F:287:ILE:HD12	1:F:290:ARG:NH2	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:148:THR:HB	1:G:168:GLY:N	2.24	0.52
1:G:264:PRO:HB3	1:G:269:MET:HE2	1.90	0.52
1:I:182:GLY:O	1:I:186:THR:HG23	2.08	0.52
1:I:264:PRO:HB3	1:I:269:MET:HE2	1.90	0.52
2:j:109:ALA:O	2:j:113:LEU:HG	2.09	0.52
2:g:53:THR:HG21	2:h:53:THR:HB	1.90	0.52
1:A:148:THR:HB	1:A:168:GLY:N	2.24	0.52
1:A:226:GLU:HA	1:A:229:THR:HG22	1.92	0.52
1:B:148:THR:HB	1:B:168:GLY:N	2.24	0.52
1:B:193:LEU:HG	1:B:198:TYR:HB2	1.91	0.52
1:D:220:ALA:HB2	1:D:255:PHE:HB2	1.90	0.52
1:E:148:THR:HB	1:E:168:GLY:N	2.23	0.52
1:G:79:TRP:HZ2	1:G:118:LYS:HE2	1.74	0.52
1:H:18:LYS:HG2	1:H:30:VAL:HG13	1.90	0.52
1:H:264:PRO:HB3	1:H:269:MET:HE2	1.90	0.52
1:J:241:GLU:OE2	1:J:245:GLY:HA2	2.10	0.52
1:O:18:LYS:HG2	1:O:30:VAL:HG13	1.90	0.52
1:O:220:ALA:HB2	1:O:255:PHE:HB2	1.90	0.52
1:P:226:GLU:HA	1:P:229:THR:HG22	1.92	0.52
1:R:79:TRP:HZ2	1:R:118:LYS:HE2	1.74	0.52
4:V:204:ARG:HH22	4:V:208:PHE:HD1	1.57	0.52
1:A:9:VAL:O	1:A:340:TRP:NE1	2.43	0.52
1:B:241:GLU:OE2	1:B:245:GLY:HA2	2.10	0.52
1:B:264:PRO:HB3	1:B:269:MET:HE2	1.90	0.52
1:E:18:LYS:HG2	1:E:30:VAL:HG13	1.90	0.52
1:E:56:ASP:OD1	1:E:56:ASP:N	2.41	0.52
1:E:264:PRO:HB3	1:E:269:MET:HE2	1.90	0.52
1:G:56:ASP:OD1	1:G:56:ASP:N	2.41	0.52
1:O:287:ILE:HD12	1:O:290:ARG:NH2	2.23	0.52
2:a:164:GLU:OE2	2:a:167:ARG:NH2	2.41	0.52
1:A:79:TRP:HZ2	1:A:118:LYS:HE2	1.74	0.52
1:F:203:THR:HA	1:F:206:ARG:HG3	1.91	0.52
1:G:226:GLU:HA	1:G:229:THR:HG22	1.92	0.52
1:H:220:ALA:HB2	1:H:255:PHE:HB2	1.90	0.52
1:H:241:GLU:OE2	1:H:245:GLY:HA2	2.10	0.52
1:I:193:LEU:HG	1:I:198:TYR:HB2	1.91	0.52
1:K:193:LEU:HG	1:K:198:TYR:HB2	1.91	0.52
1:L:349:LEU:HD22	4:V:141:ARG:HH11	1.73	0.52
1:M:241:GLU:OE2	1:M:245:GLY:HA2	2.10	0.52
1:O:103:THR:HB	1:O:132:MET:HE1	1.92	0.52
1:Q:148:THR:HB	1:Q:168:GLY:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:241:GLU:OE2	1:Q:245:GLY:HA2	2.10	0.52
1:R:226:GLU:HA	1:R:229:THR:HG22	1.92	0.52
1:R:241:GLU:OE2	1:R:245:GLY:HA2	2.10	0.52
5:U:23:ALA:HB1	5:U:47:MET:HE2	1.90	0.52
1:L:226:GLU:HA	1:L:229:THR:HG22	1.92	0.52
1:M:103:THR:HB	1:M:132:MET:HE1	1.92	0.52
1:Q:103:THR:HB	1:Q:132:MET:HE1	1.92	0.52
1:R:264:PRO:HB3	1:R:269:MET:HE2	1.90	0.52
3:Y:264:LEU:HD22	4:V:132:ILE:CD1	2.40	0.52
2:g:8:MET:SD	2:g:9:GLN:NE2	2.75	0.52
2:g:46:LEU:HG	2:h:50:LEU:HD22	1.91	0.52
1:C:226:GLU:HA	1:C:229:THR:HG22	1.92	0.52
1:G:193:LEU:HG	1:G:198:TYR:HB2	1.91	0.52
1:G:241:GLU:OE2	1:G:245:GLY:HA2	2.10	0.52
1:O:79:TRP:HZ2	1:O:118:LYS:HE2	1.74	0.52
1:O:148:THR:HB	1:O:168:GLY:N	2.24	0.52
1:P:56:ASP:OD1	1:P:56:ASP:N	2.41	0.52
2:b:104:GLU:O	2:b:108:THR:HG23	2.09	0.52
2:j:66:ASP:O	2:j:70:LYS:HG2	2.10	0.52
1:C:56:ASP:N	1:C:56:ASP:OD1	2.41	0.52
1:C:241:GLU:OE2	1:C:245:GLY:HA2	2.10	0.52
1:E:226:GLU:HA	1:E:229:THR:HG22	1.92	0.52
1:H:56:ASP:OD1	1:H:56:ASP:N	2.41	0.52
1:I:241:GLU:OE2	1:I:245:GLY:HA2	2.10	0.52
1:J:50:LYS:HE2	1:J:53:TYR:HE1	1.75	0.52
1:K:103:THR:HB	1:K:132:MET:HE1	1.92	0.52
1:K:287:ILE:HD12	1:K:290:ARG:NH2	2.23	0.52
1:L:241:GLU:OE2	1:L:245:GLY:HA2	2.10	0.52
1:M:178:LEU:HD22	1:M:277:THR:HG21	1.92	0.52
1:Q:50:LYS:HE2	1:Q:53:TYR:HE1	1.75	0.52
1:D:50:LYS:HE2	1:D:53:TYR:HE1	1.75	0.52
1:I:103:THR:HB	1:I:132:MET:HE1	1.92	0.52
1:I:226:GLU:HA	1:I:229:THR:HG22	1.92	0.52
1:J:47:MET:HB2	4:V:138:LYS:HE3	1.92	0.52
1:J:226:GLU:HA	1:J:229:THR:HG22	1.92	0.52
1:N:226:GLU:HA	1:N:229:THR:HG22	1.92	0.52
1:P:193:LEU:HG	1:P:198:TYR:HB2	1.91	0.52
3:f:260:GLU:O	3:f:264:LEU:HG	2.10	0.52
1:C:193:LEU:HG	1:C:198:TYR:HB2	1.91	0.52
1:H:50:LYS:HE2	1:H:53:TYR:HE1	1.75	0.52
1:J:193:LEU:HG	1:J:198:TYR:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:264:PRO:HB3	1:J:269:MET:HE2	1.90	0.52
1:K:50:LYS:HE2	1:K:53:TYR:HE1	1.75	0.52
1:K:241:GLU:OE2	1:K:245:GLY:HA2	2.10	0.52
1:P:264:PRO:HB3	1:P:269:MET:HE2	1.90	0.52
3:Y:269:ASN:OD1	3:Y:270:ASP:N	2.43	0.52
2:i:270:ILE:HG21	2:j:267:TYR:CE1	2.45	0.52
4:c:204:ARG:HH22	4:c:208:PHE:HD1	1.57	0.52
1:A:264:PRO:HB3	1:A:269:MET:HE2	1.90	0.51
1:B:226:GLU:HA	1:B:229:THR:HG22	1.92	0.51
1:C:244:ASP:HA	1:E:291:LYS:HB3	1.91	0.51
1:D:79:TRP:HZ2	1:D:118:LYS:HE2	1.74	0.51
1:D:193:LEU:HG	1:D:198:TYR:HB2	1.91	0.51
1:E:328:LYS:NZ	2:W:20:ASP:HB3	2.25	0.51
1:F:50:LYS:HE2	1:F:53:TYR:HE1	1.75	0.51
1:F:241:GLU:OE2	1:F:245:GLY:HA2	2.10	0.51
1:H:37:ARG:NH1	1:H:51:ASP:OD2	2.43	0.51
1:L:50:LYS:HE2	1:L:53:TYR:HE1	1.75	0.51
1:L:287:ILE:HD12	1:L:290:ARG:NH2	2.23	0.51
1:M:50:LYS:HE2	1:M:53:TYR:HE1	1.75	0.51
1:P:241:GLU:OE2	1:P:245:GLY:HA2	2.10	0.51
3:f:269:ASN:OD1	3:f:270:ASP:N	2.43	0.51
1:I:79:TRP:HZ2	1:I:118:LYS:HE2	1.74	0.51
1:L:56:ASP:N	1:L:56:ASP:OD1	2.41	0.51
1:L:264:PRO:HB3	1:L:269:MET:HE2	1.90	0.51
1:M:193:LEU:HG	1:M:198:TYR:HB2	1.91	0.51
1:O:50:LYS:HE2	1:O:53:TYR:HE1	1.75	0.51
1:P:61:LYS:HG2	1:R:167:GLU:CG	2.32	0.51
1:P:178:LEU:HD22	1:P:277:THR:HG21	1.92	0.51
1:Q:193:LEU:HG	1:Q:198:TYR:HB2	1.91	0.51
3:Y:267:ARG:NH1	4:V:132:ILE:HD13	2.25	0.51
2:i:149:LYS:O	2:i:153:HIS:ND1	2.39	0.51
2:j:104:GLU:O	2:j:108:THR:HG23	2.09	0.51
1:A:103:THR:HB	1:A:132:MET:HE1	1.92	0.51
1:A:193:LEU:HG	1:A:198:TYR:HB2	1.91	0.51
1:A:241:GLU:OE2	1:A:245:GLY:HA2	2.10	0.51
1:C:50:LYS:HE2	1:C:53:TYR:HE1	1.75	0.51
1:D:195:GLU:CB	1:E:113:LYS:HD2	2.38	0.51
1:I:287:ILE:HD12	1:I:290:ARG:NH2	2.23	0.51
1:N:264:PRO:HB3	1:N:269:MET:HE2	1.90	0.51
1:R:9:VAL:O	1:R:340:TRP:NE1	2.43	0.51
1:R:50:LYS:HE2	1:R:53:TYR:HE1	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:56:ASP:OD1	1:D:56:ASP:N	2.41	0.51
1:D:241:GLU:OE2	1:D:245:GLY:HA2	2.10	0.51
1:J:47:MET:HB3	4:V:138:LYS:HE3	1.90	0.51
1:M:79:TRP:HZ2	1:M:118:LYS:HE2	1.74	0.51
1:O:193:LEU:HG	1:O:198:TYR:HB2	1.91	0.51
1:P:99:GLU:HG3	1:P:128:ASN:HB3	1.93	0.51
2:a:270:ILE:HG21	2:b:267:TYR:HE1	1.75	0.51
5:d:2:ASP:O	5:d:6:LYS:NZ	2.44	0.51
1:D:226:GLU:HA	1:D:229:THR:HG22	1.92	0.51
1:F:193:LEU:HG	1:F:198:TYR:HB2	1.91	0.51
1:I:50:LYS:HE2	1:I:53:TYR:HE1	1.75	0.51
1:K:99:GLU:HG3	1:K:128:ASN:HB3	1.93	0.51
1:N:50:LYS:HE2	1:N:53:TYR:HE1	1.75	0.51
2:b:66:ASP:O	2:b:70:LYS:HG2	2.10	0.51
2:Z:32:ALA:O	2:Z:35:ARG:HG2	2.11	0.51
5:U:2:ASP:O	5:U:6:LYS:NZ	2.44	0.51
1:A:178:LEU:HD22	1:A:277:THR:HG21	1.93	0.51
1:C:79:TRP:HZ2	1:C:118:LYS:HE2	1.74	0.51
1:I:99:GLU:HG3	1:I:128:ASN:HB3	1.93	0.51
1:K:79:TRP:HZ2	1:K:118:LYS:HE2	1.74	0.51
1:M:99:GLU:HG3	1:M:128:ASN:HB3	1.93	0.51
1:M:287:ILE:HD12	1:M:290:ARG:NH2	2.23	0.51
1:N:9:VAL:O	1:N:340:TRP:NE1	2.43	0.51
1:N:241:GLU:OE2	1:N:245:GLY:HA2	2.10	0.51
1:O:241:GLU:OE2	1:O:245:GLY:HA2	2.10	0.51
1:Q:195:GLU:O	1:R:112:PRO:HB3	2.10	0.51
1:R:178:LEU:HD22	1:R:277:THR:HG21	1.93	0.51
2:a:141:MET:HE1	2:b:141:MET:N	2.26	0.51
1:B:50:LYS:HE2	1:B:53:TYR:HE1	1.75	0.51
1:G:178:LEU:HD22	1:G:277:THR:HG21	1.93	0.51
1:H:226:GLU:HA	1:H:229:THR:HG22	1.92	0.51
1:K:226:GLU:HA	1:K:229:THR:HG22	1.92	0.51
1:O:178:LEU:HD22	1:O:277:THR:HG21	1.93	0.51
3:Y:260:GLU:O	3:Y:264:LEU:HG	2.10	0.51
3:f:264:LEU:CD1	4:c:125:ILE:HG23	2.41	0.51
1:D:99:GLU:HG3	1:D:128:ASN:HB3	1.93	0.51
1:G:103:THR:HB	1:G:132:MET:HE1	1.92	0.51
1:M:56:ASP:OD1	1:M:56:ASP:N	2.41	0.51
1:O:56:ASP:OD1	1:O:56:ASP:N	2.41	0.51
2:i:264:LYS:HE2	2:i:264:LYS:HA	1.93	0.51
2:j:146:ILE:HA	2:j:149:LYS:HE2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:TRP:HZ2	1:B:118:LYS:HE2	1.74	0.51
1:B:287:ILE:HD12	1:B:290:ARG:NH2	2.23	0.51
1:C:99:GLU:HG3	1:C:128:ASN:HB3	1.93	0.51
1:E:50:LYS:HE2	1:E:53:TYR:HE1	1.75	0.51
1:E:241:GLU:OE2	1:E:245:GLY:HA2	2.10	0.51
1:F:64:ILE:HD11	1:H:169:TYR:CD2	2.46	0.51
1:G:99:GLU:HG3	1:G:128:ASN:HB3	1.93	0.51
1:J:39:ARG:NH1	1:J:63:GLY:O	2.44	0.51
1:M:37:ARG:HH21	1:M:53:TYR:H	1.59	0.51
1:N:178:LEU:HD22	1:N:277:THR:HG21	1.93	0.51
1:O:226:GLU:HA	1:O:229:THR:HG22	1.92	0.51
1:P:103:THR:HB	1:P:132:MET:HE1	1.92	0.51
2:a:42:GLU:HB3	2:b:43:LEU:HD11	1.92	0.51
1:A:165:ILE:HG23	1:A:169:TYR:H	1.76	0.51
1:F:36:GLY:C	1:F:37:ARG:HD2	2.36	0.51
1:F:99:GLU:HG3	1:F:128:ASN:HB3	1.93	0.51
1:F:226:GLU:HA	1:F:229:THR:HG22	1.92	0.51
1:N:39:ARG:NH1	1:N:63:GLY:O	2.44	0.51
1:N:99:GLU:HG3	1:N:128:ASN:HB3	1.93	0.51
1:N:103:THR:HB	1:N:132:MET:HE1	1.92	0.51
1:P:9:VAL:O	1:P:340:TRP:NE1	2.43	0.51
1:Q:99:GLU:HG3	1:Q:128:ASN:HB3	1.93	0.51
1:Q:226:GLU:HA	1:Q:229:THR:HG22	1.92	0.51
1:R:99:GLU:HG3	1:R:128:ASN:HB3	1.93	0.51
2:a:74:ALA:O	2:a:77:LYS:HG2	2.11	0.51
3:Y:221:ILE:HA	3:Y:224:LEU:CD1	2.41	0.51
2:i:170:VAL:O	2:i:173:GLU:HG3	2.11	0.51
1:A:39:ARG:NH1	1:A:63:GLY:O	2.44	0.50
1:G:9:VAL:O	1:G:340:TRP:NE1	2.43	0.50
1:I:44:MET:HE3	1:K:169:TYR:HD1	1.76	0.50
1:M:226:GLU:HA	1:M:229:THR:HG22	1.92	0.50
1:O:99:GLU:HG3	1:O:128:ASN:HB3	1.93	0.50
2:i:74:ALA:O	2:i:77:LYS:HG2	2.11	0.50
4:c:47:LEU:HD23	5:d:7:ALA:HB1	1.93	0.50
1:B:103:THR:HB	1:B:132:MET:HE1	1.92	0.50
1:C:103:THR:HB	1:C:132:MET:HE1	1.92	0.50
1:C:287:ILE:HD12	1:C:290:ARG:NH2	2.23	0.50
1:D:103:THR:HB	1:D:132:MET:HE1	1.92	0.50
1:F:39:ARG:NH1	1:F:63:GLY:O	2.44	0.50
1:P:50:LYS:HE2	1:P:53:TYR:HE1	1.75	0.50
1:E:9:VAL:O	1:E:340:TRP:NE1	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:99:GLU:HG3	1:J:128:ASN:HB3	1.93	0.50
1:L:99:GLU:HG3	1:L:128:ASN:HB3	1.93	0.50
1:R:103:THR:HB	1:R:132:MET:HE1	1.92	0.50
1:C:178:LEU:HD22	1:C:277:THR:HG21	1.93	0.50
1:E:99:GLU:HG3	1:E:128:ASN:HB3	1.93	0.50
1:H:99:GLU:HG3	1:H:128:ASN:HB3	1.93	0.50
1:J:9:VAL:O	1:J:340:TRP:NE1	2.43	0.50
1:K:44:MET:CE	1:M:169:TYR:CD1	2.94	0.50
1:L:44:MET:HE1	1:N:169:TYR:CD2	2.47	0.50
2:h:32:ALA:O	2:h:35:ARG:HG2	2.11	0.50
1:C:39:ARG:NH1	1:C:63:GLY:O	2.44	0.50
1:E:67:LEU:HD12	1:E:203:THR:HB	1.94	0.50
1:E:103:THR:HB	1:E:132:MET:HE1	1.92	0.50
1:F:103:THR:HB	1:F:132:MET:HE1	1.92	0.50
1:F:287:ILE:HA	1:F:290:ARG:HE	1.77	0.50
1:G:50:LYS:HE2	1:G:53:TYR:HE1	1.75	0.50
1:J:103:THR:HB	1:J:132:MET:HE1	1.92	0.50
1:J:287:ILE:HD12	1:J:290:ARG:NH2	2.23	0.50
1:O:287:ILE:HA	1:O:290:ARG:HE	1.77	0.50
1:P:67:LEU:HD12	1:P:203:THR:HB	1.94	0.50
2:b:146:ILE:HA	2:b:149:LYS:HE2	1.93	0.50
2:j:246:VAL:HG11	3:e:144:ARG:CZ	2.40	0.50
3:f:264:LEU:HD13	4:c:129:THR:OG1	2.11	0.50
1:A:287:ILE:HA	1:A:290:ARG:HE	1.77	0.50
1:H:287:ILE:HD12	1:H:290:ARG:NH2	2.23	0.50
1:L:103:THR:HB	1:L:132:MET:HE1	1.92	0.50
1:R:287:ILE:HA	1:R:290:ARG:HE	1.77	0.50
4:V:50:LYS:CD	5:U:160:VAL:HG21	2.42	0.50
1:B:99:GLU:HG3	1:B:128:ASN:HB3	1.93	0.50
1:C:9:VAL:O	1:C:340:TRP:NE1	2.43	0.50
1:C:287:ILE:HA	1:C:290:ARG:HE	1.77	0.50
1:K:64:ILE:HG12	1:M:169:TYR:CD2	2.47	0.50
1:K:67:LEU:HD12	1:K:203:THR:HB	1.94	0.50
1:P:39:ARG:NH1	1:P:63:GLY:O	2.44	0.50
1:Q:39:ARG:NH1	1:Q:63:GLY:O	2.44	0.50
1:Q:178:LEU:HD22	1:Q:277:THR:HG21	1.93	0.50
1:Q:287:ILE:HA	1:Q:290:ARG:HE	1.77	0.50
2:a:149:LYS:O	2:a:153:HIS:ND1	2.39	0.50
3:Y:253:LYS:HZ2	4:V:118:VAL:HG11	1.77	0.50
4:V:174:LYS:HG3	4:V:178:LYS:NZ	2.23	0.50
1:A:99:GLU:HG3	1:A:128:ASN:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:LEU:HD12	1:B:203:THR:HB	1.94	0.50
1:B:239:SER:HB2	1:B:249:THR:HG22	1.94	0.50
1:I:67:LEU:HD12	1:I:203:THR:HB	1.94	0.50
1:L:287:ILE:HA	1:L:290:ARG:HE	1.77	0.50
1:M:37:ARG:NE	1:M:52:SER:HA	2.27	0.50
1:N:287:ILE:HA	1:N:290:ARG:HE	1.77	0.50
2:a:148:LEU:HD11	2:a:152:LYS:HE2	1.94	0.50
2:W:29:LYS:HE3	2:W:33:GLU:OE2	2.12	0.50
4:c:44:SER:HB2	5:d:3:ASP:HB2	1.92	0.50
4:c:103:ARG:HG2	4:c:106:LYS:HZ3	1.76	0.50
1:E:287:ILE:HA	1:E:290:ARG:HE	1.77	0.50
1:G:67:LEU:HD12	1:G:203:THR:HB	1.94	0.50
1:H:103:THR:HB	1:H:132:MET:HE1	1.92	0.50
1:K:287:ILE:HA	1:K:290:ARG:HE	1.77	0.50
2:a:170:VAL:O	2:a:173:GLU:HG3	2.11	0.50
3:f:221:ILE:HA	3:f:224:LEU:CD1	2.41	0.50
1:A:50:LYS:HE2	1:A:53:TYR:HE1	1.75	0.49
1:G:114:ALA:O	1:G:118:LYS:HG2	2.12	0.49
1:H:287:ILE:HA	1:H:290:ARG:HE	1.77	0.49
1:L:9:VAL:O	1:L:340:TRP:NE1	2.43	0.49
1:M:67:LEU:HD12	1:M:203:THR:HB	1.94	0.49
1:N:32:PRO:HG2	1:N:59:GLN:HE21	1.77	0.49
5:U:97:LEU:HA	5:U:100:LEU:HD12	1.94	0.49
1:B:114:ALA:O	1:B:118:LYS:HG2	2.13	0.49
1:C:67:LEU:HD12	1:C:203:THR:HB	1.94	0.49
1:E:32:PRO:HG2	1:E:59:GLN:HE21	1.78	0.49
1:E:191:LYS:HZ1	1:F:173:HIS:HA	1.77	0.49
1:G:32:PRO:HG2	1:G:59:GLN:HE21	1.78	0.49
1:K:114:ALA:O	1:K:118:LYS:HG2	2.13	0.49
1:L:32:PRO:HG2	1:L:59:GLN:HE21	1.78	0.49
1:L:39:ARG:NH1	1:L:63:GLY:O	2.44	0.49
1:N:67:LEU:HD12	1:N:203:THR:HB	1.94	0.49
1:O:114:ALA:O	1:O:118:LYS:HG2	2.13	0.49
1:R:67:LEU:HD12	1:R:203:THR:HB	1.94	0.49
2:Z:61:SER:O	2:Z:65:LYS:HG3	2.12	0.49
2:g:29:LYS:HE3	2:g:33:GLU:OE2	2.12	0.49
3:e:110:PHE:HB3	3:e:114:LYS:HZ3	1.76	0.49
1:G:191:LYS:NZ	1:H:173:HIS:HA	2.27	0.49
1:H:39:ARG:NH1	1:H:63:GLY:O	2.44	0.49
1:M:287:ILE:HA	1:M:290:ARG:HE	1.77	0.49
1:P:287:ILE:HA	1:P:290:ARG:HE	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:243:GLU:OE2	3:X:148:ARG:HD3	2.12	0.49
1:A:32:PRO:HG2	1:A:59:GLN:HE21	1.78	0.49
1:A:221:LEU:HA	1:A:315:LYS:HZ1	1.76	0.49
1:E:39:ARG:NH1	1:E:63:GLY:O	2.44	0.49
1:I:44:MET:HE3	1:K:168:GLY:O	2.11	0.49
1:P:32:PRO:HG2	1:P:59:GLN:HE21	1.78	0.49
1:P:152:VAL:HA	1:P:298:VAL:HG23	1.95	0.49
1:Q:9:VAL:O	1:Q:340:TRP:NE1	2.43	0.49
2:a:249:LEU:HB3	2:b:253:ILE:HD11	1.94	0.49
4:V:197:ALA:HA	2:j:103:GLN:CD	2.37	0.49
1:C:32:PRO:HG2	1:C:59:GLN:HE21	1.78	0.49
1:G:287:ILE:HA	1:G:290:ARG:HE	1.77	0.49
1:I:39:ARG:NH1	1:I:63:GLY:O	2.44	0.49
1:I:287:ILE:HA	1:I:290:ARG:HE	1.77	0.49
1:J:287:ILE:HA	1:J:290:ARG:HE	1.77	0.49
1:N:152:VAL:HA	1:N:298:VAL:HG23	1.95	0.49
1:B:287:ILE:HA	1:B:290:ARG:HE	1.77	0.49
1:F:114:ALA:O	1:F:118:LYS:HG2	2.12	0.49
1:G:152:VAL:HA	1:G:298:VAL:HG23	1.95	0.49
1:H:152:VAL:HA	1:H:298:VAL:HG23	1.95	0.49
1:J:32:PRO:HG2	1:J:59:GLN:HE21	1.78	0.49
1:L:114:ALA:O	1:L:118:LYS:HG2	2.13	0.49
1:M:39:ARG:NH1	1:M:63:GLY:O	2.44	0.49
1:O:67:LEU:HD12	1:O:203:THR:HB	1.94	0.49
1:P:114:ALA:O	1:P:118:LYS:HG2	2.13	0.49
1:P:239:SER:HB2	1:P:249:THR:HG22	1.94	0.49
2:b:259:GLU:O	2:b:263:GLN:HG2	2.12	0.49
1:B:110:LEU:HB2	1:B:177:ARG:HD2	1.95	0.49
1:B:251:GLY:N	1:B:253:GLU:OE1	2.46	0.49
1:C:152:VAL:HA	1:C:298:VAL:HG23	1.95	0.49
1:C:251:GLY:N	1:C:253:GLU:OE1	2.46	0.49
1:D:32:PRO:HG2	1:D:59:GLN:HE21	1.78	0.49
1:E:110:LEU:HB2	1:E:177:ARG:HD2	1.95	0.49
1:F:152:VAL:HA	1:F:298:VAL:HG23	1.95	0.49
1:F:251:GLY:N	1:F:253:GLU:OE1	2.46	0.49
1:I:32:PRO:HG2	1:I:59:GLN:HE21	1.78	0.49
1:J:152:VAL:HA	1:J:298:VAL:HG23	1.95	0.49
1:K:39:ARG:NH1	1:K:63:GLY:O	2.44	0.49
1:L:67:LEU:HD12	1:L:203:THR:HB	1.94	0.49
1:O:39:ARG:NH1	1:O:63:GLY:O	2.44	0.49
1:O:239:SER:HB2	1:O:249:THR:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:152:VAL:HA	1:R:298:VAL:HG23	1.95	0.49
4:V:195:ILE:HD12	2:i:105:ARG:NH2	2.24	0.49
1:B:39:ARG:NH1	1:B:63:GLY:O	2.44	0.49
1:B:245:GLY:HA3	1:D:322:PRO:CB	2.43	0.49
1:G:110:LEU:HB2	1:G:177:ARG:HD2	1.95	0.49
1:H:32:PRO:HG2	1:H:59:GLN:HE21	1.78	0.49
1:I:9:VAL:O	1:I:340:TRP:NE1	2.43	0.49
1:I:251:GLY:N	1:I:253:GLU:OE1	2.46	0.49
1:L:195:GLU:HB3	1:M:113:LYS:HD2	1.95	0.49
1:M:251:GLY:N	1:M:253:GLU:OE1	2.46	0.49
1:P:110:LEU:HB2	1:P:177:ARG:HD2	1.95	0.49
1:Q:251:GLY:N	1:Q:253:GLU:OE1	2.46	0.49
1:R:114:ALA:O	1:R:118:LYS:HG2	2.13	0.49
2:a:113:LEU:HD22	2:b:112:LYS:HZ3	1.78	0.49
4:V:192:ARG:NE	2:j:110:LEU:HD11	2.27	0.49
2:j:259:GLU:O	2:j:263:GLN:HG2	2.12	0.49
1:B:9:VAL:O	1:B:340:TRP:NE1	2.43	0.49
1:D:122:ILE:HG13	1:D:123:MET:N	2.28	0.49
1:D:152:VAL:HA	1:D:298:VAL:HG23	1.95	0.49
1:E:114:ALA:O	1:E:118:LYS:HG2	2.12	0.49
1:E:152:VAL:HA	1:E:298:VAL:HG23	1.95	0.49
1:F:67:LEU:HD12	1:F:203:THR:HB	1.94	0.49
1:H:67:LEU:HD12	1:H:203:THR:HB	1.94	0.49
1:I:110:LEU:HB2	1:I:177:ARG:HD2	1.95	0.49
1:K:110:LEU:HB2	1:K:177:ARG:HD2	1.95	0.49
1:O:152:VAL:HA	1:O:298:VAL:HG23	1.95	0.49
1:Q:152:VAL:HA	1:Q:298:VAL:HG23	1.95	0.49
2:a:284:ILE:HD11	2:W:8:MET:HE2	1.94	0.49
4:V:146:ARG:HG2	4:V:149:ILE:HD12	1.95	0.49
4:V:192:ARG:CD	2:j:110:LEU:HD11	2.42	0.49
5:U:54:PRO:HB3	2:i:160:ARG:NH2	2.27	0.49
4:c:146:ARG:HG2	4:c:149:ILE:HD12	1.95	0.49
1:D:239:SER:HB2	1:D:249:THR:HG22	1.94	0.49
1:E:239:SER:HB2	1:E:249:THR:HG22	1.94	0.49
1:H:239:SER:HB2	1:H:249:THR:HG22	1.94	0.49
1:I:152:VAL:HA	1:I:298:VAL:HG23	1.95	0.49
1:K:178:LEU:HD22	1:K:277:THR:HG21	1.95	0.49
1:L:152:VAL:HA	1:L:298:VAL:HG23	1.95	0.49
1:L:221:LEU:HA	1:L:315:LYS:HZ1	1.78	0.49
1:M:152:VAL:HA	1:M:298:VAL:HG23	1.95	0.49
1:O:122:ILE:HG13	1:O:123:MET:N	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:251:GLY:N	1:O:253:GLU:OE1	2.46	0.49
1:Q:32:PRO:HG2	1:Q:59:GLN:HE21	1.78	0.49
2:a:105:ARG:HB3	4:c:195:ILE:CD1	2.42	0.49
2:a:273:GLU:HA	2:a:276:HIS:HD1	1.78	0.49
2:g:62:GLU:HA	2:g:65:LYS:HE2	1.95	0.49
1:B:152:VAL:HA	1:B:298:VAL:HG23	1.95	0.48
1:C:239:SER:HB2	1:C:249:THR:HG22	1.94	0.48
1:D:287:ILE:HA	1:D:290:ARG:HE	1.77	0.48
1:H:328:LYS:NZ	2:i:254:ASP:HA	2.28	0.48
1:J:67:LEU:HD12	1:J:203:THR:HB	1.94	0.48
1:J:251:GLY:N	1:J:253:GLU:OE1	2.46	0.48
1:K:9:VAL:O	1:K:340:TRP:NE1	2.43	0.48
1:M:239:SER:HB2	1:M:249:THR:HG22	1.94	0.48
4:V:50:LYS:HE3	5:U:156:PHE:CZ	2.48	0.48
2:i:54:GLU:HA	2:i:57:LEU:HD12	1.95	0.48
2:g:3:ALA:CB	3:e:105:LEU:HD11	2.43	0.48
1:A:238:LYS:HB2	1:A:254:ARG:HD3	1.96	0.48
1:B:32:PRO:HG2	1:B:59:GLN:HE21	1.78	0.48
1:D:251:GLY:N	1:D:253:GLU:OE1	2.46	0.48
1:G:239:SER:HB2	1:G:249:THR:HG22	1.94	0.48
1:G:251:GLY:N	1:G:253:GLU:OE1	2.46	0.48
1:H:114:ALA:O	1:H:118:LYS:HG2	2.13	0.48
1:H:122:ILE:HG13	1:H:123:MET:N	2.28	0.48
1:I:178:LEU:HD22	1:I:277:THR:HG21	1.95	0.48
1:I:239:SER:HB2	1:I:249:THR:HG22	1.94	0.48
1:L:122:ILE:HG13	1:L:123:MET:N	2.28	0.48
1:L:239:SER:HB2	1:L:249:THR:HG22	1.94	0.48
1:N:251:GLY:N	1:N:253:GLU:OE1	2.46	0.48
2:a:54:GLU:HA	2:a:57:LEU:HD12	1.95	0.48
2:j:132:SER:O	2:j:135:GLN:HG3	2.13	0.48
4:c:60:GLU:HG2	4:c:63:ARG:HH21	1.79	0.48
4:c:174:LYS:HG3	4:c:178:LYS:NZ	2.23	0.48
1:A:110:LEU:HB2	1:A:177:ARG:HD2	1.95	0.48
1:D:39:ARG:NH1	1:D:63:GLY:O	2.44	0.48
1:D:67:LEU:HD12	1:D:203:THR:HB	1.94	0.48
1:F:239:SER:HB2	1:F:249:THR:HG22	1.94	0.48
1:J:239:SER:HB2	1:J:249:THR:HG22	1.94	0.48
1:K:32:PRO:HG2	1:K:59:GLN:HE21	1.78	0.48
1:Q:239:SER:HB2	1:Q:249:THR:HG22	1.94	0.48
1:R:32:PRO:HG2	1:R:59:GLN:HE21	1.78	0.48
4:V:155:MET:C	4:V:156:GLN:NE2	2.70	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:i:105:ARG:CD	2:j:106:LEU:HD13	2.43	0.48
2:i:148:LEU:HD11	2:i:152:LYS:HE2	1.94	0.48
2:h:61:SER:O	2:h:65:LYS:HG3	2.12	0.48
1:B:122:ILE:HG13	1:B:123:MET:N	2.28	0.48
1:C:122:ILE:HG13	1:C:123:MET:N	2.28	0.48
1:F:9:VAL:O	1:F:340:TRP:NE1	2.42	0.48
1:F:32:PRO:HG2	1:F:59:GLN:HE21	1.78	0.48
1:F:110:LEU:HB2	1:F:177:ARG:HD2	1.95	0.48
1:K:152:VAL:HA	1:K:298:VAL:HG23	1.95	0.48
1:K:251:GLY:N	1:K:253:GLU:OE1	2.46	0.48
1:K:335:ARG:O	1:K:338:SER:HB2	2.14	0.48
1:N:239:SER:HB2	1:N:249:THR:HG22	1.94	0.48
1:P:251:GLY:N	1:P:253:GLU:OE1	2.46	0.48
1:P:335:ARG:O	1:P:338:SER:HB2	2.14	0.48
1:Q:67:LEU:HD12	1:Q:203:THR:HB	1.94	0.48
1:R:328:LYS:HZ3	2:j:61:SER:HB2	1.78	0.48
1:A:122:ILE:HG13	1:A:123:MET:N	2.28	0.48
1:A:152:VAL:HA	1:A:298:VAL:HG23	1.95	0.48
1:A:239:SER:HB2	1:A:249:THR:HG22	1.94	0.48
1:B:79:TRP:HE1	1:B:118:LYS:HD2	1.79	0.48
1:B:178:LEU:HD22	1:B:277:THR:HG21	1.96	0.48
1:B:335:ARG:O	1:B:338:SER:HB2	2.14	0.48
1:D:110:LEU:HB2	1:D:177:ARG:HD2	1.95	0.48
1:D:178:LEU:HD22	1:D:277:THR:HG21	1.95	0.48
1:F:335:ARG:O	1:F:338:SER:HB2	2.14	0.48
1:H:9:VAL:O	1:H:340:TRP:NE1	2.43	0.48
1:I:362:TYR:CE2	3:f:201:ARG:NH2	2.82	0.48
1:J:47:MET:HA	4:V:138:LYS:HE3	1.96	0.48
1:K:79:TRP:HE1	1:K:118:LYS:HD2	1.79	0.48
1:K:239:SER:HB2	1:K:249:THR:HG22	1.94	0.48
1:L:178:LEU:HD22	1:L:277:THR:HG21	1.96	0.48
1:L:238:LYS:HB2	1:L:254:ARG:HD3	1.96	0.48
1:N:110:LEU:HB2	1:N:177:ARG:HD2	1.95	0.48
1:N:122:ILE:HG13	1:N:123:MET:N	2.28	0.48
1:O:32:PRO:HG2	1:O:59:GLN:HE21	1.78	0.48
1:P:243:PRO:HB2	1:R:291:LYS:HD3	1.95	0.48
1:Q:114:ALA:O	1:Q:118:LYS:HG2	2.12	0.48
1:Q:122:ILE:HG13	1:Q:123:MET:N	2.28	0.48
1:Q:165:ILE:HG23	1:Q:169:TYR:O	2.13	0.48
1:R:110:LEU:HB2	1:R:177:ARG:HD2	1.95	0.48
1:R:238:LYS:HB2	1:R:254:ARG:HD3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:239:SER:HB2	1:R:249:THR:HG22	1.94	0.48
1:A:251:GLY:N	1:A:253:GLU:OE1	2.46	0.48
1:E:178:LEU:HD22	1:E:277:THR:HG21	1.96	0.48
1:F:224:GLU:HA	1:F:227:MET:HE2	1.96	0.48
1:I:114:ALA:O	1:I:118:LYS:HG2	2.13	0.48
1:I:335:ARG:O	1:I:338:SER:HB2	2.14	0.48
1:J:335:ARG:O	1:J:338:SER:HB2	2.14	0.48
1:M:110:LEU:HB2	1:M:177:ARG:HD2	1.95	0.48
1:M:224:GLU:HA	1:M:227:MET:HE2	1.96	0.48
1:N:114:ALA:O	1:N:118:LYS:HG2	2.13	0.48
1:O:79:TRP:HE1	1:O:118:LYS:HD2	1.79	0.48
1:Q:335:ARG:O	1:Q:338:SER:HB2	2.14	0.48
1:R:79:TRP:HE1	1:R:118:LYS:HD2	1.79	0.48
1:R:328:LYS:NZ	2:j:61:SER:HB2	2.28	0.48
4:V:60:GLU:HG2	4:V:63:ARG:HH21	1.78	0.48
2:i:64:LEU:HD22	2:j:60:TYR:CD1	2.48	0.48
2:j:91:ARG:HE	2:j:94:LEU:HD21	1.77	0.48
1:C:335:ARG:O	1:C:338:SER:HB2	2.14	0.48
1:G:39:ARG:NH1	1:G:63:GLY:O	2.44	0.48
1:J:110:LEU:HB2	1:J:177:ARG:HD2	1.95	0.48
1:J:178:LEU:HD22	1:J:277:THR:HG21	1.96	0.48
1:L:335:ARG:O	1:L:338:SER:HB2	2.14	0.48
1:M:114:ALA:O	1:M:118:LYS:HG2	2.13	0.48
1:M:122:ILE:HG13	1:M:123:MET:N	2.28	0.48
1:O:335:ARG:O	1:O:338:SER:HB2	2.14	0.48
1:P:79:TRP:HE1	1:P:118:LYS:HD2	1.78	0.48
2:a:45:SER:HA	2:a:48:LYS:HD2	1.96	0.48
3:X:103:GLN:O	3:X:106:ILE:HG22	2.14	0.48
4:V:145:ARG:HG2	4:V:146:ARG:H	1.77	0.48
5:U:136:LEU:HD22	5:U:156:PHE:HZ	1.78	0.48
4:c:145:ARG:HG2	4:c:146:ARG:H	1.77	0.48
5:d:99:ASP:O	5:d:102:ARG:HB3	2.14	0.48
1:D:335:ARG:O	1:D:338:SER:HB2	2.14	0.48
1:J:79:TRP:HE1	1:J:118:LYS:HD2	1.79	0.48
1:J:114:ALA:O	1:J:118:LYS:HG2	2.12	0.48
1:J:221:LEU:HA	1:J:315:LYS:HZ1	1.79	0.48
1:N:238:LYS:HB2	1:N:254:ARG:HD3	1.96	0.48
1:O:263:GLN:HB2	1:O:266:PHE:CE2	2.49	0.48
1:Q:224:GLU:HA	1:Q:227:MET:HE2	1.96	0.48
1:R:122:ILE:HG13	1:R:123:MET:N	2.28	0.48
1:R:251:GLY:N	1:R:253:GLU:OE1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:91:ARG:HE	2:b:94:LEU:HD21	1.77	0.48
2:i:106:LEU:CA	2:j:106:LEU:HD21	2.43	0.48
1:A:114:ALA:O	1:A:118:LYS:HG2	2.12	0.48
1:B:224:GLU:HA	1:B:227:MET:HE2	1.96	0.48
1:D:44:MET:HE1	1:F:169:TYR:CD1	2.45	0.48
1:D:114:ALA:O	1:D:118:LYS:HG2	2.12	0.48
1:H:238:LYS:HB2	1:H:254:ARG:HD3	1.96	0.48
1:H:251:GLY:N	1:H:253:GLU:OE1	2.46	0.48
1:M:335:ARG:O	1:M:338:SER:HB2	2.14	0.48
1:N:335:ARG:O	1:N:338:SER:HB2	2.14	0.48
1:P:122:ILE:HG13	1:P:123:MET:N	2.28	0.48
1:P:238:LYS:HB2	1:P:254:ARG:HD3	1.96	0.48
1:R:335:ARG:O	1:R:338:SER:HB2	2.14	0.48
2:a:254:ASP:HA	2:a:257:GLU:OE1	2.14	0.48
2:j:88:LEU:O	2:j:92:ILE:HG13	2.14	0.48
1:G:335:ARG:O	1:G:338:SER:HB2	2.14	0.48
1:H:79:TRP:HE1	1:H:118:LYS:HD2	1.79	0.48
1:J:122:ILE:HG13	1:J:123:MET:N	2.28	0.48
1:J:238:LYS:HB2	1:J:254:ARG:HD3	1.96	0.48
1:K:122:ILE:HG13	1:K:123:MET:N	2.28	0.48
1:M:9:VAL:O	1:M:340:TRP:NE1	2.43	0.48
1:M:367:PRO:O	1:M:370:VAL:HG12	2.14	0.48
1:R:39:ARG:NH1	1:R:63:GLY:O	2.44	0.48
4:V:199:SER:HB2	2:j:103:GLN:OE1	2.13	0.48
2:i:197:LEU:HD11	2:j:193:LEU:HB3	1.96	0.48
1:B:244:ASP:CB	1:D:290:ARG:NH2	2.77	0.47
1:E:122:ILE:HG13	1:E:123:MET:N	2.28	0.47
1:F:367:PRO:O	1:F:370:VAL:HG12	2.14	0.47
1:G:122:ILE:HG13	1:G:123:MET:N	2.28	0.47
1:H:367:PRO:O	1:H:370:VAL:HG12	2.14	0.47
1:I:224:GLU:HA	1:I:227:MET:HE2	1.96	0.47
1:K:238:LYS:HB2	1:K:254:ARG:HD3	1.96	0.47
1:L:110:LEU:HB2	1:L:177:ARG:HD2	1.95	0.47
1:L:224:GLU:HA	1:L:227:MET:HE2	1.96	0.47
1:O:224:GLU:HA	1:O:227:MET:HE2	1.96	0.47
1:Q:110:LEU:HB2	1:Q:177:ARG:HD2	1.95	0.47
2:W:62:GLU:HA	2:W:65:LYS:HE2	1.95	0.47
3:f:249:ASP:OD1	4:c:72:LYS:HD3	2.14	0.47
5:d:136:LEU:HD22	5:d:156:PHE:HZ	1.78	0.47
1:A:335:ARG:O	1:A:338:SER:HB2	2.14	0.47
1:H:335:ARG:O	1:H:338:SER:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:213:LYS:HA	1:J:217:CYS:SG	2.54	0.47
1:K:213:LYS:HA	1:K:217:CYS:SG	2.54	0.47
1:K:367:PRO:O	1:K:370:VAL:HG12	2.14	0.47
1:L:213:LYS:HA	1:L:217:CYS:SG	2.54	0.47
1:M:213:LYS:HA	1:M:217:CYS:SG	2.54	0.47
1:N:213:LYS:HA	1:N:217:CYS:SG	2.54	0.47
1:Q:213:LYS:HA	1:Q:217:CYS:SG	2.54	0.47
2:b:88:LEU:O	2:b:92:ILE:HG13	2.14	0.47
2:b:250:GLU:HB3	3:X:141:ARG:NH1	2.29	0.47
2:g:53:THR:HA	2:h:57:LEU:HD11	1.95	0.47
3:e:103:GLN:O	3:e:106:ILE:HG22	2.14	0.47
5:d:97:LEU:HA	5:d:100:LEU:HD12	1.94	0.47
5:d:136:LEU:HD22	5:d:156:PHE:CZ	2.50	0.47
1:A:79:TRP:HE1	1:A:118:LYS:HD2	1.78	0.47
1:C:224:GLU:HA	1:C:227:MET:HE2	1.96	0.47
1:E:238:LYS:HB2	1:E:254:ARG:HD3	1.96	0.47
1:F:79:TRP:HE1	1:F:118:LYS:HD2	1.79	0.47
1:G:79:TRP:HE1	1:G:118:LYS:HD2	1.79	0.47
1:H:224:GLU:HA	1:H:227:MET:HE2	1.96	0.47
1:O:110:LEU:HB2	1:O:177:ARG:HD2	1.95	0.47
1:O:213:LYS:HA	1:O:217:CYS:SG	2.54	0.47
1:R:213:LYS:HA	1:R:217:CYS:SG	2.54	0.47
2:b:257:GLU:HB2	3:X:134:ARG:NH2	2.29	0.47
3:Y:221:ILE:HA	3:Y:224:LEU:HD12	1.96	0.47
2:i:100:ASP:O	2:i:104:GLU:OE1	2.33	0.47
2:i:231:LYS:O	2:i:234:GLU:HG2	2.15	0.47
2:i:273:GLU:HA	2:i:276:HIS:HD1	1.78	0.47
2:h:53:THR:O	2:h:56:GLU:HG3	2.14	0.47
1:B:182:GLY:HA2	1:B:185:LEU:HD12	1.96	0.47
1:D:367:PRO:O	1:D:370:VAL:HG12	2.14	0.47
1:E:182:GLY:HA2	1:E:185:LEU:HD12	1.96	0.47
1:F:122:ILE:HG13	1:F:123:MET:N	2.28	0.47
1:I:122:ILE:HG13	1:I:123:MET:N	2.28	0.47
1:J:367:PRO:O	1:J:370:VAL:HG12	2.14	0.47
1:L:251:GLY:N	1:L:253:GLU:OE1	2.46	0.47
1:Q:238:LYS:HB2	1:Q:254:ARG:HD3	1.96	0.47
2:a:231:LYS:O	2:a:234:GLU:HG2	2.14	0.47
2:Z:53:THR:O	2:Z:56:GLU:HG3	2.14	0.47
3:Y:259:TYR:HA	3:Y:262:ASN:ND2	2.29	0.47
3:f:215:ARG:NH1	4:c:108:ASP:OD1	2.46	0.47
1:B:367:PRO:O	1:B:370:VAL:HG12	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:367:PRO:O	1:C:370:VAL:HG12	2.14	0.47
1:D:213:LYS:HA	1:D:217:CYS:SG	2.54	0.47
1:F:213:LYS:HA	1:F:217:CYS:SG	2.54	0.47
1:H:213:LYS:HA	1:H:217:CYS:SG	2.54	0.47
1:J:224:GLU:HA	1:J:227:MET:HE2	1.96	0.47
1:M:32:PRO:HG2	1:M:59:GLN:HE21	1.78	0.47
1:P:213:LYS:HA	1:P:217:CYS:SG	2.54	0.47
2:b:277:ALA:HA	2:Z:5:LYS:HZ2	1.80	0.47
2:Z:35:ARG:O	2:Z:38:GLN:HG3	2.15	0.47
2:h:35:ARG:O	2:h:38:GLN:HG3	2.15	0.47
4:c:56:ILE:HG13	5:d:124:THR:HG22	1.96	0.47
1:B:63:GLY:CA	1:D:286:ASP:CG	2.87	0.47
1:D:224:GLU:HA	1:D:227:MET:HE2	1.96	0.47
1:E:79:TRP:HE1	1:E:118:LYS:HD2	1.79	0.47
1:G:189:LEU:HD23	1:G:209:VAL:HB	1.97	0.47
1:G:224:GLU:HA	1:G:227:MET:HE2	1.96	0.47
1:I:125:GLU:HG2	3:f:201:ARG:NH2	2.28	0.47
1:I:213:LYS:HA	1:I:217:CYS:SG	2.54	0.47
1:I:367:PRO:O	1:I:370:VAL:HG12	2.14	0.47
1:N:185:LEU:HD21	1:N:261:LEU:HD13	1.96	0.47
1:O:367:PRO:O	1:O:370:VAL:HG12	2.14	0.47
1:P:189:LEU:HD23	1:P:209:VAL:HB	1.97	0.47
2:b:132:SER:O	2:b:135:GLN:HG3	2.13	0.47
5:U:99:ASP:O	5:U:102:ARG:HB3	2.14	0.47
2:i:245:SER:O	2:i:249:LEU:HG	2.15	0.47
1:B:189:LEU:HD23	1:B:209:VAL:HB	1.97	0.47
1:C:79:TRP:HE1	1:C:118:LYS:HD2	1.79	0.47
1:C:182:GLY:HA2	1:C:185:LEU:HD12	1.96	0.47
1:C:213:LYS:HA	1:C:217:CYS:SG	2.54	0.47
1:C:238:LYS:HB2	1:C:254:ARG:HD3	1.96	0.47
1:E:189:LEU:HD23	1:E:209:VAL:HB	1.97	0.47
1:E:213:LYS:HA	1:E:217:CYS:SG	2.54	0.47
1:F:238:LYS:HB2	1:F:254:ARG:HD3	1.96	0.47
1:G:182:GLY:HA2	1:G:185:LEU:HD12	1.96	0.47
1:G:213:LYS:HA	1:G:217:CYS:SG	2.54	0.47
1:G:367:PRO:O	1:G:370:VAL:HG12	2.14	0.47
1:H:37:ARG:HH12	1:H:84:LYS:HE3	1.78	0.47
1:H:182:GLY:HA2	1:H:185:LEU:HD12	1.96	0.47
1:I:189:LEU:HD23	1:I:209:VAL:HB	1.97	0.47
1:J:263:GLN:HB2	1:J:266:PHE:CE2	2.50	0.47
1:L:79:TRP:HE1	1:L:118:LYS:HD2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:238:LYS:HB2	1:M:254:ARG:HD3	1.96	0.47
1:N:182:GLY:HA2	1:N:185:LEU:HD12	1.96	0.47
1:N:367:PRO:O	1:N:370:VAL:HG12	2.14	0.47
1:P:182:GLY:HA2	1:P:185:LEU:HD12	1.96	0.47
1:Q:367:PRO:O	1:Q:370:VAL:HG12	2.14	0.47
1:R:182:GLY:HA2	1:R:185:LEU:HD12	1.96	0.47
1:R:224:GLU:HA	1:R:227:MET:HE2	1.96	0.47
1:R:367:PRO:O	1:R:370:VAL:HG12	2.14	0.47
5:U:41:LEU:HD11	5:U:72:VAL:HG21	1.97	0.47
2:i:254:ASP:HA	2:i:257:GLU:OE1	2.14	0.47
3:f:226:GLU:HA	4:c:90:PHE:CE1	2.50	0.47
3:f:262:ASN:O	3:f:265:ARG:HG2	2.14	0.47
4:c:194:ASN:OD1	4:c:195:ILE:N	2.48	0.47
1:C:263:GLN:HB2	1:C:266:PHE:CE2	2.50	0.47
1:G:238:LYS:HB2	1:G:254:ARG:HD3	1.96	0.47
1:H:110:LEU:HB2	1:H:177:ARG:HD2	1.95	0.47
1:K:224:GLU:HA	1:K:227:MET:HE2	1.96	0.47
3:Y:224:LEU:HD22	3:Y:228:GLN:HE21	1.80	0.47
5:U:136:LEU:HD22	5:U:156:PHE:CZ	2.50	0.47
1:B:238:LYS:HB2	1:B:254:ARG:HD3	1.96	0.47
1:D:79:TRP:HE1	1:D:118:LYS:HD2	1.79	0.47
1:E:335:ARG:O	1:E:338:SER:HB2	2.14	0.47
1:F:44:MET:HE2	1:F:44:MET:HB2	1.86	0.47
1:F:182:GLY:HA2	1:F:185:LEU:HD12	1.96	0.47
1:J:182:GLY:HA2	1:J:185:LEU:HD12	1.96	0.47
1:K:189:LEU:HD23	1:K:209:VAL:HB	1.97	0.47
1:N:79:TRP:HE1	1:N:118:LYS:HD2	1.79	0.47
1:N:224:GLU:HA	1:N:227:MET:HE2	1.96	0.47
1:O:182:GLY:HA2	1:O:185:LEU:HD12	1.96	0.47
2:a:77:LYS:HZ1	2:b:78:ALA:HB3	1.78	0.47
2:b:277:ALA:HA	2:Z:5:LYS:NZ	2.30	0.47
4:V:54:LEU:HD23	5:U:161:GLU:C	2.40	0.47
4:c:136:ARG:CZ	5:d:151:ASP:OD2	2.63	0.47
1:D:182:GLY:HA2	1:D:185:LEU:HD12	1.96	0.47
1:H:294:TYR:O	1:H:327:ILE:HG23	2.15	0.47
1:K:263:GLN:HB2	1:K:266:PHE:CE2	2.50	0.47
1:M:182:GLY:HA2	1:M:185:LEU:HD12	1.96	0.47
3:Y:262:ASN:O	3:Y:265:ARG:HG2	2.14	0.47
4:V:204:ARG:HD3	2:i:90:ARG:HD3	1.96	0.47
1:A:213:LYS:HA	1:A:217:CYS:SG	2.54	0.46
1:F:294:TYR:O	1:F:327:ILE:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:238:LYS:HB2	1:I:254:ARG:HD3	1.96	0.46
1:L:26:ALA:HB2	4:V:148:ARG:NH2	2.31	0.46
1:L:367:PRO:O	1:L:370:VAL:HG12	2.14	0.46
1:N:345:ILE:CD1	4:V:177:LYS:HG2	2.45	0.46
1:O:9:VAL:O	1:O:340:TRP:NE1	2.43	0.46
1:Q:182:GLY:HA2	1:Q:185:LEU:HD12	1.96	0.46
2:b:100:ASP:O	2:b:104:GLU:OE1	2.33	0.46
4:V:71:GLU:HA	4:V:74:ARG:HG2	1.97	0.46
2:i:125:ARG:HA	2:i:128:LYS:HZ3	1.78	0.46
5:d:41:LEU:HD11	5:d:72:VAL:HG21	1.97	0.46
1:A:182:GLY:HA2	1:A:185:LEU:HD12	1.96	0.46
1:A:189:LEU:HD23	1:A:209:VAL:HB	1.97	0.46
1:A:224:GLU:HA	1:A:227:MET:HE2	1.96	0.46
1:B:213:LYS:HA	1:B:217:CYS:SG	2.54	0.46
1:B:263:GLN:HB2	1:B:266:PHE:CE2	2.50	0.46
1:D:294:TYR:O	1:D:327:ILE:HG23	2.16	0.46
1:E:367:PRO:O	1:E:370:VAL:HG12	2.14	0.46
1:J:294:TYR:O	1:J:327:ILE:HG23	2.16	0.46
1:M:189:LEU:HD23	1:M:209:VAL:HB	1.97	0.46
1:N:189:LEU:HD23	1:N:209:VAL:HB	1.97	0.46
1:Q:203:THR:HG1	1:R:270:GLU:CD	2.22	0.46
2:a:272:GLU:C	2:a:276:HIS:HD1	2.23	0.46
4:V:114:ILE:O	4:V:118:VAL:HG23	2.15	0.46
5:U:77:PHE:O	5:U:80:MET:HG3	2.15	0.46
3:f:259:TYR:HA	3:f:262:ASN:ND2	2.29	0.46
3:f:267:ARG:HE	5:d:151:ASP:CG	2.23	0.46
1:B:64:ILE:CD1	1:D:171:LEU:CD2	2.93	0.46
1:D:9:VAL:O	1:D:340:TRP:NE1	2.43	0.46
1:M:24:ASP:CG	4:c:188:VAL:HG12	2.40	0.46
1:Q:103:THR:HB	1:Q:132:MET:SD	2.56	0.46
1:Q:263:GLN:HB2	1:Q:266:PHE:CE2	2.50	0.46
2:a:100:ASP:O	2:a:104:GLU:OE1	2.33	0.46
2:a:245:SER:O	2:a:249:LEU:HG	2.15	0.46
2:W:21:ARG:HA	2:W:24:GLN:HG3	1.98	0.46
2:j:100:ASP:O	2:j:104:GLU:OE1	2.33	0.46
1:A:103:THR:HB	1:A:132:MET:SD	2.56	0.46
1:A:198:TYR:CE2	1:A:248:ILE:HD12	2.51	0.46
1:A:367:PRO:O	1:A:370:VAL:HG12	2.14	0.46
1:D:332:PRO:O	1:D:335:ARG:NE	2.48	0.46
1:F:178:LEU:HD22	1:F:277:THR:HG21	1.96	0.46
1:H:44:MET:HE2	1:H:44:MET:HB2	1.86	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:178:LEU:HD22	1:H:277:THR:HG21	1.96	0.46
1:K:37:ARG:NH1	1:K:51:ASP:OD1	2.49	0.46
1:K:103:THR:HB	1:K:132:MET:SD	2.56	0.46
1:K:182:GLY:HA2	1:K:185:LEU:HD12	1.96	0.46
1:K:253:GLU:HG3	1:K:256:ARG:NH2	2.31	0.46
1:K:294:TYR:O	1:K:327:ILE:HG23	2.16	0.46
1:L:182:GLY:HA2	1:L:185:LEU:HD12	1.96	0.46
1:L:198:TYR:CE2	1:L:248:ILE:HD12	2.51	0.46
1:P:253:GLU:HG3	1:P:256:ARG:NH2	2.31	0.46
1:R:189:LEU:HD23	1:R:209:VAL:HB	1.97	0.46
2:W:53:THR:CG2	2:Z:53:THR:HB	2.42	0.46
3:f:208:LYS:HD2	4:c:112:TYR:CE2	2.50	0.46
3:f:224:LEU:HD22	3:f:228:GLN:HE21	1.81	0.46
1:C:253:GLU:HG3	1:C:256:ARG:NH2	2.31	0.46
1:D:263:GLN:HB2	1:D:266:PHE:CE2	2.49	0.46
1:F:40:HIS:CG	1:H:169:TYR:OH	2.69	0.46
1:F:189:LEU:HD23	1:F:209:VAL:HB	1.97	0.46
1:H:253:GLU:HG3	1:H:256:ARG:NH2	2.31	0.46
1:J:198:TYR:CE2	1:J:248:ILE:HD12	2.51	0.46
1:L:263:GLN:HB2	1:L:266:PHE:CE2	2.51	0.46
1:L:294:TYR:O	1:L:327:ILE:HG23	2.16	0.46
1:M:79:TRP:HE1	1:M:118:LYS:HD2	1.79	0.46
1:P:294:TYR:O	1:P:327:ILE:HG23	2.15	0.46
1:P:367:PRO:O	1:P:370:VAL:HG12	2.14	0.46
1:Q:44:MET:HE2	1:Q:44:MET:HB2	1.85	0.46
2:a:231:LYS:HA	2:a:234:GLU:HG2	1.97	0.46
4:V:194:ASN:OD1	4:V:195:ILE:N	2.48	0.46
3:f:229:LEU:HD23	3:f:229:LEU:HA	1.81	0.46
4:c:71:GLU:HA	4:c:74:ARG:HG2	1.97	0.46
1:A:294:TYR:O	1:A:327:ILE:HG23	2.16	0.46
1:B:198:TYR:CE2	1:B:248:ILE:HD12	2.51	0.46
1:F:253:GLU:HG3	1:F:256:ARG:NH2	2.31	0.46
1:G:253:GLU:HG3	1:G:256:ARG:NH2	2.31	0.46
1:J:253:GLU:HG3	1:J:256:ARG:NH2	2.31	0.46
1:L:253:GLU:HG3	1:L:256:ARG:NH2	2.31	0.46
1:M:103:THR:HB	1:M:132:MET:SD	2.56	0.46
1:P:224:GLU:HA	1:P:227:MET:HE2	1.96	0.46
1:Q:79:TRP:HE1	1:Q:118:LYS:HD2	1.79	0.46
1:R:263:GLN:HB2	1:R:266:PHE:CE2	2.51	0.46
2:a:39:LEU:HG	2:b:39:LEU:HB3	1.98	0.46
2:i:195:GLU:HA	2:i:198:LYS:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:i:272:GLU:C	2:i:276:HIS:HD1	2.23	0.46
1:D:44:MET:HE2	1:D:44:MET:HB2	1.86	0.46
1:D:136:ILE:O	1:D:140:LEU:HD23	2.16	0.46
1:D:238:LYS:HB2	1:D:254:ARG:HD3	1.96	0.46
1:F:263:GLN:HB2	1:F:266:PHE:CE2	2.50	0.46
1:G:136:ILE:O	1:G:140:LEU:HD23	2.16	0.46
1:H:189:LEU:HD23	1:H:209:VAL:HB	1.97	0.46
1:H:198:TYR:CE2	1:H:248:ILE:HD12	2.51	0.46
1:I:79:TRP:HE1	1:I:118:LYS:HD2	1.79	0.46
1:I:182:GLY:HA2	1:I:185:LEU:HD12	1.96	0.46
1:I:294:TYR:O	1:I:327:ILE:HG23	2.16	0.46
1:M:294:TYR:O	1:M:327:ILE:HG23	2.16	0.46
1:N:294:TYR:O	1:N:327:ILE:HG23	2.16	0.46
1:O:136:ILE:O	1:O:140:LEU:HD23	2.16	0.46
1:O:294:TYR:O	1:O:327:ILE:HG23	2.16	0.46
1:P:263:GLN:HB2	1:P:266:PHE:CE2	2.50	0.46
1:R:294:TYR:O	1:R:327:ILE:HG23	2.16	0.46
3:f:221:ILE:HA	3:f:224:LEU:HD12	1.96	0.46
4:c:114:ILE:O	4:c:118:VAL:HG23	2.15	0.46
1:A:253:GLU:HG3	1:A:256:ARG:NH2	2.31	0.46
1:C:159:VAL:HB	1:C:161:HIS:CE1	2.51	0.46
1:C:189:LEU:HD23	1:C:209:VAL:HB	1.97	0.46
1:D:253:GLU:HG3	1:D:256:ARG:NH2	2.31	0.46
1:E:224:GLU:HA	1:E:227:MET:HE2	1.96	0.46
1:E:253:GLU:HG3	1:E:256:ARG:NH2	2.31	0.46
1:I:159:VAL:HB	1:I:161:HIS:CE1	2.51	0.46
1:K:136:ILE:O	1:K:140:LEU:HD23	2.16	0.46
1:L:189:LEU:HD23	1:L:209:VAL:HB	1.97	0.46
1:M:136:ILE:O	1:M:140:LEU:HD23	2.16	0.46
1:N:136:ILE:O	1:N:140:LEU:HD23	2.16	0.46
1:N:198:TYR:CE2	1:N:248:ILE:HD12	2.51	0.46
1:N:332:PRO:O	1:N:335:ARG:NE	2.48	0.46
1:O:238:LYS:HB2	1:O:254:ARG:HD3	1.96	0.46
1:P:332:PRO:O	1:P:335:ARG:NE	2.48	0.46
2:i:78:ALA:HA	2:j:78:ALA:HB2	1.97	0.46
2:i:105:ARG:HG3	2:j:106:LEU:HD13	1.97	0.46
1:B:103:THR:HB	1:B:132:MET:SD	2.56	0.46
1:B:294:TYR:O	1:B:327:ILE:HG23	2.16	0.46
1:D:189:LEU:HD23	1:D:209:VAL:HB	1.97	0.46
1:E:251:GLY:N	1:E:253:GLU:OE1	2.46	0.46
1:F:191:LYS:HZ1	1:G:173:HIS:HA	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:103:THR:HB	1:G:132:MET:SD	2.56	0.46
1:J:165:ILE:HG23	1:J:169:TYR:O	2.16	0.46
1:N:253:GLU:HG3	1:N:256:ARG:NH2	2.31	0.46
1:O:44:MET:HE3	1:Q:169:TYR:HA	1.97	0.46
1:O:189:LEU:HD23	1:O:209:VAL:HB	1.97	0.46
1:Q:189:LEU:HD23	1:Q:209:VAL:HB	1.97	0.46
1:Q:198:TYR:CE2	1:Q:248:ILE:HD12	2.51	0.46
1:R:136:ILE:O	1:R:140:LEU:HD23	2.16	0.46
1:R:253:GLU:HG3	1:R:256:ARG:NH2	2.31	0.46
4:V:53:LEU:HD11	5:U:120:MET:HG3	1.97	0.46
5:U:96:GLU:O	5:U:99:ASP:HB2	2.15	0.46
5:U:102:ARG:HH22	5:U:108:ALA:HA	1.80	0.46
1:A:332:PRO:O	1:A:335:ARG:NE	2.48	0.46
1:C:43:VAL:CG2	1:E:374:CYS:O	2.64	0.46
1:C:136:ILE:O	1:C:140:LEU:HD23	2.16	0.46
1:C:332:PRO:O	1:C:335:ARG:NE	2.48	0.46
1:D:40:HIS:CG	1:F:169:TYR:OH	2.69	0.46
1:E:198:TYR:CE2	1:E:248:ILE:HD12	2.51	0.46
1:G:198:TYR:CE2	1:G:248:ILE:HD12	2.51	0.46
1:J:332:PRO:O	1:J:335:ARG:NE	2.48	0.46
1:K:159:VAL:HB	1:K:161:HIS:CE1	2.51	0.46
1:O:253:GLU:HG3	1:O:256:ARG:NH2	2.31	0.46
1:O:332:PRO:O	1:O:335:ARG:NE	2.48	0.46
1:P:136:ILE:O	1:P:140:LEU:HD23	2.16	0.46
2:b:91:ARG:O	2:b:95:VAL:HG23	2.16	0.46
5:U:77:PHE:CE2	5:U:81:MET:HE3	2.51	0.46
2:j:91:ARG:O	2:j:95:VAL:HG23	2.16	0.46
3:f:237:TRP:NE1	4:c:81:GLN:O	2.46	0.46
5:d:96:GLU:O	5:d:99:ASP:HB2	2.15	0.46
1:A:4:GLU:CD	1:A:5:THR:H	2.24	0.45
1:A:159:VAL:HB	1:A:161:HIS:CE1	2.51	0.45
1:C:103:THR:HB	1:C:132:MET:SD	2.56	0.45
1:C:198:TYR:CE2	1:C:248:ILE:HD12	2.51	0.45
1:E:4:GLU:CD	1:E:5:THR:H	2.24	0.45
1:E:103:THR:HB	1:E:132:MET:SD	2.56	0.45
1:E:332:PRO:O	1:E:335:ARG:NE	2.48	0.45
1:F:103:THR:HB	1:F:132:MET:SD	2.56	0.45
1:I:263:GLN:HB2	1:I:266:PHE:CE2	2.51	0.45
1:J:47:MET:CA	4:V:138:LYS:HE3	2.46	0.45
1:N:263:GLN:HB2	1:N:266:PHE:CE2	2.51	0.45
1:N:345:ILE:HD11	4:V:177:LYS:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:198:TYR:CE2	1:O:248:ILE:HD12	2.51	0.45
1:P:159:VAL:HB	1:P:161:HIS:CE1	2.51	0.45
1:Q:136:ILE:O	1:Q:140:LEU:HD23	2.16	0.45
2:a:143:ILE:O	2:a:147:GLN:HG3	2.16	0.45
2:b:109:ALA:HA	2:b:112:LYS:HE3	1.98	0.45
2:i:137:ASP:O	2:i:141:MET:HG2	2.16	0.45
3:f:200:LYS:HD3	3:f:204:GLU:CD	2.40	0.45
4:c:121:ASN:O	4:c:125:ILE:HG13	2.16	0.45
1:B:153:LEU:HD12	1:B:153:LEU:HA	1.86	0.45
1:E:159:VAL:HB	1:E:161:HIS:CE1	2.51	0.45
1:G:294:TYR:O	1:G:327:ILE:HG23	2.16	0.45
1:I:44:MET:HE3	1:K:169:TYR:CD1	2.52	0.45
1:I:136:ILE:O	1:I:140:LEU:HD23	2.16	0.45
1:J:103:THR:HB	1:J:132:MET:SD	2.56	0.45
1:L:4:GLU:CD	1:L:5:THR:H	2.25	0.45
1:M:159:VAL:HB	1:M:161:HIS:CE1	2.51	0.45
1:P:103:THR:HB	1:P:132:MET:SD	2.56	0.45
1:Q:294:TYR:O	1:Q:327:ILE:HG23	2.16	0.45
1:Q:332:PRO:O	1:Q:335:ARG:NE	2.48	0.45
1:R:332:PRO:O	1:R:335:ARG:NE	2.48	0.45
2:a:94:LEU:HD22	4:c:203:GLY:HA2	1.97	0.45
2:a:137:ASP:O	2:a:141:MET:HG2	2.16	0.45
5:d:77:PHE:O	5:d:80:MET:HG3	2.15	0.45
1:A:136:ILE:O	1:A:140:LEU:HD23	2.16	0.45
1:D:103:THR:HB	1:D:132:MET:SD	2.56	0.45
1:F:198:TYR:CE2	1:F:248:ILE:HD12	2.51	0.45
1:I:103:THR:HB	1:I:132:MET:SD	2.56	0.45
1:I:198:TYR:CE2	1:I:248:ILE:HD12	2.51	0.45
1:N:159:VAL:HB	1:N:161:HIS:CE1	2.51	0.45
1:O:103:THR:HB	1:O:132:MET:SD	2.56	0.45
1:R:159:VAL:HB	1:R:161:HIS:CE1	2.51	0.45
2:a:195:GLU:HA	2:a:198:LYS:HG2	1.98	0.45
2:a:280:ASP:HB3	2:W:8:MET:HE3	1.97	0.45
3:f:245:ALA:N	4:c:76:LEU:HD21	2.32	0.45
1:B:159:VAL:HB	1:B:161:HIS:CE1	2.51	0.45
1:C:294:TYR:O	1:C:327:ILE:HG23	2.16	0.45
1:D:4:GLU:CD	1:D:5:THR:H	2.24	0.45
1:J:136:ILE:O	1:J:140:LEU:HD23	2.16	0.45
1:J:189:LEU:HD23	1:J:209:VAL:HB	1.97	0.45
1:N:4:GLU:CD	1:N:5:THR:H	2.24	0.45
1:P:198:TYR:CE2	1:P:248:ILE:HD12	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:185:LEU:HD21	1:Q:261:LEU:HD13	1.99	0.45
1:R:4:GLU:CD	1:R:5:THR:H	2.24	0.45
1:R:198:TYR:CE2	1:R:248:ILE:HD12	2.51	0.45
5:d:102:ARG:HH22	5:d:108:ALA:HA	1.80	0.45
1:A:185:LEU:HD21	1:A:261:LEU:HD13	1.98	0.45
1:F:191:LYS:NZ	1:G:173:HIS:HA	2.32	0.45
1:F:332:PRO:O	1:F:335:ARG:NE	2.48	0.45
1:G:263:GLN:HB2	1:G:266:PHE:CE2	2.51	0.45
1:H:103:THR:HB	1:H:132:MET:SD	2.56	0.45
1:J:44:MET:HE2	1:J:44:MET:HB2	1.85	0.45
1:P:4:GLU:CD	1:P:5:THR:H	2.24	0.45
1:P:45:VAL:HG13	1:R:346:LEU:HD22	1.98	0.45
1:Q:4:GLU:CD	1:Q:5:THR:H	2.24	0.45
1:R:103:THR:HB	1:R:132:MET:SD	2.56	0.45
2:W:12:LYS:HA	2:Z:11:LEU:HD11	1.97	0.45
3:Y:200:LYS:HD3	3:Y:204:GLU:CD	2.40	0.45
4:V:50:LYS:HE3	5:U:156:PHE:CE2	2.52	0.45
2:i:71:LEU:HD22	2:j:70:LYS:CE	2.47	0.45
1:B:136:ILE:O	1:B:140:LEU:HD23	2.16	0.45
1:I:253:GLU:HG3	1:I:256:ARG:NH2	2.31	0.45
1:J:4:GLU:CD	1:J:5:THR:H	2.24	0.45
1:K:198:TYR:CE2	1:K:248:ILE:HD12	2.51	0.45
1:L:159:VAL:HB	1:L:161:HIS:CE1	2.51	0.45
1:M:263:GLN:HB2	1:M:266:PHE:CE2	2.52	0.45
5:U:53:THR:H	5:U:56:GLU:CG	2.30	0.45
2:i:99:LEU:HD22	2:j:95:VAL:HG13	1.98	0.45
2:i:231:LYS:HA	2:i:234:GLU:HG2	1.97	0.45
3:f:245:ALA:CA	4:c:76:LEU:HD21	2.45	0.45
5:d:77:PHE:CE2	5:d:81:MET:HE3	2.51	0.45
1:B:253:GLU:HG3	1:B:256:ARG:NH2	2.31	0.45
1:C:252:ASN:HA	1:C:255:PHE:CZ	2.52	0.45
1:E:64:ILE:HG12	1:G:169:TYR:CE2	2.51	0.45
1:E:294:TYR:O	1:E:327:ILE:HG23	2.16	0.45
1:G:4:GLU:CD	1:G:5:THR:H	2.25	0.45
1:G:159:VAL:HB	1:G:161:HIS:CE1	2.51	0.45
1:G:332:PRO:O	1:G:335:ARG:NE	2.48	0.45
1:J:44:MET:HE1	1:L:169:TYR:HD1	1.82	0.45
1:K:4:GLU:CD	1:K:5:THR:H	2.24	0.45
1:L:252:ASN:HA	1:L:255:PHE:CZ	2.52	0.45
1:M:198:TYR:CE2	1:M:248:ILE:HD12	2.51	0.45
1:M:253:GLU:HG3	1:M:256:ARG:NH2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:213:LYS:HG3	1:N:217:CYS:SG	2.57	0.45
1:O:239:SER:OG	1:O:247:VAL:HG22	2.17	0.45
1:R:213:LYS:HG3	1:R:217:CYS:SG	2.57	0.45
2:W:19:LEU:O	2:W:22:ALA:HB3	2.17	0.45
2:i:94:LEU:O	2:i:97:GLU:HG2	2.17	0.45
3:f:208:LYS:HD2	4:c:112:TYR:HE2	1.81	0.45
3:f:226:GLU:HA	4:c:90:PHE:CD1	2.51	0.45
1:B:213:LYS:HG3	1:B:217:CYS:SG	2.57	0.45
1:D:221:LEU:HA	1:D:315:LYS:HZ1	1.82	0.45
1:D:239:SER:OG	1:D:247:VAL:HG22	2.17	0.45
1:F:136:ILE:O	1:F:140:LEU:HD23	2.16	0.45
1:G:165:ILE:HG23	1:G:169:TYR:O	2.17	0.45
1:G:213:LYS:HG3	1:G:217:CYS:SG	2.57	0.45
1:H:136:ILE:O	1:H:140:LEU:HD23	2.16	0.45
1:J:252:ASN:HA	1:J:255:PHE:CZ	2.52	0.45
1:L:103:THR:HB	1:L:132:MET:SD	2.56	0.45
1:M:35:VAL:CG1	1:M:37:ARG:NH2	2.79	0.45
1:M:239:SER:OG	1:M:247:VAL:HG22	2.17	0.45
1:N:298:VAL:HG12	1:N:330:ILE:HG22	1.99	0.45
1:P:279:TYR:CD2	1:P:283:MET:HE1	2.52	0.45
1:P:298:VAL:HG12	1:P:330:ILE:HG22	1.99	0.45
1:Q:159:VAL:HB	1:Q:161:HIS:CE1	2.51	0.45
1:Q:253:GLU:HG3	1:Q:256:ARG:NH2	2.31	0.45
1:R:279:TYR:CD2	1:R:283:MET:HE1	2.52	0.45
2:i:143:ILE:O	2:i:147:GLN:HG3	2.16	0.45
2:j:109:ALA:HA	2:j:112:LYS:HE3	1.98	0.45
1:A:213:LYS:HG3	1:A:217:CYS:SG	2.57	0.45
1:D:159:VAL:HB	1:D:161:HIS:CE1	2.51	0.45
1:E:252:ASN:HA	1:E:255:PHE:CZ	2.52	0.45
1:E:263:GLN:HB2	1:E:266:PHE:CE2	2.52	0.45
1:F:239:SER:OG	1:F:247:VAL:HG22	2.17	0.45
1:F:252:ASN:HA	1:F:255:PHE:CZ	2.52	0.45
1:G:279:TYR:CD2	1:G:283:MET:HE1	2.52	0.45
1:H:159:VAL:HB	1:H:161:HIS:CE1	2.51	0.45
1:J:159:VAL:HB	1:J:161:HIS:CE1	2.51	0.45
1:L:213:LYS:HG3	1:L:217:CYS:SG	2.57	0.45
1:N:252:ASN:HA	1:N:255:PHE:CZ	2.52	0.45
1:O:4:GLU:CD	1:O:5:THR:H	2.24	0.45
1:O:159:VAL:HB	1:O:161:HIS:CE1	2.51	0.45
1:Q:239:SER:OG	1:Q:247:VAL:HG22	2.17	0.45
3:X:142:ASN:C	3:X:146:LYS:NZ	2.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:121:ASN:O	4:V:125:ILE:HG13	2.16	0.45
2:i:126:GLY:O	2:i:127:MET:C	2.60	0.45
2:g:57:LEU:HB2	2:h:57:LEU:HD21	1.98	0.45
1:C:4:GLU:CD	1:C:5:THR:H	2.24	0.45
1:E:136:ILE:O	1:E:140:LEU:HD23	2.16	0.45
1:F:153:LEU:HD12	1:F:153:LEU:HA	1.86	0.45
1:G:30:VAL:HG21	1:G:337:TYR:CE1	2.52	0.45
1:H:263:GLN:HB2	1:H:266:PHE:CE2	2.51	0.45
1:I:59:GLN:OE1	1:I:59:GLN:HA	2.17	0.45
1:I:180:LEU:HA	1:I:184:ASP:OD2	2.18	0.45
1:I:213:LYS:HG3	1:I:217:CYS:SG	2.57	0.45
1:L:136:ILE:O	1:L:140:LEU:HD23	2.16	0.45
1:L:279:TYR:CD2	1:L:283:MET:HE1	2.52	0.45
1:M:44:MET:CE	1:O:169:TYR:HA	2.47	0.45
1:M:332:PRO:O	1:M:335:ARG:NE	2.48	0.45
1:N:30:VAL:HG21	1:N:337:TYR:CE1	2.52	0.45
1:R:298:VAL:HG12	1:R:330:ILE:HG22	1.99	0.45
2:g:19:LEU:O	2:g:22:ALA:HB3	2.17	0.45
2:g:21:ARG:HA	2:g:24:GLN:HG3	1.98	0.45
1:A:279:TYR:CD2	1:A:283:MET:HE1	2.52	0.44
1:A:298:VAL:HG12	1:A:330:ILE:HG22	1.99	0.44
1:E:59:GLN:OE1	1:E:59:GLN:HA	2.18	0.44
1:E:279:TYR:CD2	1:E:283:MET:HE1	2.52	0.44
1:F:159:VAL:HB	1:F:161:HIS:CE1	2.51	0.44
1:G:59:GLN:HA	1:G:59:GLN:OE1	2.18	0.44
1:K:332:PRO:O	1:K:335:ARG:NE	2.48	0.44
1:L:298:VAL:HG12	1:L:330:ILE:HG22	1.99	0.44
1:M:4:GLU:CD	1:M:5:THR:H	2.24	0.44
1:N:103:THR:HB	1:N:132:MET:SD	2.56	0.44
1:N:279:TYR:CD2	1:N:283:MET:HE1	2.52	0.44
1:O:213:LYS:HG3	1:O:217:CYS:SG	2.57	0.44
1:P:59:GLN:OE1	1:P:59:GLN:HA	2.18	0.44
1:P:213:LYS:HG3	1:P:217:CYS:SG	2.57	0.44
1:R:239:SER:OG	1:R:247:VAL:HG22	2.17	0.44
2:i:178:ARG:HH21	2:i:181:GLU:CD	2.25	0.44
3:f:268:ILE:HD12	4:c:128:LEU:HD13	1.99	0.44
1:A:30:VAL:HG21	1:A:337:TYR:CE1	2.52	0.44
1:A:239:SER:OG	1:A:247:VAL:HG22	2.17	0.44
1:B:59:GLN:HA	1:B:59:GLN:OE1	2.18	0.44
1:D:30:VAL:HG21	1:D:337:TYR:CE1	2.52	0.44
1:D:198:TYR:CE2	1:D:248:ILE:HD12	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:252:ASN:HA	1:D:255:PHE:CZ	2.52	0.44
1:E:213:LYS:HG3	1:E:217:CYS:SG	2.57	0.44
1:F:4:GLU:CD	1:F:5:THR:H	2.24	0.44
1:G:76:ILE:HG12	1:G:115:ASN:HD21	1.83	0.44
1:G:298:VAL:HG12	1:G:330:ILE:HG22	1.99	0.44
1:H:180:LEU:HA	1:H:184:ASP:OD2	2.18	0.44
1:H:252:ASN:HA	1:H:255:PHE:CZ	2.52	0.44
1:H:328:LYS:NZ	2:i:257:GLU:OE1	2.42	0.44
1:J:95:ARG:HD2	3:Y:265:ARG:CZ	2.47	0.44
1:J:213:LYS:HG3	1:J:217:CYS:SG	2.57	0.44
1:J:298:VAL:HG12	1:J:330:ILE:HG22	1.99	0.44
1:K:252:ASN:HA	1:K:255:PHE:CZ	2.52	0.44
1:L:180:LEU:HA	1:L:184:ASP:OD2	2.18	0.44
1:L:239:SER:OG	1:L:247:VAL:HG22	2.17	0.44
1:M:35:VAL:HG13	1:M:37:ARG:HH22	1.82	0.44
1:M:213:LYS:HG3	1:M:217:CYS:SG	2.57	0.44
1:N:239:SER:OG	1:N:247:VAL:HG22	2.17	0.44
1:P:30:VAL:HG21	1:P:337:TYR:CE1	2.52	0.44
1:Q:213:LYS:HG3	1:Q:217:CYS:SG	2.57	0.44
1:R:252:ASN:HA	1:R:255:PHE:CZ	2.52	0.44
3:X:146:LYS:HE2	3:X:146:LYS:HB2	1.57	0.44
1:B:282:ILE:HD13	1:B:294:TYR:CE1	2.53	0.44
1:C:279:TYR:CD2	1:C:283:MET:HE1	2.52	0.44
1:E:30:VAL:HG21	1:E:337:TYR:CE1	2.52	0.44
1:F:59:GLN:OE1	1:F:59:GLN:HA	2.18	0.44
1:H:298:VAL:HG12	1:H:330:ILE:HG22	1.99	0.44
1:I:279:TYR:CD2	1:I:283:MET:HE1	2.52	0.44
1:L:227:MET:HG3	1:L:252:ASN:HB2	2.00	0.44
1:M:76:ILE:HG12	1:M:115:ASN:HD21	1.83	0.44
1:M:252:ASN:HA	1:M:255:PHE:CZ	2.52	0.44
1:N:180:LEU:HA	1:N:184:ASP:OD2	2.17	0.44
1:O:180:LEU:HA	1:O:184:ASP:OD2	2.18	0.44
1:O:227:MET:HG3	1:O:252:ASN:HB2	2.00	0.44
3:f:271:ASN:OD1	4:c:136:ARG:NH1	2.50	0.44
1:A:180:LEU:HA	1:A:184:ASP:OD2	2.18	0.44
1:A:263:GLN:HB2	1:A:266:PHE:CE2	2.53	0.44
1:B:4:GLU:CD	1:B:5:THR:H	2.24	0.44
1:B:37:ARG:CZ	1:B:37:ARG:HB2	2.48	0.44
1:B:224:GLU:H	1:B:224:GLU:CD	2.26	0.44
1:B:252:ASN:HA	1:B:255:PHE:CZ	2.52	0.44
1:C:180:LEU:HA	1:C:184:ASP:OD2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:298:VAL:HG12	1:E:330:ILE:HG22	1.99	0.44
1:F:180:LEU:HA	1:F:184:ASP:OD2	2.17	0.44
1:H:4:GLU:CD	1:H:5:THR:H	2.24	0.44
1:I:252:ASN:HA	1:I:255:PHE:CZ	2.52	0.44
1:I:282:ILE:HD13	1:I:294:TYR:CE1	2.53	0.44
1:I:332:PRO:O	1:I:335:ARG:NE	2.48	0.44
1:J:227:MET:HG3	1:J:252:ASN:HB2	2.00	0.44
1:K:239:SER:OG	1:K:247:VAL:HG22	2.17	0.44
1:L:282:ILE:HD13	1:L:294:TYR:CE1	2.53	0.44
1:P:76:ILE:HG12	1:P:115:ASN:HD21	1.83	0.44
1:P:252:ASN:HA	1:P:255:PHE:CZ	2.52	0.44
1:R:30:VAL:HG21	1:R:337:TYR:CE1	2.52	0.44
1:C:213:LYS:HG3	1:C:217:CYS:SG	2.57	0.44
1:C:298:VAL:HG12	1:C:330:ILE:HG22	1.99	0.44
1:F:227:MET:HG3	1:F:252:ASN:HB2	2.00	0.44
1:G:282:ILE:HD13	1:G:294:TYR:CE1	2.53	0.44
1:H:59:GLN:OE1	1:H:59:GLN:HA	2.18	0.44
1:I:224:GLU:H	1:I:224:GLU:CD	2.26	0.44
1:K:282:ILE:HD13	1:K:294:TYR:CE1	2.53	0.44
1:M:227:MET:HG3	1:M:252:ASN:HB2	2.00	0.44
1:N:282:ILE:HD13	1:N:294:TYR:CE1	2.53	0.44
1:O:30:VAL:HG21	1:O:337:TYR:CE1	2.52	0.44
1:R:227:MET:HG3	1:R:252:ASN:HB2	2.00	0.44
2:i:182:ARG:O	2:i:185:LEU:HG	2.18	0.44
3:f:234:LYS:HG3	4:c:83:LEU:HD13	2.00	0.44
5:d:73:ASP:O	5:d:77:PHE:HB2	2.17	0.44
1:A:39:ARG:HD3	1:B:268:GLY:HA2	1.99	0.44
1:B:279:TYR:CD2	1:B:283:MET:HE1	2.52	0.44
1:D:59:GLN:OE1	1:D:59:GLN:HA	2.18	0.44
1:D:76:ILE:HG12	1:D:115:ASN:HD21	1.83	0.44
1:D:180:LEU:HA	1:D:184:ASP:OD2	2.18	0.44
1:F:30:VAL:HG21	1:F:337:TYR:CE1	2.52	0.44
1:I:4:GLU:CD	1:I:5:THR:H	2.24	0.44
1:J:282:ILE:HD13	1:J:294:TYR:CE1	2.53	0.44
1:K:213:LYS:HG3	1:K:217:CYS:SG	2.57	0.44
1:M:30:VAL:HG21	1:M:337:TYR:CE1	2.52	0.44
1:Q:279:TYR:CD2	1:Q:283:MET:HE1	2.52	0.44
2:a:94:LEU:O	2:a:97:GLU:HG2	2.17	0.44
3:e:107:GLU:HA	3:e:110:PHE:CD2	2.53	0.44
5:d:53:THR:H	5:d:56:GLU:CG	2.30	0.44
1:A:252:ASN:HA	1:A:255:PHE:CZ	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:GLY:HA3	1:D:286:ASP:OD2	2.16	0.44
1:B:239:SER:OG	1:B:247:VAL:HG22	2.17	0.44
1:C:30:VAL:HG21	1:C:337:TYR:CE1	2.52	0.44
1:F:37:ARG:NH2	1:F:81:ASP:CG	2.76	0.44
1:G:153:LEU:HD12	1:G:153:LEU:HA	1.86	0.44
1:H:37:ARG:NH2	1:H:81:ASP:OD1	2.51	0.44
1:H:213:LYS:HG3	1:H:217:CYS:SG	2.57	0.44
1:H:239:SER:OG	1:H:247:VAL:HG22	2.17	0.44
1:K:30:VAL:HG21	1:K:337:TYR:CE1	2.52	0.44
1:M:180:LEU:HA	1:M:184:ASP:OD2	2.17	0.44
1:N:227:MET:HG3	1:N:252:ASN:HB2	2.00	0.44
1:O:224:GLU:H	1:O:224:GLU:CD	2.26	0.44
1:Q:76:ILE:HG12	1:Q:115:ASN:HD21	1.83	0.44
2:a:141:MET:HE1	2:b:141:MET:CA	2.48	0.44
5:U:73:ASP:O	5:U:77:PHE:HB2	2.17	0.44
1:A:39:ARG:HD3	1:B:268:GLY:CA	2.48	0.44
1:A:227:MET:HG3	1:A:252:ASN:HB2	2.00	0.44
1:B:76:ILE:HG12	1:B:115:ASN:HD21	1.83	0.44
1:D:227:MET:HG3	1:D:252:ASN:HB2	2.00	0.44
1:E:180:LEU:HA	1:E:184:ASP:OD2	2.18	0.44
1:E:282:ILE:HD13	1:E:294:TYR:CE1	2.53	0.44
1:F:279:TYR:CD2	1:F:283:MET:HE1	2.52	0.44
1:G:252:ASN:HA	1:G:255:PHE:CZ	2.52	0.44
1:H:279:TYR:CD2	1:H:283:MET:HE1	2.52	0.44
1:I:64:ILE:HG12	1:K:169:TYR:CE2	2.53	0.44
1:K:180:LEU:HA	1:K:184:ASP:OD2	2.17	0.44
1:K:188:TYR:O	1:K:191:LYS:HG3	2.18	0.44
1:L:44:MET:HE2	1:L:44:MET:HB2	1.85	0.44
1:L:153:LEU:HD12	1:L:153:LEU:HA	1.86	0.44
1:M:188:TYR:O	1:M:191:LYS:HG3	2.18	0.44
1:M:282:ILE:HD13	1:M:294:TYR:CE1	2.53	0.44
1:O:188:TYR:O	1:O:191:LYS:HG3	2.18	0.44
1:P:239:SER:OG	1:P:247:VAL:HG22	2.17	0.44
1:P:282:ILE:HD13	1:P:294:TYR:CE1	2.53	0.44
2:a:126:GLY:O	2:a:127:MET:C	2.60	0.44
3:X:107:GLU:HA	3:X:110:PHE:CD2	2.53	0.44
1:C:188:TYR:O	1:C:191:LYS:HG3	2.18	0.44
1:C:282:ILE:HD13	1:C:294:TYR:CE1	2.53	0.44
1:D:188:TYR:O	1:D:191:LYS:HG3	2.18	0.44
1:D:213:LYS:HG3	1:D:217:CYS:SG	2.57	0.44
1:D:282:ILE:HD13	1:D:294:TYR:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:282:ILE:HD13	1:F:294:TYR:CE1	2.53	0.44
1:G:239:SER:OG	1:G:247:VAL:HG22	2.17	0.44
1:H:227:MET:HG3	1:H:252:ASN:HB2	2.00	0.44
1:H:282:ILE:HD13	1:H:294:TYR:CE1	2.53	0.44
1:I:68:LYS:NZ	1:I:77:THR:HG21	2.33	0.44
1:J:239:SER:OG	1:J:247:VAL:HG22	2.17	0.44
1:J:279:TYR:CD2	1:J:283:MET:HE1	2.52	0.44
1:K:76:ILE:HG12	1:K:115:ASN:HD21	1.83	0.44
1:K:279:TYR:CD2	1:K:283:MET:HE1	2.52	0.44
1:Q:227:MET:HG3	1:Q:252:ASN:HB2	2.00	0.44
1:Q:252:ASN:HA	1:Q:255:PHE:CZ	2.52	0.44
2:a:182:ARG:HE	2:b:183:ALA:CB	2.31	0.44
4:V:103:ARG:HA	4:V:106:LYS:NZ	2.33	0.44
3:f:254:PHE:HE1	4:c:121:ASN:ND2	2.15	0.44
3:f:268:ILE:O	3:f:271:ASN:HB2	2.18	0.44
1:A:41:GLN:HE22	1:C:375:PHE:HB2	1.81	0.43
1:A:76:ILE:HG12	1:A:115:ASN:HD21	1.83	0.43
1:C:59:GLN:OE1	1:C:59:GLN:HA	2.18	0.43
1:E:68:LYS:NZ	1:E:77:THR:HG21	2.34	0.43
1:E:227:MET:HG3	1:E:252:ASN:HB2	2.00	0.43
1:E:239:SER:OG	1:E:247:VAL:HG22	2.17	0.43
1:G:188:TYR:O	1:G:191:LYS:HG3	2.18	0.43
1:I:30:VAL:HG21	1:I:337:TYR:CE1	2.52	0.43
1:I:76:ILE:HG12	1:I:115:ASN:HD21	1.83	0.43
1:I:188:TYR:O	1:I:191:LYS:HG3	2.18	0.43
1:I:239:SER:OG	1:I:247:VAL:HG22	2.17	0.43
1:J:30:VAL:HG21	1:J:337:TYR:CE1	2.52	0.43
1:K:227:MET:HG3	1:K:252:ASN:HB2	2.00	0.43
1:M:224:GLU:H	1:M:224:GLU:CD	2.26	0.43
1:M:279:TYR:CD2	1:M:283:MET:HE1	2.52	0.43
1:O:252:ASN:HA	1:O:255:PHE:CZ	2.52	0.43
1:P:188:TYR:O	1:P:191:LYS:HG3	2.18	0.43
1:P:227:MET:HG3	1:P:252:ASN:HB2	2.00	0.43
1:P:288:ASP:OD1	1:P:291:LYS:NZ	2.52	0.43
1:Q:180:LEU:HA	1:Q:184:ASP:OD2	2.18	0.43
1:Q:221:LEU:HA	1:Q:315:LYS:HZ1	1.83	0.43
1:R:68:LYS:NZ	1:R:77:THR:HG21	2.33	0.43
2:a:182:ARG:O	2:a:185:LEU:HG	2.18	0.43
2:b:114:GLU:HG3	4:c:192:ARG:HH22	1.82	0.43
2:i:105:ARG:HD2	2:j:106:LEU:HD13	1.99	0.43
3:e:142:ASN:C	3:e:146:LYS:NZ	2.75	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:d:94:GLU:O	5:d:150:TYR:OH	2.36	0.43
1:B:188:TYR:O	1:B:191:LYS:HG3	2.18	0.43
1:B:288:ASP:OD1	1:B:291:LYS:NZ	2.52	0.43
1:B:332:PRO:O	1:B:335:ARG:NE	2.48	0.43
1:C:227:MET:HG3	1:C:252:ASN:HB2	2.00	0.43
1:D:40:HIS:CE1	1:E:268:GLY:HA2	2.53	0.43
1:D:279:TYR:CD2	1:D:283:MET:HE1	2.52	0.43
1:E:288:ASP:OD1	1:E:291:LYS:NZ	2.52	0.43
1:F:188:TYR:O	1:F:191:LYS:HG3	2.18	0.43
1:F:213:LYS:HG3	1:F:217:CYS:SG	2.57	0.43
1:G:227:MET:HG3	1:G:252:ASN:HB2	2.00	0.43
1:I:144:ALA:CB	1:I:338:SER:HB3	2.48	0.43
1:I:298:VAL:HG12	1:I:330:ILE:HG22	1.99	0.43
1:J:160:THR:HG23	1:J:180:LEU:O	2.19	0.43
1:M:68:LYS:NZ	1:M:77:THR:HG21	2.33	0.43
1:N:68:LYS:NZ	1:N:77:THR:HG21	2.33	0.43
1:N:204:ALA:O	1:N:208:ILE:HG13	2.19	0.43
1:N:288:ASP:OD1	1:N:291:LYS:NZ	2.52	0.43
1:O:279:TYR:CD2	1:O:283:MET:HE1	2.52	0.43
1:Q:68:LYS:NZ	1:Q:77:THR:HG21	2.33	0.43
1:Q:298:VAL:HG12	1:Q:330:ILE:HG22	1.99	0.43
1:R:180:LEU:HA	1:R:184:ASP:OD2	2.18	0.43
2:a:178:ARG:HH21	2:a:181:GLU:CD	2.25	0.43
4:V:104:VAL:HA	4:V:107:VAL:HG12	2.00	0.43
3:f:261:ILE:HD11	4:c:121:ASN:HB3	2.00	0.43
1:E:76:ILE:HG12	1:E:115:ASN:HD21	1.83	0.43
1:F:305:MET:HB2	6:F:401:ADP:C2	2.54	0.43
1:G:180:LEU:HA	1:G:184:ASP:OD2	2.18	0.43
1:G:288:ASP:OD1	1:G:291:LYS:NZ	2.51	0.43
1:H:68:LYS:NZ	1:H:77:THR:HG21	2.34	0.43
1:H:288:ASP:OD1	1:H:291:LYS:NZ	2.52	0.43
1:J:204:ALA:O	1:J:208:ILE:HG13	2.19	0.43
1:K:305:MET:HB2	6:K:401:ADP:C2	2.54	0.43
1:L:160:THR:HG23	1:L:180:LEU:O	2.19	0.43
1:M:298:VAL:HG12	1:M:330:ILE:HG22	1.99	0.43
1:M:305:MET:HB2	6:M:401:ADP:C2	2.54	0.43
1:O:59:GLN:OE1	1:O:59:GLN:HA	2.18	0.43
1:O:298:VAL:HG12	1:O:330:ILE:HG22	1.99	0.43
1:P:64:ILE:HD12	1:P:64:ILE:HA	1.87	0.43
1:Q:165:ILE:HG23	1:Q:169:TYR:C	2.43	0.43
1:R:282:ILE:HD13	1:R:294:TYR:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:133:GLU:O	3:X:137:GLN:HG2	2.19	0.43
1:B:144:ALA:CB	1:B:338:SER:HB3	2.49	0.43
1:C:204:ALA:O	1:C:208:ILE:HG13	2.19	0.43
1:C:288:ASP:OD1	1:C:291:LYS:NZ	2.52	0.43
1:D:68:LYS:NZ	1:D:77:THR:HG21	2.33	0.43
1:D:160:THR:HG23	1:D:180:LEU:O	2.19	0.43
1:D:288:ASP:OD1	1:D:291:LYS:NZ	2.52	0.43
1:D:298:VAL:HG12	1:D:330:ILE:HG22	1.99	0.43
1:F:35:VAL:CG1	1:F:37:ARG:HE	2.31	0.43
1:F:160:THR:HG23	1:F:180:LEU:O	2.19	0.43
1:G:160:THR:HG23	1:G:180:LEU:O	2.19	0.43
1:H:160:THR:HG23	1:H:180:LEU:O	2.19	0.43
1:I:227:MET:HG3	1:I:252:ASN:HB2	2.00	0.43
1:I:305:MET:HB2	6:I:401:ADP:C2	2.54	0.43
1:J:180:LEU:HA	1:J:184:ASP:OD2	2.17	0.43
1:O:282:ILE:HD13	1:O:294:TYR:CE1	2.53	0.43
1:O:288:ASP:OD1	1:O:291:LYS:NZ	2.52	0.43
1:P:160:THR:HG23	1:P:180:LEU:O	2.19	0.43
1:P:180:LEU:HA	1:P:184:ASP:OD2	2.18	0.43
1:P:204:ALA:O	1:P:208:ILE:HG13	2.19	0.43
1:Q:305:MET:HB2	6:Q:401:ADP:C2	2.54	0.43
1:R:160:THR:HG23	1:R:180:LEU:O	2.19	0.43
2:b:87:SER:O	2:b:91:ARG:HG2	2.18	0.43
3:Y:268:ILE:O	3:Y:271:ASN:HB2	2.18	0.43
1:A:224:GLU:H	1:A:224:GLU:CD	2.26	0.43
1:B:30:VAL:HG21	1:B:337:TYR:CE1	2.52	0.43
1:B:204:ALA:O	1:B:208:ILE:HG13	2.19	0.43
1:B:227:MET:HG3	1:B:252:ASN:HB2	2.00	0.43
1:B:298:VAL:HG12	1:B:330:ILE:HG22	1.99	0.43
1:B:305:MET:HB2	6:B:401:ADP:C2	2.54	0.43
1:E:191:LYS:HZ3	1:F:173:HIS:HA	1.81	0.43
1:E:204:ALA:O	1:E:208:ILE:HG13	2.19	0.43
1:F:288:ASP:OD1	1:F:291:LYS:NZ	2.52	0.43
1:G:204:ALA:O	1:G:208:ILE:HG13	2.19	0.43
1:G:294:TYR:HB3	1:G:327:ILE:HG12	2.01	0.43
1:K:144:ALA:CB	1:K:338:SER:HB3	2.49	0.43
1:L:30:VAL:HG21	1:L:337:TYR:CE1	2.52	0.43
1:L:59:GLN:OE1	1:L:59:GLN:HA	2.17	0.43
1:Q:30:VAL:HG21	1:Q:337:TYR:CE1	2.52	0.43
1:Q:282:ILE:HD13	1:Q:294:TYR:CE1	2.53	0.43
1:Q:288:ASP:OD1	1:Q:291:LYS:NZ	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:188:TYR:O	1:R:191:LYS:HG3	2.18	0.43
3:e:123:LEU:O	3:e:127:ILE:HG12	2.18	0.43
4:c:103:ARG:HA	4:c:106:LYS:NZ	2.33	0.43
1:A:288:ASP:OD1	1:A:291:LYS:NZ	2.52	0.43
1:C:68:LYS:NZ	1:C:77:THR:HG21	2.34	0.43
1:C:239:SER:OG	1:C:247:VAL:HG22	2.17	0.43
1:C:294:TYR:HB3	1:C:327:ILE:HG12	2.01	0.43
1:D:305:MET:HB2	6:D:401:ADP:C2	2.54	0.43
1:F:298:VAL:HG12	1:F:330:ILE:HG22	1.99	0.43
1:J:171:LEU:O	1:J:175:ILE:HG13	2.19	0.43
1:K:59:GLN:OE1	1:K:59:GLN:HA	2.18	0.43
1:K:298:VAL:HG12	1:K:330:ILE:HG22	1.99	0.43
1:M:44:MET:HE2	1:M:44:MET:HB2	1.86	0.43
1:M:59:GLN:OE1	1:M:59:GLN:HA	2.18	0.43
1:M:160:THR:HG23	1:M:180:LEU:O	2.18	0.43
1:N:76:ILE:HG12	1:N:115:ASN:HD21	1.83	0.43
1:N:160:THR:HG23	1:N:180:LEU:O	2.19	0.43
1:N:188:TYR:O	1:N:191:LYS:HG3	2.18	0.43
1:O:160:THR:HG23	1:O:180:LEU:O	2.19	0.43
1:O:305:MET:HB2	6:O:401:ADP:C2	2.54	0.43
3:X:123:LEU:O	3:X:127:ILE:HG12	2.18	0.43
2:j:87:SER:O	2:j:91:ARG:HG2	2.18	0.43
3:e:133:GLU:O	3:e:137:GLN:HG2	2.18	0.43
3:f:268:ILE:HA	3:f:271:ASN:ND2	2.33	0.43
1:A:144:ALA:CB	1:A:338:SER:HB3	2.49	0.43
1:A:171:LEU:O	1:A:175:ILE:HG13	2.19	0.43
1:E:160:THR:HG23	1:E:180:LEU:O	2.19	0.43
1:E:294:TYR:HB3	1:E:327:ILE:HG12	2.01	0.43
1:F:221:LEU:HA	1:F:315:LYS:HZ1	1.84	0.43
1:G:68:LYS:HZ1	1:G:77:THR:HG21	1.84	0.43
1:H:221:LEU:HA	1:H:315:LYS:HZ1	1.84	0.43
1:H:294:TYR:HB3	1:H:327:ILE:HG12	2.01	0.43
1:J:59:GLN:HA	1:J:59:GLN:OE1	2.18	0.43
1:K:171:LEU:O	1:K:175:ILE:HG13	2.19	0.43
1:M:171:LEU:O	1:M:175:ILE:HG13	2.19	0.43
1:O:68:LYS:NZ	1:O:77:THR:HG21	2.34	0.43
1:Q:294:TYR:HB3	1:Q:327:ILE:HG12	2.01	0.43
1:R:332:PRO:HB3	2:j:51:LYS:CE	2.49	0.43
5:U:124:THR:OG1	5:U:126:GLU:HG2	2.19	0.43
2:j:90:ARG:O	2:j:93:GLN:HG3	2.19	0.43
1:A:68:LYS:NZ	1:A:77:THR:HG21	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:ILE:HD13	1:A:294:TYR:CE1	2.53	0.43
1:B:61:LYS:HE3	1:D:167:GLU:HG3	2.00	0.43
1:B:171:LEU:O	1:B:175:ILE:HG13	2.19	0.43
1:B:180:LEU:HA	1:B:184:ASP:OD2	2.18	0.43
1:C:305:MET:HB2	6:C:401:ADP:C2	2.54	0.43
1:D:294:TYR:HB3	1:D:327:ILE:HG12	2.01	0.43
1:E:188:TYR:O	1:E:191:LYS:HG3	2.18	0.43
1:H:30:VAL:HG21	1:H:337:TYR:CE1	2.52	0.43
1:H:76:ILE:HG12	1:H:115:ASN:HD21	1.83	0.43
1:I:294:TYR:HB3	1:I:327:ILE:HG12	2.01	0.43
1:J:172:PRO:HA	1:J:175:ILE:HD12	2.01	0.43
1:J:224:GLU:H	1:J:224:GLU:CD	2.26	0.43
1:J:294:TYR:HB3	1:J:327:ILE:HG12	2.01	0.43
1:L:68:LYS:NZ	1:L:77:THR:HG21	2.33	0.43
1:N:59:GLN:OE1	1:N:59:GLN:HA	2.18	0.43
1:O:204:ALA:O	1:O:208:ILE:HG13	2.19	0.43
1:Q:188:TYR:O	1:Q:191:LYS:HG3	2.18	0.43
1:Q:204:ALA:O	1:Q:208:ILE:HG13	2.19	0.43
1:R:204:ALA:O	1:R:208:ILE:HG13	2.19	0.43
4:V:45:ARG:O	4:V:49:LEU:HG	2.19	0.43
4:V:205:LYS:HB2	4:V:210:SER:HB2	2.00	0.43
3:f:245:ALA:HB2	4:c:76:LEU:HD11	2.01	0.43
4:c:135:LEU:HA	4:c:138:LYS:CD	2.40	0.43
4:c:205:LYS:HB2	4:c:210:SER:HB2	2.00	0.43
1:A:59:GLN:OE1	1:A:59:GLN:HA	2.18	0.43
1:A:153:LEU:HD12	1:A:153:LEU:HA	1.86	0.43
1:A:188:TYR:O	1:A:191:LYS:HG3	2.18	0.43
1:E:44:MET:HE1	1:G:169:TYR:HD1	1.84	0.43
1:F:68:LYS:NZ	1:F:77:THR:HG21	2.33	0.43
1:G:224:GLU:H	1:G:224:GLU:CD	2.26	0.43
1:H:188:TYR:O	1:H:191:LYS:HG3	2.18	0.43
1:I:171:LEU:O	1:I:175:ILE:HG13	2.19	0.43
1:J:76:ILE:HG12	1:J:115:ASN:HD21	1.83	0.43
1:J:144:ALA:CB	1:J:338:SER:HB3	2.49	0.43
1:K:294:TYR:HB3	1:K:327:ILE:HG12	2.01	0.43
1:L:76:ILE:HG12	1:L:115:ASN:HD21	1.83	0.43
1:L:144:ALA:CB	1:L:338:SER:HB3	2.49	0.43
1:L:288:ASP:OD1	1:L:291:LYS:NZ	2.52	0.43
1:M:330:ILE:HD12	1:M:330:ILE:HA	1.95	0.43
1:N:294:TYR:HB3	1:N:327:ILE:HG12	2.01	0.43
1:P:44:MET:HG3	1:R:139:VAL:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:171:LEU:O	1:P:175:ILE:HG13	2.19	0.43
1:Q:59:GLN:OE1	1:Q:59:GLN:HA	2.17	0.43
1:Q:160:THR:HG23	1:Q:180:LEU:O	2.19	0.43
1:Q:224:GLU:H	1:Q:224:GLU:CD	2.26	0.43
1:R:76:ILE:HG12	1:R:115:ASN:HD21	1.83	0.43
2:a:46:LEU:HD13	2:a:49:LYS:HE3	2.00	0.43
2:Z:12:LYS:O	2:Z:16:GLU:HG3	2.19	0.43
1:C:221:LEU:HA	1:C:315:LYS:HZ1	1.84	0.43
1:C:224:GLU:H	1:C:224:GLU:CD	2.26	0.43
1:D:153:LEU:HD12	1:D:153:LEU:HA	1.86	0.43
1:D:204:ALA:O	1:D:208:ILE:HG13	2.19	0.43
1:F:76:ILE:HG12	1:F:115:ASN:HD21	1.83	0.43
1:F:224:GLU:H	1:F:224:GLU:CD	2.26	0.43
1:F:294:TYR:HB3	1:F:327:ILE:HG12	2.01	0.43
1:G:144:ALA:CB	1:G:338:SER:HB3	2.49	0.43
1:H:144:ALA:CB	1:H:338:SER:HB3	2.49	0.43
1:H:171:LEU:O	1:H:175:ILE:HG13	2.19	0.43
1:I:204:ALA:O	1:I:208:ILE:HG13	2.19	0.43
1:K:288:ASP:OD1	1:K:291:LYS:NZ	2.51	0.43
1:M:144:ALA:CB	1:M:338:SER:HB3	2.49	0.43
1:M:288:ASP:OD1	1:M:291:LYS:NZ	2.52	0.43
1:M:294:TYR:HB3	1:M:327:ILE:HG12	2.01	0.43
1:O:76:ILE:HG12	1:O:115:ASN:HD21	1.83	0.43
1:O:171:LEU:O	1:O:175:ILE:HG13	2.19	0.43
1:R:224:GLU:H	1:R:224:GLU:CD	2.26	0.43
2:a:29:LYS:NZ	2:b:28:ASP:OD1	2.45	0.43
2:a:56:GLU:HB3	2:a:60:TYR:CE2	2.54	0.43
2:Z:7:LYS:NZ	2:Z:11:LEU:HD13	2.27	0.43
4:c:56:ILE:HG13	5:d:124:THR:HA	2.01	0.43
1:B:294:TYR:HB3	1:B:327:ILE:HG12	2.01	0.42
1:C:160:THR:HG23	1:C:180:LEU:O	2.19	0.42
1:F:204:ALA:O	1:F:208:ILE:HG13	2.19	0.42
1:H:224:GLU:H	1:H:224:GLU:CD	2.26	0.42
1:J:288:ASP:OD1	1:J:291:LYS:NZ	2.51	0.42
1:K:68:LYS:NZ	1:K:77:THR:HG21	2.33	0.42
1:L:294:TYR:HB3	1:L:327:ILE:HG12	2.01	0.42
1:N:171:LEU:O	1:N:175:ILE:HG13	2.19	0.42
1:O:294:TYR:HB3	1:O:327:ILE:HG12	2.01	0.42
1:P:68:LYS:NZ	1:P:77:THR:HG21	2.33	0.42
1:R:288:ASP:OD1	1:R:291:LYS:NZ	2.51	0.42
4:V:122:ILE:HA	4:V:125:ILE:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:i:70:LYS:O	2:i:73:LEU:HG	2.19	0.42
4:c:45:ARG:O	4:c:49:LEU:HG	2.19	0.42
4:c:104:VAL:HA	4:c:107:VAL:HG12	2.00	0.42
5:d:124:THR:OG1	5:d:126:GLU:HG2	2.19	0.42
1:A:160:THR:HG23	1:A:180:LEU:O	2.18	0.42
1:A:204:ALA:O	1:A:208:ILE:HG13	2.19	0.42
1:A:305:MET:HB2	6:A:401:ADP:C2	2.54	0.42
1:E:305:MET:HB2	6:E:401:ADP:C2	2.54	0.42
1:G:221:LEU:HA	1:G:315:LYS:HZ1	1.84	0.42
1:H:305:MET:HB2	6:H:401:ADP:C2	2.54	0.42
1:I:160:THR:HG23	1:I:180:LEU:O	2.19	0.42
1:J:68:LYS:NZ	1:J:77:THR:HG21	2.33	0.42
1:L:291:LYS:HG3	1:L:292:ASP:N	2.34	0.42
1:P:165:ILE:HG23	1:P:169:TYR:O	2.18	0.42
1:P:243:PRO:HB3	1:R:291:LYS:HE3	2.00	0.42
1:P:291:LYS:HG3	1:P:292:ASP:N	2.35	0.42
1:R:144:ALA:CB	1:R:338:SER:HB3	2.49	0.42
1:R:291:LYS:HG3	1:R:292:ASP:N	2.34	0.42
2:i:56:GLU:HB3	2:i:60:TYR:CE2	2.54	0.42
2:i:101:ARG:HB3	2:i:105:ARG:NH2	2.34	0.42
2:i:105:ARG:HG3	2:j:106:LEU:CD1	2.49	0.42
2:h:7:LYS:HZ1	2:h:11:LEU:HB2	1.83	0.42
5:d:153:PHE:CZ	5:d:157:MET:HE1	2.54	0.42
1:A:232:SER:O	1:A:233:SER:C	2.62	0.42
1:F:144:ALA:CB	1:F:338:SER:HB3	2.48	0.42
1:G:291:LYS:HG3	1:G:292:ASP:N	2.35	0.42
1:G:305:MET:HB2	6:G:401:ADP:C2	2.54	0.42
1:H:204:ALA:O	1:H:208:ILE:HG13	2.19	0.42
1:I:288:ASP:OD1	1:I:291:LYS:NZ	2.51	0.42
1:J:185:LEU:HD22	1:J:213:LYS:HE3	2.02	0.42
1:L:171:LEU:O	1:L:175:ILE:HG13	2.19	0.42
1:N:172:PRO:HA	1:N:175:ILE:HD12	2.01	0.42
1:P:144:ALA:CB	1:P:338:SER:HB3	2.48	0.42
1:R:305:MET:HB2	6:R:401:ADP:C2	2.54	0.42
2:a:249:LEU:O	2:a:253:ILE:HG13	2.20	0.42
2:W:46:LEU:HD22	2:Z:46:LEU:HG	2.01	0.42
3:X:117:GLU:O	3:X:120:LEU:HB3	2.19	0.42
4:V:54:LEU:HD23	5:U:161:GLU:OXT	2.19	0.42
5:U:56:GLU:O	5:U:60:MET:HB2	2.19	0.42
3:f:254:PHE:CD1	4:c:118:VAL:HG22	2.54	0.42
4:c:173:LEU:O	4:c:177:LYS:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:ARG:HD2	1:A:206:ARG:NH2	2.35	0.42
1:A:291:LYS:HG3	1:A:292:ASP:N	2.35	0.42
1:B:68:LYS:NZ	1:B:77:THR:HG21	2.33	0.42
1:B:183:ARG:HD2	1:B:206:ARG:NH2	2.35	0.42
1:D:144:ALA:CB	1:D:338:SER:HB3	2.49	0.42
1:F:172:PRO:HA	1:F:175:ILE:HD12	2.01	0.42
1:F:291:LYS:HG3	1:F:292:ASP:N	2.35	0.42
1:G:68:LYS:NZ	1:G:77:THR:HG21	2.33	0.42
1:G:171:LEU:O	1:G:175:ILE:HG13	2.19	0.42
1:H:169:TYR:CZ	1:H:170:ALA:O	2.73	0.42
1:J:188:TYR:O	1:J:191:LYS:HG3	2.18	0.42
1:J:328:LYS:NZ	2:j:215:SER:HB2	2.34	0.42
1:K:44:MET:HE1	1:M:169:TYR:CD1	2.48	0.42
1:K:178:LEU:HD12	1:K:178:LEU:HA	1.84	0.42
1:K:204:ALA:O	1:K:208:ILE:HG13	2.18	0.42
1:M:183:ARG:HD2	1:M:206:ARG:NH2	2.35	0.42
1:P:294:TYR:HB3	1:P:327:ILE:HG12	2.01	0.42
1:Q:144:ALA:CB	1:Q:338:SER:HB3	2.49	0.42
1:Q:171:LEU:O	1:Q:175:ILE:HG13	2.19	0.42
1:R:59:GLN:HA	1:R:59:GLN:OE1	2.18	0.42
1:R:294:TYR:HB3	1:R:327:ILE:HG12	2.01	0.42
2:a:66:ASP:O	2:a:69:GLU:HG3	2.18	0.42
2:i:192:GLU:O	2:i:195:GLU:HG3	2.20	0.42
2:g:1:MET:HB2	2:g:4:ILE:HG13	2.01	0.42
2:h:12:LYS:O	2:h:16:GLU:HG3	2.19	0.42
3:f:215:ARG:HD2	4:c:108:ASP:OD2	2.19	0.42
3:f:226:GLU:N	4:c:90:PHE:CE1	2.88	0.42
1:D:171:LEU:O	1:D:175:ILE:HG13	2.19	0.42
1:D:291:LYS:HG3	1:D:292:ASP:N	2.35	0.42
1:G:232:SER:O	1:G:233:SER:C	2.62	0.42
1:H:185:LEU:HD22	1:H:213:LYS:HE3	2.02	0.42
1:K:232:SER:O	1:K:233:SER:C	2.63	0.42
1:L:183:ARG:HD2	1:L:206:ARG:NH2	2.35	0.42
1:L:204:ALA:O	1:L:208:ILE:HG13	2.19	0.42
1:L:224:GLU:H	1:L:224:GLU:CD	2.26	0.42
2:W:1:MET:HB2	2:W:4:ILE:HG13	2.01	0.42
1:C:144:ALA:CB	1:C:338:SER:HB3	2.49	0.42
1:E:144:ALA:CB	1:E:338:SER:HB3	2.49	0.42
1:J:183:ARG:HD2	1:J:206:ARG:NH2	2.35	0.42
1:L:185:LEU:HD22	1:L:213:LYS:HE3	2.01	0.42
1:L:332:PRO:O	1:L:335:ARG:NE	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:204:ALA:O	1:M:208:ILE:HG13	2.19	0.42
1:N:44:MET:HE2	1:N:44:MET:HB2	1.85	0.42
1:N:305:MET:HB2	6:N:401:ADP:C2	2.54	0.42
1:O:144:ALA:CB	1:O:338:SER:HB3	2.49	0.42
1:R:171:LEU:O	1:R:175:ILE:HG13	2.19	0.42
1:R:172:PRO:HA	1:R:175:ILE:HD12	2.01	0.42
1:R:183:ARG:HD2	1:R:206:ARG:NH2	2.35	0.42
3:X:106:ILE:HG13	3:X:110:PHE:CZ	2.54	0.42
4:V:173:LEU:O	4:V:177:LYS:HG3	2.19	0.42
5:U:153:PHE:CZ	5:U:157:MET:HE1	2.54	0.42
3:f:221:ILE:HG22	4:c:94:GLN:OE1	2.18	0.42
5:d:56:GLU:O	5:d:60:MET:HB2	2.19	0.42
1:A:178:LEU:HD12	1:A:178:LEU:HA	1.83	0.42
1:B:160:THR:HG23	1:B:180:LEU:O	2.19	0.42
1:C:171:LEU:O	1:C:175:ILE:HG13	2.19	0.42
1:K:224:GLU:H	1:K:224:GLU:CD	2.26	0.42
1:L:305:MET:HB2	6:L:401:ADP:C2	2.54	0.42
1:O:178:LEU:HD12	1:O:178:LEU:HA	1.83	0.42
1:O:183:ARG:HD2	1:O:206:ARG:NH2	2.35	0.42
1:P:243:PRO:C	1:R:291:LYS:HD3	2.45	0.42
1:Q:185:LEU:HD22	1:Q:213:LYS:HE3	2.02	0.42
1:R:44:MET:HE2	1:R:44:MET:HB2	1.86	0.42
2:i:53:THR:O	2:i:57:LEU:HG	2.20	0.42
2:g:26:GLU:O	2:g:30:LYS:HG2	2.20	0.42
3:e:106:ILE:HG13	3:e:110:PHE:CZ	2.55	0.42
3:e:117:GLU:O	3:e:120:LEU:HB3	2.19	0.42
5:d:111:TYR:CG	5:d:147:ARG:HD2	2.55	0.42
1:B:39:ARG:HG2	1:C:268:GLY:HA2	2.02	0.42
1:B:221:LEU:HA	1:B:315:LYS:HZ1	1.84	0.42
1:E:171:LEU:O	1:E:175:ILE:HG13	2.19	0.42
1:E:291:LYS:HG3	1:E:292:ASP:N	2.35	0.42
1:F:185:LEU:HD22	1:F:213:LYS:HE3	2.02	0.42
1:G:185:LEU:HD22	1:G:213:LYS:HE3	2.01	0.42
1:H:172:PRO:HA	1:H:175:ILE:HD12	2.01	0.42
1:K:183:ARG:HD2	1:K:206:ARG:NH2	2.35	0.42
1:K:291:LYS:HG3	1:K:292:ASP:N	2.35	0.42
1:L:188:TYR:O	1:L:191:LYS:HG3	2.18	0.42
1:M:291:LYS:HG3	1:M:292:ASP:N	2.35	0.42
1:N:224:GLU:H	1:N:224:GLU:CD	2.26	0.42
2:a:70:LYS:O	2:a:73:LEU:HG	2.19	0.42
2:b:249:LEU:O	2:b:253:ILE:HG13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:97:LYS:HA	3:X:100:ASN:OD1	2.20	0.42
2:i:66:ASP:O	2:i:69:GLU:HG3	2.18	0.42
4:c:48:GLN:NE2	4:c:49:LEU:HD23	2.35	0.42
1:C:185:LEU:HD22	1:C:213:LYS:HE3	2.02	0.42
1:D:183:ARG:HD2	1:D:206:ARG:NH2	2.35	0.42
1:F:312:ARG:O	1:F:316:GLU:HG2	2.20	0.42
1:G:330:ILE:HD12	1:G:330:ILE:HA	1.95	0.42
1:H:291:LYS:HG3	1:H:292:ASP:N	2.35	0.42
1:I:155:SER:HA	1:I:160:THR:HG22	2.02	0.42
1:I:312:ARG:O	1:I:316:GLU:HG2	2.20	0.42
1:I:362:TYR:HE2	3:f:201:ARG:NH2	2.18	0.42
1:M:185:LEU:HD22	1:M:213:LYS:HE3	2.02	0.42
1:M:203:THR:O	1:M:206:ARG:HB2	2.20	0.42
1:N:144:ALA:CB	1:N:338:SER:HB3	2.49	0.42
1:P:185:LEU:HD22	1:P:213:LYS:HE3	2.02	0.42
1:P:203:THR:O	1:P:206:ARG:HB2	2.20	0.42
1:P:224:GLU:H	1:P:224:GLU:CD	2.26	0.42
1:P:305:MET:HB2	6:P:401:ADP:C2	2.54	0.42
1:Q:312:ARG:O	1:Q:316:GLU:HG2	2.20	0.42
1:R:68:LYS:HZ1	1:R:77:THR:HG21	1.84	0.42
1:R:178:LEU:HD12	1:R:178:LEU:HA	1.83	0.42
1:R:185:LEU:HD22	1:R:213:LYS:HE3	2.01	0.42
2:a:101:ARG:HB3	2:a:105:ARG:NH2	2.34	0.42
5:U:94:GLU:O	5:U:150:TYR:OH	2.36	0.42
2:g:53:THR:HG23	2:h:57:LEU:CD1	2.50	0.42
4:c:84:GLU:OE1	4:c:84:GLU:N	2.53	0.42
4:c:174:LYS:CG	4:c:178:LYS:HZ3	2.23	0.42
1:A:312:ARG:O	1:A:316:GLU:HG2	2.20	0.42
1:B:155:SER:HA	1:B:160:THR:HG22	2.02	0.42
1:B:172:PRO:HA	1:B:175:ILE:HD12	2.01	0.42
1:B:185:LEU:HD22	1:B:213:LYS:HE3	2.02	0.42
1:C:330:ILE:HD12	1:C:330:ILE:HA	1.95	0.42
1:D:172:PRO:HA	1:D:175:ILE:HD12	2.01	0.42
1:E:330:ILE:HD12	1:E:330:ILE:HA	1.95	0.42
1:F:330:ILE:HD12	1:F:330:ILE:HA	1.95	0.42
1:G:183:ARG:HD2	1:G:206:ARG:NH2	2.35	0.42
1:I:185:LEU:HD22	1:I:213:LYS:HE3	2.02	0.42
1:J:305:MET:HB2	6:J:401:ADP:C2	2.54	0.42
1:M:232:SER:O	1:M:233:SER:C	2.62	0.42
1:N:195:GLU:CB	1:O:113:LYS:HD2	2.36	0.42
1:P:221:LEU:HA	1:P:315:LYS:HZ1	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:101:ARG:HA	2:a:104:GLU:CD	2.45	0.42
2:a:172:ILE:HG22	2:b:172:ILE:HG22	2.02	0.42
4:V:173:LEU:O	4:V:176:VAL:HG22	2.20	0.42
5:U:111:TYR:CB	5:U:147:ARG:HD2	2.49	0.42
3:e:146:LYS:HB2	3:e:146:LYS:HE2	1.57	0.42
5:d:59:GLU:O	5:d:62:ASP:HB2	2.20	0.42
1:A:172:PRO:HA	1:A:175:ILE:HD12	2.01	0.41
1:B:291:LYS:HG3	1:B:292:ASP:N	2.35	0.41
1:C:172:PRO:HA	1:C:175:ILE:HD12	2.01	0.41
1:C:183:ARG:HD2	1:C:206:ARG:NH2	2.35	0.41
1:D:232:SER:O	1:D:233:SER:C	2.63	0.41
1:F:171:LEU:O	1:F:175:ILE:HG13	2.19	0.41
1:G:203:THR:O	1:G:206:ARG:HB2	2.20	0.41
1:J:291:LYS:HG3	1:J:292:ASP:N	2.35	0.41
1:K:155:SER:HA	1:K:160:THR:HG22	2.02	0.41
1:K:160:THR:HG23	1:K:180:LEU:O	2.19	0.41
1:K:185:LEU:HD22	1:K:213:LYS:HE3	2.02	0.41
1:K:330:ILE:HD12	1:K:330:ILE:HA	1.95	0.41
1:O:185:LEU:HD22	1:O:213:LYS:HE3	2.02	0.41
1:Q:172:PRO:HA	1:Q:175:ILE:HD12	2.01	0.41
1:R:203:THR:O	1:R:206:ARG:HB2	2.20	0.41
2:a:53:THR:O	2:a:57:LEU:HG	2.20	0.41
2:a:114:GLU:C	2:a:118:LYS:HZ2	2.28	0.41
3:Y:221:ILE:HA	3:Y:224:LEU:HG	2.03	0.41
4:V:103:ARG:HA	4:V:106:LYS:HZ3	1.85	0.41
5:U:111:TYR:CG	5:U:147:ARG:HD2	2.55	0.41
2:i:249:LEU:O	2:i:253:ILE:HG13	2.19	0.41
2:j:249:LEU:O	2:j:253:ILE:HG13	2.20	0.41
2:j:261:TYR:HE1	3:e:127:ILE:CD1	2.33	0.41
1:A:185:LEU:HD22	1:A:213:LYS:HE3	2.02	0.41
1:B:64:ILE:HD13	1:D:171:LEU:CD2	2.47	0.41
1:E:312:ARG:O	1:E:316:GLU:HG2	2.20	0.41
1:F:203:THR:O	1:F:206:ARG:HB2	2.20	0.41
1:I:172:PRO:HA	1:I:175:ILE:HD12	2.01	0.41
1:I:183:ARG:HD2	1:I:206:ARG:NH2	2.35	0.41
1:J:165:ILE:HG23	1:J:169:TYR:C	2.45	0.41
1:N:203:THR:O	1:N:206:ARG:HB2	2.20	0.41
1:O:203:THR:O	1:O:206:ARG:HB2	2.20	0.41
1:P:155:SER:HA	1:P:160:THR:HG22	2.02	0.41
1:Q:183:ARG:HD2	1:Q:206:ARG:NH2	2.35	0.41
2:a:182:ARG:NH2	2:b:180:GLU:HA	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:90:ARG:O	2:b:93:GLN:HG3	2.19	0.41
2:W:61:SER:HA	2:Z:60:TYR:OH	2.20	0.41
5:U:59:GLU:O	5:U:62:ASP:HB2	2.20	0.41
2:i:101:ARG:HA	2:i:104:GLU:CD	2.45	0.41
2:i:157:ASP:O	2:i:161:LYS:HG3	2.21	0.41
3:f:229:LEU:HD11	4:c:94:GLN:CD	2.45	0.41
3:f:271:ASN:HD21	4:c:136:ARG:NH1	2.19	0.41
4:c:122:ILE:HA	4:c:125:ILE:HD12	2.01	0.41
1:B:232:SER:O	1:B:233:SER:C	2.63	0.41
1:C:291:LYS:HG3	1:C:292:ASP:N	2.34	0.41
1:E:153:LEU:HD12	1:E:153:LEU:HA	1.86	0.41
1:E:155:SER:HA	1:E:160:THR:HG22	2.02	0.41
1:E:185:LEU:HD22	1:E:213:LYS:HE3	2.01	0.41
1:E:203:THR:O	1:E:206:ARG:HB2	2.20	0.41
1:F:35:VAL:HG12	1:F:37:ARG:HE	1.85	0.41
1:H:183:ARG:HD2	1:H:206:ARG:NH2	2.35	0.41
1:H:332:PRO:O	1:H:335:ARG:NE	2.48	0.41
1:I:38:PRO:HD3	1:I:51:ASP:O	2.21	0.41
1:I:203:THR:O	1:I:206:ARG:HB2	2.20	0.41
1:K:44:MET:HE2	1:K:44:MET:HB2	1.85	0.41
1:K:312:ARG:O	1:K:316:GLU:HG2	2.20	0.41
1:N:185:LEU:HD22	1:N:213:LYS:HE3	2.02	0.41
1:P:312:ARG:O	1:P:316:GLU:HG2	2.20	0.41
1:R:312:ARG:O	1:R:316:GLU:HG2	2.20	0.41
2:a:275:ASP:O	2:a:279:ASN:ND2	2.47	0.41
2:i:194:GLU:HA	2:i:197:LEU:HD12	2.02	0.41
2:g:61:SER:HA	2:h:60:TYR:CE2	2.56	0.41
3:f:234:LYS:HG3	4:c:83:LEU:CD1	2.50	0.41
5:d:111:TYR:CB	5:d:147:ARG:HD2	2.49	0.41
1:A:302:GLY:HA2	1:A:305:MET:HE2	2.03	0.41
1:B:38:PRO:HD3	1:B:51:ASP:O	2.21	0.41
1:B:203:THR:O	1:B:206:ARG:HB2	2.20	0.41
1:B:244:ASP:HB3	1:D:290:ARG:NH2	2.35	0.41
1:C:152:VAL:HB	1:C:163:VAL:CG2	2.51	0.41
1:D:185:LEU:HD22	1:D:213:LYS:HE3	2.02	0.41
1:D:312:ARG:O	1:D:316:GLU:HG2	2.20	0.41
1:K:172:PRO:HA	1:K:175:ILE:HD12	2.01	0.41
1:O:291:LYS:HG3	1:O:292:ASP:N	2.35	0.41
1:P:38:PRO:HD3	1:P:51:ASP:O	2.21	0.41
1:Q:291:LYS:HG3	1:Q:292:ASP:N	2.35	0.41
2:a:242:ALA:O	2:a:246:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:51:LYS:HD2	2:W:51:LYS:HA	1.91	0.41
4:V:50:LYS:HD3	5:U:157:MET:HA	2.02	0.41
4:V:170:ARG:HH12	4:V:174:LYS:HD3	1.85	0.41
5:U:92:LYS:CE	5:U:158:LYS:HA	2.39	0.41
4:c:170:ARG:HH12	4:c:174:LYS:HD3	1.85	0.41
1:C:155:SER:HA	1:C:160:THR:HG22	2.02	0.41
1:C:210:ARG:O	1:C:214:GLU:HG3	2.21	0.41
1:D:203:THR:O	1:D:206:ARG:HB2	2.20	0.41
1:E:172:PRO:HA	1:E:175:ILE:HD12	2.01	0.41
1:G:155:SER:HA	1:G:160:THR:HG22	2.02	0.41
1:H:203:THR:O	1:H:206:ARG:HB2	2.20	0.41
1:I:291:LYS:HG3	1:I:292:ASP:N	2.35	0.41
1:J:312:ARG:O	1:J:316:GLU:HG2	2.20	0.41
1:K:38:PRO:HD3	1:K:51:ASP:O	2.21	0.41
1:L:68:LYS:HZ1	1:L:77:THR:HG21	1.85	0.41
1:L:172:PRO:HA	1:L:175:ILE:HD12	2.01	0.41
1:N:291:LYS:HG3	1:N:292:ASP:N	2.35	0.41
1:O:312:ARG:O	1:O:316:GLU:HG2	2.20	0.41
1:P:246:GLN:HG2	1:R:322:PRO:HG2	2.02	0.41
2:i:59:LYS:HB3	2:i:59:LYS:HE2	1.88	0.41
2:i:114:GLU:C	2:i:118:LYS:HZ2	2.28	0.41
2:i:180:GLU:O	2:i:184:GLU:OE1	2.38	0.41
2:j:150:GLU:O	2:j:154:ILE:HG12	2.21	0.41
2:j:221:TYR:O	2:j:225:ILE:HG13	2.20	0.41
1:A:38:PRO:HD3	1:A:51:ASP:O	2.21	0.41
1:C:153:LEU:HD12	1:C:153:LEU:HA	1.86	0.41
1:E:183:ARG:HD2	1:E:206:ARG:NH2	2.35	0.41
1:F:68:LYS:HZ1	1:F:77:THR:HG21	1.85	0.41
1:G:38:PRO:HD3	1:G:51:ASP:O	2.21	0.41
1:G:194:THR:HG23	1:G:199:SER:OG	2.21	0.41
1:I:330:ILE:HD12	1:I:330:ILE:HA	1.95	0.41
1:J:194:THR:HG23	1:J:199:SER:OG	2.21	0.41
1:K:203:THR:O	1:K:206:ARG:HB2	2.20	0.41
1:L:194:THR:HG23	1:L:199:SER:OG	2.21	0.41
1:M:155:SER:HA	1:M:160:THR:HG22	2.02	0.41
1:M:210:ARG:O	1:M:214:GLU:HG3	2.21	0.41
1:O:210:ARG:O	1:O:214:GLU:HG3	2.21	0.41
1:O:232:SER:O	1:O:233:SER:C	2.64	0.41
1:P:172:PRO:HA	1:P:175:ILE:HD12	2.01	0.41
1:R:38:PRO:HD3	1:R:51:ASP:O	2.21	0.41
1:R:214:GLU:HA	1:R:306:TYR:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:U:4:ILE:HD12	5:U:4:ILE:HA	1.90	0.41
5:U:20:PHE:HB3	5:U:81:MET:HE1	2.03	0.41
2:i:69:GLU:HA	2:i:72:GLU:OE1	2.21	0.41
3:e:97:LYS:HA	3:e:100:ASN:OD1	2.20	0.41
3:f:224:LEU:O	4:c:90:PHE:HZ	2.03	0.41
1:A:139:VAL:HG22	1:A:143:TYR:CZ	2.56	0.41
1:A:294:TYR:HB3	1:A:327:ILE:HG12	2.01	0.41
1:G:172:PRO:HA	1:G:175:ILE:HD12	2.01	0.41
1:H:178:LEU:HA	1:H:178:LEU:HD12	1.84	0.41
1:J:203:THR:O	1:J:206:ARG:HB2	2.20	0.41
1:J:214:GLU:HA	1:J:306:TYR:CE1	2.56	0.41
1:L:302:GLY:HA2	1:L:305:MET:HE2	2.03	0.41
1:L:349:LEU:HD22	4:V:141:ARG:NH1	2.36	0.41
1:N:139:VAL:HG22	1:N:143:TYR:CZ	2.56	0.41
1:N:232:SER:O	1:N:233:SER:C	2.62	0.41
1:O:155:SER:HA	1:O:160:THR:HG22	2.02	0.41
1:O:172:PRO:HA	1:O:175:ILE:HD12	2.01	0.41
1:P:183:ARG:HD2	1:P:206:ARG:NH2	2.35	0.41
1:P:214:GLU:HA	1:P:306:TYR:CE1	2.56	0.41
1:Q:194:THR:HG23	1:Q:199:SER:OG	2.21	0.41
1:R:194:THR:HG23	1:R:199:SER:OG	2.21	0.41
2:a:165:VAL:HG21	2:b:162:TYR:CE1	2.56	0.41
2:W:26:GLU:O	2:W:30:LYS:HG2	2.20	0.41
2:W:50:LEU:O	2:W:53:THR:HB	2.21	0.41
4:V:84:GLU:N	4:V:84:GLU:OE1	2.53	0.41
2:i:59:LYS:O	2:i:62:GLU:HG3	2.20	0.41
2:i:113:LEU:HD22	2:j:112:LYS:HD3	2.02	0.41
2:g:61:SER:HA	2:h:60:TYR:HE2	1.85	0.41
1:B:312:ARG:O	1:B:316:GLU:HG2	2.20	0.41
1:C:312:ARG:O	1:C:316:GLU:HG2	2.20	0.41
1:D:224:GLU:H	1:D:224:GLU:CD	2.26	0.41
1:E:210:ARG:O	1:E:214:GLU:HG3	2.21	0.41
1:E:224:GLU:H	1:E:224:GLU:CD	2.26	0.41
1:F:183:ARG:HD2	1:F:206:ARG:NH2	2.35	0.41
1:G:152:VAL:HB	1:G:163:VAL:CG2	2.51	0.41
1:G:165:ILE:HG23	1:G:169:TYR:C	2.46	0.41
1:K:194:THR:HG23	1:K:199:SER:OG	2.21	0.41
1:M:152:VAL:HB	1:M:163:VAL:CG2	2.51	0.41
1:M:194:THR:HG23	1:M:199:SER:OG	2.21	0.41
1:N:183:ARG:HD2	1:N:206:ARG:NH2	2.35	0.41
1:O:139:VAL:HG22	1:O:143:TYR:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:152:VAL:HB	1:O:163:VAL:CG2	2.51	0.41
1:O:330:ILE:HD12	1:O:330:ILE:HA	1.95	0.41
1:P:68:LYS:HZ1	1:P:77:THR:HG21	1.86	0.41
1:P:152:VAL:HB	1:P:163:VAL:CG2	2.51	0.41
1:R:302:GLY:HA2	1:R:305:MET:HE2	2.03	0.41
2:a:53:THR:OG1	2:b:50:LEU:HD11	2.20	0.41
2:i:242:ALA:O	2:i:246:VAL:HG23	2.21	0.41
2:h:7:LYS:HZ1	2:h:11:LEU:CD1	2.25	0.41
3:f:215:ARG:HD3	4:c:111:ARG:HH21	1.80	0.41
4:c:50:LYS:HE3	5:d:156:PHE:CZ	2.56	0.41
4:c:134:ASP:O	4:c:138:LYS:HD2	2.21	0.41
1:A:152:VAL:HB	1:A:163:VAL:CG2	2.51	0.41
1:C:68:LYS:HZ1	1:C:77:THR:HG21	1.85	0.41
1:C:203:THR:O	1:C:206:ARG:HB2	2.20	0.41
1:D:38:PRO:HD3	1:D:51:ASP:O	2.21	0.41
1:D:210:ARG:O	1:D:214:GLU:HG3	2.21	0.41
1:E:152:VAL:HB	1:E:163:VAL:CG2	2.51	0.41
1:E:214:GLU:HA	1:E:306:TYR:CE1	2.56	0.41
1:F:38:PRO:HD3	1:F:51:ASP:O	2.21	0.41
1:F:138:ALA:HB1	1:F:163:VAL:HG21	2.03	0.41
1:F:155:SER:HA	1:F:160:THR:HG22	2.02	0.41
1:F:210:ARG:O	1:F:214:GLU:HG3	2.21	0.41
1:F:232:SER:O	1:F:233:SER:C	2.63	0.41
1:G:210:ARG:O	1:G:214:GLU:HG3	2.21	0.41
1:H:38:PRO:HD3	1:H:51:ASP:O	2.21	0.41
1:H:155:SER:HA	1:H:160:THR:HG22	2.02	0.41
1:H:194:THR:HG23	1:H:199:SER:OG	2.21	0.41
1:I:152:VAL:HB	1:I:163:VAL:CG2	2.51	0.41
1:J:64:ILE:HD12	1:J:64:ILE:HA	1.92	0.41
1:J:153:LEU:HD12	1:J:153:LEU:HA	1.86	0.41
1:J:302:GLY:HA2	1:J:305:MET:HE2	2.03	0.41
1:K:64:ILE:HD12	1:K:64:ILE:HA	1.92	0.41
1:K:152:VAL:HB	1:K:163:VAL:CG2	2.51	0.41
1:K:153:LEU:HD12	1:K:153:LEU:HA	1.86	0.41
1:K:210:ARG:O	1:K:214:GLU:HG3	2.21	0.41
1:L:203:THR:O	1:L:206:ARG:HB2	2.20	0.41
1:L:214:GLU:HA	1:L:306:TYR:CE1	2.56	0.41
1:L:312:ARG:O	1:L:316:GLU:HG2	2.20	0.41
1:M:38:PRO:HD3	1:M:51:ASP:O	2.21	0.41
1:M:68:LYS:HZ1	1:M:77:THR:HG21	1.85	0.41
1:M:172:PRO:HA	1:M:175:ILE:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:221:LEU:HA	1:M:315:LYS:HZ1	1.86	0.41
1:N:68:LYS:HZ1	1:N:77:THR:HG21	1.85	0.41
1:N:302:GLY:HA2	1:N:305:MET:HE2	2.03	0.41
1:N:312:ARG:O	1:N:316:GLU:HG2	2.20	0.41
1:O:194:THR:HG23	1:O:199:SER:OG	2.21	0.41
1:P:194:THR:HG23	1:P:199:SER:OG	2.21	0.41
1:P:302:GLY:HA2	1:P:305:MET:HE2	2.03	0.41
1:Q:152:VAL:HB	1:Q:163:VAL:CG2	2.51	0.41
1:Q:153:LEU:HD12	1:Q:153:LEU:HA	1.86	0.41
1:Q:155:SER:HA	1:Q:160:THR:HG22	2.02	0.41
1:R:139:VAL:HG22	1:R:143:TYR:CZ	2.56	0.41
1:R:232:SER:O	1:R:233:SER:C	2.63	0.41
2:a:69:GLU:HA	2:a:72:GLU:OE1	2.21	0.41
2:a:157:ASP:O	2:a:161:LYS:HG3	2.21	0.41
2:a:193:LEU:HD21	2:b:194:GLU:N	2.36	0.41
3:Y:246:GLU:HA	3:Y:249:ASP:HB2	2.03	0.41
4:V:134:ASP:O	4:V:138:LYS:HD2	2.21	0.41
2:h:7:LYS:O	2:h:8:MET:C	2.64	0.41
4:c:101:HIS:O	4:c:104:VAL:HG12	2.21	0.41
4:c:173:LEU:HA	4:c:176:VAL:HG22	2.03	0.41
4:c:205:LYS:HE2	4:c:210:SER:CB	2.46	0.41
5:d:20:PHE:HB3	5:d:81:MET:HE1	2.03	0.41
1:B:139:VAL:HG22	1:B:143:TYR:CZ	2.56	0.41
1:D:194:THR:HG23	1:D:199:SER:OG	2.21	0.41
1:D:302:GLY:HA2	1:D:305:MET:HE2	2.03	0.41
1:D:330:ILE:HD12	1:D:330:ILE:HA	1.95	0.41
1:G:214:GLU:HA	1:G:306:TYR:CE1	2.56	0.41
1:J:232:SER:O	1:J:233:SER:C	2.63	0.41
1:N:38:PRO:HD3	1:N:51:ASP:O	2.21	0.41
1:N:155:SER:HA	1:N:160:THR:HG22	2.02	0.41
1:O:221:LEU:HA	1:O:315:LYS:HZ1	1.86	0.41
1:O:302:GLY:HA2	1:O:305:MET:HE2	2.03	0.41
1:Q:178:LEU:HD12	1:Q:178:LEU:HA	1.83	0.41
1:Q:210:ARG:O	1:Q:214:GLU:HG3	2.21	0.41
2:a:43:LEU:CD1	2:b:39:LEU:HD22	2.51	0.41
2:a:56:GLU:HB2	2:b:57:LEU:CD1	2.48	0.41
2:a:180:GLU:O	2:a:184:GLU:OE1	2.38	0.41
2:W:1:MET:O	2:W:5:LYS:HD3	2.21	0.41
2:g:1:MET:O	2:g:5:LYS:HD3	2.21	0.41
4:c:173:LEU:O	4:c:176:VAL:HG22	2.20	0.41
5:d:38:THR:O	5:d:41:LEU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:THR:HG23	1:A:199:SER:OG	2.21	0.40
1:A:214:GLU:HA	1:A:306:TYR:CE1	2.56	0.40
1:C:194:THR:HG23	1:C:199:SER:OG	2.21	0.40
1:E:38:PRO:HD3	1:E:51:ASP:O	2.21	0.40
1:E:237:GLU:OE2	1:E:249:THR:HB	2.21	0.40
1:E:302:GLY:HA2	1:E:305:MET:HE2	2.03	0.40
1:H:138:ALA:HB1	1:H:163:VAL:HG21	2.03	0.40
1:H:210:ARG:O	1:H:214:GLU:HG3	2.21	0.40
1:H:237:GLU:OE2	1:H:249:THR:HB	2.22	0.40
1:I:139:VAL:HG22	1:I:143:TYR:CZ	2.56	0.40
1:I:210:ARG:O	1:I:214:GLU:HG3	2.21	0.40
1:L:213:LYS:HE2	1:L:257:CYS:SG	2.61	0.40
1:L:232:SER:O	1:L:233:SER:C	2.63	0.40
1:P:223:PHE:CZ	1:P:256:ARG:HG2	2.57	0.40
1:Q:38:PRO:HD3	1:Q:51:ASP:O	2.21	0.40
1:Q:139:VAL:HG22	1:Q:143:TYR:CZ	2.56	0.40
1:Q:203:THR:O	1:Q:206:ARG:HB2	2.20	0.40
1:Q:232:SER:O	1:Q:233:SER:C	2.64	0.40
1:R:155:SER:HA	1:R:160:THR:HG22	2.02	0.40
1:R:223:PHE:CZ	1:R:256:ARG:HG2	2.57	0.40
2:b:273:GLU:HB3	2:Z:1:MET:HE2	2.02	0.40
4:V:49:LEU:HD22	5:U:126:GLU:OE2	2.21	0.40
4:V:174:LYS:CG	4:V:178:LYS:HZ3	2.25	0.40
5:U:20:PHE:HB3	5:U:81:MET:SD	2.61	0.40
5:U:96:GLU:O	5:U:100:LEU:HG	2.21	0.40
2:j:90:ARG:HA	2:j:93:GLN:HG3	2.03	0.40
1:C:44:MET:HE2	1:C:44:MET:HB2	1.86	0.40
1:C:214:GLU:HA	1:C:306:TYR:CE1	2.56	0.40
1:D:68:LYS:HZ1	1:D:77:THR:HG21	1.86	0.40
1:D:155:SER:HA	1:D:160:THR:HG22	2.02	0.40
1:E:223:PHE:CZ	1:E:256:ARG:HG2	2.57	0.40
1:J:138:ALA:HB1	1:J:163:VAL:HG21	2.03	0.40
1:J:210:ARG:O	1:J:214:GLU:HG3	2.21	0.40
1:L:139:VAL:HG22	1:L:143:TYR:CZ	2.56	0.40
1:L:237:GLU:OE2	1:L:249:THR:HB	2.21	0.40
1:M:312:ARG:O	1:M:316:GLU:HG2	2.20	0.40
1:N:210:ARG:O	1:N:214:GLU:HG3	2.21	0.40
1:N:214:GLU:HA	1:N:306:TYR:CE1	2.56	0.40
1:Q:302:GLY:HA2	1:Q:305:MET:HE2	2.03	0.40
1:R:152:VAL:HB	1:R:163:VAL:CG2	2.51	0.40
2:a:192:GLU:O	2:a:195:GLU:HG3	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:90:ARG:HA	2:b:93:GLN:HG3	2.03	0.40
2:W:5:LYS:O	2:W:9:GLN:HG2	2.21	0.40
2:Z:7:LYS:HZ1	2:Z:11:LEU:CD1	2.26	0.40
4:V:205:LYS:HE2	4:V:210:SER:CB	2.46	0.40
2:i:182:ARG:HA	2:i:185:LEU:HG	2.03	0.40
1:A:221:LEU:HA	1:A:315:LYS:NZ	2.37	0.40
1:B:152:VAL:HB	1:B:163:VAL:CG2	2.51	0.40
1:C:38:PRO:HD3	1:C:51:ASP:O	2.21	0.40
1:D:138:ALA:HB1	1:D:163:VAL:HG21	2.03	0.40
1:E:194:THR:HG23	1:E:199:SER:OG	2.21	0.40
1:F:223:PHE:CZ	1:F:256:ARG:HG2	2.56	0.40
1:G:139:VAL:HG22	1:G:143:TYR:CZ	2.56	0.40
1:G:223:PHE:CZ	1:G:256:ARG:HG2	2.57	0.40
1:G:302:GLY:HA2	1:G:305:MET:HE2	2.03	0.40
1:G:312:ARG:O	1:G:316:GLU:HG2	2.20	0.40
1:H:152:VAL:HB	1:H:163:VAL:CG2	2.51	0.40
1:H:214:GLU:HA	1:H:306:TYR:CE1	2.56	0.40
1:H:221:LEU:HA	1:H:315:LYS:NZ	2.37	0.40
1:H:223:PHE:CZ	1:H:256:ARG:HG2	2.57	0.40
1:K:302:GLY:HA2	1:K:305:MET:HE2	2.03	0.40
1:M:139:VAL:HG22	1:M:143:TYR:CZ	2.56	0.40
1:M:302:GLY:HA2	1:M:305:MET:HE2	2.03	0.40
1:N:194:THR:HG23	1:N:199:SER:OG	2.21	0.40
1:N:223:PHE:CZ	1:N:256:ARG:HG2	2.57	0.40
1:O:38:PRO:HD3	1:O:51:ASP:O	2.21	0.40
2:a:182:ARG:HA	2:a:185:LEU:HG	2.03	0.40
3:Y:211:ILE:HA	3:Y:214:GLU:CD	2.47	0.40
4:V:48:GLN:NE2	4:V:49:LEU:HD23	2.35	0.40
2:g:5:LYS:O	2:g:9:GLN:HG2	2.21	0.40
1:B:210:ARG:O	1:B:214:GLU:HG3	2.21	0.40
1:B:237:GLU:OE2	1:B:249:THR:HB	2.21	0.40
1:C:139:VAL:HG22	1:C:143:TYR:CZ	2.56	0.40
1:D:64:ILE:HD12	1:D:64:ILE:HA	1.92	0.40
1:D:221:LEU:HA	1:D:315:LYS:NZ	2.37	0.40
1:F:139:VAL:HG22	1:F:143:TYR:CZ	2.56	0.40
1:F:302:GLY:HA2	1:F:305:MET:HE2	2.03	0.40
1:G:324:THR:OG1	1:G:325:MET:N	2.55	0.40
1:H:312:ARG:O	1:H:316:GLU:HG2	2.20	0.40
1:J:152:VAL:HB	1:J:163:VAL:CG2	2.51	0.40
1:J:155:SER:HA	1:J:160:THR:HG22	2.02	0.40
1:K:139:VAL:HG22	1:K:143:TYR:CZ	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:237:GLU:OE2	1:K:249:THR:HB	2.22	0.40
1:L:138:ALA:HB1	1:L:163:VAL:HG21	2.03	0.40
1:L:210:ARG:O	1:L:214:GLU:HG3	2.21	0.40
1:N:152:VAL:HB	1:N:163:VAL:CG2	2.51	0.40
1:O:123:MET:HE3	1:O:123:MET:HB3	2.01	0.40
1:P:139:VAL:HG22	1:P:143:TYR:CZ	2.56	0.40
1:Q:237:GLU:OE2	1:Q:249:THR:HB	2.21	0.40
1:R:210:ARG:O	1:R:214:GLU:HG3	2.21	0.40
2:a:43:LEU:HD11	2:b:39:LEU:HD22	2.04	0.40
3:X:103:GLN:H	3:X:103:GLN:HG3	1.62	0.40
5:U:38:THR:O	5:U:41:LEU:HB2	2.21	0.40
1:A:223:PHE:CZ	1:A:256:ARG:HG2	2.57	0.40
1:D:152:VAL:HB	1:D:163:VAL:CG2	2.51	0.40
1:E:138:ALA:HB1	1:E:163:VAL:HG21	2.03	0.40
1:F:152:VAL:HB	1:F:163:VAL:CG2	2.51	0.40
1:G:138:ALA:HB1	1:G:163:VAL:HG21	2.03	0.40
1:G:237:GLU:OE2	1:G:249:THR:HB	2.21	0.40
1:H:324:THR:OG1	1:H:325:MET:N	2.55	0.40
1:I:138:ALA:HB1	1:I:163:VAL:HG21	2.03	0.40
1:I:194:THR:HG23	1:I:199:SER:OG	2.21	0.40
1:I:232:SER:O	1:I:233:SER:C	2.64	0.40
1:J:38:PRO:HD3	1:J:51:ASP:O	2.21	0.40
1:N:237:GLU:OE2	1:N:249:THR:HB	2.21	0.40
1:O:153:LEU:HD12	1:O:153:LEU:HA	1.86	0.40
1:P:210:ARG:O	1:P:214:GLU:HG3	2.21	0.40
1:P:324:THR:OG1	1:P:325:MET:N	2.55	0.40
1:Q:138:ALA:HB1	1:Q:163:VAL:HG21	2.03	0.40
1:Q:221:LEU:HA	1:Q:315:LYS:NZ	2.37	0.40
2:b:150:GLU:O	2:b:154:ILE:HG12	2.21	0.40
4:V:190:ASP:OD1	4:V:191:TRP:N	2.45	0.40
2:g:50:LEU:O	2:g:53:THR:HB	2.21	0.40
2:h:7:LYS:NZ	2:h:11:LEU:HD13	2.26	0.40
3:f:221:ILE:HA	3:f:224:LEU:HG	2.02	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	372/377 (99%)	353 (95%)	18 (5%)	1 (0%)	36	72
1	B	372/377 (99%)	353 (95%)	18 (5%)	1 (0%)	36	72
1	C	372/377 (99%)	352 (95%)	19 (5%)	1 (0%)	36	72
1	D	372/377 (99%)	352 (95%)	19 (5%)	1 (0%)	36	72
1	E	372/377 (99%)	352 (95%)	19 (5%)	1 (0%)	36	72
1	F	372/377 (99%)	352 (95%)	19 (5%)	1 (0%)	36	72
1	G	372/377 (99%)	352 (95%)	19 (5%)	1 (0%)	36	72
1	H	372/377 (99%)	352 (95%)	19 (5%)	1 (0%)	36	72
1	I	372/377 (99%)	353 (95%)	18 (5%)	1 (0%)	36	72
1	J	372/377 (99%)	352 (95%)	19 (5%)	1 (0%)	36	72
1	K	372/377 (99%)	352 (95%)	19 (5%)	1 (0%)	36	72
1	L	372/377 (99%)	353 (95%)	18 (5%)	1 (0%)	36	72
1	M	372/377 (99%)	352 (95%)	19 (5%)	1 (0%)	36	72
1	N	372/377 (99%)	353 (95%)	18 (5%)	1 (0%)	36	72
1	O	372/377 (99%)	352 (95%)	19 (5%)	1 (0%)	36	72
1	P	372/377 (99%)	352 (95%)	19 (5%)	1 (0%)	36	72
1	Q	372/377 (99%)	352 (95%)	19 (5%)	1 (0%)	36	72
1	R	372/377 (99%)	353 (95%)	18 (5%)	1 (0%)	36	72
2	W	63/284 (22%)	63 (100%)	0	0	100	100
2	Z	63/284 (22%)	63 (100%)	0	0	100	100
2	a	255/284 (90%)	254 (100%)	1 (0%)	0	100	100
2	b	255/284 (90%)	255 (100%)	0	0	100	100
2	g	83/284 (29%)	83 (100%)	0	0	100	100
2	h	83/284 (29%)	83 (100%)	0	0	100	100
2	i	235/284 (83%)	234 (100%)	1 (0%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	j	235/284 (83%)	235 (100%)	0	0	100	100
3	X	61/288 (21%)	59 (97%)	2 (3%)	0	100	100
3	Y	72/288 (25%)	70 (97%)	2 (3%)	0	100	100
3	e	61/288 (21%)	59 (97%)	2 (3%)	0	100	100
3	f	72/288 (25%)	70 (97%)	2 (3%)	0	100	100
4	V	168/210 (80%)	156 (93%)	12 (7%)	0	100	100
4	c	168/210 (80%)	156 (93%)	12 (7%)	0	100	100
5	U	158/161 (98%)	145 (92%)	13 (8%)	0	100	100
5	d	158/161 (98%)	145 (92%)	13 (8%)	0	100	100
All	All	8886/10952 (81%)	8472 (95%)	396 (4%)	18 (0%)	44	78

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	51	ASP
1	B	51	ASP
1	C	51	ASP
1	D	51	ASP
1	E	51	ASP
1	F	51	ASP
1	G	51	ASP
1	H	51	ASP
1	I	51	ASP
1	J	51	ASP
1	K	51	ASP
1	L	51	ASP
1	M	51	ASP
1	N	51	ASP
1	O	51	ASP
1	P	51	ASP
1	Q	51	ASP
1	R	51	ASP

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	317/319 (99%)	303 (96%)	14 (4%)	25	47
1	B	317/319 (99%)	303 (96%)	14 (4%)	25	47
1	C	317/319 (99%)	305 (96%)	12 (4%)	29	50
1	D	317/319 (99%)	305 (96%)	12 (4%)	29	50
1	E	317/319 (99%)	305 (96%)	12 (4%)	29	50
1	F	317/319 (99%)	305 (96%)	12 (4%)	29	50
1	G	317/319 (99%)	305 (96%)	12 (4%)	29	50
1	H	317/319 (99%)	305 (96%)	12 (4%)	29	50
1	I	317/319 (99%)	305 (96%)	12 (4%)	29	50
1	J	317/319 (99%)	305 (96%)	12 (4%)	29	50
1	K	317/319 (99%)	305 (96%)	12 (4%)	29	50
1	L	317/319 (99%)	305 (96%)	12 (4%)	29	50
1	M	317/319 (99%)	305 (96%)	12 (4%)	29	50
1	N	317/319 (99%)	304 (96%)	13 (4%)	27	49
1	O	317/319 (99%)	305 (96%)	12 (4%)	29	50
1	P	317/319 (99%)	304 (96%)	13 (4%)	27	49
1	Q	317/319 (99%)	304 (96%)	13 (4%)	27	49
1	R	317/319 (99%)	305 (96%)	12 (4%)	29	50
2	W	56/245 (23%)	52 (93%)	4 (7%)	13	35
2	Z	56/245 (23%)	56 (100%)	0	100	100
2	a	223/245 (91%)	219 (98%)	4 (2%)	51	68
2	b	223/245 (91%)	221 (99%)	2 (1%)	70	79
2	g	71/245 (29%)	67 (94%)	4 (6%)	19	40
2	h	71/245 (29%)	71 (100%)	0	100	100
2	i	205/245 (84%)	201 (98%)	4 (2%)	48	66
2	j	205/245 (84%)	203 (99%)	2 (1%)	68	78
3	X	59/256 (23%)	53 (90%)	6 (10%)	7	23
3	Y	69/256 (27%)	68 (99%)	1 (1%)	59	72
3	e	59/256 (23%)	53 (90%)	6 (10%)	7	23
3	f	69/256 (27%)	68 (99%)	1 (1%)	59	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	V	145/176 (82%)	139 (96%)	6 (4%)	27	49
4	c	145/176 (82%)	140 (97%)	5 (3%)	32	54
5	U	141/142 (99%)	137 (97%)	4 (3%)	38	60
5	d	141/142 (99%)	138 (98%)	3 (2%)	47	65
All	All	7644/9362 (82%)	7369 (96%)	275 (4%)	32	52

All (275) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	VAL
1	A	72	GLU
1	A	113	LYS
1	A	132	MET
1	A	153	LEU
1	A	233	SER
1	A	234	SER
1	A	246	GLN
1	A	247	VAL
1	A	260	THR
1	A	299	MET
1	A	305	MET
1	A	309	ILE
1	A	325	MET
1	B	37	ARG
1	B	54	VAL
1	B	72	GLU
1	B	113	LYS
1	B	132	MET
1	B	153	LEU
1	B	233	SER
1	B	234	SER
1	B	246	GLN
1	B	247	VAL
1	B	260	THR
1	B	299	MET
1	B	305	MET
1	B	309	ILE
1	C	54	VAL
1	C	72	GLU
1	C	132	MET
1	C	153	LEU

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Mol	Chain	Res	Type
1	C	233	SER
1	C	234	SER
1	C	246	GLN
1	C	247	VAL
1	C	260	THR
1	C	299	MET
1	C	305	MET
1	C	309	ILE
1	D	54	VAL
1	D	72	GLU
1	D	113	LYS
1	D	132	MET
1	D	153	LEU
1	D	233	SER
1	D	234	SER
1	D	246	GLN
1	D	247	VAL
1	D	299	MET
1	D	305	MET
1	D	309	ILE
1	E	54	VAL
1	E	72	GLU
1	E	113	LYS
1	E	132	MET
1	E	153	LEU
1	E	233	SER
1	E	234	SER
1	E	246	GLN
1	E	247	VAL
1	E	299	MET
1	E	305	MET
1	E	309	ILE
1	F	54	VAL
1	F	72	GLU
1	F	113	LYS
1	F	132	MET
1	F	153	LEU
1	F	233	SER
1	F	234	SER
1	F	246	GLN
1	F	247	VAL
1	F	299	MET

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Mol	Chain	Res	Type
1	F	305	MET
1	F	309	ILE
1	G	54	VAL
1	G	72	GLU
1	G	113	LYS
1	G	132	MET
1	G	153	LEU
1	G	233	SER
1	G	234	SER
1	G	246	GLN
1	G	247	VAL
1	G	299	MET
1	G	305	MET
1	G	309	ILE
1	H	54	VAL
1	H	72	GLU
1	H	113	LYS
1	H	132	MET
1	H	153	LEU
1	H	233	SER
1	H	234	SER
1	H	246	GLN
1	H	247	VAL
1	H	299	MET
1	H	305	MET
1	H	309	ILE
1	I	54	VAL
1	I	72	GLU
1	I	113	LYS
1	I	132	MET
1	I	153	LEU
1	I	233	SER
1	I	234	SER
1	I	246	GLN
1	I	247	VAL
1	I	299	MET
1	I	305	MET
1	I	309	ILE
1	J	54	VAL
1	J	72	GLU
1	J	113	LYS
1	J	132	MET

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Mol	Chain	Res	Type
1	J	153	LEU
1	J	233	SER
1	J	234	SER
1	J	246	GLN
1	J	247	VAL
1	J	299	MET
1	J	305	MET
1	J	309	ILE
1	K	54	VAL
1	K	72	GLU
1	K	113	LYS
1	K	132	MET
1	K	153	LEU
1	K	233	SER
1	K	234	SER
1	K	246	GLN
1	K	247	VAL
1	K	299	MET
1	K	305	MET
1	K	309	ILE
1	L	54	VAL
1	L	72	GLU
1	L	113	LYS
1	L	132	MET
1	L	153	LEU
1	L	233	SER
1	L	234	SER
1	L	246	GLN
1	L	247	VAL
1	L	299	MET
1	L	305	MET
1	L	309	ILE
1	M	54	VAL
1	M	72	GLU
1	M	113	LYS
1	M	132	MET
1	M	153	LEU
1	M	233	SER
1	M	234	SER
1	M	246	GLN
1	M	247	VAL
1	M	299	MET

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Mol	Chain	Res	Type
1	M	305	MET
1	M	309	ILE
1	N	54	VAL
1	N	72	GLU
1	N	113	LYS
1	N	132	MET
1	N	153	LEU
1	N	233	SER
1	N	234	SER
1	N	246	GLN
1	N	247	VAL
1	N	260	THR
1	N	299	MET
1	N	305	MET
1	N	309	ILE
1	O	54	VAL
1	O	72	GLU
1	O	113	LYS
1	O	132	MET
1	O	153	LEU
1	O	233	SER
1	O	234	SER
1	O	246	GLN
1	O	247	VAL
1	O	299	MET
1	O	305	MET
1	O	309	ILE
1	P	54	VAL
1	P	64	ILE
1	P	72	GLU
1	P	113	LYS
1	P	132	MET
1	P	153	LEU
1	P	233	SER
1	P	234	SER
1	P	246	GLN
1	P	247	VAL
1	P	299	MET
1	P	305	MET
1	P	309	ILE
1	Q	54	VAL
1	Q	72	GLU

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Mol	Chain	Res	Type
1	Q	113	LYS
1	Q	132	MET
1	Q	153	LEU
1	Q	233	SER
1	Q	234	SER
1	Q	246	GLN
1	Q	247	VAL
1	Q	260	THR
1	Q	299	MET
1	Q	305	MET
1	Q	309	ILE
1	R	54	VAL
1	R	72	GLU
1	R	113	LYS
1	R	132	MET
1	R	153	LEU
1	R	233	SER
1	R	234	SER
1	R	246	GLN
1	R	247	VAL
1	R	299	MET
1	R	305	MET
1	R	309	ILE
2	a	49	LYS
2	a	51	LYS
2	a	97	GLU
2	a	281	MET
2	b	127	MET
2	b	141	MET
2	W	1	MET
2	W	8	MET
2	W	10	MET
2	W	56	GLU
3	X	89	ASP
3	X	94	ARG
3	X	97	LYS
3	X	99	LEU
3	X	103	GLN
3	X	146	LYS
3	Y	228	GLN
4	V	155	MET
4	V	156	GLN

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Mol	Chain	Res	Type
4	V	158	LEU
4	V	198	LEU
4	V	201	MET
4	V	208	PHE
5	U	60	MET
5	U	80	MET
5	U	82	VAL
5	U	103	MET
2	i	51	LYS
2	i	97	GLU
2	i	123	SER
2	i	281	MET
2	j	127	MET
2	j	141	MET
2	g	1	MET
2	g	8	MET
2	g	10	MET
2	g	56	GLU
3	e	89	ASP
3	e	93	LYS
3	e	94	ARG
3	e	97	LYS
3	e	103	GLN
3	e	146	LYS
3	f	228	GLN
4	c	155	MET
4	c	158	LEU
4	c	198	LEU
4	c	201	MET
4	c	208	PHE
5	d	60	MET
5	d	80	MET
5	d	82	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	173	HIS
1	A	354	GLN
1	B	87	HIS
1	C	173	HIS
1	D	173	HIS

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Mol	Chain	Res	Type
1	E	173	HIS
1	F	173	HIS
1	G	173	HIS
1	G	354	GLN
1	H	87	HIS
1	H	173	HIS
1	I	173	HIS
1	J	173	HIS
1	K	173	HIS
1	L	173	HIS
1	M	173	HIS
1	N	173	HIS
1	O	173	HIS
1	P	173	HIS
1	P	354	GLN
1	Q	173	HIS
1	R	173	HIS
1	R	354	GLN
2	a	111	GLN
2	a	144	GLN
2	a	210	GLN
3	Y	228	GLN
5	U	16	GLN
5	U	58	GLN
2	i	111	GLN
2	i	144	GLN
2	i	210	GLN
2	g	68	GLN
3	f	223	HIS
3	f	228	GLN
3	f	257	GLN
5	d	16	GLN
5	d	58	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

18 non-standard protein/DNA/RNA residues 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
1	HIC	C	73	1	10,11,12	1.54	1 (10%)	9,14,16	1.25	1 (11%)
1	HIC	Q	73	1	10,11,12	1.54	1 (10%)	9,14,16	1.22	1 (11%)
1	HIC	N	73	1	10,11,12	1.55	1 (10%)	9,14,16	1.21	1 (11%)
1	HIC	K	73	1	10,11,12	1.54	1 (10%)	9,14,16	1.27	1 (11%)
1	HIC	B	73	1	10,11,12	1.54	1 (10%)	9,14,16	1.26	1 (11%)
1	HIC	P	73	1	10,11,12	1.54	1 (10%)	9,14,16	1.22	1 (11%)
1	HIC	A	73	1	10,11,12	1.53	1 (10%)	9,14,16	1.26	1 (11%)
1	HIC	G	73	1	10,11,12	1.54	1 (10%)	9,14,16	1.22	1 (11%)
1	HIC	F	73	1	10,11,12	1.55	1 (10%)	9,14,16	1.23	1 (11%)
1	HIC	L	73	1	10,11,12	1.54	1 (10%)	9,14,16	1.27	1 (11%)
1	HIC	H	73	1	10,11,12	1.55	1 (10%)	9,14,16	1.26	1 (11%)
1	HIC	J	73	1	10,11,12	1.54	1 (10%)	9,14,16	1.26	1 (11%)
1	HIC	M	73	1	10,11,12	1.54	1 (10%)	9,14,16	1.24	1 (11%)
1	HIC	R	73	1	10,11,12	1.54	1 (10%)	9,14,16	1.29	1 (11%)
1	HIC	I	73	1	10,11,12	1.55	1 (10%)	9,14,16	1.24	1 (11%)
1	HIC	E	73	1	10,11,12	1.53	1 (10%)	9,14,16	1.23	1 (11%)
1	HIC	D	73	1	10,11,12	1.54	1 (10%)	9,14,16	1.25	1 (11%)
1	HIC	O	73	1	10,11,12	1.53	1 (10%)	9,14,16	1.25	1 (11%)

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
1	HIC	C	73	1	-	2/5/6/8	0/1/1/1
1	HIC	Q	73	1	-	2/5/6/8	0/1/1/1
1	HIC	N	73	1	-	2/5/6/8	0/1/1/1
1	HIC	K	73	1	-	2/5/6/8	0/1/1/1
1	HIC	B	73	1	-	2/5/6/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HIC	P	73	1	-	2/5/6/8	0/1/1/1
1	HIC	A	73	1	-	2/5/6/8	0/1/1/1
1	HIC	G	73	1	-	2/5/6/8	0/1/1/1
1	HIC	F	73	1	-	2/5/6/8	0/1/1/1
1	HIC	L	73	1	-	2/5/6/8	0/1/1/1
1	HIC	H	73	1	-	2/5/6/8	0/1/1/1
1	HIC	J	73	1	-	2/5/6/8	0/1/1/1
1	HIC	M	73	1	-	2/5/6/8	0/1/1/1
1	HIC	R	73	1	-	2/5/6/8	0/1/1/1
1	HIC	I	73	1	-	2/5/6/8	0/1/1/1
1	HIC	E	73	1	-	2/5/6/8	0/1/1/1
1	HIC	D	73	1	-	2/5/6/8	0/1/1/1
1	HIC	O	73	1	-	2/5/6/8	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	73	HIC	CD2-CG	3.14	1.41	1.36
1	P	73	HIC	CD2-CG	3.13	1.41	1.36
1	N	73	HIC	CD2-CG	3.11	1.41	1.36
1	K	73	HIC	CD2-CG	3.11	1.41	1.36
1	F	73	HIC	CD2-CG	3.10	1.41	1.36
1	D	73	HIC	CD2-CG	3.10	1.41	1.36
1	Q	73	HIC	CD2-CG	3.10	1.41	1.36
1	J	73	HIC	CD2-CG	3.09	1.41	1.36
1	L	73	HIC	CD2-CG	3.09	1.41	1.36
1	A	73	HIC	CD2-CG	3.09	1.41	1.36
1	E	73	HIC	CD2-CG	3.09	1.41	1.36
1	M	73	HIC	CD2-CG	3.09	1.41	1.36
1	I	73	HIC	CD2-CG	3.08	1.41	1.36
1	B	73	HIC	CD2-CG	3.08	1.41	1.36
1	R	73	HIC	CD2-CG	3.08	1.41	1.36
1	O	73	HIC	CD2-CG	3.07	1.41	1.36
1	C	73	HIC	CD2-CG	3.07	1.41	1.36
1	G	73	HIC	CD2-CG	3.07	1.41	1.36

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	73	HIC	NE2-CE1-ND1	-3.15	111.46	112.66
1	K	73	HIC	NE2-CE1-ND1	-3.09	111.48	112.66
1	L	73	HIC	NE2-CE1-ND1	-3.07	111.49	112.66
1	A	73	HIC	NE2-CE1-ND1	-3.05	111.49	112.66
1	B	73	HIC	NE2-CE1-ND1	-3.04	111.50	112.66
1	J	73	HIC	NE2-CE1-ND1	-3.03	111.50	112.66
1	C	73	HIC	NE2-CE1-ND1	-3.02	111.51	112.66
1	D	73	HIC	NE2-CE1-ND1	-3.02	111.51	112.66
1	H	73	HIC	NE2-CE1-ND1	-3.01	111.51	112.66
1	O	73	HIC	NE2-CE1-ND1	-2.99	111.52	112.66
1	I	73	HIC	NE2-CE1-ND1	-2.99	111.52	112.66
1	M	73	HIC	NE2-CE1-ND1	-2.97	111.53	112.66
1	F	73	HIC	NE2-CE1-ND1	-2.93	111.54	112.66
1	G	73	HIC	NE2-CE1-ND1	-2.90	111.55	112.66
1	Q	73	HIC	NE2-CE1-ND1	-2.90	111.55	112.66
1	E	73	HIC	NE2-CE1-ND1	-2.89	111.56	112.66
1	P	73	HIC	NE2-CE1-ND1	-2.89	111.56	112.66
1	N	73	HIC	NE2-CE1-ND1	-2.83	111.58	112.66

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	73	HIC	N-CA-CB-CG
1	A	73	HIC	C-CA-CB-CG
1	B	73	HIC	N-CA-CB-CG
1	B	73	HIC	C-CA-CB-CG
1	C	73	HIC	N-CA-CB-CG
1	C	73	HIC	C-CA-CB-CG
1	D	73	HIC	N-CA-CB-CG
1	D	73	HIC	C-CA-CB-CG
1	E	73	HIC	N-CA-CB-CG
1	E	73	HIC	C-CA-CB-CG
1	F	73	HIC	N-CA-CB-CG
1	F	73	HIC	C-CA-CB-CG
1	G	73	HIC	N-CA-CB-CG
1	G	73	HIC	C-CA-CB-CG
1	H	73	HIC	N-CA-CB-CG
1	H	73	HIC	C-CA-CB-CG
1	I	73	HIC	N-CA-CB-CG
1	I	73	HIC	C-CA-CB-CG
1	J	73	HIC	N-CA-CB-CG
1	J	73	HIC	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
1	K	73	HIC	N-CA-CB-CG
1	K	73	HIC	C-CA-CB-CG
1	L	73	HIC	N-CA-CB-CG
1	L	73	HIC	C-CA-CB-CG
1	M	73	HIC	N-CA-CB-CG
1	M	73	HIC	C-CA-CB-CG
1	N	73	HIC	N-CA-CB-CG
1	N	73	HIC	C-CA-CB-CG
1	O	73	HIC	N-CA-CB-CG
1	O	73	HIC	C-CA-CB-CG
1	P	73	HIC	N-CA-CB-CG
1	P	73	HIC	C-CA-CB-CG
1	Q	73	HIC	N-CA-CB-CG
1	Q	73	HIC	C-CA-CB-CG
1	R	73	HIC	N-CA-CB-CG
1	R	73	HIC	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 18 are monoatomic - leaving 18 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	ADP	E	401	7	28,29,29	1.42	4 (14%)	43,45,45	1.79	9 (20%)
6	ADP	M	401	7	28,29,29	1.42	4 (14%)	43,45,45	1.80	9 (20%)
6	ADP	Q	401	7	28,29,29	1.41	4 (14%)	43,45,45	1.79	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	ADP	J	401	7	28,29,29	1.42	4 (14%)	43,45,45	1.80	9 (20%)
6	ADP	K	401	7	28,29,29	1.41	4 (14%)	43,45,45	1.79	9 (20%)
6	ADP	N	401	7	28,29,29	1.41	4 (14%)	43,45,45	1.80	9 (20%)
6	ADP	I	401	7	28,29,29	1.42	4 (14%)	43,45,45	1.79	9 (20%)
6	ADP	F	401	7	28,29,29	1.41	4 (14%)	43,45,45	1.79	9 (20%)
6	ADP	C	401	7	28,29,29	1.42	4 (14%)	43,45,45	1.79	9 (20%)
6	ADP	O	401	7	28,29,29	1.41	4 (14%)	43,45,45	1.80	9 (20%)
6	ADP	A	401	7	28,29,29	1.42	4 (14%)	43,45,45	1.79	9 (20%)
6	ADP	P	401	7	28,29,29	1.42	4 (14%)	43,45,45	1.80	9 (20%)
6	ADP	R	401	7	28,29,29	1.41	4 (14%)	43,45,45	1.79	9 (20%)
6	ADP	H	401	7	28,29,29	1.42	4 (14%)	43,45,45	1.79	9 (20%)
6	ADP	G	401	7	28,29,29	1.42	4 (14%)	43,45,45	1.80	9 (20%)
6	ADP	B	401	7	28,29,29	1.42	4 (14%)	43,45,45	1.80	9 (20%)
6	ADP	D	401	7	28,29,29	1.42	4 (14%)	43,45,45	1.79	9 (20%)
6	ADP	L	401	7	28,29,29	1.42	4 (14%)	43,45,45	1.80	9 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ADP	E	401	7	-	2/16/32/32	0/3/3/3
6	ADP	M	401	7	-	2/16/32/32	0/3/3/3
6	ADP	Q	401	7	-	2/16/32/32	0/3/3/3
6	ADP	J	401	7	-	2/16/32/32	0/3/3/3
6	ADP	K	401	7	-	2/16/32/32	0/3/3/3
6	ADP	N	401	7	-	2/16/32/32	0/3/3/3
6	ADP	I	401	7	-	2/16/32/32	0/3/3/3
6	ADP	F	401	7	-	2/16/32/32	0/3/3/3
6	ADP	C	401	7	-	2/16/32/32	0/3/3/3
6	ADP	O	401	7	-	2/16/32/32	0/3/3/3
6	ADP	A	401	7	-	2/16/32/32	0/3/3/3
6	ADP	P	401	7	-	2/16/32/32	0/3/3/3
6	ADP	R	401	7	-	2/16/32/32	0/3/3/3
6	ADP	H	401	7	-	2/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ADP	G	401	7	-	2/16/32/32	0/3/3/3
6	ADP	B	401	7	-	2/16/32/32	0/3/3/3
6	ADP	D	401	7	-	2/16/32/32	0/3/3/3
6	ADP	L	401	7	-	2/16/32/32	0/3/3/3

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	P	401	ADP	C5-C4	4.80	1.47	1.39
6	M	401	ADP	C5-C4	4.79	1.47	1.39
6	L	401	ADP	C5-C4	4.79	1.47	1.39
6	D	401	ADP	C5-C4	4.78	1.47	1.39
6	G	401	ADP	C5-C4	4.78	1.47	1.39
6	H	401	ADP	C5-C4	4.78	1.47	1.39
6	C	401	ADP	C5-C4	4.78	1.47	1.39
6	B	401	ADP	C5-C4	4.77	1.47	1.39
6	J	401	ADP	C5-C4	4.77	1.47	1.39
6	N	401	ADP	C5-C4	4.76	1.47	1.39
6	A	401	ADP	C5-C4	4.76	1.47	1.39
6	E	401	ADP	C5-C4	4.75	1.47	1.39
6	O	401	ADP	C5-C4	4.74	1.47	1.39
6	I	401	ADP	C5-C4	4.73	1.47	1.39
6	F	401	ADP	C5-C4	4.73	1.47	1.39
6	K	401	ADP	C5-C4	4.72	1.47	1.39
6	R	401	ADP	C5-C4	4.71	1.47	1.39
6	Q	401	ADP	C5-C4	4.71	1.47	1.39
6	D	401	ADP	C5-C6	2.76	1.48	1.41
6	A	401	ADP	C5-C6	2.76	1.48	1.41
6	G	401	ADP	C5-C6	2.76	1.48	1.41
6	O	401	ADP	C5-C6	2.75	1.48	1.41
6	H	401	ADP	C5-C6	2.75	1.48	1.41
6	F	401	ADP	C5-C6	2.75	1.48	1.41
6	I	401	ADP	C5-C6	2.74	1.48	1.41
6	Q	401	ADP	C5-C6	2.74	1.48	1.41
6	J	401	ADP	C5-C6	2.74	1.48	1.41
6	K	401	ADP	C5-C6	2.74	1.48	1.41
6	C	401	ADP	C5-C6	2.74	1.48	1.41
6	E	401	ADP	C5-C6	2.73	1.48	1.41
6	N	401	ADP	C5-C6	2.73	1.48	1.41
6	M	401	ADP	C5-C6	2.73	1.48	1.41
6	P	401	ADP	C5-C6	2.73	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	R	401	ADP	C5-C6	2.73	1.48	1.41
6	L	401	ADP	C5-C6	2.73	1.48	1.41
6	B	401	ADP	C5-C6	2.73	1.48	1.41
6	P	401	ADP	C8-N7	2.37	1.36	1.31
6	C	401	ADP	C8-N7	2.35	1.36	1.31
6	E	401	ADP	C8-N7	2.35	1.36	1.31
6	Q	401	ADP	C8-N7	2.34	1.36	1.31
6	I	401	ADP	C8-N7	2.34	1.36	1.31
6	M	401	ADP	C8-N7	2.34	1.36	1.31
6	J	401	ADP	C8-N7	2.34	1.36	1.31
6	G	401	ADP	C8-N7	2.33	1.36	1.31
6	O	401	ADP	C8-N7	2.33	1.36	1.31
6	H	401	ADP	C8-N7	2.32	1.36	1.31
6	D	401	ADP	C8-N7	2.32	1.36	1.31
6	F	401	ADP	C8-N7	2.31	1.36	1.31
6	K	401	ADP	C8-N7	2.30	1.36	1.31
6	L	401	ADP	C8-N7	2.30	1.36	1.31
6	A	401	ADP	C8-N7	2.29	1.36	1.31
6	B	401	ADP	C8-N7	2.29	1.36	1.31
6	R	401	ADP	C8-N7	2.29	1.36	1.31
6	N	401	ADP	C8-N7	2.28	1.36	1.31
6	P	401	ADP	C5-N7	-2.28	1.34	1.39
6	D	401	ADP	C5-N7	-2.26	1.35	1.39
6	Q	401	ADP	C5-N7	-2.26	1.35	1.39
6	R	401	ADP	C5-N7	-2.26	1.35	1.39
6	H	401	ADP	C5-N7	-2.25	1.35	1.39
6	C	401	ADP	C5-N7	-2.25	1.35	1.39
6	F	401	ADP	C5-N7	-2.25	1.35	1.39
6	G	401	ADP	C5-N7	-2.25	1.35	1.39
6	A	401	ADP	C5-N7	-2.24	1.35	1.39
6	O	401	ADP	C5-N7	-2.24	1.35	1.39
6	E	401	ADP	C5-N7	-2.24	1.35	1.39
6	J	401	ADP	C5-N7	-2.24	1.35	1.39
6	L	401	ADP	C5-N7	-2.23	1.35	1.39
6	I	401	ADP	C5-N7	-2.23	1.35	1.39
6	B	401	ADP	C5-N7	-2.23	1.35	1.39
6	M	401	ADP	C5-N7	-2.23	1.35	1.39
6	K	401	ADP	C5-N7	-2.22	1.35	1.39
6	N	401	ADP	C5-N7	-2.21	1.35	1.39

All (162) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	N	401	ADP	C5-C4-N3	-5.84	118.67	126.72
6	B	401	ADP	C5-C4-N3	-5.83	118.69	126.72
6	K	401	ADP	C5-C4-N3	-5.83	118.69	126.72
6	M	401	ADP	C5-C4-N3	-5.83	118.69	126.72
6	L	401	ADP	C5-C4-N3	-5.83	118.69	126.72
6	E	401	ADP	C5-C4-N3	-5.82	118.70	126.72
6	I	401	ADP	C5-C4-N3	-5.82	118.71	126.72
6	J	401	ADP	C5-C4-N3	-5.82	118.71	126.72
6	O	401	ADP	C5-C4-N3	-5.82	118.71	126.72
6	Q	401	ADP	C5-C4-N3	-5.81	118.71	126.72
6	P	401	ADP	C5-C4-N3	-5.81	118.72	126.72
6	G	401	ADP	C5-C4-N3	-5.81	118.72	126.72
6	D	401	ADP	C5-C4-N3	-5.81	118.72	126.72
6	H	401	ADP	C5-C4-N3	-5.80	118.72	126.72
6	F	401	ADP	C5-C4-N3	-5.80	118.73	126.72
6	C	401	ADP	C5-C4-N3	-5.80	118.73	126.72
6	R	401	ADP	C5-C4-N3	-5.80	118.73	126.72
6	A	401	ADP	C5-C4-N3	-5.78	118.76	126.72
6	L	401	ADP	N3-C4-N9	4.65	135.07	127.17
6	D	401	ADP	N3-C4-N9	4.64	135.06	127.17
6	G	401	ADP	N3-C4-N9	4.64	135.06	127.17
6	P	401	ADP	N3-C4-N9	4.64	135.06	127.17
6	N	401	ADP	N3-C4-N9	4.64	135.06	127.17
6	H	401	ADP	N3-C4-N9	4.63	135.04	127.17
6	E	401	ADP	N3-C4-N9	4.63	135.04	127.17
6	M	401	ADP	N3-C4-N9	4.63	135.04	127.17
6	B	401	ADP	N3-C4-N9	4.62	135.03	127.17
6	J	401	ADP	N3-C4-N9	4.62	135.03	127.17
6	F	401	ADP	N3-C4-N9	4.62	135.03	127.17
6	K	401	ADP	N3-C4-N9	4.62	135.02	127.17
6	C	401	ADP	N3-C4-N9	4.62	135.02	127.17
6	O	401	ADP	N3-C4-N9	4.62	135.02	127.17
6	I	401	ADP	N3-C4-N9	4.62	135.02	127.17
6	A	401	ADP	N3-C4-N9	4.61	135.00	127.17
6	Q	401	ADP	N3-C4-N9	4.61	135.00	127.17
6	R	401	ADP	N3-C4-N9	4.60	135.00	127.17
6	O	401	ADP	C2-N3-C4	3.67	120.79	111.83
6	P	401	ADP	C2-N3-C4	3.66	120.78	111.83
6	N	401	ADP	C2-N3-C4	3.66	120.77	111.83
6	A	401	ADP	C2-N3-C4	3.66	120.76	111.83
6	J	401	ADP	C2-N3-C4	3.66	120.76	111.83
6	Q	401	ADP	C2-N3-C4	3.66	120.76	111.83
6	D	401	ADP	C2-N3-C4	3.66	120.76	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	401	ADP	C2-N3-C4	3.65	120.76	111.83
6	G	401	ADP	C2-N3-C4	3.65	120.75	111.83
6	K	401	ADP	C2-N3-C4	3.65	120.75	111.83
6	C	401	ADP	C2-N3-C4	3.65	120.74	111.83
6	E	401	ADP	C2-N3-C4	3.65	120.74	111.83
6	L	401	ADP	C2-N3-C4	3.65	120.74	111.83
6	F	401	ADP	C2-N3-C4	3.65	120.74	111.83
6	B	401	ADP	C2-N3-C4	3.64	120.73	111.83
6	R	401	ADP	C2-N3-C4	3.64	120.73	111.83
6	M	401	ADP	C2-N3-C4	3.64	120.73	111.83
6	I	401	ADP	C2-N3-C4	3.64	120.72	111.83
6	N	401	ADP	C4-C5-N7	-3.50	106.58	110.58
6	B	401	ADP	C4-C5-N7	-3.49	106.60	110.58
6	K	401	ADP	C4-C5-N7	-3.47	106.61	110.58
6	M	401	ADP	C4-C5-N7	-3.47	106.62	110.58
6	L	401	ADP	C4-C5-N7	-3.46	106.62	110.58
6	R	401	ADP	C4-C5-N7	-3.46	106.62	110.58
6	J	401	ADP	C4-C5-N7	-3.46	106.63	110.58
6	G	401	ADP	C4-C5-N7	-3.44	106.64	110.58
6	H	401	ADP	C4-C5-N7	-3.44	106.65	110.58
6	I	401	ADP	C4-C5-N7	-3.44	106.65	110.58
6	O	401	ADP	C4-C5-N7	-3.43	106.66	110.58
6	Q	401	ADP	C4-C5-N7	-3.43	106.66	110.58
6	A	401	ADP	C4-C5-N7	-3.43	106.66	110.58
6	P	401	ADP	C4-C5-N7	-3.43	106.66	110.58
6	C	401	ADP	C4-C5-N7	-3.43	106.66	110.58
6	E	401	ADP	C4-C5-N7	-3.43	106.66	110.58
6	D	401	ADP	C4-C5-N7	-3.42	106.67	110.58
6	F	401	ADP	C4-C5-N7	-3.41	106.69	110.58
6	O	401	ADP	N3-C2-N1	-3.18	123.76	128.58
6	J	401	ADP	N3-C2-N1	-3.17	123.78	128.58
6	A	401	ADP	N3-C2-N1	-3.17	123.79	128.58
6	P	401	ADP	N3-C2-N1	-3.16	123.79	128.58
6	R	401	ADP	N3-C2-N1	-3.16	123.80	128.58
6	E	401	ADP	N3-C2-N1	-3.15	123.81	128.58
6	Q	401	ADP	N3-C2-N1	-3.15	123.81	128.58
6	G	401	ADP	N3-C2-N1	-3.14	123.82	128.58
6	N	401	ADP	N3-C2-N1	-3.14	123.82	128.58
6	M	401	ADP	N3-C2-N1	-3.14	123.83	128.58
6	C	401	ADP	N3-C2-N1	-3.14	123.83	128.58
6	K	401	ADP	N3-C2-N1	-3.14	123.83	128.58
6	F	401	ADP	N3-C2-N1	-3.13	123.84	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	401	ADP	N3-C2-N1	-3.13	123.84	128.58
6	L	401	ADP	N3-C2-N1	-3.13	123.85	128.58
6	I	401	ADP	N3-C2-N1	-3.12	123.86	128.58
6	B	401	ADP	N3-C2-N1	-3.12	123.86	128.58
6	D	401	ADP	N3-C2-N1	-3.12	123.86	128.58
6	L	401	ADP	C4-N9-C8	2.66	108.53	105.74
6	N	401	ADP	C4-N9-C8	2.66	108.53	105.74
6	G	401	ADP	C4-N9-C8	2.66	108.53	105.74
6	M	401	ADP	C4-N9-C8	2.65	108.52	105.74
6	P	401	ADP	C4-N9-C8	2.65	108.52	105.74
6	E	401	ADP	C4-N9-C8	2.65	108.52	105.74
6	C	401	ADP	C4-N9-C8	2.64	108.51	105.74
6	D	401	ADP	C4-N9-C8	2.64	108.51	105.74
6	H	401	ADP	C4-N9-C8	2.64	108.51	105.74
6	I	401	ADP	C4-N9-C8	2.64	108.51	105.74
6	J	401	ADP	C4-N9-C8	2.64	108.50	105.74
6	R	401	ADP	C4-N9-C8	2.63	108.50	105.74
6	B	401	ADP	C4-N9-C8	2.62	108.49	105.74
6	Q	401	ADP	C4-N9-C8	2.62	108.49	105.74
6	F	401	ADP	C4-N9-C8	2.62	108.48	105.74
6	O	401	ADP	C4-N9-C8	2.61	108.48	105.74
6	K	401	ADP	C4-N9-C8	2.60	108.47	105.74
6	A	401	ADP	C4-N9-C8	2.58	108.45	105.74
6	N	401	ADP	C5-N7-C8	2.55	107.46	103.45
6	R	401	ADP	C5-N7-C8	2.54	107.45	103.45
6	Q	401	ADP	C5-N7-C8	2.54	107.44	103.45
6	P	401	ADP	C5-N7-C8	2.53	107.43	103.45
6	B	401	ADP	C5-N7-C8	2.53	107.43	103.45
6	H	401	ADP	C5-N7-C8	2.53	107.43	103.45
6	L	401	ADP	C5-N7-C8	2.53	107.43	103.45
6	K	401	ADP	C5-N7-C8	2.53	107.42	103.45
6	J	401	ADP	C5-N7-C8	2.52	107.42	103.45
6	M	401	ADP	C5-N7-C8	2.52	107.42	103.45
6	O	401	ADP	C5-N7-C8	2.51	107.40	103.45
6	A	401	ADP	C5-N7-C8	2.51	107.40	103.45
6	G	401	ADP	C5-N7-C8	2.51	107.39	103.45
6	D	401	ADP	C5-N7-C8	2.51	107.39	103.45
6	I	401	ADP	C5-N7-C8	2.51	107.39	103.45
6	F	401	ADP	C5-N7-C8	2.50	107.38	103.45
6	C	401	ADP	C5-N7-C8	2.49	107.36	103.45
6	E	401	ADP	C5-N7-C8	2.48	107.35	103.45
6	Q	401	ADP	C3'-C2'-C1'	2.23	105.68	101.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	401	ADP	C3'-C2'-C1'	2.22	105.66	101.46
6	N	401	ADP	C3'-C2'-C1'	2.22	105.65	101.46
6	K	401	ADP	C3'-C2'-C1'	2.21	105.65	101.46
6	O	401	ADP	C3'-C2'-C1'	2.21	105.65	101.46
6	E	401	ADP	C3'-C2'-C1'	2.21	105.65	101.46
6	J	401	ADP	C3'-C2'-C1'	2.21	105.65	101.46
6	P	401	ADP	C3'-C2'-C1'	2.21	105.64	101.46
6	L	401	ADP	C3'-C2'-C1'	2.21	105.64	101.46
6	B	401	ADP	C3'-C2'-C1'	2.21	105.64	101.46
6	M	401	ADP	C3'-C2'-C1'	2.20	105.63	101.46
6	D	401	ADP	C3'-C2'-C1'	2.20	105.63	101.46
6	H	401	ADP	C3'-C2'-C1'	2.20	105.62	101.46
6	C	401	ADP	C3'-C2'-C1'	2.20	105.62	101.46
6	A	401	ADP	C3'-C2'-C1'	2.20	105.62	101.46
6	I	401	ADP	C3'-C2'-C1'	2.19	105.61	101.46
6	R	401	ADP	C3'-C2'-C1'	2.19	105.61	101.46
6	F	401	ADP	C3'-C2'-C1'	2.18	105.59	101.46
6	J	401	ADP	C6-C5-N7	2.06	136.05	132.09
6	L	401	ADP	C6-C5-N7	2.06	136.05	132.09
6	A	401	ADP	C6-C5-N7	2.05	136.05	132.09
6	P	401	ADP	C6-C5-N7	2.05	136.05	132.09
6	B	401	ADP	C6-C5-N7	2.05	136.04	132.09
6	N	401	ADP	C6-C5-N7	2.05	136.04	132.09
6	K	401	ADP	C6-C5-N7	2.04	136.03	132.09
6	D	401	ADP	C6-C5-N7	2.04	136.03	132.09
6	G	401	ADP	C6-C5-N7	2.04	136.03	132.09
6	C	401	ADP	C6-C5-N7	2.04	136.03	132.09
6	O	401	ADP	C6-C5-N7	2.04	136.03	132.09
6	H	401	ADP	C6-C5-N7	2.04	136.02	132.09
6	M	401	ADP	C6-C5-N7	2.04	136.02	132.09
6	R	401	ADP	C6-C5-N7	2.04	136.02	132.09
6	I	401	ADP	C6-C5-N7	2.02	135.98	132.09
6	E	401	ADP	C6-C5-N7	2.02	135.97	132.09
6	Q	401	ADP	C6-C5-N7	2.01	135.97	132.09
6	F	401	ADP	C6-C5-N7	2.01	135.97	132.09

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	401	ADP	C5'-O5'-PA-O2A
6	A	401	ADP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
6	B	401	ADP	C5'-O5'-PA-O2A
6	B	401	ADP	C5'-O5'-PA-O3A
6	C	401	ADP	C5'-O5'-PA-O2A
6	C	401	ADP	C5'-O5'-PA-O3A
6	D	401	ADP	C5'-O5'-PA-O2A
6	D	401	ADP	C5'-O5'-PA-O3A
6	E	401	ADP	C5'-O5'-PA-O2A
6	E	401	ADP	C5'-O5'-PA-O3A
6	F	401	ADP	C5'-O5'-PA-O2A
6	F	401	ADP	C5'-O5'-PA-O3A
6	G	401	ADP	C5'-O5'-PA-O2A
6	G	401	ADP	C5'-O5'-PA-O3A
6	H	401	ADP	C5'-O5'-PA-O2A
6	H	401	ADP	C5'-O5'-PA-O3A
6	I	401	ADP	C5'-O5'-PA-O2A
6	I	401	ADP	C5'-O5'-PA-O3A
6	J	401	ADP	C5'-O5'-PA-O2A
6	J	401	ADP	C5'-O5'-PA-O3A
6	K	401	ADP	C5'-O5'-PA-O2A
6	K	401	ADP	C5'-O5'-PA-O3A
6	L	401	ADP	C5'-O5'-PA-O2A
6	L	401	ADP	C5'-O5'-PA-O3A
6	M	401	ADP	C5'-O5'-PA-O2A
6	M	401	ADP	C5'-O5'-PA-O3A
6	N	401	ADP	C5'-O5'-PA-O2A
6	N	401	ADP	C5'-O5'-PA-O3A
6	O	401	ADP	C5'-O5'-PA-O2A
6	O	401	ADP	C5'-O5'-PA-O3A
6	P	401	ADP	C5'-O5'-PA-O2A
6	P	401	ADP	C5'-O5'-PA-O3A
6	Q	401	ADP	C5'-O5'-PA-O2A
6	Q	401	ADP	C5'-O5'-PA-O3A
6	R	401	ADP	C5'-O5'-PA-O2A
6	R	401	ADP	C5'-O5'-PA-O3A

There are no ring outliers.

18 monomers are involved in 18 short contacts:

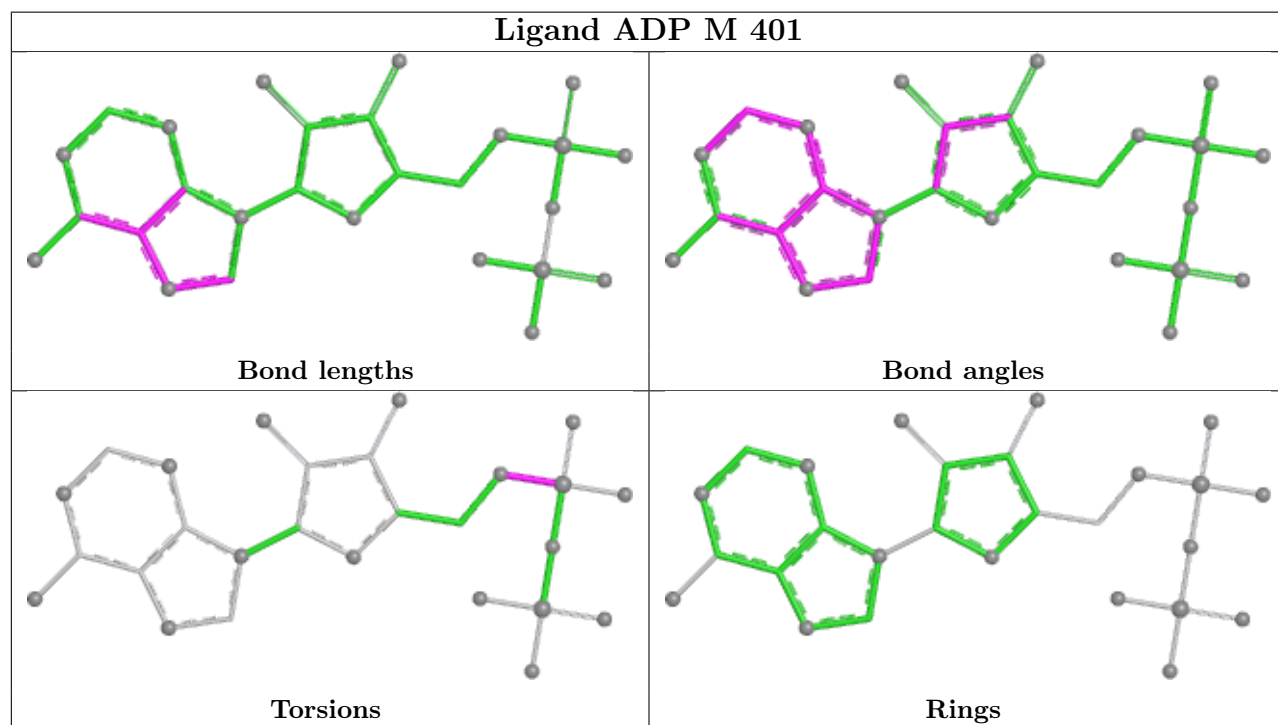
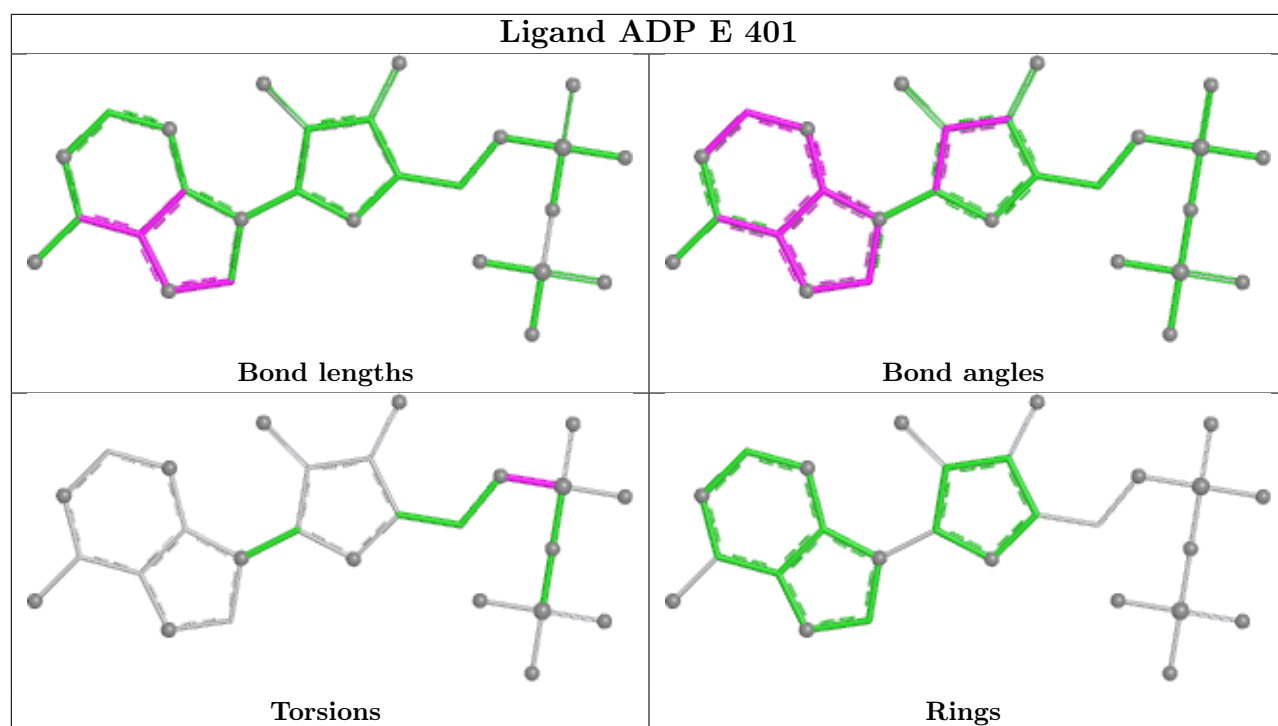
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	401	ADP	1	0
6	M	401	ADP	1	0
6	Q	401	ADP	1	0

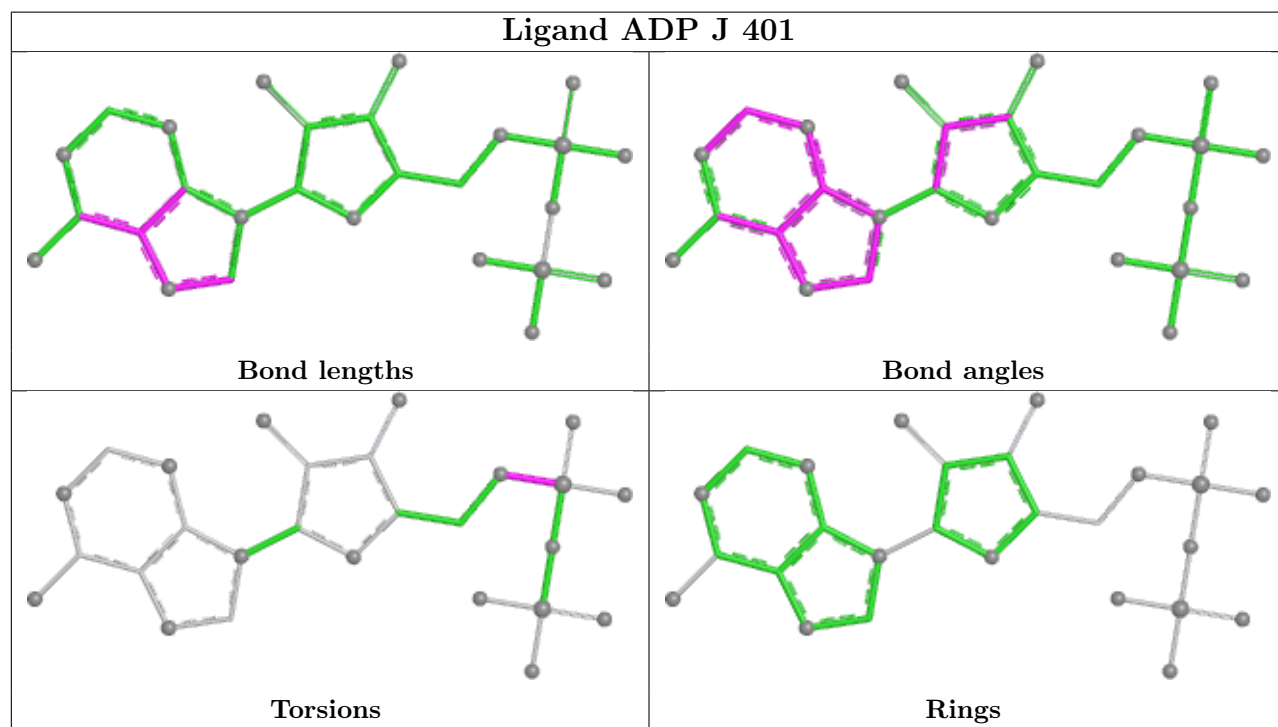
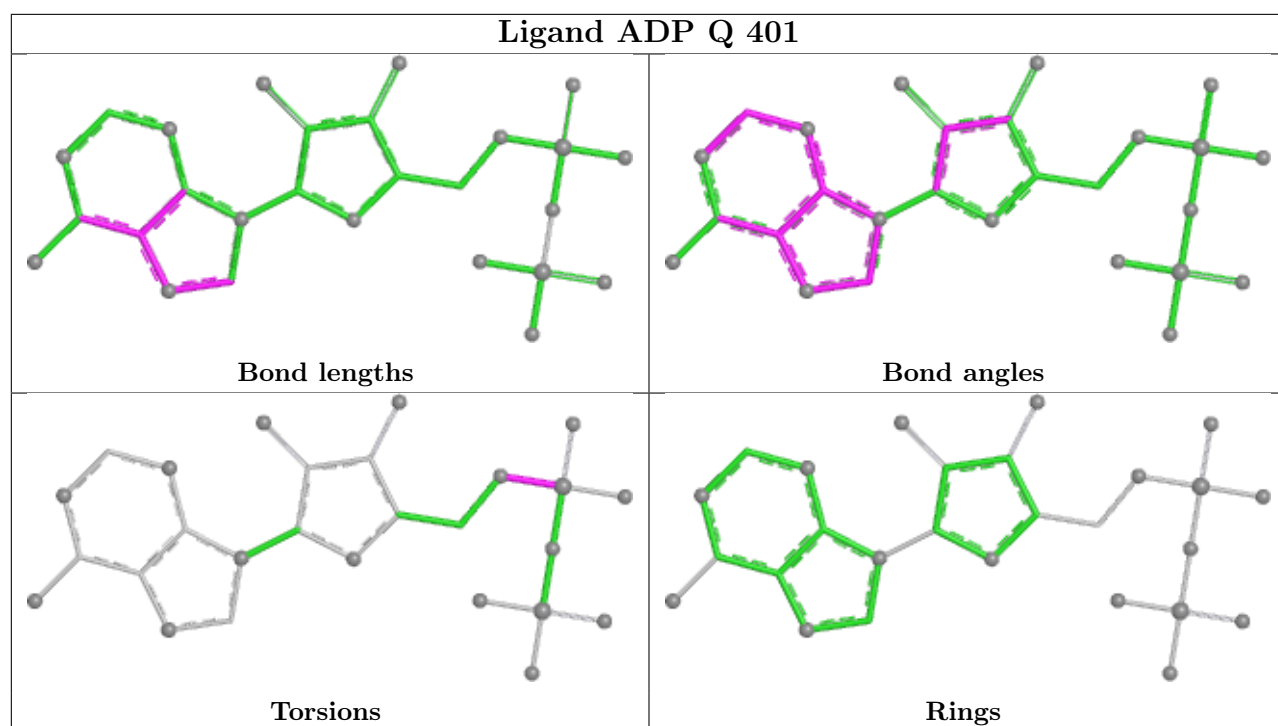
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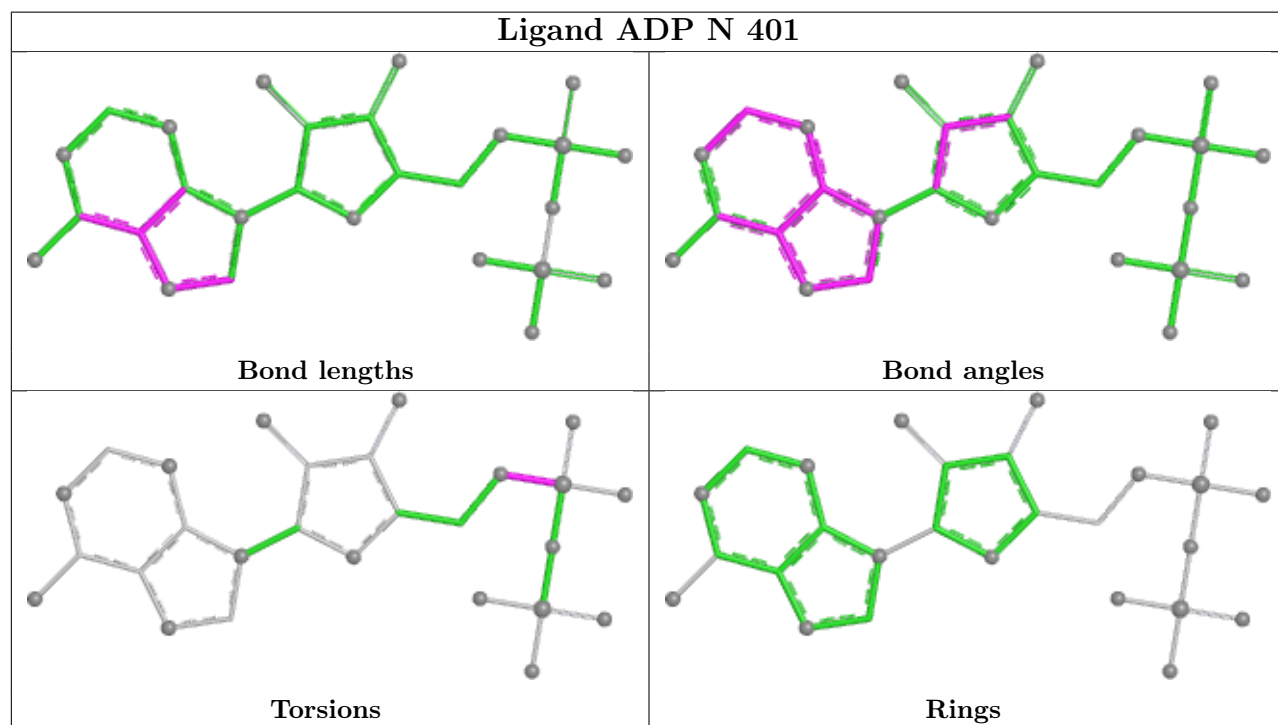
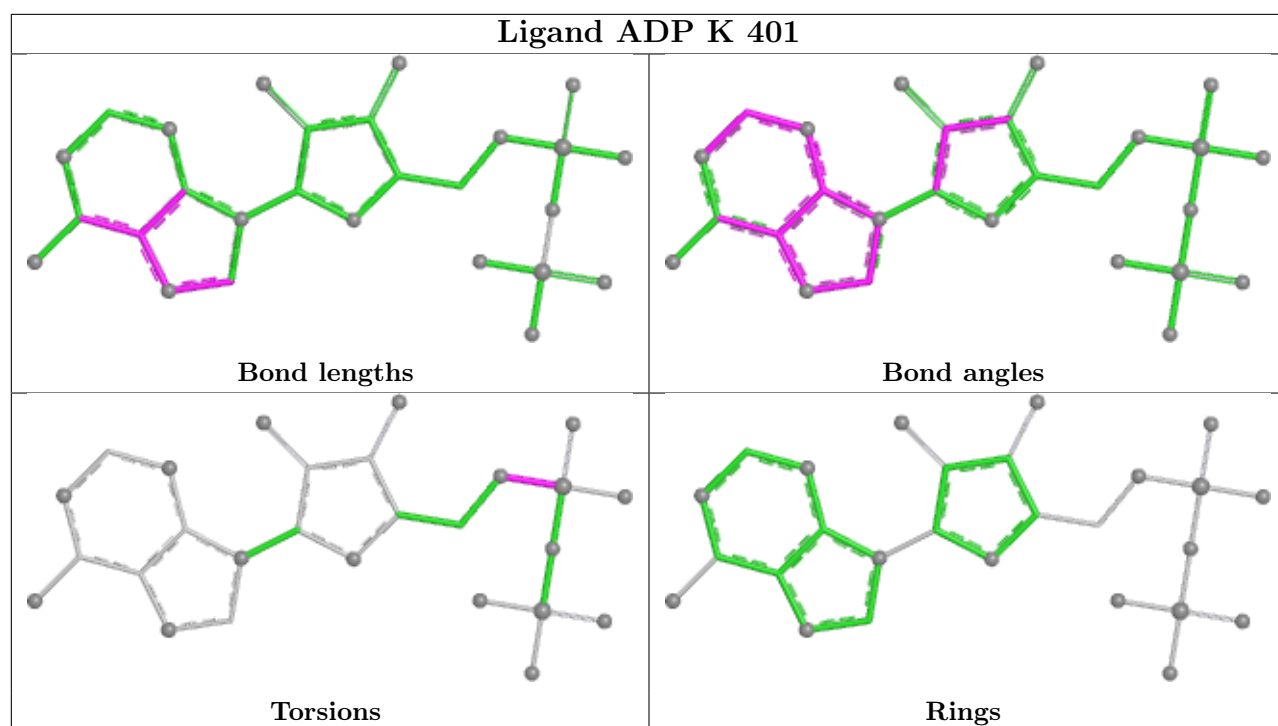
Continued from previous page...

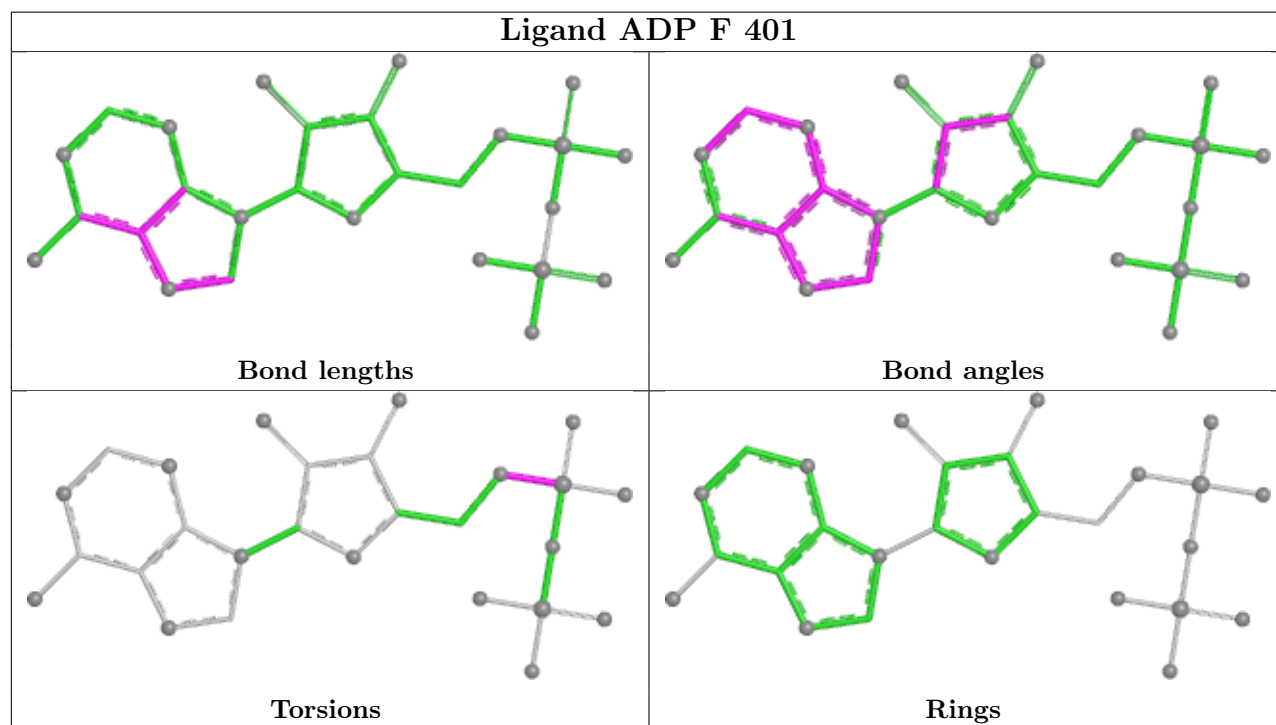
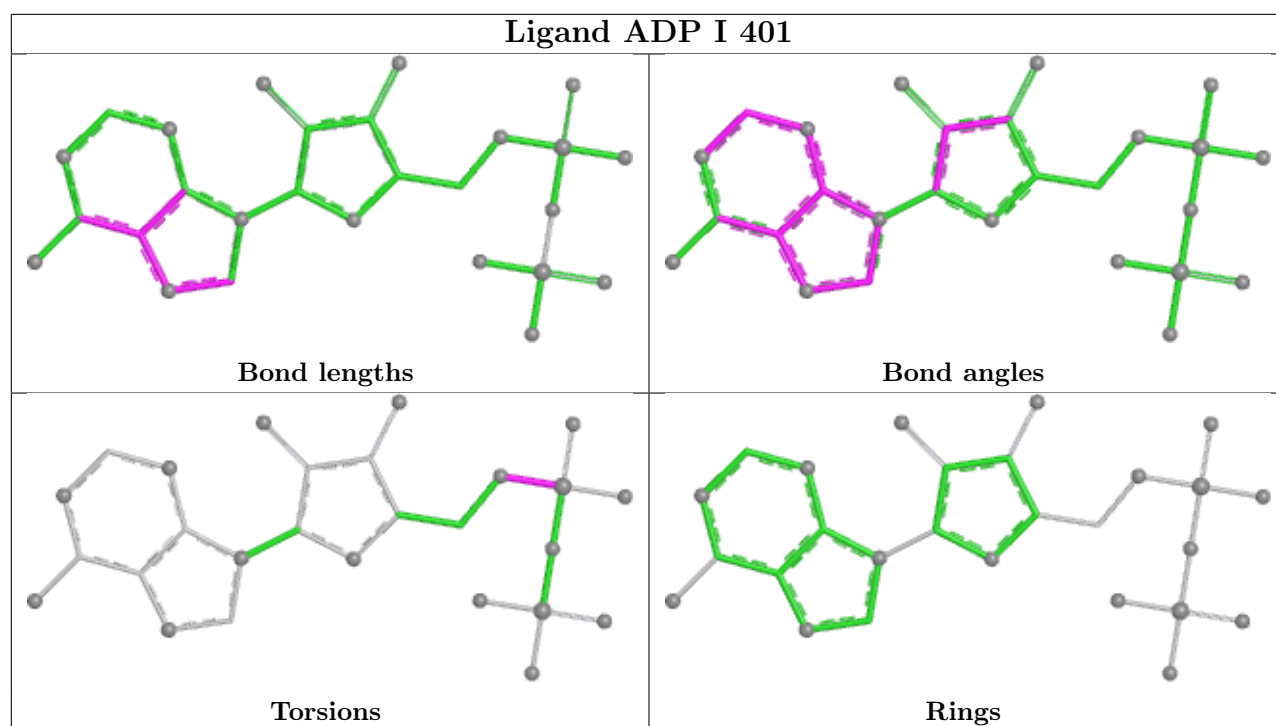
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	J	401	ADP	1	0
6	K	401	ADP	1	0
6	N	401	ADP	1	0
6	I	401	ADP	1	0
6	F	401	ADP	1	0
6	C	401	ADP	1	0
6	O	401	ADP	1	0
6	A	401	ADP	1	0
6	P	401	ADP	1	0
6	R	401	ADP	1	0
6	H	401	ADP	1	0
6	G	401	ADP	1	0
6	B	401	ADP	1	0
6	D	401	ADP	1	0
6	L	401	ADP	1	0

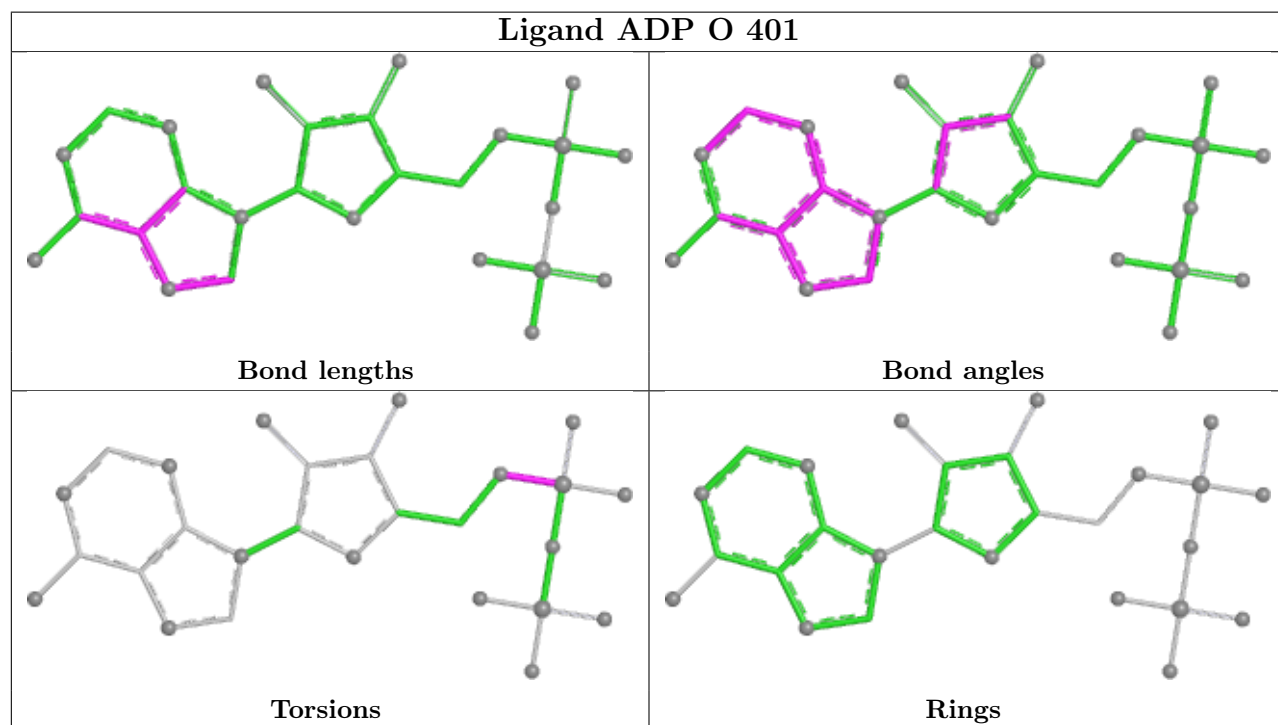
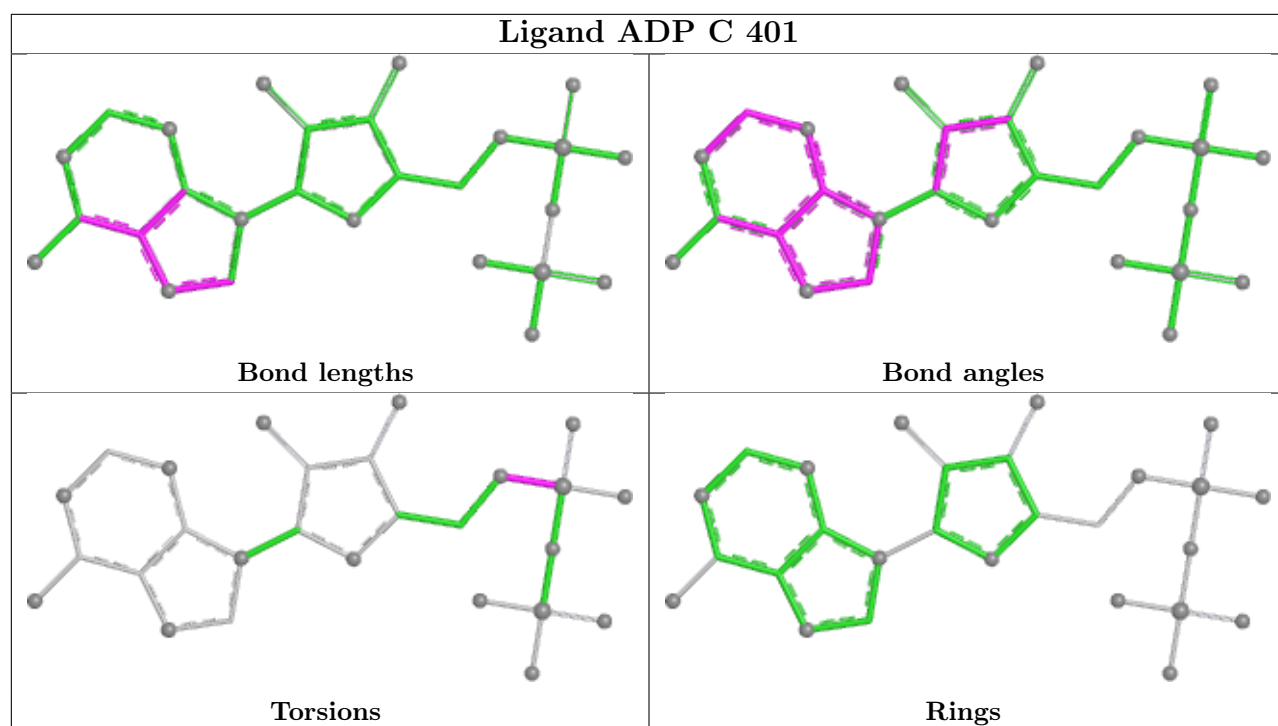
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

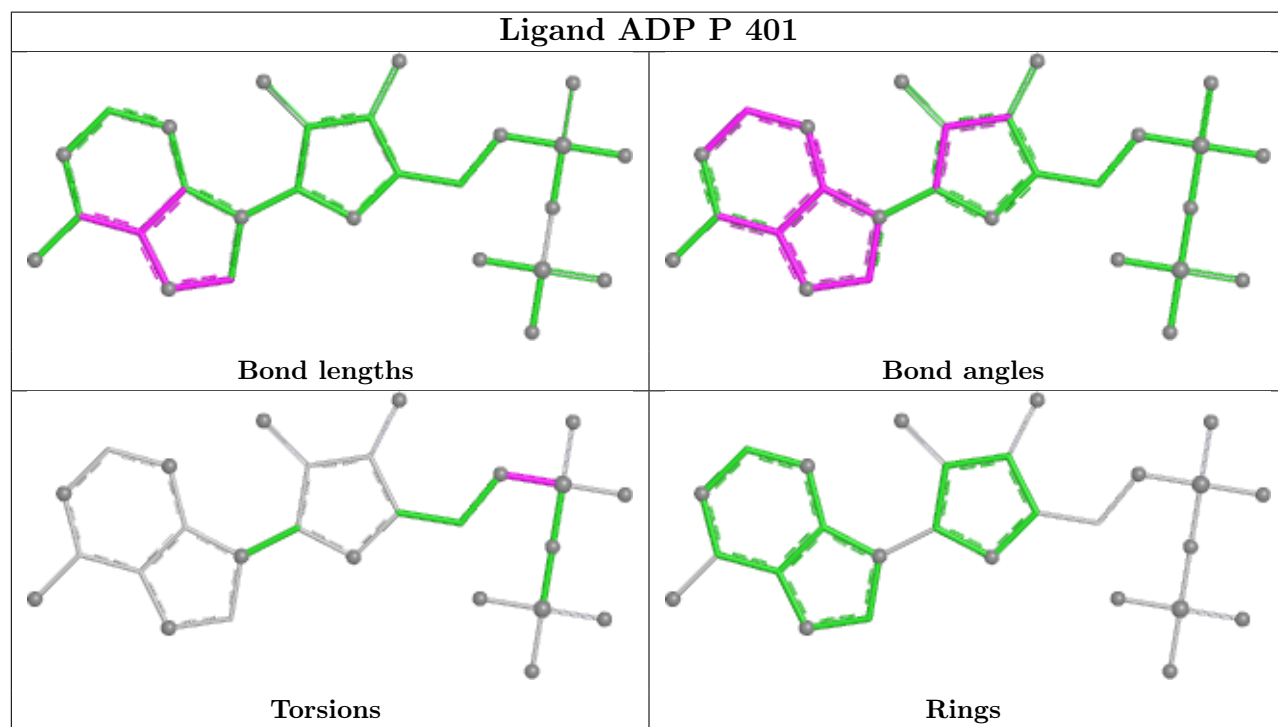
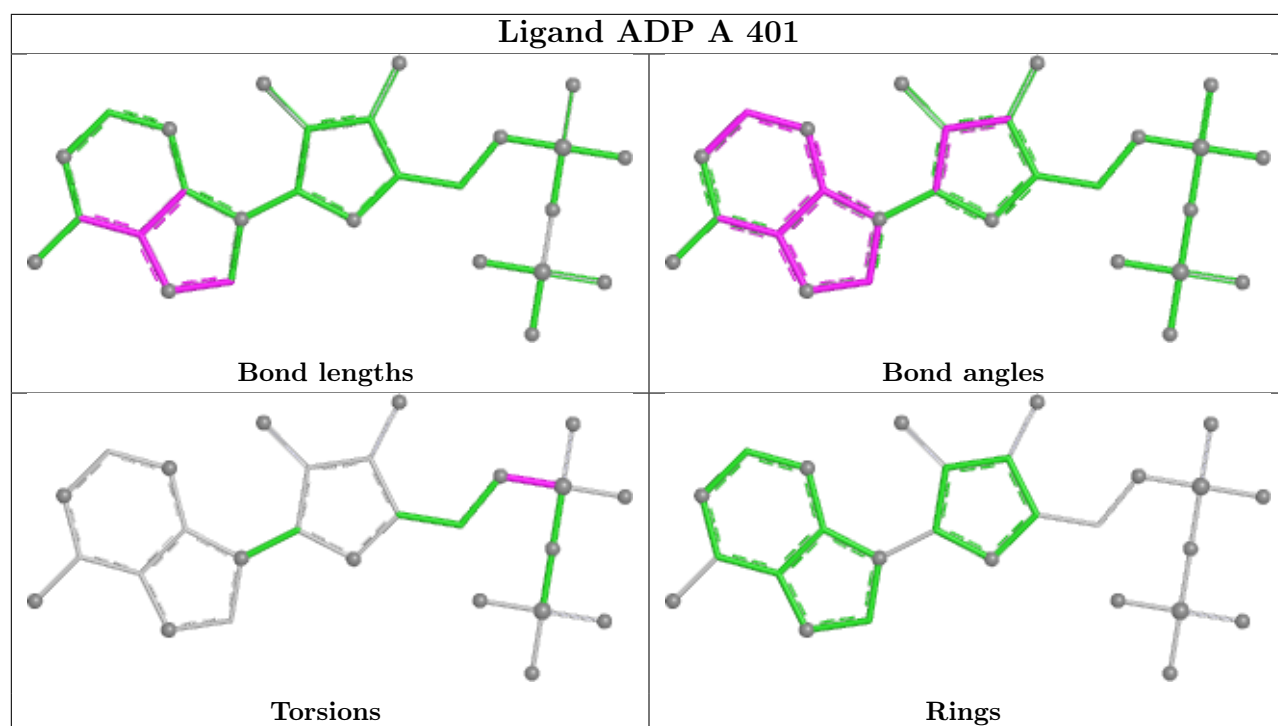


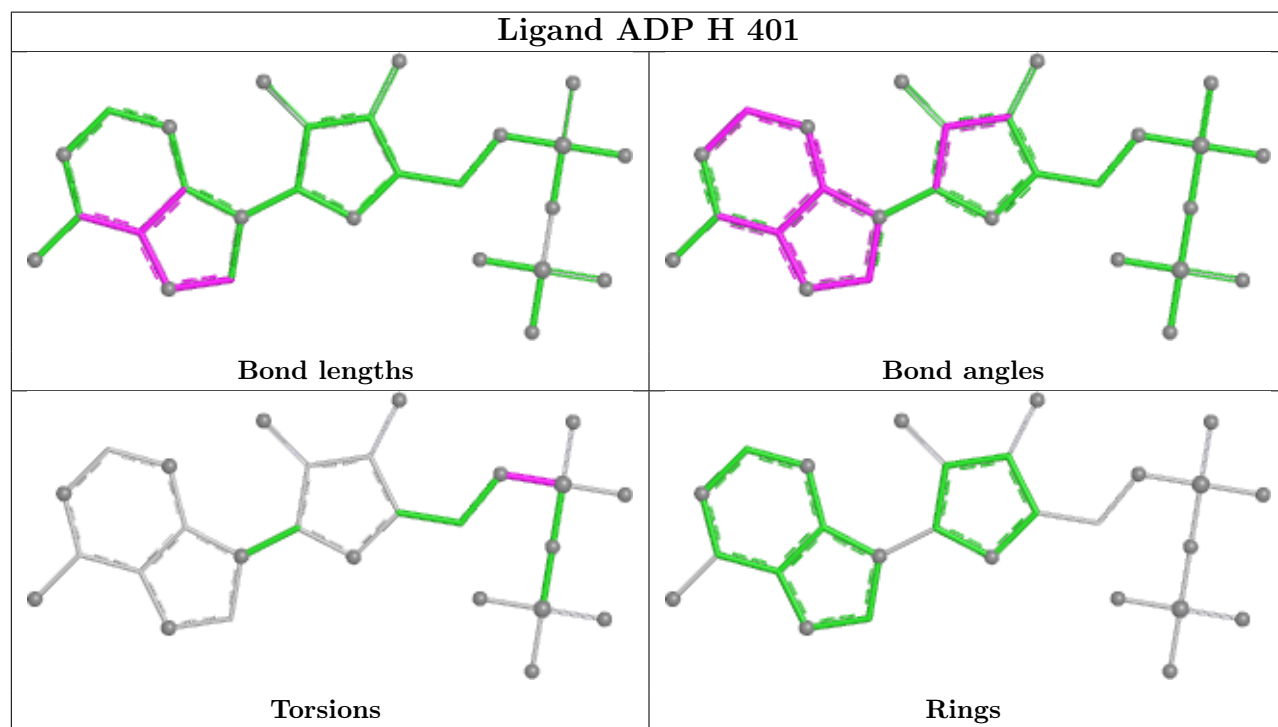
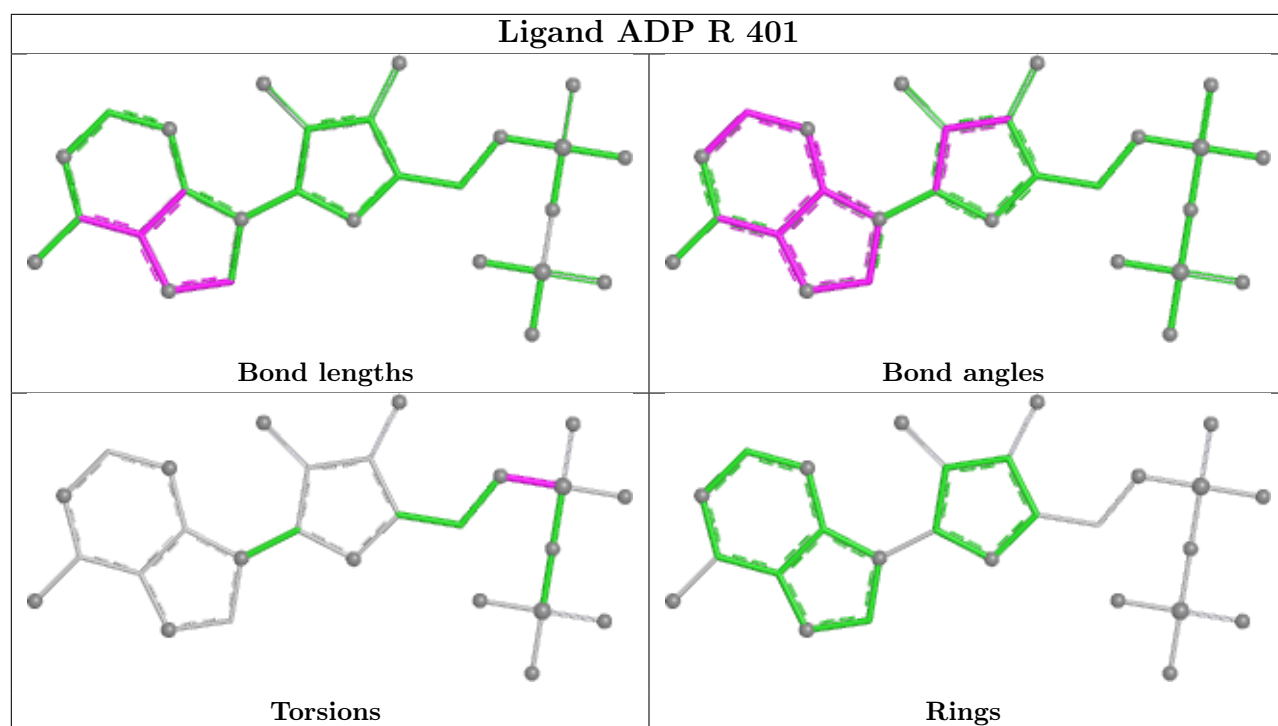


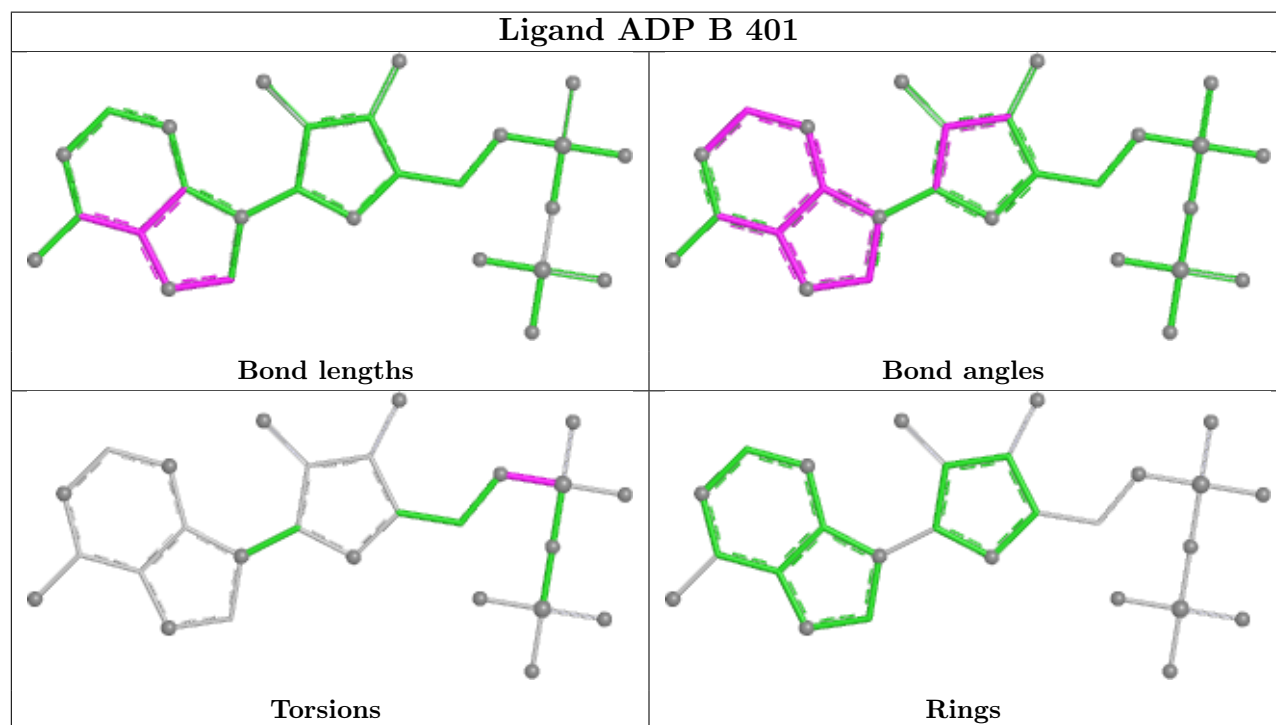
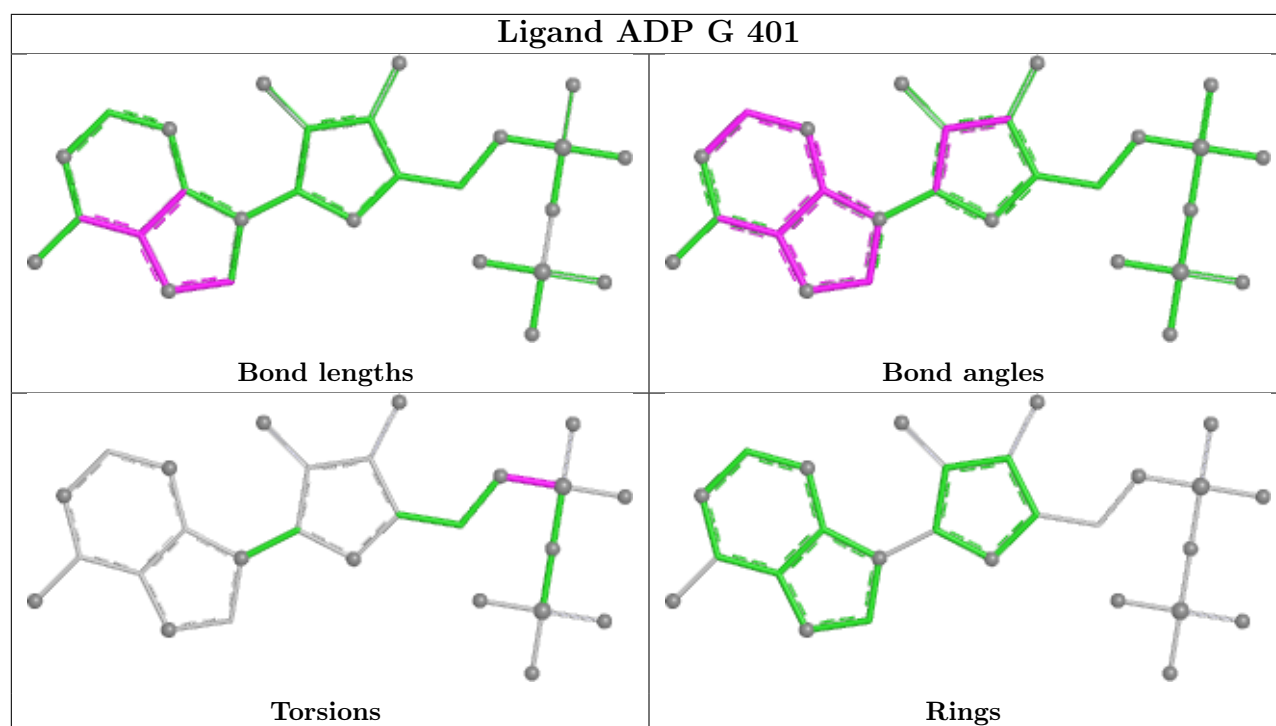


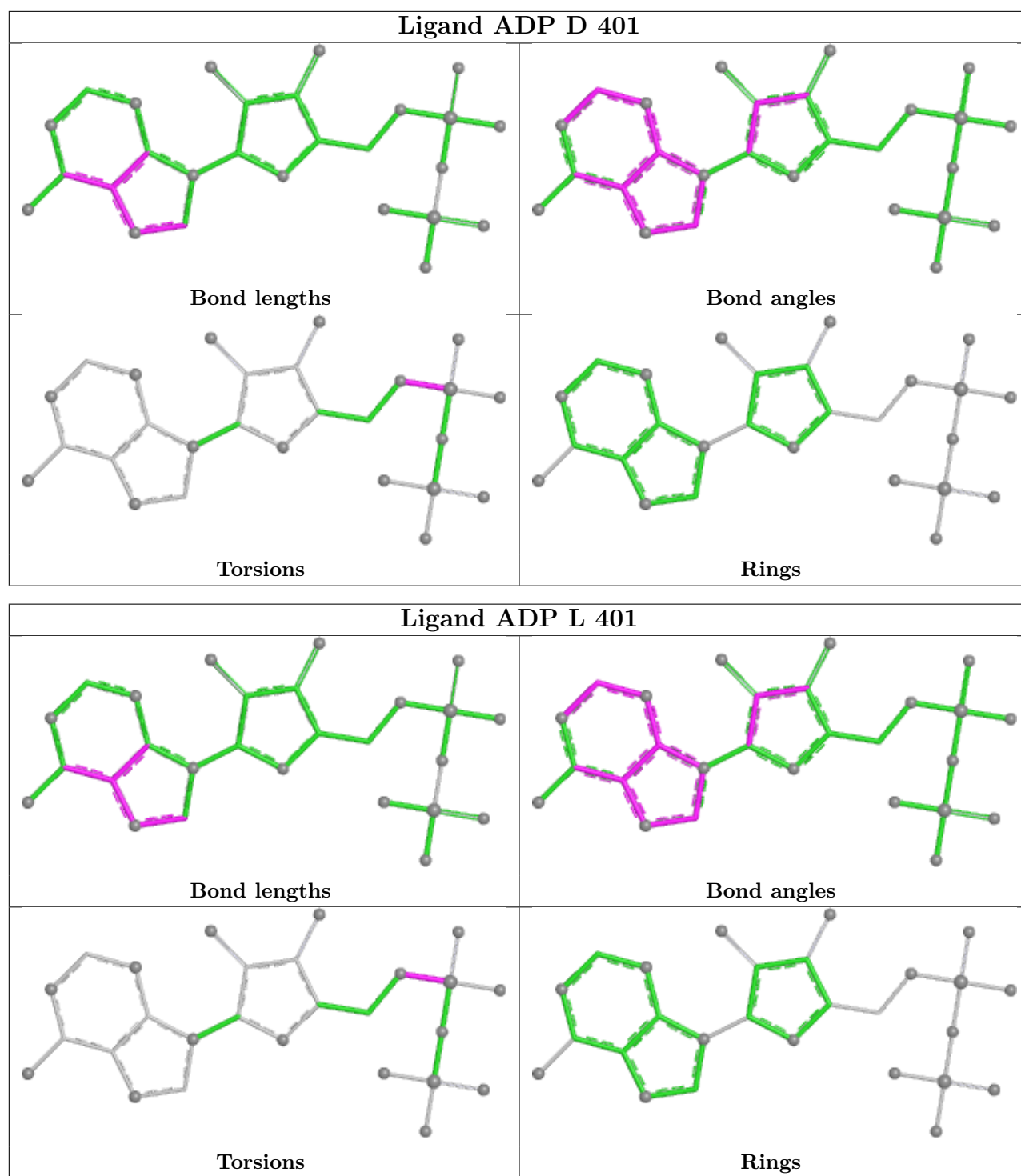












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

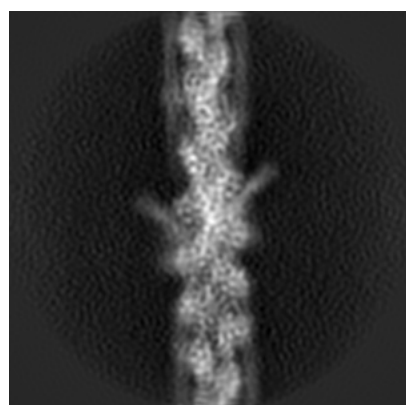
6 Map visualisation [i](#)

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.

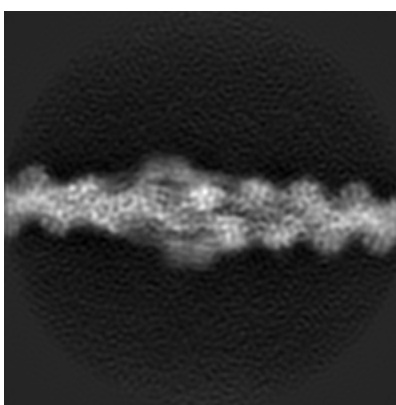
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

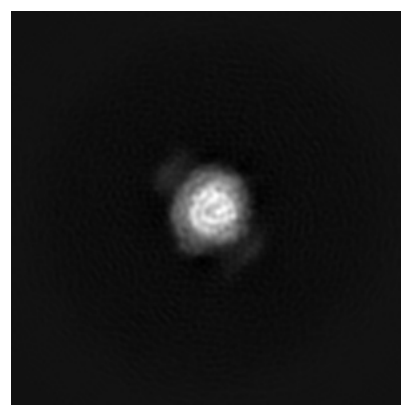
6.1.1 Primary map



X



Y

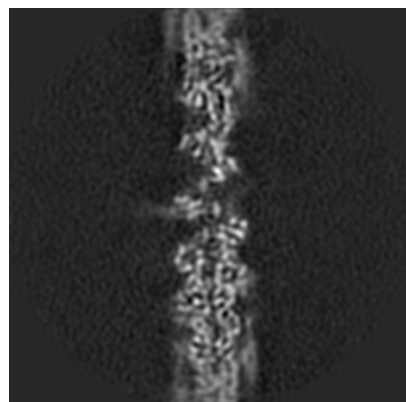


Z

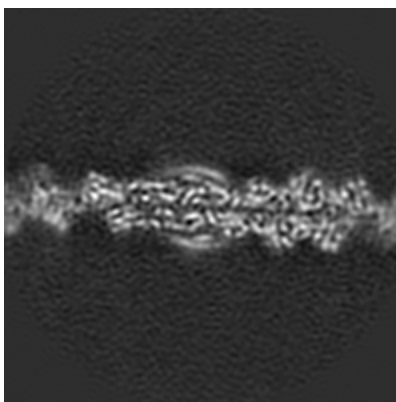
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

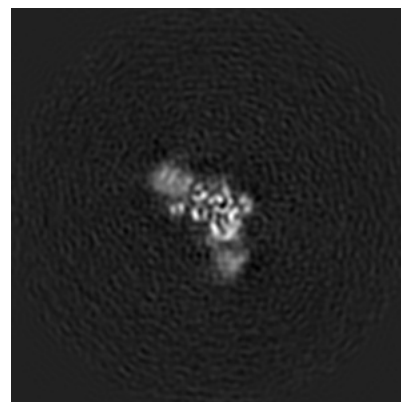
6.2.1 Primary map



X Index: 100



Y Index: 100

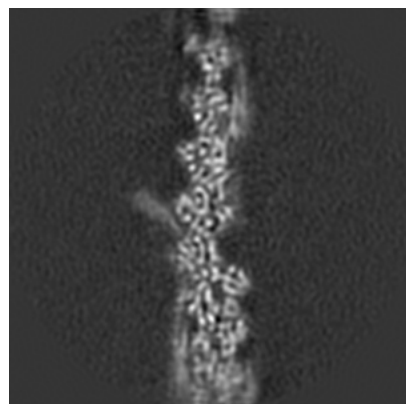


Z Index: 100

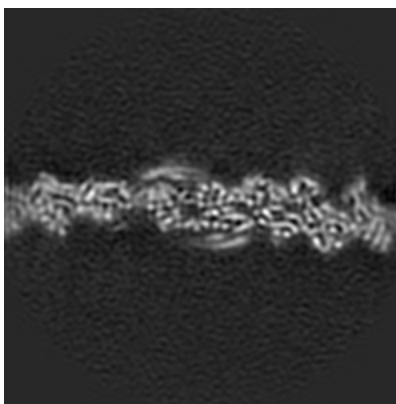
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

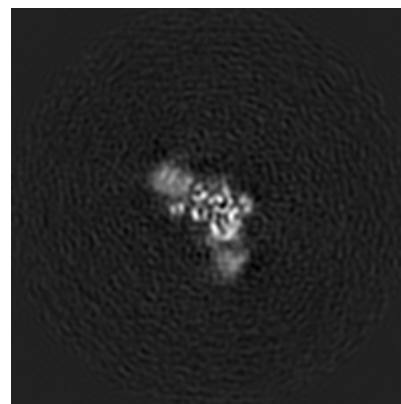
6.3.1 Primary map



X Index: 106



Y Index: 96

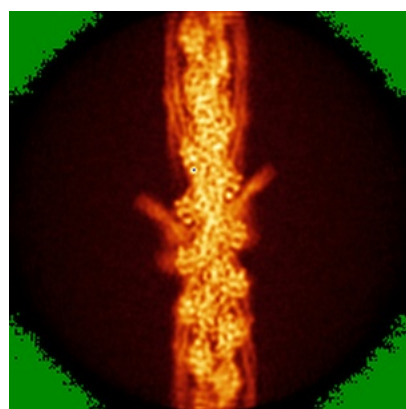


Z Index: 100

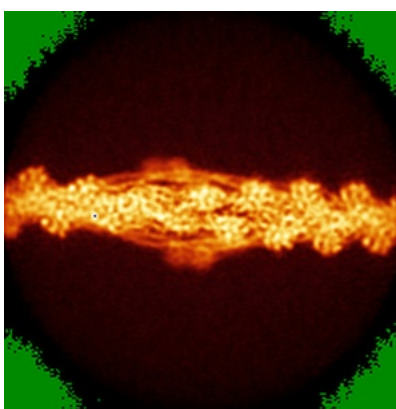
The images above show the largest variance slices of the map in three orthogonal directions.

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

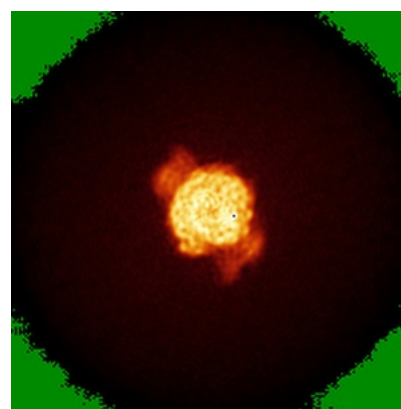
6.4.1 Primary map



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.

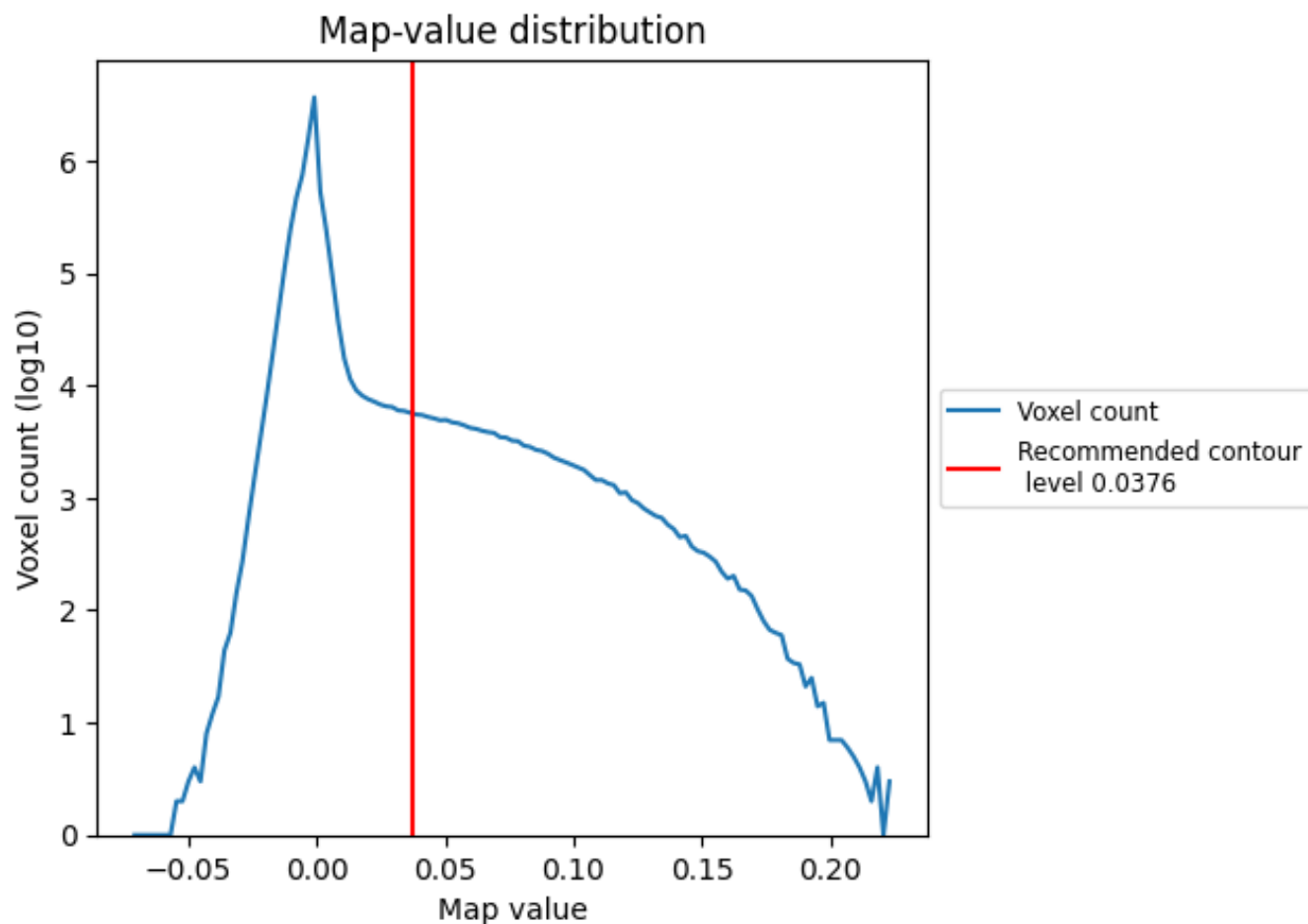
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

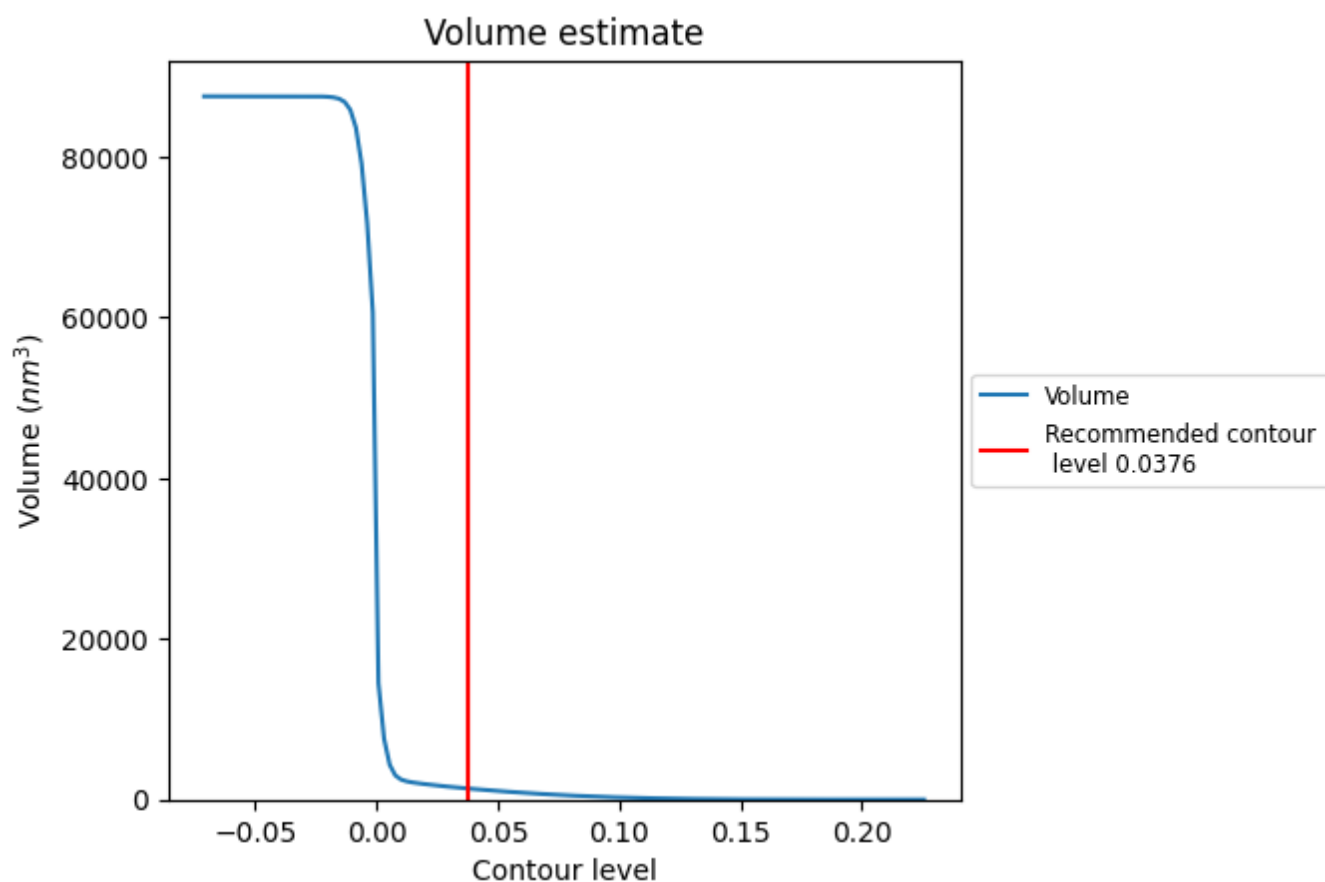
This section contains the results of statistical analysis of the map.

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.

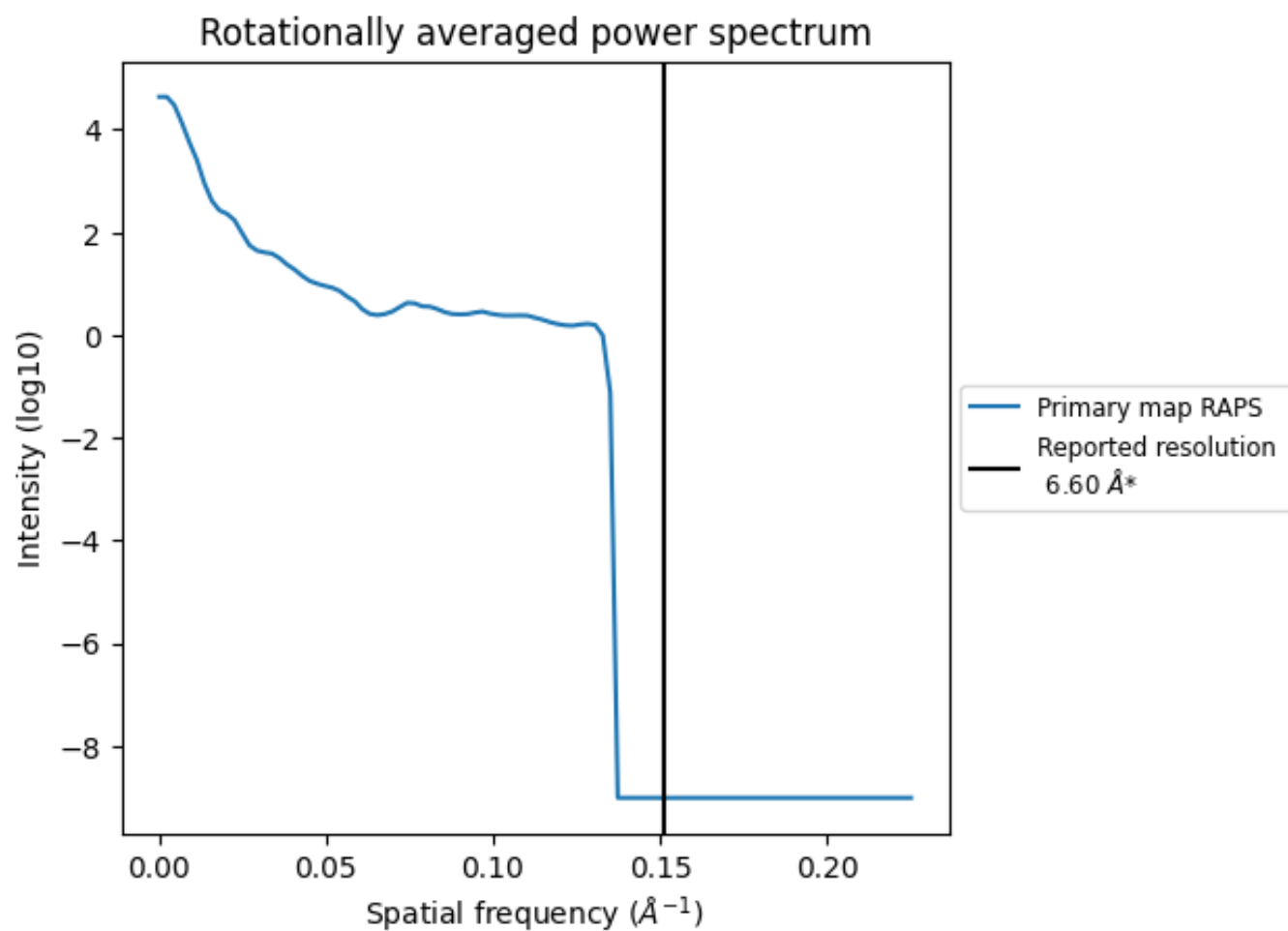
7.2 Volume estimate [i](#)



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 ⓘ

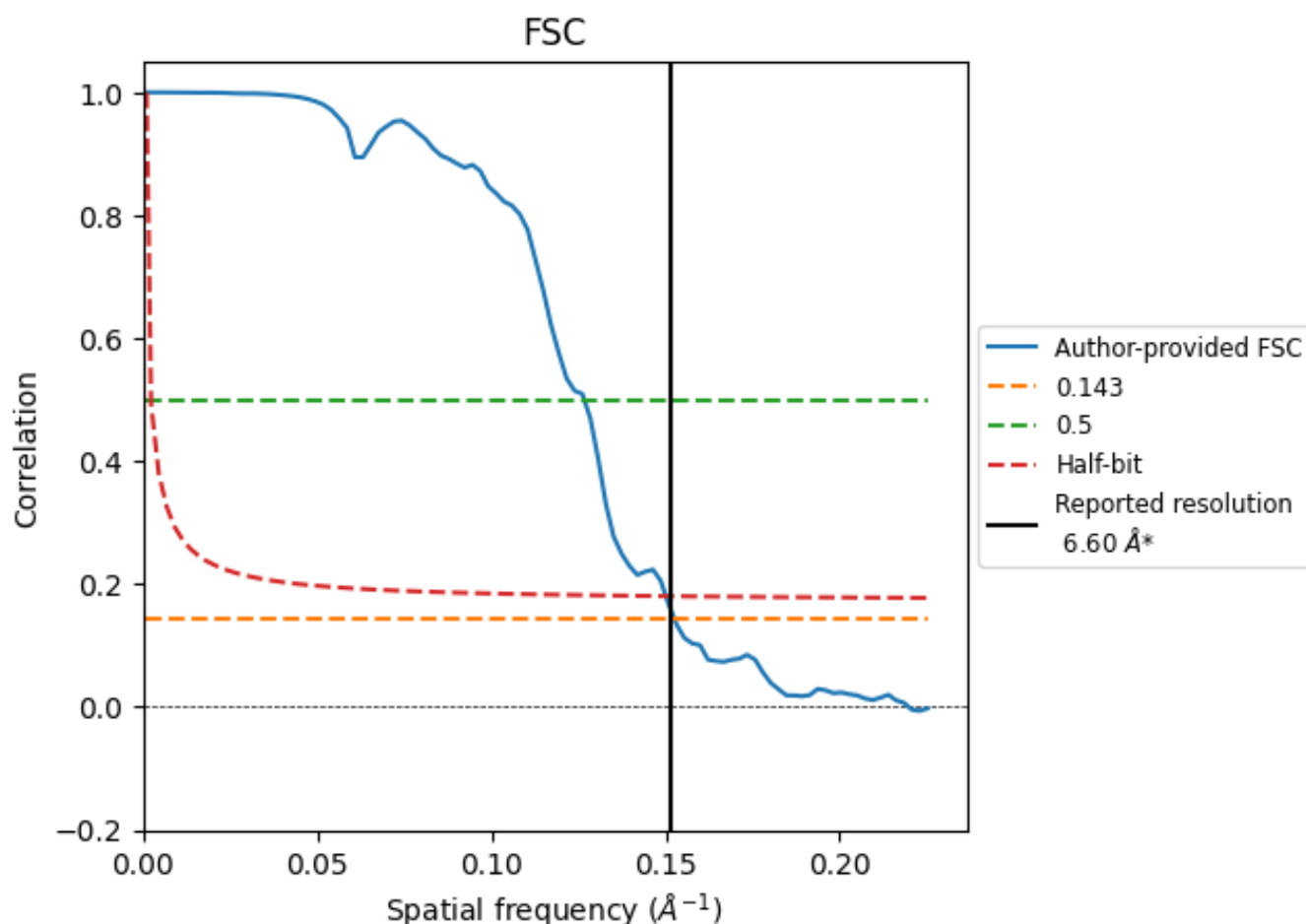


*Reported resolution corresponds to spatial frequency of 0.152 Å⁻¹

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 Å⁻¹

8.2 Resolution estimates [i](#)

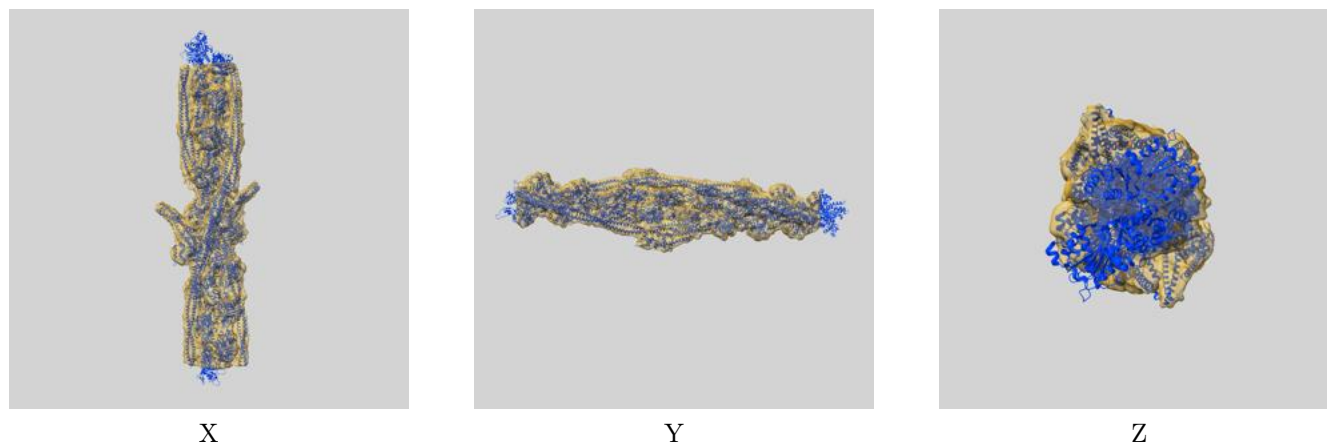
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.60	-	-
Author-provided FSC curve	6.56	7.89	6.66
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

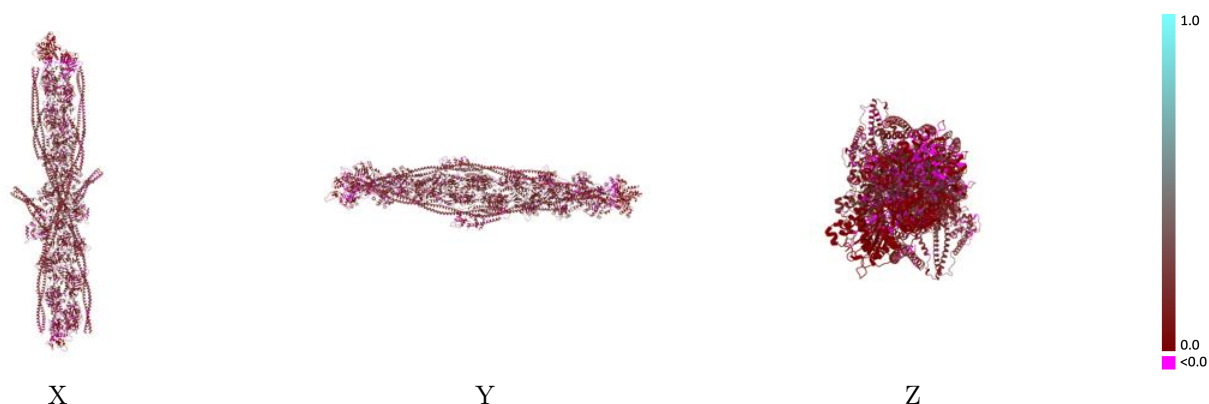
This section contains information regarding the fit between EMDB map EMD-0728 and PDB model 7UTL. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)



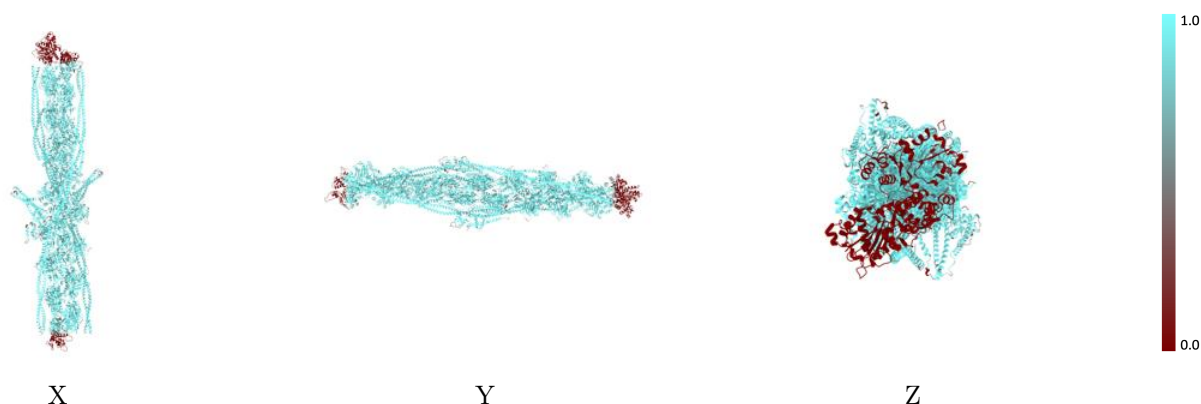
The images above show the 3D surface view of the map at the recommended contour level 0.0376 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



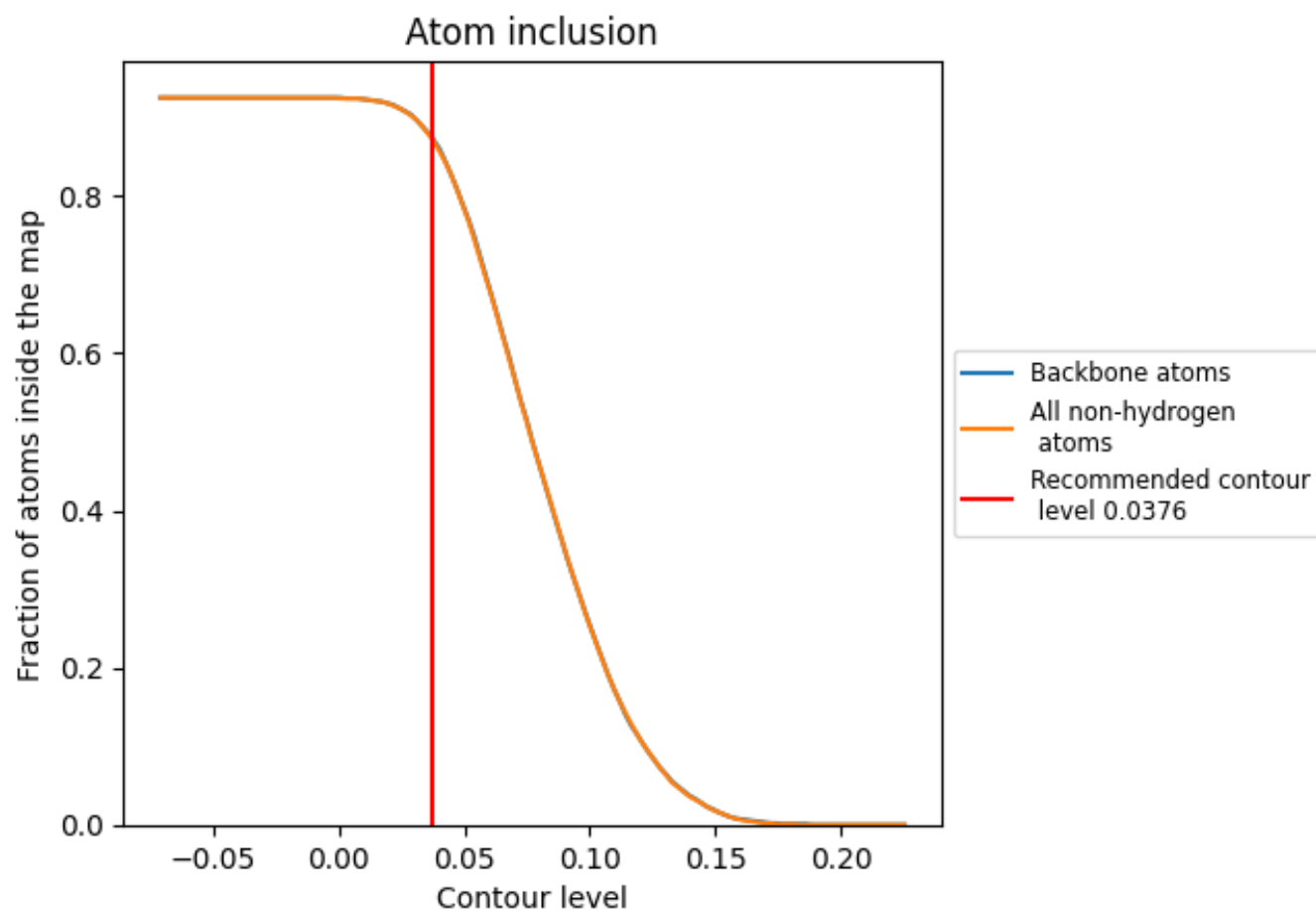
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



At the recommended contour level, 87% of all backbone atoms, 87% 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	 0.8710	 0.1320
A	 0.0580	 -0.0010
B	 0.5420	 0.0420
C	 0.9690	 0.1310
D	 0.9530	 0.1310
E	 0.9620	 0.1480
F	 0.9430	 0.1390
G	 0.9560	 0.1620
H	 0.9580	 0.1550
I	 0.9600	 0.1600
J	 0.9610	 0.1580
K	 0.9500	 0.1600
L	 0.9560	 0.1580
M	 0.9460	 0.1520
N	 0.9570	 0.1480
O	 0.9500	 0.1440
P	 0.9540	 0.1300
Q	 0.9450	 0.1200
R	 0.4680	 0.0320
U	 0.8180	 0.0840
V	 0.9100	 0.1620
W	 0.9320	 0.1550
X	 0.9660	 0.1570
Y	 0.8900	 0.1540
Z	 0.9480	 0.1480
a	 0.9530	 0.1760
b	 0.9580	 0.1730
c	 0.9120	 0.1310
d	 0.8420	 0.0840
e	 0.8970	 0.1510
f	 0.8850	 0.1290
g	 0.9550	 0.1490
h	 0.9320	 0.1370
i	 0.9510	 0.1760
j	 0.9560	 0.1690

