



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Jul 24, 2017 – 02:18 PM EDT

PDB ID : 5MPA
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 : unknown
Resolution : 4.50 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

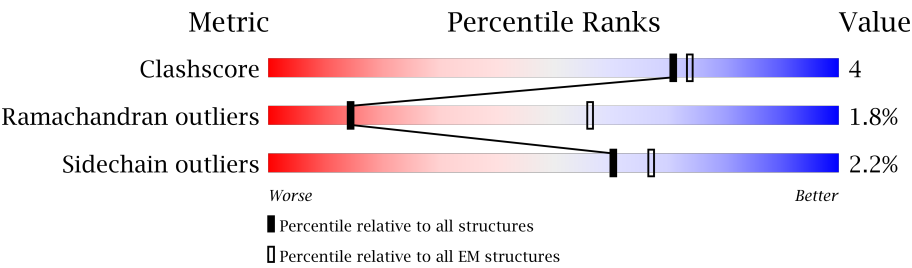
MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

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)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	252	80% 13% . .
1	a	252	81% 14% . .
2	B	250	77% 20% .
2	b	250	86% 13% .
3	C	258	74% 20% . 5%
3	c	258	83% 12% 5%
4	D	254	72% 20% . 6%
4	d	254	85% 9% 6%
5	E	260	75% 15% . . 7%

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Mol	Chain	Length	Quality of chain
5	e	260	
6	F	234	
6	f	234	
7	G	288	
7	g	288	
8	1	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	
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		

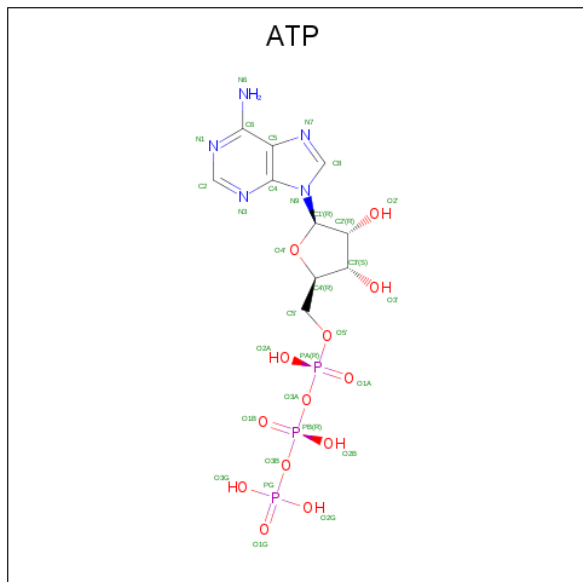
- Molecule 20 is a protein called 26S protease regulatory subunit 8 homolog.

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 (three-letter code: MG) (formula: Mg).

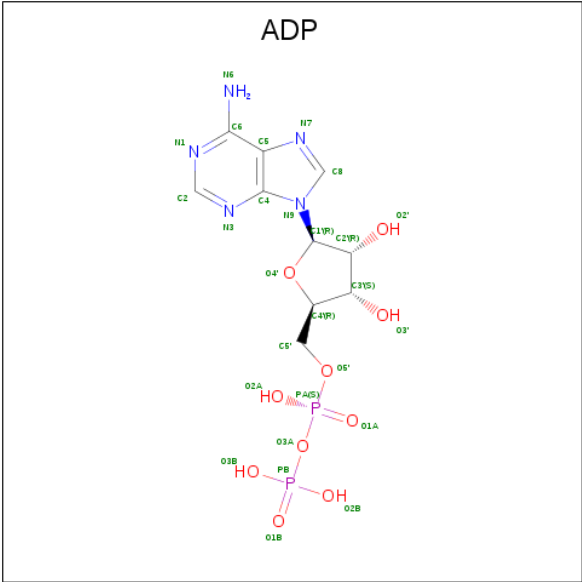
Mol	Chain	Residues	Atoms		AltConf
21	J	1	Total	Mg	0
			1	1	
21	K	1	Total	Mg	0
			1	1	
21	H	1	Total	Mg	0
			1	1	
21	I	1	Total	Mg	0
			1	1	
21	L	1	Total	Mg	0
			1	1	
21	M	1	Total	Mg	0
			1	1	

- Molecule 22 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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 (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

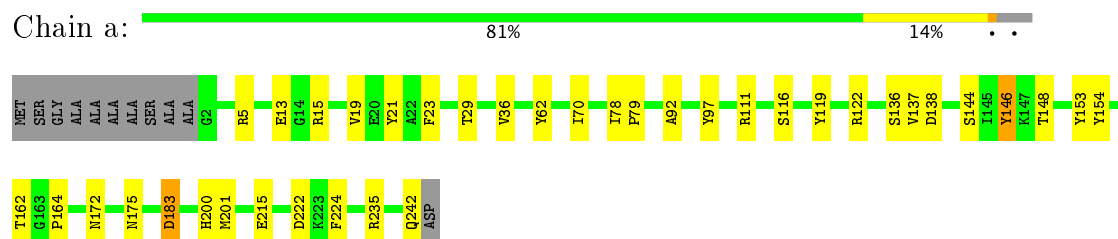


Mol	Chain	Residues	Atoms					AltConf
23	J	1	Total	C	N	O	P	0
			27	10	5	10	2	

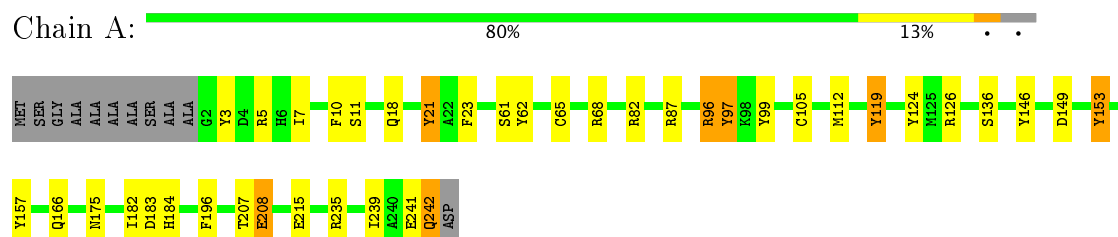
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

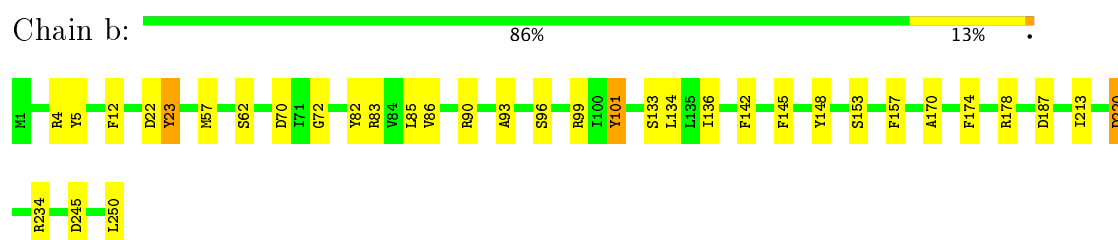
- Molecule 1: Proteasome subunit alpha type-1



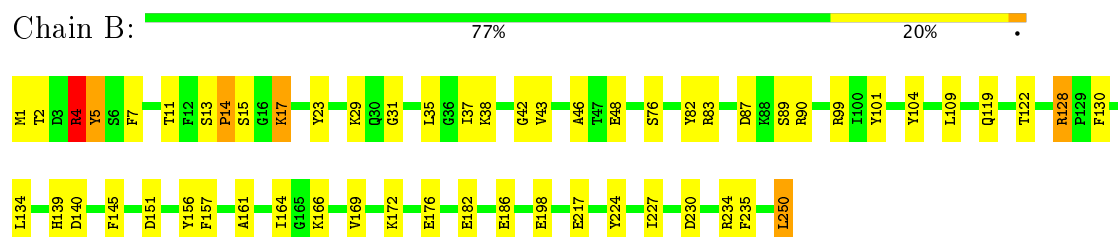
- Molecule 1: Proteasome subunit alpha type-1




- Molecule 2: Proteasome subunit alpha type-2

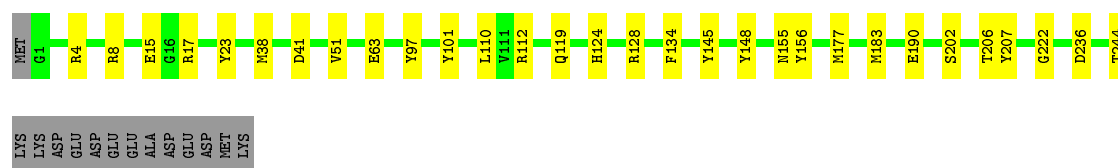


- Molecule 2: Proteasome subunit alpha type-2



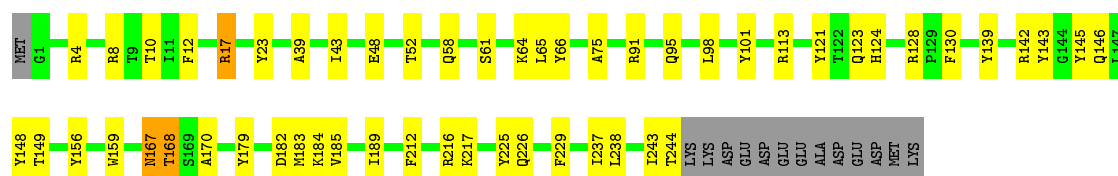
- Molecule 3: Proteasome subunit alpha type-3

Chain c: 




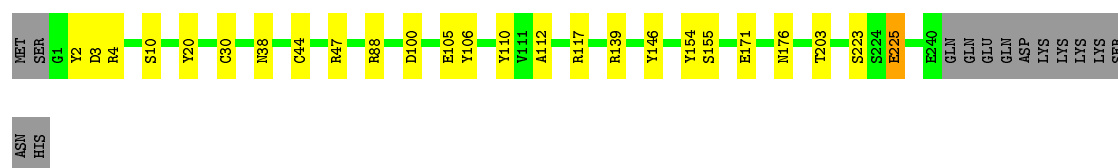
- Molecule 3: Proteasome subunit alpha type-3

Chain C: 



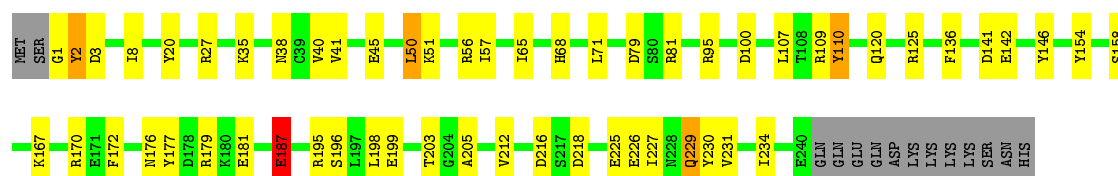
- Molecule 4: Proteasome subunit alpha type-4

Chain d: 




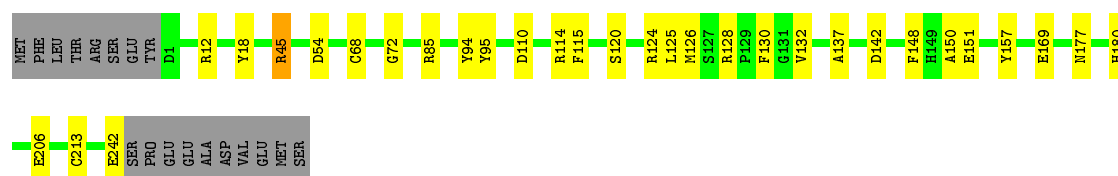
- Molecule 4: Proteasome subunit alpha type-4

Chain D: 



- Molecule 5: Proteasome subunit alpha type-5

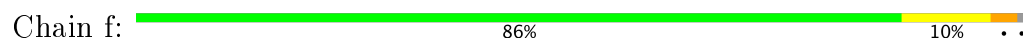
Chain e: 



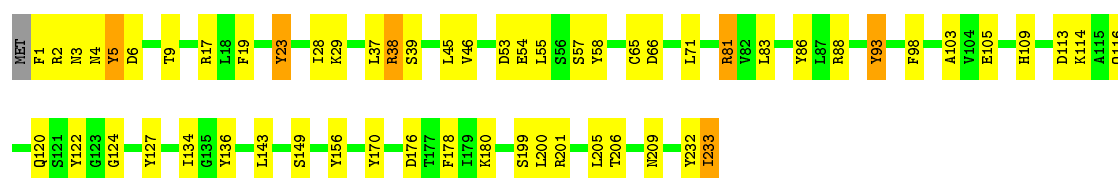
- Molecule 5: Proteasome subunit alpha type-5

Chain E: 

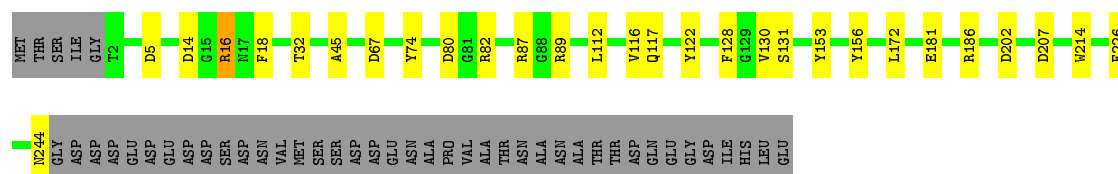
- Molecule 6: Proteasome subunit alpha type-6



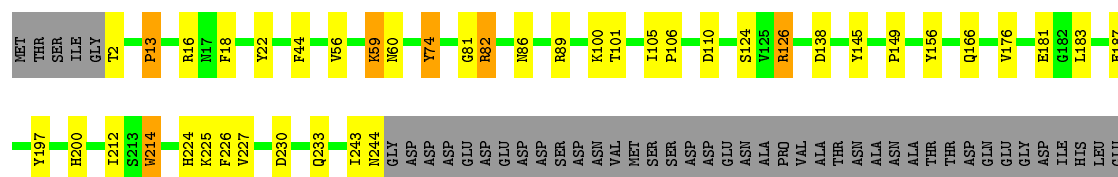
- Molecule 6: Proteasome subunit alpha type-6



- Molecule 7: Probable proteasome subunit alpha type-7



- Molecule 7: Probable proteasome subunit alpha type-7



- Molecule 8: Proteasome subunit beta type-1





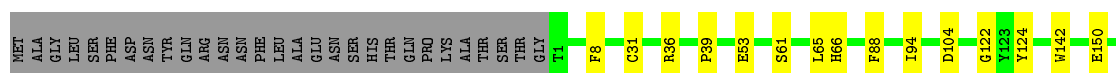
• Molecule 8: Proteasome subunit beta type-1

Chain 1: 79% 10% 9%



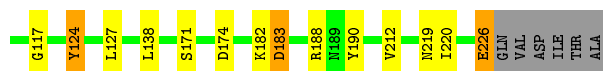
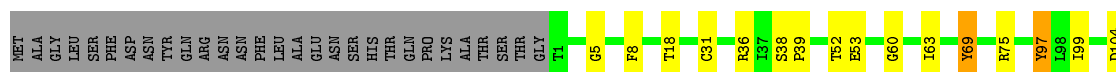
• Molecule 9: Proteasome subunit beta type-2

Chain i: 77% 9% 13%



• Molecule 9: Proteasome subunit beta type-2

Chain 2: 75% 10% 13%



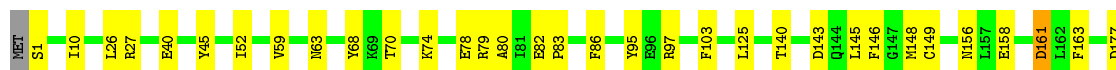
• Molecule 10: Proteasome subunit beta type-3

Chain j: 82% 17%



• Molecule 10: Proteasome subunit beta type-3

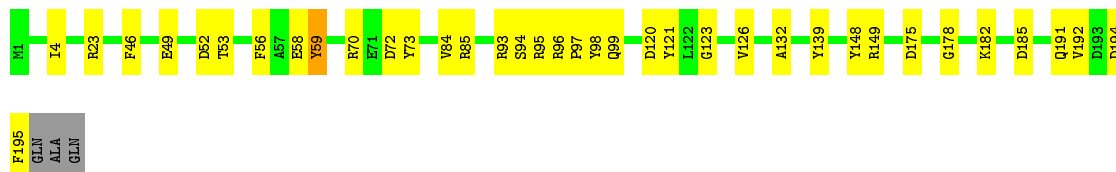
Chain 3: 80% 18%





• Molecule 11: Proteasome subunit beta type-4

Chain k: 80% 18% ..



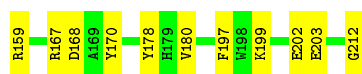
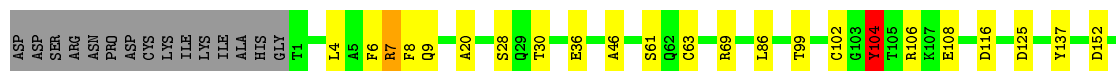
• Molecule 11: Proteasome subunit beta type-4

Chain 4: 85% 12% ..



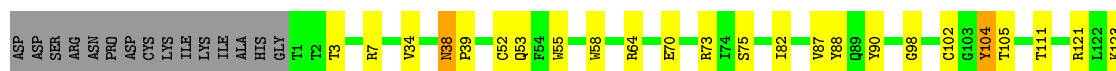
• Molecule 12: Proteasome subunit beta type-5

Chain l: 62% 11% 26%



• Molecule 12: Proteasome subunit beta type-5

Chain 5: 60% 13% 26%



• Molecule 13: Proteasome subunit beta type-6

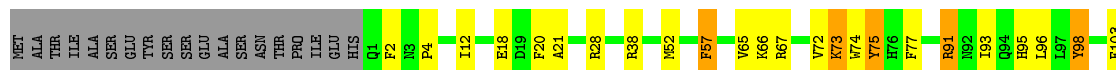
Chain m: 79% 12% 8%





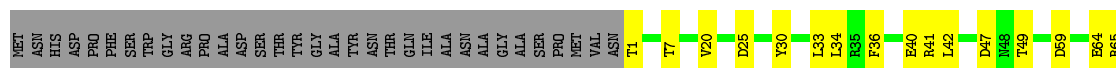
• Molecule 13: Proteasome subunit beta type-6

Chain 6: 73% 16% 8%



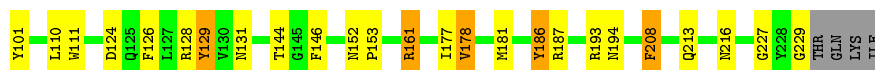
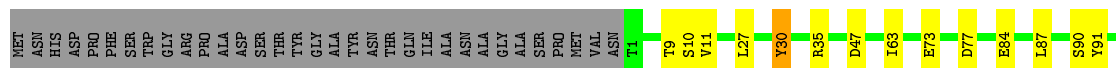
• Molecule 14: Proteasome subunit beta type-7

Chain n: 72% 14% 13%



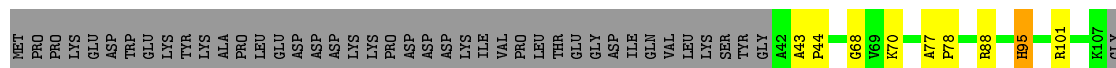
• Molecule 14: Proteasome subunit beta type-7

Chain 7: 71% 12% 14%



• Molecule 15: 26S protease regulatory subunit 7 homolog

Chain H: 71% 11% 16%

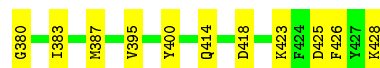


• Molecule 16: 26S protease regulatory subunit 4 homolog

12%



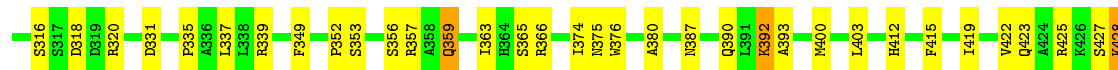
- 9%



- 11%

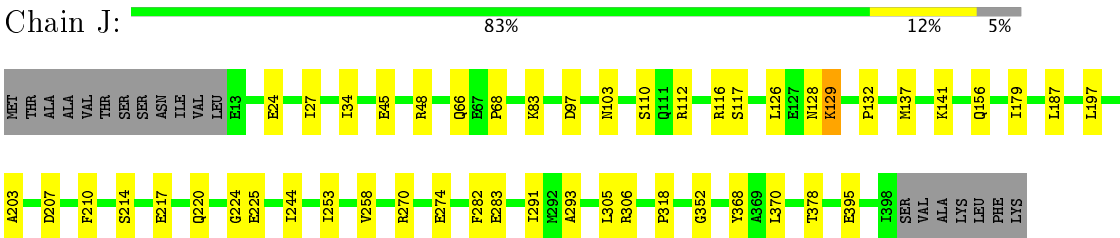


- 12%





● Molecule 20: 26S protease regulatory subunit 8 homolog



4 Experimental information

Property	Value	Source
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	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	1.34	7/1945 (0.4%)	1.49	26/2634 (1.0%)
1	a	1.34	6/1945 (0.3%)	1.51	31/2634 (1.2%)
10	3	1.33	6/1611 (0.4%)	1.43	16/2174 (0.7%)
10	j	1.50	16/1611 (1.0%)	1.49	16/2174 (0.7%)
11	4	1.34	3/1589 (0.2%)	1.40	13/2142 (0.6%)
11	k	1.50	10/1589 (0.6%)	1.61	24/2142 (1.1%)
12	5	1.49	13/1681 (0.8%)	1.56	20/2274 (0.9%)
12	l	1.50	13/1681 (0.8%)	1.59	24/2274 (1.1%)
13	6	1.41	9/1795 (0.5%)	1.49	23/2420 (1.0%)
13	m	1.50	14/1795 (0.8%)	1.55	18/2420 (0.7%)
14	7	1.41	7/1821 (0.4%)	1.49	14/2470 (0.6%)
14	n	1.49	19/1846 (1.0%)	1.48	23/2503 (0.9%)
15	H	1.06	5/3102 (0.2%)	1.05	13/4175 (0.3%)
16	I	1.10	11/3061 (0.4%)	1.03	7/4121 (0.2%)
17	K	1.07	9/3121 (0.3%)	1.06	14/4213 (0.3%)
18	L	1.04	8/3128 (0.3%)	1.02	10/4204 (0.2%)
19	M	1.06	11/3023 (0.4%)	1.01	6/4070 (0.1%)
2	B	1.34	8/1952 (0.4%)	1.45	22/2642 (0.8%)
2	b	1.41	11/1952 (0.6%)	1.49	26/2642 (1.0%)
20	J	1.04	4/3073 (0.1%)	1.02	11/4129 (0.3%)
3	C	1.36	3/1934 (0.2%)	1.49	23/2618 (0.9%)
3	c	1.41	8/1934 (0.4%)	1.44	18/2618 (0.7%)
4	D	1.32	11/1910 (0.6%)	1.39	14/2586 (0.5%)
4	d	1.36	10/1910 (0.5%)	1.45	20/2586 (0.8%)
5	E	1.43	10/1886 (0.5%)	1.52	24/2541 (0.9%)
5	e	1.41	12/1886 (0.6%)	1.51	18/2541 (0.7%)
6	F	1.39	7/1823 (0.4%)	1.47	24/2463 (1.0%)
6	f	1.37	7/1800 (0.4%)	1.50	21/2433 (0.9%)
7	G	1.28	4/1932 (0.2%)	1.36	15/2609 (0.6%)
7	g	1.41	7/1932 (0.4%)	1.41	15/2609 (0.6%)
8	l	1.45	4/1541 (0.3%)	1.59	23/2087 (1.1%)
8	h	1.50	10/1541 (0.6%)	1.55	15/2087 (0.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
9	2	1.36	6/1750 (0.3%)	1.39	8/2373 (0.3%)
9	i	1.48	11/1750 (0.6%)	1.45	8/2373 (0.3%)
All	All	1.32	300/68850 (0.4%)	1.38	603/92981 (0.6%)

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
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
2	B	0	5
2	b	0	4
20	J	0	1
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
All	All	0	88

All (300) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	7	229	GLY	C-O	-14.51	1.00	1.23
12	5	212	GLY	C-O	-14.49	1.00	1.23
12	l	212	GLY	C-O	-14.48	1.00	1.23
7	G	244	ASN	C-O	-12.11	1.00	1.23
6	f	233	ILE	C-OXT	-12.08	1.00	1.23
1	a	242	GLN	C-O	-12.08	1.00	1.23
12	5	212	GLY	C-OXT	-12.07	1.00	1.23
16	I	437	LEU	C-O	-12.07	1.00	1.23
2	b	250	LEU	C-OXT	-12.07	1.00	1.23
2	B	250	LEU	C-OXT	-12.07	1.00	1.23
3	C	244	THR	C-O	-12.07	1.00	1.23
13	6	222	ASP	C-O	-12.07	1.00	1.23
8	h	196	LEU	C-OXT	-12.07	1.00	1.23
17	K	428	LYS	C-OXT	-12.07	1.00	1.23
9	2	226	GLU	C-O	-12.07	1.00	1.23
19	M	434	ALA	C-OXT	-12.07	1.00	1.23
1	A	242	GLN	C-O	-12.06	1.00	1.23
2	B	250	LEU	C-O	-12.06	1.00	1.23
8	l	196	LEU	C-OXT	-12.06	1.00	1.23
19	M	434	ALA	C-O	-12.06	1.00	1.23
13	m	222	ASP	C-O	-12.05	1.00	1.23
2	b	250	LEU	C-O	-12.05	1.00	1.23
12	l	212	GLY	C-OXT	-12.05	1.00	1.23
6	f	233	ILE	C-O	-12.05	1.00	1.23
13	m	222	ASP	C-OXT	-12.05	1.00	1.23
8	h	196	LEU	C-O	-12.04	1.00	1.23
17	K	428	LYS	C-O	-12.05	1.00	1.23
9	i	226	GLU	C-O	-12.04	1.00	1.23
8	l	196	LEU	C-O	-12.04	1.00	1.23
11	4	195	PHE	C-O	-12.04	1.00	1.23
13	6	222	ASP	C-OXT	-12.04	1.00	1.23
15	H	467	ASN	C-O	-12.04	1.00	1.23
16	I	437	LEU	C-OXT	-12.04	1.00	1.23
5	e	242	GLU	C-O	-12.04	1.00	1.23
3	c	244	THR	C-O	-12.04	1.00	1.23
11	k	195	PHE	C-O	-12.03	1.00	1.23
18	L	436	LYS	C-O	-12.03	1.00	1.23
7	g	244	ASN	C-O	-12.03	1.00	1.23
6	F	233	ILE	C-OXT	-12.03	1.00	1.23
6	F	233	ILE	C-O	-12.03	1.00	1.23
5	E	242	GLU	C-O	-12.03	1.00	1.23
14	n	232	LYS	C-O	-12.02	1.00	1.23
15	H	467	ASN	C-OXT	-12.02	1.00	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	k	49	GLU	CG-CD	9.62	1.66	1.51
10	j	84	GLU	CG-CD	9.55	1.66	1.51
9	i	190	TYR	CD1-CE1	-8.97	1.25	1.39
3	c	207	TYR	CD1-CE1	-8.87	1.26	1.39
9	i	190	TYR	CD2-CE2	-8.84	1.26	1.39
11	k	58	GLU	CB-CG	8.80	1.68	1.52
14	n	95	TYR	CD1-CE1	-8.73	1.26	1.39
3	c	15	GLU	CG-CD	8.68	1.65	1.51
16	I	145	CYS	CB-SG	8.30	1.96	1.82
14	n	95	TYR	CD2-CE2	-8.18	1.27	1.39
2	b	187	ASP	CB-CG	8.17	1.69	1.51
13	m	106	TYR	CD1-CE1	-8.10	1.27	1.39
10	j	182	TRP	CB-CG	-7.85	1.36	1.50
15	H	467	ASN	N-CA	7.78	1.61	1.46
2	B	90	ARG	CZ-NH2	7.76	1.43	1.33
9	i	205	PHE	CB-CG	-7.71	1.38	1.51
4	d	30	CYS	CB-SG	-7.71	1.69	1.82
18	L	243	PHE	CB-CG	-7.58	1.38	1.51
14	7	73	GLU	CG-CD	7.58	1.63	1.51
7	g	226	PHE	CB-CG	-7.56	1.38	1.51
16	I	299	GLU	CG-CD	7.55	1.63	1.51
14	n	36	PHE	CB-CG	-7.53	1.38	1.51
12	5	123	LYS	CD-CE	7.52	1.70	1.51
9	2	190	TYR	CD1-CE1	-7.44	1.28	1.39
2	B	198	GLU	CG-CD	7.40	1.63	1.51
5	e	151	GLU	CD-OE1	7.38	1.33	1.25
11	k	148	TYR	CD2-CE2	-7.38	1.28	1.39
6	F	57	SER	CA-CB	7.23	1.63	1.52
11	k	148	TYR	CD1-CE1	-7.16	1.28	1.39
8	1	194	GLU	CB-CG	-6.98	1.38	1.52
12	l	159	ARG	CZ-NH2	6.90	1.42	1.33
19	M	255	TYR	CB-CG	-6.79	1.41	1.51
17	K	400	TYR	CD1-CE1	6.78	1.49	1.39
1	A	166	GLN	CG-CD	6.77	1.66	1.51
9	2	190	TYR	CD2-CE2	-6.75	1.29	1.39
3	C	17	ARG	NE-CZ	6.72	1.41	1.33
10	3	40	GLU	CG-CD	6.66	1.61	1.51
13	m	106	TYR	CB-CG	-6.65	1.41	1.51
10	j	127	GLY	CA-C	-6.63	1.41	1.51
13	6	217	TYR	CD1-CE1	-6.60	1.29	1.39
4	d	176	ASN	CB-CG	6.59	1.66	1.51
14	7	30	TYR	CD1-CE1	-6.56	1.29	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	c	15	GLU	CB-CG	6.55	1.64	1.52
12	5	58	TRP	CE2-CZ2	-6.51	1.28	1.39
2	b	145	PHE	CB-CG	-6.51	1.40	1.51
11	k	58	GLU	CG-CD	6.50	1.61	1.51
14	n	64	GLU	CD-OE1	6.49	1.32	1.25
13	6	2	PHE	CG-CD1	6.47	1.48	1.38
7	G	226	PHE	CB-CG	-6.46	1.40	1.51
14	n	30	TYR	CD1-CE1	-6.46	1.29	1.39
2	b	142	PHE	CE1-CZ	6.46	1.49	1.37
12	l	168	ASP	CB-CG	6.44	1.65	1.51
12	l	202	GLU	CG-CD	-6.43	1.42	1.51
3	c	145	TYR	CD1-CE1	-6.41	1.29	1.39
8	h	47	GLY	CA-C	-6.41	1.41	1.51
5	E	210	GLN	CG-CD	6.40	1.65	1.51
14	n	146	PHE	CB-CG	-6.39	1.40	1.51
16	I	90	GLU	CG-CD	6.38	1.61	1.51
13	m	106	TYR	CD2-CE2	-6.37	1.29	1.39
4	d	10	SER	CA-CB	6.36	1.62	1.52
2	B	4	ARG	N-CA	-6.36	1.33	1.46
10	3	79	ARG	CZ-NH2	6.33	1.41	1.33
13	m	39	TYR	CD2-CE2	-6.33	1.29	1.39
18	L	279	PHE	CE2-CZ	6.32	1.49	1.37
5	e	85	ARG	NE-CZ	6.32	1.41	1.33
10	j	97	ARG	CZ-NH2	6.30	1.41	1.33
14	7	208	PHE	CD1-CE1	-6.30	1.26	1.39
5	e	124	ARG	CD-NE	6.28	1.57	1.46
19	M	392	LYS	CB-CG	6.27	1.69	1.52
15	H	298	ALA	CA-CB	-6.24	1.39	1.52
8	h	72	THR	C-N	-6.22	1.22	1.34
8	h	174	ARG	NE-CZ	6.20	1.41	1.33
14	n	208	PHE	CB-CG	-6.18	1.40	1.51
14	n	219	TRP	CB-CG	6.17	1.61	1.50
13	m	75	TYR	CZ-OH	6.16	1.48	1.37
16	I	433	GLU	CB-CG	-6.16	1.40	1.52
20	J	66	GLN	CG-CD	-6.16	1.36	1.51
10	j	36	SER	CA-CB	-6.13	1.43	1.52
14	n	65	ARG	CG-CD	6.12	1.67	1.51
9	i	150	GLU	CB-CG	-6.09	1.40	1.52
17	K	171	TYR	CE2-CZ	6.08	1.46	1.38
20	J	270	ARG	NE-CZ	6.06	1.41	1.33
8	h	84	GLU	CG-CD	6.03	1.60	1.51
5	e	12	ARG	NE-CZ	6.03	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	c	207	TYR	CD2-CE2	-6.03	1.30	1.39
6	F	65	CYS	CB-SG	6.03	1.92	1.82
14	n	40	GLU	CB-CG	6.03	1.63	1.52
4	D	187	GLU	CB-CG	6.02	1.63	1.52
6	f	106	ARG	CD-NE	6.02	1.56	1.46
12	5	172	GLY	N-CA	-6.01	1.37	1.46
14	n	30	TYR	CD2-CE2	-6.00	1.30	1.39
13	6	28	ARG	NE-CZ	5.98	1.40	1.33
9	i	173	VAL	CB-CG2	-5.98	1.40	1.52
4	D	1	GLY	N-CA	5.97	1.55	1.46
19	M	29	GLU	CG-CD	5.96	1.60	1.51
12	5	102	CYS	CB-SG	-5.96	1.72	1.81
13	6	221	ARG	CD-NE	5.93	1.56	1.46
17	K	369	ASP	CB-CG	5.93	1.64	1.51
2	B	83	ARG	CD-NE	5.91	1.56	1.46
4	D	167	LYS	CD-CE	5.91	1.66	1.51
18	L	279	PHE	CG-CD1	5.91	1.47	1.38
13	m	39	TYR	CD1-CE1	-5.88	1.30	1.39
1	A	208	GLU	CG-CD	5.88	1.60	1.51
11	k	72	ASP	CB-CG	5.88	1.64	1.51
9	i	190	TYR	CB-CG	-5.87	1.42	1.51
8	h	36	ARG	CG-CD	5.84	1.66	1.51
17	K	51	LEU	CA-CB	-5.83	1.40	1.53
10	j	79	ARG	CZ-NH2	5.82	1.40	1.33
7	G	89	ARG	CZ-NH1	5.82	1.40	1.33
5	e	95	TYR	CG-CD1	5.81	1.46	1.39
17	K	176	GLY	N-CA	-5.81	1.37	1.46
14	7	90	SER	CA-CB	5.78	1.61	1.52
5	e	114	ARG	CZ-NH1	5.78	1.40	1.33
4	D	146	TYR	CE2-CZ	5.77	1.46	1.38
7	g	89	ARG	CZ-NH2	5.76	1.40	1.33
16	I	314	ASP	CB-CG	5.75	1.63	1.51
6	f	147	GLN	CB-CG	-5.74	1.37	1.52
4	D	170	ARG	CZ-NH1	5.74	1.40	1.33
3	c	222	GLY	CA-C	-5.73	1.42	1.51
14	n	36	PHE	CD2-CE2	-5.73	1.27	1.39
9	i	218	VAL	CB-CG2	5.71	1.64	1.52
14	n	73	GLU	CB-CG	-5.66	1.41	1.52
13	6	157	LYS	CD-CE	5.65	1.65	1.51
4	d	117	ARG	CZ-NH2	5.63	1.40	1.33
4	D	95	ARG	NE-CZ	5.63	1.40	1.33
5	E	123	GLU	CD-OE2	5.63	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	5	144	TYR	CB-CG	-5.62	1.43	1.51
19	M	129	LEU	C-N	5.62	1.45	1.34
4	d	225	GLU	CG-CD	5.61	1.60	1.51
19	M	255	TYR	CD1-CE1	-5.60	1.30	1.39
18	L	245	PHE	CB-CG	5.59	1.60	1.51
6	F	149	SER	CA-CB	5.59	1.61	1.52
4	d	106	TYR	CZ-OH	5.55	1.47	1.37
5	e	68	CYS	CB-SG	-5.55	1.72	1.81
19	M	320	ARG	NE-CZ	5.55	1.40	1.33
12	l	203	GLU	CB-CG	-5.55	1.41	1.52
7	g	153	TYR	CE1-CZ	5.54	1.45	1.38
12	5	7	ARG	CZ-NH2	5.54	1.40	1.33
19	M	331	ASP	CB-CG	5.53	1.63	1.51
10	j	34	GLY	N-CA	-5.52	1.37	1.46
8	h	61	TYR	CE1-CZ	-5.51	1.31	1.38
14	7	30	TYR	CD2-CE2	-5.51	1.31	1.39
8	h	185	ARG	CZ-NH2	5.50	1.40	1.33
1	A	5	ARG	NE-CZ	5.50	1.40	1.33
12	5	144	TYR	CD1-CE1	-5.50	1.31	1.39
18	L	243	PHE	CA-CB	-5.50	1.41	1.53
4	d	88	ARG	CZ-NH2	5.50	1.40	1.33
9	i	53	GLU	CG-CD	5.50	1.60	1.51
3	C	179	TYR	CE1-CZ	5.50	1.45	1.38
11	k	98	TYR	CG-CD2	5.49	1.46	1.39
6	f	211	SER	CA-CB	5.47	1.61	1.52
12	5	58	TRP	CE3-CZ3	-5.46	1.29	1.38
18	L	195	GLU	CG-CD	5.46	1.60	1.51
12	l	108	GLU	C-N	5.45	1.42	1.33
13	m	193	GLU	CG-CD	5.45	1.60	1.51
1	a	13	GLU	CG-CD	-5.44	1.43	1.51
12	l	69	ARG	CD-NE	5.43	1.55	1.46
11	4	96	ARG	CZ-NH1	5.43	1.40	1.33
20	J	274	GLU	CG-CD	5.42	1.60	1.51
8	1	29	ARG	NE-CZ	5.42	1.40	1.33
12	l	178	TYR	CE1-CZ	-5.42	1.31	1.38
1	a	70	ILE	C-N	5.41	1.42	1.33
13	6	67	ARG	CZ-NH2	5.41	1.40	1.33
2	b	153	SER	CA-CB	5.41	1.61	1.52
13	m	137	ARG	CZ-NH2	5.41	1.40	1.33
10	3	97	ARG	CZ-NH2	5.41	1.40	1.33
2	b	96	SER	CA-CB	5.40	1.61	1.52
4	d	171	GLU	CG-CD	5.40	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	j	58	ASP	CB-CG	5.40	1.63	1.51
12	l	69	ARG	CZ-NH2	5.40	1.40	1.33
4	D	56	ARG	CZ-NH2	5.40	1.40	1.33
8	h	48	SER	CB-OG	5.38	1.49	1.42
13	m	187	SER	CB-OG	5.38	1.49	1.42
9	2	219	ASN	CB-CG	5.37	1.63	1.51
12	l	180	VAL	CB-CG2	-5.36	1.41	1.52
12	5	88	TYR	CE2-CZ	-5.35	1.31	1.38
7	g	186	ARG	CB-CG	-5.35	1.38	1.52
3	c	145	TYR	CD2-CE2	-5.34	1.31	1.39
14	n	175	GLU	CG-CD	-5.34	1.44	1.51
2	b	90	ARG	CZ-NH2	5.33	1.40	1.33
10	j	45	TYR	CD1-CE1	-5.33	1.31	1.39
16	I	351	GLU	CB-CG	5.33	1.62	1.52
1	a	5	ARG	NE-CZ	5.32	1.40	1.33
19	M	50	ARG	NE-CZ	5.32	1.40	1.33
5	E	79	SER	CA-CB	5.31	1.60	1.52
5	E	174	GLU	CG-CD	5.30	1.59	1.51
2	b	90	ARG	CZ-NH1	5.29	1.40	1.33
13	m	74	TRP	CG-CD1	5.29	1.44	1.36
10	3	82	GLU	CG-CD	5.29	1.59	1.51
5	E	78	ARG	CZ-NH2	5.29	1.40	1.33
5	E	114	ARG	CD-NE	5.28	1.55	1.46
7	g	87	ARG	NE-CZ	5.28	1.40	1.33
10	j	105	GLY	C-N	-5.28	1.24	1.34
13	m	215	GLU	CB-CG	5.28	1.62	1.52
1	A	126	ARG	NE-CZ	5.27	1.40	1.33
7	G	16	ARG	CZ-NH1	5.27	1.40	1.33
12	l	180	VAL	CB-CG1	-5.27	1.41	1.52
10	3	197	ARG	CD-NE	5.27	1.55	1.46
4	d	105	GLU	CD-OE1	5.27	1.31	1.25
1	A	87	ARG	CZ-NH2	5.27	1.39	1.33
4	d	47	ARG	NE-CZ	5.26	1.39	1.33
12	5	121	ARG	NE-CZ	5.26	1.39	1.33
2	B	89	SER	CA-CB	5.26	1.60	1.52
13	6	166	GLY	CA-C	-5.25	1.43	1.51
6	f	106	ARG	CZ-NH2	5.24	1.39	1.33
14	n	40	GLU	CG-CD	5.24	1.59	1.51
14	7	129	TYR	CD2-CE2	5.24	1.47	1.39
1	A	11	SER	CA-CB	5.22	1.60	1.52
11	4	23	ARG	NE-CZ	5.22	1.39	1.33
9	i	142	TRP	NE1-CE2	-5.21	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	81	ARG	CZ-NH2	5.21	1.39	1.33
9	2	183	ASP	CB-CG	-5.21	1.40	1.51
5	E	124	ARG	NE-CZ	5.21	1.39	1.33
17	K	400	TYR	CD2-CE2	5.21	1.47	1.39
10	j	49	PHE	CB-CG	-5.20	1.42	1.51
4	D	170	ARG	CD-NE	5.20	1.55	1.46
4	D	110	TYR	CD1-CE1	5.18	1.47	1.39
5	e	114	ARG	NE-CZ	5.18	1.39	1.33
10	j	130	ASP	CB-CG	5.17	1.62	1.51
9	2	75	ARG	CZ-NH2	5.17	1.39	1.33
20	J	395	GLU	CB-CG	-5.17	1.42	1.52
10	j	198	TYR	CD2-CE2	-5.17	1.31	1.39
6	f	201	ARG	CG-CD	5.17	1.64	1.51
12	l	28	SER	CA-CB	5.16	1.60	1.52
16	I	199	GLU	CB-CG	-5.16	1.42	1.52
14	n	41	ARG	CZ-NH1	5.15	1.39	1.33
11	k	121	TYR	CZ-OH	5.15	1.46	1.37
11	k	182	LYS	CE-NZ	5.14	1.61	1.49
5	e	115	PHE	CG-CD2	5.14	1.46	1.38
10	j	135	PHE	CG-CD2	5.13	1.46	1.38
7	g	128	PHE	CB-CG	-5.13	1.42	1.51
1	a	146	TYR	CE1-CZ	5.13	1.45	1.38
14	n	190	ARG	CB-CG	-5.13	1.38	1.52
2	b	72	GLY	N-CA	-5.12	1.38	1.46
5	e	72	GLY	CA-C	-5.12	1.43	1.51
4	D	20	TYR	CG-CD1	5.12	1.45	1.39
19	M	162	GLU	CG-CD	5.12	1.59	1.51
1	a	183	ASP	CB-CG	-5.11	1.41	1.51
5	e	94	TYR	CD1-CE1	5.10	1.47	1.39
14	n	102	GLN	CB-CG	-5.09	1.38	1.52
13	m	185	ARG	CZ-NH2	5.08	1.39	1.33
5	E	124	ARG	CZ-NH2	5.08	1.39	1.33
16	I	200	LEU	C-N	5.08	1.43	1.34
15	H	101	ARG	CZ-NH1	5.07	1.39	1.33
9	i	53	GLU	CB-CG	5.06	1.61	1.52
5	E	157	TYR	N-CA	-5.06	1.36	1.46
18	L	331	ASP	CB-CG	5.06	1.62	1.51
10	j	102	TYR	CB-CG	5.06	1.59	1.51
17	K	270	PHE	CB-CG	5.04	1.59	1.51
10	j	68	TYR	CE1-CZ	5.04	1.45	1.38
2	B	130	PHE	C-N	5.03	1.42	1.33
16	I	406	GLU	CG-CD	5.02	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	3	1	SER	CA-CB	5.02	1.60	1.52
2	b	62	SER	CA-CB	5.01	1.60	1.52
4	D	2	TYR	CG-CD2	5.00	1.45	1.39
12	5	132	GLY	N-CA	-5.00	1.38	1.46
6	F	1	PHE	CA-C	5.00	1.66	1.52

All (603) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	7	187	ARG	NE-CZ-NH2	16.79	128.70	120.30
12	5	104	TYR	CB-CG-CD2	-13.38	112.97	121.00
12	5	187	TYR	CB-CG-CD1	12.91	128.75	121.00
12	5	121	ARG	NE-CZ-NH1	12.88	126.74	120.30
12	l	159	ARG	NE-CZ-NH1	12.35	126.48	120.30
12	l	170	TYR	CB-CG-CD2	-11.91	113.85	121.00
1	A	21	TYR	CB-CG-CD1	11.65	127.99	121.00
12	l	69	ARG	NE-CZ-NH2	-11.42	114.59	120.30
3	C	156	TYR	CB-CG-CD2	-11.40	114.16	121.00
12	5	104	TYR	CB-CG-CD1	11.30	127.78	121.00
6	F	170	TYR	CB-CG-CD1	11.19	127.72	121.00
4	d	88	ARG	NE-CZ-NH1	11.17	125.89	120.30
6	F	170	TYR	CB-CG-CD2	-11.13	114.32	121.00
17	K	336	ARG	NE-CZ-NH1	11.09	125.84	120.30
5	E	12	ARG	NE-CZ-NH1	11.03	125.81	120.30
12	5	90	TYR	CB-CG-CD2	-10.99	114.41	121.00
4	d	47	ARG	NE-CZ-NH1	10.98	125.79	120.30
12	5	187	TYR	CB-CG-CD2	-10.89	114.46	121.00
13	6	38	ARG	NE-CZ-NH2	-10.84	114.88	120.30
14	n	190	ARG	NE-CZ-NH2	-10.79	114.90	120.30
20	J	368	TYR	CB-CG-CD1	-10.62	114.63	121.00
17	K	51	LEU	CA-CB-CG	-10.51	91.13	115.30
8	1	25	TYR	CB-CG-CD2	-10.46	114.72	121.00
3	C	101	TYR	CB-CG-CD1	10.45	127.27	121.00
12	5	197	PHE	CB-CG-CD2	-10.43	113.50	120.80
9	2	188	ARG	NE-CZ-NH1	10.40	125.50	120.30
17	K	51	LEU	CB-CA-C	10.34	129.84	110.20
13	m	77	PHE	CB-CG-CD1	10.16	127.91	120.80
14	n	193	ARG	NE-CZ-NH1	10.02	125.31	120.30
4	d	117	ARG	NE-CZ-NH1	9.88	125.24	120.30
14	7	35	ARG	NE-CZ-NH2	9.85	125.23	120.30
6	f	173	ARG	NE-CZ-NH2	9.84	125.22	120.30
5	e	128	ARG	NE-CZ-NH2	9.83	125.21	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	22	ASP	CB-CG-OD2	-9.74	109.53	118.30
13	m	133	ARG	NE-CZ-NH2	-9.68	115.46	120.30
18	L	243	PHE	CB-CG-CD1	-9.63	114.06	120.80
10	3	197	ARG	NE-CZ-NH1	9.62	125.11	120.30
6	f	12	PHE	CB-CG-CD1	9.62	127.53	120.80
6	f	127	TYR	CB-CG-CD1	-9.61	115.24	121.00
6	f	12	PHE	CB-CG-CD2	-9.57	114.10	120.80
12	l	116	ASP	CB-CG-OD1	9.53	126.88	118.30
11	k	23	ARG	NE-CZ-NH2	9.52	125.06	120.30
4	D	20	TYR	CB-CG-CD1	9.47	126.68	121.00
14	n	185	TYR	CB-CG-CD1	-9.33	115.40	121.00
2	b	220	ASP	CB-CG-OD1	-9.26	109.96	118.30
11	k	56	PHE	CB-CG-CD2	-9.25	114.32	120.80
9	i	36	ARG	NE-CZ-NH1	9.17	124.89	120.30
14	7	186	TYR	CB-CG-CD2	-9.17	115.50	121.00
7	G	126	ARG	NE-CZ-NH1	9.15	124.88	120.30
1	a	122	ARG	NE-CZ-NH2	-9.14	115.73	120.30
7	g	87	ARG	NE-CZ-NH1	-9.14	115.73	120.30
2	b	220	ASP	CB-CG-OD2	9.11	126.50	118.30
11	k	149	ARG	NE-CZ-NH1	9.08	124.84	120.30
12	l	104	TYR	CB-CG-CD2	-9.04	115.58	121.00
8	l	191	ASP	CB-CG-OD1	9.04	126.44	118.30
5	E	2	ARG	NE-CZ-NH1	-8.98	115.81	120.30
7	G	18	PHE	CB-CG-CD2	-8.98	114.51	120.80
12	l	63	CYS	CA-CB-SG	-8.93	97.93	114.00
2	b	99	ARG	NE-CZ-NH1	8.89	124.75	120.30
8	l	191	ASP	CB-CG-OD2	-8.82	110.36	118.30
1	A	21	TYR	CB-CG-CD2	-8.79	115.72	121.00
14	n	185	TYR	CB-CG-CD2	8.77	126.26	121.00
9	i	36	ARG	NE-CZ-NH2	-8.75	115.92	120.30
10	j	43	PHE	CB-CG-CD1	-8.74	114.68	120.80
12	l	116	ASP	CB-CG-OD2	-8.72	110.45	118.30
1	a	21	TYR	CB-CG-CD2	-8.69	115.79	121.00
3	C	216	ARG	NE-CZ-NH2	-8.68	115.96	120.30
20	J	368	TYR	CB-CG-CD2	8.66	126.19	121.00
8	h	19	ARG	NE-CZ-NH2	-8.65	115.97	120.30
20	J	282	PHE	CB-CG-CD1	8.58	126.81	120.80
5	e	94	TYR	CB-CG-CD2	-8.56	115.86	121.00
3	C	101	TYR	CB-CG-CD2	-8.54	115.87	121.00
4	D	110	TYR	CB-CG-CD2	-8.52	115.89	121.00
12	5	90	TYR	CB-CG-CD1	8.52	126.11	121.00
6	F	98	PHE	CB-CG-CD1	-8.50	114.85	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	d	20	TYR	CB-CG-CD1	8.46	126.07	121.00
11	k	46	PHE	CB-CG-CD2	-8.44	114.89	120.80
8	l	82	PHE	CB-CG-CD2	-8.42	114.91	120.80
1	A	10	PHE	CB-CG-CD2	-8.39	114.93	120.80
1	a	5	ARG	NE-CZ-NH2	-8.38	116.11	120.30
13	m	133	ARG	NE-CZ-NH1	8.35	124.47	120.30
11	k	59	TYR	CB-CG-CD2	-8.34	116.00	121.00
8	l	45	ARG	NE-CZ-NH1	8.32	124.46	120.30
8	l	25	TYR	CB-CG-CD1	8.32	125.99	121.00
8	l	111	TYR	CB-CG-CD2	-8.31	116.01	121.00
5	E	159	TYR	CB-CG-CD2	-8.30	116.02	121.00
13	6	57	PHE	CB-CG-CD2	-8.30	114.99	120.80
7	G	18	PHE	CB-CG-CD1	8.28	126.60	120.80
1	A	157	TYR	CB-CG-CD2	-8.24	116.06	121.00
13	m	105	TYR	CB-CG-CD1	-8.22	116.07	121.00
1	a	146	TYR	CB-CG-CD1	-8.19	116.09	121.00
5	e	130	PHE	CB-CG-CD1	-8.18	115.08	120.80
5	e	157	TYR	CB-CG-CD1	-8.16	116.10	121.00
11	k	56	PHE	CB-CG-CD1	8.16	126.51	120.80
5	e	157	TYR	CB-CG-CD2	8.16	125.90	121.00
5	E	124	ARG	NE-CZ-NH2	-8.13	116.24	120.30
4	D	195	ARG	NE-CZ-NH2	8.07	124.34	120.30
8	h	45	ARG	NE-CZ-NH2	-8.07	116.27	120.30
8	h	45	ARG	NE-CZ-NH1	8.07	124.33	120.30
4	D	195	ARG	NE-CZ-NH1	-8.06	116.27	120.30
8	h	51	ASP	CB-CG-OD2	-8.06	111.05	118.30
7	g	18	PHE	CB-CG-CD1	8.03	126.42	120.80
4	D	110	TYR	CB-CG-CD1	7.98	125.79	121.00
3	c	128	ARG	NE-CZ-NH2	-7.97	116.32	120.30
5	E	77	ALA	O-C-N	-7.96	109.97	122.70
14	n	41	ARG	NE-CZ-NH1	7.95	124.28	120.30
13	6	91	ARG	NE-CZ-NH2	-7.94	116.33	120.30
2	B	157	PHE	CB-CG-CD1	-7.94	115.24	120.80
11	k	95	ARG	NE-CZ-NH1	7.93	124.27	120.30
2	b	4	ARG	NE-CZ-NH2	7.91	124.26	120.30
3	C	66	TYR	CB-CG-CD2	-7.89	116.27	121.00
2	B	99	ARG	NE-CZ-NH1	7.89	124.24	120.30
12	l	170	TYR	CB-CG-CD1	7.87	125.72	121.00
14	7	47	ASP	CB-CG-OD1	7.86	125.37	118.30
11	4	141	PHE	CB-CG-CD1	7.82	126.28	120.80
2	B	82	TYR	CB-CG-CD1	7.80	125.68	121.00
5	e	18	TYR	CB-CG-CD1	7.78	125.67	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	H	467	ASN	N-CA-C	7.75	131.94	111.00
14	7	186	TYR	CB-CG-CD1	7.73	125.64	121.00
8	1	70	TYR	CB-CG-CD1	7.72	125.63	121.00
7	G	156	TYR	CB-CG-CD1	7.72	125.63	121.00
12	l	46	ALA	N-CA-CB	7.71	120.89	110.10
2	b	23	TYR	CB-CG-CD1	7.68	125.61	121.00
5	E	145	TYR	CB-CG-CD1	-7.67	116.40	121.00
6	F	23	TYR	CB-CG-CD2	-7.67	116.40	121.00
9	i	188	ARG	NE-CZ-NH1	7.66	124.13	120.30
5	e	45	ARG	NE-CZ-NH1	7.58	124.09	120.30
2	b	22	ASP	CB-CG-OD1	7.55	125.09	118.30
11	k	96	ARG	NE-CZ-NH1	7.54	124.07	120.30
6	f	66	ASP	CB-CG-OD1	-7.52	111.53	118.30
5	e	125	LEU	CB-CG-CD2	7.48	123.72	111.00
12	l	167	ARG	NE-CZ-NH1	7.45	124.02	120.30
10	j	65	MET	CG-SD-CE	7.42	112.06	100.20
4	d	20	TYR	CB-CG-CD2	-7.39	116.57	121.00
18	L	261	ARG	NE-CZ-NH1	7.36	123.98	120.30
20	J	116	ARG	NE-CZ-NH1	-7.34	116.63	120.30
11	4	117	TYR	CB-CG-CD2	-7.33	116.61	121.00
3	c	112	ARG	NE-CZ-NH2	7.32	123.96	120.30
6	f	170	TYR	CB-CG-CD1	7.32	125.39	121.00
2	B	5	TYR	CB-CG-CD1	-7.32	116.61	121.00
10	3	27	ARG	NE-CZ-NH1	7.32	123.96	120.30
5	e	18	TYR	CB-CG-CD2	-7.30	116.62	121.00
2	b	23	TYR	CB-CG-CD2	-7.28	116.63	121.00
5	E	128	ARG	NE-CZ-NH1	-7.26	116.67	120.30
14	n	161	ARG	NE-CZ-NH2	-7.25	116.67	120.30
2	B	17	LYS	N-CA-CB	7.24	123.64	110.60
10	j	80	ALA	N-CA-CB	7.24	120.24	110.10
2	B	90	ARG	NE-CZ-NH2	-7.21	116.69	120.30
13	6	137	ARG	NE-CZ-NH1	-7.20	116.70	120.30
13	6	67	ARG	NE-CZ-NH1	7.17	123.88	120.30
15	H	319	PHE	CB-CG-CD1	7.14	125.80	120.80
4	d	146	TYR	CB-CG-CD1	-7.13	116.72	121.00
6	f	19	PHE	CB-CG-CD1	7.11	125.77	120.80
9	2	188	ARG	NE-CZ-NH2	-7.11	116.75	120.30
2	b	5	TYR	CB-CG-CD2	-7.09	116.74	121.00
10	3	97	ARG	NE-CZ-NH1	7.09	123.84	120.30
9	i	8	PHE	CB-CG-CD2	-7.07	115.85	120.80
2	B	130	PHE	CB-CG-CD1	7.07	125.75	120.80
5	E	70	MET	CG-SD-CE	7.04	111.47	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	J	282	PHE	CB-CG-CD2	-7.04	115.87	120.80
8	1	70	TYR	CB-CG-CD2	-7.04	116.78	121.00
12	l	159	ARG	NE-CZ-NH2	-7.03	116.78	120.30
1	A	96	ARG	NE-CZ-NH2	-7.02	116.79	120.30
14	7	77	ASP	CB-CG-OD2	-7.02	111.98	118.30
13	m	101	ARG	NE-CZ-NH2	-7.00	116.80	120.30
11	k	70	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	a	153	TYR	CG-CD2-CE2	-6.99	115.71	121.30
6	F	19	PHE	CB-CG-CD2	-6.98	115.91	120.80
7	g	16	ARG	NE-CZ-NH2	6.97	123.79	120.30
6	f	127	TYR	CB-CG-CD2	6.96	125.18	121.00
10	3	70	THR	CA-CB-CG2	-6.96	102.66	112.40
14	n	190	ARG	NE-CZ-NH1	6.94	123.77	120.30
4	D	3	ASP	CB-CG-OD2	-6.94	112.06	118.30
11	4	70	ARG	NE-CZ-NH1	6.93	123.77	120.30
5	E	2	ARG	NH1-CZ-NH2	6.89	126.98	119.40
3	C	156	TYR	CG-CD2-CE2	-6.88	115.80	121.30
12	5	111	THR	CA-CB-CG2	-6.87	102.79	112.40
3	C	130	PHE	CB-CG-CD2	6.86	125.60	120.80
14	7	181	MET	N-CA-CB	6.84	122.92	110.60
4	d	106	TYR	CD1-CE1-CZ	-6.81	113.67	119.80
10	3	187	TYR	CB-CG-CD1	-6.80	116.92	121.00
7	g	156	TYR	CB-CG-CD2	-6.78	116.93	121.00
1	A	65	CYS	CA-CB-SG	6.78	126.21	114.00
7	g	18	PHE	CB-CG-CD2	-6.78	116.05	120.80
1	a	146	TYR	CB-CG-CD2	6.78	125.06	121.00
6	f	173	ARG	NE-CZ-NH1	-6.77	116.91	120.30
14	n	193	ARG	NE-CZ-NH2	-6.77	116.91	120.30
2	b	234	ARG	NE-CZ-NH1	6.77	123.69	120.30
13	m	213	ARG	NE-CZ-NH1	6.77	123.68	120.30
6	f	232	TYR	CG-CD2-CE2	-6.76	115.89	121.30
6	F	38	ARG	NE-CZ-NH2	6.76	123.68	120.30
19	M	366	ARG	NE-CZ-NH1	6.75	123.67	120.30
3	C	148	TYR	CB-CG-CD2	-6.74	116.95	121.00
6	f	201	ARG	NE-CZ-NH2	6.74	123.67	120.30
1	a	136	SER	N-CA-CB	6.73	120.59	110.50
6	F	232	TYR	CB-CG-CD1	-6.73	116.97	121.00
9	i	8	PHE	CB-CG-CD1	6.71	125.50	120.80
12	l	106	ARG	NE-CZ-NH1	6.71	123.66	120.30
6	f	93	TYR	CB-CG-CD1	-6.68	116.99	121.00
11	k	98	TYR	CB-CG-CD2	-6.68	116.99	121.00
12	5	64	ARG	NE-CZ-NH1	-6.66	116.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	2	ARG	NE-CZ-NH2	-6.65	116.97	120.30
13	6	98	TYR	CB-CG-CD1	-6.65	117.01	121.00
5	e	85	ARG	NE-CZ-NH1	-6.65	116.98	120.30
13	m	142	ALA	CB-CA-C	-6.64	100.14	110.10
4	D	81	ARG	NE-CZ-NH2	-6.61	117.00	120.30
7	G	82	ARG	NE-CZ-NH2	6.60	123.60	120.30
1	a	122	ARG	NE-CZ-NH1	6.58	123.59	120.30
2	b	148	TYR	CG-CD1-CE1	-6.55	116.06	121.30
7	g	153	TYR	CB-CG-CD2	6.55	124.93	121.00
6	F	2	ARG	NE-CZ-NH1	6.54	123.57	120.30
8	1	61	TYR	CB-CG-CD2	-6.54	117.08	121.00
2	B	130	PHE	CB-CG-CD2	-6.53	116.23	120.80
1	a	62	TYR	CB-CG-CD1	-6.53	117.08	121.00
2	B	235	PHE	CB-CG-CD1	6.53	125.37	120.80
1	a	19	VAL	CA-CB-CG2	-6.52	101.11	110.90
6	F	98	PHE	CB-CG-CD2	6.52	125.37	120.80
13	6	95	HIS	O-C-N	-6.52	112.26	122.70
17	K	141	ARG	NE-CZ-NH2	6.51	123.56	120.30
4	d	3	ASP	CB-CG-OD1	-6.51	112.44	118.30
1	A	62	TYR	CG-CD1-CE1	-6.49	116.11	121.30
18	L	338	LEU	CA-CB-CG	6.49	130.23	115.30
8	h	66	TYR	CB-CG-CD2	-6.49	117.11	121.00
3	C	4	ARG	NE-CZ-NH1	6.48	123.54	120.30
3	C	156	TYR	CG-CD1-CE1	-6.47	116.12	121.30
14	7	229	GLY	CA-C-O	-6.46	108.96	120.60
5	E	2	ARG	NE-CZ-NH2	-6.46	117.07	120.30
13	m	137	ARG	NE-CZ-NH2	6.45	123.53	120.30
1	a	154	TYR	CG-CD2-CE2	-6.44	116.15	121.30
12	l	212	GLY	CA-C-O	-6.44	109.01	120.60
12	5	212	GLY	CA-C-O	-6.44	109.01	120.60
3	C	148	TYR	CB-CG-CD1	6.43	124.86	121.00
10	3	97	ARG	NE-CZ-NH2	-6.43	117.08	120.30
10	j	67	ARG	NE-CZ-NH2	-6.43	117.09	120.30
3	c	97	TYR	CB-CG-CD2	-6.41	117.15	121.00
4	d	223	SER	N-CA-CB	6.40	120.10	110.50
12	l	69	ARG	NE-CZ-NH1	6.38	123.49	120.30
20	J	270	ARG	NE-CZ-NH2	-6.37	117.11	120.30
6	f	19	PHE	CB-CG-CD2	-6.37	116.34	120.80
1	A	97	TYR	CB-CG-CD2	6.37	124.82	121.00
11	4	98	TYR	CB-CG-CD2	-6.37	117.18	121.00
3	C	113	ARG	NE-CZ-NH2	-6.35	117.12	120.30
13	m	75	TYR	CB-CG-CD2	-6.35	117.19	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	12	PHE	CB-CG-CD2	-6.34	116.36	120.80
14	n	182	ARG	NE-CZ-NH1	-6.34	117.13	120.30
8	h	57	ASP	CB-CG-OD2	6.33	124.00	118.30
8	1	129	SER	N-CA-CB	6.33	119.99	110.50
6	f	163	ARG	NE-CZ-NH2	6.32	123.46	120.30
10	3	161	ASP	CB-CG-OD2	-6.32	112.61	118.30
2	B	82	TYR	CB-CG-CD2	-6.32	117.21	121.00
8	h	174	ARG	NE-CZ-NH2	-6.30	117.15	120.30
3	c	148	TYR	CB-CG-CD1	-6.30	117.22	121.00
1	A	3	TYR	CB-CG-CD2	-6.29	117.22	121.00
4	D	2	TYR	CG-CD1-CE1	-6.28	116.27	121.30
13	m	90	ALA	N-CA-CB	6.28	118.89	110.10
5	e	130	PHE	CB-CG-CD2	6.25	125.17	120.80
8	h	189	TYR	CG-CD1-CE1	-6.25	116.30	121.30
14	n	7	THR	CA-CB-CG2	-6.25	103.66	112.40
1	A	99	TYR	CB-CG-CD2	-6.24	117.26	121.00
1	A	10	PHE	CB-CG-CD1	6.23	125.16	120.80
6	f	106	ARG	NE-CZ-NH1	6.21	123.41	120.30
12	l	167	ARG	NE-CZ-NH2	-6.21	117.19	120.30
3	C	91	ARG	NE-CZ-NH2	-6.21	117.19	120.30
11	4	20	ALA	N-CA-CB	6.21	118.80	110.10
13	m	105	TYR	CB-CG-CD2	6.20	124.72	121.00
2	b	170	ALA	N-CA-CB	6.18	118.76	110.10
13	m	149	PHE	CB-CG-CD1	-6.17	116.48	120.80
8	1	66	TYR	CB-CG-CD1	-6.17	117.30	121.00
17	K	253	MET	CG-SD-CE	6.16	110.06	100.20
13	m	60	ASP	CB-CG-OD1	-6.16	112.76	118.30
2	B	4	ARG	NE-CZ-NH1	-6.16	117.22	120.30
8	1	87	TYR	CZ-CE2-CD2	-6.16	114.26	119.80
12	l	152	ASP	CB-CG-OD1	-6.15	112.77	118.30
4	D	218	ASP	CB-CG-OD1	6.15	123.83	118.30
14	7	128	ARG	NE-CZ-NH2	6.15	123.38	120.30
10	j	132	ALA	N-CA-CB	6.15	118.71	110.10
11	k	139	TYR	CB-CG-CD2	-6.15	117.31	121.00
3	c	17	ARG	NE-CZ-NH1	6.13	123.37	120.30
5	e	12	ARG	NE-CZ-NH1	6.13	123.36	120.30
3	c	128	ARG	NE-CZ-NH1	6.13	123.36	120.30
10	j	45	TYR	CB-CG-CD1	-6.13	117.32	121.00
6	F	83	LEU	CB-CG-CD2	6.13	121.42	111.00
1	a	5	ARG	NE-CZ-NH1	6.12	123.36	120.30
4	d	117	ARG	NE-CZ-NH2	-6.10	117.25	120.30
12	5	121	ARG	NE-CZ-NH2	-6.10	117.25	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	3	68	TYR	CB-CG-CD1	6.10	124.66	121.00
13	6	221	ARG	NE-CZ-NH2	-6.09	117.25	120.30
11	4	121	TYR	CB-CG-CD1	-6.09	117.35	121.00
2	b	178	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	A	23	PHE	CB-CG-CD2	-6.07	116.55	120.80
7	g	82	ARG	NE-CZ-NH1	6.05	123.33	120.30
14	n	59	ASP	CB-CG-OD1	-6.04	112.86	118.30
5	E	158	ARG	NE-CZ-NH1	-6.04	117.28	120.30
1	a	15	ARG	CG-CD-NE	6.04	124.48	111.80
3	c	15	GLU	OE1-CD-OE2	-6.04	116.06	123.30
14	n	33	LEU	CB-CG-CD1	6.03	121.24	111.00
14	n	190	ARG	CG-CD-NE	-6.03	99.14	111.80
9	i	88	PHE	CB-CG-CD1	6.00	125.00	120.80
2	B	87	ASP	CB-CG-OD1	5.99	123.69	118.30
3	C	4	ARG	NE-CZ-NH2	-5.97	117.32	120.30
1	a	15	ARG	NE-CZ-NH1	5.97	123.28	120.30
17	K	257	VAL	CA-CB-CG2	-5.97	101.95	110.90
4	D	170	ARG	NE-CZ-NH1	-5.96	117.32	120.30
6	F	103	ALA	N-CA-CB	5.96	118.44	110.10
4	d	155	SER	N-CA-CB	5.94	119.41	110.50
12	l	7	ARG	NE-CZ-NH2	5.94	123.27	120.30
12	5	102	CYS	CA-CB-SG	-5.94	103.31	114.00
10	j	201	MET	CB-CG-SD	-5.93	94.60	112.40
17	K	307	ASP	CB-CG-OD1	-5.93	112.96	118.30
3	C	23	TYR	CG-CD2-CE2	-5.92	116.56	121.30
5	e	148	PHE	CG-CD2-CE2	5.92	127.31	120.80
13	6	74	TRP	CG-CD2-CE3	-5.90	128.59	133.90
6	F	5	TYR	CB-CG-CD2	-5.89	117.46	121.00
9	2	75	ARG	NE-CZ-NH1	5.89	123.25	120.30
2	B	101	TYR	CG-CD1-CE1	5.88	126.01	121.30
13	6	168	VAL	CG1-CB-CG2	-5.87	101.52	110.90
14	7	187	ARG	NH1-CZ-NH2	-5.87	112.95	119.40
10	j	36	SER	CB-CA-C	-5.86	98.97	110.10
12	5	3	THR	N-CA-C	-5.86	95.18	111.00
5	E	95	TYR	CB-CG-CD2	5.85	124.51	121.00
10	3	140	THR	CA-CB-CG2	-5.85	104.21	112.40
1	A	215	GLU	N-CA-CB	5.85	121.13	110.60
2	b	86	VAL	CA-CB-CG2	-5.84	102.14	110.90
7	G	156	TYR	CB-CG-CD2	-5.84	117.50	121.00
14	7	111	TRP	CD1-CG-CD2	-5.84	101.63	106.30
14	7	126	PHE	CB-CG-CD1	-5.83	116.72	120.80
3	c	23	TYR	CB-CG-CD1	5.83	124.50	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	e	150	ALA	CB-CA-C	-5.83	101.36	110.10
7	G	110	ASP	CB-CG-OD1	5.81	123.53	118.30
2	B	101	TYR	CB-CG-CD1	5.81	124.48	121.00
2	b	4	ARG	NE-CZ-NH1	-5.80	117.40	120.30
2	B	23	TYR	CB-CG-CD2	-5.80	117.52	121.00
1	A	87	ARG	NE-CZ-NH1	5.79	123.20	120.30
9	2	36	ARG	NE-CZ-NH1	5.78	123.19	120.30
17	K	152	PRO	CA-N-CD	5.78	119.79	111.70
7	G	22	TYR	CB-CG-CD2	-5.78	117.53	121.00
13	6	185	ARG	NE-CZ-NH1	-5.78	117.41	120.30
8	h	14	LEU	CB-CG-CD2	-5.77	101.19	111.00
1	a	153	TYR	CB-CG-CD1	-5.76	117.54	121.00
7	G	74	TYR	CB-CG-CD2	-5.76	117.54	121.00
17	K	51	LEU	CB-CG-CD1	5.75	120.78	111.00
8	h	124	TYR	CB-CG-CD1	-5.72	117.57	121.00
12	l	197	PHE	CB-CG-CD1	-5.72	116.80	120.80
12	l	125	ASP	CA-CB-CG	-5.72	100.82	113.40
20	J	318	PRO	CA-N-CD	5.72	119.70	111.70
10	3	187	TYR	CA-CB-CG	-5.71	102.56	113.40
12	5	64	ARG	NE-CZ-NH2	5.70	123.15	120.30
3	c	101	TYR	CB-CG-CD1	5.70	124.42	121.00
6	F	93	TYR	CB-CG-CD2	-5.70	117.58	121.00
3	C	156	TYR	CD1-CG-CD2	5.69	124.16	117.90
4	d	106	TYR	CG-CD1-CE1	5.68	125.84	121.30
1	a	78	ILE	CA-C-N	5.68	132.99	117.10
10	3	79	ARG	NE-CZ-NH2	-5.67	117.46	120.30
12	5	73	ARG	NE-CZ-NH1	5.67	123.14	120.30
10	3	26	LEU	CB-CG-CD2	5.66	120.62	111.00
2	b	99	ARG	NE-CZ-NH2	-5.65	117.47	120.30
8	h	82	PHE	CB-CG-CD2	-5.65	116.84	120.80
10	j	86	PHE	CB-CG-CD2	-5.64	116.85	120.80
11	4	98	TYR	CB-CG-CD1	5.64	124.38	121.00
1	A	112	MET	CG-SD-CE	-5.63	91.19	100.20
10	j	187	TYR	CB-CG-CD1	5.63	124.38	121.00
16	I	171	MET	CG-SD-CE	-5.63	91.19	100.20
13	6	2	PHE	CB-CG-CD2	-5.63	116.86	120.80
15	H	410	LEU	CA-CB-CG	5.63	128.24	115.30
4	d	4	ARG	NE-CZ-NH1	5.62	123.11	120.30
5	E	77	ALA	CA-C-N	5.62	129.56	117.20
20	J	210	PHE	CB-CG-CD1	-5.62	116.87	120.80
3	c	101	TYR	CB-CG-CD2	-5.61	117.63	121.00
8	1	36	ARG	NE-CZ-NH1	-5.61	117.49	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	M	154	LEU	N-CA-CB	5.60	121.60	110.40
3	C	48	GLU	N-CA-CB	-5.60	100.53	110.60
7	G	145	TYR	CB-CG-CD2	-5.60	117.64	121.00
8	1	45	ARG	NE-CZ-NH2	-5.60	117.50	120.30
2	b	157	PHE	CB-CG-CD1	5.59	124.71	120.80
8	h	25	TYR	CB-CG-CD1	-5.59	117.65	121.00
5	E	114	ARG	NE-CZ-NH2	5.58	123.09	120.30
16	I	293	ASP	CB-CG-OD1	5.58	123.32	118.30
6	f	232	TYR	CB-CG-CD1	-5.58	117.66	121.00
2	B	169	VAL	CG1-CB-CG2	5.57	119.82	110.90
4	d	110	TYR	CB-CG-CD2	5.56	124.34	121.00
3	c	23	TYR	CB-CG-CD2	-5.56	117.66	121.00
1	A	119	TYR	CB-CG-CD2	-5.56	117.67	121.00
6	F	66	ASP	CB-CG-OD2	-5.56	113.30	118.30
7	g	80	ASP	CB-CG-OD1	-5.55	113.30	118.30
14	n	1	THR	CA-CB-CG2	-5.55	104.63	112.40
11	k	59	TYR	CB-CG-CD1	5.55	124.33	121.00
6	F	127	TYR	CB-CG-CD2	-5.54	117.67	121.00
1	A	61	SER	N-CA-CB	5.54	118.81	110.50
13	6	77	PHE	CB-CG-CD1	-5.53	116.93	120.80
1	A	96	ARG	NE-CZ-NH1	5.53	123.06	120.30
8	h	104	ASP	CB-CG-OD2	-5.53	113.33	118.30
13	6	57	PHE	CB-CG-CD1	5.53	124.67	120.80
1	a	97	TYR	CB-CG-CD2	-5.52	117.69	121.00
5	E	157	TYR	CB-CG-CD2	-5.51	117.69	121.00
12	5	87	VAL	CA-CB-CG2	5.51	119.16	110.90
12	l	6	PHE	CB-CG-CD1	5.51	124.65	120.80
8	1	153	ASP	CB-CG-OD2	5.51	123.26	118.30
2	b	136	ILE	CA-CB-CG2	-5.50	99.89	110.90
6	F	180	LYS	O-C-N	-5.50	113.90	122.70
1	a	29	THR	CA-CB-CG2	-5.50	104.70	112.40
9	2	174	ASP	CB-CG-OD1	5.50	123.25	118.30
4	d	139	ARG	NE-CZ-NH1	5.49	123.05	120.30
2	B	235	PHE	CB-CG-CD2	-5.49	116.96	120.80
2	b	82	TYR	CB-CG-CD1	-5.49	117.71	121.00
6	f	103	ALA	N-CA-CB	5.48	117.78	110.10
2	B	104	TYR	CB-CG-CD1	-5.48	117.71	121.00
4	d	154	TYR	CG-CD1-CE1	-5.47	116.92	121.30
8	1	153	ASP	O-C-N	-5.47	113.95	122.70
4	d	110	TYR	CB-CG-CD1	-5.47	117.72	121.00
13	m	48	ASP	CB-CG-OD1	-5.46	113.38	118.30
14	n	69	ASP	CB-CG-OD2	-5.46	113.39	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	153	TYR	CG-CD1-CE1	-5.46	116.93	121.30
16	I	369	MET	CG-SD-CE	-5.46	91.47	100.20
13	6	21	ALA	N-CA-CB	5.46	117.74	110.10
14	7	124	ASP	CB-CG-OD2	5.45	123.21	118.30
3	c	183	MET	CG-SD-CE	5.45	108.92	100.20
6	f	170	TYR	CB-CG-CD2	-5.45	117.73	121.00
13	6	20	PHE	CB-CG-CD2	-5.45	116.98	120.80
4	d	112	ALA	N-CA-CB	5.45	117.73	110.10
6	F	66	ASP	CB-CG-OD1	5.43	123.19	118.30
11	4	152	MET	CG-SD-CE	-5.43	91.51	100.20
11	k	139	TYR	CB-CA-C	-5.42	99.55	110.40
17	K	335	ASP	CB-CG-OD1	5.42	123.18	118.30
15	H	243	PRO	CA-N-CD	5.42	119.28	111.70
2	b	101	TYR	N-CA-CB	5.41	120.34	110.60
16	I	216	PRO	CA-N-CD	5.41	119.28	111.70
3	C	12	PHE	CB-CA-C	-5.41	99.58	110.40
11	k	84	VAL	CG1-CB-CG2	-5.40	102.25	110.90
13	6	218	GLU	OE1-CD-OE2	5.40	129.78	123.30
9	2	69	TYR	CB-CG-CD1	5.40	124.24	121.00
13	6	151	ASP	CB-CG-OD1	-5.39	113.44	118.30
5	e	110	ASP	CB-CG-OD2	5.39	123.15	118.30
13	m	81	ASP	N-CA-CB	5.38	120.29	110.60
13	6	105	TYR	CD1-CE1-CZ	5.38	124.64	119.80
1	a	224	PHE	CB-CG-CD2	5.37	124.56	120.80
17	K	262	ARG	NE-CZ-NH2	-5.37	117.62	120.30
14	n	161	ARG	NE-CZ-NH1	5.36	122.98	120.30
14	n	86	ALA	N-CA-CB	5.34	117.58	110.10
8	1	66	TYR	CG-CD1-CE1	-5.34	117.03	121.30
11	k	93	ARG	NE-CZ-NH2	5.34	122.97	120.30
11	k	132	ALA	CB-CA-C	-5.34	102.09	110.10
1	A	196	PHE	CB-CG-CD2	5.33	124.53	120.80
2	B	161	ALA	N-CA-CB	5.33	117.56	110.10
1	a	92	ALA	N-CA-CB	5.32	117.55	110.10
1	a	116	SER	N-CA-CB	5.32	118.48	110.50
10	j	1	SER	O-C-N	-5.32	114.19	122.70
3	c	236	ASP	N-CA-CB	5.32	120.17	110.60
16	I	437	LEU	CA-C-O	-5.32	108.94	120.10
13	m	210	ASP	CB-CG-OD1	5.31	123.08	118.30
5	E	242	GLU	CA-C-O	-5.31	108.94	120.10
8	1	196	LEU	CA-C-O	-5.31	108.95	120.10
1	A	242	GLN	CA-C-O	-5.31	108.95	120.10
7	G	101	THR	N-CA-C	-5.31	96.67	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	9	THR	CA-CB-CG2	-5.31	104.97	112.40
9	2	226	GLU	CA-C-O	-5.30	108.97	120.10
13	6	222	ASP	CA-C-O	-5.30	108.97	120.10
15	H	178	ARG	NE-CZ-NH2	-5.30	117.65	120.30
11	4	195	PHE	CA-C-O	-5.30	108.97	120.10
8	h	196	LEU	CA-C-O	-5.30	108.98	120.10
14	n	42	LEU	CB-CG-CD2	5.30	120.00	111.00
3	C	244	THR	CA-C-O	-5.30	108.98	120.10
7	G	244	ASN	CA-C-O	-5.30	108.98	120.10
15	H	467	ASN	CA-C-O	-5.30	108.98	120.10
19	M	434	ALA	CA-C-O	-5.30	108.98	120.10
5	e	137	ALA	CB-CA-C	-5.29	102.16	110.10
2	b	250	LEU	CA-C-O	-5.29	108.98	120.10
11	k	195	PHE	CA-C-O	-5.29	108.98	120.10
7	g	244	ASN	CA-C-O	-5.29	108.99	120.10
9	i	226	GLU	CA-C-O	-5.29	108.99	120.10
3	C	39	ALA	CB-CA-C	5.29	118.04	110.10
6	F	233	ILE	CA-C-O	-5.29	108.99	120.10
15	H	247	LEU	CA-CB-CG	5.29	127.47	115.30
5	e	94	TYR	CB-CG-CD1	5.29	124.17	121.00
9	i	122	GLY	N-CA-C	-5.29	99.88	113.10
12	l	125	ASP	CB-CG-OD2	5.29	123.06	118.30
14	n	232	LYS	CA-C-O	-5.29	109.00	120.10
1	A	149	ASP	CB-CG-OD2	-5.29	113.54	118.30
18	L	436	LYS	CA-C-O	-5.29	109.00	120.10
1	a	242	GLN	CA-C-O	-5.28	109.01	120.10
3	c	244	THR	CA-C-O	-5.28	109.00	120.10
10	3	83	PRO	CA-N-CD	5.28	119.10	111.70
1	a	215	GLU	N-CA-C	-5.28	96.74	111.00
12	l	102	CYS	CA-CB-SG	-5.28	104.49	114.00
13	m	222	ASP	CA-C-O	-5.28	109.01	120.10
17	K	428	LYS	CA-C-O	-5.28	109.01	120.10
5	e	242	GLU	CA-C-O	-5.28	109.01	120.10
7	g	45	ALA	N-CA-CB	5.28	117.49	110.10
12	l	8	PHE	CB-CG-CD1	-5.28	117.10	120.80
2	B	250	LEU	CA-C-O	-5.28	109.02	120.10
2	b	82	TYR	CG-CD1-CE1	-5.27	117.08	121.30
12	5	75	SER	N-CA-CB	5.27	118.41	110.50
11	k	120	ASP	CB-CG-OD1	5.27	123.04	118.30
6	f	233	ILE	CA-C-O	-5.26	109.05	120.10
7	g	130	VAL	CG1-CB-CG2	-5.26	102.49	110.90
5	E	18	TYR	CB-CG-CD1	5.26	124.16	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	J	132	PRO	CA-N-CD	5.26	119.06	111.70
3	c	156	TYR	CG-CD1-CE1	-5.25	117.10	121.30
10	j	28	LEU	N-CA-CB	5.25	120.90	110.40
16	I	135	PHE	N-CA-CB	5.25	120.05	110.60
8	l	87	TYR	CD1-CE1-CZ	-5.25	115.08	119.80
1	a	137	VAL	CA-CB-CG2	-5.24	103.05	110.90
5	E	148	PHE	CB-CG-CD2	-5.23	117.14	120.80
1	a	222	ASP	N-CA-CB	5.23	120.02	110.60
7	g	112	LEU	CB-CA-C	-5.23	100.27	110.20
14	n	25	ASP	CB-CG-OD1	-5.23	113.59	118.30
5	E	130	PHE	CD1-CE1-CZ	5.23	126.37	120.10
6	F	205	LEU	CB-CG-CD1	5.22	119.87	111.00
7	G	2	THR	CA-CB-CG2	-5.22	105.09	112.40
19	M	131	MET	CG-SD-CE	-5.21	91.86	100.20
6	F	65	CYS	CA-CB-SG	5.21	123.38	114.00
8	l	120	HIS	N-CA-CB	5.21	119.97	110.60
17	K	102	PRO	CA-N-CD	5.20	118.99	111.70
14	7	161	ARG	NE-CZ-NH2	-5.20	117.70	120.30
15	H	432	ARG	NE-CZ-NH1	-5.19	117.70	120.30
2	b	93	ALA	CB-CA-C	-5.19	102.32	110.10
1	a	119	TYR	CB-CG-CD1	5.19	124.11	121.00
11	k	97	PRO	N-CA-CB	5.19	109.52	103.30
1	A	3	TYR	CG-CD1-CE1	-5.18	117.15	121.30
8	l	189	TYR	CB-CG-CD1	-5.18	117.89	121.00
1	A	196	PHE	CB-CG-CD1	-5.18	117.17	120.80
4	D	136	PHE	CB-CG-CD1	-5.18	117.17	120.80
15	H	204	PRO	CA-N-CD	5.18	118.95	111.70
3	C	66	TYR	CB-CG-CD1	5.18	124.11	121.00
15	H	95	HIS	CA-CB-CG	-5.18	104.80	113.60
16	I	145	CYS	CA-CB-SG	5.18	123.32	114.00
1	a	79	PRO	CA-N-CD	-5.17	104.26	111.50
1	A	87	ARG	NE-CZ-NH2	-5.17	117.71	120.30
4	D	20	TYR	CB-CG-CD2	-5.17	117.90	121.00
4	D	81	ARG	NE-CZ-NH1	5.17	122.89	120.30
15	H	165	PRO	CA-N-CD	5.17	118.94	111.70
18	L	165	PRO	CA-N-CD	5.17	118.94	111.70
1	a	21	TYR	CB-CG-CD1	5.17	124.10	121.00
12	l	20	ALA	N-CA-CB	5.17	117.34	110.10
10	j	79	ARG	NE-CZ-NH2	-5.17	117.72	120.30
20	J	68	PRO	CA-N-CD	5.17	118.93	111.70
1	a	23	PHE	CB-CG-CD2	-5.17	117.19	120.80
7	g	67	ASP	CB-CG-OD1	5.16	122.94	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	2	97	TYR	CB-CG-CD2	-5.16	117.91	121.00
15	H	466	TYR	C-N-CA	5.15	134.58	121.70
1	A	157	TYR	CG-CD1-CE1	-5.15	117.18	121.30
5	E	223	TYR	CB-CG-CD1	5.15	124.09	121.00
7	g	74	TYR	CG-CD2-CE2	-5.14	117.18	121.30
13	m	103	PHE	CB-CG-CD2	-5.14	117.20	120.80
6	F	88	ARG	NE-CZ-NH1	5.14	122.87	120.30
7	g	186	ARG	CG-CD-NE	-5.14	101.01	111.80
11	k	191	GLN	CB-CA-C	-5.13	100.13	110.40
12	5	98	GLY	N-CA-C	-5.13	100.27	113.10
15	H	186	PRO	CA-N-CD	5.13	118.88	111.70
3	c	38	MET	CG-SD-CE	5.12	108.40	100.20
19	M	221	TYR	CB-CG-CD2	-5.12	117.93	121.00
11	k	99	GLN	CB-CA-C	5.12	120.64	110.40
5	E	94	TYR	CB-CG-CD1	5.12	124.07	121.00
4	d	3	ASP	CB-CG-OD2	5.12	122.91	118.30
2	B	109	LEU	N-CA-CB	5.12	120.63	110.40
7	G	13	PRO	CA-N-CD	5.12	118.86	111.70
10	3	103	PHE	CB-CG-CD2	-5.12	117.22	120.80
17	K	48	TYR	CB-CG-CD2	-5.11	117.93	121.00
8	h	57	ASP	CB-CG-OD1	-5.11	113.70	118.30
3	c	156	TYR	CD1-CE1-CZ	5.11	124.40	119.80
5	E	89	VAL	CA-CB-CG2	-5.10	103.25	110.90
11	4	67	TYR	CB-CG-CD1	5.10	124.06	121.00
18	L	137	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	a	111	ARG	CG-CD-NE	-5.09	101.11	111.80
13	6	75	TYR	CG-CD2-CE2	-5.09	117.23	121.30
6	F	114	LYS	CB-CA-C	-5.09	100.22	110.40
13	6	103	PHE	N-CA-C	-5.09	97.26	111.00
4	d	2	TYR	CB-CG-CD1	-5.09	117.95	121.00
10	j	163	PHE	CB-CG-CD1	5.08	124.36	120.80
11	4	181	VAL	CG1-CB-CG2	5.08	119.03	110.90
1	a	172	ASN	N-CA-CB	5.08	119.74	110.60
2	B	14	PRO	CA-N-CD	5.08	118.81	111.70
6	f	88	ARG	NE-CZ-NH1	5.08	122.84	120.30
10	j	43	PHE	CB-CG-CD2	5.08	124.35	120.80
11	4	2	ASP	CB-CG-OD1	-5.08	113.73	118.30
18	L	141	LYS	N-CA-CB	5.07	119.73	110.60
11	k	185	ASP	CB-CG-OD1	5.07	122.86	118.30
6	f	98	PHE	CB-CA-C	-5.06	100.27	110.40
4	D	154	TYR	CZ-CE2-CD2	-5.06	115.24	119.80
5	E	124	ARG	CB-CG-CD	5.06	124.75	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	234	ARG	NE-CZ-NH2	-5.05	117.77	120.30
14	n	214	VAL	CA-CB-CG2	-5.05	103.32	110.90
5	E	124	ARG	NE-CZ-NH1	5.05	122.83	120.30
7	G	126	ARG	NH1-CZ-NH2	-5.05	113.85	119.40
10	3	80	ALA	N-CA-CB	5.05	117.17	110.10
18	L	352	PRO	CA-N-CD	5.04	118.76	111.70
3	c	112	ARG	NE-CZ-NH1	-5.04	117.78	120.30
18	L	104	LEU	CB-CG-CD1	-5.04	102.44	111.00
2	b	174	PHE	CB-CG-CD1	-5.04	117.28	120.80
11	4	173	PRO	CA-N-CD	5.03	118.75	111.70
11	k	192	VAL	CG1-CB-CG2	-5.03	102.85	110.90
20	J	368	TYR	CG-CD2-CE2	-5.03	117.28	121.30
10	3	86	PHE	CB-CG-CD2	-5.03	117.28	120.80
10	j	84	GLU	OE1-CD-OE2	-5.02	117.28	123.30
11	k	85	ARG	NE-CZ-NH2	-5.02	117.79	120.30
14	n	65	ARG	NE-CZ-NH2	5.02	122.81	120.30
19	M	337	LEU	CB-CG-CD2	5.02	119.53	111.00
3	C	130	PHE	CB-CA-C	-5.02	100.37	110.40
18	L	223	PRO	CA-N-CD	5.02	118.72	111.70
8	1	124	TYR	CB-CG-CD2	5.01	124.01	121.00
13	6	108	HIS	N-CA-C	-5.01	97.47	111.00
12	5	105	THR	CA-CB-CG2	-5.01	105.39	112.40
14	n	34	LEU	CB-CG-CD2	5.01	119.51	111.00
3	C	168	THR	CA-CB-CG2	-5.01	105.39	112.40

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

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Mol	Chain	Res	Type	Group
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	Mainchain,Peptide
5	E	130	PHE	Sidechain
5	E	157	TYR	Sidechain
5	E	2	ARG	Sidechain
6	F	136	TYR	Sidechain
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

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Mol	Chain	Res	Type	Group
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	Sidechain,Peptide
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
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 ⓘ

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	8	0
1	a	1907	0	1901	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1915	0	1929	39	0
2	b	1915	0	1928	0	0
3	C	1904	0	1904	28	0
3	c	1904	0	1904	0	0
4	D	1881	0	1895	29	0
4	d	1881	0	1895	0	0
5	E	1861	0	1839	24	0
5	e	1861	0	1839	0	0
6	F	1795	0	1800	22	0
6	f	1773	0	1775	0	0
7	G	1892	0	1883	27	0
7	g	1892	0	1883	0	0
8	1	1512	0	1481	5	0
8	h	1512	0	1481	0	0
9	2	1719	0	1719	14	0
9	i	1719	0	1719	0	0
10	3	1581	0	1574	15	0
10	j	1581	0	1574	0	0
11	4	1561	0	1569	8	0
11	k	1561	0	1569	0	0
12	5	1644	0	1595	13	0
12	l	1644	0	1595	0	0
13	6	1757	0	1711	12	0
13	m	1757	0	1711	0	0
14	7	1790	0	1793	13	0
14	n	1815	0	1821	0	0
15	H	3053	0	3126	24	0
16	I	3022	0	3090	40	0
17	K	3078	0	3141	27	0
18	L	3082	0	3156	43	0
19	M	2986	0	3054	54	0
20	J	3033	0	3153	26	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	M	31	0	12	3	0
23	J	27	0	11	6	0
All	All	67883	0	67979	440	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 4.

All (440) 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	6.94	0.91
18:L:183:ILE:CD1	22:L:501:ATP:HN62	1.80	0.89
2:B:4:ARG:NH2	5:E:117:GLU:CB	7.86	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
20:J:197:LEU:HD11	23:J:501:ADP:C2'	2.08	0.83
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	5.03	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:OE1	5:E:217:GLN:N	2.17	0.77
16:I:337:ALA:O	16:I:343:ARG:NH1	2.18	0.76
10:3:95:TYR:CD2	10:3:95:TYR:O	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	4.22	0.73
20:J:197:LEU:HD13	23:J:501:ADP:H2'	1.71	0.72
5:E:206:GLU:N	5:E:206:GLU:OE1	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:227:ILE:HG23	2:B:230:ASP:OD2	4.99	0.71
19:M:352:PRO:CA	19:M:356:SER:HB2	2.20	0.71
10:3:95:TYR:CG	10:3:95:TYR:O	2.44	0.71
16:I:436:TYR:C	16:I:437:LEU:O	2.28	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
14:7:131:ASN:OD1	14:7:131:ASN:C	2.31	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	2.38	0.67
4:D:45:GLU:HG3	4:D:45:GLU:O	1.92	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:O	11:4:120:ASP:OD1	2.12	0.67
19:M:352:PRO:HB2	19:M:356:SER:HB2	1.77	0.66
2:B:227:ILE:O	2:B:227:ILE:HG23	3.88	0.65
3:C:229:PHE:N	3:C:229:PHE:CD1	2.64	0.65
8:1:193:TYR:O	8:1:196:LEU:O	2.14	0.65
14:7:63:ILE:HG22	14:7:63:ILE:O	1.96	0.65
18:L:241:ALA:O	18:L:243:PHE:CE1	2.50	0.64
18:L:241:ALA:O	18:L:243:PHE:CZ	2.49	0.64
19:M:374:ILE:CG2	19:M:376:TRP:CE2	2.80	0.64
3:C:237:ILE:O	3:C:237:ILE:HG22	4.46	0.64
16:I:190:GLN:N	16:I:190:GLN:OE1	2.31	0.64
15:H:328:GLU:OE1	15:H:328:GLU:N	2.29	0.64
2:B:139:HIS:C	2:B:139:HIS:ND1	3.51	0.63
18:L:432:ILE:O	18:L:432:ILE:HG22	1.97	0.63
4:D:226:GLU:N	4:D:226:GLU:OE1	2.24	0.63
2:B:139:HIS:ND1	2:B:139:HIS:O	4.27	0.62
6:F:233:ILE:HG22	6:F:233:ILE:OXT	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	7.31	0.62
11:4:120:ASP:C	11:4:120:ASP:OD1	2.32	0.62
6:F:54:GLU:N	6:F:54:GLU:OE1	2.30	0.61
18:L:399:GLY:O	18:L:403:ILE:HG13	2.00	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	7.86	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4:ARG:HH22	5:E:117:GLU:CB	7.57	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
15:H:458:SER:O	15:H:461:SER:N	2.35	0.60
9:2:138:LEU:HD13	9:2:138:LEU:C	2.22	0.60
15:H:458:SER:O	15:H:459:SER:C	2.39	0.60
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
19:M:283:LEU:HG	19:M:283:LEU:O	2.03	0.59
7:G:197:TYR:HD1	7:G:197:TYR:N	2.01	0.59
19:M:387:ASN:OD1	19:M:387:ASN:C	2.41	0.59
19:M:359:GLN:O	19:M:363:ILE:HG12	2.03	0.59
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	4.28	0.58
16:I:339:ILE:HD12	16:I:339:ILE:C	2.24	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	7.79	0.58
2:B:4:ARG:HH21	5:E:117:GLU:HB3	7.48	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
12:5:207:PHE:O	12:5:208:ASN:C	2.43	0.57
9:2:220:ILE:C	9:2:220:ILE:HD12	2.25	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	3.41	0.56
18:L:426:LYS:O	18:L:426:LYS:HG2	2.05	0.56
14:7:152:ASN:HB3	14:7:153:PRO:HD3	1.87	0.56
2:B:48:GLU:OE1	2:B:48:GLU:N	2.34	0.56
18:L:167:VAL:O	18:L:167:VAL:HG22	2.06	0.56
13:6:91:ARG:O	13:6:91:ARG:HG3	2.05	0.56
7:G:197:TYR:CD1	7:G:197:TYR:N	2.71	0.56
22:H:502:ATP:O1G	16:I:340:ARG:NH1	2.40	0.55
9:2:124:TYR:CG	9:2:138:LEU:HG	2.40	0.55
5:E:217:GLN:HA	5:E:217:GLN:OE1	3.48	0.55
19:M:81:ASN:C	19:M:81:ASN:OD1	2.44	0.55
17:K:274:VAL:HG23	17:K:274:VAL:O	2.07	0.55
2:B:1:MET:O	6:F:122:TYR:HB3	8.09	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:I:184:ILE:C	16:I:184:ILE:HD12	2.27	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
15:H:335:GLU:OE1	15:H:335:GLU:HA	2.08	0.54
18:L:256:ILE:HD11	19:M:256:ILE:HD12	1.89	0.54
2:B:186:GLU:N	2:B:186:GLU:OE2	4.11	0.54
8:1:144:GLU:N	8:1:144:GLU:OE1	2.35	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
18:L:361:PHE:CE1	18:L:391:ILE:HG23	2.44	0.53
2:B:13:SER:O	2:B:15:SER:N	2.79	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
20:J:34:ILE:O	20:J:34:ILE:HG22	2.08	0.52
18:L:207:PHE:N	18:L:207:PHE:CD1	2.77	0.52
18:L:236:ALA:O	18:L:243:PHE:CZ	2.62	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
12:5:193:VAL:CG1	12:5:193:VAL:O	2.58	0.52
2:B:35:LEU:C	2:B:35:LEU:HD12	2.30	0.52
3:C:237:ILE:O	3:C:237:ILE:CG2	4.30	0.52
19:M:182:ASP:O	19:M:363:ILE:HG21	2.09	0.52
18:L:188:GLU:OE1	18:L:188:GLU:HA	2.09	0.52
19:M:142:PRO:O	19:M:143:ASN:HB2	2.10	0.52
14:7:194:ASN:OD1	14:7:194:ASN:C	2.47	0.52
7:G:230:ASP:O	7:G:233:GLN:N	3.14	0.52
18:L:137:ARG:HB3	18:L:137:ARG:CZ	2.38	0.52
14:7:63:ILE:CG2	14:7:63:ILE:O	2.58	0.51
16:I:344:ILE:HD12	16:I:344:ILE:C	2.30	0.51
4:D:198:LEU:HD21	4:D:231:VAL:HG13	3.96	0.51
4:D:40:VAL:HG12	4:D:41:VAL:N	4.52	0.51
6:F:206:THR:OG1	6:F:209:ASN:HB2	2.09	0.51
6:F:233:ILE:CG2	6:F:233:ILE:OXT	2.59	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
10:3:10: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:J:103:ASN:C	20:J:103:ASN:OD1	2.49	0.51
19:M:352:PRO:HB3	19:M:356:SER:HB3	1.91	0.51
16:I:425:LYS:HB3	16:I:429:GLU:OE2	2.11	0.51
10:3:203:GLN:OE1	10:3:203:GLN:CA	2.55	0.51
7:G:214:TRP:O	7:G:214:TRP:CD1	2.63	0.51
3:C:64:LYS:O	3:C:65:LEU:HD12	5.51	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	4.96	0.50
2:B:182:GLU:HA	2:B:182:GLU:OE1	2.10	0.50
20:J:156:GLN:N	20:J:156:GLN:OE1	2.45	0.50
19:M:199:LEU:N	19:M:200:PRO:HD2	2.25	0.50
2:B:186:GLU:CA	2:B:186:GLU:OE2	3.54	0.50
7:G:56:VAL:HG23	7:G:59:LYS:HB2	1.94	0.50
20:J:97:ASP:C	20:J:97:ASP:OD1	2.46	0.50
5:E:13:LEU:O	5:E:14:PHE:C	2.49	0.50
16:I:247:ILE:HG22	16:I:248:VAL:O	2.11	0.50
16:I:339:ILE:HD12	16:I:339:ILE:O	2.11	0.50
7:G:214:TRP:N	7:G:214:TRP:CD1	2.78	0.49
6:F:28:ILE:HG13	6:F:29:LYS:N	4.74	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:N	1:A:183:ASP:OD1	4.34	0.49
14:7:177:ILE:O	14:7:178:VAL:C	2.48	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
18:L:383:SER:O	18:L:384:ASP:O	2.31	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	2.98	0.48
6:F:37:LEU:HD23	6:F:37:LEU:H	1.78	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
7:G:166:GLN:H	7:G:166:GLN:CD	3.76	0.48
16:I:300:ARG:HA	16:I:300:ARG:NE	2.28	0.48
5:E:128:ARG:H	5:E:129:PRO:HD3	1.77	0.48
5:E:83:HIS:CE1	5:E:111:LEU:HD21	5.13	0.48
16:I:160:LEU:HG	16:I:160:LEU:O	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
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
17:K:221:MET:CE	22:K:501:ATP:C6	2.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:2:18:THR:HB	9:2:31:CYS:H	1.78	0.48
14:7:131:ASN:OD1	14:7:131:ASN:O	2.32	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
12:5:52:CYS:O	12:5:53:GLN:C	2.51	0.48
2:B:172:LYS:O	2:B:176:GLU:OE1	2.30	0.48
4:D:230:TYR:O	4:D:234:ILE:HG13	2.70	0.48
16:I:378:GLU:N	16:I:378:GLU:OE1	2.35	0.48
12:5:200:VAL:HG12	12:5:200:VAL:O	2.13	0.48
2:B:139:HIS:CE1	2:B:140:ASP:O	2.89	0.48
18:L:283:VAL:O	18:L:283:VAL:HG22	2.14	0.48
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:HA	15:H:331:ARG:NE	2.29	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
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
2:B:4:ARG:NH2	5:E:117:GLU:CA	8.24	0.47
14:7:91:TYR:N	14:7:91:TYR:CD1	2.77	0.47
19:M:400:MET:O	19:M:403:LEU:N	2.47	0.47
1:A:182:ILE:HD12	1:A:184:HIS:O	3.63	0.47
4:D:172:PHE:O	4:D:176:ASN:ND2	2.47	0.47
4:D:68:HIS:CD2	4:D:68:HIS:H	2.33	0.47
4:D:109:ARG:HH12	12:5:70:GLU:HA	1.78	0.47
15:H:396:MET:HA	16:I:211:MET:O	2.14	0.47
19:M:230:LEU:HD13	19:M:230:LEU:C	2.36	0.47
20:J:253:ILE:HG22	20:J:258:VAL:HG23	1.96	0.47
19:M:352:PRO:HA	19:M:356:SER:CB	2.45	0.47
3:C:212:PHE:CD2	3:C:229:PHE:CD1	3.41	0.47
13:6:72:VAL:O	13:6:73:LYS:O	2.32	0.46
2:B:7:PHE:CD1	2:B:7:PHE:O	3.41	0.46
19:M:374:ILE:HD13	19:M:412:HIS:HB3	1.96	0.46
10:3:184:ALA:HB3	10:3:199:LEU:HB2	1.98	0.46
5:E:38:VAL:O	5:E:213:CYS:HB2	2.64	0.46
18:L:350:PRO:O	18:L:351:LEU:C	2.53	0.46
3:C:128:ARG:HD2	3:C:128:ARG:C	2.35	0.46
3:C:146:GLN:HE21	4:D:57:ILE:HG21	5.29	0.46
6:F:6:ASP:N	6:F:6:ASP:OD1	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:3:95:TYR:C	10:3:95:TYR:CD2	2.87	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
3:C:225:TYR:CD2	3:C:226:GLN:O	2.69	0.46
4:D:50:LEU:O	4:D:51:LYS:C	2.55	0.46
6:F:37:LEU:HD23	6:F:37:LEU:N	2.31	0.46
19:M:186:LEU:HD23	19:M:186:LEU:N	2.30	0.46
2:B:2:THR:HG21	5:E:117:GLU:HG3	8.71	0.46
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:64:LYS:O	3:C:75:ALA:HA	2.27	0.45
7:G:166:GLN:H	7:G:166:GLN:NE2	4.95	0.45
17:K:380:GLY:HA3	22:K:501:ATP:C8	2.52	0.45
6:F:105:GLU:HG2	6:F:109:HIS:CE1	2.51	0.45
15:H:382:LEU:O	15:H:382:LEU:HG	2.16	0.45
16:I:161:GLN:CD	16:I:161:GLN:N	2.70	0.45
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:O	3:C:217:LYS:HD3	5.18	0.45
6:F:45:LEU:HG	6:F:134:ILE:HD13	2.18	0.45
18:L:361:PHE:CD1	18:L:391:ILE:HG23	2.52	0.45
10:3:45:TYR:OH	10:3:63:ASN:OD1	2.34	0.45
6:F:199:SER:O	6:F:201:ARG:N	2.49	0.45
13:6:146:ILE:O	13:6:147:MET:C	2.49	0.44
3:C:182:ASP:O	3:C:183:MET:O	2.87	0.44
6:F:143:LEU:O	6:F:143:LEU:HG	3.18	0.44
19:M:349:PHE:N	19:M:349:PHE:CD1	2.85	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
11:4:138:PHE:N	11:4:138:PHE:CD1	2.85	0.44
3:C:58:GLN:N	3:C:58:GLN:OE1	2.36	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
19:M:289:LYS:HG2	19:M:335:PRO:HD3	1.99	0.44
4:D:229:GLN:OE1	4:D:229:GLN:N	2.50	0.44
4:D:41:VAL:HG22	4:D:212:VAL:HG22	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:71:LEU:C	6:F:71:LEU:HD12	2.38	0.44
20:J:220:GLN:HG3	20:J:224:GLY:H	1.81	0.44
10:3:74:LYS:O	10:3:78:GLU:HA	2.16	0.44
6:F:55:LEU:H	6:F:55:LEU:HD22	4.66	0.44
18:L:291:PHE:N	18:L:291:PHE:CD1	2.85	0.44
4:D:50:LEU:O	4:D:51:LYS:HD3	6.71	0.44
5:E:149:HIS:CD2	5:E:162:LYS:HE2	2.53	0.44
4:D:141:ASP:OD1	4:D:142:GLU:N	2.88	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
20:J:244:ILE:HG23	20:J:291:ILE:HG13	2.00	0.43
17:K:395:VAL:O	17:K:395:VAL:HG12	2.17	0.43
17:K:55:GLU:O	17:K:59:GLU:HG2	2.18	0.43
8:1:100:ALA:HB2	8:1:110:VAL:HG22	2.00	0.43
2:B:139:HIS:CE1	2:B:234:ARG:CZ	3.54	0.43
9:2:97:TYR:HB3	9:2:127:LEU:HD21	1.99	0.43
2:B:7:PHE:HD1	2:B:7:PHE:O	3.29	0.43
3:C:185:VAL:O	3:C:189:ILE:HG13	2.37	0.43
4:D:35:LYS:CG	4:D:35:LYS:O	3.56	0.43
19:M:415:PHE:O	19:M:419:ILE:HG13	2.18	0.43
3:C:139:TYR:CD1	3:C:139:TYR:C	3.67	0.43
3:C:95:GLN:HE22	3:C:98:LEU:HD23	3.48	0.43
7:G:44:PHE:N	7:G:44:PHE:CD1	3.14	0.43
7:G:56:VAL:H	7:G:56:VAL:HG22	1.60	0.43
12:5:157:GLY:O	12:5:158:LYS:C	2.56	0.43
2:B:42:GLY:HA2	2:B:145:PHE:CE2	2.83	0.43
3:C:167:ASN:HB2	3:C:170:ALA:HB3	2.00	0.43
3:C:182:ASP:O	3:C:183:MET:C	2.72	0.43
4:D:177:TYR:CD1	4:D:177:TYR:C	4.16	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
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
7:G:138:ASP:C	7:G:138:ASP:OD1	2.57	0.43
17:K:221:MET:HE1	22:K:501:ATP:C5	2.54	0.43
19:M:375:ASN:OD1	19:M:375:ASN:C	2.57	0.43
19:M:374:ILE:HD13	19:M:412:HIS:CB	2.49	0.43
1:A:175:ASN:N	1:A:175:ASN:OD1	4.41	0.43
6:F:53:ASP:C	6:F:53:ASP:OD1	2.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:186:GLU:OE2	2:B:186:GLU:HA	2.89	0.43
3:C:212:PHE:CD2	3:C:229:PHE:CE1	3.96	0.43
7:G:176:VAL:O	7:G:176:VAL:HG12	2.19	0.43
10:3:143:ASP:N	10:3:143:ASP:OD1	2.52	0.42
11:4:138:PHE:HD1	11:4:138:PHE:N	2.17	0.42
20:J:197:LEU:HD12	23:J:501:ADP:C8	2.54	0.42
19:M:374:ILE:CD1	19:M:412:HIS:HA	2.49	0.42
19:M:374:ILE:HD13	19:M:412:HIS:CA	2.48	0.42
19:M:428:LYS:HE2	19:M:429:SER:HB3	2.00	0.42
8:1:8:PHE:CE1	8:1:10:ASP:HB2	2.55	0.42
12:5:137:TYR:HD1	12:5:137:TYR:HA	1.66	0.42
13:6:52:MET:HE3	13:6:65:VAL:HG22	2.01	0.42
3:C:145:TYR:OH	3:C:217:LYS:HB3	4.47	0.42
17:K:158:ILE:HG12	17:K:159:SER:O	2.19	0.42
18:L:351:LEU:O	18:L:352:PRO:C	2.56	0.42
4:D:35:LYS:HE2	4:D:158:SER:HA	2.52	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
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
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
9:2:182:LYS:O	9:2:183:ASP:C	2.54	0.42
1:A:21:TYR:CD1	7:G:13:PRO:HA	2.90	0.42
6:F:113:ASP:CG	7:G:86:ASN:HD21	2.22	0.42
15:H:88:ARG:NE	15:H:88:ARG:HA	2.35	0.42
16:I:194:ILE:CG2	16:I:236:VAL:HG11	2.50	0.42
20:J:179:ILE:HG23	20:J:179:ILE:O	2.19	0.42
19:M:154:LEU:HA	19:M:154:LEU:HD13	1.95	0.42
19:M:365:SER:CB	19:M:376:TRP:CH2	3.02	0.42
4:D:125:ARG:O	4:D:125:ARG:HG3	2.54	0.42
17:K:51:LEU:HA	17:K:51:LEU:HD23	1.32	0.42
9:2:99:ILE:HD11	9:2:127:LEU:HD22	2.02	0.42
2:B:119:GLN:O	2:B:122:THR:HG22	4.72	0.42
5:E:51:LEU:HD23	5:E:51:LEU:C	2.39	0.42
7:G:56:VAL:HG22	7:G:60:ASN:HD21	1.85	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
14:7:146:PHE:CG	14:7:146:PHE:O	2.72	0.42
14:7:193:ARG:O	14:7:213:GLN:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:224:HIS:O	7:G:225:LYS:HG3	3.08	0.42
15:H:191:ILE:HG13	15:H:191:ILE:O	2.20	0.42
17:K:146:LEU:C	17:K:146:LEU:HD23	2.40	0.42
17:K:221:MET:HE3	22:K:501:ATP:C6	2.54	0.42
18:L:384:ASP:OD1	18:L:384:ASP:C	2.56	0.42
18:L:392:ARG:HG3	18:L:392:ARG:O	2.20	0.41
12:5:140:LEU:O	12:5:144:TYR:HB2	2.20	0.41
2:B:250:LEU:OXT	2:B:250:LEU:CD1	4.69	0.41
3:C:139:TYR:CD1	3:C:139:TYR:O	4.61	0.41
3:C:43:ILE:HD11	3:C:145:TYR:HB3	2.39	0.41
4:D:40:VAL:HG12	4:D:41:VAL:H	4.21	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
9:2:138:LEU:C	9:2:138:LEU:HD22	2.37	0.41
13:6:194:ARG:HD3	13:6:194:ARG:HA	1.87	0.41
1:A:105:CYS:HB2	1:A:136:SER:OG	3.60	0.41
1:A:241:GLU:C	1:A:242:GLN:O	3.54	0.41
2:B:37:ILE:O	2:B:43:VAL:CG1	3.51	0.41
2:B:38:LYS:HA	2:B:43:VAL:HG13	2.77	0.41
3:C:149:THR:HG22	3:C:159:TRP:HE1	4.29	0.41
16:I:338:LEU:O	16:I:344:ILE:HG12	2.20	0.41
13:6:12:ILE:HD13	13:6:110:ILE:HG21	2.03	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
12:5:34:VAL:HG21	12:5:178:TYR:CE1	2.56	0.41
7:G:214:TRP:H	7:G:214:TRP:HD1	1.67	0.41
10:3:163:PHE:CZ	10:3:197:ARG:HD3	2.56	0.41
11:4:49:GLU:O	11:4:50:ALA:C	2.59	0.41
1:A:18:GLN:HA	1:A:21:TYR:CD2	3.46	0.41
4:D:27:ARG:HB3	4:D:27:ARG:NH1	5.01	0.41
5:E:114:ARG:HB2	5:E:126:MET:SD	4.47	0.41
17:K:356:ILE:CG2	17:K:387:MET:HG3	2.51	0.41
17:K:43:VAL:O	17:K:47:ILE:HG13	2.20	0.41
18:L:401:PHE:CE2	18:L:417:LYS:HB3	2.56	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
3:C:123:GLN:HB3	3:C:124:HIS:CE1	3.48	0.41
16:I:148:LEU:HD23	16:I:148:LEU:HA	1.86	0.41
17:K:426:PHE:CD1	17:K:426:PHE:N	2.89	0.41
19:M:40:GLU:C	19:M:40:GLU:OE2	5.06	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:217:GLN:CA	5:E:217:GLN:OE1	2.95	0.41
6:F:178:PHE:C	6:F:178:PHE:CD1	3.24	0.41
6:F:122:TYR:HB2	7:G:124:SER:O	2.31	0.41
7:G:212:ILE:CG1	7:G:227:VAL:HB	2.50	0.41
16:I:96:LEU:HD23	16:I:135:PHE:CG	2.56	0.41
16:I:316:PHE:CD1	16:I:316:PHE:O	2.73	0.41
17:K:395:VAL:O	17:K:395:VAL:CG1	2.69	0.41
10:3:52:ILE:CG2	10:3:59:VAL:HG13	2.51	0.41
2:B:140:ASP:OD1	2:B:140:ASP:C	2.59	0.41
6:F:206:THR:O	6:F:233:ILE:HD11	5.84	0.41
17:K:51:LEU:HD12	20:J:27:ILE:HD12	2.03	0.41
9:2:5:GLY:O	9:2:124:TYR:CD1	2.74	0.41
4:D:65:ILE:HG21	4:D:107:LEU:HD21	2.03	0.41
7:G:105:ILE:HB	7:G:106:PRO:HD3	2.36	0.41
7:G:243:ILE:O	7:G:243:ILE:CG1	2.68	0.41
22:H:502:ATP:PB	16:I:340:ARG:HH12	2.42	0.41
10:3:158:GLU:O	10:3:161:ASP:N	2.54	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:HA	20:J:217:GLU:OE1	2.20	0.41
1:A:235:ARG:O	1:A:239:ILE:HG13	3.00	0.40
4:D:45:GLU:CG	4:D:45:GLU:O	2.64	0.40
6:F:38:ARG:HD3	6:F:39:SER:O	4.83	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
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:HG23	19:M:127:VAL:O	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	2.80	0.40
7:G:200:HIS:CG	7:G:200:HIS:O	2.74	0.40
17:K:383:ILE:O	17:K:383:ILE:HG22	2.20	0.40
2:B:13:SER:O	2:B:14:PRO:C	3.00	0.40
15:H:43:ALA:HB3	15:H:44:PRO:HD3	2.03	0.40
10:3:148:MET:O	10:3:149:CYS:C	2.59	0.40
4:D:27:ARG:HB3	4:D:27:ARG:HH11	4.76	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%)	38	77
1	a	239/252 (95%)	221 (92%)	17 (7%)	1 (0%)	38	77
2	B	248/250 (99%)	232 (94%)	14 (6%)	2 (1%)	22	66
2	b	248/250 (99%)	223 (90%)	24 (10%)	1 (0%)	38	77
3	C	242/258 (94%)	225 (93%)	14 (6%)	3 (1%)	15	58
3	c	242/258 (94%)	217 (90%)	21 (9%)	4 (2%)	11	52
4	D	238/254 (94%)	215 (90%)	17 (7%)	6 (2%)	6	43
4	d	238/254 (94%)	221 (93%)	15 (6%)	2 (1%)	22	66
5	E	240/260 (92%)	223 (93%)	9 (4%)	8 (3%)	4	37
5	e	240/260 (92%)	222 (92%)	14 (6%)	4 (2%)	11	52
6	F	231/234 (99%)	211 (91%)	15 (6%)	5 (2%)	8	46
6	f	229/234 (98%)	207 (90%)	21 (9%)	1 (0%)	38	77
7	G	241/288 (84%)	223 (92%)	17 (7%)	1 (0%)	38	77
7	g	241/288 (84%)	221 (92%)	17 (7%)	3 (1%)	15	58
8	1	194/215 (90%)	186 (96%)	8 (4%)	0	100	100
8	h	194/215 (90%)	176 (91%)	17 (9%)	1 (0%)	32	74
9	2	224/261 (86%)	204 (91%)	18 (8%)	2 (1%)	20	63
9	i	224/261 (86%)	200 (89%)	17 (8%)	7 (3%)	5	39
10	3	202/205 (98%)	187 (93%)	12 (6%)	3 (2%)	12	54
10	j	202/205 (98%)	174 (86%)	23 (11%)	5 (2%)	6	43
11	4	193/198 (98%)	175 (91%)	13 (7%)	5 (3%)	6	42
11	k	193/198 (98%)	169 (88%)	19 (10%)	5 (3%)	6	42
12	5	210/287 (73%)	194 (92%)	14 (7%)	2 (1%)	18	61
12	l	210/287 (73%)	193 (92%)	17 (8%)	0	100	100
13	6	220/241 (91%)	193 (88%)	23 (10%)	4 (2%)	10	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	m	220/241 (91%)	196 (89%)	18 (8%)	6 (3%)	6	42
14	7	227/266 (85%)	202 (89%)	19 (8%)	6 (3%)	6	42
14	n	230/266 (86%)	205 (89%)	21 (9%)	4 (2%)	11	52
15	H	386/467 (83%)	333 (86%)	33 (8%)	20 (5%)	2	27
16	I	383/437 (88%)	345 (90%)	32 (8%)	6 (2%)	11	53
17	K	387/428 (90%)	350 (90%)	28 (7%)	9 (2%)	7	45
18	L	386/437 (88%)	343 (89%)	36 (9%)	7 (2%)	10	50
19	M	377/434 (87%)	339 (90%)	27 (7%)	11 (3%)	5	40
20	J	384/405 (95%)	347 (90%)	30 (8%)	7 (2%)	10	50
All	All	8602/9546 (90%)	7790 (91%)	660 (8%)	152 (2%)	14	50

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	70	86
1	a	206/210 (98%)	197 (96%)	9 (4%)	33	65
2	B	209/209 (100%)	205 (98%)	4 (2%)	62	82
2	b	209/209 (100%)	203 (97%)	6 (3%)	48	73
3	C	203/216 (94%)	202 (100%)	1 (0%)	91	95
3	c	203/216 (94%)	195 (96%)	8 (4%)	37	67
4	D	212/226 (94%)	206 (97%)	6 (3%)	49	74
4	d	212/226 (94%)	209 (99%)	3 (1%)	71	86
5	E	198/215 (92%)	193 (98%)	5 (2%)	53	77
5	e	198/215 (92%)	191 (96%)	7 (4%)	41	70
6	F	192/193 (100%)	190 (99%)	2 (1%)	80	90
6	f	190/193 (98%)	179 (94%)	11 (6%)	23	57
7	G	201/239 (84%)	198 (98%)	3 (2%)	70	86
7	g	201/239 (84%)	192 (96%)	9 (4%)	32	64
8	1	162/178 (91%)	161 (99%)	1 (1%)	89	94
8	h	162/178 (91%)	159 (98%)	3 (2%)	62	82
9	2	185/214 (86%)	184 (100%)	1 (0%)	91	95
9	i	185/214 (86%)	182 (98%)	3 (2%)	68	85
10	3	172/173 (99%)	171 (99%)	1 (1%)	89	94
10	j	172/173 (99%)	168 (98%)	4 (2%)	56	79
11	4	173/175 (99%)	171 (99%)	2 (1%)	75	88
11	k	173/175 (99%)	168 (97%)	5 (3%)	48	73
12	5	169/235 (72%)	167 (99%)	2 (1%)	75	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	l	169/235 (72%)	159 (94%)	10 (6%)	23	57
13	6	185/201 (92%)	184 (100%)	1 (0%)	91	95
13	m	185/201 (92%)	181 (98%)	4 (2%)	57	79
14	7	195/224 (87%)	192 (98%)	3 (2%)	70	86
14	n	198/224 (88%)	191 (96%)	7 (4%)	41	70
15	H	330/399 (83%)	326 (99%)	4 (1%)	75	88
16	I	342/385 (89%)	333 (97%)	9 (3%)	51	76
17	K	342/374 (91%)	338 (99%)	4 (1%)	75	88
18	L	332/377 (88%)	328 (99%)	4 (1%)	75	88
19	M	329/375 (88%)	322 (98%)	7 (2%)	59	80
20	J	336/352 (96%)	330 (98%)	6 (2%)	64	84
All	All	7336/8078 (91%)	7178 (98%)	158 (2%)	60	79

All (158) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	36	VAL
1	a	138	ASP
1	a	144	SER
1	a	162	THR
1	a	175	ASN
1	a	183	ASP
1	a	200	HIS
1	a	201	MET
1	a	235	ARG
2	b	57	MET
2	b	70	ASP
2	b	85	LEU
2	b	133	SER
2	b	220	ASP
2	b	245	ASP
3	c	41	ASP
3	c	110	LEU
3	c	119	GLN
3	c	124	HIS
3	c	155	ASN
3	c	177	MET
3	c	190	GLU

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Mol	Chain	Res	Type
3	c	206	THR
4	d	44	CYS
4	d	100	ASP
4	d	225	GLU
5	e	54	ASP
5	e	126	MET
5	e	169	GLU
5	e	177	ASN
5	e	180	HIS
5	e	206	GLU
5	e	213	CYS
6	f	10	VAL
6	f	12	PHE
6	f	53	ASP
6	f	65	CYS
6	f	71	LEU
6	f	73	LEU
6	f	87	LEU
6	f	116	GLN
6	f	143	LEU
6	f	188	LEU
6	f	202	ASP
7	g	5	ASP
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
7	g	214	TRP
8	h	30	VAL
8	h	72	THR
8	h	148	LYS
9	i	61	SER
9	i	183	ASP
9	i	214	LYS
10	j	143	ASP
10	j	146	PHE
10	j	148	MET
10	j	151	SER
11	k	52	ASP

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Mol	Chain	Res	Type
11	k	53	THR
11	k	126	VAL
11	k	175	ASP
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
12	l	104	TYR
12	l	137	TYR
12	l	199	LYS
13	m	40	GLU
13	m	101	ARG
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	162	GLU
14	n	184	LEU
14	n	208	PHE
1	A	124	TYR
1	A	207	THR
1	A	208	GLU
2	B	11	THR
2	B	128	ARG
2	B	151	ASP
2	B	217	GLU
3	C	168	THR
4	D	71	LEU
4	D	79	ASP
4	D	181	GLU
4	D	187	GLU
4	D	225	GLU
4	D	229	GLN
5	E	105	THR
5	E	115	PHE
5	E	128	ARG

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Mol	Chain	Res	Type
5	E	129	PRO
5	E	132	VAL
6	F	46	VAL
6	F	176	ASP
7	G	149	PRO
7	G	181	GLU
7	G	214	TRP
8	1	153	ASP
9	2	212	VAL
10	3	146	PHE
11	4	87	GLU
11	4	166	GLN
12	5	104	TYR
12	5	182	GLU
13	6	150	LEU
14	7	30	TYR
14	7	161	ARG
14	7	208	PHE
15	H	271	PHE
15	H	319	PHE
15	H	367	ARG
15	H	392	HIS
16	I	111	GLU
16	I	230	THR
16	I	256	TYR
16	I	293	ASP
16	I	305	THR
16	I	314	ASP
16	I	328	THR
16	I	410	GLN
16	I	428	VAL
17	K	264	ASN
17	K	337	LYS
17	K	369	ASP
17	K	425	ASP
18	L	67	HIS
18	L	107	GLU
18	L	313	ASP
18	L	427	LYS
19	M	161	SER
19	M	162	GLU
19	M	186	LEU

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Mol	Chain	Res	Type
19	M	359	GLN
19	M	392	LYS
19	M	428	LYS
19	M	433	TYR
20	J	110	SER
20	J	137	MET
20	J	225	GLU
20	J	305	LEU
20	J	306	ARG
20	J	370	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	176	HIS
3	c	95	GLN
3	c	146	GLN
4	d	94	HIS
8	h	38	HIS
10	j	47	HIS
10	j	88	GLN
10	j	112	ASN
11	k	133	HIS
12	l	66	HIS
14	n	102	GLN
14	n	120	GLN
14	n	211	ASN
14	n	231	GLN
2	B	123	GLN
3	C	96	ASN
3	C	226	GLN
4	D	176	ASN
5	E	149	HIS
6	F	109	HIS
6	F	116	GLN
7	G	86	ASN
11	4	99	GLN
12	5	166	HIS
15	H	98	GLN
15	H	392	HIS
16	I	295	ASN
16	I	352	ASN

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Mol	Chain	Res	Type
17	K	238	ASN
20	J	66	GLN
20	J	331	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	ATP	H	502	21	27,33,33	1.26	3 (11%)	25,52,52	3.68	9 (36%)
22	ATP	I	501	21	27,33,33	1.65	6 (22%)	25,52,52	2.86	8 (32%)
23	ADP	J	501	21	25,29,29	1.80	4 (16%)	24,45,45	3.37	6 (25%)
22	ATP	K	501	21	27,33,33	1.54	5 (18%)	25,52,52	3.21	6 (24%)
22	ATP	L	501	21	27,33,33	1.34	3 (11%)	25,52,52	2.67	8 (32%)
22	ATP	M	501	21	27,33,33	1.05	1 (3%)	25,52,52	3.14	8 (32%)

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	H	502	21	-	0/18/38/38	0/3/3/3
22	ATP	I	501	21	-	0/18/38/38	0/3/3/3
23	ADP	J	501	21	-	0/12/32/32	0/3/3/3
22	ATP	K	501	21	-	0/18/38/38	0/3/3/3
22	ATP	L	501	21	-	0/18/38/38	0/3/3/3
22	ATP	M	501	21	-	0/18/38/38	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	H	502	ATP	C2-N3	2.06	1.35	1.32
23	J	501	ADP	C5-C4	2.10	1.45	1.40
22	H	502	ATP	C4-N3	2.18	1.38	1.35
22	K	501	ATP	C5-C4	2.31	1.45	1.40
23	J	501	ADP	C4-N3	2.44	1.39	1.35
22	I	501	ATP	C2-N1	2.47	1.38	1.33
22	I	501	ATP	C4-N3	2.52	1.39	1.35
22	K	501	ATP	O4'-C1'	2.57	1.44	1.41
22	I	501	ATP	O4'-C1'	2.72	1.45	1.41
22	L	501	ATP	C2-N3	2.80	1.36	1.32
23	J	501	ADP	C2-N3	2.80	1.36	1.32
22	L	501	ATP	O4'-C1'	2.83	1.45	1.41
22	M	501	ATP	PG-O3B	2.92	1.64	1.60
22	K	501	ATP	C4-N3	2.95	1.39	1.35
22	I	501	ATP	C5-C4	3.03	1.47	1.40
22	K	501	ATP	C2-N3	3.22	1.37	1.32
22	I	501	ATP	C2-N3	3.53	1.38	1.32
22	L	501	ATP	PG-O3B	3.86	1.66	1.60
22	K	501	ATP	PG-O3B	4.00	1.66	1.60
22	H	502	ATP	PG-O3B	4.18	1.66	1.60
22	I	501	ATP	PG-O3B	4.32	1.67	1.60
23	J	501	ADP	PB-O3A	6.43	1.70	1.60

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	H	502	ATP	N3-C2-N1	-15.89	115.02	128.86
23	J	501	ADP	N3-C2-N1	-15.17	115.64	128.86
22	K	501	ATP	N3-C2-N1	-14.39	116.32	128.86
22	M	501	ATP	N3-C2-N1	-13.52	117.09	128.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	L	501	ATP	N3-C2-N1	-10.78	119.47	128.86
22	I	501	ATP	N3-C2-N1	-10.77	119.48	128.86
22	H	502	ATP	C5-C6-N6	-4.31	111.69	120.47
22	I	501	ATP	C4-C5-N7	-3.88	105.66	109.41
22	M	501	ATP	C1'-N9-C4	-3.28	120.96	126.64
22	H	502	ATP	C1'-N9-C4	-3.14	121.20	126.64
22	K	501	ATP	C5-C6-N6	-2.96	114.43	120.47
22	M	501	ATP	C4'-O4'-C1'	-2.95	106.63	109.77
23	J	501	ADP	C1'-N9-C4	-2.74	121.89	126.64
22	L	501	ATP	C5-C6-N6	-2.74	114.88	120.47
23	J	501	ADP	C5-C6-N6	-2.71	114.94	120.47
22	L	501	ATP	O2'-C2'-C1'	-2.52	103.72	111.61
22	I	501	ATP	O5'-C5'-C4'	-2.51	100.11	109.00
22	H	502	ATP	O5'-PA-O1A	-2.45	99.37	109.25
22	L	501	ATP	O5'-PA-O1A	-2.42	99.49	109.25
22	L	501	ATP	O3B-PG-O1G	-2.23	97.74	111.44
22	M	501	ATP	O5'-PA-O1A	-2.18	100.47	109.25
22	L	501	ATP	O4'-C4'-C3'	-2.11	100.97	105.17
22	M	501	ATP	O2'-C2'-C1'	-2.11	105.02	111.61
22	M	501	ATP	O3G-PG-O2G	2.05	115.88	107.61
22	M	501	ATP	O2A-PA-O1A	2.05	122.89	112.28
22	H	502	ATP	O5'-C5'-C4'	2.08	116.38	109.00
22	K	501	ATP	N6-C6-N1	2.08	122.90	118.77
22	H	502	ATP	C5-C6-N1	2.10	126.06	119.70
23	J	501	ADP	N6-C6-N1	2.14	123.02	118.77
22	L	501	ATP	O2G-PG-O1G	2.17	118.99	110.50
22	H	502	ATP	O2A-PA-O1A	2.21	123.72	112.28
22	I	501	ATP	O4'-C4'-C5'	2.21	116.88	109.40
23	J	501	ADP	O5'-C5'-C4'	2.24	116.95	109.00
22	K	501	ATP	C4'-O4'-C1'	2.41	112.33	109.77
22	L	501	ATP	O3'-C3'-C2'	2.44	119.65	111.83
22	K	501	ATP	O4'-C4'-C5'	2.60	118.19	109.40
22	I	501	ATP	N6-C6-N1	2.69	124.09	118.77
22	K	501	ATP	O5'-C5'-C4'	2.72	118.63	109.00
23	J	501	ADP	C2-N1-C6	2.73	123.54	118.77
22	I	501	ATP	O2'-C2'-C3'	2.91	121.16	111.83
22	H	502	ATP	C4'-O4'-C1'	2.93	112.89	109.77
22	I	501	ATP	C2-N1-C6	2.94	123.92	118.77
22	H	502	ATP	O2G-PG-O1G	3.56	124.42	110.50
22	I	501	ATP	O3'-C3'-C2'	3.78	123.93	111.83
22	M	501	ATP	C2-N1-C6	3.88	125.57	118.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 27 short contacts:

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

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.