



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 06:21 AM UTC

PDB ID : 5MPA / pdb_00005mpa
EMDB ID : EMD-3535
Title : 26S proteasome in presence of ATP (s2)
Authors : Wehmer, M.; Rudack, T.; Beck, F.; Aufderheide, A.; Pfeifer, G.; Plitzko, J.M.;
Foerster, F.; Schulten, K.; Baumeister, W.; Sakata, E.
Deposited on : 2016-12-16
Resolution : 4.50 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:

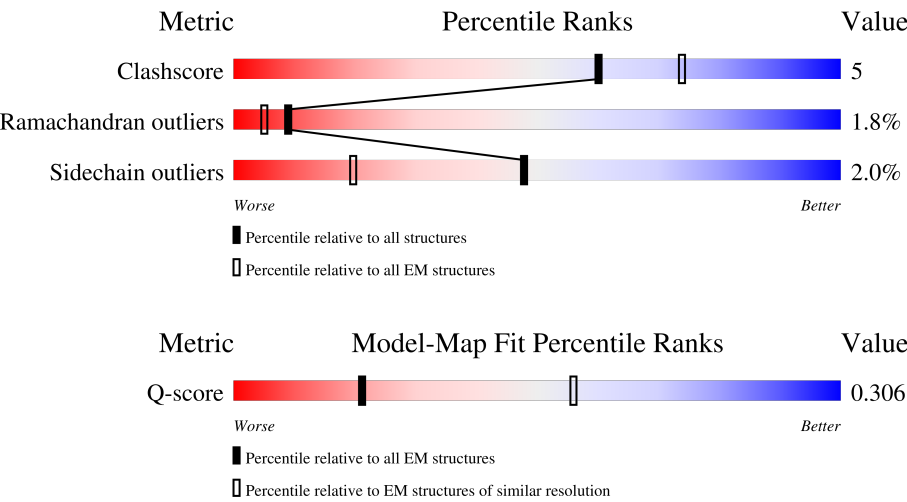
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 4.50 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.



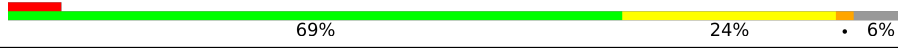
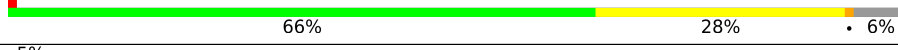
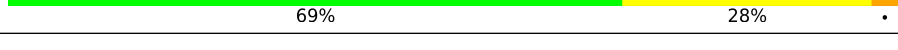
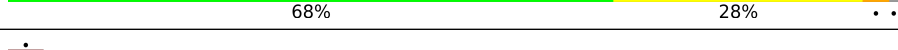
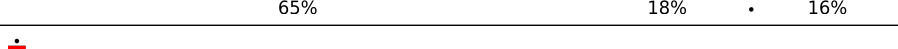
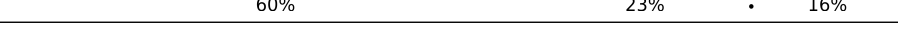
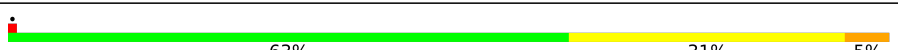
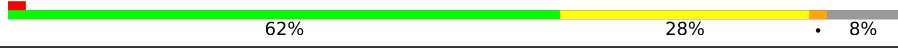
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2937 (4.00 - 5.00)

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	5% 73% 23% .
1	a	252	. 70% 23% . .
2	B	250	. 76% 21% .
2	b	250	. 65% 32% .

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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	H	467	

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Mol	Chain	Length	Quality of chain
16	I	437	
17	K	428	
18	L	437	
19	M	434	
20	J	405	

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 67883 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	250	Total	C	N	O	S	0	0
			1915	1219	315	377	4		
2	B	250	Total	C	N	O	S	0	0
			1915	1219	315	377	4		

- 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	240	Total	C	N	O	S	0	0
			1881	1176	329	372	4		
4	D	240	Total	C	N	O	S	0	0
			1881	1176	329	372	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	242	Total	C	N	O	S	0	0
			1861	1162	314	378	7		
5	E	242	Total	C	N	O	S	0	0
			1861	1162	314	378	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	233	Total	C	N	O	S	0	0
			1795	1129	312	350	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	243	Total	C	N	O	S	0	0
			1892	1203	329	356	4		
7	G	243	Total	C	N	O	S	0	0
			1892	1203	329	356	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	232	Total	C	N	O	S	0	0
			1815	1148	311	349	7		
14	7	229	Total	C	N	O	S	0	0
			1790	1133	306	344	7		

- Molecule 15 is a protein called 26S protease regulatory subunit 7 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	H	390	Total	C	N	O	S	0	0
			3053	1920	546	570	17		

- Molecule 16 is a protein called 26S protease regulatory subunit 4 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	385	Total	C	N	O	S	0	0
			3022	1899	508	598	17		

- Molecule 17 is a protein called 26S protease regulatory subunit 6B homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	K	389	Total	C	N	O	S	0	0
			3078	1933	540	595	10		

- Molecule 18 is a protein called 26S protease subunit RPT4.

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

- Molecule 19 is a protein called 26S protease regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	M	381	Total	C	N	O	S	0	0
			2986	1870	524	580	12		

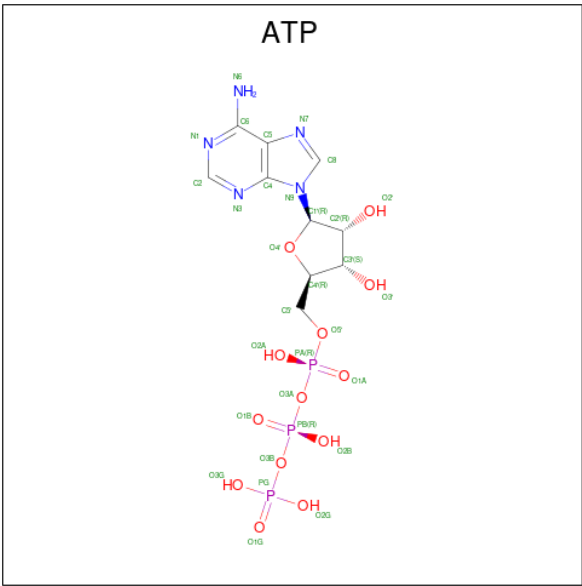
- Molecule 20 is a protein called 26S protease regulatory subunit 8 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	J	386	Total	C	N	O	S	0	0
			3033	1906	543	567	17		

- Molecule 21 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 22 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

- Molecule 23 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

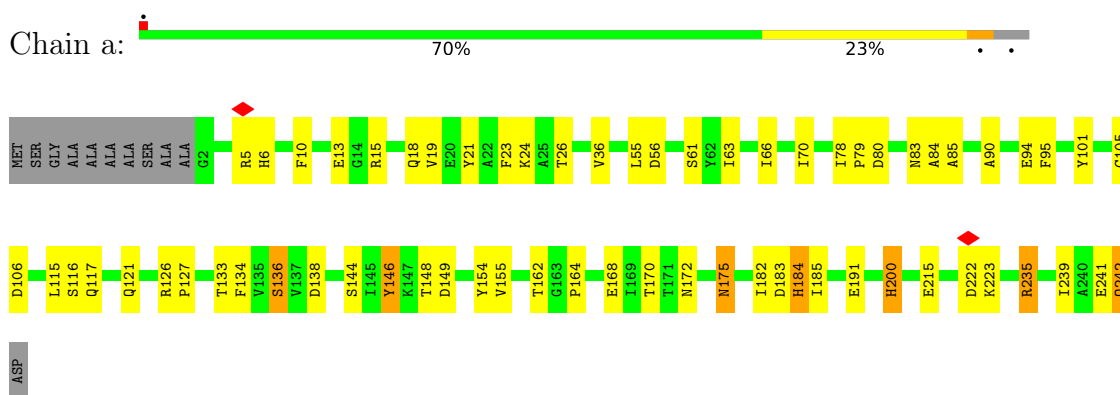


Mol	Chain	Residues	Atoms					AltConf
23	J	1	Total	C	N	O	P	0
			27	10	5	10	2	

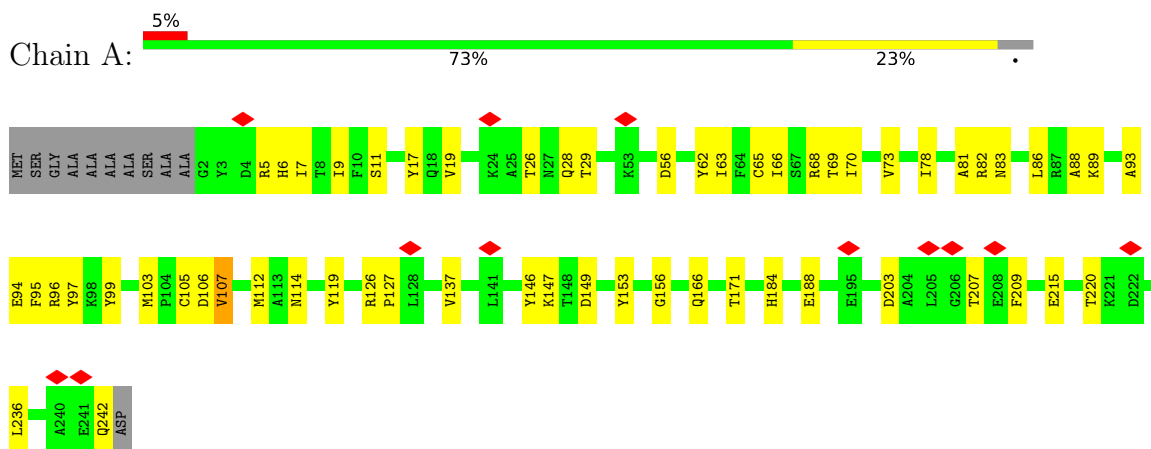
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

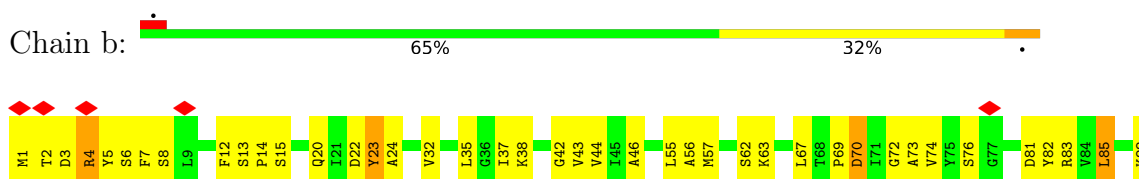
- Molecule 1: Proteasome subunit alpha type-1

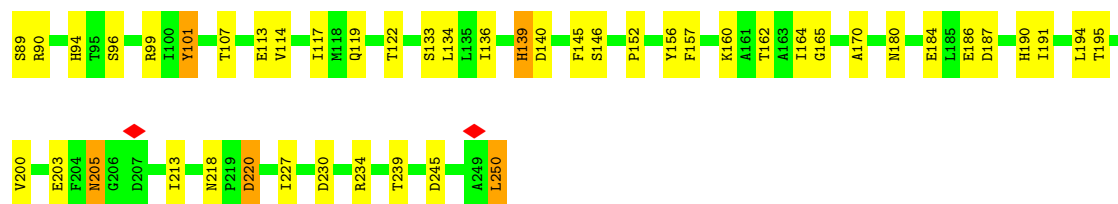


- Molecule 1: Proteasome subunit alpha type-1

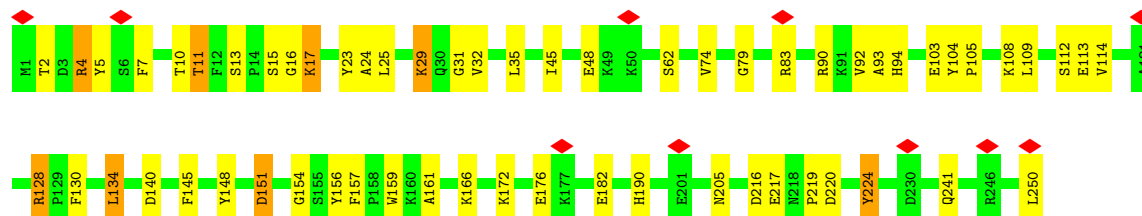
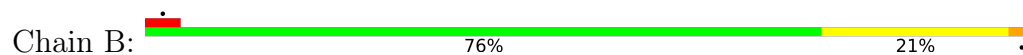


- Molecule 2: Proteasome subunit alpha type-2

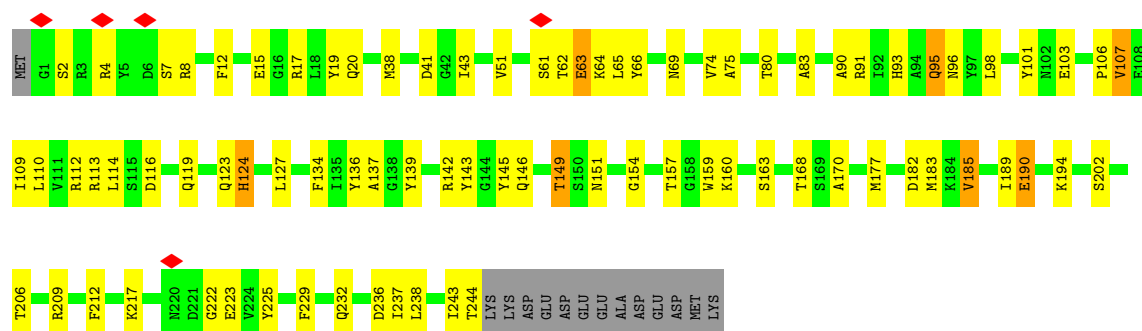




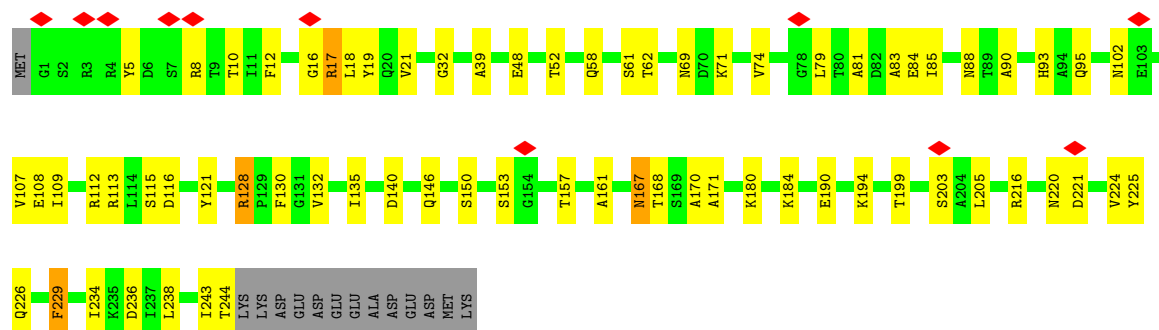
• Molecule 2: Proteasome subunit alpha type-2



• Molecule 3: Proteasome subunit alpha type-3



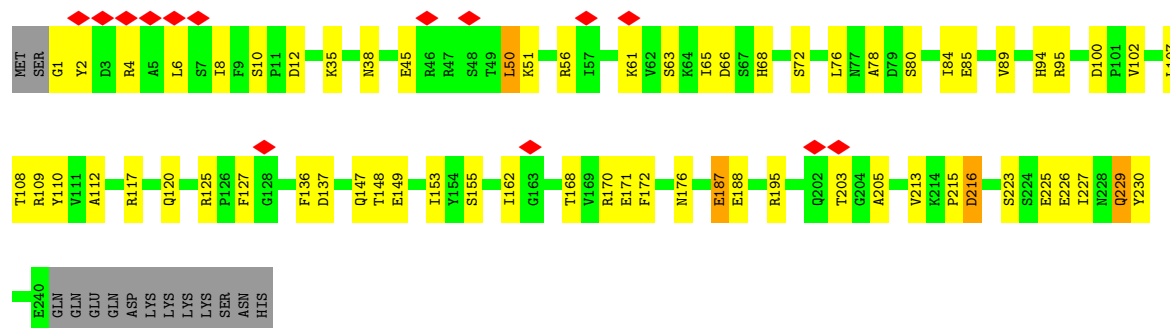
• Molecule 3: Proteasome subunit alpha type-3



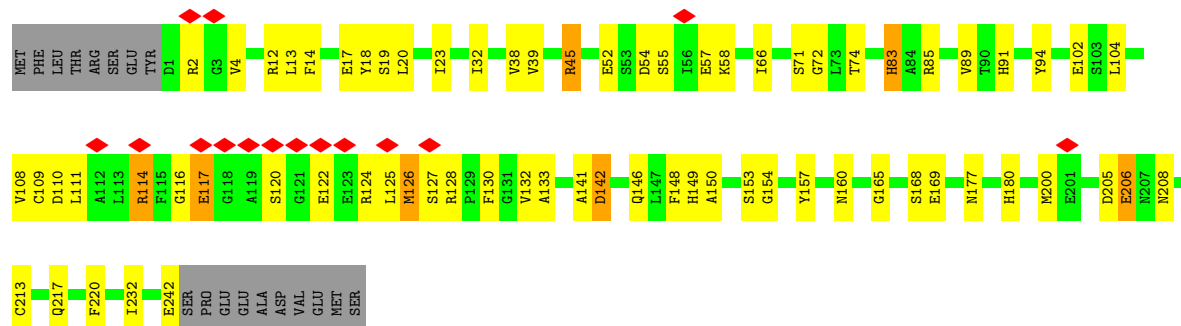
• Molecule 4: Proteasome subunit alpha type-4



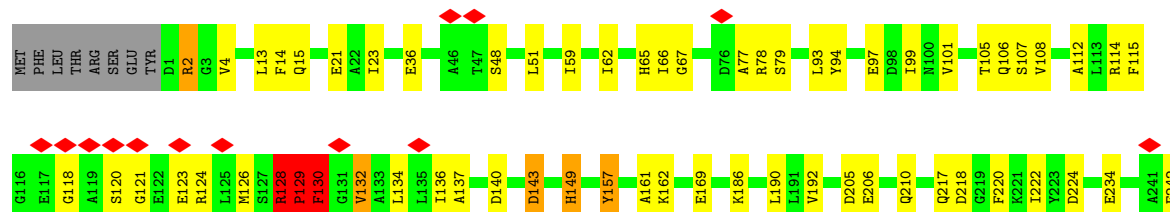
- Molecule 4: Proteasome subunit alpha type-4



- Molecule 5: Proteasome subunit alpha type-5



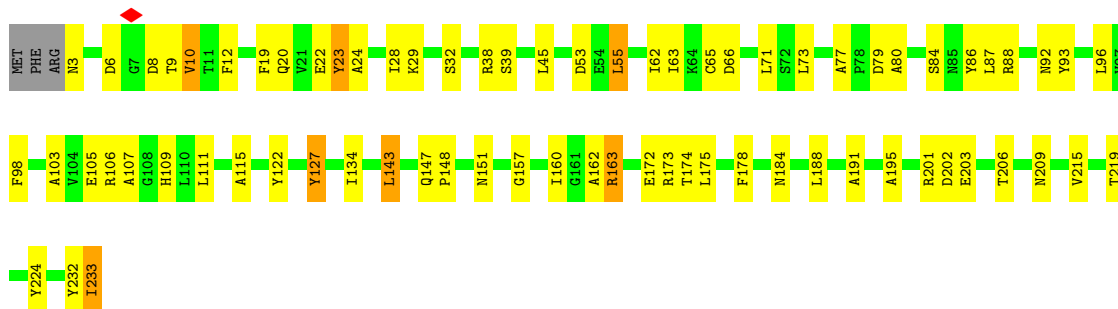
- Molecule 5: Proteasome subunit alpha type-5



SER
PRO
PHE
GLU
GLU
ALA
ASP
VAL
GLU
MET
SER

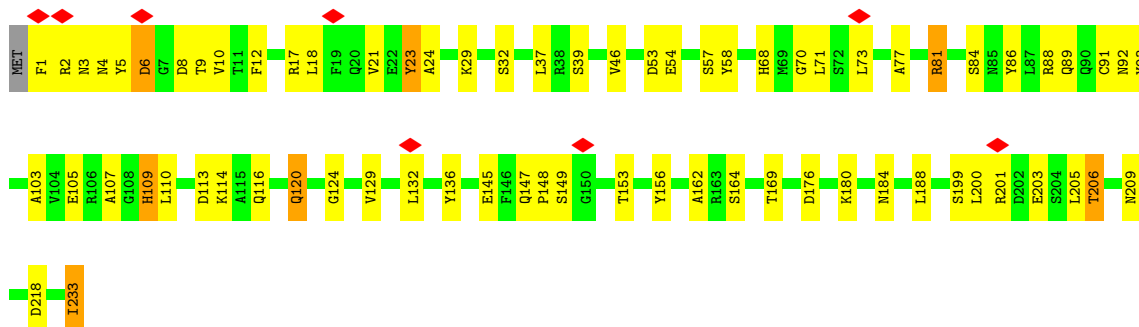
• Molecule 6: Proteasome subunit alpha type-6

Chain f:  68% 28% . .



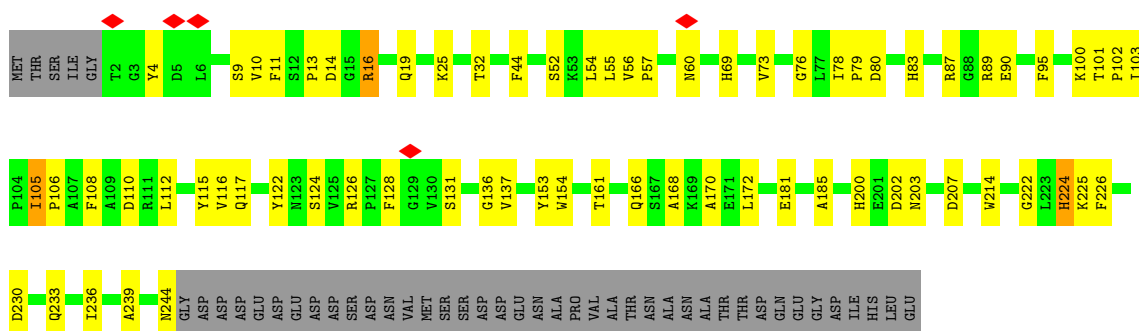
• Molecule 6: Proteasome subunit alpha type-6

Chain F:  69% 28% .



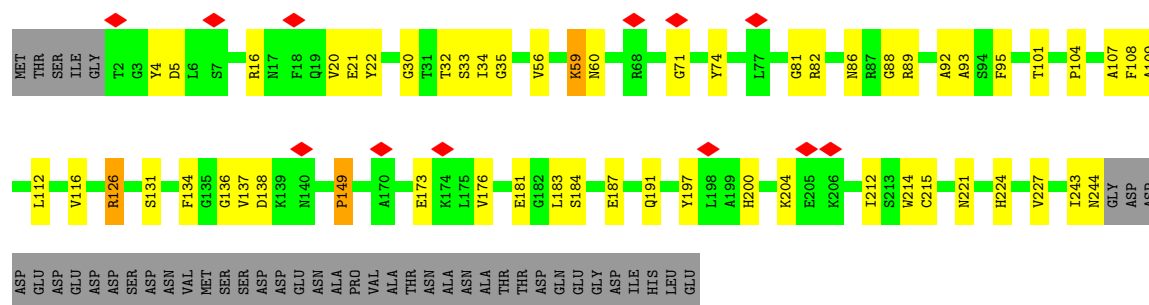
• Molecule 7: Probable proteasome subunit alpha type-7

Chain g:  60% 23% 16%



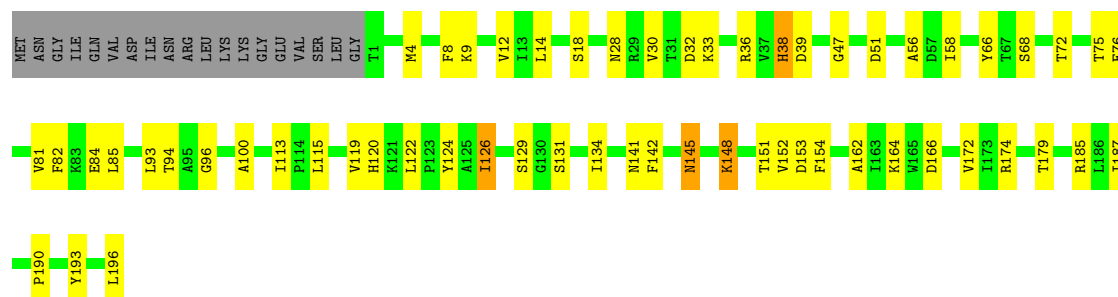
• Molecule 7: Probable proteasome subunit alpha type-7

Chain G:  65% 18% 16%



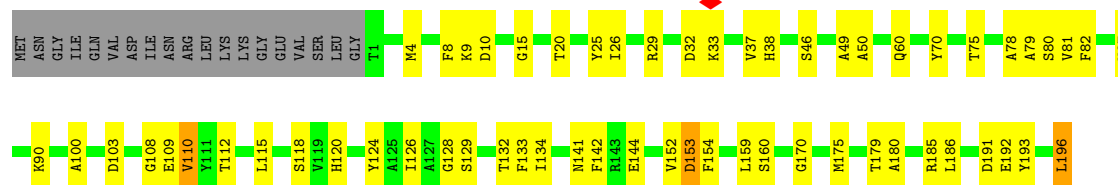
- Molecule 8: Proteasome subunit beta type-1

Chain h: 64% 26% 9%



- Molecule 8: Proteasome subunit beta type-1

Chain 1: 63% 27% 9%



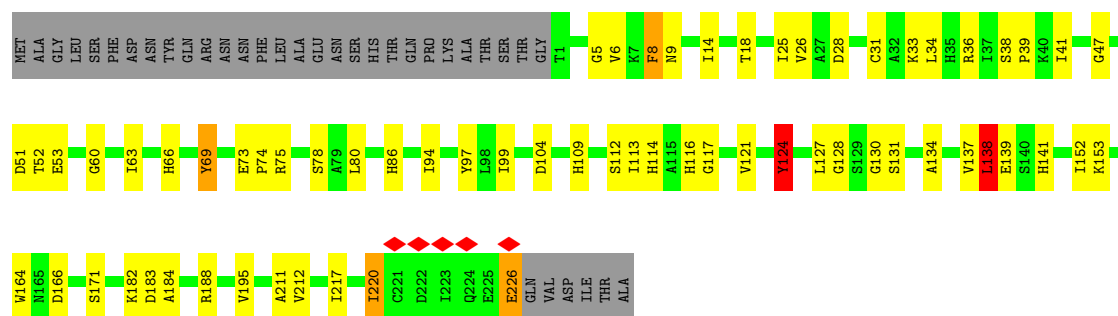
- Molecule 9: Proteasome subunit beta type-2

Chain i: 56% 28% 13%



- Molecule 9: Proteasome subunit beta type-2

Chain 2: 



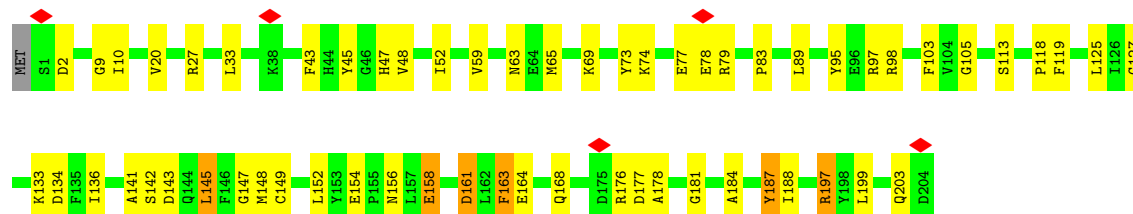
- Molecule 10: Proteasome subunit beta type-3

Chain j: 



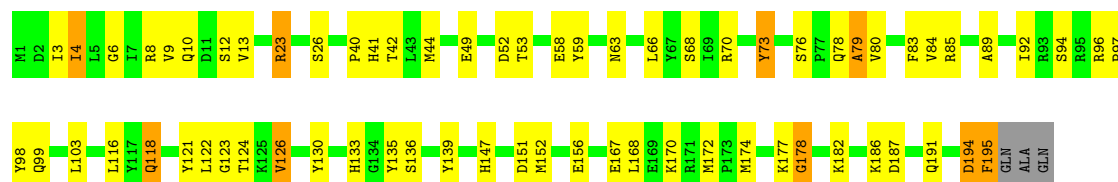
- Molecule 10: Proteasome subunit beta type-3

Chain 3: 

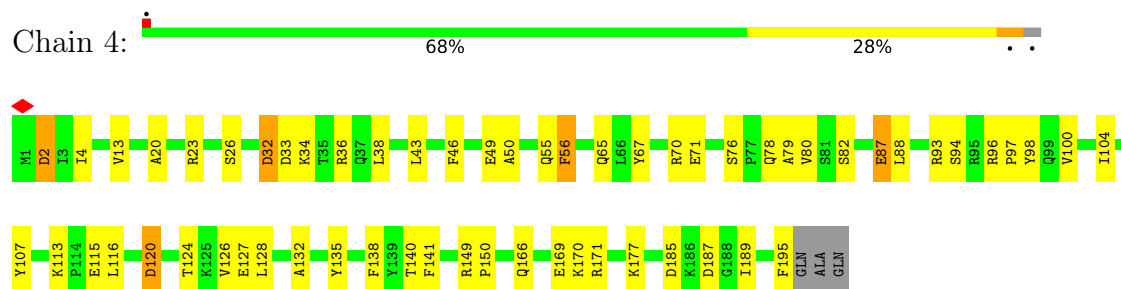


- Molecule 11: Proteasome subunit beta type-4

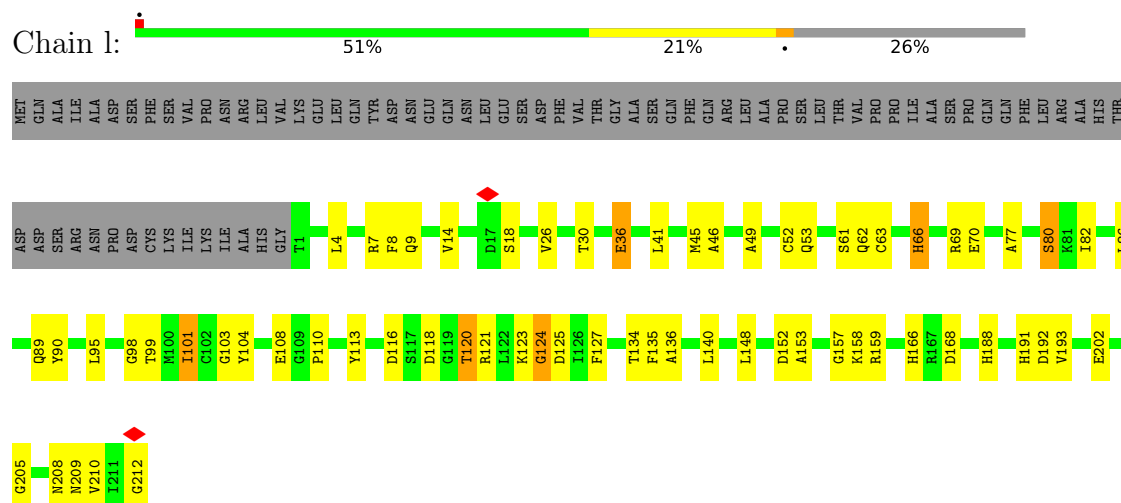
Chain k: 



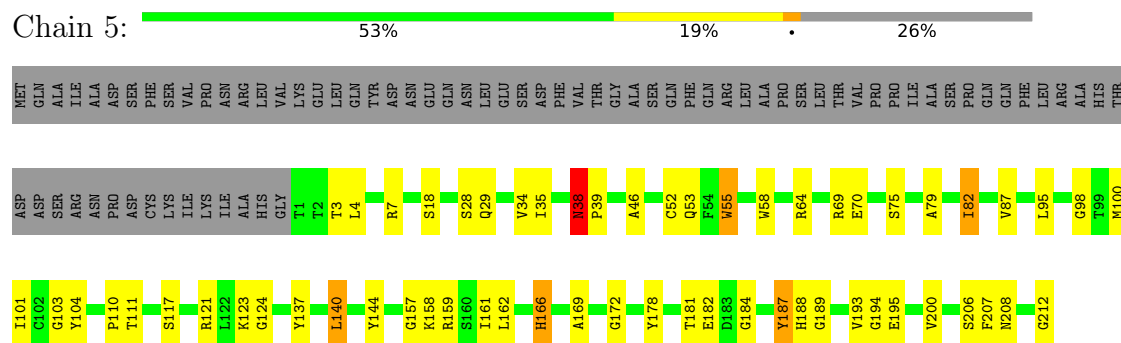
- Molecule 11: Proteasome subunit beta type-4



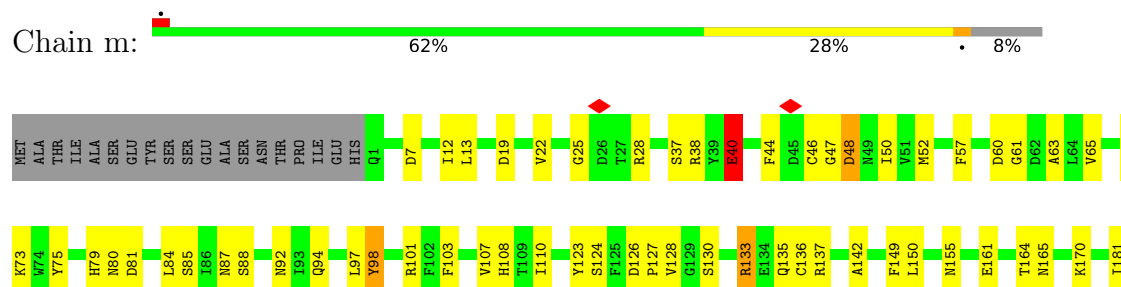
• Molecule 12: Proteasome subunit beta type-5

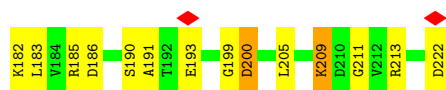


• Molecule 12: Proteasome subunit beta type-5



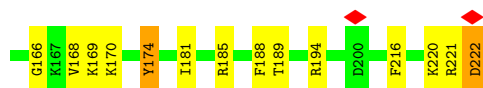
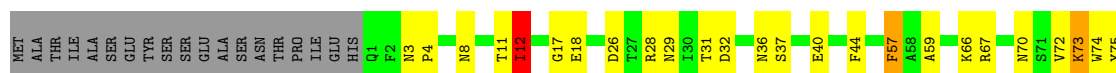
• Molecule 13: Proteasome subunit beta type-6





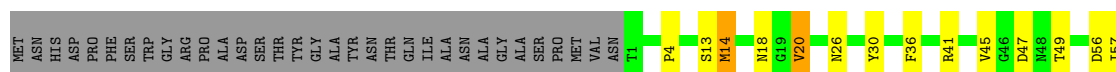
• Molecule 13: Proteasome subunit beta type-6

Chain 6: 59% 29% 8%



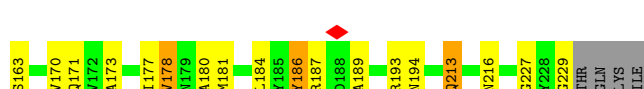
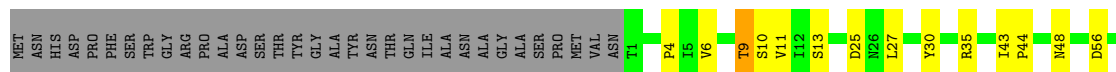
• Molecule 14: Proteasome subunit beta type-7

Chain n: 64% 20% 13%



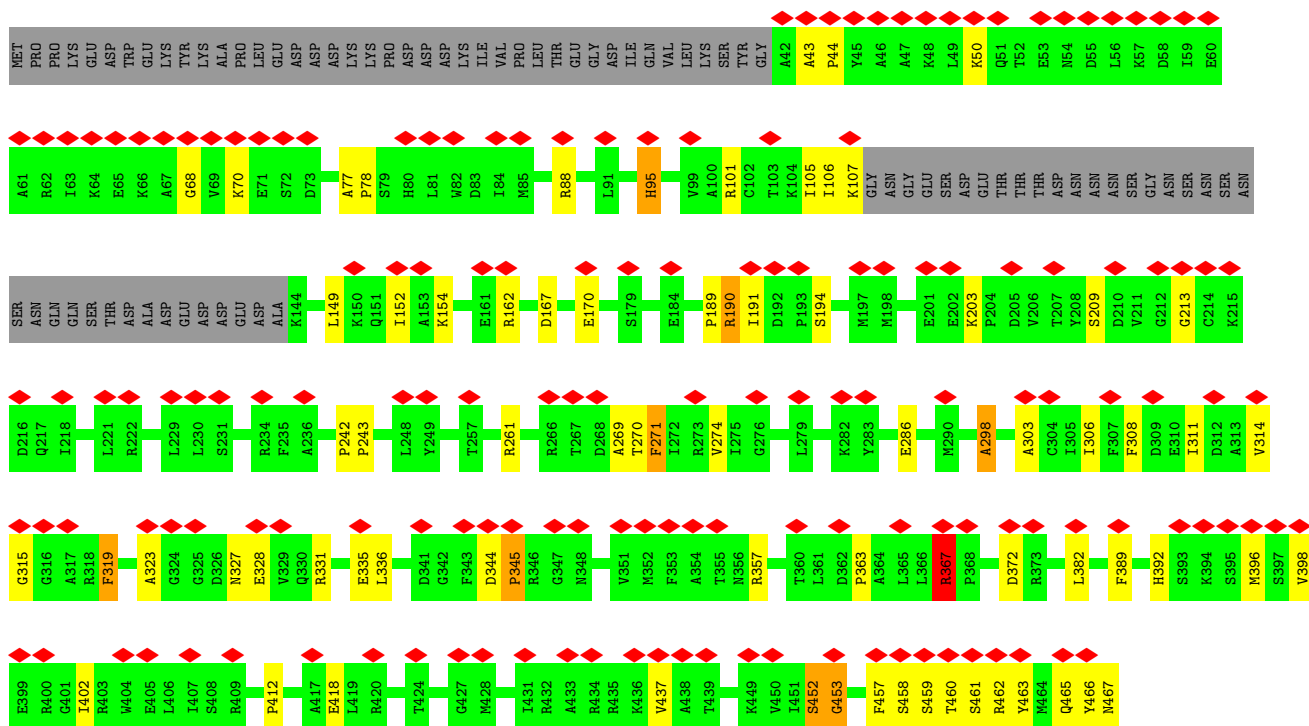
• Molecule 14: Proteasome subunit beta type-7

Chain 7: 61% 22% 14%

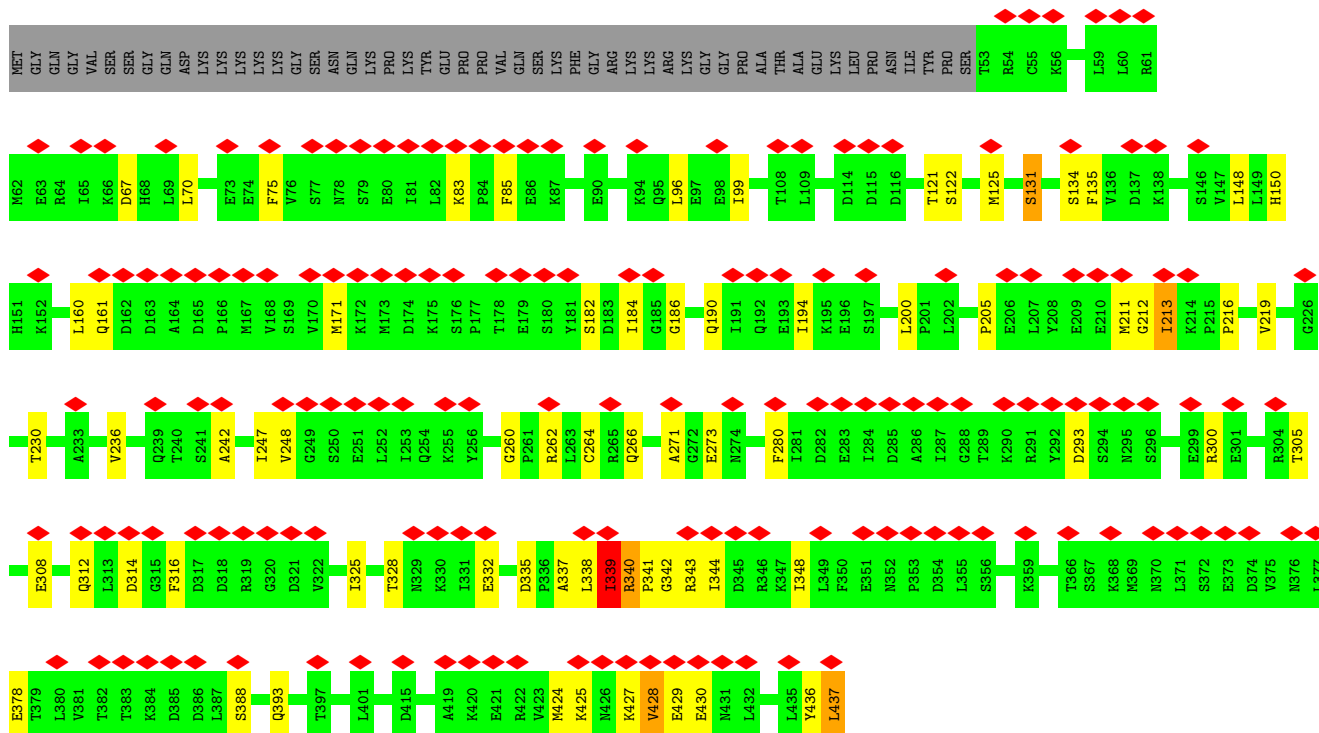


• Molecule 15: 26S protease regulatory subunit 7 homolog

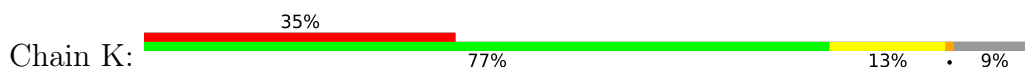
Chain H: 33% 67% 14% 16%

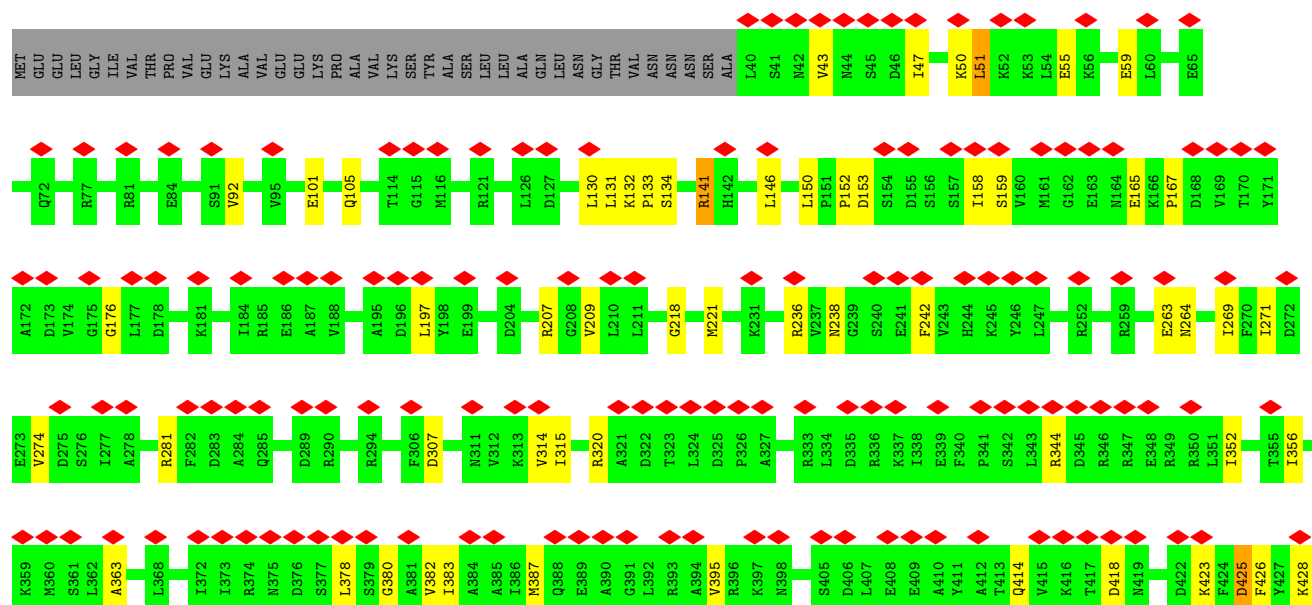


• Molecule 16: 26S protease regulatory subunit 4 homolog

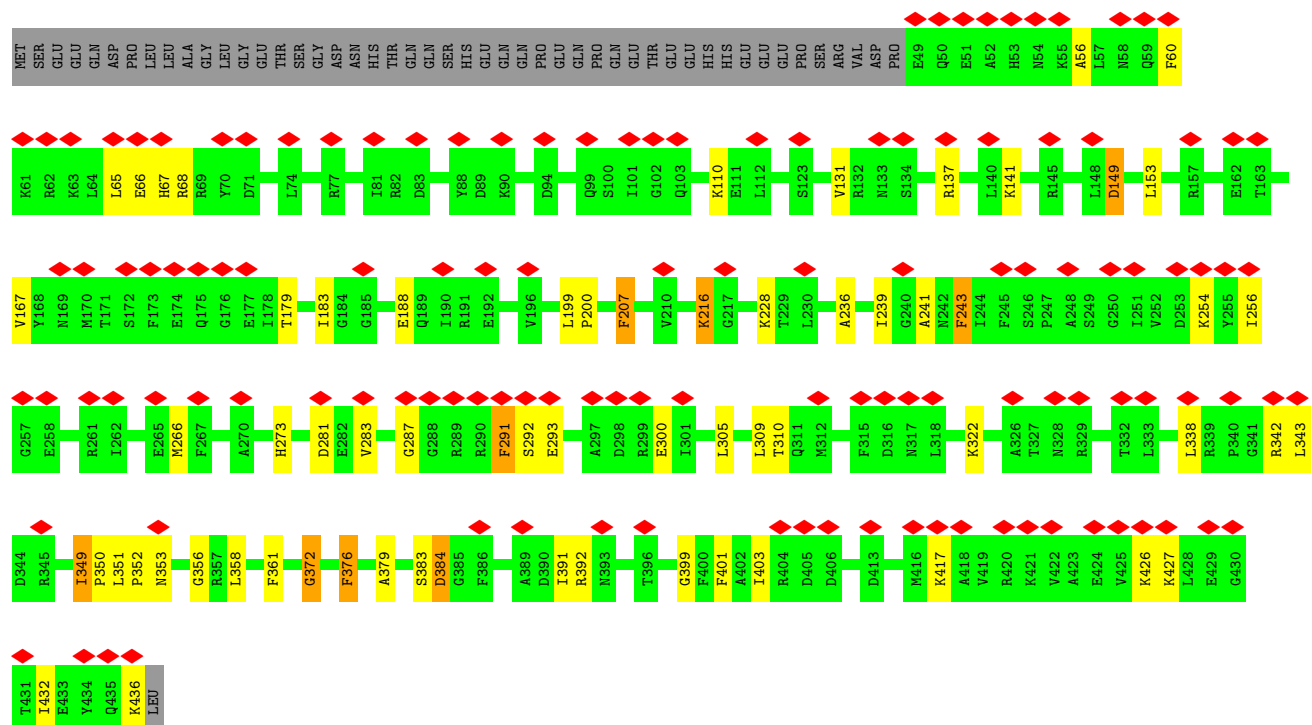
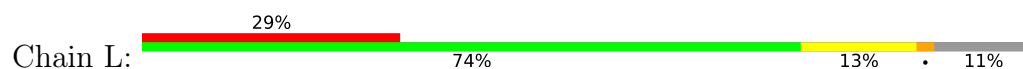


• Molecule 17: 26S protease regulatory subunit 6B homolog

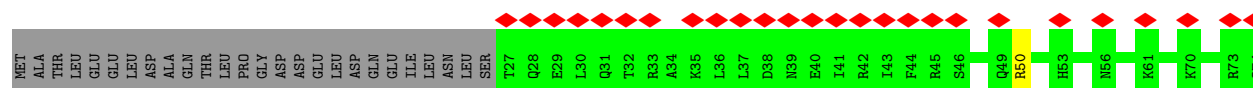


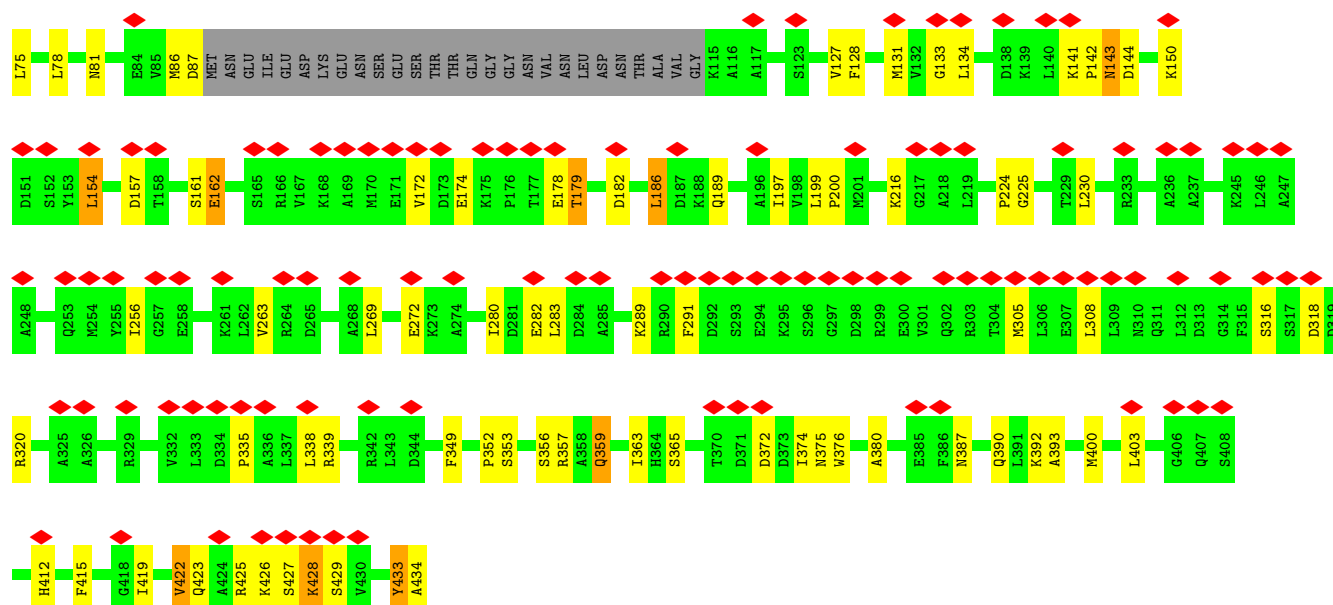


• Molecule 18: 26S protease subunit RPT4

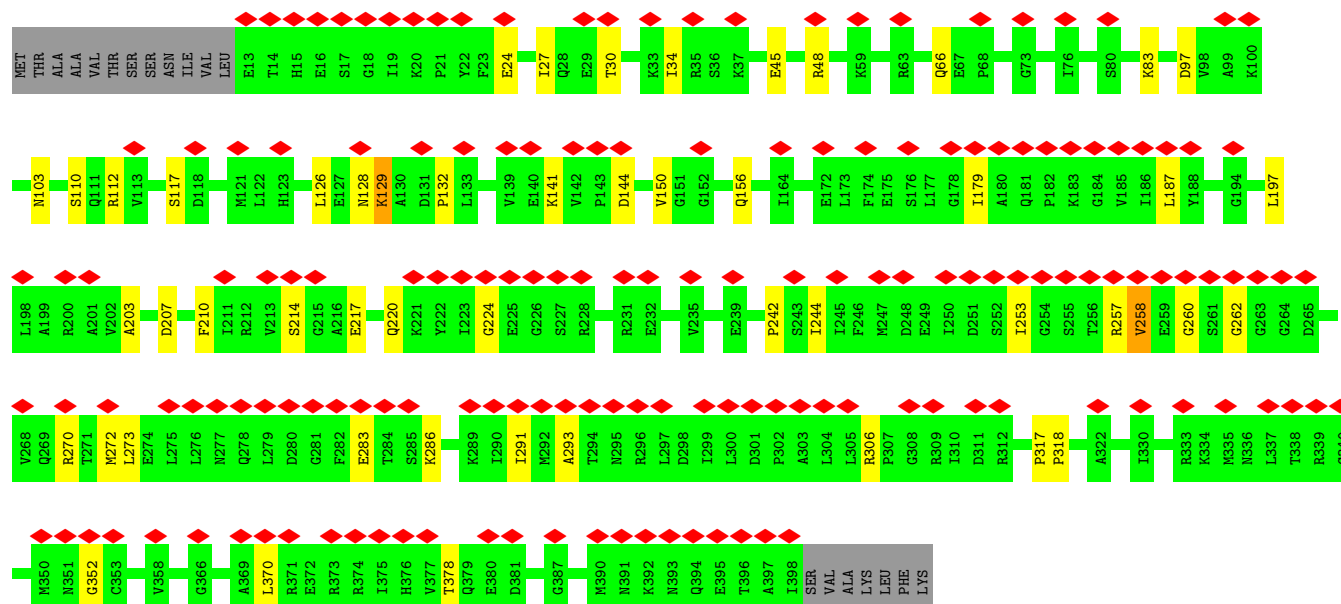
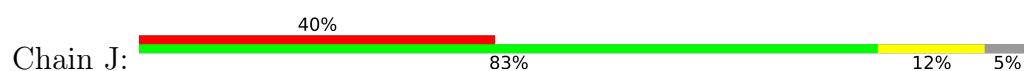


• Molecule 19: 26S protease regulatory subunit 6A





- Molecule 20: 26S protease regulatory subunit 8 homolog



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	193337	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 ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.131	Depositor
Minimum map value	-0.092	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.017	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: ATP, ADP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.67	25/1945 (1.3%)	1.82	39/2634 (1.5%)
1	a	1.67	22/1945 (1.1%)	1.79	41/2634 (1.6%)
2	B	1.69	26/1952 (1.3%)	1.75	41/2642 (1.6%)
2	b	1.73	30/1952 (1.5%)	1.80	55/2642 (2.1%)
3	C	1.73	29/1934 (1.5%)	1.82	45/2618 (1.7%)
3	c	1.68	20/1934 (1.0%)	1.77	45/2618 (1.7%)
4	D	1.67	21/1910 (1.1%)	1.75	38/2586 (1.5%)
4	d	1.71	32/1910 (1.7%)	1.75	39/2586 (1.5%)
5	E	1.79	25/1886 (1.3%)	1.92	54/2541 (2.1%)
5	e	1.78	35/1886 (1.9%)	1.89	53/2541 (2.1%)
6	F	1.75	28/1823 (1.5%)	1.76	41/2463 (1.7%)
6	f	1.73	24/1800 (1.3%)	1.81	43/2433 (1.8%)
7	G	1.65	20/1932 (1.0%)	1.78	39/2609 (1.5%)
7	g	1.75	23/1932 (1.2%)	1.78	46/2609 (1.8%)
8	1	1.81	21/1541 (1.4%)	1.81	35/2087 (1.7%)
8	h	1.83	31/1541 (2.0%)	1.84	24/2087 (1.1%)
9	2	1.77	31/1750 (1.8%)	1.76	27/2373 (1.1%)
9	i	1.84	33/1750 (1.9%)	1.82	45/2373 (1.9%)
10	3	1.68	20/1611 (1.2%)	1.79	39/2174 (1.8%)
10	j	1.83	33/1611 (2.0%)	1.85	39/2174 (1.8%)
11	4	1.76	26/1589 (1.6%)	1.80	38/2142 (1.8%)
11	k	1.77	21/1589 (1.3%)	1.77	28/2142 (1.3%)
12	5	1.81	30/1681 (1.8%)	1.76	35/2274 (1.5%)
12	l	1.78	25/1681 (1.5%)	1.79	31/2274 (1.4%)
13	6	1.77	36/1795 (2.0%)	1.84	47/2420 (1.9%)
13	m	1.78	26/1795 (1.4%)	1.83	36/2420 (1.5%)
14	7	1.74	21/1821 (1.2%)	1.81	50/2470 (2.0%)
14	n	1.73	20/1846 (1.1%)	1.75	32/2503 (1.3%)
15	H	1.19	18/3102 (0.6%)	1.22	16/4175 (0.4%)
16	I	1.23	15/3061 (0.5%)	1.25	11/4121 (0.3%)
17	K	1.16	14/3121 (0.4%)	1.22	18/4213 (0.4%)
18	L	1.13	7/3128 (0.2%)	1.19	12/4204 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
19	M	1.18	12/3023 (0.4%)	1.23	14/4070 (0.3%)
20	J	1.13	8/3073 (0.3%)	1.19	9/4129 (0.2%)
All	All	1.61	808/68850 (1.2%)	1.66	1205/92981 (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	7
1	a	0	2
2	B	0	5
2	b	0	4
3	C	0	4
3	c	0	3
4	D	0	2
5	E	0	5
6	F	0	8
6	f	0	7
7	G	0	2
7	g	0	1
8	1	0	2
9	2	0	4
9	i	0	1
10	3	0	1
10	j	0	1
11	4	0	4
11	k	0	1
12	l	0	2
13	6	0	2
13	m	0	1
14	7	0	4
14	n	0	2
15	H	0	1
16	I	0	4
17	K	0	1
18	L	0	5
19	M	0	1
20	J	0	1
All	All	0	88

All (808) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	b	67	LEU	CA-C	-12.32	1.41	1.53
7	g	137	VAL	C-N	11.84	1.43	1.33
7	G	244	ASN	C-O	-11.61	1.00	1.23
6	f	233	ILE	C-OXT	-11.58	1.00	1.23
1	a	242	GLN	C-O	-11.57	1.00	1.23
12	5	212	GLY	C-OXT	-11.57	1.00	1.23
16	I	437	LEU	C-O	-11.57	1.00	1.23
2	b	250	LEU	C-OXT	-11.57	1.00	1.23
2	B	250	LEU	C-OXT	-11.57	1.00	1.23
3	C	244	THR	C-O	-11.57	1.00	1.23
13	6	222	ASP	C-O	-11.57	1.00	1.23
8	h	196	LEU	C-OXT	-11.57	1.00	1.23
17	K	428	LYS	C-OXT	-11.57	1.00	1.23
9	2	226	GLU	C-O	-11.56	1.00	1.23
19	M	434	ALA	C-OXT	-11.56	1.00	1.23
14	7	229	GLY	C-O	-11.56	1.00	1.23
1	A	242	GLN	C-O	-11.55	1.00	1.23
2	B	250	LEU	C-O	-11.55	1.00	1.23
8	1	196	LEU	C-OXT	-11.56	1.00	1.23
19	M	434	ALA	C-O	-11.55	1.00	1.23
2	b	250	LEU	C-O	-11.55	1.00	1.23
12	l	212	GLY	C-OXT	-11.55	1.00	1.23
13	m	222	ASP	C-O	-11.55	1.00	1.23
6	f	233	ILE	C-O	-11.54	1.00	1.23
13	m	222	ASP	C-OXT	-11.54	1.00	1.23
12	5	212	GLY	C-O	-11.55	1.00	1.23
8	h	196	LEU	C-O	-11.54	1.00	1.23
17	K	428	LYS	C-O	-11.54	1.00	1.23
13	6	222	ASP	C-OXT	-11.54	1.00	1.23
9	i	226	GLU	C-O	-11.54	1.00	1.23
8	1	196	LEU	C-O	-11.54	1.00	1.23
11	4	195	PHE	C-O	-11.54	1.00	1.23
15	H	467	ASN	C-O	-11.54	1.00	1.23
16	I	437	LEU	C-OXT	-11.54	1.00	1.23
3	c	244	THR	C-O	-11.53	1.00	1.23
5	e	242	GLU	C-O	-11.54	1.00	1.23
11	k	195	PHE	C-O	-11.53	1.00	1.23
12	l	212	GLY	C-O	-11.53	1.00	1.23
18	L	436	LYS	C-O	-11.53	1.00	1.23
7	g	244	ASN	C-O	-11.53	1.00	1.23
5	E	242	GLU	C-O	-11.53	1.00	1.23
6	F	233	ILE	C-O	-11.53	1.00	1.23
6	F	233	ILE	C-OXT	-11.53	1.00	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	n	232	LYS	C-O	-11.52	1.00	1.23
15	H	467	ASN	C-OXT	-11.52	1.00	1.23
11	4	128	LEU	CA-C	-9.87	1.43	1.52
5	E	134	LEU	CA-C	-9.87	1.40	1.52
6	F	145	GLU	CA-C	-9.36	1.41	1.52
10	j	121	ALA	CA-C	-9.33	1.41	1.52
8	h	47	GLY	CA-C	-9.26	1.41	1.52
10	j	103	PHE	CA-C	-9.11	1.43	1.53
7	G	22	TYR	CA-C	-9.05	1.41	1.52
18	L	141	LYS	CA-C	-8.89	1.42	1.52
15	H	367	ARG	CA-C	8.88	1.62	1.53
7	G	35	GLY	CA-C	-8.82	1.44	1.51
4	D	149	GLU	C-N	-8.63	1.25	1.33
15	H	357	ARG	C-N	8.40	1.40	1.33
15	H	298	ALA	CA-CB	-8.39	1.39	1.53
2	B	216	ASP	CA-C	-8.30	1.41	1.53
17	K	51	LEU	CA-CB	-8.30	1.40	1.53
1	A	106	ASP	CA-C	-8.26	1.41	1.52
15	H	467	ASN	N-CA	8.24	1.61	1.46
4	d	218	ASP	CA-C	-8.23	1.42	1.53
12	l	66	HIS	ND1-CE1	8.21	1.40	1.32
7	g	236	ILE	N-CA	-8.19	1.36	1.46
5	E	136	ILE	CA-CB	-8.19	1.44	1.54
12	l	26	VAL	N-CA	-8.15	1.36	1.46
9	2	86	HIS	ND1-CE1	8.09	1.40	1.32
12	5	82	ILE	CA-C	-8.09	1.42	1.52
7	g	153	TYR	CA-C	-8.07	1.42	1.52
1	a	117	GLN	C-N	8.00	1.43	1.34
13	m	101	ARG	CA-C	-7.99	1.42	1.52
5	e	125	LEU	CA-C	-7.99	1.43	1.52
14	7	76	TYR	CA-C	-7.99	1.42	1.52
6	f	209	ASN	CA-C	-7.97	1.41	1.52
9	i	43	CYS	CA-C	-7.96	1.42	1.52
9	2	94	ILE	N-CA	-7.96	1.38	1.46
3	C	17	ARG	NE-CZ	7.95	1.41	1.33
8	h	38	HIS	ND1-CE1	7.94	1.40	1.32
9	i	125	LEU	CA-C	-7.93	1.43	1.52
16	I	200	LEU	C-N	7.85	1.43	1.34
7	g	170	ALA	CA-C	-7.82	1.42	1.52
15	H	270	THR	CA-C	-7.78	1.42	1.52
2	b	200	VAL	CA-C	-7.77	1.43	1.52
5	e	124	ARG	CD-NE	7.76	1.57	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	j	122	GLY	CA-C	-7.76	1.45	1.52
6	f	111	LEU	C-N	7.76	1.43	1.33
12	5	172	GLY	N-CA	-7.69	1.37	1.45
8	1	4	MET	N-CA	-7.69	1.37	1.46
2	B	62	SER	CA-C	-7.63	1.43	1.52
9	i	103	VAL	CA-C	-7.61	1.43	1.53
12	l	103	GLY	CA-C	-7.61	1.44	1.51
5	E	157	TYR	N-CA	-7.61	1.36	1.45
6	f	96	LEU	CA-C	-7.59	1.43	1.52
10	j	127	GLY	CA-C	-7.54	1.41	1.51
1	A	6	HIS	N-CA	-7.53	1.37	1.46
16	I	99	ILE	N-CA	-7.53	1.37	1.46
12	l	18	SER	CA-C	7.50	1.61	1.52
14	7	108	ASN	CA-C	-7.47	1.43	1.52
5	e	180	HIS	ND1-CE1	7.47	1.40	1.32
5	e	85	ARG	NE-CZ	7.46	1.41	1.33
14	n	191	SER	CA-C	-7.46	1.43	1.52
9	i	90	TYR	CA-CB	7.46	1.65	1.53
2	B	90	ARG	CZ-NH2	7.45	1.43	1.33
6	f	106	ARG	CD-NE	7.45	1.56	1.46
3	c	80	THR	CA-C	-7.40	1.43	1.52
2	B	103	GLU	CA-C	-7.38	1.43	1.53
13	6	221	ARG	CD-NE	7.34	1.56	1.46
10	j	105	GLY	C-N	-7.34	1.24	1.33
8	h	174	ARG	NE-CZ	7.33	1.41	1.33
2	B	83	ARG	CD-NE	7.32	1.56	1.46
1	A	95	PHE	C-N	7.31	1.43	1.33
1	a	136	SER	CA-C	-7.30	1.44	1.52
5	e	122	GLU	CA-C	-7.29	1.43	1.53
11	4	132	ALA	CA-C	-7.29	1.43	1.52
9	2	116	HIS	ND1-CE1	7.28	1.39	1.32
9	2	195	VAL	CA-CB	-7.25	1.46	1.54
2	b	117	ILE	CA-C	-7.24	1.44	1.52
13	6	37	SER	CA-C	-7.24	1.43	1.52
3	c	163	SER	CA-C	-7.21	1.43	1.52
14	7	6	VAL	CA-C	-7.21	1.43	1.52
12	5	4	LEU	CA-C	-7.19	1.43	1.52
7	G	21	GLU	CA-C	-7.18	1.43	1.52
20	J	270	ARG	NE-CZ	7.16	1.41	1.33
12	5	101	ILE	N-CA	-7.16	1.37	1.46
2	b	23	TYR	CA-C	-7.14	1.43	1.52
11	4	115	GLU	C-N	7.14	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	173	GLU	CA-C	-7.14	1.43	1.52
3	c	168	THR	CA-C	-7.13	1.43	1.52
5	e	12	ARG	NE-CZ	7.13	1.40	1.33
11	4	189	ILE	N-CA	-7.13	1.37	1.46
3	c	127	LEU	CA-C	-7.12	1.43	1.52
2	B	4	ARG	N-CA	-7.11	1.33	1.46
12	5	166	HIS	ND1-CE1	7.07	1.39	1.32
13	6	28	ARG	NE-CZ	7.07	1.40	1.33
14	n	112	ASN	CA-C	-7.07	1.43	1.52
10	j	129	ILE	CA-C	-7.05	1.45	1.52
13	6	101	ARG	CA-C	-7.05	1.42	1.52
2	b	74	VAL	N-CA	-7.02	1.38	1.46
4	D	56	ARG	C-N	6.98	1.42	1.33
9	2	114	HIS	ND1-CE1	6.98	1.39	1.32
10	j	14	MET	N-CA	-6.98	1.37	1.45
9	i	82	MET	CA-C	-6.97	1.43	1.52
9	2	36	ARG	C-N	6.97	1.42	1.33
4	D	155	SER	C-N	6.96	1.43	1.33
11	k	126	VAL	CA-C	-6.96	1.43	1.52
12	l	116	ASP	CA-C	-6.96	1.44	1.52
17	K	176	GLY	N-CA	-6.92	1.37	1.45
6	f	105	GLU	N-CA	-6.91	1.38	1.46
14	7	116	VAL	CA-C	-6.91	1.44	1.52
5	e	220	PHE	CA-CB	6.90	1.63	1.53
1	a	222	ASP	C-N	6.89	1.42	1.33
3	C	236	ASP	N-CA	-6.88	1.37	1.46
9	i	4	VAL	CA-C	-6.84	1.44	1.52
6	F	110	LEU	N-CA	-6.84	1.38	1.46
7	g	101	THR	CA-C	-6.83	1.45	1.52
5	E	136	ILE	CA-C	-6.83	1.44	1.52
4	d	5	ALA	CA-C	-6.80	1.43	1.52
8	h	12	VAL	N-CA	-6.80	1.37	1.46
1	a	115	LEU	N-CA	-6.79	1.38	1.46
5	E	59	ILE	C-N	6.79	1.42	1.33
12	l	140	LEU	CA-C	-6.77	1.44	1.52
12	5	124	GLY	CA-C	-6.76	1.44	1.51
10	j	13	ALA	N-CA	-6.75	1.37	1.45
2	b	187	ASP	CB-CG	6.74	1.69	1.52
12	l	69	ARG	CD-NE	6.74	1.55	1.46
14	7	97	ALA	CA-C	-6.74	1.43	1.52
7	g	115	TYR	N-CA	-6.73	1.37	1.46
2	b	32	VAL	N-CA	-6.72	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	d	80	SER	N-CA	-6.72	1.37	1.46
5	E	161	ALA	C-N	6.70	1.42	1.33
1	a	85	ALA	CA-C	-6.70	1.44	1.52
8	h	100	ALA	CA-C	-6.69	1.44	1.52
12	5	195	GLU	CA-C	-6.68	1.43	1.52
15	H	311	ILE	CA-C	-6.67	1.46	1.53
10	j	23	ALA	CA-C	-6.66	1.44	1.52
18	L	287	GLY	C-N	6.66	1.41	1.33
16	I	171	MET	C-N	6.66	1.42	1.33
4	D	95	ARG	NE-CZ	6.66	1.40	1.33
12	l	134	THR	C-N	6.65	1.43	1.33
2	B	134	LEU	CA-C	-6.65	1.45	1.52
12	5	111	THR	CA-C	-6.64	1.44	1.52
9	2	47	GLY	CA-C	-6.63	1.45	1.52
8	h	126	ILE	CA-C	-6.61	1.44	1.52
13	6	108	HIS	CA-C	-6.61	1.44	1.52
13	6	126	ASP	CA-C	-6.60	1.46	1.53
12	l	159	ARG	CZ-NH2	6.59	1.42	1.33
7	g	239	ALA	CA-C	-6.59	1.44	1.52
2	B	105	PRO	CA-CB	-6.59	1.48	1.54
20	J	273	LEU	C-N	6.57	1.43	1.34
5	e	133	ALA	CA-C	-6.57	1.44	1.52
6	f	109	HIS	ND1-CE1	6.57	1.39	1.32
8	l	110	VAL	CA-C	-6.56	1.44	1.52
19	M	320	ARG	NE-CZ	6.56	1.40	1.33
5	E	114	ARG	CD-NE	6.56	1.55	1.46
1	A	93	ALA	CA-C	-6.55	1.44	1.52
6	F	57	SER	CA-CB	6.55	1.63	1.53
10	3	197	ARG	CD-NE	6.54	1.55	1.46
10	j	80	ALA	CA-C	-6.52	1.45	1.52
9	i	186	TYR	CA-CB	6.52	1.62	1.53
13	m	13	LEU	CA-C	-6.52	1.44	1.52
1	A	5	ARG	NE-CZ	6.51	1.40	1.33
2	b	72	GLY	N-CA	-6.50	1.38	1.44
7	g	161	THR	CA-C	-6.50	1.44	1.52
1	A	171	THR	C-N	6.49	1.41	1.33
2	B	220	ASP	CA-C	-6.49	1.44	1.52
8	h	124	TYR	N-CA	-6.48	1.37	1.46
2	b	73	ALA	C-N	6.47	1.41	1.33
4	D	170	ARG	CD-NE	6.46	1.55	1.46
8	h	122	LEU	CA-C	-6.45	1.45	1.52
3	c	113	ARG	C-O	-6.45	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	n	117	ALA	C-N	6.44	1.41	1.33
8	1	20	THR	CA-C	6.43	1.59	1.52
6	F	68	HIS	ND1-CE1	6.42	1.39	1.32
11	4	170	LYS	N-CA	-6.42	1.38	1.46
7	g	200	HIS	ND1-CE1	6.42	1.39	1.32
16	I	150	HIS	ND1-CE1	6.41	1.39	1.32
9	i	59	ILE	N-CA	-6.41	1.38	1.46
16	I	242	ALA	CA-C	-6.41	1.44	1.53
5	e	72	GLY	CA-C	-6.40	1.43	1.52
8	1	29	ARG	NE-CZ	6.40	1.40	1.33
6	f	80	ALA	CA-C	-6.39	1.44	1.52
10	3	48	VAL	N-CA	6.38	1.53	1.46
7	g	11	PHE	CA-C	-6.36	1.44	1.52
7	g	102	PRO	CA-C	-6.36	1.45	1.52
5	E	137	ALA	N-CA	6.36	1.53	1.45
1	a	6	HIS	ND1-CE1	6.35	1.39	1.32
1	a	66	ILE	C-N	6.35	1.41	1.33
13	m	108	HIS	CA-C	-6.34	1.45	1.52
17	K	363	ALA	CA-C	-6.34	1.45	1.53
14	n	14	MET	CA-C	-6.33	1.44	1.52
3	C	205	LEU	N-CA	-6.32	1.38	1.46
10	3	161	ASP	C-N	6.32	1.42	1.33
15	H	50	LYS	C-N	6.32	1.42	1.33
4	D	168	THR	N-CA	6.32	1.53	1.46
14	7	90	SER	C-N	6.31	1.41	1.33
9	2	109	HIS	CA-C	-6.31	1.44	1.52
13	6	28	ARG	CA-CB	6.31	1.61	1.53
7	g	90	GLU	CA-C	-6.30	1.44	1.52
3	C	150	SER	CA-C	-6.30	1.45	1.52
1	a	5	ARG	NE-CZ	6.29	1.40	1.33
12	l	108	GLU	C-N	6.29	1.42	1.33
19	M	50	ARG	NE-CZ	6.29	1.40	1.33
9	i	161	ALA	CA-C	-6.28	1.44	1.52
8	h	113	ILE	N-CA	-6.28	1.40	1.46
11	k	79	ALA	CA-C	-6.28	1.44	1.52
5	E	220	PHE	CA-C	-6.27	1.44	1.52
6	F	9	THR	CA-C	-6.26	1.44	1.52
14	7	76	TYR	N-CA	-6.26	1.38	1.46
10	3	136	ILE	CA-C	-6.25	1.45	1.52
11	4	140	THR	C-N	6.25	1.42	1.33
7	g	87	ARG	NE-CZ	6.24	1.40	1.33
1	A	126	ARG	NE-CZ	6.23	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	137	VAL	CA-C	-6.23	1.47	1.53
4	d	47	ARG	NE-CZ	6.22	1.39	1.33
4	d	89	VAL	CA-C	-6.22	1.45	1.52
10	j	125	LEU	C-N	6.22	1.41	1.33
13	6	170	LYS	CA-CB	6.22	1.62	1.53
13	m	110	ILE	N-CA	-6.21	1.38	1.46
12	5	121	ARG	NE-CZ	6.21	1.39	1.33
2	b	165	GLY	C-O	-6.21	1.20	1.24
8	h	179	THR	C-N	6.21	1.42	1.34
5	e	58	LYS	CA-CB	-6.20	1.43	1.53
10	j	44	HIS	ND1-CE1	6.20	1.38	1.32
6	F	1	PHE	CA-C	6.20	1.66	1.52
14	7	120	GLN	CA-C	-6.19	1.45	1.53
3	C	32	GLY	C-N	6.18	1.42	1.33
5	E	67	GLY	C-N	6.18	1.41	1.33
9	2	112	SER	CA-C	-6.18	1.45	1.52
13	6	142	ALA	CA-C	-6.17	1.44	1.52
8	h	141	ASN	CA-CB	6.17	1.63	1.53
5	e	12	ARG	CA-C	-6.17	1.44	1.53
3	C	153	SER	C-N	6.17	1.40	1.33
11	4	26	SER	N-CA	-6.17	1.37	1.45
4	d	62	VAL	N-CA	-6.17	1.39	1.46
11	4	23	ARG	NE-CZ	6.17	1.39	1.33
5	E	124	ARG	NE-CZ	6.16	1.39	1.33
13	6	97	LEU	CA-C	-6.15	1.44	1.52
14	7	128	ARG	CA-C	-6.15	1.44	1.52
11	4	87	GLU	C-N	6.15	1.41	1.33
8	h	81	VAL	CA-C	-6.15	1.45	1.52
1	A	156	GLY	C-N	6.15	1.41	1.33
4	d	86	LYS	CA-C	-6.15	1.44	1.52
3	c	149	THR	CA-C	-6.14	1.45	1.52
17	K	131	LEU	N-CA	-6.14	1.38	1.46
13	6	181	ILE	CA-C	-6.13	1.44	1.52
5	E	99	ILE	CA-C	-6.13	1.45	1.52
4	d	218	ASP	CA-CB	6.12	1.62	1.53
1	A	112	MET	N-CA	-6.12	1.38	1.46
5	e	114	ARG	NE-CZ	6.12	1.39	1.33
13	6	74	TRP	C-N	6.11	1.41	1.33
15	H	101	ARG	CD-NE	6.11	1.54	1.46
5	e	85	ARG	C-N	6.11	1.41	1.33
2	B	157	PHE	CA-C	-6.11	1.46	1.52
14	7	170	VAL	C-O	-6.10	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	I	339	ILE	CA-C	6.09	1.60	1.53
9	i	3	ILE	N-CA	6.09	1.53	1.46
5	e	74	THR	C-N	6.09	1.41	1.33
3	C	85	ILE	CA-C	-6.09	1.45	1.52
9	2	34	LEU	N-CA	-6.09	1.38	1.46
4	D	4	ARG	CA-CB	6.08	1.63	1.53
12	5	29	GLN	C-N	6.08	1.42	1.33
2	b	96	SER	CA-C	-6.07	1.44	1.52
7	g	60	ASN	CA-CB	6.07	1.61	1.53
10	3	98	ARG	CD-NE	6.07	1.54	1.46
11	4	88	LEU	CA-C	-6.07	1.45	1.52
17	K	101	GLU	C-N	6.07	1.40	1.33
9	i	142	TRP	NE1-CE2	-6.07	1.30	1.37
20	J	66	GLN	CG-CD	-6.07	1.36	1.52
10	j	104	VAL	N-CA	-6.06	1.36	1.45
2	b	90	ARG	CD-NE	6.06	1.54	1.46
10	j	191	LYS	C-N	6.06	1.42	1.33
12	l	103	GLY	N-CA	-6.05	1.39	1.45
9	2	33	LYS	CA-C	-6.04	1.44	1.52
14	n	111	TRP	CA-C	-6.04	1.46	1.53
5	e	20	LEU	C-N	6.03	1.41	1.33
3	C	39	ALA	CA-C	-6.03	1.45	1.52
10	3	79	ARG	CZ-NH2	6.03	1.41	1.33
3	c	223	GLU	N-CA	-6.01	1.38	1.46
14	7	109	PRO	N-CA	-6.01	1.40	1.46
10	j	97	ARG	CZ-NH2	6.00	1.41	1.33
8	h	56	ALA	N-CA	-5.99	1.38	1.46
4	D	35	LYS	N-CA	-5.99	1.39	1.46
13	6	169	LYS	CA-C	-5.99	1.44	1.52
4	d	188	GLU	CA-C	-5.98	1.45	1.52
14	n	57	ILE	C-N	5.98	1.41	1.33
4	d	6	LEU	CA-C	-5.97	1.46	1.52
8	1	9	LYS	N-CA	5.97	1.53	1.46
12	l	124	GLY	CA-C	-5.97	1.46	1.51
20	J	260	GLY	C-N	5.97	1.42	1.33
10	j	166	ILE	N-CA	-5.97	1.37	1.46
8	h	142	PHE	C-N	5.96	1.42	1.33
9	2	78	SER	N-CA	-5.96	1.39	1.46
6	F	89	GLN	N-CA	-5.96	1.39	1.46
12	5	104	TYR	N-CA	-5.96	1.39	1.46
11	4	124	THR	CA-CB	-5.95	1.44	1.53
6	F	148	PRO	C-N	5.94	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	d	136	PHE	CA-C	-5.94	1.45	1.52
15	H	105	ILE	CA-C	-5.94	1.46	1.53
10	j	68	TYR	N-CA	-5.93	1.38	1.46
19	M	134	LEU	C-N	5.93	1.40	1.33
12	l	8	PHE	CA-CB	5.92	1.61	1.53
4	D	85	GLU	N-CA	-5.92	1.39	1.46
8	h	32	ASP	CA-C	-5.92	1.45	1.52
6	F	92	ASN	CA-CB	5.92	1.62	1.53
10	j	25	ASP	CA-C	-5.92	1.45	1.52
1	a	106	ASP	CA-CB	5.92	1.63	1.53
14	n	20	VAL	C-N	5.91	1.41	1.33
9	2	9	ASN	CA-CB	5.91	1.64	1.53
11	4	116	LEU	N-CA	-5.91	1.38	1.46
4	D	1	GLY	N-CA	5.91	1.55	1.45
8	h	66	TYR	C-N	5.91	1.41	1.33
12	l	135	PHE	CA-C	-5.91	1.44	1.52
14	7	67	LEU	CA-C	-5.90	1.45	1.52
2	B	130	PHE	C-N	5.89	1.42	1.33
2	B	92	VAL	CA-C	-5.88	1.44	1.52
6	F	188	LEU	C-N	5.88	1.41	1.33
9	2	152	ILE	CA-C	-5.88	1.44	1.52
4	D	216	ASP	CA-CB	5.88	1.63	1.53
9	i	35	HIS	ND1-CE1	5.87	1.38	1.32
4	d	10	SER	CA-CB	5.87	1.62	1.53
13	6	166	GLY	CA-C	-5.87	1.43	1.51
7	G	93	ALA	N-CA	-5.87	1.39	1.46
12	5	123	LYS	CD-CE	5.87	1.70	1.52
3	C	19	TYR	N-CA	-5.86	1.39	1.46
3	C	108	GLU	N-CA	-5.86	1.39	1.46
15	H	319	PHE	CA-CB	5.86	1.63	1.53
8	1	15	GLY	CA-C	-5.86	1.45	1.51
13	6	17	GLY	CA-C	-5.85	1.46	1.52
9	i	21	THR	N-CA	-5.85	1.39	1.45
7	G	33	SER	CA-C	-5.85	1.45	1.52
5	e	180	HIS	N-CA	-5.85	1.39	1.45
12	5	187	TYR	C-N	5.83	1.41	1.33
7	G	126	ARG	NE-CZ	5.83	1.39	1.33
1	A	166	GLN	CG-CD	5.83	1.66	1.52
16	I	262	ARG	CA-C	5.82	1.60	1.52
13	m	80	ASN	C-N	5.82	1.41	1.33
9	2	69	TYR	CA-C	-5.81	1.44	1.52
1	a	185	ILE	CA-C	-5.81	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	84	ALA	C-N	5.81	1.41	1.33
11	k	103	LEU	N-CA	-5.81	1.39	1.46
12	l	77	ALA	CA-C	-5.79	1.45	1.52
19	M	133	GLY	C-N	5.79	1.41	1.33
16	I	271	ALA	CA-C	-5.79	1.45	1.52
5	E	130	PHE	CA-CB	5.78	1.63	1.53
10	j	197	ARG	NE-CZ	5.78	1.39	1.33
1	A	83	ASN	CA-CB	5.77	1.62	1.53
4	D	63	SER	N-CA	-5.77	1.39	1.45
9	2	124	TYR	CA-C	-5.77	1.45	1.52
12	5	69	ARG	NE-CZ	5.77	1.39	1.33
7	g	203	ASN	N-CA	-5.77	1.39	1.46
13	6	100	LYS	CA-C	-5.76	1.46	1.53
2	b	152	PRO	C-O	-5.75	1.17	1.24
3	C	21	VAL	C-N	5.74	1.41	1.33
7	G	20	VAL	CA-CB	5.74	1.61	1.54
2	b	156	TYR	CA-C	-5.73	1.45	1.52
11	k	49	GLU	CG-CD	5.73	1.66	1.52
1	A	86	LEU	CA-C	-5.73	1.45	1.52
3	c	222	GLY	CA-C	-5.73	1.42	1.51
2	B	154	GLY	C-N	5.73	1.41	1.33
13	m	185	ARG	CD-NE	5.73	1.54	1.46
14	n	41	ARG	CD-NE	5.73	1.54	1.46
17	K	165	GLU	C-N	5.72	1.41	1.33
16	I	266	GLN	CA-C	-5.71	1.45	1.52
2	B	2	THR	C-N	5.71	1.41	1.33
3	c	101	TYR	CA-C	5.71	1.60	1.52
6	f	191	ALA	CA-C	-5.71	1.45	1.52
5	E	121	GLY	C-N	5.71	1.41	1.33
14	7	44	PRO	CA-C	-5.71	1.45	1.52
10	3	2	ASP	CA-C	5.70	1.60	1.53
5	e	117	GLU	N-CA	-5.70	1.38	1.45
4	d	56	ARG	CD-NE	5.69	1.54	1.46
10	j	84	GLU	CG-CD	5.69	1.66	1.52
4	D	148	THR	C-N	5.69	1.41	1.33
5	e	18	TYR	C-N	5.69	1.41	1.33
5	e	153	SER	CA-C	-5.68	1.45	1.52
14	n	128	ARG	NE-CZ	5.68	1.39	1.33
11	k	174	MET	CA-C	-5.68	1.45	1.52
14	n	45	VAL	C-N	5.68	1.41	1.33
19	M	392	LYS	CB-CG	5.68	1.69	1.52
3	C	74	VAL	CA-C	-5.68	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	m	25	GLY	CA-C	-5.67	1.45	1.51
11	4	171	ARG	NE-CZ	5.67	1.39	1.33
12	5	159	ARG	NE-CZ	5.67	1.39	1.33
15	H	261	ARG	NE-CZ	5.67	1.39	1.33
8	1	37	VAL	N-CA	5.66	1.53	1.46
4	d	176	ASN	CB-CG	5.66	1.66	1.52
6	F	162	ALA	C-N	5.66	1.42	1.33
5	E	2	ARG	NE-CZ	5.66	1.39	1.33
13	6	185	ARG	NE-CZ	5.65	1.39	1.33
4	D	95	ARG	CA-C	-5.65	1.45	1.52
1	a	223	LYS	CA-C	-5.64	1.45	1.52
5	E	124	ARG	CA-CB	5.64	1.61	1.53
4	d	129	VAL	CA-C	-5.64	1.45	1.52
5	e	153	SER	C-N	5.64	1.40	1.32
9	i	213	LEU	N-CA	-5.64	1.39	1.46
10	3	187	TYR	C-N	5.64	1.40	1.33
4	d	150	PRO	C-N	5.63	1.41	1.33
17	K	130	LEU	C-N	5.63	1.41	1.33
8	1	33	LYS	CA-C	-5.63	1.45	1.52
10	3	2	ASP	CA-CB	5.63	1.61	1.53
9	i	42	TRP	NE1-CE2	5.62	1.43	1.37
7	G	89	ARG	CZ-NH1	5.62	1.40	1.32
9	2	116	HIS	CA-C	-5.62	1.45	1.52
5	E	161	ALA	CA-C	-5.62	1.45	1.52
2	B	10	THR	N-CA	-5.62	1.39	1.46
7	G	136	GLY	CA-C	-5.62	1.46	1.51
15	H	167	ASP	C-N	5.61	1.39	1.33
6	f	127	TYR	N-CA	-5.61	1.39	1.46
9	i	116	HIS	N-CA	-5.61	1.38	1.46
12	5	98	GLY	CA-C	-5.60	1.44	1.51
13	m	155	ASN	CA-C	-5.60	1.44	1.52
5	e	32	ILE	CA-C	-5.60	1.46	1.52
9	2	113	ILE	N-CA	-5.60	1.39	1.46
10	3	89	LEU	N-CA	-5.60	1.39	1.46
3	c	95	GLN	N-CA	-5.60	1.39	1.46
1	A	89	LYS	CA-C	-5.60	1.45	1.52
8	h	145	ASN	CA-C	-5.59	1.45	1.52
4	d	216	ASP	CA-C	-5.59	1.45	1.52
8	1	159	LEU	N-CA	-5.59	1.38	1.46
20	J	257	ARG	CD-NE	5.58	1.54	1.46
5	e	114	ARG	CZ-NH1	5.58	1.40	1.32
8	1	79	ALA	CA-C	-5.58	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	4	65	GLN	C-N	5.58	1.41	1.33
6	f	88	ARG	CD-NE	5.57	1.54	1.46
8	h	120	HIS	CB-CG	-5.57	1.42	1.50
8	h	38	HIS	C-N	5.55	1.42	1.33
3	C	132	VAL	N-CA	-5.55	1.39	1.46
12	5	79	ALA	CA-C	-5.55	1.45	1.52
6	F	29	LYS	C-N	5.55	1.41	1.33
2	b	3	ASP	N-CA	-5.54	1.39	1.46
11	k	44	MET	CA-C	-5.54	1.46	1.52
4	D	170	ARG	CZ-NH1	5.54	1.40	1.32
9	2	80	LEU	CA-CB	5.54	1.61	1.53
11	4	71	GLU	C-N	5.54	1.40	1.33
2	B	74	VAL	N-CA	-5.54	1.40	1.46
3	C	18	LEU	CA-C	-5.54	1.45	1.53
6	f	157	GLY	CA-C	-5.54	1.45	1.51
14	n	114	ILE	N-CA	-5.54	1.39	1.46
13	m	181	ILE	CA-C	-5.53	1.45	1.52
13	m	92	ASN	C-N	5.53	1.40	1.34
11	4	104	ILE	CA-C	-5.53	1.45	1.52
10	j	36	SER	C-N	5.52	1.41	1.33
11	k	6	GLY	CA-C	-5.52	1.47	1.51
11	4	4	ILE	N-CA	-5.52	1.39	1.46
6	F	153	THR	N-CA	-5.52	1.39	1.45
4	d	214	LYS	C-N	5.52	1.40	1.33
9	i	124	TYR	N-CA	-5.52	1.39	1.46
14	n	137	TYR	C-N	-5.52	1.25	1.33
1	A	107	VAL	CA-CB	-5.52	1.47	1.54
5	e	45	ARG	CD-NE	5.52	1.53	1.46
10	j	79	ARG	CZ-NH2	5.52	1.40	1.33
12	5	169	ALA	CA-C	-5.52	1.45	1.52
2	b	96	SER	CA-CB	5.51	1.61	1.53
8	1	134	ILE	N-CA	-5.51	1.40	1.46
2	b	239	THR	CA-C	-5.51	1.45	1.53
3	c	116	ASP	CA-CB	5.51	1.62	1.53
7	g	136	GLY	N-CA	-5.51	1.40	1.45
3	C	199	THR	C-N	5.51	1.41	1.33
3	C	69	ASN	CA-C	-5.50	1.46	1.53
14	n	103	ARG	NE-CZ	5.50	1.39	1.33
3	C	5	TYR	N-CA	-5.50	1.38	1.46
8	h	96	GLY	CA-C	-5.49	1.44	1.51
5	E	48	SER	CA-C	-5.49	1.46	1.52
10	j	15	THR	CA-C	-5.49	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	210	GLN	CG-CD	5.49	1.65	1.52
11	k	80	VAL	C-N	5.49	1.41	1.33
5	e	109	CYS	CA-C	-5.48	1.45	1.52
4	D	188	GLU	CA-C	5.48	1.59	1.52
19	M	320	ARG	CD-NE	5.48	1.53	1.46
12	l	103	GLY	C-N	5.48	1.40	1.33
9	2	116	HIS	C-N	5.48	1.41	1.33
3	C	112	ARG	CD-NE	5.48	1.53	1.46
13	6	36	ASN	C-N	5.48	1.40	1.33
4	d	209	GLU	CA-C	-5.47	1.45	1.52
6	f	201	ARG	NE-CZ	5.47	1.39	1.33
11	k	58	GLU	CB-CG	5.47	1.68	1.52
3	C	113	ARG	NE-CZ	5.47	1.39	1.33
13	m	79	HIS	ND1-CE1	5.47	1.38	1.32
2	b	4	ARG	NE-CZ	5.47	1.39	1.33
15	H	149	LEU	C-N	5.47	1.41	1.33
10	3	163	PHE	CA-C	-5.46	1.45	1.52
7	g	56	VAL	CA-C	-5.46	1.48	1.53
10	j	98	ARG	CA-C	-5.46	1.45	1.52
11	k	116	LEU	N-CA	-5.46	1.39	1.46
10	3	168	GLN	CA-C	-5.46	1.46	1.52
6	F	68	HIS	CB-CG	5.46	1.57	1.50
2	b	165	GLY	CA-C	-5.45	1.45	1.52
1	A	236	LEU	C-N	5.45	1.40	1.33
10	j	6	ILE	C-N	5.45	1.41	1.33
7	G	224	HIS	ND1-CE1	5.45	1.38	1.32
2	b	184	GLU	CA-C	-5.45	1.45	1.52
7	g	89	ARG	CZ-NH2	5.45	1.40	1.33
16	I	171	MET	CA-C	-5.45	1.46	1.52
10	j	25	ASP	N-CA	-5.45	1.39	1.45
12	l	41	LEU	C-N	5.45	1.41	1.33
6	F	120	GLN	C-N	5.45	1.41	1.33
14	7	98	THR	C-N	5.45	1.40	1.33
11	k	186	LYS	C-N	5.45	1.40	1.33
9	i	132	LEU	CA-C	5.44	1.60	1.52
3	C	216	ARG	NE-CZ	5.44	1.39	1.33
1	A	6	HIS	ND1-CE1	5.43	1.38	1.32
12	5	64	ARG	CD-NE	5.43	1.53	1.46
13	m	127	PRO	C-N	5.43	1.40	1.33
10	j	89	LEU	CA-C	-5.43	1.45	1.52
7	G	224	HIS	N-CA	-5.42	1.39	1.46
14	7	189	ALA	C-N	5.42	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	f	201	ARG	CD-NE	5.42	1.53	1.46
14	7	13	SER	C-N	5.42	1.40	1.33
8	1	124	TYR	CA-C	-5.42	1.45	1.52
8	h	187	ILE	C-N	5.42	1.41	1.33
9	i	37	ILE	CA-C	-5.42	1.46	1.52
11	4	46	PHE	C-N	5.42	1.40	1.33
8	h	12	VAL	C-N	5.42	1.40	1.33
3	c	83	ALA	C-N	5.41	1.40	1.33
12	5	161	ILE	CA-C	-5.41	1.45	1.52
12	5	103	GLY	CA-C	-5.41	1.45	1.51
14	7	161	ARG	CD-NE	5.41	1.53	1.46
7	G	131	SER	CA-C	-5.40	1.46	1.52
9	i	205	PHE	CB-CG	-5.40	1.38	1.50
13	m	12	ILE	C-N	5.40	1.40	1.33
8	h	141	ASN	C-N	5.39	1.41	1.33
8	1	26	ILE	C-N	5.39	1.41	1.33
13	6	139	GLY	CA-C	-5.39	1.45	1.51
14	7	173	ALA	CA-C	-5.39	1.45	1.52
4	d	155	SER	CA-C	-5.39	1.46	1.52
5	e	116	GLY	N-CA	5.39	1.50	1.45
13	6	59	ALA	CA-C	-5.38	1.46	1.52
9	2	25	ILE	N-CA	-5.38	1.39	1.46
4	d	169	VAL	CA-C	-5.38	1.46	1.52
7	G	131	SER	N-CA	-5.38	1.39	1.46
11	4	169	GLU	CA-C	-5.38	1.45	1.52
11	k	68	SER	C-N	5.38	1.40	1.33
12	l	14	VAL	CA-CB	-5.38	1.47	1.54
2	b	94	HIS	ND1-CE1	5.38	1.38	1.32
20	J	242	PRO	C-N	5.37	1.40	1.33
7	G	137	VAL	CA-C	-5.37	1.46	1.52
5	e	108	VAL	C-N	5.37	1.41	1.34
9	i	135	MET	CA-CB	5.37	1.62	1.53
9	i	97	TYR	CA-C	-5.37	1.47	1.53
8	h	75	THR	C-N	5.37	1.40	1.33
5	E	97	GLU	CA-C	-5.36	1.45	1.52
8	1	46	SER	N-CA	-5.36	1.39	1.46
13	6	32	ASP	CA-C	-5.36	1.47	1.52
2	B	79	GLY	N-CA	5.36	1.52	1.44
15	H	154	LYS	C-N	5.36	1.41	1.33
13	6	168	VAL	CA-C	-5.36	1.45	1.52
4	d	171	GLU	N-CA	-5.35	1.40	1.46
11	4	124	THR	CA-C	-5.35	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	M	269	LEU	N-CA	-5.35	1.39	1.46
5	e	19	SER	CA-C	-5.35	1.45	1.52
13	6	185	ARG	CD-NE	5.35	1.53	1.46
13	m	211	GLY	CA-C	-5.35	1.45	1.52
13	6	174	TYR	N-CA	-5.35	1.39	1.46
3	C	83	ALA	N-CA	-5.35	1.40	1.46
10	3	69	LYS	CA-C	-5.35	1.46	1.52
13	m	124	SER	CA-C	-5.34	1.46	1.52
6	F	88	ARG	NE-CZ	5.34	1.39	1.33
9	2	153	LYS	CA-C	-5.34	1.46	1.52
5	E	128	ARG	CA-C	5.34	1.59	1.52
16	I	205	PRO	N-CA	-5.34	1.40	1.47
1	a	106	ASP	C-N	5.34	1.40	1.33
8	1	124	TYR	CA-CB	5.34	1.62	1.53
4	d	236	GLN	C-N	5.34	1.41	1.34
17	K	263	GLU	N-CA	-5.34	1.39	1.46
18	L	273	HIS	CE1-NE2	5.33	1.37	1.32
4	d	117	ARG	CZ-NH2	5.33	1.40	1.33
7	g	170	ALA	CA-CB	5.33	1.61	1.53
12	5	58	TRP	CE2-CZ2	-5.32	1.28	1.39
1	a	80	ASP	N-CA	-5.31	1.39	1.46
6	f	20	GLN	C-N	5.31	1.40	1.33
4	d	132	LEU	CA-C	-5.31	1.46	1.52
5	e	126	MET	C-N	5.31	1.41	1.33
2	B	90	ARG	CD-NE	5.31	1.53	1.46
19	M	131	MET	C-N	5.30	1.39	1.33
5	e	180	HIS	CA-C	-5.30	1.46	1.52
13	m	137	ARG	NE-CZ	5.30	1.38	1.33
9	2	8	PHE	CA-CB	5.30	1.61	1.53
6	F	24	ALA	C-N	5.30	1.40	1.33
10	j	110	GLY	C-N	5.30	1.41	1.33
8	1	185	ARG	CA-C	-5.30	1.46	1.52
18	L	243	PHE	CB-CG	-5.30	1.38	1.50
6	f	195	ALA	C-N	5.29	1.40	1.33
11	k	118	GLN	CA-C	-5.29	1.46	1.52
15	H	170	GLU	C-N	5.29	1.41	1.33
1	a	121	GLN	CA-C	-5.29	1.45	1.52
11	k	12	SER	N-CA	-5.29	1.39	1.45
12	l	168	ASP	CB-CG	5.29	1.65	1.52
5	e	55	SER	C-N	5.29	1.40	1.33
10	j	94	LEU	CA-C	-5.29	1.45	1.52
7	g	226	PHE	CB-CG	-5.29	1.38	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	c	95	GLN	C-O	-5.28	1.17	1.24
9	2	138	LEU	CA-CB	-5.28	1.45	1.53
10	j	98	ARG	CD-NE	5.28	1.53	1.46
19	M	272	GLU	N-CA	-5.28	1.40	1.46
3	C	221	ASP	CA-CB	5.27	1.61	1.53
19	M	422	VAL	C-N	5.27	1.41	1.33
5	E	222	ILE	CA-CB	-5.27	1.47	1.54
6	F	12	PHE	N-CA	-5.27	1.39	1.46
8	1	25	TYR	N-CA	5.27	1.52	1.46
15	H	319	PHE	CA-C	-5.27	1.45	1.52
1	a	126	ARG	CD-NE	5.27	1.53	1.46
8	1	90	LYS	CA-C	-5.26	1.45	1.52
14	n	36	PHE	CB-CG	-5.26	1.38	1.50
14	n	65	ARG	CD-NE	5.26	1.53	1.46
2	b	56	ALA	N-CA	-5.26	1.39	1.46
11	4	96	ARG	CZ-NH1	5.25	1.40	1.32
4	d	223	SER	N-CA	-5.25	1.39	1.46
6	F	169	THR	CA-C	-5.25	1.46	1.52
9	2	166	ASP	C-N	5.25	1.41	1.33
13	6	29	ASN	C-N	5.25	1.40	1.33
16	I	131	SER	C-N	5.25	1.39	1.33
13	m	136	CYS	N-CA	-5.25	1.40	1.46
4	D	108	THR	N-CA	-5.24	1.40	1.46
10	3	9	GLY	CA-C	-5.24	1.46	1.52
8	h	68	SER	N-CA	-5.24	1.39	1.46
10	j	141	ALA	CA-C	-5.24	1.46	1.53
12	5	7	ARG	CZ-NH2	5.23	1.40	1.33
3	C	157	THR	CA-C	-5.23	1.46	1.52
1	a	146	TYR	CA-C	-5.22	1.46	1.52
9	i	26	VAL	C-N	5.22	1.41	1.33
11	k	42	THR	N-CA	5.22	1.52	1.46
2	B	145	PHE	N-CA	-5.22	1.39	1.46
18	L	322	LYS	CA-C	-5.22	1.46	1.52
9	i	79	ALA	CA-C	-5.22	1.46	1.52
5	e	57	GLU	CA-C	-5.22	1.46	1.52
9	2	128	GLY	CA-C	-5.21	1.46	1.52
13	6	101	ARG	CD-NE	5.21	1.53	1.46
9	i	69	TYR	C-N	5.21	1.41	1.33
3	c	209	ARG	NE-CZ	5.21	1.38	1.33
8	h	119	VAL	N-CA	-5.21	1.40	1.46
4	d	151	SER	N-CA	-5.21	1.40	1.46
20	J	257	ARG	NE-CZ	5.21	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	c	232	GLN	CA-C	-5.21	1.45	1.52
2	B	23	TYR	N-CA	-5.20	1.40	1.46
10	3	77	GLU	C-N	5.20	1.41	1.33
1	A	94	GLU	C-N	5.20	1.41	1.34
11	4	107	TYR	CA-C	-5.20	1.46	1.52
6	f	9	THR	N-CA	-5.20	1.39	1.46
7	G	32	THR	CA-C	-5.20	1.46	1.52
18	L	243	PHE	CA-CB	-5.20	1.41	1.53
8	h	185	ARG	CZ-NH2	5.20	1.40	1.33
7	g	55	LEU	C-N	5.20	1.37	1.33
6	F	81	ARG	NE-CZ	5.20	1.38	1.33
5	e	102	GLU	N-CA	-5.19	1.40	1.46
4	d	88	ARG	CZ-NH2	5.19	1.40	1.33
9	i	179	GLU	CA-C	-5.19	1.46	1.52
17	K	281	ARG	NE-CZ	5.19	1.38	1.33
3	C	109	ILE	N-CA	-5.19	1.40	1.46
1	A	209	PHE	CA-CB	5.18	1.62	1.53
6	F	180	LYS	C-N	5.18	1.38	1.33
20	J	210	PHE	CA-CB	5.18	1.59	1.52
8	h	120	HIS	C-O	-5.18	1.17	1.23
8	1	180	ALA	N-CA	-5.18	1.39	1.46
11	k	26	SER	C-N	5.18	1.38	1.33
9	i	123	TYR	C-N	5.18	1.40	1.33
2	B	108	LYS	CA-C	-5.18	1.45	1.52
12	5	140	LEU	N-CA	-5.18	1.39	1.46
13	m	107	VAL	CA-C	-5.17	1.46	1.52
1	A	203	ASP	CA-C	-5.17	1.46	1.52
14	n	109	PRO	CA-C	-5.17	1.47	1.52
6	F	129	VAL	CA-C	-5.17	1.46	1.52
5	e	232	ILE	CA-C	-5.17	1.46	1.52
3	c	15	GLU	CG-CD	5.17	1.65	1.52
9	i	105	PRO	CA-C	-5.17	1.44	1.52
14	n	181	MET	N-CA	-5.17	1.40	1.46
14	7	128	ARG	CD-NE	5.17	1.53	1.46
4	D	95	ARG	CD-NE	5.17	1.53	1.46
12	5	87	VAL	CA-CB	-5.17	1.48	1.54
10	3	98	ARG	CA-C	-5.16	1.46	1.52
6	F	84	SER	C-N	5.16	1.40	1.33
4	d	61	LYS	C-N	5.16	1.40	1.33
6	f	107	ALA	CA-C	-5.16	1.45	1.52
17	K	363	ALA	C-O	-5.16	1.17	1.23
13	m	191	ALA	C-N	5.15	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	45	ILE	N-CA	-5.15	1.40	1.46
3	C	171	ALA	N-CA	-5.15	1.40	1.46
3	c	109	ILE	N-CA	-5.15	1.40	1.46
17	K	307	ASP	CA-C	-5.15	1.46	1.52
6	F	149	SER	CA-CB	5.15	1.61	1.53
11	4	141	PHE	C-N	5.15	1.41	1.33
9	i	66	HIS	N-CA	5.14	1.52	1.46
6	f	62	ILE	C-N	5.14	1.39	1.33
1	A	11	SER	CA-CB	5.14	1.60	1.53
7	G	95	PHE	CA-C	5.14	1.59	1.52
1	a	83	ASN	CA-C	-5.14	1.46	1.52
9	i	68	LEU	N-CA	-5.14	1.40	1.46
7	G	4	TYR	C-N	5.13	1.41	1.33
13	6	57	PHE	CA-CB	5.13	1.59	1.53
13	6	153	GLN	CA-C	-5.13	1.46	1.52
13	m	28	ARG	C-N	5.13	1.40	1.33
6	f	147	GLN	CB-CG	-5.13	1.37	1.52
5	e	127	SER	CA-C	5.13	1.60	1.52
11	k	12	SER	C-N	5.13	1.40	1.33
1	a	154	TYR	CA-CB	5.13	1.61	1.53
2	b	90	ARG	CZ-NH1	5.13	1.40	1.32
1	A	147	LYS	C-N	5.13	1.40	1.33
9	i	2	THR	CA-C	-5.12	1.46	1.52
14	n	74	ASN	CA-CB	5.12	1.61	1.53
2	b	70	ASP	C-N	5.12	1.39	1.33
12	l	121	ARG	NE-CZ	5.12	1.38	1.33
17	K	141	ARG	NE-CZ	5.12	1.38	1.33
2	B	94	HIS	CD2-NE2	5.12	1.43	1.37
9	2	188	ARG	NE-CZ	5.12	1.38	1.33
11	4	78	GLN	N-CA	-5.12	1.40	1.46
10	j	33	LEU	C-N	5.11	1.38	1.33
5	E	123	GLU	CA-CB	5.11	1.59	1.52
13	6	31	THR	C-O	-5.11	1.17	1.23
7	G	16	ARG	CZ-NH1	5.11	1.40	1.32
16	I	262	ARG	N-CA	-5.11	1.40	1.46
13	6	8	ASN	N-CA	-5.11	1.41	1.46
13	6	67	ARG	CZ-NH2	5.11	1.40	1.33
13	m	137	ARG	CZ-NH2	5.10	1.40	1.33
13	6	122	VAL	N-CA	-5.10	1.40	1.46
10	3	97	ARG	CZ-NH2	5.10	1.40	1.33
13	m	181	ILE	CA-CB	-5.10	1.47	1.54
12	l	69	ARG	CZ-NH2	5.09	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	56	ARG	CZ-NH2	5.09	1.40	1.33
6	F	73	LEU	CA-CB	5.09	1.61	1.53
12	5	181	THR	CA-C	-5.09	1.46	1.53
10	3	188	ILE	CA-C	-5.09	1.46	1.52
13	6	136	CYS	C-N	5.09	1.40	1.33
1	A	114	ASN	CA-C	-5.09	1.46	1.52
12	l	8	PHE	C-N	5.08	1.41	1.33
3	C	113	ARG	CA-C	-5.08	1.45	1.52
10	3	145	LEU	C-N	5.08	1.40	1.33
12	l	98	GLY	C-N	5.08	1.40	1.33
2	b	205	ASN	CA-C	-5.08	1.46	1.52
4	d	109	ARG	N-CA	-5.08	1.40	1.46
12	5	166	HIS	CE1-NE2	-5.08	1.27	1.32
3	c	7	SER	C-N	5.08	1.40	1.33
9	2	164	TRP	CA-C	-5.08	1.45	1.52
7	g	168	ALA	CA-C	-5.07	1.46	1.52
2	b	8	SER	CA-C	-5.07	1.46	1.52
13	m	103	PHE	N-CA	-5.07	1.41	1.46
13	m	213	ARG	NE-CZ	5.07	1.38	1.33
1	A	188	GLU	CA-C	-5.07	1.46	1.52
2	B	114	VAL	CA-C	-5.06	1.46	1.52
13	6	26	ASP	C-N	5.06	1.40	1.33
10	3	163	PHE	N-CA	-5.06	1.40	1.46
6	f	10	VAL	N-CA	-5.06	1.40	1.46
4	D	147	GLN	C-N	5.06	1.40	1.33
2	b	62	SER	CA-C	-5.05	1.46	1.52
4	d	169	VAL	CA-CB	-5.05	1.48	1.54
10	j	176	ARG	CD-NE	-5.05	1.39	1.46
12	5	18	SER	N-CA	-5.04	1.40	1.46
1	a	215	GLU	CA-C	-5.04	1.46	1.52
6	F	2	ARG	NE-CZ	5.04	1.38	1.33
9	i	87	LEU	C-N	5.03	1.40	1.33
5	E	79	SER	N-CA	-5.03	1.40	1.46
11	k	8	ARG	NE-CZ	5.03	1.38	1.33
1	a	26	THR	CA-C	-5.03	1.46	1.52
8	h	14	LEU	CA-C	-5.02	1.46	1.52
9	2	6	VAL	N-CA	-5.02	1.41	1.46
9	2	211	ALA	N-CA	-5.02	1.40	1.46
2	b	90	ARG	CZ-NH2	5.02	1.40	1.33
3	c	107	VAL	CA-CB	-5.02	1.48	1.54
11	k	13	VAL	CA-CB	-5.02	1.48	1.54
3	C	79	LEU	CA-C	-5.02	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	7	133	LEU	N-CA	5.01	1.52	1.46
4	d	195	ARG	NE-CZ	5.01	1.38	1.33
3	C	153	SER	CA-C	-5.01	1.46	1.52
6	f	203	GLU	CA-C	5.01	1.58	1.53
14	n	65	ARG	NE-CZ	5.01	1.38	1.33
4	D	76	LEU	CA-C	5.01	1.59	1.52
11	4	97	PRO	CA-C	-5.01	1.47	1.52
6	f	103	ALA	CA-C	-5.00	1.46	1.52
11	k	135	TYR	N-CA	-5.00	1.39	1.46

All (1205) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	l	125	ASP	CA-CB-CG	-11.78	100.82	112.60
17	K	51	LEU	CB-CA-C	11.48	129.84	110.79
18	L	243	PHE	CA-CB-CG	-11.13	102.67	113.80
14	7	187	ARG	NE-CZ-NH2	10.55	128.70	119.20
2	B	151	ASP	CA-C-O	-10.22	111.40	120.60
5	E	77	ALA	O-C-N	-10.00	109.97	122.27
8	h	8	PHE	CA-CB-CG	9.78	123.58	113.80
13	m	7	ASP	CA-CB-CG	9.62	122.22	112.60
13	6	86	ILE	CA-C-N	9.56	133.09	120.28
13	6	86	ILE	C-N-CA	9.56	133.09	120.28
1	A	28	GLN	N-CA-C	-9.55	103.73	114.62
3	C	229	PHE	CA-CB-CG	-9.55	104.25	113.80
9	i	103	VAL	CA-C-O	-9.47	112.63	121.72
7	G	221	ASN	CA-CB-CG	-9.20	103.40	112.60
5	E	205	ASP	CA-CB-CG	-9.20	103.40	112.60
7	G	104	PRO	CA-C-N	9.13	125.99	120.24
7	G	104	PRO	C-N-CA	9.13	125.99	120.24
11	4	76	SER	CA-C-N	9.09	129.14	119.05
11	4	76	SER	C-N-CA	9.09	129.14	119.05
15	H	95	HIS	CA-CB-CG	-9.00	104.80	113.80
14	7	77	ASP	CA-CB-CG	-8.93	103.67	112.60
10	j	103	PHE	CA-CB-CG	-8.92	104.88	113.80
13	6	135	GLN	N-CA-C	-8.74	103.20	114.04
7	g	60	ASN	CA-CB-CG	-8.71	103.89	112.60
14	7	181	MET	N-CA-CB	8.71	122.92	110.12
19	M	150	LYS	CA-C-N	8.66	131.70	120.44
19	M	150	LYS	C-N-CA	8.66	131.70	120.44
12	5	75	SER	CA-C-N	8.51	131.45	120.56
12	5	75	SER	C-N-CA	8.51	131.45	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	g	101	THR	O-C-N	-8.42	115.90	121.88
4	D	136	PHE	CA-CB-CG	-8.40	105.40	113.80
5	E	101	VAL	CA-C-N	8.26	131.17	120.44
5	E	101	VAL	C-N-CA	8.26	131.17	120.44
15	H	372	ASP	CA-CB-CG	-8.24	104.36	112.60
1	A	106	ASP	CA-CB-CG	8.19	120.78	112.60
7	G	92	ALA	CA-C-N	8.15	131.20	120.28
7	G	92	ALA	C-N-CA	8.15	131.20	120.28
13	6	146	ILE	CA-C-N	-8.13	109.87	120.44
13	6	146	ILE	C-N-CA	-8.13	109.87	120.44
12	l	127	PHE	CA-CB-CG	-8.12	105.67	113.80
8	h	113	ILE	N-CA-C	-8.12	100.11	108.15
3	c	232	GLN	OE1-CD-NE2	8.06	130.66	122.60
5	E	149	HIS	CE1-NE2-CD2	-8.04	100.96	109.00
12	5	55	TRP	N-CA-C	7.97	122.43	112.87
5	e	180	HIS	CG-CD2-NE2	7.94	115.14	107.20
3	c	19	TYR	N-CA-C	7.90	119.52	111.07
16	I	335	ASP	O-C-N	-7.88	114.92	121.38
11	4	187	ASP	CA-CB-CG	-7.81	104.79	112.60
2	B	17	LYS	N-CA-CB	7.78	123.64	110.49
1	A	184	HIS	CA-CB-CG	-7.77	106.03	113.80
13	6	95	HIS	O-C-N	-7.67	112.26	122.23
5	E	126	MET	N-CA-C	-7.66	97.67	109.24
11	4	141	PHE	CA-CB-CG	-7.66	106.14	113.80
12	5	3	THR	N-CA-C	-7.63	95.18	108.69
12	l	191	HIS	ND1-CE1-NE2	7.62	116.02	108.40
8	1	142	PHE	CA-CB-CG	-7.59	106.21	113.80
6	f	84	SER	N-CA-C	7.58	121.62	112.38
10	j	44	HIS	CE1-NE2-CD2	-7.53	101.47	109.00
9	2	134	ALA	CA-C-N	7.52	130.68	120.38
9	2	134	ALA	C-N-CA	7.52	130.68	120.38
8	h	120	HIS	CE1-NE2-CD2	-7.51	101.49	109.00
10	3	33	LEU	CA-C-N	7.49	128.81	121.62
10	3	33	LEU	C-N-CA	7.49	128.81	121.62
2	b	162	THR	O-C-N	-7.48	115.81	123.29
13	m	108	HIS	CB-CG-CD2	-7.48	121.47	131.20
15	H	467	ASN	N-CA-C	7.48	131.94	111.00
5	e	2	ARG	CA-C-N	7.45	127.07	119.92
5	e	2	ARG	C-N-CA	7.45	127.07	119.92
9	i	122	GLY	N-CA-C	-7.44	99.88	110.75
8	1	115	LEU	N-CA-C	7.44	119.39	111.28
4	d	88	ARG	CA-C-N	7.41	129.96	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	d	88	ARG	C-N-CA	7.41	129.96	120.70
14	7	131	ASN	CA-C-N	7.37	131.87	120.82
14	7	131	ASN	C-N-CA	7.37	131.87	120.82
3	C	88	ASN	CA-CB-CG	-7.36	105.25	112.60
6	f	79	ASP	CA-C-N	7.34	130.42	120.44
6	f	79	ASP	C-N-CA	7.34	130.42	120.44
19	M	197	ILE	CA-C-O	-7.31	113.71	120.73
1	A	88	ALA	CA-C-N	7.30	130.39	120.54
1	A	88	ALA	C-N-CA	7.30	130.39	120.54
5	e	149	HIS	CE1-NE2-CD2	-7.30	101.70	109.00
4	D	66	ASP	N-CA-C	-7.30	98.53	108.38
7	g	112	LEU	CA-C-N	7.28	128.02	119.94
7	g	112	LEU	C-N-CA	7.28	128.02	119.94
2	b	70	ASP	CA-CB-CG	7.27	119.87	112.60
8	h	120	HIS	ND1-CE1-NE2	7.27	115.67	108.40
14	n	56	ASP	CA-C-N	7.25	129.84	120.56
14	n	56	ASP	C-N-CA	7.25	129.84	120.56
9	2	78	SER	CA-C-N	7.25	129.86	120.44
9	2	78	SER	C-N-CA	7.25	129.86	120.44
6	F	218	ASP	CA-CB-CG	-7.23	105.37	112.60
10	3	154	GLU	N-CA-C	-7.20	97.84	109.58
2	b	190	HIS	CE1-NE2-CD2	-7.20	101.80	109.00
4	d	125	ARG	CA-C-N	7.19	127.24	119.90
4	d	125	ARG	C-N-CA	7.19	127.24	119.90
17	K	51	LEU	CA-CB-CG	-7.19	91.13	116.30
9	i	38	SER	CA-C-N	7.19	128.83	119.84
9	i	38	SER	C-N-CA	7.19	128.83	119.84
10	j	154	GLU	CA-C-O	-7.18	114.00	119.32
5	e	39	VAL	N-CA-CB	7.18	121.32	111.41
12	l	63	CYS	CA-CB-SG	-7.16	97.93	114.40
13	6	216	PHE	CA-CB-CG	-7.16	106.64	113.80
15	H	466	TYR	CA-C-N	7.16	134.58	121.70
15	H	466	TYR	C-N-CA	7.16	134.58	121.70
7	g	11	PHE	CA-CB-CG	-7.15	106.65	113.80
7	g	19	GLN	CA-C-N	7.15	129.71	120.56
7	g	19	GLN	C-N-CA	7.15	129.71	120.56
6	f	23	TYR	CA-C-N	7.14	130.18	120.54
6	f	23	TYR	C-N-CA	7.14	130.18	120.54
9	i	8	PHE	CA-CB-CG	7.14	120.94	113.80
13	6	95	HIS	CA-C-N	7.14	130.15	120.44
13	6	95	HIS	C-N-CA	7.14	130.15	120.44
6	f	19	PHE	CA-CB-CG	-7.12	106.68	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	4	127	GLU	CA-C-O	-7.11	113.20	121.16
4	d	115	GLN	CA-C-N	7.10	130.10	120.38
4	d	115	GLN	C-N-CA	7.10	130.10	120.38
13	m	46	CYS	N-CA-C	-7.10	103.18	112.41
13	6	82	LYS	N-CA-C	-7.08	99.33	109.96
4	D	112	ALA	CA-C-N	7.08	127.99	119.99
4	D	112	ALA	C-N-CA	7.08	127.99	119.99
13	6	80	ASN	OD1-CG-ND2	7.08	129.68	122.60
5	E	220	PHE	CA-CB-CG	-7.08	106.72	113.80
2	B	109	LEU	N-CA-CB	7.08	120.63	110.16
12	l	89	GLN	CA-C-O	7.07	128.24	120.82
5	e	66	ILE	CB-CA-C	-7.07	103.24	111.09
9	i	141	HIS	ND1-CE1-NE2	7.06	115.46	108.40
14	n	224	ASP	CA-C-N	7.06	130.02	120.63
14	n	224	ASP	C-N-CA	7.06	130.02	120.63
5	E	94	TYR	CA-C-O	-7.05	111.02	119.27
5	E	48	SER	O-C-N	-7.05	116.92	121.85
20	J	262	GLY	N-CA-C	-7.03	105.10	115.72
2	B	24	ALA	O-C-N	-7.03	114.83	122.07
5	E	128	ARG	O-C-N	-7.03	113.23	121.32
4	d	167	LYS	CA-C-N	7.03	129.58	120.44
4	d	167	LYS	C-N-CA	7.03	129.58	120.44
3	C	95	GLN	N-CA-C	7.02	118.93	111.28
10	j	2	ASP	CA-CB-CG	-7.02	105.58	112.60
10	j	71	ASN	CA-CB-CG	-7.02	105.58	112.60
9	2	26	VAL	CA-C-N	7.01	129.67	120.28
9	2	26	VAL	C-N-CA	7.01	129.67	120.28
4	D	108	THR	CA-C-N	6.99	129.95	120.38
4	D	108	THR	C-N-CA	6.99	129.95	120.38
8	1	38	HIS	CA-CB-CG	-6.98	106.82	113.80
5	E	242	GLU	CA-C-O	-6.97	108.94	120.80
12	5	110	PRO	CA-C-O	-6.97	113.77	121.23
1	A	242	GLN	CA-C-O	-6.97	108.95	120.80
3	C	194	LYS	CA-C-N	6.97	130.90	120.31
3	C	194	LYS	C-N-CA	6.97	130.90	120.31
11	k	187	ASP	N-CA-C	-6.96	103.89	112.88
1	A	220	THR	N-CA-C	-6.96	99.04	108.86
1	a	78	ILE	O-C-N	-6.96	113.17	121.10
9	2	226	GLU	CA-C-O	-6.96	108.97	120.80
11	4	195	PHE	CA-C-O	-6.96	108.97	120.80
7	G	244	ASN	CA-C-O	-6.96	108.98	120.80
3	C	244	THR	CA-C-O	-6.95	108.98	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	k	195	PHE	CA-C-O	-6.95	108.98	120.80
6	F	153	THR	CA-C-N	6.95	131.44	121.50
6	F	153	THR	C-N-CA	6.95	131.44	121.50
15	H	327	ASN	CA-CB-CG	-6.95	105.65	112.60
2	b	63	LYS	N-CA-C	-6.95	103.99	113.30
7	g	244	ASN	CA-C-O	-6.95	108.99	120.80
9	i	226	GLU	CA-C-O	-6.95	108.99	120.80
14	n	232	LYS	CA-C-O	-6.94	109.00	120.80
18	L	436	LYS	CA-C-O	-6.94	109.00	120.80
3	c	244	THR	CA-C-O	-6.94	109.00	120.80
1	a	242	GLN	CA-C-O	-6.94	109.01	120.80
5	e	242	GLU	CA-C-O	-6.94	109.01	120.80
1	A	93	ALA	CA-C-N	6.94	131.22	120.82
1	A	93	ALA	C-N-CA	6.94	131.22	120.82
6	F	184	ASN	O-C-N	-6.92	115.63	121.23
3	C	93	HIS	CA-C-N	6.91	129.42	120.44
3	C	93	HIS	C-N-CA	6.91	129.42	120.44
5	e	180	HIS	CE1-NE2-CD2	-6.91	102.09	109.00
8	1	179	THR	CA-C-N	6.91	130.22	120.28
8	1	179	THR	C-N-CA	6.91	130.22	120.28
8	1	191	ASP	CA-CB-CG	-6.90	105.70	112.60
10	3	97	ARG	CA-C-N	6.90	129.85	120.54
10	3	97	ARG	C-N-CA	6.90	129.85	120.54
6	f	219	THR	O-C-N	-6.90	113.52	120.83
6	f	6	ASP	CA-CB-CG	6.89	119.50	112.60
9	i	86	HIS	CE1-NE2-CD2	-6.88	102.12	109.00
5	E	66	ILE	O-C-N	-6.88	116.78	122.97
14	7	43	ILE	CA-C-N	6.87	127.41	119.99
14	7	43	ILE	C-N-CA	6.87	127.41	119.99
7	g	69	HIS	CA-C-O	-6.87	113.51	119.97
7	G	71	GLY	CA-C-O	-6.86	115.33	121.64
1	a	155	VAL	N-CA-C	-6.85	99.35	107.70
12	l	36	GLU	CA-C-N	6.84	129.83	120.46
12	l	36	GLU	C-N-CA	6.84	129.83	120.46
4	d	19	GLU	CA-C-N	6.84	130.00	120.29
4	d	19	GLU	C-N-CA	6.84	130.00	120.29
1	A	105	CYS	CA-C-N	6.80	129.70	120.38
1	A	105	CYS	C-N-CA	6.80	129.70	120.38
6	F	91	CYS	CA-C-N	6.80	129.40	120.28
6	F	91	CYS	C-N-CA	6.80	129.40	120.28
19	M	272	GLU	N-CA-C	6.80	118.48	111.14
4	d	223	SER	N-CA-CB	6.80	120.10	109.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	2	66	HIS	CA-C-N	6.80	129.28	120.44
9	2	66	HIS	C-N-CA	6.80	129.28	120.44
1	a	215	GLU	N-CA-C	-6.78	96.74	107.93
13	m	186	ASP	CA-CB-CG	-6.78	105.82	112.60
10	3	73	TYR	O-C-N	-6.78	114.77	122.09
9	i	116	HIS	ND1-CE1-NE2	6.78	115.18	108.40
4	D	171	GLU	CA-C-O	-6.77	113.37	120.55
12	l	14	VAL	N-CA-C	-6.77	98.73	108.48
5	E	106	GLN	OE1-CD-NE2	6.76	129.37	122.60
17	K	134	SER	N-CA-C	6.76	120.30	110.42
3	c	236	ASP	N-CA-CB	6.76	120.17	110.16
4	d	171	GLU	CA-C-N	6.75	129.65	120.54
4	d	171	GLU	C-N-CA	6.75	129.65	120.54
6	F	77	ALA	CA-C-N	6.73	126.19	118.85
6	F	77	ALA	C-N-CA	6.73	126.19	118.85
16	I	150	HIS	CA-CB-CG	6.73	120.53	113.80
4	D	137	ASP	CA-C-O	-6.71	113.19	120.17
2	b	22	ASP	CA-CB-CG	-6.70	105.90	112.60
7	G	184	SER	CA-C-N	6.70	129.93	120.28
7	G	184	SER	C-N-CA	6.70	129.93	120.28
14	7	35	ARG	NE-CZ-NH2	6.70	125.23	119.20
3	C	81	ALA	CA-C-O	-6.69	113.79	120.82
6	f	173	ARG	NE-CZ-NH2	6.69	125.22	119.20
13	m	38	ARG	N-CA-C	-6.68	103.47	111.69
5	e	128	ARG	NE-CZ-NH2	6.68	125.21	119.20
13	6	79	HIS	CA-CB-CG	-6.67	107.13	113.80
11	k	97	PRO	N-CA-CB	6.67	109.52	103.19
1	a	101	TYR	CA-C-O	-6.66	114.11	121.23
7	g	101	THR	CA-C-N	6.66	126.68	119.89
7	g	101	THR	C-N-CA	6.66	126.68	119.89
11	4	34	LYS	N-CA-C	-6.64	101.80	111.30
12	l	116	ASP	CA-C-N	6.64	129.07	120.44
12	l	116	ASP	C-N-CA	6.64	129.07	120.44
4	d	103	THR	N-CA-C	-6.64	99.39	109.95
7	g	224	HIS	CA-CB-CG	6.64	120.44	113.80
2	b	88	LYS	CA-C-N	6.64	129.07	120.44
2	b	88	LYS	C-N-CA	6.64	129.07	120.44
4	D	127	PHE	CB-CA-C	-6.64	100.83	110.06
10	j	9	GLY	N-CA-C	-6.64	103.03	111.72
3	C	224	VAL	N-CA-C	-6.63	98.81	108.89
13	6	78	ASP	CA-CB-CG	-6.63	105.97	112.60
13	6	128	VAL	N-CA-C	-6.62	104.40	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	j	28	LEU	N-CA-CB	6.62	120.90	110.84
13	m	126	ASP	N-CA-CB	6.61	119.22	110.29
5	e	89	VAL	N-CA-C	6.60	117.36	110.62
12	5	35	ILE	CA-C-O	6.60	126.09	120.22
14	n	57	ILE	CA-C-O	-6.59	113.74	121.05
7	g	4	TYR	N-CA-C	-6.59	105.06	113.23
1	a	172	ASN	N-CA-CB	6.58	119.74	109.94
10	j	59	VAL	CB-CA-C	-6.58	103.55	111.97
8	1	129	SER	N-CA-CB	6.57	119.99	110.20
1	A	149	ASP	CA-CB-CG	6.56	119.16	112.60
2	b	220	ASP	CA-C-O	6.56	127.52	120.24
14	7	78	ASN	CA-C-N	6.56	126.14	119.19
14	7	78	ASN	C-N-CA	6.56	126.14	119.19
2	B	104	TYR	CA-C-N	6.55	124.38	119.66
2	B	104	TYR	C-N-CA	6.55	124.38	119.66
4	d	17	GLN	CA-C-N	6.55	130.11	120.74
4	d	17	GLN	C-N-CA	6.55	130.11	120.74
8	1	170	GLY	N-CA-C	-6.55	101.67	110.97
10	j	132	ALA	CA-C-O	6.55	128.32	121.38
11	4	26	SER	CA-C-N	6.54	131.50	122.93
11	4	26	SER	C-N-CA	6.54	131.50	122.93
2	b	114	VAL	CA-C-N	6.54	129.57	120.29
2	b	114	VAL	C-N-CA	6.54	129.57	120.29
14	n	88	GLU	CA-C-O	-6.54	113.57	120.70
1	a	24	LYS	CA-C-N	6.54	129.69	120.28
1	a	24	LYS	C-N-CA	6.54	129.69	120.28
14	n	18	ASN	CA-CB-CG	-6.53	106.07	112.60
9	i	26	VAL	N-CA-CB	6.53	118.95	111.90
6	F	77	ALA	O-C-N	-6.53	113.81	121.32
12	l	191	HIS	CA-CB-CG	-6.52	107.28	113.80
14	n	4	PRO	CA-C-O	-6.52	113.72	121.67
11	k	23	ARG	NE-CZ-NH2	6.51	125.06	119.20
8	1	118	SER	CA-C-O	-6.51	114.46	121.36
11	k	98	TYR	N-CA-C	-6.50	101.16	110.59
12	5	189	GLY	CA-C-N	6.48	132.13	123.05
12	5	189	GLY	C-N-CA	6.48	132.13	123.05
5	e	116	GLY	CA-C-O	-6.48	115.34	122.14
7	g	126	ARG	CA-C-O	-6.47	112.36	119.61
5	E	107	SER	CA-C-N	6.47	128.72	120.56
5	E	107	SER	C-N-CA	6.47	128.72	120.56
11	k	78	GLN	O-C-N	-6.47	115.26	122.12
10	3	113	SER	CA-C-N	6.45	129.45	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	3	113	SER	C-N-CA	6.45	129.45	120.29
11	k	124	THR	CA-C-N	6.45	130.03	120.87
11	k	124	THR	C-N-CA	6.45	130.03	120.87
2	b	5	TYR	N-CA-C	-6.45	103.75	112.26
5	e	154	GLY	N-CA-C	-6.43	105.46	116.01
8	h	164	LYS	N-CA-C	6.43	118.29	111.28
14	n	123	GLY	CA-C-N	6.43	130.24	121.05
14	n	123	GLY	C-N-CA	6.43	130.24	121.05
3	c	69	ASN	N-CA-C	-6.43	99.38	108.96
10	j	121	ALA	CA-C-N	6.42	128.29	121.48
10	j	121	ALA	C-N-CA	6.42	128.29	121.48
7	g	16	ARG	N-CA-C	6.42	119.08	110.35
2	B	109	LEU	CA-C-O	6.42	127.22	120.42
5	E	93	LEU	N-CA-C	-6.41	104.15	112.23
8	1	15	GLY	CA-C-O	-6.41	115.70	121.47
10	j	75	LEU	CA-C-O	-6.40	112.61	119.97
6	F	109	HIS	CE1-NE2-CD2	-6.40	102.60	109.00
12	l	101	ILE	CB-CA-C	-6.40	102.98	110.91
1	a	95	PHE	CA-C-N	6.39	129.71	120.38
1	a	95	PHE	C-N-CA	6.39	129.71	120.38
13	m	87	ASN	OD1-CG-ND2	6.39	128.99	122.60
3	C	48	GLU	N-CA-CB	-6.39	100.53	110.55
8	h	82	PHE	CA-CB-CG	-6.38	107.42	113.80
10	j	132	ALA	O-C-N	-6.38	116.56	123.26
13	m	57	PHE	CA-C-N	6.38	129.12	120.38
13	m	57	PHE	C-N-CA	6.38	129.12	120.38
11	4	55	GLN	CA-C-N	6.38	131.37	120.72
11	4	55	GLN	C-N-CA	6.38	131.37	120.72
13	6	108	HIS	CE1-NE2-CD2	-6.38	102.62	109.00
2	b	180	ASN	N-CA-C	-6.36	99.48	108.96
5	e	149	HIS	ND1-CE1-NE2	6.36	114.76	108.40
13	m	108	HIS	CA-CB-CG	-6.36	107.44	113.80
2	b	94	HIS	CG-CD2-NE2	6.36	113.56	107.20
2	b	160	LYS	CA-C-O	6.36	127.47	119.78
2	b	194	LEU	CA-C-N	6.36	128.80	120.28
2	b	194	LEU	C-N-CA	6.36	128.80	120.28
8	h	33	LYS	N-CA-C	-6.36	104.78	113.30
14	7	71	VAL	CB-CA-C	-6.35	103.73	112.24
5	E	62	ILE	N-CA-C	-6.34	106.36	111.81
5	E	149	HIS	ND1-CE1-NE2	6.34	114.74	108.40
2	B	224	TYR	CA-C-N	6.34	130.48	121.42
2	B	224	TYR	C-N-CA	6.34	130.48	121.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	j	59	VAL	N-CA-CB	6.33	117.95	110.55
13	6	3	ASN	CA-C-O	-6.33	113.96	119.72
3	C	203	SER	N-CA-C	6.32	118.17	111.28
8	1	128	GLY	CA-C-O	-6.32	116.51	122.13
14	7	88	GLU	CA-C-N	6.31	125.81	119.24
14	7	88	GLU	C-N-CA	6.31	125.81	119.24
1	a	155	VAL	N-CA-CB	6.31	118.16	109.84
10	3	187	TYR	CA-CB-CG	-6.30	102.56	113.90
5	e	83	HIS	CE1-NE2-CD2	-6.30	102.70	109.00
6	f	6	ASP	CA-C-N	6.30	131.57	120.74
6	f	6	ASP	C-N-CA	6.30	131.57	120.74
7	g	105	ILE	CA-C-N	6.30	125.92	119.56
7	g	105	ILE	C-N-CA	6.30	125.92	119.56
13	6	76	HIS	N-CA-C	6.30	119.81	111.75
9	2	75	ARG	CA-C-N	6.29	128.62	120.56
9	2	75	ARG	C-N-CA	6.29	128.62	120.56
2	b	99	ARG	O-C-N	6.29	129.34	122.11
7	g	57	PRO	CA-C-N	6.29	133.54	121.54
7	g	57	PRO	C-N-CA	6.29	133.54	121.54
5	e	128	ARG	CA-C-O	-6.28	113.50	119.91
15	H	242	PRO	N-CA-C	6.28	118.36	110.70
14	7	112	ASN	CA-C-N	6.28	132.41	122.62
14	7	112	ASN	C-N-CA	6.28	132.41	122.62
20	J	150	VAL	O-C-N	6.28	127.87	122.16
12	l	89	GLN	OE1-CD-NE2	6.27	128.87	122.60
8	h	28	ASN	CA-CB-CG	6.26	118.86	112.60
2	b	218	ASN	CA-C-O	-6.26	112.31	119.32
12	5	184	GLY	O-C-N	-6.26	116.95	123.58
13	6	70	ASN	CA-CB-CG	-6.26	106.34	112.60
9	i	35	HIS	CE1-NE2-CD2	-6.25	102.75	109.00
2	b	136	ILE	CA-CB-CG2	-6.24	99.89	110.50
1	a	63	ILE	N-CA-C	-6.24	99.44	108.17
4	D	137	ASP	CA-CB-CG	-6.24	106.36	112.60
5	e	18	TYR	O-C-N	-6.23	114.93	122.22
3	c	103	GLU	N-CA-C	-6.22	99.27	108.79
4	d	108	THR	CA-C-O	-6.22	114.29	120.70
9	i	116	HIS	CE1-NE2-CD2	-6.22	102.78	109.00
3	c	194	LYS	O-C-N	-6.22	115.53	122.12
5	e	94	TYR	N-CA-C	6.22	120.70	113.18
8	1	153	ASP	O-C-N	-6.21	113.95	122.46
14	7	152	ASN	CA-C-O	-6.21	111.66	120.16
9	i	160	GLN	CA-C-N	6.20	128.50	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	i	160	GLN	C-N-CA	6.20	128.50	120.44
6	F	180	LYS	O-C-N	-6.20	113.90	122.46
9	2	184	ALA	O-C-N	-6.20	115.95	122.96
2	b	190	HIS	ND1-CE1-NE2	6.20	114.59	108.40
9	i	35	HIS	ND1-CE1-NE2	6.19	114.59	108.40
2	b	94	HIS	CE1-NE2-CD2	-6.18	102.82	109.00
6	f	98	PHE	CB-CA-C	-6.18	100.27	110.72
14	7	139	SER	N-CA-CB	6.18	117.08	111.27
7	g	11	PHE	N-CA-CB	6.17	119.15	109.83
1	a	10	PHE	N-CA-CB	6.17	119.15	109.83
4	D	72	SER	N-CA-C	-6.17	99.67	109.23
7	g	73	VAL	CA-C-O	-6.17	114.74	121.28
11	k	121	TYR	CA-C-N	6.17	128.54	120.28
11	k	121	TYR	C-N-CA	6.17	128.54	120.28
3	c	106	PRO	CA-C-N	6.16	128.90	120.46
3	c	106	PRO	C-N-CA	6.16	128.90	120.46
7	g	79	PRO	CA-C-N	6.16	128.86	120.54
7	g	79	PRO	C-N-CA	6.16	128.86	120.54
9	i	90	TYR	N-CA-C	6.16	120.82	112.88
12	l	66	HIS	CE1-NE2-CD2	-6.16	102.84	109.00
12	l	166	HIS	CA-C-O	-6.16	114.03	120.55
3	c	96	ASN	CA-C-N	6.15	128.85	120.54
3	c	96	ASN	C-N-CA	6.15	128.85	120.54
13	6	88	SER	CA-C-N	6.15	130.05	120.82
13	6	88	SER	C-N-CA	6.15	130.05	120.82
13	6	108	HIS	ND1-CE1-NE2	6.15	114.55	108.40
9	i	141	HIS	CE1-NE2-CD2	-6.14	102.86	109.00
10	3	141	ALA	N-CA-C	-6.14	103.16	110.41
1	A	137	VAL	O-C-N	-6.14	116.16	122.30
5	e	205	ASP	O-C-N	-6.14	116.81	123.26
2	b	22	ASP	CA-C-N	6.14	128.50	120.28
2	b	22	ASP	C-N-CA	6.14	128.50	120.28
1	A	62	TYR	N-CA-C	-6.13	103.96	112.30
2	b	170	ALA	CA-C-N	6.13	129.33	120.38
2	b	170	ALA	C-N-CA	6.13	129.33	120.38
7	g	112	LEU	CB-CA-C	-6.13	100.27	110.68
19	M	134	LEU	CA-C-O	6.12	126.91	120.42
3	c	190	GLU	N-CA-C	6.12	117.95	111.28
12	l	191	HIS	CE1-NE2-CD2	-6.12	102.88	109.00
2	b	55	LEU	CA-C-N	6.12	129.81	120.82
2	b	55	LEU	C-N-CA	6.12	129.81	120.82
6	F	110	LEU	N-CA-C	6.12	117.95	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	3	134	ASP	N-CA-C	-6.11	102.24	111.34
8	1	38	HIS	N-CA-C	-6.11	99.68	108.60
20	J	317	PRO	N-CA-CB	-6.11	100.04	103.22
11	4	2	ASP	CA-CB-CG	6.10	118.70	112.60
1	A	83	ASN	CA-C-N	6.09	128.94	120.29
1	A	83	ASN	C-N-CA	6.09	128.94	120.29
12	l	66	HIS	CA-C-O	6.09	126.98	120.10
8	1	81	VAL	CA-C-N	6.09	129.26	120.79
8	1	81	VAL	C-N-CA	6.09	129.26	120.79
2	b	20	GLN	CA-C-N	6.09	128.81	120.46
2	b	20	GLN	C-N-CA	6.09	128.81	120.46
4	D	6	LEU	N-CA-C	-6.09	105.81	113.72
4	D	10	SER	N-CA-C	-6.08	102.39	109.93
2	b	191	ILE	CA-C-O	-6.08	114.41	120.85
8	h	94	THR	CA-CB-OG1	6.08	118.72	109.60
12	5	46	ALA	N-CA-C	-6.08	100.09	109.14
3	c	62	THR	N-CA-C	-6.07	97.55	108.48
5	e	165	GLY	N-CA-C	-6.07	104.89	111.21
9	2	74	PRO	CA-C-O	-6.07	114.70	121.32
3	c	151	ASN	CA-C-N	6.07	126.19	119.87
3	c	151	ASN	C-N-CA	6.07	126.19	119.87
2	b	195	THR	N-CA-CB	6.07	119.04	110.12
8	1	108	GLY	CA-C-O	-6.07	116.12	121.58
6	f	12	PHE	CA-CB-CG	6.07	119.86	113.80
7	g	80	ASP	CA-C-N	6.06	126.71	119.98
7	g	80	ASP	C-N-CA	6.06	126.71	119.98
5	E	97	GLU	CA-C-N	6.06	129.37	120.82
5	E	97	GLU	C-N-CA	6.06	129.37	120.82
5	e	109	CYS	CA-C-N	6.05	129.00	120.28
5	e	109	CYS	C-N-CA	6.05	129.00	120.28
19	M	197	ILE	O-C-N	6.05	127.36	121.98
6	F	68	HIS	CB-CG-CD2	-6.05	123.34	131.20
7	G	88	GLY	CA-C-N	6.05	128.70	120.54
7	G	88	GLY	C-N-CA	6.05	128.70	120.54
6	f	103	ALA	CA-C-O	-6.04	114.39	121.16
13	m	110	ILE	N-CA-C	-6.04	99.42	108.12
14	n	97	ALA	CA-C-O	-6.04	113.95	121.02
10	3	142	SER	CA-C-N	6.04	128.37	120.28
10	3	142	SER	C-N-CA	6.04	128.37	120.28
10	j	201	MET	CB-CG-SD	-6.03	94.60	112.70
9	i	109	HIS	ND1-CE1-NE2	6.03	114.43	108.40
14	7	180	ALA	CA-C-N	6.03	128.36	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	7	180	ALA	C-N-CA	6.03	128.36	120.28
3	c	91	ARG	N-CA-CB	6.03	118.92	109.94
12	5	162	LEU	CA-C-N	6.03	129.17	120.79
12	5	162	LEU	C-N-CA	6.03	129.17	120.79
20	J	272	MET	CB-CA-C	-6.03	100.73	110.74
12	5	82	ILE	CA-C-N	6.02	129.85	120.82
12	5	82	ILE	C-N-CA	6.02	129.85	120.82
3	c	2	SER	CA-C-N	6.02	128.26	120.44
3	c	2	SER	C-N-CA	6.02	128.26	120.44
8	1	75	THR	O-C-N	6.02	128.50	122.12
6	f	63	ILE	CA-C-O	6.02	126.97	120.53
12	l	136	ALA	CA-C-O	-6.01	114.49	120.80
4	d	149	GLU	CA-C-O	-6.01	114.69	120.64
5	e	160	ASN	CA-CB-CG	-6.00	106.60	112.60
3	C	81	ALA	O-C-N	6.00	128.25	122.07
2	B	105	PRO	CA-C-O	-6.00	115.99	120.73
6	F	109	HIS	CG-CD2-NE2	6.00	113.20	107.20
7	g	200	HIS	CE1-NE2-CD2	-6.00	103.00	109.00
13	m	40	GLU	O-C-N	-6.00	114.42	121.32
5	e	17	GLU	CA-C-N	6.00	128.91	120.28
5	e	17	GLU	C-N-CA	6.00	128.91	120.28
4	D	78	ALA	CA-C-N	5.99	129.42	120.31
4	D	78	ALA	C-N-CA	5.99	129.42	120.31
14	n	88	GLU	CA-C-N	5.99	125.19	118.97
14	n	88	GLU	C-N-CA	5.99	125.19	118.97
1	A	9	ILE	N-CA-C	5.98	116.57	110.05
14	7	108	ASN	CA-CB-CG	-5.98	106.62	112.60
13	m	142	ALA	CB-CA-C	-5.98	100.14	110.72
5	e	168	SER	CA-C-N	5.98	129.40	120.31
5	e	168	SER	C-N-CA	5.98	129.40	120.31
9	i	3	ILE	N-CA-C	-5.98	98.87	107.78
14	7	43	ILE	CA-C-O	-5.98	114.84	119.20
13	m	126	ASP	N-CA-C	-5.98	102.54	110.07
2	B	104	TYR	O-C-N	-5.97	114.85	121.66
1	A	215	GLU	N-CA-CB	5.97	121.13	110.80
8	1	80	SER	CA-C-O	-5.97	112.27	119.49
18	L	349	ILE	N-CA-C	-5.95	103.51	108.63
7	G	101	THR	N-CA-C	-5.95	96.67	109.81
6	F	203	GLU	N-CA-C	-5.94	98.17	108.69
8	h	47	GLY	O-C-N	-5.94	117.79	122.90
10	3	164	GLU	N-CA-CB	5.94	118.85	110.12
10	j	80	ALA	N-CA-CB	5.93	120.24	110.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	6	108	HIS	N-CA-C	-5.93	97.47	108.02
14	7	122	ASN	CA-C-O	5.93	126.69	119.11
12	5	35	ILE	O-C-N	-5.92	117.64	122.97
8	h	9	LYS	CB-CA-C	-5.92	100.96	110.79
6	f	92	ASN	CA-CB-CG	-5.92	106.68	112.60
6	F	205	LEU	O-C-N	5.92	129.94	123.13
11	4	33	ASP	N-CA-CB	5.91	118.66	109.97
5	E	2	ARG	NH1-CZ-NH2	5.91	126.98	119.30
10	3	158	GLU	CA-C-N	5.91	126.32	119.47
10	3	158	GLU	C-N-CA	5.91	126.32	119.47
2	B	148	TYR	O-C-N	-5.90	116.66	123.33
4	D	80	SER	CA-C-N	5.90	129.00	120.38
4	D	80	SER	C-N-CA	5.90	129.00	120.38
7	g	200	HIS	CG-CD2-NE2	5.90	113.10	107.20
3	C	236	ASP	CA-CB-CG	-5.90	106.70	112.60
6	F	147	GLN	CA-C-N	5.90	125.77	119.28
6	F	147	GLN	C-N-CA	5.90	125.77	119.28
13	6	141	ALA	N-CA-C	5.89	117.70	111.28
6	f	162	ALA	N-CA-C	5.89	118.79	109.96
13	m	47	GLY	O-C-N	5.89	130.36	122.70
3	C	84	GLU	CA-C-N	5.89	128.49	120.77
3	C	84	GLU	C-N-CA	5.89	128.49	120.77
1	a	200	HIS	CE1-NE2-CD2	-5.88	103.12	109.00
4	d	4	ARG	CA-C-N	5.88	129.73	121.02
4	d	4	ARG	C-N-CA	5.88	129.73	121.02
2	B	25	LEU	N-CA-C	5.88	118.17	111.11
10	3	154	GLU	CA-C-N	5.88	125.79	119.85
10	3	154	GLU	C-N-CA	5.88	125.79	119.85
14	n	74	ASN	OD1-CG-ND2	-5.88	116.72	122.60
3	c	93	HIS	CE1-NE2-CD2	-5.88	103.12	109.00
1	a	116	SER	N-CA-CB	5.87	118.48	109.91
4	D	12	ASP	N-CA-C	-5.87	105.70	112.92
2	B	219	PRO	CA-C-O	5.87	125.61	118.92
4	d	231	VAL	CA-C-N	5.86	128.06	120.44
4	d	231	VAL	C-N-CA	5.86	128.06	120.44
5	e	91	HIS	CG-CD2-NE2	5.86	113.06	107.20
5	E	99	ILE	CA-C-O	-5.86	114.96	121.23
19	M	154	LEU	N-CA-CB	5.86	121.60	111.00
13	6	44	PHE	CA-C-N	5.86	129.19	120.87
13	6	44	PHE	C-N-CA	5.86	129.19	120.87
10	3	154	GLU	O-C-N	-5.85	116.77	121.80
5	E	124	ARG	CB-CG-CD	5.85	124.75	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	c	93	HIS	CG-CD2-NE2	5.85	113.05	107.20
2	b	218	ASN	CA-C-N	5.84	127.78	121.00
2	b	218	ASN	C-N-CA	5.84	127.78	121.00
3	C	16	GLY	N-CA-C	-5.84	107.26	115.32
10	j	200	LYS	CA-C-N	-5.84	111.64	121.75
10	j	200	LYS	C-N-CA	-5.84	111.64	121.75
14	n	190	ARG	CG-CD-NE	-5.84	99.14	112.00
7	g	83	HIS	ND1-CE1-NE2	5.84	114.24	108.40
2	b	101	TYR	N-CA-CB	5.83	120.34	110.49
10	3	145	LEU	CA-C-N	5.83	128.41	120.54
10	3	145	LEU	C-N-CA	5.83	128.41	120.54
10	3	20	VAL	CA-C-O	-5.83	116.31	121.09
9	i	29	LYS	N-CA-CB	5.83	118.69	110.12
1	a	56	ASP	CA-C-N	5.82	126.33	120.04
1	a	56	ASP	C-N-CA	5.82	126.33	120.04
2	b	113	GLU	CA-C-O	-5.82	114.71	120.70
9	i	55	VAL	CA-C-N	5.82	128.07	120.28
9	i	55	VAL	C-N-CA	5.82	128.07	120.28
13	6	141	ALA	CA-C-O	-5.81	114.39	120.55
1	a	78	ILE	CA-C-N	5.81	127.10	119.84
1	a	78	ILE	C-N-CA	5.81	127.10	119.84
7	g	222	GLY	N-CA-C	-5.81	107.37	114.92
9	2	139	GLU	N-CA-C	5.81	119.84	112.87
6	f	32	SER	CA-C-N	5.80	128.98	120.91
6	f	32	SER	C-N-CA	5.80	128.98	120.91
4	D	89	VAL	O-C-N	5.80	127.74	121.94
13	m	81	ASP	N-CA-CB	5.80	120.29	110.49
13	m	88	SER	CA-C-N	5.80	128.05	120.28
13	m	88	SER	C-N-CA	5.80	128.05	120.28
9	2	217	ILE	O-C-N	-5.80	116.92	123.18
5	e	154	GLY	CA-C-O	5.80	124.22	118.77
9	2	220	ILE	CA-C-O	5.80	128.03	120.78
11	4	56	PHE	CA-CB-CG	-5.80	108.00	113.80
3	C	220	ASN	CA-CB-CG	-5.79	106.81	112.60
8	1	103	ASP	N-CA-C	-5.79	100.70	109.85
12	l	135	PHE	CA-CB-CG	-5.79	108.01	113.80
11	4	195	PHE	CA-CB-CG	-5.79	108.01	113.80
2	b	89	SER	CA-C-N	5.79	128.35	120.54
2	b	89	SER	C-N-CA	5.79	128.35	120.54
3	c	17	ARG	N-CA-C	-5.79	100.70	108.86
10	3	118	PRO	CB-CA-C	5.79	118.91	111.21
4	D	102	VAL	O-C-N	5.78	128.57	122.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	g	87	ARG	NE-CZ-NH1	-5.77	115.73	121.50
14	7	4	PRO	CA-C-O	-5.77	115.06	121.23
7	g	9	SER	N-CA-C	5.77	119.35	111.39
2	B	29	LYS	O-C-N	-5.77	114.70	122.43
3	c	114	LEU	N-CA-C	5.76	118.34	111.71
2	B	190	HIS	ND1-CE1-NE2	5.76	114.17	108.40
3	C	115	SER	CA-CB-OG	5.76	122.63	111.10
2	b	107	THR	N-CA-CB	5.76	118.58	109.82
5	e	117	GLU	CA-C-N	5.76	131.47	120.07
5	e	117	GLU	C-N-CA	5.76	131.47	120.07
6	F	103	ALA	N-CA-CB	5.76	118.44	109.97
13	6	12	ILE	CA-CB-CG1	5.76	120.19	110.40
13	m	37	SER	N-CA-C	-5.75	99.96	108.99
15	H	269	ALA	N-CA-C	-5.75	100.52	109.72
13	m	161	GLU	CA-C-N	5.74	126.03	119.83
13	m	161	GLU	C-N-CA	5.74	126.03	119.83
16	I	67	ASP	CA-CB-CG	-5.74	106.86	112.60
2	b	139	HIS	CB-CA-C	-5.74	102.30	110.34
9	i	64	GLU	N-CA-CB	5.74	118.62	110.13
18	L	207	PHE	CA-CB-CG	-5.74	108.06	113.80
11	k	136	SER	CA-C-O	-5.74	114.80	120.82
7	G	126	ARG	CA-C-N	5.74	126.02	119.83
7	G	126	ARG	C-N-CA	5.74	126.02	119.83
3	C	161	ALA	O-C-N	-5.73	117.24	123.26
5	E	23	ILE	O-C-N	5.73	127.53	121.91
8	l	154	PHE	CA-CB-CG	5.73	119.53	113.80
2	b	12	PHE	CA-CB-CG	-5.73	108.07	113.80
1	A	73	VAL	N-CA-CB	5.72	116.96	110.72
2	B	113	GLU	CB-CA-C	-5.72	101.29	110.79
6	F	114	LYS	CB-CA-C	-5.72	100.22	110.70
14	n	67	LEU	CA-C-O	-5.72	114.81	120.70
16	I	280	PHE	CA-CB-CG	5.72	119.52	113.80
12	5	75	SER	N-CA-CB	5.72	118.41	110.17
11	k	70	ARG	O-C-N	-5.72	115.23	122.27
5	e	130	PHE	N-CA-C	5.71	118.12	110.35
15	H	271	PHE	CA-CB-CG	-5.71	108.08	113.80
3	C	88	ASN	CA-C-N	5.71	128.40	120.29
3	C	88	ASN	C-N-CA	5.71	128.40	120.29
4	D	195	ARG	NE-CZ-NH2	5.71	124.34	119.20
10	j	128	CYS	CA-C-N	5.71	128.74	120.98
10	j	128	CYS	C-N-CA	5.71	128.74	120.98
2	b	81	ASP	CA-CB-CG	-5.70	106.90	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	164	SER	CA-C-N	5.70	128.19	120.38
6	F	164	SER	C-N-CA	5.70	128.19	120.38
9	i	59	ILE	N-CA-C	-5.70	105.26	113.07
10	j	37	ASN	CA-CB-CG	5.70	118.30	112.60
3	C	93	HIS	CE1-NE2-CD2	-5.70	103.30	109.00
7	G	116	VAL	CA-C-N	5.70	128.70	120.38
7	G	116	VAL	C-N-CA	5.70	128.70	120.38
5	E	2	ARG	NE-CZ-NH1	-5.69	115.81	121.50
13	m	44	PHE	CA-CB-CG	-5.69	108.11	113.80
20	J	30	THR	CA-C-N	5.69	128.37	120.29
20	J	30	THR	C-N-CA	5.69	128.37	120.29
7	G	108	PHE	CA-CB-CG	-5.68	108.11	113.80
13	6	103	PHE	N-CA-C	-5.68	97.26	109.81
1	a	15	ARG	CG-CD-NE	5.67	124.48	112.00
3	c	136	TYR	N-CA-CB	5.67	119.48	110.57
11	4	120	ASP	CA-CB-CG	-5.67	106.93	112.60
12	l	90	TYR	CB-CA-C	-5.67	104.19	111.22
2	B	32	VAL	O-C-N	-5.67	116.78	122.62
14	n	71	VAL	CA-C-N	5.66	127.87	120.28
14	n	71	VAL	C-N-CA	5.66	127.87	120.28
3	C	146	GLN	N-CA-C	-5.66	100.45	109.23
10	3	43	PHE	N-CA-C	-5.66	101.14	109.81
11	k	122	LEU	N-CA-C	-5.66	105.11	111.28
5	E	78	ARG	CA-C-O	-5.66	114.55	120.55
7	G	204	LYS	CA-C-N	5.66	128.12	120.65
7	G	204	LYS	C-N-CA	5.66	128.12	120.65
14	7	186	TYR	O-C-N	5.66	128.14	122.03
8	h	47	GLY	N-CA-C	-5.65	103.91	112.84
6	f	215	VAL	N-CA-C	-5.65	99.64	108.86
2	b	191	ILE	O-C-N	5.65	127.65	121.83
5	E	192	VAL	CB-CA-C	-5.65	104.74	111.97
16	I	260	GLY	CA-C-N	5.65	126.02	119.47
16	I	260	GLY	C-N-CA	5.65	126.02	119.47
10	j	104	VAL	N-CA-C	-5.64	101.94	108.82
2	B	16	GLY	CA-C-N	5.64	132.31	121.54
2	B	16	GLY	C-N-CA	5.64	132.31	121.54
8	1	78	ALA	CA-C-N	5.64	128.09	120.65
8	1	78	ALA	C-N-CA	5.64	128.09	120.65
13	m	48	ASP	CA-C-N	5.64	130.13	122.07
13	m	48	ASP	C-N-CA	5.64	130.13	122.07
14	7	229	GLY	CA-C-O	-5.64	108.96	120.80
2	b	89	SER	CA-C-O	-5.63	114.90	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	e	150	ALA	CB-CA-C	-5.63	101.36	110.77
13	m	75	TYR	CA-C-O	-5.63	115.10	120.90
1	A	6	HIS	CE1-NE2-CD2	-5.63	103.36	109.00
3	C	130	PHE	CB-CA-C	-5.63	100.37	109.72
7	G	109	ALA	CA-C-O	-5.63	114.90	120.82
6	F	107	ALA	CA-C-N	5.63	126.19	119.94
6	F	107	ALA	C-N-CA	5.63	126.19	119.94
8	h	18	SER	N-CA-C	-5.63	104.21	113.50
8	l	120	HIS	N-CA-CB	5.63	119.97	110.79
10	j	47	HIS	CE1-NE2-CD2	-5.63	103.37	109.00
13	6	79	HIS	CA-C-N	5.63	130.35	122.36
13	6	79	HIS	C-N-CA	5.63	130.35	122.36
1	A	99	TYR	N-CA-C	-5.62	106.09	114.64
7	G	30	GLY	N-CA-C	5.62	118.52	112.33
20	J	258	VAL	CB-CA-C	-5.62	104.46	112.22
2	b	24	ALA	CA-C-O	-5.62	114.59	120.55
5	E	21	GLU	CA-C-N	5.62	128.38	120.28
5	E	21	GLU	C-N-CA	5.62	128.38	120.28
7	G	191	GLN	CA-C-N	5.62	127.75	120.44
7	G	191	GLN	C-N-CA	5.62	127.75	120.44
2	b	4	ARG	NE-CZ-NH2	5.62	124.26	119.20
6	F	8	ASP	CA-CB-CG	5.62	118.22	112.60
14	7	115	ILE	N-CA-C	-5.62	100.39	108.53
5	e	148	PHE	CA-CB-CG	-5.61	108.19	113.80
11	k	41	HIS	CA-CB-CG	-5.61	108.19	113.80
4	D	215	PRO	N-CA-CB	5.61	108.55	103.33
3	C	102	ASN	CA-C-N	5.61	130.67	121.58
3	C	102	ASN	C-N-CA	5.61	130.67	121.58
9	2	141	HIS	CG-CD2-NE2	5.61	112.81	107.20
8	l	126	ILE	N-CA-C	-5.61	100.15	108.45
1	a	90	ALA	CA-C-N	5.61	127.73	120.44
1	a	90	ALA	C-N-CA	5.61	127.73	120.44
5	e	91	HIS	CE1-NE2-CD2	-5.61	103.39	109.00
1	A	127	PRO	CA-C-O	-5.61	115.03	121.36
4	d	6	LEU	N-CA-C	-5.60	105.48	112.93
5	E	124	ARG	CB-CA-C	-5.60	101.72	110.74
14	7	110	LEU	N-CA-C	-5.60	99.39	108.41
6	f	115	ALA	CA-C-N	5.60	132.24	121.54
6	f	115	ALA	C-N-CA	5.60	132.24	121.54
10	j	44	HIS	CG-CD2-NE2	5.60	112.80	107.20
14	7	93	PHE	CA-CB-CG	-5.60	108.20	113.80
3	c	95	GLN	N-CA-C	5.60	118.11	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	K	269	ILE	CA-C-O	-5.60	114.58	120.57
4	D	94	HIS	N-CA-C	5.59	117.06	111.07
5	e	83	HIS	ND1-CE1-NE2	5.59	113.99	108.40
2	B	205	ASN	N-CA-C	-5.59	100.44	108.60
11	4	80	VAL	CA-C-N	5.59	127.71	120.44
11	4	80	VAL	C-N-CA	5.59	127.71	120.44
11	4	100	VAL	CA-C-O	5.59	126.21	120.96
10	j	64	GLU	N-CA-C	-5.59	106.42	113.18
15	H	319	PHE	CA-CB-CG	5.59	119.39	113.80
7	g	103	ILE	N-CA-CB	5.58	115.27	110.08
3	C	180	LYS	CA-C-O	-5.58	114.69	121.28
5	E	136	ILE	N-CA-C	-5.58	99.85	107.99
5	E	132	VAL	N-CA-C	-5.58	100.19	107.88
13	6	79	HIS	ND1-CE1-NE2	5.58	113.98	108.40
9	i	155	ALA	CA-C-O	-5.57	114.97	120.82
6	f	172	GLU	N-CA-C	-5.57	106.32	113.23
8	h	8	PHE	CA-C-N	5.57	127.74	120.28
8	h	8	PHE	C-N-CA	5.57	127.74	120.28
6	F	23	TYR	CA-C-N	5.57	128.01	120.38
6	F	23	TYR	C-N-CA	5.57	128.01	120.38
2	B	159	TRP	CA-C-N	5.57	128.19	120.29
2	B	159	TRP	C-N-CA	5.57	128.19	120.29
17	K	152	PRO	CA-N-CD	5.57	119.79	112.00
19	M	263	VAL	N-CA-C	5.57	115.76	110.53
8	h	115	LEU	CA-C-N	5.57	126.16	119.98
8	h	115	LEU	C-N-CA	5.57	126.16	119.98
5	e	12	ARG	N-CA-C	-5.56	101.94	109.95
8	h	166	ASP	CA-CB-CG	5.56	118.16	112.60
11	4	82	SER	CA-C-O	-5.56	114.95	120.90
14	7	43	ILE	O-C-N	-5.56	117.13	121.46
3	C	128	ARG	O-C-N	-5.56	115.53	121.42
5	E	4	VAL	CA-C-N	5.56	127.66	120.44
5	E	4	VAL	C-N-CA	5.56	127.66	120.44
14	n	138	SER	N-CA-C	-5.55	101.98	110.14
2	B	109	LEU	CB-CA-C	-5.55	101.42	110.85
3	C	234	ILE	CA-C-N	5.55	128.74	120.31
3	C	234	ILE	C-N-CA	5.55	128.74	120.31
14	7	6	VAL	N-CA-C	-5.54	99.16	107.37
2	B	113	GLU	N-CA-CB	5.54	118.27	110.12
13	6	103	PHE	CA-CB-CG	-5.54	108.26	113.80
7	G	93	ALA	CA-C-N	5.54	127.70	120.28
7	G	93	ALA	C-N-CA	5.54	127.70	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	132	LEU	CA-C-O	-5.54	114.86	120.84
19	M	426	LYS	CA-C-N	5.54	132.11	121.54
19	M	426	LYS	C-N-CA	5.54	132.11	121.54
5	E	149	HIS	CG-CD2-NE2	5.53	112.73	107.20
8	1	133	PHE	CA-CB-CG	-5.53	108.27	113.80
1	a	79	PRO	CA-N-CD	-5.53	104.26	112.00
5	e	83	HIS	CA-C-N	5.53	127.95	120.65
5	e	83	HIS	C-N-CA	5.53	127.95	120.65
11	4	38	LEU	N-CA-C	-5.53	104.16	111.96
7	G	109	ALA	O-C-N	5.53	127.76	122.07
7	g	154	TRP	CA-C-N	5.53	126.18	120.60
7	g	154	TRP	C-N-CA	5.53	126.18	120.60
12	l	46	ALA	N-CA-CB	5.53	120.89	111.66
1	A	73	VAL	CA-C-O	-5.52	114.47	120.71
4	D	153	ILE	N-CA-C	-5.52	104.03	110.05
6	f	77	ALA	CA-C-N	5.52	124.71	118.97
6	f	77	ALA	C-N-CA	5.52	124.71	118.97
8	1	82	PHE	O-C-N	5.52	127.98	122.08
12	5	28	SER	CB-CA-C	-5.52	101.11	109.99
7	g	185	ALA	N-CA-C	5.51	116.98	110.97
5	E	224	ASP	N-CA-C	-5.51	102.32	110.48
17	K	281	ARG	CB-CA-C	-5.51	101.32	110.14
12	l	188	HIS	CE1-NE2-CD2	-5.51	103.49	109.00
6	F	70	GLY	N-CA-C	-5.51	102.23	110.38
10	j	1	SER	O-C-N	-5.51	114.19	123.00
6	f	127	TYR	CA-C-O	-5.50	114.11	120.49
20	J	318	PRO	CA-N-CD	5.50	119.70	112.00
7	G	215	CYS	CA-C-O	-5.50	114.42	120.24
11	4	2	ASP	CA-C-N	5.50	129.81	122.01
11	4	2	ASP	C-N-CA	5.50	129.81	122.01
11	k	70	ARG	CA-C-O	5.49	126.29	119.97
9	i	17	ASP	CA-C-N	5.49	130.85	122.23
9	i	17	ASP	C-N-CA	5.49	130.85	122.23
9	i	131	SER	O-C-N	-5.49	115.29	122.59
2	B	93	ALA	CA-C-N	5.49	127.63	120.28
2	B	93	ALA	O-C-N	-5.49	116.42	122.07
2	B	93	ALA	C-N-CA	5.49	127.63	120.28
5	E	218	ASP	CA-CB-CG	-5.48	107.12	112.60
8	1	109	GLU	N-CA-C	-5.48	100.73	109.23
8	1	160	SER	O-C-N	-5.48	115.90	122.15
12	5	95	LEU	O-C-N	-5.48	116.77	122.96
1	a	184	HIS	CE1-NE2-CD2	-5.48	103.52	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	e	83	HIS	O-C-N	5.48	128.39	122.15
13	6	87	ASN	CB-CA-C	-5.48	101.70	110.79
11	4	32	ASP	N-CA-C	-5.47	99.14	110.80
3	c	170	ALA	N-CA-C	5.46	117.24	111.28
9	i	8	PHE	CA-C-N	5.46	127.87	120.38
9	i	8	PHE	C-N-CA	5.46	127.87	120.38
1	A	66	ILE	N-CA-C	5.46	115.71	110.74
9	i	109	HIS	CA-CB-CG	-5.46	108.34	113.80
14	n	67	LEU	CA-C-N	5.46	128.36	120.38
14	n	67	LEU	C-N-CA	5.46	128.36	120.38
1	a	19	VAL	CA-CB-CG2	-5.46	101.11	110.40
3	c	223	GLU	N-CA-CB	5.46	118.12	109.71
11	4	13	VAL	N-CA-CB	5.46	117.55	110.99
3	C	69	ASN	N-CA-C	-5.46	100.54	108.07
16	I	273	GLU	CA-C-O	5.46	126.39	120.55
10	j	59	VAL	CA-C-O	-5.45	115.39	121.17
10	3	145	LEU	CA-C-O	-5.45	115.06	120.90
6	f	184	ASN	N-CA-CB	5.45	117.85	111.09
12	5	29	GLN	N-CA-C	-5.45	104.90	113.02
12	5	98	GLY	N-CA-C	-5.45	100.27	113.18
5	e	4	VAL	N-CA-CB	5.44	117.17	110.64
9	2	41	ILE	N-CA-C	-5.44	98.02	109.34
11	k	122	LEU	CA-C-O	5.44	126.32	120.55
13	m	133	ARG	N-CA-CB	5.44	118.10	109.51
5	E	190	LEU	CA-C-N	5.43	128.01	120.29
5	E	190	LEU	C-N-CA	5.43	128.01	120.29
7	G	149	PRO	CA-C-N	5.43	127.56	120.28
7	G	149	PRO	C-N-CA	5.43	127.56	120.28
6	f	88	ARG	CA-C-N	5.43	127.87	120.54
6	f	88	ARG	C-N-CA	5.43	127.87	120.54
14	n	18	ASN	OD1-CG-ND2	-5.43	117.17	122.60
4	D	89	VAL	CA-C-N	5.43	127.87	120.54
4	D	89	VAL	C-N-CA	5.43	127.87	120.54
3	c	185	VAL	CB-CA-C	-5.43	103.31	112.16
4	d	136	PHE	CA-C-N	5.42	128.03	120.65
4	d	136	PHE	C-N-CA	5.42	128.03	120.65
3	C	108	GLU	CA-C-N	5.42	127.48	120.70
3	C	108	GLU	C-N-CA	5.42	127.48	120.70
13	6	93	ILE	N-CA-C	-5.42	104.67	110.36
1	A	17	TYR	CA-C-N	5.42	127.86	120.54
1	A	17	TYR	C-N-CA	5.42	127.86	120.54
3	c	119	GLN	CA-C-O	5.42	126.48	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	K	271	ILE	CA-C-N	5.42	127.54	120.28
17	K	271	ILE	C-N-CA	5.42	127.54	120.28
8	h	162	ALA	CA-C-N	5.41	127.38	120.56
8	h	162	ALA	C-N-CA	5.41	127.38	120.56
6	F	88	ARG	N-CA-CB	5.41	117.81	109.91
7	g	83	HIS	CE1-NE2-CD2	-5.41	103.59	109.00
2	B	128	ARG	CA-C-N	5.41	126.60	119.84
2	B	128	ARG	C-N-CA	5.41	126.60	119.84
3	C	116	ASP	CA-CB-CG	-5.41	107.19	112.60
7	G	107	ALA	CA-C-N	5.41	127.53	120.28
7	G	107	ALA	C-N-CA	5.41	127.53	120.28
14	7	78	ASN	O-C-N	-5.41	115.10	121.32
5	e	157	TYR	CA-C-N	5.40	128.54	120.87
5	e	157	TYR	C-N-CA	5.40	128.54	120.87
14	n	77	ASP	CA-CB-CG	-5.40	107.20	112.60
17	K	242	PHE	CA-CB-CG	-5.40	108.40	113.80
1	a	19	VAL	CA-C-O	-5.40	115.66	121.27
5	E	169	GLU	N-CA-C	-5.39	104.82	111.40
4	d	84	ILE	CA-C-N	-5.39	111.36	120.58
4	d	84	ILE	C-N-CA	-5.39	111.36	120.58
8	h	9	LYS	N-CA-C	5.39	117.16	111.28
11	k	41	HIS	CE1-NE2-CD2	-5.39	103.61	109.00
13	m	126	ASP	CA-CB-CG	-5.39	107.21	112.60
5	E	118	GLY	CA-C-O	5.39	125.82	119.46
5	E	108	VAL	CA-C-N	5.39	128.04	120.28
5	E	108	VAL	C-N-CA	5.39	128.04	120.28
11	4	113	LYS	O-C-N	-5.39	115.12	121.32
4	D	117	ARG	CD-NE-CZ	-5.39	116.86	124.40
13	m	79	HIS	CA-C-O	-5.38	113.43	119.95
5	E	136	ILE	N-CA-CB	5.38	117.51	111.21
13	m	94	GLN	N-CA-CB	5.38	118.61	110.28
10	j	110	GLY	N-CA-C	-5.38	103.39	111.19
11	k	80	VAL	CA-C-N	5.38	127.49	120.28
11	k	80	VAL	C-N-CA	5.38	127.49	120.28
12	5	4	LEU	CA-C-O	5.37	127.13	121.33
3	C	12	PHE	CB-CA-C	-5.37	99.58	109.46
11	4	32	ASP	N-CA-CB	5.37	119.57	110.49
18	L	141	LYS	N-CA-CB	5.37	119.73	111.46
1	a	136	SER	N-CA-CB	5.37	120.59	111.57
14	7	184	LEU	CA-C-N	5.36	128.46	120.31
14	7	184	LEU	C-N-CA	5.36	128.46	120.31
14	7	25	ASP	CA-C-O	-5.36	115.88	121.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	c	137	ALA	CA-C-O	-5.36	115.03	120.71
9	i	141	HIS	N-CA-C	5.36	118.03	111.82
5	E	108	VAL	N-CA-CB	5.36	116.82	110.55
7	G	134	PHE	O-C-N	-5.36	117.37	123.48
10	3	152	LEU	CA-C-N	5.36	129.92	121.56
10	3	152	LEU	C-N-CA	5.36	129.92	121.56
9	i	93	HIS	O-C-N	-5.35	116.31	122.09
11	k	139	TYR	CB-CA-C	-5.35	99.55	109.29
14	7	9	THR	CA-C-N	5.35	131.76	121.54
14	7	9	THR	C-N-CA	5.35	131.76	121.54
13	m	57	PHE	CA-CB-CG	5.35	119.15	113.80
13	m	108	HIS	CA-C-O	-5.35	114.50	120.54
12	l	110	PRO	CB-CA-C	5.34	118.38	111.64
4	D	223	SER	CA-C-N	5.34	127.76	120.54
4	D	223	SER	C-N-CA	5.34	127.76	120.54
5	e	71	SER	N-CA-C	-5.34	99.98	109.06
1	a	200	HIS	ND1-CE1-NE2	5.34	113.74	108.40
14	n	155	LEU	CB-CA-C	-5.34	101.61	110.68
2	b	85	LEU	CA-C-N	5.33	128.90	120.47
2	b	85	LEU	C-N-CA	5.33	128.90	120.47
3	C	135	ILE	CA-C-O	-5.33	114.86	120.57
1	A	56	ASP	CA-C-N	5.33	125.02	119.64
1	A	56	ASP	C-N-CA	5.33	125.02	119.64
14	7	146	PHE	CA-CB-CG	-5.33	108.47	113.80
7	g	108	PHE	CA-C-N	5.33	129.69	120.58
7	g	108	PHE	C-N-CA	5.33	129.69	120.58
4	D	223	SER	N-CA-C	-5.33	102.16	110.42
1	a	149	ASP	CA-C-N	5.32	126.49	119.84
1	a	149	ASP	C-N-CA	5.32	126.49	119.84
12	l	101	ILE	N-CA-CB	5.32	116.52	110.72
2	B	112	SER	CA-C-N	5.32	127.41	120.28
2	B	112	SER	C-N-CA	5.32	127.41	120.28
15	H	363	PRO	N-CA-CB	5.32	108.41	103.46
5	e	110	ASP	CA-C-N	5.32	128.39	120.31
5	e	110	ASP	C-N-CA	5.32	128.39	120.31
11	4	93	ARG	CA-C-N	5.32	131.69	121.54
11	4	93	ARG	C-N-CA	5.32	131.69	121.54
14	7	213	GLN	CB-CG-CD	-5.31	103.57	112.60
18	L	149	ASP	CA-C-N	5.31	127.25	120.56
18	L	149	ASP	C-N-CA	5.31	127.25	120.56
5	e	18	TYR	CA-C-O	5.31	126.10	120.10
5	e	108	VAL	CA-C-O	5.31	126.57	121.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	f	103	ALA	N-CA-CB	5.31	117.78	109.97
13	6	74	TRP	CG-CD2-CE3	-5.31	128.59	133.90
9	2	141	HIS	CB-CG-ND1	5.30	130.65	122.70
12	5	187	TYR	CB-CG-CD1	5.30	128.75	120.80
14	7	171	GLN	CA-C-N	5.30	127.34	120.56
14	7	171	GLN	C-N-CA	5.30	127.34	120.56
3	c	69	ASN	CA-C-N	5.30	129.16	120.63
3	c	69	ASN	C-N-CA	5.30	129.16	120.63
5	e	168	SER	CA-C-O	-5.30	115.24	120.70
15	H	209	SER	CA-C-N	5.30	127.38	120.28
15	H	209	SER	C-N-CA	5.30	127.38	120.28
10	j	86	PHE	CA-CB-CG	-5.29	108.51	113.80
11	k	191	GLN	CB-CG-CD	-5.29	103.60	112.60
3	c	12	PHE	N-CA-CB	5.29	117.82	110.04
3	c	112	ARG	NE-CZ-NH2	5.29	123.96	119.20
9	i	124	TYR	N-CA-CB	5.29	119.32	110.59
11	4	150	PRO	N-CA-CB	-5.29	99.26	102.81
4	d	79	ASP	CB-CA-C	-5.29	102.01	110.79
4	d	111	VAL	CA-C-N	5.29	127.68	120.54
4	d	111	VAL	C-N-CA	5.29	127.68	120.54
7	g	95	PHE	CA-CB-CG	-5.29	108.51	113.80
7	g	128	PHE	CB-CA-C	-5.29	101.62	110.29
9	i	114	HIS	CE1-NE2-CD2	-5.29	103.71	109.00
11	k	191	GLN	CB-CA-C	-5.29	100.13	109.70
3	c	7	SER	CA-C-N	5.28	131.63	121.54
3	c	7	SER	C-N-CA	5.28	131.63	121.54
7	G	112	LEU	O-C-N	5.28	128.40	122.22
11	4	32	ASP	CA-CB-CG	-5.28	107.32	112.60
3	c	61	SER	N-CA-C	5.28	117.69	110.24
14	7	122	ASN	CA-CB-CG	-5.28	107.32	112.60
7	g	25	LYS	CA-C-O	5.28	126.14	120.55
3	C	71	LYS	CA-C-N	-5.28	115.10	122.75
3	C	71	LYS	C-N-CA	-5.28	115.10	122.75
10	3	103	PHE	CA-CB-CG	-5.27	108.53	113.80
18	L	349	ILE	N-CA-CB	5.27	115.87	110.23
6	F	39	SER	CA-C-O	-5.27	115.10	121.32
14	n	94	GLU	CB-CG-CD	-5.26	103.65	112.60
6	f	3	ASN	OD1-CG-ND2	-5.26	117.34	122.60
12	5	100	MET	N-CA-CB	5.26	118.81	110.55
14	7	48	ASN	CA-CB-CG	5.26	117.86	112.60
5	E	77	ALA	CA-C-N	5.26	127.33	120.28
5	E	77	ALA	C-N-CA	5.26	127.33	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	1	141	ASN	CB-CG-ND2	5.26	124.29	116.40
6	f	22	GLU	CA-C-N	5.26	129.57	120.58
6	f	22	GLU	C-N-CA	5.26	129.57	120.58
4	D	137	ASP	CA-C-N	5.26	125.56	119.93
4	D	137	ASP	C-N-CA	5.26	125.56	119.93
12	5	117	SER	N-CA-C	5.26	117.76	111.71
4	d	78	ALA	CA-C-N	5.26	127.32	120.28
4	d	78	ALA	C-N-CA	5.26	127.32	120.28
14	n	97	ALA	O-C-N	5.26	128.56	122.20
6	f	148	PRO	N-CA-C	-5.25	107.18	114.27
6	f	151	ASN	N-CA-CB	5.25	117.80	109.71
7	g	76	GLY	CA-C-O	-5.25	117.05	122.25
11	k	41	HIS	ND1-CE1-NE2	5.25	113.65	108.40
5	e	146	GLN	OE1-CD-NE2	5.25	127.85	122.60
10	3	127	GLY	CA-C-N	5.25	130.39	122.99
10	3	127	GLY	C-N-CA	5.25	130.39	122.99
13	6	40	GLU	N-CA-C	-5.25	98.20	109.81
14	7	114	ILE	O-C-N	-5.25	117.48	123.10
15	H	286	GLU	N-CA-CB	5.25	117.93	110.16
2	b	5	TYR	CA-CB-CG	-5.25	104.45	113.90
6	f	8	ASP	CA-C-O	-5.25	115.18	121.11
6	f	160	ILE	CA-C-O	-5.25	116.44	121.63
9	i	164	TRP	N-CA-CB	5.25	118.02	110.20
3	c	66	TYR	O-C-N	-5.24	116.96	123.36
10	j	115	SER	N-CA-C	-5.24	108.14	114.75
14	7	86	ALA	CA-C-N	5.24	131.55	121.54
14	7	86	ALA	C-N-CA	5.24	131.55	121.54
6	f	12	PHE	CA-C-N	5.24	128.65	120.68
6	f	12	PHE	C-N-CA	5.24	128.65	120.68
12	5	121	ARG	NE-CZ-NH1	5.24	126.74	121.50
1	a	70	ILE	CB-CA-C	-5.24	104.50	110.73
10	j	187	TYR	N-CA-CB	5.24	118.96	110.43
14	n	227	GLY	O-C-N	-5.24	115.89	122.70
10	3	176	ARG	O-C-N	-5.23	116.06	122.34
11	4	36	ARG	CA-C-N	5.23	128.20	120.82
11	4	36	ARG	C-N-CA	5.23	128.20	120.82
11	k	139	TYR	CA-CB-CG	-5.23	104.48	113.90
4	D	195	ARG	NE-CZ-NH1	-5.23	116.27	121.50
1	A	19	VAL	N-CA-C	-5.23	105.28	110.62
5	E	4	VAL	CB-CA-C	-5.23	105.00	112.22
4	d	112	ALA	N-CA-CB	5.23	117.73	109.94
5	E	66	ILE	CA-C-O	5.23	124.87	120.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	k	170	LYS	CB-CA-C	-5.23	102.67	110.88
6	F	6	ASP	CA-CB-CG	-5.23	107.37	112.60
17	K	363	ALA	CA-C-O	-5.22	115.01	120.70
3	c	63	GLU	N-CA-CB	5.22	119.31	110.49
2	B	7	PHE	CA-C-N	5.22	128.12	120.71
2	B	7	PHE	C-N-CA	5.22	128.12	120.71
1	A	26	THR	N-CA-C	5.22	117.38	111.02
12	5	104	TYR	CB-CG-CD2	-5.22	112.97	120.80
1	A	65	CYS	CB-CA-C	5.21	118.35	109.80
9	i	116	HIS	CA-CB-CG	-5.21	108.59	113.80
6	F	206	THR	N-CA-CB	5.20	118.68	110.56
1	A	6	HIS	CG-CD2-NE2	5.20	112.40	107.20
9	2	9	ASN	CA-CB-CG	-5.20	107.40	112.60
15	H	243	PRO	CA-N-CD	5.20	119.28	112.00
16	I	216	PRO	CA-N-CD	5.20	119.28	112.00
16	I	271	ALA	CA-C-O	-5.20	114.91	120.42
4	D	213	VAL	CA-C-O	5.19	125.84	120.39
14	7	56	ASP	CA-C-N	5.19	127.20	120.56
14	7	56	ASP	C-N-CA	5.19	127.20	120.56
8	h	129	SER	CB-CA-C	-5.18	102.04	110.85
13	m	94	GLN	CB-CA-C	-5.18	100.72	110.67
6	F	21	VAL	CA-C-N	5.18	127.23	120.28
6	F	21	VAL	C-N-CA	5.18	127.23	120.28
12	5	181	THR	CA-CB-OG1	5.18	117.38	109.60
3	C	190	GLU	CA-C-O	-5.18	114.93	120.42
9	2	86	HIS	CE1-NE2-CD2	-5.18	103.82	109.00
19	M	144	ASP	CA-CB-CG	-5.18	107.42	112.60
4	d	116	GLN	CA-C-O	5.18	126.22	120.63
6	f	163	ARG	CA-C-N	5.18	129.37	120.72
6	f	163	ARG	C-N-CA	5.18	129.37	120.72
8	1	152	VAL	N-CA-C	5.18	115.90	110.62
19	M	141	LYS	CA-C-O	-5.18	115.33	120.66
3	C	107	VAL	CA-C-N	5.17	127.21	120.28
3	C	107	VAL	C-N-CA	5.17	127.21	120.28
10	3	105	GLY	CA-C-N	5.17	125.58	119.99
10	3	105	GLY	C-N-CA	5.17	125.58	119.99
18	L	281	ASP	CA-C-O	-5.17	114.74	120.38
7	G	71	GLY	O-C-N	5.17	128.24	122.96
1	a	61	SER	N-CA-C	-5.17	101.05	108.60
1	a	170	THR	N-CA-CB	5.17	118.51	109.72
19	M	150	LYS	N-CA-CB	5.17	117.56	110.07
11	k	96	ARG	N-CA-CB	5.17	119.38	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	2	14	ILE	O-C-N	-5.16	117.49	123.07
1	a	127	PRO	CA-C-N	5.16	128.88	121.50
1	a	127	PRO	C-N-CA	5.16	128.88	121.50
12	l	113	TYR	CA-CB-CG	-5.16	104.61	113.90
9	2	9	ASN	CB-CG-ND2	-5.16	108.66	116.40
12	l	80	SER	N-CA-CB	5.16	117.49	110.01
2	B	105	PRO	N-CA-CB	5.16	105.90	103.22
3	c	20	GLN	CA-C-N	5.16	127.75	120.42
3	c	20	GLN	C-N-CA	5.16	127.75	120.42
13	m	164	THR	N-CA-C	-5.16	107.16	113.50
10	3	133	LYS	N-CA-C	-5.16	104.75	112.54
16	I	293	ASP	N-CA-CB	5.16	119.21	110.49
12	5	35	ILE	N-CA-C	-5.16	98.26	107.18
1	A	81	ALA	O-C-N	-5.16	116.73	122.09
10	3	20	VAL	CB-CA-C	-5.16	104.13	111.40
2	B	105	PRO	CA-C-N	5.15	126.28	119.84
2	B	105	PRO	C-N-CA	5.15	126.28	119.84
12	5	87	VAL	CA-CB-CG2	5.15	119.16	110.40
8	h	8	PHE	O-C-N	-5.15	116.89	122.92
1	A	88	ALA	O-C-N	-5.15	116.47	122.03
10	j	134	ASP	CA-CB-CG	5.15	117.75	112.60
6	f	24	ALA	CA-C-N	5.15	127.69	120.28
6	f	24	ALA	C-N-CA	5.15	127.69	120.28
6	F	32	SER	CA-C-N	5.15	127.50	120.35
6	F	32	SER	C-N-CA	5.15	127.50	120.35
2	B	62	SER	N-CA-C	-5.14	100.06	108.76
9	2	116	HIS	CE1-NE2-CD2	-5.14	103.86	109.00
3	c	154	GLY	CA-C-N	5.14	128.97	121.31
3	c	154	GLY	C-N-CA	5.14	128.97	121.31
9	2	73	GLU	O-C-N	-5.14	117.46	121.47
10	j	106	PRO	CA-C-N	5.14	130.20	122.75
10	j	106	PRO	C-N-CA	5.14	130.20	122.75
11	k	99	GLN	CB-CA-C	5.14	120.64	110.42
14	n	119	VAL	N-CA-CB	5.14	119.86	111.44
1	A	65	CYS	CA-CB-SG	5.13	126.21	114.40
13	6	116	GLU	CB-CA-C	-5.13	102.27	110.79
16	I	70	LEU	CB-CA-C	-5.13	102.27	110.79
11	4	79	ALA	CA-C-N	5.13	127.22	120.60
11	4	79	ALA	C-N-CA	5.13	127.22	120.60
10	j	44	HIS	ND1-CE1-NE2	5.12	113.52	108.40
13	6	125	PHE	CA-CB-CG	-5.12	108.68	113.80
12	l	69	ARG	NE-CZ-NH2	-5.12	114.59	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	94	GLU	N-CA-C	5.12	117.27	111.02
1	a	191	GLU	CA-C-N	5.12	127.45	120.54
1	a	191	GLU	C-N-CA	5.12	127.45	120.54
13	6	220	LYS	N-CA-C	-5.12	102.70	110.28
17	K	425	ASP	CA-C-N	5.12	129.04	120.70
17	K	425	ASP	C-N-CA	5.12	129.04	120.70
3	C	62	THR	N-CA-C	-5.12	101.81	109.95
17	K	307	ASP	CA-C-N	5.12	129.82	122.35
17	K	307	ASP	C-N-CA	5.12	129.82	122.35
13	6	189	THR	CA-C-O	5.11	125.91	120.24
18	L	372	GLY	N-CA-C	-5.11	101.07	113.18
2	b	3	ASP	CA-C-O	-5.11	114.65	120.58
14	n	79	PRO	CB-CA-C	-5.11	104.59	111.85
1	a	134	PHE	CA-CB-CG	-5.11	108.69	113.80
15	H	336	LEU	N-CA-CB	5.11	118.19	110.28
8	1	32	ASP	N-CA-C	-5.10	100.92	109.24
12	5	194	GLY	O-C-N	-5.10	116.28	122.71
5	e	125	LEU	N-CA-C	-5.10	106.61	114.16
7	g	110	ASP	CA-C-O	-5.10	115.45	120.70
1	A	149	ASP	CB-CA-C	5.10	117.88	109.97
2	B	11	THR	O-C-N	-5.10	117.96	123.42
13	m	170	LYS	CA-C-N	5.10	125.39	119.93
13	m	170	LYS	C-N-CA	5.10	125.39	119.93
9	2	51	ASP	CA-CB-CG	5.10	117.70	112.60
10	3	27	ARG	N-CA-C	5.10	117.83	110.28
7	g	16	ARG	NE-CZ-NH2	5.10	123.79	119.20
4	D	61	LYS	CA-C-O	5.10	125.80	119.12
14	n	26	ASN	CA-CB-CG	-5.09	107.51	112.60
3	C	90	ALA	O-C-N	5.09	127.31	122.07
6	F	10	VAL	CA-C-O	-5.09	115.40	121.05
7	G	5	ASP	CA-CB-CG	5.09	117.69	112.60
12	5	140	LEU	CA-C-O	-5.09	114.35	120.10
17	K	150	LEU	CB-CA-C	-5.09	101.25	108.88
17	K	197	LEU	CA-C-O	-5.09	115.03	120.42
4	D	216	ASP	CA-C-N	5.09	131.26	121.54
4	D	216	ASP	C-N-CA	5.09	131.26	121.54
11	k	66	LEU	O-C-N	-5.09	116.73	122.12
13	6	131	TYR	O-C-N	-5.08	118.42	123.46
9	i	102	GLY	N-CA-C	5.08	117.93	111.37
8	1	115	LEU	O-C-N	5.08	127.51	122.12
10	3	47	HIS	CE1-NE2-CD2	-5.08	103.92	109.00
5	e	149	HIS	CG-CD2-NE2	5.08	112.28	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	5	188	HIS	ND1-CE1-NE2	5.08	113.48	108.40
1	A	70	ILE	O-C-N	5.08	129.67	122.97
14	7	163	SER	N-CA-C	-5.08	107.26	113.50
17	K	167	PRO	CA-C-N	5.08	129.31	120.68
17	K	167	PRO	C-N-CA	5.08	129.31	120.68
9	i	16	ALA	CA-C-O	-5.07	115.98	121.36
9	i	66	HIS	CE1-NE2-CD2	-5.07	103.93	109.00
10	j	65	MET	CG-SD-CE	5.07	112.06	100.90
10	3	83	PRO	CA-N-CD	5.07	119.10	112.00
13	6	77	PHE	CB-CA-C	-5.07	102.23	110.85
4	d	103	THR	CA-C-O	-5.07	115.43	121.16
4	d	155	SER	N-CA-CB	5.07	119.41	111.56
10	j	82	GLU	CA-C-N	5.07	125.10	119.32
10	j	82	GLU	C-N-CA	5.07	125.10	119.32
2	b	190	HIS	CG-CD2-NE2	5.07	112.27	107.20
1	a	13	GLU	CB-CG-CD	-5.06	103.99	112.60
2	b	69	PRO	CB-CA-C	5.06	119.92	111.56
3	c	74	VAL	N-CA-C	-5.06	100.62	108.81
10	3	119	PHE	O-C-N	-5.06	117.22	123.44
4	D	84	ILE	N-CA-C	5.06	115.78	110.62
9	2	28	ASP	CB-CA-C	-5.06	103.26	110.34
1	A	29	THR	CA-C-O	-5.05	113.84	120.00
20	J	132	PRO	CA-N-CD	5.05	119.06	112.00
5	E	234	GLU	CA-C-N	5.04	127.04	120.28
5	E	234	GLU	C-N-CA	5.04	127.04	120.28
5	e	23	ILE	CA-C-N	5.04	127.97	120.31
5	e	23	ILE	C-N-CA	5.04	127.97	120.31
12	5	140	LEU	N-CA-C	5.04	117.51	111.71
8	h	96	GLY	N-CA-C	-5.04	101.24	113.18
12	l	125	ASP	CB-CA-C	-5.04	101.00	109.27
6	F	18	LEU	N-CA-CB	5.04	118.50	110.84
4	d	160	GLN	CA-C-O	-5.04	115.71	121.40
6	F	88	ARG	CA-C-N	5.04	127.34	120.54
6	F	88	ARG	C-N-CA	5.04	127.34	120.54
7	G	89	ARG	CA-C-N	5.04	127.03	120.28
7	G	89	ARG	C-N-CA	5.04	127.03	120.28
1	a	23	PHE	N-CA-CB	5.03	117.52	110.12
1	A	78	ILE	O-C-N	-5.03	115.36	121.10
8	1	192	GLU	CB-CG-CD	-5.03	104.04	112.60
12	5	111	THR	O-C-N	-5.03	117.25	123.44
7	G	34	ILE	CA-C-N	5.03	125.48	121.61
7	G	34	ILE	C-N-CA	5.03	125.48	121.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	4	43	LEU	O-C-N	-5.03	117.13	123.27
8	1	132	THR	N-CA-CB	5.03	118.74	110.39
2	b	157	PHE	O-C-N	5.03	125.45	121.88
2	B	161	ALA	N-CA-C	-5.03	100.50	108.14
13	6	11	THR	CA-C-N	5.03	129.76	122.77
13	6	11	THR	C-N-CA	5.03	129.76	122.77
13	6	161	GLU	CB-CG-CD	-5.03	104.05	112.60
2	b	6	SER	CA-C-N	5.03	127.99	120.95
2	b	6	SER	C-N-CA	5.03	127.99	120.95
12	l	82	ILE	CA-C-N	5.03	127.42	120.29
12	l	82	ILE	C-N-CA	5.03	127.42	120.29
8	1	112	THR	CA-CB-OG1	5.03	117.14	109.60
9	i	86	HIS	ND1-CE1-NE2	5.02	113.42	108.40
13	m	98	TYR	CA-CB-CG	-5.02	104.86	113.90
11	4	46	PHE	CA-CB-CG	-5.02	108.78	113.80
9	i	222	ASP	CA-C-N	5.02	127.42	120.49
9	i	222	ASP	C-N-CA	5.02	127.42	120.49
14	n	77	ASP	CA-C-O	-5.02	111.23	119.21
13	6	32	ASP	CB-CA-C	-5.02	110.41	117.23
7	g	78	ILE	CA-C-O	-5.01	113.23	119.95
2	B	105	PRO	N-CA-C	-5.01	105.21	110.58
14	7	139	SER	CA-C-N	5.01	124.70	119.64
14	7	139	SER	C-N-CA	5.01	124.70	119.64
3	C	116	ASP	CB-CA-C	-5.01	102.47	110.79
19	M	372	ASP	CA-CB-CG	-5.01	107.59	112.60
12	l	118	ASP	N-CA-CB	5.01	117.48	110.12
11	4	20	ALA	N-CA-CB	5.01	118.80	110.63
9	i	75	ARG	N-CA-C	-5.01	101.71	109.72
9	i	213	LEU	O-C-N	5.01	129.06	122.30
10	j	22	ILE	O-C-N	-5.01	117.74	123.10
18	L	293	GLU	N-CA-C	-5.01	107.85	114.31
4	d	202	GLN	CA-C-N	5.00	131.10	121.54
4	d	202	GLN	C-N-CA	5.00	131.10	121.54
2	b	82	TYR	O-C-N	-5.00	116.82	122.12
3	c	90	ALA	CA-C-N	5.00	127.29	120.54
3	c	90	ALA	C-N-CA	5.00	127.29	120.54
5	E	112	ALA	CA-C-N	5.00	127.23	120.38
5	E	112	ALA	C-N-CA	5.00	127.23	120.38
5	E	129	PRO	O-C-N	5.00	129.39	122.64
12	5	38	ASN	O-C-N	-5.00	115.57	121.32
13	6	188	PHE	CA-CB-CG	-5.00	108.80	113.80
18	L	293	GLU	O-C-N	-5.00	116.84	122.34

There are no chirality outliers.

All (88) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	1	70	TYR	Sidechain
8	1	87	TYR	Sidechain
9	2	124	TYR	Sidechain
9	2	171	SER	Peptide
9	2	69	TYR	Sidechain
9	2	8	PHE	Sidechain
10	3	187	TYR	Sidechain
11	4	135	TYR	Sidechain
11	4	67	TYR	Sidechain
11	4	70	ARG	Sidechain
11	4	98	TYR	Sidechain
13	6	57	PHE	Sidechain
13	6	75	TYR	Sidechain
14	7	101	TYR	Sidechain
14	7	129	TYR	Sidechain
14	7	186	TYR	Sidechain
14	7	9	THR	Peptide
1	A	119	TYR	Sidechain
1	A	146	TYR	Sidechain
1	A	153	TYR	Sidechain
1	A	68	ARG	Sidechain
1	A	82	ARG	Sidechain
1	A	96	ARG	Sidechain
1	A	97	TYR	Sidechain
2	B	134	LEU	Peptide
2	B	156	TYR	Sidechain
2	B	224	TYR	Sidechain
2	B	4	ARG	Sidechain
2	B	5	TYR	Sidechain
3	C	121	TYR	Sidechain
3	C	17	ARG	Sidechain
3	C	61	SER	Peptide
3	C	8	ARG	Sidechain
4	D	110	TYR	Sidechain
4	D	2	TYR	Sidechain
5	E	128	ARG	Peptide,Mainchain
5	E	130	PHE	Sidechain
5	E	157	TYR	Sidechain
5	E	2	ARG	Sidechain
6	F	136	TYR	Sidechain

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Mol	Chain	Res	Type	Group
6	F	156	TYR	Sidechain
6	F	17	ARG	Sidechain
6	F	23	TYR	Sidechain
6	F	5	TYR	Sidechain
6	F	81	ARG	Sidechain
6	F	86	TYR	Sidechain
6	F	93	TYR	Sidechain
7	G	126	ARG	Sidechain
7	G	82	ARG	Sidechain
15	H	367	ARG	Peptide
16	I	182	SER	Peptide
16	I	186	GLY	Peptide
16	I	339	ILE	Peptide
16	I	342	GLY	Peptide
20	J	378	THR	Peptide
17	K	320	ARG	Sidechain
18	L	131	VAL	Peptide
18	L	292	SER	Peptide
18	L	338	LEU	Peptide
18	L	342	ARG	Peptide
18	L	376	PHE	Peptide
19	M	291	PHE	Peptide
1	a	146	TYR	Sidechain
1	a	148	THR	Peptide
2	b	134	LEU	Peptide
2	b	213	ILE	Peptide
2	b	23	TYR	Sidechain
2	b	83	ARG	Sidechain
3	c	134	PHE	Peptide,Sidechain
3	c	4	ARG	Sidechain
6	f	127	TYR	Sidechain
6	f	163	ARG	Sidechain
6	f	224	TYR	Sidechain
6	f	23	TYR	Sidechain
6	f	232	TYR	Sidechain
6	f	86	TYR	Sidechain
6	f	93	TYR	Sidechain
7	g	16	ARG	Sidechain
9	i	124	TYR	Sidechain
10	j	68	TYR	Sidechain
11	k	59	TYR	Sidechain
12	l	104	TYR	Sidechain

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Mol	Chain	Res	Type	Group
12	l	7	ARG	Sidechain
13	m	98	TYR	Sidechain
14	n	101	TYR	Sidechain
14	n	77	ASP	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1907	0	1901	1	0
1	a	1907	0	1901	8	0
2	B	1915	0	1929	9	0
2	b	1915	0	1928	34	0
3	C	1904	0	1904	10	0
3	c	1904	0	1904	24	0
4	D	1881	0	1895	13	0
4	d	1881	0	1895	17	0
5	E	1861	0	1839	11	0
5	e	1861	0	1839	19	0
6	F	1795	0	1800	13	0
6	f	1773	0	1775	12	0
7	G	1892	0	1883	19	0
7	g	1892	0	1883	11	0
8	1	1512	0	1481	7	0
8	h	1512	0	1481	20	0
9	2	1719	0	1719	17	0
9	i	1719	0	1719	16	0
10	3	1581	0	1574	18	0
10	j	1581	0	1574	19	0
11	4	1561	0	1569	9	0
11	k	1561	0	1569	22	0
12	5	1644	0	1595	15	0
12	l	1644	0	1595	19	0
13	6	1757	0	1711	13	0
13	m	1757	0	1711	18	0
14	7	1790	0	1793	14	0
14	n	1815	0	1821	18	0
15	H	3053	0	3126	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	I	3022	0	3090	44	0
17	K	3078	0	3141	27	0
18	L	3082	0	3156	46	0
19	M	2986	0	3054	61	0
20	J	3033	0	3153	27	0
21	H	1	0	0	0	0
21	I	1	0	0	0	0
21	J	1	0	0	0	0
21	K	1	0	0	0	0
21	L	1	0	0	0	0
21	M	1	0	0	0	0
22	H	31	0	12	4	0
22	I	31	0	12	0	0
22	K	31	0	12	6	0
22	L	31	0	12	8	0
22	M	31	0	12	3	0
23	J	27	0	11	6	0
All	All	67883	0	67979	615	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 5.

All (615) 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)
18:L:183:ILE:CD1	22:L:501:ATP:N6	1.74	1.49
18:L:183:ILE:HD13	22:L:501:ATP:N6	1.41	1.17
20:J:197:LEU:HD11	23:J:501:ADP:H2'	1.24	1.15
19:M:374:ILE:HG21	19:M:376:TRP:CZ2	1.81	1.15
20:J:197:LEU:CD1	23:J:501:ADP:H2'	1.80	1.11
18:L:183:ILE:CD1	22:L:501:ATP:HN61	1.46	1.10
18:L:183:ILE:HD12	22:L:501:ATP:HN61	1.01	1.06
20:J:197:LEU:HG	23:J:501:ADP:O1A	1.59	1.02
18:L:183:ILE:HD12	22:L:501:ATP:N6	1.51	1.02
16:I:436:TYR:O	16:I:437:LEU:O	1.86	0.92
2:b:4:ARG:NH2	5:e:117:GLU:HB3	1.85	0.91
18:L:183:ILE:CD1	22:L:501:ATP:HN62	1.80	0.89
17:K:221:MET:HE1	22:K:501:ATP:C6	2.08	0.89
2:b:4:ARG:NH2	5:e:117:GLU:CB	2.39	0.86
19:M:357:ARG:NH1	19:M:380:ALA:O	2.09	0.86
18:L:183:ILE:HD13	22:L:501:ATP:HN62	1.35	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:J:197:LEU:HD11	23:J:501:ADP:C2'	2.08	0.83
8:h:126:ILE:HG13	8:h:131:SER:HB2	1.61	0.82
16:I:312:GLN:HA	16:I:312:GLN:OE1	1.82	0.80
19:M:374:ILE:CG2	19:M:376:TRP:CZ2	2.64	0.80
2:b:250:LEU:OXT	2:b:250:LEU:HD13	1.82	0.80
19:M:374:ILE:HG21	19:M:376:TRP:CH2	2.16	0.80
10:3:203:GLN:HA	10:3:203:GLN:OE1	1.82	0.79
16:I:212:GLY:O	16:I:213:ILE:O	2.01	0.78
19:M:352:PRO:CB	19:M:356:SER:HB2	2.13	0.78
5:E:143:ASP:OD1	5:E:143:ASP:O	2.01	0.77
5:E:217:GLN:N	5:E:217:GLN:OE1	2.17	0.77
16:I:337:ALA:O	16:I:343:ARG:NH1	2.18	0.76
16:I:436:TYR:C	16:I:437:LEU:O	2.28	0.75
10:3:95:TYR:O	10:3:95:TYR:CD2	2.40	0.74
13:6:222:ASP:OXT	13:6:222:ASP:OD1	2.06	0.74
2:b:227:ILE:CG2	2:b:230:ASP:OD2	2.36	0.73
14:7:131:ASN:OD1	14:7:131:ASN:C	2.31	0.72
20:J:197:LEU:HD13	23:J:501:ADP:H2'	1.71	0.72
8:h:126:ILE:CG1	8:h:131:SER:HB2	2.19	0.72
5:E:206:GLU:OE1	5:E:206:GLU:N	2.19	0.72
2:b:227:ILE:HG23	2:b:230:ASP:OD2	1.90	0.71
19:M:352:PRO:CA	19:M:356:SER:HB2	2.20	0.71
10:3:95:TYR:O	10:3:95:TYR:CG	2.44	0.71
18:L:236:ALA:O	18:L:243:PHE:CE1	2.43	0.70
16:I:424:MET:O	16:I:428:VAL:HB	1.91	0.70
19:M:280:ILE:HG22	19:M:282:GLU:O	1.91	0.70
19:M:352:PRO:CB	19:M:356:SER:CB	2.70	0.69
17:K:238:ASN:ND2	18:L:310:THR:OG1	2.25	0.69
2:b:139:HIS:ND1	2:b:139:HIS:C	2.51	0.68
8:h:51:ASP:OD2	8:h:93:LEU:HA	1.94	0.68
8:h:38:HIS:CD2	8:h:39:ASP:H	2.11	0.68
13:m:60:ASP:O	13:m:63:ALA:N	2.26	0.68
17:K:221:MET:HE1	22:K:501:ATP:N6	2.08	0.68
14:7:84:GLU:N	14:7:84:GLU:OE1	2.27	0.67
7:g:100:LYS:O	7:g:100:LYS:HG2	1.93	0.67
11:k:152:MET:HG2	11:k:156:GLU:OE2	1.95	0.67
19:M:387:ASN:OD1	19:M:387:ASN:O	2.12	0.67
17:K:352:ILE:HG22	17:K:383:ILE:HG21	1.77	0.67
11:4:120:ASP:OD1	11:4:120:ASP:O	2.12	0.67
11:4:120:ASP:OD1	11:4:120:ASP:C	2.32	0.66
4:D:45:GLU:O	4:D:45:GLU:HG3	1.92	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:l:152:ASP:OD1	12:l:152:ASP:N	2.25	0.66
19:M:352:PRO:HB2	19:M:356:SER:HB2	1.77	0.66
3:C:229:PHE:CD1	3:C:229:PHE:N	2.64	0.65
8:1:193:TYR:O	8:1:196:LEU:O	2.14	0.65
9:2:138:LEU:HD13	9:2:138:LEU:C	2.22	0.65
14:7:63:ILE:HG22	14:7:63:ILE:O	1.96	0.65
15:H:458:SER:O	15:H:459:SER:C	2.39	0.64
18:L:241:ALA:O	18:L:243:PHE:CZ	2.49	0.64
18:L:241:ALA:O	18:L:243:PHE:CE1	2.50	0.64
19:M:374:ILE:CG2	19:M:376:TRP:CE2	2.80	0.64
3:c:237:ILE:HG22	3:c:237:ILE:O	1.98	0.64
2:b:227:ILE:HG23	2:b:227:ILE:O	1.96	0.64
16:I:190:GLN:N	16:I:190:GLN:OE1	2.31	0.64
11:k:194:ASP:O	11:k:195:PHE:O	2.16	0.64
15:H:328:GLU:OE1	15:H:328:GLU:N	2.29	0.64
19:M:387:ASN:OD1	19:M:387:ASN:C	2.41	0.63
14:n:231:GLN:HE22	8:1:60:GLN:HE22	1.46	0.63
18:L:432:ILE:O	18:L:432:ILE:HG22	1.97	0.63
9:i:130:GLY:O	9:i:131:SER:C	2.40	0.63
12:l:208:ASN:O	12:l:209:ASN:C	2.38	0.63
4:D:226:GLU:OE1	4:D:226:GLU:N	2.24	0.63
16:I:339:ILE:C	16:I:339:ILE:HD12	2.24	0.63
2:b:139:HIS:ND1	2:b:139:HIS:O	2.32	0.62
10:j:47:HIS:CD2	10:j:47:HIS:H	2.16	0.62
6:F:233:ILE:OXT	6:F:233:ILE:HG22	2.00	0.62
9:2:124:TYR:CD1	9:2:138:LEU:HG	2.35	0.62
2:b:76:SER:OG	2:b:164:ILE:HG23	1.99	0.62
12:5:207:PHE:O	12:5:208:ASN:C	2.43	0.62
6:F:54:GLU:OE1	6:F:54:GLU:N	2.30	0.61
18:L:399:GLY:O	18:L:403:ILE:HG13	2.00	0.61
9:2:220:ILE:C	9:2:220:ILE:HD12	2.25	0.61
15:H:398:VAL:HB	15:H:402:ILE:HD12	1.82	0.61
2:B:29:LYS:O	2:B:166:LYS:HA	1.99	0.61
15:H:95:HIS:CD2	16:I:131:SER:HB2	2.36	0.61
2:b:4:ARG:HH22	5:e:117:GLU:HA	1.65	0.61
2:b:4:ARG:HH22	5:e:117:GLU:CB	2.15	0.60
18:L:65:LEU:O	18:L:68:ARG:HB2	1.99	0.60
22:H:502:ATP:O3B	16:I:340:ARG:NH1	2.34	0.60
13:m:22:VAL:HG23	13:m:22:VAL:O	2.00	0.60
15:H:458:SER:O	15:H:461:SER:N	2.35	0.60
19:M:81:ASN:OD1	19:M:81:ASN:C	2.44	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:J:112:ARG:O	20:J:126:LEU:HB3	2.02	0.60
17:K:209:VAL:HB	17:K:315:ILE:HG12	1.84	0.60
18:L:183:ILE:HD13	22:L:501:ATP:C6	2.29	0.60
19:M:225:GLY:O	22:M:501:ATP:C8	2.54	0.60
8:h:190:PRO:HA	8:h:193:TYR:CE2	2.36	0.59
16:I:184:ILE:C	16:I:184:ILE:HD12	2.27	0.59
19:M:283:LEU:O	19:M:283:LEU:HG	2.03	0.59
7:G:197:TYR:HD1	7:G:197:TYR:N	2.01	0.59
19:M:359:GLN:O	19:M:363:ILE:HG12	2.03	0.59
6:f:233:ILE:HG22	6:f:233:ILE:OXT	2.01	0.58
13:6:93:ILE:O	13:6:96:LEU:N	2.36	0.58
3:C:229:PHE:HD1	3:C:229:PHE:H	1.51	0.58
3:c:142:ARG:O	3:c:143:TYR:CG	2.56	0.58
7:G:243:ILE:HG12	7:G:243:ILE:O	2.02	0.58
2:b:4:ARG:HH22	5:e:117:GLU:CA	2.17	0.58
2:b:4:ARG:HH21	5:e:117:GLU:HB3	1.68	0.57
19:M:374:ILE:HG22	19:M:376:TRP:CE2	2.39	0.57
11:4:126:VAL:HG13	11:4:126:VAL:O	2.05	0.57
12:5:55:TRP:NE1	13:6:98:TYR:OH	2.38	0.57
12:5:193:VAL:HG12	12:5:193:VAL:O	2.03	0.57
17:K:221:MET:HE1	22:K:501:ATP:C5	2.40	0.57
9:i:58:LEU:HD23	9:i:58:LEU:O	2.05	0.56
14:7:194:ASN:OD1	14:7:194:ASN:C	2.47	0.56
18:L:376:PHE:O	18:L:379:ALA:N	2.38	0.56
2:b:227:ILE:HG21	2:b:230:ASP:OD2	2.04	0.56
2:B:35:LEU:C	2:B:35:LEU:HD12	2.30	0.56
18:L:426:LYS:HG2	18:L:426:LYS:O	2.05	0.56
10:j:44:HIS:HB3	10:j:49:PHE:CE2	2.40	0.56
14:7:152:ASN:HB3	14:7:153:PRO:HD3	1.87	0.56
16:I:436:TYR:O	16:I:437:LEU:C	2.48	0.56
2:B:48:GLU:OE1	2:B:48:GLU:N	2.34	0.56
16:I:344:ILE:HD12	16:I:344:ILE:C	2.30	0.56
18:L:167:VAL:HG22	18:L:167:VAL:O	2.06	0.56
20:J:103:ASN:C	20:J:103:ASN:OD1	2.49	0.56
7:G:197:TYR:N	7:G:197:TYR:CD1	2.71	0.56
13:6:91:ARG:O	13:6:91:ARG:HG3	2.05	0.56
22:H:502:ATP:O1G	16:I:340:ARG:NH1	2.40	0.55
5:e:217:GLN:HA	5:e:217:GLN:OE1	2.06	0.55
9:i:159:ILE:HG21	9:i:173:VAL:HG13	1.87	0.55
9:2:124:TYR:CG	9:2:138:LEU:HG	2.40	0.55
17:K:274:VAL:HG23	17:K:274:VAL:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:l:80:SER:HA	12:l:101:ILE:HD12	1.88	0.55
2:b:1:MET:O	6:f:122:TYR:HB3	2.07	0.55
10:j:39:PHE:CD1	10:j:39:PHE:C	2.84	0.55
5:E:13:LEU:O	5:E:14:PHE:C	2.49	0.55
20:J:97:ASP:C	20:J:97:ASP:OD1	2.46	0.55
2:B:128:ARG:O	2:B:128:ARG:HD3	2.07	0.54
14:7:11:VAL:N	14:7:144:THR:OG1	2.40	0.54
12:l:45:MET:SD	12:l:49:ALA:HA	2.47	0.54
13:m:52:MET:HE2	13:m:65:VAL:HG22	1.90	0.54
15:H:335:GLU:HA	15:H:335:GLU:OE1	2.08	0.54
18:L:256:ILE:HD11	19:M:256:ILE:HD12	1.89	0.54
2:b:186:GLU:OE2	2:b:186:GLU:N	2.41	0.54
14:7:177:ILE:O	14:7:178:VAL:C	2.48	0.54
11:k:84:VAL:O	11:k:85:ARG:C	2.51	0.53
8:1:144:GLU:OE1	8:1:144:GLU:N	2.35	0.53
8:h:76:GLU:C	8:h:76:GLU:CD	2.76	0.53
9:i:130:GLY:O	9:i:132:LEU:N	2.42	0.53
4:D:120:GLN:HG2	5:E:128:ARG:HH21	1.73	0.53
16:I:219:VAL:HG12	16:I:325:ILE:HD13	1.90	0.53
19:M:423:GLN:O	19:M:425:ARG:HG3	2.08	0.53
3:C:10:THR:HG22	4:D:125:ARG:HB3	1.91	0.53
15:H:77:ALA:N	15:H:78:PRO:HD2	2.24	0.53
7:g:166:GLN:CD	7:g:166:GLN:H	2.16	0.53
12:l:148:LEU:HD23	12:l:153:ALA:HB2	1.91	0.53
5:e:13:LEU:O	5:e:14:PHE:C	2.51	0.53
18:L:361:PHE:CE1	18:L:391:ILE:HG23	2.44	0.53
2:b:13:SER:O	2:b:15:SER:N	2.42	0.53
12:5:52:CYS:O	12:5:53:GLN:C	2.51	0.53
15:H:298:ALA:CB	15:H:306:ILE:HD11	2.39	0.53
7:G:212:ILE:HG13	7:G:227:VAL:HB	1.90	0.52
18:L:207:PHE:CD1	18:L:207:PHE:N	2.77	0.52
18:L:236:ALA:O	18:L:243:PHE:CZ	2.62	0.52
20:J:34:ILE:O	20:J:34:ILE:HG22	2.08	0.52
6:F:116:GLN:HE21	6:F:120:GLN:HG3	1.73	0.52
17:K:51:LEU:HB3	20:J:27:ILE:HB	1.90	0.52
14:n:231:GLN:OE1	14:n:231:GLN:HA	2.08	0.52
12:5:193:VAL:O	12:5:193:VAL:CG1	2.58	0.52
3:c:237:ILE:O	3:c:237:ILE:CG2	2.57	0.52
12:l:52:CYS:O	12:l:53:GLN:C	2.50	0.52
19:M:182:ASP:O	19:M:363:ILE:HG21	2.09	0.52
18:L:188:GLU:HA	18:L:188:GLU:OE1	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:M:142:PRO:O	19:M:143:ASN:HB2	2.10	0.52
7:g:230:ASP:O	7:g:233:GLN:N	2.43	0.52
11:k:23:ARG:HE	12:l:120:THR:HG21	1.75	0.52
11:k:63:ASN:OD1	11:k:83:PHE:CZ	2.63	0.52
18:L:137:ARG:HB3	18:L:137:ARG:CZ	2.38	0.52
14:7:63:ILE:O	14:7:63:ILE:CG2	2.58	0.51
4:d:40:VAL:HG12	4:d:41:VAL:N	2.25	0.51
4:d:198:LEU:HD21	4:d:231:VAL:HG13	1.91	0.51
6:f:233:ILE:OXT	6:f:233:ILE:CG2	2.59	0.51
6:F:206:THR:OG1	6:F:209:ASN:HB2	2.09	0.51
19:M:352:PRO:CB	19:M:356:SER:HB3	2.40	0.51
3:C:225:TYR:CD2	9:2:226:GLU:HG3	2.45	0.51
10:j:131:GLU:OE1	10:j:131:GLU:HA	2.10	0.51
14:n:30:TYR:O	14:n:30:TYR:CG	2.64	0.51
13:m:209:LYS:H	13:m:209:LYS:CD	2.22	0.51
10:3:10:ILE:HD12	10:3:145:LEU:HD11	1.93	0.51
12:5:38:ASN:HB2	12:5:39:PRO:HD2	1.91	0.51
13:6:137:ARG:HG2	13:6:138:ALA:O	2.10	0.51
18:L:350:PRO:O	18:L:351:LEU:C	2.53	0.51
19:M:352:PRO:HB3	19:M:356:SER:HB3	1.91	0.51
3:C:128:ARG:HD2	3:C:128:ARG:C	2.35	0.51
16:I:425:LYS:HB3	16:I:429:GLU:OE2	2.11	0.51
19:M:230:LEU:C	19:M:230:LEU:HD13	2.36	0.51
12:l:157:GLY:O	12:l:158:LYS:C	2.53	0.51
10:3:95:TYR:CD2	10:3:95:TYR:C	2.87	0.51
7:G:214:TRP:O	7:G:214:TRP:CD1	2.63	0.51
10:3:203:GLN:OE1	10:3:203:GLN:CA	2.55	0.51
3:c:64:LYS:O	3:c:65:LEU:HD12	2.11	0.50
16:I:219:VAL:HG21	16:I:348:ILE:CD1	2.41	0.50
4:d:196:SER:HA	4:d:199:GLU:OE1	2.11	0.50
4:D:50:LEU:O	4:D:51:LYS:C	2.55	0.50
2:B:182:GLU:OE1	2:B:182:GLU:HA	2.10	0.50
19:M:199:LEU:N	19:M:200:PRO:HD2	2.25	0.50
20:J:156:GLN:OE1	20:J:156:GLN:N	2.45	0.50
2:b:186:GLU:OE2	2:b:186:GLU:CA	2.58	0.50
7:G:56:VAL:HG23	7:G:59:LYS:HB2	1.94	0.50
6:F:233:ILE:OXT	6:F:233:ILE:CG2	2.59	0.50
16:I:247:ILE:HG22	16:I:248:VAL:O	2.11	0.50
16:I:161:GLN:N	16:I:161:GLN:CD	2.70	0.50
16:I:339:ILE:HD12	16:I:339:ILE:O	2.11	0.50
9:i:39:PRO:O	9:i:40:LYS:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:214:TRP:CD1	7:G:214:TRP:N	2.78	0.49
6:f:28:ILE:HG13	6:f:29:LYS:N	2.26	0.49
9:i:207:ARG:NH1	10:j:160:GLU:HB2	2.28	0.49
10:j:181:GLY:HA2	10:j:201:MET:CE	2.42	0.49
13:6:147:MET:N	13:6:148:PRO:HD2	2.27	0.49
15:H:306:ILE:HG22	15:H:308:PHE:CE2	2.46	0.49
1:a:183:ASP:OD1	1:a:183:ASP:N	2.43	0.49
3:c:142:ARG:NH1	11:k:73:TYR:CD2	2.81	0.49
15:H:418:GLU:HG2	16:I:341:PRO:HG2	1.94	0.49
16:I:85:PHE:CD1	16:I:85:PHE:N	2.81	0.49
13:6:146:ILE:O	13:6:147:MET:C	2.49	0.49
18:L:383:SER:O	18:L:384:ASP:O	2.31	0.49
13:m:60:ASP:O	13:m:61:GLY:C	2.56	0.49
13:m:149:PHE:HA	10:3:148:MET:SD	2.53	0.49
19:M:422:VAL:HG12	19:M:422:VAL:O	2.11	0.49
2:b:35:LEU:HD11	2:b:46:ALA:HB3	1.95	0.48
6:F:37:LEU:H	6:F:37:LEU:HD23	1.78	0.48
6:F:71:LEU:HD12	6:F:71:LEU:C	2.38	0.48
7:G:183:LEU:HG	7:G:187:GLU:HB2	1.95	0.48
15:H:459:SER:HB2	16:I:339:ILE:HD11	1.95	0.48
14:n:157:LYS:O	14:n:157:LYS:HG2	2.12	0.48
16:I:300:ARG:HA	16:I:300:ARG:NE	2.28	0.48
5:e:83:HIS:CE1	5:e:111:LEU:HD21	2.48	0.48
5:E:128:ARG:H	5:E:129:PRO:HD3	1.77	0.48
9:i:131:SER:O	9:i:132:LEU:C	2.57	0.48
16:I:160:LEU:O	16:I:160:LEU:HG	2.13	0.48
17:K:51:LEU:CD1	20:J:27:ILE:HD12	2.44	0.48
19:M:428:LYS:HD3	19:M:429:SER:H	1.79	0.48
8:h:131:SER:O	8:h:134:ILE:HG12	2.13	0.48
14:n:95:TYR:O	14:n:99:VAL:HG23	2.12	0.48
13:m:209:LYS:H	13:m:209:LYS:HD2	1.77	0.48
9:2:60:GLY:O	9:2:63:ILE:HG22	2.12	0.48
15:H:43:ALA:N	15:H:44:PRO:CD	2.76	0.48
3:c:139:TYR:CD1	3:c:139:TYR:C	2.90	0.48
9:2:18:THR:HB	9:2:31:CYS:H	1.78	0.48
15:H:298:ALA:HB1	15:H:306:ILE:HD11	1.96	0.48
19:M:352:PRO:CA	19:M:356:SER:CB	2.91	0.48
4:d:230:TYR:O	4:d:234:ILE:HG13	2.14	0.48
2:B:172:LYS:O	2:B:176:GLU:OE1	2.30	0.48
12:5:157:GLY:O	12:5:158:LYS:C	2.56	0.48
14:7:131:ASN:OD1	14:7:131:ASN:O	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:182:ASP:O	3:c:183:MET:C	2.57	0.48
11:k:147:HIS:O	11:k:152:MET:HE3	2.14	0.48
16:I:378:GLU:OE1	16:I:378:GLU:N	2.35	0.48
2:b:139:HIS:CE1	2:b:140:ASP:O	2.66	0.48
8:h:126:ILE:HD11	8:h:134:ILE:HD11	1.94	0.48
12:5:200:VAL:HG12	12:5:200:VAL:O	2.13	0.48
18:L:283:VAL:O	18:L:283:VAL:HG22	2.14	0.48
9:i:130:GLY:O	9:i:133:ALA:N	2.46	0.47
7:G:138:ASP:OD1	7:G:138:ASP:C	2.57	0.47
15:H:460:THR:HA	16:I:332:GLU:O	2.14	0.47
19:M:352:PRO:HB2	19:M:356:SER:CB	2.40	0.47
15:H:331:ARG:NE	15:H:331:ARG:HA	2.29	0.47
12:l:66:HIS:CE1	12:l:70:GLU:HG3	2.49	0.47
4:d:177:TYR:CD1	4:d:177:TYR:C	2.92	0.47
10:j:28:LEU:HD13	10:j:39:PHE:CE2	2.50	0.47
5:E:13:LEU:O	5:E:15:GLN:N	2.48	0.47
16:I:343:ARG:HB3	16:I:344:ILE:HG23	1.95	0.47
19:M:375:ASN:C	19:M:375:ASN:OD1	2.57	0.47
12:l:192:ASP:OD1	12:l:193:VAL:N	2.47	0.47
18:L:351:LEU:O	18:L:352:PRO:C	2.56	0.47
2:b:4:ARG:NH2	5:e:117:GLU:CA	2.76	0.47
6:F:113:ASP:CG	7:G:86:ASN:HD21	2.22	0.47
11:4:56:PHE:CD2	11:4:56:PHE:O	2.67	0.47
11:4:56:PHE:O	11:4:56:PHE:CG	2.67	0.47
1:a:182:ILE:HD12	1:a:184:HIS:O	2.14	0.47
8:h:58:ILE:HG21	8:h:85:LEU:HD11	1.97	0.47
8:h:151:THR:O	8:h:152:VAL:C	2.58	0.47
4:D:68:HIS:H	4:D:68:HIS:CD2	2.33	0.47
4:D:172:PHE:O	4:D:176:ASN:ND2	2.47	0.47
14:7:91:TYR:CD1	14:7:91:TYR:N	2.77	0.47
19:M:400:MET:O	19:M:403:LEU:N	2.47	0.47
4:D:109:ARG:HH12	12:5:70:GLU:HA	1.78	0.47
9:2:182:LYS:O	9:2:183:ASP:C	2.54	0.47
15:H:396:MET:HA	16:I:211:MET:O	2.14	0.47
19:M:352:PRO:HA	19:M:356:SER:CB	2.45	0.47
20:J:253:ILE:HG22	20:J:258:VAL:HG23	1.96	0.47
3:c:212:PHE:CD2	3:c:229:PHE:CD1	3.03	0.47
9:i:52:THR:OG1	9:i:53:GLU:N	2.48	0.47
10:j:58:ASP:OD2	10:j:102:TYR:HA	2.14	0.47
5:E:51:LEU:HD23	5:E:51:LEU:C	2.39	0.46
13:6:72:VAL:O	13:6:73:LYS:O	2.32	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:7:PHE:O	2:b:7:PHE:CD1	2.67	0.46
14:n:178:VAL:O	14:n:179:ASN:C	2.58	0.46
6:F:53:ASP:OD1	6:F:53:ASP:C	2.57	0.46
17:K:146:LEU:C	17:K:146:LEU:HD23	2.40	0.46
18:L:384:ASP:C	18:L:384:ASP:OD1	2.56	0.46
19:M:374:ILE:HD13	19:M:412:HIS:HB3	1.96	0.46
5:e:38:VAL:O	5:e:213:CYS:HB2	2.15	0.46
7:G:214:TRP:CD1	7:G:214:TRP:H	2.33	0.46
10:3:184:ALA:HB3	10:3:199:LEU:HB2	1.98	0.46
3:c:146:GLN:HE21	4:d:57:ILE:HG21	1.80	0.46
14:n:178:VAL:O	14:n:181:MET:N	2.48	0.46
14:n:190:ARG:CD	14:n:190:ARG:N	2.78	0.46
1:a:241:GLU:C	1:a:242:GLN:O	2.53	0.46
12:l:62:GLN:HA	12:l:62:GLN:OE1	2.14	0.46
20:J:187:LEU:O	20:J:293:ALA:HA	2.15	0.46
10:3:177:ASP:OD1	10:3:178:ALA:N	2.48	0.46
12:l:95:LEU:HD12	12:l:95:LEU:N	2.31	0.46
11:4:49:GLU:O	11:4:50:ALA:C	2.59	0.46
17:K:218:GLY:HA2	22:K:501:ATP:O1A	2.15	0.46
9:2:52:THR:OG1	9:2:53:GLU:N	2.49	0.46
9:2:138:LEU:C	9:2:138:LEU:HD22	2.37	0.46
19:M:376:TRP:CD1	19:M:376:TRP:H	2.34	0.46
11:k:10:GLN:OE1	11:k:151:ASP:O	2.34	0.46
3:C:225:TYR:CD2	3:C:226:GLN:O	2.69	0.46
6:F:37:LEU:HD23	6:F:37:LEU:N	2.31	0.46
19:M:186:LEU:N	19:M:186:LEU:HD23	2.30	0.46
2:b:2:THR:HG21	5:e:117:GLU:HG3	1.98	0.46
5:e:141:ALA:C	5:e:142:ASP:CG	2.84	0.46
6:f:178:PHE:CD1	6:f:178:PHE:C	2.93	0.46
2:B:140:ASP:OD1	2:B:140:ASP:C	2.59	0.45
9:2:38:SER:HB2	9:2:39:PRO:HD2	1.97	0.45
19:M:305:MET:O	19:M:308:LEU:HB3	2.16	0.45
3:c:38:MET:HE3	3:c:160:LYS:HA	1.97	0.45
3:c:64:LYS:O	3:c:75:ALA:HA	2.17	0.45
7:g:166:GLN:H	7:g:166:GLN:NE2	2.14	0.45
14:n:178:VAL:O	14:n:180:ALA:N	2.49	0.45
17:K:380:GLY:HA3	22:K:501:ATP:C8	2.52	0.45
13:m:40:GLU:OE2	13:m:40:GLU:C	2.59	0.45
13:m:182:LYS:O	13:m:183:LEU:C	2.60	0.45
6:F:105:GLU:HG2	6:F:109:HIS:CE1	2.51	0.45
15:H:382:LEU:HG	15:H:382:LEU:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:I:427:LYS:HA	16:I:430:GLU:OE1	2.17	0.45
17:K:378:LEU:HD13	17:K:383:ILE:HD11	1.97	0.45
3:c:217:LYS:HD3	3:c:217:LYS:O	2.16	0.45
6:f:45:LEU:HG	6:f:134:ILE:HD13	1.99	0.45
18:L:361:PHE:CD1	18:L:391:ILE:HG23	2.52	0.45
2:b:13:SER:O	2:b:14:PRO:C	2.59	0.45
6:F:199:SER:O	6:F:201:ARG:N	2.49	0.45
10:3:45:TYR:OH	10:3:63:ASN:OD1	2.34	0.45
13:m:205:LEU:HD12	13:m:205:LEU:N	2.32	0.45
14:n:227:GLY:HA3	14:n:231:GLN:HB2	1.99	0.45
14:n:190:ARG:N	14:n:190:ARG:HD2	2.31	0.45
13:m:199:GLY:O	13:m:200:ASP:HB3	2.17	0.45
19:M:423:GLN:C	19:M:425:ARG:HG3	2.41	0.45
3:c:182:ASP:O	3:c:183:MET:O	2.36	0.44
6:f:143:LEU:HG	6:f:143:LEU:O	2.15	0.44
10:j:23:ALA:HB1	10:j:170:LEU:HD22	2.00	0.44
19:M:349:PHE:N	19:M:349:PHE:CD1	2.85	0.44
11:k:76:SER:O	11:k:79:ALA:N	2.47	0.44
4:D:187:GLU:HB3	4:D:230:TYR:OH	2.16	0.44
16:I:194:ILE:HG21	16:I:236:VAL:HG11	1.99	0.44
20:J:34:ILE:O	20:J:34:ILE:CG2	2.64	0.44
3:C:58:GLN:OE1	3:C:58:GLN:N	2.36	0.44
11:4:138:PHE:CD1	11:4:138:PHE:N	2.85	0.44
16:I:75:PHE:CD1	16:I:75:PHE:C	2.96	0.44
17:K:153:ASP:O	18:L:110:LYS:NZ	2.48	0.44
17:K:218:GLY:HA2	22:K:501:ATP:PA	2.58	0.44
18:L:305:LEU:O	18:L:309:LEU:HG	2.18	0.44
19:M:178:GLU:O	19:M:179:THR:OG1	2.31	0.44
12:l:205:GLY:O	11:4:149:ARG:CZ	2.65	0.44
1:A:103:MET:HE2	1:A:107:VAL:HG12	1.99	0.44
19:M:289:LYS:HG2	19:M:335:PRO:HD3	1.99	0.44
14:n:127:LEU:HG	14:n:142:LEU:HD12	1.99	0.44
4:D:229:GLN:N	4:D:229:GLN:OE1	2.50	0.44
10:3:65:MET:SD	10:3:65:MET:C	3.01	0.44
4:d:41:VAL:HG22	4:d:212:VAL:HG22	2.00	0.44
16:I:264:CYS:HB3	16:I:308:GLU:HG2	1.99	0.44
18:L:352:PRO:HB3	18:L:356:GLY:O	2.17	0.44
8:h:84:GLU:O	8:h:84:GLU:HG3	2.18	0.44
20:J:220:GLN:HG3	20:J:224:GLY:H	1.81	0.44
6:f:55:LEU:HD22	6:f:55:LEU:H	1.83	0.44
12:l:208:ASN:C	12:l:210:VAL:N	2.72	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:3:74:LYS:O	10:3:78:GLU:HA	2.16	0.44
18:L:291:PHE:CD1	18:L:291:PHE:N	2.85	0.44
4:d:50:LEU:O	4:d:51:LYS:HD3	2.18	0.44
8:h:4:MET:HB3	8:h:126:ILE:HD12	2.00	0.44
11:k:118:GLN:HG3	11:k:133:HIS:CE1	2.53	0.44
5:E:149:HIS:CD2	5:E:162:LYS:HE2	2.53	0.44
3:c:142:ARG:CZ	11:k:73:TYR:CD2	3.01	0.43
4:d:141:ASP:OD1	4:d:142:GLU:N	2.50	0.43
7:G:74:TYR:CE1	7:G:81:GLY:HA3	2.52	0.43
22:H:502:ATP:PG	16:I:340:ARG:HH12	2.41	0.43
17:K:55:GLU:O	17:K:59:GLU:HG2	2.18	0.43
17:K:395:VAL:O	17:K:395:VAL:HG12	2.17	0.43
20:J:244:ILE:HG23	20:J:291:ILE:HG13	2.00	0.43
2:b:139:HIS:CE1	2:b:234:ARG:CZ	3.00	0.43
8:1:100:ALA:HB2	8:1:110:VAL:HG22	2.00	0.43
2:b:7:PHE:O	2:b:7:PHE:HD1	2.02	0.43
3:c:185:VAL:O	3:c:189:ILE:HG13	2.18	0.43
4:d:35:LYS:O	4:d:35:LYS:CG	2.65	0.43
8:h:193:TYR:CD1	8:h:193:TYR:C	2.96	0.43
2:B:241:GLN:CD	2:B:241:GLN:C	2.86	0.43
9:2:97:TYR:HB3	9:2:127:LEU:HD21	1.99	0.43
19:M:415:PHE:O	19:M:419:ILE:HG13	2.18	0.43
2:b:13:SER:C	2:b:15:SER:N	2.75	0.43
3:c:95:GLN:HE22	3:c:98:LEU:HD23	1.82	0.43
7:g:44:PHE:N	7:g:44:PHE:CD1	2.86	0.43
13:m:150:LEU:HD13	13:m:150:LEU:HA	1.85	0.43
7:G:56:VAL:H	7:G:56:VAL:HG22	1.60	0.43
19:M:128:PHE:C	19:M:128:PHE:CD2	2.96	0.43
10:j:203:GLN:HE21	12:5:166:HIS:HE1	1.67	0.43
11:k:4:ILE:O	11:k:4:ILE:HG23	2.19	0.43
11:k:151:ASP:O	11:k:152:MET:C	2.61	0.43
2:b:42:GLY:HA2	2:b:145:PHE:CE2	2.54	0.43
6:f:174:THR:O	6:f:175:LEU:C	2.60	0.43
3:C:167:ASN:HB2	3:C:170:ALA:HB3	2.00	0.43
19:M:352:PRO:HA	19:M:356:SER:HB2	1.97	0.43
19:M:390:GLN:O	19:M:393:ALA:HB3	2.19	0.43
8:h:151:THR:O	8:h:154:PHE:N	2.52	0.43
8:h:151:THR:C	8:h:153:ASP:N	2.75	0.43
13:m:84:LEU:O	13:m:85:SER:C	2.61	0.43
17:K:132:LYS:N	17:K:133:PRO:HD2	2.33	0.43
18:L:149:ASP:HB3	18:L:153:LEU:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1:49:ALA:O	8:1:50:ALA:C	2.61	0.43
19:M:374:ILE:HD13	19:M:412:HIS:CB	2.49	0.43
1:a:175:ASN:OD1	1:a:175:ASN:N	2.52	0.43
4:d:40:VAL:C	4:d:41:VAL:HG23	2.44	0.43
9:i:59:ILE:O	9:i:63:ILE:HG12	2.18	0.43
20:J:128:ASN:O	20:J:129:LYS:HB2	2.19	0.43
20:J:203:ALA:HB2	20:J:244:ILE:HD12	2.00	0.43
2:b:186:GLU:OE2	2:b:186:GLU:HA	2.19	0.43
3:c:212:PHE:CD2	3:c:229:PHE:CE1	3.07	0.43
5:e:206:GLU:CD	5:e:206:GLU:H	2.27	0.43
8:h:126:ILE:HG13	8:h:131:SER:CB	2.39	0.43
12:l:45:MET:HG3	12:l:52:CYS:CB	2.48	0.43
7:G:176:VAL:O	7:G:176:VAL:HG12	2.19	0.43
11:4:138:PHE:N	11:4:138:PHE:HD1	2.17	0.42
19:M:374:ILE:HD13	19:M:412:HIS:CA	2.48	0.42
19:M:374:ILE:CD1	19:M:412:HIS:HA	2.49	0.42
19:M:428:LYS:HE2	19:M:429:SER:HB3	2.00	0.42
20:J:197:LEU:HD12	23:J:501:ADP:C8	2.54	0.42
3:c:145:TYR:OH	3:c:217:LYS:HB3	2.19	0.42
7:g:214:TRP:O	7:g:214:TRP:CD1	2.72	0.42
9:i:175:VAL:HG12	9:i:176:CYS:N	2.34	0.42
11:k:130:TYR:CD1	11:k:130:TYR:C	2.98	0.42
8:1:8:PHE:CE1	8:1:10:ASP:HB2	2.55	0.42
10:3:148:MET:O	10:3:149:CYS:C	2.59	0.42
12:5:137:TYR:HD1	12:5:137:TYR:HA	1.66	0.42
17:K:158:ILE:HG12	17:K:159:SER:O	2.19	0.42
18:L:66:GLU:C	18:L:68:ARG:N	2.77	0.42
19:M:75:LEU:HD12	19:M:75:LEU:C	2.43	0.42
2:b:13:SER:C	2:b:15:SER:H	2.28	0.42
4:d:35:LYS:HE2	4:d:158:SER:HA	2.01	0.42
5:e:200:MET:HE1	5:e:208:ASN:OD1	2.19	0.42
15:H:398:VAL:HB	15:H:402:ILE:CD1	2.48	0.42
20:J:83:LYS:HA	20:J:97:ASP:HA	2.01	0.42
10:3:143:ASP:N	10:3:143:ASP:OD1	2.52	0.42
14:7:63:ILE:HD11	14:7:110:LEU:HD13	2.01	0.42
18:L:228:LYS:HG2	18:L:349:ILE:HD12	2.01	0.42
10:j:36:SER:OG	10:j:37:ASN:N	2.46	0.42
14:n:173:ALA:O	14:n:174:GLU:C	2.60	0.42
3:C:238:LEU:HD12	3:C:243:ILE:HD12	2.01	0.42
4:D:205:ALA:HB1	4:D:227:ILE:HG22	2.00	0.42
5:E:186:LYS:O	5:E:186:LYS:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:2:138:LEU:C	9:2:138:LEU:CD1	2.89	0.42
1:a:21:TYR:CD1	7:g:13:PRO:HA	2.55	0.42
8:h:151:THR:O	8:h:153:ASP:N	2.53	0.42
14:n:208:PHE:C	14:n:208:PHE:CD1	2.97	0.42
15:H:88:ARG:HA	15:H:88:ARG:NE	2.35	0.42
16:I:194:ILE:CG2	16:I:236:VAL:HG11	2.50	0.42
19:M:154:LEU:HD13	19:M:154:LEU:HA	1.95	0.42
19:M:365:SER:CB	19:M:376:TRP:CH2	3.02	0.42
20:J:179:ILE:O	20:J:179:ILE:HG23	2.19	0.42
4:d:125:ARG:O	4:d:125:ARG:HG3	2.19	0.42
11:k:194:ASP:C	11:k:195:PHE:O	2.61	0.42
14:n:13:SER:O	14:n:155:LEU:HD13	2.19	0.42
9:2:130:GLY:O	9:2:131:SER:C	2.63	0.42
17:K:51:LEU:HA	17:K:51:LEU:HD23	1.32	0.42
2:b:119:GLN:O	2:b:122:THR:HG22	2.20	0.42
8:h:148:LYS:HD2	8:h:148:LYS:O	2.20	0.42
9:i:135:MET:HA	9:i:138:LEU:HD12	2.02	0.42
7:G:56:VAL:HG22	7:G:60:ASN:HD21	1.85	0.42
9:2:99:ILE:HD11	9:2:127:LEU:HD22	2.02	0.42
10:3:147:GLY:O	10:3:148:MET:C	2.62	0.42
16:I:219:VAL:HG12	16:I:325:ILE:CD1	2.49	0.42
19:M:224:PRO:HB3	22:M:501:ATP:O3G	2.20	0.42
20:J:144:ASP:OD1	20:J:144:ASP:C	2.63	0.42
9:i:72:ARG:O	9:i:73:GLU:C	2.60	0.42
10:j:146:PHE:HD1	10:j:146:PHE:O	2.03	0.42
11:k:177:LYS:O	11:k:178:GLY:O	2.37	0.42
14:7:193:ARG:O	14:7:213:GLN:HA	2.20	0.42
3:c:238:LEU:HD12	3:c:243:ILE:HD12	2.01	0.42
7:g:224:HIS:O	7:g:225:LYS:HG3	2.20	0.42
12:l:123:LYS:CG	12:l:124:GLY:N	2.83	0.42
15:H:191:ILE:HG13	15:H:191:ILE:O	2.20	0.42
19:M:86:MET:O	19:M:87:ASP:C	2.63	0.42
7:g:52:SER:C	7:g:54:LEU:H	2.28	0.41
11:k:89:ALA:O	11:k:92:ILE:HG12	2.20	0.41
13:6:12:ILE:C	13:6:12:ILE:HD12	2.45	0.41
18:L:392:ARG:O	18:L:392:ARG:HG3	2.20	0.41
2:b:250:LEU:OXT	2:b:250:LEU:CD1	2.62	0.41
3:c:43:ILE:HD11	3:c:145:TYR:HB3	2.02	0.41
3:c:139:TYR:CD1	3:c:139:TYR:O	2.73	0.41
4:d:40:VAL:HG12	4:d:41:VAL:H	1.83	0.41
10:j:181:GLY:HA2	10:j:201:MET:HE1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:140:ASP:OD1	3:C:140:ASP:C	2.63	0.41
12:5:140:LEU:O	12:5:144:TYR:HB2	2.20	0.41
18:L:167:VAL:HB	18:L:266:MET:HE1	2.00	0.41
18:L:199:LEU:N	18:L:200:PRO:HD2	2.35	0.41
19:M:225:GLY:O	22:M:501:ATP:N7	2.52	0.41
1:a:105:CYS:HB2	1:a:136:SER:OG	2.20	0.41
2:b:37:ILE:O	2:b:43:VAL:CG1	2.68	0.41
2:b:38:LYS:HA	2:b:43:VAL:HG13	2.02	0.41
3:c:149:THR:HG22	3:c:159:TRP:HE1	1.85	0.41
13:6:194:ARG:HA	13:6:194:ARG:HD3	1.87	0.41
16:I:338:LEU:O	16:I:344:ILE:HG12	2.20	0.41
10:j:120:ILE:HD12	10:j:136:ILE:HG12	2.02	0.41
13:m:190:SER:O	13:m:193:GLU:N	2.45	0.41
2:B:13:SER:C	2:B:15:SER:H	2.28	0.41
13:6:12:ILE:HD13	13:6:110:ILE:HG21	2.03	0.41
13:6:131:TYR:CD1	13:6:131:TYR:C	2.98	0.41
14:7:146:PHE:O	14:7:146:PHE:CG	2.72	0.41
15:H:344:ASP:O	15:H:345:PRO:O	2.38	0.41
18:L:239:ILE:HG22	18:L:241:ALA:H	1.85	0.41
18:L:254:LYS:HA	19:M:256:ILE:O	2.19	0.41
11:k:9:VAL:HG12	11:k:10:GLN:H	1.84	0.41
13:m:50:ILE:HG23	13:m:50:ILE:O	2.18	0.41
7:G:214:TRP:H	7:G:214:TRP:HD1	1.67	0.41
12:5:34:VAL:HG21	12:5:178:TYR:CE1	2.56	0.41
1:a:18:GLN:HA	1:a:21:TYR:CD2	2.55	0.41
4:d:27:ARG:NH1	4:d:27:ARG:HB3	2.35	0.41
5:e:114:ARG:HB2	5:e:126:MET:SD	2.60	0.41
9:i:220:ILE:HG22	10:j:44:HIS:CE1	2.55	0.41
10:j:193:GLU:O	10:j:193:GLU:HG3	2.18	0.41
12:l:45:MET:HG3	12:l:52:CYS:HB2	2.03	0.41
10:3:163:PHE:CZ	10:3:197:ARG:HD3	2.56	0.41
12:5:206:SER:O	12:5:207:PHE:C	2.63	0.41
17:K:43:VAL:O	17:K:47:ILE:HG13	2.20	0.41
17:K:356:ILE:CG2	17:K:387:MET:HG3	2.51	0.41
18:L:401:PHE:CE2	18:L:417:LYS:HB3	2.56	0.41
3:c:123:GLN:HB3	3:c:124:HIS:CE1	2.55	0.41
3:c:225:TYR:OH	9:i:225:GLU:HB3	2.21	0.41
5:e:104:LEU:HD13	5:e:104:LEU:C	2.46	0.41
11:k:3:ILE:HD11	11:k:172:MET:HE2	2.03	0.41
12:l:123:LYS:CG	12:l:124:GLY:H	2.33	0.41
14:n:14:MET:HG2	14:n:177:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:n:63:ILE:O	14:n:63:ILE:HG22	2.20	0.41
8:1:175:MET:HB2	8:1:186:LEU:HB2	2.03	0.41
12:5:178:TYR:CE2	12:5:187:TYR:CD1	3.08	0.41
16:I:148:LEU:HD23	16:I:148:LEU:HA	1.86	0.41
17:K:426:PHE:N	17:K:426:PHE:CD1	2.89	0.41
5:e:217:GLN:OE1	5:e:217:GLN:CA	2.69	0.41
6:f:122:TYR:HB2	7:g:124:SER:O	2.20	0.41
11:k:118:GLN:CG	11:k:133:HIS:CE1	3.04	0.41
12:l:202:GLU:O	12:l:202:GLU:HG2	2.20	0.41
14:n:151:ALA:O	14:n:152:ASN:C	2.64	0.41
7:G:212:ILE:CG1	7:G:227:VAL:HB	2.50	0.41
15:H:106:ILE:O	15:H:107:LYS:C	2.63	0.41
16:I:96:LEU:HD23	16:I:135:PHE:CG	2.56	0.41
16:I:316:PHE:O	16:I:316:PHE:CD1	2.73	0.41
17:K:395:VAL:O	17:K:395:VAL:CG1	2.69	0.41
19:M:189:GLN:N	19:M:189:GLN:CD	2.79	0.41
6:f:206:THR:O	6:f:233:ILE:HD11	2.20	0.41
7:g:105:ILE:HB	7:g:106:PRO:HD3	2.02	0.41
11:k:10:GLN:O	11:k:10:GLN:CG	2.69	0.41
4:D:65:ILE:HG21	4:D:107:LEU:HD21	2.03	0.41
7:G:243:ILE:O	7:G:243:ILE:CG1	2.68	0.41
9:2:5:GLY:O	9:2:124:TYR:CD1	2.74	0.41
10:3:52:ILE:CG2	10:3:59:VAL:HG13	2.51	0.41
22:H:502:ATP:PB	16:I:340:ARG:HH12	2.42	0.41
16:I:393:GLN:CD	16:I:393:GLN:O	2.64	0.41
17:K:51:LEU:HD12	20:J:27:ILE:HD12	2.03	0.41
18:L:300:GLU:CD	18:L:300:GLU:C	2.88	0.41
8:h:172:VAL:HG12	8:h:190:PRO:HD3	2.02	0.41
10:3:158:GLU:O	10:3:161:ASP:N	2.54	0.41
14:7:30:TYR:C	14:7:30:TYR:CD1	2.98	0.41
15:H:452:SER:OG	15:H:453:GLY:N	2.54	0.41
16:I:121:THR:HG22	16:I:122:SER:O	2.20	0.41
20:J:217:GLU:OE1	20:J:217:GLU:HA	2.20	0.41
1:a:235:ARG:O	1:a:239:ILE:HG13	2.21	0.40
6:f:38:ARG:HD3	6:f:39:SER:O	2.21	0.40
8:h:36:ARG:HG2	8:h:38:HIS:O	2.21	0.40
10:j:60:THR:O	10:j:61:THR:C	2.62	0.40
4:D:45:GLU:O	4:D:45:GLU:CG	2.64	0.40
20:J:24:GLU:HA	20:J:27:ILE:HG12	2.03	0.40
20:J:45:GLU:HA	20:J:48:ARG:HG2	2.02	0.40
10:j:44:HIS:HB3	10:j:49:PHE:CD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:m:72:VAL:O	13:m:73:LYS:C	2.64	0.40
6:F:6:ASP:N	6:F:6:ASP:OD1	2.48	0.40
13:6:18:GLU:HG3	13:6:174:TYR:HB3	2.03	0.40
15:H:189:PRO:O	15:H:190:ARG:O	2.39	0.40
18:L:216:LYS:O	18:L:216:LYS:HG3	2.21	0.40
19:M:127:VAL:O	19:M:127:VAL:HG23	2.20	0.40
19:M:142:PRO:O	19:M:143:ASN:CB	2.69	0.40
4:d:179:ARG:HH22	5:e:52:GLU:HA	1.87	0.40
13:m:199:GLY:O	13:m:200:ASP:CB	2.69	0.40
5:E:140:ASP:OD1	5:E:140:ASP:C	2.64	0.40
7:G:200:HIS:O	7:G:200:HIS:CG	2.74	0.40
9:2:137:VAL:O	9:2:138:LEU:C	2.64	0.40
16:I:339:ILE:C	16:I:339:ILE:CD1	2.94	0.40
17:K:383:ILE:O	17:K:383:ILE:HG22	2.20	0.40
19:M:157:ASP:OD1	19:M:157:ASP:C	2.64	0.40
19:M:338:LEU:HD23	19:M:338:LEU:C	2.46	0.40
13:m:123:TYR:CE1	13:m:133:ARG:HB2	2.57	0.40
15:H:43:ALA:HB3	15:H:44:PRO:HD3	2.03	0.40
4:d:27:ARG:HB3	4:d:27:ARG:HH11	1.86	0.40
9:i:146:LEU:HD22	9:i:150:GLU:OE2	2.21	0.40
10:j:28:LEU:HD13	10:j:39:PHE:CD2	2.57	0.40
11:k:167:GLU:O	11:k:168:LEU:C	2.65	0.40
17:K:158:ILE:HD13	17:K:236:ARG:O	2.21	0.40
18:L:56:ALA:O	18:L:60:PHE:CD2	2.75	0.40
19:M:216:LYS:NZ	19:M:318:ASP:O	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	239/252 (95%)	218 (91%)	20 (8%)	1 (0%)	30 67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	239/252 (95%)	221 (92%)	17 (7%)	1 (0%)	30	67
2	B	248/250 (99%)	232 (94%)	14 (6%)	2 (1%)	16	53
2	b	248/250 (99%)	223 (90%)	24 (10%)	1 (0%)	30	67
3	C	242/258 (94%)	225 (93%)	14 (6%)	3 (1%)	10	43
3	c	242/258 (94%)	217 (90%)	21 (9%)	4 (2%)	7	35
4	D	238/254 (94%)	215 (90%)	17 (7%)	6 (2%)	4	26
4	d	238/254 (94%)	221 (93%)	15 (6%)	2 (1%)	16	53
5	E	240/260 (92%)	223 (93%)	9 (4%)	8 (3%)	3	21
5	e	240/260 (92%)	222 (92%)	14 (6%)	4 (2%)	7	35
6	F	231/234 (99%)	211 (91%)	15 (6%)	5 (2%)	5	29
6	f	229/234 (98%)	207 (90%)	21 (9%)	1 (0%)	30	67
7	G	241/288 (84%)	223 (92%)	17 (7%)	1 (0%)	30	67
7	g	241/288 (84%)	221 (92%)	17 (7%)	3 (1%)	10	43
8	1	194/215 (90%)	186 (96%)	8 (4%)	0	100	100
8	h	194/215 (90%)	176 (91%)	17 (9%)	1 (0%)	24	63
9	2	224/261 (86%)	204 (91%)	18 (8%)	2 (1%)	14	49
9	i	224/261 (86%)	200 (89%)	17 (8%)	7 (3%)	3	22
10	3	202/205 (98%)	187 (93%)	12 (6%)	3 (2%)	8	38
10	j	202/205 (98%)	174 (86%)	23 (11%)	5 (2%)	4	26
11	4	193/198 (98%)	175 (91%)	13 (7%)	5 (3%)	4	26
11	k	193/198 (98%)	169 (88%)	19 (10%)	5 (3%)	4	26
12	5	210/287 (73%)	194 (92%)	14 (7%)	2 (1%)	12	47
12	l	210/287 (73%)	193 (92%)	17 (8%)	0	100	100
13	6	220/241 (91%)	193 (88%)	23 (10%)	4 (2%)	6	33
13	m	220/241 (91%)	196 (89%)	18 (8%)	6 (3%)	4	25
14	7	227/266 (85%)	202 (89%)	19 (8%)	6 (3%)	4	26
14	n	230/266 (86%)	205 (89%)	21 (9%)	4 (2%)	7	35
15	H	386/467 (83%)	333 (86%)	33 (8%)	20 (5%)	1	15
16	I	383/437 (88%)	345 (90%)	32 (8%)	6 (2%)	7	37
17	K	387/428 (90%)	350 (90%)	28 (7%)	9 (2%)	5	28
18	L	386/437 (88%)	343 (89%)	36 (9%)	7 (2%)	6	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	M	377/434 (87%)	339 (90%)	27 (7%)	11 (3%)	3	23
20	J	384/405 (95%)	347 (90%)	30 (8%)	7 (2%)	6	33
All	All	8602/9546 (90%)	7790 (91%)	660 (8%)	152 (2%)	9	33

All (152) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	d	203	THR
9	i	39	PRO
9	i	104	ASP
10	j	6	ILE
10	j	203	GLN
4	D	50	LEU
5	E	129	PRO
5	E	130	PHE
10	3	125	LEU
11	4	94	SER
13	6	66	LYS
14	7	10	SER
15	H	190	ARG
15	H	194	SER
15	H	452	SER
16	I	125	MET
16	I	134	SER
16	I	213	ILE
17	K	344	ARG
18	L	343	LEU
18	L	353	ASN
18	L	384	ASP
19	M	316	SER
19	M	427	SER
3	c	8	ARG
3	c	202	SER
4	d	38	ASN
5	e	45	ARG
9	i	31	CYS
9	i	65	LEU
9	i	66	HIS
11	k	178	GLY
13	m	48	ASP
14	n	227	GLY

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Mol	Chain	Res	Type
2	B	17	LYS
2	B	31	GLY
5	E	36	GLU
5	E	65	HIS
5	E	115	PHE
5	E	120	SER
6	F	124	GLY
6	F	200	LEU
13	6	73	LYS
14	7	216	ASN
14	7	227	GLY
15	H	68	GLY
15	H	70	LYS
15	H	453	GLY
15	H	462	ARG
17	K	418	ASP
17	K	423	LYS
18	L	216	LYS
18	L	372	GLY
20	J	129	LYS
5	e	120	SER
7	g	207	ASP
10	j	7	ASN
10	j	39	PHE
11	k	73	TYR
11	k	94	SER
13	m	19	ASP
13	m	200	ASP
14	n	47	ASP
3	C	184	LYS
4	D	203	THR
5	E	128	ARG
6	F	4	ASN
7	G	59	LYS
10	3	156	ASN
11	4	2	ASP
11	4	177	LYS
12	5	82	ILE
14	7	27	LEU
14	7	87	LEU
15	H	162	ARG
15	H	203	LYS

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Mol	Chain	Res	Type
15	H	213	GLY
15	H	303	ALA
15	H	457	PHE
16	I	83	LYS
17	K	105	GLN
19	M	78	LEU
19	M	143	ASN
19	M	162	GLU
19	M	339	ARG
3	c	63	GLU
5	e	142	ASP
7	g	117	GLN
13	m	165	ASN
14	n	86	ALA
3	C	52	THR
4	D	38	ASN
6	F	3	ASN
6	F	58	TYR
10	3	181	GLY
15	H	315	GLY
15	H	323	ALA
15	H	345	PRO
15	H	463	TYR
17	K	141	ARG
17	K	207	ARG
17	K	414	GLN
18	L	179	THR
18	L	291	PHE
19	M	174	GLU
20	J	117	SER
20	J	141	LYS
2	b	101	TYR
8	h	145	ASN
10	j	155	PRO
13	m	97	LEU
4	D	216	ASP
11	4	32	ASP
11	4	185	ASP
13	6	4	PRO
15	H	389	PHE
16	I	388	SER
19	M	179	THR

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Mol	Chain	Res	Type
19	M	353	SER
19	M	433	TYR
20	J	214	SER
1	a	164	PRO
6	f	66	ASP
13	m	130	SER
3	C	167	ASN
4	D	100	ASP
5	E	143	ASP
9	2	104	ASP
12	5	38	ASN
13	6	129	GLY
15	H	152	ILE
17	K	92	VAL
17	K	314	VAL
20	J	207	ASP
20	J	283	GLU
9	i	94	ILE
9	i	193	PRO
9	2	117	GLY
20	J	352	GLY
5	e	132	VAL
4	D	8	ILE
15	H	314	VAL
15	H	412	PRO
16	I	340	ARG
7	g	116	VAL
3	c	51	VAL
11	k	123	GLY
14	n	178	VAL
14	7	178	VAL
19	M	172	VAL
11	k	4	ILE
1	A	7	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	206/210 (98%)	203 (98%)	3 (2%)	57	70
1	a	206/210 (98%)	196 (95%)	10 (5%)	22	44
2	B	209/209 (100%)	206 (99%)	3 (1%)	59	71
2	b	209/209 (100%)	199 (95%)	10 (5%)	23	45
3	C	203/216 (94%)	202 (100%)	1 (0%)	81	81
3	c	203/216 (94%)	195 (96%)	8 (4%)	28	50
4	D	212/226 (94%)	208 (98%)	4 (2%)	50	66
4	d	212/226 (94%)	207 (98%)	5 (2%)	43	63
5	E	198/215 (92%)	194 (98%)	4 (2%)	48	65
5	e	198/215 (92%)	194 (98%)	4 (2%)	48	65
6	F	192/193 (100%)	190 (99%)	2 (1%)	68	76
6	f	190/193 (98%)	180 (95%)	10 (5%)	20	42
7	G	201/239 (84%)	199 (99%)	2 (1%)	68	76
7	g	201/239 (84%)	193 (96%)	8 (4%)	28	49
8	1	162/178 (91%)	161 (99%)	1 (1%)	78	80
8	h	162/178 (91%)	159 (98%)	3 (2%)	50	66
9	2	185/214 (86%)	182 (98%)	3 (2%)	55	69
9	i	185/214 (86%)	184 (100%)	1 (0%)	81	81
10	3	172/173 (99%)	172 (100%)	0	100	100
10	j	172/173 (99%)	168 (98%)	4 (2%)	44	63
11	4	173/175 (99%)	171 (99%)	2 (1%)	63	73
11	k	173/175 (99%)	167 (96%)	6 (4%)	32	53
12	5	169/235 (72%)	168 (99%)	1 (1%)	78	80
12	l	169/235 (72%)	161 (95%)	8 (5%)	23	45
13	6	185/201 (92%)	183 (99%)	2 (1%)	65	74
13	m	185/201 (92%)	181 (98%)	4 (2%)	45	64
14	7	195/224 (87%)	195 (100%)	0	100	100
14	n	198/224 (88%)	192 (97%)	6 (3%)	36	57
15	H	330/399 (83%)	323 (98%)	7 (2%)	47	65
16	I	342/385 (89%)	337 (98%)	5 (2%)	57	70
17	K	342/374 (91%)	338 (99%)	4 (1%)	63	73
18	L	332/377 (88%)	329 (99%)	3 (1%)	70	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
19	M	329/375 (88%)	323 (98%)	6 (2%)	51 67
20	J	336/352 (96%)	332 (99%)	4 (1%)	63 73
All	All	7336/8078 (91%)	7192 (98%)	144 (2%)	48 65

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	36	VAL
1	a	55	LEU
1	a	133	THR
1	a	138	ASP
1	a	144	SER
1	a	162	THR
1	a	168	GLU
1	a	175	ASN
1	a	200	HIS
1	a	235	ARG
2	b	44	VAL
2	b	57	MET
2	b	70	ASP
2	b	85	LEU
2	b	133	SER
2	b	146	SER
2	b	203	GLU
2	b	205	ASN
2	b	220	ASP
2	b	245	ASP
3	c	41	ASP
3	c	107	VAL
3	c	110	LEU
3	c	124	HIS
3	c	157	THR
3	c	177	MET
3	c	190	GLU
3	c	206	THR
4	d	44	CYS
4	d	107	LEU
4	d	162	ILE
4	d	220	VAL
4	d	225	GLU
5	e	54	ASP

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Mol	Chain	Res	Type
5	e	169	GLU
5	e	177	ASN
5	e	206	GLU
6	f	10	VAL
6	f	53	ASP
6	f	55	LEU
6	f	65	CYS
6	f	71	LEU
6	f	73	LEU
6	f	87	LEU
6	f	143	LEU
6	f	188	LEU
6	f	202	ASP
7	g	10	VAL
7	g	14	ASP
7	g	32	THR
7	g	122	TYR
7	g	131	SER
7	g	172	LEU
7	g	181	GLU
7	g	202	ASP
8	h	30	VAL
8	h	72	THR
8	h	148	LYS
9	i	183	ASP
10	j	11	VAL
10	j	108	VAL
10	j	143	ASP
10	j	171	LEU
11	k	40	PRO
11	k	52	ASP
11	k	53	THR
11	k	126	VAL
11	k	182	LYS
11	k	194	ASP
12	l	4	LEU
12	l	9	GLN
12	l	30	THR
12	l	36	GLU
12	l	61	SER
12	l	86	LEU
12	l	99	THR

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Mol	Chain	Res	Type
12	l	120	THR
13	m	40	GLU
13	m	128	VAL
13	m	135	GLN
13	m	209	LYS
14	n	20	VAL
14	n	49	THR
14	n	84	GLU
14	n	137	TYR
14	n	154	LEU
14	n	184	LEU
1	A	63	ILE
1	A	69	THR
1	A	207	THR
2	B	11	THR
2	B	151	ASP
2	B	217	GLU
3	C	168	THR
4	D	162	ILE
4	D	187	GLU
4	D	225	GLU
4	D	229	GLN
5	E	105	THR
5	E	128	ARG
5	E	129	PRO
5	E	132	VAL
6	F	46	VAL
6	F	176	ASP
7	G	149	PRO
7	G	181	GLU
8	1	153	ASP
9	2	121	VAL
9	2	138	LEU
9	2	212	VAL
11	4	87	GLU
11	4	166	GLN
12	5	182	GLU
13	6	12	ILE
13	6	150	LEU
15	H	271	PHE
15	H	274	VAL
15	H	319	PHE

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Mol	Chain	Res	Type
15	H	367	ARG
15	H	392	HIS
15	H	437	VAL
15	H	465	GLN
16	I	230	THR
16	I	305	THR
16	I	314	ASP
16	I	328	THR
16	I	428	VAL
17	K	50	LYS
17	K	264	ASN
17	K	382	VAL
17	K	425	ASP
18	L	67	HIS
18	L	358	LEU
18	L	427	LYS
19	M	161	SER
19	M	162	GLU
19	M	186	LEU
19	M	359	GLN
19	M	428	LYS
19	M	433	TYR
20	J	110	SER
20	J	286	LYS
20	J	306	ARG
20	J	370	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (124) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	32	ASN
1	a	121	GLN
1	a	167	GLN
1	a	176	HIS
2	b	20	GLN
2	b	30	GLN
3	c	93	HIS
3	c	95	GLN
3	c	96	ASN
3	c	119	GLN
3	c	146	GLN
3	c	172	GLN

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Mol	Chain	Res	Type
3	c	226	GLN
4	d	94	HIS
4	d	147	GLN
5	e	83	HIS
5	e	149	HIS
5	e	207	ASN
6	f	20	GLN
6	f	30	GLN
6	f	59	GLN
6	f	90	GLN
6	f	120	GLN
7	g	8	ASN
7	g	19	GLN
7	g	83	HIS
7	g	114	GLN
7	g	117	GLN
7	g	123	ASN
7	g	179	HIS
7	g	224	HIS
8	h	28	ASN
8	h	38	HIS
8	h	89	ASN
8	h	106	ASN
8	h	141	ASN
8	h	145	ASN
9	i	9	ASN
9	i	10	ASN
9	i	116	HIS
9	i	141	HIS
10	j	7	ASN
10	j	37	ASN
10	j	47	HIS
10	j	88	GLN
10	j	112	ASN
10	j	172	ASN
11	k	10	GLN
11	k	61	GLN
11	k	101	ASN
11	k	118	GLN
11	k	133	HIS
12	l	29	GLN
12	l	66	HIS

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Mol	Chain	Res	Type
12	l	85	ASN
12	l	179	HIS
13	m	70	ASN
13	m	87	ASN
13	m	197	GLN
14	n	18	ASN
14	n	48	ASN
14	n	102	GLN
14	n	152	ASN
14	n	203	ASN
14	n	211	ASN
14	n	231	GLN
1	A	6	HIS
1	A	200	HIS
2	B	123	GLN
3	C	226	GLN
5	E	15	GLN
5	E	149	HIS
5	E	180	HIS
6	F	68	HIS
6	F	85	ASN
6	F	92	ASN
6	F	109	HIS
6	F	116	GLN
6	F	165	GLN
7	G	86	ASN
7	G	166	GLN
7	G	179	HIS
7	G	191	GLN
7	G	200	HIS
8	1	28	ASN
8	1	141	ASN
9	2	114	HIS
10	3	168	GLN
11	4	101	ASN
11	4	133	HIS
11	4	146	HIS
12	5	38	ASN
12	5	166	HIS
12	5	176	ASN
12	5	190	ASN
13	6	3	ASN

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Mol	Chain	Res	Type
13	6	29	ASN
13	6	70	ASN
13	6	79	HIS
13	6	152	ASN
14	7	61	GLN
14	7	62	HIS
15	H	98	GLN
15	H	182	ASN
15	H	348	ASN
15	H	359	ASN
16	I	151	HIS
16	I	295	ASN
16	I	352	ASN
16	I	370	ASN
16	I	376	ASN
17	K	142	HIS
17	K	238	ASN
17	K	264	ASN
17	K	311	ASN
17	K	419	ASN
18	L	242	ASN
18	L	302	GLN
18	L	353	ASN
18	L	409	HIS
19	M	238	GLN
19	M	364	HIS
20	J	66	GLN
20	J	331	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 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
22	ATP	K	501	21	32,33,33	2.47	8 (25%)	48,52,52	2.80	21 (43%)
22	ATP	H	502	21	32,33,33	2.14	8 (25%)	48,52,52	2.82	20 (41%)
23	ADP	J	501	21	28,29,29	2.64	5 (17%)	43,45,45	2.79	18 (41%)
22	ATP	M	501	21	32,33,33	1.90	7 (21%)	48,52,52	2.72	16 (33%)
22	ATP	I	501	21	32,33,33	2.25	10 (31%)	48,52,52	2.98	22 (45%)
22	ATP	L	501	21	32,33,33	2.06	6 (18%)	48,52,52	2.61	19 (39%)

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
22	ATP	K	501	21	-	4/22/38/38	0/3/3/3
22	ATP	H	502	21	-	7/22/38/38	0/3/3/3
23	ADP	J	501	21	-	2/16/32/32	0/3/3/3
22	ATP	M	501	21	-	7/22/38/38	0/3/3/3
22	ATP	I	501	21	-	3/22/38/38	0/3/3/3
22	ATP	L	501	21	-	8/22/38/38	0/3/3/3

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	J	501	ADP	PA-O3A	11.62	1.72	1.59
22	H	502	ATP	PB-O3B	7.71	1.67	1.59
22	K	501	ATP	PB-O3B	7.42	1.67	1.59
22	I	501	ATP	PB-O3B	6.90	1.66	1.59
22	K	501	ATP	PA-O3A	6.11	1.66	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	L	501	ATP	PB-O3B	6.07	1.66	1.59
22	K	501	ATP	PB-O3A	5.95	1.65	1.59
22	M	501	ATP	PB-O3A	5.59	1.65	1.59
22	L	501	ATP	PA-O3A	5.55	1.65	1.59
22	L	501	ATP	PB-O3A	5.16	1.65	1.59
22	M	501	ATP	PA-O3A	4.97	1.64	1.59
22	H	502	ATP	PB-O3A	4.66	1.64	1.59
22	I	501	ATP	C5-C4	4.62	1.47	1.39
22	I	501	ATP	PA-O3A	4.45	1.64	1.59
22	M	501	ATP	PB-O3B	3.85	1.63	1.59
22	I	501	ATP	C5-C6	3.85	1.51	1.41
22	I	501	ATP	PB-O3A	3.84	1.63	1.59
22	K	501	ATP	C5-C4	3.71	1.45	1.39
22	H	502	ATP	PA-O3A	3.62	1.63	1.59
23	J	501	ADP	C5-C4	3.45	1.45	1.39
22	K	501	ATP	C5-C6	3.32	1.50	1.41
22	M	501	ATP	C5-C4	3.15	1.44	1.39
22	K	501	ATP	C8-N7	3.10	1.37	1.31
22	H	502	ATP	C5-C4	3.07	1.44	1.39
22	L	501	ATP	C5-C4	3.05	1.44	1.39
22	K	501	ATP	C4-N3	2.94	1.39	1.34
23	J	501	ADP	C5-C6	2.84	1.48	1.41
22	H	502	ATP	C8-N7	2.79	1.37	1.31
23	J	501	ADP	C8-N7	2.76	1.37	1.31
22	M	501	ATP	C5-C6	2.69	1.48	1.41
22	H	502	ATP	C1'-N9	2.64	1.53	1.46
22	I	501	ATP	C4-N3	2.60	1.39	1.34
22	I	501	ATP	C2-N1	2.60	1.38	1.33
23	J	501	ADP	C4-N3	2.54	1.39	1.34
22	I	501	ATP	C6-N6	2.50	1.40	1.34
22	I	501	ATP	C8-N7	2.49	1.36	1.31
22	M	501	ATP	C4-N9	-2.39	1.32	1.37
22	L	501	ATP	C5-C6	2.36	1.47	1.41
22	H	502	ATP	C5-C6	2.35	1.47	1.41
22	H	502	ATP	C4-N3	2.33	1.38	1.34
22	I	501	ATP	C2-N3	2.32	1.38	1.33
22	M	501	ATP	C8-N7	2.31	1.36	1.31
22	L	501	ATP	C8-N7	2.28	1.36	1.31
22	K	501	ATP	C2-N3	2.03	1.37	1.33

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	M	501	ATP	C4-N9-C8	9.02	115.20	105.74
22	H	502	ATP	N3-C2-N1	-8.96	115.02	128.58
23	J	501	ADP	N3-C2-N1	-8.55	115.64	128.58
22	K	501	ATP	N3-C2-N1	-8.10	116.32	128.58
22	M	501	ATP	N3-C2-N1	-7.59	117.09	128.58
22	L	501	ATP	C5-C4-N3	-7.24	116.75	126.72
22	K	501	ATP	C5-C4-N3	-7.03	117.04	126.72
22	L	501	ATP	N3-C4-N9	7.01	139.09	127.17
22	I	501	ATP	C4-N9-C8	6.89	112.98	105.74
22	K	501	ATP	C2-N3-C4	6.84	128.54	111.83
23	J	501	ADP	C4-N9-C8	6.77	112.85	105.74
22	H	502	ATP	C2-N3-C4	6.52	127.76	111.83
22	I	501	ATP	N3-C4-N9	6.39	138.04	127.17
22	I	501	ATP	C5-C4-N3	-6.22	118.15	126.72
22	M	501	ATP	N9-C8-N7	-6.14	105.22	113.94
22	I	501	ATP	N9-C8-N7	-6.13	105.24	113.94
22	L	501	ATP	N3-C2-N1	-6.02	119.47	128.58
22	I	501	ATP	N3-C2-N1	-6.01	119.48	128.58
22	H	502	ATP	C6-C5-C4	-6.01	108.97	117.18
22	K	501	ATP	N3-C4-N9	5.98	137.33	127.17
22	L	501	ATP	C2-N3-C4	5.69	125.74	111.83
22	I	501	ATP	C5-N7-C8	5.63	112.31	103.45
23	J	501	ADP	C2-N3-C4	5.59	125.49	111.83
22	H	502	ATP	O3A-PB-O1B	-5.22	95.01	110.70
22	I	501	ATP	C2-N3-C4	4.90	123.80	111.83
23	J	501	ADP	N9-C8-N7	-4.82	107.10	113.94
22	H	502	ATP	C5-C6-N6	-4.68	111.69	123.29
23	J	501	ADP	N3-C4-N9	4.64	135.05	127.17
22	L	501	ATP	C4-N9-C8	4.55	110.52	105.74
22	H	502	ATP	C6-C5-N7	4.37	140.51	132.09
22	H	502	ATP	C5-C4-N3	-4.33	120.75	126.72
22	I	501	ATP	C4-C5-N7	-4.30	105.66	110.58
22	M	501	ATP	C2-N3-C4	4.24	122.19	111.83
23	J	501	ADP	C6-C5-C4	-4.18	111.47	117.18
22	M	501	ATP	C2-N1-C6	4.16	125.57	118.73
22	H	502	ATP	N3-C4-N9	4.11	134.15	127.17
22	K	501	ATP	C3'-C2'-C1'	4.07	109.17	101.46
23	J	501	ADP	O3A-PA-O1A	4.07	122.95	110.70
22	I	501	ATP	O2B-PB-O3A	-3.92	96.67	107.27
22	M	501	ATP	N3-C4-N9	3.92	133.84	127.17
22	I	501	ATP	O3'-C3'-C2'	3.78	123.93	111.82
23	J	501	ADP	C6-C5-N7	3.76	139.34	132.09
22	K	501	ATP	N9-C8-N7	-3.67	108.73	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	L	501	ATP	N9-C8-N7	-3.66	108.74	113.94
22	M	501	ATP	C6-C5-N7	3.58	139.00	132.09
22	K	501	ATP	C5-C6-N6	-3.58	114.43	123.29
22	K	501	ATP	O2B-PB-O3B	3.57	116.93	107.27
23	J	501	ADP	C5-C4-N3	-3.56	121.82	126.72
22	M	501	ATP	C6-C5-C4	-3.51	112.39	117.18
22	H	502	ATP	O2G-PG-O1G	3.49	124.42	110.83
22	K	501	ATP	C4-N9-C8	3.45	109.36	105.74
22	M	501	ATP	C5-N7-C8	3.40	108.80	103.45
22	L	501	ATP	C5-C6-N6	-3.40	114.88	123.29
23	J	501	ADP	C5-C6-N6	-3.37	114.94	123.29
22	H	502	ATP	C5-C6-N1	3.37	126.06	117.51
22	K	501	ATP	C5-N7-C8	3.37	108.74	103.45
22	I	501	ATP	O2A-PA-O3A	3.36	116.36	107.27
22	M	501	ATP	C5-C4-N9	-3.35	102.16	105.81
22	K	501	ATP	C6-C5-N7	3.32	138.50	132.09
22	K	501	ATP	O4'-C1'-N9	3.27	114.37	108.09
22	I	501	ATP	C2-N1-C6	3.16	123.92	118.73
22	L	501	ATP	C1'-N9-C8	-3.13	120.15	127.09
22	M	501	ATP	O2B-PB-O3A	3.03	115.45	107.27
22	L	501	ATP	O3G-PG-O3B	3.00	114.71	104.64
22	L	501	ATP	C5-N7-C8	2.95	108.09	103.45
23	J	501	ADP	C2-N1-C6	2.93	123.54	118.73
22	I	501	ATP	O2'-C2'-C3'	2.91	121.16	111.82
22	I	501	ATP	C1'-N9-C8	-2.85	120.76	127.09
22	H	502	ATP	O3G-PG-O3B	2.85	114.19	104.64
22	K	501	ATP	O5'-C5'-C4'	2.83	118.63	108.99
22	I	501	ATP	O2B-PB-O3B	2.77	114.75	107.27
22	H	502	ATP	C4-N9-C8	2.77	108.64	105.74
22	K	501	ATP	O4'-C4'-C5'	2.77	118.19	109.33
23	J	501	ADP	C5-N7-C8	2.73	107.74	103.45
22	K	501	ATP	C4-C5-N7	-2.65	107.55	110.58
22	K	501	ATP	O3A-PA-O1A	2.65	118.67	110.70
22	I	501	ATP	O2G-PG-O3B	2.62	113.42	104.64
22	H	502	ATP	N9-C8-N7	-2.62	110.22	113.94
22	I	501	ATP	O5'-C5'-C4'	-2.61	100.11	108.99
22	M	501	ATP	O4'-C1'-N9	-2.61	103.08	108.09
22	H	502	ATP	O2B-PB-O3A	2.57	114.22	107.27
22	I	501	ATP	N6-C6-N1	2.57	124.09	118.38
22	L	501	ATP	O3B-PG-O1G	-2.53	97.74	111.04
23	J	501	ADP	C5-C4-N9	-2.48	103.11	105.81
22	L	501	ATP	O3'-C3'-C2'	2.44	119.65	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	I	501	ATP	C2'-C1'-N9	-2.44	107.24	113.30
22	M	501	ATP	C4-N9-C1'	-2.42	120.96	126.63
22	H	502	ATP	O2A-PA-O1A	2.42	123.72	112.44
22	H	502	ATP	O5'-PA-O1A	-2.41	99.37	108.94
22	L	501	ATP	O5'-PA-O1A	-2.38	99.49	108.94
22	K	501	ATP	C6-C5-C4	-2.36	113.95	117.18
22	I	501	ATP	O4'-C4'-C5'	2.36	116.88	109.33
23	J	501	ADP	O5'-C5'-C4'	2.34	116.95	108.99
22	H	502	ATP	O2B-PB-O3B	2.33	113.57	107.27
22	H	502	ATP	C4-N9-C1'	-2.32	121.20	126.63
22	H	502	ATP	O3A-PA-O1A	-2.31	103.76	110.70
22	K	501	ATP	O2G-PG-O3B	2.29	112.30	104.64
22	M	501	ATP	O2A-PA-O1A	2.25	122.89	112.44
23	J	501	ADP	C2'-C1'-N9	-2.23	107.75	113.30
22	I	501	ATP	C6-C5-N7	2.17	136.28	132.09
22	H	502	ATP	O5'-C5'-C4'	2.17	116.38	108.99
22	I	501	ATP	O3B-PG-O1G	-2.16	99.66	111.04
22	M	501	ATP	O3G-PG-O2G	2.15	115.88	107.80
22	M	501	ATP	O5'-PA-O1A	-2.14	100.47	108.94
22	L	501	ATP	O2B-PB-O3B	2.13	113.03	107.27
22	L	501	ATP	C6-C5-N7	2.12	136.18	132.09
22	L	501	ATP	O4'-C4'-C3'	-2.11	100.97	105.15
22	L	501	ATP	O2G-PG-O1G	2.09	118.99	110.83
23	J	501	ADP	N6-C6-N1	2.08	123.02	118.38
22	L	501	ATP	O4'-C4'-C5'	2.06	115.94	109.33
22	L	501	ATP	C5-C6-N1	2.04	122.70	117.51
22	K	501	ATP	C5-C6-N1	2.03	122.67	117.51
22	K	501	ATP	N6-C6-N1	2.03	122.90	118.38
23	J	501	ADP	C4-N9-C1'	-2.03	121.89	126.63
22	K	501	ATP	O3G-PG-O3B	-2.02	97.86	104.64
23	J	501	ADP	O2B-PB-O3A	2.01	111.36	104.64

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	H	502	ATP	C5'-O5'-PA-O2A
22	H	502	ATP	C5'-O5'-PA-O3A
22	I	501	ATP	C5'-O5'-PA-O1A
22	I	501	ATP	C5'-O5'-PA-O2A
22	I	501	ATP	C5'-O5'-PA-O3A
22	K	501	ATP	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
22	L	501	ATP	PB-O3B-PG-O2G
22	L	501	ATP	C5'-O5'-PA-O2A
22	L	501	ATP	C5'-O5'-PA-O3A
22	M	501	ATP	PB-O3B-PG-O2G
22	M	501	ATP	C5'-O5'-PA-O2A
22	M	501	ATP	C5'-O5'-PA-O3A
23	J	501	ADP	C5'-O5'-PA-O3A
22	H	502	ATP	PG-O3B-PB-O2B
23	J	501	ADP	O4'-C4'-C5'-O5'
22	K	501	ATP	C5'-O5'-PA-O1A
22	K	501	ATP	C5'-O5'-PA-O3A
22	L	501	ATP	PB-O3B-PG-O1G
22	L	501	ATP	O4'-C4'-C5'-O5'
22	L	501	ATP	PG-O3B-PB-O2B
22	K	501	ATP	C4'-C5'-O5'-PA
22	L	501	ATP	PA-O3A-PB-O1B
22	M	501	ATP	PG-O3B-PB-O1B
22	H	502	ATP	PB-O3B-PG-O3G
22	M	501	ATP	PB-O3B-PG-O3G
22	H	502	ATP	PA-O3A-PB-O2B
22	L	501	ATP	PG-O3B-PB-O1B
22	H	502	ATP	PB-O3B-PG-O1G
22	M	501	ATP	PB-O3B-PG-O1G
22	H	502	ATP	PG-O3B-PB-O1B
22	M	501	ATP	PG-O3B-PB-O2B

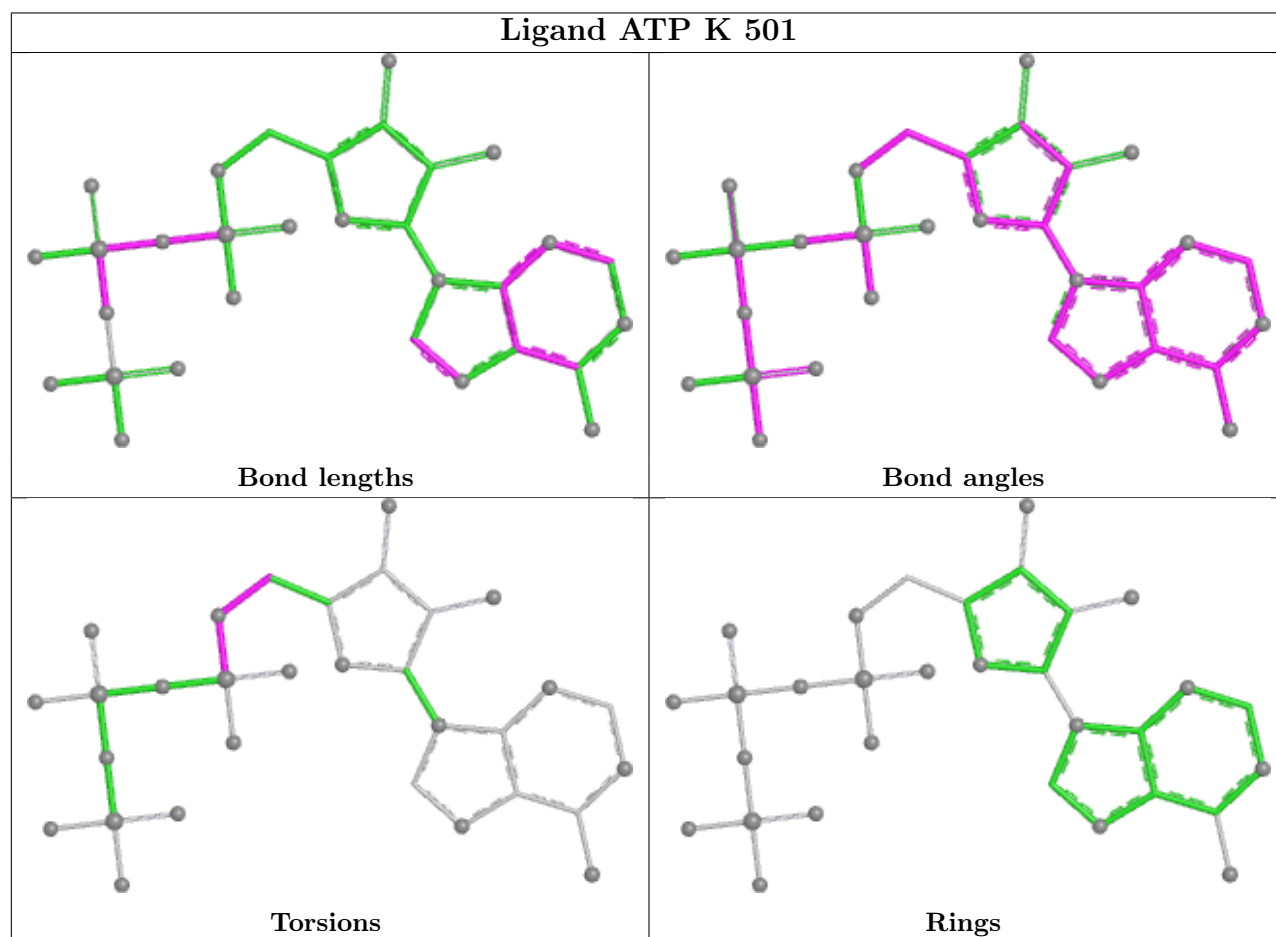
There are no ring outliers.

5 monomers are involved in 27 short contacts:

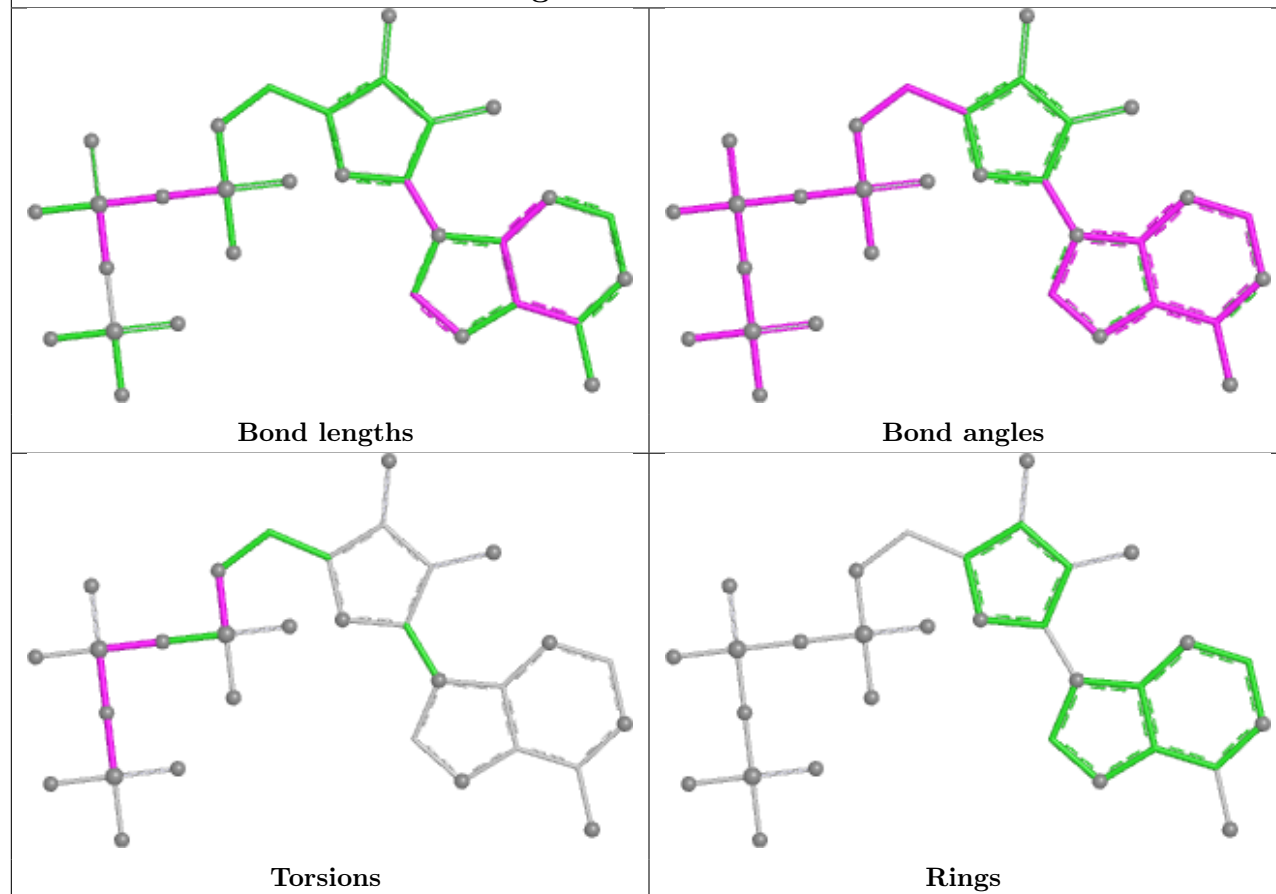
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	K	501	ATP	6	0
22	H	502	ATP	4	0
23	J	501	ADP	6	0
22	M	501	ATP	3	0
22	L	501	ATP	8	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

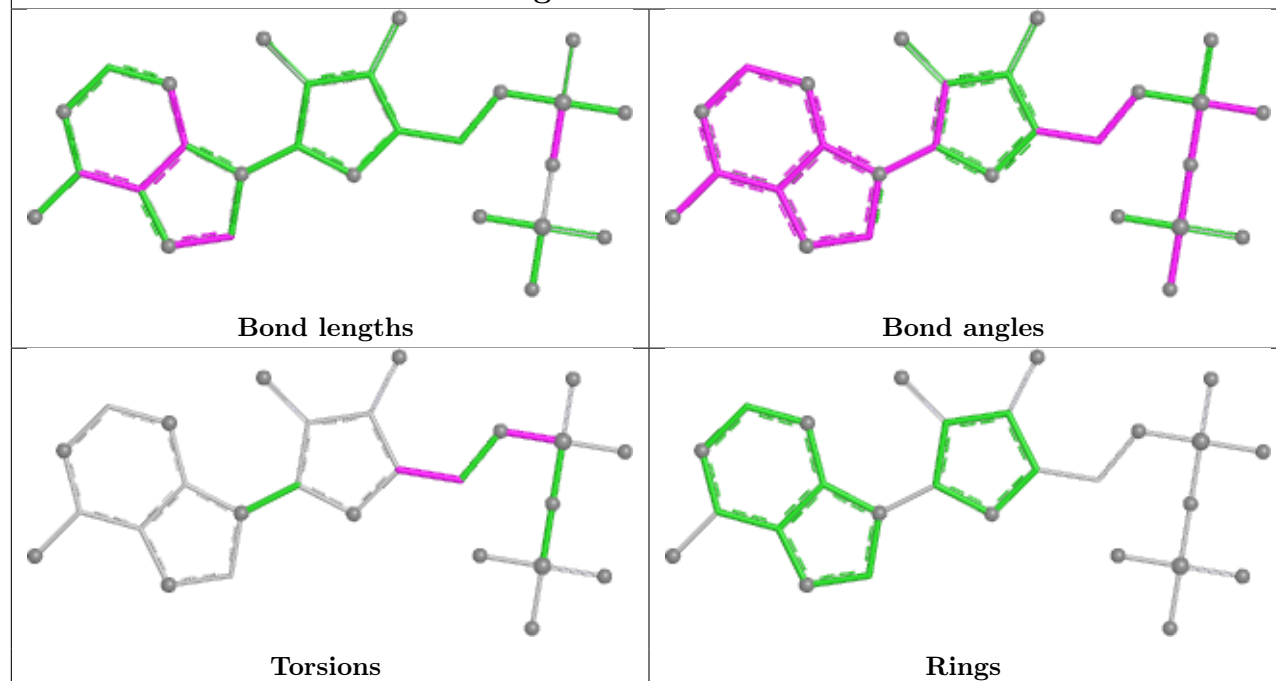
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

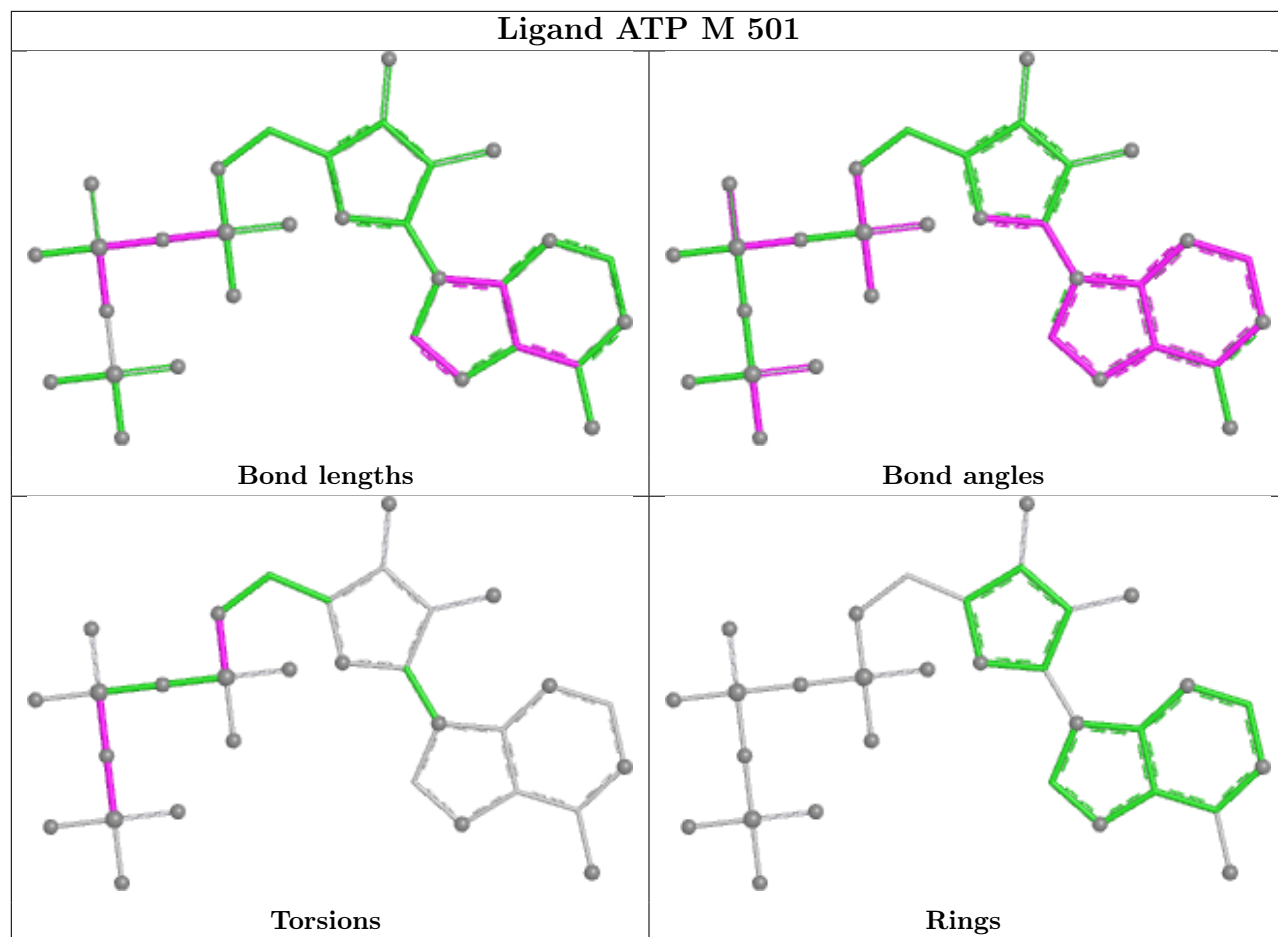


Ligand ATP H 502

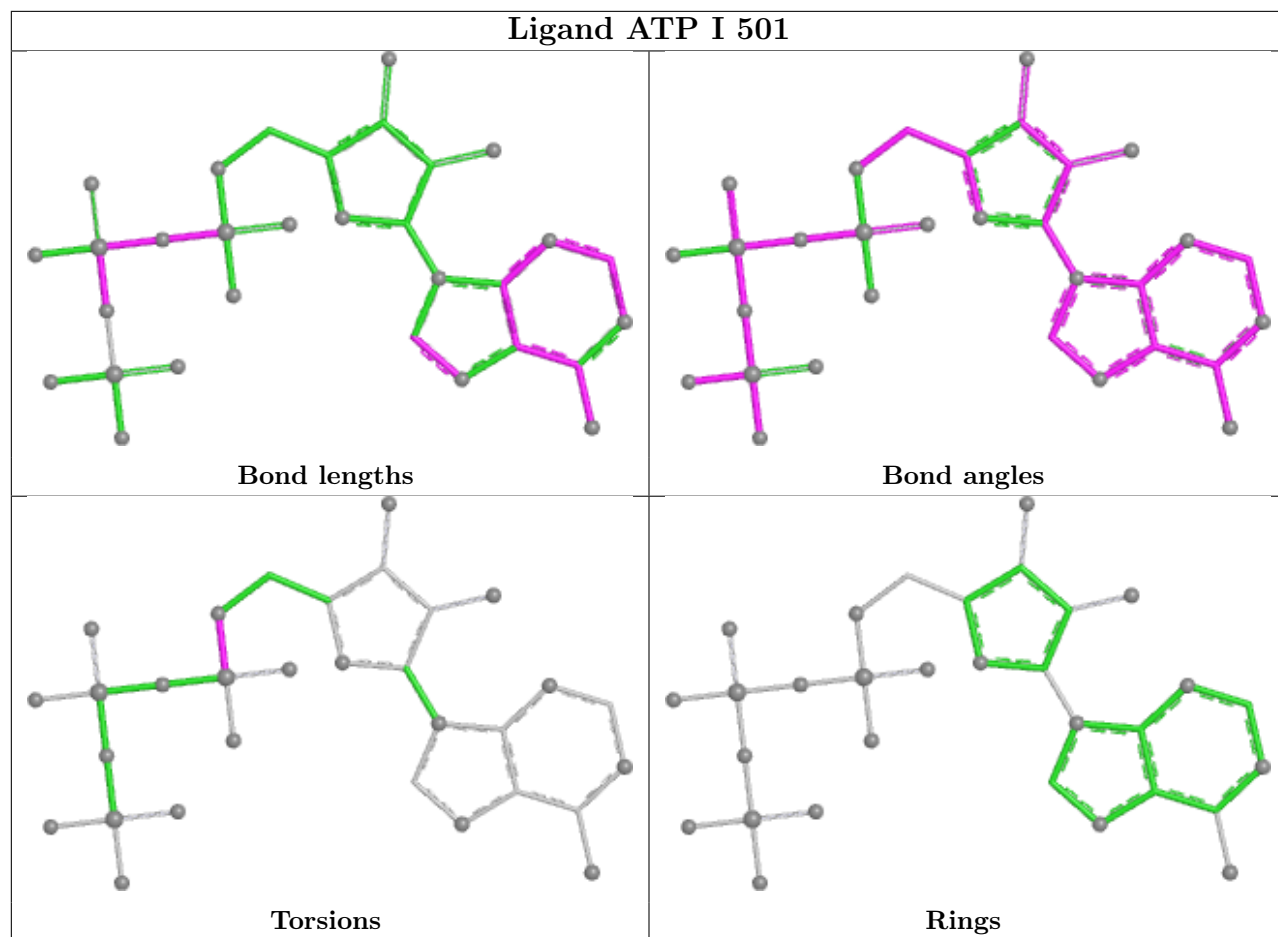


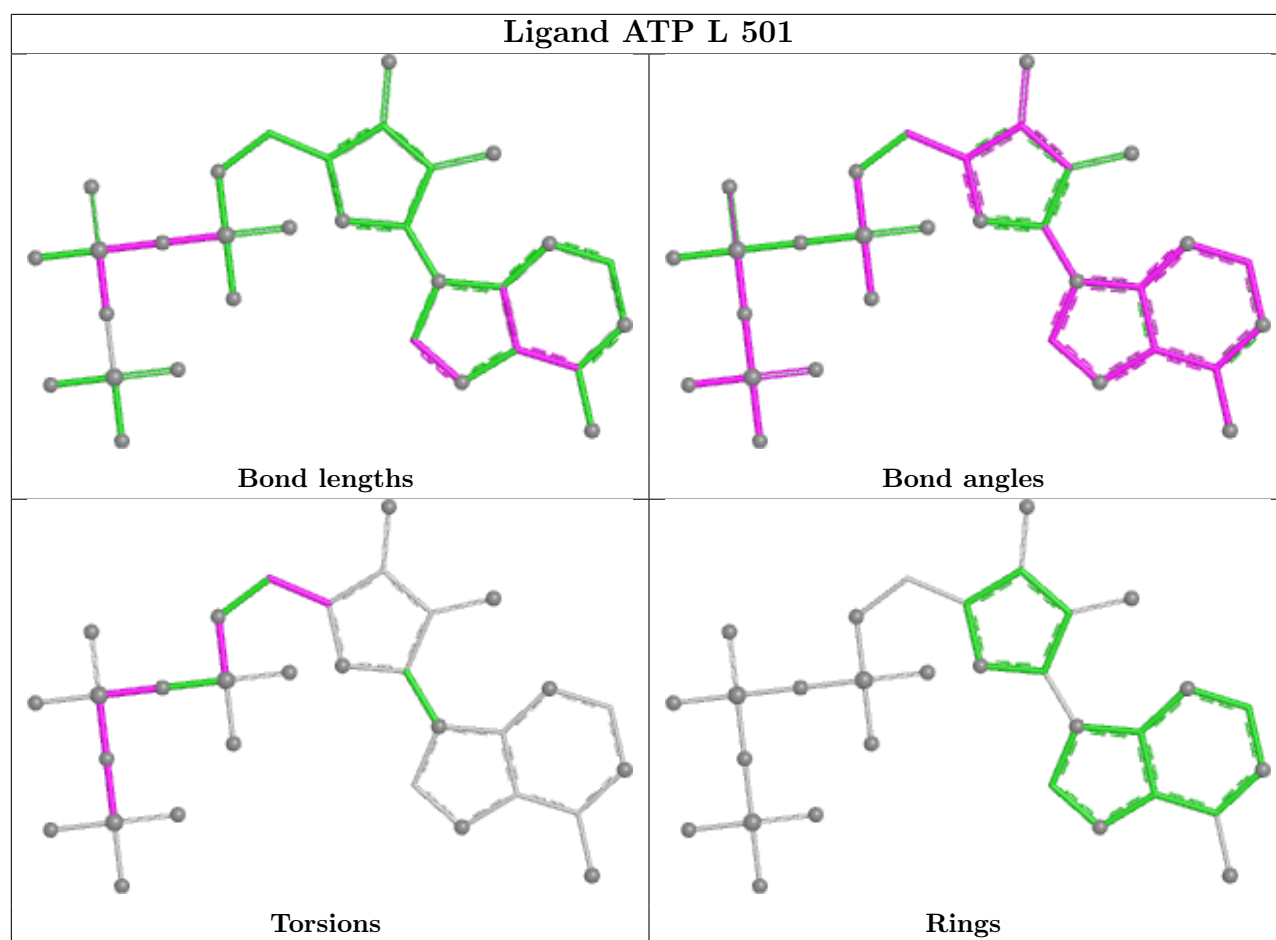
Ligand ADP J 501





Ligand ATP I 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.

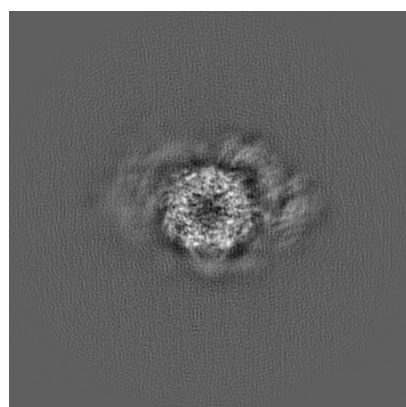
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3535. These allow visual inspection of the internal detail of the map and identification of artifacts.

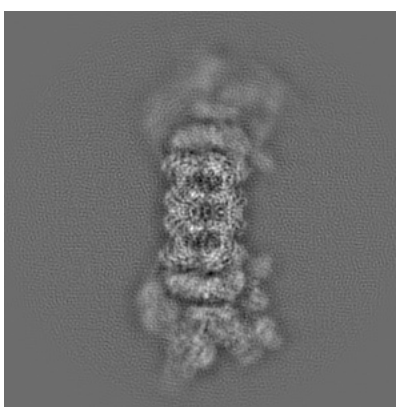
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

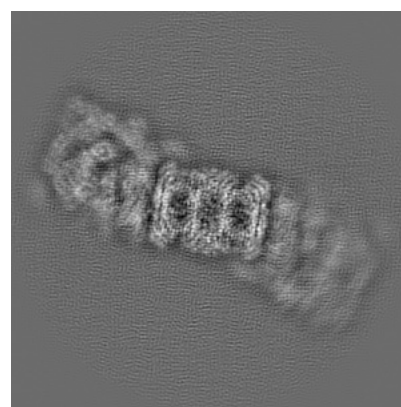
6.1.1 Primary map



X



Y

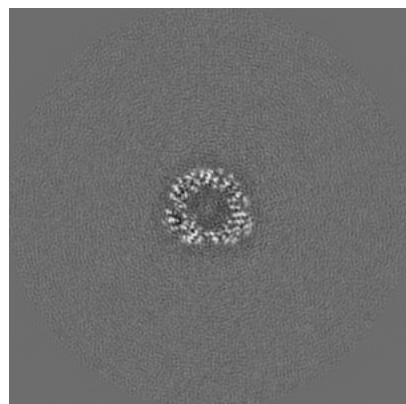


Z

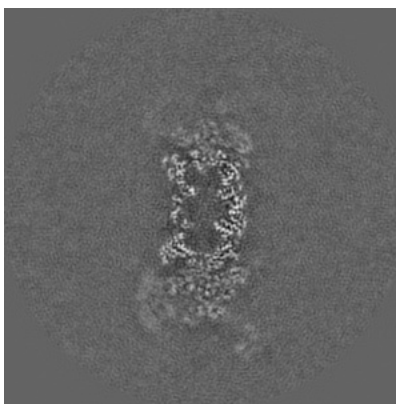
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

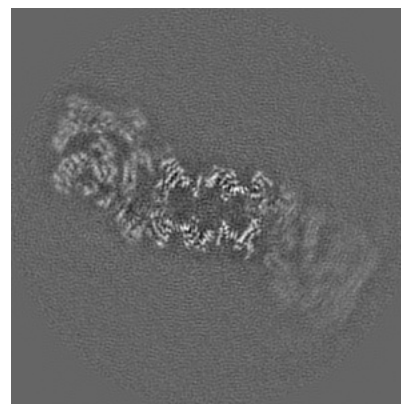
6.2.1 Primary map



X Index: 192



Y Index: 192

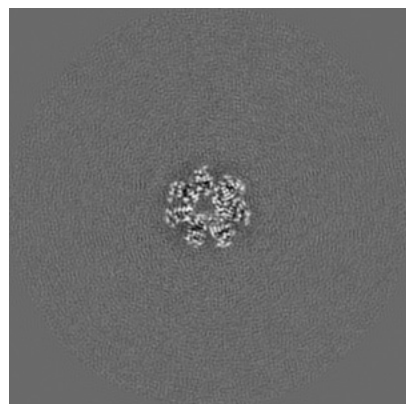


Z Index: 192

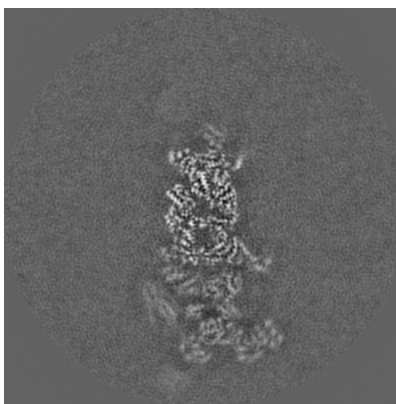
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

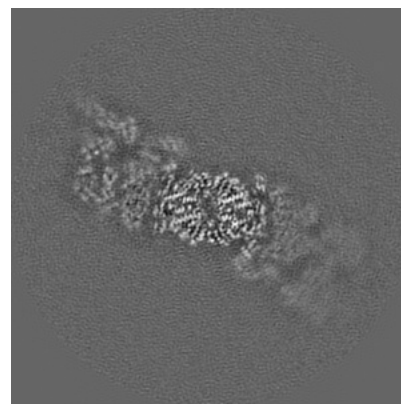
6.3.1 Primary map



X Index: 206



Y Index: 210

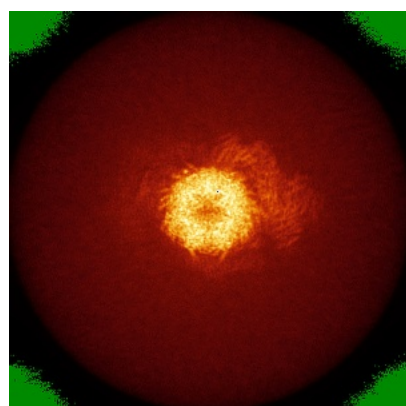


Z Index: 210

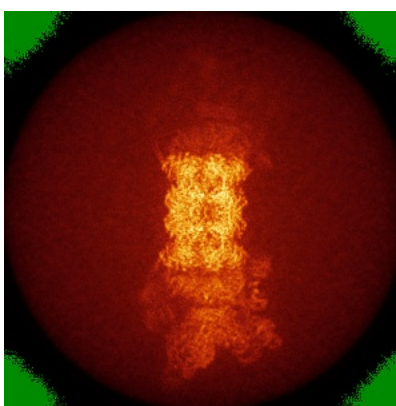
The images above show the largest variance slices of the map in three orthogonal directions.

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

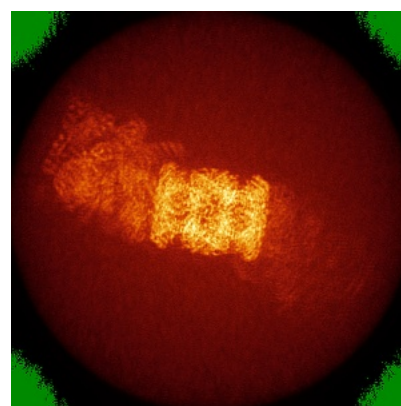
6.4.1 Primary map



X



Y

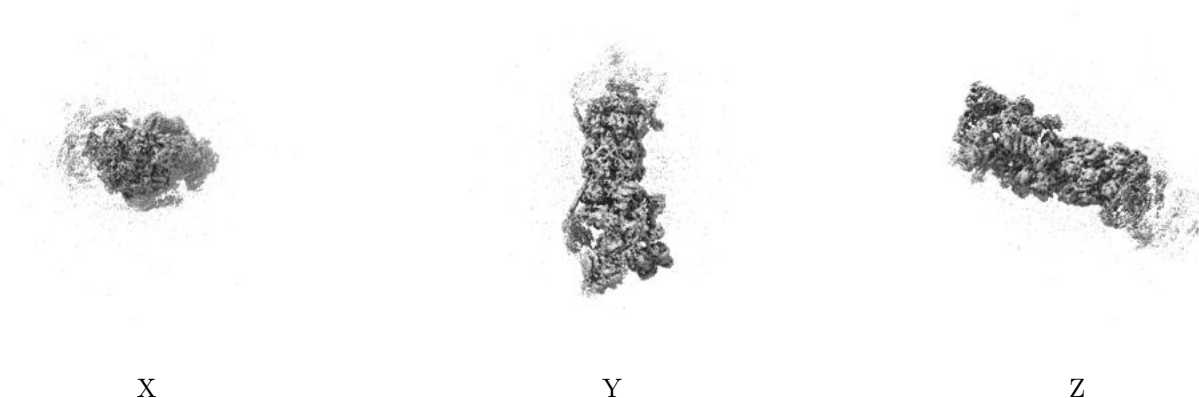


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.017. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

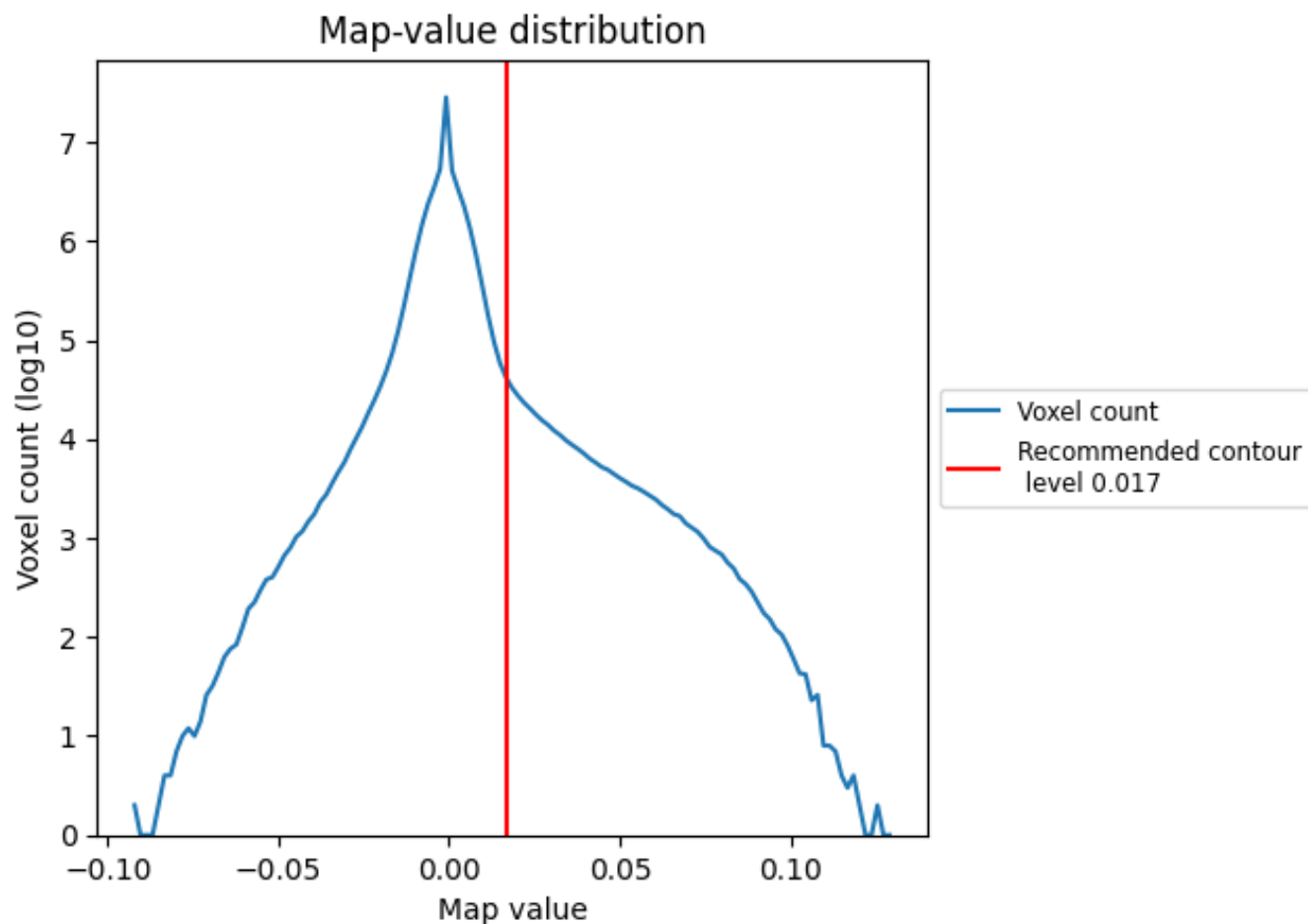
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

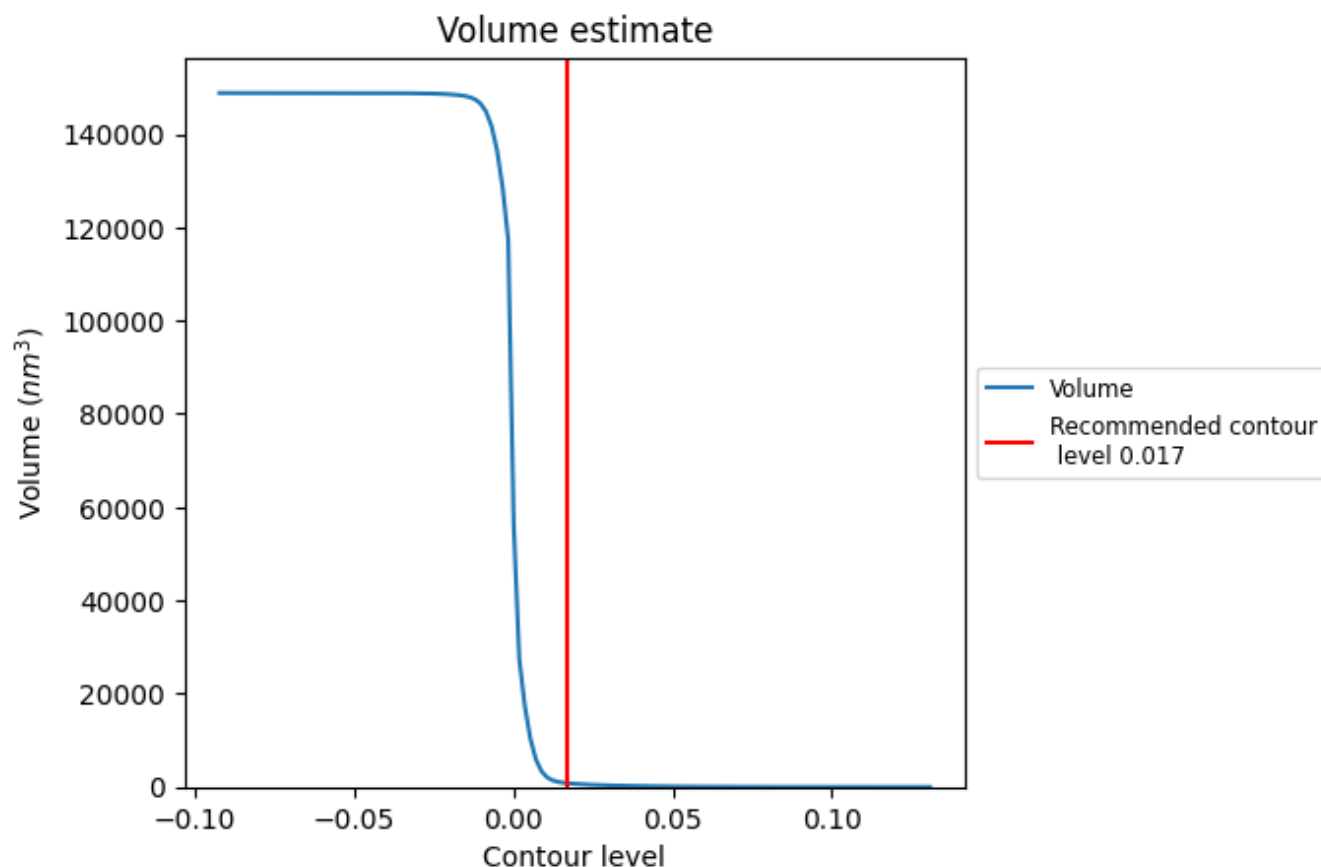
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

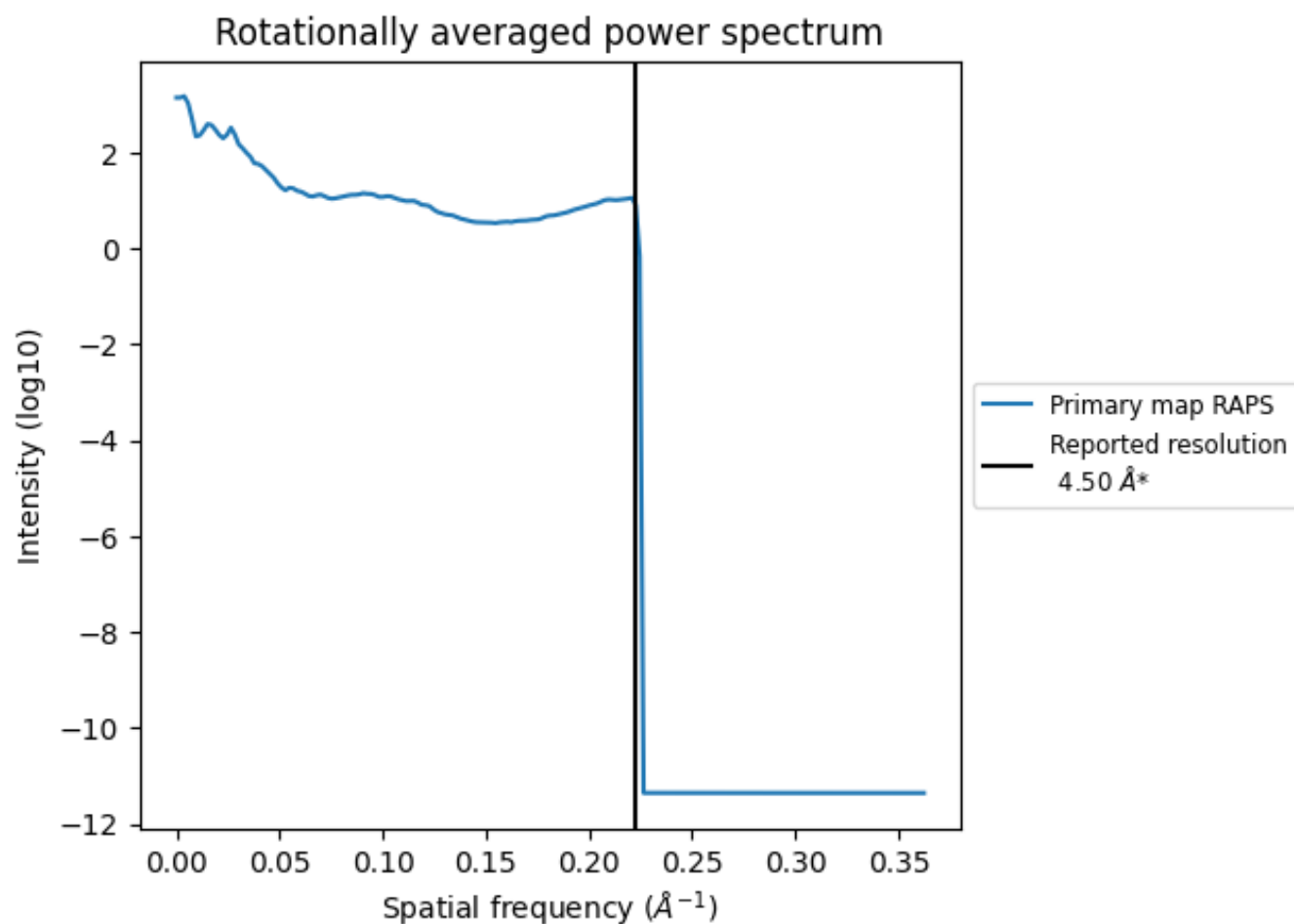
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 813 nm³; this corresponds to an approximate mass of 734 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 0.222 Å⁻¹

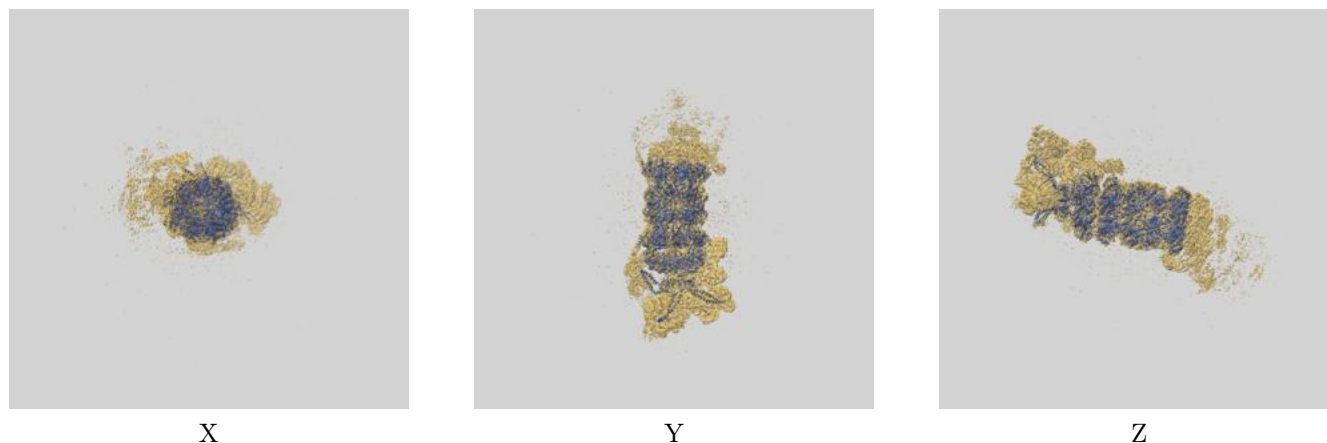
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

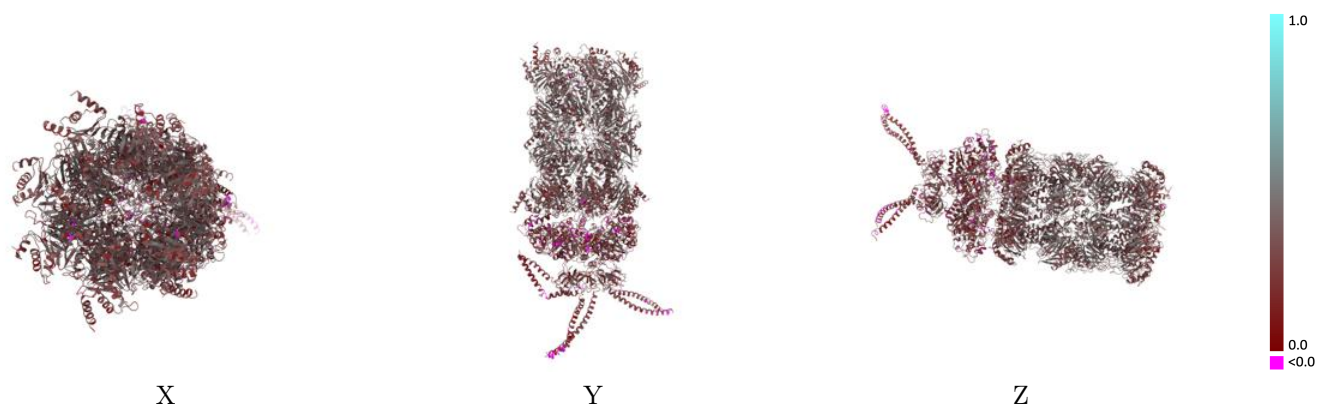
This section contains information regarding the fit between EMDB map EMD-3535 and PDB model 5MPA. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.017 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](#)

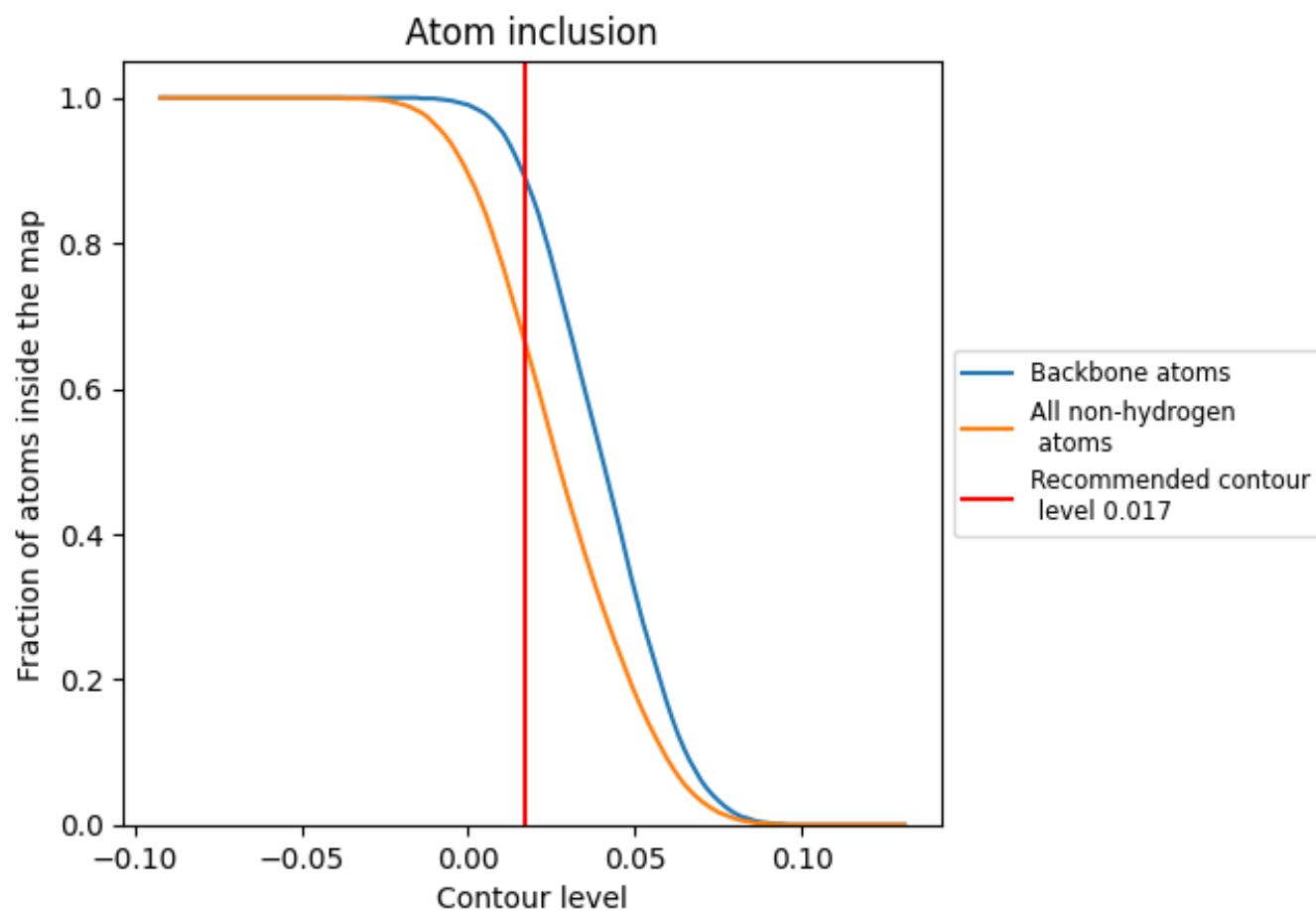


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 66% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.017) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6640	 0.3060
1	 0.7710	 0.3550
2	 0.7400	 0.3430
3	 0.7330	 0.3550
4	 0.7560	 0.3550
5	 0.7750	 0.3620
6	 0.7580	 0.3580
7	 0.7750	 0.3630
A	 0.6940	 0.3060
B	 0.6800	 0.3050
C	 0.6950	 0.3060
D	 0.7020	 0.3090
E	 0.6880	 0.2970
F	 0.7100	 0.3030
G	 0.7080	 0.3080
H	 0.4730	 0.2260
I	 0.4390	 0.2080
J	 0.4480	 0.2020
K	 0.4850	 0.2280
L	 0.5090	 0.2390
M	 0.4890	 0.2480
a	 0.7240	 0.3270
b	 0.7160	 0.3240
c	 0.7310	 0.3180
d	 0.7240	 0.3150
e	 0.7050	 0.3080
f	 0.7340	 0.3340
g	 0.7400	 0.3320
h	 0.7830	 0.3660
i	 0.7730	 0.3710
j	 0.7450	 0.3640
k	 0.7680	 0.3670
l	 0.7820	 0.3660
m	 0.7620	 0.3610
n	 0.7670	 0.3660

