



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 02:07 PM UTC

PDB ID : 7QO5 / pdb_00007qo5
EMDB ID : EMD-14084
Title : 26S proteasome Rpt1-RK -Ubp6-UbVS complex in the si state
Authors : Hung, K.Y.S.; Klumpe, S.; Eisele, M.R.; Elsassner, S.; Geng, T.T.; Cheng, T.C.; Joshi, T.; Rudack, T.; Sakata, E.; Finley, D.
Deposited on : 2021-12-23
Resolution : 6.00 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

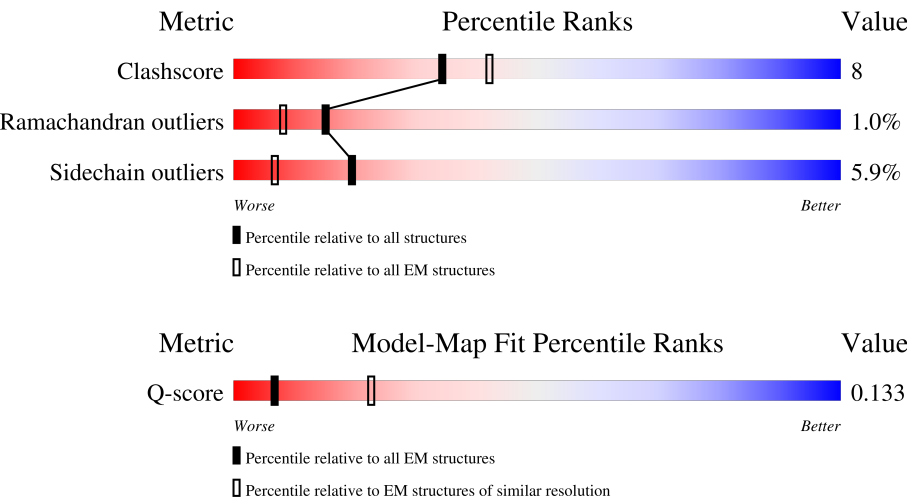
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 6.00 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	525 (5.50 - 6.50)

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	252	
1	a	252	
2	B	250	
2	b	250	

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Mol	Chain	Length	Quality of chain
3	C	258	
3	c	258	
4	D	254	
4	d	254	
5	E	260	
5	e	260	
6	F	234	
6	f	234	
7	G	288	
7	g	288	
8	l	215	
8	h	215	
9	2	261	
9	i	261	
10	3	205	
10	j	205	
11	4	198	
11	k	198	
12	5	287	
12	l	287	
13	6	241	
13	m	241	
14	7	266	
14	n	266	
15	W	268	

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Mol	Chain	Length	Quality of chain
16	V	306	
17	T	274	
18	X	156	
19	Y	89	
20	Z	993	
21	N	945	
22	S	523	
23	P	445	
24	Q	434	
25	R	429	
26	U	338	
27	O	393	
28	H	467	
29	I	437	
30	K	428	
31	L	437	
32	M	434	
33	J	405	
34	8	499	
35	9	76	

2 Entry composition [i](#)

There are 38 unique types of molecules in this entry. The entry contains 112834 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	241	Total	C	N	O	S	0	0
			1907	1214	320	365	8		
1	A	241	Total	C	N	O	S	0	0
			1907	1214	320	365	8		

- Molecule 2 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	249	Total	C	N	O	S	0	0
			1907	1214	314	376	3		
2	B	249	Total	C	N	O	S	0	0
			1907	1214	314	376	3		

- Molecule 3 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	244	Total	C	N	O	S	0	0
			1904	1201	321	379	3		
3	C	244	Total	C	N	O	S	0	0
			1904	1201	321	379	3		

- Molecule 4 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	236	Total	C	N	O	S	0	0
			1850	1158	323	365	4		
4	D	236	Total	C	N	O	S	0	0
			1850	1158	323	365	4		

- Molecule 5 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	244	Total	C	N	O	S	0	0
			1882	1176	316	383	7		
5	E	244	Total	C	N	O	S	0	0
			1882	1176	316	383	7		

- Molecule 6 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	231	Total	C	N	O	S	0	0
			1773	1114	307	348	4		
6	F	231	Total	C	N	O	S	0	0
			1773	1114	307	348	4		

- Molecule 7 is a protein called Probable proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	242	Total	C	N	O	S	0	0
			1885	1199	328	354	4		
7	G	242	Total	C	N	O	S	0	0
			1885	1199	328	354	4		

- Molecule 8 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	196	Total	C	N	O	S	0	0
			1512	955	250	300	7		
8	1	196	Total	C	N	O	S	0	0
			1512	955	250	300	7		

- Molecule 9 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	226	Total	C	N	O	S	0	0
			1719	1082	298	332	7		
9	2	226	Total	C	N	O	S	0	0
			1719	1082	298	332	7		

- Molecule 10 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	204	Total	C	N	O	S	0	0
			1581	1010	258	305	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	3	204	Total	C	N	O	S	0	0
			1581	1010	258	305	8		

- Molecule 11 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	195	Total	C	N	O	S	0	0
			1561	992	264	299	6		
11	4	195	Total	C	N	O	S	0	0
			1561	992	264	299	6		

- Molecule 12 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	l	212	Total	C	N	O	S	0	0
			1644	1045	280	312	7		
12	5	212	Total	C	N	O	S	0	0
			1644	1045	280	312	7		

- Molecule 13 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	m	222	Total	C	N	O	S	0	0
			1757	1115	303	335	4		
13	6	222	Total	C	N	O	S	0	0
			1757	1115	303	335	4		

- Molecule 14 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	n	229	Total	C	N	O	S	0	0
			1790	1133	306	344	7		
14	7	229	Total	C	N	O	S	0	0
			1790	1133	306	344	7		

- Molecule 15 is a protein called 26S proteasome regulatory subunit RPN10.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	W	197	Total	C	N	O	S	0	0
			1534	962	269	300	3		

- Molecule 16 is a protein called Ubiquitin carboxyl-terminal hydrolase RPN11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	V	289	Total	C	N	O	S	0	0
			2274	1425	389	446	14		

- Molecule 17 is a protein called 26S proteasome regulatory subunit RPN12.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	266	Total	C	N	O	S	0	0
			2192	1405	349	432	6		

- Molecule 18 is a protein called 26S proteasome regulatory subunit RPN13.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	X	127	Total	C	N	O	S	0	0
			1032	664	169	195	4		

- Molecule 19 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Y	89	Total	C	N	O	S	0	0
			731	447	119	164	1		

- Molecule 20 is a protein called 26S proteasome regulatory subunit RPN1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Z	906	Total	C	N	O	S	0	0
			7005	4416	1150	1409	30		

- Molecule 21 is a protein called 26S proteasome regulatory subunit RPN2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	N	832	Total	C	N	O	S	0	0
			6418	4078	1077	1238	25		

- Molecule 22 is a protein called 26S proteasome regulatory subunit RPN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	S	475	Total	C	N	O	S	0	0
			3894	2488	653	738	15		

- Molecule 23 is a protein called 26S proteasome regulatory subunit RPN5.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	P	440	Total	C	N	O	S	0	0
			3608	2297	604	697	10		

- Molecule 24 is a protein called 26S proteasome regulatory subunit RPN6.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Q	434	Total	C	N	O	S	0	0
			3499	2225	577	681	16		

- Molecule 25 is a protein called 26S proteasome regulatory subunit RPN7.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	R	405	Total	C	N	O	S	0	0
			3258	2077	535	636	10		

- Molecule 26 is a protein called 26S proteasome regulatory subunit RPN8.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	U	290	Total	C	N	O	S	0	0
			2306	1454	392	453	7		

- Molecule 27 is a protein called 26S proteasome regulatory subunit RPN9.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	O	388	Total	C	N	O	S	0	0
			3186	2051	519	608	8		

- Molecule 28 is a protein called 26S proteasome regulatory subunit 7 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	H	391	Total	C	N	O	S	0	0
			3064	1927	551	569	17		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	164	ARG	SER	variant	UNP P33299
H	166	LYS	THR	variant	UNP P33299

- Molecule 29 is a protein called 26S proteasome regulatory subunit 4 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	I	384	Total	C	N	O	S	0	0
			3015	1895	507	596	17		

- Molecule 30 is a protein called 26S proteasome regulatory subunit 6B homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	K	394	Total	C	N	O	S	0	0
			3113	1951	548	604	10		

- Molecule 31 is a protein called 26S proteasome subunit RPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	L	388	Total	C	N	O	S	0	0
			3082	1942	548	580	12		

- Molecule 32 is a protein called 26S proteasome regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	M	421	Total	C	N	O	S	0	0
			3285	2043	573	656	13		

- Molecule 33 is a protein called 26S proteasome regulatory subunit 8 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	J	405	Total	C	N	O	S	0	0
			3171	1995	565	593	18		

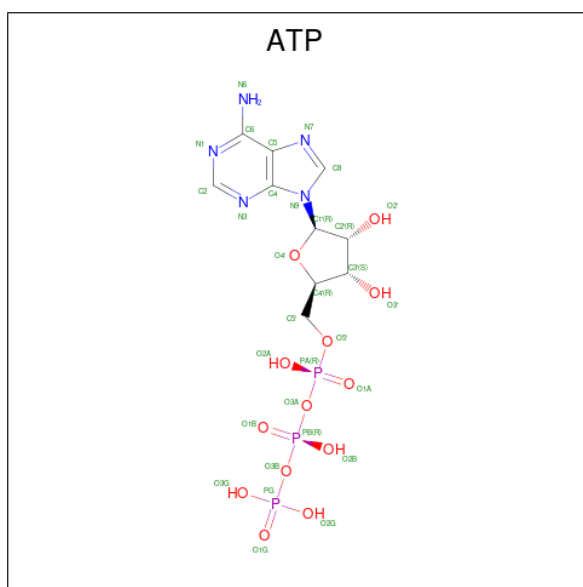
- Molecule 34 is a protein called Ubiquitin carboxyl-terminal hydrolase 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	8	372	Total	C	N	O	S	0	0
			3034	1918	521	583	12		

- Molecule 35 is a protein called Polyubiquitin-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	9	76	Total	C	N	O	S	0	0
			601	378	105	117	1		

- Molecule 36 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

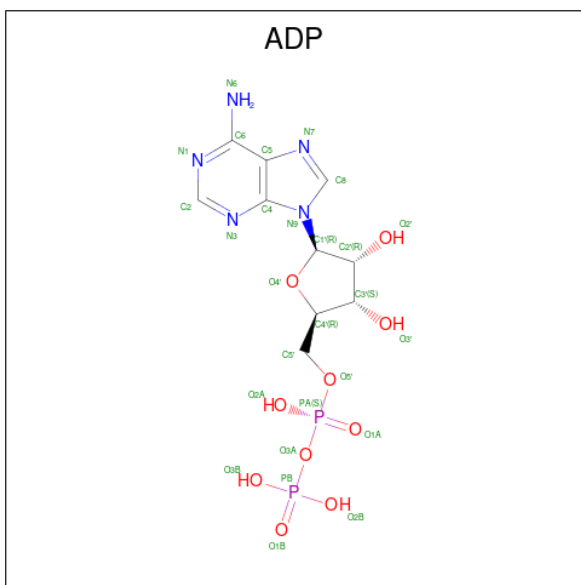


Mol	Chain	Residues	Atoms					AltConf
36	H	1	Total 31	C 10	N 5	O 13	P 3	0
36	I	1	Total 31	C 10	N 5	O 13	P 3	0
36	K	1	Total 31	C 10	N 5	O 13	P 3	0
36	L	1	Total 31	C 10	N 5	O 13	P 3	0
36	M	1	Total 31	C 10	N 5	O 13	P 3	0

- Molecule 37 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
37	H	1	Total 1	Mg 1	0
37	I	1	Total 1	Mg 1	0
37	K	1	Total 1	Mg 1	0
37	L	1	Total 1	Mg 1	0
37	M	1	Total 1	Mg 1	0
37	J	1	Total 1	Mg 1	0

- Molecule 38 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

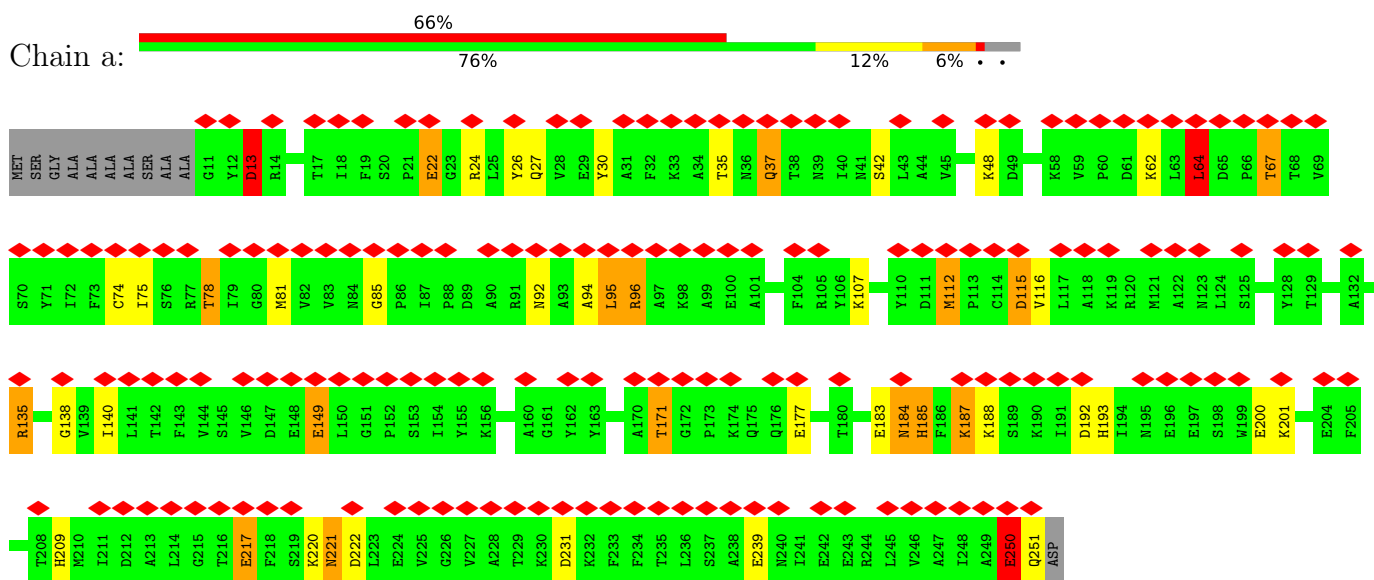


Mol	Chain	Residues	Atoms					AltConf
38	J	1	Total	C	N	O	P	0
			27	10	5	10	2	

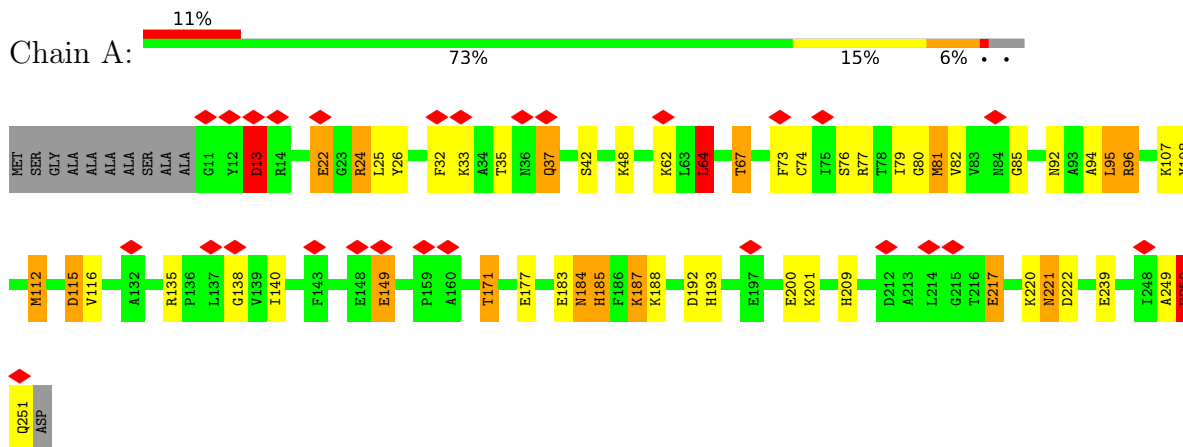
3 Residue-property plots

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.

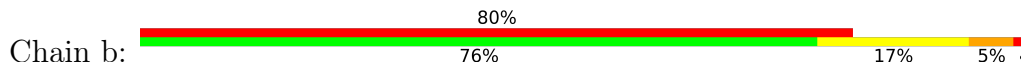
• Molecule 1: Proteasome subunit alpha type-1

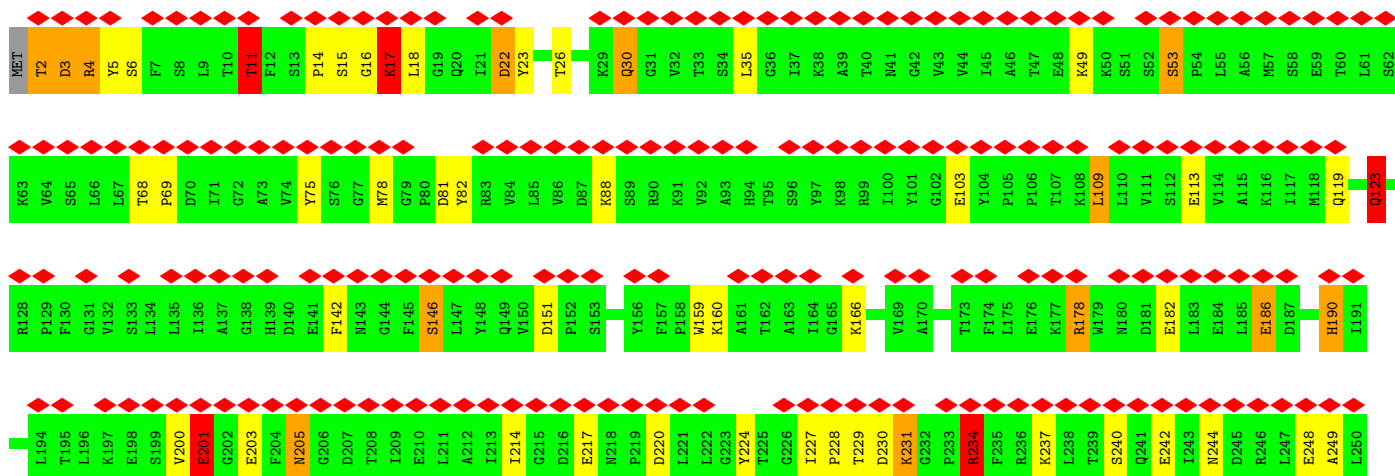


• Molecule 1: Proteasome subunit alpha type-1

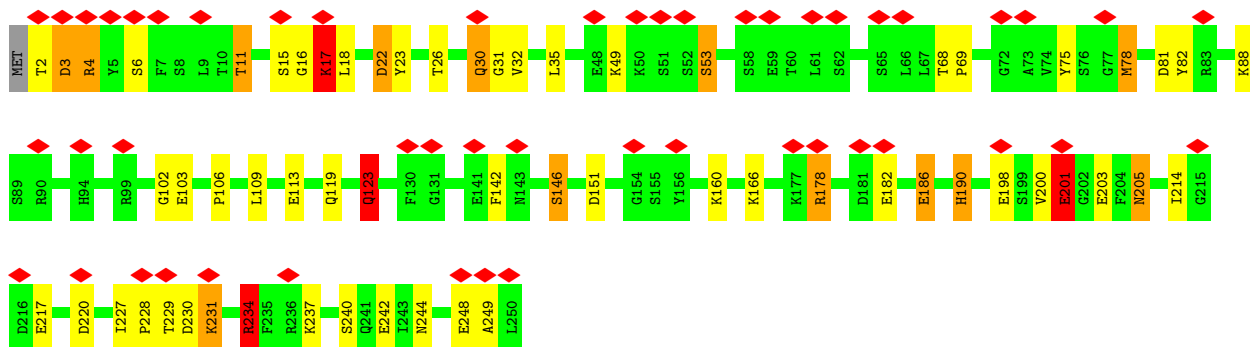
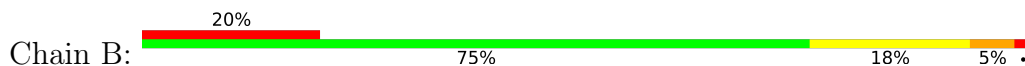


• Molecule 2: Proteasome subunit alpha type-2

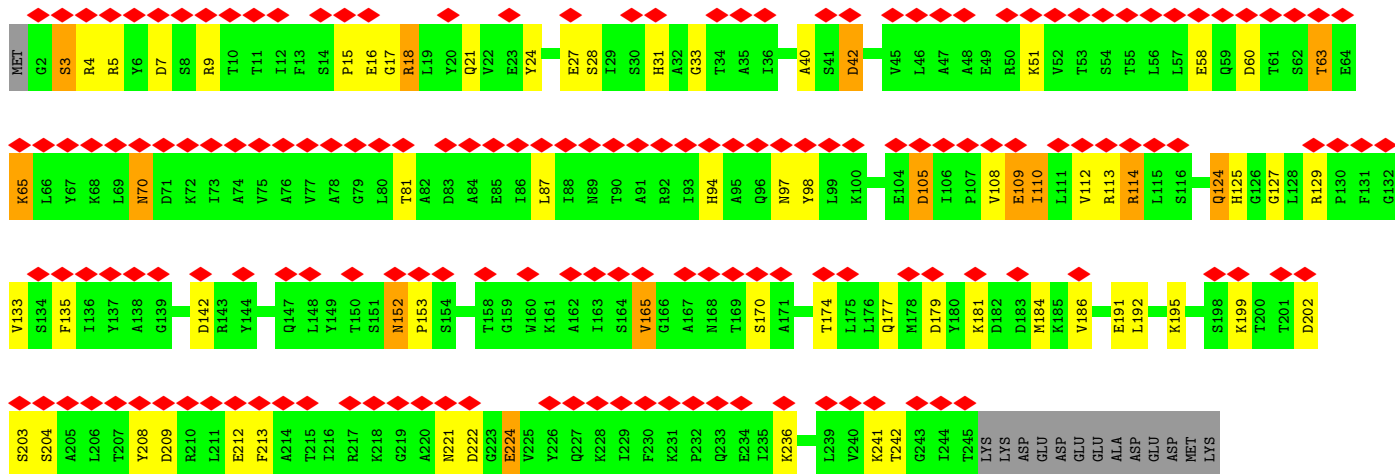




• Molecule 2: Proteasome subunit alpha type-2

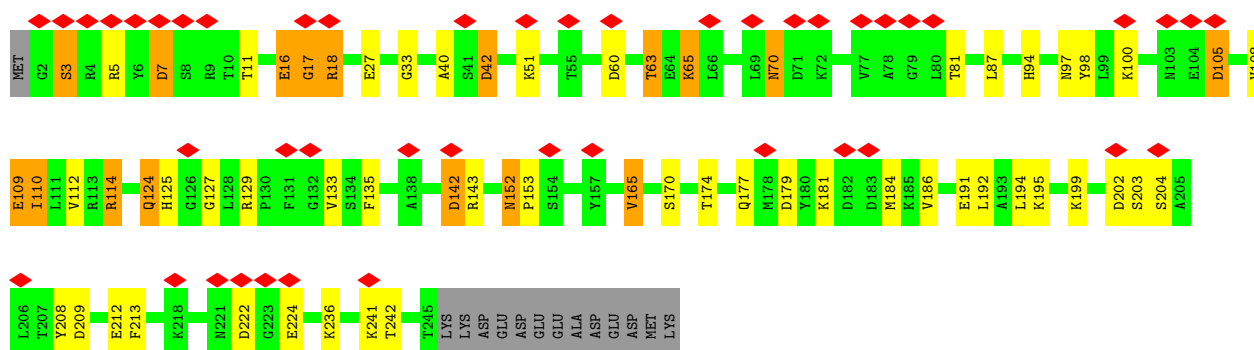


• Molecule 3: Proteasome subunit alpha type-3



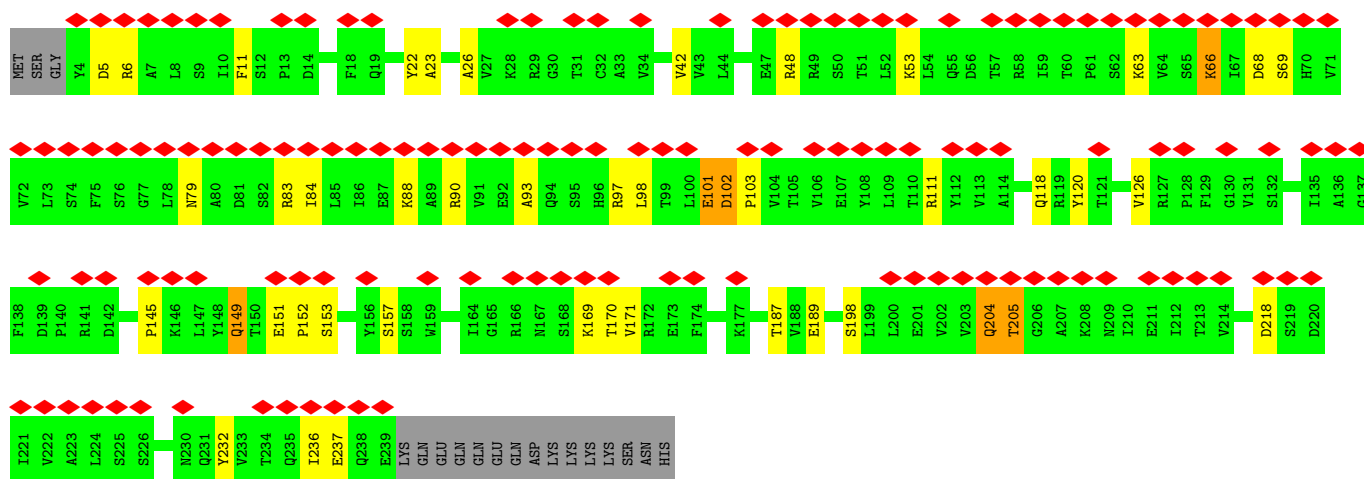
• Molecule 3: Proteasome subunit alpha type-3

Chain C: 17% 70% 18% 7% 5%



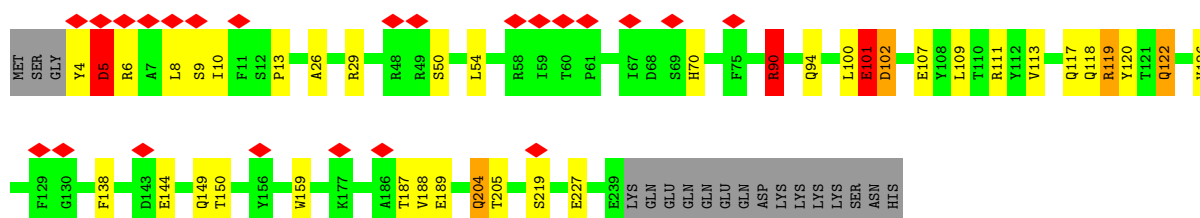
• Molecule 4: Proteasome subunit alpha type-4

Chain d: 54% 75% 16% 7%



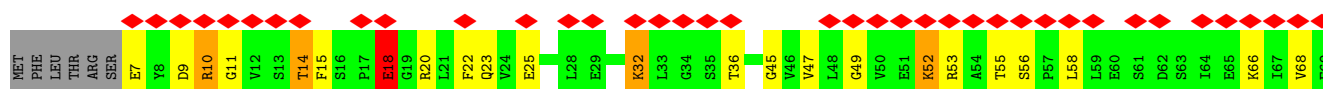
• Molecule 4: Proteasome subunit alpha type-4

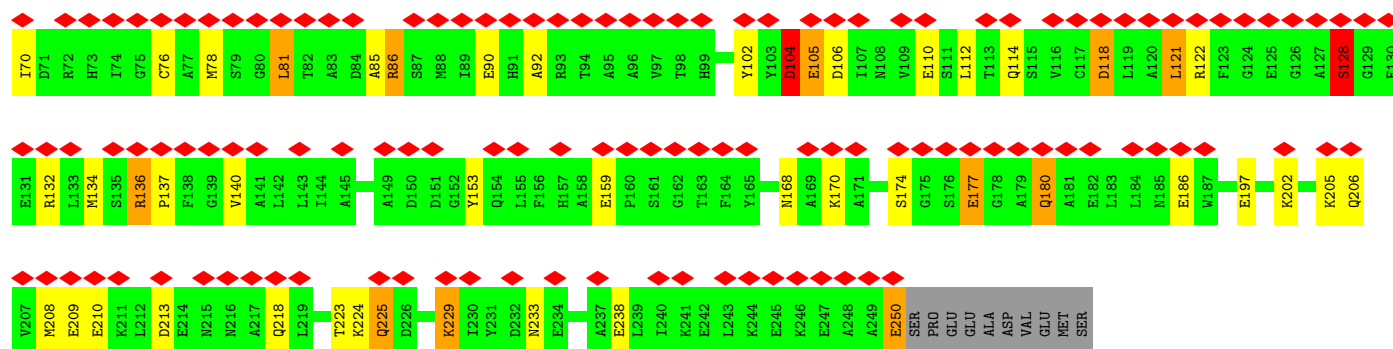
Chain D: 9% 78% 13% 7%



• Molecule 5: Proteasome subunit alpha type-5

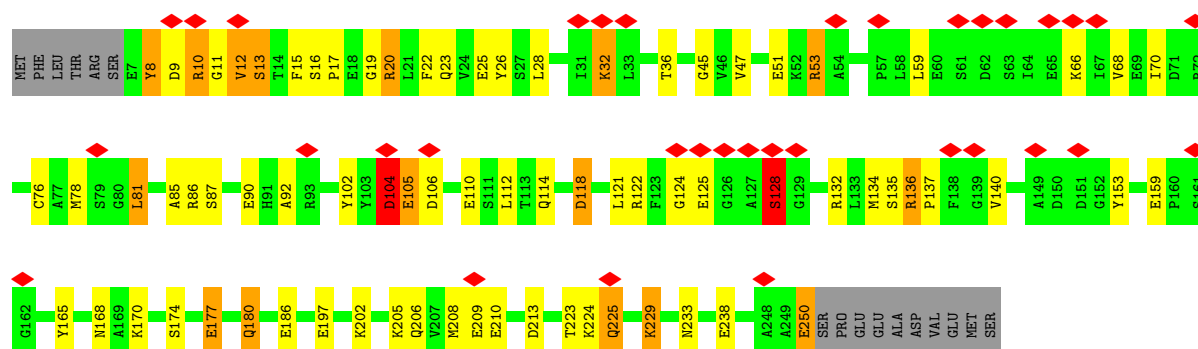
Chain e: 62% 67% 20% 6% 6%





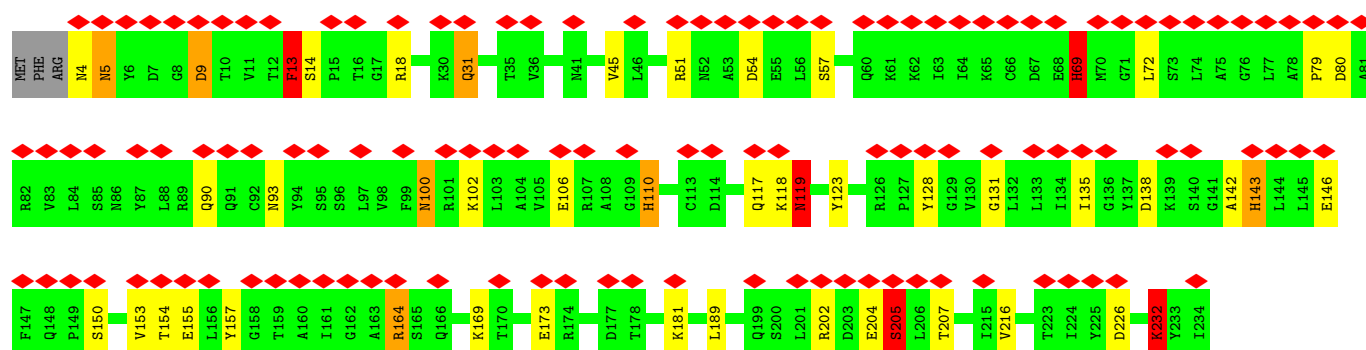
• Molecule 5: Proteasome subunit alpha type-5

Chain E: 13% 64% 23% 6% • 6%



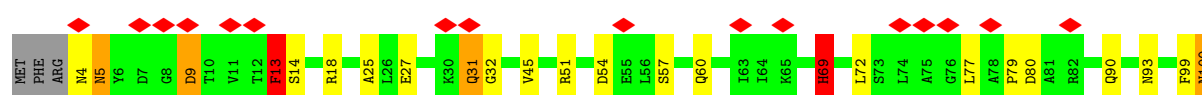
• Molecule 6: Proteasome subunit alpha type-6

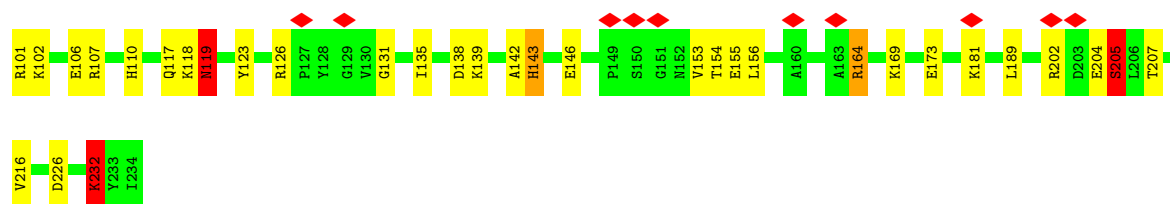
Chain f: 52% 78% 16% • •



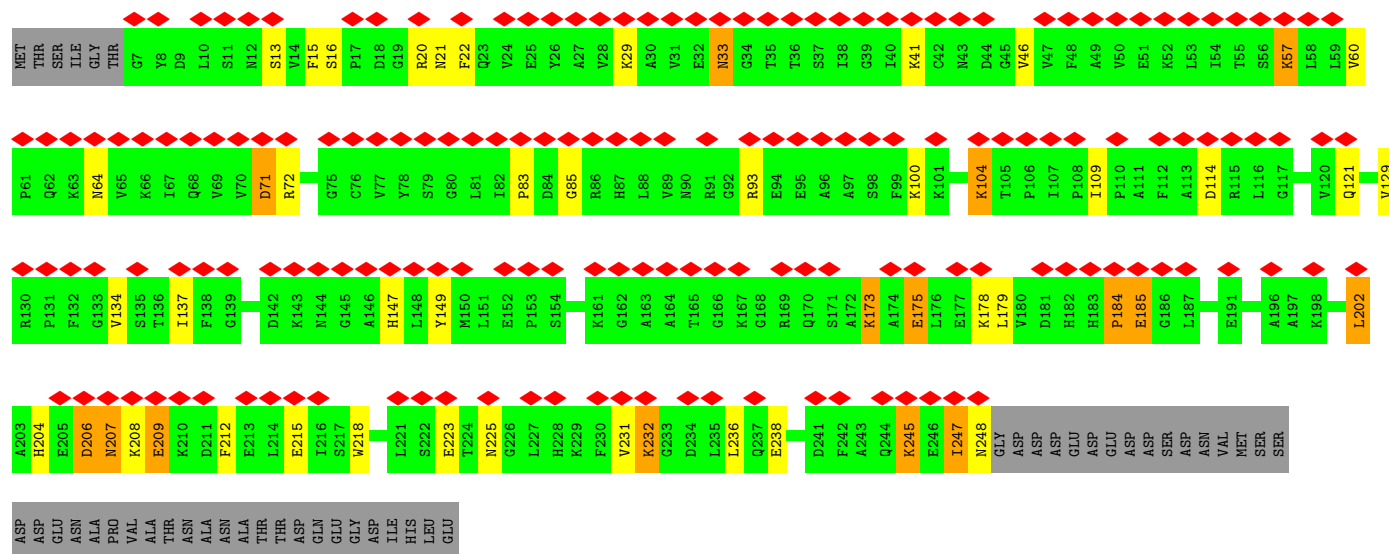
• Molecule 6: Proteasome subunit alpha type-6

Chain F: 11% 74% 20% • •

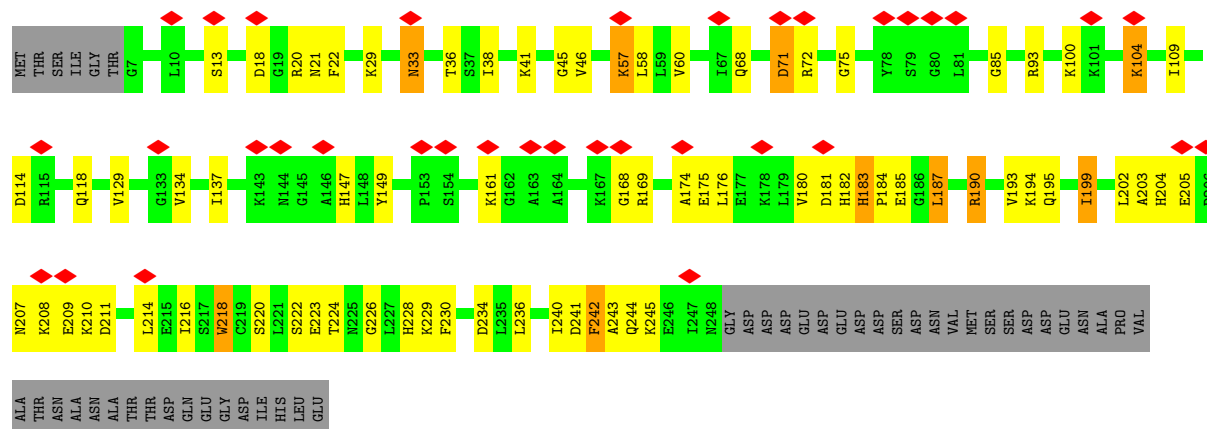




• Molecule 7: Probable proteasome subunit alpha type-7

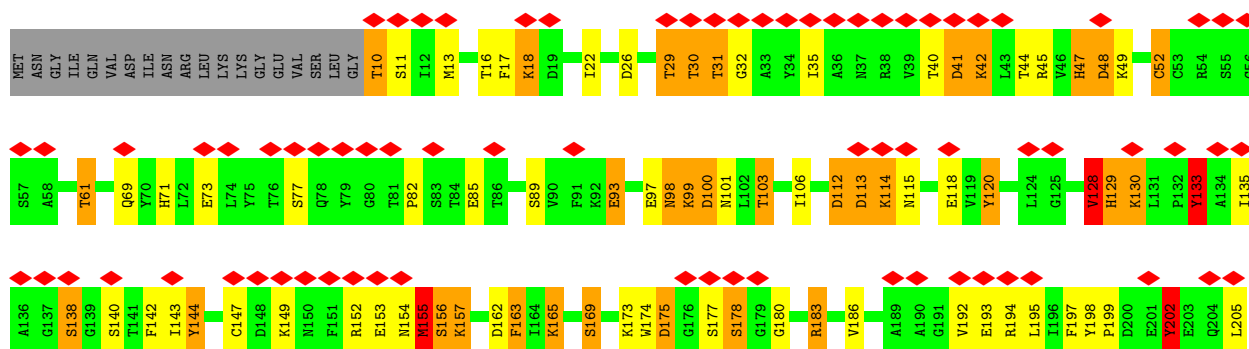


• Molecule 7: Probable proteasome subunit alpha type-7

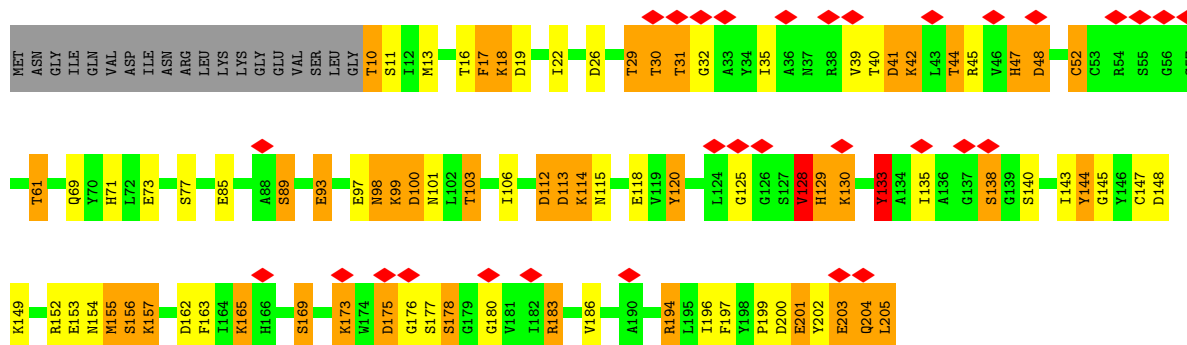


• Molecule 8: Proteasome subunit beta type-1

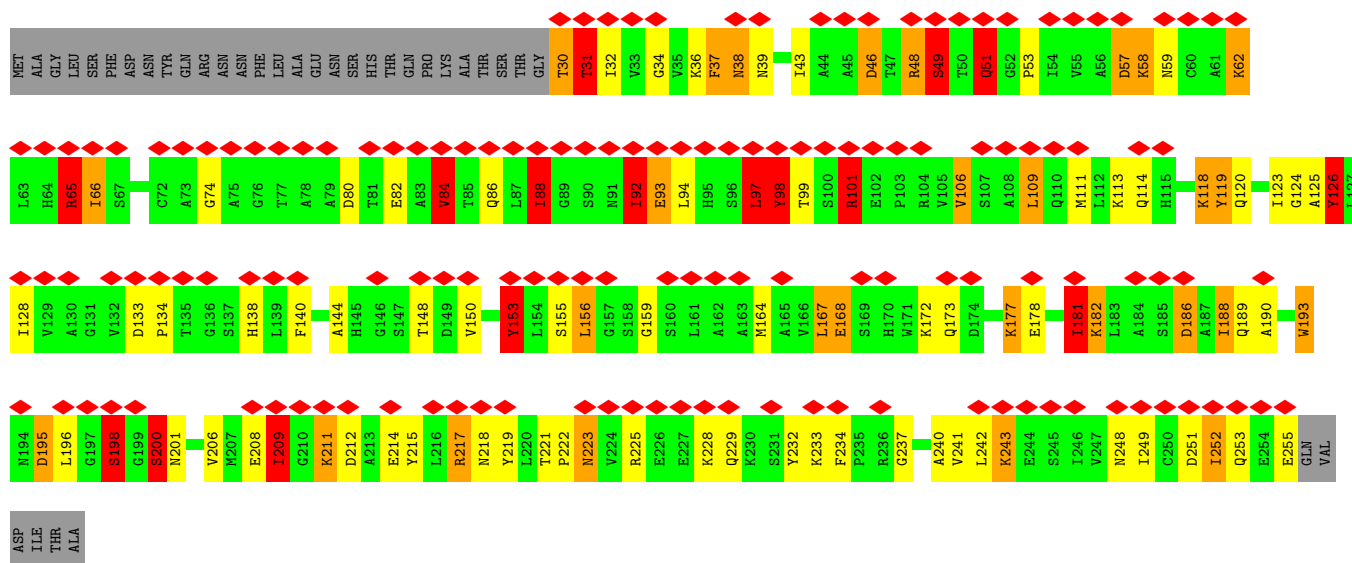




• Molecule 8: Proteasome subunit beta type-1

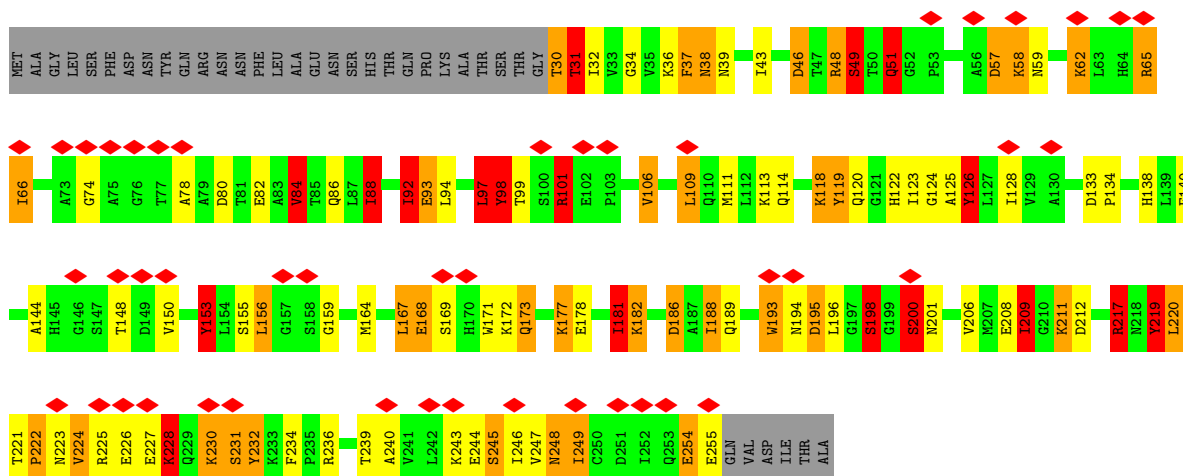


• Molecule 9: Proteasome subunit beta type-2

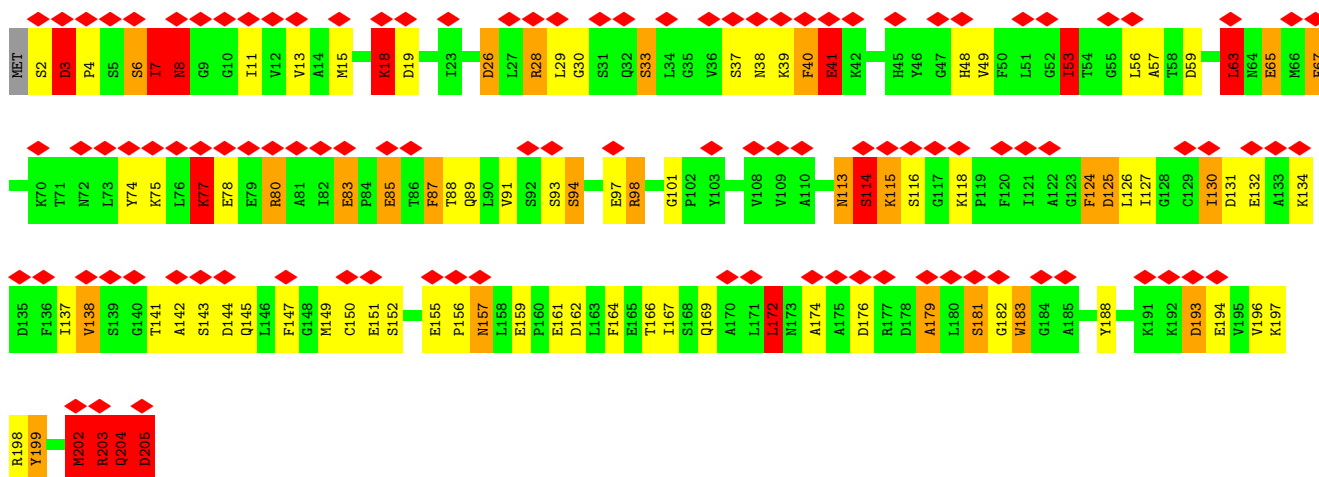


• Molecule 9: Proteasome subunit beta type-2

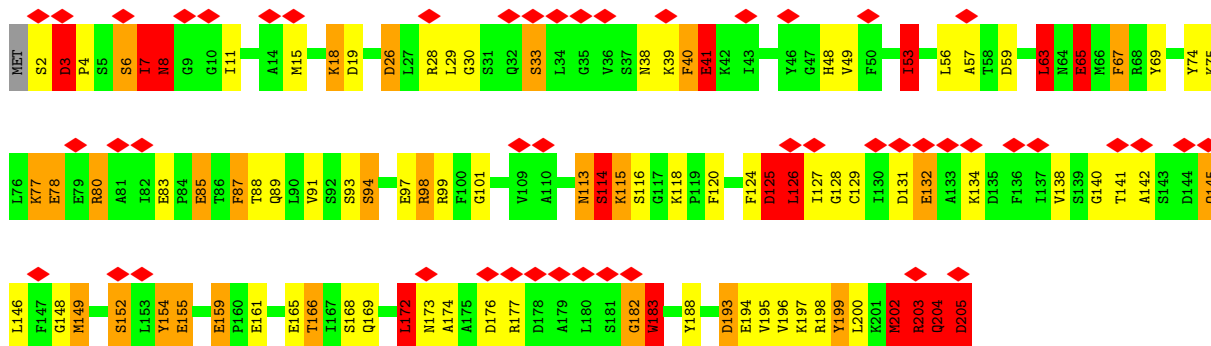




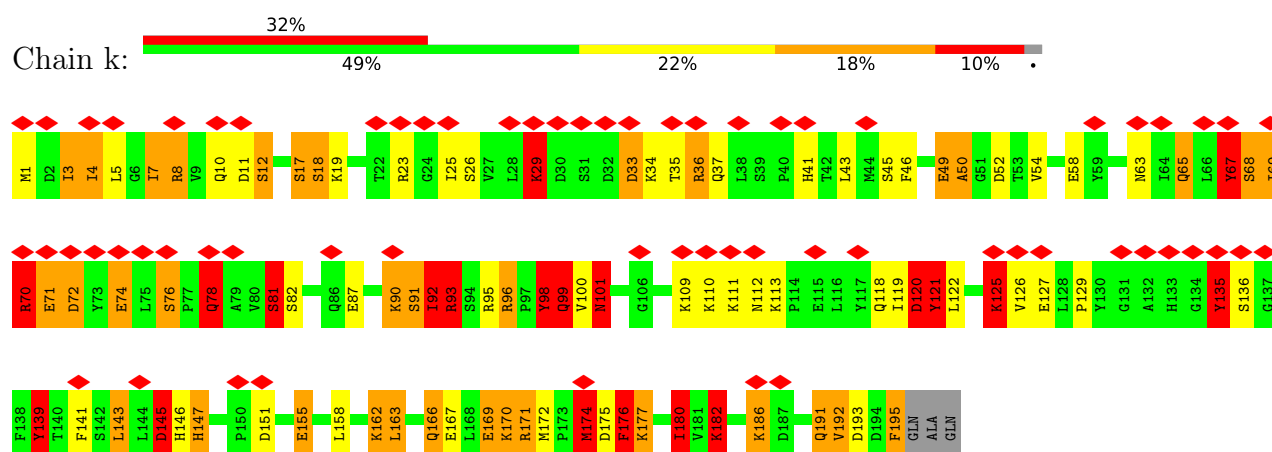
• Molecule 10: Proteasome subunit beta type-3



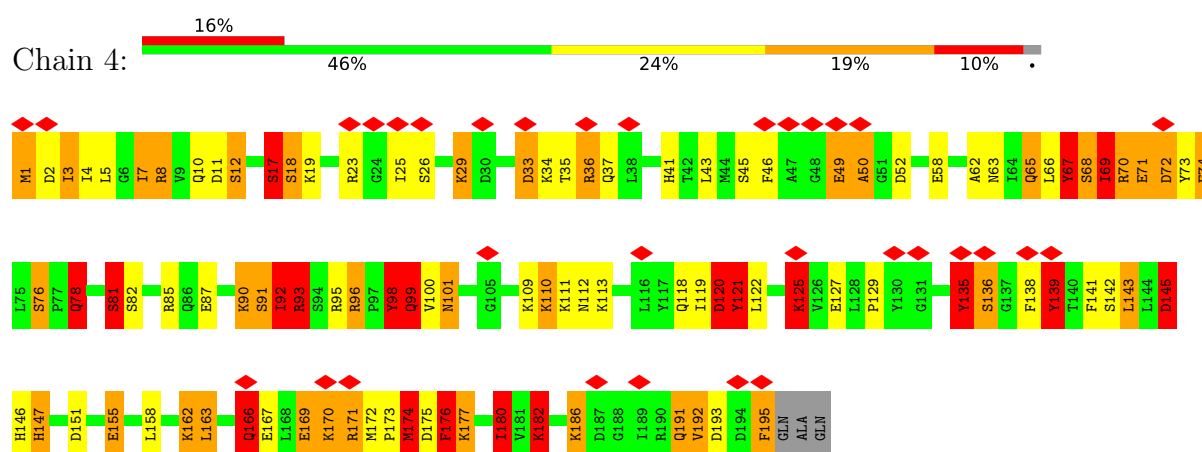
• Molecule 10: Proteasome subunit beta type-3



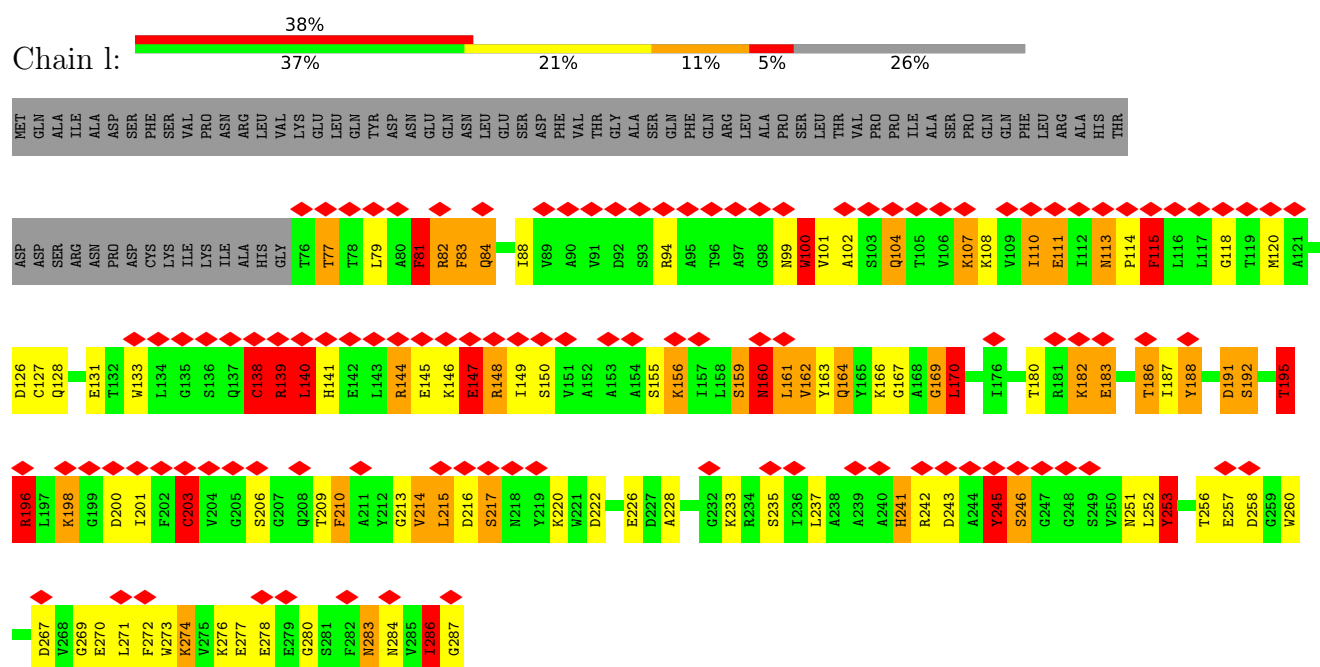
• Molecule 11: Proteasome subunit beta type-4



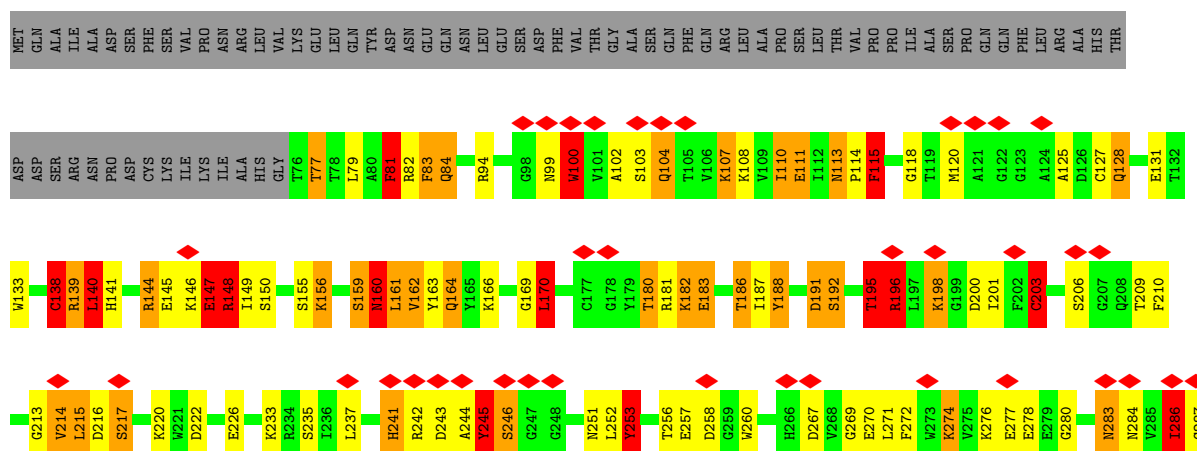
• Molecule 11: Proteasome subunit beta type-4



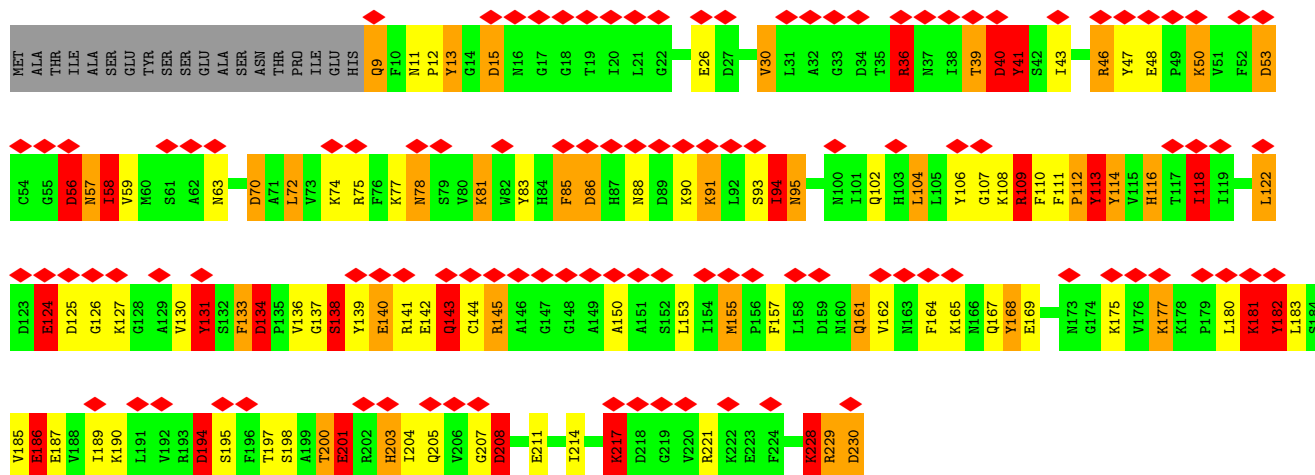
• Molecule 12: Proteasome subunit beta type-5



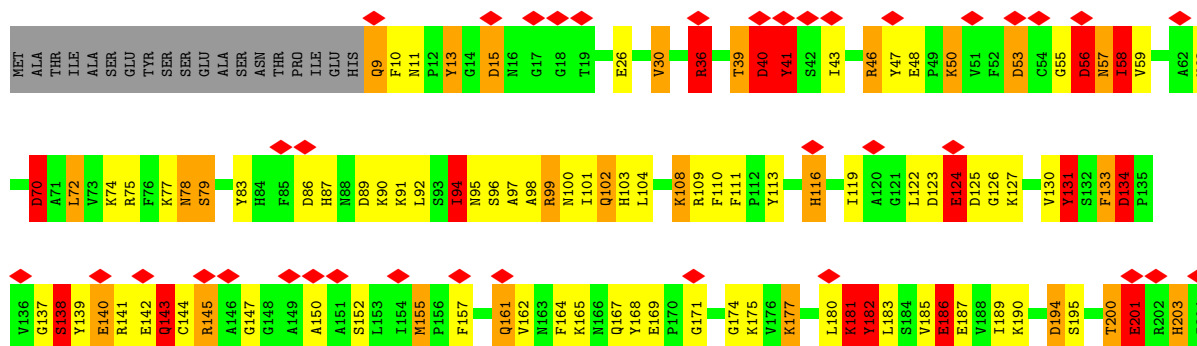
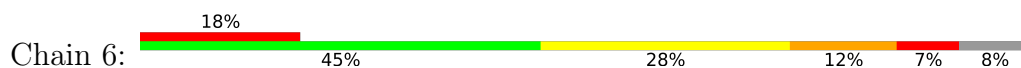
• Molecule 12: Proteasome subunit beta type-5



• Molecule 13: Proteasome subunit beta type-6

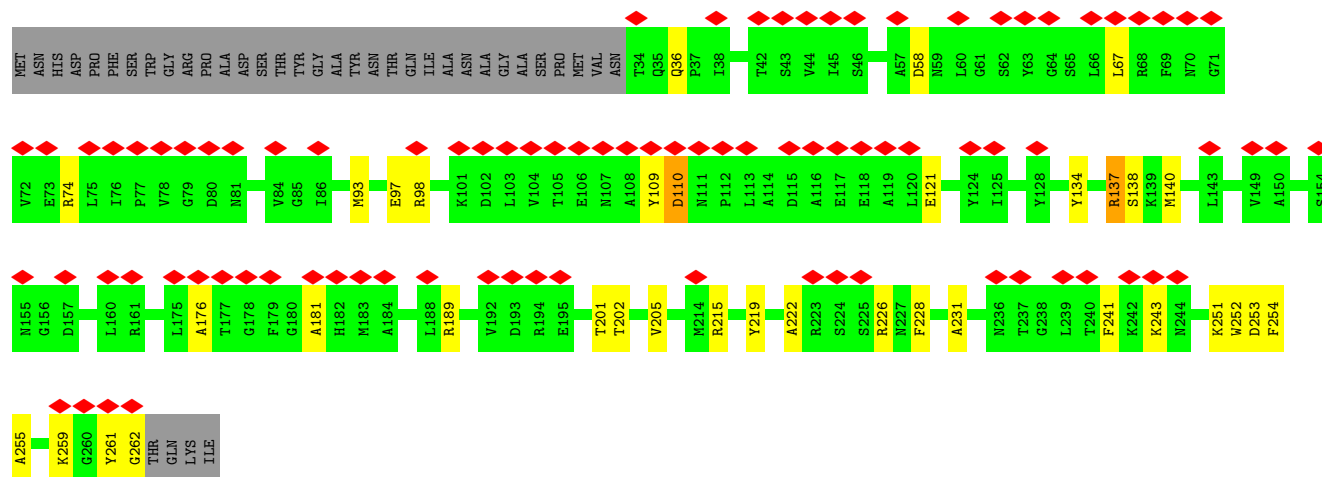


• Molecule 13: Proteasome subunit beta type-6

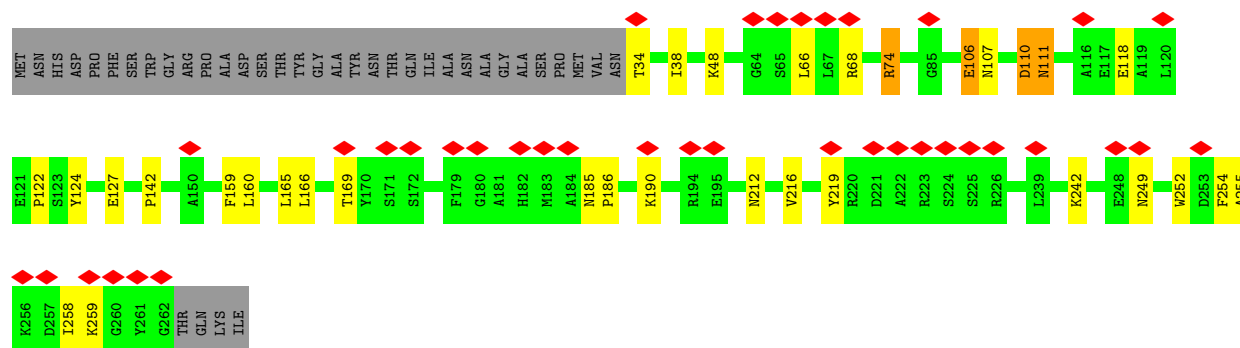
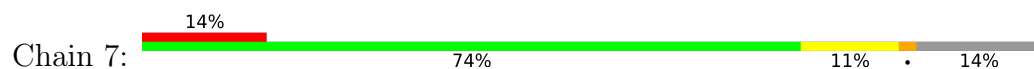




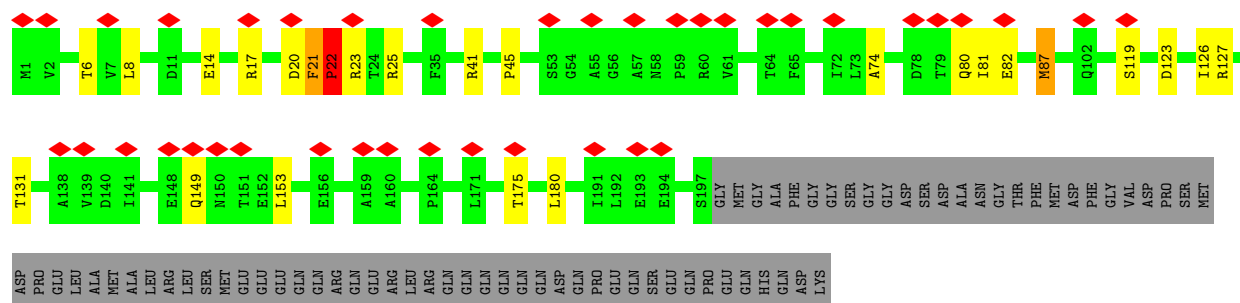
• Molecule 14: Proteasome subunit beta type-7



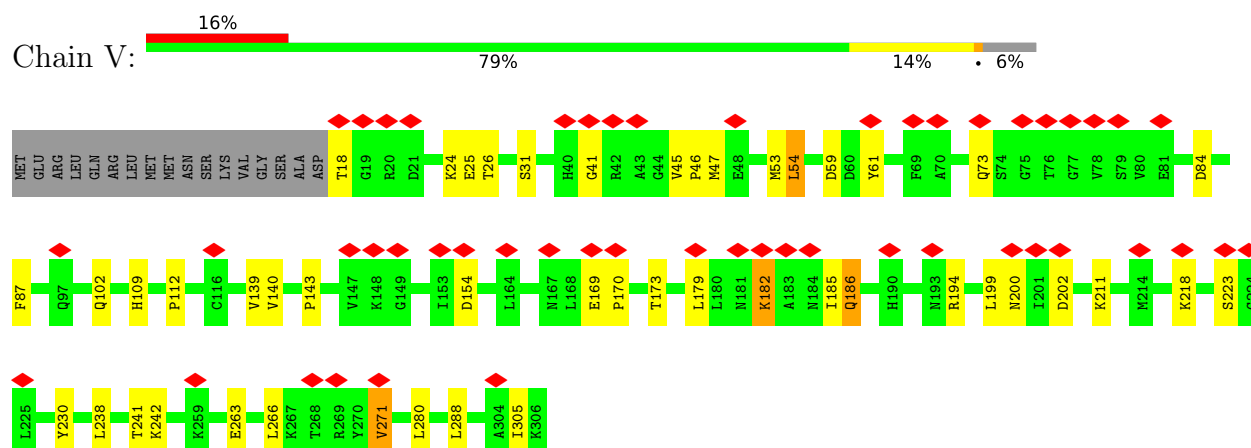
• Molecule 14: Proteasome subunit beta type-7



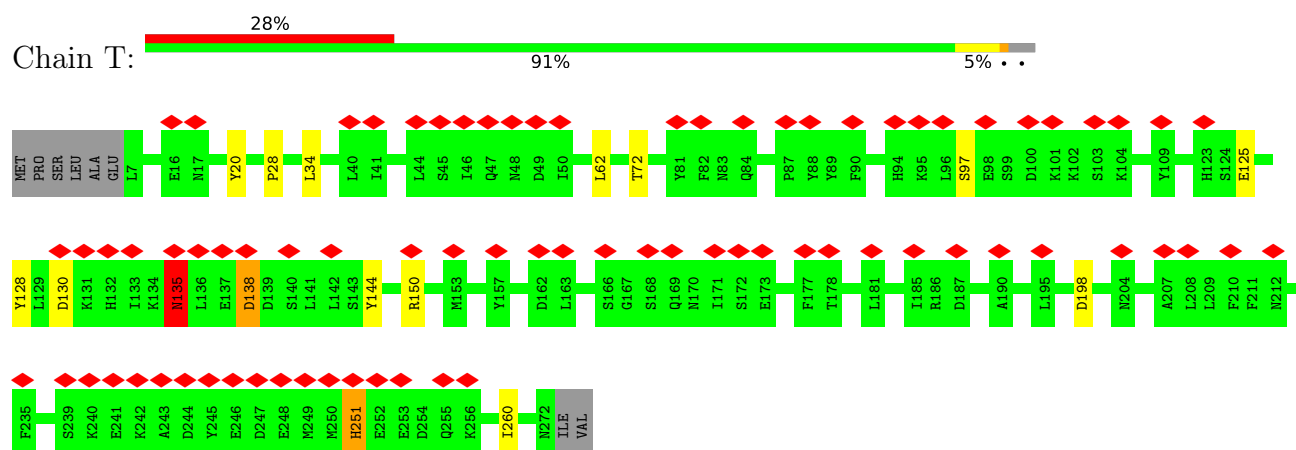
• Molecule 15: 26S proteasome regulatory subunit RPN10



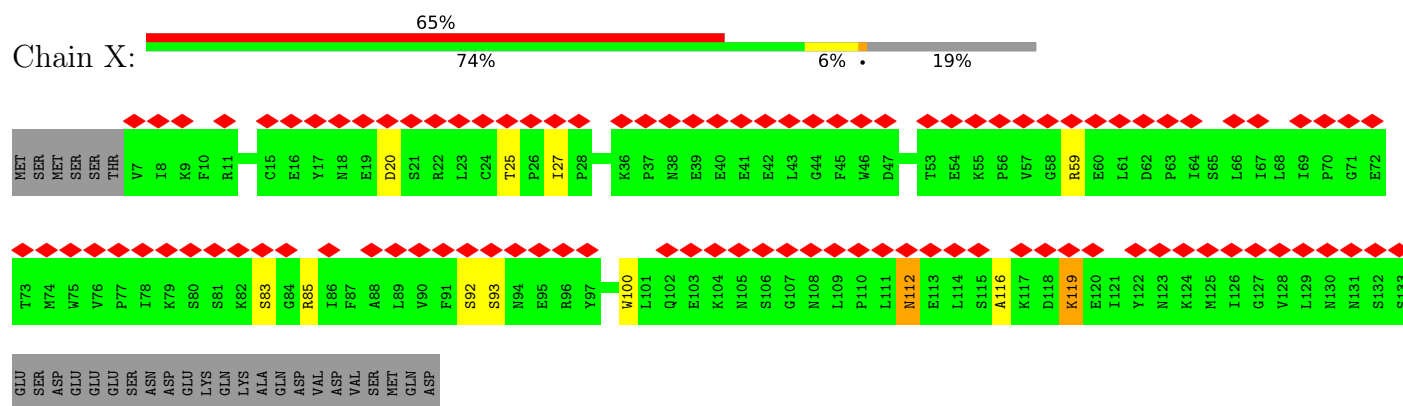
- Molecule 16: Ubiquitin carboxyl-terminal hydrolase RPN11



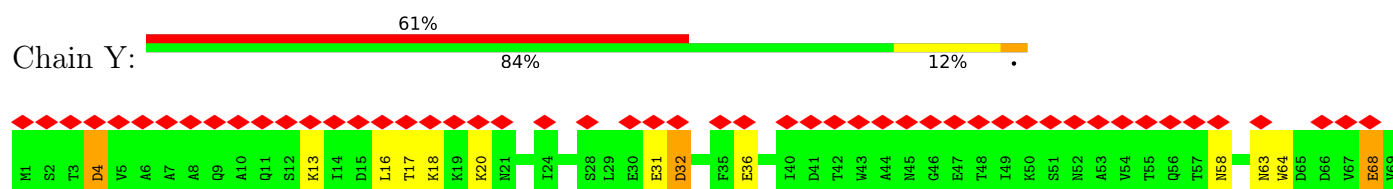
- Molecule 17: 26S proteasome regulatory subunit RPN12

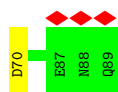


- Molecule 18: 26S proteasome regulatory subunit RPN13

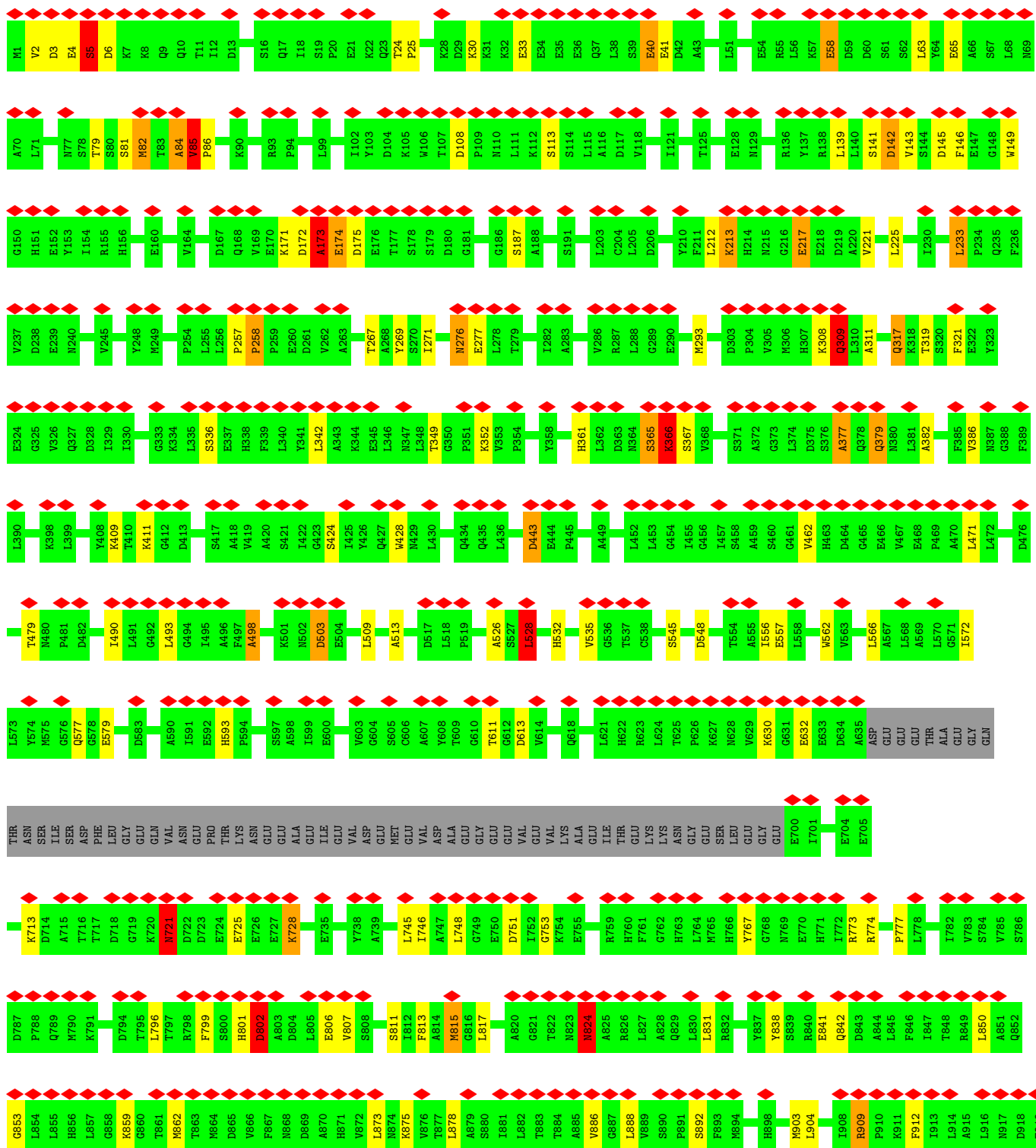
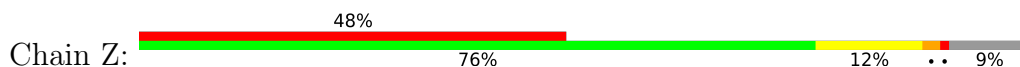


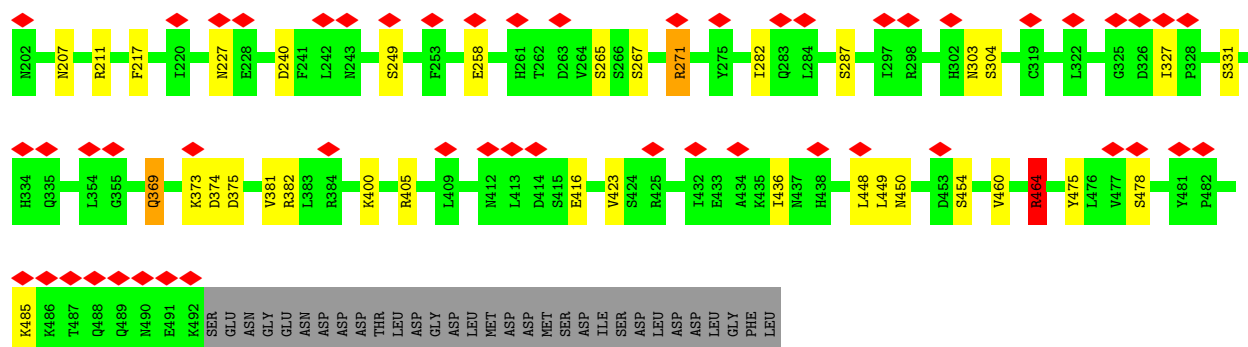
- Molecule 19: 26S proteasome complex subunit SEM1



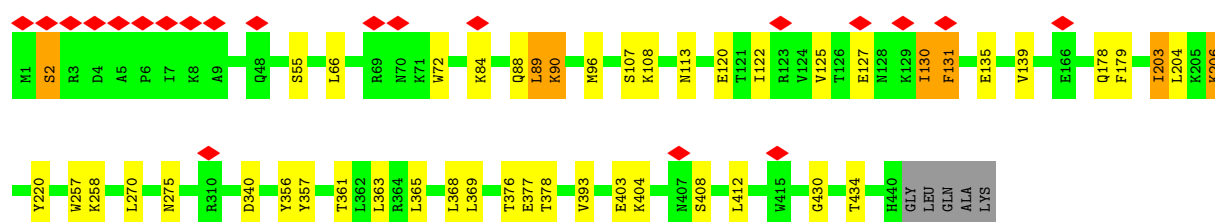
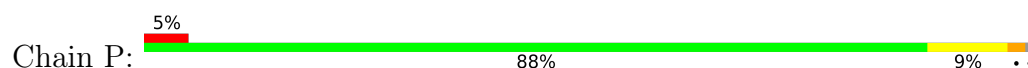


- Molecule 20: 26S proteasome regulatory subunit RPN1

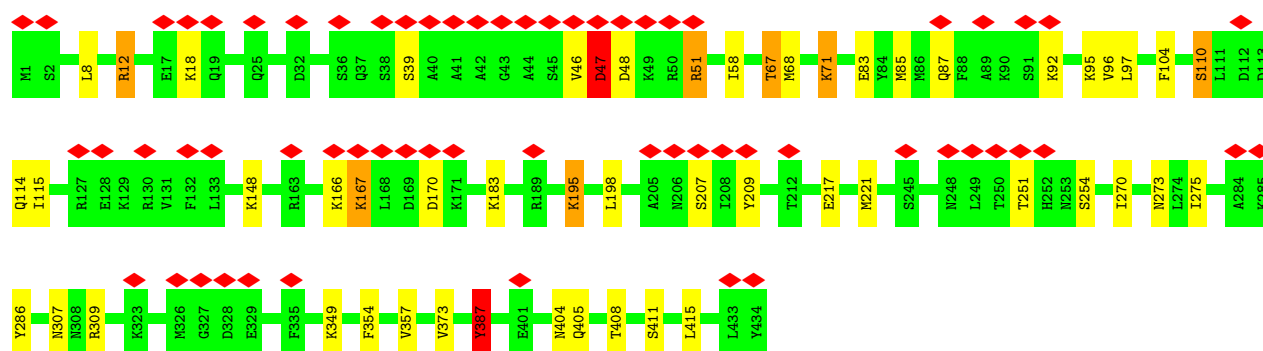
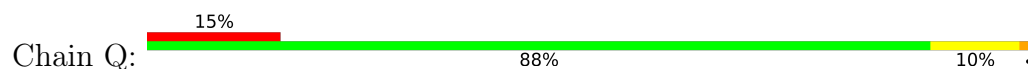




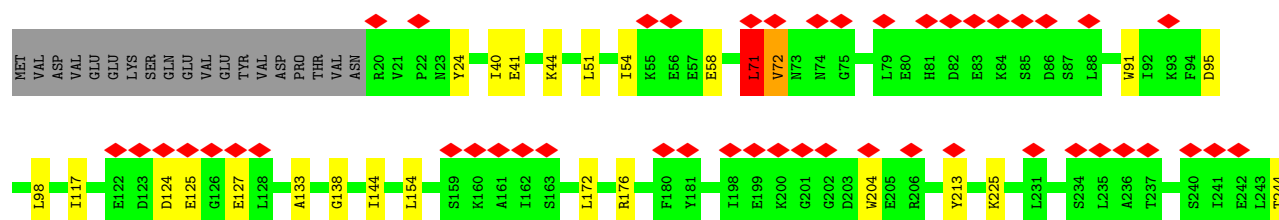
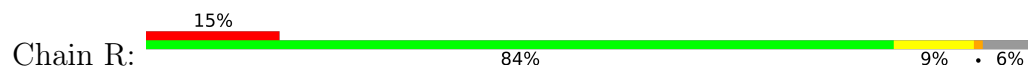
• Molecule 23: 26S proteasome regulatory subunit RPN5

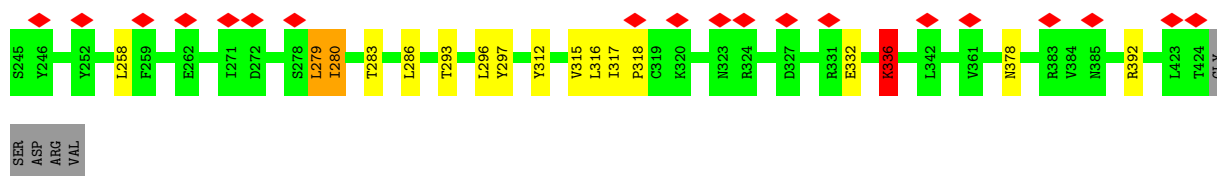


• Molecule 24: 26S proteasome regulatory subunit RPN6

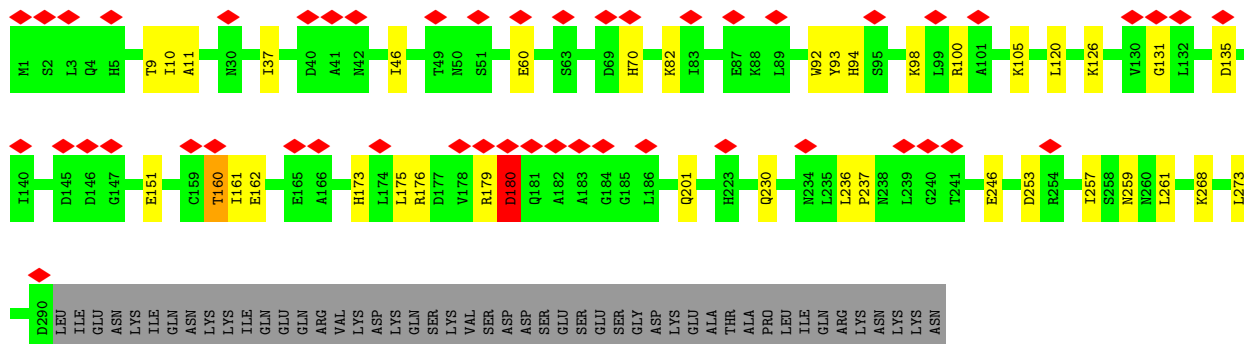
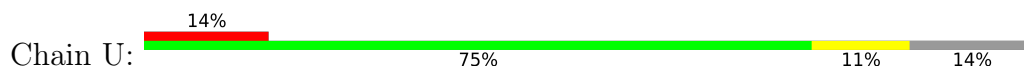


• Molecule 25: 26S proteasome regulatory subunit RPN7





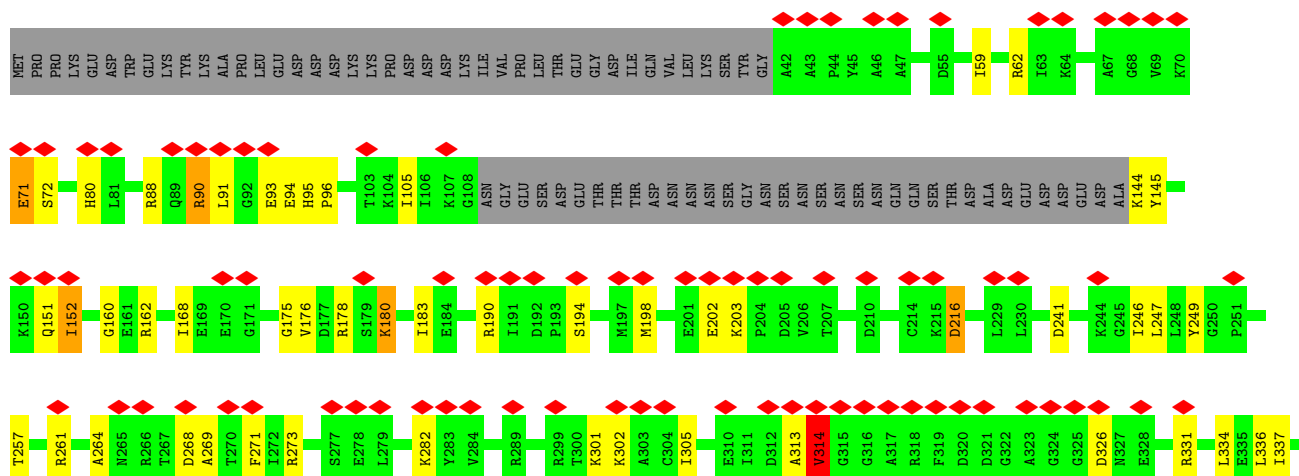
• Molecule 26: 26S proteasome regulatory subunit RPN8

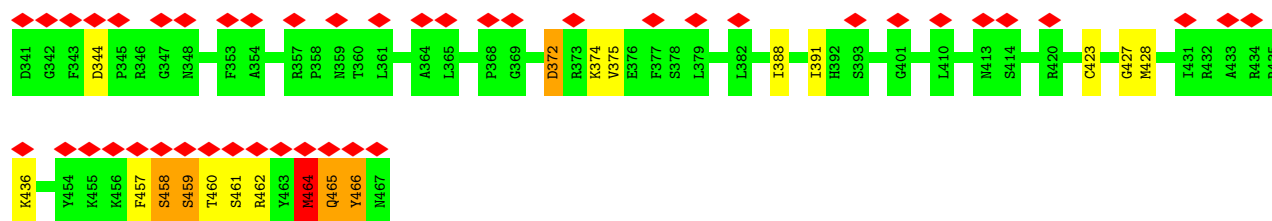


• Molecule 27: 26S proteasome regulatory subunit RPN9

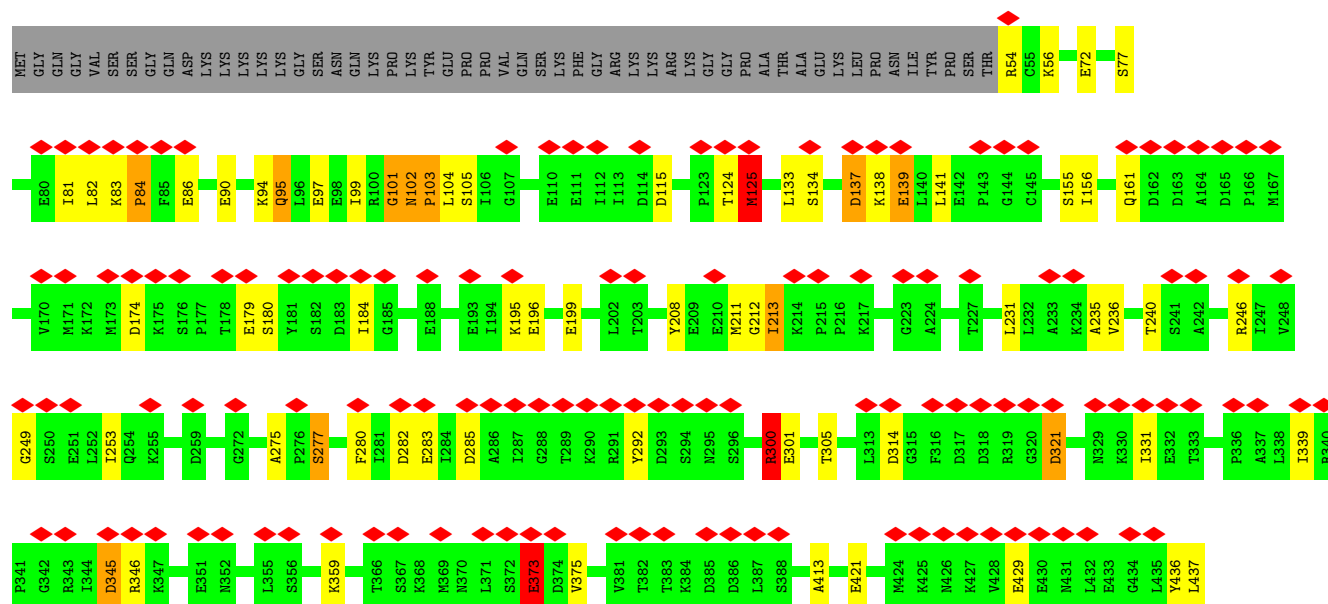


• Molecule 28: 26S proteasome regulatory subunit 7 homolog

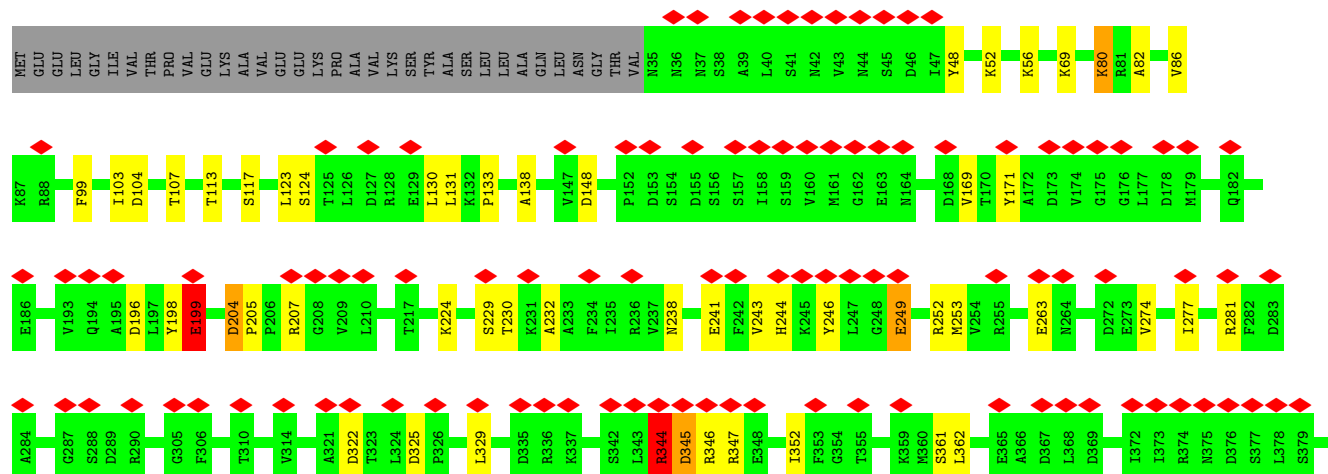
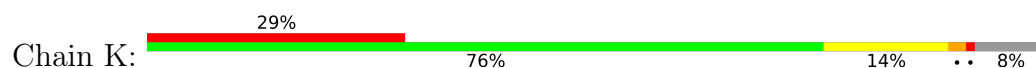




- Molecule 29: 26S proteasome regulatory subunit 4 homolog



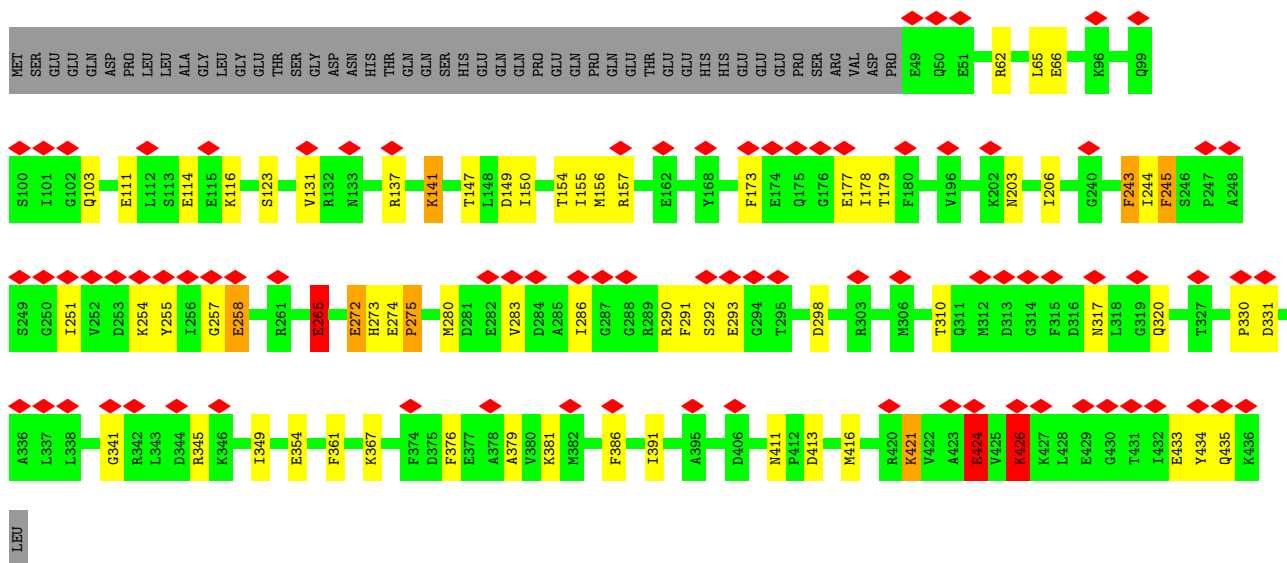
- Molecule 30: 26S proteasome regulatory subunit 6B homolog





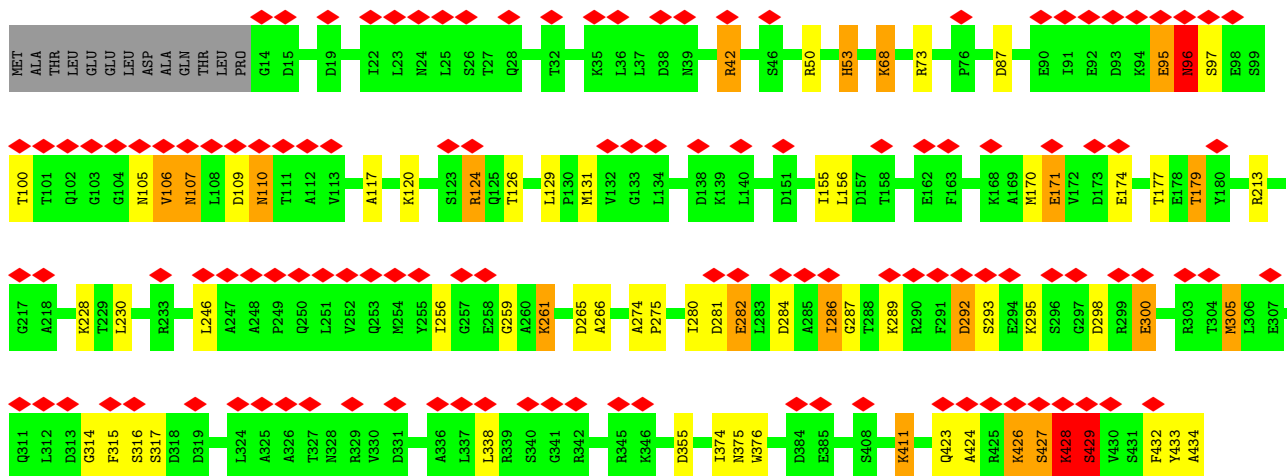
• Molecule 31: 26S proteasome subunit RPT4

Chain L: 19% 73% 14% .. 11%



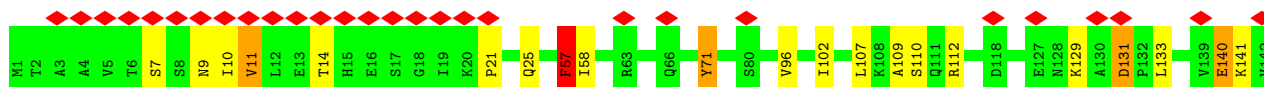
• Molecule 32: 26S proteasome regulatory subunit 6A

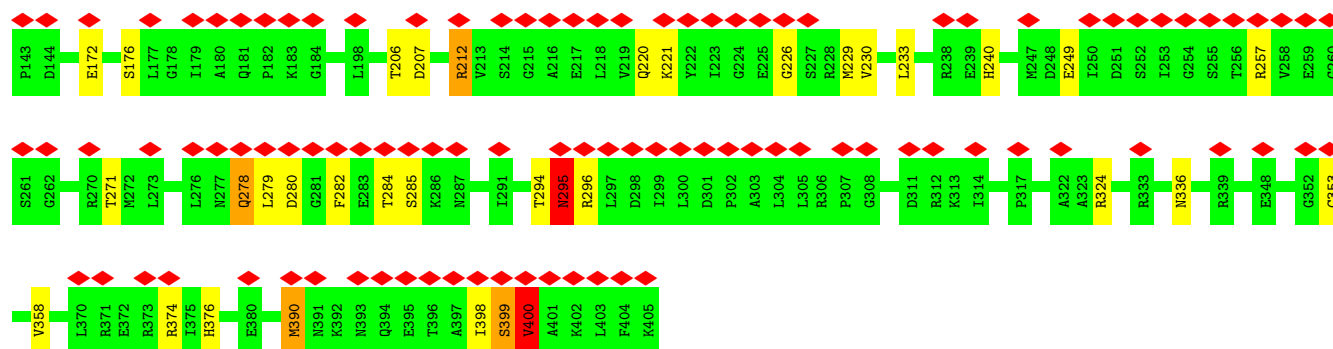
Chain M: 28% 81% 11%



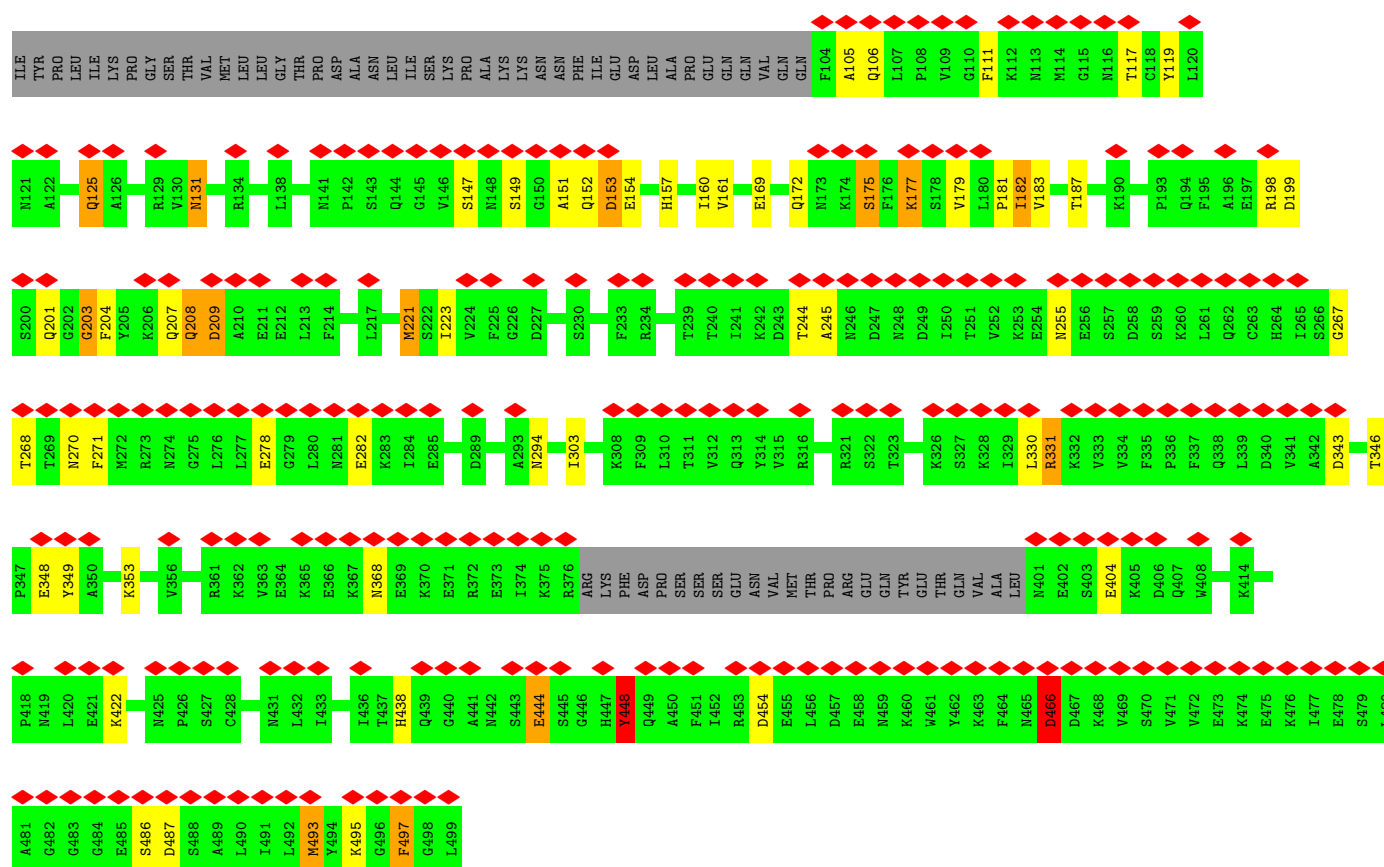
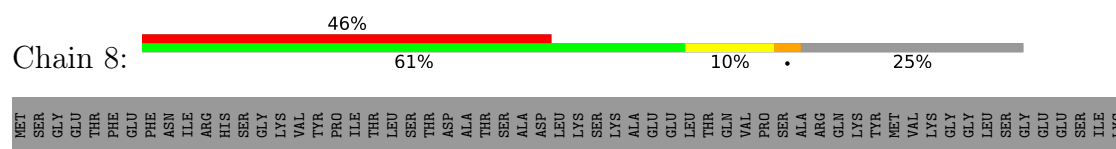
• Molecule 33: 26S proteasome regulatory subunit 8 homolog

Chain J: 32% 86% 11% ..





• Molecule 34: Ubiquitin carboxyl-terminal hydrolase 6



• Molecule 35: Polyubiquitin-B





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	64766	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	35	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	25.895	Depositor
Minimum map value	-17.249	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.920	Depositor
Recommended contour level	4.8	Depositor
Map size (Å)	529.92, 529.92, 529.92	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.38, 1.38, 1.38	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.44	46/1945 (2.4%)	1.46	35/2634 (1.3%)
1	a	1.43	45/1945 (2.3%)	1.41	30/2634 (1.1%)
2	B	1.38	38/1944 (2.0%)	1.40	29/2632 (1.1%)
2	b	1.38	38/1944 (2.0%)	1.40	29/2632 (1.1%)
3	C	1.34	38/1934 (2.0%)	1.44	32/2618 (1.2%)
3	c	1.34	38/1934 (2.0%)	1.44	32/2618 (1.2%)
4	D	0.66	1/1879 (0.1%)	1.22	10/2546 (0.4%)
4	d	0.66	0/1879	1.14	5/2546 (0.2%)
5	E	1.46	41/1908 (2.1%)	1.59	43/2571 (1.7%)
5	e	1.58	49/1908 (2.6%)	1.64	54/2571 (2.1%)
6	F	1.21	22/1800 (1.2%)	1.24	14/2433 (0.6%)
6	f	1.21	23/1800 (1.3%)	1.24	14/2433 (0.6%)
7	G	1.61	39/1925 (2.0%)	1.77	51/2599 (2.0%)
7	g	1.33	33/1925 (1.7%)	1.41	25/2599 (1.0%)
8	1	2.42	87/1541 (5.6%)	2.00	76/2087 (3.6%)
8	h	2.39	79/1541 (5.1%)	1.99	77/2087 (3.7%)
9	2	2.88	137/1750 (7.8%)	2.53	113/2373 (4.8%)
9	i	2.64	118/1750 (6.7%)	2.48	97/2373 (4.1%)
10	3	2.86	119/1611 (7.4%)	2.18	89/2174 (4.1%)
10	j	2.62	88/1611 (5.5%)	2.33	111/2174 (5.1%)
11	4	3.29	141/1589 (8.9%)	2.35	102/2142 (4.8%)
11	k	3.29	141/1589 (8.9%)	2.35	103/2142 (4.8%)
12	5	2.72	111/1681 (6.6%)	2.14	98/2274 (4.3%)
12	l	2.74	113/1681 (6.7%)	2.16	100/2274 (4.4%)
13	6	3.17	161/1795 (9.0%)	2.38	131/2420 (5.4%)
13	m	3.25	173/1795 (9.6%)	2.39	130/2420 (5.4%)
14	7	0.60	0/1821	1.10	3/2470 (0.1%)
14	n	0.66	0/1821	1.15	6/2470 (0.2%)
15	W	0.70	0/1557	1.31	9/2111 (0.4%)
16	V	0.63	0/2309	1.25	13/3115 (0.4%)
17	T	0.68	2/2235 (0.1%)	1.23	10/3017 (0.3%)
18	X	0.61	0/1058	1.29	6/1432 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
19	Y	0.57	0/741	1.27	2/1000 (0.2%)
20	Z	0.65	3/7122 (0.0%)	1.34	55/9645 (0.6%)
21	N	0.61	1/6521 (0.0%)	1.15	14/8824 (0.2%)
22	S	0.60	1/3966 (0.0%)	1.29	21/5355 (0.4%)
23	P	0.60	0/3663	1.12	5/4940 (0.1%)
24	Q	0.61	0/3556	1.27	18/4787 (0.4%)
25	R	0.64	1/3313 (0.0%)	1.27	8/4469 (0.2%)
26	U	0.65	0/2340	1.19	9/3168 (0.3%)
27	O	0.58	0/3247	1.11	6/4380 (0.1%)
28	H	0.66	0/3113	1.27	22/4187 (0.5%)
29	I	0.69	2/3054 (0.1%)	1.46	24/4111 (0.6%)
30	K	0.65	0/3156	1.30	17/4261 (0.4%)
31	L	0.74	4/3128 (0.1%)	1.50	37/4204 (0.9%)
32	M	0.74	4/3323 (0.1%)	1.50	29/4478 (0.6%)
33	J	0.64	0/3212	1.26	16/4316 (0.4%)
34	8	0.75	5/3089 (0.2%)	1.35	25/4144 (0.6%)
35	9	0.61	0/603	1.25	3/811 (0.4%)
All	All	1.45	1942/114552 (1.7%)	1.54	1988/154701 (1.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	a	0	2
2	B	0	1
2	b	0	1
3	C	0	3
3	c	0	3
4	D	0	4
4	d	0	4
5	E	0	4
5	e	0	4
6	F	0	3
6	f	0	3
7	G	0	6
7	g	0	4
8	1	0	1
8	h	0	1
9	2	0	6

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Mol	Chain	#Chirality outliers	#Planarity outliers
9	i	0	7
10	3	0	2
10	j	0	1
11	4	0	1
11	k	0	1
12	5	0	3
12	l	0	3
13	6	0	5
13	m	0	8
14	7	0	2
15	W	0	4
16	V	0	1
17	T	0	3
19	Y	0	3
20	Z	0	22
21	N	0	5
22	S	0	5
23	P	0	2
24	Q	0	6
25	R	0	2
26	U	0	5
27	O	0	2
28	H	0	9
29	I	0	15
30	K	0	7
31	L	0	10
32	M	0	20
33	J	0	7
34	8	0	15
35	9	0	1
All	All	0	230

All (1942) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	6	181	LYS	CB-CG	-23.16	0.82	1.52
13	m	181	LYS	CB-CG	-23.14	0.83	1.52
11	k	70	ARG	CZ-NH2	-21.60	1.05	1.33
11	4	70	ARG	CZ-NH2	-21.58	1.05	1.33
10	3	146	LEU	C-N	19.34	1.59	1.33
13	6	141	ARG	CZ-NH1	-19.16	1.05	1.32
13	m	141	ARG	CZ-NH1	-19.14	1.05	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	l	170	LEU	CG-CD2	-19.11	0.89	1.52
12	5	170	LEU	CG-CD2	-19.10	0.89	1.52
9	i	101	ARG	CD-NE	-19.01	1.19	1.46
9	2	101	ARG	CD-NE	-18.99	1.19	1.46
13	m	46	ARG	CZ-NH2	-18.78	1.09	1.33
13	6	46	ARG	CZ-NH2	-18.75	1.09	1.33
12	l	115	PHE	CE2-CZ	-18.46	0.83	1.38
9	i	65	ARG	CZ-NH1	-18.46	1.06	1.32
12	5	115	PHE	CE2-CZ	-18.46	0.83	1.38
13	m	181	LYS	CG-CD	-18.41	0.97	1.52
13	6	181	LYS	CG-CD	-18.38	0.97	1.52
9	2	65	ARG	CZ-NH1	-18.37	1.07	1.32
5	e	11	GLY	C-N	18.00	1.56	1.33
10	j	40	PHE	CG-CD2	-17.86	1.01	1.38
10	3	40	PHE	CG-CD2	-17.84	1.01	1.38
11	k	176	PHE	CG-CD1	-17.75	1.01	1.38
9	i	101	ARG	CZ-NH2	-17.75	1.10	1.33
11	4	176	PHE	CG-CD1	-17.73	1.01	1.38
9	2	101	ARG	CZ-NH2	-17.72	1.10	1.33
8	h	48	ASP	C-N	17.71	1.58	1.33
10	3	118	LYS	CD-CE	-17.71	0.99	1.52
10	j	118	LYS	CD-CE	-17.71	0.99	1.52
13	m	145	ARG	CZ-NH2	-17.62	1.10	1.33
13	6	145	ARG	CZ-NH2	-17.61	1.10	1.33
11	k	176	PHE	CE2-CZ	-17.55	0.86	1.38
13	6	46	ARG	CD-NE	-17.54	1.21	1.46
13	m	46	ARG	CD-NE	-17.54	1.21	1.46
12	l	115	PHE	CG-CD1	-17.52	1.02	1.38
11	4	176	PHE	CE2-CZ	-17.51	0.86	1.38
12	5	115	PHE	CG-CD1	-17.50	1.02	1.38
9	2	217	ARG	CZ-NH1	-17.48	1.08	1.32
11	4	135	TYR	CG-CD1	-17.45	1.02	1.39
11	k	135	TYR	CG-CD1	-17.42	1.02	1.39
9	2	119	TYR	CG-CD1	-17.38	1.02	1.39
9	i	119	TYR	CG-CD1	-17.35	1.02	1.39
11	k	96	ARG	CZ-NH2	-17.26	1.11	1.33
11	4	96	ARG	CZ-NH2	-17.25	1.11	1.33
11	4	96	ARG	CD-NE	-17.22	1.22	1.46
11	k	96	ARG	CD-NE	-17.16	1.22	1.46
12	5	81	PHE	CE2-CZ	-17.09	0.87	1.38
11	4	70	ARG	CZ-NH1	-17.09	1.08	1.32
12	l	81	PHE	CE2-CZ	-17.08	0.87	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	k	70	ARG	CZ-NH1	-17.03	1.08	1.32
9	2	232	TYR	CG-CD1	-17.02	1.03	1.39
11	4	67	TYR	CG-CD2	-16.92	1.03	1.39
11	k	67	TYR	CG-CD2	-16.91	1.03	1.39
11	k	93	ARG	CZ-NH2	-16.91	1.11	1.33
11	4	93	ARG	CZ-NH2	-16.88	1.11	1.33
11	k	67	TYR	CE1-CZ	-16.86	0.97	1.38
9	2	232	TYR	CE2-CZ	-16.85	0.97	1.38
11	4	67	TYR	CE1-CZ	-16.85	0.97	1.38
11	4	78	GLN	CG-CD	-16.84	1.09	1.52
11	k	8	ARG	CZ-NH1	-16.83	1.09	1.32
11	4	8	ARG	CZ-NH1	-16.82	1.09	1.32
11	k	78	GLN	CG-CD	-16.80	1.10	1.52
11	4	49	GLU	CG-CD	-16.61	1.10	1.52
11	k	49	GLU	CG-CD	-16.60	1.10	1.52
9	2	153	TYR	CD1-CE1	-16.56	0.89	1.38
9	i	153	TYR	CD1-CE1	-16.54	0.89	1.38
10	3	40	PHE	CE1-CZ	-16.50	0.89	1.38
10	3	127	ILE	C-N	16.50	1.57	1.33
10	j	40	PHE	CE1-CZ	-16.47	0.89	1.38
10	3	118	LYS	CG-CD	-16.45	1.03	1.52
10	j	118	LYS	CG-CD	-16.42	1.03	1.52
8	h	133	TYR	CE2-CZ	-16.32	0.99	1.38
8	1	133	TYR	CE2-CZ	-16.31	0.99	1.38
9	i	119	TYR	CE2-CZ	-16.21	0.99	1.38
9	2	119	TYR	CE2-CZ	-16.20	0.99	1.38
9	2	126	TYR	CG-CD2	-16.05	1.05	1.39
11	k	99	GLN	CB-CG	-16.05	1.04	1.52
10	3	154	TYR	CE1-CZ	-16.04	0.99	1.38
9	i	126	TYR	CG-CD2	-16.03	1.05	1.39
11	k	96	ARG	CG-CD	-16.03	1.04	1.52
11	4	99	GLN	CB-CG	-16.03	1.04	1.52
9	i	126	TYR	CE1-CZ	-16.01	0.99	1.38
11	4	96	ARG	CG-CD	-16.00	1.04	1.52
9	2	126	TYR	CE1-CZ	-15.99	0.99	1.38
8	1	133	TYR	CG-CD1	-15.90	1.05	1.39
8	h	133	TYR	CG-CD1	-15.89	1.05	1.39
8	1	45	ARG	CD-NE	-15.86	1.24	1.46
8	h	45	ARG	CD-NE	-15.85	1.24	1.46
32	M	96	ASN	CG-OD1	-15.84	0.93	1.23
13	m	133	PHE	CE2-CZ	-15.83	0.91	1.38
13	6	133	PHE	CE2-CZ	-15.83	0.91	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	234	ARG	CZ-NH1	-15.82	1.10	1.32
2	b	234	ARG	CZ-NH1	-15.81	1.10	1.32
12	l	139	ARG	CD-NE	-15.61	1.24	1.46
13	6	131	TYR	CG-CD2	-15.60	1.06	1.39
12	5	139	ARG	CD-NE	-15.59	1.24	1.46
12	l	81	PHE	CG-CD1	-15.58	1.06	1.38
10	3	154	TYR	CG-CD2	-15.54	1.06	1.39
13	m	131	TYR	CG-CD2	-15.54	1.06	1.39
12	5	81	PHE	CG-CD1	-15.54	1.06	1.38
11	k	110	LYS	CG-CD	-15.46	1.06	1.52
11	k	182	LYS	CD-CE	-15.45	1.06	1.52
11	4	182	LYS	CD-CE	-15.45	1.06	1.52
11	4	110	LYS	CG-CD	-15.45	1.06	1.52
13	m	131	TYR	CE1-CZ	-15.42	1.01	1.38
13	6	131	TYR	CE1-CZ	-15.39	1.01	1.38
8	h	10	THR	CB-CG2	-15.10	1.02	1.52
8	1	10	THR	CB-CG2	-15.08	1.02	1.52
11	4	182	LYS	CE-NZ	-15.04	1.04	1.49
11	k	182	LYS	CE-NZ	-15.02	1.04	1.49
12	l	188	TYR	CG-CD2	-14.98	1.07	1.39
11	4	10	GLN	CG-CD	-14.94	1.14	1.52
12	5	188	TYR	CG-CD2	-14.94	1.07	1.39
11	k	10	GLN	CG-CD	-14.91	1.14	1.52
12	l	164	GLN	CB-CG	-14.90	1.07	1.52
8	h	26	ASP	CB-CG	-14.89	1.14	1.52
11	k	135	TYR	CE2-CZ	-14.87	1.02	1.38
8	1	26	ASP	CB-CG	-14.86	1.14	1.52
12	5	164	GLN	CB-CG	-14.86	1.07	1.52
13	6	133	PHE	CG-CD1	-14.86	1.07	1.38
11	4	135	TYR	CE2-CZ	-14.86	1.02	1.38
13	m	133	PHE	CG-CD1	-14.83	1.07	1.38
10	j	74	TYR	CG-CD1	-14.81	1.08	1.39
10	3	74	TYR	CG-CD1	-14.81	1.08	1.39
9	2	153	TYR	CB-CG	-14.79	1.19	1.51
9	i	153	TYR	CB-CG	-14.75	1.19	1.51
11	k	121	TYR	CG-CD2	-14.73	1.08	1.39
11	4	121	TYR	CG-CD2	-14.73	1.08	1.39
11	k	121	TYR	CE1-CZ	-14.70	1.02	1.38
11	4	121	TYR	CE1-CZ	-14.69	1.02	1.38
8	1	120	TYR	CG-CD1	-14.63	1.08	1.39
8	h	120	TYR	CG-CD1	-14.61	1.08	1.39
11	k	121	TYR	CE2-CZ	-14.58	1.03	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	4	121	TYR	CE2-CZ	-14.57	1.03	1.38
12	l	81	PHE	CE1-CZ	-14.54	0.95	1.38
12	5	81	PHE	CE1-CZ	-14.54	0.95	1.38
13	6	47	TYR	CE1-CZ	-14.51	1.03	1.38
13	6	145	ARG	CD-NE	-14.51	1.25	1.46
13	m	47	TYR	CE1-CZ	-14.48	1.03	1.38
13	m	145	ARG	CD-NE	-14.45	1.26	1.46
8	1	120	TYR	CE2-CZ	-14.44	1.03	1.38
8	h	120	TYR	CE2-CZ	-14.43	1.03	1.38
10	j	67	PHE	CE2-CZ	-14.42	0.95	1.38
11	4	121	TYR	CG-CD1	-14.40	1.09	1.39
10	3	67	PHE	CE2-CZ	-14.40	0.95	1.38
11	k	139	TYR	CG-CD2	-14.37	1.09	1.39
11	k	121	TYR	CG-CD1	-14.37	1.09	1.39
11	4	139	TYR	CG-CD2	-14.35	1.09	1.39
11	k	70	ARG	CD-NE	-14.28	1.26	1.46
11	4	70	ARG	CD-NE	-14.26	1.26	1.46
11	4	113	LYS	CE-NZ	-14.23	1.06	1.49
11	k	113	LYS	CE-NZ	-14.21	1.06	1.49
13	m	182	TYR	CE2-CZ	-14.19	1.04	1.38
12	l	245	TYR	CE1-CZ	-14.18	1.04	1.38
13	6	182	TYR	CE2-CZ	-14.17	1.04	1.38
12	5	245	TYR	CE1-CZ	-14.16	1.04	1.38
11	k	139	TYR	CE1-CZ	-14.15	1.04	1.38
11	4	139	TYR	CE1-CZ	-14.13	1.04	1.38
12	5	115	PHE	CE1-CZ	-14.07	0.96	1.38
12	5	188	TYR	CE1-CZ	-14.07	1.04	1.38
12	l	115	PHE	CE1-CZ	-14.05	0.96	1.38
12	l	188	TYR	CE1-CZ	-14.04	1.04	1.38
13	m	85	PHE	CE2-CZ	-14.02	0.96	1.38
10	j	74	TYR	CE2-CZ	-13.99	1.04	1.38
12	l	245	TYR	CG-CD2	-13.99	1.09	1.39
10	3	74	TYR	CE2-CZ	-13.99	1.04	1.38
12	5	245	TYR	CG-CD2	-13.98	1.09	1.39
12	5	77	THR	CB-CG2	-13.97	1.06	1.52
10	j	204	GLN	CB-CG	-13.97	1.10	1.52
12	l	77	THR	CB-CG2	-13.96	1.06	1.52
13	m	85	PHE	CE1-CZ	-13.96	0.96	1.38
10	3	204	GLN	CB-CG	-13.95	1.10	1.52
8	h	45	ARG	CZ-NH2	-13.94	1.15	1.33
7	g	207	ASN	CG-ND2	-13.93	1.03	1.33
8	h	49	LYS	C-N	13.93	1.50	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	h	16	THR	C-N	13.91	1.47	1.33
8	1	45	ARG	CZ-NH2	-13.90	1.15	1.33
5	e	10	ARG	CZ-NH1	-13.90	1.13	1.32
9	i	126	TYR	CG-CD1	-13.83	1.10	1.39
8	1	133	TYR	CE1-CZ	-13.82	1.05	1.38
9	2	126	TYR	CG-CD1	-13.81	1.10	1.39
8	h	133	TYR	CE1-CZ	-13.79	1.05	1.38
8	h	133	TYR	CG-CD2	-13.79	1.10	1.39
8	1	133	TYR	CG-CD2	-13.78	1.10	1.39
13	6	168	TYR	CG-CD1	-13.75	1.10	1.39
13	m	168	TYR	CG-CD1	-13.74	1.10	1.39
13	6	47	TYR	CG-CD1	-13.71	1.10	1.39
13	m	47	TYR	CG-CD1	-13.71	1.10	1.39
10	3	154	TYR	CE2-CZ	-13.68	1.05	1.38
8	1	183	ARG	CZ-NH2	-13.65	1.15	1.33
9	i	126	TYR	CE2-CZ	-13.64	1.05	1.38
12	5	82	ARG	CZ-NH2	-13.64	1.15	1.33
13	6	145	ARG	NE-CZ	-13.64	1.18	1.33
9	2	126	TYR	CE2-CZ	-13.63	1.05	1.38
8	h	183	ARG	CZ-NH2	-13.62	1.15	1.33
12	l	82	ARG	CZ-NH2	-13.61	1.15	1.33
20	Z	361	HIS	CE1-NE2	-13.61	1.19	1.32
13	m	145	ARG	NE-CZ	-13.61	1.18	1.33
9	2	248	ASN	CB-CG	-13.60	1.18	1.52
13	6	47	TYR	CG-CD2	-13.56	1.10	1.39
13	m	47	TYR	CG-CD2	-13.55	1.10	1.39
10	j	87	PHE	CE1-CZ	-13.49	0.98	1.38
10	3	87	PHE	CE1-CZ	-13.48	0.98	1.38
13	m	85	PHE	CG-CD2	-13.48	1.10	1.38
13	6	217	LYS	CB-CG	-13.47	1.12	1.52
5	E	53	ARG	CZ-NH1	-13.47	1.13	1.32
13	m	217	LYS	CB-CG	-13.45	1.12	1.52
11	4	67	TYR	CE2-CZ	-13.42	1.06	1.38
11	k	67	TYR	CE2-CZ	-13.41	1.06	1.38
12	5	274	LYS	CE-NZ	-13.41	1.09	1.49
12	l	274	LYS	CE-NZ	-13.41	1.09	1.49
10	3	154	TYR	CG-CD1	-13.39	1.11	1.39
12	5	245	TYR	CG-CD1	-13.39	1.11	1.39
12	l	245	TYR	CG-CD1	-13.32	1.11	1.39
9	i	153	TYR	CG-CD1	-13.30	1.11	1.39
9	2	153	TYR	CG-CD1	-13.29	1.11	1.39
9	2	153	TYR	CD2-CE2	-13.27	0.98	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	i	153	TYR	CD2-CE2	-13.27	0.98	1.38
13	6	161	GLN	CD-NE2	-13.24	1.05	1.33
13	m	131	TYR	CG-CD1	-13.24	1.11	1.39
13	m	161	GLN	CD-NE2	-13.22	1.05	1.33
13	6	131	TYR	CG-CD1	-13.16	1.11	1.39
10	j	67	PHE	CG-CD1	-13.16	1.11	1.38
10	3	67	PHE	CG-CD1	-13.14	1.11	1.38
13	m	47	TYR	CE2-CZ	-13.01	1.07	1.38
9	2	230	LYS	CE-NZ	-12.99	1.10	1.49
13	6	47	TYR	CE2-CZ	-12.98	1.07	1.38
10	3	75	LYS	CG-CD	-12.97	1.13	1.52
9	i	88	ILE	CG1-CD1	-12.97	1.01	1.51
10	j	75	LYS	CG-CD	-12.97	1.13	1.52
9	2	88	ILE	CG1-CD1	-12.96	1.01	1.51
11	4	139	TYR	CG-CD1	-12.94	1.12	1.39
13	m	131	TYR	CE2-CZ	-12.93	1.07	1.38
13	6	131	TYR	CE2-CZ	-12.93	1.07	1.38
11	k	139	TYR	CG-CD1	-12.92	1.12	1.39
2	B	231	LYS	CE-NZ	-12.92	1.10	1.49
13	m	133	PHE	CE1-CZ	-12.91	0.99	1.38
2	b	231	LYS	CE-NZ	-12.90	1.10	1.49
1	a	96	ARG	CZ-NH1	-12.89	1.14	1.32
11	k	67	TYR	CG-CD1	-12.89	1.12	1.39
13	6	133	PHE	CE1-CZ	-12.89	0.99	1.38
11	4	67	TYR	CG-CD1	-12.89	1.12	1.39
1	A	96	ARG	CZ-NH1	-12.87	1.14	1.32
10	3	113	ASN	CB-CG	-12.83	1.20	1.52
10	3	199	TYR	CE1-CZ	-12.82	1.07	1.38
10	j	199	TYR	CE1-CZ	-12.81	1.07	1.38
12	l	245	TYR	CE2-CZ	-12.79	1.07	1.38
12	5	245	TYR	CE2-CZ	-12.79	1.07	1.38
10	j	113	ASN	CB-CG	-12.78	1.20	1.52
13	m	36	ARG	CZ-NH2	-12.77	1.16	1.33
12	l	108	LYS	CE-NZ	-12.77	1.11	1.49
9	i	119	TYR	CE1-CZ	-12.74	1.07	1.38
11	k	139	TYR	CE2-CZ	-12.74	1.07	1.38
13	6	143	GLN	CG-CD	-12.73	1.20	1.52
11	4	139	TYR	CE2-CZ	-12.73	1.07	1.38
12	5	108	LYS	CE-NZ	-12.73	1.11	1.49
13	6	36	ARG	CZ-NH2	-12.73	1.17	1.33
13	m	143	GLN	CG-CD	-12.72	1.20	1.52
9	2	119	TYR	CE1-CZ	-12.71	1.07	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	4	163	LEU	CG-CD1	-12.71	1.10	1.52
11	k	163	LEU	CG-CD1	-12.69	1.10	1.52
8	1	120	TYR	CE1-CZ	-12.67	1.07	1.38
8	h	120	TYR	CE1-CZ	-12.65	1.07	1.38
6	f	169	LYS	CE-NZ	-12.63	1.11	1.49
13	m	83	TYR	CG-CD2	-12.60	1.12	1.39
6	F	169	LYS	CE-NZ	-12.59	1.11	1.49
13	m	83	TYR	CE1-CZ	-12.56	1.08	1.38
13	m	9	GLN	CD-NE2	-12.55	1.06	1.33
2	B	237	LYS	CE-NZ	-12.54	1.11	1.49
2	b	237	LYS	CE-NZ	-12.54	1.11	1.49
13	m	167	GLN	CD-NE2	-12.54	1.06	1.33
13	6	167	GLN	CD-NE2	-12.54	1.06	1.33
13	6	9	GLN	CD-NE2	-12.54	1.06	1.33
12	l	139	ARG	CZ-NH2	-12.52	1.17	1.33
8	1	153	GLU	CB-CG	-12.51	1.15	1.52
8	h	153	GLU	CB-CG	-12.51	1.15	1.52
10	3	199	TYR	CG-CD2	-12.51	1.13	1.39
10	3	87	PHE	CE2-CZ	-12.50	1.01	1.38
10	j	87	PHE	CE2-CZ	-12.47	1.01	1.38
10	j	199	TYR	CG-CD2	-12.46	1.13	1.39
12	5	139	ARG	CZ-NH2	-12.46	1.17	1.33
5	e	10	ARG	CZ-NH2	-12.45	1.17	1.33
13	m	85	PHE	CG-CD1	-12.43	1.12	1.38
11	4	46	PHE	CG-CD2	-12.42	1.12	1.38
9	2	101	ARG	NE-CZ	-12.41	1.19	1.33
11	k	46	PHE	CG-CD2	-12.40	1.12	1.38
1	a	74	CYS	C-N	12.38	1.51	1.33
12	5	253	TYR	CG-CD1	-12.37	1.13	1.39
12	l	253	TYR	CG-CD1	-12.35	1.13	1.39
11	k	98	TYR	CG-CD2	-12.35	1.13	1.39
9	i	101	ARG	NE-CZ	-12.34	1.19	1.33
8	h	120	TYR	CG-CD2	-12.33	1.13	1.39
13	m	83	TYR	CE2-CZ	-12.32	1.08	1.38
11	4	98	TYR	CG-CD2	-12.32	1.13	1.39
11	4	93	ARG	CD-NE	-12.31	1.29	1.46
12	5	81	PHE	CG-CD2	-12.31	1.12	1.38
8	1	120	TYR	CG-CD2	-12.31	1.13	1.39
12	5	82	ARG	CD-NE	-12.31	1.29	1.46
11	k	93	ARG	CD-NE	-12.29	1.29	1.46
8	h	183	ARG	CD-NE	-12.28	1.29	1.46
12	5	115	PHE	CG-CD2	-12.27	1.13	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	l	82	ARG	CD-NE	-12.26	1.29	1.46
12	l	81	PHE	CG-CD2	-12.25	1.13	1.38
8	1	183	ARG	CD-NE	-12.24	1.29	1.46
11	k	99	GLN	CG-CD	-12.24	1.21	1.52
12	l	156	LYS	CE-NZ	-12.23	1.12	1.49
13	m	83	TYR	CG-CD1	-12.23	1.13	1.39
11	4	99	GLN	CG-CD	-12.23	1.21	1.52
12	5	156	LYS	CE-NZ	-12.23	1.12	1.49
13	6	181	LYS	CA-CB	-12.23	1.33	1.53
13	m	221	ARG	CZ-NH2	-12.21	1.17	1.33
12	l	115	PHE	CG-CD2	-12.21	1.13	1.38
13	6	221	ARG	CZ-NH2	-12.20	1.17	1.33
13	m	181	LYS	CA-CB	-12.18	1.33	1.53
13	m	187	GLU	CB-CG	-12.16	1.16	1.52
1	a	184	ASN	CG-ND2	-12.14	1.07	1.33
13	6	187	GLU	CB-CG	-12.13	1.16	1.52
13	m	50	LYS	CG-CD	-12.12	1.16	1.52
13	6	50	LYS	CG-CD	-12.12	1.16	1.52
3	C	241	LYS	CD-CE	-12.11	1.16	1.52
8	1	194	ARG	CZ-NH1	-12.11	1.15	1.32
8	1	196	ILE	C-N	12.11	1.48	1.33
1	A	184	ASN	CG-ND2	-12.11	1.07	1.33
9	i	37	PHE	CG-CD2	-12.10	1.13	1.38
9	2	37	PHE	CG-CD2	-12.10	1.13	1.38
3	c	241	LYS	CD-CE	-12.10	1.16	1.52
13	6	182	TYR	CD1-CE1	-12.09	1.02	1.38
13	m	182	TYR	CD1-CE1	-12.07	1.02	1.38
11	k	98	TYR	CE1-CZ	-12.04	1.09	1.38
11	4	98	TYR	CE1-CZ	-12.03	1.09	1.38
12	5	182	LYS	CB-CG	-12.02	1.16	1.52
10	j	75	LYS	CB-CG	-12.01	1.16	1.52
12	l	182	LYS	CB-CG	-12.01	1.16	1.52
9	2	220	LEU	CG-CD2	-12.01	1.12	1.52
10	j	87	PHE	CG-CD2	-12.00	1.13	1.38
5	E	53	ARG	NE-CZ	-12.00	1.19	1.33
10	3	75	LYS	CB-CG	-12.00	1.16	1.52
10	3	87	PHE	CG-CD2	-11.98	1.13	1.38
8	1	201	GLU	CG-CD	-11.91	1.22	1.52
10	3	161	GLU	CG-CD	-11.91	1.22	1.52
10	3	87	PHE	CG-CD1	-11.87	1.14	1.38
10	j	87	PHE	CG-CD1	-11.87	1.14	1.38
9	2	119	TYR	CG-CD2	-11.87	1.14	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	2	228	LYS	CE-NZ	-11.87	1.13	1.49
9	i	119	TYR	CG-CD2	-11.86	1.14	1.39
8	1	130	LYS	CE-NZ	-11.86	1.13	1.49
13	m	190	LYS	CE-NZ	-11.83	1.13	1.49
13	6	190	LYS	CE-NZ	-11.83	1.13	1.49
8	h	130	LYS	CE-NZ	-11.82	1.13	1.49
9	2	36	LYS	CD-CE	-11.79	1.17	1.52
13	m	221	ARG	CG-CD	-11.79	1.17	1.52
9	i	36	LYS	CD-CE	-11.78	1.17	1.52
11	4	143	LEU	CG-CD1	-11.78	1.13	1.52
13	6	221	ARG	CG-CD	-11.77	1.17	1.52
11	k	143	LEU	CG-CD1	-11.75	1.13	1.52
13	m	41	TYR	CE1-CZ	-11.72	1.10	1.38
13	m	221	ARG	CZ-NH1	-11.71	1.16	1.32
13	6	41	TYR	CE1-CZ	-11.70	1.10	1.38
9	i	86	GLN	CD-NE2	-11.69	1.08	1.33
11	k	93	ARG	CZ-NH1	-11.68	1.16	1.32
11	4	93	ARG	CZ-NH1	-11.67	1.16	1.32
13	6	221	ARG	CZ-NH1	-11.66	1.16	1.32
9	2	86	GLN	CD-NE2	-11.66	1.08	1.33
10	j	80	ARG	CZ-NH1	-11.64	1.16	1.32
12	5	226	GLU	CB-CG	-11.64	1.17	1.52
12	1	226	GLU	CB-CG	-11.61	1.17	1.52
10	3	80	ARG	CZ-NH1	-11.58	1.16	1.32
9	2	255	GLU	C-O	-11.56	1.00	1.23
10	j	199	TYR	CG-CD1	-11.50	1.15	1.39
11	4	46	PHE	CE1-CZ	-11.50	1.04	1.38
10	3	199	TYR	CG-CD1	-11.50	1.15	1.39
13	m	142	GLU	CG-CD	-11.49	1.23	1.52
13	6	142	GLU	CG-CD	-11.49	1.23	1.52
11	k	46	PHE	CE1-CZ	-11.46	1.04	1.38
8	1	194	ARG	CZ-NH2	-11.44	1.18	1.33
13	m	168	TYR	CE2-CZ	-11.43	1.10	1.38
7	G	33	ASN	CG-ND2	-11.43	1.09	1.33
13	6	133	PHE	CG-CD2	-11.42	1.14	1.38
12	5	253	TYR	CE2-CZ	-11.42	1.10	1.38
12	1	253	TYR	CE2-CZ	-11.42	1.10	1.38
13	m	133	PHE	CG-CD2	-11.42	1.14	1.38
13	6	168	TYR	CE2-CZ	-11.42	1.10	1.38
7	g	248	ASN	CG-ND2	-11.41	1.09	1.33
7	g	33	ASN	CG-ND2	-11.40	1.09	1.33
11	k	176	PHE	CE1-CZ	-11.39	1.04	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	5	196	ARG	CD-NE	-11.38	1.30	1.46
11	4	176	PHE	CE1-CZ	-11.38	1.04	1.38
12	l	196	ARG	CD-NE	-11.34	1.30	1.46
11	4	95	ARG	CD-NE	-11.33	1.30	1.46
13	m	155	MET	SD-CE	-11.32	1.51	1.79
11	k	95	ARG	CD-NE	-11.30	1.30	1.46
13	6	155	MET	SD-CE	-11.29	1.51	1.79
10	3	80	ARG	NE-CZ	-11.29	1.20	1.33
10	j	80	ARG	NE-CZ	-11.26	1.20	1.33
9	2	227	GLU	CB-CG	-11.24	1.18	1.52
10	3	118	LYS	CB-CG	-11.23	1.18	1.52
12	l	83	PHE	C-N	11.23	1.50	1.33
6	F	119	ASN	CG-ND2	-11.23	1.09	1.33
10	j	118	LYS	CB-CG	-11.22	1.18	1.52
12	l	253	TYR	CE1-CZ	-11.21	1.11	1.38
6	f	119	ASN	CG-ND2	-11.21	1.09	1.33
12	5	253	TYR	CE1-CZ	-11.20	1.11	1.38
11	k	96	ARG	NE-CZ	-11.19	1.20	1.33
11	4	96	ARG	NE-CZ	-11.17	1.20	1.33
6	F	169	LYS	CD-CE	-11.16	1.19	1.52
1	a	62	LYS	CE-NZ	-11.15	1.16	1.49
1	A	62	LYS	CE-NZ	-11.15	1.16	1.49
6	f	169	LYS	CD-CE	-11.14	1.19	1.52
9	i	153	TYR	CE2-CZ	-11.05	1.11	1.38
13	m	221	ARG	CD-NE	-11.05	1.30	1.46
10	3	159	GLU	CG-CD	-11.04	1.24	1.52
9	2	153	TYR	CE2-CZ	-11.04	1.11	1.38
13	6	221	ARG	CD-NE	-11.04	1.30	1.46
9	2	232	TYR	CE1-CZ	-11.02	1.11	1.38
9	2	232	TYR	CG-CD2	-11.02	1.16	1.39
9	i	39	ASN	CG-ND2	-10.99	1.10	1.33
9	2	39	ASN	CG-ND2	-10.97	1.10	1.33
9	2	109	LEU	CG-CD1	-10.94	1.16	1.52
9	i	109	LEU	CG-CD1	-10.94	1.16	1.52
10	j	98	ARG	CZ-NH2	-10.93	1.19	1.33
10	3	98	ARG	CZ-NH2	-10.88	1.19	1.33
13	m	182	TYR	CB-CG	-10.87	1.27	1.51
11	4	163	LEU	CB-CG	-10.86	1.31	1.53
11	4	49	GLU	CB-CG	-10.85	1.20	1.52
11	k	49	GLU	CB-CG	-10.84	1.20	1.52
13	6	182	TYR	CB-CG	-10.84	1.27	1.51
11	k	163	LEU	CB-CG	-10.83	1.31	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	m	41	TYR	CG-CD2	-10.82	1.16	1.39
8	h	152	ARG	CG-CD	-10.81	1.20	1.52
8	1	152	ARG	CG-CD	-10.81	1.20	1.52
13	6	41	TYR	CG-CD2	-10.79	1.16	1.39
13	m	58	ILE	CB-CG2	-10.77	1.17	1.52
11	k	96	ARG	CB-CG	-10.77	1.20	1.52
13	6	58	ILE	CB-CG2	-10.77	1.17	1.52
11	4	96	ARG	CB-CG	-10.77	1.20	1.52
13	6	77	LYS	CD-CE	-10.69	1.20	1.52
10	j	63	LEU	CG-CD2	-10.69	1.17	1.52
13	m	77	LYS	CD-CE	-10.69	1.20	1.52
10	3	63	LEU	CG-CD2	-10.67	1.17	1.52
12	5	188	TYR	CG-CD1	-10.58	1.17	1.39
9	2	219	TYR	CG-CD1	-10.56	1.17	1.39
12	1	188	TYR	CG-CD1	-10.54	1.17	1.39
9	2	37	PHE	CE1-CZ	-10.53	1.07	1.38
10	3	199	TYR	CE2-CZ	-10.51	1.13	1.38
9	i	37	PHE	CE1-CZ	-10.51	1.07	1.38
10	j	199	TYR	CE2-CZ	-10.50	1.13	1.38
8	1	204	GLN	CB-CG	-10.49	1.21	1.52
8	h	114	LYS	CE-NZ	-10.48	1.18	1.49
13	m	36	ARG	CZ-NH1	-10.46	1.18	1.32
8	1	114	LYS	CE-NZ	-10.45	1.18	1.49
13	6	36	ARG	CZ-NH1	-10.44	1.18	1.32
13	m	58	ILE	CB-CG1	-10.42	1.32	1.53
13	6	58	ILE	CB-CG1	-10.40	1.32	1.53
3	c	114	ARG	NE-CZ	-10.40	1.21	1.33
5	e	168	ASN	CG-ND2	-10.39	1.11	1.33
12	5	82	ARG	CZ-NH1	-10.39	1.18	1.32
5	E	168	ASN	CG-ND2	-10.39	1.11	1.33
9	2	101	ARG	CB-CG	-10.37	1.21	1.52
9	i	101	ARG	CB-CG	-10.37	1.21	1.52
8	1	17	PHE	C-N	10.36	1.47	1.33
12	1	82	ARG	CZ-NH1	-10.35	1.18	1.32
3	C	114	ARG	NE-CZ	-10.35	1.21	1.33
10	3	75	LYS	CD-CE	-10.34	1.21	1.52
9	2	219	TYR	CG-CD2	-10.32	1.17	1.39
10	3	67	PHE	CE1-CZ	-10.31	1.07	1.38
10	j	67	PHE	CE1-CZ	-10.31	1.07	1.38
10	j	75	LYS	CD-CE	-10.30	1.21	1.52
11	4	36	ARG	CZ-NH1	-10.30	1.18	1.32
11	k	36	ARG	CZ-NH1	-10.30	1.18	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	g	175	GLU	CG-CD	-10.29	1.26	1.52
9	2	243	LYS	CE-NZ	-10.28	1.18	1.49
3	C	124	GLN	CD-NE2	-10.28	1.11	1.33
3	c	124	GLN	CD-NE2	-10.26	1.11	1.33
8	h	18	LYS	CD-CE	-10.26	1.21	1.52
13	m	13	TYR	CE2-CZ	-10.25	1.13	1.38
8	1	18	LYS	CD-CE	-10.25	1.21	1.52
2	b	234	ARG	CZ-NH2	-10.24	1.20	1.33
10	j	80	ARG	CZ-NH2	-10.24	1.20	1.33
2	B	234	ARG	CZ-NH2	-10.24	1.20	1.33
13	6	13	TYR	CE2-CZ	-10.24	1.13	1.38
9	2	249	ILE	CA-CB	-10.23	1.40	1.54
10	3	80	ARG	CZ-NH2	-10.22	1.20	1.33
9	2	219	TYR	CE2-CZ	-10.21	1.13	1.38
13	m	177	LYS	C-N	10.20	1.54	1.33
13	6	177	LYS	C-N	10.20	1.54	1.33
13	m	63	ASN	CG-ND2	-10.20	1.11	1.33
10	j	75	LYS	CE-NZ	-10.19	1.18	1.49
13	6	63	ASN	CG-ND2	-10.17	1.11	1.33
1	A	95	LEU	CG-CD2	-10.17	1.19	1.52
13	6	201	GLU	CG-CD	-10.17	1.26	1.52
10	3	75	LYS	CE-NZ	-10.16	1.18	1.49
1	a	95	LEU	CG-CD2	-10.14	1.19	1.52
13	m	201	GLU	CG-CD	-10.14	1.26	1.52
2	b	231	LYS	CB-CG	-10.13	1.22	1.52
10	j	40	PHE	CE2-CZ	-10.13	1.08	1.38
2	B	231	LYS	CB-CG	-10.12	1.22	1.52
13	6	182	TYR	CG-CD1	-10.12	1.18	1.39
13	6	75	ARG	CZ-NH2	-10.11	1.20	1.33
10	3	40	PHE	CE2-CZ	-10.11	1.08	1.38
12	l	82	ARG	C-N	-10.11	1.25	1.33
10	3	74	TYR	CE1-CZ	-10.11	1.14	1.38
10	3	98	ARG	CD-NE	-10.10	1.32	1.46
13	m	182	TYR	CD2-CE2	-10.10	1.08	1.38
13	m	182	TYR	CG-CD1	-10.10	1.18	1.39
10	j	74	TYR	CE1-CZ	-10.09	1.14	1.38
13	m	78	ASN	CG-ND2	-10.09	1.12	1.33
13	6	78	ASN	CG-ND2	-10.08	1.12	1.33
13	6	182	TYR	CD2-CE2	-10.08	1.08	1.38
5	e	229	LYS	CD-CE	-10.08	1.22	1.52
13	m	46	ARG	CG-CD	-10.08	1.22	1.52
5	E	229	LYS	CD-CE	-10.06	1.22	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	6	46	ARG	CG-CD	-10.06	1.22	1.52
9	2	167	LEU	CG-CD1	-10.05	1.19	1.52
13	m	75	ARG	CZ-NH2	-10.04	1.20	1.33
7	G	100	LYS	CB-CG	-10.02	1.22	1.52
10	j	98	ARG	CD-NE	-10.02	1.32	1.46
9	i	167	LEU	CG-CD1	-10.02	1.19	1.52
7	g	100	LYS	CB-CG	-10.01	1.22	1.52
11	4	63	ASN	CG-ND2	-10.01	1.12	1.33
11	k	63	ASN	CG-ND2	-9.96	1.12	1.33
12	l	233	LYS	CD-CE	-9.95	1.22	1.52
12	5	233	LYS	CD-CE	-9.95	1.22	1.52
13	6	75	ARG	CD-NE	-9.93	1.32	1.46
10	3	115	LYS	CD-CE	-9.92	1.22	1.52
10	j	115	LYS	CD-CE	-9.92	1.22	1.52
10	j	8	ASN	CB-CG	-9.89	1.27	1.52
13	m	75	ARG	CD-NE	-9.87	1.32	1.46
6	F	110	HIS	CE1-NE2	-9.87	1.22	1.32
10	3	8	ASN	CB-CG	-9.87	1.27	1.52
6	f	110	HIS	CE1-NE2	-9.87	1.22	1.32
17	T	130	ASP	CG-OD1	-9.87	1.06	1.25
9	2	62	LYS	CG-CD	-9.87	1.22	1.52
9	i	62	LYS	CG-CD	-9.86	1.22	1.52
11	4	171	ARG	CZ-NH2	-9.86	1.20	1.33
13	6	41	TYR	CG-CD1	-9.85	1.18	1.39
11	4	176	PHE	CG-CD2	-9.85	1.18	1.38
12	l	188	TYR	CE2-CZ	-9.84	1.14	1.38
11	k	171	ARG	CZ-NH2	-9.83	1.20	1.33
12	5	188	TYR	CE2-CZ	-9.83	1.14	1.38
11	k	176	PHE	CG-CD2	-9.82	1.18	1.38
13	m	41	TYR	CG-CD1	-9.82	1.18	1.39
9	2	189	GLN	CG-CD	-9.82	1.27	1.52
9	2	156	LEU	CG-CD2	-9.82	1.20	1.52
9	i	156	LEU	CG-CD2	-9.80	1.20	1.52
13	6	13	TYR	CG-CD2	-9.79	1.18	1.39
9	i	189	GLN	CG-CD	-9.79	1.27	1.52
13	m	13	TYR	CG-CD2	-9.79	1.18	1.39
10	3	125	ASP	CB-CG	-9.75	1.27	1.52
12	l	140	LEU	CG-CD2	-9.73	1.20	1.52
11	4	95	ARG	CZ-NH2	-9.72	1.20	1.33
12	5	140	LEU	CG-CD2	-9.72	1.20	1.52
8	h	98	ASN	CG-ND2	-9.71	1.12	1.33
13	m	90	LYS	CE-NZ	-9.71	1.20	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	k	95	ARG	CZ-NH2	-9.71	1.20	1.33
8	1	98	ASN	CG-ND2	-9.70	1.12	1.33
1	a	188	LYS	CE-NZ	-9.69	1.20	1.49
9	2	246	ILE	CG1-CD1	-9.68	1.14	1.51
1	A	188	LYS	CE-NZ	-9.67	1.20	1.49
11	4	111	LYS	CE-NZ	-9.67	1.20	1.49
2	b	160	LYS	CE-NZ	-9.66	1.20	1.49
1	a	95	LEU	CG-CD1	-9.65	1.20	1.52
11	k	111	LYS	CE-NZ	-9.65	1.20	1.49
1	a	107	LYS	CE-NZ	-9.65	1.20	1.49
1	A	95	LEU	CG-CD1	-9.65	1.20	1.52
2	B	160	LYS	CE-NZ	-9.65	1.20	1.49
12	5	286	ILE	CB-CG2	-9.64	1.20	1.52
1	A	107	LYS	CE-NZ	-9.63	1.20	1.49
1	A	201	LYS	CD-CE	-9.63	1.23	1.52
13	6	228	LYS	CE-NZ	-9.63	1.20	1.49
10	j	77	LYS	CE-NZ	-9.62	1.20	1.49
13	m	228	LYS	CE-NZ	-9.62	1.20	1.49
10	3	77	LYS	CE-NZ	-9.62	1.20	1.49
1	a	201	LYS	CD-CE	-9.61	1.23	1.52
12	l	286	ILE	CB-CG2	-9.61	1.20	1.52
9	2	211	LYS	CB-CG	-9.60	1.23	1.52
9	i	211	LYS	CB-CG	-9.59	1.23	1.52
3	c	165	VAL	CB-CG2	-9.58	1.21	1.52
10	j	53	ILE	CB-CG2	-9.58	1.21	1.52
10	3	53	ILE	CB-CG2	-9.57	1.21	1.52
13	m	13	TYR	CG-CD1	-9.56	1.19	1.39
11	k	135	TYR	CB-CG	-9.55	1.30	1.51
3	C	165	VAL	CB-CG2	-9.55	1.21	1.52
11	4	135	TYR	CB-CG	-9.55	1.30	1.51
13	6	13	TYR	CG-CD1	-9.54	1.19	1.39
13	m	94	ILE	CB-CG2	-9.52	1.21	1.52
13	m	186	GLU	CB-CG	-9.51	1.24	1.52
13	6	186	GLU	CB-CG	-9.49	1.24	1.52
13	6	57	ASN	CG-ND2	-9.49	1.13	1.33
12	5	139	ARG	NE-CZ	-9.48	1.22	1.33
8	h	103	THR	CB-CG2	-9.48	1.21	1.52
13	6	134	ASP	CG-OD1	-9.47	1.07	1.25
12	l	139	ARG	NE-CZ	-9.46	1.22	1.33
8	1	194	ARG	CG-CD	-9.46	1.24	1.52
13	m	134	ASP	CG-OD1	-9.46	1.07	1.25
8	1	103	THR	CB-CG2	-9.45	1.21	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	m	57	ASN	CG-ND2	-9.45	1.13	1.33
11	k	95	ARG	NE-CZ	-9.43	1.22	1.33
11	4	95	ARG	NE-CZ	-9.41	1.22	1.33
12	5	226	GLU	CD-OE2	-9.40	1.07	1.25
9	2	219	TYR	CE1-CZ	-9.40	1.15	1.38
9	2	84	VAL	CB-CG1	-9.39	1.21	1.52
9	i	84	VAL	CB-CG1	-9.37	1.21	1.52
9	i	106	VAL	CB-CG2	-9.37	1.21	1.52
9	2	106	VAL	CB-CG2	-9.37	1.21	1.52
10	3	131	ASP	C-N	9.36	1.46	1.33
12	l	160	ASN	CG-ND2	-9.35	1.13	1.33
6	F	5	ASN	CG-ND2	-9.35	1.13	1.33
9	2	230	LYS	CD-CE	-9.34	1.24	1.52
12	5	160	ASN	CG-ND2	-9.34	1.13	1.33
6	f	5	ASN	CG-ND2	-9.34	1.13	1.33
13	m	41	TYR	CE2-CZ	-9.33	1.15	1.38
12	l	226	GLU	CD-OE2	-9.33	1.07	1.25
13	6	41	TYR	CE2-CZ	-9.32	1.15	1.38
9	i	51	GLN	CB-CG	-9.32	1.24	1.52
11	k	8	ARG	CZ-NH2	-9.32	1.21	1.33
12	l	274	LYS	CB-CG	-9.32	1.24	1.52
12	5	274	LYS	CB-CG	-9.30	1.24	1.52
13	m	102	GLN	CD-OE1	-9.30	1.05	1.23
9	2	51	GLN	CB-CG	-9.30	1.24	1.52
11	4	8	ARG	CZ-NH2	-9.29	1.21	1.33
11	k	182	LYS	CG-CD	-9.28	1.24	1.52
13	6	228	LYS	CG-CD	-9.27	1.24	1.52
13	6	13	TYR	CE1-CZ	-9.27	1.16	1.38
13	m	228	LYS	CG-CD	-9.26	1.24	1.52
11	4	182	LYS	CG-CD	-9.26	1.24	1.52
13	m	88	ASN	CG-ND2	-9.25	1.13	1.33
8	1	204	GLN	C-N	9.25	1.46	1.33
13	m	208	ASP	CB-CG	-9.24	1.28	1.52
13	6	208	ASP	CB-CG	-9.24	1.28	1.52
13	m	13	TYR	CE1-CZ	-9.24	1.16	1.38
8	1	42	LYS	CE-NZ	-9.22	1.21	1.49
8	h	42	LYS	CE-NZ	-9.21	1.21	1.49
13	m	91	LYS	CG-CD	-9.20	1.24	1.52
1	a	48	LYS	CE-NZ	-9.20	1.21	1.49
1	A	48	LYS	CE-NZ	-9.19	1.21	1.49
6	f	131	GLY	CA-C	-9.17	1.45	1.52
11	k	174	MET	SD-CE	-9.16	1.56	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	131	GLY	CA-C	-9.15	1.45	1.52
11	4	112	ASN	CG-ND2	-9.14	1.14	1.33
11	4	174	MET	SD-CE	-9.14	1.56	1.79
9	i	59	ASN	CB-CG	-9.13	1.29	1.52
9	2	59	ASN	CB-CG	-9.12	1.29	1.52
11	k	112	ASN	CG-ND2	-9.11	1.14	1.33
9	2	220	LEU	CB-CG	-9.11	1.35	1.53
5	E	32	LYS	CE-NZ	-9.08	1.22	1.49
8	1	153	GLU	CG-CD	-9.08	1.29	1.52
5	e	23	GLN	CD-NE2	-9.07	1.14	1.33
5	E	23	GLN	CD-NE2	-9.06	1.14	1.33
9	i	173	GLN	CD-NE2	-9.06	1.14	1.33
8	h	153	GLU	CG-CD	-9.06	1.29	1.52
9	i	58	LYS	CD-CE	-9.05	1.25	1.52
9	2	58	LYS	CD-CE	-9.05	1.25	1.52
5	e	32	LYS	CE-NZ	-9.04	1.22	1.49
9	2	173	GLN	CD-NE2	-9.04	1.14	1.33
12	5	148	ARG	CZ-NH2	-8.97	1.21	1.33
2	b	231	LYS	CD-CE	-8.96	1.25	1.52
2	B	231	LYS	CD-CE	-8.96	1.25	1.52
17	T	130	ASP	CG-OD2	-8.95	1.08	1.25
12	l	148	ARG	CZ-NH2	-8.95	1.21	1.33
10	3	169	GLN	CG-CD	-8.94	1.29	1.52
12	5	100	TRP	CZ2-CH2	-8.93	1.20	1.37
10	3	67	PHE	CG-CD2	-8.92	1.20	1.38
12	l	100	TRP	CZ2-CH2	-8.92	1.20	1.37
13	6	205	GLN	CG-CD	-8.91	1.29	1.52
10	j	67	PHE	CG-CD2	-8.91	1.20	1.38
5	e	225	GLN	CD-NE2	-8.89	1.14	1.33
9	i	98	TYR	CB-CG	-8.89	1.32	1.51
12	l	278	GLU	CB-CG	-8.89	1.25	1.52
5	E	225	GLN	CD-NE2	-8.89	1.14	1.33
9	2	98	TYR	CB-CG	-8.88	1.32	1.51
13	m	205	GLN	CG-CD	-8.88	1.29	1.52
12	5	278	GLU	CB-CG	-8.88	1.25	1.52
13	m	141	ARG	CG-CD	-8.87	1.25	1.52
10	j	193	ASP	CG-OD1	-8.84	1.08	1.25
9	i	177	LYS	CE-NZ	-8.84	1.22	1.49
13	6	141	ARG	CG-CD	-8.84	1.25	1.52
9	2	177	LYS	CE-NZ	-8.82	1.22	1.49
6	F	31	GLN	CD-NE2	-8.82	1.14	1.33
6	f	31	GLN	CD-NE2	-8.82	1.14	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	213	PHE	CG-CD1	-8.82	1.20	1.38
5	E	20	ARG	C-N	8.81	1.45	1.33
13	m	113	TYR	C-N	-8.81	1.22	1.33
3	c	213	PHE	CG-CD1	-8.80	1.20	1.38
10	3	193	ASP	CG-OD1	-8.80	1.08	1.25
9	i	65	ARG	NE-CZ	-8.79	1.23	1.33
11	k	111	LYS	CB-CG	-8.78	1.26	1.52
12	l	104	GLN	CD-OE1	-8.78	1.06	1.23
11	4	111	LYS	CB-CG	-8.77	1.26	1.52
11	k	170	LYS	CB-CG	-8.76	1.26	1.52
9	2	168	GLU	CG-CD	-8.76	1.30	1.52
11	4	170	LYS	CB-CG	-8.76	1.26	1.52
12	5	104	GLN	CD-OE1	-8.74	1.06	1.23
9	i	168	GLU	CG-CD	-8.74	1.30	1.52
10	j	77	LYS	CG-CD	-8.74	1.26	1.52
12	5	251	ASN	CG-OD1	-8.73	1.06	1.23
10	3	77	LYS	CG-CD	-8.73	1.26	1.52
9	2	65	ARG	NE-CZ	-8.72	1.23	1.33
11	4	5	LEU	C-N	8.71	1.45	1.32
12	5	270	GLU	CG-CD	-8.72	1.30	1.52
11	4	118	GLN	CD-NE2	-8.71	1.15	1.33
12	l	270	GLU	CG-CD	-8.70	1.30	1.52
12	l	148	ARG	CD-NE	-8.69	1.34	1.46
12	l	251	ASN	CG-OD1	-8.69	1.07	1.23
3	c	97	ASN	CG-ND2	-8.69	1.15	1.33
13	m	58	ILE	CG1-CD1	-8.69	1.17	1.51
11	k	118	GLN	CD-NE2	-8.69	1.15	1.33
13	6	58	ILE	CG1-CD1	-8.69	1.17	1.51
13	6	134	ASP	CB-CG	-8.68	1.30	1.52
7	g	100	LYS	CD-CE	-8.68	1.26	1.52
13	m	134	ASP	CB-CG	-8.67	1.30	1.52
12	5	148	ARG	CD-NE	-8.67	1.34	1.46
11	4	180	ILE	CB-CG2	-8.66	1.24	1.52
3	C	97	ASN	CG-ND2	-8.66	1.15	1.33
11	4	69	ILE	CG1-CD1	-8.65	1.18	1.51
7	G	100	LYS	CD-CE	-8.65	1.26	1.52
13	6	155	MET	CG-SD	-8.64	1.59	1.80
11	k	69	ILE	CG1-CD1	-8.64	1.18	1.51
11	k	180	ILE	CB-CG2	-8.64	1.24	1.52
5	e	177	GLU	CB-CG	-8.63	1.26	1.52
1	a	24	ARG	CG-CD	-8.62	1.26	1.52
20	Z	361	HIS	CG-CD2	-8.62	1.26	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	24	ARG	CG-CD	-8.62	1.26	1.52
13	m	155	MET	CG-SD	-8.61	1.59	1.80
5	E	177	GLU	CB-CG	-8.60	1.26	1.52
9	i	37	PHE	CE2-CZ	-8.60	1.12	1.38
9	2	37	PHE	CE2-CZ	-8.59	1.12	1.38
11	k	127	GLU	CD-OE1	-8.57	1.09	1.25
9	2	172	LYS	CE-NZ	-8.57	1.23	1.49
11	4	127	GLU	CD-OE1	-8.56	1.09	1.25
9	i	172	LYS	CE-NZ	-8.56	1.23	1.49
1	A	64	LEU	CG-CD1	-8.53	1.24	1.52
2	b	205	ASN	CG-ND2	-8.53	1.15	1.33
8	1	128	VAL	CB-CG1	-8.53	1.24	1.52
1	a	64	LEU	CG-CD1	-8.52	1.24	1.52
10	3	173	ASN	CG-ND2	-8.50	1.15	1.33
3	c	213	PHE	CE2-CZ	-8.50	1.13	1.38
3	C	213	PHE	CE2-CZ	-8.50	1.13	1.38
8	h	128	VAL	CB-CG1	-8.49	1.24	1.52
8	1	112	ASP	CB-CG	-8.49	1.30	1.52
12	5	128	GLN	CD-OE1	-8.49	1.07	1.23
12	l	128	GLN	CD-OE1	-8.48	1.07	1.23
13	6	70	ASP	CB-CG	-8.48	1.30	1.52
8	h	112	ASP	CB-CG	-8.48	1.30	1.52
2	B	205	ASN	CG-ND2	-8.46	1.15	1.33
5	e	7	GLU	CG-CD	-8.46	1.30	1.52
9	i	38	ASN	CG-ND2	-8.45	1.15	1.33
11	k	34	LYS	CG-CD	-8.45	1.27	1.52
13	m	70	ASP	CB-CG	-8.45	1.30	1.52
11	k	46	PHE	CE2-CZ	-8.44	1.13	1.38
7	g	57	LYS	CG-CD	-8.44	1.27	1.52
9	2	38	ASN	CG-ND2	-8.44	1.15	1.33
11	4	46	PHE	CE2-CZ	-8.43	1.13	1.38
7	g	209	GLU	CG-CD	-8.43	1.30	1.52
8	1	128	VAL	CB-CG2	-8.43	1.24	1.52
8	h	128	VAL	CB-CG2	-8.43	1.24	1.52
7	G	57	LYS	CG-CD	-8.43	1.27	1.52
11	4	34	LYS	CG-CD	-8.41	1.27	1.52
5	e	180	GLN	CD-OE1	-8.41	1.07	1.23
5	E	13	SER	CA-C	-8.40	1.45	1.53
2	b	30	GLN	CD-NE2	-8.39	1.15	1.33
2	B	30	GLN	CD-NE2	-8.39	1.15	1.33
7	g	202	LEU	CG-CD1	-8.39	1.24	1.52
5	E	180	GLN	CD-OE1	-8.39	1.07	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	g	33	ASN	CG-OD1	-8.38	1.07	1.23
11	4	113	LYS	CD-CE	-8.38	1.27	1.52
7	G	33	ASN	CG-OD1	-8.37	1.07	1.23
2	B	201	GLU	CD-OE1	-8.37	1.09	1.25
11	k	113	LYS	CD-CE	-8.37	1.27	1.52
12	l	99	ASN	CB-CG	-8.35	1.31	1.52
10	3	97	GLU	CG-CD	-8.35	1.31	1.52
10	3	74	TYR	CG-CD2	-8.35	1.21	1.39
10	j	74	TYR	CG-CD2	-8.35	1.21	1.39
12	5	99	ASN	CB-CG	-8.35	1.31	1.52
13	6	230	ASP	CA-C	-8.35	1.35	1.52
2	B	186	GLU	CG-CD	-8.34	1.31	1.52
11	k	69	ILE	CB-CG2	-8.34	1.25	1.52
5	E	229	LYS	CE-NZ	-8.34	1.24	1.49
2	b	201	GLU	CD-OE1	-8.34	1.09	1.25
10	j	205	ASP	CB-CG	-8.33	1.31	1.52
12	l	100	TRP	CD2-CE3	-8.33	1.26	1.40
10	3	205	ASP	CB-CG	-8.33	1.31	1.52
10	j	97	GLU	CG-CD	-8.32	1.31	1.52
11	4	69	ILE	CB-CG2	-8.32	1.25	1.52
5	e	229	LYS	CE-NZ	-8.32	1.24	1.49
10	3	173	ASN	CG-OD1	-8.32	1.07	1.23
2	b	186	GLU	CG-CD	-8.31	1.31	1.52
12	5	100	TRP	CD2-CE3	-8.31	1.26	1.40
13	m	230	ASP	CA-C	-8.31	1.35	1.52
12	5	84	GLN	CG-CD	-8.30	1.31	1.52
8	1	115	ASN	CG-OD1	-8.29	1.07	1.23
1	a	13	ASP	CB-CG	-8.28	1.31	1.52
9	2	82	GLU	CB-CG	-8.28	1.27	1.52
9	i	82	GLU	CB-CG	-8.27	1.27	1.52
3	c	70	ASN	CG-ND2	-8.27	1.15	1.33
1	A	13	ASP	CB-CG	-8.27	1.31	1.52
3	C	109	GLU	CG-CD	-8.27	1.31	1.52
12	l	84	GLN	CG-CD	-8.26	1.31	1.52
3	C	70	ASN	CG-ND2	-8.26	1.16	1.33
9	i	153	TYR	CA-CB	-8.26	1.40	1.53
12	5	148	ARG	CB-CG	-8.26	1.27	1.52
8	h	115	ASN	CG-OD1	-8.25	1.07	1.23
9	i	84	VAL	CB-CG2	-8.25	1.25	1.52
12	l	148	ARG	CB-CG	-8.25	1.27	1.52
12	l	267	ASP	CB-CG	-8.25	1.31	1.52
12	5	267	ASP	CB-CG	-8.25	1.31	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	2	84	VAL	CB-CG2	-8.24	1.25	1.52
3	c	109	GLU	CG-CD	-8.23	1.31	1.52
9	2	153	TYR	CA-CB	-8.23	1.40	1.53
12	5	104	GLN	CG-CD	-8.22	1.31	1.52
8	h	162	ASP	C-N	8.20	1.45	1.33
12	l	104	GLN	CG-CD	-8.20	1.31	1.52
11	k	166	GLN	CD-OE1	-8.20	1.07	1.23
10	3	159	GLU	CD-OE1	-8.19	1.09	1.25
11	4	166	GLN	CD-OE1	-8.19	1.07	1.23
11	k	71	GLU	CG-CD	-8.19	1.31	1.52
34	8	268	THR	C-N	8.17	1.45	1.33
11	4	71	GLU	CG-CD	-8.16	1.31	1.52
10	j	205	ASP	CG-OD1	-8.15	1.09	1.25
12	l	84	GLN	CB-CG	-8.15	1.28	1.52
5	E	20	ARG	CA-C	-8.15	1.42	1.52
11	4	49	GLU	CD-OE1	-8.15	1.09	1.25
13	6	50	LYS	CE-NZ	-8.15	1.25	1.49
12	l	287	GLY	C-O	-8.14	1.07	1.23
12	5	287	GLY	C-O	-8.14	1.07	1.23
8	h	152	ARG	CD-NE	-8.14	1.34	1.46
11	k	49	GLU	CD-OE1	-8.14	1.09	1.25
12	5	84	GLN	CB-CG	-8.14	1.28	1.52
3	C	97	ASN	CG-OD1	-8.14	1.08	1.23
3	c	97	ASN	CG-OD1	-8.13	1.08	1.23
8	1	203	GLU	CB-CG	-8.13	1.28	1.52
13	m	50	LYS	CE-NZ	-8.12	1.25	1.49
8	1	152	ARG	CD-NE	-8.12	1.34	1.46
10	3	205	ASP	CG-OD1	-8.12	1.09	1.25
9	2	211	LYS	CD-CE	-8.12	1.28	1.52
32	M	96	ASN	CG-ND2	-8.12	1.16	1.33
11	4	125	LYS	CB-CG	-8.11	1.28	1.52
11	k	125	LYS	CB-CG	-8.11	1.28	1.52
13	6	177	LYS	CG-CD	-8.11	1.28	1.52
9	i	211	LYS	CD-CE	-8.10	1.28	1.52
6	F	181	LYS	CE-NZ	-8.09	1.25	1.49
6	f	181	LYS	CE-NZ	-8.08	1.25	1.49
13	m	177	LYS	CG-CD	-8.08	1.28	1.52
12	5	82	ARG	C-N	8.08	1.44	1.33
12	5	253	TYR	CG-CD2	-8.08	1.22	1.39
12	l	198	LYS	CB-CG	-8.08	1.28	1.52
2	B	205	ASN	CG-OD1	-8.08	1.08	1.23
12	l	253	TYR	CG-CD2	-8.07	1.22	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	h	69	GLN	CG-CD	-8.07	1.31	1.52
12	5	198	LYS	CB-CG	-8.06	1.28	1.52
2	b	205	ASN	CG-OD1	-8.06	1.08	1.23
10	j	40	PHE	CG-CD1	-8.06	1.22	1.38
8	1	48	ASP	C-N	-8.06	1.21	1.34
10	3	40	PHE	CG-CD1	-8.06	1.22	1.38
8	1	69	GLN	CG-CD	-8.05	1.31	1.52
13	m	181	LYS	CD-CE	-8.04	1.28	1.52
13	m	187	GLU	CG-CD	-8.04	1.31	1.52
13	6	181	LYS	CD-CE	-8.04	1.28	1.52
9	2	227	GLU	CG-CD	-8.04	1.31	1.52
5	E	90	GLU	CG-CD	-8.03	1.31	1.52
13	6	187	GLU	CG-CD	-8.03	1.31	1.52
5	e	90	GLU	CG-CD	-8.00	1.32	1.52
10	j	113	ASN	CG-OD1	-8.00	1.08	1.23
13	6	168	TYR	CE1-CZ	-7.98	1.19	1.38
11	k	163	LEU	CG-CD2	-7.98	1.26	1.52
10	3	113	ASN	CG-OD1	-7.96	1.08	1.23
9	2	92	ILE	CG1-CD1	-7.96	1.20	1.51
13	m	168	TYR	CE1-CZ	-7.96	1.19	1.38
9	i	92	ILE	CG1-CD1	-7.95	1.20	1.51
11	4	163	LEU	CG-CD2	-7.95	1.26	1.52
5	E	159	GLU	CD-OE1	-7.95	1.10	1.25
5	e	159	GLU	CD-OE1	-7.94	1.10	1.25
8	h	113	ASP	CG-OD2	-7.94	1.10	1.25
7	g	175	GLU	CB-CG	-7.94	1.28	1.52
9	2	173	GLN	CB-CG	-7.93	1.28	1.52
9	i	173	GLN	CB-CG	-7.93	1.28	1.52
8	1	113	ASP	CG-OD2	-7.92	1.10	1.25
9	i	101	ARG	CG-CD	-7.91	1.28	1.52
9	2	101	ARG	CG-CD	-7.91	1.28	1.52
13	m	124	GLU	CD-OE1	-7.91	1.10	1.25
8	1	149	LYS	CE-NZ	-7.91	1.25	1.49
9	2	182	LYS	CE-NZ	-7.90	1.25	1.49
1	A	250	GLU	CD-OE2	-7.90	1.10	1.25
12	5	164	GLN	CG-CD	-7.90	1.32	1.52
8	1	101	ASN	CB-CG	-7.90	1.32	1.52
1	A	81	MET	CA-C	-7.90	1.43	1.52
8	h	101	ASN	CB-CG	-7.89	1.32	1.52
8	h	154	ASN	CG-ND2	-7.89	1.16	1.33
13	6	124	GLU	CD-OE1	-7.89	1.10	1.25
8	h	149	LYS	CE-NZ	-7.88	1.25	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	l	164	GLN	CG-CD	-7.88	1.32	1.52
3	c	3	SER	C-N	7.87	1.46	1.33
1	a	250	GLU	CD-OE2	-7.87	1.10	1.25
9	i	182	LYS	CE-NZ	-7.87	1.25	1.49
3	C	3	SER	C-N	7.86	1.46	1.33
12	5	251	ASN	CG-ND2	-7.86	1.16	1.33
12	l	100	TRP	CE2-CZ2	-7.86	1.23	1.39
12	l	162	VAL	CB-CG1	-7.85	1.26	1.52
8	1	154	ASN	CG-ND2	-7.85	1.16	1.33
12	5	162	VAL	CB-CG1	-7.85	1.26	1.52
1	A	135	ARG	CZ-NH1	-7.84	1.21	1.32
10	3	28	ARG	CZ-NH1	-7.84	1.21	1.32
5	e	10	ARG	CD-NE	-7.84	1.35	1.46
9	2	249	ILE	CA-C	-7.83	1.42	1.52
7	g	209	GLU	CD-OE1	-7.83	1.10	1.25
12	l	251	ASN	CG-ND2	-7.83	1.16	1.33
13	6	90	LYS	CA-C	-7.82	1.43	1.52
11	k	174	MET	CB-CG	-7.82	1.28	1.52
10	j	28	ARG	CZ-NH1	-7.82	1.21	1.32
12	l	257	GLU	CG-CD	-7.82	1.32	1.52
10	3	155	GLU	CB-CG	-7.81	1.29	1.52
12	5	100	TRP	CE2-CZ2	-7.81	1.23	1.39
12	l	241	HIS	CE1-NE2	-7.80	1.24	1.32
9	2	97	LEU	CG-CD1	-7.80	1.26	1.52
11	4	174	MET	CB-CG	-7.80	1.29	1.52
12	5	241	HIS	CE1-NE2	-7.80	1.24	1.32
9	i	97	LEU	CG-CD1	-7.79	1.26	1.52
12	5	257	GLU	CG-CD	-7.79	1.32	1.52
13	6	108	LYS	CA-C	7.79	1.62	1.52
10	3	205	ASP	C-OXT	-7.79	1.07	1.23
7	G	182	HIS	C-N	7.77	1.39	1.33
12	l	147	GLU	CB-CG	-7.77	1.29	1.52
8	h	154	ASN	CG-OD1	-7.77	1.08	1.23
12	5	147	GLU	CB-CG	-7.77	1.29	1.52
1	a	135	ARG	CZ-NH1	-7.76	1.21	1.32
10	j	115	LYS	CB-CG	-7.76	1.29	1.52
10	3	115	LYS	CB-CG	-7.75	1.29	1.52
13	6	201	GLU	CD-OE1	-7.75	1.10	1.25
10	j	205	ASP	C-OXT	-7.75	1.08	1.23
8	h	115	ASN	CG-ND2	-7.75	1.17	1.33
8	1	154	ASN	CG-OD1	-7.74	1.08	1.23
13	m	11	ASN	CG-ND2	-7.74	1.17	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	5	141	HIS	CE1-NE2	-7.73	1.24	1.32
13	m	125	ASP	CG-OD1	-7.73	1.10	1.25
13	6	109	ARG	CA-C	-7.72	1.42	1.52
13	6	11	ASN	CG-ND2	-7.72	1.17	1.33
10	3	41	GLU	CB-CG	-7.72	1.29	1.52
8	1	115	ASN	CG-ND2	-7.71	1.17	1.33
10	j	41	GLU	CB-CG	-7.71	1.29	1.52
8	h	71	HIS	CE1-NE2	-7.71	1.24	1.32
13	m	201	GLU	CD-OE1	-7.70	1.10	1.25
13	6	125	ASP	CG-OD1	-7.70	1.10	1.25
13	6	230	ASP	C-O	-7.70	1.08	1.23
5	e	104	ASP	CG-OD2	-7.68	1.10	1.25
5	e	58	LEU	C-N	7.68	1.43	1.33
9	i	93	GLU	CG-CD	-7.68	1.32	1.52
13	m	230	ASP	C-O	-7.68	1.08	1.23
2	b	2	THR	C-O	-7.68	1.08	1.23
13	m	175	LYS	CB-CG	-7.67	1.29	1.52
13	6	175	LYS	CB-CG	-7.67	1.29	1.52
2	B	2	THR	C-O	-7.67	1.08	1.23
12	l	141	HIS	CE1-NE2	-7.66	1.24	1.32
10	j	80	ARG	CD-NE	-7.65	1.35	1.46
5	E	104	ASP	CG-OD2	-7.65	1.10	1.25
13	m	95	ASN	CB-CG	-7.64	1.32	1.52
3	c	70	ASN	CG-OD1	-7.64	1.09	1.23
8	1	71	HIS	CE1-NE2	-7.64	1.25	1.32
10	3	80	ARG	CD-NE	-7.63	1.35	1.46
9	2	93	GLU	CG-CD	-7.63	1.32	1.52
3	C	70	ASN	CG-OD1	-7.62	1.09	1.23
9	i	153	TYR	CZ-OH	-7.62	1.22	1.38
11	4	135	TYR	CD1-CE1	-7.61	1.15	1.38
9	2	153	TYR	CZ-OH	-7.61	1.22	1.38
11	k	135	TYR	CD1-CE1	-7.60	1.15	1.38
10	j	113	ASN	CG-ND2	-7.60	1.17	1.33
10	3	113	ASN	CG-ND2	-7.60	1.17	1.33
5	e	7	GLU	CD-OE2	-7.59	1.10	1.25
10	3	159	GLU	CD-OE2	-7.59	1.10	1.25
13	m	40	ASP	CG-OD1	-7.57	1.10	1.25
2	B	244	ASN	CB-CG	-7.56	1.33	1.52
9	i	120	GLN	CG-CD	-7.55	1.33	1.52
9	2	120	GLN	CG-CD	-7.55	1.33	1.52
7	G	104	LYS	CE-NZ	-7.54	1.26	1.49
8	1	69	GLN	CD-NE2	-7.54	1.17	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	b	244	ASN	CB-CG	-7.54	1.33	1.52
13	6	40	ASP	CG-OD1	-7.54	1.11	1.25
13	m	63	ASN	CG-OD1	-7.54	1.09	1.23
13	6	30	VAL	CB-CG1	-7.54	1.27	1.52
11	k	118	GLN	CD-OE1	-7.54	1.09	1.23
13	6	63	ASN	CG-OD1	-7.53	1.09	1.23
11	4	118	GLN	CD-OE1	-7.53	1.09	1.23
13	m	30	VAL	CB-CG1	-7.52	1.27	1.52
7	g	104	LYS	CE-NZ	-7.52	1.26	1.49
8	h	69	GLN	CD-NE2	-7.52	1.17	1.33
11	4	93	ARG	CB-CG	-7.52	1.29	1.52
11	k	109	LYS	CD-CE	-7.51	1.29	1.52
8	h	101	ASN	CG-OD1	-7.50	1.09	1.23
12	5	110	ILE	CG1-CD1	-7.49	1.22	1.51
12	5	100	TRP	CB-CG	-7.49	1.27	1.50
9	i	37	PHE	CG-CD1	-7.49	1.23	1.38
12	l	110	ILE	CG1-CD1	-7.49	1.22	1.51
8	1	101	ASN	CG-OD1	-7.49	1.09	1.23
9	2	254	GLU	CA-CB	-7.49	1.41	1.53
11	4	109	LYS	CD-CE	-7.48	1.30	1.52
11	k	93	ARG	CB-CG	-7.48	1.30	1.52
12	l	100	TRP	CB-CG	-7.48	1.27	1.50
12	5	195	THR	CB-CG2	-7.48	1.27	1.52
12	l	107	LYS	CE-NZ	-7.48	1.26	1.49
13	m	211	GLU	CG-CD	-7.48	1.33	1.52
12	5	107	LYS	CE-NZ	-7.47	1.26	1.49
3	C	165	VAL	CB-CG1	-7.47	1.27	1.52
3	c	165	VAL	CB-CG1	-7.47	1.27	1.52
12	l	195	THR	CB-CG2	-7.47	1.27	1.52
9	i	98	TYR	CD1-CE1	-7.47	1.16	1.38
9	2	37	PHE	CG-CD1	-7.45	1.23	1.38
9	i	156	LEU	CG-CD1	-7.45	1.27	1.52
13	6	211	GLU	CG-CD	-7.44	1.33	1.52
1	A	217	GLU	CD-OE1	-7.44	1.11	1.25
9	2	156	LEU	CG-CD1	-7.44	1.28	1.52
12	l	162	VAL	CB-CG2	-7.43	1.28	1.52
9	2	98	TYR	CD1-CE1	-7.43	1.16	1.38
12	5	162	VAL	CB-CG2	-7.43	1.28	1.52
12	5	128	GLN	CG-CD	-7.43	1.33	1.52
1	a	217	GLU	CD-OE1	-7.43	1.11	1.25
11	4	112	ASN	CG-OD1	-7.43	1.09	1.23
10	3	65	GLU	CB-CG	-7.42	1.30	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	k	112	ASN	CG-OD1	-7.42	1.09	1.23
12	l	222	ASP	CB-CG	-7.42	1.33	1.52
9	2	109	LEU	CG-CD2	-7.42	1.28	1.52
12	l	128	GLN	CG-CD	-7.42	1.33	1.52
3	C	65	LYS	CE-NZ	-7.42	1.27	1.49
9	i	109	LEU	CG-CD2	-7.41	1.28	1.52
10	j	65	GLU	CB-CG	-7.41	1.30	1.52
3	c	65	LYS	CE-NZ	-7.40	1.27	1.49
12	l	138	CYS	CB-SG	-7.39	1.56	1.81
11	k	180	ILE	CB-CG1	-7.38	1.38	1.53
11	4	180	ILE	CB-CG1	-7.38	1.38	1.53
12	5	222	ASP	CB-CG	-7.37	1.33	1.52
12	5	138	CYS	CB-SG	-7.37	1.56	1.81
11	k	63	ASN	CG-OD1	-7.37	1.09	1.23
1	A	13	ASP	CG-OD1	-7.35	1.11	1.25
9	i	173	GLN	CD-OE1	-7.34	1.09	1.23
1	a	13	ASP	CG-OD1	-7.34	1.11	1.25
9	i	182	LYS	CB-CG	-7.33	1.30	1.52
10	3	202	MET	CB-CG	-7.33	1.30	1.52
10	j	202	MET	CB-CG	-7.32	1.30	1.52
9	2	182	LYS	CB-CG	-7.32	1.30	1.52
9	i	113	LYS	CD-CE	-7.31	1.30	1.52
9	2	113	LYS	CD-CE	-7.31	1.30	1.52
7	g	57	LYS	CE-NZ	-7.31	1.27	1.49
9	2	173	GLN	CD-OE1	-7.31	1.09	1.23
12	l	161	LEU	CB-CG	-7.30	1.38	1.53
13	m	90	LYS	CG-CD	-7.30	1.30	1.52
6	F	100	ASN	CG-ND2	-7.30	1.18	1.33
12	5	161	LEU	CB-CG	-7.30	1.38	1.53
13	m	30	VAL	CB-CG2	-7.30	1.28	1.52
13	m	88	ASN	CG-OD1	-7.30	1.09	1.23
2	B	78	MET	SD-CE	-7.29	1.61	1.79
2	b	78	MET	SD-CE	-7.29	1.61	1.79
3	c	199	LYS	CG-CD	-7.29	1.30	1.52
11	4	63	ASN	CG-OD1	-7.29	1.09	1.23
7	G	57	LYS	CE-NZ	-7.29	1.27	1.49
7	G	181	ASP	N-CA	-7.28	1.36	1.46
9	2	138	HIS	CE1-NE2	-7.28	1.25	1.32
13	6	30	VAL	CB-CG2	-7.28	1.28	1.52
9	i	138	HIS	CE1-NE2	-7.28	1.25	1.32
8	1	194	ARG	CD-NE	-7.27	1.36	1.46
6	f	100	ASN	CG-ND2	-7.27	1.18	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	3	166	THR	CB-CG2	-7.26	1.28	1.52
3	C	199	LYS	CG-CD	-7.25	1.30	1.52
13	6	127	LYS	CE-NZ	-7.25	1.27	1.49
7	g	225	ASN	CG-ND2	-7.24	1.18	1.33
9	i	223	ASN	C-N	7.23	1.40	1.33
12	5	203	CYS	CB-SG	-7.22	1.57	1.81
13	6	194	ASP	CB-CG	-7.20	1.34	1.52
13	m	127	LYS	CE-NZ	-7.20	1.27	1.49
11	k	186	LYS	CE-NZ	-7.20	1.27	1.49
11	4	186	LYS	CE-NZ	-7.20	1.27	1.49
12	l	203	CYS	CB-SG	-7.19	1.57	1.81
13	6	98	ALA	CA-C	-7.19	1.43	1.52
11	4	110	LYS	CB-CG	-7.19	1.30	1.52
11	k	110	LYS	CB-CG	-7.18	1.30	1.52
13	m	194	ASP	CB-CG	-7.18	1.34	1.52
5	E	205	LYS	CE-NZ	-7.18	1.27	1.49
5	e	205	LYS	CE-NZ	-7.17	1.27	1.49
8	h	165	LYS	CD-CE	-7.17	1.30	1.52
12	5	215	LEU	CG-CD1	-7.17	1.28	1.52
13	6	177	LYS	CE-NZ	-7.17	1.27	1.49
11	k	166	GLN	CB-CG	-7.16	1.30	1.52
13	m	177	LYS	CE-NZ	-7.16	1.27	1.49
11	4	166	GLN	CB-CG	-7.16	1.30	1.52
12	l	215	LEU	CG-CD1	-7.16	1.28	1.52
10	3	182	GLY	C-N	-7.15	1.23	1.33
13	m	168	TYR	CG-CD2	-7.15	1.24	1.39
8	1	165	LYS	CD-CE	-7.14	1.31	1.52
10	j	3	ASP	C-N	-7.13	1.27	1.34
10	3	3	ASP	C-N	-7.13	1.27	1.34
13	6	144	CYS	CB-SG	-7.12	1.57	1.81
13	6	168	TYR	CG-CD2	-7.12	1.24	1.39
13	6	86	ASP	C-N	7.12	1.44	1.33
10	3	161	GLU	CD-OE2	-7.11	1.11	1.25
9	i	51	GLN	CD-OE1	-7.10	1.10	1.23
13	m	144	CYS	CB-SG	-7.10	1.57	1.81
9	2	51	GLN	CD-OE1	-7.10	1.10	1.23
13	m	203	HIS	CE1-NE2	-7.09	1.25	1.32
13	m	118	ILE	CB-CG2	-7.09	1.29	1.52
6	F	93	ASN	CG-ND2	-7.09	1.18	1.33
13	m	86	ASP	CG-OD1	-7.08	1.11	1.25
10	3	115	LYS	CE-NZ	-7.07	1.28	1.49
6	f	93	ASN	CG-ND2	-7.07	1.18	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	5	146	LYS	C-N	-7.07	1.24	1.33
12	l	146	LYS	C-N	-7.07	1.24	1.33
10	j	115	LYS	CE-NZ	-7.05	1.28	1.49
10	j	63	LEU	CG-CD1	-7.05	1.29	1.52
10	3	6	SER	C-N	-7.05	1.24	1.33
11	4	10	GLN	CB-CG	-7.05	1.31	1.52
10	3	63	LEU	CG-CD1	-7.04	1.29	1.52
5	e	7	GLU	CA-CB	-7.04	1.39	1.53
13	m	15	ASP	CG-OD1	-7.04	1.11	1.25
11	k	10	GLN	CB-CG	-7.03	1.31	1.52
13	6	15	ASP	CG-OD1	-7.03	1.11	1.25
12	l	100	TRP	CG-CD2	-7.03	1.31	1.43
9	i	209	ILE	CB-CG2	-7.02	1.29	1.52
3	C	124	GLN	CD-OE1	-7.01	1.10	1.23
12	5	100	TRP	CG-CD2	-7.01	1.31	1.43
34	8	183	VAL	N-CA	-7.01	1.37	1.46
12	l	144	ARG	CZ-NH2	-7.01	1.24	1.33
9	2	209	ILE	CB-CG2	-7.01	1.29	1.52
11	k	7	ILE	CB-CG2	-7.00	1.29	1.52
10	3	126	LEU	C-N	-7.00	1.25	1.34
9	2	66	ILE	CG1-CD1	-7.00	1.24	1.51
3	c	124	GLN	CD-OE1	-7.00	1.10	1.23
8	1	99	LYS	CE-NZ	-7.00	1.28	1.49
8	h	178	SER	CB-OG	-6.99	1.28	1.42
11	4	7	ILE	CB-CG2	-6.99	1.29	1.52
8	h	99	LYS	CE-NZ	-6.99	1.28	1.49
10	j	197	LYS	CD-CE	-6.99	1.31	1.52
9	i	66	ILE	CG1-CD1	-6.99	1.24	1.51
8	1	178	SER	CB-OG	-6.99	1.28	1.42
13	m	118	ILE	CB-CG1	-6.98	1.39	1.53
13	6	100	ASN	C-N	-6.98	1.42	1.33
10	j	6	SER	C-N	-6.98	1.24	1.33
13	m	143	GLN	CB-CG	-6.98	1.31	1.52
8	1	113	ASP	CB-CG	-6.97	1.34	1.52
10	3	197	LYS	CD-CE	-6.97	1.31	1.52
13	6	203	HIS	CE1-NE2	-6.97	1.25	1.32
12	5	144	ARG	CZ-NH2	-6.96	1.24	1.33
8	h	113	ASP	CB-CG	-6.96	1.34	1.52
9	2	254	GLU	N-CA	-6.95	1.36	1.45
32	M	261	LYS	CG-CD	-6.95	1.31	1.52
13	6	143	GLN	CB-CG	-6.95	1.31	1.52
7	g	245	LYS	CE-NZ	-6.94	1.28	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	1	162	ASP	C-N	-6.93	1.24	1.33
3	c	241	LYS	CE-NZ	-6.92	1.28	1.49
3	c	195	LYS	CG-CD	-6.91	1.31	1.52
3	C	195	LYS	CG-CD	-6.91	1.31	1.52
3	C	241	LYS	CE-NZ	-6.90	1.28	1.49
8	h	17	PHE	CA-C	-6.90	1.44	1.53
11	k	166	GLN	CD-NE2	-6.87	1.18	1.33
11	4	166	GLN	CD-NE2	-6.85	1.18	1.33
9	i	106	VAL	CB-CG1	-6.85	1.29	1.52
5	E	186	GLU	CD-OE1	-6.85	1.12	1.25
11	k	69	ILE	CB-CG1	-6.85	1.39	1.53
5	e	186	GLU	CD-OE1	-6.84	1.12	1.25
9	2	106	VAL	CB-CG1	-6.83	1.29	1.52
11	4	69	ILE	CB-CG1	-6.83	1.39	1.53
5	E	104	ASP	CB-CG	-6.83	1.34	1.52
12	l	144	ARG	CD-NE	-6.82	1.36	1.46
7	g	41	LYS	CE-NZ	-6.81	1.28	1.49
3	c	16	GLU	CD-OE1	-6.81	1.12	1.25
5	e	104	ASP	CB-CG	-6.81	1.35	1.52
3	C	16	GLU	CD-OE1	-6.81	1.12	1.25
6	F	31	GLN	CD-OE1	-6.80	1.10	1.23
1	a	251	GLN	C-O	-6.80	1.09	1.23
7	G	41	LYS	CE-NZ	-6.79	1.28	1.49
9	i	188	ILE	CG1-CD1	-6.79	1.25	1.51
9	2	188	ILE	CG1-CD1	-6.79	1.25	1.51
13	m	112	PRO	N-CA	6.79	1.55	1.47
2	B	242	GLU	CD-OE1	-6.79	1.12	1.25
11	k	145	ASP	CB-CG	-6.79	1.35	1.52
1	A	251	GLN	C-O	-6.79	1.09	1.23
11	4	191	GLN	CB-CG	-6.78	1.32	1.52
11	k	90	LYS	CE-NZ	-6.78	1.29	1.49
11	4	72	ASP	CB-CG	-6.78	1.35	1.52
11	4	90	LYS	CE-NZ	-6.78	1.29	1.49
11	k	191	GLN	CB-CG	-6.77	1.32	1.52
11	k	72	ASP	CB-CG	-6.77	1.35	1.52
12	5	144	ARG	CD-NE	-6.77	1.36	1.46
12	l	192	SER	CB-OG	-6.77	1.28	1.42
3	C	224	GLU	CD-OE2	-6.77	1.12	1.25
6	f	31	GLN	CD-OE1	-6.76	1.10	1.23
11	4	145	ASP	CB-CG	-6.75	1.35	1.52
12	5	192	SER	CB-OG	-6.75	1.28	1.42
13	m	81	LYS	CD-CE	-6.75	1.32	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	b	242	GLU	CD-OE1	-6.75	1.12	1.25
3	c	224	GLU	CD-OE2	-6.74	1.12	1.25
12	5	241	HIS	CG-CD2	-6.74	1.28	1.35
2	B	49	LYS	CE-NZ	-6.74	1.29	1.49
2	b	49	LYS	CE-NZ	-6.74	1.29	1.49
13	m	167	GLN	CG-CD	-6.73	1.35	1.52
1	A	221	ASN	CG-ND2	-6.73	1.19	1.33
8	1	163	PHE	C-N	-6.73	1.25	1.33
13	6	167	GLN	CG-CD	-6.72	1.35	1.52
1	a	221	ASN	CG-ND2	-6.72	1.19	1.33
11	k	177	LYS	CG-CD	-6.70	1.32	1.52
11	4	177	LYS	CG-CD	-6.70	1.32	1.52
11	4	147	HIS	CE1-NE2	-6.69	1.25	1.32
1	a	37	GLN	CD-NE2	-6.69	1.19	1.33
12	l	241	HIS	CG-CD2	-6.69	1.28	1.35
11	k	186	LYS	CB-CG	-6.69	1.32	1.52
11	4	186	LYS	CB-CG	-6.68	1.32	1.52
1	A	37	GLN	CD-NE2	-6.68	1.19	1.33
9	2	249	ILE	CG1-CD1	-6.67	1.25	1.51
8	h	118	GLU	CG-CD	-6.66	1.35	1.52
7	G	202	LEU	C-N	6.66	1.43	1.33
8	1	118	GLU	CG-CD	-6.66	1.35	1.52
9	i	195	ASP	CG-OD1	-6.65	1.12	1.25
11	4	74	GLU	CB-CG	-6.65	1.32	1.52
11	k	147	HIS	CE1-NE2	-6.64	1.25	1.32
9	2	195	ASP	CG-OD1	-6.63	1.12	1.25
10	3	138	VAL	CA-C	-6.63	1.44	1.52
11	k	74	GLU	CB-CG	-6.63	1.32	1.52
10	3	127	ILE	CA-CB	-6.63	1.46	1.54
7	g	209	GLU	CD-OE2	-6.62	1.12	1.25
11	4	192	VAL	CB-CG1	-6.62	1.30	1.52
8	h	73	GLU	CG-CD	-6.62	1.35	1.52
10	j	78	GLU	CG-CD	-6.62	1.35	1.52
10	3	78	GLU	CG-CD	-6.62	1.35	1.52
11	k	192	VAL	CB-CG1	-6.62	1.30	1.52
13	6	104	LEU	C-N	6.61	1.41	1.33
8	1	129	HIS	CE1-NE2	-6.61	1.25	1.32
1	A	250	GLU	CG-CD	-6.60	1.35	1.52
12	l	226	GLU	CG-CD	-6.60	1.35	1.52
10	3	128	GLY	C-O	-6.60	1.15	1.23
5	e	15	PHE	CA-C	-6.60	1.44	1.52
8	1	73	GLU	CG-CD	-6.59	1.35	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	250	GLU	CG-CD	-6.59	1.35	1.52
9	i	241	VAL	CA-C	-6.59	1.44	1.52
13	6	87	HIS	CG-ND1	6.59	1.45	1.38
11	4	29	LYS	CB-CG	-6.59	1.32	1.52
11	k	29	LYS	CB-CG	-6.59	1.32	1.52
8	1	205	LEU	N-CA	6.58	1.58	1.46
13	6	95	ASN	CA-C	-6.58	1.44	1.52
9	i	208	GLU	CD-OE1	-6.58	1.12	1.25
9	2	208	GLU	CG-CD	-6.58	1.35	1.52
9	2	230	LYS	CB-CG	-6.58	1.32	1.52
9	i	98	TYR	CD2-CE2	-6.57	1.19	1.38
10	3	131	ASP	CG-OD1	-6.57	1.12	1.25
11	k	7	ILE	CB-CG1	-6.57	1.40	1.53
9	2	208	GLU	CD-OE1	-6.56	1.12	1.25
12	l	215	LEU	CG-CD2	-6.56	1.30	1.52
12	5	226	GLU	CG-CD	-6.56	1.35	1.52
8	h	129	HIS	CE1-NE2	-6.56	1.25	1.32
9	2	98	TYR	CD2-CE2	-6.56	1.19	1.38
12	l	83	PHE	CA-CB	6.55	1.60	1.54
12	5	215	LEU	CG-CD2	-6.55	1.30	1.52
13	6	57	ASN	CG-OD1	-6.55	1.11	1.23
13	6	228	LYS	CB-CG	-6.55	1.32	1.52
13	m	57	ASN	CG-OD1	-6.55	1.11	1.23
11	4	7	ILE	CB-CG1	-6.55	1.40	1.53
13	6	142	GLU	CD-OE1	-6.55	1.12	1.25
13	m	228	LYS	CB-CG	-6.55	1.32	1.52
12	5	258	ASP	CG-OD1	-6.55	1.12	1.25
10	3	161	GLU	CD-OE1	-6.54	1.12	1.25
8	h	183	ARG	CZ-NH1	-6.53	1.23	1.32
11	k	171	ARG	CZ-NH1	-6.53	1.23	1.32
3	C	202	ASP	CG-OD2	-6.53	1.12	1.25
9	i	208	GLU	CG-CD	-6.53	1.35	1.52
12	l	258	ASP	CG-OD1	-6.53	1.12	1.25
3	c	202	ASP	CG-OD2	-6.53	1.12	1.25
11	k	10	GLN	CD-NE2	-6.53	1.19	1.33
29	I	139	GLU	CB-CG	-6.53	1.32	1.52
8	1	52	CYS	CB-SG	-6.53	1.59	1.81
11	k	171	ARG	CD-NE	-6.52	1.37	1.46
10	3	193	ASP	CB-CG	-6.52	1.35	1.52
13	m	142	GLU	CD-OE1	-6.52	1.12	1.25
13	6	145	ARG	CG-CD	-6.51	1.32	1.52
10	j	193	ASP	CB-CG	-6.51	1.35	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	1	183	ARG	CZ-NH1	-6.51	1.23	1.32
8	h	52	CYS	CB-SG	-6.51	1.59	1.81
11	4	10	GLN	CD-NE2	-6.51	1.19	1.33
11	4	171	ARG	CZ-NH1	-6.50	1.23	1.32
13	m	145	ARG	CG-CD	-6.50	1.32	1.52
9	i	46	ASP	CG-OD2	-6.50	1.13	1.25
2	B	190	HIS	CE1-NE2	-6.50	1.26	1.32
9	2	209	ILE	CB-CG1	-6.50	1.40	1.53
10	j	198	ARG	CZ-NH1	-6.49	1.23	1.32
9	2	46	ASP	CG-OD2	-6.48	1.13	1.25
5	E	102	TYR	CG-CD2	-6.48	1.25	1.39
9	2	65	ARG	CB-CG	-6.48	1.33	1.52
13	m	56	ASP	CB-CG	-6.47	1.35	1.52
9	i	65	ARG	CB-CG	-6.47	1.33	1.52
2	b	234	ARG	CD-NE	-6.46	1.37	1.46
9	i	209	ILE	CB-CG1	-6.46	1.40	1.53
2	B	182	GLU	CD-OE2	-6.46	1.13	1.25
13	m	175	LYS	CD-CE	-6.46	1.33	1.52
1	a	239	GLU	CD-OE2	-6.45	1.13	1.25
5	e	102	TYR	CG-CD2	-6.45	1.25	1.39
9	i	114	GLN	CD-OE1	-6.45	1.11	1.23
12	5	214	VAL	CB-CG2	-6.45	1.31	1.52
13	6	175	LYS	CD-CE	-6.45	1.33	1.52
1	A	239	GLU	CD-OE2	-6.45	1.13	1.25
11	4	87	GLU	CD-OE1	-6.45	1.13	1.25
10	3	198	ARG	CZ-NH1	-6.44	1.23	1.32
2	B	234	ARG	CD-NE	-6.44	1.37	1.46
13	6	56	ASP	CB-CG	-6.44	1.35	1.52
5	E	224	LYS	CD-CE	-6.44	1.33	1.52
11	4	171	ARG	CD-NE	-6.44	1.37	1.46
1	A	222	ASP	CG-OD2	-6.44	1.13	1.25
2	b	182	GLU	CD-OE2	-6.43	1.13	1.25
11	k	87	GLU	CD-OE1	-6.43	1.13	1.25
12	l	214	VAL	CB-CG2	-6.43	1.31	1.52
5	E	225	GLN	CG-CD	-6.43	1.35	1.52
5	e	224	LYS	CD-CE	-6.42	1.33	1.52
5	e	225	GLN	CG-CD	-6.42	1.35	1.52
1	a	222	ASP	CG-OD2	-6.42	1.13	1.25
5	e	238	GLU	CB-CG	-6.41	1.33	1.52
12	l	217	SER	CB-OG	-6.41	1.29	1.42
12	5	217	SER	CB-OG	-6.41	1.29	1.42
9	i	178	GLU	CG-CD	-6.41	1.36	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	2	114	GLN	CD-OE1	-6.41	1.11	1.23
9	2	178	GLU	CG-CD	-6.39	1.36	1.52
2	b	190	HIS	CE1-NE2	-6.39	1.26	1.32
6	f	90	GLN	CD-NE2	-6.38	1.19	1.33
5	E	238	GLU	CB-CG	-6.37	1.33	1.52
8	h	114	LYS	CB-CG	-6.37	1.33	1.52
10	j	204	GLN	N-CA	-6.37	1.38	1.46
13	m	169	GLU	CD-OE1	-6.36	1.13	1.25
6	F	90	GLN	CD-NE2	-6.35	1.20	1.33
9	i	92	ILE	CB-CG1	-6.35	1.40	1.53
9	i	167	LEU	CB-CG	-6.35	1.40	1.53
8	1	114	LYS	CB-CG	-6.35	1.33	1.52
13	m	114	TYR	CE2-CZ	-6.34	1.23	1.38
7	G	185	GLU	N-CA	-6.34	1.41	1.47
9	2	254	GLU	CD-OE1	-6.34	1.13	1.25
10	3	18	LYS	CD-CE	-6.34	1.33	1.52
10	j	19	ASP	CG-OD1	-6.33	1.13	1.25
10	j	198	ARG	CZ-NH2	-6.33	1.25	1.33
10	3	204	GLN	N-CA	-6.33	1.38	1.46
8	h	112	ASP	CG-OD1	-6.32	1.13	1.25
10	j	18	LYS	CD-CE	-6.32	1.33	1.52
10	j	98	ARG	NE-CZ	-6.31	1.26	1.33
9	2	92	ILE	CB-CG1	-6.31	1.40	1.53
9	2	167	LEU	CB-CG	-6.31	1.40	1.53
5	e	104	ASP	CG-OD1	-6.31	1.13	1.25
13	6	169	GLU	CD-OE1	-6.31	1.13	1.25
5	E	104	ASP	CG-OD1	-6.30	1.13	1.25
8	1	112	ASP	CG-OD1	-6.30	1.13	1.25
9	i	168	GLU	CD-OE1	-6.29	1.13	1.25
10	3	19	ASP	CG-OD1	-6.29	1.13	1.25
10	3	98	ARG	NE-CZ	-6.29	1.26	1.33
12	5	100	TRP	NE1-CE2	-6.29	1.30	1.37
13	6	56	ASP	CG-OD1	-6.29	1.13	1.25
13	6	180	LEU	C-N	-6.29	1.24	1.33
5	E	86	ARG	CG-CD	-6.28	1.33	1.52
13	m	180	LEU	C-N	-6.28	1.24	1.33
8	1	100	ASP	CG-OD1	-6.28	1.13	1.25
5	e	86	ARG	CG-CD	-6.27	1.33	1.52
9	2	39	ASN	CG-OD1	-6.27	1.11	1.23
10	j	126	LEU	C-N	6.27	1.41	1.33
9	2	181	ILE	CB-CG1	-6.27	1.41	1.53
5	E	78	MET	SD-CE	-6.26	1.63	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	192	ASP	CG-OD1	-6.26	1.13	1.25
10	3	198	ARG	CZ-NH2	-6.26	1.25	1.33
13	m	15	ASP	CB-CG	-6.26	1.36	1.52
11	k	46	PHE	CG-CD1	-6.25	1.25	1.38
12	l	100	TRP	NE1-CE2	-6.25	1.30	1.37
13	m	56	ASP	CG-OD1	-6.25	1.13	1.25
13	m	72	LEU	CG-CD2	-6.25	1.31	1.52
9	i	39	ASN	CG-OD1	-6.25	1.11	1.23
9	i	181	ILE	CB-CG1	-6.25	1.41	1.53
13	6	72	LEU	CG-CD2	-6.25	1.31	1.52
5	e	78	MET	SD-CE	-6.25	1.64	1.79
9	i	86	GLN	CD-OE1	-6.25	1.11	1.23
9	2	86	GLN	CD-OE1	-6.24	1.11	1.23
8	h	100	ASP	CG-OD1	-6.24	1.13	1.25
11	4	46	PHE	CG-CD1	-6.24	1.25	1.38
9	2	168	GLU	CD-OE1	-6.24	1.13	1.25
11	4	92	ILE	CG1-CD1	-6.24	1.27	1.51
13	6	15	ASP	CB-CG	-6.24	1.36	1.52
8	h	114	LYS	CD-CE	-6.23	1.33	1.52
11	k	92	ILE	CG1-CD1	-6.23	1.27	1.51
2	b	4	ARG	CZ-NH2	-6.23	1.25	1.33
1	a	149	GLU	CD-OE1	-6.23	1.13	1.25
1	a	192	ASP	CG-OD1	-6.23	1.13	1.25
1	A	149	GLU	CD-OE1	-6.22	1.13	1.25
2	B	4	ARG	CZ-NH2	-6.22	1.25	1.33
10	3	172	LEU	CG-CD1	-6.22	1.32	1.52
8	1	114	LYS	CD-CE	-6.22	1.33	1.52
1	A	222	ASP	CG-OD1	-6.20	1.13	1.25
2	B	17	LYS	CB-CG	6.20	1.71	1.52
1	a	222	ASP	CG-OD1	-6.20	1.13	1.25
8	1	152	ARG	NE-CZ	-6.20	1.26	1.33
13	6	87	HIS	CE1-NE2	6.19	1.38	1.32
11	k	19	LYS	CE-NZ	-6.18	1.30	1.49
11	4	19	LYS	CE-NZ	-6.18	1.30	1.49
11	4	36	ARG	CG-CD	-6.18	1.33	1.52
11	k	36	ARG	CG-CD	-6.17	1.33	1.52
2	b	17	LYS	CB-CG	6.17	1.71	1.52
8	h	152	ARG	NE-CZ	-6.16	1.26	1.33
7	G	175	GLU	N-CA	-6.15	1.37	1.46
8	1	17	PHE	CA-CB	6.14	1.65	1.53
13	m	72	LEU	CG-CD1	-6.14	1.32	1.52
9	i	38	ASN	CG-OD1	-6.14	1.11	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	2	38	ASN	CG-OD1	-6.12	1.11	1.23
11	4	109	LYS	CG-CD	-6.12	1.34	1.52
13	6	72	LEU	CG-CD1	-6.12	1.32	1.52
6	F	143	HIS	CE1-NE2	-6.10	1.26	1.32
11	4	41	HIS	CE1-NE2	-6.10	1.26	1.32
12	5	191	ASP	CG-OD2	-6.09	1.13	1.25
8	1	45	ARG	CG-CD	-6.09	1.34	1.52
11	k	109	LYS	CG-CD	-6.09	1.34	1.52
12	5	169	GLY	C-N	-6.09	1.24	1.33
12	l	169	GLY	C-N	-6.09	1.24	1.33
11	4	98	TYR	CE2-CZ	-6.09	1.23	1.38
8	h	45	ARG	CG-CD	-6.08	1.34	1.52
8	1	29	THR	CB-CG2	-6.08	1.32	1.52
11	4	111	LYS	CD-CE	-6.08	1.34	1.52
12	l	191	ASP	CG-OD2	-6.08	1.13	1.25
9	2	177	LYS	CB-CG	-6.08	1.34	1.52
7	g	202	LEU	CG-CD2	-6.07	1.32	1.52
11	k	98	TYR	CE2-CZ	-6.07	1.23	1.38
11	k	41	HIS	CE1-NE2	-6.07	1.26	1.32
8	h	29	THR	CB-CG2	-6.07	1.32	1.52
10	j	53	ILE	CB-CG1	-6.06	1.41	1.53
8	1	98	ASN	CG-OD1	-6.06	1.12	1.23
1	A	185	HIS	CE1-NE2	-6.06	1.26	1.32
2	B	103	GLU	CD-OE1	-6.06	1.13	1.25
3	C	142	ASP	CG-OD2	-6.06	1.13	1.25
7	G	242	PHE	CA-CB	6.06	1.62	1.53
13	6	15	ASP	CG-OD2	-6.06	1.13	1.25
5	e	202	LYS	CE-NZ	-6.05	1.31	1.49
5	E	202	LYS	CE-NZ	-6.05	1.31	1.49
5	e	58	LEU	N-CA	-6.05	1.37	1.45
11	k	111	LYS	CD-CE	-6.05	1.34	1.52
9	2	224	VAL	CB-CG2	-6.05	1.32	1.52
3	c	142	ASP	CG-OD2	-6.04	1.13	1.25
9	i	177	LYS	CB-CG	-6.04	1.34	1.52
10	3	53	ILE	CB-CG1	-6.04	1.41	1.53
1	A	217	GLU	CB-CG	-6.04	1.34	1.52
8	h	98	ASN	CG-OD1	-6.04	1.12	1.23
2	b	220	ASP	CG-OD1	-6.04	1.13	1.25
2	b	103	GLU	CD-OE1	-6.03	1.13	1.25
3	c	222	ASP	CG-OD1	-6.03	1.13	1.25
2	B	220	ASP	CG-OD1	-6.03	1.13	1.25
31	L	273	HIS	ND1-CE1	6.03	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	i	228	LYS	CA-C	-6.03	1.45	1.53
11	k	143	LEU	CG-CD2	-6.03	1.32	1.52
3	C	222	ASP	CG-OD1	-6.03	1.14	1.25
11	4	143	LEU	CG-CD2	-6.02	1.32	1.52
1	a	217	GLU	CB-CG	-6.02	1.34	1.52
6	f	143	HIS	CE1-NE2	-6.02	1.26	1.32
11	k	11	ASP	CG-OD2	-6.02	1.14	1.25
13	m	15	ASP	CG-OD2	-6.02	1.14	1.25
2	B	217	GLU	CD-OE2	-6.02	1.14	1.25
2	b	248	GLU	CD-OE1	-6.01	1.14	1.25
13	m	94	ILE	CB-CG1	-6.01	1.41	1.53
8	1	130	LYS	CG-CD	-6.01	1.34	1.52
11	4	11	ASP	CG-OD2	-6.01	1.14	1.25
7	G	104	LYS	CD-CE	-6.00	1.34	1.52
8	h	130	LYS	CG-CD	-6.00	1.34	1.52
11	4	92	ILE	CB-CG2	-6.00	1.32	1.52
7	g	104	LYS	CD-CE	-5.99	1.34	1.52
2	B	248	GLU	CD-OE1	-5.99	1.14	1.25
3	c	142	ASP	CG-OD1	-5.98	1.14	1.25
3	C	142	ASP	CG-OD1	-5.98	1.14	1.25
2	B	228	PRO	C-N	-5.98	1.26	1.33
13	6	74	LYS	CE-NZ	-5.98	1.31	1.49
11	k	92	ILE	CB-CG2	-5.98	1.32	1.52
3	c	209	ASP	CG-OD2	-5.98	1.14	1.25
2	b	217	GLU	CD-OE2	-5.97	1.14	1.25
13	m	74	LYS	CE-NZ	-5.97	1.31	1.49
1	a	185	HIS	CE1-NE2	-5.96	1.26	1.32
3	C	209	ASP	CG-OD2	-5.96	1.14	1.25
3	C	222	ASP	CG-OD2	-5.96	1.14	1.25
13	m	114	TYR	CG-CD2	-5.96	1.26	1.39
1	A	184	ASN	CG-OD1	-5.95	1.12	1.23
10	j	83	GLU	CD-OE2	-5.95	1.14	1.25
10	3	77	LYS	CB-CG	-5.95	1.34	1.52
2	b	228	PRO	C-N	-5.95	1.26	1.33
3	c	222	ASP	CG-OD2	-5.95	1.14	1.25
8	h	155	MET	CB-CG	-5.95	1.34	1.52
1	a	184	ASN	CG-OD1	-5.94	1.12	1.23
10	3	83	GLU	CD-OE2	-5.94	1.14	1.25
5	e	118	ASP	CG-OD2	-5.94	1.14	1.25
5	e	18	GLU	C-N	5.94	1.42	1.33
1	A	112	MET	CG-SD	-5.93	1.66	1.80
11	k	41	HIS	CG-CD2	-5.93	1.29	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	1	155	MET	CB-CG	-5.93	1.34	1.52
10	j	77	LYS	CB-CG	-5.93	1.34	1.52
11	k	120	ASP	CB-CG	-5.93	1.37	1.52
3	c	7	ASP	CA-C	-5.93	1.45	1.52
10	j	205	ASP	CA-CB	-5.93	1.41	1.53
3	C	7	ASP	CA-C	-5.92	1.45	1.52
7	G	194	LYS	CA-C	5.92	1.60	1.52
9	2	51	GLN	CG-CD	-5.92	1.37	1.52
13	m	102	GLN	CD-NE2	-5.92	1.20	1.33
7	g	114	ASP	CG-OD1	-5.91	1.14	1.25
11	4	120	ASP	CB-CG	-5.91	1.37	1.52
13	m	122	LEU	CG-CD2	-5.91	1.33	1.52
5	E	118	ASP	CG-OD2	-5.91	1.14	1.25
10	3	205	ASP	CA-CB	-5.91	1.41	1.53
13	6	122	LEU	CG-CD2	-5.91	1.33	1.52
6	f	69	HIS	CE1-NE2	-5.90	1.26	1.32
1	a	112	MET	CG-SD	-5.89	1.66	1.80
7	G	114	ASP	CG-OD1	-5.89	1.14	1.25
9	2	254	GLU	CA-C	-5.89	1.45	1.53
9	i	51	GLN	CG-CD	-5.89	1.37	1.52
8	1	41	ASP	CG-OD2	-5.89	1.14	1.25
8	1	16	THR	C-N	-5.89	1.26	1.33
6	F	69	HIS	CE1-NE2	-5.88	1.26	1.32
12	5	278	GLU	CD-OE2	-5.88	1.14	1.25
32	M	261	LYS	CA-CB	-5.88	1.43	1.53
11	k	33	ASP	CB-CG	-5.88	1.37	1.52
8	h	41	ASP	CG-OD2	-5.87	1.14	1.25
12	l	183	GLU	CB-CG	-5.87	1.34	1.52
12	5	183	GLU	CB-CG	-5.87	1.34	1.52
3	c	114	ARG	CZ-NH1	-5.86	1.24	1.32
9	2	57	ASP	CG-OD2	-5.86	1.14	1.25
11	4	37	GLN	CB-CG	-5.86	1.34	1.52
10	3	131	ASP	CG-OD2	-5.86	1.14	1.25
11	4	33	ASP	CB-CG	-5.86	1.37	1.52
13	6	56	ASP	CG-OD2	-5.86	1.14	1.25
12	l	278	GLU	CD-OE2	-5.86	1.14	1.25
11	k	37	GLN	CB-CG	-5.85	1.34	1.52
9	i	233	LYS	CA-C	-5.85	1.45	1.52
10	j	15	MET	CB-CG	-5.85	1.34	1.52
10	3	63	LEU	CB-CG	-5.85	1.41	1.53
9	i	57	ASP	CG-OD2	-5.84	1.14	1.25
10	3	15	MET	CB-CG	-5.84	1.34	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	f	93	ASN	CG-OD1	-5.84	1.12	1.23
6	f	226	ASP	CB-CG	-5.84	1.37	1.52
7	G	57	LYS	CD-CE	-5.83	1.34	1.52
13	6	143	GLN	CD-NE2	-5.83	1.21	1.33
8	1	26	ASP	CG-OD2	-5.83	1.14	1.25
11	4	41	HIS	CG-CD2	-5.83	1.29	1.35
10	j	63	LEU	CB-CG	-5.83	1.41	1.53
12	l	277	GLU	CD-OE1	-5.82	1.14	1.25
5	E	213	ASP	CG-OD2	-5.82	1.14	1.25
6	F	93	ASN	CG-OD1	-5.82	1.12	1.23
2	b	49	LYS	CD-CE	-5.82	1.34	1.52
12	l	148	ARG	NE-CZ	-5.82	1.26	1.33
13	m	143	GLN	CD-NE2	-5.82	1.21	1.33
12	5	148	ARG	NE-CZ	-5.82	1.26	1.33
3	C	114	ARG	CZ-NH1	-5.81	1.24	1.32
8	1	61	THR	CB-CG2	-5.81	1.33	1.52
7	g	57	LYS	CD-CE	-5.81	1.35	1.52
8	h	61	THR	CB-CG2	-5.81	1.33	1.52
9	i	120	GLN	CD-NE2	-5.81	1.21	1.33
9	i	31	THR	CB-CG2	-5.81	1.33	1.52
13	m	205	GLN	CD-OE1	-5.81	1.12	1.23
13	6	205	GLN	CD-OE1	-5.80	1.12	1.23
10	3	165	GLU	CD-OE2	-5.80	1.14	1.25
12	5	277	GLU	CD-OE1	-5.80	1.14	1.25
8	h	26	ASP	CG-OD2	-5.79	1.14	1.25
13	m	56	ASP	CG-OD2	-5.79	1.14	1.25
13	m	116	HIS	CB-CG	-5.79	1.42	1.50
2	B	49	LYS	CD-CE	-5.79	1.35	1.52
9	2	31	THR	CB-CG2	-5.79	1.33	1.52
12	5	160	ASN	CG-OD1	-5.79	1.12	1.23
9	2	120	GLN	CD-NE2	-5.79	1.21	1.33
13	m	53	ASP	CG-OD1	-5.79	1.14	1.25
8	1	175	ASP	CG-OD2	-5.79	1.14	1.25
13	6	113	TYR	CA-CB	5.79	1.61	1.53
8	h	175	ASP	CG-OD2	-5.79	1.14	1.25
9	i	242	LEU	CA-CB	5.78	1.62	1.53
2	B	123	GLN	CB-CG	-5.78	1.35	1.52
13	6	53	ASP	CG-OD1	-5.78	1.14	1.25
7	g	173	LYS	CD-CE	-5.78	1.35	1.52
6	F	226	ASP	CB-CG	-5.78	1.37	1.52
7	G	222	SER	CA-C	5.78	1.60	1.52
10	3	6	SER	CB-OG	-5.78	1.30	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	4	195	PHE	CB-CG	-5.78	1.37	1.50
5	e	213	ASP	CG-OD2	-5.77	1.14	1.25
11	k	195	PHE	CB-CG	-5.77	1.37	1.50
13	6	182	TYR	CG-CD2	-5.77	1.27	1.39
9	i	92	ILE	CB-CG2	-5.76	1.33	1.52
2	b	123	GLN	CB-CG	-5.76	1.35	1.52
7	G	169	ARG	NE-CZ	5.76	1.39	1.33
5	E	16	SER	CA-C	5.76	1.60	1.52
10	j	6	SER	CB-OG	-5.75	1.30	1.42
1	A	22	GLU	CG-CD	-5.75	1.37	1.52
9	2	92	ILE	CB-CG2	-5.75	1.33	1.52
9	2	220	LEU	CG-CD1	-5.75	1.33	1.52
13	m	182	TYR	CG-CD2	-5.74	1.27	1.39
8	1	47	HIS	CE1-NE2	-5.74	1.26	1.32
5	e	233	ASN	CG-OD1	-5.74	1.12	1.23
34	8	201	GLN	CD-NE2	5.74	1.45	1.33
12	5	286	ILE	CB-CG1	-5.73	1.42	1.53
12	l	286	ILE	CB-CG1	-5.73	1.42	1.53
8	h	47	HIS	CE1-NE2	-5.73	1.26	1.32
2	B	11	THR	CB-CG2	-5.73	1.33	1.52
7	G	22	PHE	CA-C	-5.73	1.46	1.52
5	E	105	GLU	CD-OE1	-5.73	1.14	1.25
5	e	105	GLU	CD-OE1	-5.73	1.14	1.25
10	3	176	ASP	CG-OD1	-5.73	1.14	1.25
12	l	140	LEU	CG-CD1	-5.73	1.33	1.52
12	l	160	ASN	CG-OD1	-5.72	1.12	1.23
12	5	139	ARG	CG-CD	-5.72	1.35	1.52
9	i	30	THR	CB-CG2	-5.72	1.33	1.52
7	g	223	GLU	CD-OE2	-5.71	1.14	1.25
7	G	114	ASP	CG-OD2	-5.71	1.14	1.25
12	5	140	LEU	CG-CD1	-5.71	1.33	1.52
1	a	22	GLU	CG-CD	-5.71	1.37	1.52
7	g	114	ASP	CG-OD2	-5.70	1.14	1.25
7	g	22	PHE	CA-C	-5.70	1.46	1.52
12	l	139	ARG	CG-CD	-5.70	1.35	1.52
5	E	233	ASN	CG-OD1	-5.70	1.12	1.23
2	b	11	THR	CB-CG2	-5.70	1.33	1.52
9	2	30	THR	CB-CG2	-5.70	1.33	1.52
11	k	101	ASN	CG-ND2	-5.69	1.21	1.33
13	m	75	ARG	NE-CZ	-5.68	1.26	1.33
7	G	208	LYS	C-N	5.68	1.41	1.33
9	i	243	LYS	C-N	5.67	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	j	98	ARG	CG-CD	-5.67	1.35	1.52
11	4	90	LYS	CB-CG	-5.67	1.35	1.52
10	3	205	ASP	CA-C	-5.67	1.41	1.52
1	a	22	GLU	CD-OE1	-5.67	1.14	1.25
10	3	98	ARG	CG-CD	-5.67	1.35	1.52
11	4	101	ASN	CG-ND2	-5.67	1.21	1.33
11	k	90	LYS	CB-CG	-5.67	1.35	1.52
13	m	169	GLU	CD-OE2	-5.67	1.14	1.25
13	6	169	GLU	CD-OE2	-5.67	1.14	1.25
13	m	201	GLU	CB-CG	-5.66	1.35	1.52
5	e	213	ASP	CG-OD1	-5.66	1.14	1.25
12	l	146	LYS	CA-C	-5.65	1.45	1.52
1	A	22	GLU	CD-OE1	-5.65	1.14	1.25
25	R	225	LYS	CG-CD	-5.65	1.35	1.52
9	i	211	LYS	C-N	5.65	1.41	1.33
13	m	78	ASN	CB-CG	-5.65	1.38	1.52
11	4	49	GLU	C-O	-5.65	1.16	1.23
12	5	146	LYS	CA-C	-5.65	1.45	1.52
11	k	162	LYS	CG-CD	-5.65	1.35	1.52
10	j	205	ASP	CA-C	-5.64	1.41	1.52
9	2	178	GLU	CD-OE2	-5.64	1.14	1.25
2	B	113	GLU	CD-OE1	-5.64	1.14	1.25
13	6	201	GLU	CB-CG	-5.64	1.35	1.52
11	k	49	GLU	C-O	-5.63	1.16	1.23
13	6	78	ASN	CB-CG	-5.63	1.38	1.52
2	b	113	GLU	CD-OE1	-5.63	1.14	1.25
9	2	57	ASP	CG-OD1	-5.63	1.14	1.25
11	4	162	LYS	CG-CD	-5.63	1.35	1.52
13	m	114	TYR	CG-CD1	-5.63	1.27	1.39
3	c	109	GLU	CD-OE2	-5.62	1.14	1.25
3	c	109	GLU	CD-OE1	-5.62	1.14	1.25
13	6	75	ARG	NE-CZ	-5.62	1.26	1.33
9	i	178	GLU	CD-OE2	-5.61	1.14	1.25
13	6	103	HIS	CD2-NE2	5.60	1.44	1.37
12	5	186	THR	CB-CG2	-5.60	1.34	1.52
3	C	109	GLU	CD-OE1	-5.60	1.14	1.25
9	2	224	VAL	CB-CG1	-5.60	1.34	1.52
10	3	114	SER	CB-OG	-5.60	1.30	1.42
12	5	147	GLU	N-CA	-5.60	1.39	1.45
5	E	213	ASP	CG-OD1	-5.59	1.14	1.25
7	G	180	VAL	CA-C	-5.59	1.44	1.52
10	j	114	SER	CB-OG	-5.59	1.30	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	3	125	ASP	CG-OD2	-5.59	1.14	1.25
9	2	114	GLN	CG-CD	-5.58	1.38	1.52
12	l	147	GLU	N-CA	-5.58	1.39	1.45
9	i	114	GLN	CG-CD	-5.58	1.38	1.52
3	C	105	ASP	CG-OD1	-5.58	1.14	1.25
9	i	57	ASP	CG-OD1	-5.57	1.14	1.25
12	l	186	THR	CB-CG2	-5.57	1.34	1.52
3	C	109	GLU	CD-OE2	-5.57	1.14	1.25
3	c	105	ASP	CG-OD1	-5.57	1.14	1.25
6	f	5	ASN	CB-CG	-5.57	1.38	1.52
7	g	248	ASN	CG-OD1	-5.57	1.12	1.23
8	1	93	GLU	CD-OE2	-5.57	1.14	1.25
1	A	74	CYS	C-N	5.56	1.41	1.33
8	h	129	HIS	CG-CD2	-5.56	1.29	1.35
9	i	88	ILE	CB-CG2	-5.55	1.34	1.52
13	m	181	LYS	CA-C	-5.55	1.45	1.53
34	8	201	GLN	CA-C	5.55	1.60	1.52
11	4	34	LYS	CE-NZ	-5.55	1.32	1.49
10	3	176	ASP	CG-OD2	-5.54	1.14	1.25
9	2	88	ILE	CB-CG2	-5.54	1.34	1.52
13	m	182	TYR	CZ-OH	-5.54	1.26	1.38
8	1	129	HIS	CG-CD2	-5.54	1.29	1.35
6	F	5	ASN	CB-CG	-5.53	1.38	1.52
8	h	31	THR	CB-CG2	-5.53	1.34	1.52
5	E	102	TYR	CE1-CZ	-5.53	1.25	1.38
1	a	115	ASP	CG-OD1	-5.53	1.14	1.25
7	G	205	GLU	C-N	5.53	1.41	1.33
11	k	34	LYS	CE-NZ	-5.52	1.32	1.49
11	k	110	LYS	CD-CE	-5.52	1.35	1.52
5	e	102	TYR	CE1-CZ	-5.52	1.25	1.38
10	3	155	GLU	CD-OE1	-5.52	1.14	1.25
8	h	93	GLU	CD-OE2	-5.52	1.14	1.25
9	i	118	LYS	CB-CG	-5.51	1.35	1.52
10	j	26	ASP	CG-OD2	-5.51	1.14	1.25
8	1	31	THR	CB-CG2	-5.51	1.34	1.52
11	4	110	LYS	CD-CE	-5.51	1.35	1.52
13	6	182	TYR	CE1-CZ	-5.51	1.25	1.38
2	B	234	ARG	CG-CD	-5.51	1.35	1.52
13	m	182	TYR	CE1-CZ	-5.51	1.25	1.38
7	g	238	GLU	CD-OE2	-5.50	1.14	1.25
9	2	118	LYS	CB-CG	-5.50	1.35	1.52
2	b	234	ARG	CG-CD	-5.50	1.35	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	25	GLU	CB-CG	-5.50	1.35	1.52
13	6	182	TYR	CZ-OH	-5.50	1.26	1.38
9	2	98	TYR	CG-CD1	-5.49	1.27	1.39
12	l	83	PHE	CA-C	-5.49	1.48	1.53
9	i	98	TYR	CG-CD1	-5.48	1.27	1.39
10	3	7	ILE	CB-CG1	-5.48	1.42	1.53
13	m	40	ASP	CG-OD2	-5.48	1.15	1.25
12	l	156	LYS	CG-CD	-5.48	1.36	1.52
13	6	40	ASP	CG-OD2	-5.48	1.15	1.25
7	G	182	HIS	CB-CG	5.47	1.57	1.50
12	5	156	LYS	CG-CD	-5.47	1.36	1.52
5	e	25	GLU	CB-CG	-5.47	1.36	1.52
10	j	7	ILE	CB-CG1	-5.47	1.42	1.53
1	a	188	LYS	CD-CE	-5.46	1.36	1.52
13	6	9	GLN	CD-OE1	-5.46	1.13	1.23
2	B	81	ASP	CG-OD2	-5.46	1.15	1.25
8	h	93	GLU	CD-OE1	-5.46	1.15	1.25
13	6	181	LYS	CA-C	-5.46	1.45	1.53
1	A	188	LYS	CD-CE	-5.46	1.36	1.52
1	A	115	ASP	CG-OD1	-5.45	1.15	1.25
9	2	155	SER	CB-OG	-5.45	1.31	1.42
8	1	93	GLU	CD-OE1	-5.45	1.15	1.25
10	3	26	ASP	CG-OD2	-5.45	1.15	1.25
13	m	9	GLN	CD-OE1	-5.45	1.13	1.23
6	f	138	ASP	CG-OD1	-5.45	1.15	1.25
11	4	155	GLU	CD-OE1	-5.45	1.15	1.25
2	b	81	ASP	CG-OD2	-5.44	1.15	1.25
6	f	119	ASN	CG-OD1	-5.44	1.13	1.23
7	G	180	VAL	N-CA	5.44	1.53	1.46
7	g	223	GLU	CD-OE1	-5.44	1.15	1.25
10	j	203	ARG	C-N	-5.44	1.26	1.33
11	k	155	GLU	CD-OE1	-5.43	1.15	1.25
10	3	202	MET	SD-CE	-5.43	1.66	1.79
10	j	202	MET	SD-CE	-5.43	1.66	1.79
9	2	186	ASP	CB-CG	-5.43	1.38	1.52
8	h	152	ARG	CB-CG	-5.42	1.36	1.52
9	i	155	SER	CB-OG	-5.42	1.31	1.42
11	k	99	GLN	CD-NE2	-5.42	1.21	1.33
13	m	108	LYS	CA-C	-5.42	1.47	1.53
6	F	119	ASN	CG-OD1	-5.42	1.13	1.23
10	3	203	ARG	C-N	-5.42	1.26	1.33
13	6	181	LYS	N-CA	-5.42	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	1	152	ARG	CB-CG	-5.42	1.36	1.52
12	l	150	SER	C-N	-5.42	1.27	1.33
9	i	186	ASP	CB-CG	-5.41	1.38	1.52
7	G	168	GLY	C-N	5.41	1.41	1.33
11	4	99	GLN	CD-NE2	-5.41	1.21	1.33
11	k	74	GLU	CD-OE2	-5.41	1.15	1.25
3	c	27	GLU	CD-OE2	-5.41	1.15	1.25
13	m	181	LYS	N-CA	-5.41	1.38	1.45
8	h	100	ASP	CG-OD2	-5.40	1.15	1.25
11	4	74	GLU	CD-OE2	-5.39	1.15	1.25
31	L	317	ASN	N-CA	-5.39	1.39	1.46
10	j	151	GLU	CA-C	-5.39	1.46	1.52
6	F	138	ASP	CG-OD1	-5.39	1.15	1.25
1	a	67	THR	CB-CG2	-5.39	1.34	1.52
10	3	145	GLN	N-CA	-5.38	1.40	1.46
3	c	18	ARG	CG-CD	-5.38	1.36	1.52
2	B	4	ARG	CZ-NH1	-5.38	1.25	1.32
7	g	207	ASN	CG-OD1	-5.38	1.13	1.23
13	m	107	GLY	CA-C	-5.37	1.46	1.52
12	5	150	SER	C-N	-5.37	1.27	1.33
13	6	103	HIS	CB-CG	-5.37	1.42	1.50
1	a	112	MET	SD-CE	-5.37	1.66	1.79
3	C	18	ARG	CG-CD	-5.37	1.36	1.52
7	G	183	HIS	CB-CG	5.37	1.57	1.50
1	A	239	GLU	CD-OE1	-5.37	1.15	1.25
1	A	67	THR	CB-CG2	-5.37	1.34	1.52
8	1	100	ASP	CG-OD2	-5.37	1.15	1.25
29	I	54	ARG	NE-CZ	5.37	1.39	1.33
11	k	135	TYR	CD2-CE2	-5.36	1.22	1.38
11	4	127	GLU	CG-CD	-5.36	1.38	1.52
9	i	215	TYR	CA-CB	5.36	1.60	1.53
11	4	135	TYR	CD2-CE2	-5.36	1.22	1.38
5	e	9	ASP	CG-OD1	-5.36	1.15	1.25
1	a	239	GLU	CD-OE1	-5.36	1.15	1.25
5	e	9	ASP	CG-OD2	-5.36	1.15	1.25
9	i	252	ILE	CA-C	-5.35	1.46	1.52
9	2	186	ASP	CG-OD2	-5.35	1.15	1.25
3	C	27	GLU	CD-OE2	-5.35	1.15	1.25
9	i	186	ASP	CG-OD2	-5.35	1.15	1.25
11	4	78	GLN	CD-OE1	-5.35	1.13	1.23
13	6	53	ASP	CG-OD2	-5.34	1.15	1.25
1	A	112	MET	SD-CE	-5.34	1.66	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	m	141	ARG	NE-CZ	-5.34	1.27	1.33
13	m	124	GLU	CG-CD	-5.33	1.38	1.52
11	k	78	GLN	CD-OE1	-5.33	1.13	1.23
9	2	58	LYS	CE-NZ	-5.33	1.33	1.49
7	G	241	ASP	CA-CB	5.33	1.61	1.53
8	h	163	PHE	C-N	5.32	1.40	1.33
13	6	124	GLU	CG-CD	-5.32	1.38	1.52
2	b	4	ARG	CZ-NH1	-5.32	1.25	1.32
9	i	58	LYS	CE-NZ	-5.32	1.33	1.49
7	G	204	HIS	C-N	5.32	1.40	1.33
10	3	132	GLU	C-N	5.32	1.40	1.33
1	A	74	CYS	CA-C	-5.32	1.46	1.52
11	k	127	GLU	CG-CD	-5.31	1.38	1.52
6	f	138	ASP	CG-OD2	-5.31	1.15	1.25
8	1	152	ARG	CZ-NH2	-5.31	1.26	1.33
9	i	214	GLU	CA-C	-5.30	1.46	1.52
13	m	53	ASP	CG-OD2	-5.30	1.15	1.25
8	1	106	ILE	CG1-CD1	-5.30	1.31	1.51
9	2	254	GLU	C-O	-5.30	1.16	1.23
11	4	33	ASP	CG-OD2	-5.30	1.15	1.25
11	4	109	LYS	CE-NZ	-5.30	1.33	1.49
1	a	217	GLU	CD-OE2	-5.30	1.15	1.25
8	h	106	ILE	CG1-CD1	-5.30	1.31	1.51
12	5	220	LYS	CB-CG	-5.29	1.36	1.52
8	h	129	HIS	CG-ND1	-5.29	1.32	1.38
34	8	198	ARG	C-N	-5.29	1.25	1.33
11	4	135	TYR	CA-CB	-5.29	1.44	1.53
6	F	138	ASP	CG-OD2	-5.29	1.15	1.25
1	A	217	GLU	CD-OE2	-5.28	1.15	1.25
2	B	22	ASP	CG-OD1	-5.28	1.15	1.25
13	6	89	ASP	CA-C	-5.28	1.46	1.53
11	k	109	LYS	CE-NZ	-5.28	1.33	1.49
12	l	220	LYS	CB-CG	-5.28	1.36	1.52
8	h	152	ARG	CZ-NH2	-5.27	1.26	1.33
13	m	182	TYR	CA-C	-5.27	1.46	1.52
13	6	97	ALA	CA-C	-5.27	1.46	1.52
13	6	141	ARG	NE-CZ	-5.27	1.27	1.33
7	G	210	LYS	CA-C	-5.26	1.45	1.53
12	5	257	GLU	CD-OE1	-5.25	1.15	1.25
10	j	142	ALA	N-CA	-5.25	1.40	1.46
13	m	114	TYR	CE1-CZ	-5.25	1.25	1.38
11	4	11	ASP	CG-OD1	-5.25	1.15	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	110	GLU	CD-OE1	-5.25	1.15	1.25
1	A	200	GLU	CD-OE2	-5.25	1.15	1.25
3	C	152	ASN	CG-ND2	-5.25	1.22	1.33
4	D	119	ARG	CB-CG	-5.25	1.36	1.52
13	6	165	LYS	CE-NZ	-5.25	1.33	1.49
11	k	11	ASP	CG-OD1	-5.24	1.15	1.25
11	k	33	ASP	CG-OD2	-5.24	1.15	1.25
8	1	129	HIS	CG-ND1	-5.24	1.32	1.38
5	e	110	GLU	CD-OE1	-5.23	1.15	1.25
13	6	111	PHE	N-CA	-5.23	1.41	1.46
3	c	152	ASN	CG-ND2	-5.23	1.22	1.33
11	k	135	TYR	CA-CB	-5.23	1.44	1.53
12	l	257	GLU	CD-OE1	-5.23	1.15	1.25
12	5	83	PHE	CA-CB	5.23	1.62	1.53
5	E	170	LYS	CE-NZ	-5.23	1.33	1.49
11	k	37	GLN	CD-OE1	-5.22	1.13	1.23
13	m	229	ARG	CB-CG	-5.22	1.36	1.52
13	6	182	TYR	CA-C	-5.22	1.46	1.52
5	e	58	LEU	CA-CB	5.22	1.62	1.54
1	a	37	GLN	CD-OE1	-5.22	1.13	1.23
5	E	110	GLU	CD-OE2	-5.22	1.15	1.25
5	e	23	GLN	CD-OE1	-5.22	1.13	1.23
10	j	38	ASN	C-N	5.21	1.41	1.33
10	3	38	ASN	C-N	5.21	1.41	1.33
2	b	22	ASP	CG-OD1	-5.21	1.15	1.25
11	k	3	ILE	N-CA	-5.21	1.40	1.46
13	m	122	LEU	CG-CD1	-5.21	1.35	1.52
13	m	165	LYS	CE-NZ	-5.21	1.33	1.49
2	b	103	GLU	CD-OE2	-5.21	1.15	1.25
2	B	103	GLU	CD-OE2	-5.21	1.15	1.25
10	3	125	ASP	CG-OD1	-5.21	1.15	1.25
1	a	200	GLU	CD-OE2	-5.21	1.15	1.25
5	e	110	GLU	CD-OE2	-5.21	1.15	1.25
13	m	205	GLN	CD-NE2	-5.21	1.22	1.33
13	6	205	GLN	CD-NE2	-5.21	1.22	1.33
1	A	37	GLN	CD-OE1	-5.21	1.13	1.23
6	F	69	HIS	CG-CD2	-5.21	1.30	1.35
5	e	170	LYS	CE-NZ	-5.20	1.33	1.49
13	6	122	LEU	CG-CD1	-5.20	1.35	1.52
5	E	23	GLN	CD-OE1	-5.19	1.13	1.23
6	F	118	LYS	CE-NZ	-5.19	1.33	1.49
11	4	37	GLN	CD-OE1	-5.19	1.13	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	f	69	HIS	CG-CD2	-5.19	1.30	1.35
6	f	118	LYS	CE-NZ	-5.19	1.33	1.49
1	A	183	GLU	CD-OE2	-5.19	1.15	1.25
3	C	110	ILE	CG1-CD1	-5.19	1.31	1.51
11	4	92	ILE	CB-CG1	-5.18	1.43	1.53
7	G	41	LYS	CG-CD	-5.18	1.36	1.52
3	c	110	ILE	CG1-CD1	-5.18	1.31	1.51
12	5	216	ASP	CB-CG	-5.18	1.39	1.52
13	6	229	ARG	CB-CG	-5.18	1.36	1.52
11	k	92	ILE	CB-CG1	-5.17	1.43	1.53
7	G	182	HIS	CA-CB	5.17	1.61	1.53
13	m	39	THR	CB-CG2	-5.17	1.35	1.52
7	G	224	THR	CA-C	-5.17	1.45	1.52
9	i	212	ASP	N-CA	-5.17	1.39	1.46
12	l	216	ASP	CB-CG	-5.16	1.39	1.52
7	g	41	LYS	CG-CD	-5.16	1.36	1.52
7	g	129	VAL	C-N	5.16	1.45	1.33
13	m	167	GLN	CB-CG	-5.16	1.36	1.52
13	6	39	THR	CB-CG2	-5.16	1.35	1.52
13	6	167	GLN	CB-CG	-5.15	1.36	1.52
3	c	179	ASP	CG-OD1	-5.14	1.15	1.25
13	6	99	ARG	NE-CZ	5.14	1.38	1.33
7	G	129	VAL	C-N	5.14	1.45	1.33
3	C	179	ASP	CG-OD1	-5.14	1.15	1.25
12	l	191	ASP	CG-OD1	-5.13	1.15	1.25
1	a	183	GLU	CD-OE2	-5.13	1.15	1.25
21	N	282	TYR	CD2-CE2	-5.13	1.23	1.38
10	3	140	GLY	C-N	5.12	1.40	1.33
1	a	75	ILE	CA-C	-5.12	1.46	1.52
12	5	100	TRP	CE3-CZ3	-5.12	1.23	1.38
31	L	421	LYS	CD-CE	-5.12	1.37	1.52
20	Z	40	GLU	CB-CG	-5.11	1.37	1.52
22	S	43	LYS	CB-CG	-5.11	1.37	1.52
11	k	169	GLU	CB-CG	-5.11	1.37	1.52
12	5	191	ASP	CG-OD1	-5.11	1.15	1.25
1	a	187	LYS	CB-CG	-5.10	1.37	1.52
5	e	224	LYS	CG-CD	-5.10	1.37	1.52
7	G	216	ILE	CA-C	-5.10	1.46	1.52
11	4	91	SER	CB-OG	-5.10	1.31	1.42
1	A	177	GLU	CD-OE1	-5.09	1.15	1.25
5	E	224	LYS	CG-CD	-5.09	1.37	1.52
12	l	100	TRP	CE3-CZ3	-5.09	1.23	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	L	317	ASN	CA-C	-5.09	1.46	1.52
9	i	215	TYR	C-N	5.09	1.39	1.33
6	f	143	HIS	CG-ND1	-5.08	1.32	1.38
11	4	169	GLU	CB-CG	-5.08	1.37	1.52
1	a	177	GLU	CD-OE1	-5.08	1.15	1.25
11	k	91	SER	CB-OG	-5.08	1.31	1.42
13	m	78	ASN	CG-OD1	-5.08	1.13	1.23
9	2	97	LEU	CG-CD2	-5.08	1.35	1.52
3	c	7	ASP	C-N	-5.08	1.26	1.33
9	i	97	LEU	CG-CD2	-5.08	1.35	1.52
9	2	156	LEU	CB-CG	-5.08	1.43	1.53
10	j	131	ASP	C-N	5.07	1.40	1.33
7	G	187	LEU	C-N	5.07	1.40	1.33
13	6	208	ASP	CG-OD2	-5.07	1.15	1.25
8	h	194	ARG	N-CA	-5.07	1.39	1.46
13	m	208	ASP	CG-OD2	-5.07	1.15	1.25
1	A	187	LYS	CB-CG	-5.07	1.37	1.52
1	A	115	ASP	CG-OD2	-5.07	1.15	1.25
13	6	78	ASN	CG-OD1	-5.07	1.14	1.23
10	j	65	GLU	CD-OE1	-5.06	1.15	1.25
9	i	156	LEU	CB-CG	-5.06	1.43	1.53
3	C	7	ASP	C-N	-5.06	1.26	1.33
9	i	181	ILE	CB-CG2	-5.05	1.35	1.52
2	B	22	ASP	CG-OD2	-5.05	1.15	1.25
9	2	181	ILE	CB-CG2	-5.05	1.35	1.52
2	b	22	ASP	CG-OD2	-5.05	1.15	1.25
3	c	87	LEU	CG-CD1	-5.05	1.35	1.52
2	B	248	GLU	CD-OE2	-5.04	1.15	1.25
2	b	248	GLU	CD-OE2	-5.04	1.15	1.25
3	C	87	LEU	CG-CD1	-5.04	1.35	1.52
8	h	202	TYR	CA-CB	5.04	1.62	1.54
7	G	223	GLU	CA-C	-5.03	1.46	1.52
13	6	96	SER	C-O	-5.03	1.18	1.24
7	g	215	GLU	CD-OE1	-5.03	1.15	1.25
9	i	217	ARG	CD-NE	5.03	1.53	1.46
10	3	8	ASN	CG-ND2	-5.03	1.22	1.33
5	e	66	LYS	CD-CE	-5.03	1.37	1.52
10	j	8	ASN	CG-ND2	-5.03	1.22	1.33
9	2	228	LYS	CB-CG	-5.03	1.37	1.52
5	E	66	LYS	CD-CE	-5.03	1.37	1.52
9	i	249	ILE	C-N	5.02	1.40	1.33
1	a	115	ASP	CG-OD2	-5.02	1.15	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	3	65	GLU	CD-OE1	-5.01	1.15	1.25
13	6	79	SER	C-N	-5.01	1.27	1.33
10	j	164	PHE	N-CA	-5.00	1.40	1.46

All (1988) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	L	421	LYS	CG-CD-CE	26.52	172.30	111.30
31	L	367	LYS	CB-CG-CD	25.64	170.28	111.30
32	M	68	LYS	CG-CD-CE	25.56	170.09	111.30
9	i	65	ARG	NE-CZ-NH2	25.29	141.96	119.20
9	2	65	ARG	NE-CZ-NH2	25.25	141.93	119.20
9	2	220	LEU	CD1-CG-CD2	-25.18	55.41	110.80
9	i	65	ARG	NE-CZ-NH1	-24.37	97.13	121.50
9	2	65	ARG	NE-CZ-NH1	-24.34	97.17	121.50
22	S	43	LYS	CB-CG-CD	23.89	166.25	111.30
25	R	225	LYS	CG-CD-CE	23.55	165.46	111.30
9	2	51	GLN	CB-CG-CD	23.36	152.32	112.60
9	i	51	GLN	CB-CG-CD	23.31	152.22	112.60
29	I	139	GLU	CB-CG-CD	22.64	151.10	112.60
32	M	261	LYS	CA-CB-CG	22.58	159.27	114.10
10	j	39	LYS	CB-CG-CD	21.87	161.60	111.30
10	3	39	LYS	CB-CG-CD	21.85	161.55	111.30
9	i	211	LYS	CB-CG-CD	21.45	160.63	111.30
9	2	211	LYS	CB-CG-CD	21.41	160.54	111.30
20	Z	632	GLU	CB-CG-CD	21.28	148.78	112.60
10	j	124	PHE	O-C-N	21.13	147.20	123.33
9	i	51	GLN	CA-CB-CG	20.60	155.29	114.10
9	2	51	GLN	CA-CB-CG	20.57	155.24	114.10
24	Q	166	LYS	CB-CG-CD	19.82	156.88	111.30
5	E	53	ARG	NE-CZ-NH1	-19.66	101.84	121.50
29	I	139	GLU	CA-CB-CG	19.37	152.84	114.10
9	2	156	LEU	CD1-CG-CD2	-19.17	68.62	110.80
9	i	156	LEU	CD1-CG-CD2	-19.17	68.62	110.80
11	4	170	LYS	CB-CG-CD	18.76	154.44	111.30
11	k	170	LYS	CB-CG-CD	18.75	154.41	111.30
15	W	87	MET	CB-CG-SD	18.70	168.79	112.70
24	Q	166	LYS	CA-CB-CG	18.52	151.13	114.10
11	k	93	ARG	NH1-CZ-NH2	-18.00	95.90	119.30
11	4	93	ARG	NH1-CZ-NH2	-17.99	95.92	119.30
11	4	70	ARG	NE-CZ-NH1	17.95	139.45	121.50
11	k	70	ARG	NE-CZ-NH1	17.90	139.40	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	4	163	LEU	CD1-CG-CD2	-17.86	71.51	110.80
10	j	41	GLU	CA-CB-CG	17.84	149.77	114.10
11	k	163	LEU	CD1-CG-CD2	-17.83	71.57	110.80
10	3	41	GLU	CA-CB-CG	17.82	149.75	114.10
24	Q	166	LYS	CG-CD-CE	17.76	152.15	111.30
11	4	143	LEU	CD1-CG-CD2	-17.65	71.98	110.80
11	k	143	LEU	CD1-CG-CD2	-17.62	72.03	110.80
9	2	220	LEU	CB-CG-CD2	17.58	163.43	110.70
13	m	104	LEU	O-C-N	-17.20	99.38	122.43
31	L	367	LYS	CG-CD-CE	16.75	149.83	111.30
13	m	113	TYR	CA-C-N	-16.54	98.36	122.67
13	m	113	TYR	C-N-CA	-16.54	98.36	122.67
9	2	101	ARG	NE-CZ-NH2	-16.47	104.38	119.20
9	i	101	ARG	NE-CZ-NH2	-16.44	104.40	119.20
5	e	18	GLU	O-C-N	16.27	144.22	122.59
7	G	57	LYS	CB-CG-CD	16.15	148.44	111.30
7	g	57	LYS	CB-CG-CD	16.14	148.43	111.30
8	h	183	ARG	NE-CZ-NH1	16.08	137.58	121.50
8	1	183	ARG	NE-CZ-NH1	16.07	137.57	121.50
9	2	217	ARG	NE-CZ-NH2	15.94	133.55	119.20
13	m	141	ARG	NE-CZ-NH2	15.83	133.45	119.20
13	6	141	ARG	NE-CZ-NH2	15.76	133.39	119.20
9	i	109	LEU	CD1-CG-CD2	-15.76	76.14	110.80
9	2	109	LEU	CD1-CG-CD2	-15.74	76.16	110.80
8	1	130	LYS	CD-CE-NZ	15.73	162.25	111.90
29	I	373	GLU	CG-CD-OE1	15.71	154.54	118.40
8	h	130	LYS	CD-CE-NZ	15.71	162.17	111.90
9	2	88	ILE	CB-CG1-CD1	-15.68	80.88	113.80
9	i	88	ILE	CB-CG1-CD1	-15.65	80.92	113.80
12	5	220	LYS	CD-CE-NZ	-15.50	62.30	111.90
12	l	220	LYS	CD-CE-NZ	-15.50	62.31	111.90
22	S	43	LYS	CA-CB-CG	15.42	144.94	114.10
32	M	261	LYS	CB-CG-CD	15.38	146.68	111.30
11	k	70	ARG	NH1-CZ-NH2	-15.33	99.38	119.30
12	l	82	ARG	NH1-CZ-NH2	-15.27	99.44	119.30
12	5	82	ARG	NH1-CZ-NH2	-15.27	99.45	119.30
11	4	70	ARG	NH1-CZ-NH2	-15.25	99.47	119.30
5	E	20	ARG	O-C-N	-15.17	107.19	123.42
3	c	241	LYS	CD-CE-NZ	15.13	160.31	111.90
9	2	30	THR	OG1-CB-CG2	-15.13	79.05	109.30
9	i	30	THR	OG1-CB-CG2	-15.12	79.06	109.30
3	C	241	LYS	CD-CE-NZ	15.12	160.28	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	m	104	LEU	CA-C-N	14.94	154.08	121.80
13	m	104	LEU	C-N-CA	14.94	154.08	121.80
9	2	211	LYS	CA-CB-CG	14.94	143.97	114.10
9	i	211	LYS	CA-CB-CG	14.92	143.93	114.10
11	4	174	MET	CG-SD-CE	-14.90	68.13	100.90
11	k	174	MET	CG-SD-CE	-14.89	68.14	100.90
10	3	126	LEU	O-C-N	-14.88	102.81	122.59
3	C	114	ARG	NE-CZ-NH1	-14.78	106.72	121.50
3	c	114	ARG	NE-CZ-NH1	-14.77	106.73	121.50
32	M	261	LYS	CG-CD-CE	14.68	145.05	111.30
13	6	181	LYS	CD-CE-NZ	-14.64	65.03	111.90
13	m	181	LYS	CD-CE-NZ	-14.64	65.06	111.90
8	1	114	LYS	CD-CE-NZ	-14.62	65.13	111.90
13	m	142	GLU	CB-CG-CD	14.61	137.43	112.60
8	h	114	LYS	CD-CE-NZ	-14.60	65.17	111.90
13	6	142	GLU	CB-CG-CD	14.59	137.40	112.60
2	B	49	LYS	CD-CE-NZ	14.45	158.15	111.90
2	b	49	LYS	CD-CE-NZ	14.45	158.13	111.90
20	Z	632	GLU	CA-CB-CG	-14.44	85.23	114.10
13	m	46	ARG	NE-CZ-NH1	14.27	135.77	121.50
13	6	46	ARG	NE-CZ-NH1	14.24	135.74	121.50
13	m	141	ARG	NE-CZ-NH1	-14.09	107.41	121.50
13	m	145	ARG	CD-NE-CZ	-14.09	104.68	124.40
8	1	10	THR	OG1-CB-CG2	-14.06	81.18	109.30
13	6	145	ARG	CD-NE-CZ	-14.06	104.72	124.40
13	6	141	ARG	NE-CZ-NH1	-14.05	107.45	121.50
8	h	10	THR	OG1-CB-CG2	-14.04	81.22	109.30
32	M	96	ASN	CB-CG-ND2	14.00	137.40	116.40
12	5	139	ARG	NE-CZ-NH2	-13.89	106.69	119.20
2	B	234	ARG	NH1-CZ-NH2	-13.85	101.30	119.30
2	b	234	ARG	NH1-CZ-NH2	-13.84	101.30	119.30
12	l	139	ARG	NE-CZ-NH2	-13.84	106.75	119.20
13	m	46	ARG	NE-CZ-NH2	-13.67	106.90	119.20
13	6	46	ARG	NE-CZ-NH2	-13.57	106.99	119.20
29	I	373	GLU	CG-CD-OE2	-13.47	87.41	118.40
13	6	228	LYS	CD-CE-NZ	-13.35	69.19	111.90
13	m	228	LYS	CD-CE-NZ	-13.34	69.21	111.90
29	I	373	GLU	OE1-CD-OE2	-13.17	91.30	122.90
9	i	153	TYR	CB-CG-CD1	-13.10	101.16	120.80
9	2	153	TYR	CB-CG-CD1	-13.08	101.19	120.80
12	l	156	LYS	CD-CE-NZ	13.03	153.59	111.90
12	5	156	LYS	CD-CE-NZ	13.03	153.59	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	l	104	GLN	CA-CB-CG	12.98	140.06	114.10
12	5	104	GLN	CA-CB-CG	12.98	140.05	114.10
10	3	98	ARG	NE-CZ-NH2	-12.94	107.56	119.20
12	5	170	LEU	CD1-CG-CD2	-12.94	82.34	110.80
10	j	98	ARG	NE-CZ-NH2	-12.93	107.56	119.20
12	l	170	LEU	CD1-CG-CD2	-12.92	82.38	110.80
8	1	194	ARG	NH1-CZ-NH2	-12.91	102.51	119.30
31	L	421	LYS	CB-CG-CD	12.91	140.99	111.30
11	k	93	ARG	NE-CZ-NH1	12.81	134.31	121.50
9	i	92	ILE	CB-CG1-CD1	12.78	140.63	113.80
9	2	92	ILE	CB-CG1-CD1	12.77	140.62	113.80
11	4	93	ARG	NE-CZ-NH1	12.73	134.23	121.50
17	T	130	ASP	OD1-CG-OD2	-12.71	92.41	122.90
8	1	114	LYS	CG-CD-CE	12.69	140.48	111.30
8	h	114	LYS	CG-CD-CE	12.67	140.44	111.30
8	1	42	LYS	CD-CE-NZ	12.60	152.23	111.90
8	h	42	LYS	CD-CE-NZ	12.59	152.20	111.90
10	3	39	LYS	CA-CB-CG	12.57	139.24	114.10
10	j	39	LYS	CA-CB-CG	12.56	139.22	114.10
13	m	221	ARG	CB-CG-CD	12.56	140.19	111.30
13	6	221	ARG	CB-CG-CD	12.56	140.18	111.30
12	l	144	ARG	CG-CD-NE	-12.46	84.58	112.00
12	5	144	ARG	CG-CD-NE	-12.46	84.58	112.00
1	A	73	PHE	CA-C-N	-12.46	106.65	122.84
1	A	73	PHE	C-N-CA	-12.46	106.65	122.84
5	e	224	LYS	CG-CD-CE	12.41	139.85	111.30
5	E	224	LYS	CG-CD-CE	12.41	139.85	111.30
8	1	152	ARG	CG-CD-NE	-12.38	84.75	112.00
5	E	53	ARG	NE-CZ-NH2	12.36	130.33	119.20
8	h	152	ARG	CG-CD-NE	-12.35	84.82	112.00
10	3	63	LEU	CD1-CG-CD2	-12.31	83.72	110.80
22	S	43	LYS	CG-CD-CE	12.31	139.61	111.30
10	j	63	LEU	CD1-CG-CD2	-12.30	83.73	110.80
9	2	230	LYS	CD-CE-NZ	12.30	151.27	111.90
11	4	74	GLU	CB-CG-CD	12.24	133.41	112.60
32	M	96	ASN	CB-CG-OD1	-12.23	96.35	120.80
11	k	74	GLU	CB-CG-CD	12.21	133.36	112.60
8	h	45	ARG	NE-CZ-NH1	12.06	133.56	121.50
8	1	45	ARG	NE-CZ-NH1	12.06	133.56	121.50
2	B	234	ARG	CG-CD-NE	12.02	138.44	112.00
13	m	50	LYS	CB-CG-CD	12.00	138.91	111.30
13	6	50	LYS	CB-CG-CD	11.98	138.86	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	234	ARG	CG-CD-NE	11.98	138.35	112.00
28	H	464	MET	CB-CG-SD	11.97	148.63	112.70
5	e	229	LYS	CG-CD-CE	11.96	138.81	111.30
5	E	229	LYS	CG-CD-CE	11.94	138.77	111.30
10	j	98	ARG	NE-CZ-NH1	11.90	133.41	121.50
10	3	98	ARG	NE-CZ-NH1	11.88	133.38	121.50
11	k	36	ARG	NE-CZ-NH2	11.77	129.79	119.20
24	Q	51	ARG	N-CA-CB	-11.75	90.64	110.49
11	4	36	ARG	NE-CZ-NH2	11.74	129.77	119.20
12	5	257	GLU	CB-CG-CD	11.72	132.53	112.60
13	6	36	ARG	NH1-CZ-NH2	-11.72	104.06	119.30
12	l	257	GLU	CB-CG-CD	11.71	132.51	112.60
13	m	36	ARG	NH1-CZ-NH2	-11.69	104.10	119.30
11	k	99	GLN	CB-CG-CD	11.65	132.40	112.60
11	4	99	GLN	CB-CG-CD	11.65	132.40	112.60
10	3	131	ASP	O-C-N	11.64	138.15	123.01
12	5	170	LEU	CB-CG-CD1	11.63	145.58	110.70
12	l	170	LEU	CB-CG-CD1	11.60	145.50	110.70
28	H	314	VAL	N-CA-C	-11.57	85.27	109.34
25	R	225	LYS	CB-CG-CD	11.56	137.90	111.30
1	A	96	ARG	NE-CZ-NH2	11.43	129.49	119.20
34	8	182	ILE	N-CA-C	-11.40	100.84	111.67
1	a	96	ARG	NE-CZ-NH2	11.40	129.46	119.20
13	6	177	LYS	CB-CG-CD	11.36	137.42	111.30
1	a	75	ILE	N-CA-C	-11.35	101.80	111.56
13	m	177	LYS	CB-CG-CD	11.34	137.39	111.30
11	k	170	LYS	CA-CB-CG	11.32	136.74	114.10
11	4	170	LYS	CA-CB-CG	11.31	136.72	114.10
10	j	118	LYS	CB-CG-CD	11.30	137.30	111.30
10	3	118	LYS	CB-CG-CD	11.29	137.27	111.30
11	k	110	LYS	CD-CE-NZ	-11.25	75.90	111.90
11	4	110	LYS	CD-CE-NZ	-11.24	75.93	111.90
32	M	68	LYS	CB-CG-CD	11.22	137.10	111.30
13	6	72	LEU	CD1-CG-CD2	-11.20	86.17	110.80
1	a	250	GLU	CG-CD-OE1	11.19	144.15	118.40
1	A	250	GLU	CG-CD-OE1	11.19	144.14	118.40
13	6	187	GLU	CB-CG-CD	11.18	131.61	112.60
10	j	98	ARG	CG-CD-NE	-11.18	87.41	112.00
13	m	72	LEU	CD1-CG-CD2	-11.18	86.21	110.80
13	m	187	GLU	CB-CG-CD	11.18	131.60	112.60
8	l	10	THR	CA-CB-CG2	11.16	129.47	110.50
8	h	10	THR	CA-CB-CG2	11.16	129.47	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	3	98	ARG	CG-CD-NE	-11.15	87.48	112.00
32	M	171	GLU	CG-CD-OE2	-11.07	92.94	118.40
11	k	8	ARG	NE-CZ-NH2	11.03	129.12	119.20
9	i	211	LYS	O-C-N	11.02	135.81	123.25
12	5	196	ARG	CD-NE-CZ	11.01	139.81	124.40
12	5	140	LEU	CD1-CG-CD2	-11.00	86.60	110.80
2	b	234	ARG	NE-CZ-NH2	10.99	129.09	119.20
11	4	8	ARG	NE-CZ-NH2	10.99	129.09	119.20
10	j	124	PHE	CA-C-N	-10.98	99.54	122.82
10	j	124	PHE	C-N-CA	-10.98	99.54	122.82
2	B	234	ARG	NE-CZ-NH2	10.98	129.08	119.20
12	l	196	ARG	CD-NE-CZ	10.98	139.77	124.40
12	l	140	LEU	CD1-CG-CD2	-10.97	86.66	110.80
8	h	197	PHE	CA-CB-CG	-10.97	102.83	113.80
13	m	46	ARG	CD-NE-CZ	-10.92	109.11	124.40
12	5	226	GLU	CA-CB-CG	10.90	135.89	114.10
13	6	46	ARG	CD-NE-CZ	-10.89	109.15	124.40
12	l	215	LEU	CD1-CG-CD2	-10.87	86.89	110.80
12	5	215	LEU	CD1-CG-CD2	-10.87	86.89	110.80
32	M	171	GLU	CG-CD-OE1	10.87	143.39	118.40
12	l	226	GLU	CA-CB-CG	10.85	135.80	114.10
11	4	8	ARG	NH1-CZ-NH2	-10.83	105.22	119.30
11	k	8	ARG	NH1-CZ-NH2	-10.81	105.25	119.30
12	l	139	ARG	CD-NE-CZ	-10.78	109.31	124.40
13	m	221	ARG	NH1-CZ-NH2	-10.78	105.29	119.30
13	6	221	ARG	NH1-CZ-NH2	-10.78	105.29	119.30
12	5	139	ARG	CD-NE-CZ	-10.76	109.34	124.40
9	2	227	GLU	CB-CG-CD	10.75	130.88	112.60
5	e	250	GLU	CA-C-O	10.70	138.99	120.80
5	E	250	GLU	CA-C-O	10.68	138.95	120.80
11	4	69	ILE	CB-CG1-CD1	10.63	136.13	113.80
13	m	181	LYS	N-CA-C	10.62	124.23	110.53
11	k	69	ILE	CB-CG1-CD1	10.62	136.10	113.80
31	L	367	LYS	CA-CB-CG	10.62	135.34	114.10
13	6	181	LYS	N-CA-C	10.61	124.22	110.53
12	l	226	GLU	CG-CD-OE1	10.57	142.72	118.40
12	5	226	GLU	CG-CD-OE1	10.57	142.72	118.40
30	K	399	ARG	CB-CG-CD	10.55	135.57	111.30
7	g	57	LYS	CG-CD-CE	10.54	135.53	111.30
7	G	57	LYS	CG-CD-CE	10.51	135.47	111.30
9	2	222	PRO	CA-C-N	10.51	138.32	122.77
9	2	222	PRO	C-N-CA	10.51	138.32	122.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	5	82	ARG	NE-CZ-NH2	10.46	128.61	119.20
12	l	82	ARG	NE-CZ-NH2	10.45	128.61	119.20
1	A	250	GLU	CG-CD-OE2	-10.44	94.39	118.40
12	l	164	GLN	CB-CG-CD	10.44	130.34	112.60
7	g	245	LYS	CD-CE-NZ	-10.44	78.50	111.90
1	a	250	GLU	CG-CD-OE2	-10.43	94.41	118.40
9	i	101	ARG	CD-NE-CZ	-10.42	109.81	124.40
9	2	101	ARG	CD-NE-CZ	-10.42	109.81	124.40
12	5	164	GLN	CB-CG-CD	10.40	130.29	112.60
12	l	147	GLU	CA-CB-CG	10.38	134.85	114.10
12	5	147	GLU	CA-CB-CG	10.37	134.85	114.10
10	3	77	LYS	CD-CE-NZ	-10.37	78.73	111.90
10	j	77	LYS	CD-CE-NZ	-10.35	78.78	111.90
9	2	31	THR	OG1-CB-CG2	-10.34	88.62	109.30
9	i	31	THR	OG1-CB-CG2	-10.33	88.65	109.30
20	Z	143	VAL	N-CA-C	-10.28	102.68	112.96
12	l	82	ARG	NE-CZ-NH1	10.27	131.77	121.50
12	5	82	ARG	NE-CZ-NH1	10.26	131.76	121.50
8	1	17	PHE	O-C-N	-10.25	111.31	123.10
9	i	209	ILE	CB-CG1-CD1	10.25	135.32	113.80
9	2	209	ILE	CB-CG1-CD1	10.25	135.32	113.80
13	m	211	GLU	CB-CG-CD	10.23	130.00	112.60
13	6	211	GLU	CB-CG-CD	10.23	129.99	112.60
10	3	118	LYS	CG-CD-CE	10.22	134.80	111.30
16	V	194	ARG	CG-CD-NE	10.22	134.48	112.00
10	j	118	LYS	CG-CD-CE	10.22	134.80	111.30
9	2	153	TYR	OH-CZ-CE2	-10.21	89.28	119.90
7	g	57	LYS	CA-CB-CG	10.20	134.51	114.10
7	G	57	LYS	CA-CB-CG	10.20	134.49	114.10
9	i	153	TYR	OH-CZ-CE2	-10.16	89.42	119.90
11	4	186	LYS	CB-CG-CD	10.11	134.56	111.30
11	k	186	LYS	CB-CG-CD	10.11	134.56	111.30
9	i	84	VAL	CG1-CB-CG2	-10.08	88.62	110.80
13	m	111	PHE	CA-C-N	10.08	130.17	119.89
13	m	111	PHE	C-N-CA	10.08	130.17	119.89
9	2	84	VAL	CG1-CB-CG2	-10.07	88.66	110.80
10	3	78	GLU	CB-CG-CD	10.05	129.69	112.60
11	4	109	LYS	CG-CD-CE	10.05	134.41	111.30
5	e	10	ARG	NH1-CZ-NH2	-10.05	106.24	119.30
10	j	78	GLU	CB-CG-CD	10.04	129.67	112.60
12	5	161	LEU	CB-CG-CD2	-10.04	80.57	110.70
11	k	109	LYS	CG-CD-CE	10.04	134.39	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	l	161	LEU	CB-CG-CD2	-10.04	80.59	110.70
13	6	111	PHE	CA-C-N	9.98	130.08	119.90
13	6	111	PHE	C-N-CA	9.98	130.08	119.90
7	G	207	ASN	CA-CB-CG	-9.97	102.63	112.60
25	R	225	LYS	CD-CE-NZ	-9.95	80.06	111.90
11	4	113	LYS	CD-CE-NZ	9.90	143.57	111.90
11	k	113	LYS	CD-CE-NZ	9.88	143.53	111.90
11	4	96	ARG	NE-CZ-NH2	-9.86	110.33	119.20
1	A	135	ARG	NE-CZ-NH1	-9.84	111.66	121.50
1	a	135	ARG	NE-CZ-NH1	-9.84	111.66	121.50
11	k	96	ARG	NE-CZ-NH2	-9.84	110.34	119.20
1	a	135	ARG	NE-CZ-NH2	9.82	128.04	119.20
12	5	107	LYS	CD-CE-NZ	9.82	143.32	111.90
12	l	107	LYS	CD-CE-NZ	9.80	143.25	111.90
11	k	7	ILE	CG1-CB-CG2	-9.77	81.38	110.70
5	E	229	LYS	CD-CE-NZ	9.77	143.16	111.90
11	4	7	ILE	CG1-CB-CG2	-9.77	81.40	110.70
32	M	286	ILE	N-CA-C	-9.77	103.91	112.12
5	e	229	LYS	CD-CE-NZ	9.75	143.11	111.90
1	A	135	ARG	NE-CZ-NH2	9.74	127.97	119.20
20	Z	824	ASN	CA-CB-CG	9.74	122.34	112.60
13	6	58	ILE	CB-CG1-CD1	9.71	134.18	113.80
9	i	218	ASN	CA-C-N	9.71	133.06	120.44
9	i	218	ASN	C-N-CA	9.71	133.06	120.44
11	4	109	LYS	CD-CE-NZ	9.70	142.95	111.90
13	m	58	ILE	CB-CG1-CD1	9.70	134.16	113.80
12	5	233	LYS	CG-CD-CE	9.69	133.59	111.30
11	k	109	LYS	CD-CE-NZ	9.69	142.91	111.90
12	l	233	LYS	CG-CD-CE	9.68	133.56	111.30
20	Z	40	GLU	CB-CG-CD	9.64	128.99	112.60
11	k	143	LEU	CB-CG-CD2	9.64	139.62	110.70
11	4	143	LEU	CB-CG-CD2	9.63	139.59	110.70
10	3	77	LYS	CG-CD-CE	9.63	133.44	111.30
10	j	77	LYS	CG-CD-CE	9.62	133.43	111.30
5	e	58	LEU	O-C-N	-9.60	110.54	122.35
13	m	181	LYS	CG-CD-CE	-9.57	89.28	111.30
11	k	36	ARG	NE-CZ-NH1	-9.57	111.93	121.50
4	D	119	ARG	CB-CG-CD	9.57	133.31	111.30
13	6	181	LYS	CG-CD-CE	-9.57	89.30	111.30
11	4	36	ARG	NE-CZ-NH1	-9.55	111.95	121.50
3	c	109	GLU	CB-CG-CD	9.53	128.80	112.60
3	C	109	GLU	CB-CG-CD	9.53	128.80	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	2	155	SER	CA-CB-OG	9.52	130.14	111.10
9	i	155	SER	CA-CB-OG	9.51	130.13	111.10
3	C	63	THR	CA-C-N	-9.49	107.19	121.99
3	C	63	THR	C-N-CA	-9.49	107.19	121.99
9	2	36	LYS	CG-CD-CE	9.49	133.12	111.30
9	i	36	LYS	CG-CD-CE	9.46	133.06	111.30
3	c	63	THR	CA-C-N	-9.45	107.25	121.99
3	c	63	THR	C-N-CA	-9.45	107.25	121.99
29	I	300	ARG	CB-CG-CD	9.42	132.96	111.30
13	m	143	GLN	CA-CB-CG	9.39	132.88	114.10
13	6	143	GLN	CA-CB-CG	9.36	132.82	114.10
10	3	63	LEU	CB-CG-CD1	9.35	138.76	110.70
3	C	114	ARG	NE-CZ-NH2	9.35	127.61	119.20
10	j	63	LEU	CB-CG-CD1	9.34	138.73	110.70
32	M	171	GLU	OE1-CD-OE2	-9.34	100.47	122.90
8	h	183	ARG	NE-CZ-NH2	-9.32	110.81	119.20
3	c	114	ARG	NE-CZ-NH2	9.32	127.58	119.20
9	i	167	LEU	CB-CG-CD1	-9.30	82.81	110.70
8	1	183	ARG	NE-CZ-NH2	-9.29	110.84	119.20
9	2	167	LEU	CB-CG-CD1	-9.29	82.82	110.70
13	6	46	ARG	CG-CD-NE	9.27	132.40	112.00
10	j	176	ASP	N-CA-C	-9.27	101.67	113.72
13	m	46	ARG	CG-CD-NE	9.26	132.37	112.00
10	3	65	GLU	CB-CG-CD	9.25	128.33	112.60
12	l	81	PHE	CD1-CG-CD2	-9.25	104.73	118.60
10	j	65	GLU	CB-CG-CD	9.23	128.30	112.60
30	K	399	ARG	CA-CB-CG	9.23	132.55	114.10
12	5	81	PHE	CD1-CG-CD2	-9.21	104.78	118.60
2	b	237	LYS	CD-CE-NZ	9.21	141.36	111.90
2	B	237	LYS	CD-CE-NZ	9.20	141.34	111.90
20	Z	366	LYS	CB-CG-CD	9.19	132.43	111.30
32	M	124	ARG	CG-CD-NE	-9.17	91.82	112.00
8	h	153	GLU	CB-CG-CD	9.16	128.18	112.60
8	1	153	GLU	CB-CG-CD	9.16	128.17	112.60
13	m	75	ARG	NE-CZ-NH2	-9.15	110.97	119.20
20	Z	58	GLU	CA-CB-CG	-9.13	95.83	114.10
1	a	95	LEU	CD1-CG-CD2	-9.12	90.73	110.80
13	6	75	ARG	NE-CZ-NH2	-9.12	110.99	119.20
20	Z	943	LYS	CA-CB-CG	9.12	132.34	114.10
1	A	73	PHE	O-C-N	9.11	135.07	123.23
12	l	220	LYS	CG-CD-CE	9.11	132.24	111.30
1	A	95	LEU	CD1-CG-CD2	-9.09	90.80	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	2	230	LYS	CG-CD-CE	9.09	132.21	111.30
12	5	220	LYS	CG-CD-CE	9.09	132.20	111.30
13	6	36	ARG	NE-CZ-NH1	9.08	130.58	121.50
13	m	221	ARG	CG-CD-NE	9.08	131.97	112.00
13	m	36	ARG	NE-CZ-NH1	9.07	130.57	121.50
13	6	221	ARG	CG-CD-NE	9.07	131.95	112.00
34	8	466	ASP	N-CA-CB	-9.04	95.21	110.49
9	2	153	TYR	CB-CG-CD2	9.04	134.36	120.80
6	F	51	ARG	NE-CZ-NH2	9.03	127.33	119.20
11	4	135	TYR	CA-CB-CG	9.03	130.16	113.90
8	h	17	PHE	O-C-N	9.03	133.26	122.88
8	1	42	LYS	CG-CD-CE	9.01	132.02	111.30
8	h	42	LYS	CG-CD-CE	9.00	132.00	111.30
11	k	135	TYR	CA-CB-CG	8.99	130.09	113.90
9	i	153	TYR	CB-CG-CD2	8.99	134.29	120.80
32	M	42	ARG	NE-CZ-NH2	-8.98	111.11	119.20
5	e	10	ARG	NE-CZ-NH1	8.97	130.47	121.50
12	l	206	SER	CA-CB-OG	8.97	129.05	111.10
6	f	51	ARG	NE-CZ-NH2	8.97	127.27	119.20
12	5	206	SER	CA-CB-OG	8.96	129.02	111.10
32	M	42	ARG	CD-NE-CZ	8.96	136.94	124.40
4	D	90	ARG	CB-CG-CD	8.95	131.89	111.30
9	2	246	ILE	CB-CG1-CD1	8.94	132.58	113.80
5	e	7	GLU	CG-CD-OE2	-8.91	97.89	118.40
8	h	45	ARG	NE-CZ-NH2	-8.91	111.18	119.20
9	2	101	ARG	NE-CZ-NH1	8.89	130.39	121.50
11	k	29	LYS	CA-CB-CG	8.88	131.86	114.10
8	h	18	LYS	CG-CD-CE	8.87	131.70	111.30
8	h	192	VAL	O-C-N	-8.87	114.43	123.03
11	4	29	LYS	CA-CB-CG	8.85	131.80	114.10
8	1	18	LYS	CG-CD-CE	8.84	131.63	111.30
9	2	156	LEU	CB-CG-CD1	8.84	137.21	110.70
9	i	101	ARG	NE-CZ-NH1	8.83	130.33	121.50
8	1	45	ARG	NE-CZ-NH2	-8.83	111.25	119.20
9	i	156	LEU	CB-CG-CD1	8.83	137.19	110.70
9	2	230	LYS	CA-CB-CG	8.82	131.74	114.10
10	j	115	LYS	CB-CG-CD	8.82	131.58	111.30
12	5	162	VAL	CG1-CB-CG2	-8.82	91.40	110.80
10	3	115	LYS	CB-CG-CD	8.81	131.57	111.30
10	3	8	ASN	CB-CG-ND2	-8.81	103.19	116.40
13	m	141	ARG	CG-CD-NE	8.80	131.36	112.00
12	l	162	VAL	CG1-CB-CG2	-8.80	91.44	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	l	77	THR	OG1-CB-CG2	-8.80	91.71	109.30
10	j	8	ASN	CB-CG-ND2	-8.79	103.21	116.40
13	6	141	ARG	CG-CD-NE	8.78	131.30	112.00
12	5	77	THR	OG1-CB-CG2	-8.76	91.78	109.30
8	1	197	PHE	O-C-N	8.75	134.48	123.28
23	P	88	GLN	CA-C-N	8.75	138.25	121.54
23	P	88	GLN	C-N-CA	8.75	138.25	121.54
12	l	115	PHE	CD1-CG-CD2	-8.74	105.49	118.60
12	5	115	PHE	CD1-CG-CD2	-8.74	105.50	118.60
8	1	194	ARG	CB-CG-CD	8.72	131.36	111.30
11	k	17	SER	CA-CB-OG	8.72	128.54	111.10
13	6	116	HIS	CA-CB-CG	-8.71	105.09	113.80
8	1	194	ARG	NE-CZ-NH2	8.70	127.03	119.20
11	4	17	SER	CA-CB-OG	8.70	128.50	111.10
3	C	109	GLU	CA-CB-CG	8.68	131.47	114.10
3	c	109	GLU	CA-CB-CG	8.67	131.44	114.10
5	e	18	GLU	N-CA-CB	8.65	125.10	110.49
8	h	18	LYS	CD-CE-NZ	8.64	139.55	111.90
8	1	18	LYS	CD-CE-NZ	8.64	139.54	111.90
11	4	163	LEU	CA-CB-CG	8.61	146.45	116.30
11	k	163	LEU	CA-CB-CG	8.60	146.42	116.30
12	l	286	ILE	CB-CG1-CD1	-8.60	95.74	113.80
12	5	286	ILE	CB-CG1-CD1	-8.60	95.75	113.80
35	9	31	GLN	CA-CB-CG	8.57	131.24	114.10
8	1	17	PHE	CA-CB-CG	8.57	122.37	113.80
5	E	180	GLN	CG-CD-NE2	8.54	129.20	116.40
8	h	45	ARG	CD-NE-CZ	-8.52	112.48	124.40
34	8	221	MET	CB-CG-SD	8.52	138.25	112.70
5	e	180	GLN	CG-CD-NE2	8.50	129.15	116.40
11	4	81	SER	CA-CB-OG	8.50	128.10	111.10
11	k	10	GLN	CB-CG-CD	8.48	127.02	112.60
11	k	81	SER	CA-CB-OG	8.48	128.06	111.10
7	g	245	LYS	CG-CD-CE	8.47	130.79	111.30
8	1	45	ARG	CD-NE-CZ	-8.47	112.55	124.40
13	6	182	TYR	OH-CZ-CE2	-8.46	94.51	119.90
10	j	125	ASP	CA-C-N	8.46	132.30	120.29
10	j	125	ASP	C-N-CA	8.46	132.30	120.29
11	4	10	GLN	CB-CG-CD	8.45	126.97	112.60
13	m	182	TYR	OH-CZ-CE2	-8.44	94.57	119.90
10	3	131	ASP	CA-C-N	-8.43	110.30	122.19
10	3	131	ASP	C-N-CA	-8.43	110.30	122.19
20	Z	187	SER	N-CA-C	-8.41	100.49	110.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	2	227	GLU	CA-CB-CG	8.37	130.84	114.10
11	4	2	ASP	CA-CB-CG	8.37	120.97	112.60
20	Z	217	GLU	CA-CB-CG	8.35	130.79	114.10
2	b	6	SER	CA-CB-OG	8.33	127.77	111.10
9	i	248	ASN	CA-C-N	8.33	133.19	121.53
9	i	248	ASN	C-N-CA	8.33	133.19	121.53
9	i	84	VAL	CA-CB-CG2	8.33	124.56	110.40
9	2	84	VAL	CA-CB-CG2	8.31	124.52	110.40
13	m	230	ASP	CA-C-O	-8.30	96.08	121.00
11	4	176	PHE	CD1-CG-CD2	-8.30	106.14	118.60
13	6	230	ASP	CA-C-O	-8.30	96.11	121.00
2	B	6	SER	CA-CB-OG	8.29	127.68	111.10
11	k	8	ARG	CD-NE-CZ	8.28	136.00	124.40
11	k	176	PHE	CD1-CG-CD2	-8.28	106.18	118.60
11	k	5	LEU	CA-C-N	8.28	137.63	121.41
11	k	5	LEU	C-N-CA	8.28	137.63	121.41
10	3	3	ASP	CA-CB-CG	8.27	120.87	112.60
11	k	125	LYS	CB-CG-CD	8.27	130.31	111.30
11	4	125	LYS	CB-CG-CD	8.27	130.31	111.30
12	l	148	ARG	CG-CD-NE	8.26	130.17	112.00
1	A	96	ARG	CB-CG-CD	8.26	130.30	111.30
11	4	8	ARG	CD-NE-CZ	8.26	135.97	124.40
13	6	133	PHE	CD1-CG-CD2	-8.26	106.21	118.60
1	a	96	ARG	CB-CG-CD	8.26	130.29	111.30
10	j	80	ARG	NE-CZ-NH2	8.25	126.63	119.20
13	m	133	PHE	CD1-CG-CD2	-8.25	106.22	118.60
12	5	148	ARG	CG-CD-NE	8.24	130.14	112.00
11	k	96	ARG	CB-CG-CD	8.24	130.26	111.30
10	j	3	ASP	CA-CB-CG	8.24	120.84	112.60
11	4	96	ARG	CB-CG-CD	8.24	130.25	111.30
10	3	80	ARG	NE-CZ-NH2	8.24	126.61	119.20
10	3	87	PHE	CD1-CG-CD2	-8.21	106.29	118.60
5	e	49	GLY	CA-C-N	-8.20	110.42	122.23
5	e	49	GLY	C-N-CA	-8.20	110.42	122.23
10	j	87	PHE	CD1-CG-CD2	-8.20	106.30	118.60
30	K	344	ARG	N-CA-CB	-8.20	96.63	110.49
9	2	211	LYS	CG-CD-CE	8.19	130.14	111.30
12	l	83	PHE	O-C-N	8.18	129.25	123.11
5	e	15	PHE	CA-CB-CG	-8.18	105.62	113.80
20	Z	943	LYS	CB-CG-CD	8.18	130.11	111.30
10	j	78	GLU	CA-CB-CG	-8.17	97.75	114.10
9	i	211	LYS	CG-CD-CE	8.17	130.09	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	180	GLN	CA-CB-CG	8.17	130.44	114.10
10	3	78	GLU	CA-CB-CG	-8.16	97.78	114.10
5	e	180	GLN	CA-CB-CG	8.15	130.40	114.10
13	6	177	LYS	CD-CE-NZ	8.15	137.99	111.90
7	G	243	ALA	CA-C-N	8.15	131.20	120.28
7	G	243	ALA	C-N-CA	8.15	131.20	120.28
10	3	40	PHE	CB-CG-CD1	8.14	134.54	120.70
10	j	40	PHE	CB-CG-CD1	8.14	134.54	120.70
11	k	5	LEU	N-CA-C	-8.14	96.90	109.52
13	m	177	LYS	CD-CE-NZ	8.13	137.92	111.90
9	i	153	TYR	CA-CB-CG	8.12	128.52	113.90
11	4	93	ARG	CG-CD-NE	8.12	129.85	112.00
9	i	212	ASP	CA-CB-CG	8.11	120.71	112.60
4	d	149	GLN	CA-CB-CG	8.11	130.31	114.10
9	i	234	PHE	CA-C-O	-8.10	111.93	120.28
9	2	153	TYR	CA-CB-CG	8.10	128.48	113.90
11	4	5	LEU	O-C-N	8.10	133.15	123.27
13	m	85	PHE	CD1-CG-CD2	-8.10	106.45	118.60
11	k	93	ARG	CG-CD-NE	8.09	129.80	112.00
10	3	126	LEU	CA-C-N	8.09	134.43	121.09
10	3	126	LEU	C-N-CA	8.09	134.43	121.09
31	L	367	LYS	CD-CE-NZ	-8.08	86.04	111.90
11	k	110	LYS	CB-CG-CD	8.08	129.88	111.30
7	G	226	GLY	N-CA-C	-8.08	103.37	115.32
11	4	110	LYS	CB-CG-CD	8.07	129.87	111.30
8	h	128	VAL	CG1-CB-CG2	-8.05	93.08	110.80
8	1	128	VAL	CG1-CB-CG2	-8.04	93.12	110.80
13	m	86	ASP	OD1-CG-OD2	-8.03	103.62	122.90
13	m	167	GLN	CG-CD-NE2	-8.01	104.39	116.40
11	4	93	ARG	NE-CZ-NH2	8.01	126.41	119.20
13	6	167	GLN	CG-CD-NE2	-8.00	104.39	116.40
11	k	93	ARG	NE-CZ-NH2	7.98	126.38	119.20
5	e	18	GLU	CA-C-N	-7.98	109.17	122.25
5	e	18	GLU	C-N-CA	-7.98	109.17	122.25
13	6	97	ALA	CA-C-N	7.96	130.79	120.44
13	6	97	ALA	C-N-CA	7.96	130.79	120.44
20	Z	366	LYS	N-CA-CB	7.96	123.93	110.49
9	2	249	ILE	CA-CB-CG1	-7.94	96.90	110.40
5	E	86	ARG	CB-CG-CD	7.94	129.56	111.30
5	e	86	ARG	CB-CG-CD	7.93	129.54	111.30
12	l	210	PHE	CA-CB-CG	-7.92	105.88	113.80
11	4	96	ARG	CD-NE-CZ	-7.91	113.33	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	5	108	LYS	CD-CE-NZ	7.91	137.20	111.90
13	6	211	GLU	CG-CD-OE1	-7.90	100.22	118.40
8	1	112	ASP	CA-CB-CG	7.90	120.50	112.60
12	l	108	LYS	CD-CE-NZ	7.90	137.17	111.90
13	m	211	GLU	CG-CD-OE1	-7.90	100.24	118.40
11	k	96	ARG	CD-NE-CZ	-7.88	113.38	124.40
11	4	176	PHE	CB-CG-CD2	7.87	134.07	120.70
8	h	112	ASP	CA-CB-CG	7.87	120.47	112.60
20	Z	174	GLU	N-CA-CB	-7.85	97.22	110.49
9	2	209	ILE	CA-CB-CG2	7.85	123.84	110.50
10	j	53	ILE	CG1-CB-CG2	-7.85	87.16	110.70
10	3	53	ILE	CG1-CB-CG2	-7.84	87.17	110.70
11	4	171	ARG	NE-CZ-NH1	7.84	129.34	121.50
11	k	176	PHE	CB-CG-CD2	7.84	134.02	120.70
13	6	122	LEU	CD1-CG-CD2	-7.83	93.56	110.80
22	S	36	LYS	CG-CD-CE	7.82	129.29	111.30
10	j	205	ASP	CA-C-O	7.82	144.46	121.00
8	1	133	TYR	CD1-CG-CD2	-7.82	106.37	118.10
9	i	209	ILE	CA-CB-CG2	7.82	123.79	110.50
13	m	195	SER	CA-CB-OG	7.82	126.73	111.10
11	k	171	ARG	NE-CZ-NH1	7.81	129.31	121.50
10	3	205	ASP	CA-C-O	7.81	144.43	121.00
8	h	133	TYR	CD1-CG-CD2	-7.81	106.39	118.10
13	m	122	LEU	CD1-CG-CD2	-7.80	93.64	110.80
13	6	195	SER	CA-CB-OG	7.80	126.70	111.10
35	9	31	GLN	CB-CG-CD	7.79	125.85	112.60
13	6	95	ASN	CA-CB-CG	-7.78	104.82	112.60
13	6	186	GLU	CA-CB-CG	7.76	129.62	114.10
9	i	66	ILE	CB-CG1-CD1	7.76	130.09	113.80
13	m	113	TYR	O-C-N	7.76	131.63	122.94
13	m	186	GLU	CA-CB-CG	7.75	129.60	114.10
9	2	66	ILE	CB-CG1-CD1	7.75	130.06	113.80
1	A	82	VAL	O-C-N	-7.74	115.24	123.14
8	1	178	SER	CA-CB-OG	7.74	126.58	111.10
20	Z	173	ALA	CA-C-N	7.74	136.32	121.54
20	Z	173	ALA	C-N-CA	7.74	136.32	121.54
4	d	66	LYS	CB-CG-CD	-7.73	93.52	111.30
8	h	178	SER	CA-CB-OG	7.73	126.55	111.10
8	1	17	PHE	CA-C-N	7.72	130.63	120.28
8	1	17	PHE	C-N-CA	7.72	130.63	120.28
17	T	198	ASP	N-CA-C	-7.72	105.02	114.75
15	W	87	MET	CA-CB-CG	7.72	129.54	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	k	163	LEU	CB-CG-CD2	7.71	133.84	110.70
12	l	226	GLU	CB-CG-CD	7.71	125.71	112.60
8	1	113	ASP	CB-CG-OD1	7.71	136.12	118.40
11	4	163	LEU	CB-CG-CD2	7.71	133.82	110.70
29	I	125	MET	N-CA-C	7.71	126.84	109.81
12	5	226	GLU	CB-CG-CD	7.69	125.68	112.60
13	6	103	HIS	ND1-CE1-NE2	7.69	116.09	108.40
13	m	201	GLU	CB-CG-CD	7.68	125.65	112.60
8	h	113	ASP	CB-CG-OD1	7.68	136.06	118.40
16	V	182	LYS	CB-CG-CD	7.68	128.96	111.30
30	K	80	LYS	CB-CG-CD	7.67	128.95	111.30
13	6	201	GLU	CB-CG-CD	7.67	125.63	112.60
10	j	75	LYS	CD-CE-NZ	7.66	136.40	111.90
10	3	75	LYS	CD-CE-NZ	7.64	136.36	111.90
12	5	226	GLU	CG-CD-OE2	-7.64	100.82	118.40
8	h	17	PHE	CA-CB-CG	7.63	121.44	113.80
12	l	226	GLU	CG-CD-OE2	-7.63	100.84	118.40
13	6	182	TYR	N-CA-C	7.63	121.09	108.96
13	m	140	GLU	CB-CG-CD	7.62	125.56	112.60
15	W	20	ASP	CA-C-N	7.62	134.12	121.92
15	W	20	ASP	C-N-CA	7.62	134.12	121.92
10	3	8	ASN	CA-CB-CG	7.62	120.22	112.60
13	6	140	GLU	CB-CG-CD	7.62	125.56	112.60
31	L	274	GLU	CA-C-N	7.61	129.35	119.84
31	L	274	GLU	C-N-CA	7.61	129.35	119.84
9	2	228	LYS	CD-CE-NZ	7.60	136.23	111.90
24	Q	166	LYS	CD-CE-NZ	-7.60	87.58	111.90
16	V	271	VAL	N-CA-CB	-7.60	98.69	111.23
8	1	113	ASP	CB-CG-OD2	-7.59	100.95	118.40
8	h	113	ASP	CB-CG-OD2	-7.58	100.95	118.40
11	4	91	SER	CA-CB-OG	7.58	126.27	111.10
10	j	8	ASN	CA-CB-CG	7.58	120.18	112.60
13	m	182	TYR	N-CA-C	7.58	121.01	108.96
32	M	95	GLU	CA-C-N	7.58	136.01	121.54
32	M	95	GLU	C-N-CA	7.58	136.01	121.54
9	2	156	LEU	CB-CG-CD2	7.58	133.43	110.70
9	i	156	LEU	CB-CG-CD2	7.57	133.40	110.70
9	i	172	LYS	CD-CE-NZ	7.57	136.11	111.90
11	k	91	SER	CA-CB-OG	7.56	126.22	111.10
9	2	172	LYS	CD-CE-NZ	7.55	136.07	111.90
11	4	135	TYR	CE1-CZ-OH	7.55	142.56	119.90
8	1	203	GLU	CA-CB-CG	-7.55	99.00	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	2	37	PHE	CD1-CG-CD2	-7.55	107.27	118.60
11	k	135	TYR	CE1-CZ-OH	7.55	142.54	119.90
20	Z	361	HIS	CB-CG-ND1	7.55	134.02	122.70
12	5	164	GLN	CG-CD-NE2	7.54	127.72	116.40
12	l	164	GLN	CG-CD-NE2	7.54	127.70	116.40
10	3	205	ASP	CB-CA-C	-7.54	95.78	110.10
10	j	205	ASP	CB-CA-C	-7.53	95.80	110.10
3	C	3	SER	CA-C-N	7.53	133.73	121.99
3	C	3	SER	C-N-CA	7.53	133.73	121.99
12	l	286	ILE	CA-CB-CG1	7.53	123.19	110.40
29	I	300	ARG	CA-CB-CG	7.52	129.14	114.10
10	3	145	GLN	CA-C-N	7.52	130.57	120.65
10	3	145	GLN	C-N-CA	7.52	130.57	120.65
10	3	149	MET	CA-CB-CG	7.51	129.12	114.10
10	3	154	TYR	CD1-CG-CD2	-7.51	106.83	118.10
5	e	58	LEU	CA-C-N	7.51	131.53	120.87
5	e	58	LEU	C-N-CA	7.51	131.53	120.87
9	i	37	PHE	CD1-CG-CD2	-7.51	107.34	118.60
12	5	286	ILE	CA-CB-CG1	7.51	123.16	110.40
3	c	3	SER	CA-C-N	7.50	133.69	121.99
3	c	3	SER	C-N-CA	7.50	133.69	121.99
22	S	192	GLU	CB-CG-CD	7.49	125.34	112.60
11	4	121	TYR	CD1-CG-CD2	-7.49	106.87	118.10
6	f	169	LYS	CG-CD-CE	7.49	128.52	111.30
4	D	119	ARG	CA-CB-CG	7.49	129.07	114.10
10	j	125	ASP	CA-CB-CG	7.48	120.08	112.60
11	k	121	TYR	CD1-CG-CD2	-7.48	106.88	118.10
6	F	169	LYS	CG-CD-CE	7.48	128.51	111.30
9	i	198	SER	CA-CB-OG	7.47	126.04	111.10
13	m	40	ASP	OD1-CG-OD2	-7.47	104.97	122.90
20	Z	909	ARG	CB-CG-CD	7.47	128.48	111.30
13	6	40	ASP	OD1-CG-OD2	-7.46	104.98	122.90
11	k	70	ARG	CD-NE-CZ	7.46	134.85	124.40
28	H	372	ASP	N-CA-CB	-7.46	97.88	110.49
9	2	198	SER	CA-CB-OG	7.45	126.00	111.10
9	i	97	LEU	CD1-CG-CD2	-7.43	94.45	110.80
11	4	70	ARG	CD-NE-CZ	7.43	134.80	124.40
2	B	2	THR	O-C-N	-7.42	111.13	123.00
12	l	192	SER	CA-CB-OG	7.41	125.92	111.10
10	j	202	MET	CA-CB-CG	7.41	128.92	114.10
9	2	97	LEU	CD1-CG-CD2	-7.41	94.50	110.80
12	l	100	TRP	CA-CB-CG	7.41	127.67	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	5	192	SER	CA-CB-OG	7.40	125.91	111.10
21	N	455	MET	CB-CG-SD	7.40	134.91	112.70
8	1	45	ARG	CG-CD-NE	7.40	128.28	112.00
12	5	148	ARG	CD-NE-CZ	-7.40	114.04	124.40
10	3	202	MET	CA-CB-CG	7.40	128.89	114.10
12	l	148	ARG	CD-NE-CZ	-7.39	114.05	124.40
11	4	169	GLU	CB-CG-CD	-7.39	100.04	112.60
31	L	426	LYS	CB-CG-CD	7.39	128.29	111.30
8	h	114	LYS	CB-CG-CD	7.38	128.28	111.30
5	E	205	LYS	CD-CE-NZ	7.38	135.53	111.90
12	5	100	TRP	CA-CB-CG	7.38	127.63	113.60
5	e	205	LYS	CD-CE-NZ	7.38	135.53	111.90
2	b	2	THR	O-C-N	-7.38	111.19	123.00
8	h	45	ARG	CG-CD-NE	7.38	128.22	112.00
9	i	242	LEU	N-CA-C	-7.38	103.90	113.12
9	i	234	PHE	O-C-N	7.37	127.11	121.88
11	4	67	TYR	CD1-CG-CD2	-7.37	107.05	118.10
13	m	47	TYR	CD1-CG-CD2	-7.36	107.05	118.10
22	S	464	ARG	CB-CG-CD	7.36	128.23	111.30
8	1	114	LYS	CB-CG-CD	7.36	128.23	111.30
11	k	67	TYR	CD1-CG-CD2	-7.36	107.06	118.10
11	k	169	GLU	CB-CG-CD	-7.35	100.11	112.60
6	F	169	LYS	CD-CE-NZ	-7.35	88.39	111.90
10	j	147	PHE	CA-C-N	7.34	127.94	119.94
10	j	147	PHE	C-N-CA	7.34	127.94	119.94
6	f	169	LYS	CD-CE-NZ	-7.34	88.41	111.90
13	m	95	ASN	CA-CB-CG	7.33	119.94	112.60
11	4	121	TYR	CE1-CZ-CE2	-7.33	105.63	120.30
16	V	182	LYS	CA-CB-CG	7.33	128.76	114.10
9	i	188	ILE	CB-CG1-CD1	7.33	129.19	113.80
9	2	188	ILE	CB-CG1-CD1	7.33	129.18	113.80
11	k	121	TYR	CE1-CZ-CE2	-7.32	105.67	120.30
8	h	133	TYR	CE1-CZ-CE2	-7.31	105.68	120.30
13	6	47	TYR	CD1-CG-CD2	-7.30	107.15	118.10
5	e	7	GLU	CG-CD-OE1	7.30	135.18	118.40
9	2	36	LYS	CD-CE-NZ	7.30	135.25	111.90
12	5	110	ILE	CB-CG1-CD1	7.29	129.11	113.80
27	O	80	LYS	CA-CB-CG	7.29	128.68	114.10
10	3	67	PHE	CD1-CG-CD2	-7.29	107.67	118.60
10	j	67	PHE	CD1-CG-CD2	-7.29	107.67	118.60
8	1	133	TYR	CE1-CZ-CE2	-7.28	105.73	120.30
12	l	110	ILE	CB-CG1-CD1	7.28	129.09	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	i	36	LYS	CD-CE-NZ	7.28	135.18	111.90
34	8	270	ASN	CA-CB-CG	-7.27	105.33	112.60
7	g	202	LEU	CD1-CG-CD2	-7.26	94.83	110.80
1	a	115	ASP	OD1-CG-OD2	-7.25	105.49	122.90
10	j	157	ASN	OD1-CG-ND2	7.25	129.85	122.60
7	G	209	GLU	CA-C-O	-7.25	112.86	120.55
11	4	99	GLN	CA-CB-CG	-7.25	99.60	114.10
12	l	196	ARG	NE-CZ-NH1	-7.25	114.25	121.50
1	A	115	ASP	OD1-CG-OD2	-7.25	105.51	122.90
20	Z	213	LYS	CB-CG-CD	7.23	127.93	111.30
11	k	99	GLN	CA-CB-CG	-7.23	99.64	114.10
2	b	205	ASN	CB-CG-ND2	7.22	127.23	116.40
10	3	75	LYS	CB-CG-CD	7.22	127.91	111.30
2	B	205	ASN	CB-CG-ND2	7.22	127.23	116.40
10	3	40	PHE	CD1-CG-CD2	-7.21	107.78	118.60
12	5	196	ARG	NE-CZ-NH1	-7.21	114.28	121.50
29	I	373	GLU	CB-CG-CD	7.21	124.86	112.60
10	j	75	LYS	CB-CG-CD	7.21	127.88	111.30
8	h	128	VAL	CA-CB-CG1	7.21	122.65	110.40
10	j	137	ILE	N-CA-C	-7.20	97.65	108.17
15	W	21	PHE	CA-CB-CG	-7.20	106.60	113.80
12	5	140	LEU	CB-CG-CD1	7.20	132.30	110.70
12	l	140	LEU	CB-CG-CD1	7.20	132.29	110.70
12	5	242	ARG	NE-CZ-NH2	7.20	125.68	119.20
34	8	204	PHE	CA-C-N	7.20	131.79	121.50
34	8	204	PHE	C-N-CA	7.20	131.79	121.50
26	U	105	LYS	CG-CD-CE	7.20	127.85	111.30
3	c	105	ASP	OD1-CG-OD2	-7.19	105.63	122.90
31	L	421	LYS	CD-CE-NZ	-7.19	88.88	111.90
10	j	40	PHE	CD1-CG-CD2	-7.19	107.81	118.60
11	k	110	LYS	CG-CD-CE	-7.18	94.78	111.30
12	l	242	ARG	NE-CZ-NH2	7.18	125.67	119.20
8	1	128	VAL	CA-CB-CG1	7.18	122.61	110.40
10	j	147	PHE	CA-C-O	-7.18	112.94	120.55
3	C	105	ASP	OD1-CG-OD2	-7.18	105.67	122.90
11	4	110	LYS	CG-CD-CE	-7.17	94.80	111.30
9	2	119	TYR	CE1-CZ-CE2	-7.17	105.97	120.30
7	G	22	PHE	O-C-N	7.16	131.77	122.03
7	g	22	PHE	O-C-N	7.16	131.77	122.03
22	S	36	LYS	CB-CG-CD	7.15	127.75	111.30
12	5	82	ARG	CG-CD-NE	7.14	127.72	112.00
1	A	96	ARG	NE-CZ-NH1	-7.14	114.36	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	3	205	ASP	CB-CG-OD2	7.14	134.82	118.40
9	i	119	TYR	CE1-CZ-CE2	-7.14	106.03	120.30
10	j	118	LYS	CD-CE-NZ	-7.14	89.06	111.90
12	l	82	ARG	CG-CD-NE	7.14	127.70	112.00
8	1	10	THR	CA-CB-OG1	7.14	120.31	109.60
10	3	154	TYR	CE1-CZ-CE2	-7.14	106.03	120.30
8	h	10	THR	CA-CB-OG1	7.13	120.30	109.60
11	4	111	LYS	CD-CE-NZ	7.13	134.72	111.90
5	e	136	ARG	CB-CG-CD	7.12	127.68	111.30
10	j	205	ASP	CB-CG-OD2	7.12	134.79	118.40
10	3	118	LYS	CD-CE-NZ	-7.12	89.10	111.90
13	m	182	TYR	CB-CG-CD1	-7.12	110.12	120.80
1	a	96	ARG	NE-CZ-NH1	-7.10	114.40	121.50
10	j	33	SER	CA-CB-OG	7.10	125.30	111.10
5	E	136	ARG	CB-CG-CD	7.10	127.63	111.30
11	k	111	LYS	CD-CE-NZ	7.09	134.60	111.90
30	K	199	GLU	CG-CD-OE2	-7.09	102.08	118.40
10	3	33	SER	CA-CB-OG	7.09	125.28	111.10
13	m	36	ARG	CD-NE-CZ	7.09	134.32	124.40
10	3	172	LEU	CD1-CG-CD2	-7.08	95.22	110.80
15	W	87	MET	CG-SD-CE	7.08	116.48	100.90
10	j	145	GLN	CA-C-N	7.08	129.76	120.28
10	j	145	GLN	C-N-CA	7.08	129.76	120.28
12	l	270	GLU	CB-CG-CD	7.08	124.63	112.60
13	6	182	TYR	CB-CG-CD1	-7.08	110.19	120.80
13	6	36	ARG	CD-NE-CZ	7.07	134.30	124.40
31	L	141	LYS	CB-CG-CD	7.07	127.55	111.30
12	5	270	GLU	CB-CG-CD	7.05	124.59	112.60
9	i	126	TYR	CD1-CG-CD2	-7.05	107.52	118.10
12	l	214	VAL	CG1-CB-CG2	-7.05	95.29	110.80
13	m	145	ARG	NE-CZ-NH2	-7.05	112.86	119.20
22	S	303	ASN	N-CA-C	7.04	119.66	110.43
9	2	126	TYR	CD1-CG-CD2	-7.04	107.54	118.10
20	Z	174	GLU	N-CA-C	7.04	125.79	110.80
12	5	214	VAL	CG1-CB-CG2	-7.04	95.32	110.80
11	k	177	LYS	CG-CD-CE	7.03	127.47	111.30
8	1	201	GLU	CG-CD-OE2	-7.03	102.23	118.40
11	4	177	LYS	CG-CD-CE	7.02	127.44	111.30
2	b	3	ASP	N-CA-CB	7.01	122.34	110.49
31	L	341	GLY	N-CA-C	-7.01	105.18	115.63
9	i	51	GLN	N-CA-CB	7.00	122.28	110.87
2	B	3	ASP	N-CA-CB	7.00	122.33	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	2	51	GLN	N-CA-CB	7.00	122.28	110.87
2	b	201	GLU	CG-CD-OE2	7.00	134.50	118.40
13	6	145	ARG	NE-CZ-NH2	-7.00	112.90	119.20
2	B	201	GLU	CG-CD-OE2	7.00	134.49	118.40
7	G	193	VAL	CB-CA-C	-6.99	102.70	112.14
8	1	156	SER	CA-CB-OG	6.99	125.08	111.10
13	6	131	TYR	CD1-CG-CD2	-6.99	107.62	118.10
27	O	160	LYS	CG-CD-CE	6.99	127.37	111.30
9	i	119	TYR	CD1-CG-CD2	-6.98	107.63	118.10
11	k	139	TYR	CD1-CG-CD2	-6.98	107.63	118.10
1	A	250	GLU	CB-CG-CD	6.98	124.46	112.60
11	4	139	TYR	CD1-CG-CD2	-6.97	107.64	118.10
8	h	156	SER	CA-CB-OG	6.97	125.04	111.10
11	k	67	TYR	CE1-CZ-CE2	-6.97	106.36	120.30
11	4	67	TYR	CE1-CZ-CE2	-6.97	106.36	120.30
1	a	250	GLU	CB-CG-CD	6.96	124.43	112.60
2	b	242	GLU	OE1-CD-OE2	-6.96	106.20	122.90
5	E	11	GLY	O-C-N	-6.96	116.94	123.48
5	e	86	ARG	CG-CD-NE	6.95	127.30	112.00
9	2	255	GLU	CA-C-O	-6.95	108.98	120.80
9	2	119	TYR	CD1-CG-CD2	-6.95	107.68	118.10
9	2	208	GLU	CB-CG-CD	6.95	124.41	112.60
13	m	131	TYR	CD1-CG-CD2	-6.94	107.69	118.10
5	E	86	ARG	CG-CD-NE	6.94	127.26	112.00
24	Q	167	LYS	CG-CD-CE	6.94	127.25	111.30
2	B	242	GLU	OE1-CD-OE2	-6.93	106.25	122.90
13	m	141	ARG	CD-NE-CZ	6.93	134.10	124.40
13	6	131	TYR	CE1-CZ-CE2	-6.93	106.44	120.30
7	g	104	LYS	CD-CE-NZ	-6.93	89.74	111.90
9	i	208	GLU	CB-CG-CD	6.93	124.38	112.60
25	R	336	LYS	CB-CG-CD	6.92	127.22	111.30
13	6	47	TYR	CE1-CZ-CE2	-6.92	106.46	120.30
5	e	55	THR	N-CA-C	-6.92	104.12	114.64
5	E	12	VAL	O-C-N	6.92	128.32	122.09
7	G	104	LYS	CD-CE-NZ	-6.91	89.78	111.90
13	m	47	TYR	CE1-CZ-CE2	-6.91	106.47	120.30
20	Z	175	ASP	CB-CA-C	6.91	122.15	111.02
2	B	220	ASP	OD1-CG-OD2	-6.91	106.31	122.90
10	j	114	SER	CA-CB-OG	6.90	124.89	111.10
1	a	22	GLU	CG-CD-OE1	-6.89	102.54	118.40
13	6	141	ARG	CD-NE-CZ	6.89	134.05	124.40
1	A	22	GLU	CG-CD-OE1	-6.89	102.55	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	220	ASP	OD1-CG-OD2	-6.89	106.37	122.90
9	2	126	TYR	CE1-CZ-CE2	-6.89	106.52	120.30
12	l	214	VAL	CA-CB-CG1	6.89	122.11	110.40
10	3	114	SER	CA-CB-OG	6.89	124.87	111.10
34	8	270	ASN	N-CA-CB	-6.88	101.75	110.90
13	m	131	TYR	CE1-CZ-CE2	-6.88	106.54	120.30
12	5	198	LYS	CB-CG-CD	6.88	127.12	111.30
9	2	217	ARG	NH1-CZ-NH2	-6.88	110.36	119.30
28	H	152	ILE	N-CA-CB	-6.86	99.91	111.23
9	2	232	TYR	CE1-CZ-CE2	-6.86	106.58	120.30
12	5	214	VAL	CA-CB-CG1	6.86	122.06	110.40
9	i	126	TYR	CE1-CZ-CE2	-6.86	106.59	120.30
13	m	138	SER	CA-CB-OG	6.85	124.81	111.10
12	l	198	LYS	CB-CG-CD	6.85	127.06	111.30
7	G	100	LYS	CG-CD-CE	6.85	127.05	111.30
13	6	94	ILE	CA-C-N	6.84	130.01	120.29
13	6	94	ILE	C-N-CA	6.84	130.01	120.29
5	E	20	ARG	CA-C-N	6.84	130.59	120.87
5	E	20	ARG	C-N-CA	6.84	130.59	120.87
13	6	138	SER	CA-CB-OG	6.84	124.78	111.10
7	g	100	LYS	CG-CD-CE	6.84	127.03	111.30
13	6	182	TYR	CE1-CZ-OH	6.83	140.39	119.90
11	k	135	TYR	OH-CZ-CE2	-6.83	99.42	119.90
11	4	135	TYR	OH-CZ-CE2	-6.82	99.44	119.90
8	1	204	GLN	CA-C-N	6.81	133.96	121.70
8	1	204	GLN	C-N-CA	6.81	133.96	121.70
13	m	182	TYR	CE1-CZ-OH	6.81	140.33	119.90
34	8	270	ASN	CA-C-O	6.81	126.33	118.77
8	h	192	VAL	CA-C-N	6.81	132.58	123.05
8	h	192	VAL	C-N-CA	6.81	132.58	123.05
9	2	208	GLU	CG-CD-OE1	-6.80	102.76	118.40
9	i	208	GLU	CG-CD-OE1	-6.80	102.77	118.40
12	l	251	ASN	CB-CG-ND2	6.80	126.59	116.40
13	m	181	LYS	CB-CA-C	-6.80	96.33	110.40
12	5	81	PHE	CB-CG-CD2	6.80	132.25	120.70
13	6	181	LYS	CB-CA-C	-6.80	96.33	110.40
4	D	5	ASP	CB-CA-C	6.79	123.94	110.42
11	4	95	ARG	CD-NE-CZ	-6.79	114.89	124.40
11	k	95	ARG	CD-NE-CZ	-6.79	114.89	124.40
1	A	112	MET	CG-SD-CE	6.78	115.82	100.90
1	a	112	MET	CG-SD-CE	6.78	115.82	100.90
9	2	227	GLU	CG-CD-OE2	-6.78	102.80	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	5	209	THR	O-C-N	6.78	131.04	122.23
17	T	251	HIS	N-CA-C	-6.77	103.73	113.21
12	l	81	PHE	CB-CG-CD2	6.77	132.21	120.70
9	2	232	TYR	CD1-CE1-CZ	6.77	131.78	119.60
12	l	182	LYS	CA-CB-CG	6.76	127.63	114.10
12	5	182	LYS	CA-CB-CG	6.75	127.61	114.10
12	5	251	ASN	CB-CG-ND2	6.75	126.53	116.40
5	E	20	ARG	CA-C-O	6.75	128.45	121.23
12	l	245	TYR	CE1-CZ-CE2	-6.75	106.81	120.30
9	2	254	GLU	CA-CB-CG	6.74	127.59	114.10
8	h	195	LEU	N-CA-C	-6.74	99.07	109.52
31	L	280	MET	CB-CG-SD	6.74	132.92	112.70
4	d	66	LYS	CG-CD-CE	6.74	126.80	111.30
9	2	181	ILE	CA-CB-CG2	6.74	121.95	110.50
11	k	5	LEU	O-C-N	-6.73	114.40	123.15
8	1	152	ARG	CB-CG-CD	6.73	126.78	111.30
8	h	152	ARG	CB-CG-CD	6.72	126.77	111.30
11	4	76	SER	CA-CB-OG	6.72	124.55	111.10
9	i	181	ILE	CA-CB-CG2	6.72	121.93	110.50
1	A	76	SER	O-C-N	6.72	132.44	122.76
10	3	152	SER	CA-CB-OG	6.72	124.54	111.10
12	5	245	TYR	CE1-CZ-CE2	-6.72	106.85	120.30
12	5	245	TYR	CD1-CG-CD2	-6.72	108.02	118.10
13	6	144	CYS	CA-CB-SG	6.72	129.86	114.40
11	k	76	SER	CA-CB-OG	6.72	124.54	111.10
32	M	429	SER	N-CA-C	-6.71	96.50	110.80
13	m	77	LYS	CD-CE-NZ	6.71	133.38	111.90
13	m	144	CYS	CA-CB-SG	6.71	129.82	114.40
13	6	77	LYS	CD-CE-NZ	6.71	133.36	111.90
33	J	71	TYR	N-CA-C	-6.70	96.52	110.80
9	2	118	LYS	CA-CB-CG	6.70	127.50	114.10
9	i	118	LYS	CA-CB-CG	6.70	127.50	114.10
13	6	143	GLN	CB-CA-C	-6.70	98.51	109.56
12	l	245	TYR	CD1-CG-CD2	-6.69	108.06	118.10
8	1	52	CYS	CA-CB-SG	6.69	129.79	114.40
8	h	52	CYS	CA-CB-SG	6.69	129.79	114.40
24	Q	71	LYS	CG-CD-CE	6.69	126.68	111.30
11	4	139	TYR	CE1-CZ-CE2	-6.68	106.93	120.30
30	K	199	GLU	CG-CD-OE1	6.68	133.78	118.40
8	1	120	TYR	CD1-CG-CD2	-6.68	108.08	118.10
11	k	139	TYR	CE1-CZ-CE2	-6.68	106.94	120.30
1	a	64	LEU	CB-CG-CD2	6.68	130.73	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	5	284	ASN	N-CA-C	-6.68	105.76	114.04
13	m	143	GLN	CB-CA-C	-6.67	98.55	109.56
13	6	167	GLN	CG-CD-OE1	6.67	134.14	120.80
8	h	138	SER	CA-CB-OG	6.67	124.44	111.10
13	m	102	GLN	CG-CD-NE2	6.67	126.40	116.40
5	E	213	ASP	OD1-CG-OD2	-6.67	106.89	122.90
8	1	138	SER	CA-CB-OG	6.67	124.44	111.10
10	j	2	SER	N-CA-C	-6.66	92.35	111.00
1	A	64	LEU	CB-CG-CD2	6.66	130.68	110.70
5	e	213	ASP	OD1-CG-OD2	-6.66	106.92	122.90
13	6	168	TYR	CD1-CE1-CZ	6.65	131.58	119.60
2	b	88	LYS	CG-CD-CE	6.65	126.60	111.30
13	m	167	GLN	CG-CD-OE1	6.65	134.10	120.80
8	h	120	TYR	CD1-CG-CD2	-6.65	108.13	118.10
12	l	284	ASN	N-CA-C	-6.65	105.80	114.04
26	U	98	LYS	O-C-N	6.65	129.94	123.29
10	3	2	SER	N-CA-C	-6.64	92.39	111.00
9	2	119	TYR	CD1-CE1-CZ	6.64	131.55	119.60
13	m	169	GLU	OE1-CD-OE2	-6.64	106.97	122.90
2	B	88	LYS	CG-CD-CE	6.64	126.56	111.30
31	L	265	GLU	CB-CG-CD	6.64	123.88	112.60
20	Z	40	GLU	N-CA-CB	-6.63	100.08	110.30
13	m	168	TYR	CD1-CE1-CZ	6.63	131.54	119.60
13	6	169	GLU	OE1-CD-OE2	-6.63	106.98	122.90
10	3	128	GLY	CA-C-N	6.62	134.19	121.54
10	3	128	GLY	C-N-CA	6.62	134.19	121.54
9	2	153	TYR	CE1-CZ-OH	6.62	139.75	119.90
20	Z	824	ASN	CB-CG-OD1	-6.61	107.58	120.80
9	i	119	TYR	CD1-CE1-CZ	6.61	131.50	119.60
8	1	120	TYR	CE1-CZ-CE2	-6.60	107.09	120.30
9	i	153	TYR	CE1-CZ-OH	6.59	139.68	119.90
8	h	120	TYR	CE1-CZ-CE2	-6.59	107.12	120.30
21	N	861	TYR	N-CA-C	-6.59	96.76	110.80
31	L	275	PRO	CA-C-N	6.59	130.07	120.71
31	L	275	PRO	C-N-CA	6.59	130.07	120.71
10	j	205	ASP	CB-CG-OD1	-6.59	103.25	118.40
12	l	148	ARG	CA-CB-CG	6.59	127.28	114.10
10	3	205	ASP	CB-CG-OD1	-6.59	103.25	118.40
17	T	130	ASP	CB-CG-OD1	6.59	133.55	118.40
24	Q	195	LYS	CG-CD-CE	6.58	126.45	111.30
10	j	150	CYS	CA-C-N	6.58	129.00	120.44
10	j	150	CYS	C-N-CA	6.58	129.00	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	2	232	TYR	CD1-CG-CD2	-6.58	108.23	118.10
12	l	120	MET	CB-CG-SD	6.57	132.42	112.70
11	k	195	PHE	CA-CB-CG	-6.57	107.23	113.80
12	5	148	ARG	CA-CB-CG	6.57	127.24	114.10
29	I	56	LYS	CA-C-N	6.57	129.38	120.38
29	I	56	LYS	C-N-CA	6.57	129.38	120.38
11	4	195	PHE	CA-CB-CG	-6.57	107.23	113.80
9	i	177	LYS	CA-CB-CG	6.56	127.22	114.10
9	2	177	LYS	CA-CB-CG	6.56	127.23	114.10
30	K	69	LYS	CG-CD-CE	-6.56	96.21	111.30
8	1	194	ARG	CG-CD-NE	6.56	126.44	112.00
12	5	115	PHE	CB-CG-CD2	6.56	131.85	120.70
30	K	344	ARG	CB-CG-CD	6.56	126.38	111.30
12	5	120	MET	CB-CG-SD	6.55	132.34	112.70
12	l	209	THR	CA-C-N	6.54	132.58	121.14
12	l	209	THR	C-N-CA	6.54	132.58	121.14
9	2	178	GLU	CB-CG-CD	6.54	123.72	112.60
7	G	181	ASP	N-CA-C	-6.54	105.12	113.23
9	i	178	GLU	CB-CG-CD	6.54	123.71	112.60
12	l	115	PHE	CB-CG-CD2	6.54	131.81	120.70
1	a	107	LYS	CG-CD-CE	6.53	126.32	111.30
22	S	369	GLN	CG-CD-NE2	-6.53	106.61	116.40
5	e	49	GLY	O-C-N	6.53	131.18	122.70
9	2	177	LYS	CB-CG-CD	6.52	126.30	111.30
13	6	119	ILE	O-C-N	6.52	129.81	122.97
9	i	118	LYS	CG-CD-CE	6.51	126.27	111.30
1	A	107	LYS	CG-CD-CE	6.51	126.27	111.30
10	j	141	THR	N-CA-C	-6.51	105.97	114.04
9	2	118	LYS	CG-CD-CE	6.51	126.27	111.30
9	i	177	LYS	CB-CG-CD	6.50	126.24	111.30
34	8	331	ARG	N-CA-C	-6.50	96.96	110.80
11	4	67	TYR	CZ-CE2-CD2	6.49	131.29	119.60
11	k	67	TYR	CZ-CE2-CD2	6.49	131.28	119.60
3	C	195	LYS	CB-CG-CD	6.49	126.22	111.30
11	4	37	GLN	CB-CG-CD	6.48	123.62	112.60
30	K	241	GLU	OE1-CD-OE2	-6.48	107.34	122.90
10	3	205	ASP	N-CA-C	6.48	129.14	111.00
3	c	195	LYS	CB-CG-CD	6.47	126.19	111.30
13	6	124	GLU	CG-CD-OE2	6.47	133.28	118.40
16	V	185	ILE	CA-C-N	6.47	133.90	121.54
16	V	185	ILE	C-N-CA	6.47	133.90	121.54
13	m	124	GLU	CG-CD-OE2	6.46	133.27	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	L	245	PHE	N-CA-C	-6.46	97.03	110.80
1	A	222	ASP	OD1-CG-OD2	-6.46	107.39	122.90
9	2	38	ASN	OD1-CG-ND2	-6.46	116.14	122.60
1	A	22	GLU	CG-CD-OE2	6.46	133.25	118.40
10	j	18	LYS	CB-CG-CD	6.46	126.15	111.30
10	j	205	ASP	N-CA-C	6.46	129.08	111.00
11	k	37	GLN	CB-CG-CD	6.46	123.58	112.60
20	Z	40	GLU	CA-CB-CG	6.46	127.01	114.10
10	3	18	LYS	CB-CG-CD	6.45	126.14	111.30
17	T	128	TYR	CA-CB-CG	6.45	125.52	113.90
1	a	222	ASP	OD1-CG-OD2	-6.45	107.42	122.90
22	S	153	GLU	N-CA-CB	-6.45	99.59	110.49
5	e	9	ASP	OD1-CG-OD2	-6.44	107.44	122.90
1	a	22	GLU	CG-CD-OE2	6.43	133.19	118.40
9	i	38	ASN	OD1-CG-ND2	-6.43	116.17	122.60
12	5	198	LYS	CA-CB-CG	6.42	126.95	114.10
10	j	3	ASP	CB-CA-C	6.42	118.09	109.42
9	i	113	LYS	CG-CD-CE	6.42	126.06	111.30
13	6	109	ARG	NE-CZ-NH2	-6.42	113.42	119.20
9	2	113	LYS	CG-CD-CE	6.42	126.05	111.30
12	5	164	GLN	CG-CD-OE1	-6.41	107.97	120.80
20	Z	5	SER	CA-C-N	6.41	131.84	122.41
20	Z	5	SER	C-N-CA	6.41	131.84	122.41
11	4	37	GLN	CA-CB-CG	6.41	126.92	114.10
33	J	390	MET	CG-SD-CE	-6.41	86.80	100.90
11	4	11	ASP	OD1-CG-OD2	-6.41	107.52	122.90
12	5	115	PHE	CD1-CE1-CZ	6.40	131.53	120.00
22	S	152	LEU	CA-C-N	6.40	133.77	121.54
22	S	152	LEU	C-N-CA	6.40	133.77	121.54
14	n	109	TYR	CA-C-N	6.40	133.76	121.54
14	n	109	TYR	C-N-CA	6.40	133.76	121.54
10	3	142	ALA	N-CA-C	-6.40	104.09	112.41
12	l	115	PHE	CD1-CE1-CZ	6.40	131.51	120.00
11	k	11	ASP	OD1-CG-OD2	-6.39	107.56	122.90
12	l	164	GLN	CG-CD-OE1	-6.39	108.01	120.80
2	B	53	SER	CA-CB-OG	6.39	123.88	111.10
29	I	345	ASP	N-CA-CB	-6.39	99.69	110.49
11	k	37	GLN	CA-CB-CG	6.39	126.87	114.10
13	6	134	ASP	CB-CG-OD1	-6.39	103.71	118.40
2	b	53	SER	CA-CB-OG	6.38	123.87	111.10
3	c	202	ASP	OD1-CG-OD2	-6.38	107.58	122.90
12	l	198	LYS	CA-CB-CG	6.38	126.86	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	202	ASP	OD1-CG-OD2	-6.38	107.59	122.90
8	1	11	SER	CA-CB-OG	6.38	123.86	111.10
10	3	3	ASP	CB-CA-C	6.38	118.03	109.42
10	3	127	ILE	O-C-N	-6.38	113.78	122.26
13	m	94	ILE	CA-CB-CG1	6.38	121.24	110.40
8	h	11	SER	CA-CB-OG	6.37	123.83	111.10
13	m	134	ASP	CB-CG-OD1	-6.37	103.76	118.40
18	X	119	LYS	CA-CB-CG	6.36	126.82	114.10
31	L	424	GLU	CA-CB-CG	-6.36	101.38	114.10
11	4	12	SER	CA-CB-OG	6.35	123.80	111.10
10	3	155	GLU	OE1-CD-OE2	-6.35	107.67	122.90
10	3	176	ASP	OD1-CG-OD2	-6.35	107.67	122.90
11	k	12	SER	CA-CB-OG	6.34	123.78	111.10
28	H	71	GLU	CB-CG-CD	6.33	123.36	112.60
33	J	10	ILE	CA-C-N	6.33	133.36	121.97
33	J	10	ILE	C-N-CA	6.33	133.36	121.97
10	j	203	ARG	CB-CG-CD	6.32	125.84	111.30
34	8	255	ASN	N-CA-C	-6.32	105.61	113.38
5	e	14	THR	N-CA-C	-6.32	98.91	108.96
11	k	135	TYR	CB-CG-CD1	-6.32	111.33	120.80
11	k	176	PHE	CD1-CE1-CZ	6.31	131.37	120.00
13	m	83	TYR	CD1-CG-CD2	-6.31	108.63	118.10
11	k	186	LYS	CD-CE-NZ	6.31	132.08	111.90
11	4	176	PHE	CD1-CE1-CZ	6.31	131.35	120.00
10	3	203	ARG	CB-CG-CD	6.30	125.80	111.30
10	j	74	TYR	CB-CG-CD2	6.30	130.25	120.80
22	S	97	THR	N-CA-C	6.30	124.22	110.80
22	S	36	LYS	CD-CE-NZ	6.29	132.04	111.90
6	f	13	PHE	CA-C-N	6.29	133.01	121.70
6	f	13	PHE	C-N-CA	6.29	133.01	121.70
10	j	78	GLU	CG-CD-OE1	-6.29	103.94	118.40
5	E	20	ARG	NE-CZ-NH2	-6.29	113.54	119.20
7	G	22	PHE	CA-C-N	6.29	128.99	120.38
7	G	22	PHE	C-N-CA	6.29	128.99	120.38
10	3	74	TYR	CB-CG-CD2	6.29	130.23	120.80
11	4	186	LYS	CD-CE-NZ	6.28	132.01	111.90
13	6	100	ASN	CA-CB-CG	6.28	118.88	112.60
12	l	220	LYS	CA-CB-CG	6.28	126.67	114.10
10	3	78	GLU	CG-CD-OE1	-6.28	103.95	118.40
8	h	31	THR	CA-CB-CG2	6.27	121.16	110.50
7	g	22	PHE	CA-C-N	6.27	128.97	120.38
7	g	22	PHE	C-N-CA	6.27	128.97	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	1	31	THR	CA-CB-CG2	6.26	121.15	110.50
6	F	13	PHE	CA-C-N	6.26	132.97	121.70
6	F	13	PHE	C-N-CA	6.26	132.97	121.70
11	4	135	TYR	CB-CG-CD1	-6.26	111.41	120.80
32	M	96	ASN	OD1-CG-ND2	-6.26	116.34	122.60
8	h	101	ASN	CB-CA-C	-6.26	100.96	109.28
2	B	123	GLN	CA-CB-CG	6.25	126.60	114.10
15	W	22	PRO	O-C-N	-6.25	114.20	122.64
20	Z	721	ASN	CB-CG-OD1	-6.25	108.31	120.80
8	1	101	ASN	CB-CA-C	-6.25	100.97	109.28
12	5	220	LYS	CA-CB-CG	6.25	126.59	114.10
17	T	135	ASN	N-CA-C	-6.24	105.15	114.64
2	b	123	GLN	CA-CB-CG	6.24	126.58	114.10
7	G	245	LYS	O-C-N	-6.24	114.60	122.27
28	H	216	ASP	CA-CB-CG	6.23	118.83	112.60
7	G	224	THR	N-CA-C	-6.23	105.36	114.39
25	R	71	LEU	CA-C-N	6.23	133.18	121.97
25	R	71	LEU	C-N-CA	6.23	133.18	121.97
7	g	114	ASP	OD1-CG-OD2	-6.22	107.96	122.90
20	Z	5	SER	N-CA-C	6.22	124.06	110.80
12	l	104	GLN	CG-CD-NE2	6.22	125.72	116.40
7	G	114	ASP	OD1-CG-OD2	-6.22	107.98	122.90
12	5	104	GLN	CG-CD-NE2	6.21	125.72	116.40
12	l	188	TYR	CE1-CZ-CE2	-6.21	107.88	120.30
11	4	67	TYR	CB-CG-CD1	6.21	130.11	120.80
1	a	217	GLU	OE1-CD-OE2	-6.20	108.01	122.90
21	N	81	TYR	CA-CB-CG	-6.20	102.74	113.90
31	L	273	HIS	CB-CG-CD2	-6.20	123.14	131.20
10	3	74	TYR	CE1-CZ-CE2	-6.20	107.91	120.30
20	Z	85	VAL	N-CA-CB	-6.20	102.54	111.21
31	L	272	GLU	N-CA-C	-6.19	104.79	112.90
5	e	11	GLY	O-C-N	6.19	132.06	123.03
20	Z	943	LYS	CG-CD-CE	-6.18	97.08	111.30
11	k	67	TYR	CB-CG-CD1	6.18	130.07	120.80
11	k	135	TYR	CB-CA-C	-6.18	97.08	109.99
13	6	142	GLU	CG-CD-OE2	-6.18	104.19	118.40
28	H	80	HIS	N-CA-C	-6.18	105.25	114.64
12	5	188	TYR	CE1-CZ-CE2	-6.18	107.94	120.30
8	h	199	PRO	CA-C-N	6.18	129.17	120.28
8	h	199	PRO	C-N-CA	6.18	129.17	120.28
1	A	217	GLU	OE1-CD-OE2	-6.17	108.08	122.90
11	4	135	TYR	CB-CA-C	-6.17	97.09	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	j	74	TYR	CE1-CZ-CE2	-6.17	107.97	120.30
13	6	77	LYS	CG-CD-CE	6.16	125.48	111.30
13	m	142	GLU	CG-CD-OE2	-6.16	104.23	118.40
13	m	77	LYS	CG-CD-CE	6.16	125.46	111.30
9	i	57	ASP	OD1-CG-OD2	-6.15	108.14	122.90
5	e	81	LEU	CB-CA-C	-6.14	101.31	110.16
10	3	19	ASP	CB-CG-OD2	6.14	132.52	118.40
5	e	66	LYS	CG-CD-CE	6.14	125.42	111.30
1	A	95	LEU	CB-CG-CD2	6.14	129.11	110.70
24	Q	170	ASP	N-CA-C	-6.14	103.37	113.50
1	a	95	LEU	CB-CG-CD2	6.14	129.11	110.70
5	E	66	LYS	CG-CD-CE	6.14	125.42	111.30
10	j	19	ASP	CB-CG-OD2	6.13	132.51	118.40
10	j	169	GLN	CA-C-N	6.13	128.49	120.28
10	j	169	GLN	C-N-CA	6.13	128.49	120.28
9	i	173	GLN	CB-CG-CD	6.12	123.01	112.60
5	E	81	LEU	CB-CA-C	-6.12	101.34	110.16
1	A	64	LEU	CB-CG-CD1	-6.12	92.33	110.70
7	G	193	VAL	N-CA-CB	6.12	118.87	110.54
27	O	157	LEU	CB-CA-C	-6.12	101.27	110.88
9	2	57	ASP	OD1-CG-OD2	-6.12	108.21	122.90
13	6	58	ILE	CA-CB-CG2	6.12	120.90	110.50
1	a	64	LEU	CB-CG-CD1	-6.12	92.34	110.70
12	l	77	THR	CA-CB-OG1	6.12	118.78	109.60
10	3	149	MET	CB-CG-SD	6.12	131.05	112.70
9	2	173	GLN	CB-CG-CD	6.12	123.00	112.60
34	8	177	LYS	CB-CG-CD	6.11	125.36	111.30
13	m	58	ILE	CA-CB-CG2	6.11	120.88	110.50
22	S	43	LYS	CD-CE-NZ	-6.11	92.36	111.90
22	S	192	GLU	CG-CD-OE1	6.11	132.44	118.40
13	m	26	GLU	CB-CG-CD	6.10	122.98	112.60
10	j	181	SER	N-CA-C	-6.10	100.05	109.14
7	G	218	TRP	CA-C-O	-6.09	114.16	120.99
11	4	96	ARG	NE-CZ-NH1	6.09	127.59	121.50
12	5	183	GLU	CB-CG-CD	6.09	122.95	112.60
13	6	182	TYR	CA-CB-CG	-6.09	102.94	113.90
13	6	116	HIS	N-CA-C	-6.09	97.37	108.02
13	m	182	TYR	CA-CB-CG	-6.08	102.95	113.90
12	5	77	THR	CA-CB-OG1	6.08	118.72	109.60
13	6	26	GLU	CB-CG-CD	6.08	122.94	112.60
4	D	90	ARG	N-CA-CB	-6.08	101.19	110.12
1	a	239	GLU	OE1-CD-OE2	-6.08	108.32	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	2	231	SER	CA-CB-OG	6.08	123.25	111.10
12	l	183	GLU	CB-CG-CD	6.07	122.92	112.60
29	I	292	TYR	CA-C-O	6.07	121.46	117.94
32	M	411	LYS	CA-CB-CG	6.06	126.23	114.10
11	k	96	ARG	NE-CZ-NH1	6.06	127.56	121.50
1	A	239	GLU	OE1-CD-OE2	-6.06	108.35	122.90
20	Z	276	ASN	CA-CB-CG	6.06	118.66	112.60
22	S	192	GLU	CG-CD-OE2	-6.06	104.45	118.40
9	i	49	SER	CA-CB-OG	6.05	123.21	111.10
13	m	95	ASN	CB-CG-ND2	-6.05	107.32	116.40
11	4	125	LYS	CA-CB-CG	6.05	126.21	114.10
12	l	107	LYS	CB-CG-CD	6.05	125.22	111.30
8	1	157	LYS	CG-CD-CE	6.05	125.22	111.30
13	m	187	GLU	CA-CB-CG	-6.05	102.01	114.10
16	V	194	ARG	CD-NE-CZ	6.05	132.87	124.40
9	2	49	SER	CA-CB-OG	6.04	123.19	111.10
13	6	98	ALA	CA-C-O	-6.04	114.47	120.82
13	6	187	GLU	CA-CB-CG	-6.04	102.02	114.10
28	H	460	THR	CA-C-N	6.04	129.48	120.17
28	H	460	THR	C-N-CA	6.04	129.48	120.17
4	d	149	GLN	CB-CG-CD	6.04	122.86	112.60
11	k	125	LYS	CA-CB-CG	6.04	126.17	114.10
28	H	71	GLU	CA-CB-CG	6.03	126.17	114.10
12	5	107	LYS	CB-CG-CD	6.03	125.17	111.30
8	h	169	SER	CA-CB-OG	6.03	123.16	111.10
9	i	195	ASP	OD1-CG-OD2	-6.03	108.43	122.90
13	m	230	ASP	CB-CA-C	-6.03	98.65	110.10
20	Z	806	GLU	N-CA-C	-6.03	104.04	112.12
8	h	157	LYS	CG-CD-CE	6.03	125.16	111.30
10	3	41	GLU	N-CA-CB	-6.03	100.58	110.52
10	j	162	ASP	CA-C-N	6.02	128.27	120.44
10	j	162	ASP	C-N-CA	6.02	128.27	120.44
7	G	204	HIS	N-CA-C	-6.02	105.51	112.92
10	j	41	GLU	N-CA-CB	-6.02	100.59	110.52
9	2	195	ASP	OD1-CG-OD2	-6.02	108.46	122.90
7	G	211	ASP	CA-CB-CG	6.01	118.61	112.60
10	j	40	PHE	CZ-CE2-CD2	6.01	130.82	120.00
13	6	217	LYS	CG-CD-CE	-6.01	97.48	111.30
10	j	28	ARG	NE-CZ-NH2	6.00	124.60	119.20
12	5	159	SER	CA-CB-OG	6.00	123.11	111.10
30	K	347	ARG	NE-CZ-NH2	6.00	124.60	119.20
5	e	225	GLN	CG-CD-NE2	-6.00	107.40	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	l	188	TYR	CD1-CG-CD2	-6.00	109.10	118.10
5	E	53	ARG	NH1-CZ-NH2	6.00	127.10	119.30
5	E	225	GLN	CG-CD-NE2	-6.00	107.40	116.40
8	h	194	ARG	CA-C-O	-6.00	114.03	120.92
13	6	221	ARG	NE-CZ-NH2	6.00	124.60	119.20
2	B	103	GLU	OE1-CD-OE2	-6.00	108.51	122.90
8	1	169	SER	CA-CB-OG	5.99	123.09	111.10
10	3	131	ASP	OD1-CG-OD2	-5.99	108.52	122.90
13	6	230	ASP	CB-CA-C	-5.99	98.71	110.10
13	6	102	GLN	OE1-CD-NE2	-5.99	116.61	122.60
13	m	94	ILE	CG1-CB-CG2	-5.99	92.74	110.70
7	G	216	ILE	O-C-N	-5.99	116.40	123.05
10	j	199	TYR	CE1-CZ-CE2	-5.99	108.33	120.30
12	5	188	TYR	CD1-CG-CD2	-5.98	109.12	118.10
12	l	104	GLN	CG-CD-OE1	-5.98	108.83	120.80
13	m	217	LYS	CG-CD-CE	-5.98	97.54	111.30
13	6	53	ASP	OD1-CG-OD2	-5.98	108.54	122.90
15	W	82	GLU	N-CA-C	-5.98	105.81	113.23
13	m	221	ARG	NE-CZ-NH2	5.98	124.58	119.20
11	4	127	GLU	CG-CD-OE2	5.98	132.16	118.40
17	T	130	ASP	CB-CG-OD2	5.98	132.16	118.40
13	m	53	ASP	OD1-CG-OD2	-5.98	108.56	122.90
10	3	40	PHE	CZ-CE2-CD2	5.98	130.76	120.00
1	a	74	CYS	CA-C-N	5.97	129.11	123.08
1	a	74	CYS	C-N-CA	5.97	129.11	123.08
30	K	80	LYS	CD-CE-NZ	-5.97	92.78	111.90
7	G	214	LEU	CA-C-O	5.97	127.29	120.54
8	1	112	ASP	CB-CA-C	-5.97	99.95	109.80
12	l	159	SER	CA-CB-OG	5.97	123.04	111.10
2	b	103	GLU	OE1-CD-OE2	-5.97	108.58	122.90
8	h	112	ASP	CB-CA-C	-5.97	99.95	109.80
8	h	198	TYR	CA-C-O	-5.97	114.19	120.88
3	C	209	ASP	OD1-CG-OD2	-5.97	108.58	122.90
16	V	186	GLN	CB-CA-C	-5.96	98.55	110.42
10	3	199	TYR	CE1-CZ-CE2	-5.96	108.38	120.30
11	k	127	GLU	CG-CD-OE2	5.96	132.11	118.40
12	5	104	GLN	CG-CD-OE1	-5.96	108.88	120.80
29	I	124	THR	CA-C-N	5.96	136.34	121.80
29	I	124	THR	C-N-CA	5.96	136.34	121.80
9	i	106	VAL	CA-CB-CG1	5.96	120.53	110.40
11	k	166	GLN	CA-CB-CG	5.96	126.01	114.10
10	3	74	TYR	CD1-CE1-CZ	5.95	130.32	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	i	232	TYR	CA-CB-CG	-5.95	103.19	113.90
10	3	28	ARG	NE-CZ-NH2	5.95	124.56	119.20
31	L	426	LYS	CD-CE-NZ	5.95	130.94	111.90
10	j	141	THR	CA-CB-CG2	-5.95	100.39	110.50
9	2	106	VAL	CA-CB-CG1	5.95	120.51	110.40
3	c	209	ASP	OD1-CG-OD2	-5.94	108.63	122.90
11	4	166	GLN	CA-CB-CG	5.94	125.97	114.10
8	1	183	ARG	NH1-CZ-NH2	-5.94	111.58	119.30
13	6	30	VAL	CG1-CB-CG2	-5.94	97.74	110.80
10	j	142	ALA	N-CA-C	-5.93	104.43	112.26
9	i	58	LYS	CD-CE-NZ	-5.93	92.92	111.90
12	l	191	ASP	OD1-CG-OD2	-5.93	108.67	122.90
12	5	191	ASP	OD1-CG-OD2	-5.93	108.67	122.90
17	T	135	ASN	CB-CG-ND2	-5.93	107.51	116.40
11	k	92	ILE	CA-CB-CG1	5.92	120.47	110.40
7	g	202	LEU	CB-CG-CD2	5.92	128.47	110.70
8	h	183	ARG	NH1-CZ-NH2	-5.92	111.60	119.30
10	j	74	TYR	CD1-CE1-CZ	5.92	130.26	119.60
3	c	222	ASP	OD1-CG-OD2	-5.92	108.69	122.90
11	4	92	ILE	CA-CB-CG1	5.92	120.46	110.40
30	K	246	TYR	CA-CB-CG	-5.92	103.25	113.90
9	2	58	LYS	CD-CE-NZ	-5.92	92.97	111.90
8	1	149	LYS	CD-CE-NZ	5.91	130.82	111.90
11	k	46	PHE	CZ-CE2-CD2	5.91	130.64	120.00
13	m	83	TYR	CE1-CZ-CE2	-5.91	108.48	120.30
12	l	257	GLU	CG-CD-OE1	-5.91	104.81	118.40
3	C	222	ASP	OD1-CG-OD2	-5.91	108.72	122.90
22	S	36	LYS	CA-CB-CG	5.91	125.92	114.10
13	m	30	VAL	CG1-CB-CG2	-5.90	97.81	110.80
21	N	87	ASP	N-CA-CB	5.90	120.47	110.49
11	4	46	PHE	CZ-CE2-CD2	5.90	130.62	120.00
12	5	257	GLU	CG-CD-OE1	-5.90	104.82	118.40
13	6	119	ILE	CB-CA-C	-5.90	103.11	111.19
8	h	149	LYS	CD-CE-NZ	5.90	130.78	111.90
13	m	228	LYS	CB-CG-CD	-5.89	97.74	111.30
13	6	228	LYS	CB-CG-CD	-5.89	97.75	111.30
20	Z	366	LYS	CA-CB-CG	5.89	125.88	114.10
10	j	162	ASP	N-CA-C	-5.89	104.94	111.36
34	8	493	MET	CG-SD-CE	-5.89	87.95	100.90
11	k	23	ARG	NE-CZ-NH2	5.88	124.50	119.20
3	C	224	GLU	CG-CD-OE1	5.88	131.93	118.40
3	c	224	GLU	CG-CD-OE1	5.88	131.93	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	101	GLU	N-CA-CB	-5.88	100.55	110.49
13	6	168	TYR	CE1-CZ-CE2	-5.88	108.54	120.30
6	F	138	ASP	OD1-CG-OD2	-5.88	108.79	122.90
11	4	145	ASP	CA-CB-CG	5.88	118.48	112.60
13	m	168	TYR	CE1-CZ-CE2	-5.88	108.55	120.30
1	A	80	GLY	N-CA-C	-5.88	103.61	112.89
28	H	216	ASP	CB-CA-C	-5.88	98.25	109.95
34	8	270	ASN	N-CA-C	-5.88	106.73	114.31
11	4	23	ARG	NE-CZ-NH2	5.87	124.48	119.20
24	Q	71	LYS	CB-CG-CD	5.87	124.80	111.30
11	k	145	ASP	CA-CB-CG	5.87	118.47	112.60
8	1	153	GLU	CA-CB-CG	-5.87	102.37	114.10
8	h	100	ASP	OD1-CG-OD2	-5.86	108.83	122.90
5	E	104	ASP	OD1-CG-OD2	-5.86	108.83	122.90
3	c	142	ASP	OD1-CG-OD2	-5.86	108.84	122.90
4	D	119	ARG	CB-CA-C	-5.86	101.68	110.88
17	T	97	SER	N-CA-C	-5.86	107.37	114.75
2	b	160	LYS	CD-CE-NZ	5.86	130.65	111.90
13	m	58	ILE	CA-CB-CG1	-5.86	100.44	110.40
8	h	153	GLU	CA-CB-CG	-5.86	102.39	114.10
11	k	191	GLN	CA-CB-CG	5.85	125.81	114.10
24	Q	167	LYS	CD-CE-NZ	5.85	130.63	111.90
28	H	216	ASP	N-CA-CB	5.85	120.25	110.41
13	6	58	ILE	CA-CB-CG1	-5.85	100.45	110.40
10	j	199	TYR	CD1-CG-CD2	-5.85	109.32	118.10
31	L	275	PRO	CA-N-CD	-5.85	103.81	112.00
8	1	100	ASP	OD1-CG-OD2	-5.85	108.86	122.90
11	4	68	SER	CA-CB-OG	5.85	122.80	111.10
9	i	219	TYR	O-C-N	5.85	128.09	122.07
2	B	160	LYS	CD-CE-NZ	5.85	130.61	111.90
22	S	70	ASN	N-CA-C	-5.85	107.14	114.56
5	e	104	ASP	OD1-CG-OD2	-5.85	108.87	122.90
6	f	138	ASP	OD1-CG-OD2	-5.85	108.87	122.90
11	k	68	SER	CA-CB-OG	5.85	122.79	111.10
3	C	142	ASP	OD1-CG-OD2	-5.84	108.87	122.90
7	G	100	LYS	CB-CG-CD	5.84	124.73	111.30
14	7	74	ARG	CG-CD-NE	-5.84	99.15	112.00
10	3	199	TYR	CD1-CG-CD2	-5.84	109.34	118.10
5	e	110	GLU	OE1-CD-OE2	-5.84	108.89	122.90
10	3	118	LYS	CA-CB-CG	5.83	125.77	114.10
11	4	191	GLN	CA-CB-CG	5.83	125.77	114.10
16	V	182	LYS	N-CA-CB	-5.83	101.44	110.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	1	203	GLU	CB-CG-CD	5.83	122.51	112.60
11	4	33	ASP	CA-CB-CG	5.83	118.43	112.60
30	K	80	LYS	CG-CD-CE	5.83	124.71	111.30
7	g	100	LYS	CB-CG-CD	5.83	124.70	111.30
13	m	116	HIS	CB-CG-CD2	-5.83	123.63	131.20
13	6	127	LYS	CD-CE-NZ	5.82	130.54	111.90
13	6	168	TYR	CE1-CZ-OH	5.82	137.37	119.90
10	j	118	LYS	CA-CB-CG	5.82	125.74	114.10
11	k	33	ASP	CA-CB-CG	5.82	118.42	112.60
13	m	127	LYS	CD-CE-NZ	5.82	130.52	111.90
9	2	168	GLU	CG-CD-OE1	-5.82	105.01	118.40
32	M	106	VAL	N-CA-CB	-5.82	101.63	111.23
13	m	13	TYR	CE1-CZ-CE2	-5.81	108.67	120.30
5	E	10	ARG	NH1-CZ-NH2	5.81	126.86	119.30
13	m	168	TYR	CE1-CZ-OH	5.81	137.34	119.90
13	6	13	TYR	CE1-CZ-CE2	-5.81	108.68	120.30
3	c	129	ARG	CG-CD-NE	5.81	124.78	112.00
13	m	50	LYS	CG-CD-CE	5.81	124.66	111.30
26	U	98	LYS	CA-C-N	5.81	130.62	121.56
26	U	98	LYS	C-N-CA	5.81	130.62	121.56
5	e	128	SER	CA-C-N	5.81	127.66	120.34
5	e	128	SER	C-N-CA	5.81	127.66	120.34
5	E	110	GLU	OE1-CD-OE2	-5.81	108.96	122.90
16	V	154	ASP	N-CA-C	-5.80	100.47	109.24
5	E	128	SER	CA-C-N	5.80	127.65	120.34
5	E	128	SER	C-N-CA	5.80	127.65	120.34
7	G	209	GLU	O-C-N	5.80	128.27	122.12
3	C	129	ARG	CG-CD-NE	5.80	124.77	112.00
10	j	98	ARG	CB-CG-CD	5.80	124.64	111.30
5	E	10	ARG	NE-CZ-NH1	-5.80	115.70	121.50
15	W	87	MET	N-CA-CB	-5.80	101.37	110.30
9	i	168	GLU	CG-CD-OE1	-5.80	105.07	118.40
24	Q	195	LYS	CB-CG-CD	5.79	124.63	111.30
11	k	135	TYR	CB-CG-CD2	5.79	129.49	120.80
10	3	98	ARG	CB-CG-CD	5.79	124.62	111.30
13	6	125	ASP	CB-CG-OD2	5.79	131.71	118.40
9	2	245	SER	CA-CB-OG	5.79	122.67	111.10
13	m	109	ARG	N-CA-C	-5.79	106.20	113.72
13	6	50	LYS	CG-CD-CE	5.78	124.60	111.30
7	G	184	PRO	N-CA-CB	5.78	109.32	103.25
34	8	203	GLY	CA-C-N	5.78	132.57	121.54
34	8	203	GLY	C-N-CA	5.78	132.57	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	k	175	ASP	CA-CB-CG	5.77	118.37	112.60
20	Z	361	HIS	CB-CG-CD2	-5.77	123.70	131.20
13	m	125	ASP	CB-CG-OD2	5.77	131.66	118.40
3	c	204	SER	N-CA-C	-5.76	106.87	114.31
8	h	155	MET	CB-CG-SD	5.76	130.00	112.70
8	l	155	MET	CB-CG-SD	5.76	130.00	112.70
8	h	155	MET	CA-CB-CG	5.76	125.63	114.10
3	C	16	GLU	CG-CD-OE2	5.76	131.66	118.40
8	l	155	MET	CA-CB-CG	5.76	125.62	114.10
3	c	16	GLU	CG-CD-OE2	5.76	131.64	118.40
13	m	75	ARG	NE-CZ-NH1	5.76	127.26	121.50
27	O	80	LYS	CB-CG-CD	5.76	124.54	111.30
3	C	204	SER	N-CA-C	-5.75	106.89	114.31
10	j	127	ILE	N-CA-C	-5.75	104.59	113.16
20	Z	824	ASN	N-CA-CB	5.75	118.65	111.00
9	i	193	TRP	CA-C-N	-5.75	113.02	121.99
9	i	193	TRP	C-N-CA	-5.75	113.02	121.99
12	5	160	ASN	OD1-CG-ND2	-5.75	116.85	122.60
11	4	135	TYR	CB-CG-CD2	5.75	129.42	120.80
13	6	94	ILE	N-CA-CB	5.74	118.35	110.54
21	N	632	LYS	CG-CD-CE	5.74	124.50	111.30
9	i	120	GLN	CB-CG-CD	5.74	122.35	112.60
34	8	271	PHE	CA-C-N	5.73	128.28	120.54
34	8	271	PHE	C-N-CA	5.73	128.28	120.54
9	2	120	GLN	CB-CG-CD	5.73	122.34	112.60
2	B	248	GLU	OE1-CD-OE2	-5.72	109.16	122.90
11	4	175	ASP	CA-CB-CG	5.72	118.32	112.60
16	V	186	GLN	N-CA-C	5.72	122.99	110.80
11	k	171	ARG	NH1-CZ-NH2	-5.72	111.86	119.30
12	l	160	ASN	OD1-CG-ND2	-5.72	116.88	122.60
2	b	248	GLU	OE1-CD-OE2	-5.72	109.17	122.90
13	6	110	PHE	CA-CB-CG	5.72	119.52	113.80
13	6	75	ARG	NE-CZ-NH1	5.72	127.22	121.50
2	b	178	ARG	CB-CG-CD	5.71	124.44	111.30
2	B	178	ARG	CB-CG-CD	5.71	124.44	111.30
28	H	190	ARG	N-CA-C	5.71	122.97	110.80
7	g	209	GLU	CB-CG-CD	5.71	122.31	112.60
26	U	100	ARG	NE-CZ-NH2	-5.71	114.07	119.20
12	l	111	GLU	CB-CG-CD	5.70	122.30	112.60
9	2	193	TRP	CA-C-N	-5.70	113.09	121.99
9	2	193	TRP	C-N-CA	-5.70	113.09	121.99
5	e	238	GLU	CA-CB-CG	5.70	125.50	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	i	233	LYS	N-CA-C	-5.70	100.39	109.23
5	E	238	GLU	CA-CB-CG	5.70	125.50	114.10
5	E	9	ASP	CA-CB-CG	5.70	118.30	112.60
21	N	716	GLN	CA-CB-CG	5.70	125.50	114.10
8	h	162	ASP	CA-C-N	5.70	128.38	120.29
8	h	162	ASP	C-N-CA	5.70	128.38	120.29
8	l	17	PHE	N-CA-C	-5.70	100.47	108.96
8	h	175	ASP	OD1-CG-OD2	-5.69	109.24	122.90
18	X	119	LYS	CB-CG-CD	5.69	124.39	111.30
9	i	181	ILE	CG1-CB-CG2	-5.69	93.63	110.70
32	M	53	HIS	CA-CB-CG	5.69	119.49	113.80
12	l	253	TYR	CE1-CZ-CE2	-5.69	108.93	120.30
28	H	314	VAL	CB-CA-C	5.69	120.61	111.29
11	4	171	ARG	NH1-CZ-NH2	-5.68	111.91	119.30
28	H	175	GLY	N-CA-C	-5.68	101.06	110.95
10	j	80	ARG	NE-CZ-NH1	-5.68	115.82	121.50
9	2	181	ILE	CG1-CB-CG2	-5.68	93.65	110.70
12	5	111	GLU	CB-CG-CD	5.68	122.25	112.60
7	G	204	HIS	CG-CD2-NE2	5.68	112.88	107.20
19	Y	36	GLU	N-CA-C	-5.68	107.35	114.56
8	h	193	GLU	N-CA-CB	5.67	119.46	110.55
10	j	8	ASN	CB-CG-OD1	5.67	132.15	120.80
33	J	11	VAL	N-CA-C	5.67	121.14	109.34
10	3	80	ARG	NE-CZ-NH1	-5.67	115.83	121.50
20	Z	632	GLU	CG-CD-OE2	-5.67	105.36	118.40
5	E	134	MET	CA-CB-CG	5.67	125.43	114.10
30	K	199	GLU	CB-CG-CD	5.67	122.23	112.60
12	5	253	TYR	CE1-CZ-CE2	-5.66	108.98	120.30
11	k	120	ASP	CA-CB-CG	5.66	118.26	112.60
10	j	74	TYR	CD1-CG-CD2	-5.65	109.62	118.10
2	B	244	ASN	CA-CB-CG	5.65	118.25	112.60
7	G	244	GLN	OE1-CD-NE2	5.65	128.25	122.60
24	Q	51	ARG	NE-CZ-NH1	5.65	127.15	121.50
32	M	96	ASN	N-CA-CB	-5.65	100.94	110.49
5	e	134	MET	CA-CB-CG	5.65	125.40	114.10
31	L	349	ILE	N-CA-C	-5.65	101.29	107.73
8	l	175	ASP	OD1-CG-OD2	-5.64	109.35	122.90
7	G	182	HIS	CA-C-O	5.64	126.50	120.24
5	e	58	LEU	N-CA-C	-5.63	106.39	113.72
13	6	94	ILE	N-CA-C	-5.63	104.87	110.62
20	Z	528	LEU	CB-CA-C	-5.63	101.79	110.81
10	3	8	ASN	CB-CG-OD1	5.63	132.06	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	Z	84	ALA	CA-C-N	5.63	132.55	122.13
20	Z	84	ALA	C-N-CA	5.63	132.55	122.13
8	h	133	TYR	CD1-CE1-CZ	5.63	129.73	119.60
12	l	253	TYR	CD1-CE1-CZ	5.63	129.73	119.60
2	b	201	GLU	OE1-CD-OE2	-5.63	109.39	122.90
13	m	133	PHE	CB-CG-CD2	5.63	130.27	120.70
13	6	133	PHE	CB-CG-CD2	5.63	130.26	120.70
8	1	133	TYR	CD1-CE1-CZ	5.62	129.72	119.60
9	2	46	ASP	OD1-CG-OD2	-5.62	109.41	122.90
13	6	99	ARG	CD-NE-CZ	-5.62	116.53	124.40
10	j	174	ALA	CA-C-N	5.62	130.97	121.14
10	j	174	ALA	C-N-CA	5.62	130.97	121.14
10	3	74	TYR	CD1-CG-CD2	-5.62	109.67	118.10
12	5	276	LYS	CD-CE-NZ	5.62	129.88	111.90
13	6	131	TYR	CZ-CE2-CD2	5.62	129.71	119.60
11	4	120	ASP	CA-CB-CG	5.62	118.22	112.60
4	D	117	GLN	CA-C-N	5.61	127.80	120.28
4	D	117	GLN	C-N-CA	5.61	127.80	120.28
10	3	154	TYR	CZ-CE2-CD2	5.61	129.71	119.60
20	Z	85	VAL	N-CA-C	5.61	121.01	108.88
5	e	186	GLU	CG-CD-OE2	5.61	131.30	118.40
12	l	276	LYS	CD-CE-NZ	5.61	129.86	111.90
3	C	16	GLU	OE1-CD-OE2	-5.61	109.44	122.90
29	I	359	LYS	CB-CG-CD	5.61	124.20	111.30
16	V	202	ASP	N-CA-C	-5.61	100.99	109.85
2	b	244	ASN	CA-CB-CG	5.61	118.21	112.60
9	i	46	ASP	OD1-CG-OD2	-5.61	109.44	122.90
1	A	149	GLU	OE1-CD-OE2	-5.61	109.44	122.90
2	B	201	GLU	OE1-CD-OE2	-5.61	109.44	122.90
7	G	229	LYS	N-CA-CB	5.61	120.70	111.62
5	e	10	ARG	CD-NE-CZ	5.60	132.25	124.40
2	b	3	ASP	N-CA-C	-5.60	98.87	110.80
9	i	119	TYR	CB-CG-CD2	5.60	129.20	120.80
12	5	253	TYR	CD1-CE1-CZ	5.60	129.68	119.60
8	h	194	ARG	NE-CZ-NH2	-5.60	114.16	119.20
13	m	131	TYR	CZ-CE2-CD2	5.60	129.68	119.60
14	n	97	GLU	CA-CB-CG	5.60	125.29	114.10
1	a	149	GLU	OE1-CD-OE2	-5.59	109.47	122.90
5	E	186	GLU	CG-CD-OE2	5.59	131.27	118.40
13	6	108	LYS	N-CA-CB	5.59	119.33	110.55
33	J	221	LYS	CG-CD-CE	-5.59	98.43	111.30
3	c	16	GLU	OE1-CD-OE2	-5.59	109.48	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	Z	233	LEU	N-CA-C	5.59	122.17	109.81
9	i	219	TYR	CA-C-O	-5.59	114.95	120.82
7	G	234	ASP	CA-CB-CG	5.59	118.19	112.60
1	A	192	ASP	OD1-CG-OD2	-5.59	109.49	122.90
8	1	204	GLN	CA-CB-CG	5.59	125.28	114.10
13	6	125	ASP	OD1-CG-OD2	-5.59	109.49	122.90
2	B	3	ASP	N-CA-C	-5.58	98.90	110.80
25	R	125	GLU	N-CA-C	5.58	122.69	110.80
10	3	165	GLU	OE1-CD-OE2	-5.58	109.50	122.90
7	g	20	ARG	NE-CZ-NH2	5.57	124.22	119.20
7	g	184	PRO	O-C-N	-5.57	115.12	122.64
14	n	121	GLU	N-CA-C	-5.57	102.03	110.50
7	G	240	ILE	N-CA-C	-5.57	104.94	110.62
1	a	192	ASP	OD1-CG-OD2	-5.57	109.54	122.90
3	c	124	GLN	OE1-CD-NE2	-5.57	117.03	122.60
9	2	119	TYR	CB-CG-CD2	5.56	129.15	120.80
12	5	81	PHE	CD1-CE1-CZ	5.56	130.01	120.00
8	h	41	ASP	OD1-CG-OD2	-5.56	109.55	122.90
13	m	125	ASP	OD1-CG-OD2	-5.56	109.55	122.90
10	j	161	GLU	N-CA-CB	5.56	118.30	110.90
20	Z	379	GLN	CG-CD-NE2	-5.55	108.07	116.40
13	6	50	LYS	CA-CB-CG	5.55	125.20	114.10
9	2	217	ARG	CG-CD-NE	5.55	124.21	112.00
8	1	41	ASP	OD1-CG-OD2	-5.55	109.59	122.90
20	Z	611	THR	N-CA-C	-5.55	104.35	113.50
11	4	5	LEU	CA-C-N	-5.54	117.88	121.65
11	4	5	LEU	C-N-CA	-5.54	117.88	121.65
11	4	121	TYR	CZ-CE2-CD2	5.53	129.56	119.60
33	J	140	GLU	CA-C-N	5.53	132.11	121.54
33	J	140	GLU	C-N-CA	5.53	132.11	121.54
7	G	20	ARG	NE-CZ-NH2	5.53	124.18	119.20
12	l	81	PHE	CD1-CE1-CZ	5.53	129.96	120.00
31	L	272	GLU	CA-C-O	5.53	126.07	119.60
3	C	124	GLN	OE1-CD-NE2	-5.53	117.07	122.60
8	1	16	THR	O-C-N	5.53	129.13	122.94
13	m	41	TYR	CD1-CG-CD2	-5.52	109.81	118.10
8	1	201	GLU	CA-CB-CG	-5.52	103.05	114.10
13	m	50	LYS	CA-CB-CG	5.52	125.14	114.10
21	N	862	SER	N-CA-C	-5.52	100.89	109.72
31	L	320	GLN	N-CA-C	-5.52	107.80	114.75
9	i	114	GLN	CG-CD-NE2	5.52	124.67	116.40
7	G	229	LYS	N-CA-C	-5.52	100.92	109.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	6	124	GLU	CG-CD-OE1	-5.52	105.71	118.40
12	5	182	LYS	CB-CG-CD	5.52	123.99	111.30
12	l	182	LYS	CB-CG-CD	5.51	123.98	111.30
20	Z	909	ARG	CA-CB-CG	5.51	125.13	114.10
12	l	241	HIS	CB-CG-ND1	5.51	130.97	122.70
12	l	233	LYS	CD-CE-NZ	-5.51	94.27	111.90
10	j	138	VAL	N-CA-C	-5.51	99.89	108.81
8	1	26	ASP	CB-CG-OD2	-5.50	105.74	118.40
10	j	172	LEU	CA-C-N	5.50	128.10	120.29
10	j	172	LEU	C-N-CA	5.50	128.10	120.29
11	k	121	TYR	CZ-CE2-CD2	5.50	129.51	119.60
3	c	199	LYS	CB-CG-CD	5.50	123.95	111.30
13	6	41	TYR	CD1-CG-CD2	-5.50	109.85	118.10
29	I	275	ALA	CA-C-O	-5.50	112.62	120.16
9	2	114	GLN	CG-CD-NE2	5.50	124.65	116.40
12	5	104	GLN	CB-CG-CD	5.50	121.95	112.60
12	5	233	LYS	CD-CE-NZ	-5.50	94.30	111.90
8	h	26	ASP	CB-CG-OD2	-5.50	105.76	118.40
33	J	96	VAL	CA-C-N	5.50	129.05	120.75
33	J	96	VAL	C-N-CA	5.50	129.05	120.75
12	l	104	GLN	CB-CG-CD	5.50	121.94	112.60
3	C	199	LYS	CB-CG-CD	5.50	123.94	111.30
5	e	177	GLU	CB-CG-CD	5.49	121.94	112.60
13	m	124	GLU	CG-CD-OE1	-5.49	105.77	118.40
13	6	100	ASN	OD1-CG-ND2	5.49	128.09	122.60
13	6	187	GLU	CG-CD-OE2	-5.49	105.77	118.40
1	a	22	GLU	CB-CG-CD	5.49	121.93	112.60
13	6	203	HIS	CB-CG-ND1	5.49	130.93	122.70
34	8	199	ASP	N-CA-C	-5.49	100.35	109.46
13	m	187	GLU	CG-CD-OE2	-5.48	105.80	118.40
10	j	149	MET	CA-C-N	5.48	128.17	120.28
10	j	149	MET	C-N-CA	5.48	128.17	120.28
13	m	203	HIS	CB-CG-ND1	5.47	130.91	122.70
1	A	22	GLU	CB-CG-CD	5.47	121.90	112.60
13	m	141	ARG	CB-CG-CD	5.47	123.87	111.30
9	2	217	ARG	NE-CZ-NH1	-5.46	116.04	121.50
20	Z	853	GLY	N-CA-C	-5.46	106.12	115.08
2	b	146	SER	CA-CB-OG	5.46	122.02	111.10
8	h	154	ASN	CB-CG-ND2	5.46	124.59	116.40
7	G	175	GLU	N-CA-C	-5.46	106.46	113.23
5	E	177	GLU	CB-CG-CD	5.46	121.87	112.60
8	1	154	ASN	CB-CG-ND2	5.46	124.58	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	118	ASP	OD1-CG-OD2	-5.45	109.82	122.90
12	5	241	HIS	CB-CG-ND1	5.45	130.88	122.70
9	2	228	LYS	CA-CB-CG	5.45	125.00	114.10
13	6	134	ASP	CA-CB-CG	5.45	118.05	112.60
29	I	321	ASP	CB-CA-C	5.45	118.43	110.26
6	f	181	LYS	CD-CE-NZ	5.45	129.33	111.90
9	i	134	PRO	CA-C-N	-5.45	113.56	122.54
9	i	134	PRO	C-N-CA	-5.45	113.56	122.54
9	2	134	PRO	CA-C-N	-5.44	113.56	122.54
9	2	134	PRO	C-N-CA	-5.44	113.56	122.54
9	2	219	TYR	CD1-CG-CD2	-5.44	109.94	118.10
5	e	52	LYS	CA-C-N	5.44	131.93	121.54
5	e	52	LYS	C-N-CA	5.44	131.93	121.54
5	E	8	TYR	N-CA-C	-5.44	105.29	113.89
6	F	181	LYS	CD-CE-NZ	5.44	129.31	111.90
10	3	182	GLY	O-C-N	-5.44	115.63	122.70
9	2	248	ASN	CB-CG-ND2	-5.43	108.25	116.40
10	3	113	ASN	CB-CG-ND2	5.43	124.55	116.40
20	Z	498	ALA	N-CA-CB	-5.43	101.31	110.49
10	j	144	ASP	CA-C-N	5.43	127.50	120.44
10	j	144	ASP	C-N-CA	5.43	127.50	120.44
7	G	230	PHE	N-CA-C	-5.43	100.85	109.76
20	Z	802	ASP	N-CA-CB	-5.43	101.31	110.49
32	M	426	LYS	N-CA-C	-5.43	101.68	110.32
5	e	118	ASP	OD1-CG-OD2	-5.43	109.87	122.90
35	9	34	GLU	N-CA-C	-5.43	107.31	114.04
20	Z	613	ASP	N-CA-C	-5.43	107.67	114.56
10	3	41	GLU	CB-CA-C	5.43	118.60	109.48
3	c	17	GLY	N-CA-C	-5.42	107.11	116.01
34	8	149	SER	N-CA-C	-5.42	106.14	114.16
8	1	101	ASN	CA-CB-CG	5.42	118.02	112.60
9	2	243	LYS	CD-CE-NZ	5.42	129.24	111.90
13	6	141	ARG	CB-CG-CD	5.42	123.77	111.30
13	m	134	ASP	CA-CB-CG	5.42	118.02	112.60
3	C	17	GLY	N-CA-C	-5.42	107.12	116.01
21	N	123	PHE	N-CA-C	-5.42	104.36	112.54
10	3	77	LYS	CB-CG-CD	5.42	123.76	111.30
2	B	146	SER	CA-CB-OG	5.41	121.93	111.10
8	1	120	TYR	CD1-CE1-CZ	5.41	129.34	119.60
27	O	80	LYS	N-CA-CB	-5.41	101.58	110.40
2	B	217	GLU	OE1-CD-OE2	-5.41	109.92	122.90
8	h	115	ASN	CB-CG-ND2	5.41	124.51	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	244	ASN	CB-CG-ND2	-5.40	108.29	116.40
10	j	41	GLU	CB-CA-C	5.40	118.56	109.48
9	2	126	TYR	CZ-CE2-CD2	5.40	129.32	119.60
9	i	126	TYR	CZ-CE2-CD2	5.40	129.31	119.60
2	B	244	ASN	CB-CG-ND2	-5.40	108.31	116.40
2	b	217	GLU	OE1-CD-OE2	-5.39	109.95	122.90
8	h	120	TYR	CD1-CE1-CZ	5.39	129.30	119.60
10	j	77	LYS	CB-CG-CD	5.39	123.69	111.30
8	1	115	ASN	CB-CG-ND2	5.39	124.48	116.40
34	8	125	GLN	CA-CB-CG	5.39	124.87	114.10
1	a	184	ASN	OD1-CG-ND2	-5.38	117.22	122.60
14	7	259	LYS	CB-CG-CD	-5.38	98.93	111.30
10	j	113	ASN	CB-CG-ND2	5.38	124.47	116.40
30	K	346	ARG	CB-CG-CD	5.38	123.67	111.30
13	m	228	LYS	CA-CB-CG	5.38	124.85	114.10
7	G	20	ARG	NE-CZ-NH1	-5.37	116.13	121.50
13	6	90	LYS	N-CA-C	-5.37	100.42	108.96
25	R	297	TYR	CA-CB-CG	5.37	123.57	113.90
9	2	30	THR	CA-CB-CG2	5.37	119.63	110.50
6	f	9	ASP	OD1-CG-OD2	-5.37	110.02	122.90
10	j	159	GLU	CA-C-O	-5.37	114.64	120.87
12	l	84	GLN	CB-CG-CD	-5.37	103.47	112.60
13	6	228	LYS	CA-CB-CG	5.37	124.84	114.10
9	i	30	THR	CA-CB-CG2	5.37	119.62	110.50
34	8	209	ASP	N-CA-C	-5.37	99.37	110.80
26	U	135	ASP	N-CA-C	-5.36	101.83	110.14
11	4	186	LYS	CG-CD-CE	-5.36	98.97	111.30
7	g	20	ARG	NE-CZ-NH1	-5.36	116.14	121.50
5	E	180	GLN	CG-CD-OE1	-5.36	110.08	120.80
12	l	222	ASP	CA-CB-CG	5.36	117.96	112.60
4	d	169	LYS	CB-CG-CD	5.36	123.62	111.30
5	e	177	GLU	CA-CB-CG	5.36	124.81	114.10
7	g	223	GLU	OE1-CD-OE2	-5.36	110.04	122.90
5	e	180	GLN	CG-CD-OE1	-5.36	110.09	120.80
8	h	93	GLU	OE1-CD-OE2	-5.36	110.05	122.90
6	F	9	ASP	OD1-CG-OD2	-5.36	110.05	122.90
3	c	42	ASP	N-CA-C	-5.35	106.13	113.30
33	J	400	VAL	N-CA-C	-5.35	98.21	109.34
34	8	267	GLY	N-CA-C	-5.35	107.40	115.32
2	b	22	ASP	OD1-CG-OD2	-5.35	110.07	122.90
12	5	222	ASP	CA-CB-CG	5.35	117.95	112.60
13	6	104	LEU	CA-C-N	5.35	128.22	120.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	6	104	LEU	C-N-CA	5.35	128.22	120.79
31	L	258	GLU	N-CA-C	-5.35	106.92	113.50
7	G	204	HIS	CE1-NE2-CD2	-5.35	103.65	109.00
7	g	185	GLU	CA-C-N	-5.34	113.25	123.03
7	g	185	GLU	C-N-CA	-5.34	113.25	123.03
11	k	186	LYS	CG-CD-CE	-5.34	99.01	111.30
8	l	93	GLU	OE1-CD-OE2	-5.34	110.08	122.90
31	L	137	ARG	CG-CD-NE	5.34	123.75	112.00
5	E	177	GLU	CA-CB-CG	5.34	124.77	114.10
12	5	84	GLN	CB-CG-CD	-5.34	103.53	112.60
26	U	180	ASP	N-CA-C	-5.33	106.66	114.39
13	m	131	TYR	CB-CG-CD1	5.33	128.80	120.80
14	n	137	ARG	NE-CZ-NH2	5.33	124.00	119.20
31	L	265	GLU	CA-CB-CG	-5.33	103.43	114.10
12	l	188	TYR	CZ-CE2-CD2	5.33	129.20	119.60
3	C	42	ASP	N-CA-C	-5.33	106.16	113.30
13	m	112	PRO	CA-N-CD	-5.33	104.54	112.00
8	h	101	ASN	CA-CB-CG	5.33	117.93	112.60
11	k	65	GLN	CB-CG-CD	5.33	121.66	112.60
1	A	76	SER	CA-C-O	-5.33	114.54	121.73
12	5	139	ARG	NE-CZ-NH1	5.33	126.83	121.50
2	B	22	ASP	OD1-CG-OD2	-5.32	110.13	122.90
11	4	65	GLN	CB-CG-CD	5.32	121.64	112.60
1	A	184	ASN	OD1-CG-ND2	-5.32	117.28	122.60
20	Z	40	GLU	CG-CD-OE2	-5.32	106.17	118.40
23	P	404	LYS	N-CA-C	-5.32	102.96	110.29
9	i	214	GLU	N-CA-C	-5.31	100.07	108.73
12	l	139	ARG	NE-CZ-NH1	5.31	126.81	121.50
32	M	106	VAL	N-CA-C	5.31	120.39	109.34
6	f	232	LYS	CA-CB-CG	5.31	124.71	114.10
6	F	232	LYS	CA-CB-CG	5.30	124.71	114.10
13	m	181	LYS	N-CA-CB	-5.30	102.86	110.44
12	5	188	TYR	CZ-CE2-CD2	5.30	129.14	119.60
10	j	130	ILE	CA-C-O	-5.29	115.00	121.04
11	k	19	LYS	CG-CD-CE	5.29	123.48	111.30
13	6	26	GLU	CG-CD-OE2	-5.29	106.22	118.40
20	Z	309	GLN	N-CA-C	5.29	122.07	110.80
13	6	40	ASP	CB-CG-OD2	5.29	130.57	118.40
31	L	150	ILE	N-CA-C	-5.29	106.27	111.77
33	J	285	SER	N-CA-C	5.29	122.07	110.80
5	e	209	GLU	OE1-CD-OE2	-5.29	110.20	122.90
11	4	19	LYS	CG-CD-CE	5.29	123.46	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	6	26	GLU	CG-CD-OE1	5.29	130.56	118.40
6	f	69	HIS	CB-CG-ND1	5.29	130.63	122.70
10	j	143	SER	O-C-N	5.29	128.41	122.22
11	k	163	LEU	CB-CG-CD1	5.29	126.56	110.70
13	m	40	ASP	CB-CG-OD2	5.29	130.56	118.40
5	E	209	GLU	OE1-CD-OE2	-5.29	110.22	122.90
11	4	163	LEU	CB-CG-CD1	5.29	126.56	110.70
31	L	426	LYS	CA-CB-CG	-5.28	103.53	114.10
12	5	242	ARG	NE-CZ-NH1	-5.28	116.22	121.50
13	6	131	TYR	CB-CG-CD1	5.28	128.72	120.80
28	H	180	LYS	CG-CD-CE	5.28	123.45	111.30
12	5	164	GLN	CA-CB-CG	-5.28	103.54	114.10
11	4	155	GLU	OE1-CD-OE2	-5.27	110.24	122.90
13	m	26	GLU	CG-CD-OE2	-5.27	106.27	118.40
5	E	105	GLU	CG-CD-OE2	5.27	130.53	118.40
7	G	182	HIS	N-CA-CB	5.27	118.06	110.20
5	e	105	GLU	CG-CD-OE2	5.27	130.52	118.40
10	3	97	GLU	CB-CG-CD	5.27	121.56	112.60
3	c	109	GLU	CG-CD-OE1	-5.26	106.29	118.40
13	6	181	LYS	N-CA-CB	-5.26	102.91	110.44
33	J	278	GLN	CA-CB-CG	5.26	124.63	114.10
8	1	73	GLU	CG-CD-OE2	-5.26	106.30	118.40
13	6	87	HIS	CE1-NE2-CD2	-5.26	103.74	109.00
12	5	188	TYR	CB-CG-CD1	5.26	128.69	120.80
10	j	97	GLU	CB-CG-CD	5.26	121.54	112.60
11	k	155	GLU	OE1-CD-OE2	-5.26	110.28	122.90
9	i	48	ARG	NE-CZ-NH2	5.26	123.93	119.20
13	m	26	GLU	CG-CD-OE1	5.26	130.49	118.40
8	h	73	GLU	CG-CD-OE2	-5.25	106.31	118.40
9	i	215	TYR	N-CA-C	-5.25	99.22	108.20
6	F	69	HIS	CB-CG-ND1	5.25	130.58	122.70
20	Z	82	MET	N-CA-CB	-5.25	101.67	110.65
11	k	63	ASN	OD1-CG-ND2	-5.25	117.35	122.60
12	l	242	ARG	NE-CZ-NH1	-5.25	116.25	121.50
9	2	48	ARG	NE-CZ-NH2	5.25	123.93	119.20
9	i	229	GLN	OE1-CD-NE2	5.25	127.85	122.60
12	l	164	GLN	CA-CB-CG	-5.25	103.61	114.10
33	J	57	PHE	CA-CB-CG	5.25	119.05	113.80
7	G	176	LEU	N-CA-CB	-5.24	101.69	110.39
11	4	63	ASN	OD1-CG-ND2	-5.24	117.36	122.60
12	l	161	LEU	CA-CB-CG	5.24	134.65	116.30
12	5	161	LEU	CA-CB-CG	5.24	134.64	116.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	Z	40	GLU	CG-CD-OE1	5.24	130.45	118.40
29	I	125	MET	CB-CA-C	-5.24	99.85	110.17
12	l	128	GLN	CB-CG-CD	5.24	121.51	112.60
12	5	128	GLN	CB-CG-CD	5.24	121.50	112.60
10	j	97	GLU	CG-CD-OE1	-5.23	106.36	118.40
29	I	246	ARG	NE-CZ-NH1	-5.23	116.27	121.50
12	l	188	TYR	CB-CG-CD1	5.23	128.65	120.80
7	g	247	ILE	CB-CG1-CD1	5.23	124.78	113.80
20	Z	379	GLN	CB-CG-CD	5.23	121.49	112.60
32	M	300	GLU	CA-CB-CG	5.23	124.56	114.10
3	C	195	LYS	CG-CD-CE	5.23	123.32	111.30
32	M	293	SER	N-CA-C	-5.23	98.71	108.02
5	e	18	GLU	N-CA-C	-5.23	99.67	110.80
10	j	94	SER	CA-CB-OG	5.23	121.55	111.10
13	m	133	PHE	CD1-CE1-CZ	5.22	129.41	120.00
6	F	164	ARG	NE-CZ-NH2	5.22	123.90	119.20
10	3	97	GLU	CG-CD-OE1	-5.22	106.39	118.40
10	3	94	SER	CA-CB-OG	5.22	121.54	111.10
33	J	221	LYS	N-CA-C	-5.22	105.19	112.03
3	c	195	LYS	CG-CD-CE	5.22	123.31	111.30
11	k	4	ILE	N-CA-C	-5.22	98.49	109.34
11	k	49	GLU	CB-CA-C	-5.22	102.97	111.68
3	C	109	GLU	CG-CD-OE1	-5.22	106.40	118.40
9	2	224	VAL	CG1-CB-CG2	-5.22	99.32	110.80
11	4	110	LYS	CA-CB-CG	5.22	124.53	114.10
5	e	56	SER	CA-C-O	-5.21	115.54	120.34
11	k	110	LYS	CA-CB-CG	5.21	124.53	114.10
5	E	32	LYS	CD-CE-NZ	5.21	128.59	111.90
9	2	208	GLU	CG-CD-OE2	5.21	130.38	118.40
18	X	112	ASN	CA-CB-CG	5.21	117.81	112.60
26	U	131	GLY	N-CA-C	-5.21	100.83	113.18
20	Z	841	GLU	N-CA-C	-5.21	101.27	109.50
22	S	271	ARG	CB-CG-CD	5.21	123.28	111.30
14	7	106	GLU	CB-CA-C	-5.21	102.71	110.88
11	4	49	GLU	CB-CA-C	-5.20	102.99	111.68
18	X	20	ASP	CA-C-N	5.20	129.18	120.70
18	X	20	ASP	C-N-CA	5.20	129.18	120.70
31	L	413	ASP	N-CA-C	-5.20	105.67	112.23
12	l	144	ARG	CB-CG-CD	5.20	123.26	111.30
33	J	284	THR	N-CA-C	5.20	121.87	110.80
7	G	195	GLN	CA-C-N	5.20	127.67	120.29
7	G	195	GLN	C-N-CA	5.20	127.67	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	j	179	ALA	CA-C-O	-5.19	114.00	119.97
13	m	91	LYS	CG-CD-CE	5.19	123.24	111.30
5	e	32	LYS	CD-CE-NZ	5.19	128.51	111.90
9	i	208	GLU	CG-CD-OE2	5.19	130.34	118.40
8	l	101	ASN	CB-CG-ND2	5.19	124.19	116.40
13	6	133	PHE	CD1-CE1-CZ	5.19	129.34	120.00
19	Y	68	GLU	N-CA-CB	5.19	119.26	110.49
1	A	79	ILE	CA-C-O	-5.19	115.23	120.31
11	k	121	TYR	CD1-CE1-CZ	5.18	128.93	119.60
12	5	258	ASP	OD1-CG-OD2	-5.18	110.46	122.90
2	B	205	ASN	OD1-CG-ND2	-5.18	117.42	122.60
11	4	19	LYS	CD-CE-NZ	-5.18	95.31	111.90
28	H	180	LYS	CB-CG-CD	5.18	123.22	111.30
34	8	268	THR	N-CA-C	-5.18	106.36	113.30
12	5	144	ARG	CB-CG-CD	5.18	123.22	111.30
1	A	149	GLU	CG-CD-OE2	5.18	130.31	118.40
5	E	105	GLU	OE1-CD-OE2	-5.18	110.47	122.90
7	G	185	GLU	CA-C-N	5.18	137.72	120.42
7	G	185	GLU	C-N-CA	5.18	137.72	120.42
13	m	107	GLY	CA-C-N	5.18	129.26	122.06
13	m	107	GLY	C-N-CA	5.18	129.26	122.06
8	h	101	ASN	CB-CG-ND2	5.18	124.17	116.40
13	m	13	TYR	CZ-CE2-CD2	5.18	128.92	119.60
13	6	13	TYR	CZ-CE2-CD2	5.18	128.92	119.60
3	c	109	GLU	CG-CD-OE2	5.17	130.30	118.40
5	e	105	GLU	OE1-CD-OE2	-5.17	110.48	122.90
10	j	167	ILE	CA-C-N	5.17	127.48	120.44
10	j	167	ILE	C-N-CA	5.17	127.48	120.44
12	l	83	PHE	CA-CB-CG	5.17	118.97	113.80
3	C	179	ASP	OD1-CG-OD2	-5.17	110.48	122.90
13	6	47	TYR	CD1-CE1-CZ	5.17	128.91	119.60
13	6	102	GLN	CA-C-O	5.17	126.03	120.55
13	m	208	ASP	CB-CG-OD2	-5.17	106.50	118.40
11	4	98	TYR	CB-CG-CD1	5.17	128.56	120.80
2	b	205	ASN	OD1-CG-ND2	-5.17	117.43	122.60
21	N	471	TYR	CA-CB-CG	5.17	123.20	113.90
34	8	199	ASP	N-CA-CB	5.17	118.69	110.16
6	f	164	ARG	NE-CZ-NH2	5.17	123.85	119.20
3	C	109	GLU	CG-CD-OE2	5.17	130.28	118.40
11	k	19	LYS	CD-CE-NZ	-5.17	95.37	111.90
12	l	258	ASP	OD1-CG-OD2	-5.16	110.51	122.90
11	4	121	TYR	CD1-CE1-CZ	5.16	128.89	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	149	GLU	CG-CD-OE2	5.16	130.27	118.40
23	P	275	ASN	CA-C-N	5.16	127.50	120.54
23	P	275	ASN	C-N-CA	5.16	127.50	120.54
3	c	179	ASP	OD1-CG-OD2	-5.16	110.52	122.90
10	3	74	TYR	CE1-CZ-OH	5.16	135.37	119.90
12	5	210	PHE	CA-C-N	5.16	127.14	120.44
12	5	210	PHE	C-N-CA	5.16	127.14	120.44
32	M	305	MET	CB-CG-SD	5.16	128.16	112.70
9	2	34	GLY	N-CA-C	-5.15	100.97	113.18
10	j	74	TYR	CE1-CZ-OH	5.15	135.35	119.90
13	m	47	TYR	CD1-CE1-CZ	5.15	128.86	119.60
20	Z	593	HIS	N-CA-C	-5.15	102.28	108.25
7	g	71	ASP	N-CA-CB	-5.15	101.79	110.49
11	k	98	TYR	CB-CG-CD1	5.14	128.52	120.80
13	6	208	ASP	CB-CG-OD2	-5.14	106.57	118.40
6	f	205	SER	N-CA-CB	5.14	119.18	110.49
14	n	110	ASP	CB-CA-C	-5.14	100.20	110.42
2	B	151	ASP	OD1-CG-OD2	-5.14	110.57	122.90
7	G	199	ILE	CA-CB-CG1	5.14	119.13	110.40
24	Q	167	LYS	CB-CG-CD	5.13	123.11	111.30
3	c	127	GLY	N-CA-C	-5.13	108.17	115.30
9	i	34	GLY	N-CA-C	-5.13	101.02	113.18
6	F	205	SER	N-CA-CB	5.13	119.16	110.49
2	b	151	ASP	OD1-CG-OD2	-5.13	110.58	122.90
8	h	197	PHE	CD1-CG-CD2	-5.13	110.90	118.60
7	G	185	GLU	O-C-N	5.13	126.62	121.85
1	a	201	LYS	CG-CD-CE	5.13	123.09	111.30
2	b	81	ASP	OD1-CG-OD2	-5.13	110.59	122.90
28	H	458	SER	CA-C-N	5.13	131.34	121.54
28	H	458	SER	C-N-CA	5.13	131.34	121.54
7	G	71	ASP	N-CA-CB	-5.13	101.83	110.49
21	N	689	LYS	CG-CD-CE	5.13	123.09	111.30
24	Q	273	ASN	N-CA-C	-5.12	105.87	113.40
27	O	80	LYS	CB-CA-C	5.12	120.70	109.99
17	T	144	TYR	CA-CB-CG	5.12	123.12	113.90
8	h	205	LEU	N-CA-CB	5.12	119.21	110.50
1	A	201	LYS	CG-CD-CE	5.12	123.08	111.30
3	C	127	GLY	N-CA-C	-5.12	108.18	115.30
2	B	81	ASP	OD1-CG-OD2	-5.12	110.62	122.90
28	H	344	ASP	N-CA-CB	5.12	120.22	110.49
13	6	103	HIS	CE1-NE2-CD2	-5.11	103.89	109.00
13	m	30	VAL	CA-CB-CG2	5.11	119.09	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	183	HIS	ND1-CE1-NE2	5.11	113.51	108.40
21	N	895	LYS	CA-C-N	5.11	128.36	121.05
21	N	895	LYS	C-N-CA	5.11	128.36	121.05
24	Q	47	ASP	CA-C-N	5.11	131.30	121.54
24	Q	47	ASP	C-N-CA	5.11	131.30	121.54
12	l	170	LEU	N-CA-C	-5.11	101.78	109.85
29	I	161	GLN	CB-CA-C	-5.11	102.83	110.90
8	1	29	THR	CA-CB-CG2	5.11	119.18	110.50
4	D	50	SER	N-CA-C	-5.10	105.35	112.03
13	m	13	TYR	CD1-CG-CD2	-5.10	110.45	118.10
13	m	90	LYS	CB-CG-CD	5.10	123.03	111.30
7	G	174	ALA	O-C-N	5.10	128.18	122.22
3	C	165	VAL	CG1-CB-CG2	-5.09	99.59	110.80
34	8	348	GLU	CG-CD-OE1	-5.09	106.68	118.40
10	j	151	GLU	CA-C-O	5.09	126.17	120.82
12	l	251	ASN	OD1-CG-ND2	-5.09	117.51	122.60
3	c	165	VAL	CG1-CB-CG2	-5.09	99.60	110.80
8	h	163	PHE	O-C-N	5.09	127.95	122.15
13	6	30	VAL	CA-CB-CG2	5.09	119.05	110.40
31	L	273	HIS	CA-C-N	5.09	127.49	120.67
31	L	273	HIS	C-N-CA	5.09	127.49	120.67
16	V	218	LYS	N-CA-C	-5.09	106.76	113.17
9	2	228	LYS	CB-CG-CD	5.08	122.99	111.30
12	5	170	LEU	N-CA-C	-5.08	101.82	109.85
21	N	175	ASP	N-CA-C	-5.08	106.64	114.16
13	m	94	ILE	CB-CG1-CD1	5.08	124.47	113.80
7	G	224	THR	CA-C-O	-5.08	112.85	118.69
11	k	33	ASP	CB-CA-C	-5.08	101.29	109.72
11	4	33	ASP	CB-CA-C	-5.07	101.30	109.72
7	g	232	LYS	CD-CE-NZ	5.07	128.13	111.90
13	m	110	PHE	N-CA-C	-5.07	106.34	112.88
13	6	13	TYR	CD1-CG-CD2	-5.07	110.49	118.10
9	i	208	GLU	CA-CB-CG	5.07	124.24	114.10
9	i	211	LYS	CB-CA-C	-5.07	99.56	110.45
6	F	80	ASP	OD1-CG-OD2	-5.07	110.75	122.90
9	2	211	LYS	CB-CA-C	-5.07	99.56	110.45
10	3	198	ARG	NH1-CZ-NH2	-5.07	112.71	119.30
21	N	689	LYS	N-CA-C	-5.07	105.80	112.94
26	U	126	LYS	N-CA-C	-5.07	107.08	114.12
9	i	39	ASN	CB-CG-ND2	5.06	124.00	116.40
10	j	134	LYS	CB-CA-C	-5.06	102.55	110.85
9	2	208	GLU	CA-CB-CG	5.06	124.22	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	L	141	LYS	CA-CB-CG	5.06	124.22	114.10
8	h	29	THR	CA-CB-CG2	5.06	119.10	110.50
9	2	51	GLN	CB-CA-C	-5.06	103.38	111.17
9	i	51	GLN	CB-CA-C	-5.06	103.38	111.17
29	I	300	ARG	N-CA-CB	-5.06	102.69	110.12
31	L	206	ILE	N-CA-C	-5.06	105.63	113.16
8	h	61	THR	OG1-CB-CG2	-5.05	99.19	109.30
9	2	232	TYR	CB-CG-CD2	5.05	128.38	120.80
32	M	259	GLY	N-CA-C	-5.05	106.28	113.86
10	j	166	THR	CA-CB-OG1	5.05	117.18	109.60
11	k	180	ILE	CG1-CB-CG2	-5.05	95.54	110.70
8	1	61	THR	OG1-CB-CG2	-5.05	99.20	109.30
9	2	227	GLU	CG-CD-OE1	5.05	130.01	118.40
29	I	277	SER	N-CA-C	5.05	117.63	108.69
3	c	60	ASP	OD1-CG-OD2	-5.05	110.79	122.90
24	Q	51	ARG	CD-NE-CZ	5.05	131.47	124.40
18	X	83	SER	N-CA-C	-5.04	101.41	109.23
9	2	39	ASN	CB-CG-ND2	5.04	123.97	116.40
8	h	133	TYR	CZ-CE2-CD2	5.04	128.67	119.60
11	4	180	ILE	CG1-CB-CG2	-5.04	95.58	110.70
3	c	202	ASP	CB-CG-OD1	5.04	129.98	118.40
6	f	80	ASP	OD1-CG-OD2	-5.04	110.81	122.90
10	j	15	MET	CA-CB-CG	5.03	124.17	114.10
32	M	411	LYS	CB-CG-CD	5.03	122.88	111.30
9	2	219	TYR	CE1-CZ-CE2	-5.03	110.24	120.30
12	5	251	ASN	OD1-CG-ND2	-5.03	117.57	122.60
13	6	143	GLN	N-CA-C	-5.03	106.83	113.12
30	K	123	LEU	CA-C-N	5.03	127.99	120.90
30	K	123	LEU	C-N-CA	5.03	127.99	120.90
13	m	134	ASP	CB-CG-OD2	5.03	129.97	118.40
10	3	173	ASN	CB-CG-ND2	5.03	123.94	116.40
20	Z	774	ARG	CG-CD-NE	-5.03	100.94	112.00
10	j	198	ARG	NH1-CZ-NH2	-5.03	112.76	119.30
13	6	175	LYS	CG-CD-CE	5.03	122.86	111.30
31	L	331	ASP	N-CA-C	-5.02	105.25	113.19
13	m	175	LYS	CG-CD-CE	5.02	122.85	111.30
31	L	411	ASN	N-CA-C	-5.02	103.22	110.40
7	g	206	ASP	OD1-CG-OD2	-5.02	110.86	122.90
1	A	192	ASP	CB-CG-OD2	5.02	129.94	118.40
13	m	81	LYS	CG-CD-CE	5.02	122.84	111.30
1	a	192	ASP	CB-CG-OD2	5.01	129.94	118.40
3	C	60	ASP	OD1-CG-OD2	-5.01	110.87	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	173	GLU	OE1-CD-OE2	-5.01	110.86	122.90
12	5	146	LYS	CA-C-N	-5.01	112.97	121.85
12	5	146	LYS	C-N-CA	-5.01	112.97	121.85
9	i	218	ASN	CA-CB-CG	-5.01	107.59	112.60
3	C	202	ASP	CB-CG-OD1	5.01	129.93	118.40
28	H	90	ARG	CA-C-N	5.01	131.11	121.54
28	H	90	ARG	C-N-CA	5.01	131.11	121.54
29	I	196	GLU	N-CA-C	-5.01	105.27	113.19
6	f	173	GLU	OE1-CD-OE2	-5.01	110.88	122.90
9	2	86	GLN	OE1-CD-NE2	-5.01	117.59	122.60
13	6	134	ASP	CB-CG-OD2	5.01	129.92	118.40
10	j	155	GLU	CA-C-N	5.01	126.10	119.84
10	j	155	GLU	C-N-CA	5.01	126.10	119.84
9	i	120	GLN	CA-CB-CG	-5.01	104.09	114.10
12	l	146	LYS	CA-C-N	-5.01	112.99	121.85
12	l	146	LYS	C-N-CA	-5.01	112.99	121.85
9	2	120	GLN	CA-CB-CG	-5.01	104.08	114.10
10	3	15	MET	CA-CB-CG	5.01	124.11	114.10
13	m	143	GLN	N-CA-C	-5.00	106.87	113.12
9	i	86	GLN	OE1-CD-NE2	-5.00	117.60	122.60
22	S	485	LYS	CG-CD-CE	5.00	122.80	111.30

There are no chirality outliers.

All (230) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	1	201	GLU	Sidechain
9	2	124	GLY	Mainchain
9	2	200	SER	Mainchain
9	2	248	ASN	Sidechain
9	2	37	PHE	Sidechain
9	2	38	ASN	Sidechain
9	2	51	GLN	Sidechain
10	3	126	LEU	Mainchain
10	3	85	GLU	Sidechain
11	4	78	GLN	Sidechain
12	5	147	GLU	Sidechain
12	5	196	ARG	Sidechain
12	5	83	PHE	Mainchain
13	6	13	TYR	Sidechain
13	6	181	LYS	Mainchain
13	6	182	TYR	Sidechain

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Mol	Chain	Res	Type	Group
13	6	36	ARG	Sidechain
13	6	70	ASP	Sidechain
14	7	106	GLU	Sidechain
14	7	74	ARG	Sidechain
34	8	131	ASN	Sidechain
34	8	152	GLN	Sidechain
34	8	153	ASP	Sidechain
34	8	175	SER	Peptide
34	8	181	PRO	Peptide
34	8	208	GLN	Peptide
34	8	244	THR	Peptide
34	8	282	GLU	Sidechain
34	8	330	LEU	Peptide
34	8	343	ASP	Sidechain
34	8	368	ASN	Sidechain
34	8	444	GLU	Sidechain
34	8	448	TYR	Peptide
34	8	466	ASP	Sidechain
34	8	497	PHE	Mainchain
35	9	75	GLY	Peptide
1	A	115	ASP	Sidechain
1	A	250	GLU	Sidechain
1	A	77	ARG	Sidechain
2	B	234	ARG	Sidechain
3	C	105	ASP	Sidechain
3	C	109	GLU	Sidechain
3	C	63	THR	Mainchain
4	D	102	ASP	Mainchain
4	D	122	GLN	Sidechain
4	D	204	GLN	Mainchain
4	D	5	ASP	Sidechain
5	E	104	ASP	Sidechain
5	E	106	ASP	Sidechain
5	E	17	PRO	Peptide
5	E	206	GLN	Sidechain
6	F	13	PHE	Peptide
6	F	18	ARG	Peptide
6	F	205	SER	Mainchain
7	G	13	SER	Peptide
7	G	183	HIS	Sidechain
7	G	190	ARG	Sidechain
7	G	21	ASN	Peptide

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Mol	Chain	Res	Type	Group
7	G	242	PHE	Sidechain
7	G	72	ARG	Sidechain
28	H	151	GLN	Peptide
28	H	160	GLY	Peptide
28	H	241	ASP	Sidechain
28	H	313	ALA	Peptide
28	H	326	ASP	Sidechain
28	H	466	TYR	Mainchain
28	H	93	GLU	Sidechain
28	H	94	GLU	Peptide
28	H	96	PRO	Peptide
29	I	101	GLY	Peptide
29	I	104	LEU	Peptide
29	I	137	ASP	Sidechain
29	I	174	ASP	Sidechain
29	I	179	GLU	Sidechain
29	I	280	PHE	Sidechain
29	I	282	ASP	Sidechain
29	I	285	ASP	Sidechain
29	I	300	ARG	Sidechain
29	I	314	ASP	Sidechain
29	I	321	ASP	Sidechain
29	I	339	ILE	Peptide
29	I	373	GLU	Sidechain
29	I	421	GLU	Sidechain
29	I	429	GLU	Peptide
33	J	131	ASP	Sidechain
33	J	172	GLU	Sidechain
33	J	212	ARG	Sidechain
33	J	280	ASP	Sidechain
33	J	295	ASN	Sidechain
33	J	399	SER	Peptide
33	J	9	ASN	Sidechain
30	K	196	ASP	Sidechain
30	K	199	GLU	Sidechain
30	K	204	ASP	Sidechain
30	K	244	HIS	Sidechain
30	K	345	ASP	Sidechain
30	K	414	GLN	Sidechain
30	K	415	VAL	Mainchain
31	L	173	PHE	Peptide
31	L	243	PHE	Sidechain

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Mol	Chain	Res	Type	Group
31	L	244	ILE	Peptide
31	L	265	GLU	Sidechain
31	L	292	SER	Peptide
31	L	293	GLU	Sidechain
31	L	298	ASP	Sidechain
31	L	376	PHE	Peptide
31	L	386	PHE	Sidechain
31	L	433	GLU	Sidechain
32	M	105	ASN	Peptide,Sidechain
32	M	107	ASN	Sidechain
32	M	171	GLU	Sidechain
32	M	179	THR	Mainchain
32	M	265	ASP	Sidechain
32	M	282	GLU	Mainchain
32	M	284	ASP	Sidechain
32	M	292	ASP	Sidechain
32	M	298	ASP	Sidechain
32	M	300	GLU	Sidechain
32	M	314	GLY	Peptide
32	M	315	PHE	Peptide
32	M	355	ASP	Sidechain
32	M	42	ARG	Sidechain
32	M	423	GLN	Peptide
32	M	428	LYS	Mainchain,Peptide
32	M	95	GLU	Sidechain
32	M	96	ASN	Sidechain
21	N	346	ASN	Sidechain
21	N	361	ASN	Mainchain
21	N	437	GLU	Sidechain
21	N	86	LYS	Mainchain
21	N	887	ASP	Sidechain
27	O	225	ASP	Sidechain
27	O	50	ASP	Sidechain
23	P	127	GLU	Sidechain
23	P	131	PHE	Sidechain
24	Q	110	SER	Mainchain
24	Q	217	GLU	Sidechain
24	Q	387	TYR	Mainchain
24	Q	47	ASP	Mainchain
24	Q	48	ASP	Mainchain
24	Q	67	THR	Peptide
25	R	127	GLU	Sidechain

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Mol	Chain	Res	Type	Group
25	R	279	LEU	Peptide
22	S	153	GLU	Sidechain
22	S	192	GLU	Sidechain
22	S	217	PHE	Sidechain
22	S	227	ASN	Sidechain
22	S	369	GLN	Sidechain
17	T	135	ASN	Sidechain
17	T	138	ASP	Mainchain
17	T	251	HIS	Peptide
26	U	151	GLU	Peptide
26	U	230	GLN	Sidechain
26	U	246	GLU	Sidechain
26	U	60	GLU	Sidechain
26	U	70	HIS	Sidechain
16	V	61	TYR	Sidechain
15	W	14	GLU	Sidechain
15	W	149	GLN	Sidechain
15	W	23	ARG	Peptide
15	W	80	GLN	Sidechain
19	Y	4	ASP	Mainchain
19	Y	58	ASN	Sidechain
19	Y	70	ASP	Sidechain
20	Z	108	ASP	Sidechain
20	Z	276	ASN	Sidechain
20	Z	321	PHE	Sidechain
20	Z	33	GLU	Sidechain
20	Z	365	SER	Mainchain
20	Z	377	ALA	Mainchain
20	Z	379	GLN	Sidechain
20	Z	443	ASP	Mainchain,Sidechain
20	Z	5	SER	Peptide
20	Z	503	ASP	Sidechain
20	Z	6	ASP	Sidechain
20	Z	65	GLU	Sidechain
20	Z	721	ASN	Sidechain
20	Z	728	LYS	Mainchain
20	Z	751	ASP	Sidechain
20	Z	802	ASP	Mainchain
20	Z	807	VAL	Peptide
20	Z	824	ASN	Sidechain
20	Z	84	ALA	Peptide
20	Z	959	HIS	Sidechain

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Mol	Chain	Res	Type	Group
20	Z	961	GLU	Sidechain
1	a	115	ASP	Sidechain
1	a	250	GLU	Sidechain
2	b	234	ARG	Sidechain
3	c	105	ASP	Sidechain
3	c	109	GLU	Sidechain
3	c	63	THR	Mainchain
4	d	102	ASP	Mainchain
4	d	204	GLN	Mainchain
4	d	237	GLU	Sidechain
4	d	79	ASN	Sidechain
5	e	104	ASP	Sidechain
5	e	106	ASP	Sidechain
5	e	18	GLU	Mainchain
5	e	206	GLN	Sidechain
6	f	13	PHE	Peptide
6	f	18	ARG	Peptide
6	f	205	SER	Mainchain
7	g	13	SER	Peptide
7	g	184	PRO	Mainchain
7	g	21	ASN	Peptide
7	g	72	ARG	Sidechain
8	h	202	TYR	Sidechain
9	i	124	GLY	Mainchain
9	i	200	SER	Mainchain
9	i	217	ARG	Sidechain
9	i	225	ARG	Sidechain
9	i	37	PHE	Sidechain
9	i	38	ASN	Sidechain
9	i	51	GLN	Sidechain
10	j	85	GLU	Sidechain
11	k	78	GLN	Sidechain
12	l	147	GLU	Sidechain
12	l	196	ARG	Sidechain
12	l	82	ARG	Mainchain
13	m	104	LEU	Mainchain
13	m	113	TYR	Mainchain
13	m	13	TYR	Sidechain
13	m	181	LYS	Mainchain
13	m	182	TYR	Sidechain
13	m	36	ARG	Sidechain
13	m	70	ASP	Sidechain

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Mol	Chain	Res	Type	Group
13	m	86	ASP	Sidechain

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	1907	0	1901	33	0
1	a	1907	0	1901	33	0
2	B	1907	0	1917	31	0
2	b	1907	0	1917	35	0
3	C	1904	0	1901	48	0
3	c	1904	0	1901	48	0
4	D	1850	0	1862	40	0
4	d	1850	0	1862	30	0
5	E	1882	0	1851	42	0
5	e	1882	0	1851	27	0
6	F	1773	0	1771	54	0
6	f	1773	0	1772	32	0
7	G	1885	0	1876	24	0
7	g	1885	0	1873	32	0
8	1	1512	0	1474	51	0
8	h	1512	0	1474	35	0
9	2	1719	0	1715	117	0
9	i	1719	0	1715	95	0
10	3	1581	0	1571	107	0
10	j	1581	0	1570	92	0
11	4	1561	0	1567	114	0
11	k	1561	0	1567	81	0
12	5	1644	0	1590	79	0
12	l	1644	0	1590	84	0
13	6	1757	0	1703	110	0
13	m	1757	0	1701	127	0
14	7	1790	0	1790	29	0
14	n	1790	0	1790	55	0
15	W	1534	0	1542	13	0
16	V	2274	0	2273	29	0
17	T	2192	0	2161	6	0
18	X	1032	0	1017	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	Y	731	0	675	6	0
20	Z	7005	0	6932	72	0
21	N	6418	0	6487	53	0
22	S	3894	0	3938	31	0
23	P	3608	0	3694	33	0
24	Q	3499	0	3524	24	0
25	R	3258	0	3263	38	0
26	U	2306	0	2331	24	0
27	O	3186	0	3213	21	0
28	H	3064	0	3144	33	0
29	I	3015	0	3084	54	0
30	K	3113	0	3169	46	0
31	L	3082	0	3157	33	0
32	M	3285	0	3323	43	0
33	J	3171	0	3313	30	0
34	8	3034	0	3005	21	0
35	9	601	0	630	5	0
36	H	31	0	12	0	0
36	I	31	0	12	0	0
36	K	31	0	12	0	0
36	L	31	0	12	0	0
36	M	31	0	12	0	0
37	H	1	0	0	0	0
37	I	1	0	0	0	0
37	J	1	0	0	0	0
37	K	1	0	0	0	0
37	L	1	0	0	0	0
37	M	1	0	0	0	0
38	J	27	0	11	0	0
All	All	112834	0	112919	1835	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 8.

All (1835) 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)
13:m:109:ARG:HG3	13:m:136:VAL:CG1	1.26	1.54
13:m:109:ARG:CG	13:m:136:VAL:HG11	1.46	1.41
13:m:109:ARG:CG	13:m:136:VAL:CG1	1.99	1.39
11:k:35:THR:HG21	11:k:182:LYS:NZ	1.33	1.38

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:4:35:THR:HG21	11:4:182:LYS:NZ	1.33	1.38
12:l:102:ALA:O	13:m:145:ARG:NH2	1.58	1.33
13:m:145:ARG:NH1	13:m:155:MET:HE1	1.51	1.24
13:6:145:ARG:NH1	13:6:155:MET:HE1	1.51	1.23
11:4:96:ARG:NH2	12:5:166:LYS:HD3	1.51	1.23
13:m:164:PHE:CE2	13:m:181:LYS:HD3	1.76	1.21
13:m:145:ARG:NH1	13:m:155:MET:CE	2.04	1.20
13:6:164:PHE:CE2	13:6:181:LYS:HD3	1.76	1.20
9:i:48:ARG:NH2	13:6:230:ASP:OD2	1.74	1.20
14:n:137:ARG:NH1	14:n:138:SER:OG	1.76	1.18
13:6:145:ARG:NH1	13:6:155:MET:CE	2.04	1.18
2:b:142:PHE:CD1	10:j:80:ARG:NH2	2.12	1.18
9:2:153:TYR:CZ	9:2:167:LEU:HD13	1.78	1.18
9:i:153:TYR:CZ	9:i:167:LEU:HD13	1.78	1.17
10:3:63:LEU:HD23	10:3:67:PHE:HE2	1.10	1.16
21:N:280:GLN:NE2	21:N:282:TYR:OH	1.79	1.15
10:3:98:ARG:HH22	11:4:93:ARG:NE	1.45	1.15
13:6:145:ARG:HH11	13:6:155:MET:HE1	0.96	1.12
3:C:5:ARG:NH2	6:F:9:ASP:OD2	1.82	1.12
13:m:168:TYR:HE1	9:2:240:ALA:HB2	1.06	1.12
13:m:58:ILE:HD11	13:m:94:ILE:HD12	1.31	1.10
3:c:9:ARG:HD2	4:d:6:ARG:NH1	1.65	1.09
10:j:63:LEU:HD23	10:j:67:PHE:HE2	1.10	1.08
3:c:110:ILE:HD11	11:k:71:GLU:CD	1.78	1.08
13:m:145:ARG:HH11	13:m:155:MET:HE1	0.96	1.08
13:m:113:TYR:O	13:m:114:TYR:CD1	2.05	1.07
11:k:96:ARG:NH2	12:l:166:LYS:HD3	1.70	1.07
10:3:98:ARG:NH2	11:4:93:ARG:HE	1.51	1.06
9:i:48:ARG:CZ	13:6:230:ASP:OD2	2.04	1.06
5:E:51:GLU:OE1	5:E:53:ARG:NH2	1.88	1.05
4:D:90:ARG:CZ	11:4:69:ILE:HG21	1.86	1.05
10:3:63:LEU:HD23	10:3:67:PHE:CE2	1.93	1.04
10:j:63:LEU:HD23	10:j:67:PHE:CE2	1.93	1.02
10:j:204:GLN:HG2	12:5:272:PHE:CE2	1.94	1.02
13:m:113:TYR:O	13:m:114:TYR:HD1	1.41	1.02
13:m:168:TYR:CE1	9:2:240:ALA:HB2	1.94	1.02
13:m:58:ILE:HD11	13:m:94:ILE:CD1	1.90	1.02
9:2:153:TYR:CE1	9:2:167:LEU:HD13	1.95	1.01
2:b:142:PHE:HD1	10:j:80:ARG:NH2	1.55	1.01
11:k:96:ARG:HH21	12:l:166:LYS:HD3	1.22	1.01
13:m:109:ARG:HG3	13:m:136:VAL:HG12	1.35	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:n:255:ALA:O	8:1:183:ARG:NH2	1.92	1.01
9:i:153:TYR:CE1	9:i:167:LEU:HD13	1.95	1.01
14:n:215:ARG:HH12	9:2:169:SER:HA	1.24	1.00
11:k:35:THR:CG2	11:k:182:LYS:NZ	2.25	0.99
1:A:24:ARG:NH1	30:K:427:TYR:CD2	2.28	0.99
13:m:113:TYR:C	13:m:114:TYR:HD1	1.70	0.99
8:h:183:ARG:NH2	14:7:255:ALA:O	1.95	0.99
5:E:12:VAL:HB	5:E:135:SER:O	1.61	0.99
11:4:35:THR:CG2	11:4:182:LYS:NZ	2.25	0.99
13:6:164:PHE:CZ	13:6:181:LYS:NZ	2.32	0.98
13:m:164:PHE:CZ	13:m:181:LYS:NZ	2.32	0.98
9:2:153:TYR:CZ	9:2:167:LEU:CD1	2.46	0.98
3:C:110:ILE:HD11	11:4:71:GLU:CD	1.88	0.98
10:3:101:GLY:O	11:4:93:ARG:NH2	1.97	0.97
9:i:153:TYR:CZ	9:i:167:LEU:CD1	2.46	0.97
3:c:110:ILE:CD1	11:k:71:GLU:OE1	2.12	0.96
1:a:149:GLU:HB3	9:i:101:ARG:NH1	1.79	0.96
13:m:230:ASP:OD1	13:m:230:ASP:O	1.84	0.95
10:j:8:ASN:ND2	10:j:57:ALA:HB2	1.82	0.95
14:n:259:LYS:HB3	8:1:194:ARG:NH1	1.81	0.95
10:j:63:LEU:CD2	10:j:67:PHE:HE2	1.78	0.95
10:3:63:LEU:CD2	10:3:67:PHE:HE2	1.78	0.95
11:4:96:ARG:HH21	12:5:166:LYS:HD3	1.26	0.95
13:m:164:PHE:HE2	13:m:181:LYS:HD3	1.19	0.94
10:3:8:ASN:ND2	10:3:57:ALA:HB2	1.82	0.94
13:6:150:ALA:HB2	13:6:203:HIS:HD2	1.32	0.94
13:6:230:ASP:O	13:6:230:ASP:OD1	1.84	0.94
13:6:164:PHE:HE2	13:6:181:LYS:HD3	1.19	0.94
13:m:145:ARG:HH12	13:m:155:MET:CE	1.79	0.94
3:C:142:ASP:OD1	11:4:110:LYS:HE3	1.66	0.94
13:6:145:ARG:HH12	13:6:155:MET:CE	1.79	0.94
3:C:5:ARG:NH2	6:F:9:ASP:CG	2.26	0.94
1:a:149:GLU:CB	9:i:101:ARG:HH12	1.81	0.93
12:5:102:ALA:C	13:6:145:ARG:HH22	1.74	0.93
13:6:46:ARG:HH21	13:6:229:ARG:HE	1.15	0.93
21:N:280:GLN:NE2	21:N:282:TYR:CZ	2.36	0.93
13:m:109:ARG:HG2	13:m:136:VAL:HG11	1.48	0.93
13:m:150:ALA:HB2	13:m:203:HIS:HD2	1.32	0.92
11:4:35:THR:HG21	11:4:182:LYS:HZ1	1.33	0.92
5:E:104:ASP:OD2	13:6:99:ARG:NH2	2.02	0.92
14:n:259:LYS:HB3	8:1:194:ARG:HH12	1.33	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:4:35:THR:HG21	11:4:182:LYS:HZ3	0.95	0.91
16:V:41:GLY:O	16:V:45:VAL:HG23	1.69	0.91
3:C:110:ILE:CD1	11:4:71:GLU:CD	2.44	0.90
29:I:115:ASP:HB2	34:8:486:SER:OG	1.70	0.90
14:n:219:TYR:CE2	9:2:168:GLU:OE1	2.25	0.90
11:k:170:LYS:HE3	11:k:171:ARG:HH21	1.38	0.89
10:3:67:PHE:HE1	10:3:91:VAL:HG22	1.37	0.89
13:6:124:GLU:N	13:6:124:GLU:OE1	2.05	0.89
10:3:183:TRP:CD1	10:3:204:GLN:OE1	2.25	0.89
20:Z:145:ASP:HA	20:Z:149:TRP:HE1	1.38	0.89
11:k:35:THR:HG21	11:k:182:LYS:HZ1	1.22	0.89
10:j:67:PHE:HE1	10:j:91:VAL:HG22	1.37	0.89
13:m:46:ARG:HH21	13:m:229:ARG:HE	1.15	0.89
13:6:145:ARG:HH11	13:6:155:MET:CE	1.78	0.89
13:m:124:GLU:OE1	13:m:124:GLU:N	2.05	0.88
13:m:81:LYS:O	13:m:85:PHE:HD2	1.56	0.88
11:4:170:LYS:HE3	11:4:171:ARG:HH21	1.37	0.88
14:n:134:TYR:O	14:n:137:ARG:HD3	1.72	0.88
5:E:12:VAL:CB	5:E:135:SER:O	2.21	0.87
11:k:35:THR:HG21	11:k:182:LYS:HZ3	1.05	0.87
4:D:90:ARG:HD3	11:4:69:ILE:HG22	1.57	0.87
13:m:109:ARG:HG3	13:m:136:VAL:HG11	0.88	0.87
12:5:102:ALA:O	13:6:145:ARG:NH2	2.07	0.87
8:1:128:VAL:O	8:1:129:HIS:HD2	1.58	0.86
13:m:109:ARG:CG	13:m:136:VAL:HG13	2.05	0.86
14:n:219:TYR:CD2	9:2:168:GLU:OE1	2.29	0.86
2:b:201:GLU:OE1	2:b:201:GLU:N	2.09	0.86
13:m:157:PHE:CZ	9:2:232:TYR:HE1	1.94	0.85
14:n:134:TYR:O	14:n:137:ARG:CD	2.23	0.85
8:h:128:VAL:O	8:h:129:HIS:HD2	1.58	0.85
10:3:98:ARG:HH22	11:4:93:ARG:HE	1.06	0.85
2:B:201:GLU:OE1	2:B:201:GLU:N	2.09	0.85
12:l:169:GLY:O	13:m:109:ARG:NH2	2.10	0.85
10:3:125:ASP:OD2	10:3:126:LEU:N	2.10	0.85
1:A:22:GLU:OE1	30:K:420:THR:HG22	1.75	0.84
9:i:240:ALA:HB2	13:6:174:GLY:CA	2.07	0.84
3:c:110:ILE:HD11	11:k:71:GLU:OE1	1.73	0.84
11:k:3:ILE:HG13	11:k:176:PHE:HD1	1.42	0.84
13:6:164:PHE:CE2	13:6:181:LYS:CD	2.61	0.84
14:n:137:ARG:HH12	14:n:138:SER:HG	1.25	0.84
5:E:20:ARG:HH21	6:F:31:GLN:HB2	1.43	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:4:35:THR:CG2	11:4:182:LYS:HZ3	1.86	0.84
9:i:201:ASN:OD1	9:i:221:THR:HG23	1.78	0.83
10:3:65:GLU:OE2	11:4:85:ARG:NH2	2.10	0.83
13:6:230:ASP:O	13:6:230:ASP:CG	2.06	0.83
1:a:149:GLU:HB3	9:i:101:ARG:HH12	1.41	0.83
10:3:8:ASN:HD21	10:3:57:ALA:HB2	1.41	0.83
10:j:179:ALA:HB1	12:5:244:ALA:HB1	1.60	0.83
14:n:241:PHE:HE2	14:n:243:LYS:HG2	1.42	0.83
2:B:78:MET:CE	30:K:426:PHE:HE2	1.92	0.83
8:1:157:LYS:HE3	8:1:186:VAL:HG11	1.60	0.82
10:j:183:TRP:CD1	10:j:204:GLN:OE1	2.33	0.82
9:2:153:TYR:CE2	9:2:167:LEU:CD1	2.63	0.82
9:i:80:ASP:O	9:i:84:VAL:HG23	1.80	0.82
11:k:35:THR:CG2	11:k:182:LYS:HZ1	1.86	0.82
9:2:80:ASP:O	9:2:84:VAL:HG23	1.80	0.82
9:i:153:TYR:CE2	9:i:167:LEU:CD1	2.62	0.82
23:P:89:LEU:O	23:P:90:LYS:HG2	1.80	0.81
3:c:9:ARG:HD2	4:d:6:ARG:HH12	1.42	0.81
8:h:157:LYS:HE3	8:h:186:VAL:HG11	1.60	0.81
13:m:230:ASP:O	13:m:230:ASP:CG	2.06	0.81
11:k:135:TYR:HE1	11:4:25:ILE:HG12	1.44	0.81
9:i:240:ALA:HB2	13:6:174:GLY:HA3	1.62	0.81
20:Z:490:ILE:HD12	20:Z:526:ALA:HA	1.60	0.81
12:l:94:ARG:NH2	10:3:205:ASP:OD2	2.13	0.81
13:6:70:ASP:OD2	14:7:169:THR:OG1	1.98	0.81
10:j:8:ASN:HD21	10:j:57:ALA:HB2	1.41	0.81
10:3:98:ARG:HH22	11:4:93:ARG:CZ	1.93	0.81
3:c:15:PRO:HA	4:d:22:TYR:CE1	2.15	0.81
13:m:168:TYR:HE1	9:2:240:ALA:CB	1.90	0.81
13:m:164:PHE:HE2	13:m:181:LYS:CD	1.94	0.81
10:3:49:VAL:HG11	10:3:87:PHE:HD1	1.45	0.81
3:c:224:GLU:CB	9:i:252:ILE:HG21	2.10	0.80
13:m:164:PHE:CE2	13:m:181:LYS:CD	2.61	0.80
12:l:102:ALA:C	13:m:145:ARG:NH2	2.40	0.80
10:3:98:ARG:NH2	11:4:93:ARG:NE	2.15	0.80
10:j:49:VAL:HG11	10:j:87:PHE:HD1	1.45	0.80
9:2:201:ASN:OD1	9:2:221:THR:HG23	1.82	0.80
14:n:253:ASP:O	9:2:173:GLN:OE1	2.00	0.80
12:l:272:PHE:CZ	10:3:204:GLN:HG2	2.17	0.79
13:m:164:PHE:CZ	13:m:181:LYS:HD3	2.18	0.79
31:L:283:VAL:HG23	31:L:286:ILE:HG13	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:N:742:TRP:CD1	21:N:744:PRO:HD2	2.18	0.79
10:j:204:GLN:HG2	12:5:272:PHE:CD2	2.18	0.79
21:N:736:PHE:O	21:N:739:PHE:HD1	1.66	0.79
12:l:213:GLY:HA2	11:4:167:GLU:OE2	1.82	0.79
13:m:157:PHE:CE1	9:2:232:TYR:HE1	2.01	0.79
28:H:145:TYR:HE2	28:H:168:ILE:HG21	1.47	0.79
3:C:5:ARG:NH2	6:F:9:ASP:OD1	2.15	0.79
10:3:183:TRP:HD1	10:3:204:GLN:OE1	1.64	0.78
12:5:100:TRP:CE2	13:6:152:SER:HB3	2.18	0.78
8:1:128:VAL:C	8:1:129:HIS:HD2	1.91	0.78
13:m:164:PHE:HZ	13:m:181:LYS:NZ	1.79	0.78
9:2:219:TYR:C	9:2:219:TYR:HD1	1.91	0.78
13:m:143:GLN:NE2	13:m:143:GLN:N	2.32	0.78
12:5:100:TRP:CZ2	13:6:152:SER:HB3	2.17	0.78
8:h:128:VAL:C	8:h:129:HIS:HD2	1.91	0.78
25:R:41:GLU:HA	25:R:44:LYS:HZ3	1.46	0.78
13:6:164:PHE:HE2	13:6:181:LYS:CD	1.94	0.78
13:m:112:PRO:HG2	13:m:114:TYR:HE1	1.47	0.78
10:3:67:PHE:CE1	10:3:91:VAL:HG22	2.19	0.78
1:A:13:ASP:N	1:A:13:ASP:OD1	2.13	0.77
13:6:143:GLN:N	13:6:143:GLN:NE2	2.32	0.77
13:6:164:PHE:HZ	13:6:181:LYS:NZ	1.79	0.77
21:N:277:LEU:CD2	21:N:282:TYR:CE2	2.68	0.77
13:m:164:PHE:HE2	13:m:181:LYS:HB2	1.50	0.77
10:3:29:LEU:HD22	10:3:40:PHE:CD2	2.20	0.77
20:Z:221:VAL:HG12	20:Z:267:THR:HG21	1.67	0.77
24:Q:275:ILE:HD12	24:Q:307:ASN:HB2	1.65	0.77
20:Z:562:TRP:O	20:Z:566:LEU:HD23	1.83	0.77
2:b:224:TYR:CZ	9:i:65:ARG:NH1	2.51	0.77
10:j:29:LEU:HD22	10:j:40:PHE:CD2	2.20	0.77
11:k:25:ILE:HG12	11:4:135:TYR:CE1	2.20	0.77
11:k:135:TYR:CE1	11:4:25:ILE:HG12	2.20	0.77
7:g:104:LYS:HZ1	14:n:98:ARG:HH11	1.32	0.77
32:M:117:ALA:O	32:M:129:LEU:HD23	1.85	0.77
10:j:11:ILE:CD1	10:j:181:SER:HB3	2.15	0.76
8:h:142:PHE:CE1	14:7:66:LEU:HD13	2.19	0.76
12:l:237:LEU:HD13	12:l:271:LEU:HD23	1.67	0.76
12:5:237:LEU:HD13	12:5:271:LEU:HD23	1.67	0.76
25:R:40:ILE:HG22	25:R:44:LYS:HZ2	1.50	0.76
9:i:48:ARG:NH1	13:6:230:ASP:OD1	2.18	0.76
10:j:204:GLN:HG2	12:5:272:PHE:CZ	2.19	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:n:241:PHE:CE2	14:n:243:LYS:HG2	2.20	0.76
13:6:164:PHE:HE2	13:6:181:LYS:HB2	1.50	0.76
10:j:67:PHE:CE1	10:j:91:VAL:HG22	2.19	0.76
1:A:42:SER:OG	1:A:171:THR:OG1	2.04	0.76
4:D:90:ARG:HD3	11:4:69:ILE:CG2	2.16	0.76
16:V:25:GLU:O	16:V:199:LEU:HD12	1.85	0.76
5:e:121:LEU:HD13	6:f:79:PRO:HB2	1.67	0.76
13:m:230:ASP:HB2	9:2:223:ASN:ND2	2.01	0.76
1:a:42:SER:OG	1:a:171:THR:OG1	2.04	0.76
13:m:197:THR:HG21	9:2:226:GLU:HG3	1.68	0.76
11:4:81:SER:HB3	11:4:119:ILE:HD11	1.68	0.75
13:m:109:ARG:CB	13:m:136:VAL:CG1	2.65	0.75
28:H:145:TYR:HE2	28:H:168:ILE:CG2	1.99	0.75
1:a:149:GLU:CD	9:i:101:ARG:HH12	1.95	0.75
1:A:149:GLU:HB3	9:2:101:ARG:HH12	1.51	0.75
5:E:12:VAL:CG1	5:E:135:SER:O	2.35	0.75
13:6:164:PHE:CZ	13:6:181:LYS:HD3	2.18	0.75
20:Z:366:LYS:O	20:Z:842:GLN:NE2	2.19	0.75
20:Z:528:LEU:HD12	20:Z:532:HIS:NE2	2.02	0.74
13:m:126:GLY:HA2	13:m:217:LYS:NZ	2.02	0.74
3:C:110:ILE:CD1	11:4:71:GLU:OE1	2.36	0.74
5:e:18:GLU:HG2	5:e:20:ARG:HG2	1.68	0.74
9:i:223:ASN:HD22	13:6:230:ASP:HB2	1.51	0.74
7:G:29:LYS:O	7:G:33:ASN:OD1	2.05	0.74
11:k:67:TYR:O	11:k:67:TYR:HD2	1.71	0.74
11:k:81:SER:HB3	11:k:119:ILE:HD11	1.68	0.74
4:D:90:ARG:CZ	11:4:69:ILE:CG2	2.64	0.74
28:H:105:ILE:HG23	28:H:145:TYR:CE1	2.23	0.74
22:S:207:ASN:O	22:S:211:ARG:HG2	1.89	0.73
13:m:113:TYR:C	13:m:114:TYR:CD1	2.56	0.73
13:m:150:ALA:HB2	13:m:203:HIS:CD2	2.22	0.73
1:a:13:ASP:N	1:a:13:ASP:OD1	2.13	0.73
13:m:157:PHE:CZ	9:2:232:TYR:CE1	2.76	0.73
13:6:126:GLY:HA2	13:6:217:LYS:NZ	2.02	0.73
10:j:11:ILE:HG12	10:j:26:ASP:OD2	1.88	0.73
29:I:249:GLY:HA3	29:I:283:GLU:O	1.88	0.73
13:6:46:ARG:HH21	13:6:229:ARG:NE	1.86	0.73
13:m:126:GLY:HA2	13:m:217:LYS:HZ3	1.53	0.73
15:W:6:THR:HG22	15:W:8:LEU:HD23	1.70	0.73
29:I:208:TYR:HD2	29:I:211:MET:HE2	1.53	0.73
11:4:67:TYR:HD2	11:4:67:TYR:O	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:J:398:ILE:HG13	33:J:399:SER:N	2.04	0.73
11:k:67:TYR:HD2	11:k:67:TYR:C	1.97	0.72
29:I:133:LEU:HD22	29:I:155:SER:OG	1.89	0.72
8:h:133:TYR:HD2	8:h:133:TYR:O	1.73	0.72
9:2:249:ILE:HD13	10:3:195:VAL:HG21	1.71	0.72
3:C:110:ILE:HD11	11:4:71:GLU:OE2	1.89	0.72
10:3:11:ILE:HG12	10:3:26:ASP:OD2	1.88	0.72
12:5:200:ASP:O	12:5:201:ILE:HG13	1.90	0.72
13:m:112:PRO:HG2	13:m:114:TYR:CE1	2.24	0.72
9:i:243:LYS:NZ	10:j:199:TYR:CE2	2.58	0.72
11:k:3:ILE:HG13	11:k:176:PHE:CD1	2.24	0.72
12:l:113:ASN:HB2	12:l:114:PRO:CD	2.20	0.72
12:l:144:ARG:HG3	12:l:144:ARG:NH1	1.96	0.72
11:4:3:ILE:CG2	11:4:136:SER:HB2	2.19	0.72
10:j:172:LEU:CD1	10:j:202:MET:HE3	2.20	0.72
31:L:254:LYS:HG2	32:M:256:ILE:O	1.90	0.72
7:g:29:LYS:O	7:g:33:ASN:OD1	2.05	0.72
10:j:8:ASN:HD21	10:j:57:ALA:CB	2.03	0.72
13:m:81:LYS:O	13:m:85:PHE:CD2	2.43	0.72
2:B:78:MET:CE	30:K:426:PHE:CE2	2.71	0.72
11:4:35:THR:CG2	11:4:182:LYS:HZ1	1.97	0.72
13:m:46:ARG:CA	13:m:208:ASP:OD2	2.38	0.72
9:2:219:TYR:HD1	9:2:219:TYR:O	1.73	0.72
11:4:67:TYR:HD2	11:4:67:TYR:C	1.97	0.71
11:4:96:ARG:HD3	12:5:166:LYS:O	1.90	0.71
12:5:113:ASN:HB2	12:5:114:PRO:CD	2.20	0.71
13:m:46:ARG:HH21	13:m:229:ARG:NE	1.86	0.71
28:H:145:TYR:CE2	28:H:168:ILE:HG21	2.25	0.71
9:i:88:ILE:HG21	9:i:111:MET:HB3	1.73	0.71
10:3:98:ARG:NH2	11:4:93:ARG:CZ	2.52	0.71
10:j:11:ILE:HG23	10:j:181:SER:OG	1.90	0.71
11:4:3:ILE:HG23	11:4:136:SER:HB2	1.73	0.71
11:4:3:ILE:HG23	11:4:136:SER:OG	1.89	0.71
8:1:133:TYR:O	8:1:133:TYR:HD2	1.73	0.71
10:3:8:ASN:HD21	10:3:57:ALA:CB	2.03	0.71
5:E:20:ARG:HH21	6:F:31:GLN:CB	2.04	0.71
28:H:246:ILE:HD11	28:H:375:VAL:HG12	1.72	0.71
11:4:3:ILE:HG23	11:4:136:SER:CB	2.20	0.71
13:6:46:ARG:CA	13:6:208:ASP:OD2	2.38	0.71
25:R:41:GLU:HA	25:R:44:LYS:NZ	2.05	0.71
29:I:101:GLY:HA3	29:I:102:ASN:O	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Z:382:ALA:O	20:Z:386:VAL:HG23	1.89	0.71
11:k:1:MET:HE1	11:k:101:ASN:ND2	2.06	0.71
1:a:149:GLU:CB	9:i:101:ARG:NH1	2.47	0.70
2:b:142:PHE:CD1	10:j:80:ARG:CZ	2.75	0.70
12:l:200:ASP:O	12:l:201:ILE:HG13	1.90	0.70
9:2:88:ILE:HG21	9:2:111:MET:HB3	1.73	0.70
21:N:277:LEU:HD22	21:N:282:TYR:CE2	2.26	0.70
7:g:104:LYS:NZ	14:n:98:ARG:HH11	1.90	0.70
13:m:145:ARG:HH11	13:m:155:MET:CE	1.78	0.70
13:6:164:PHE:CE2	13:6:181:LYS:NZ	2.57	0.70
12:5:144:ARG:HG3	12:5:144:ARG:NH1	1.96	0.70
3:c:224:GLU:HB3	9:i:252:ILE:HG21	1.74	0.70
13:m:109:ARG:CB	13:m:136:VAL:HG13	2.20	0.70
1:A:149:GLU:HB3	9:2:101:ARG:NH1	2.06	0.70
11:4:3:ILE:HG12	11:4:136:SER:OG	1.91	0.70
13:m:230:ASP:OD2	9:2:48:ARG:NH2	2.24	0.70
13:6:101:ILE:HG21	13:6:133:PHE:CE1	2.25	0.70
11:4:33:ASP:HA	11:4:180:ILE:HD11	1.72	0.70
10:j:205:ASP:OD2	12:5:94:ARG:NH2	2.25	0.69
34:8:438:HIS:CE1	34:8:448:TYR:CE2	2.80	0.69
2:b:186:GLU:O	2:b:190:HIS:ND1	2.25	0.69
11:k:33:ASP:HA	11:k:180:ILE:HD11	1.72	0.69
13:6:143:GLN:NE2	13:6:143:GLN:H	1.90	0.69
25:R:40:ILE:O	25:R:44:LYS:HG3	1.92	0.69
4:D:101:GLU:OE2	12:5:196:ARG:NH1	2.25	0.69
8:1:133:TYR:HD2	8:1:133:TYR:C	1.99	0.69
21:N:277:LEU:O	21:N:282:TYR:HD2	1.74	0.69
2:b:224:TYR:CE2	9:i:65:ARG:NH1	2.61	0.69
21:N:277:LEU:HD23	21:N:282:TYR:CE2	2.27	0.69
12:l:245:TYR:N	12:l:245:TYR:HD1	1.91	0.69
12:l:269:GLY:HA3	10:3:203:ARG:HE	1.57	0.69
3:C:110:ILE:HD13	11:4:71:GLU:OE1	1.93	0.69
25:R:40:ILE:C	25:R:44:LYS:HZ3	2.01	0.69
13:m:204:ILE:HD12	9:2:196:LEU:HB3	1.74	0.69
14:n:226:ARG:NH1	8:1:200:ASP:OD2	2.26	0.69
8:h:133:TYR:HD2	8:h:133:TYR:C	1.99	0.69
7:G:18:ASP:OD2	31:L:434:TYR:CD2	2.45	0.69
33:J:398:ILE:HG13	33:J:399:SER:H	1.58	0.69
1:a:149:GLU:CD	9:i:101:ARG:HH22	2.00	0.69
7:g:104:LYS:HZ1	14:n:98:ARG:NH1	1.91	0.69
12:5:125:ALA:HA	13:6:138:SER:HB3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:186:GLU:O	2:B:190:HIS:ND1	2.25	0.69
8:h:165:LYS:HE3	8:h:202:TYR:HB3	1.74	0.68
6:F:164:ARG:NH2	6:F:204:GLU:OE2	2.26	0.68
13:6:181:LYS:HG3	13:6:182:TYR:N	2.08	0.68
5:e:18:GLU:OE1	5:e:22:PHE:HE1	1.75	0.68
6:f:164:ARG:NH2	6:f:204:GLU:OE2	2.26	0.68
11:4:1:MET:N	11:4:18:SER:HB3	2.08	0.68
12:5:245:TYR:N	12:5:245:TYR:HD1	1.91	0.68
3:C:18:ARG:NH2	29:I:436:TYR:CD1	2.60	0.68
6:F:77:LEU:HB3	32:M:433:TYR:CE2	2.28	0.68
12:l:140:LEU:HD23	12:l:144:ARG:HH21	1.57	0.68
13:m:46:ARG:NH2	13:m:229:ARG:HE	1.91	0.68
8:1:199:PRO:HA	8:1:202:TYR:CZ	2.28	0.68
13:6:126:GLY:HA2	13:6:217:LYS:HZ3	1.58	0.68
13:6:150:ALA:HB2	13:6:203:HIS:CD2	2.22	0.68
10:j:205:ASP:OXT	10:j:205:ASP:OD1	2.11	0.68
10:3:205:ASP:OD1	10:3:205:ASP:OXT	2.11	0.68
25:R:40:ILE:C	25:R:44:LYS:NZ	2.51	0.68
4:D:4:TYR:O	4:D:5:ASP:HB3	1.93	0.68
34:8:119:TYR:HA	34:8:448:TYR:CD1	2.28	0.68
4:D:70:HIS:CD2	4:D:138:PHE:O	2.46	0.68
8:1:85:GLU:HA	8:1:120:TYR:HE1	1.58	0.68
9:2:46:ASP:OD2	9:2:198:SER:HA	1.94	0.68
8:h:85:GLU:HA	8:h:120:TYR:HE1	1.59	0.68
9:i:46:ASP:OD2	9:i:198:SER:HA	1.94	0.68
9:i:240:ALA:CB	13:6:174:GLY:HA3	2.24	0.68
10:j:183:TRP:HZ2	12:5:241:HIS:NE2	1.92	0.68
12:l:102:ALA:O	13:m:145:ARG:CZ	2.36	0.68
2:B:198:GLU:OE2	24:Q:209:TYR:HB2	1.94	0.68
3:C:18:ARG:HH21	29:I:436:TYR:HD1	1.35	0.68
12:5:140:LEU:HD23	12:5:144:ARG:HH21	1.57	0.68
2:b:142:PHE:HD1	10:j:80:ARG:CZ	2.06	0.67
32:M:432:PHE:CE2	32:M:433:TYR:CD1	2.83	0.67
9:i:126:TYR:HE1	9:i:144:ALA:HB2	1.59	0.67
14:n:259:LYS:CB	8:1:194:ARG:NH1	2.55	0.67
1:a:116:VAL:HG21	9:i:99:THR:HG22	1.75	0.67
10:j:11:ILE:HG12	10:j:181:SER:HB3	1.75	0.67
13:m:181:LYS:HG3	13:m:182:TYR:N	2.08	0.67
11:k:96:ARG:NH2	12:l:166:LYS:CD	2.55	0.67
9:2:217:ARG:HH11	9:2:217:ARG:CG	2.07	0.67
13:m:143:GLN:NE2	13:m:143:GLN:H	1.90	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:n:241:PHE:HE2	14:n:243:LYS:CG	2.07	0.67
13:6:101:ILE:HG21	13:6:133:PHE:HE1	1.60	0.67
10:j:28:ARG:HB2	10:j:182:GLY:O	1.95	0.67
13:m:161:GLN:OE1	13:m:161:GLN:HA	1.95	0.67
28:H:144:LYS:O	28:H:145:TYR:HD1	1.78	0.67
1:A:149:GLU:CB	9:2:101:ARG:HH12	2.08	0.67
11:4:96:ARG:HH22	12:5:166:LYS:HD3	1.53	0.67
20:Z:367:SER:HA	20:Z:842:GLN:NE2	2.10	0.66
13:m:112:PRO:CG	13:m:114:TYR:HE1	2.08	0.66
4:D:111:ARG:NH1	12:5:145:GLU:OE2	2.20	0.66
9:2:249:ILE:HD13	10:3:195:VAL:CG2	2.26	0.66
22:S:68:LEU:O	22:S:69:LEU:O	2.13	0.66
12:l:280:GLY:O	12:l:283:ASN:ND2	2.28	0.66
8:1:128:VAL:O	8:1:129:HIS:CD2	2.46	0.66
16:V:45:VAL:HG13	16:V:46:PRO:HA	1.77	0.66
20:Z:813:PHE:CE1	20:Z:817:LEU:HD21	2.30	0.66
25:R:40:ILE:O	25:R:44:LYS:NZ	2.27	0.66
10:3:98:ARG:NH2	11:4:93:ARG:NH2	2.44	0.66
10:3:98:ARG:CZ	11:4:93:ARG:HE	2.07	0.66
20:Z:748:LEU:HA	29:I:86:GLU:OE1	1.95	0.66
3:c:110:ILE:HD13	11:k:71:GLU:OE1	1.94	0.66
10:3:98:ARG:NH2	11:4:93:ARG:HH21	1.94	0.66
12:5:170:LEU:HD23	12:5:170:LEU:HA	1.77	0.66
29:I:115:ASP:CB	34:8:486:SER:OG	2.44	0.66
6:F:139:LYS:HD2	14:7:118:GLU:O	1.96	0.66
12:5:252:LEU:C	12:5:253:TYR:HD1	2.04	0.66
13:6:116:HIS:HD2	13:6:147:GLY:HA3	1.60	0.66
12:l:252:LEU:C	12:l:253:TYR:HD1	2.03	0.66
1:A:116:VAL:HG21	9:2:99:THR:HG22	1.77	0.66
11:k:155:GLU:OE1	11:k:158:LEU:HD12	1.96	0.66
13:m:164:PHE:CE2	13:m:181:LYS:NZ	2.57	0.66
32:M:281:ASP:O	32:M:282:GLU:HB2	1.94	0.66
13:m:157:PHE:HZ	9:2:232:TYR:CE1	2.13	0.66
13:6:161:GLN:OE1	13:6:161:GLN:HA	1.95	0.65
33:J:206:THR:O	33:J:207:ASP:HB2	1.96	0.65
14:n:134:TYR:CZ	14:n:137:ARG:NH2	2.65	0.65
32:M:432:PHE:CE2	32:M:433:TYR:CE1	2.84	0.65
9:i:92:ILE:CG1	9:i:111:MET:HE1	2.26	0.65
14:n:231:ALA:HB2	14:n:241:PHE:HD1	1.61	0.65
8:h:47:HIS:ND1	8:h:48:ASP:N	2.45	0.65
8:h:128:VAL:O	8:h:129:HIS:CD2	2.46	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:i:125:ALA:C	9:i:126:TYR:HD1	2.05	0.65
5:E:20:ARG:NE	6:F:31:GLN:OE1	2.29	0.65
4:d:101:GLU:OE1	12:l:156:LYS:HD3	1.96	0.65
9:i:196:LEU:HD21	13:6:43:ILE:HD11	1.79	0.65
12:l:170:LEU:HA	12:l:170:LEU:HD23	1.77	0.65
8:1:47:HIS:ND1	8:1:48:ASP:N	2.45	0.65
3:C:142:ASP:OD1	11:4:110:LYS:CE	2.41	0.65
11:4:1:MET:H3	11:4:18:SER:HB3	1.61	0.65
13:m:201:GLU:OE1	9:2:58:LYS:HE3	1.96	0.65
3:C:11:THR:OG1	4:D:8:LEU:HD13	1.96	0.65
25:R:40:ILE:HG22	25:R:44:LYS:NZ	2.11	0.65
4:d:118:GLN:OE1	5:e:86:ARG:HB2	1.97	0.65
8:h:128:VAL:C	8:h:129:HIS:CD2	2.75	0.65
9:2:181:ILE:HG23	9:2:219:TYR:HE2	1.62	0.65
5:e:128:SER:HA	6:f:119:ASN:ND2	2.11	0.65
8:h:135:ILE:HD11	8:h:144:TYR:CD2	2.32	0.65
1:A:24:ARG:HD3	30:K:427:TYR:CE2	2.32	0.65
3:C:152:ASN:HD21	29:I:437:LEU:HD22	1.61	0.65
9:2:125:ALA:C	9:2:126:TYR:HD1	2.05	0.65
11:4:155:GLU:OE1	11:4:158:LEU:HD12	1.96	0.65
12:l:272:PHE:CE2	10:3:204:GLN:HG2	2.31	0.64
1:A:37:GLN:OE1	1:A:37:GLN:HA	1.97	0.64
9:2:92:ILE:CG1	9:2:111:MET:HE1	2.26	0.64
12:5:280:GLY:O	12:5:283:ASN:ND2	2.28	0.64
11:4:146:HIS:ND1	11:4:147:HIS:CE1	2.66	0.64
20:Z:850:LEU:HD23	20:Z:859:LYS:HA	1.79	0.64
11:k:146:HIS:ND1	11:k:147:HIS:CE1	2.65	0.64
9:2:51:GLN:HE22	10:3:125:ASP:HB3	1.62	0.64
9:2:126:TYR:HE1	9:2:144:ALA:HB2	1.59	0.64
10:3:204:GLN:HA	10:3:204:GLN:NE2	1.99	0.64
13:6:46:ARG:NH2	13:6:229:ARG:HE	1.91	0.64
21:N:277:LEU:HD22	21:N:282:TYR:CZ	2.31	0.64
2:B:106:PRO:HG2	10:3:78:GLU:OE2	1.98	0.64
9:2:51:GLN:HE22	10:3:125:ASP:CB	2.10	0.64
12:l:126:ASP:HA	13:m:106:TYR:OH	1.97	0.64
8:1:135:ILE:HD11	8:1:144:TYR:CD2	2.32	0.64
32:M:426:LYS:O	32:M:427:SER:O	2.16	0.64
10:j:204:GLN:NE2	10:j:204:GLN:HA	1.98	0.64
8:1:128:VAL:C	8:1:129:HIS:CD2	2.75	0.64
29:I:125:MET:O	29:I:125:MET:HG2	1.95	0.64
2:B:102:GLY:HA3	10:3:89:GLN:HE21	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:101:GLU:OE2	12:5:196:ARG:CZ	2.46	0.64
4:d:205:THR:HG22	4:d:205:THR:O	1.98	0.63
5:e:68:VAL:HG23	5:e:76:CYS:HB3	1.80	0.63
34:8:208:GLN:HG3	34:8:208:GLN:O	1.98	0.63
3:c:221:ASN:HB2	9:i:253:GLN:HB2	1.80	0.63
10:j:63:LEU:CD2	10:j:67:PHE:CE2	2.68	0.63
11:k:120:ASP:OD1	11:k:120:ASP:N	2.30	0.63
6:F:77:LEU:HD22	32:M:433:TYR:CE2	2.32	0.63
2:b:17:LYS:HG3	3:c:31:HIS:CE1	2.33	0.63
11:4:3:ILE:HD12	11:4:176:PHE:HD1	1.62	0.63
2:b:142:PHE:CE1	10:j:80:ARG:NH2	2.66	0.63
29:I:125:MET:O	29:I:125:MET:CG	2.45	0.63
5:E:165:TYR:CE2	6:F:60:GLN:HB2	2.34	0.63
10:3:154:TYR:HD1	10:3:155:GLU:N	1.96	0.63
13:6:94:ILE:HG22	13:6:123:ASP:HA	1.80	0.63
23:P:204:LEU:HD11	31:L:203:ASN:OD1	1.99	0.63
1:a:37:GLN:OE1	1:a:37:GLN:HA	1.97	0.63
10:j:172:LEU:HD12	10:j:202:MET:HE3	1.80	0.63
13:m:46:ARG:O	13:m:208:ASP:OD2	2.17	0.63
13:m:145:ARG:HH12	13:m:155:MET:HE3	1.63	0.63
1:A:24:ARG:HA	30:K:427:TYR:CE1	2.34	0.63
12:5:102:ALA:C	13:6:145:ARG:NH2	2.52	0.63
32:M:432:PHE:CD2	32:M:433:TYR:HD1	2.17	0.63
9:i:48:ARG:CZ	13:6:230:ASP:CG	2.72	0.63
10:j:203:ARG:HE	12:5:269:GLY:HA3	1.64	0.63
10:3:29:LEU:HD22	10:3:40:PHE:HD2	1.63	0.62
13:6:46:ARG:O	13:6:208:ASP:OD2	2.17	0.62
5:E:51:GLU:OE1	5:E:53:ARG:CZ	2.47	0.62
5:E:68:VAL:HG23	5:E:76:CYS:HB3	1.80	0.62
9:2:78:ALA:HB1	10:3:129:CYS:SG	2.39	0.62
13:m:109:ARG:HG2	13:m:136:VAL:CG1	2.13	0.62
9:2:51:GLN:NE2	10:3:125:ASP:CB	2.62	0.62
10:3:49:VAL:HG11	10:3:87:PHE:CD1	2.32	0.62
13:m:46:ARG:HA	13:m:208:ASP:OD2	2.00	0.62
4:D:149:GLN:NE2	4:D:150:THR:O	2.32	0.62
6:F:106:GLU:HG3	6:F:143:HIS:CD2	2.34	0.62
6:f:106:GLU:HG3	6:f:143:HIS:CD2	2.34	0.62
10:j:29:LEU:HD22	10:j:40:PHE:HD2	1.63	0.62
14:n:137:ARG:HH11	14:n:138:SER:N	1.98	0.62
13:m:201:GLU:OE1	9:2:58:LYS:CE	2.47	0.62
9:i:153:TYR:CE1	9:i:167:LEU:CD1	2.77	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:23:TYR:O	2:B:26:THR:OG1	2.16	0.62
3:C:18:ARG:NE	29:I:436:TYR:CE1	2.67	0.62
29:I:195:LYS:HE3	29:I:199:GLU:OE1	1.99	0.62
10:3:63:LEU:CD2	10:3:67:PHE:CE2	2.68	0.62
13:6:145:ARG:HH12	13:6:155:MET:HE3	1.63	0.62
10:j:88:THR:HG22	10:j:130:ILE:HG12	1.81	0.61
13:m:134:ASP:N	13:m:134:ASP:OD1	2.14	0.61
14:n:67:LEU:HD12	8:1:173:LYS:O	2.00	0.61
30:K:130:LEU:O	30:K:133:PRO:HD2	2.00	0.61
11:k:3:ILE:CG1	11:k:176:PHE:HD1	2.10	0.61
12:5:170:LEU:HD23	12:5:170:LEU:CA	2.22	0.61
23:P:361:THR:HG22	23:P:363:LEU:H	1.65	0.61
12:l:272:PHE:CE1	10:3:204:GLN:HG2	2.35	0.61
13:m:194:ASP:OD1	9:2:228:LYS:HB3	1.99	0.61
9:2:219:TYR:C	9:2:219:TYR:CD1	2.70	0.61
4:D:90:ARG:NE	11:4:69:ILE:HG21	2.15	0.61
8:1:120:TYR:HE2	8:1:130:LYS:HG3	1.65	0.61
25:R:44:LYS:HD3	25:R:91:TRP:CZ2	2.35	0.61
3:C:5:ARG:HH22	6:F:9:ASP:CG	2.08	0.61
3:C:177:GLN:HA	4:D:54:LEU:HD11	1.82	0.61
25:R:44:LYS:HG2	25:R:91:TRP:CE2	2.34	0.61
3:C:7:ASP:OD2	4:D:6:ARG:HD2	2.00	0.61
4:D:111:ARG:HH12	12:5:145:GLU:CD	2.08	0.61
1:a:149:GLU:CG	9:i:101:ARG:HH12	2.12	0.61
11:k:18:SER:OG	11:k:176:PHE:HB2	2.01	0.61
13:m:228:LYS:HE2	9:2:225:ARG:HA	1.82	0.61
10:3:98:ARG:HH21	11:4:93:ARG:HH21	1.49	0.61
5:e:18:GLU:OE1	5:e:22:PHE:CE1	2.54	0.61
3:C:18:ARG:NH2	29:I:436:TYR:CE1	2.65	0.61
25:R:44:LYS:HG2	25:R:91:TRP:CZ2	2.35	0.61
25:R:204:TRP:HB2	33:J:336:ASN:HD22	1.64	0.61
9:i:48:ARG:NH1	13:6:230:ASP:CG	2.59	0.60
9:2:92:ILE:HG13	9:2:111:MET:SD	2.41	0.60
16:V:45:VAL:CG1	16:V:46:PRO:HA	2.31	0.60
9:i:92:ILE:HG13	9:i:111:MET:SD	2.41	0.60
10:j:11:ILE:CG1	10:j:181:SER:HB3	2.32	0.60
10:3:98:ARG:HH12	11:4:93:ARG:CG	2.14	0.60
6:f:142:ALA:C	6:f:143:HIS:HD1	2.09	0.60
4:D:90:ARG:CD	11:4:69:ILE:CG2	2.79	0.60
8:1:85:GLU:HA	8:1:120:TYR:CE1	2.36	0.60
22:S:89:LYS:HE3	22:S:93:LEU:HD11	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:142:PHE:HB3	10:j:80:ARG:NE	2.17	0.60
8:h:85:GLU:HA	8:h:120:TYR:CE1	2.36	0.60
8:h:120:TYR:HE2	8:h:130:LYS:HG3	1.65	0.60
12:l:114:PRO:C	12:l:115:PHE:HD2	2.10	0.60
2:B:142:PHE:CD1	10:3:80:ARG:NH2	2.70	0.60
5:E:15:PHE:HE1	6:F:126:ARG:HD2	1.67	0.60
13:6:46:ARG:HA	13:6:208:ASP:OD2	2.00	0.60
17:T:150:ARG:HH21	22:S:381:VAL:HG23	1.66	0.60
31:L:254:LYS:CG	32:M:256:ILE:O	2.49	0.60
20:Z:912:PHE:CD1	20:Z:920:GLY:HA2	2.36	0.60
22:S:405:ARG:HD3	22:S:416:GLU:HG2	1.82	0.60
31:L:290:ARG:HE	32:M:295:LYS:HE2	1.66	0.60
2:b:159:TRP:HA	3:c:58:GLU:H	1.66	0.60
9:i:153:TYR:HE2	9:i:164:MET:SD	2.24	0.60
12:5:163:TYR:O	12:5:166:LYS:HB3	2.02	0.60
7:g:206:ASP:C	7:g:207:ASN:HD22	2.10	0.60
13:m:157:PHE:CE1	9:2:232:TYR:CE1	2.88	0.60
3:C:3:SER:H	6:F:123:TYR:HE2	1.50	0.60
12:5:114:PRO:C	12:5:115:PHE:HD2	2.10	0.60
10:3:8:ASN:HD21	10:3:57:ALA:N	2.00	0.60
11:4:18:SER:OG	11:4:176:PHE:HB2	2.01	0.60
13:6:101:ILE:CG2	13:6:133:PHE:CE1	2.85	0.59
16:V:242:LYS:HA	16:V:242:LYS:HE3	1.84	0.59
4:d:90:ARG:HD3	11:k:70:ARG:HA	1.84	0.59
12:l:163:TYR:O	12:l:166:LYS:HB3	2.02	0.59
13:m:145:ARG:NH1	13:m:155:MET:HE3	2.13	0.59
21:N:277:LEU:CD2	21:N:282:TYR:CZ	2.85	0.59
9:2:153:TYR:CE1	9:2:167:LEU:CD1	2.77	0.59
25:R:41:GLU:CA	25:R:44:LYS:HZ3	2.15	0.59
9:2:57:ASP:OD2	10:3:132:GLU:O	2.20	0.59
20:Z:528:LEU:HG	20:Z:532:HIS:CE1	2.38	0.59
21:N:303:LEU:HD13	21:N:342:GLY:HA3	1.84	0.59
34:8:154:GLU:HA	34:8:157:HIS:CD2	2.38	0.59
1:A:22:GLU:HG3	1:A:22:GLU:O	2.03	0.59
14:n:259:LYS:CG	8:1:194:ARG:NH1	2.66	0.59
9:2:153:TYR:HE2	9:2:164:MET:SD	2.24	0.59
20:Z:141:SER:O	20:Z:142:ASP:O	2.21	0.59
9:i:92:ILE:HG13	9:i:111:MET:HE1	1.85	0.59
11:k:135:TYR:CE1	11:4:25:ILE:CG1	2.86	0.59
10:3:172:LEU:HD11	10:3:200:LEU:HD13	1.85	0.59
28:H:331:ARG:HA	28:H:331:ARG:HE	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:g:104:LYS:HE3	14:n:98:ARG:CG	2.33	0.59
10:j:49:VAL:HG11	10:j:87:PHE:CD1	2.32	0.59
9:i:201:ASN:CG	9:i:221:THR:HG23	2.26	0.59
9:2:92:ILE:HG13	9:2:111:MET:HE1	1.85	0.59
9:2:247:VAL:O	10:3:195:VAL:O	2.20	0.59
12:5:133:TRP:CH2	12:5:161:LEU:HD21	2.37	0.59
22:S:112:ASN:O	22:S:114:TYR:CD2	2.55	0.59
26:U:175:LEU:C	26:U:176:ARG:HD2	2.28	0.59
10:j:8:ASN:HD21	10:j:57:ALA:N	1.99	0.59
20:Z:862:MET:HB3	20:Z:886:VAL:HG23	1.84	0.59
22:S:282:ILE:HA	22:S:382:ARG:HH12	1.68	0.59
12:l:133:TRP:CH2	12:l:161:LEU:HD21	2.37	0.58
6:F:142:ALA:C	6:F:143:HIS:HD1	2.09	0.58
11:4:120:ASP:N	11:4:120:ASP:OD1	2.30	0.58
10:j:152:SER:HB3	13:6:157:PHE:CZ	2.39	0.58
20:Z:308:LYS:O	20:Z:309:GLN:O	2.20	0.58
28:H:247:LEU:HD23	28:H:249:TYR:CD1	2.38	0.58
7:G:38:ILE:HD13	7:G:199:ILE:HD11	1.84	0.58
25:R:378:ASN:HD22	25:R:392:ARG:HG3	1.68	0.58
22:S:34:LEU:HD11	22:S:137:PHE:CD2	2.39	0.58
3:c:42:ASP:HB3	3:c:186:VAL:HG13	1.86	0.58
8:h:30:THR:HG22	8:h:32:GLY:O	2.02	0.58
12:l:286:ILE:HD11	10:3:199:TYR:CE2	2.38	0.58
11:4:3:ILE:CG2	11:4:136:SER:CB	2.80	0.58
25:R:117:ILE:HD12	25:R:133:ALA:HB1	1.85	0.58
10:j:11:ILE:CG2	10:j:181:SER:OG	2.52	0.58
1:A:249:ALA:O	23:P:84:LYS:CE	2.51	0.58
15:W:153:LEU:H	15:W:153:LEU:HD12	1.69	0.58
2:b:23:TYR:O	2:b:26:THR:OG1	2.16	0.58
13:m:58:ILE:HD11	13:m:94:ILE:HD13	1.83	0.58
21:N:672:ASN:HB3	21:N:675:VAL:HG23	1.85	0.58
1:a:22:GLU:HG3	1:a:22:GLU:O	2.03	0.58
3:C:42:ASP:HB3	3:C:186:VAL:HG13	1.86	0.58
7:G:18:ASP:CG	31:L:434:TYR:CD1	2.81	0.58
8:1:30:THR:HG22	8:1:32:GLY:O	2.03	0.58
30:K:415:VAL:O	30:K:416:LYS:O	2.21	0.58
12:5:140:LEU:CD2	12:5:144:ARG:HH21	2.17	0.58
23:P:204:LEU:HD13	23:P:206:LYS:HE2	1.85	0.58
11:k:96:ARG:HH21	12:l:166:LYS:CD	2.06	0.58
5:E:20:ARG:NH2	6:F:31:GLN:HB2	2.17	0.58
27:O:115:ARG:HH11	27:O:115:ARG:HG2	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:121:LEU:HD13	6:f:79:PRO:CB	2.33	0.57
10:j:11:ILE:CD1	10:j:181:SER:CB	2.81	0.57
2:B:78:MET:HE3	30:K:427:TYR:CE1	2.39	0.57
13:6:145:ARG:NH1	13:6:155:MET:HE3	2.13	0.57
29:I:77:SER:O	29:I:81:ILE:HG13	2.04	0.57
29:I:212:GLY:O	29:I:213:ILE:O	2.20	0.57
10:j:85:GLU:OE1	10:j:113:ASN:ND2	2.38	0.57
12:l:140:LEU:CD2	12:l:144:ARG:HH21	2.17	0.57
13:m:204:ILE:HD12	9:2:196:LEU:CB	2.34	0.57
11:4:4:ILE:HG22	11:4:17:SER:HB3	1.86	0.57
9:i:48:ARG:NH2	13:6:230:ASP:CG	2.58	0.57
9:i:88:ILE:HG21	9:i:111:MET:CB	2.34	0.57
29:I:102:ASN:O	29:I:103:PRO:C	2.48	0.57
8:h:142:PHE:CZ	14:7:66:LEU:HD13	2.39	0.57
9:i:237:GLY:HA3	13:6:171:GLY:H	1.69	0.57
9:i:243:LYS:NZ	10:j:199:TYR:HE2	2.02	0.57
7:G:18:ASP:OD2	31:L:434:TYR:CG	2.56	0.57
10:j:3:ASP:OD2	10:j:6:SER:HB2	2.05	0.57
12:l:170:LEU:HD23	12:l:170:LEU:CA	2.22	0.57
13:m:124:GLU:OE1	13:m:124:GLU:CA	2.48	0.57
13:m:201:GLU:CD	9:2:58:LYS:HE2	2.30	0.57
5:E:12:VAL:HG11	5:E:135:SER:O	2.03	0.57
9:2:88:ILE:HG21	9:2:111:MET:CB	2.34	0.57
33:J:133:LEU:HD22	33:J:240:HIS:CB	2.34	0.57
2:b:17:LYS:HG3	3:c:31:HIS:ND1	2.19	0.57
13:m:137:GLY:O	13:m:138:SER:O	2.23	0.57
8:1:199:PRO:HA	8:1:202:TYR:CE2	2.40	0.57
2:b:224:TYR:OH	9:i:65:ARG:NH1	2.20	0.57
1:A:249:ALA:O	23:P:84:LYS:NZ	2.37	0.57
10:3:3:ASP:OD2	10:3:6:SER:HB2	2.05	0.57
11:4:96:ARG:NH2	12:5:166:LYS:CD	2.46	0.57
30:K:104:ASP:HB3	30:K:107:THR:OG1	2.04	0.57
8:h:155:MET:HE1	8:h:163:PHE:CD1	2.40	0.57
12:l:155:SER:HG	12:l:188:TYR:HD2	1.51	0.57
1:A:249:ALA:O	23:P:84:LYS:HE2	2.05	0.57
9:2:249:ILE:CD1	10:3:195:VAL:HG23	2.35	0.57
13:6:101:ILE:CG2	13:6:133:PHE:HE1	2.18	0.57
25:R:40:ILE:H	25:R:40:ILE:HD12	1.69	0.57
9:i:181:ILE:HD11	9:i:206:VAL:HG21	1.87	0.57
19:Y:17:THR:HA	19:Y:20:LYS:HD2	1.86	0.57
13:6:94:ILE:HG21	13:6:123:ASP:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Q:46:VAL:O	24:Q:47:ASP:HB2	2.04	0.57
3:c:65:LYS:HB2	3:c:212:GLU:OE2	2.05	0.56
14:n:231:ALA:HB2	14:n:241:PHE:CD1	2.39	0.56
10:3:85:GLU:OE1	10:3:113:ASN:ND2	2.38	0.56
12:5:100:TRP:CH2	13:6:152:SER:HB3	2.40	0.56
1:a:78:THR:CG2	1:a:231:ASP:HA	2.35	0.56
5:E:20:ARG:HE	6:F:31:GLN:CD	2.12	0.56
9:2:181:ILE:HD11	9:2:206:VAL:HG21	1.87	0.56
25:R:71:LEU:HD12	25:R:72:VAL:H	1.70	0.56
10:j:8:ASN:HB3	10:j:30:GLY:O	2.06	0.56
8:1:13:MET:HB3	8:1:135:ILE:HG22	1.88	0.56
19:Y:31:GLU:HG3	19:Y:31:GLU:O	2.04	0.56
21:N:498:ILE:HG23	21:N:535:LEU:HD22	1.88	0.56
13:6:46:ARG:C	13:6:208:ASP:OD2	2.49	0.56
21:N:360:GLN:O	21:N:361:ASN:C	2.48	0.56
8:h:13:MET:HB3	8:h:135:ILE:HG22	1.88	0.56
8:h:174:TRP:HE1	8:1:145:GLY:HA2	1.70	0.56
13:m:46:ARG:C	13:m:208:ASP:OD2	2.49	0.56
9:2:123:ILE:HA	10:3:99:ARG:HH11	1.70	0.56
4:d:98:LEU:O	12:l:156:LYS:HE2	2.05	0.56
11:k:139:TYR:CD1	11:k:171:ARG:HB2	2.41	0.56
12:l:79:LEU:HB3	12:l:203:CYS:SG	2.46	0.56
3:C:65:LYS:HB2	3:C:212:GLU:OE2	2.05	0.56
6:F:155:GLU:HG3	7:G:60:VAL:HG21	1.88	0.56
32:M:286:ILE:HG13	32:M:287:GLY:N	2.18	0.56
3:c:5:ARG:NH2	6:f:9:ASP:OD2	2.39	0.56
10:3:8:ASN:HB3	10:3:30:GLY:O	2.06	0.56
12:5:155:SER:HG	12:5:188:TYR:HD2	1.53	0.56
22:S:211:ARG:NH1	22:S:240:ASP:HB3	2.20	0.56
5:e:128:SER:HB3	6:f:128:TYR:OH	2.05	0.56
11:4:139:TYR:CD1	11:4:171:ARG:HB2	2.41	0.56
12:5:79:LEU:HB3	12:5:203:CYS:SG	2.46	0.56
13:6:137:GLY:O	13:6:138:SER:O	2.23	0.56
6:f:119:ASN:N	6:f:119:ASN:OD1	2.37	0.56
16:V:45:VAL:HG21	16:V:143:PRO:CG	2.35	0.56
16:V:54:LEU:HD21	16:V:102:GLN:H	1.70	0.56
10:3:125:ASP:CG	10:3:126:LEU:N	2.61	0.55
16:V:18:THR:HG23	21:N:397:SER:HA	1.88	0.55
20:Z:959:HIS:H	20:Z:961:GLU:HG3	1.72	0.55
29:I:77:SER:HA	29:I:81:ILE:HD11	1.87	0.55
30:K:82:ALA:O	30:K:86:VAL:HG23	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:191:GLU:HG3	3:c:242:THR:HG22	1.89	0.55
10:3:29:LEU:HD22	10:3:40:PHE:CE2	2.42	0.55
12:5:245:TYR:N	12:5:245:TYR:CD1	2.67	0.55
13:6:124:GLU:OE1	13:6:124:GLU:CA	2.48	0.55
20:Z:171:LYS:HD3	20:Z:171:LYS:N	2.21	0.55
12:5:128:GLN:OE1	13:6:102:GLN:OE1	2.24	0.55
17:T:260:ILE:HD12	17:T:260:ILE:H	1.71	0.55
3:c:224:GLU:HB2	9:i:252:ILE:HG21	1.88	0.55
13:m:41:TYR:N	13:m:41:TYR:HD1	2.05	0.55
7:G:18:ASP:OD2	31:L:434:TYR:CE2	2.58	0.55
3:C:11:THR:OG1	4:D:8:LEU:CD1	2.54	0.55
1:A:81:MET:HE1	1:A:94:ALA:HA	1.89	0.55
3:C:191:GLU:HG3	3:C:242:THR:HG22	1.89	0.55
12:5:102:ALA:O	13:6:145:ARG:CZ	2.54	0.55
34:8:444:GLU:H	35:9:73:LEU:HD12	1.72	0.55
9:i:223:ASN:ND2	13:6:230:ASP:HB2	2.21	0.55
11:k:121:TYR:HD1	11:k:122:LEU:N	2.05	0.55
15:W:22:PRO:HG3	15:W:180:LEU:CD2	2.36	0.55
15:W:127:ARG:O	15:W:131:THR:HG23	2.06	0.55
12:l:79:LEU:HD21	12:l:235:SER:HB2	1.89	0.55
29:I:138:LYS:O	29:I:141:LEU:CD2	2.55	0.55
2:b:17:LYS:H	3:c:28:SER:HB3	1.71	0.55
5:e:18:GLU:CD	5:e:22:PHE:HE1	2.14	0.55
12:5:79:LEU:HD21	12:5:235:SER:HB2	1.89	0.55
9:i:243:LYS:NZ	10:j:199:TYR:CD2	2.70	0.55
10:j:89:GLN:OE1	10:j:130:ILE:HD11	2.06	0.55
6:F:119:ASN:OD1	6:F:119:ASN:N	2.37	0.55
20:Z:713:LYS:HE3	20:Z:746:ILE:HD11	1.89	0.55
14:n:219:TYR:HE2	9:2:168:GLU:OE1	1.84	0.54
8:1:144:TYR:OH	14:7:68:ARG:HA	2.07	0.54
14:n:252:TRP:CZ2	8:1:199:PRO:HG2	2.42	0.54
24:Q:39:SER:HB3	24:Q:87:GLN:HE21	1.72	0.54
2:b:4:ARG:HG2	4:d:5:ASP:OD1	2.06	0.54
12:l:111:GLU:HG2	12:l:260:TRP:CZ2	2.42	0.54
10:3:182:GLY:O	10:3:183:TRP:C	2.49	0.54
13:6:134:ASP:OD1	13:6:134:ASP:N	2.14	0.54
20:Z:142:ASP:C	20:Z:142:ASP:OD1	2.51	0.54
20:Z:721:ASN:OD1	20:Z:767:TYR:HB3	2.07	0.54
21:N:242:PHE:HB3	21:N:282:TYR:OH	2.07	0.54
23:P:130:ILE:HD12	23:P:131:PHE:H	1.72	0.54
14:n:215:ARG:NH1	9:2:169:SER:HA	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:18:ASP:CG	31:L:434:TYR:CG	2.85	0.54
11:4:96:ARG:CZ	11:4:96:ARG:HB3	2.37	0.54
20:Z:850:LEU:CD2	20:Z:859:LYS:HA	2.36	0.54
21:N:301:THR:HG22	21:N:920:VAL:HG23	1.89	0.54
21:N:553:PHE:O	21:N:557:LEU:HD12	2.06	0.54
27:O:266:PHE:O	27:O:270:ILE:HG12	2.07	0.54
2:b:123:GLN:OE1	2:b:123:GLN:HA	2.08	0.54
10:3:4:PRO:O	10:3:56:LEU:HB2	2.08	0.54
12:5:138:CYS:SG	12:5:149:ILE:HG21	2.48	0.54
16:V:25:GLU:HB2	16:V:199:LEU:HD11	1.88	0.54
14:n:254:PHE:CE2	8:1:39:VAL:HG11	2.42	0.54
6:F:155:GLU:HG3	7:G:60:VAL:CG2	2.37	0.54
10:3:8:ASN:HD21	10:3:57:ALA:CA	2.20	0.54
10:j:8:ASN:HD21	10:j:57:ALA:CA	2.21	0.54
10:j:29:LEU:HD22	10:j:40:PHE:CE2	2.42	0.54
6:F:101:ARG:NH1	14:7:107:ASN:HD21	2.06	0.54
20:Z:773:ARG:HG2	20:Z:799:PHE:CZ	2.43	0.54
24:Q:275:ILE:CD1	24:Q:307:ASN:HB2	2.35	0.54
25:R:315:VAL:C	25:R:318:PRO:HD2	2.33	0.54
13:6:41:TYR:N	13:6:41:TYR:HD1	2.05	0.54
12:l:138:CYS:SG	12:l:149:ILE:HG21	2.48	0.54
13:m:201:GLU:CD	9:2:58:LYS:CE	2.81	0.54
11:4:121:TYR:HD1	11:4:122:LEU:N	2.05	0.54
12:5:111:GLU:HG2	12:5:260:TRP:CZ2	2.42	0.54
32:M:432:PHE:CE2	32:M:433:TYR:HD1	2.25	0.54
16:V:241:THR:HG23	24:Q:415:LEU:HD22	1.90	0.54
6:F:139:LYS:CD	14:7:118:GLU:O	2.56	0.53
10:3:125:ASP:OD2	10:3:126:LEU:HD12	2.08	0.53
19:Y:31:GLU:O	19:Y:32:ASP:CB	2.56	0.53
11:k:96:ARG:HB3	11:k:96:ARG:CZ	2.37	0.53
11:4:170:LYS:HE3	11:4:171:ARG:NH2	2.16	0.53
16:V:288:LEU:HB2	26:U:261:LEU:HD23	1.90	0.53
16:V:305:ILE:HG22	26:U:236:LEU:HG	1.89	0.53
25:R:71:LEU:HD12	25:R:72:VAL:N	2.23	0.53
14:n:36:GLN:H	14:n:36:GLN:CD	2.16	0.53
2:B:78:MET:HE3	30:K:426:PHE:CE2	2.44	0.53
8:1:17:PHE:CE1	8:1:19:ASP:HB2	2.43	0.53
9:2:78:ALA:CB	10:3:129:CYS:SG	2.96	0.53
28:H:457:PHE:CE2	29:I:331:ILE:HD12	2.43	0.53
7:g:104:LYS:NZ	14:n:98:ARG:NH1	2.54	0.53
9:i:92:ILE:HG13	9:i:111:MET:CE	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:j:11:ILE:HG12	10:j:181:SER:CB	2.38	0.53
11:k:25:ILE:O	11:4:173:PRO:HD3	2.08	0.53
11:k:121:TYR:HD1	11:k:121:TYR:C	2.16	0.53
11:k:170:LYS:HE3	11:k:171:ARG:NH2	2.16	0.53
5:E:47:VAL:HG11	5:E:197:GLU:HG3	1.89	0.53
13:6:36:ARG:HH11	13:6:207:GLY:HA3	1.73	0.53
31:L:290:ARG:NE	32:M:295:LYS:HE2	2.22	0.53
12:l:241:HIS:CD2	10:3:183:TRP:HE1	2.27	0.53
9:2:51:GLN:NE2	10:3:125:ASP:HB3	2.23	0.53
11:4:96:ARG:HB3	11:4:96:ARG:NH1	2.24	0.53
16:V:230:TYR:CD1	23:P:412:LEU:HB3	2.42	0.53
21:N:39:ILE:HG13	21:N:39:ILE:O	2.09	0.53
4:d:120:TYR:HA	4:d:126:VAL:CG2	2.39	0.53
10:j:37:SER:HB3	11:k:126:VAL:HG11	1.91	0.53
11:k:96:ARG:HB3	11:k:96:ARG:NH1	2.23	0.53
12:l:187:ILE:C	12:l:188:TYR:HD1	2.17	0.53
2:B:123:GLN:OE1	2:B:123:GLN:HA	2.08	0.53
11:4:121:TYR:HD1	11:4:121:TYR:C	2.16	0.53
12:5:113:ASN:HB2	12:5:114:PRO:HD2	1.89	0.53
26:U:82:LYS:HG2	32:M:68:LYS:HE3	1.91	0.53
34:8:131:ASN:H	34:8:495:LYS:HZ1	1.56	0.53
5:e:47:VAL:HG11	5:e:197:GLU:HG3	1.89	0.53
9:i:181:ILE:HD11	9:i:206:VAL:CG2	2.39	0.53
10:j:26:ASP:OD2	10:j:181:SER:HB3	2.08	0.53
9:2:92:ILE:HG13	9:2:111:MET:CE	2.38	0.53
28:H:144:LYS:O	28:H:145:TYR:CD1	2.60	0.53
3:c:5:ARG:NH2	6:f:9:ASP:CG	2.67	0.53
9:i:88:ILE:CG2	9:i:111:MET:HB3	2.37	0.53
5:e:18:GLU:O	6:f:31:GLN:NE2	2.42	0.53
10:j:4:PRO:O	10:j:56:LEU:HB2	2.08	0.53
2:B:16:GLY:O	2:B:17:LYS:HB2	2.08	0.53
7:G:104:LYS:CG	8:1:89:SER:HB3	2.39	0.53
26:U:175:LEU:O	26:U:176:ARG:NH1	2.42	0.53
3:c:98:TYR:HH	11:k:67:TYR:HE1	1.51	0.53
10:j:11:ILE:HD13	10:j:181:SER:CB	2.39	0.53
6:F:146:GLU:O	6:F:153:VAL:HA	2.09	0.53
13:6:126:GLY:CA	13:6:217:LYS:NZ	2.72	0.53
30:K:352:ILE:HG22	30:K:383:ILE:HG21	1.91	0.53
6:f:146:GLU:O	6:f:153:VAL:HA	2.09	0.52
1:A:185:HIS:ND1	1:A:209:HIS:CE1	2.77	0.52
5:E:15:PHE:CE1	6:F:126:ARG:HD2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:2:181:ILE:HD11	9:2:206:VAL:CG2	2.39	0.52
15:W:6:THR:CG2	15:W:8:LEU:HD23	2.38	0.52
22:S:267:SER:O	22:S:271:ARG:HG3	2.09	0.52
25:R:204:TRP:HB2	33:J:336:ASN:ND2	2.23	0.52
1:a:81:MET:HE1	1:a:94:ALA:HA	1.91	0.52
4:D:159:TRP:CH2	5:E:59:LEU:HD13	2.44	0.52
11:4:49:GLU:O	11:4:50:ALA:C	2.51	0.52
27:O:169:ASN:OD1	27:O:198:THR:HG23	2.09	0.52
29:I:138:LYS:O	29:I:141:LEU:HD21	2.09	0.52
30:K:322:ASP:CG	31:L:290:ARG:HH11	2.18	0.52
33:J:133:LEU:HD22	33:J:240:HIS:CG	2.44	0.52
1:a:185:HIS:ND1	1:a:209:HIS:CE1	2.77	0.52
2:b:14:PRO:HA	3:c:24:TYR:CD1	2.45	0.52
9:i:243:LYS:HZ1	10:j:199:TYR:HE2	1.48	0.52
1:A:35:THR:HG22	1:A:138:GLY:O	2.09	0.52
4:D:94:GLN:HE21	11:4:62:ALA:HA	1.75	0.52
6:F:77:LEU:HD13	32:M:433:TYR:CE2	2.44	0.52
8:1:125:GLY:CA	14:7:38:ILE:HG13	2.40	0.52
9:2:88:ILE:CG2	9:2:111:MET:HB3	2.37	0.52
12:5:187:ILE:C	12:5:188:TYR:HD1	2.17	0.52
14:n:176:ALA:HB3	14:n:181:ALA:HA	1.92	0.52
2:B:32:VAL:HG13	30:K:428:LYS:OXT	2.10	0.52
9:2:249:ILE:CD1	10:3:195:VAL:CG2	2.87	0.52
7:g:204:HIS:CE1	7:g:212:PHE:HD1	2.28	0.52
20:Z:813:PHE:CD1	20:Z:817:LEU:HD21	2.45	0.52
9:i:190:ALA:HB2	14:7:190:LYS:HE2	1.90	0.52
33:J:324:ARG:HG3	33:J:358:VAL:HG11	1.91	0.52
8:h:30:THR:CG2	8:h:32:GLY:O	2.58	0.52
12:l:113:ASN:HB2	12:l:114:PRO:HD2	1.89	0.52
13:m:36:ARG:HH11	13:m:207:GLY:HA3	1.73	0.52
2:B:190:HIS:CE1	24:Q:95:LYS:HE2	2.44	0.52
8:1:30:THR:CG2	8:1:32:GLY:O	2.58	0.52
11:4:3:ILE:HG21	11:4:136:SER:HB2	1.90	0.52
29:I:301:GLU:O	29:I:305:THR:HG23	2.10	0.52
13:m:126:GLY:CA	13:m:217:LYS:NZ	2.72	0.52
13:m:197:THR:HG21	9:2:226:GLU:CG	2.39	0.52
12:5:103:SER:OG	13:6:145:ARG:NH2	2.42	0.52
13:6:186:GLU:OE1	13:6:186:GLU:HA	2.10	0.52
33:J:220:GLN:HE22	33:J:226:GLY:HA2	1.74	0.52
8:h:99:LYS:HG3	8:h:100:ASP:OD2	2.10	0.52
14:n:222:ALA:HA	8:1:35:ILE:HD11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:4:170:LYS:CE	11:4:171:ARG:HH21	2.18	0.52
8:h:180:GLY:HA2	14:7:252:TRP:CZ3	2.45	0.52
13:m:186:GLU:OE1	13:m:186:GLU:HA	2.10	0.52
10:3:168:SER:O	10:3:172:LEU:HD12	2.10	0.52
13:6:101:ILE:HG21	13:6:133:PHE:CD1	2.43	0.52
20:Z:221:VAL:HG12	20:Z:267:THR:CG2	2.38	0.52
23:P:89:LEU:O	23:P:90:LYS:CG	2.57	0.52
4:d:171:VAL:HG13	4:d:198:SER:HB3	1.92	0.51
11:k:174:MET:HE3	11:4:173:PRO:O	2.10	0.51
2:B:4:ARG:NH2	5:E:125:GLU:HB2	2.25	0.51
20:Z:4:GLU:O	20:Z:5:SER:O	2.28	0.51
20:Z:428:TRP:CE3	20:Z:888:LEU:HD12	2.46	0.51
26:U:176:ARG:HD2	26:U:176:ARG:N	2.24	0.51
33:J:399:SER:O	33:J:400:VAL:HG23	2.10	0.51
2:b:16:GLY:O	2:b:17:LYS:HB2	2.08	0.51
8:1:99:LYS:HG3	8:1:100:ASP:OD2	2.10	0.51
21:N:709:GLY:HA3	21:N:713:VAL:HG22	1.91	0.51
2:b:30:GLN:OE1	2:b:30:GLN:HA	2.10	0.51
9:i:92:ILE:HD11	9:i:111:MET:CE	2.40	0.51
1:a:35:THR:HG22	1:a:138:GLY:O	2.09	0.51
11:k:35:THR:CG2	11:k:182:LYS:HZ3	1.98	0.51
4:D:187:THR:HG22	4:D:189:GLU:H	1.75	0.51
16:V:238:LEU:HB2	24:Q:408:THR:HG22	1.93	0.51
30:K:230:THR:HG23	30:K:232:ALA:H	1.76	0.51
1:a:135:ARG:NH1	7:g:15:PHE:CE2	2.78	0.51
28:H:462:ARG:HH21	28:H:465:GLN:NE2	2.09	0.51
35:9:15:LEU:HG	35:9:17:VAL:HG23	1.93	0.51
11:k:67:TYR:O	11:k:67:TYR:CD2	2.59	0.51
9:2:92:ILE:HD11	9:2:111:MET:CE	2.40	0.51
18:X:85:ARG:HH21	18:X:100:TRP:HE1	1.59	0.51
8:h:97:GLU:C	8:h:98:ASN:OD1	2.54	0.51
10:j:183:TRP:CZ2	12:5:241:HIS:CD2	2.99	0.51
10:3:48:HIS:CE1	10:3:114:SER:OG	2.64	0.51
11:4:67:TYR:O	11:4:67:TYR:CD2	2.59	0.51
29:I:101:GLY:HA3	29:I:102:ASN:C	2.35	0.51
31:L:426:LYS:HE3	32:M:338:LEU:O	2.11	0.51
32:M:428:LYS:O	32:M:429:SER:HB2	2.09	0.51
13:m:189:ILE:HD11	13:m:214:ILE:HD11	1.92	0.51
8:1:144:TYR:OH	14:7:68:ARG:HG3	2.11	0.51
3:c:221:ASN:HB2	9:i:253:GLN:CB	2.41	0.51
10:j:183:TRP:HD1	10:j:204:GLN:OE1	1.86	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:79:PRO:HD2	32:M:433:TYR:HD2	1.75	0.51
8:l:133:TYR:C	8:l:133:TYR:CD2	2.77	0.51
20:Z:767:TYR:CG	20:Z:850:LEU:HD13	2.46	0.51
21:N:360:GLN:O	21:N:361:ASN:O	2.29	0.51
24:Q:115:ILE:HD11	24:Q:148:LYS:HG3	1.93	0.51
26:U:10:ILE:HD12	26:U:160:THR:O	2.11	0.51
11:k:49:GLU:O	11:k:50:ALA:C	2.51	0.50
20:Z:713:LYS:HE3	20:Z:746:ILE:CD1	2.41	0.50
20:Z:746:ILE:HG21	20:Z:753:GLY:C	2.36	0.50
1:a:149:GLU:OE1	9:i:101:ARG:NH2	2.42	0.50
10:j:48:HIS:CE1	10:j:114:SER:OG	2.64	0.50
14:n:222:ALA:O	8:l:176:GLY:O	2.30	0.50
13:6:200:THR:HG22	13:6:230:ASP:OXT	2.11	0.50
34:8:111:PHE:CZ	34:8:179:VAL:HG11	2.46	0.50
14:n:189:ARG:HD2	9:2:194:ASN:OD1	2.11	0.50
4:D:90:ARG:NE	11:4:69:ILE:CG2	2.74	0.50
1:a:78:THR:HG23	1:a:231:ASP:HA	1.93	0.50
9:i:153:TYR:OH	9:i:167:LEU:CD1	2.59	0.50
13:m:46:ARG:HB3	13:m:208:ASP:OD2	2.12	0.50
2:B:30:GLN:OE1	2:B:30:GLN:HA	2.11	0.50
20:Z:725:GLU:OE1	20:Z:850:LEU:HD22	2.11	0.50
21:N:280:GLN:CD	21:N:282:TYR:OH	2.49	0.50
8:h:133:TYR:C	8:h:133:TYR:CD2	2.77	0.50
9:2:153:TYR:OH	9:2:167:LEU:CD1	2.59	0.50
13:6:189:ILE:HD11	13:6:214:ILE:HD11	1.92	0.50
19:Y:31:GLU:O	19:Y:32:ASP:HB2	2.11	0.50
30:K:274:VAL:HG12	30:K:277:ILE:HD12	1.93	0.50
9:i:153:TYR:C	9:i:153:TYR:CD2	2.90	0.50
13:m:200:THR:HG22	13:m:230:ASP:OXT	2.11	0.50
3:C:152:ASN:HB2	3:C:153:PRO:HD2	1.94	0.50
6:F:45:VAL:HG21	6:F:189:LEU:HB3	1.94	0.50
30:K:56:LYS:O	30:K:56:LYS:HG2	2.12	0.50
30:K:138:ALA:HB3	30:K:148:ASP:HB3	1.94	0.50
5:e:52:LYS:HE3	5:e:218:GLN:HB2	1.94	0.50
12:5:140:LEU:HD23	12:5:144:ARG:NH2	2.25	0.50
20:Z:462:VAL:HG13	20:Z:462:VAL:O	2.11	0.50
29:I:101:GLY:CA	29:I:102:ASN:O	2.58	0.50
3:c:152:ASN:HB2	3:c:153:PRO:HD2	1.94	0.50
10:3:87:PHE:HD2	10:3:87:PHE:O	1.95	0.50
29:I:133:LEU:HD23	29:I:156:ILE:O	2.10	0.50
31:L:283:VAL:HG13	31:L:283:VAL:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:9:31:GLN:HB2	35:9:36:ILE:O	2.12	0.50
8:1:97:GLU:C	8:1:98:ASN:OD1	2.54	0.50
2:B:200:VAL:C	2:B:201:GLU:OE1	2.55	0.49
6:F:107:ARG:CG	14:7:111:ASN:OD1	2.60	0.49
20:Z:146:PHE:CD1	20:Z:149:TRP:HD1	2.30	0.49
10:3:11:ILE:CG1	10:3:26:ASP:OD2	2.60	0.49
11:4:172:MET:HE2	11:4:174:MET:HB2	1.95	0.49
17:T:150:ARG:NH2	22:S:381:VAL:HG23	2.28	0.49
28:H:90:ARG:HG2	28:H:91:LEU:H	1.77	0.49
11:k:172:MET:HE2	11:k:174:MET:HB2	1.95	0.49
4:D:107:GLU:HG2	4:D:111:ARG:HH11	1.77	0.49
20:Z:309:GLN:C	20:Z:311:ALA:N	2.69	0.49
25:R:138:GLY:HA3	25:R:154:LEU:HG	1.94	0.49
28:H:203:LYS:HD2	28:H:264:ALA:O	2.12	0.49
32:M:117:ALA:O	32:M:129:LEU:CD2	2.57	0.49
9:2:94:LEU:O	9:2:98:TYR:HB2	2.13	0.49
9:2:153:TYR:C	9:2:153:TYR:CD2	2.90	0.49
10:3:120:PHE:CD1	10:3:134:LYS:HE3	2.47	0.49
16:V:45:VAL:HG21	16:V:143:PRO:HG2	1.94	0.49
2:b:203:GLU:OE1	2:b:205:ASN:OD1	2.30	0.49
9:i:92:ILE:HD11	9:i:111:MET:HE1	1.95	0.49
10:j:89:GLN:OE1	10:j:130:ILE:CD1	2.60	0.49
10:j:101:GLY:C	11:k:93:ARG:HH21	2.20	0.49
1:A:249:ALA:HB1	23:P:84:LYS:HB3	1.94	0.49
5:E:20:ARG:NH2	6:F:31:GLN:CB	2.74	0.49
16:V:45:VAL:HG21	16:V:143:PRO:HG3	1.93	0.49
12:l:83:PHE:CE1	12:l:88:ILE:HG12	2.47	0.49
12:l:286:ILE:HD11	10:3:199:TYR:CD2	2.47	0.49
13:m:57:ASN:N	13:m:57:ASN:OD1	2.43	0.49
1:A:108:TYR:CE1	9:2:111:MET:HE2	2.47	0.49
3:C:143:ARG:CZ	11:4:73:TYR:HB2	2.42	0.49
13:6:46:ARG:HB3	13:6:208:ASP:OD2	2.12	0.49
15:W:123:ASP:O	15:W:126:ILE:HG22	2.12	0.49
20:Z:24:THR:HB	20:Z:25:PRO:HD3	1.94	0.49
22:S:475:TYR:CD1	26:U:273:LEU:HB2	2.48	0.49
9:i:49:SER:OG	9:i:62:LYS:NZ	2.45	0.49
11:k:139:TYR:HD1	11:k:171:ARG:HB2	1.77	0.49
9:2:92:ILE:HD11	9:2:111:MET:HE1	1.95	0.49
9:2:126:TYR:CE1	9:2:144:ALA:HB2	2.45	0.49
24:Q:12:ARG:HA	24:Q:12:ARG:HH11	1.77	0.49
26:U:173:HIS:O	26:U:176:ARG:NH1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:L:131:VAL:HG12	31:L:155:ILE:HD12	1.94	0.49
32:M:432:PHE:CZ	32:M:433:TYR:HE1	2.31	0.49
2:b:200:VAL:C	2:b:201:GLU:OE1	2.55	0.49
9:i:153:TYR:CD2	9:i:167:LEU:CD1	2.94	0.49
14:n:137:ARG:NH1	14:n:138:SER:CB	2.74	0.49
2:B:203:GLU:OE1	2:B:205:ASN:OD1	2.30	0.49
4:D:10:ILE:HG21	5:E:10:ARG:HH21	1.76	0.49
16:V:25:GLU:C	16:V:199:LEU:HD12	2.37	0.49
21:N:530:GLU:OE1	21:N:530:GLU:N	2.39	0.49
24:Q:67:THR:HB	24:Q:68:MET:HA	1.94	0.49
1:a:92:ASN:HD22	7:g:121:GLN:HE22	1.61	0.49
28:H:388:ILE:HA	28:H:391:ILE:HD12	1.93	0.49
29:I:208:TYR:CD2	29:I:211:MET:HE2	2.40	0.49
1:a:149:GLU:CD	9:i:101:ARG:NH1	2.67	0.48
4:d:93:ALA:HB1	4:d:97:ARG:HH21	1.78	0.48
6:f:45:VAL:HG21	6:f:189:LEU:HB3	1.94	0.48
7:g:204:HIS:CE1	7:g:212:PHE:CD1	3.01	0.48
12:l:94:ARG:NH2	10:3:205:ASP:CG	2.71	0.48
5:E:13:SER:OG	5:E:124:GLY:HA2	2.12	0.48
20:Z:850:LEU:HD23	20:Z:850:LEU:O	2.13	0.48
32:M:129:LEU:CD1	32:M:155:ILE:H	2.25	0.48
10:j:18:LYS:HB2	10:j:157:ASN:HB3	1.95	0.48
10:j:205:ASP:CG	12:5:94:ARG:NH2	2.71	0.48
4:D:100:LEU:O	4:D:101:GLU:O	2.31	0.48
10:3:145:GLN:HB2	10:3:174:ALA:HB1	1.95	0.48
20:Z:85:VAL:HB	20:Z:86:PRO:CD	2.43	0.48
9:i:94:LEU:O	9:i:98:TYR:HB2	2.13	0.48
10:j:87:PHE:O	10:j:87:PHE:HD2	1.95	0.48
11:k:98:TYR:N	11:k:98:TYR:CD1	2.80	0.48
13:m:109:ARG:HA	13:m:136:VAL:HG13	1.95	0.48
9:2:49:SER:OG	9:2:62:LYS:NZ	2.45	0.48
12:5:113:ASN:CB	12:5:114:PRO:CD	2.90	0.48
12:5:155:SER:OG	12:5:188:TYR:HD2	1.96	0.48
13:6:101:ILE:CG2	13:6:133:PHE:CD1	2.97	0.48
26:U:37:ILE:HD11	26:U:93:TYR:CA	2.43	0.48
1:a:30:TYR:HB3	7:g:16:SER:O	2.13	0.48
9:i:109:LEU:HD11	9:i:148:THR:HG21	1.94	0.48
11:k:121:TYR:C	11:k:121:TYR:CD1	2.90	0.48
12:l:126:ASP:HA	13:m:106:TYR:CE1	2.48	0.48
13:m:201:GLU:OE2	9:2:58:LYS:CE	2.61	0.48
6:F:99:PHE:O	14:7:124:TYR:HA	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:4:98:TYR:N	11:4:98:TYR:CD1	2.80	0.48
20:Z:817:LEU:HD23	20:Z:817:LEU:N	2.26	0.48
33:J:109:ALA:O	33:J:110:SER:HB2	2.12	0.48
3:c:177:GLN:HE21	4:d:53:LYS:HB2	1.78	0.48
12:l:140:LEU:HD23	12:l:144:ARG:NH2	2.25	0.48
16:V:26:THR:HG23	16:V:200:ASN:O	2.13	0.48
24:Q:104:PHE:CE2	24:Q:114:GLN:HA	2.49	0.48
24:Q:309:ARG:HH12	24:Q:349:LYS:HD2	1.79	0.48
27:O:26:PHE:HA	27:O:29:PHE:CE2	2.48	0.48
12:l:187:ILE:O	12:l:188:TYR:HD1	1.96	0.48
14:n:134:TYR:O	14:n:137:ARG:NE	2.46	0.48
9:2:109:LEU:HD11	9:2:148:THR:HG21	1.94	0.48
24:Q:83:GLU:OE2	24:Q:83:GLU:N	2.47	0.48
10:j:28:ARG:CB	10:j:182:GLY:O	2.61	0.48
27:O:36:LYS:HA	27:O:38:TRP:CE2	2.48	0.48
29:I:99:ILE:HD13	29:I:133:LEU:HG	1.96	0.48
4:d:232:TYR:O	4:d:236:ILE:HD12	2.14	0.48
11:k:71:GLU:O	11:k:72:ASP:HB2	2.13	0.48
12:l:100:TRP:CE3	10:3:145:GLN:NE2	2.82	0.48
11:4:121:TYR:C	11:4:121:TYR:CD1	2.90	0.48
11:4:193:ASP:O	11:4:195:PHE:CZ	2.67	0.48
20:Z:317:GLN:HE21	20:Z:317:GLN:HA	1.79	0.48
21:N:246:LYS:HE2	21:N:246:LYS:HA	1.95	0.48
26:U:236:LEU:HD23	26:U:237:PRO:O	2.14	0.48
30:K:249:GLU:O	30:K:252:ARG:HG2	2.12	0.48
3:c:4:ARG:HG2	4:d:6:ARG:HG2	1.94	0.48
3:c:133:VAL:HG11	3:c:135:PHE:CZ	2.48	0.48
9:i:31:THR:OG1	9:i:159:GLY:C	2.57	0.48
9:i:153:TYR:OH	9:i:167:LEU:HD13	2.04	0.48
13:m:197:THR:CG2	9:2:226:GLU:HG3	2.42	0.48
3:C:133:VAL:HG11	3:C:135:PHE:CZ	2.48	0.48
5:E:8:TYR:HD1	5:E:22:PHE:CE2	2.32	0.48
20:Z:745:LEU:HD12	20:Z:746:ILE:HG13	1.95	0.48
8:h:41:ASP:HB2	8:h:183:ARG:HH11	1.79	0.48
9:i:240:ALA:HB2	13:6:174:GLY:N	2.29	0.48
12:l:155:SER:OG	12:l:188:TYR:HD2	1.96	0.48
14:n:251:LYS:HE2	9:2:171:TRP:O	2.12	0.48
18:X:27:ILE:H	18:X:59:ARG:HH22	1.60	0.48
20:Z:875:LYS:HB2	20:Z:878:LEU:HD23	1.95	0.48
11:k:49:GLU:O	11:k:50:ALA:O	2.32	0.47
6:F:106:GLU:CG	6:F:143:HIS:CD2	2.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1:175:ASP:OD2	8:1:177:SER:N	2.47	0.47
9:2:153:TYR:OH	9:2:167:LEU:HD13	2.04	0.47
11:4:49:GLU:O	11:4:50:ALA:O	2.32	0.47
12:5:187:ILE:O	12:5:188:TYR:HD1	1.96	0.47
13:6:9:GLN:OE1	13:6:9:GLN:HA	2.14	0.47
13:6:79:SER:O	13:6:83:TYR:HB2	2.13	0.47
20:Z:801:HIS:O	20:Z:802:ASP:C	2.57	0.47
22:S:114:TYR:HB3	22:S:115:PRO:HD2	1.96	0.47
25:R:258:LEU:HD21	25:R:293:THR:HA	1.94	0.47
27:O:58:ARG:NH1	27:O:85:SER:OG	2.46	0.47
34:8:117:THR:O	34:8:117:THR:HG22	2.13	0.47
10:j:88:THR:HG23	10:j:124:PHE:HZ	1.79	0.47
11:k:193:ASP:O	11:k:195:PHE:CZ	2.67	0.47
5:E:53:ARG:HE	5:E:53:ARG:HB2	1.40	0.47
9:2:31:THR:OG1	9:2:159:GLY:C	2.57	0.47
13:6:94:ILE:CG2	13:6:123:ASP:HA	2.44	0.47
27:O:76:LEU:O	27:O:80:LYS:HB2	2.14	0.47
32:M:129:LEU:HD23	32:M:129:LEU:H	1.79	0.47
10:j:11:ILE:HD11	10:j:181:SER:HB3	1.93	0.47
11:k:43:LEU:HD21	11:k:182:LYS:HE2	1.96	0.47
9:2:153:TYR:CD2	9:2:167:LEU:CD1	2.94	0.47
10:3:59:ASP:O	10:3:63:LEU:HB2	2.15	0.47
33:J:324:ARG:CG	33:J:358:VAL:HG11	2.44	0.47
5:e:121:LEU:CD1	6:f:79:PRO:HB2	2.40	0.47
13:m:162:VAL:HG13	13:m:183:LEU:HD11	1.97	0.47
10:3:88:THR:HG23	10:3:124:PHE:HZ	1.79	0.47
10:3:88:THR:HG23	10:3:124:PHE:CZ	2.50	0.47
11:4:98:TYR:N	11:4:98:TYR:HD1	2.12	0.47
11:4:151:ASP:OD2	11:4:151:ASP:N	2.48	0.47
13:6:56:ASP:OD1	13:6:91:LYS:HG2	2.14	0.47
15:W:22:PRO:HG3	15:W:180:LEU:HD22	1.96	0.47
20:Z:85:VAL:HB	20:Z:86:PRO:HD3	1.96	0.47
21:N:546:LEU:H	21:N:546:LEU:HD22	1.80	0.47
26:U:37:ILE:CD1	26:U:92:TRP:C	2.87	0.47
26:U:257:ILE:O	26:U:261:LEU:HD13	2.14	0.47
28:H:176:VAL:HG12	28:H:183:ILE:HA	1.95	0.47
30:K:281:ARG:HH11	33:J:257:ARG:HH22	1.62	0.47
34:8:111:PHE:CE1	34:8:179:VAL:HG11	2.49	0.47
3:c:110:ILE:CD1	11:k:71:GLU:CD	2.59	0.47
6:f:106:GLU:HG3	6:f:143:HIS:NE2	2.30	0.47
9:i:193:TRP:NE1	13:6:229:ARG:HD3	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:j:63:LEU:O	10:j:67:PHE:HD2	1.98	0.47
10:j:172:LEU:HG	10:j:202:MET:HE3	1.97	0.47
14:n:219:TYR:HD2	9:2:168:GLU:OE1	1.91	0.47
3:C:18:ARG:NH2	29:I:436:TYR:HD1	2.08	0.47
11:4:71:GLU:O	11:4:72:ASP:HB2	2.13	0.47
13:6:162:VAL:HG13	13:6:183:LEU:HD11	1.97	0.47
23:P:270:LEU:HD22	23:P:340:ASP:HB3	1.97	0.47
32:M:432:PHE:CE2	32:M:433:TYR:HE1	2.31	0.47
6:f:106:GLU:CG	6:f:143:HIS:CD2	2.97	0.47
10:j:88:THR:HG23	10:j:124:PHE:CZ	2.50	0.47
11:k:25:ILE:HG12	11:4:135:TYR:CD1	2.47	0.47
7:G:36:THR:HG21	7:G:203:ALA:HB1	1.97	0.47
10:3:63:LEU:O	10:3:67:PHE:HD2	1.98	0.47
13:6:57:ASN:OD1	13:6:57:ASN:N	2.43	0.47
14:7:212:ASN:O	14:7:216:VAL:HG23	2.15	0.47
20:Z:903:MET:HG2	20:Z:904:LEU:H	1.79	0.47
27:O:17:GLU:HG2	27:O:57:LEU:HD21	1.97	0.47
33:J:230:VAL:HG11	33:J:271:THR:HG22	1.97	0.47
8:h:175:ASP:OD2	8:h:177:SER:N	2.47	0.47
10:j:11:ILE:CG1	10:j:26:ASP:OD2	2.60	0.47
5:E:136:ARG:HB2	5:E:137:PRO:HD2	1.96	0.47
10:3:154:TYR:CD1	10:3:154:TYR:C	2.93	0.47
13:6:126:GLY:CA	13:6:217:LYS:HZ1	2.28	0.47
14:7:48:LYS:HE3	14:7:160:LEU:HB3	1.95	0.47
25:R:172:LEU:HD22	25:R:213:TYR:CD1	2.50	0.47
25:R:317:ILE:N	25:R:318:PRO:CD	2.78	0.47
28:H:257:THR:HG22	28:H:261:ARG:HE	1.79	0.47
29:I:102:ASN:HB3	29:I:103:PRO:CD	2.45	0.47
14:n:259:LYS:HG3	8:1:194:ARG:NH1	2.30	0.47
1:A:64:LEU:HD12	1:A:64:LEU:HA	1.64	0.47
6:F:77:LEU:HD22	32:M:433:TYR:CZ	2.49	0.47
25:R:279:LEU:O	25:R:280:ILE:O	2.33	0.47
26:U:9:THR:HG21	26:U:162:GLU:HG3	1.97	0.47
29:I:195:LYS:HE3	29:I:199:GLU:CD	2.39	0.47
33:J:57:PHE:HD1	33:J:58:ILE:N	2.13	0.47
5:e:208:MET:HG3	5:e:210:GLU:H	1.80	0.47
11:k:151:ASP:OD2	11:k:151:ASP:N	2.48	0.47
5:E:208:MET:HG3	5:E:210:GLU:H	1.80	0.47
6:F:77:LEU:HB3	32:M:433:TYR:CD2	2.49	0.47
7:G:68:GLN:NE2	14:7:110:ASP:OD2	2.48	0.47
5:e:136:ARG:HB2	5:e:137:PRO:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:f:150:SER:HB3	7:g:83:PRO:HG2	1.96	0.47
11:k:98:TYR:N	11:k:98:TYR:HD1	2.12	0.47
13:m:150:ALA:CB	13:m:203:HIS:HD2	2.16	0.47
14:n:201:THR:HG22	14:n:202:THR:N	2.30	0.47
14:n:261:TYR:O	9:2:150:VAL:HG23	2.15	0.47
6:F:79:PRO:HD2	32:M:433:TYR:CD2	2.50	0.47
20:Z:225:LEU:HD12	20:Z:271:ILE:HG13	1.97	0.47
21:N:858:LYS:HE3	21:N:860:LYS:HZ1	1.79	0.47
26:U:236:LEU:HG	26:U:237:PRO:HD2	1.96	0.47
4:d:120:TYR:HA	4:d:126:VAL:HG21	1.98	0.46
5:e:136:ARG:HB2	5:e:137:PRO:CD	2.45	0.46
7:g:218:TRP:CD1	7:g:231:VAL:CG2	2.97	0.46
11:4:139:TYR:HD1	11:4:171:ARG:HB2	1.77	0.46
22:S:173:LEU:H	22:S:176:LEU:HD12	1.80	0.46
22:S:423:VAL:HB	22:S:436:ILE:HD11	1.96	0.46
25:R:24:TYR:CD2	25:R:244:THR:HA	2.50	0.46
35:9:15:LEU:HG	35:9:17:VAL:CG2	2.45	0.46
2:b:22:ASP:O	2:b:26:THR:HG23	2.16	0.46
5:e:18:GLU:CD	5:e:22:PHE:CE1	2.93	0.46
10:j:59:ASP:O	10:j:63:LEU:HB2	2.15	0.46
13:m:198:SER:OG	9:2:225:ARG:NH2	2.48	0.46
8:1:165:LYS:NZ	8:1:205:LEU:HD12	2.30	0.46
21:N:875:LEU:HB3	21:N:876:PRO:HD2	1.97	0.46
23:P:430:GLY:O	23:P:434:THR:HG23	2.15	0.46
29:I:94:LYS:O	29:I:95:GLN:CB	2.63	0.46
29:I:141:LEU:H	29:I:141:LEU:HD23	1.81	0.46
29:I:199:GLU:HG3	29:I:240:THR:HG23	1.96	0.46
30:K:113:THR:HG22	30:K:252:ARG:HD2	1.97	0.46
1:a:27:GLN:HE22	7:g:15:PHE:N	2.13	0.46
2:b:11:THR:HG22	3:c:21:GLN:OE1	2.16	0.46
7:g:232:LYS:HA	7:g:236:LEU:HB2	1.98	0.46
8:h:35:ILE:HD12	14:7:219:TYR:O	2.15	0.46
12:l:113:ASN:CB	12:l:114:PRO:CD	2.90	0.46
13:m:9:GLN:OE1	13:m:9:GLN:HA	2.14	0.46
13:m:46:ARG:CB	13:m:208:ASP:OD2	2.64	0.46
3:C:100:LYS:HD2	10:3:69:TYR:HB2	1.98	0.46
7:G:38:ILE:HD13	7:G:199:ILE:CD1	2.45	0.46
8:1:41:ASP:HB2	8:1:183:ARG:HH11	1.79	0.46
9:2:249:ILE:HD11	10:3:195:VAL:HG23	1.96	0.46
11:4:43:LEU:HD21	11:4:182:LYS:HE2	1.96	0.46
14:7:185:ASN:HB3	14:7:186:PRO:HD3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Z:319:THR:OG1	20:Z:349:THR:HG23	2.15	0.46
20:Z:493:LEU:HD23	20:Z:509:LEU:HD21	1.98	0.46
25:R:296:LEU:HD23	25:R:296:LEU:C	2.41	0.46
30:K:397:LYS:O	30:K:398:ASN:HB2	2.16	0.46
31:L:147:THR:HG22	31:L:157:ARG:H	1.80	0.46
31:L:178:ILE:HG13	31:L:179:THR:H	1.79	0.46
32:M:50:ARG:HA	32:M:53:HIS:CD2	2.50	0.46
9:i:92:ILE:HG12	9:i:111:MET:HE1	1.98	0.46
12:l:160:ASN:N	12:l:160:ASN:HD22	2.14	0.46
2:B:22:ASP:O	2:B:26:THR:HG23	2.16	0.46
2:B:75:TYR:CD2	2:B:82:TYR:CD2	3.03	0.46
6:F:107:ARG:HG2	14:7:111:ASN:OD1	2.16	0.46
20:Z:813:PHE:O	20:Z:817:LEU:HG	2.15	0.46
33:J:295:ASN:O	33:J:296:ARG:HG2	2.15	0.46
9:i:58:LYS:HE2	13:6:201:GLU:OE2	2.15	0.46
5:E:15:PHE:CE2	6:F:25:ALA:HA	2.50	0.46
14:7:122:PRO:HB2	14:7:159:PHE:CG	2.51	0.46
17:T:34:LEU:HD11	17:T:62:LEU:HD21	1.97	0.46
33:J:398:ILE:CG1	33:J:399:SER:N	2.78	0.46
2:b:75:TYR:CD2	2:b:82:TYR:CD2	3.03	0.46
12:5:191:ASP:HB2	12:5:195:THR:OG1	2.16	0.46
16:V:280:LEU:HD13	26:U:268:LYS:HE2	1.98	0.46
24:Q:58:ILE:HG12	24:Q:96:VAL:HG11	1.98	0.46
1:a:35:THR:HG21	1:a:140:ILE:HG13	1.98	0.46
7:g:175:GLU:OE1	7:g:178:LYS:HE2	2.16	0.46
4:D:118:GLN:NE2	5:E:87:SER:HB2	2.31	0.46
5:E:136:ARG:HB2	5:E:137:PRO:CD	2.45	0.46
9:2:122:HIS:O	10:3:99:ARG:NH1	2.49	0.46
13:6:58:ILE:HG21	13:6:92:LEU:HD21	1.97	0.46
20:Z:309:GLN:C	20:Z:311:ALA:H	2.24	0.46
21:N:288:ASN:O	21:N:291:SER:OG	2.25	0.46
21:N:355:TRP:HA	21:N:358:LYS:HE2	1.98	0.46
21:N:672:ASN:HB3	21:N:675:VAL:CG2	2.46	0.46
3:c:15:PRO:HA	4:d:22:TYR:CD1	2.49	0.46
10:j:205:ASP:OD1	12:5:94:ARG:NH2	2.48	0.46
12:l:118:GLY:HA3	12:l:131:GLU:OE2	2.16	0.46
12:l:144:ARG:NH1	12:l:144:ARG:CG	2.64	0.46
6:F:106:GLU:HG3	6:F:143:HIS:NE2	2.30	0.46
9:2:126:TYR:HD1	9:2:126:TYR:N	2.12	0.46
9:2:232:TYR:HD2	9:2:232:TYR:N	2.14	0.46
11:4:92:ILE:HG21	11:4:92:ILE:HD12	1.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:5:118:GLY:HA3	12:5:131:GLU:OE2	2.16	0.46
13:6:46:ARG:CB	13:6:208:ASP:OD2	2.64	0.46
16:V:169:GLU:HB2	16:V:170:PRO:HD3	1.98	0.46
20:Z:172:ASP:O	20:Z:173:ALA:O	2.34	0.46
29:I:102:ASN:CB	29:I:103:PRO:CD	2.93	0.46
3:c:177:GLN:NE2	4:d:53:LYS:HB2	2.31	0.46
11:k:135:TYR:HE1	11:4:25:ILE:CG1	2.19	0.46
9:2:225:ARG:HH12	9:2:228:LYS:HD3	1.81	0.46
11:4:7:ILE:HD13	11:4:7:ILE:HG21	1.50	0.46
12:5:160:ASN:HD22	12:5:160:ASN:N	2.14	0.46
12:5:241:HIS:CD2	12:5:241:HIS:C	2.93	0.46
20:Z:811:SER:O	20:Z:815:MET:HB2	2.16	0.46
21:N:277:LEU:O	21:N:282:TYR:CD2	2.60	0.46
22:S:258:GLU:OE1	22:S:258:GLU:N	2.49	0.46
31:L:255:TYR:HB2	31:L:258:GLU:CB	2.45	0.46
9:i:88:ILE:HG22	9:i:111:MET:SD	2.57	0.46
9:i:153:TYR:OH	9:i:167:LEU:HB3	2.16	0.46
12:l:164:GLN:C	12:l:166:LYS:H	2.24	0.46
3:C:17:GLY:HA3	4:D:26:ALA:HB2	1.97	0.46
12:5:128:GLN:OE1	13:6:138:SER:HA	2.16	0.46
3:c:224:GLU:CB	9:i:252:ILE:CG2	2.91	0.45
6:f:135:ILE:HD12	6:f:216:VAL:HG12	1.98	0.45
7:g:204:HIS:CD2	7:g:212:PHE:CE1	3.04	0.45
8:h:93:GLU:OE1	8:h:93:GLU:HA	2.16	0.45
12:l:210:PHE:CE1	11:4:138:PHE:O	2.69	0.45
4:D:159:TRP:CE3	5:E:59:LEU:HA	2.51	0.45
11:4:96:ARG:HH21	12:5:166:LYS:CD	2.12	0.45
12:5:102:ALA:O	13:6:145:ARG:NH1	2.49	0.45
15:W:17:ARG:HH21	15:W:81:ILE:HG13	1.81	0.45
28:H:334:LEU:HA	28:H:337:ILE:HD12	1.98	0.45
30:K:99:PHE:CD2	30:K:131:LEU:O	2.69	0.45
30:K:399:ARG:HA	30:K:399:ARG:HE	1.81	0.45
32:M:170:MET:HE1	32:M:266:ALA:HB2	1.98	0.45
12:l:191:ASP:HB2	12:l:195:THR:OG1	2.16	0.45
15:W:22:PRO:HG3	15:W:180:LEU:HD23	1.98	0.45
28:H:464:MET:O	28:H:465:GLN:O	2.33	0.45
13:m:197:THR:CG2	9:2:226:GLU:CG	2.95	0.45
1:A:184:ASN:N	1:A:184:ASN:HD22	2.14	0.45
5:E:19:GLY:HA3	6:F:27:GLU:HB2	1.98	0.45
9:2:140:PHE:HD1	9:2:150:VAL:HG22	1.82	0.45
11:4:180:ILE:HD13	11:4:180:ILE:HG21	1.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:6:185:VAL:O	13:6:189:ILE:HG13	2.16	0.45
16:V:47:MET:SD	16:V:73:GLN:HB3	2.56	0.45
20:Z:79:THR:C	20:Z:81:SER:H	2.25	0.45
27:O:14:LEU:HB3	27:O:57:LEU:HD12	1.97	0.45
28:H:271:PHE:O	28:H:273:ARG:NH1	2.49	0.45
8:h:174:TRP:HZ2	8:1:148:ASP:HB2	1.81	0.45
10:j:204:GLN:HB2	12:5:272:PHE:CD2	2.51	0.45
8:1:144:TYR:CE1	14:7:66:LEU:HD11	2.52	0.45
9:2:88:ILE:HG22	9:2:111:MET:SD	2.56	0.45
9:2:153:TYR:CZ	9:2:167:LEU:HB3	2.51	0.45
21:N:359:ALA:C	21:N:360:GLN:CD	2.84	0.45
32:M:107:ASN:HB3	32:M:110:ASN:HB2	1.99	0.45
34:8:169:GLU:HA	34:8:172:GLN:HE21	1.80	0.45
9:i:51:GLN:HE22	10:j:125:ASP:HB3	1.81	0.45
13:m:228:LYS:CE	9:2:225:ARG:HA	2.46	0.45
28:H:271:PHE:CE2	28:H:305:ILE:HD13	2.52	0.45
30:K:48:TYR:CE1	30:K:52:LYS:HE2	2.51	0.45
7:g:104:LYS:HE3	14:n:98:ARG:HG3	1.98	0.45
9:i:57:ASP:OD2	10:j:132:GLU:O	2.34	0.45
9:i:153:TYR:CZ	9:i:167:LEU:HB3	2.51	0.45
11:k:49:GLU:HB2	11:k:99:GLN:HB3	1.98	0.45
11:k:96:ARG:HD3	12:l:166:LYS:O	2.17	0.45
13:m:201:GLU:OE2	9:2:58:LYS:HE2	2.16	0.45
20:Z:535:VAL:HG22	20:Z:572:ILE:O	2.16	0.45
25:R:312:TYR:HA	25:R:316:LEU:HD12	1.97	0.45
25:R:332:GLU:C	25:R:336:LYS:HZ2	2.25	0.45
30:K:103:ILE:HG13	30:K:107:THR:OG1	2.17	0.45
33:J:249:GLU:OE2	33:J:294:THR:HB	2.16	0.45
4:d:48:ARG:HA	4:d:63:LYS:HE2	1.99	0.45
10:j:172:LEU:CG	10:j:202:MET:HE3	2.46	0.45
12:l:243:ASP:HB3	12:l:246:SER:HB2	1.99	0.45
13:m:41:TYR:N	13:m:41:TYR:CD1	2.80	0.45
13:m:53:ASP:HA	13:m:59:VAL:HG12	1.99	0.45
9:2:153:TYR:OH	9:2:167:LEU:HB3	2.16	0.45
20:Z:336:SER:HA	20:Z:342:LEU:HD22	1.98	0.45
23:P:361:THR:HG22	23:P:363:LEU:N	2.31	0.45
33:J:102:ILE:HD12	33:J:107:LEU:HD11	1.98	0.45
34:8:147:SER:H	34:8:223:ILE:HG23	1.82	0.45
2:b:227:ILE:HG22	2:b:230:ASP:H	1.82	0.45
7:g:109:ILE:HG21	7:g:147:HIS:HB2	1.98	0.45
10:j:3:ASP:HA	10:j:4:PRO:HD3	1.77	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:THR:HG21	1:A:140:ILE:HG13	1.98	0.45
8:1:93:GLU:OE1	8:1:93:GLU:HA	2.16	0.45
9:2:239:THR:HG22	9:2:240:ALA:N	2.32	0.45
10:3:65:GLU:OE2	11:4:85:ARG:CZ	2.64	0.45
22:S:47:THR:HG22	22:S:178:LEU:HD11	1.98	0.45
25:R:44:LYS:CG	25:R:91:TRP:CZ2	2.99	0.45
26:U:37:ILE:HD11	26:U:93:TYR:N	2.32	0.45
29:I:101:GLY:C	29:I:102:ASN:O	2.60	0.45
2:b:214:ILE:HG22	2:b:234:ARG:HG2	1.99	0.45
3:c:15:PRO:CA	4:d:22:TYR:CE1	2.96	0.45
9:i:243:LYS:NZ	12:5:286:ILE:HD11	2.31	0.45
6:F:32:GLY:HA2	32:M:434:ALA:HB1	1.98	0.45
9:2:92:ILE:HG12	9:2:111:MET:HE1	1.98	0.45
21:N:525:ASN:HA	21:N:528:ARG:HE	1.82	0.45
30:K:325:ASP:O	30:K:329:LEU:HD23	2.16	0.45
31:L:103:GLN:HB3	31:L:147:THR:OG1	2.17	0.45
12:l:126:ASP:HA	13:m:106:TYR:CZ	2.51	0.45
7:G:68:GLN:HG2	14:7:110:ASP:OD1	2.17	0.45
13:6:53:ASP:HA	13:6:59:VAL:HG12	1.99	0.45
14:7:165:LEU:HD12	14:7:166:LEU:N	2.32	0.45
22:S:139:HIS:HB2	22:S:183:LEU:HD11	1.98	0.45
25:R:44:LYS:HG2	25:R:91:TRP:CH2	2.52	0.45
9:i:126:TYR:HD1	9:i:126:TYR:N	2.12	0.44
12:l:210:PHE:HB3	11:4:142:SER:HB3	1.99	0.44
14:n:67:LEU:HD12	8:1:173:LYS:C	2.42	0.44
6:F:135:ILE:HD12	6:F:216:VAL:HG12	1.98	0.44
7:G:109:ILE:HG21	7:G:147:HIS:HB2	1.98	0.44
12:5:164:GLN:C	12:5:166:LYS:H	2.24	0.44
13:6:9:GLN:N	14:7:34:THR:HG23	2.31	0.44
23:P:357:TYR:HA	27:O:341:ILE:HB	1.99	0.44
24:Q:92:LYS:HA	24:Q:95:LYS:HZ3	1.82	0.44
28:H:428:MET:HE1	29:I:346:ARG:HD2	1.99	0.44
30:K:344:ARG:HH11	30:K:344:ARG:HD3	1.56	0.44
1:a:184:ASN:HD22	1:a:184:ASN:N	2.14	0.44
2:b:190:HIS:CD2	2:b:249:ALA:O	2.71	0.44
9:i:140:PHE:HD1	9:i:150:VAL:HG22	1.81	0.44
13:m:109:ARG:CA	13:m:136:VAL:HG13	2.46	0.44
13:m:185:VAL:O	13:m:189:ILE:HG13	2.16	0.44
2:B:227:ILE:HG22	2:B:230:ASP:H	1.82	0.44
3:C:208:TYR:CZ	3:C:236:LYS:HD2	2.52	0.44
15:W:74:ALA:HB2	32:M:53:HIS:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:M:120:LYS:HB2	32:M:126:THR:HG22	1.99	0.44
4:d:84:ILE:O	4:d:88:LYS:HG3	2.18	0.44
5:e:85:ALA:HB2	5:e:140:VAL:HG21	2.00	0.44
2:B:214:ILE:HG22	2:B:234:ARG:HG2	1.99	0.44
10:3:101:GLY:C	11:4:93:ARG:NH2	2.74	0.44
13:6:10:PHE:CE2	14:7:142:PRO:HG3	2.53	0.44
15:W:153:LEU:H	15:W:153:LEU:CD1	2.30	0.44
3:c:208:TYR:CZ	3:c:236:LYS:HD2	2.52	0.44
11:k:170:LYS:CE	11:k:171:ARG:HH21	2.18	0.44
5:E:105:GLU:OE1	5:E:105:GLU:HA	2.17	0.44
9:2:217:ARG:HH11	9:2:217:ARG:HG2	1.82	0.44
13:6:41:TYR:N	13:6:41:TYR:CD1	2.80	0.44
23:P:135:GLU:O	23:P:139:VAL:HG23	2.17	0.44
28:H:423:CYS:HB3	29:I:213:ILE:HD13	1.98	0.44
9:i:119:TYR:CD1	9:i:123:ILE:CD1	3.01	0.44
8:1:133:TYR:O	8:1:133:TYR:CD2	2.62	0.44
11:4:49:GLU:HB2	11:4:99:GLN:HB3	1.98	0.44
21:N:387:ALA:HB3	21:N:388:PRO:HD3	1.99	0.44
21:N:581:ASP:HB3	21:N:616:HIS:CD2	2.52	0.44
25:R:95:ASP:H	25:R:98:LEU:HD12	1.83	0.44
25:R:117:ILE:CD1	25:R:133:ALA:HB1	2.46	0.44
5:e:32:LYS:HA	5:e:174:SER:HA	2.00	0.44
5:e:105:GLU:OE1	5:e:105:GLU:HA	2.18	0.44
6:f:13:PHE:HA	6:f:14:SER:CB	2.48	0.44
7:g:232:LYS:CA	7:g:236:LEU:HB2	2.47	0.44
10:j:172:LEU:HD12	10:j:202:MET:CE	2.46	0.44
11:k:93:ARG:HD2	11:k:93:ARG:HA	1.63	0.44
13:m:12:PRO:HD3	14:n:140:MET:HE1	2.00	0.44
12:5:156:LYS:O	12:5:160:ASN:ND2	2.51	0.44
12:5:243:ASP:HB3	12:5:246:SER:HB2	1.99	0.44
23:P:356:TYR:CE1	27:O:332:ILE:CG2	3.00	0.44
30:K:171:TYR:HD1	30:K:229:SER:HG	1.59	0.44
4:d:111:ARG:NH1	12:l:145:GLU:OE2	2.47	0.44
7:g:204:HIS:O	7:g:208:LYS:HB3	2.18	0.44
12:l:156:LYS:O	12:l:160:ASN:ND2	2.51	0.44
13:m:40:ASP:C	13:m:41:TYR:HD1	2.26	0.44
5:E:85:ALA:HB2	5:E:140:VAL:HG21	2.00	0.44
31:L:147:THR:HG23	31:L:156:MET:H	1.83	0.44
33:J:112:ARG:HE	33:J:129:LYS:HA	1.82	0.44
3:c:98:TYR:OH	11:k:67:TYR:CE1	2.66	0.44
6:f:232:LYS:HE2	6:f:232:LYS:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:k:3:ILE:HG12	11:k:18:SER:OG	2.18	0.44
2:B:190:HIS:CD2	2:B:249:ALA:O	2.71	0.44
20:Z:409:LYS:O	20:Z:411:LYS:HE2	2.18	0.44
23:P:203:ILE:HD11	23:P:220:TYR:CE1	2.52	0.44
25:R:44:LYS:CD	25:R:91:TRP:CZ2	3.01	0.44
33:J:279:LEU:HG	33:J:279:LEU:O	2.18	0.44
10:3:53:ILE:HG21	10:3:53:ILE:HD13	1.50	0.44
31:L:361:PHE:CE1	31:L:391:ILE:HG23	2.53	0.44
34:8:203:GLY:O	34:8:207:GLN:NE2	2.51	0.44
9:i:93:GLU:O	9:i:97:LEU:HD12	2.18	0.43
12:l:133:TRP:CH2	12:l:161:LEU:CD2	3.01	0.43
6:F:232:LYS:HE2	6:F:232:LYS:HA	1.99	0.43
12:5:133:TRP:CH2	12:5:161:LEU:CD2	3.01	0.43
12:5:283:ASN:HD22	12:5:283:ASN:N	2.16	0.43
21:N:43:LEU:HD12	21:N:46:ILE:HD13	2.00	0.43
21:N:858:LYS:HE3	21:N:860:LYS:NZ	2.33	0.43
22:S:460:VAL:O	22:S:464:ARG:HG3	2.18	0.43
23:P:72:TRP:CH2	23:P:113:ASN:HA	2.52	0.43
24:Q:85:MET:HE2	24:Q:97:LEU:HD22	1.99	0.43
28:H:59:ILE:HA	28:H:62:ARG:HE	1.83	0.43
11:k:25:ILE:HG12	11:4:135:TYR:HE1	1.76	0.43
1:A:92:ASN:HA	7:G:118:GLN:OE1	2.19	0.43
2:B:198:GLU:OE2	24:Q:209:TYR:CB	2.63	0.43
6:F:69:HIS:NE2	6:F:102:LYS:HB2	2.33	0.43
8:1:22:ILE:HG12	8:1:186:VAL:HG13	2.00	0.43
11:4:8:ARG:HH21	11:4:129:PRO:HB3	1.83	0.43
12:5:286:ILE:HD13	12:5:286:ILE:HG21	1.59	0.43
13:6:150:ALA:CB	13:6:203:HIS:HD2	2.17	0.43
20:Z:777:PRO:HA	20:Z:796:LEU:HD22	1.98	0.43
20:Z:875:LYS:CG	20:Z:878:LEU:HD23	2.49	0.43
21:N:318:LYS:HD3	21:N:352:ASN:ND2	2.33	0.43
3:c:70:ASN:OD1	3:c:70:ASN:C	2.62	0.43
6:f:164:ARG:HH11	6:f:202:ARG:HH21	1.65	0.43
12:l:241:HIS:CD2	10:3:183:TRP:CZ2	3.07	0.43
14:n:58:ASP:HA	14:n:228:PHE:HA	1.99	0.43
1:A:25:LEU:HD12	2:B:78:MET:HE1	2.00	0.43
9:2:153:TYR:OH	9:2:168:GLU:HG2	2.18	0.43
20:Z:577:GLN:HG3	20:Z:579:GLU:H	1.83	0.43
23:P:377:GLU:OE2	23:P:378:THR:N	2.51	0.43
25:R:58:GLU:O	25:R:144:ILE:HG22	2.18	0.43
5:e:128:SER:HA	6:f:119:ASN:HD21	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:l:241:HIS:CD2	10:3:183:TRP:HZ2	2.36	0.43
13:m:94:ILE:HG22	13:m:95:ASN:N	2.31	0.43
4:D:70:HIS:NE2	4:D:138:PHE:O	2.50	0.43
7:G:68:GLN:NE2	14:7:110:ASP:OD1	2.52	0.43
9:2:119:TYR:CD1	9:2:123:ILE:CD1	3.01	0.43
10:3:3:ASP:HA	10:3:4:PRO:HD3	1.77	0.43
10:3:98:ARG:HH12	11:4:93:ARG:HG3	1.82	0.43
22:S:475:TYR:HD1	26:U:273:LEU:HB2	1.82	0.43
23:P:122:ILE:HA	23:P:125:VAL:HG22	1.99	0.43
13:6:40:ASP:C	13:6:41:TYR:HD1	2.26	0.43
18:X:92:SER:O	18:X:93:SER:HB2	2.17	0.43
21:N:711:ARG:O	21:N:873:ARG:HD2	2.18	0.43
22:S:49:ASP:HB2	22:S:50:PRO:HD3	2.00	0.43
22:S:89:LYS:HE3	22:S:93:LEU:CD1	2.48	0.43
27:O:112:LYS:O	27:O:115:ARG:NH1	2.52	0.43
3:c:184:MET:HE1	3:c:192:LEU:HD23	2.01	0.43
8:h:22:ILE:HG12	8:h:186:VAL:HG13	2.00	0.43
12:l:245:TYR:N	12:l:245:TYR:CD1	2.66	0.43
14:n:74:ARG:HA	14:n:93:MET:HE1	2.00	0.43
3:C:184:MET:HE1	3:C:192:LEU:HD23	2.01	0.43
5:E:32:LYS:HA	5:E:174:SER:HA	2.00	0.43
6:F:164:ARG:HH11	6:F:202:ARG:HH21	1.65	0.43
12:5:252:LEU:O	12:5:253:TYR:HD1	2.02	0.43
21:N:553:PHE:O	21:N:557:LEU:CD1	2.66	0.43
23:P:365:LEU:HA	23:P:368:LEU:HD12	1.99	0.43
26:U:180:ASP:OD1	26:U:180:ASP:N	2.52	0.43
34:8:303:ILE:O	34:8:346:THR:HG23	2.18	0.43
10:j:98:ARG:HH22	11:k:93:ARG:HE	1.67	0.43
11:k:54:VAL:HG21	12:l:195:THR:HG22	2.00	0.43
6:F:13:PHE:HA	6:F:14:SER:CB	2.48	0.43
9:2:181:ILE:HG21	9:2:181:ILE:HD13	1.63	0.43
15:W:41:ARG:HD2	15:W:45:PRO:HA	1.99	0.43
21:N:735:MET:HG3	21:N:748:PHE:CE2	2.53	0.43
23:P:130:ILE:O	23:P:131:PHE:HB2	2.19	0.43
1:a:135:ARG:NH1	7:g:15:PHE:CD2	2.86	0.43
5:e:114:GLN:O	5:e:118:ASP:OD1	2.36	0.43
9:i:153:TYR:OH	9:i:168:GLU:HG2	2.18	0.43
11:k:8:ARG:HH21	11:k:129:PRO:HB3	1.83	0.43
13:m:112:PRO:CB	13:m:114:TYR:HE1	2.31	0.43
2:B:31:GLY:HA2	30:K:427:TYR:O	2.18	0.43
3:C:208:TYR:CE2	3:C:236:LYS:HD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:28:LEU:HD11	32:M:432:PHE:CD2	2.54	0.43
5:E:114:GLN:O	5:E:118:ASP:OD1	2.36	0.43
12:5:148:ARG:HH11	12:5:148:ARG:HD2	1.39	0.43
21:N:736:PHE:O	21:N:739:PHE:CD1	2.57	0.43
22:S:282:ILE:HG12	22:S:382:ARG:HH22	1.83	0.43
25:R:283:THR:HG23	25:R:286:LEU:H	1.82	0.43
29:I:180:SER:HA	29:I:235:ALA:HB1	2.00	0.43
1:a:13:ASP:O	1:a:26:TYR:HD1	2.02	0.43
4:d:187:THR:HG22	4:d:189:GLU:H	1.84	0.43
6:f:157:TYR:CE2	7:g:60:VAL:HG22	2.54	0.43
12:l:241:HIS:CD2	12:l:241:HIS:C	2.94	0.43
4:D:109:LEU:O	4:D:113:VAL:HG23	2.18	0.43
9:2:234:PHE:O	9:2:236:ARG:NH1	2.51	0.43
21:N:307:LYS:NZ	21:N:343:THR:HB	2.34	0.43
28:H:271:PHE:HB3	28:H:273:ARG:CZ	2.48	0.43
28:H:457:PHE:HE2	29:I:331:ILE:HD12	1.81	0.43
33:J:229:MET:HE3	33:J:233:LEU:HD13	2.01	0.43
1:a:220:LYS:HG3	1:a:221:ASN:OD1	2.18	0.43
3:c:113:ARG:HG3	4:d:83:ARG:NH1	2.34	0.43
3:c:208:TYR:CE2	3:c:236:LYS:HD2	2.54	0.43
5:e:45:GLY:HA2	5:e:153:TYR:CE2	2.54	0.43
7:g:104:LYS:HD3	14:n:98:ARG:HD3	2.00	0.43
12:l:283:ASN:HD22	12:l:283:ASN:N	2.16	0.43
3:C:16:GLU:O	4:D:29:ARG:HD2	2.19	0.43
11:4:166:GLN:HE21	11:4:166:GLN:HB3	1.62	0.43
19:Y:63:ASN:O	19:Y:64:TRP:CB	2.66	0.43
21:N:298:TYR:O	21:N:301:THR:OG1	2.35	0.43
24:Q:183:LYS:HA	24:Q:221:MET:CE	2.49	0.43
25:R:51:LEU:HA	25:R:54:ILE:HD12	2.01	0.43
28:H:162:ARG:HG2	28:H:162:ARG:HH11	1.84	0.43
2:b:5:TYR:CE1	3:c:3:SER:HA	2.54	0.42
3:c:124:GLN:OE1	3:c:124:GLN:HA	2.19	0.42
4:d:23:ALA:O	4:d:26:ALA:HB3	2.19	0.42
10:j:13:VAL:HG23	10:j:138:VAL:HG12	2.01	0.42
11:k:193:ASP:O	11:k:195:PHE:CE2	2.72	0.42
7:G:45:GLY:HA3	7:G:220:SER:HB3	2.01	0.42
10:3:154:TYR:CD1	10:3:155:GLU:N	2.83	0.42
28:H:203:LYS:NZ	28:H:268:ASP:HA	2.34	0.42
32:M:96:ASN:OD1	32:M:96:ASN:N	2.48	0.42
33:J:282:PHE:N	33:J:282:PHE:CD1	2.87	0.42
6:f:69:HIS:NE2	6:f:102:LYS:HB2	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:f:110:HIS:CD2	14:n:110:ASP:HB3	2.54	0.42
10:j:183:TRP:CZ2	12:5:241:HIS:NE2	2.79	0.42
1:A:13:ASP:O	1:A:26:TYR:HD1	2.02	0.42
1:A:220:LYS:HG3	1:A:221:ASN:OD1	2.18	0.42
5:E:45:GLY:HA2	5:E:153:TYR:CE2	2.54	0.42
10:3:7:ILE:HD13	10:3:7:ILE:HG21	1.76	0.42
16:V:242:LYS:CD	24:Q:411:SER:HB3	2.49	0.42
27:O:307:MET:CE	27:O:347:LEU:HD22	2.49	0.42
29:I:77:SER:HA	29:I:81:ILE:CG1	2.49	0.42
33:J:398:ILE:CG1	33:J:399:SER:H	2.28	0.42
12:l:81:PHE:O	12:l:81:PHE:HD2	2.02	0.42
12:l:252:LEU:O	12:l:253:TYR:HD1	2.01	0.42
2:B:68:THR:HB	2:B:69:PRO:CD	2.50	0.42
4:D:90:ARG:NH1	11:4:69:ILE:CG2	2.82	0.42
6:F:32:GLY:CA	32:M:434:ALA:HB1	2.49	0.42
6:F:156:LEU:HA	7:G:58:LEU:O	2.19	0.42
11:4:141:PHE:O	11:4:145:ASP:HB3	2.20	0.42
21:N:671:LEU:HD13	21:N:860:LYS:HE2	2.02	0.42
29:I:115:ASP:O	34:8:486:SER:OG	2.29	0.42
31:L:354:GLU:OE1	31:L:381:LYS:O	2.36	0.42
1:a:78:THR:HG21	1:a:231:ASP:HA	2.01	0.42
4:d:68:ASP:CG	4:d:69:SER:H	2.27	0.42
4:d:90:ARG:CD	11:k:70:ARG:HA	2.49	0.42
9:i:133:ASP:O	9:i:209:ILE:HD11	2.19	0.42
10:j:204:GLN:CG	12:5:272:PHE:CD2	2.98	0.42
12:l:83:PHE:HE1	12:l:88:ILE:HG12	1.84	0.42
13:m:133:PHE:CD2	13:m:139:TYR:HB3	2.55	0.42
5:E:70:ILE:HD13	5:E:92:ALA:HB1	2.01	0.42
9:2:123:ILE:HA	10:3:99:ARG:NH1	2.33	0.42
11:4:193:ASP:O	11:4:195:PHE:CE2	2.72	0.42
13:6:126:GLY:HA2	13:6:217:LYS:HZ1	1.79	0.42
20:Z:2:VAL:HG22	20:Z:3:ASP:H	1.85	0.42
20:Z:212:LEU:HD22	20:Z:221:VAL:HG22	2.02	0.42
23:P:178:GLN:OE1	23:P:179:PHE:N	2.52	0.42
28:H:462:ARG:HH21	28:H:465:GLN:CD	2.27	0.42
29:I:94:LYS:O	29:I:95:GLN:HB2	2.18	0.42
31:L:255:TYR:HB2	31:L:258:GLU:HB3	2.00	0.42
32:M:50:ARG:HA	32:M:53:HIS:NE2	2.34	0.42
3:c:94:HIS:CD2	3:c:114:ARG:HG2	2.54	0.42
4:d:120:TYR:HA	4:d:126:VAL:HG23	2.01	0.42
11:k:3:ILE:H	11:k:18:SER:HB2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:100:LYS:O	10:3:65:GLU:OE1	2.37	0.42
6:F:77:LEU:HB3	32:M:433:TYR:HE2	1.78	0.42
7:G:75:GLY:HA3	7:G:228:HIS:CD2	2.54	0.42
9:2:93:GLU:O	9:2:97:LEU:HD12	2.18	0.42
9:2:195:ASP:OD1	9:2:196:LEU:N	2.53	0.42
11:4:36:ARG:HD2	11:4:58:GLU:OE1	2.19	0.42
12:5:81:PHE:HD2	12:5:81:PHE:O	2.02	0.42
21:N:546:LEU:HD22	21:N:546:LEU:N	2.35	0.42
23:P:130:ILE:HD12	23:P:131:PHE:N	2.33	0.42
23:P:369:LEU:HD12	23:P:376:THR:HG23	2.01	0.42
24:Q:270:ILE:HA	24:Q:275:ILE:HG22	2.01	0.42
30:K:169:VAL:HB	30:K:224:LYS:HB3	2.01	0.42
1:a:64:LEU:HD12	1:a:64:LEU:HA	1.64	0.42
9:i:80:ASP:O	9:i:84:VAL:CG2	2.60	0.42
11:k:92:ILE:HG23	11:k:92:ILE:HD13	1.67	0.42
1:A:24:ARG:HD3	30:K:427:TYR:CZ	2.54	0.42
11:4:96:ARG:HH11	11:4:96:ARG:HD2	1.58	0.42
16:V:242:LYS:HA	16:V:242:LYS:CE	2.49	0.42
20:Z:365:SER:HA	28:H:436:LYS:HE2	2.02	0.42
21:N:899:ASN:CG	21:N:900:ASN:H	2.28	0.42
23:P:356:TYR:CE1	27:O:332:ILE:HG22	2.55	0.42
33:J:14:THR:HG22	33:J:14:THR:O	2.19	0.42
2:b:68:THR:HB	2:b:69:PRO:CD	2.50	0.42
10:j:53:ILE:HD13	10:j:53:ILE:HG21	1.49	0.42
11:k:7:ILE:HD13	11:k:7:ILE:HG21	1.50	0.42
12:l:94:ARG:CZ	10:3:205:ASP:OD1	2.68	0.42
4:D:90:ARG:NH1	11:4:66:LEU:HA	2.34	0.42
9:2:133:ASP:O	9:2:209:ILE:HD11	2.20	0.42
11:4:3:ILE:CG2	11:4:136:SER:OG	2.62	0.42
20:Z:269:TYR:CE2	20:Z:293:MET:SD	3.13	0.42
22:S:19:HIS:CE1	22:S:101:LYS:HD2	2.55	0.42
22:S:211:ARG:CD	22:S:240:ASP:OD1	2.68	0.42
23:P:257:TRP:CZ3	23:P:258:LYS:HG2	2.55	0.42
29:I:83:LYS:N	29:I:84:PRO:HD3	2.34	0.42
29:I:199:GLU:HG3	29:I:240:THR:CG2	2.49	0.42
31:L:147:THR:HG21	31:L:157:ARG:HG2	2.02	0.42
34:8:160:ILE:HG13	34:8:187:THR:HG22	2.01	0.42
34:8:448:TYR:N	34:8:448:TYR:CD2	2.88	0.42
8:h:133:TYR:O	8:h:133:TYR:CD2	2.62	0.42
12:l:101:VAL:HB	10:3:177:ARG:HA	2.01	0.42
3:C:17:GLY:CA	4:D:26:ALA:HB2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:94:HIS:CD2	3:C:114:ARG:HG2	2.54	0.42
3:C:194:LEU:HD23	3:C:194:LEU:HA	1.84	0.42
12:5:180:THR:HB	12:5:181:ARG:H	1.70	0.42
17:T:20:TYR:HB2	17:T:72:THR:HG23	2.01	0.42
22:S:374:ASP:O	22:S:375:ASP:CG	2.63	0.42
27:O:115:ARG:HH11	27:O:115:ARG:CG	2.33	0.42
30:K:249:GLU:O	30:K:252:ARG:CG	2.68	0.42
31:L:424:GLU:O	31:L:424:GLU:HG3	2.20	0.42
6:f:100:ASN:OD1	6:f:100:ASN:O	2.37	0.42
6:f:142:ALA:O	6:f:143:HIS:ND1	2.45	0.42
6:f:155:GLU:H	7:g:64:ASN:HD21	1.67	0.42
7:g:104:LYS:HZ3	7:g:104:LYS:HG3	1.53	0.42
9:i:153:TYR:CD2	9:i:167:LEU:HD11	2.55	0.42
13:m:153:LEU:HB3	10:3:148:GLY:HA3	2.02	0.42
14:n:261:TYR:HE2	8:1:44:THR:CG2	2.32	0.42
3:C:124:GLN:OE1	3:C:124:GLN:HA	2.19	0.42
27:O:112:LYS:HA	27:O:115:ARG:NH1	2.34	0.42
30:K:198:TYR:CD2	30:K:205:PRO:HA	2.55	0.42
32:M:73:ARG:HA	32:M:156:LEU:HD21	2.02	0.42
3:c:98:TYR:CE2	11:k:67:TYR:HE1	2.38	0.42
9:i:195:ASP:OD1	9:i:196:LEU:N	2.53	0.42
12:l:83:PHE:CZ	12:l:228:ALA:CB	3.03	0.42
12:l:286:ILE:HD11	10:3:199:TYR:HE2	1.81	0.42
4:D:13:PRO:HA	5:E:26:TYR:CG	2.54	0.42
7:G:161:LYS:NZ	23:P:2:SER:HB2	2.35	0.42
9:2:153:TYR:CD2	9:2:167:LEU:HD11	2.55	0.42
13:6:181:LYS:HG3	13:6:182:TYR:H	1.82	0.42
21:N:610:SER:HB3	21:N:621:THR:HG21	2.01	0.42
24:Q:404:ASN:O	24:Q:405:GLN:HB2	2.19	0.42
30:K:352:ILE:HG22	30:K:383:ILE:CG2	2.50	0.42
31:L:147:THR:O	31:L:155:ILE:HA	2.20	0.42
32:M:246:LEU:HD23	32:M:280:ILE:HG12	2.02	0.42
4:d:151:GLU:HB2	4:d:152:PRO:HD2	2.02	0.41
7:g:85:GLY:N	7:g:134:VAL:HG11	2.35	0.41
1:A:32:PHE:HB2	30:K:424:PHE:CE2	2.55	0.41
13:6:133:PHE:CD2	13:6:139:TYR:HB3	2.55	0.41
16:V:263:GLU:HA	16:V:266:LEU:HD12	2.01	0.41
30:K:207:ARG:HG2	30:K:207:ARG:HH11	1.85	0.41
32:M:274:ALA:HA	32:M:275:PRO:C	2.45	0.41
32:M:374:ILE:HG13	32:M:375:ASN:N	2.35	0.41
32:M:376:TRP:CD1	32:M:376:TRP:H	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:g:175:GLU:OE1	7:g:175:GLU:HA	2.20	0.41
9:i:32:ILE:HD11	9:i:74:GLY:C	2.45	0.41
13:m:43:ILE:HD12	9:2:193:TRP:O	2.20	0.41
3:C:11:THR:CB	4:D:8:LEU:HD13	2.51	0.41
6:F:100:ASN:OD1	6:F:100:ASN:O	2.37	0.41
20:Z:293:MET:HE2	20:Z:293:MET:HA	2.02	0.41
21:N:83:LEU:HG	21:N:132:LYS:HG3	2.02	0.41
22:S:47:THR:O	22:S:51:ARG:HG2	2.20	0.41
22:S:464:ARG:HE	26:U:259:ASN:HD21	1.69	0.41
29:I:82:LEU:O	29:I:83:LYS:HG3	2.20	0.41
31:L:62:ARG:HA	31:L:65:LEU:HD21	2.02	0.41
2:b:142:PHE:HB3	10:j:80:ARG:CZ	2.50	0.41
10:j:40:PHE:HD1	10:j:41:GLU:N	2.18	0.41
11:k:141:PHE:O	11:k:145:ASP:HB3	2.20	0.41
13:m:56:ASP:O	13:m:91:LYS:NZ	2.54	0.41
13:m:126:GLY:CA	13:m:217:LYS:HZ1	2.32	0.41
7:G:85:GLY:N	7:G:134:VAL:HG11	2.35	0.41
23:P:356:TYR:HB3	27:O:341:ILE:HD12	2.02	0.41
23:P:393:VAL:H	24:Q:354:PHE:HA	1.85	0.41
28:H:301:LYS:O	28:H:302:LYS:HD3	2.20	0.41
31:L:65:LEU:HD12	31:L:66:GLU:N	2.35	0.41
34:8:438:HIS:CE1	34:8:448:TYR:CZ	3.08	0.41
9:i:119:TYR:CD1	9:i:123:ILE:HD12	2.55	0.41
11:k:36:ARG:HD2	11:k:58:GLU:OE1	2.19	0.41
12:l:253:TYR:HD1	12:l:253:TYR:N	2.18	0.41
1:A:42:SER:HG	1:A:171:THR:HG1	1.60	0.41
3:C:7:ASP:HB3	4:D:6:ARG:HE	1.85	0.41
3:C:108:VAL:O	3:C:112:VAL:HG23	2.20	0.41
5:E:128:SER:H	6:F:119:ASN:HD22	1.66	0.41
5:E:136:ARG:NH1	5:E:137:PRO:O	2.54	0.41
6:F:54:ASP:H	6:F:57:SER:HB3	1.86	0.41
9:2:119:TYR:CD1	9:2:123:ILE:HD12	2.55	0.41
11:4:92:ILE:H	11:4:92:ILE:HG12	1.70	0.41
12:5:253:TYR:HD1	12:5:253:TYR:N	2.18	0.41
20:Z:257:PRO:O	20:Z:258:PRO:C	2.63	0.41
26:U:37:ILE:HD12	26:U:92:TRP:C	2.44	0.41
26:U:94:HIS:HB3	26:U:120:LEU:HD11	2.02	0.41
29:I:375:VAL:HA	29:I:413:ALA:HB2	2.02	0.41
1:a:30:TYR:CD2	7:g:15:PHE:O	2.74	0.41
3:c:108:VAL:O	3:c:112:VAL:HG23	2.20	0.41
8:h:183:ARG:HH12	14:7:258:ILE:HB	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:PHE:HB2	30:K:424:PHE:CD2	2.54	0.41
2:B:78:MET:HE1	30:K:426:PHE:HE2	1.78	0.41
13:6:10:PHE:CZ	14:7:142:PRO:HG3	2.55	0.41
13:6:48:GLU:HG3	13:6:48:GLU:O	2.21	0.41
20:Z:513:ALA:O	20:Z:548:ASP:OD1	2.39	0.41
21:N:906:ARG:HA	21:N:906:ARG:NE	2.34	0.41
23:P:107:SER:O	23:P:108:LYS:HB2	2.20	0.41
24:Q:251:THR:HA	24:Q:254:SER:HB2	2.01	0.41
28:H:203:LYS:HZ3	28:H:269:ALA:N	2.19	0.41
3:c:18:ARG:HH11	3:c:18:ARG:HD2	1.72	0.41
5:e:136:ARG:NH1	5:e:137:PRO:O	2.54	0.41
14:n:202:THR:OG1	14:n:205:VAL:HG23	2.21	0.41
3:C:18:ARG:HH11	3:C:18:ARG:HD2	1.71	0.41
4:D:187:THR:HG22	4:D:188:VAL:N	2.35	0.41
7:G:187:LEU:H	7:G:187:LEU:HD23	1.85	0.41
8:1:140:SER:HA	8:1:143:ILE:HG12	2.03	0.41
11:4:82:SER:OG	11:4:125:LYS:HE2	2.21	0.41
16:V:24:LYS:HE2	16:V:173:THR:HA	2.03	0.41
25:R:41:GLU:CA	25:R:44:LYS:NZ	2.78	0.41
30:K:362:LEU:HA	30:K:402:ILE:H	1.84	0.41
5:e:70:ILE:HD13	5:e:92:ALA:HB1	2.01	0.41
6:f:54:ASP:H	6:f:57:SER:HB3	1.86	0.41
9:i:126:TYR:CE1	9:i:144:ALA:HB2	2.45	0.41
11:k:139:TYR:CD2	11:k:139:TYR:N	2.88	0.41
13:m:130:VAL:C	13:m:131:TYR:HD1	2.29	0.41
14:n:137:ARG:NH1	14:n:138:SER:CA	2.84	0.41
9:2:32:ILE:HD11	9:2:74:GLY:C	2.45	0.41
19:Y:16:LEU:O	19:Y:20:LYS:HD2	2.21	0.41
21:N:83:LEU:HG	21:N:132:LYS:CG	2.51	0.41
30:K:243:VAL:HG21	31:L:257:GLY:HA3	2.01	0.41
34:8:349:TYR:CZ	34:8:353:LYS:HE3	2.55	0.41
3:c:181:LYS:HB2	3:c:184:MET:HG3	2.03	0.41
11:k:82:SER:OG	11:k:125:LYS:HE2	2.21	0.41
11:k:167:GLU:OE2	12:5:213:GLY:HA2	2.21	0.41
13:m:145:ARG:HH11	13:m:145:ARG:HD2	1.38	0.41
8:1:180:GLY:O	8:1:202:TYR:OH	2.39	0.41
11:4:3:ILE:HD12	11:4:176:PHE:CD1	2.47	0.41
13:6:36:ARG:NH1	13:6:207:GLY:HA3	2.34	0.41
13:6:145:ARG:HH11	13:6:145:ARG:HD2	1.38	0.41
15:W:21:PHE:HB2	15:W:25:ARG:HG2	2.02	0.41
20:Z:139:LEU:O	20:Z:149:TRP:CZ3	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Z:875:LYS:CB	20:Z:878:LEU:HD23	2.51	0.41
22:S:122:ASN:CB	22:S:128:ILE:HD11	2.50	0.41
29:I:77:SER:HA	29:I:81:ILE:CD1	2.51	0.41
29:I:90:GLU:O	29:I:94:LYS:HG3	2.20	0.41
2:b:109:LEU:CD2	10:j:77:LYS:HE3	2.51	0.41
5:e:122:ARG:HA	5:e:132:ARG:HH11	1.85	0.41
6:f:69:HIS:CD2	6:f:102:LYS:HB2	2.56	0.41
7:g:109:ILE:HG22	7:g:149:TYR:CE2	2.56	0.41
7:g:218:TRP:CD1	7:g:231:VAL:HG23	2.56	0.41
9:i:53:PRO:HB2	13:6:203:HIS:CE1	2.56	0.41
9:i:126:TYR:N	9:i:126:TYR:CD1	2.87	0.41
13:m:106:TYR:HA	13:m:136:VAL:O	2.20	0.41
13:m:118:ILE:HD13	13:m:118:ILE:HG21	1.63	0.41
14:n:259:LYS:HG3	8:1:194:ARG:HH11	1.86	0.41
3:C:70:ASN:OD1	3:C:70:ASN:C	2.62	0.41
6:F:4:ASN:OD1	6:F:4:ASN:C	2.64	0.41
10:3:40:PHE:HD1	10:3:41:GLU:N	2.18	0.41
10:3:126:LEU:H	10:3:126:LEU:HG	1.71	0.41
10:3:145:GLN:HB3	10:3:174:ALA:HA	2.02	0.41
13:6:55:GLY:O	13:6:56:ASP:HB2	2.21	0.41
16:V:53:MET:HE1	16:V:139:VAL:HG21	2.01	0.41
20:Z:58:GLU:HB3	20:Z:63:LEU:HD21	2.03	0.41
20:Z:556:ILE:HD12	20:Z:556:ILE:O	2.21	0.41
21:N:743:PHE:N	21:N:744:PRO:CD	2.83	0.41
29:I:184:ILE:HD11	29:I:231:LEU:HG	2.03	0.41
30:K:252:ARG:HG3	30:K:253:MET:N	2.35	0.41
31:L:111:GLU:OE2	31:L:116:LYS:O	2.39	0.41
31:L:149:ASP:H	31:L:154:THR:H	1.68	0.41
35:9:72:ARG:HB3	35:9:73:LEU:H	1.66	0.41
12:l:286:ILE:HG21	12:l:286:ILE:HD13	1.59	0.41
13:m:36:ARG:NH1	13:m:207:GLY:HA3	2.34	0.41
3:C:181:LYS:HB2	3:C:184:MET:HG3	2.03	0.41
6:F:142:ALA:O	6:F:143:HIS:ND1	2.45	0.41
16:V:84:ASP:HB3	16:V:87:PHE:CD2	2.56	0.41
20:Z:838:TYR:CD1	20:Z:838:TYR:C	2.99	0.41
26:U:10:ILE:HG22	26:U:11:ALA:O	2.21	0.41
27:O:205:ILE:N	27:O:205:ILE:HD12	2.36	0.41
27:O:305:ILE:O	27:O:305:ILE:HG13	2.21	0.41
29:I:199:GLU:OE1	29:I:236:VAL:HG12	2.21	0.41
3:c:33:GLY:H	3:c:51:LYS:HB3	1.87	0.40
10:j:7:ILE:HG22	10:j:8:ASN:OD1	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:m:122:LEU:HD22	13:m:217:LYS:HE3	2.03	0.40
2:B:18:LEU:O	2:B:22:ASP:OD2	2.38	0.40
2:B:78:MET:HE2	30:K:426:PHE:CE2	2.54	0.40
6:F:69:HIS:CD2	6:F:102:LYS:HB2	2.56	0.40
9:2:80:ASP:O	9:2:84:VAL:CG2	2.60	0.40
10:3:8:ASN:HD21	10:3:57:ALA:H	1.69	0.40
10:3:204:GLN:NE2	10:3:204:GLN:CA	2.65	0.40
11:4:139:TYR:CD2	11:4:139:TYR:N	2.88	0.40
13:6:130:VAL:C	13:6:131:TYR:HD1	2.29	0.40
17:T:150:ARG:CZ	22:S:382:ARG:HA	2.50	0.40
26:U:253:ASP:O	26:U:257:ILE:HG12	2.21	0.40
28:H:459:SER:HA	28:H:462:ARG:HD3	2.03	0.40
29:I:133:LEU:O	29:I:134:SER:OG	2.36	0.40
33:J:133:LEU:HD22	33:J:240:HIS:HB2	2.01	0.40
33:J:140:GLU:HG2	33:J:212:ARG:HB3	2.03	0.40
1:a:35:THR:HA	1:a:85:GLY:HA2	2.02	0.40
2:b:2:THR:OG1	6:f:123:TYR:O	2.25	0.40
10:j:7:ILE:HG21	10:j:7:ILE:HD13	1.76	0.40
12:l:126:ASP:OD1	13:m:109:ARG:NH1	2.53	0.40
12:l:139:ARG:HH11	12:l:139:ARG:HD3	1.41	0.40
4:D:111:ARG:NH1	12:5:145:GLU:CD	2.77	0.40
7:G:109:ILE:HG22	7:G:149:TYR:CE2	2.56	0.40
29:I:133:LEU:CD2	29:I:155:SER:OG	2.63	0.40
33:J:21:PRO:O	33:J:25:GLN:HG3	2.21	0.40
2:b:18:LEU:O	2:b:22:ASP:OD2	2.38	0.40
8:h:140:SER:HA	8:h:143:ILE:HG12	2.03	0.40
10:j:83:GLU:OE2	10:j:83:GLU:HA	2.21	0.40
11:k:96:ARG:HD3	12:l:167:GLY:HA3	2.03	0.40
12:l:272:PHE:CE1	10:3:204:GLN:CG	3.04	0.40
13:m:48:GLU:HG3	13:m:48:GLU:O	2.21	0.40
13:m:181:LYS:HG3	13:m:182:TYR:H	1.82	0.40
3:C:33:GLY:H	3:C:51:LYS:HB3	1.87	0.40
3:C:133:VAL:HG11	3:C:135:PHE:CE1	2.57	0.40
10:3:183:TRP:HD1	10:3:204:GLN:CD	2.26	0.40
16:V:109:HIS:CE1	16:V:140:VAL:HG22	2.57	0.40
20:Z:30:LYS:HD2	20:Z:41:GLU:HG2	2.04	0.40
20:Z:545:SER:HA	20:Z:548:ASP:OD1	2.21	0.40
27:O:268:SER:HA	27:O:271:LYS:HE3	2.03	0.40
28:H:427:GLY:HA3	29:I:211:MET:SD	2.62	0.40
30:K:238:ASN:ND2	31:L:310:THR:HG21	2.36	0.40
3:c:133:VAL:HG11	3:c:135:PHE:CE1	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:h:47:HIS:HD2	8:h:82:PRO:HG3	1.86	0.40
14:n:262:GLY:HA2	9:2:150:VAL:CG2	2.52	0.40
1:A:35:THR:HA	1:A:85:GLY:HA2	2.02	0.40
3:C:98:TYR:HE2	11:4:67:TYR:HE1	1.69	0.40
4:D:90:ARG:HH12	11:4:66:LEU:HA	1.87	0.40
5:E:122:ARG:HA	5:E:132:ARG:HH11	1.85	0.40
27:O:136:THR:HG22	27:O:140:LYS:HE2	2.03	0.40
33:J:7:SER:HB2	33:J:14:THR:OG1	2.22	0.40
34:8:105:ALA:HB2	34:8:454:ASP:OD2	2.21	0.40
1:a:149:GLU:CD	9:i:101:ARG:NH2	2.74	0.40
4:d:42:VAL:HG13	4:d:145:PRO:HB3	2.04	0.40
6:f:4:ASN:OD1	6:f:4:ASN:C	2.64	0.40
9:i:92:ILE:CD1	9:i:111:MET:HE1	2.51	0.40
9:i:243:LYS:HZ1	10:j:199:TYR:HD2	1.57	0.40
11:k:29:LYS:HA	11:k:29:LYS:HD2	1.93	0.40
12:l:140:LEU:CD2	12:l:144:ARG:NH2	2.84	0.40
12:l:191:ASP:CB	12:l:195:THR:OG1	2.70	0.40
12:l:273:TRP:HZ2	10:3:202:MET:O	2.05	0.40
1:A:33:LYS:HE3	30:K:424:PHE:CE1	2.57	0.40
4:D:120:TYR:HA	4:D:126:VAL:CG2	2.51	0.40
9:2:92:ILE:CD1	9:2:111:MET:HE1	2.51	0.40
16:V:24:LYS:CE	16:V:173:THR:HA	2.52	0.40
21:N:246:LYS:HA	21:N:246:LYS:CE	2.52	0.40
22:S:153:GLU:HB2	22:S:154:GLN:H	1.69	0.40
23:P:55:SER:HB2	23:P:96:MET:HE3	2.03	0.40
31:L:379:ALA:HB3	31:L:416:MET:CE	2.51	0.40
33:J:374:ARG:HG2	33:J:376:HIS:H	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	239/252 (95%)	229 (96%)	10 (4%)	0	100	100
1	a	239/252 (95%)	228 (95%)	11 (5%)	0	100	100
2	B	247/250 (99%)	237 (96%)	8 (3%)	2 (1%)	16	54
2	b	247/250 (99%)	237 (96%)	8 (3%)	2 (1%)	16	54
3	C	242/258 (94%)	233 (96%)	8 (3%)	1 (0%)	30	67
3	c	242/258 (94%)	233 (96%)	8 (3%)	1 (0%)	30	67
4	D	234/254 (92%)	219 (94%)	10 (4%)	5 (2%)	5	29
4	d	234/254 (92%)	218 (93%)	11 (5%)	5 (2%)	5	29
5	E	242/260 (93%)	227 (94%)	14 (6%)	1 (0%)	30	67
5	e	242/260 (93%)	224 (93%)	15 (6%)	3 (1%)	10	44
6	F	229/234 (98%)	222 (97%)	6 (3%)	1 (0%)	30	67
6	f	229/234 (98%)	222 (97%)	6 (3%)	1 (0%)	30	67
7	G	240/288 (83%)	225 (94%)	14 (6%)	1 (0%)	30	67
7	g	240/288 (83%)	227 (95%)	12 (5%)	1 (0%)	30	67
8	1	194/215 (90%)	187 (96%)	7 (4%)	0	100	100
8	h	194/215 (90%)	185 (95%)	9 (5%)	0	100	100
9	2	224/261 (86%)	213 (95%)	9 (4%)	2 (1%)	14	50
9	i	224/261 (86%)	209 (93%)	12 (5%)	3 (1%)	9	42
10	3	202/205 (98%)	191 (95%)	9 (4%)	2 (1%)	12	48
10	j	202/205 (98%)	193 (96%)	7 (4%)	2 (1%)	12	48
11	4	193/198 (98%)	183 (95%)	9 (5%)	1 (0%)	24	63
11	k	193/198 (98%)	183 (95%)	8 (4%)	2 (1%)	12	48
12	5	210/287 (73%)	199 (95%)	10 (5%)	1 (0%)	24	63
12	l	210/287 (73%)	198 (94%)	11 (5%)	1 (0%)	24	63
13	6	220/241 (91%)	206 (94%)	12 (6%)	2 (1%)	14	50
13	m	220/241 (91%)	206 (94%)	12 (6%)	2 (1%)	14	50
14	7	227/266 (85%)	206 (91%)	18 (8%)	3 (1%)	9	42
14	n	227/266 (85%)	210 (92%)	17 (8%)	0	100	100
15	W	195/268 (73%)	177 (91%)	17 (9%)	1 (0%)	24	63
16	V	287/306 (94%)	261 (91%)	22 (8%)	4 (1%)	9	40
17	T	264/274 (96%)	239 (90%)	24 (9%)	1 (0%)	30	67
18	X	125/156 (80%)	107 (86%)	17 (14%)	1 (1%)	16	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	Y	87/89 (98%)	77 (88%)	7 (8%)	3 (3%)	3	21
20	Z	902/993 (91%)	822 (91%)	63 (7%)	17 (2%)	6	32
21	N	828/945 (88%)	796 (96%)	28 (3%)	4 (0%)	24	63
22	S	473/523 (90%)	437 (92%)	27 (6%)	9 (2%)	6	32
23	P	438/445 (98%)	418 (95%)	17 (4%)	3 (1%)	18	56
24	Q	432/434 (100%)	397 (92%)	30 (7%)	5 (1%)	10	44
25	R	403/429 (94%)	377 (94%)	23 (6%)	3 (1%)	18	56
26	U	288/338 (85%)	276 (96%)	11 (4%)	1 (0%)	36	72
27	O	386/393 (98%)	372 (96%)	14 (4%)	0	100	100
28	H	387/467 (83%)	355 (92%)	25 (6%)	7 (2%)	6	34
29	I	382/437 (87%)	331 (87%)	42 (11%)	9 (2%)	4	27
30	K	392/428 (92%)	360 (92%)	30 (8%)	2 (0%)	24	63
31	L	386/437 (88%)	349 (90%)	33 (8%)	4 (1%)	12	48
32	M	419/434 (96%)	374 (89%)	35 (8%)	10 (2%)	4	27
33	J	403/405 (100%)	356 (88%)	42 (10%)	5 (1%)	10	44
34	8	368/499 (74%)	329 (89%)	30 (8%)	9 (2%)	4	27
35	9	74/76 (97%)	70 (95%)	4 (5%)	0	100	100
All	All	14205/15714 (90%)	13230 (93%)	832 (6%)	143 (1%)	15	48

All (143) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	b	3	ASP
4	d	204	GLN
5	e	128	SER
9	i	200	SER
9	i	222	PRO
11	k	50	ALA
13	m	138	SER
2	B	3	ASP
4	D	101	GLU
4	D	204	GLN
5	E	128	SER
9	2	200	SER
10	3	126	LEU
10	3	183	TRP

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Mol	Chain	Res	Type
11	4	50	ALA
13	6	138	SER
14	7	110	ASP
16	V	59	ASP
16	V	271	VAL
17	T	138	ASP
19	Y	4	ASP
19	Y	32	ASP
20	Z	5	SER
20	Z	142	ASP
20	Z	173	ALA
20	Z	174	GLU
20	Z	309	GLN
20	Z	366	LYS
20	Z	443	ASP
20	Z	498	ALA
20	Z	728	LYS
20	Z	802	ASP
20	Z	926	ASN
21	N	87	ASP
21	N	361	ASN
21	N	529	GLN
22	S	69	LEU
22	S	449	LEU
24	Q	387	TYR
25	R	71	LEU
25	R	72	VAL
25	R	280	ILE
28	H	95	HIS
28	H	152	ILE
28	H	314	VAL
28	H	372	ASP
28	H	465	GLN
28	H	466	TYR
29	I	102	ASN
29	I	125	MET
29	I	213	ILE
29	I	345	ASP
30	K	344	ARG
30	K	416	LYS
31	L	275	PRO
31	L	291	PHE

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Mol	Chain	Res	Type
32	M	96	ASN
32	M	106	VAL
32	M	179	THR
32	M	316	SER
32	M	427	SER
32	M	429	SER
33	J	71	TYR
33	J	400	VAL
34	8	209	ASP
34	8	245	ALA
34	8	497	PHE
5	e	18	GLU
9	i	251	ASP
13	m	40	ASP
4	D	5	ASP
9	2	222	PRO
13	6	40	ASP
20	Z	85	VAL
20	Z	939	ALA
22	S	153	GLU
22	S	450	ASN
23	P	90	LYS
24	Q	51	ARG
32	M	97	SER
32	M	424	ALA
33	J	11	VAL
34	8	466	ASP
2	b	17	LYS
3	c	40	ALA
4	d	205	THR
6	f	205	SER
7	g	71	ASP
2	B	17	LYS
3	C	40	ALA
6	F	205	SER
7	G	71	ASP
16	V	112	PRO
16	V	186	GLN
18	X	116	ALA
19	Y	68	GLU
20	Z	377	ALA
26	U	179	ARG

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Mol	Chain	Res	Type
28	H	459	SER
29	I	103	PRO
29	I	105	SER
31	L	245	PHE
34	8	331	ARG
4	d	102	ASP
5	e	53	ARG
20	Z	963	ALA
22	S	84	ASP
23	P	403	GLU
31	L	114	GLU
32	M	87	ASP
34	8	106	GLN
34	8	487	ASP
4	d	101	GLU
4	D	102	ASP
4	D	205	THR
21	N	861	TYR
22	S	112	ASN
22	S	327	ILE
23	P	89	LEU
24	Q	47	ASP
24	Q	110	SER
24	Q	286	TYR
32	M	317	SER
33	J	141	LYS
34	8	151	ALA
4	d	103	PRO
10	j	156	PRO
10	j	183	TRP
14	7	111	ASN
14	7	249	ASN
29	I	95	GLN
29	I	137	ASP
33	J	353	CYS
34	8	294	ASN
20	Z	233	LEU
15	W	22	PRO
20	Z	940	GLY
12	l	113	ASN
22	S	83	PRO
29	I	84	PRO

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Mol	Chain	Res	Type
11	k	4	ILE
12	5	113	ASN
22	S	115	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	206/210 (98%)	195 (95%)	11 (5%)	20	41
1	a	206/210 (98%)	194 (94%)	12 (6%)	18	40
2	B	208/209 (100%)	194 (93%)	14 (7%)	15	36
2	b	208/209 (100%)	194 (93%)	14 (7%)	15	36
3	C	203/216 (94%)	197 (97%)	6 (3%)	36	57
3	c	203/216 (94%)	197 (97%)	6 (3%)	36	57
4	D	209/226 (92%)	202 (97%)	7 (3%)	33	55
4	d	209/226 (92%)	202 (97%)	7 (3%)	33	55
5	E	200/215 (93%)	189 (94%)	11 (6%)	19	41
5	e	200/215 (93%)	187 (94%)	13 (6%)	15	37
6	F	190/193 (98%)	182 (96%)	8 (4%)	26	48
6	f	190/193 (98%)	182 (96%)	8 (4%)	26	48
7	G	200/239 (84%)	193 (96%)	7 (4%)	32	53
7	g	200/239 (84%)	189 (94%)	11 (6%)	19	41
8	l	162/178 (91%)	134 (83%)	28 (17%)	2	9
8	h	162/178 (91%)	136 (84%)	26 (16%)	2	11
9	2	185/214 (86%)	146 (79%)	39 (21%)	1	6
9	i	185/214 (86%)	156 (84%)	29 (16%)	2	12
10	3	172/173 (99%)	141 (82%)	31 (18%)	2	9
10	j	172/173 (99%)	148 (86%)	24 (14%)	3	13
11	4	173/175 (99%)	127 (73%)	46 (27%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	k	173/175 (99%)	129 (75%)	44 (25%)	0	3
12	5	169/235 (72%)	132 (78%)	37 (22%)	1	6
12	l	169/235 (72%)	132 (78%)	37 (22%)	1	6
13	6	185/201 (92%)	159 (86%)	26 (14%)	3	13
13	m	185/201 (92%)	156 (84%)	29 (16%)	2	12
14	7	195/224 (87%)	192 (98%)	3 (2%)	57	72
14	n	195/224 (87%)	195 (100%)	0	100	100
15	W	171/230 (74%)	167 (98%)	4 (2%)	44	64
16	V	253/268 (94%)	247 (98%)	6 (2%)	43	63
17	T	249/256 (97%)	246 (99%)	3 (1%)	63	75
18	X	116/144 (81%)	113 (97%)	3 (3%)	40	61
19	Y	81/81 (100%)	79 (98%)	2 (2%)	42	62
20	Z	773/850 (91%)	748 (97%)	25 (3%)	34	56
21	N	698/797 (88%)	685 (98%)	13 (2%)	50	67
22	S	447/489 (91%)	431 (96%)	16 (4%)	31	52
23	P	412/415 (99%)	405 (98%)	7 (2%)	53	69
24	Q	391/391 (100%)	380 (97%)	11 (3%)	38	60
25	R	356/379 (94%)	353 (99%)	3 (1%)	73	80
26	U	263/308 (85%)	258 (98%)	5 (2%)	50	67
27	O	363/368 (99%)	359 (99%)	4 (1%)	65	76
28	H	330/399 (83%)	314 (95%)	16 (5%)	23	44
29	I	341/385 (89%)	334 (98%)	7 (2%)	47	65
30	K	346/374 (92%)	332 (96%)	14 (4%)	28	49
31	L	332/377 (88%)	319 (96%)	13 (4%)	28	49
32	M	364/375 (97%)	346 (95%)	18 (5%)	22	43
33	J	352/352 (100%)	346 (98%)	6 (2%)	53	69
34	8	337/449 (75%)	325 (96%)	12 (4%)	31	52
35	9	68/68 (100%)	67 (98%)	1 (2%)	57	72
All	All	12357/13571 (91%)	11634 (94%)	723 (6%)	19	39

All (723) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	13	ASP
1	a	64	LEU
1	a	67	THR
1	a	78	THR
1	a	95	LEU
1	a	96	ARG
1	a	112	MET
1	a	171	THR
1	a	187	LYS
1	a	193	HIS
1	a	217	GLU
1	a	250	GLU
2	b	11	THR
2	b	15	SER
2	b	35	LEU
2	b	53	SER
2	b	109	LEU
2	b	119	GLN
2	b	123	GLN
2	b	146	SER
2	b	166	LYS
2	b	178	ARG
2	b	201	GLU
2	b	229	THR
2	b	231	LYS
2	b	240	SER
3	c	81	THR
3	c	125	HIS
3	c	165	VAL
3	c	170	SER
3	c	174	THR
3	c	203	SER
4	d	11	PHE
4	d	66	LYS
4	d	149	GLN
4	d	153	SER
4	d	157	SER
4	d	170	THR
4	d	218	ASP
5	e	10	ARG
5	e	14	THR
5	e	36	THR
5	e	81	LEU

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Mol	Chain	Res	Type
5	e	104	ASP
5	e	112	LEU
5	e	121	LEU
5	e	177	GLU
5	e	180	GLN
5	e	223	THR
5	e	225	GLN
5	e	229	LYS
5	e	250	GLU
6	f	5	ASN
6	f	69	HIS
6	f	72	LEU
6	f	117	GLN
6	f	119	ASN
6	f	154	THR
6	f	207	THR
6	f	232	LYS
7	g	46	VAL
7	g	57	LYS
7	g	93	ARG
7	g	137	ILE
7	g	173	LYS
7	g	179	LEU
7	g	185	GLU
7	g	202	LEU
7	g	209	GLU
7	g	245	LYS
7	g	247	ILE
8	h	10	THR
8	h	18	LYS
8	h	29	THR
8	h	30	THR
8	h	31	THR
8	h	40	THR
8	h	42	LYS
8	h	44	THR
8	h	52	CYS
8	h	61	THR
8	h	77	SER
8	h	89	SER
8	h	103	THR
8	h	112	ASP

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Mol	Chain	Res	Type
8	h	113	ASP
8	h	114	LYS
8	h	128	VAL
8	h	133	TYR
8	h	138	SER
8	h	144	TYR
8	h	147	CYS
8	h	155	MET
8	h	156	SER
8	h	169	SER
8	h	173	LYS
8	h	178	SER
9	i	30	THR
9	i	31	THR
9	i	43	ILE
9	i	49	SER
9	i	51	GLN
9	i	65	ARG
9	i	66	ILE
9	i	84	VAL
9	i	88	ILE
9	i	92	ILE
9	i	97	LEU
9	i	98	TYR
9	i	101	ARG
9	i	106	VAL
9	i	118	LYS
9	i	126	TYR
9	i	128	ILE
9	i	153	TYR
9	i	156	LEU
9	i	177	LYS
9	i	181	ILE
9	i	182	LYS
9	i	186	ASP
9	i	188	ILE
9	i	198	SER
9	i	200	SER
9	i	209	ILE
9	i	211	LYS
9	i	255	GLU
10	j	3	ASP

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Mol	Chain	Res	Type
10	j	7	ILE
10	j	8	ASN
10	j	18	LYS
10	j	33	SER
10	j	41	GLU
10	j	53	ILE
10	j	63	LEU
10	j	65	GLU
10	j	77	LYS
10	j	93	SER
10	j	94	SER
10	j	114	SER
10	j	115	LYS
10	j	116	SER
10	j	172	LEU
10	j	188	TYR
10	j	193	ASP
10	j	194	GLU
10	j	196	VAL
10	j	202	MET
10	j	203	ARG
10	j	204	GLN
10	j	205	ASP
11	k	12	SER
11	k	17	SER
11	k	18	SER
11	k	26	SER
11	k	29	LYS
11	k	45	SER
11	k	52	ASP
11	k	65	GLN
11	k	67	TYR
11	k	68	SER
11	k	69	ILE
11	k	70	ARG
11	k	74	GLU
11	k	76	SER
11	k	78	GLN
11	k	81	SER
11	k	90	LYS
11	k	91	SER
11	k	92	ILE

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Mol	Chain	Res	Type
11	k	93	ARG
11	k	98	TYR
11	k	99	GLN
11	k	100	VAL
11	k	101	ASN
11	k	120	ASP
11	k	121	TYR
11	k	125	LYS
11	k	135	TYR
11	k	136	SER
11	k	139	TYR
11	k	143	LEU
11	k	145	ASP
11	k	162	LYS
11	k	163	LEU
11	k	166	GLN
11	k	169	GLU
11	k	174	MET
11	k	176	PHE
11	k	177	LYS
11	k	180	ILE
11	k	182	LYS
11	k	186	LYS
11	k	191	GLN
11	k	192	VAL
12	l	77	THR
12	l	81	PHE
12	l	84	GLN
12	l	100	TRP
12	l	104	GLN
12	l	107	LYS
12	l	110	ILE
12	l	115	PHE
12	l	127	CYS
12	l	138	CYS
12	l	139	ARG
12	l	140	LEU
12	l	147	GLU
12	l	148	ARG
12	l	159	SER
12	l	160	ASN
12	l	162	VAL

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Mol	Chain	Res	Type
12	l	170	LEU
12	l	180	THR
12	l	182	LYS
12	l	183	GLU
12	l	186	THR
12	l	192	SER
12	l	195	THR
12	l	196	ARG
12	l	198	LYS
12	l	203	CYS
12	l	214	VAL
12	l	215	LEU
12	l	217	SER
12	l	245	TYR
12	l	246	SER
12	l	253	TYR
12	l	256	THR
12	l	274	LYS
12	l	283	ASN
12	l	286	ILE
13	m	15	ASP
13	m	30	VAL
13	m	39	THR
13	m	41	TYR
13	m	50	LYS
13	m	56	ASP
13	m	58	ILE
13	m	72	LEU
13	m	78	ASN
13	m	93	SER
13	m	94	ILE
13	m	109	ARG
13	m	116	HIS
13	m	118	ILE
13	m	124	GLU
13	m	131	TYR
13	m	134	ASP
13	m	138	SER
13	m	140	GLU
13	m	143	GLN
13	m	177	LYS
13	m	181	LYS

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Mol	Chain	Res	Type
13	m	186	GLU
13	m	194	ASP
13	m	200	THR
13	m	201	GLU
13	m	208	ASP
13	m	217	LYS
13	m	228	LYS
1	A	13	ASP
1	A	64	LEU
1	A	67	THR
1	A	95	LEU
1	A	96	ARG
1	A	112	MET
1	A	171	THR
1	A	187	LYS
1	A	193	HIS
1	A	217	GLU
1	A	250	GLU
2	B	11	THR
2	B	15	SER
2	B	35	LEU
2	B	53	SER
2	B	109	LEU
2	B	119	GLN
2	B	123	GLN
2	B	146	SER
2	B	166	LYS
2	B	178	ARG
2	B	201	GLU
2	B	229	THR
2	B	231	LYS
2	B	240	SER
3	C	81	THR
3	C	125	HIS
3	C	165	VAL
3	C	170	SER
3	C	174	THR
3	C	203	SER
4	D	9	SER
4	D	90	ARG
4	D	119	ARG
4	D	122	GLN

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Mol	Chain	Res	Type
4	D	144	GLU
4	D	219	SER
4	D	227	GLU
5	E	36	THR
5	E	81	LEU
5	E	104	ASP
5	E	112	LEU
5	E	121	LEU
5	E	177	GLU
5	E	180	GLN
5	E	223	THR
5	E	225	GLN
5	E	229	LYS
5	E	250	GLU
6	F	5	ASN
6	F	69	HIS
6	F	72	LEU
6	F	117	GLN
6	F	119	ASN
6	F	154	THR
6	F	207	THR
6	F	232	LYS
7	G	46	VAL
7	G	57	LYS
7	G	93	ARG
7	G	137	ILE
7	G	190	ARG
7	G	218	TRP
7	G	236	LEU
8	1	10	THR
8	1	18	LYS
8	1	29	THR
8	1	30	THR
8	1	31	THR
8	1	40	THR
8	1	42	LYS
8	1	44	THR
8	1	52	CYS
8	1	61	THR
8	1	77	SER
8	1	89	SER
8	1	103	THR

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Mol	Chain	Res	Type
8	1	112	ASP
8	1	113	ASP
8	1	114	LYS
8	1	128	VAL
8	1	133	TYR
8	1	138	SER
8	1	144	TYR
8	1	147	CYS
8	1	155	MET
8	1	156	SER
8	1	169	SER
8	1	173	LYS
8	1	178	SER
8	1	203	GLU
8	1	204	GLN
9	2	30	THR
9	2	31	THR
9	2	43	ILE
9	2	49	SER
9	2	51	GLN
9	2	65	ARG
9	2	66	ILE
9	2	84	VAL
9	2	88	ILE
9	2	92	ILE
9	2	97	LEU
9	2	98	TYR
9	2	101	ARG
9	2	106	VAL
9	2	118	LYS
9	2	126	TYR
9	2	128	ILE
9	2	153	TYR
9	2	156	LEU
9	2	177	LYS
9	2	181	ILE
9	2	182	LYS
9	2	186	ASP
9	2	188	ILE
9	2	198	SER
9	2	200	SER
9	2	209	ILE

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Mol	Chain	Res	Type
9	2	211	LYS
9	2	212	ASP
9	2	217	ARG
9	2	219	TYR
9	2	220	LEU
9	2	224	VAL
9	2	228	LYS
9	2	230	LYS
9	2	231	SER
9	2	244	GLU
9	2	245	SER
9	2	254	GLU
10	3	3	ASP
10	3	7	ILE
10	3	8	ASN
10	3	18	LYS
10	3	33	SER
10	3	41	GLU
10	3	53	ILE
10	3	63	LEU
10	3	65	GLU
10	3	77	LYS
10	3	93	SER
10	3	94	SER
10	3	114	SER
10	3	115	LYS
10	3	116	SER
10	3	125	ASP
10	3	141	THR
10	3	149	MET
10	3	152	SER
10	3	159	GLU
10	3	166	THR
10	3	172	LEU
10	3	183	TRP
10	3	188	TYR
10	3	193	ASP
10	3	194	GLU
10	3	196	VAL
10	3	202	MET
10	3	203	ARG
10	3	204	GLN

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Mol	Chain	Res	Type
10	3	205	ASP
11	4	1	MET
11	4	3	ILE
11	4	12	SER
11	4	17	SER
11	4	18	SER
11	4	26	SER
11	4	29	LYS
11	4	45	SER
11	4	52	ASP
11	4	65	GLN
11	4	67	TYR
11	4	68	SER
11	4	69	ILE
11	4	70	ARG
11	4	74	GLU
11	4	76	SER
11	4	78	GLN
11	4	81	SER
11	4	90	LYS
11	4	91	SER
11	4	92	ILE
11	4	93	ARG
11	4	98	TYR
11	4	99	GLN
11	4	100	VAL
11	4	101	ASN
11	4	120	ASP
11	4	121	TYR
11	4	125	LYS
11	4	135	TYR
11	4	136	SER
11	4	139	TYR
11	4	143	LEU
11	4	145	ASP
11	4	162	LYS
11	4	163	LEU
11	4	166	GLN
11	4	169	GLU
11	4	174	MET
11	4	176	PHE
11	4	177	LYS

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Mol	Chain	Res	Type
11	4	180	ILE
11	4	182	LYS
11	4	186	LYS
11	4	191	GLN
11	4	192	VAL
12	5	77	THR
12	5	81	PHE
12	5	84	GLN
12	5	100	TRP
12	5	104	GLN
12	5	107	LYS
12	5	110	ILE
12	5	115	PHE
12	5	127	CYS
12	5	138	CYS
12	5	139	ARG
12	5	140	LEU
12	5	147	GLU
12	5	148	ARG
12	5	159	SER
12	5	160	ASN
12	5	162	VAL
12	5	170	LEU
12	5	180	THR
12	5	182	LYS
12	5	183	GLU
12	5	186	THR
12	5	192	SER
12	5	195	THR
12	5	196	ARG
12	5	198	LYS
12	5	203	CYS
12	5	214	VAL
12	5	215	LEU
12	5	217	SER
12	5	245	TYR
12	5	246	SER
12	5	253	TYR
12	5	256	THR
12	5	274	LYS
12	5	283	ASN
12	5	286	ILE

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Mol	Chain	Res	Type
13	6	15	ASP
13	6	30	VAL
13	6	39	THR
13	6	41	TYR
13	6	50	LYS
13	6	56	ASP
13	6	58	ILE
13	6	72	LEU
13	6	78	ASN
13	6	94	ILE
13	6	108	LYS
13	6	124	GLU
13	6	131	TYR
13	6	134	ASP
13	6	138	SER
13	6	140	GLU
13	6	143	GLN
13	6	177	LYS
13	6	181	LYS
13	6	186	GLU
13	6	194	ASP
13	6	200	THR
13	6	201	GLU
13	6	208	ASP
13	6	217	LYS
13	6	228	LYS
14	7	127	GLU
14	7	242	LYS
14	7	254	PHE
15	W	22	PRO
15	W	87	MET
15	W	119	SER
15	W	175	THR
16	V	31	SER
16	V	54	LEU
16	V	179	LEU
16	V	182	LYS
16	V	211	LYS
16	V	223	SER
17	T	28	PRO
17	T	125	GLU
17	T	135	ASN

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Mol	Chain	Res	Type
18	X	25	THR
18	X	112	ASN
18	X	119	LYS
19	Y	13	LYS
19	Y	18	LYS
20	Z	40	GLU
20	Z	82	MET
20	Z	113	SER
20	Z	213	LYS
20	Z	217	GLU
20	Z	258	PRO
20	Z	277	GLU
20	Z	309	GLN
20	Z	317	GLN
20	Z	352	LYS
20	Z	366	LYS
20	Z	424	SER
20	Z	471	LEU
20	Z	479	THR
20	Z	503	ASP
20	Z	528	LEU
20	Z	557	GLU
20	Z	630	LYS
20	Z	815	MET
20	Z	824	ASN
20	Z	831	LEU
20	Z	873	LEU
20	Z	892	SER
20	Z	909	ARG
20	Z	943	LYS
21	N	39	ILE
21	N	42	GLU
21	N	210	SER
21	N	269	LEU
21	N	311	ILE
21	N	330	THR
21	N	417	ARG
21	N	479	GLU
21	N	490	LEU
21	N	632	LYS
21	N	671	LEU
21	N	716	GLN

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Mol	Chain	Res	Type
21	N	747	HIS
22	S	36	LYS
22	S	43	LYS
22	S	101	LYS
22	S	138	MET
22	S	192	GLU
22	S	249	SER
22	S	265	SER
22	S	287	SER
22	S	304	SER
22	S	331	SER
22	S	373	LYS
22	S	400	LYS
22	S	448	LEU
22	S	454	SER
22	S	464	ARG
22	S	478	SER
23	P	2	SER
23	P	66	LEU
23	P	120	GLU
23	P	130	ILE
23	P	203	ILE
23	P	206	LYS
23	P	408	SER
24	Q	8	LEU
24	Q	12	ARG
24	Q	18	LYS
24	Q	71	LYS
24	Q	167	LYS
24	Q	195	LYS
24	Q	198	LEU
24	Q	207	SER
24	Q	357	VAL
24	Q	373	VAL
24	Q	387	TYR
25	R	124	ASP
25	R	176	ARG
25	R	336	LYS
26	U	46	ILE
26	U	160	THR
26	U	161	ILE
26	U	180	ASP

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Mol	Chain	Res	Type
26	U	201	GLN
27	O	80	LYS
27	O	112	LYS
27	O	157	LEU
27	O	285	SER
28	H	71	GLU
28	H	72	SER
28	H	88	ARG
28	H	178	ARG
28	H	180	LYS
28	H	194	SER
28	H	198	MET
28	H	202	GLU
28	H	216	ASP
28	H	282	LYS
28	H	314	VAL
28	H	336	LEU
28	H	374	LYS
28	H	458	SER
28	H	461	SER
28	H	464	MET
29	I	72	GLU
29	I	97	GLU
29	I	139	GLU
29	I	253	ILE
29	I	277	SER
29	I	300	ARG
29	I	373	GLU
30	K	80	LYS
30	K	117	SER
30	K	124	SER
30	K	199	GLU
30	K	204	ASP
30	K	249	GLU
30	K	263	GLU
30	K	344	ARG
30	K	345	ASP
30	K	361	SER
30	K	387	MET
30	K	399	ARG
30	K	405	SER
30	K	414	GLN

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Mol	Chain	Res	Type
31	L	123	SER
31	L	141	LYS
31	L	177	GLU
31	L	243	PHE
31	L	251	ILE
31	L	265	GLU
31	L	272	GLU
31	L	330	PRO
31	L	345	ARG
31	L	421	LYS
31	L	424	GLU
31	L	426	LYS
31	L	435	GLN
32	M	96	ASN
32	M	100	THR
32	M	109	ASP
32	M	110	ASN
32	M	124	ARG
32	M	131	MET
32	M	174	GLU
32	M	177	THR
32	M	213	ARG
32	M	228	LYS
32	M	230	LEU
32	M	261	LYS
32	M	289	LYS
32	M	292	ASP
32	M	305	MET
32	M	411	LYS
32	M	428	LYS
32	M	429	SER
33	J	57	PHE
33	J	131	ASP
33	J	176	SER
33	J	278	GLN
33	J	295	ASN
33	J	390	MET
34	8	125	GLN
34	8	153	ASP
34	8	161	VAL
34	8	175	SER
34	8	177	LYS

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Mol	Chain	Res	Type
34	8	182	ILE
34	8	221	MET
34	8	278	GLU
34	8	404	GLU
34	8	422	LYS
34	8	448	TYR
34	8	493	MET
35	9	31	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (254) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	56	GLN
1	a	92	ASN
1	a	184	ASN
1	a	209	HIS
1	a	251	GLN
2	b	218	ASN
2	b	244	ASN
3	c	94	HIS
3	c	152	ASN
3	c	156	ASN
3	c	177	GLN
3	c	227	GLN
3	c	233	GLN
4	d	19	GLN
4	d	79	ASN
4	d	94	GLN
4	d	96	HIS
4	d	122	GLN
4	d	231	GLN
5	e	154	GLN
5	e	185	ASN
5	e	188	HIS
6	f	100	ASN
6	f	121	GLN
6	f	148	GLN
6	f	185	ASN
7	g	64	ASN
7	g	68	GLN
7	g	204	HIS
7	g	207	ASN

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Mol	Chain	Res	Type
8	h	129	HIS
8	h	154	ASN
8	h	170	GLN
9	i	51	GLN
9	i	173	GLN
9	i	223	ASN
10	j	8	ASN
10	j	48	HIS
10	j	145	GLN
10	j	173	ASN
10	j	204	GLN
11	k	61	GLN
11	k	147	HIS
11	k	166	GLN
12	l	160	ASN
12	l	251	ASN
13	m	16	ASN
13	m	78	ASN
13	m	88	ASN
13	m	100	ASN
13	m	143	GLN
13	m	163	ASN
13	m	203	HIS
14	n	59	ASN
14	n	94	GLN
14	n	111	ASN
14	n	204	GLN
14	n	236	ASN
14	n	246	GLN
1	A	56	GLN
1	A	184	ASN
1	A	209	HIS
1	A	251	GLN
2	B	94	HIS
2	B	119	GLN
2	B	218	ASN
3	C	89	ASN
3	C	94	HIS
3	C	152	ASN
3	C	173	GLN
3	C	221	ASN
3	C	227	GLN

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Mol	Chain	Res	Type
3	C	233	GLN
4	D	16	HIS
4	D	70	HIS
4	D	118	GLN
4	D	149	GLN
5	E	114	GLN
5	E	154	GLN
5	E	185	ASN
5	E	188	HIS
6	F	100	ASN
6	F	148	GLN
6	F	185	ASN
7	G	23	GLN
7	G	68	GLN
7	G	182	HIS
7	G	195	GLN
7	G	204	HIS
7	G	228	HIS
8	1	69	GLN
8	1	78	GLN
8	1	129	HIS
8	1	154	ASN
9	2	51	GLN
9	2	91	ASN
9	2	122	HIS
9	2	173	GLN
9	2	223	ASN
10	3	8	ASN
10	3	48	HIS
10	3	89	GLN
10	3	145	GLN
11	4	61	GLN
11	4	147	HIS
11	4	166	GLN
12	5	160	ASN
12	5	251	ASN
12	5	254	HIS
12	5	284	ASN
13	6	16	ASN
13	6	78	ASN
13	6	84	HIS
13	6	87	HIS

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Mol	Chain	Res	Type
13	6	88	ASN
13	6	100	ASN
13	6	116	HIS
13	6	143	GLN
13	6	163	ASN
13	6	203	HIS
14	7	70	ASN
14	7	107	ASN
15	W	86	HIS
15	W	107	HIS
16	V	111	HIS
16	V	131	GLN
16	V	237	ASN
16	V	274	GLN
17	T	17	ASN
17	T	74	ASN
17	T	93	ASN
17	T	123	HIS
17	T	127	GLN
18	X	94	ASN
18	X	130	ASN
18	X	131	ASN
19	Y	52	ASN
20	Z	26	ASN
20	Z	327	GLN
20	Z	361	HIS
20	Z	380	ASN
20	Z	391	ASN
20	Z	403	ASN
20	Z	427	GLN
20	Z	434	GLN
20	Z	766	HIS
20	Z	769	ASN
20	Z	823	ASN
20	Z	833	GLN
20	Z	874	ASN
20	Z	926	ASN
21	N	34	GLN
21	N	122	GLN
21	N	176	GLN
21	N	268	GLN
21	N	280	GLN

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Mol	Chain	Res	Type
21	N	306	ASN
21	N	340	HIS
21	N	512	ASN
21	N	525	ASN
21	N	573	HIS
21	N	580	ASN
21	N	613	HIS
21	N	614	ASN
21	N	616	HIS
21	N	635	GLN
21	N	747	HIS
21	N	899	ASN
22	S	112	ASN
22	S	139	HIS
22	S	177	ASN
22	S	205	ASN
22	S	206	GLN
22	S	339	GLN
22	S	386	ASN
22	S	488	GLN
23	P	88	GLN
23	P	98	GLN
23	P	164	GLN
23	P	285	GLN
23	P	375	GLN
23	P	417	HIS
24	Q	145	HIS
24	Q	147	GLN
24	Q	252	HIS
24	Q	315	ASN
24	Q	371	GLN
24	Q	379	GLN
24	Q	394	ASN
24	Q	404	ASN
24	Q	420	ASN
25	R	42	GLN
25	R	340	GLN
25	R	378	ASN
25	R	401	HIS
26	U	21	HIS
26	U	62	ASN
26	U	75	ASN

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Mol	Chain	Res	Type
26	U	77	ASN
26	U	84	ASN
26	U	216	ASN
26	U	230	GLN
26	U	262	GLN
27	O	40	GLN
27	O	75	GLN
27	O	141	ASN
27	O	177	GLN
27	O	183	ASN
27	O	244	ASN
27	O	247	ASN
27	O	256	ASN
27	O	318	HIS
27	O	323	ASN
28	H	89	GLN
28	H	98	GLN
29	I	102	ASN
29	I	150	HIS
29	I	190	GLN
29	I	254	GLN
29	I	274	ASN
29	I	365	HIS
29	I	370	ASN
30	K	72	GLN
30	K	194	GLN
31	L	169	ASN
31	L	273	HIS
31	L	320	GLN
31	L	393	ASN
32	M	24	ASN
32	M	31	GLN
32	M	65	ASN
32	M	72	ASN
32	M	96	ASN
32	M	107	ASN
32	M	125	GLN
32	M	143	ASN
32	M	149	ASN
32	M	302	GLN
32	M	328	ASN
32	M	377	GLN

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Mol	Chain	Res	Type
32	M	423	GLN
33	J	9	ASN
33	J	89	GLN
33	J	287	ASN
33	J	295	ASN
33	J	376	HIS
33	J	391	ASN
33	J	393	ASN
34	8	113	ASN
34	8	121	ASN
34	8	157	HIS
34	8	172	GLN
34	8	313	GLN
35	9	62	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
35	GLZ	9	76	35	3,3,3	0.29	0	1,2,2	0.65	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	GLZ	9	76	35	-	0/0/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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
36	ATP	K	501	37	32,33,33	2.24	5 (15%)	48,52,52	1.49	11 (22%)
36	ATP	L	501	37	32,33,33	2.09	6 (18%)	48,52,52	1.47	12 (25%)
36	ATP	M	501	-	32,33,33	2.71	8 (25%)	48,52,52	1.18	2 (4%)
36	ATP	H	501	37	32,33,33	2.40	4 (12%)	48,52,52	1.63	10 (20%)
38	ADP	J	501	-	28,29,29	2.05	7 (25%)	43,45,45	1.04	4 (9%)
36	ATP	I	501	37	32,33,33	3.34	7 (21%)	48,52,52	1.18	4 (8%)

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
36	ATP	K	501	37	-	7/22/38/38	0/3/3/3
36	ATP	L	501	37	-	4/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	ATP	M	501	-	-	2/22/38/38	0/3/3/3
36	ATP	H	501	37	-	5/22/38/38	0/3/3/3
38	ADP	J	501	-	-	2/16/32/32	0/3/3/3
36	ATP	I	501	37	-	9/22/38/38	0/3/3/3

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	I	501	ATP	PB-O3A	11.78	1.72	1.59
36	I	501	ATP	PA-O3A	11.29	1.71	1.59
36	M	501	ATP	PB-O3A	11.21	1.71	1.59
36	H	501	ATP	PA-O3A	10.35	1.70	1.59
36	K	501	ATP	PB-O3B	8.44	1.68	1.59
36	L	501	ATP	PA-O3A	6.51	1.66	1.59
36	I	501	ATP	PB-O3B	6.28	1.66	1.59
38	J	501	ADP	PA-O3A	6.21	1.66	1.59
36	L	501	ATP	PB-O3A	5.88	1.65	1.59
36	M	501	ATP	PB-O3B	5.52	1.65	1.59
36	K	501	ATP	PA-O3A	5.18	1.65	1.59
36	K	501	ATP	PB-O3A	5.01	1.64	1.59
36	H	501	ATP	C5-N7	-4.31	1.31	1.39
36	H	501	ATP	PB-O3A	4.21	1.64	1.59
36	M	501	ATP	PA-O3A	4.13	1.64	1.59
36	L	501	ATP	PB-O3B	4.10	1.63	1.59
38	J	501	ADP	O4'-C4'	-4.10	1.35	1.45
36	M	501	ATP	O4'-C1'	3.67	1.50	1.42
38	J	501	ADP	O2'-C2'	-3.62	1.34	1.43
36	M	501	ATP	C8-N9	3.08	1.42	1.37
36	H	501	ATP	PB-O3B	3.04	1.62	1.59
36	K	501	ATP	C4-N9	3.01	1.43	1.37
36	M	501	ATP	C4-N3	-3.01	1.28	1.34
38	J	501	ADP	C2-N1	2.95	1.39	1.33
38	J	501	ADP	C5-C4	2.95	1.44	1.39
36	M	501	ATP	C8-N7	-2.89	1.26	1.31
38	J	501	ADP	C2-N3	2.76	1.38	1.33
36	I	501	ATP	C4-N3	2.75	1.39	1.34
36	K	501	ATP	C8-N7	-2.70	1.26	1.31
36	L	501	ATP	PG-O1G	2.55	1.58	1.50
36	I	501	ATP	C5'-C4'	2.51	1.59	1.51
36	I	501	ATP	C5-C4	2.44	1.43	1.39
36	L	501	ATP	C2-N1	2.33	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	J	501	ADP	C3'-C4'	2.27	1.58	1.53
36	I	501	ATP	C1'-N9	2.23	1.52	1.46
36	L	501	ATP	C8-N9	2.10	1.41	1.37
36	M	501	ATP	C2-N1	2.04	1.37	1.33

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	H	501	ATP	C5-C4-N3	-4.39	120.68	126.72
36	H	501	ATP	C6-C5-C4	3.82	122.39	117.18
36	K	501	ATP	N6-C6-N1	3.81	126.86	118.38
36	I	501	ATP	C4-C5-N7	-3.74	106.31	110.58
36	I	501	ATP	C5-C4-N9	3.35	109.47	105.81
36	H	501	ATP	C5-N7-C8	3.15	108.39	103.45
36	H	501	ATP	C4-C5-N7	-2.92	107.24	110.58
36	K	501	ATP	O3G-PG-O2G	2.87	118.56	107.80
36	L	501	ATP	O3G-PG-O2G	2.86	118.51	107.80
36	I	501	ATP	C5-C4-N3	-2.83	122.82	126.72
36	L	501	ATP	C5-C4-N3	-2.71	122.98	126.72
36	K	501	ATP	C6-C5-C4	2.68	120.84	117.18
36	L	501	ATP	C6-C5-C4	2.65	120.80	117.18
36	M	501	ATP	O5'-C5'-C4'	2.62	117.91	108.99
36	H	501	ATP	O2A-PA-O3A	2.59	114.27	107.27
36	K	501	ATP	N3-C4-N9	2.55	131.50	127.17
36	H	501	ATP	O2B-PB-O1B	2.55	124.29	112.44
38	J	501	ADP	C4'-O4'-C1'	2.51	115.02	109.47
36	K	501	ATP	C5-C4-N3	-2.49	123.29	126.72
36	L	501	ATP	N3-C4-N9	2.45	131.33	127.17
36	M	501	ATP	O3B-PG-O1G	-2.39	98.44	111.04
36	K	501	ATP	N3-C2-N1	-2.38	124.98	128.58
38	J	501	ADP	O3'-C3'-C4'	2.35	117.84	111.08
36	K	501	ATP	C5-C6-N6	-2.35	117.46	123.29
36	L	501	ATP	N9-C8-N7	-2.34	110.61	113.94
36	H	501	ATP	O3B-PG-O1G	-2.28	99.04	111.04
36	L	501	ATP	C2'-C3'-C4'	-2.27	98.23	102.61
36	K	501	ATP	O4'-C4'-C5'	2.26	116.58	109.33
36	H	501	ATP	C5-C4-N9	2.25	108.27	105.81
38	J	501	ADP	O5'-C5'-C4'	2.22	116.56	108.99
36	K	501	ATP	O3G-PG-O3B	-2.21	97.22	104.64
36	K	501	ATP	O4'-C1'-N9	2.20	112.31	108.09
36	L	501	ATP	O4'-C1'-C2'	-2.15	102.01	106.62
38	J	501	ADP	N3-C2-N1	-2.14	125.34	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	H	501	ATP	N3-C4-N9	2.14	130.80	127.17
36	L	501	ATP	O2B-PB-O3B	2.14	113.05	107.27
36	H	501	ATP	O2A-PA-O5'	-2.13	97.92	107.57
36	L	501	ATP	O3'-C3'-C4'	2.07	117.03	111.08
36	L	501	ATP	C3'-C2'-C1'	2.07	105.38	101.46
36	L	501	ATP	C5-N7-C8	2.07	106.70	103.45
36	K	501	ATP	C4-N9-C8	-2.06	103.58	105.74
36	I	501	ATP	O2B-PB-O1B	2.04	121.93	112.44
36	L	501	ATP	C6-C5-N7	-2.00	128.23	132.09

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
36	H	501	ATP	PB-O3B-PG-O2G
36	H	501	ATP	C5'-O5'-PA-O2A
36	H	501	ATP	C5'-O5'-PA-O3A
36	I	501	ATP	PB-O3B-PG-O2G
36	I	501	ATP	C5'-O5'-PA-O1A
36	I	501	ATP	C5'-O5'-PA-O2A
36	I	501	ATP	C5'-O5'-PA-O3A
36	K	501	ATP	PB-O3B-PG-O2G
36	K	501	ATP	PB-O3B-PG-O3G
36	K	501	ATP	C5'-O5'-PA-O3A
36	L	501	ATP	C5'-O5'-PA-O2A
36	L	501	ATP	C5'-O5'-PA-O3A
36	M	501	ATP	C5'-O5'-PA-O1A
38	J	501	ADP	C5'-O5'-PA-O3A
36	I	501	ATP	PB-O3A-PA-O5'
36	K	501	ATP	C5'-O5'-PA-O1A
38	J	501	ADP	C5'-O5'-PA-O1A
36	L	501	ATP	PA-O3A-PB-O1B
36	I	501	ATP	PB-O3A-PA-O1A
36	H	501	ATP	O4'-C4'-C5'-O5'
36	M	501	ATP	C4'-C5'-O5'-PA
36	K	501	ATP	PB-O3B-PG-O1G
36	H	501	ATP	PB-O3B-PG-O3G
36	I	501	ATP	PB-O3B-PG-O3G
36	K	501	ATP	PG-O3B-PB-O2B
36	I	501	ATP	PB-O3B-PG-O1G
36	I	501	ATP	PA-O3A-PB-O2B
36	K	501	ATP	PG-O3B-PB-O1B

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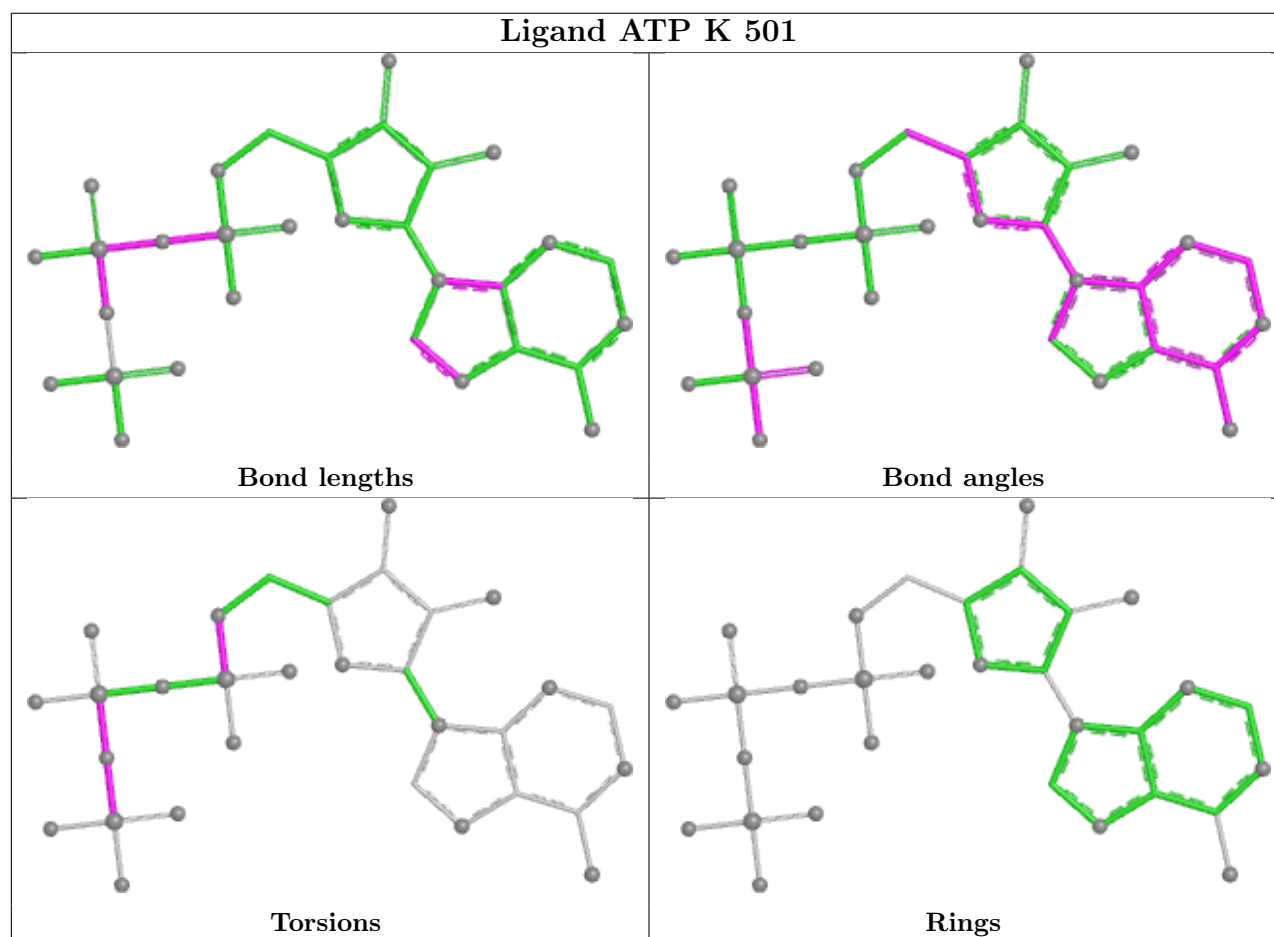
Continued from previous page...

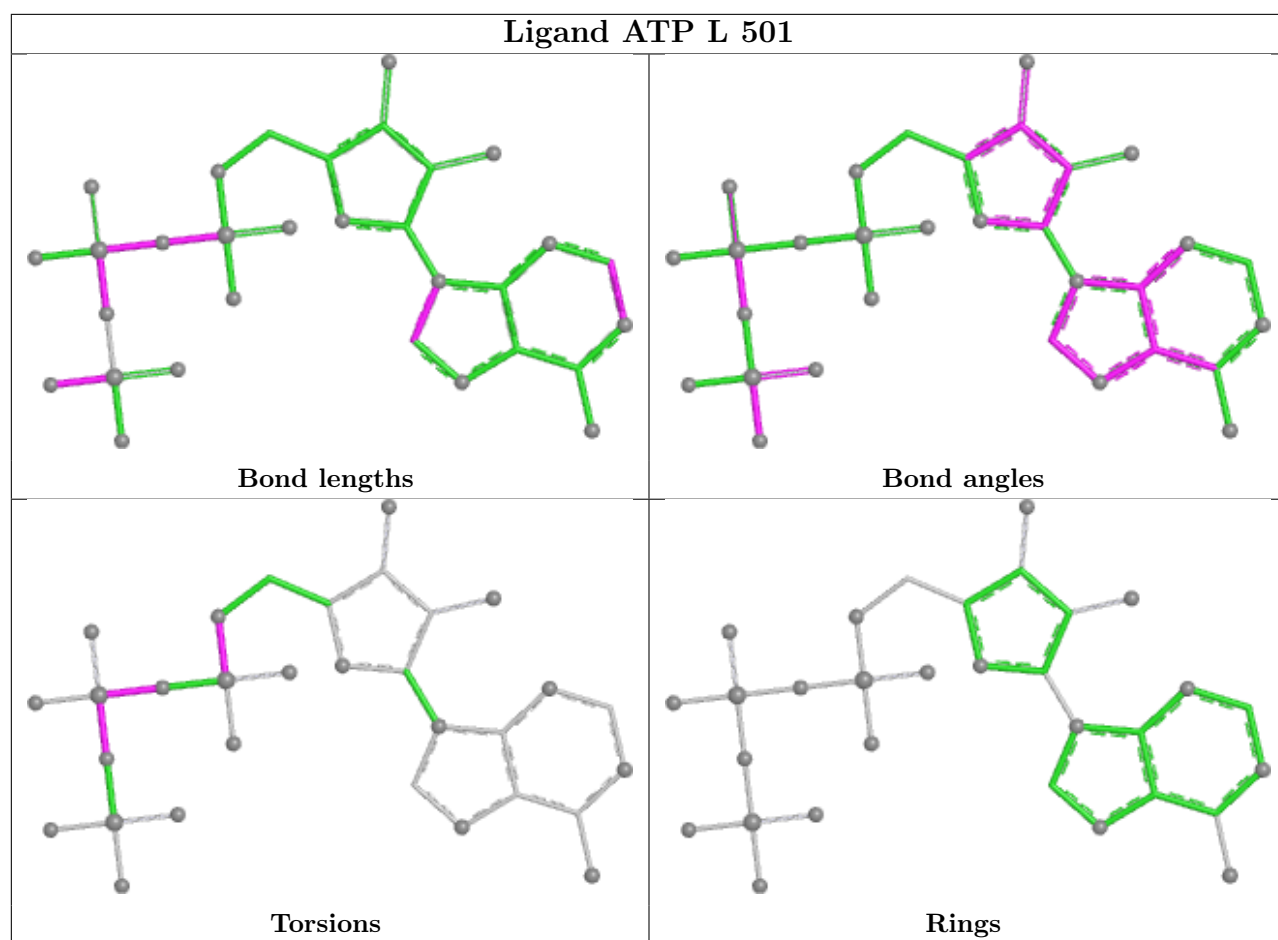
Mol	Chain	Res	Type	Atoms
36	L	501	ATP	PG-O3B-PB-O2B

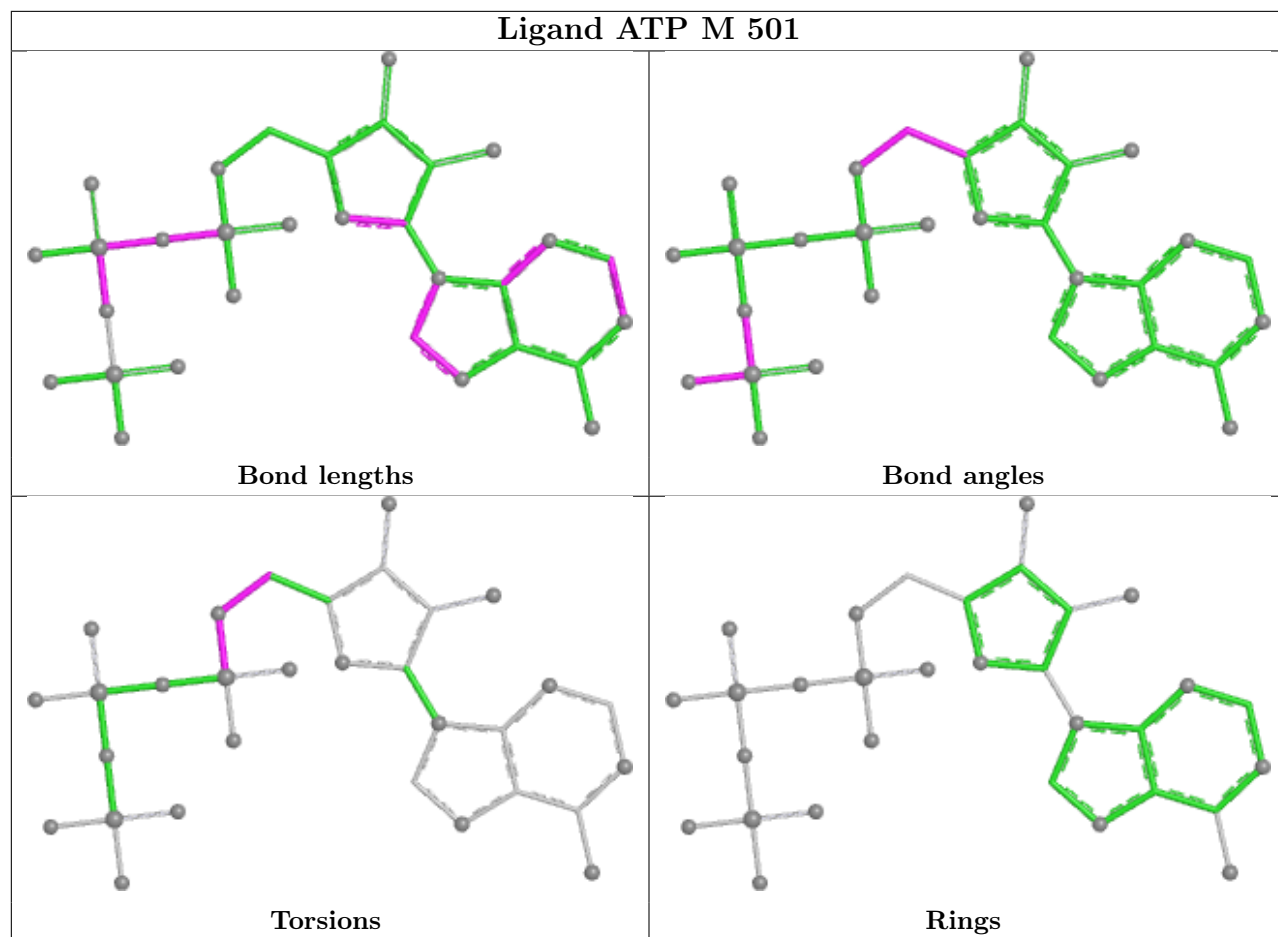
There are no ring outliers.

No monomer is involved in short contacts.

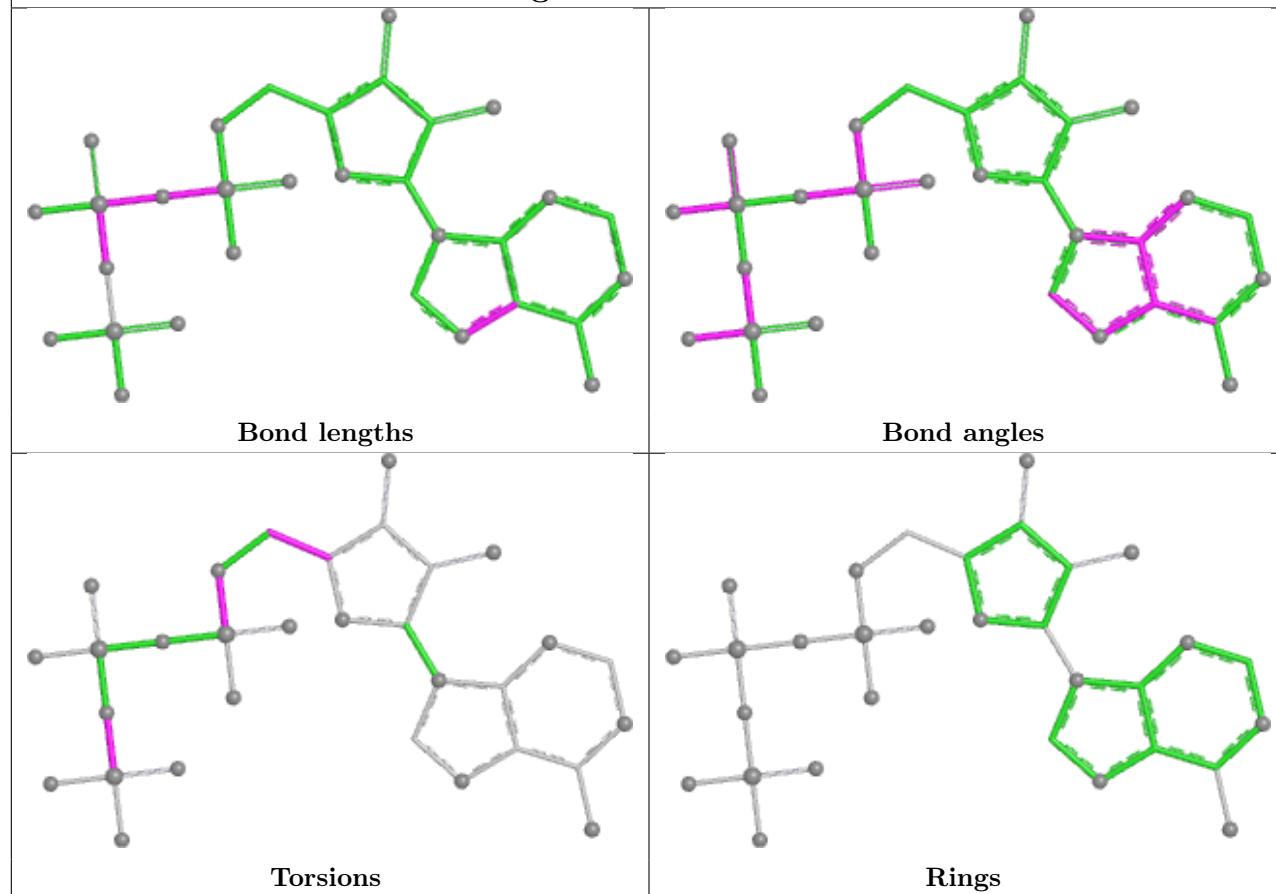
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



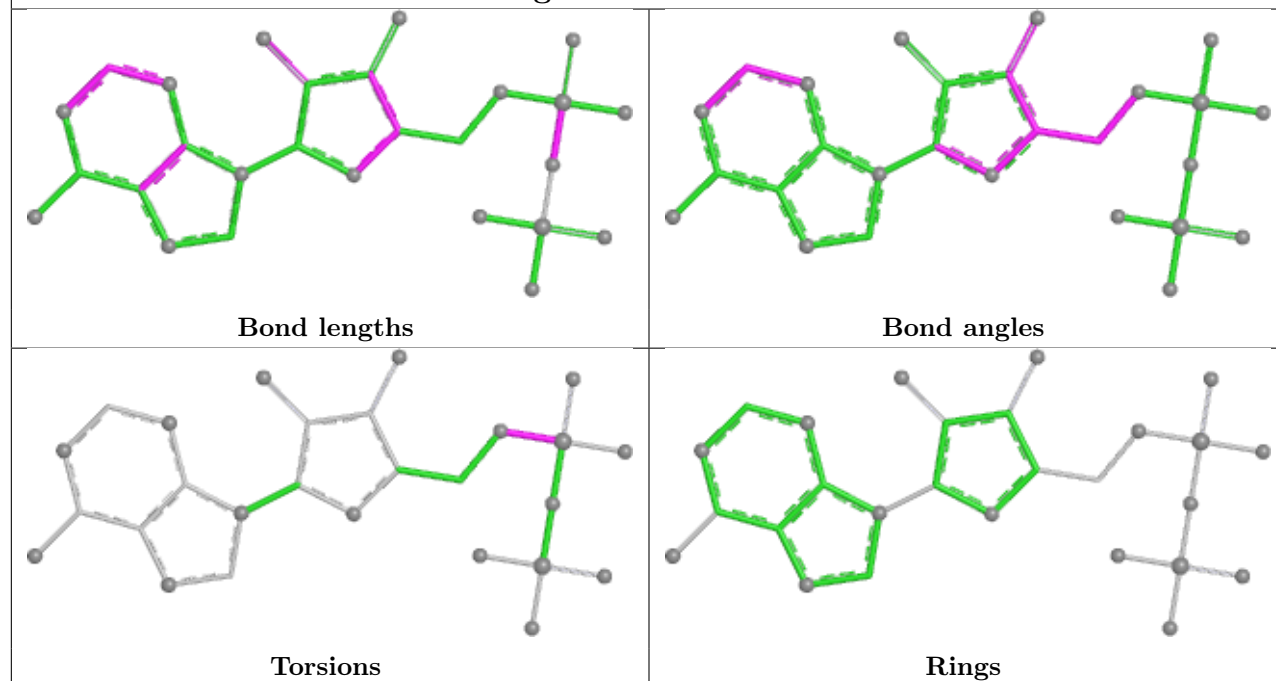


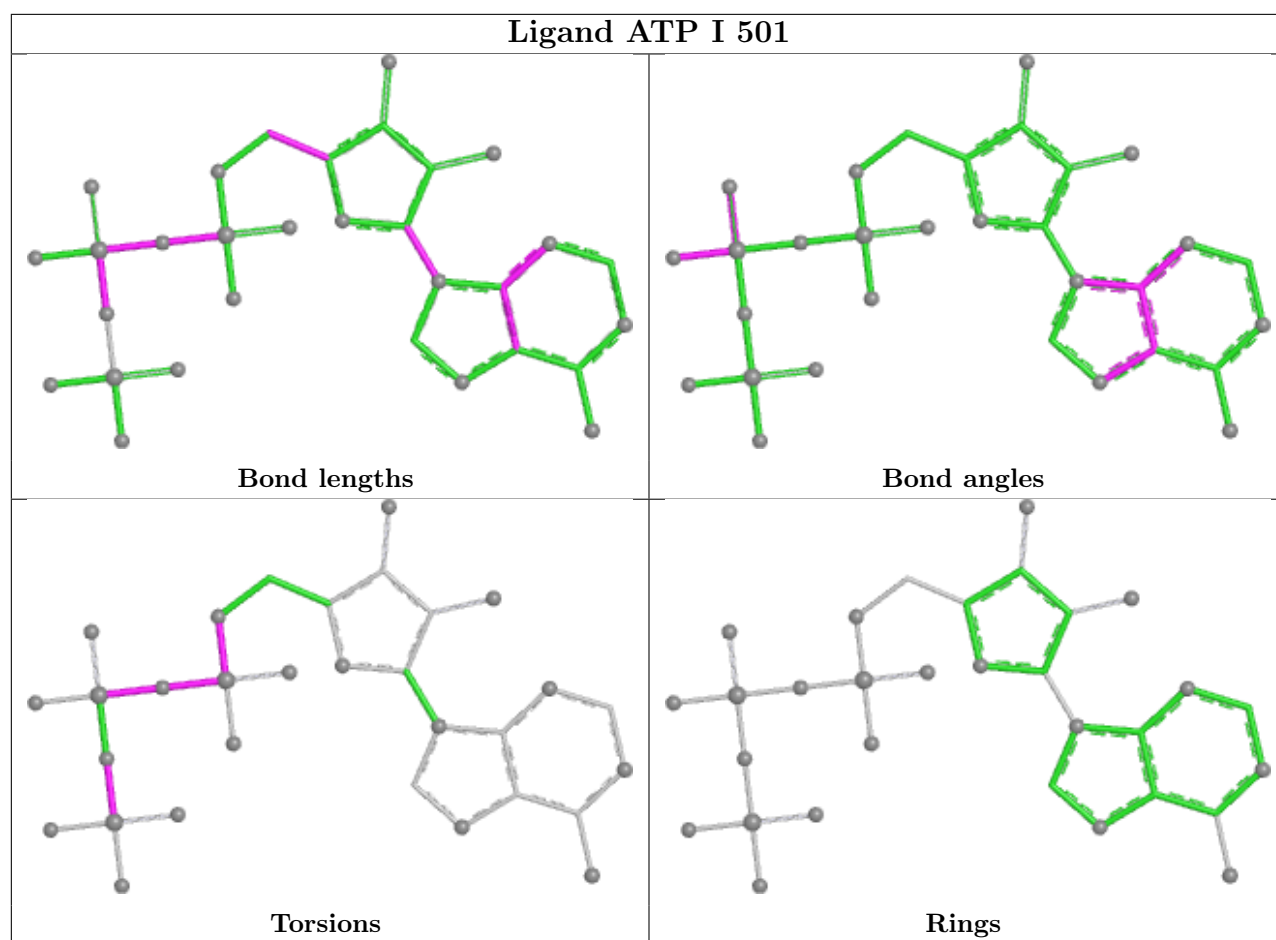


Ligand ATP H 501



Ligand ADP J 501





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

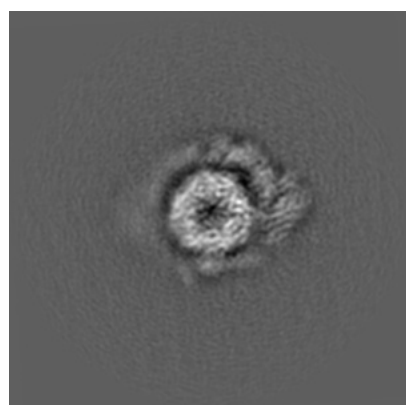
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14084. These allow visual inspection of the internal detail of the map and identification of artifacts.

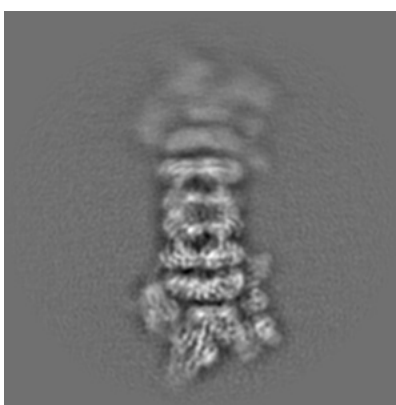
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

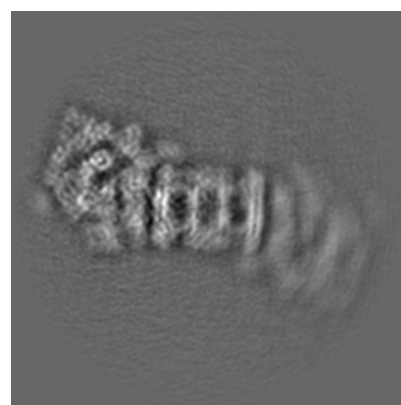
6.1.1 Primary map



X



Y

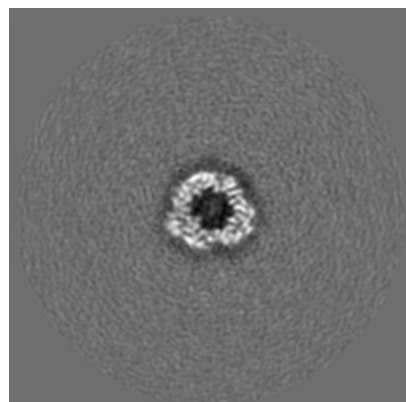


Z

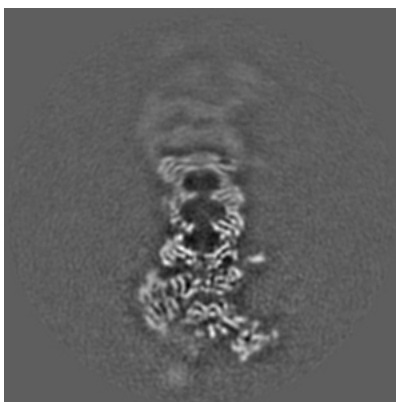
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

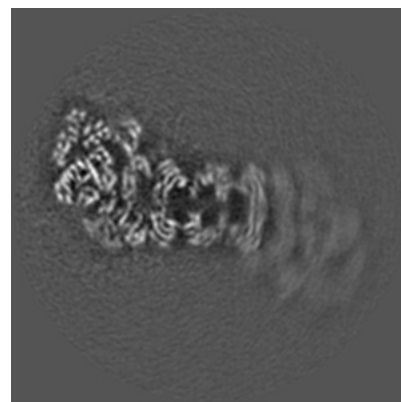
6.2.1 Primary map



X Index: 192



Y Index: 192

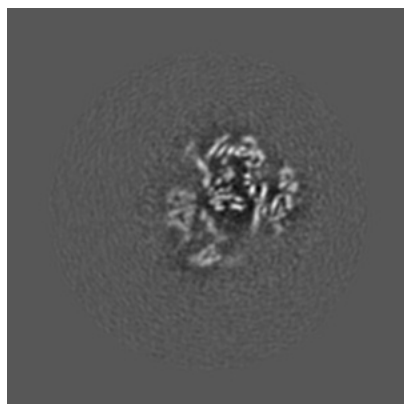


Z Index: 192

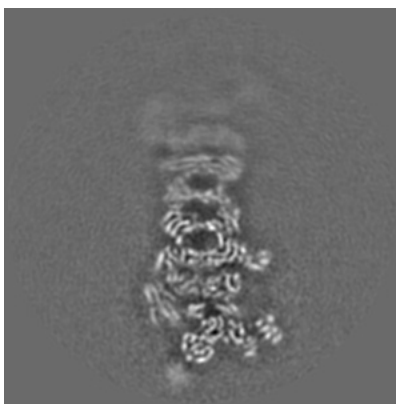
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

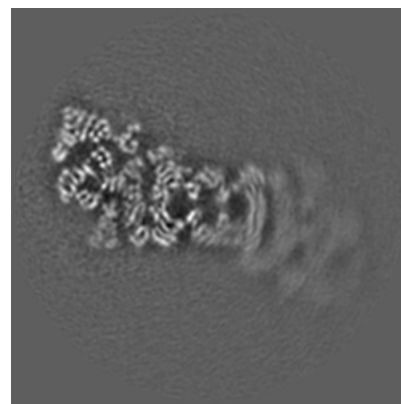
6.3.1 Primary map



X Index: 82



Y Index: 204

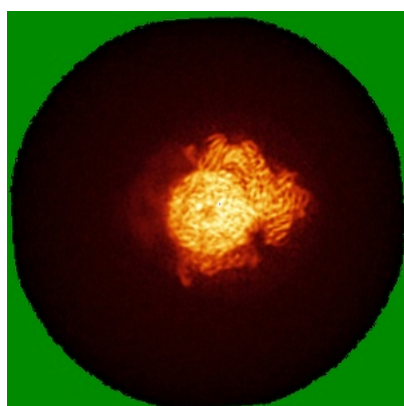


Z Index: 197

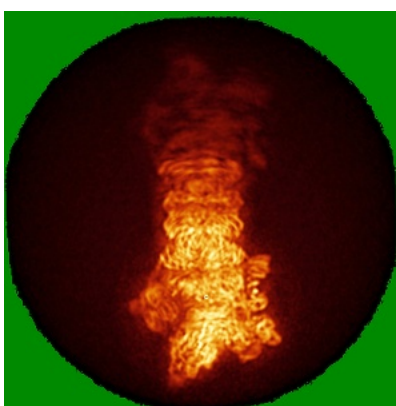
The images above show the largest variance slices of the map in three orthogonal directions.

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

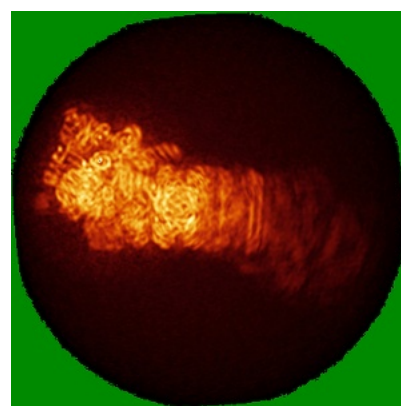
6.4.1 Primary map



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

This section was not generated.

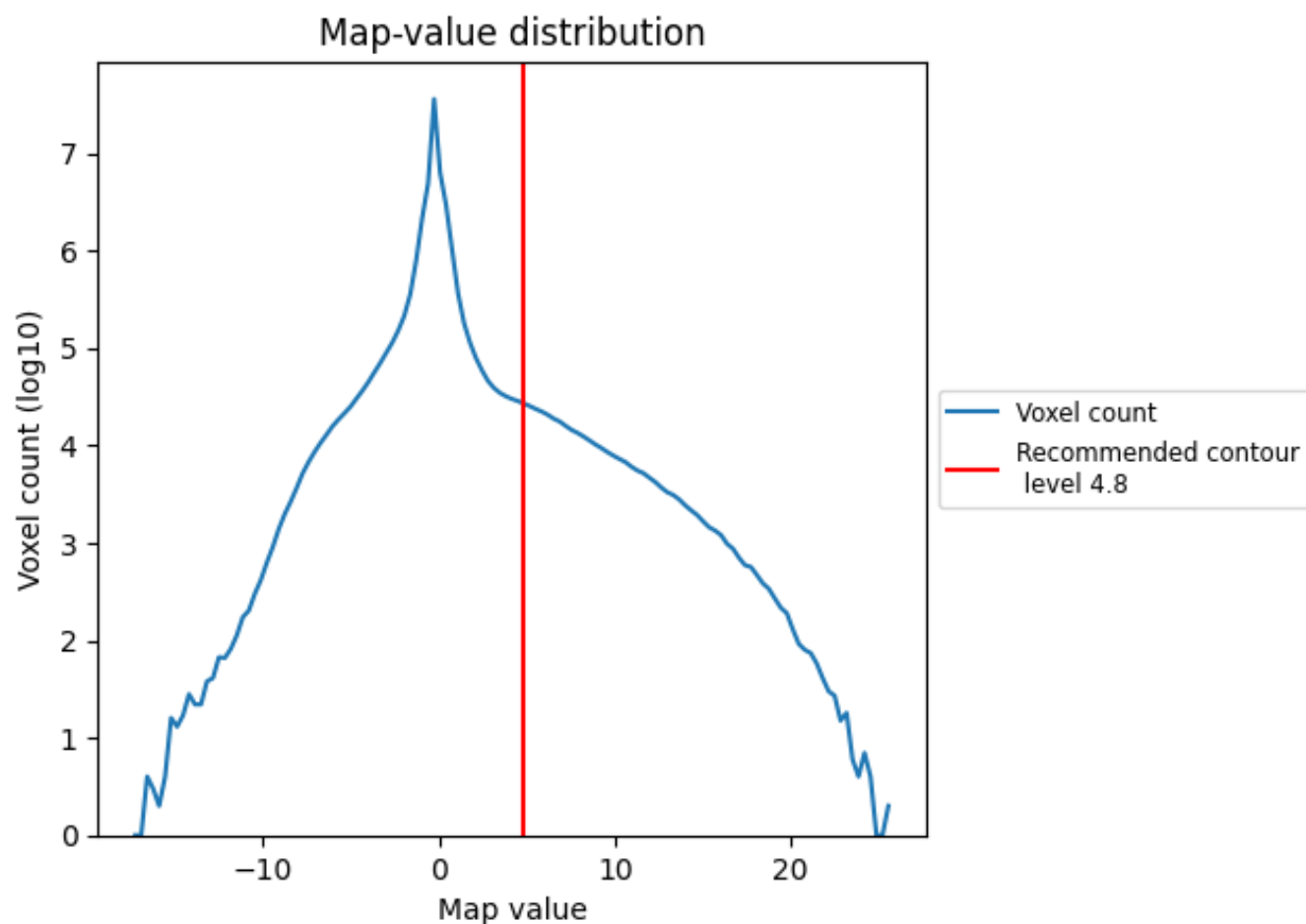
6.6 Mask visualisation

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

7 Map analysis [i](#)

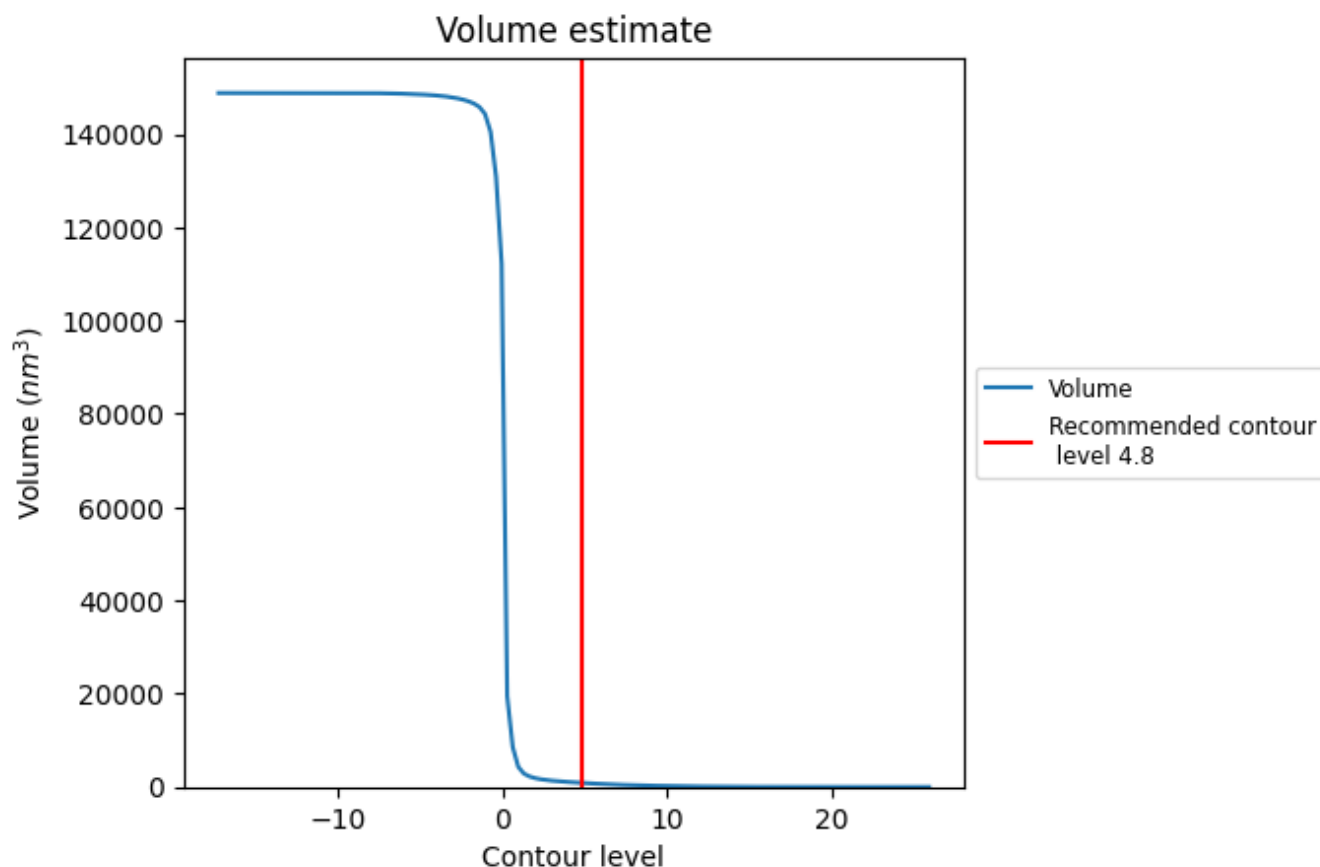
This section contains the results of statistical analysis of the map.

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.

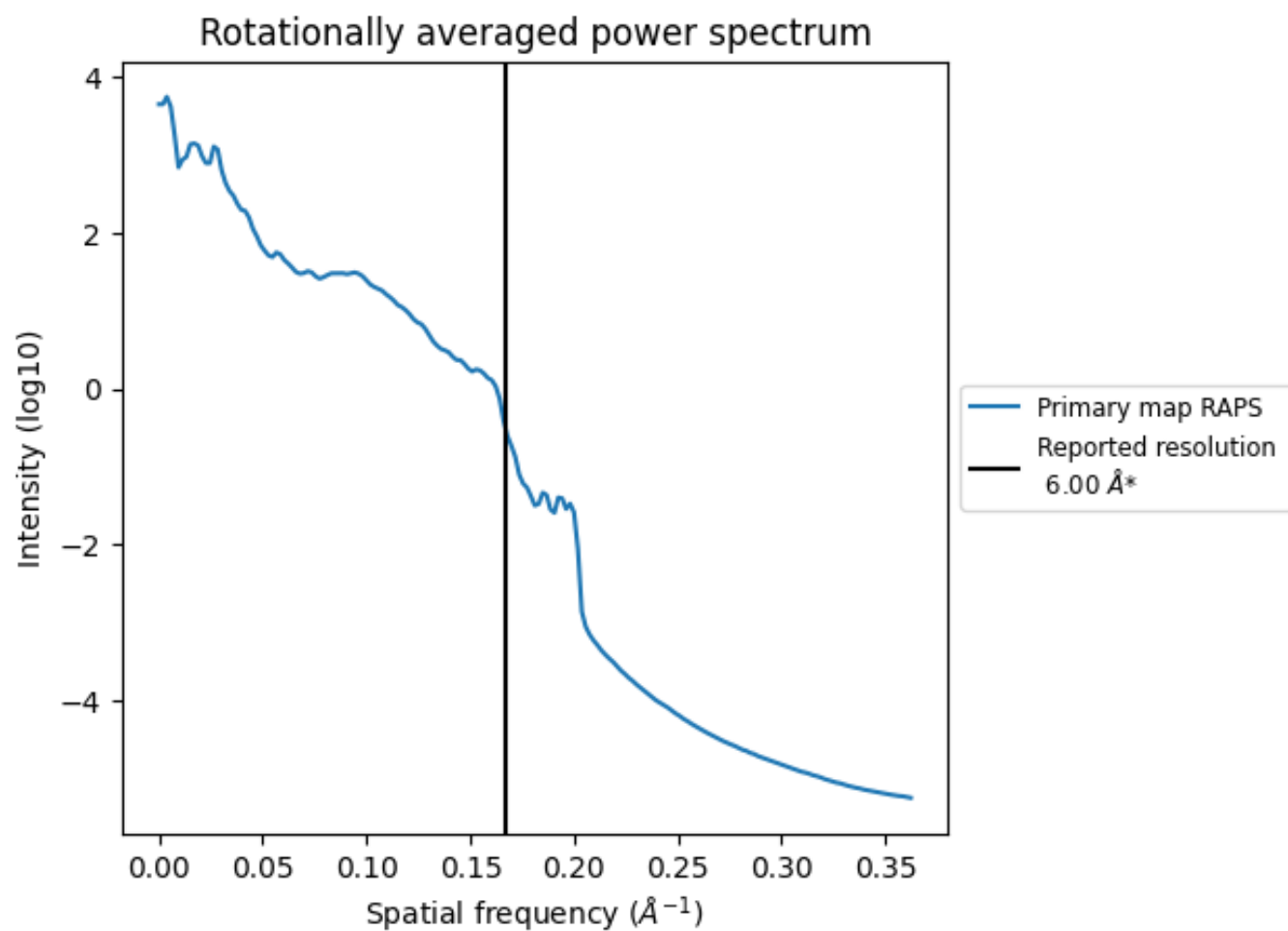
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 874 nm^3 ; this corresponds to an approximate mass of 789 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 0.167 Å⁻¹

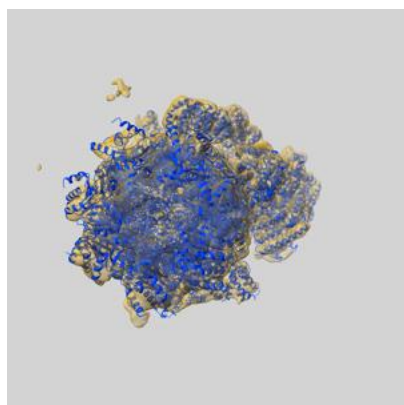
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

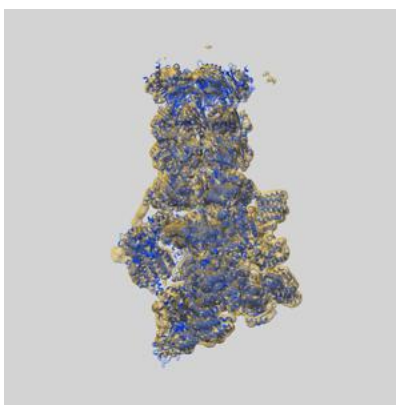
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14084 and PDB model 7QO5. Per-residue inclusion information can be found in section 3 on page 13.

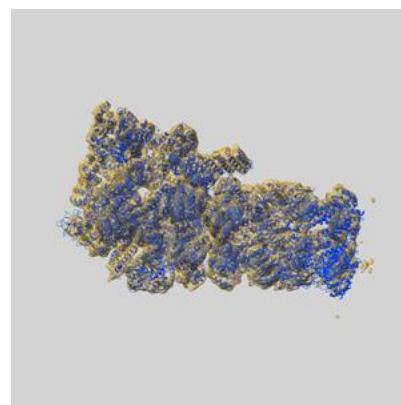
9.1 Map-model overlay [i](#)



X



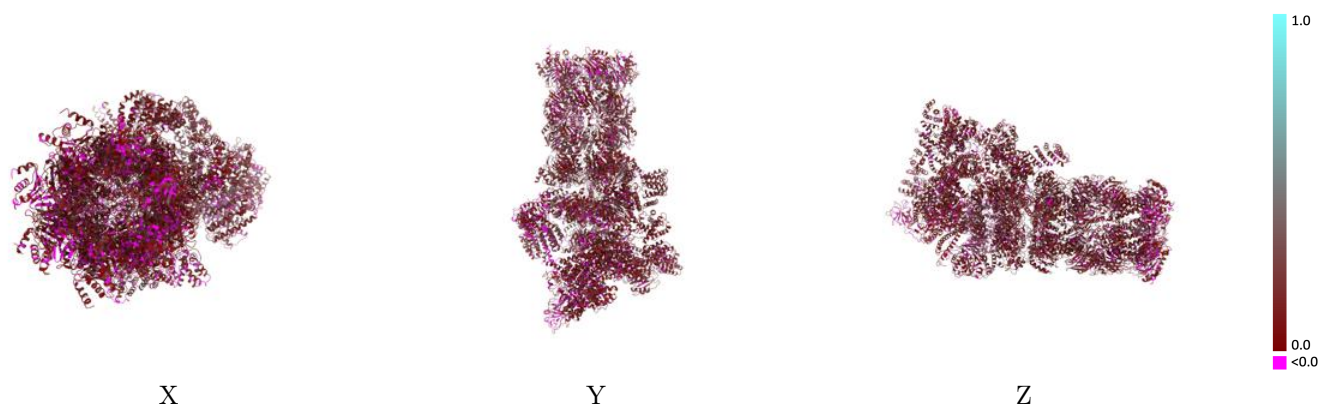
Y



Z

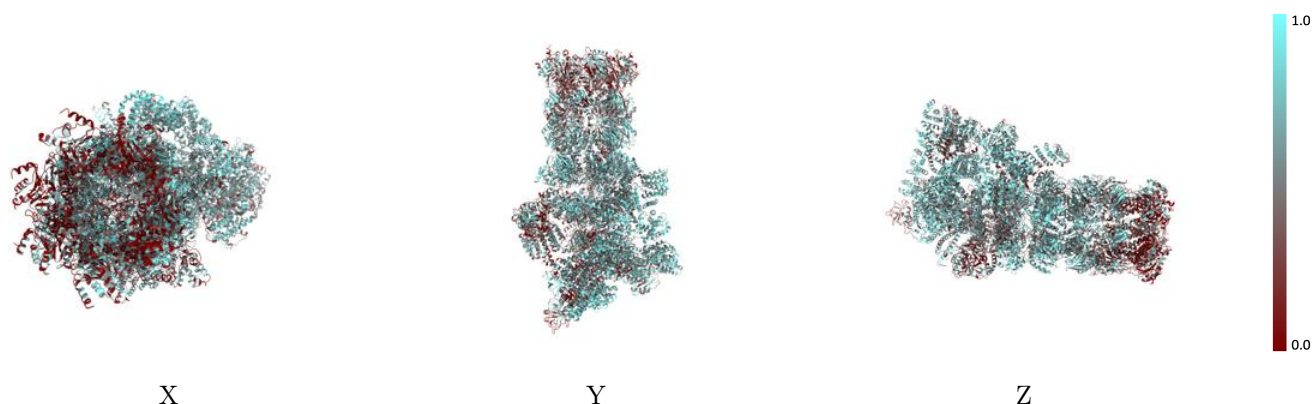
The images above show the 3D surface view of the map at the recommended contour level 4.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



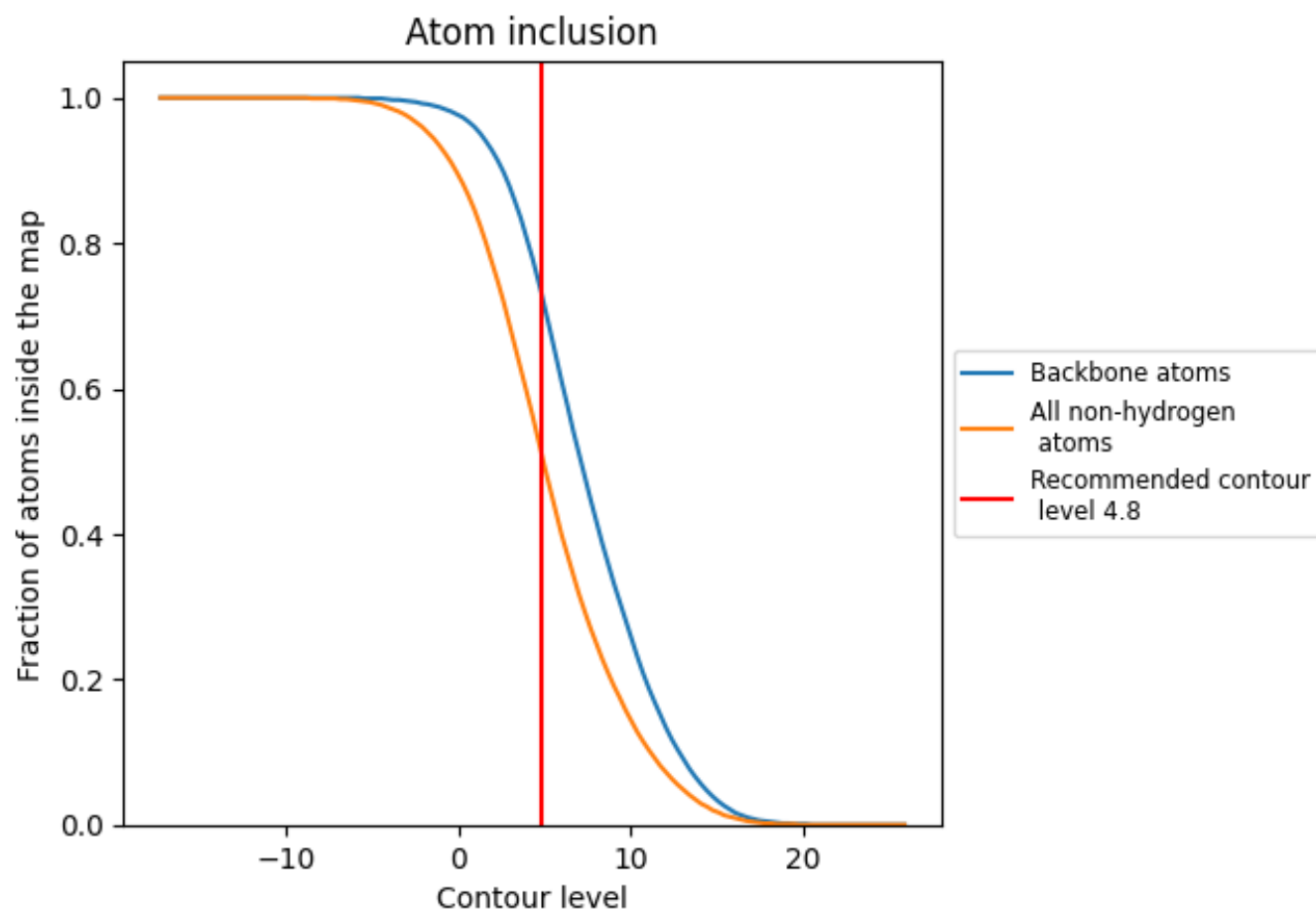
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4.8).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 52% 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 (4.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5150	 0.1330
1	 0.6410	 0.1550
2	 0.6090	 0.1530
3	 0.5650	 0.1330
4	 0.6210	 0.1550
5	 0.6130	 0.1530
6	 0.5860	 0.1500
7	 0.5990	 0.1490
8	 0.3040	 0.1120
9	 0.3020	 0.1250
A	 0.6290	 0.1590
B	 0.5580	 0.1500
C	 0.6000	 0.1460
D	 0.6320	 0.1530
E	 0.6200	 0.1490
F	 0.6450	 0.1570
G	 0.6290	 0.1600
H	 0.5030	 0.1450
I	 0.4680	 0.1390
J	 0.5020	 0.1300
K	 0.4930	 0.1430
L	 0.5570	 0.1430
M	 0.5360	 0.1370
N	 0.6430	 0.1440
O	 0.6650	 0.1500
P	 0.7180	 0.1500
Q	 0.6420	 0.1430
R	 0.6200	 0.1310
S	 0.5580	 0.1340
T	 0.5420	 0.1320
U	 0.5840	 0.1430
V	 0.5940	 0.1540
W	 0.6180	 0.1360
X	 0.1950	 0.0320
Y	 0.3330	 0.0640



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Chain	Atom inclusion	Q-score
Z	 0.3950	 0.0860
a	 0.2820	 0.1120
b	 0.1850	 0.0940
c	 0.3020	 0.1030
d	 0.3610	 0.1140
e	 0.2930	 0.1050
f	 0.3810	 0.1130
g	 0.2860	 0.1080
h	 0.4920	 0.1430
i	 0.3480	 0.1300
j	 0.3780	 0.1250
k	 0.5120	 0.1370
l	 0.4380	 0.1230
m	 0.4310	 0.1250
n	 0.4890	 0.1440