



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 01:56 PM UTC

PDB ID : 5FMG / pdb_00005fmg
EMDB ID : EMD-3231
Title : Structure and function based design of Plasmodium-selective proteasome inhibitors
Authors : Li, H.; O'Donoghue, A.J.; van der Linden, W.A.; Xie, S.C.; Yoo, E.; Foe, I.T.; Tilley, L.; Craik, C.S.; da Fonseca, P.C.A.; Bogyo, M.
Deposited on : 2015-11-04
Resolution : 3.60 Å (reported)
Based on initial model : 1IRU

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

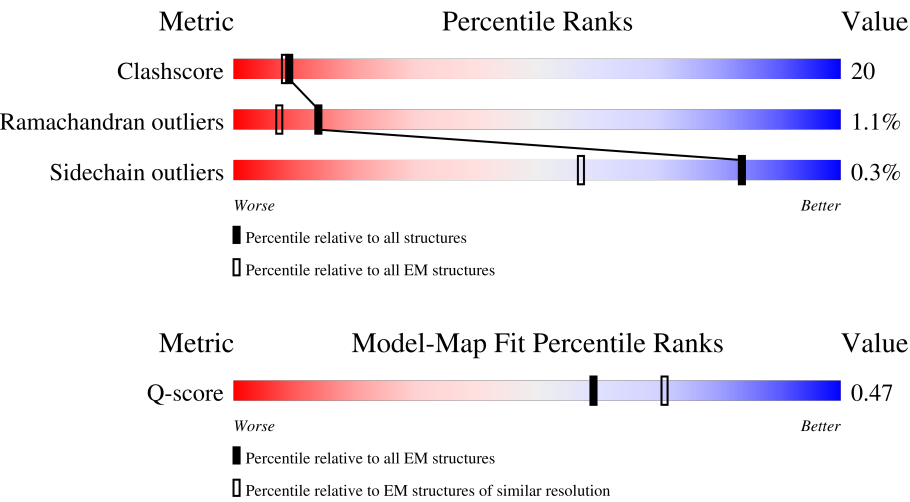
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



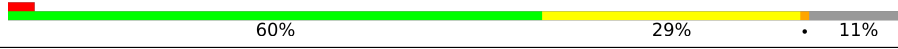
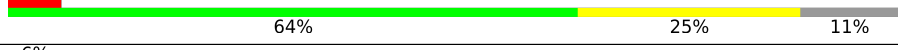
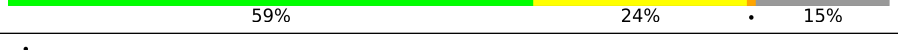
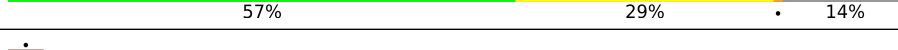
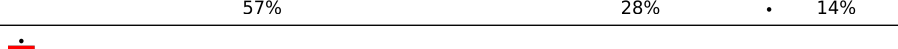
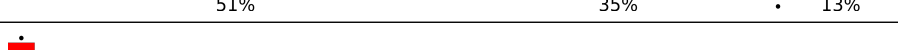
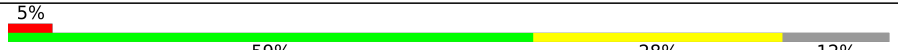
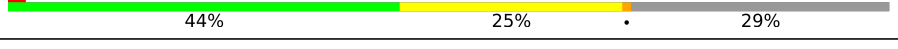
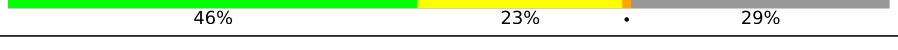
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12797 (3.10 - 4.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	260	61%23%16%
1	O	260	60%23%16%
2	B	235	5% 64%25%10%

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Mol	Chain	Length	Quality of chain
2	P	235	
3	C	246	
3	Q	246	
4	D	241	
4	R	241	
5	E	256	
5	S	256	
6	F	254	
6	T	254	
7	G	252	
7	U	252	
8	H	252	
8	V	252	
9	I	229	
9	W	229	
10	J	218	
10	X	218	
11	K	195	
11	Y	195	
12	L	211	
12	Z	211	
13	M	240	
13	a	240	
14	N	265	
14	b	265	

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 39334 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, PUTATIVE.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	219	Total	C	N	O	S	0	0
			1440	907	251	274	8		
1	O	219	Total	C	N	O	S	0	0
			1440	907	251	274	8		

- Molecule 2 is a protein called PROTEASOME SUBUNIT ALPHA TYPE 2, PUTATIVE.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	212	Total	C	N	O	S	0	0
			1381	895	232	250	4		
2	P	212	Total	C	N	O	S	0	0
			1381	895	232	250	4		

- Molecule 3 is a protein called PROTEASOME SUBUNIT ALPHA TYPE.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	220	Total	C	N	O	S	0	0
			1527	984	251	289	3		
3	Q	220	Total	C	N	O	S	0	0
			1527	984	251	289	3		

- Molecule 4 is a protein called PROTEASOME SUBUNIT ALPHA TYPE.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	215	Total	C	N	O	S	0	0
			1409	904	241	259	5		
4	R	215	Total	C	N	O	S	0	0
			1409	904	241	259	5		

- Molecule 5 is a protein called PROTEASOME SUBUNIT ALPHA TYPE.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	217	Total	C	N	O	S	0	0
			1440	914	241	277	8		
5	S	217	Total	C	N	O	S	0	0
			1440	914	241	277	8		

- Molecule 6 is a protein called PROTEOSOME SUBUNIT ALPHA TYPE 1, PUTATIVE.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	219	Total	C	N	O	S	0	0
			1492	956	244	287	5		
6	T	219	Total	C	N	O	S	0	0
			1492	956	244	287	5		

- Molecule 7 is a protein called PROTEASOME COMPONENT C8, PUTATIVE.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	219	Total	C	N	O	S	0	0
			1542	988	265	281	8		
7	U	219	Total	C	N	O	S	0	0
			1542	988	265	281	8		

- Molecule 8 is a protein called PROTEASOME, PUTATIVE.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	191	Total	C	N	O	S	0	0
			1316	832	224	253	7		
8	V	191	Total	C	N	O	S	0	0
			1316	832	224	253	7		

- Molecule 9 is a protein called PROTEASOME SUBUNIT BETA TYPE.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	186	Total	C	N	O	S	0	0
			1241	774	218	236	13		
9	W	186	Total	C	N	O	S	0	0
			1241	774	218	236	13		

- Molecule 10 is a protein called BETA3 PROTEASOME SUBUNIT, PUTATIVE.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	191	Total	C	N	O	S	0	0
			1273	803	215	243	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	191	Total	C	N	O	S	0	0
			1273	803	215	243	12		

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	1	MET	-	initiating methionine	UNP Q8I261
J	2	GLY	-	expression tag	UNP Q8I261
J	3	SER	-	expression tag	UNP Q8I261
J	4	ILE	-	expression tag	UNP Q8I261
J	5	TYR	-	expression tag	UNP Q8I261
J	6	ASN	-	expression tag	UNP Q8I261
J	7	TYR	-	expression tag	UNP Q8I261
J	8	ASN	-	expression tag	UNP Q8I261
J	9	GLY	-	expression tag	UNP Q8I261
J	10	GLY	-	expression tag	UNP Q8I261
J	11	CYS	-	expression tag	UNP Q8I261
J	12	VAL	-	expression tag	UNP Q8I261
J	13	LEU	-	expression tag	UNP Q8I261
J	14	GLY	-	expression tag	UNP Q8I261
X	1	MET	-	initiating methionine	UNP Q8I261
X	2	GLY	-	expression tag	UNP Q8I261
X	3	SER	-	expression tag	UNP Q8I261
X	4	ILE	-	expression tag	UNP Q8I261
X	5	TYR	-	expression tag	UNP Q8I261
X	6	ASN	-	expression tag	UNP Q8I261
X	7	TYR	-	expression tag	UNP Q8I261
X	8	ASN	-	expression tag	UNP Q8I261
X	9	GLY	-	expression tag	UNP Q8I261
X	10	GLY	-	expression tag	UNP Q8I261
X	11	CYS	-	expression tag	UNP Q8I261
X	12	VAL	-	expression tag	UNP Q8I261
X	13	LEU	-	expression tag	UNP Q8I261
X	14	GLY	-	expression tag	UNP Q8I261

- Molecule 11 is a protein called PROTEASOME SUBUNIT BETA TYPE.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	194	Total	C	N	O	S	0	0
			1452	932	240	273	7		
11	Y	194	Total	C	N	O	S	0	0
			1452	932	240	273	7		

- Molecule 12 is a protein called PROTEASOME SUBUNIT BETA TYPE.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	189	Total	C	N	O	S	0	0
			1355	870	223	256	6		
12	Z	189	Total	C	N	O	S	0	0
			1355	870	223	256	6		

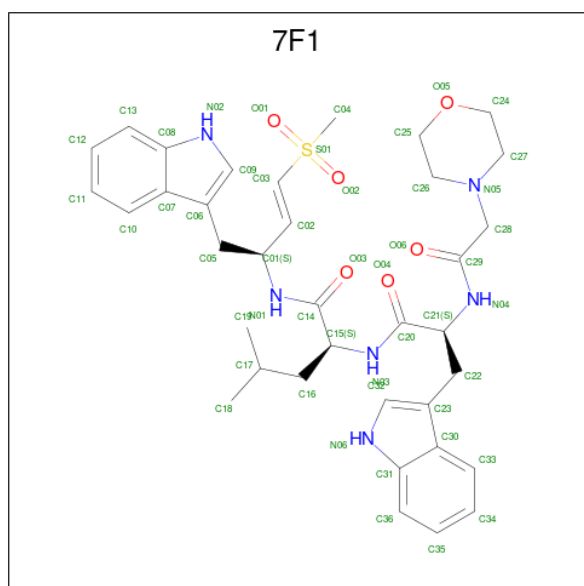
- Molecule 13 is a protein called PROTEASOME SUBUNIT BETA TYPE.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	199	Total	C	N	O	S	0	0
			1413	908	236	263	6		
13	a	199	Total	C	N	O	S	0	0
			1413	908	236	263	6		

- Molecule 14 is a protein called PROTEASOME SUBUNIT BETA TYPE.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	187	Total	C	N	O	S	0	0
			1337	852	233	249	3		
14	b	187	Total	C	N	O	S	0	0
			1337	852	233	249	3		

- Molecule 15 is (2S)-N-[(E,2S)-1-(1H-indol-3-yl)-4-methylsulfonyl-but-3-en-2-yl]-2-[[[(2S)-3-(1H-indol-3-yl)-2-(2-morpholin-4-ylethanoylamino)propanoyl]amino]-4-methyl-pentanamide (CCD ID: 7F1) (formula: C₃₆H₄₆N₆O₆S).

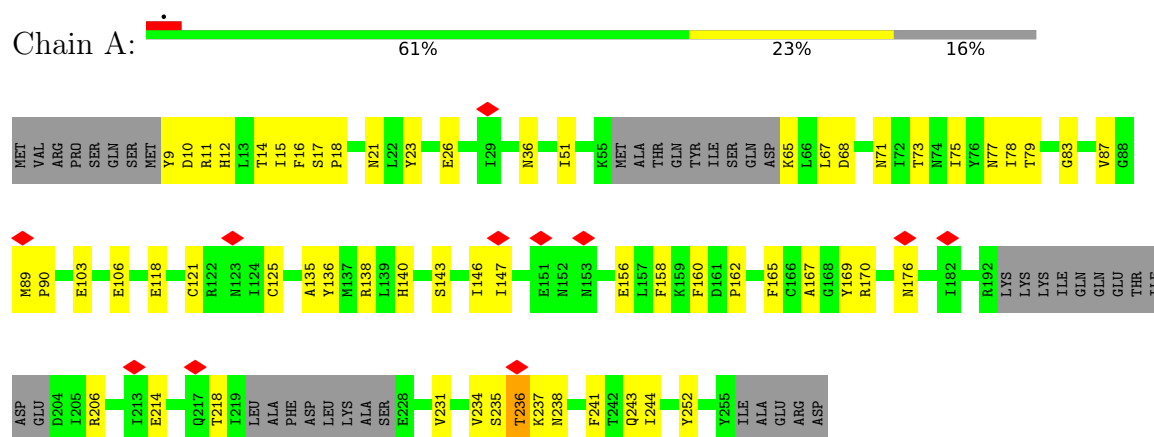


Mol	Chain	Residues	Atoms					AltConf
15	I	1	Total 49	C 36	N 6	O 6	S 1	0
15	W	1	Total 49	C 36	N 6	O 6	S 1	0

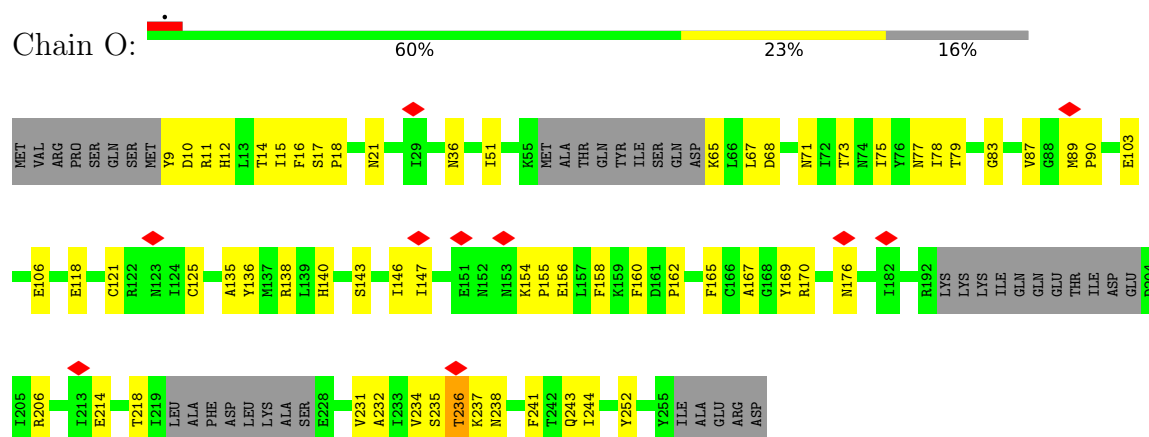
3 Residue-property plots

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

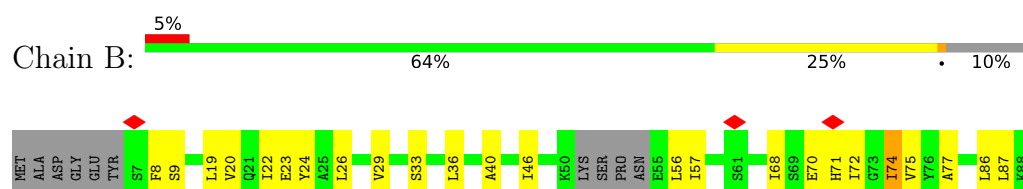
- Molecule 1: PROTEASOME SUBUNIT ALPHA, PUTATIVE

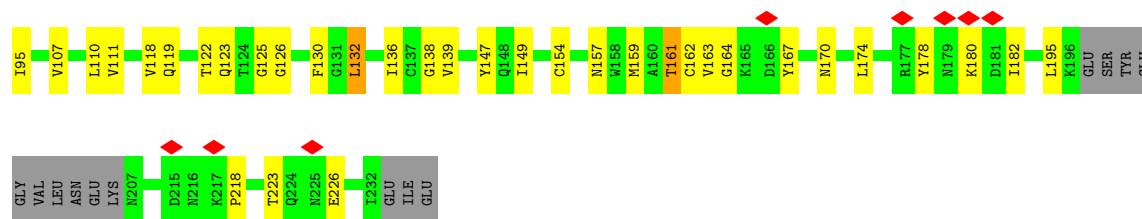


- Molecule 1: PROTEASOME SUBUNIT ALPHA, PUTATIVE



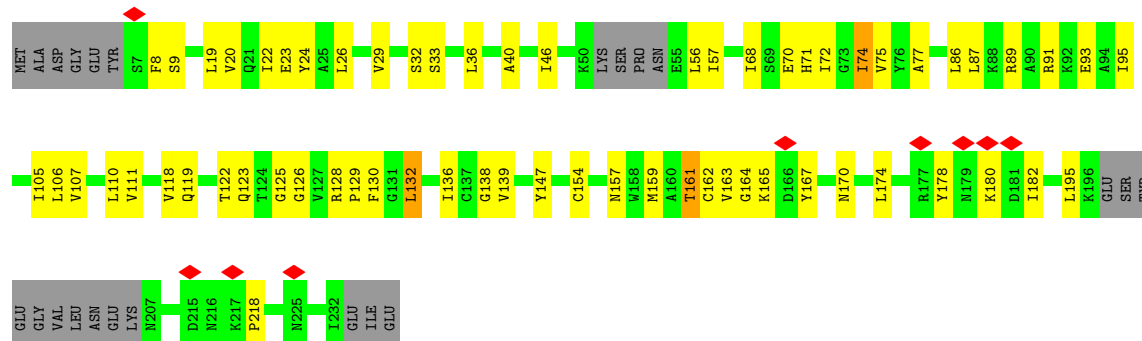
- Molecule 2: PROTEASOME SUBUNIT ALPHA TYPE 2, PUTATIVE





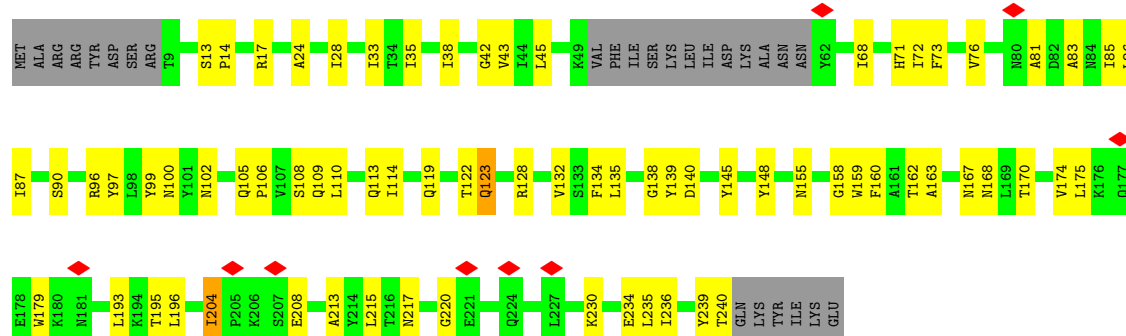
• Molecule 2: PROTEASOME SUBUNIT ALPHA TYPE 2, PUTATIVE

Chain P: 63% 26% 10%



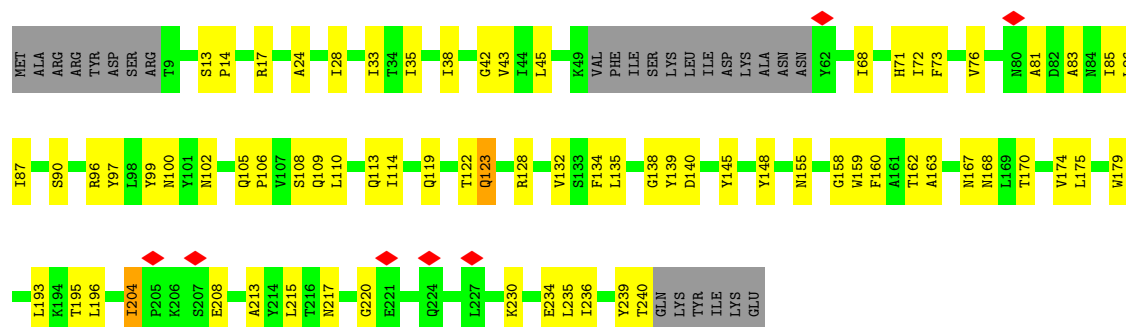
• Molecule 3: PROTEASOME SUBUNIT ALPHA TYPE

Chain C: 60% 29% 11%

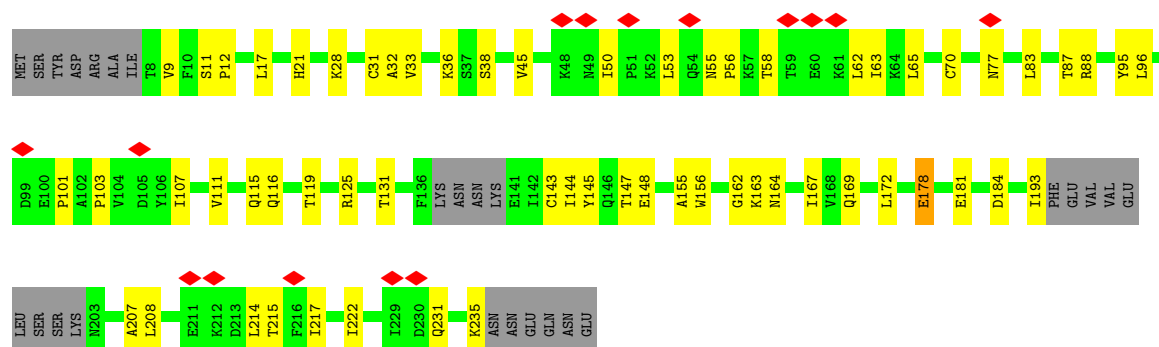


• Molecule 3: PROTEASOME SUBUNIT ALPHA TYPE

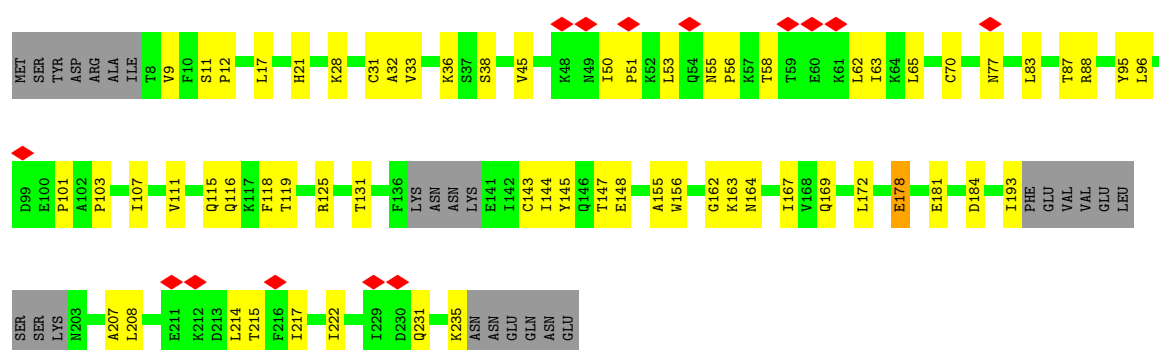
Chain Q: 60% 29% 11%



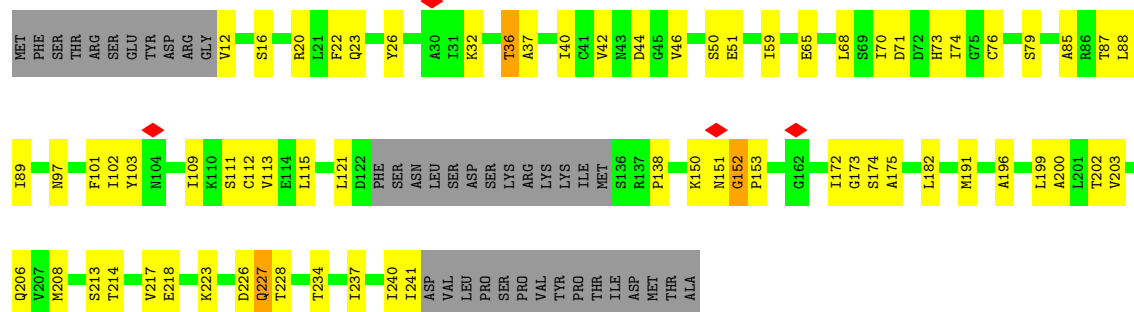
Chain D: 6% 64% 25% 11%



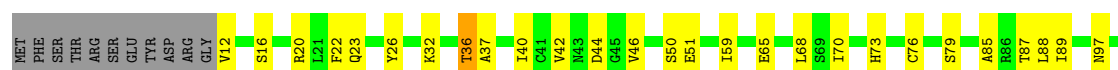
Chain R:

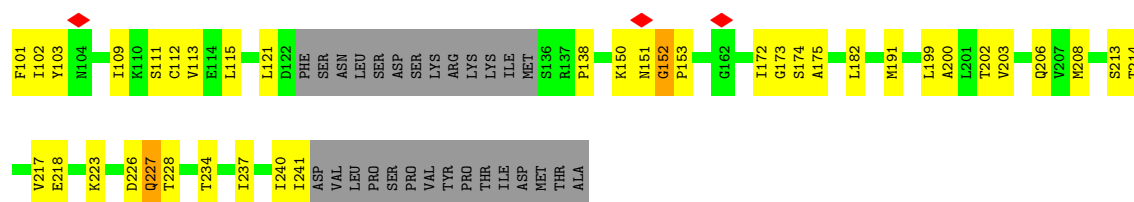


Chain E: 58% 25% 15%



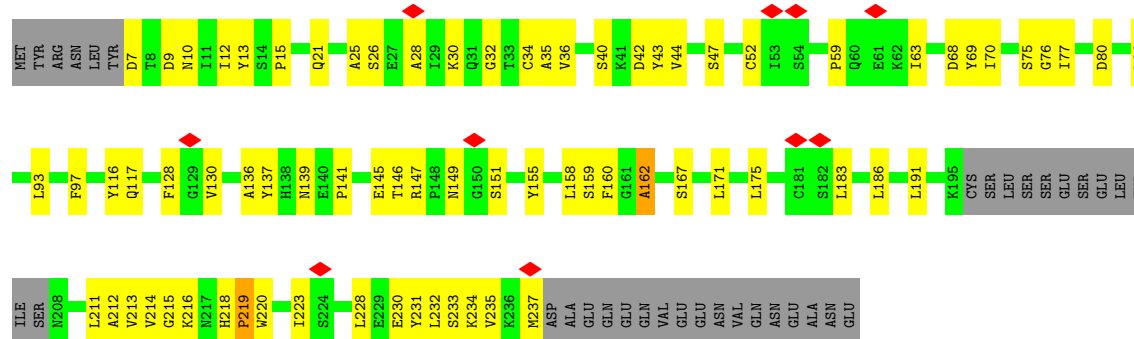
Chain S:





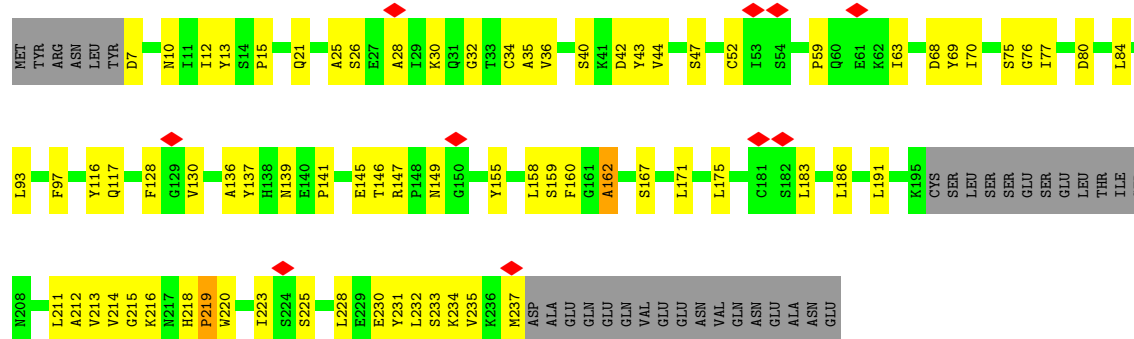
• Molecule 6: PROTEOSOME SUBUNIT ALPHA TYPE 1, PUTATIVE

Chain F: 57% 29% 14%



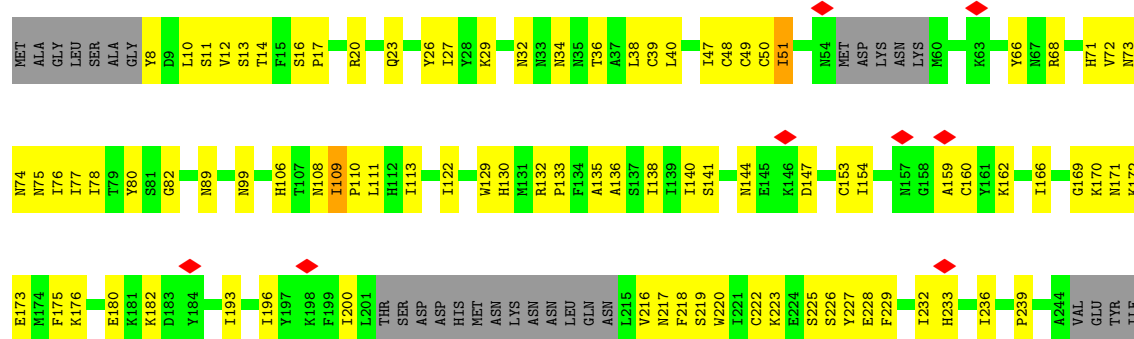
• Molecule 6: PROTEOSOME SUBUNIT ALPHA TYPE 1, PUTATIVE

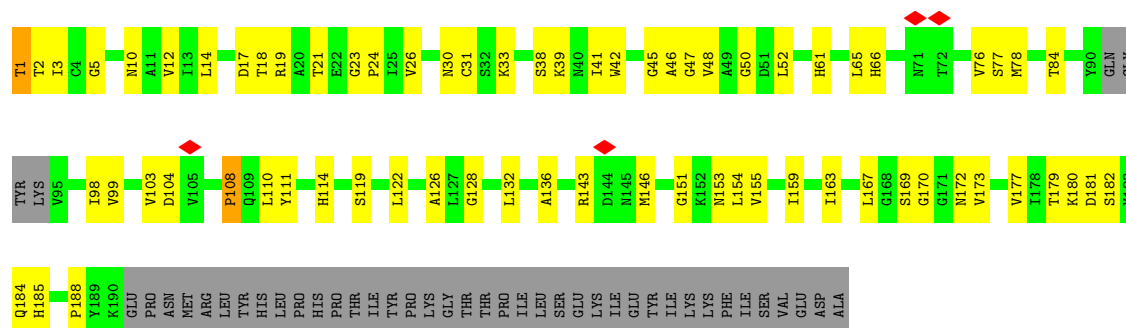
Chain T: 57% 28% 14%



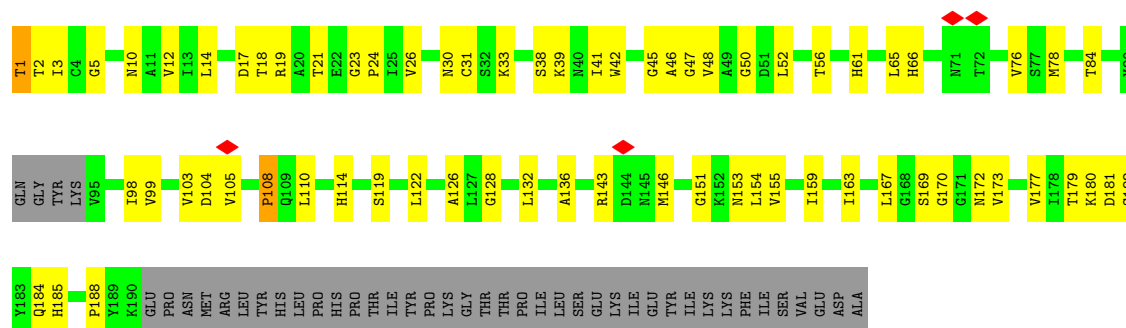
• Molecule 7: PROTEASOME COMPONENT C8, PUTATIVE

Chain G: 51% 35% 13%

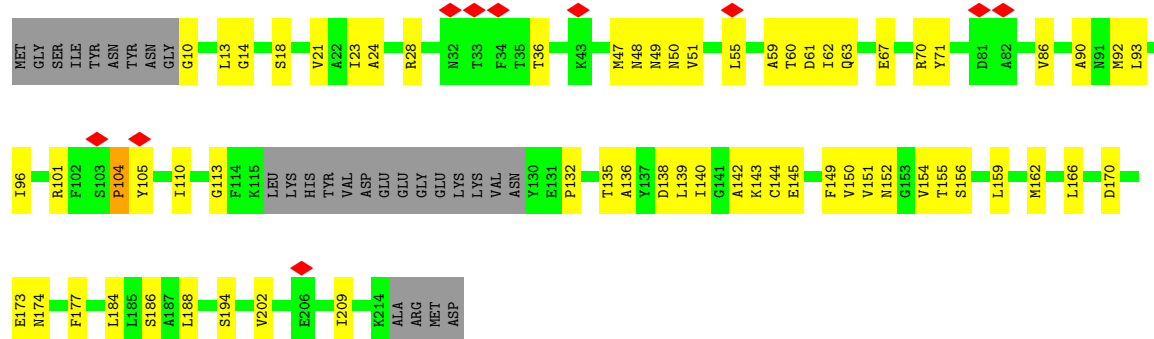




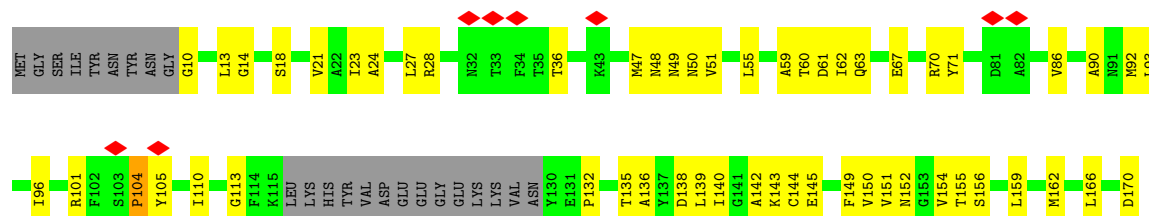
• Molecule 9: PROTEASOME SUBUNIT BETA TYPE



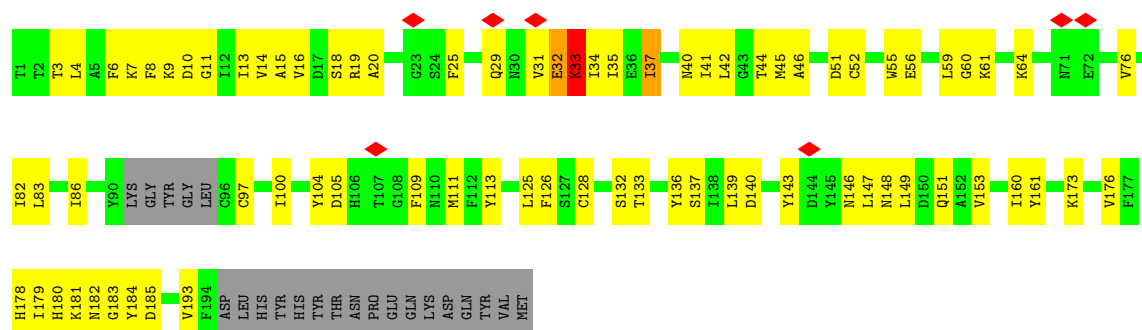
• Molecule 10: BETA3 PROTEASOME SUBUNIT, PUTATIVE



• Molecule 10: BETA3 PROTEASOME SUBUNIT, PUTATIVE

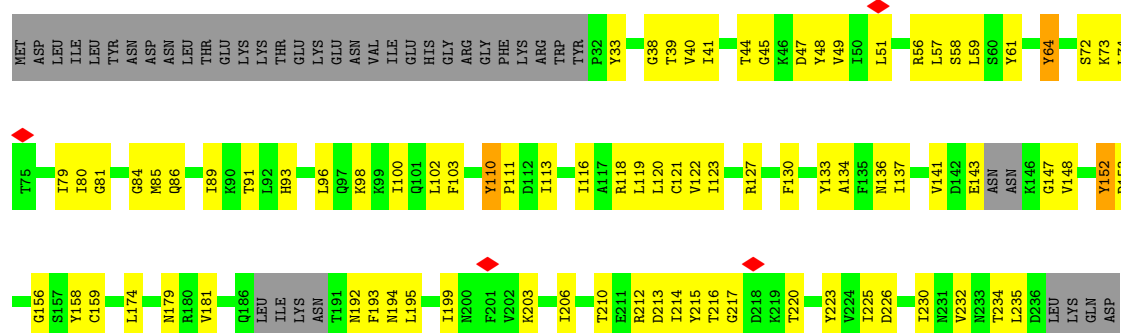






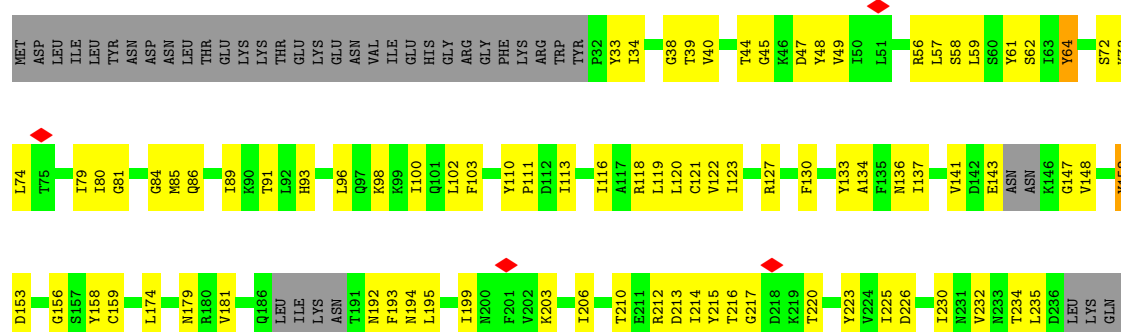
• Molecule 13: PROTEASOME SUBUNIT BETA TYPE

Chain M: 48% 34% 17%



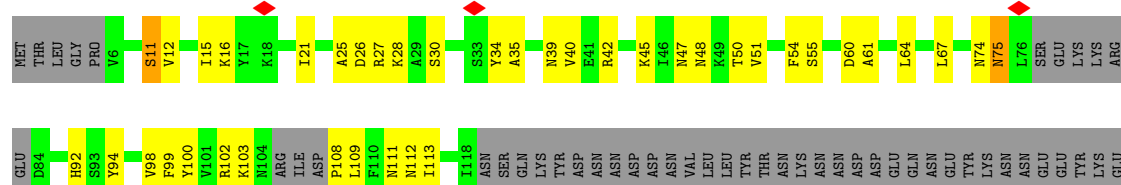
• Molecule 13: PROTEASOME SUBUNIT BETA TYPE

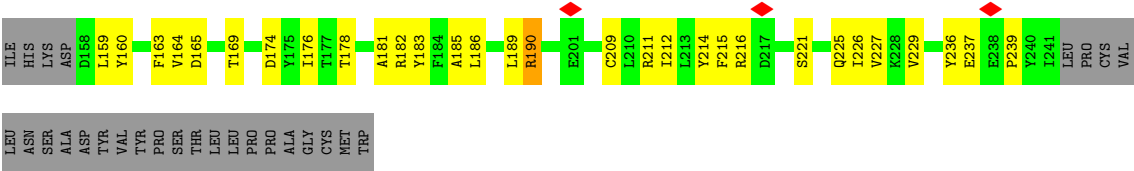
Chain a: 48% 34% 17%



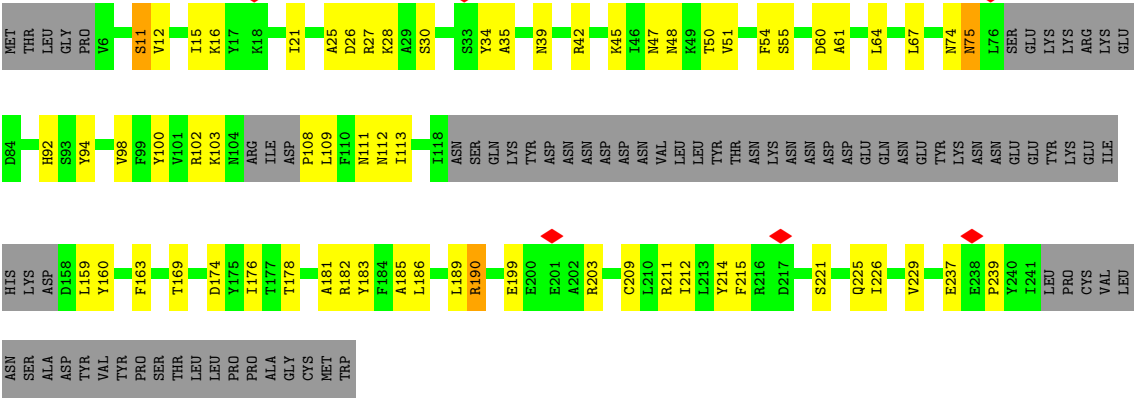
• Molecule 14: PROTEASOME SUBUNIT BETA TYPE

Chain N: 44% 25% 29%





● Molecule 14: PROTEASOME SUBUNIT BETA TYPE



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	97720	Depositor
Resolution determination method	Not provided	
CTF correction method	FULL RECORDED IMAGE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	4.8	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	3200	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	15.982	Depositor
Minimum map value	-10.651	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	3	Depositor
Map size ($\text{\AA}$)	266.24, 266.24, 266.24	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.04, 1.04, 1.04	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 7F1

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.65	0/1455	0.95	4/1988 (0.2%)
1	O	0.65	0/1455	0.95	4/1988 (0.2%)
2	B	0.66	0/1400	1.01	7/1921 (0.4%)
2	P	0.66	0/1400	1.01	7/1921 (0.4%)
3	C	0.64	0/1554	0.97	5/2131 (0.2%)
3	Q	0.64	0/1554	0.97	5/2131 (0.2%)
4	D	0.66	0/1427	0.95	5/1964 (0.3%)
4	R	0.66	0/1427	0.95	5/1964 (0.3%)
5	E	0.65	0/1457	0.97	4/1997 (0.2%)
5	S	0.65	0/1457	0.97	4/1997 (0.2%)
6	F	0.64	0/1519	0.92	1/2082 (0.0%)
6	T	0.64	0/1519	0.92	1/2082 (0.0%)
7	G	0.66	0/1571	0.95	4/2150 (0.2%)
7	U	0.66	0/1571	0.95	4/2150 (0.2%)
8	H	0.72	0/1332	0.95	2/1814 (0.1%)
8	V	0.72	0/1332	0.95	2/1814 (0.1%)
9	I	1.05	1/1257 (0.1%)	1.03	9/1721 (0.5%)
9	W	1.05	1/1257 (0.1%)	1.03	9/1721 (0.5%)
10	J	0.71	0/1283	0.97	2/1751 (0.1%)
10	X	0.71	0/1283	0.97	2/1751 (0.1%)
11	K	0.69	0/1482	0.97	4/2017 (0.2%)
11	Y	0.69	0/1482	0.97	4/2017 (0.2%)
12	L	0.68	0/1378	1.02	4/1866 (0.2%)
12	Z	0.68	0/1378	1.02	4/1866 (0.2%)
13	M	0.69	0/1434	0.96	5/1956 (0.3%)
13	a	0.69	0/1434	0.96	5/1956 (0.3%)
14	N	0.72	0/1355	0.96	2/1844 (0.1%)
14	b	0.72	0/1355	0.96	2/1844 (0.1%)
All	All	0.70	2/39808 (0.0%)	0.97	116/54404 (0.2%)

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	1
1	O	0	1
11	K	0	1
11	Y	0	1
12	L	0	2
12	Z	0	2
All	All	0	8

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	1	THR	C-N	26.84	1.69	1.33
9	W	1	THR	C-N	26.84	1.69	1.33

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	1	THR	O-C-N	-13.24	101.81	123.00
9	W	1	THR	O-C-N	-13.24	101.81	123.00
12	L	32	GLU	O-C-N	-9.78	111.73	123.27
12	Z	32	GLU	O-C-N	-9.78	111.73	123.27
13	M	152	TYR	N-CA-C	8.62	121.25	108.14
13	a	152	TYR	N-CA-C	8.62	121.25	108.14
12	L	33	LYS	CA-C-N	-8.07	110.52	121.66
12	L	33	LYS	C-N-CA	-8.07	110.52	121.66
12	Z	33	LYS	CA-C-N	-8.07	110.52	121.66
12	Z	33	LYS	C-N-CA	-8.07	110.52	121.66
5	E	152	GLY	CA-C-N	7.99	128.00	119.78
5	E	152	GLY	C-N-CA	7.99	128.00	119.78
5	S	152	GLY	CA-C-N	7.99	128.00	119.78
5	S	152	GLY	C-N-CA	7.99	128.00	119.78
3	C	128	ARG	CA-C-N	7.64	127.64	119.78
3	C	128	ARG	C-N-CA	7.64	127.64	119.78
3	Q	128	ARG	CA-C-N	7.64	127.64	119.78
3	Q	128	ARG	C-N-CA	7.64	127.64	119.78
2	B	33	SER	N-CA-C	7.23	119.01	109.83
2	P	33	SER	N-CA-C	7.23	119.01	109.83
9	I	1	THR	CA-C-N	7.21	130.95	120.71
9	I	1	THR	C-N-CA	7.21	130.95	120.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	W	1	THR	CA-C-N	7.21	130.95	120.71
9	W	1	THR	C-N-CA	7.21	130.95	120.71
12	L	33	LYS	O-C-N	7.10	131.07	122.48
12	Z	33	LYS	O-C-N	7.10	131.07	122.48
2	B	33	SER	CA-C-N	6.93	126.92	119.78
2	B	33	SER	C-N-CA	6.93	126.92	119.78
2	P	33	SER	CA-C-N	6.93	126.92	119.78
2	P	33	SER	C-N-CA	6.93	126.92	119.78
7	G	217	ASN	N-CA-C	6.65	119.46	108.49
7	U	217	ASN	N-CA-C	6.65	119.46	108.49
11	K	96	ASN	CA-C-N	-6.36	113.23	119.78
11	K	96	ASN	C-N-CA	-6.36	113.23	119.78
11	Y	96	ASN	CA-C-N	-6.36	113.23	119.78
11	Y	96	ASN	C-N-CA	-6.36	113.23	119.78
1	A	167	ALA	CB-CA-C	-6.21	109.39	116.54
1	O	167	ALA	CB-CA-C	-6.21	109.39	116.54
2	B	125	GLY	N-CA-C	6.12	118.51	111.36
2	P	125	GLY	N-CA-C	6.12	118.51	111.36
5	E	112	CYS	N-CA-C	-6.06	104.59	111.07
5	S	112	CYS	N-CA-C	-6.06	104.59	111.07
3	C	204	ILE	CB-CA-C	-6.02	107.98	113.70
3	Q	204	ILE	CB-CA-C	-6.02	107.98	113.70
13	M	130	PHE	CA-C-N	5.86	125.81	119.78
13	M	130	PHE	C-N-CA	5.86	125.81	119.78
13	a	130	PHE	CA-C-N	5.86	125.81	119.78
13	a	130	PHE	C-N-CA	5.86	125.81	119.78
2	B	132	LEU	N-CA-C	5.73	118.11	109.23
2	P	132	LEU	N-CA-C	5.73	118.11	109.23
3	C	132	VAL	N-CA-C	5.66	116.03	108.11
3	Q	132	VAL	N-CA-C	5.66	116.03	108.11
4	D	55	ASN	CA-C-N	5.64	125.48	119.28
4	D	55	ASN	C-N-CA	5.64	125.48	119.28
4	R	55	ASN	CA-C-N	5.64	125.48	119.28
4	R	55	ASN	C-N-CA	5.64	125.48	119.28
4	D	148	GLU	CA-C-N	5.56	125.39	119.28
4	D	148	GLU	C-N-CA	5.56	125.39	119.28
4	R	148	GLU	CA-C-N	5.56	125.39	119.28
4	R	148	GLU	C-N-CA	5.56	125.39	119.28
8	H	151	LEU	N-CA-C	5.54	116.69	108.60
8	V	151	LEU	N-CA-C	5.54	116.69	108.60
14	N	11	SER	N-CA-C	5.47	117.40	108.76
14	b	11	SER	N-CA-C	5.47	117.40	108.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	96	ASN	N-CA-C	5.39	121.72	109.81
11	Y	96	ASN	N-CA-C	5.39	121.72	109.81
6	F	175	LEU	N-CA-C	-5.38	102.91	110.50
6	T	175	LEU	N-CA-C	-5.38	102.91	110.50
9	I	114	HIS	CA-C-N	5.36	125.18	119.28
9	I	114	HIS	C-N-CA	5.36	125.18	119.28
9	W	114	HIS	CA-C-N	5.36	125.18	119.28
9	W	114	HIS	C-N-CA	5.36	125.18	119.28
13	M	110	TYR	CA-C-N	5.29	125.23	119.78
13	M	110	TYR	C-N-CA	5.29	125.23	119.78
13	a	110	TYR	CA-C-N	5.29	125.23	119.78
13	a	110	TYR	C-N-CA	5.29	125.23	119.78
9	I	99	VAL	CA-C-N	-5.21	115.65	122.99
9	I	99	VAL	C-N-CA	-5.21	115.65	122.99
9	W	99	VAL	CA-C-N	-5.21	115.65	122.99
9	W	99	VAL	C-N-CA	-5.21	115.65	122.99
11	K	12	PHE	N-CA-C	5.20	116.43	108.52
11	Y	12	PHE	N-CA-C	5.20	116.43	108.52
4	D	58	THR	N-CA-C	-5.20	106.71	113.16
10	J	209	ILE	N-CA-C	5.20	114.27	106.42
4	R	58	THR	N-CA-C	-5.20	106.71	113.16
10	X	209	ILE	N-CA-C	5.20	114.27	106.42
8	H	172	SER	N-CA-C	5.17	116.95	108.52
8	V	172	SER	N-CA-C	5.17	116.95	108.52
1	A	89	MET	CA-C-N	5.14	124.76	119.05
1	A	89	MET	C-N-CA	5.14	124.76	119.05
1	O	89	MET	CA-C-N	5.14	124.76	119.05
1	O	89	MET	C-N-CA	5.14	124.76	119.05
2	B	161	THR	N-CA-C	5.13	116.09	108.60
2	P	161	THR	N-CA-C	5.13	116.09	108.60
5	E	36	THR	N-CA-C	5.12	117.29	110.53
7	G	109	ILE	CA-C-N	-5.12	114.51	119.78
7	G	109	ILE	C-N-CA	-5.12	114.51	119.78
5	S	36	THR	N-CA-C	5.12	117.29	110.53
7	U	109	ILE	CA-C-N	-5.12	114.51	119.78
7	U	109	ILE	C-N-CA	-5.12	114.51	119.78
9	I	122	LEU	CA-C-N	5.06	124.84	119.28
9	I	122	LEU	C-N-CA	5.06	124.84	119.28
9	W	122	LEU	CA-C-N	5.06	124.84	119.28
9	W	122	LEU	C-N-CA	5.06	124.84	119.28
1	A	237	LYS	N-CA-C	-5.05	101.72	109.76
1	O	237	LYS	N-CA-C	-5.05	101.72	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	33	ILE	N-CA-C	5.05	116.09	109.58
14	N	190	ARG	N-CA-C	-5.05	106.97	113.23
3	Q	33	ILE	N-CA-C	5.05	116.09	109.58
14	b	190	ARG	N-CA-C	-5.05	106.97	113.23
2	B	74	ILE	N-CA-C	5.05	117.28	108.90
2	P	74	ILE	N-CA-C	5.05	117.28	108.90
7	G	136	ALA	N-CA-C	5.03	116.58	108.34
7	U	136	ALA	N-CA-C	5.03	116.58	108.34
10	J	105	TYR	N-CA-C	-5.00	105.96	111.71
10	X	105	TYR	N-CA-C	-5.00	105.96	111.71

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	236	THR	Peptide
11	K	12	PHE	Peptide
12	L	32	GLU	Mainchain
12	L	33	LYS	Mainchain
1	O	236	THR	Peptide
11	Y	12	PHE	Peptide
12	Z	32	GLU	Mainchain
12	Z	33	LYS	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1440	0	1220	40	0
1	O	1440	0	1220	40	0
2	B	1381	0	1212	47	0
2	P	1381	0	1212	48	0
3	C	1527	0	1339	65	0
3	Q	1527	0	1339	63	0
4	D	1409	0	1210	47	0
4	R	1409	0	1210	48	0
5	E	1440	0	1279	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	S	1440	0	1279	43	0
6	F	1492	0	1278	56	0
6	T	1492	0	1278	53	0
7	G	1542	0	1357	80	0
7	U	1542	0	1357	81	0
8	H	1316	0	1153	62	0
8	V	1316	0	1153	61	0
9	I	1241	0	1143	53	0
9	W	1241	0	1143	53	0
10	J	1273	0	1171	53	0
10	X	1273	0	1171	52	0
11	K	1452	0	1292	96	0
11	Y	1452	0	1292	95	0
12	L	1355	0	1254	73	0
12	Z	1355	0	1254	77	0
13	M	1413	0	1334	71	0
13	a	1413	0	1334	69	0
14	N	1337	0	1220	57	0
14	b	1337	0	1220	55	0
15	I	49	0	0	18	0
15	W	49	0	0	17	0
All	All	39334	0	34924	1518	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 20.

All (1518) 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)
9:I:1:THR:C	9:I:2:THR:N	1.69	1.48
9:W:1:THR:C	9:W:2:THR:N	1.69	1.48
8:H:4:ILE:HD11	8:H:193:LEU:CD1	1.69	1.23
8:V:4:ILE:HD11	8:V:193:LEU:CD1	1.69	1.20
12:Z:20:ALA:HB2	12:Z:31:VAL:HG21	1.29	1.12
12:L:20:ALA:HB2	12:L:31:VAL:HG21	1.29	1.10
12:Z:33:LYS:CE	12:Z:45:MET:HE2	1.80	1.10
12:L:33:LYS:CE	12:L:45:MET:HE2	1.80	1.09
12:L:33:LYS:HE3	12:L:45:MET:HE2	1.33	1.09
15:W:300:7F1:C34	10:X:144:CYS:HB2	1.84	1.07
15:I:300:7F1:C34	10:J:144:CYS:HB2	1.84	1.06
12:Z:33:LYS:HE3	12:Z:45:MET:HE2	1.33	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:33:LYS:NZ	12:Z:45:MET:HE2	1.75	1.01
11:K:170:ARG:HH12	12:Z:140:ASP:HB2	1.24	1.01
12:L:140:ASP:HB2	11:Y:170:ARG:HH12	1.24	0.99
11:K:148:HIS:HB2	11:K:151:LEU:HB2	1.41	0.99
11:Y:148:HIS:HB2	11:Y:151:LEU:HB2	1.41	0.99
8:H:4:ILE:HD11	8:H:193:LEU:HD13	1.44	0.99
12:L:33:LYS:NZ	12:L:45:MET:HE2	1.75	0.98
14:b:42:ARG:H	14:b:225:GLN:HE22	1.13	0.96
8:V:4:ILE:HD11	8:V:193:LEU:HD13	1.44	0.96
14:N:42:ARG:H	14:N:225:GLN:HE22	1.13	0.92
12:L:18:SER:O	12:L:31:VAL:HG22	1.70	0.91
9:I:163:ILE:HG23	9:I:170:GLY:HA2	1.52	0.91
14:b:28:LYS:HB2	14:b:221:SER:HB2	1.53	0.91
15:W:300:7F1:C28	10:X:138:ASP:OD2	2.18	0.91
12:Z:18:SER:O	12:Z:31:VAL:CG2	2.19	0.91
8:V:4:ILE:HD11	8:V:193:LEU:HD11	1.52	0.91
15:I:300:7F1:C28	10:J:138:ASP:OD2	2.18	0.90
12:L:18:SER:O	12:L:31:VAL:CG2	2.19	0.90
9:W:163:ILE:HG23	9:W:170:GLY:HA2	1.52	0.90
14:N:28:LYS:HB2	14:N:221:SER:HB2	1.53	0.89
14:b:92:HIS:HD1	14:b:160:TYR:HH	1.17	0.89
12:Z:18:SER:O	12:Z:31:VAL:HG22	1.70	0.89
12:Z:14:VAL:HG21	12:Z:42:LEU:HD11	1.55	0.89
13:a:152:TYR:HB3	13:a:158:TYR:HA	1.55	0.89
12:L:14:VAL:HG21	12:L:42:LEU:HD11	1.55	0.88
13:M:152:TYR:HB3	13:M:158:TYR:HA	1.55	0.88
12:L:20:ALA:CB	12:L:31:VAL:HG21	2.04	0.88
14:N:92:HIS:HD1	14:N:160:TYR:HH	1.18	0.88
8:H:4:ILE:HD11	8:H:193:LEU:HD11	1.52	0.87
11:K:69:GLN:HE21	11:K:76:MET:H	1.21	0.86
12:Z:20:ALA:CB	12:Z:31:VAL:HG21	2.04	0.86
3:C:236:ILE:HA	3:C:239:TYR:HB3	1.57	0.86
8:H:4:ILE:CD1	8:H:193:LEU:CD1	2.53	0.86
8:V:4:ILE:CD1	8:V:193:LEU:CD1	2.53	0.85
9:W:31:CYS:SG	9:W:33:LYS:NZ	2.50	0.85
8:H:31:SER:OG	8:H:33:LYS:NZ	2.11	0.84
3:Q:236:ILE:HA	3:Q:239:TYR:HB3	1.57	0.84
11:Y:69:GLN:HE21	11:Y:76:MET:H	1.21	0.84
9:I:31:CYS:SG	9:I:33:LYS:NZ	2.50	0.83
14:N:47:ASN:HB3	14:N:50:THR:HB	1.59	0.83
5:E:73:HIS:ND1	5:E:227:GLN:O	2.12	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:31:SER:OG	8:V:33:LYS:NZ	2.11	0.82
9:W:52:LEU:HD13	15:W:300:7F1:C10	2.10	0.81
14:b:47:ASN:HB3	14:b:50:THR:HB	1.59	0.81
9:I:52:LEU:HD13	15:I:300:7F1:C10	2.10	0.81
9:I:132:LEU:HB3	14:b:183:TYR:HB3	1.63	0.81
5:S:73:HIS:ND1	5:S:227:GLN:O	2.12	0.81
14:N:183:TYR:HB3	9:W:132:LEU:HB3	1.63	0.80
11:Y:16:ALA:HB1	11:Y:164:PHE:HZ	1.46	0.79
5:E:51:GLU:HG3	5:E:208:MET:HE1	1.63	0.79
11:K:20:TYR:HB3	11:K:28:LEU:HD22	1.64	0.79
13:a:79:ILE:HG12	13:a:225:ILE:HD11	1.65	0.79
11:K:16:ALA:HB1	11:K:164:PHE:HZ	1.46	0.79
13:M:79:ILE:HG12	13:M:225:ILE:HD11	1.65	0.79
14:b:16:LYS:HE2	14:b:174:ASP:HA	1.65	0.79
9:I:5:GLY:HA3	9:I:14:LEU:HD23	1.65	0.78
7:G:78:ILE:HG12	7:G:140:ILE:HG12	1.64	0.78
5:S:51:GLU:HG3	5:S:208:MET:HE1	1.63	0.78
7:U:99:ASN:ND2	14:b:74:ASN:OD1	2.17	0.78
14:N:16:LYS:HE2	14:N:174:ASP:HA	1.65	0.78
9:W:21:THR:HG22	9:W:23:GLY:H	1.49	0.77
8:H:76:PHE:CE1	8:H:163:GLN:HB2	2.20	0.77
11:K:166:GLU:OE1	11:K:170:ARG:NH2	2.18	0.77
12:L:3:THR:OG1	12:L:128:CYS:SG	2.43	0.77
13:M:113:ILE:HA	13:M:116:ILE:HD12	1.65	0.77
7:G:99:ASN:ND2	14:N:74:ASN:OD1	2.17	0.77
9:I:21:THR:HG22	9:I:23:GLY:H	1.49	0.77
8:V:76:PHE:CE1	8:V:163:GLN:HB2	2.20	0.77
12:Z:3:THR:OG1	12:Z:128:CYS:SG	2.43	0.77
13:a:113:ILE:HA	13:a:116:ILE:HD12	1.65	0.77
7:U:78:ILE:HG12	7:U:140:ILE:HG12	1.64	0.77
8:V:203:LYS:HD2	8:V:232:ASN:HD21	1.50	0.77
11:Y:20:TYR:HB3	11:Y:28:LEU:HD22	1.64	0.77
11:Y:40:HIS:CD2	11:Y:69:GLN:HE22	2.03	0.77
11:K:40:HIS:CD2	11:K:69:GLN:HE22	2.03	0.77
9:W:5:GLY:HA3	9:W:14:LEU:HD23	1.65	0.77
10:X:173:GLU:HB2	10:X:202:VAL:HG11	1.68	0.76
10:J:173:GLU:HB2	10:J:202:VAL:HG11	1.68	0.76
11:Y:166:GLU:OE1	11:Y:170:ARG:NH2	2.18	0.76
8:H:203:LYS:HD2	8:H:232:ASN:HD21	1.50	0.76
11:Y:47:LEU:HD23	11:Y:102:CYS:HB3	1.68	0.76
11:K:47:LEU:HD23	11:K:102:CYS:HB3	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:W:300:7F1:C24	10:X:140:ILE:HB	2.16	0.75
15:I:300:7F1:C24	10:J:140:ILE:HB	2.16	0.75
10:J:188:LEU:HG	10:J:194:SER:HB3	1.69	0.75
8:H:4:ILE:HG13	8:H:181:VAL:HG22	1.69	0.74
8:V:4:ILE:HG13	8:V:181:VAL:HG22	1.69	0.74
15:W:300:7F1:C35	10:X:144:CYS:HB2	2.18	0.74
7:U:144:ASN:HB2	7:U:147:ASP:HB3	1.69	0.74
11:Y:42:ASN:HB3	11:Y:107:TYR:HB3	1.70	0.74
11:K:42:ASN:HB3	11:K:107:TYR:HB3	1.70	0.73
15:I:300:7F1:C35	10:J:144:CYS:HB2	2.18	0.73
10:X:188:LEU:HG	10:X:194:SER:HB3	1.69	0.73
13:M:212:ARG:HD3	9:W:26:VAL:HG22	1.69	0.73
11:K:170:ARG:HH12	12:Z:140:ASP:CB	2.01	0.73
12:L:6:PHE:HA	12:L:111:MET:HE1	1.71	0.73
7:G:144:ASN:HB2	7:G:147:ASP:HB3	1.69	0.73
9:I:26:VAL:HG22	13:a:212:ARG:HD3	1.69	0.72
11:K:129:LYS:HE3	11:K:144:ASP:HA	1.70	0.72
11:Y:129:LYS:HE3	11:Y:144:ASP:HA	1.70	0.72
4:D:62:LEU:HD12	4:D:207:ALA:HB3	1.72	0.72
13:a:199:ILE:HG22	13:a:203:LYS:HE3	1.72	0.72
13:M:199:ILE:HG22	13:M:203:LYS:HE3	1.72	0.72
12:L:136:TYR:CZ	11:Y:170:ARG:HD2	2.25	0.71
12:Z:6:PHE:HA	12:Z:111:MET:HE1	1.71	0.71
14:N:15:ILE:HD12	14:N:189:LEU:HD11	1.73	0.71
9:W:17:ASP:OD1	9:W:18:THR:N	2.24	0.71
11:K:170:ARG:HD2	12:Z:136:TYR:CZ	2.25	0.71
4:R:62:LEU:HD12	4:R:207:ALA:HB3	1.72	0.71
14:b:26:ASP:OD2	14:b:221:SER:N	2.24	0.71
4:D:12:PRO:HA	5:E:26:TYR:HD1	1.56	0.71
12:L:140:ASP:CB	11:Y:170:ARG:HH12	2.01	0.71
12:L:29:GLN:O	12:L:173:LYS:NZ	2.23	0.70
9:I:17:ASP:OD1	9:I:18:THR:N	2.24	0.70
12:L:33:LYS:NZ	12:L:45:MET:CE	2.54	0.70
4:R:12:PRO:HA	5:S:26:TYR:HD1	1.56	0.70
12:Z:153:VAL:HB	12:Z:178:HIS:HE2	1.57	0.70
14:b:186:LEU:O	14:b:190:ARG:N	2.25	0.69
11:K:13:VAL:HG11	11:K:105:ALA:HB1	1.75	0.69
12:L:33:LYS:HE3	12:L:45:MET:CE	2.18	0.69
10:X:24:ALA:HB1	10:X:184:LEU:HD11	1.73	0.69
12:Z:29:GLN:O	12:Z:173:LYS:NZ	2.23	0.69
14:b:15:ILE:HD12	14:b:189:LEU:HD11	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:b:182:ARG:O	14:b:186:LEU:HB3	1.92	0.69
9:I:167:LEU:HD11	13:a:58:SER:HB3	1.74	0.69
14:N:186:LEU:O	14:N:190:ARG:N	2.25	0.69
1:O:214:GLU:O	1:O:218:THR:N	2.25	0.69
10:J:18:SER:HB2	10:J:170:ASP:HB3	1.74	0.69
14:N:182:ARG:O	14:N:186:LEU:HB3	1.92	0.69
10:J:24:ALA:HB1	10:J:184:LEU:HD11	1.73	0.69
11:K:170:ARG:HH21	12:Z:137:SER:HA	1.57	0.69
12:L:137:SER:HA	11:Y:170:ARG:HH21	1.57	0.69
13:M:80:ILE:HD11	13:M:136:ASN:HD21	1.57	0.69
10:X:18:SER:HB2	10:X:170:ASP:HB3	1.74	0.69
8:H:76:PHE:HE1	8:H:163:GLN:HB2	1.58	0.68
11:Y:13:VAL:HG11	11:Y:105:ALA:HB1	1.75	0.68
12:Z:33:LYS:NZ	12:Z:45:MET:CE	2.54	0.68
14:N:26:ASP:OD2	14:N:221:SER:N	2.24	0.68
6:T:13:TYR:OH	7:U:132:ARG:NH1	2.26	0.68
6:F:13:TYR:OH	7:G:132:ARG:NH1	2.26	0.68
12:L:153:VAL:HB	12:L:178:HIS:HE2	1.57	0.68
1:O:65:LYS:HD2	1:O:67:LEU:HD23	1.76	0.68
11:K:46:LEU:HD23	11:K:103:LEU:HD12	1.76	0.68
14:N:26:ASP:OD1	14:N:42:ARG:NH2	2.27	0.68
11:Y:46:LEU:HD23	11:Y:103:LEU:HD12	1.76	0.68
12:L:18:SER:O	12:L:31:VAL:HG23	1.94	0.67
6:F:36:VAL:HG23	6:F:159:SER:HB3	1.76	0.67
11:K:40:HIS:HD2	11:K:69:GLN:HE22	1.41	0.67
14:b:26:ASP:OD1	14:b:42:ARG:NH2	2.27	0.67
11:K:170:ARG:HD2	12:Z:136:TYR:CE2	2.29	0.67
12:L:136:TYR:CE2	11:Y:170:ARG:HD2	2.29	0.67
13:M:58:SER:HB3	9:W:167:LEU:HD11	1.74	0.67
4:R:65:LEU:HD13	4:R:87:THR:HG21	1.75	0.67
6:F:10:ASN:HB3	6:F:21:GLN:HB2	1.77	0.67
5:S:214:THR:HG22	5:S:237:ILE:HB	1.76	0.67
10:X:48:ASN:OD1	10:X:49:ASN:N	2.27	0.67
12:Z:18:SER:O	12:Z:31:VAL:HG23	1.94	0.67
3:Q:114:ILE:HG21	3:Q:134:PHE:HZ	1.59	0.66
6:T:36:VAL:HG23	6:T:159:SER:HB3	1.76	0.66
13:M:85:MET:H	13:M:133:TYR:HD2	1.43	0.66
11:Y:40:HIS:HD2	11:Y:69:GLN:HE22	1.41	0.66
3:C:114:ILE:HG21	3:C:134:PHE:HZ	1.59	0.66
13:a:85:MET:H	13:a:133:TYR:HD2	1.43	0.66
1:A:65:LYS:HD2	1:A:67:LEU:HD23	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:117:GLN:HG2	7:G:89:ASN:OD1	1.96	0.66
10:J:48:ASN:OD1	10:J:49:ASN:N	2.27	0.66
14:N:163:PHE:HB2	14:N:176:ILE:HG21	1.78	0.66
10:X:47:MET:HE1	10:X:70:ARG:HA	1.78	0.66
1:A:214:GLU:O	1:A:218:THR:N	2.25	0.66
4:D:65:LEU:HD13	4:D:87:THR:HG21	1.75	0.66
5:E:102:ILE:HD12	13:M:122:VAL:HG22	1.78	0.66
5:E:214:THR:HG22	5:E:237:ILE:HB	1.76	0.66
6:T:10:ASN:HB3	6:T:21:GLN:HB2	1.77	0.66
6:T:117:GLN:HG2	7:U:89:ASN:OD1	1.96	0.66
2:B:9:SER:OG	2:B:123:GLN:O	2.12	0.66
4:D:28:LYS:HA	4:D:163:LYS:HD3	1.78	0.66
2:B:159:MET:O	2:B:178:TYR:OH	2.12	0.66
10:J:162:MET:HE3	10:J:166:LEU:HD22	1.77	0.66
6:F:137:TYR:HB3	6:F:141:PRO:HA	1.78	0.66
8:V:76:PHE:HE1	8:V:163:GLN:HB2	1.58	0.66
13:a:80:ILE:HD11	13:a:136:ASN:HD21	1.57	0.66
14:b:45:LYS:HA	14:b:51:VAL:HG12	1.78	0.66
14:b:163:PHE:HB2	14:b:176:ILE:HG21	1.78	0.65
8:H:191:SER:OG	8:V:188:TYR:O	2.14	0.65
12:L:44:THR:HG22	12:L:100:ILE:HB	1.78	0.65
6:T:147:ARG:O	6:T:149:ASN:N	2.28	0.65
7:U:36:THR:HA	7:U:169:GLY:HA3	1.79	0.65
11:Y:40:HIS:HE2	11:Y:75:ASP:HB2	1.61	0.65
13:a:203:LYS:HE2	13:a:235:LEU:HD13	1.78	0.65
10:J:47:MET:HE1	10:J:70:ARG:HA	1.78	0.65
10:J:48:ASN:HB3	10:J:51:VAL:HB	1.79	0.65
2:P:159:MET:O	2:P:178:TYR:OH	2.12	0.65
12:Z:44:THR:HG22	12:Z:100:ILE:HB	1.78	0.65
9:W:52:LEU:HD22	15:W:300:7F1:C11	2.27	0.65
6:F:147:ARG:O	6:F:149:ASN:N	2.28	0.65
13:M:225:ILE:HG23	13:M:230:ILE:HG13	1.78	0.65
4:R:28:LYS:HA	4:R:163:LYS:HD3	1.78	0.65
6:T:137:TYR:HB3	6:T:141:PRO:HA	1.78	0.65
8:V:233:ILE:HD13	8:V:239:GLU:HG3	1.78	0.65
7:G:36:THR:HA	7:G:169:GLY:HA3	1.79	0.65
13:M:203:LYS:HE2	13:M:235:LEU:HD13	1.78	0.65
4:R:116:GLN:NE2	5:S:87:THR:OG1	2.30	0.65
11:K:40:HIS:HE2	11:K:75:ASP:HB2	1.61	0.65
2:P:9:SER:OG	2:P:123:GLN:O	2.12	0.65
6:T:44:VAL:HG23	6:T:141:PRO:HB3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:31:VAL:HG12	13:a:159:CYS:SG	2.37	0.65
14:b:26:ASP:HB2	14:b:221:SER:HB3	1.79	0.65
9:I:52:LEU:HD22	15:I:300:7F1:C11	2.27	0.65
11:K:93:LEU:O	11:K:97:PRO:HD3	1.97	0.65
14:N:26:ASP:HB2	14:N:221:SER:HB3	1.79	0.65
14:N:45:LYS:HA	14:N:51:VAL:HG12	1.78	0.65
5:S:36:THR:HB	5:S:175:ALA:HB3	1.79	0.65
10:X:48:ASN:HB3	10:X:51:VAL:HB	1.79	0.65
12:Z:33:LYS:HE3	12:Z:45:MET:CE	2.18	0.65
8:H:233:ILE:HD13	8:H:239:GLU:HG3	1.78	0.64
10:X:162:MET:HE3	10:X:166:LEU:HD22	1.77	0.64
8:H:188:TYR:O	8:V:191:SER:OG	2.14	0.64
9:I:1:THR:O	9:I:128:GLY:HA3	1.97	0.64
12:L:31:VAL:HG12	13:M:159:CYS:SG	2.37	0.64
11:Y:93:LEU:O	11:Y:97:PRO:HD3	1.97	0.64
8:H:18:SER:OG	8:H:31:SER:N	2.30	0.64
5:S:102:ILE:HD12	13:a:122:VAL:HG22	1.78	0.64
4:D:116:GLN:NE2	5:E:87:THR:OG1	2.30	0.64
4:D:181:GLU:HB2	4:D:184:ASP:HB3	1.80	0.64
13:M:179:ASN:ND2	10:X:186:SER:OG	2.31	0.64
8:V:18:SER:OG	8:V:31:SER:N	2.30	0.64
3:C:108:SER:HG	3:C:148:TYR:HH	1.46	0.63
6:T:47:SER:HB2	6:T:211:LEU:HD13	1.81	0.63
13:a:225:ILE:HG23	13:a:230:ILE:HG13	1.78	0.63
3:Q:14:PRO:HA	4:R:21:HIS:CD2	2.33	0.63
9:W:1:THR:O	9:W:128:GLY:HA3	1.97	0.63
3:C:14:PRO:HA	4:D:21:HIS:CD2	2.33	0.63
1:O:18:PRO:HA	2:P:24:TYR:CE1	2.34	0.63
5:E:36:THR:HB	5:E:175:ALA:HB3	1.79	0.63
6:F:44:VAL:HG23	6:F:141:PRO:HB3	1.79	0.63
3:Q:122:THR:O	4:R:125:ARG:NH1	2.32	0.63
8:H:4:ILE:CD1	8:H:193:LEU:HD13	2.26	0.63
10:J:186:SER:OG	13:a:179:ASN:ND2	2.31	0.63
10:J:63:GLN:HB2	11:K:86:ARG:NH2	2.13	0.63
10:J:138:ASP:OD1	10:J:139:LEU:N	2.31	0.63
7:U:222:CYS:H	7:U:225:SER:HB2	1.64	0.63
3:C:122:THR:O	4:D:125:ARG:NH1	2.32	0.62
6:F:47:SER:HB2	6:F:211:LEU:HD13	1.81	0.62
3:Q:160:PHE:H	4:R:53:LEU:HD12	1.64	0.62
1:A:103:GLU:O	1:A:106:GLU:HG2	2.00	0.62
3:C:159:TRP:CE3	4:D:53:LEU:HG	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:63:GLN:HB2	11:Y:86:ARG:NH2	2.13	0.62
3:Q:159:TRP:CE3	4:R:53:LEU:HG	2.34	0.62
3:C:160:PHE:H	4:D:53:LEU:HD12	1.64	0.62
7:G:222:CYS:SG	7:G:225:SER:OG	2.52	0.62
11:Y:129:LYS:HD2	11:Y:143:LEU:HB3	1.82	0.62
1:O:103:GLU:O	1:O:106:GLU:HG2	2.00	0.62
1:A:231:VAL:HG23	1:A:244:ILE:HB	1.82	0.62
9:I:104:ASP:N	9:I:104:ASP:OD1	2.32	0.62
2:P:87:LEU:HD11	2:P:91:ARG:HE	1.65	0.62
5:S:46:VAL:HG23	5:S:153:PRO:HB3	1.82	0.62
2:B:87:LEU:HD11	2:B:91:ARG:HE	1.65	0.62
3:C:96:ARG:O	3:C:100:ASN:ND2	2.33	0.62
9:I:1:THR:CB	15:I:300:7F1:C02	2.77	0.62
11:K:129:LYS:HD2	11:K:143:LEU:HB3	1.82	0.61
4:R:181:GLU:HB2	4:R:184:ASP:HB3	1.80	0.61
9:W:104:ASP:N	9:W:104:ASP:OD1	2.32	0.61
2:B:46:ILE:HD12	2:B:75:VAL:HG23	1.82	0.61
9:I:39:LYS:NZ	9:I:181:ASP:O	2.33	0.61
7:U:129:TRP:H	7:U:129:TRP:HE3	1.47	0.61
1:A:18:PRO:HA	2:B:24:TYR:CE1	2.34	0.61
3:C:76:VAL:HG13	3:C:134:PHE:HB3	1.83	0.61
12:L:33:LYS:HZ1	12:L:45:MET:HE2	1.64	0.61
8:H:18:SER:HG	8:H:31:SER:HG	1.47	0.61
9:W:1:THR:CB	15:W:300:7F1:C02	2.77	0.61
5:E:46:VAL:HG23	5:E:153:PRO:HB3	1.82	0.61
7:G:222:CYS:H	7:G:225:SER:HB2	1.64	0.61
13:M:103:PHE:CD2	13:M:111:PRO:HG3	2.36	0.61
3:Q:96:ARG:O	3:Q:100:ASN:ND2	2.33	0.61
9:W:39:LYS:NZ	9:W:181:ASP:O	2.33	0.61
13:a:103:PHE:CD2	13:a:111:PRO:HG3	2.36	0.61
1:A:17:SER:OG	1:A:21:ASN:N	2.33	0.61
8:H:17:ASP:OD2	8:H:225:GLY:N	2.31	0.61
9:I:18:THR:OG1	9:I:172:ASN:O	2.14	0.61
3:Q:174:VAL:HB	3:Q:195:THR:HG22	1.83	0.61
5:E:85:ALA:O	5:E:89:ILE:HG12	2.00	0.61
7:G:129:TRP:HE3	7:G:129:TRP:H	1.47	0.61
7:G:233:HIS:HB3	7:G:236:ILE:HG12	1.83	0.61
9:I:1:THR:O	9:I:2:THR:N	2.28	0.61
2:P:46:ILE:HD12	2:P:75:VAL:HG23	1.82	0.61
3:C:174:VAL:HB	3:C:195:THR:HG22	1.83	0.60
5:S:85:ALA:O	5:S:89:ILE:HG12	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:179:THR:OG1	9:W:182:SER:O	2.13	0.60
1:O:17:SER:OG	1:O:21:ASN:N	2.33	0.60
1:O:147:ILE:HD12	1:O:156:GLU:O	2.02	0.60
3:Q:138:GLY:HA2	3:Q:215:LEU:HD21	1.83	0.60
9:W:1:THR:O	9:W:2:THR:N	2.28	0.60
13:M:136:ASN:OD1	13:M:137:ILE:N	2.35	0.60
7:U:233:HIS:HB3	7:U:236:ILE:HG12	1.83	0.60
8:V:17:ASP:OD2	8:V:225:GLY:N	2.31	0.60
1:O:231:VAL:HG23	1:O:244:ILE:HB	1.82	0.60
2:P:118:VAL:HA	2:P:130:PHE:CE2	2.37	0.60
3:Q:76:VAL:HG13	3:Q:134:PHE:HB3	1.83	0.60
6:T:70:ILE:HA	6:T:136:ALA:HB2	1.83	0.60
2:B:118:VAL:HA	2:B:130:PHE:HE2	1.67	0.60
6:F:52:CYS:HB3	6:F:59:PRO:HG3	1.84	0.60
10:J:90:ALA:HB1	10:J:143:LYS:HE3	1.84	0.60
9:W:143:ARG:O	9:W:146:MET:HG3	2.01	0.60
14:b:47:ASN:OD1	14:b:48:ASN:N	2.35	0.60
2:B:118:VAL:HA	2:B:130:PHE:CE2	2.37	0.60
9:I:179:THR:OG1	9:I:182:SER:O	2.13	0.60
10:J:10:GLY:O	10:J:154:VAL:N	2.32	0.60
8:V:4:ILE:CD1	8:V:193:LEU:HD13	2.26	0.60
1:A:118:GLU:HB3	1:A:158:PHE:CZ	2.37	0.60
14:N:47:ASN:OD1	14:N:48:ASN:N	2.35	0.60
7:G:175:PHE:HE1	7:G:200:ILE:HA	1.67	0.60
1:O:143:SER:HA	1:O:160:PHE:CE1	2.37	0.60
2:P:118:VAL:HA	2:P:130:PHE:HE2	1.67	0.60
6:F:70:ILE:HA	6:F:136:ALA:HB2	1.83	0.60
11:K:8:ARG:NH2	11:K:128:ASN:OD1	2.35	0.60
7:U:175:PHE:HE1	7:U:200:ILE:HA	1.67	0.60
3:C:138:GLY:HA2	3:C:215:LEU:HD21	1.83	0.59
1:A:143:SER:HA	1:A:160:PHE:CE1	2.37	0.59
13:a:136:ASN:OD1	13:a:137:ILE:N	2.35	0.59
7:G:111:LEU:HD11	7:G:140:ILE:HG22	1.84	0.59
11:K:18:ASP:OD1	11:K:19:THR:N	2.36	0.59
10:X:10:GLY:O	10:X:154:VAL:N	2.32	0.59
13:a:152:TYR:CB	13:a:158:TYR:HA	2.29	0.59
1:A:147:ILE:HD12	1:A:156:GLU:O	2.02	0.59
9:I:143:ARG:O	9:I:146:MET:HG3	2.01	0.59
11:K:19:THR:HB	11:K:32:ASP:HA	1.85	0.59
4:D:231:GLN:O	4:D:235:LYS:N	2.33	0.59
10:X:138:ASP:OD1	10:X:139:LEU:N	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:19:THR:HB	11:Y:32:ASP:HA	1.85	0.59
1:O:118:GLU:HB3	1:O:158:PHE:CZ	2.37	0.59
11:Y:8:ARG:NH2	11:Y:128:ASN:OD1	2.35	0.59
11:K:72:ASN:OD1	11:K:73:ASN:N	2.35	0.58
11:K:108:ASP:OD1	11:K:109:LYS:N	2.35	0.58
10:X:51:VAL:HG22	10:X:86:VAL:HG22	1.85	0.58
10:X:90:ALA:HB1	10:X:143:LYS:HE3	1.84	0.58
11:Y:108:ASP:OD1	11:Y:109:LYS:N	2.35	0.58
11:Y:18:ASP:OD1	11:Y:19:THR:N	2.36	0.58
14:b:30:SER:HA	14:b:35:ALA:HA	1.85	0.58
5:E:150:LYS:O	5:E:152:GLY:N	2.37	0.58
13:M:152:TYR:CB	13:M:158:TYR:HA	2.29	0.58
3:Q:71:HIS:CD2	3:Q:72:ILE:HG13	2.38	0.58
5:S:150:LYS:O	5:S:152:GLY:N	2.37	0.58
7:U:218:PHE:HB2	7:U:232:ILE:HG21	1.86	0.58
6:T:52:CYS:HB3	6:T:59:PRO:HG3	1.84	0.58
9:W:103:VAL:HG12	9:W:180:LYS:HB3	1.86	0.58
5:E:16:SER:OG	5:E:20:ARG:O	2.15	0.58
2:P:167:TYR:HA	2:P:170:ASN:HB3	1.85	0.58
3:C:71:HIS:CD2	3:C:72:ILE:HG13	2.38	0.58
8:H:219:HIS:HD2	8:V:194:GLN:HE22	1.51	0.58
13:M:73:LYS:HA	13:M:79:ILE:HG22	1.85	0.58
2:B:167:TYR:HA	2:B:170:ASN:HB3	1.85	0.58
7:G:106:HIS:HB2	8:H:81:THR:HG21	1.86	0.58
11:Y:72:ASN:OD1	11:Y:73:ASN:N	2.35	0.58
13:a:72:SER:HB2	13:a:93:HIS:HD2	1.69	0.58
13:a:73:LYS:HA	13:a:79:ILE:HG22	1.85	0.58
13:M:72:SER:HB2	13:M:93:HIS:HD2	1.69	0.58
3:Q:13:SER:N	3:Q:17:ARG:O	2.34	0.58
10:X:13:LEU:HG	10:X:151:VAL:HG12	1.86	0.58
8:H:194:GLN:HE22	8:V:219:HIS:HD2	1.51	0.58
10:J:51:VAL:HG22	10:J:86:VAL:HG22	1.85	0.58
9:W:103:VAL:CG1	9:W:180:LYS:HB3	2.34	0.58
12:Z:3:THR:HG1	12:Z:128:CYS:HG	1.29	0.58
9:I:103:VAL:HG12	9:I:180:LYS:HB3	1.86	0.57
14:N:30:SER:HA	14:N:35:ALA:HA	1.85	0.57
15:W:300:7F1:C35	10:X:144:CYS:CB	2.82	0.57
11:Y:14:VAL:HG12	11:Y:182:ILE:HG12	1.86	0.57
12:Z:147:LEU:HD13	12:Z:151:GLN:HG2	1.85	0.57
12:L:3:THR:HG1	12:L:128:CYS:HG	1.31	0.57
3:Q:106:PRO:HA	3:Q:140:ASP:HB3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:111:LEU:HD11	7:U:140:ILE:HG22	1.84	0.57
7:G:218:PHE:HB2	7:G:232:ILE:HG21	1.86	0.57
11:K:14:VAL:HG12	11:K:182:ILE:HG12	1.86	0.57
14:b:25:ALA:HB1	14:b:42:ARG:NH2	2.19	0.57
5:S:202:THR:O	5:S:206:GLN:HG2	2.05	0.57
7:U:27:ILE:HG23	7:U:135:ALA:HA	1.87	0.57
13:a:103:PHE:HD2	13:a:111:PRO:HG3	1.69	0.57
14:N:25:ALA:HB1	14:N:42:ARG:NH2	2.19	0.57
8:H:89:ASP:OD1	8:H:89:ASP:N	2.38	0.57
4:R:88:ARG:NH1	11:Y:70:TYR:O	2.37	0.57
7:U:222:CYS:H	7:U:225:SER:CB	2.18	0.57
8:V:53:GLN:HA	8:V:56:ILE:HD12	1.87	0.57
4:D:88:ARG:NH1	11:K:70:TYR:O	2.37	0.57
12:L:147:LEU:HD13	12:L:151:GLN:HG2	1.85	0.57
6:T:63:ILE:HG23	6:T:220:TRP:HZ2	1.70	0.57
15:I:300:7F1:C35	10:J:144:CYS:CB	2.82	0.57
10:J:13:LEU:HG	10:J:151:VAL:HG12	1.86	0.57
13:M:45:GLY:N	13:M:48:TYR:O	2.35	0.57
5:S:23:GLN:HG3	5:S:138:PRO:HG3	1.87	0.57
7:U:38:LEU:HB3	7:U:49:CYS:SG	2.45	0.57
3:C:108:SER:OG	3:C:148:TYR:OH	2.21	0.57
9:I:103:VAL:CG1	9:I:180:LYS:HB3	2.34	0.57
10:J:92:MET:O	10:J:96:ILE:HG13	2.05	0.57
13:M:72:SER:HB2	13:M:93:HIS:CD2	2.40	0.57
14:N:92:HIS:ND1	14:N:160:TYR:OH	2.22	0.57
2:P:29:VAL:HG22	2:P:132:LEU:HA	1.87	0.57
3:C:106:PRO:HA	3:C:140:ASP:HB3	1.85	0.56
7:G:38:LEU:HB3	7:G:49:CYS:SG	2.45	0.56
7:G:222:CYS:H	7:G:225:SER:CB	2.18	0.56
10:X:138:ASP:HB3	10:X:142:ALA:HB3	1.86	0.56
13:a:72:SER:HB2	13:a:93:HIS:CD2	2.40	0.56
3:C:83:ALA:O	3:C:87:ILE:HG12	2.05	0.56
4:D:11:SER:HB3	4:D:12:PRO:HD2	1.87	0.56
5:E:202:THR:O	5:E:206:GLN:HG2	2.05	0.56
4:R:11:SER:HB3	4:R:12:PRO:HD2	1.87	0.56
6:T:43:TYR:CG	6:T:183:LEU:HD21	2.40	0.56
7:U:106:HIS:HB2	8:V:81:THR:HG21	1.86	0.56
8:V:89:ASP:N	8:V:89:ASP:OD1	2.38	0.56
10:X:13:LEU:O	10:X:23:ILE:HG13	2.06	0.56
13:a:141:VAL:HG12	13:a:143:GLU:H	1.70	0.56
8:H:53:GLN:HA	8:H:56:ILE:HD12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:40:SER:HB2	6:T:186:LEU:HD13	1.88	0.56
2:B:119:GLN:O	2:B:122:THR:OG1	2.18	0.56
6:F:63:ILE:HG23	6:F:220:TRP:HZ2	1.70	0.56
7:G:39:CYS:HA	7:G:48:CYS:HA	1.87	0.56
13:M:103:PHE:HD2	13:M:111:PRO:HG3	1.69	0.56
13:M:141:VAL:HG12	13:M:143:GLU:H	1.70	0.56
3:Q:236:ILE:O	3:Q:240:THR:N	2.36	0.56
5:S:16:SER:OG	5:S:20:ARG:O	2.15	0.56
8:V:189:ILE:HG13	8:V:217:ALA:HB2	1.87	0.56
9:W:18:THR:OG1	9:W:172:ASN:O	2.14	0.56
5:E:23:GLN:HG3	5:E:138:PRO:HG3	1.87	0.56
15:I:300:7F1:C27	10:J:138:ASP:OD2	2.54	0.56
2:P:147:TYR:HD1	2:P:157:ASN:HA	1.71	0.56
8:V:18:SER:HG	8:V:31:SER:H	1.52	0.56
1:A:71:ASN:HB2	7:G:162:LYS:HE2	1.87	0.56
3:C:235:LEU:O	3:C:239:TYR:N	2.38	0.56
6:F:43:TYR:CG	6:F:183:LEU:HD21	2.40	0.56
8:V:19:ARG:HB2	8:V:225:GLY:HA2	1.88	0.56
10:X:92:MET:O	10:X:96:ILE:HG13	2.05	0.56
3:Q:83:ALA:O	3:Q:87:ILE:HG12	2.05	0.56
7:U:39:CYS:HA	7:U:48:CYS:HA	1.87	0.56
8:H:181:VAL:HG12	8:H:186:SER:HB2	1.88	0.56
12:L:8:PHE:HE1	12:L:13:ILE:HG21	1.70	0.56
12:Z:15:ALA:HB1	12:Z:160:ILE:HD11	1.88	0.56
8:H:19:ARG:HE	8:H:225:GLY:HA2	1.71	0.56
10:J:13:LEU:O	10:J:23:ILE:HG13	2.06	0.56
10:J:138:ASP:HB3	10:J:142:ALA:HB3	1.86	0.56
8:V:232:ASN:O	8:V:239:GLU:HB2	2.06	0.56
6:F:40:SER:HB2	6:F:186:LEU:HD13	1.88	0.55
13:M:113:ILE:HG21	13:M:148:VAL:HG21	1.87	0.55
3:Q:230:LYS:O	3:Q:234:GLU:N	2.40	0.55
7:U:153:CYS:HB2	7:U:166:ILE:HG21	1.88	0.55
7:U:236:ILE:C	7:U:239:PRO:HD2	2.31	0.55
15:W:300:7F1:C27	10:X:138:ASP:OD2	2.54	0.55
2:B:29:VAL:HG22	2:B:132:LEU:HA	1.87	0.55
7:G:27:ILE:HG23	7:G:135:ALA:HA	1.87	0.55
7:G:236:ILE:C	7:G:239:PRO:HD2	2.31	0.55
9:W:3:ILE:HD12	9:W:46:ALA:HB2	1.88	0.55
2:B:95:ILE:HG13	9:I:65:LEU:HB2	1.88	0.55
3:C:13:SER:N	3:C:17:ARG:O	2.34	0.55
5:E:214:THR:HG21	5:E:234:THR:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:8:PHE:HE1	12:Z:13:ILE:HG21	1.70	0.55
13:a:45:GLY:N	13:a:48:TYR:O	2.35	0.55
12:L:37:ILE:HG23	12:L:60:GLY:HA2	1.89	0.55
2:B:147:TYR:HD1	2:B:157:ASN:HA	1.71	0.55
8:H:19:ARG:HB2	8:H:225:GLY:HA2	1.88	0.55
8:H:189:ILE:HG13	8:H:217:ALA:HB2	1.87	0.55
8:H:232:ASN:O	8:H:239:GLU:HB2	2.06	0.55
5:S:214:THR:HG21	5:S:234:THR:O	2.06	0.55
11:Y:20:TYR:HE2	11:Y:174:THR:HA	1.71	0.55
12:Z:16:VAL:HB	12:Z:34:ILE:HD11	1.88	0.55
12:Z:33:LYS:HZ2	12:Z:45:MET:HE2	1.70	0.55
3:C:230:LYS:O	3:C:234:GLU:N	2.40	0.55
7:G:153:CYS:HB2	7:G:166:ILE:HG21	1.88	0.55
7:U:75:ASN:HD21	7:U:108:ASN:HD22	1.55	0.55
11:Y:37:TYR:CE1	11:Y:47:LEU:HD12	2.41	0.55
12:L:16:VAL:HB	12:L:34:ILE:HD11	1.88	0.55
3:Q:215:LEU:O	3:Q:215:LEU:HD12	2.06	0.55
9:I:3:ILE:HD12	9:I:46:ALA:HB2	1.88	0.55
11:K:20:TYR:HE2	11:K:174:THR:HA	1.71	0.55
6:F:12:ILE:HG21	7:G:10:LEU:O	2.07	0.55
12:L:15:ALA:HB1	12:L:160:ILE:HD11	1.88	0.55
7:U:40:LEU:HB3	7:U:47:ILE:HG13	1.89	0.55
12:Z:46:ALA:O	12:Z:97:CYS:HB2	2.07	0.55
3:C:215:LEU:O	3:C:215:LEU:HD12	2.06	0.54
7:G:75:ASN:HD21	7:G:108:ASN:HD22	1.55	0.54
8:H:6:ILE:HD11	8:H:193:LEU:HD11	1.89	0.54
8:V:19:ARG:HE	8:V:225:GLY:HA2	1.71	0.54
11:K:37:TYR:CE1	11:K:47:LEU:HD12	2.41	0.54
3:Q:97:TYR:OH	11:Y:68:TYR:OH	2.21	0.54
8:V:181:VAL:HG12	8:V:186:SER:HB2	1.88	0.54
13:a:113:ILE:HG21	13:a:148:VAL:HG21	1.87	0.54
4:D:96:LEU:HA	11:K:63:LYS:HE2	1.89	0.54
7:U:74:ASN:O	7:U:229:PHE:N	2.33	0.54
1:O:71:ASN:HB2	7:U:162:LYS:HE2	1.87	0.54
7:U:50:CYS:HB3	7:U:68:ARG:HH11	1.73	0.54
13:a:84:GLY:HA3	13:a:134:ALA:HA	1.89	0.54
7:G:236:ILE:O	7:G:239:PRO:HD2	2.08	0.54
4:R:96:LEU:HA	11:Y:63:LYS:HE2	1.89	0.54
1:A:206:ARG:HA	1:A:252:TYR:HE1	1.73	0.54
3:C:114:ILE:HG21	3:C:134:PHE:CZ	2.42	0.54
3:Q:135:LEU:HD21	3:Q:162:THR:OG1	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:235:LEU:O	3:Q:239:TYR:N	2.38	0.54
7:U:40:LEU:HD23	7:U:47:ILE:HD11	1.90	0.54
7:U:106:HIS:O	7:U:106:HIS:ND1	2.41	0.54
11:Y:33:ASN:OD1	11:Y:34:THR:N	2.40	0.54
7:G:40:LEU:HB3	7:G:47:ILE:HG13	1.89	0.54
8:H:80:GLU:HA	8:H:153:PHE:CE2	2.43	0.54
12:Z:37:ILE:HG23	12:Z:60:GLY:HA2	1.89	0.54
13:a:45:GLY:HA3	13:a:48:TYR:CE1	2.43	0.54
13:M:45:GLY:HA3	13:M:48:TYR:CE1	2.43	0.54
13:M:84:GLY:HA3	13:M:134:ALA:HA	1.89	0.54
4:R:231:GLN:O	4:R:235:LYS:N	2.33	0.54
6:T:76:GLY:HA3	6:T:130:VAL:HA	1.90	0.54
11:Y:4:LEU:HB2	11:Y:132:HIS:HB2	1.90	0.54
9:I:45:GLY:HA2	9:I:98:ILE:HA	1.90	0.54
12:L:46:ALA:O	12:L:97:CYS:HB2	2.07	0.54
2:P:23:GLU:HA	2:P:26:LEU:HD12	1.89	0.54
1:A:234:VAL:HG22	1:A:241:PHE:HD1	1.73	0.53
6:F:76:GLY:HA3	6:F:130:VAL:HA	1.90	0.53
1:O:206:ARG:HA	1:O:252:TYR:HE1	1.73	0.53
2:P:68:ILE:HD11	2:P:74:ILE:HD13	1.90	0.53
2:P:95:ILE:HG13	9:W:65:LEU:HB2	1.88	0.53
8:V:203:LYS:HD2	8:V:232:ASN:ND2	2.22	0.53
9:W:45:GLY:HA2	9:W:98:ILE:HA	1.90	0.53
2:B:23:GLU:HA	2:B:26:LEU:HD12	1.89	0.53
2:B:68:ILE:HD11	2:B:74:ILE:HD13	1.90	0.53
3:C:135:LEU:HD21	3:C:162:THR:OG1	2.08	0.53
7:G:50:CYS:HB3	7:G:68:ARG:HH11	1.73	0.53
10:J:135:THR:HB	10:J:143:LYS:HE2	1.90	0.53
12:L:161:TYR:CE1	12:L:193:VAL:HG22	2.43	0.53
8:V:80:GLU:HA	8:V:153:PHE:CE2	2.43	0.53
10:X:135:THR:HB	10:X:143:LYS:HE2	1.90	0.53
13:a:96:LEU:HD22	13:a:120:LEU:HD21	1.89	0.53
1:A:83:GLY:HA3	1:A:241:PHE:CE2	2.43	0.53
7:U:129:TRP:CE2	7:U:130:HIS:HD2	2.26	0.53
8:V:6:ILE:HD11	8:V:193:LEU:HD11	1.89	0.53
11:Y:16:ALA:HA	11:Y:180:LEU:HB3	1.91	0.53
7:G:40:LEU:HD23	7:G:47:ILE:HD11	1.90	0.53
7:G:106:HIS:O	7:G:106:HIS:ND1	2.41	0.53
11:K:33:ASN:OD1	11:K:34:THR:N	2.40	0.53
1:O:9:TYR:HB2	1:O:12:HIS:CD2	2.43	0.53
7:U:236:ILE:O	7:U:239:PRO:HD2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:161:TYR:CE1	12:Z:193:VAL:HG22	2.43	0.53
14:b:55:SER:HB3	14:b:178:THR:HG22	1.89	0.53
13:M:96:LEU:HD22	13:M:120:LEU:HD21	1.89	0.53
2:P:107:VAL:O	2:P:111:VAL:HG23	2.09	0.53
3:C:68:ILE:HG21	3:C:110:LEU:HD21	1.91	0.53
9:I:42:TRP:HH2	9:I:185:HIS:HB2	1.74	0.53
11:K:16:ALA:HA	11:K:180:LEU:HB3	1.91	0.53
6:T:12:ILE:HG21	7:U:10:LEU:O	2.07	0.53
1:A:9:TYR:HB2	1:A:12:HIS:CD2	2.43	0.53
7:G:220:TRP:HB3	7:G:225:SER:OG	2.09	0.53
2:P:87:LEU:HD21	2:P:91:ARG:NH2	2.24	0.53
2:P:119:GLN:O	2:P:122:THR:OG1	2.18	0.53
5:E:102:ILE:HD12	13:M:122:VAL:CG2	2.39	0.53
1:O:234:VAL:HG22	1:O:241:PHE:HD1	1.73	0.53
9:W:42:TRP:HH2	9:W:185:HIS:HB2	1.74	0.53
14:b:181:ALA:O	14:b:185:ALA:N	2.42	0.53
2:B:87:LEU:HD21	2:B:91:ARG:NH2	2.24	0.52
10:J:28:ARG:HG3	10:J:36:THR:HG23	1.91	0.52
14:N:55:SER:HB3	14:N:178:THR:HG22	1.89	0.52
1:O:83:GLY:HA3	1:O:241:PHE:CE2	2.43	0.52
14:b:102:ARG:HG2	14:b:109:LEU:HG	1.91	0.52
5:E:182:LEU:HB2	5:E:203:VAL:HG13	1.91	0.52
12:L:7:LYS:O	12:L:143:TYR:OH	2.27	0.52
4:D:217:ILE:HG21	4:D:222:ILE:HD11	1.92	0.52
3:Q:68:ILE:HG21	3:Q:110:LEU:HD21	1.91	0.52
1:A:10:ASP:OD1	1:A:11:ARG:N	2.42	0.52
2:B:29:VAL:HG13	2:B:77:ALA:HB3	1.92	0.52
3:C:159:TRP:HE3	4:D:53:LEU:HG	1.74	0.52
14:N:94:TYR:O	14:N:98:VAL:HG23	2.10	0.52
6:T:137:TYR:OH	6:T:216:LYS:N	2.43	0.52
9:W:3:ILE:O	9:W:126:ALA:HA	2.10	0.52
10:J:156:SER:HA	10:J:159:LEU:HD12	1.92	0.52
12:L:137:SER:HA	11:Y:170:ARG:NH2	2.25	0.52
13:M:181:VAL:O	13:M:192:ASN:ND2	2.43	0.52
5:S:182:LEU:HB2	5:S:203:VAL:HG13	1.91	0.52
7:U:220:TRP:HB3	7:U:225:SER:OG	2.09	0.52
14:b:94:TYR:O	14:b:98:VAL:HG23	2.10	0.52
2:B:107:VAL:O	2:B:111:VAL:HG23	2.09	0.52
2:B:119:GLN:NE2	3:C:81:ALA:O	2.43	0.52
7:G:129:TRP:CE2	7:G:130:HIS:HD2	2.26	0.52
2:P:119:GLN:NE2	3:Q:81:ALA:O	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:204:ILE:O	3:Q:208:GLU:N	2.42	0.52
10:X:55:LEU:HB3	10:X:62:ILE:HG12	1.91	0.52
6:F:15:PRO:O	7:G:29:LYS:NZ	2.24	0.52
9:I:3:ILE:O	9:I:126:ALA:HA	2.10	0.52
11:K:57:PHE:HZ	11:K:85:THR:HG23	1.75	0.52
3:C:105:GLN:HE21	3:C:109:GLN:HB3	1.75	0.52
11:K:37:TYR:HB3	11:K:39:ILE:HD11	1.91	0.52
12:Z:7:LYS:O	12:Z:143:TYR:OH	2.27	0.52
6:F:137:TYR:OH	6:F:216:LYS:N	2.43	0.52
11:K:4:LEU:HB2	11:K:132:HIS:HB2	1.90	0.52
1:O:10:ASP:OD1	1:O:11:ARG:N	2.42	0.52
5:S:102:ILE:HD12	13:a:122:VAL:CG2	2.39	0.52
13:a:181:VAL:O	13:a:192:ASN:ND2	2.43	0.52
5:E:70:ILE:HG13	5:E:76:CYS:SG	2.50	0.51
10:J:55:LEU:HB3	10:J:62:ILE:HG12	1.91	0.51
11:K:104:ILE:HB	11:K:116:TYR:HB2	1.91	0.51
14:b:92:HIS:ND1	14:b:160:TYR:OH	2.22	0.51
4:D:208:LEU:O	4:D:215:THR:HG22	2.10	0.51
8:H:230:ILE:O	8:H:241:PHE:HB3	2.10	0.51
3:Q:159:TRP:HE3	4:R:53:LEU:HG	1.74	0.51
4:R:83:LEU:HD11	4:R:111:VAL:HG13	1.92	0.51
5:S:70:ILE:HG13	5:S:76:CYS:SG	2.50	0.51
8:V:9:ASP:N	8:V:201:MET:O	2.43	0.51
11:Y:37:TYR:HB3	11:Y:39:ILE:HD11	1.91	0.51
8:H:182:SER:C	8:H:186:SER:HB3	2.36	0.51
2:P:95:ILE:HG23	9:W:61:HIS:HB3	1.93	0.51
10:X:110:ILE:HD11	10:X:152:ASN:H	1.76	0.51
8:H:19:ARG:HB2	8:H:225:GLY:CA	2.40	0.51
11:K:118:CYS:SG	11:K:119:ASP:N	2.84	0.51
9:W:38:SER:HB2	9:W:41:ILE:HG23	1.92	0.51
7:G:32:ASN:O	7:G:170:LYS:HA	2.11	0.51
7:U:32:ASN:O	7:U:170:LYS:HA	2.11	0.51
7:U:220:TRP:HB3	7:U:225:SER:HG	1.75	0.51
8:V:19:ARG:HB2	8:V:225:GLY:CA	2.40	0.51
3:C:204:ILE:O	3:C:208:GLU:N	2.42	0.51
9:I:41:ILE:O	9:I:42:TRP:HD1	1.94	0.51
11:K:86:ARG:HD2	11:K:122:SER:OG	2.11	0.51
4:R:50:ILE:HB	4:R:53:LEU:HD23	1.92	0.51
6:T:137:TYR:CE1	6:T:215:GLY:HA2	2.46	0.51
11:Y:104:ILE:HB	11:Y:116:TYR:HB2	1.91	0.51
11:Y:151:LEU:HD11	11:Y:155:GLU:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:83:LEU:HD11	4:D:111:VAL:HG13	1.92	0.51
15:I:300:7F1:C32	15:I:300:7F1:N04	2.73	0.51
14:N:102:ARG:HG2	14:N:109:LEU:HG	1.91	0.51
4:R:208:LEU:O	4:R:215:THR:HG22	2.10	0.51
4:R:217:ILE:HG21	4:R:222:ILE:HD11	1.92	0.51
8:V:182:SER:C	8:V:186:SER:HB3	2.36	0.51
12:Z:45:MET:HB2	12:Z:52:CYS:HB3	1.93	0.51
3:C:236:ILE:O	3:C:240:THR:N	2.36	0.51
6:T:233:SER:O	6:T:237:MET:N	2.44	0.51
10:X:28:ARG:HG3	10:X:36:THR:HG23	1.91	0.51
13:a:113:ILE:HG21	13:a:148:VAL:CG2	2.41	0.51
7:G:50:CYS:HB3	7:G:68:ARG:NH1	2.26	0.51
8:H:9:ASP:N	8:H:201:MET:O	2.43	0.51
9:I:38:SER:HB2	9:I:41:ILE:HG23	1.92	0.51
2:P:111:VAL:HG21	2:P:147:TYR:HD2	1.76	0.51
4:R:17:LEU:O	4:R:21:HIS:ND1	2.40	0.51
15:W:300:7F1:C32	15:W:300:7F1:N04	2.73	0.51
12:Z:82:ILE:O	12:Z:86:ILE:HG12	2.11	0.51
10:J:110:ILE:HD11	10:J:152:ASN:H	1.76	0.51
11:K:151:LEU:HD11	11:K:155:GLU:HB2	1.92	0.51
12:L:82:ILE:O	12:L:86:ILE:HG12	2.11	0.51
13:M:113:ILE:HG21	13:M:148:VAL:CG2	2.41	0.51
1:A:169:TYR:HA	2:B:57:ILE:HA	1.93	0.50
8:H:203:LYS:HD2	8:H:232:ASN:ND2	2.22	0.50
11:K:170:ARG:NH2	12:Z:137:SER:HA	2.25	0.50
3:Q:105:GLN:HE21	3:Q:109:GLN:HB3	1.75	0.50
11:Y:57:PHE:HZ	11:Y:85:THR:HG23	1.75	0.50
11:Y:86:ARG:HD2	11:Y:122:SER:OG	2.11	0.50
6:F:167:SER:O	6:F:171:LEU:HG	2.11	0.50
4:R:131:THR:OG1	4:R:147:THR:HB	2.11	0.50
3:Q:109:GLN:HE21	11:Y:72:ASN:HB2	1.77	0.50
10:X:156:SER:HA	10:X:159:LEU:HD12	1.92	0.50
4:D:131:THR:OG1	4:D:147:THR:HB	2.11	0.50
8:H:192:TYR:HD1	8:V:192:TYR:HD1	1.58	0.50
12:L:45:MET:HB2	12:L:52:CYS:HB3	1.93	0.50
2:P:29:VAL:HG13	2:P:77:ALA:HB3	1.92	0.50
6:T:167:SER:O	6:T:171:LEU:HG	2.11	0.50
14:b:237:GLU:HB3	14:b:239:PRO:HD2	1.94	0.50
4:D:32:ALA:HA	4:D:45:VAL:HA	1.93	0.50
6:F:137:TYR:CE1	6:F:215:GLY:HA2	2.46	0.50
1:O:68:ASP:OD2	7:U:162:LYS:HE3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:169:TYR:HA	2:P:57:ILE:HA	1.93	0.50
4:R:115:GLN:O	4:R:119:THR:HG23	2.12	0.50
8:V:245:ASN:OD1	8:V:245:ASN:O	2.30	0.50
1:A:170:ARG:N	2:B:56:LEU:O	2.35	0.50
2:B:111:VAL:HG21	2:B:147:TYR:HD2	1.76	0.50
14:N:64:LEU:HD23	14:N:67:LEU:HD12	1.94	0.50
12:Z:179:ILE:HG23	12:Z:183:GLY:O	2.11	0.50
14:b:11:SER:H	14:b:42:ARG:HH12	1.59	0.50
4:D:50:ILE:HB	4:D:53:LEU:HD23	1.92	0.50
14:N:237:GLU:HB3	14:N:239:PRO:HD2	1.94	0.50
3:Q:96:ARG:O	3:Q:99:TYR:HB3	2.12	0.50
4:R:169:GLN:O	4:R:172:LEU:HB3	2.12	0.50
11:Y:108:ASP:HB3	11:Y:112:GLY:N	2.27	0.50
2:B:95:ILE:HG23	9:I:61:HIS:HB3	1.93	0.50
6:F:214:VAL:HB	6:F:220:TRP:HA	1.94	0.50
8:V:230:ILE:O	8:V:241:PHE:HB3	2.10	0.50
9:W:41:ILE:O	9:W:42:TRP:HD1	1.94	0.50
11:Y:47:LEU:HB3	11:Y:54:ARG:HB2	1.94	0.50
11:Y:65:VAL:HG21	11:Y:81:PHE:CD1	2.47	0.50
2:B:72:ILE:HG12	2:B:107:VAL:HG22	1.94	0.50
6:F:84:LEU:HD21	6:F:128:PHE:HE2	1.77	0.50
8:H:4:ILE:HG12	8:H:5:GLY:N	2.27	0.50
11:K:47:LEU:HB3	11:K:54:ARG:HB2	1.94	0.50
12:L:179:ILE:HG23	12:L:183:GLY:O	2.11	0.50
13:M:47:ASP:OD1	13:M:48:TYR:HD2	1.94	0.50
3:Q:195:THR:OG1	3:Q:196:LEU:N	2.45	0.50
12:Z:104:TYR:HB2	12:Z:109:PHE:CD2	2.46	0.50
10:J:60:THR:O	11:K:86:ARG:NH2	2.44	0.49
10:J:93:LEU:HA	10:J:96:ILE:HD12	1.93	0.49
13:M:56:ARG:HB3	13:M:217:GLY:HA3	1.93	0.49
3:Q:114:ILE:HG21	3:Q:134:PHE:CZ	2.42	0.49
11:Y:118:CYS:SG	11:Y:119:ASP:N	2.84	0.49
3:C:195:THR:OG1	3:C:196:LEU:N	2.45	0.49
6:F:233:SER:O	6:F:237:MET:N	2.44	0.49
11:K:108:ASP:HB3	11:K:112:GLY:N	2.27	0.49
7:U:50:CYS:HB3	7:U:68:ARG:NH1	2.26	0.49
8:V:4:ILE:HG12	8:V:5:GLY:N	2.27	0.49
14:b:54:PHE:CG	14:b:61:ALA:HB1	2.47	0.49
3:C:14:PRO:HA	4:D:21:HIS:HD2	1.77	0.49
8:H:245:ASN:OD1	8:H:245:ASN:O	2.30	0.49
11:K:65:VAL:HG21	11:K:81:PHE:CD1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:63:ILE:HD13	6:T:212:ALA:HB2	1.95	0.49
10:X:93:LEU:HA	10:X:96:ILE:HD12	1.93	0.49
1:A:68:ASP:OD2	7:G:162:LYS:HE3	2.12	0.49
12:L:104:TYR:HB2	12:L:109:PHE:CD2	2.46	0.49
13:M:223:TYR:CE2	13:M:232:VAL:HG22	2.47	0.49
3:Q:108:SER:OG	3:Q:148:TYR:OH	2.21	0.49
3:Q:167:ASN:HB3	3:Q:170:THR:HB	1.94	0.49
6:T:214:VAL:HB	6:T:220:TRP:HA	1.94	0.49
13:a:56:ARG:HB3	13:a:217:GLY:HA3	1.93	0.49
13:a:223:TYR:CE2	13:a:232:VAL:HG22	2.47	0.49
6:F:63:ILE:HD13	6:F:212:ALA:HB2	1.95	0.49
12:Z:25:PHE:HZ	13:a:174:LEU:HD12	1.78	0.49
13:a:47:ASP:OD1	13:a:48:TYR:HD2	1.94	0.49
14:b:64:LEU:HD23	14:b:67:LEU:HD12	1.94	0.49
3:C:167:ASN:HB3	3:C:170:THR:HB	1.94	0.49
5:E:240:ILE:HG23	5:E:241:ILE:HG13	1.95	0.49
11:K:57:PHE:CZ	11:K:85:THR:HG23	2.47	0.49
13:a:62:SER:HG	14:b:183:TYR:HH	1.59	0.49
4:D:115:GLN:O	4:D:119:THR:HG23	2.12	0.49
4:D:169:GLN:O	4:D:172:LEU:HB3	2.12	0.49
7:G:8:TYR:CZ	7:G:17:PRO:HG3	2.48	0.49
5:S:37:ALA:HA	5:S:50:SER:HA	1.95	0.49
9:W:42:TRP:HZ3	9:W:185:HIS:ND1	2.11	0.49
14:b:226:ILE:HG23	14:b:237:GLU:HB2	1.95	0.49
14:N:181:ALA:O	14:N:185:ALA:N	2.42	0.49
4:R:32:ALA:HA	4:R:45:VAL:HA	1.93	0.49
6:T:84:LEU:HD21	6:T:128:PHE:HE2	1.77	0.49
6:T:230:GLU:OE2	6:T:234:LYS:NZ	2.46	0.49
7:G:220:TRP:HE1	7:G:232:ILE:HG13	1.78	0.49
9:I:167:LEU:HD12	13:a:61:TYR:HA	1.95	0.49
13:M:61:TYR:HA	9:W:167:LEU:HD12	1.95	0.49
9:W:30:ASN:OD1	9:W:31:CYS:N	2.46	0.49
11:Y:57:PHE:CZ	11:Y:85:THR:HG23	2.47	0.49
9:I:42:TRP:HZ3	9:I:185:HIS:ND1	2.11	0.49
11:K:83:PHE:O	11:K:86:ARG:HB3	2.13	0.49
14:N:11:SER:H	14:N:42:ARG:HH12	1.59	0.49
2:B:118:VAL:HG13	2:B:130:PHE:HD2	1.78	0.48
3:C:96:ARG:O	3:C:99:TYR:HB3	2.12	0.48
5:E:37:ALA:HA	5:E:50:SER:HA	1.95	0.48
7:G:74:ASN:O	7:G:229:PHE:N	2.33	0.48
9:I:48:VAL:HG12	9:I:50:GLY:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:54:PHE:CG	14:N:61:ALA:HB1	2.47	0.48
10:X:135:THR:HG22	10:X:145:GLU:HA	1.95	0.48
11:Y:143:LEU:O	11:Y:147:TYR:HB2	2.13	0.48
12:Z:111:MET:HG2	12:Z:126:PHE:HD2	1.78	0.48
13:a:213:ASP:OD1	13:a:214:ILE:N	2.46	0.48
9:I:30:ASN:OD1	9:I:31:CYS:N	2.46	0.48
10:J:186:SER:CB	13:a:179:ASN:HD21	2.25	0.48
12:L:8:PHE:CE2	12:L:10:ASP:HB2	2.49	0.48
1:O:51:ILE:HG22	1:O:231:VAL:HG12	1.95	0.48
7:U:8:TYR:CZ	7:U:17:PRO:HG3	2.48	0.48
9:W:45:GLY:C	9:W:52:LEU:HD11	2.38	0.48
3:C:119:GLN:NE2	3:C:123:GLN:HB2	2.27	0.48
12:L:25:PHE:HZ	13:M:174:LEU:HD12	1.78	0.48
2:P:72:ILE:HG12	2:P:107:VAL:HG22	1.94	0.48
3:Q:119:GLN:NE2	3:Q:123:GLN:HB2	2.27	0.48
15:W:300:7F1:N04	10:X:138:ASP:OD2	2.46	0.48
4:D:17:LEU:O	4:D:21:HIS:ND1	2.40	0.48
11:K:143:LEU:O	11:K:147:TYR:HB2	2.13	0.48
3:Q:42:GLY:HA3	3:Q:215:LEU:O	2.13	0.48
9:W:33:LYS:HG2	15:W:300:7F1:C10	2.43	0.48
12:Z:6:PHE:CA	12:Z:111:MET:HE1	2.43	0.48
3:C:109:GLN:HE21	11:K:72:ASN:HB2	1.77	0.48
9:I:45:GLY:C	9:I:52:LEU:HD11	2.38	0.48
13:M:120:LEU:HB3	13:M:152:TYR:OH	2.14	0.48
4:R:17:LEU:HD22	4:R:21:HIS:HE1	1.78	0.48
9:W:48:VAL:HG12	9:W:50:GLY:H	1.78	0.48
4:D:178:GLU:OE1	4:D:178:GLU:N	2.46	0.48
6:F:32:GLY:O	6:F:162:ALA:N	2.47	0.48
10:J:63:GLN:HB2	11:K:86:ARG:HH21	1.78	0.48
3:Q:73:PHE:CE2	3:Q:215:LEU:HD23	2.48	0.48
12:Z:105:ASP:OD1	12:Z:105:ASP:N	2.46	0.48
3:C:42:GLY:HA3	3:C:215:LEU:O	2.13	0.48
4:D:36:LYS:HB2	4:D:144:ILE:HD12	1.96	0.48
6:F:230:GLU:OE2	6:F:234:LYS:NZ	2.46	0.48
8:H:8:TYR:CD1	8:H:9:ASP:N	2.82	0.48
9:I:19:ARG:HH21	9:I:169:SER:C	2.22	0.48
13:M:74:LEU:HD22	13:M:100:ILE:HD12	1.96	0.48
13:M:179:ASN:HD21	10:X:186:SER:CB	2.25	0.48
13:M:213:ASP:OD1	13:M:214:ILE:N	2.46	0.48
5:S:97:ASN:HD21	12:Z:64:LYS:HB3	1.79	0.48
12:Z:8:PHE:CE2	12:Z:10:ASP:HB2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:40:ILE:HD12	5:E:200:ALA:HB2	1.96	0.48
7:G:49:CYS:HB2	7:G:218:PHE:CD1	2.49	0.48
7:G:68:ARG:HD3	7:G:80:TYR:O	2.13	0.48
9:I:12:VAL:HG13	9:I:110:LEU:HD12	1.95	0.48
3:Q:109:GLN:O	3:Q:113:GLN:HG2	2.13	0.48
4:R:36:LYS:HB2	4:R:144:ILE:HD12	1.96	0.48
6:T:32:GLY:O	6:T:162:ALA:N	2.47	0.48
3:C:86:LEU:O	3:C:90:SER:OG	2.14	0.48
5:E:97:ASN:HD21	12:L:64:LYS:HB3	1.79	0.48
9:I:33:LYS:HG2	15:I:300:7F1:C10	2.43	0.48
15:I:300:7F1:N04	10:J:138:ASP:OD2	2.46	0.48
3:Q:213:ALA:HB1	3:Q:220:GLY:HA3	1.96	0.48
8:V:8:TYR:CD1	8:V:9:ASP:N	2.82	0.48
5:E:65:GLU:HA	5:E:218:GLU:OE1	2.14	0.48
3:Q:14:PRO:HA	4:R:21:HIS:HD2	1.77	0.48
4:R:36:LYS:HD2	4:R:143:CYS:HA	1.96	0.48
5:S:40:ILE:HD12	5:S:200:ALA:HB2	1.96	0.48
7:U:220:TRP:HE1	7:U:232:ILE:HG13	1.78	0.48
11:Y:35:LYS:HE2	11:Y:54:ARG:HH12	1.79	0.48
3:C:109:GLN:O	3:C:113:GLN:HG2	2.13	0.47
3:C:213:ALA:HB1	3:C:220:GLY:HA3	1.96	0.47
4:D:17:LEU:HD22	4:D:21:HIS:HE1	1.78	0.47
14:N:226:ILE:HG23	14:N:237:GLU:HB2	1.95	0.47
2:P:22:ILE:O	2:P:26:LEU:HG	2.14	0.47
2:P:118:VAL:HG13	2:P:130:PHE:HD2	1.78	0.47
5:S:65:GLU:HA	5:S:218:GLU:OE1	2.14	0.47
1:A:51:ILE:HG22	1:A:231:VAL:HG12	1.95	0.47
2:B:22:ILE:O	2:B:26:LEU:HG	2.14	0.47
12:L:19:ARG:HA	12:L:29:GLN:HA	1.97	0.47
12:L:132:SER:O	12:L:136:TYR:HB2	2.14	0.47
5:S:223:LYS:HB2	5:S:226:ASP:HB3	1.96	0.47
9:W:19:ARG:HH21	9:W:169:SER:C	2.22	0.47
11:Y:83:PHE:O	11:Y:86:ARG:HB3	2.13	0.47
12:Z:19:ARG:HA	12:Z:29:GLN:HA	1.97	0.47
8:H:153:PHE:HB2	8:H:165:TYR:HB2	1.97	0.47
14:N:27:ARG:NH2	14:N:39:ASN:O	2.47	0.47
2:P:154:CYS:SG	3:Q:81:ALA:HB2	2.54	0.47
8:V:19:ARG:HH11	8:V:26:ILE:HD13	1.79	0.47
8:V:153:PHE:HB2	8:V:165:TYR:HB2	1.97	0.47
10:X:60:THR:O	11:Y:86:ARG:NH2	2.44	0.47
12:Z:132:SER:O	12:Z:136:TYR:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:73:PHE:CE2	3:C:215:LEU:HD23	2.48	0.47
5:E:223:LYS:HB2	5:E:226:ASP:HB3	1.96	0.47
5:E:226:ASP:C	5:E:228:THR:H	2.22	0.47
9:I:159:ILE:HG21	9:I:173:VAL:HG13	1.95	0.47
9:W:12:VAL:HG13	9:W:110:LEU:HD12	1.95	0.47
9:W:159:ILE:HG21	9:W:173:VAL:HG13	1.95	0.47
12:Z:7:LYS:HE3	12:Z:109:PHE:H	1.80	0.47
5:E:109:ILE:O	5:E:113:VAL:HG23	2.14	0.47
9:I:167:LEU:HD13	13:a:215:TYR:HD1	1.79	0.47
12:L:7:LYS:HE3	12:L:109:PHE:H	1.80	0.47
12:L:105:ASP:N	12:L:105:ASP:OD1	2.46	0.47
4:R:95:TYR:CD2	11:Y:63:LYS:HE3	2.49	0.47
5:S:109:ILE:O	5:S:113:VAL:HG23	2.14	0.47
5:S:240:ILE:HG23	5:S:241:ILE:HG13	1.95	0.47
7:U:49:CYS:HB2	7:U:218:PHE:CD1	2.49	0.47
7:U:222:CYS:SG	7:U:225:SER:OG	2.52	0.47
11:Y:39:ILE:HG23	11:Y:62:ARG:HA	1.96	0.47
4:D:95:TYR:CD2	11:K:63:LYS:HE3	2.49	0.47
10:J:101:ARG:O	10:J:104:PRO:HD2	2.15	0.47
12:L:111:MET:HG2	12:L:126:PHE:HD2	1.78	0.47
13:M:215:TYR:HD1	9:W:167:LEU:HD13	1.79	0.47
14:N:11:SER:OG	14:N:181:ALA:HB2	2.15	0.47
7:U:68:ARG:HD3	7:U:80:TYR:O	2.13	0.47
10:X:101:ARG:O	10:X:104:PRO:HD2	2.15	0.47
1:A:138:ARG:HB3	7:G:13:SER:HB2	1.97	0.47
2:B:164:GLY:O	2:B:167:TYR:HB3	2.15	0.47
3:C:73:PHE:CD2	3:C:215:LEU:HD23	2.50	0.47
3:C:99:TYR:HA	10:J:67:GLU:OE2	2.15	0.47
10:J:135:THR:HG22	10:J:145:GLU:HA	1.95	0.47
11:K:39:ILE:HG23	11:K:62:ARG:HA	1.96	0.47
1:O:138:ARG:HB3	7:U:13:SER:HB2	1.97	0.47
6:T:75:SER:HB3	6:T:160:PHE:CE2	2.50	0.47
13:a:120:LEU:HB3	13:a:152:TYR:OH	2.14	0.47
14:b:11:SER:OG	14:b:181:ALA:HB2	2.15	0.47
14:b:21:ILE:CG2	14:b:229:VAL:HB	2.45	0.47
3:C:97:TYR:OH	11:K:68:TYR:OH	2.21	0.47
11:K:35:LYS:HE2	11:K:54:ARG:HH12	1.79	0.47
13:M:86:GLN:HB3	14:N:169:THR:HG23	1.97	0.47
14:N:34:TYR:CG	8:V:188:TYR:OH	2.68	0.47
1:O:235:SER:HA	1:O:238:ASN:HA	1.97	0.47
3:Q:86:LEU:O	3:Q:90:SER:OG	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:108:SER:HG	3:Q:148:TYR:HH	1.49	0.47
5:S:68:LEU:HD12	5:S:89:ILE:HG13	1.96	0.47
6:T:191:LEU:HD21	6:T:211:LEU:HD22	1.97	0.47
8:V:76:PHE:CZ	8:V:163:GLN:HB2	2.50	0.47
12:Z:125:LEU:HD12	12:Z:125:LEU:O	2.15	0.47
13:a:74:LEU:HD22	13:a:100:ILE:HD12	1.96	0.47
14:b:27:ARG:NH2	14:b:39:ASN:O	2.47	0.47
6:F:191:LEU:HD21	6:F:211:LEU:HD22	1.97	0.47
8:H:19:ARG:HH11	8:H:26:ILE:HD13	1.79	0.47
13:M:210:THR:HG22	13:M:216:THR:HG22	1.96	0.47
1:O:51:ILE:CG2	1:O:231:VAL:HG12	2.45	0.47
2:P:164:GLY:O	2:P:167:TYR:HB3	2.15	0.47
4:R:178:GLU:OE1	4:R:178:GLU:N	2.46	0.47
5:S:237:ILE:HA	5:S:240:ILE:HG22	1.96	0.47
12:Z:20:ALA:HB3	12:Z:31:VAL:HG11	1.97	0.47
11:K:29:LYS:O	12:L:136:TYR:OH	2.32	0.47
11:Y:29:LYS:O	12:Z:136:TYR:OH	2.32	0.47
2:B:154:CYS:SG	3:C:81:ALA:HB2	2.54	0.46
11:K:40:HIS:NE2	11:K:75:ASP:HB2	2.29	0.46
12:L:125:LEU:HD12	12:L:125:LEU:O	2.15	0.46
5:S:226:ASP:C	5:S:228:THR:H	2.22	0.46
7:U:109:ILE:HG12	7:U:110:PRO:O	2.15	0.46
1:A:140:HIS:O	1:A:162:PRO:HB3	2.16	0.46
4:D:36:LYS:HD2	4:D:143:CYS:HA	1.96	0.46
7:G:129:TRP:CZ2	7:G:130:HIS:HD2	2.32	0.46
8:H:44:CYS:HB2	8:H:152:ILE:HB	1.97	0.46
7:U:129:TRP:CZ2	7:U:130:HIS:HD2	2.32	0.46
1:A:121:CYS:SG	1:A:146:ILE:HD12	2.56	0.46
8:H:20:THR:HG1	8:H:33:LYS:HZ1	1.60	0.46
11:K:164:PHE:CD2	11:K:178:TYR:HD2	2.33	0.46
2:P:111:VAL:HG21	2:P:147:TYR:CD2	2.50	0.46
12:Z:40:ASN:ND2	12:Z:104:TYR:HB3	2.30	0.46
7:G:40:LEU:HD22	7:G:196:ILE:HD11	1.98	0.46
7:G:109:ILE:HG12	7:G:110:PRO:O	2.15	0.46
11:K:37:TYR:CD1	11:K:47:LEU:HD12	2.50	0.46
12:L:20:ALA:HB3	12:L:31:VAL:HG11	1.97	0.46
12:L:41:ILE:CD1	12:L:76:VAL:HG13	2.46	0.46
2:P:36:LEU:HD13	2:P:195:LEU:HD13	1.98	0.46
1:A:51:ILE:CG2	1:A:231:VAL:HG12	2.45	0.46
5:E:68:LEU:HD12	5:E:89:ILE:HG13	1.96	0.46
6:F:34:CYS:HA	6:F:160:PHE:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:232:LEU:O	6:F:235:VAL:HG22	2.16	0.46
8:H:188:TYR:OH	14:b:34:TYR:CG	2.68	0.46
11:K:171:PHE:CG	11:K:172:LEU:N	2.84	0.46
12:L:40:ASN:ND2	12:L:104:TYR:HB3	2.30	0.46
8:V:2:THR:HG22	8:V:185:GLY:HA3	1.98	0.46
11:Y:37:TYR:CD1	11:Y:47:LEU:HD12	2.50	0.46
13:a:40:VAL:HG21	13:a:81:GLY:HA3	1.98	0.46
13:a:152:TYR:HD1	13:a:153:ASP:O	1.98	0.46
13:a:210:THR:HG22	13:a:216:THR:HG22	1.96	0.46
5:E:111:SER:O	5:E:115:LEU:HG	2.15	0.46
14:N:21:ILE:CG2	14:N:229:VAL:HB	2.45	0.46
3:Q:109:GLN:HG3	11:Y:72:ASN:ND2	2.30	0.46
5:S:111:SER:O	5:S:115:LEU:HG	2.15	0.46
7:U:40:LEU:HD22	7:U:196:ILE:HD11	1.98	0.46
1:A:235:SER:HA	1:A:238:ASN:HA	1.97	0.46
4:R:31:CYS:HA	4:R:162:GLY:HA3	1.98	0.46
6:T:30:LYS:HA	6:T:30:LYS:HD3	1.63	0.46
5:E:237:ILE:HA	5:E:240:ILE:HG22	1.96	0.46
6:F:13:TYR:HB2	7:G:23:GLN:OE1	2.16	0.46
11:K:183:MET:SD	11:K:188:VAL:HG12	2.56	0.46
13:M:152:TYR:HD1	13:M:153:ASP:O	1.98	0.46
1:O:121:CYS:SG	1:O:146:ILE:HD12	2.56	0.46
1:O:140:HIS:O	1:O:162:PRO:HB3	2.16	0.46
6:T:116:TYR:CE1	6:T:146:THR:HG21	2.51	0.46
11:Y:40:HIS:CD2	11:Y:69:GLN:NE2	2.80	0.46
11:Y:77:PHE:O	11:Y:80:SER:N	2.48	0.46
11:Y:171:PHE:CG	11:Y:172:LEU:N	2.84	0.46
12:Z:41:ILE:CD1	12:Z:76:VAL:HG13	2.46	0.46
12:Z:147:LEU:HD13	12:Z:151:GLN:CG	2.46	0.46
13:a:45:GLY:HA3	13:a:48:TYR:CZ	2.50	0.46
3:C:155:ASN:HD22	4:D:77:ASN:HB3	1.81	0.46
6:F:116:TYR:CE1	6:F:146:THR:HG21	2.51	0.46
6:T:13:TYR:HB2	7:U:23:GLN:OE1	2.16	0.46
8:V:44:CYS:HB2	8:V:152:ILE:HB	1.97	0.46
10:X:155:THR:HG21	10:X:194:SER:OG	2.16	0.46
12:Z:51:ASP:O	12:Z:55:TRP:HD1	1.99	0.46
12:Z:125:LEU:HD13	12:Z:139:LEU:HB3	1.98	0.46
4:D:101:PRO:O	4:D:103:PRO:HD3	2.16	0.46
5:E:50:SER:O	5:E:217:VAL:HA	2.16	0.46
6:F:145:GLU:HB2	6:F:158:LEU:HD22	1.97	0.46
8:H:2:THR:HG22	8:H:185:GLY:HA3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:74:ILE:HD11	2:P:87:LEU:HD13	1.98	0.46
2:P:107:VAL:HG21	2:P:138:GLY:HA3	1.98	0.46
3:Q:73:PHE:CD2	3:Q:215:LEU:HD23	2.50	0.46
4:R:101:PRO:O	4:R:103:PRO:HD3	2.16	0.46
6:T:34:CYS:HA	6:T:160:PHE:O	2.16	0.46
6:T:232:LEU:O	6:T:235:VAL:HG22	2.16	0.46
11:Y:103:LEU:HG	11:Y:132:HIS:CD2	2.51	0.46
11:Y:164:PHE:CD2	11:Y:178:TYR:HD2	2.33	0.46
2:B:36:LEU:HD13	2:B:195:LEU:HD13	1.98	0.45
6:F:75:SER:HB3	6:F:160:PHE:CE2	2.50	0.45
10:J:21:VAL:CG1	10:J:132:PRO:HB3	2.46	0.45
11:K:77:PHE:O	11:K:80:SER:N	2.48	0.45
12:L:6:PHE:CA	12:L:111:MET:HE1	2.43	0.45
12:L:125:LEU:HD13	12:L:139:LEU:HB3	1.98	0.45
13:M:40:VAL:HG21	13:M:81:GLY:HA3	1.98	0.45
3:Q:155:ASN:HD22	4:R:77:ASN:HB3	1.81	0.45
6:T:15:PRO:O	7:U:29:LYS:NZ	2.24	0.45
10:X:63:GLN:HB2	11:Y:86:ARG:HH21	1.78	0.45
13:a:86:GLN:HB3	14:b:169:THR:HG23	1.97	0.45
8:H:43:VAL:HG22	8:H:153:PHE:CD1	2.51	0.45
6:T:15:PRO:HA	7:U:26:TYR:CZ	2.51	0.45
6:T:145:GLU:HB2	6:T:158:LEU:HD22	1.97	0.45
8:V:49:SER:O	8:V:53:GLN:HG3	2.17	0.45
10:X:21:VAL:CG1	10:X:132:PRO:HB3	2.46	0.45
3:C:109:GLN:HG3	11:K:72:ASN:ND2	2.30	0.45
3:C:163:ALA:O	3:C:168:ASN:HA	2.16	0.45
4:D:31:CYS:HA	4:D:162:GLY:HA3	1.98	0.45
11:K:103:LEU:HG	11:K:132:HIS:CD2	2.51	0.45
13:M:45:GLY:HA3	13:M:48:TYR:CZ	2.50	0.45
14:N:54:PHE:HB3	14:N:113:ILE:HG12	1.99	0.45
3:Q:13:SER:HB3	3:Q:17:ARG:H	1.81	0.45
3:Q:99:TYR:HA	10:X:67:GLU:OE2	2.15	0.45
8:V:4:ILE:CG1	8:V:5:GLY:N	2.79	0.45
11:Y:183:MET:SD	11:Y:188:VAL:HG12	2.56	0.45
2:B:111:VAL:HG21	2:B:147:TYR:CD2	2.50	0.45
6:F:228:LEU:HA	6:F:231:TYR:CD2	2.52	0.45
7:G:220:TRP:NE1	7:G:232:ILE:HG13	2.32	0.45
8:H:4:ILE:CG1	8:H:5:GLY:N	2.79	0.45
1:O:170:ARG:N	2:P:56:LEU:O	2.35	0.45
6:T:63:ILE:HD13	6:T:212:ALA:CB	2.46	0.45
8:V:232:ASN:O	8:V:234:THR:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:63:ILE:HD13	6:F:212:ALA:CB	2.46	0.45
7:G:175:PHE:CE1	7:G:200:ILE:HA	2.49	0.45
7:G:226:SER:C	7:G:228:GLU:H	2.25	0.45
8:H:214:VAL:HG11	8:H:228:ILE:HG21	1.98	0.45
6:T:223:ILE:O	6:T:228:LEU:HD22	2.17	0.45
7:U:220:TRP:NE1	7:U:232:ILE:HG13	2.32	0.45
8:V:214:VAL:HG11	8:V:228:ILE:HG21	1.98	0.45
10:X:13:LEU:HD13	10:X:184:LEU:HD21	1.98	0.45
11:Y:18:ASP:HA	11:Y:178:TYR:CD1	2.52	0.45
3:C:13:SER:HB3	3:C:17:ARG:N	2.32	0.45
6:F:15:PRO:HA	7:G:26:TYR:CZ	2.51	0.45
10:J:155:THR:HG21	10:J:194:SER:OG	2.16	0.45
7:U:172:LYS:O	7:U:176:LYS:HG3	2.17	0.45
8:V:43:VAL:HG22	8:V:153:PHE:CD1	2.51	0.45
10:X:14:GLY:O	10:X:149:PHE:HA	2.17	0.45
13:a:44:THR:HG23	13:a:147:GLY:H	1.82	0.45
8:H:76:PHE:CZ	8:H:163:GLN:HB2	2.50	0.45
8:H:179:PHE:HZ	8:H:194:GLN:HB3	1.81	0.45
11:K:90:ALA:HB2	11:K:122:SER:CB	2.47	0.45
12:L:147:LEU:HD13	12:L:151:GLN:CG	2.46	0.45
12:L:179:ILE:HG12	12:L:184:TYR:HB3	1.97	0.45
12:L:180:HIS:CD2	12:L:181:LYS:H	2.35	0.45
6:T:7:ASP:HA	6:T:12:ILE:HD11	1.99	0.45
8:V:179:PHE:HZ	8:V:194:GLN:HB3	1.81	0.45
12:Z:180:HIS:CD2	12:Z:181:LYS:H	2.35	0.45
14:b:42:ARG:N	14:b:225:GLN:HE22	1.97	0.45
6:T:93:LEU:HD13	13:a:102:LEU:HB2	1.98	0.45
9:W:1:THR:OG1	15:W:300:7F1:C01	2.61	0.45
10:X:60:THR:HG22	11:Y:123:ASN:N	2.32	0.45
1:A:65:LYS:HB2	1:A:67:LEU:HG	1.99	0.45
2:B:107:VAL:HG21	2:B:138:GLY:HA3	1.98	0.45
3:C:13:SER:HB3	3:C:17:ARG:H	1.81	0.45
6:F:149:ASN:OD1	6:F:151:SER:OG	2.20	0.45
8:H:232:ASN:O	8:H:234:THR:N	2.49	0.45
14:N:212:ILE:HG21	9:W:136:ALA:HA	1.99	0.45
3:Q:163:ALA:O	3:Q:168:ASN:HA	2.16	0.45
4:R:116:GLN:O	4:R:119:THR:OG1	2.24	0.45
7:U:193:ILE:HD12	7:U:218:PHE:CD2	2.52	0.45
7:U:226:SER:C	7:U:228:GLU:H	2.25	0.45
7:G:193:ILE:HD12	7:G:218:PHE:CD2	2.52	0.45
13:M:44:THR:HG23	13:M:147:GLY:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:110:TYR:HA	13:M:111:PRO:HD3	1.78	0.45
2:P:68:ILE:HG21	2:P:110:LEU:HD21	1.99	0.45
6:T:228:LEU:HA	6:T:231:TYR:CD2	2.52	0.45
7:U:72:VAL:HG22	7:U:76:ILE:HB	1.99	0.45
12:Z:179:ILE:HG12	12:Z:184:TYR:HB3	1.97	0.45
1:A:125:CYS:SG	1:A:165:PHE:N	2.91	0.44
2:B:86:LEU:HD12	2:B:132:LEU:HD11	1.99	0.44
3:C:193:LEU:HD23	3:C:196:LEU:HD22	1.99	0.44
7:G:129:TRP:CE3	7:G:129:TRP:N	2.80	0.44
15:I:300:7F1:C24	10:J:140:ILE:CB	2.92	0.44
10:J:13:LEU:HD13	10:J:184:LEU:HD21	1.98	0.44
6:T:68:ASP:O	6:T:219:PRO:HB2	2.17	0.44
9:W:84:THR:HG21	9:W:119:SER:HB2	2.00	0.44
15:W:300:7F1:C29	10:X:138:ASP:OD2	2.65	0.44
11:Y:40:HIS:NE2	11:Y:75:ASP:HB2	2.29	0.44
11:Y:90:ALA:HB2	11:Y:122:SER:CB	2.47	0.44
13:a:121:CYS:HB2	13:a:158:TYR:HD2	1.82	0.44
7:G:72:VAL:HG22	7:G:76:ILE:HB	1.99	0.44
7:G:193:ILE:HG23	7:G:218:PHE:CE2	2.53	0.44
12:L:51:ASP:O	12:L:55:TRP:HD1	1.99	0.44
9:W:42:TRP:CZ3	9:W:185:HIS:ND1	2.85	0.44
9:W:153:ASN:OD1	9:W:154:LEU:N	2.50	0.44
13:a:127:ARG:HG2	13:a:127:ARG:O	2.18	0.44
6:F:30:LYS:HA	6:F:30:LYS:HD3	1.63	0.44
7:G:172:LYS:O	7:G:176:LYS:HG3	2.17	0.44
9:I:1:THR:OG1	15:I:300:7F1:C01	2.61	0.44
9:I:153:ASN:OD1	9:I:154:LEU:N	2.50	0.44
10:J:14:GLY:O	10:J:149:PHE:HA	2.17	0.44
7:U:193:ILE:HG23	7:U:218:PHE:CE2	2.53	0.44
1:A:234:VAL:HA	1:A:241:PHE:HA	1.99	0.44
2:B:74:ILE:HD11	2:B:87:LEU:HD13	1.98	0.44
7:G:138:ILE:HG22	7:G:140:ILE:HG13	2.00	0.44
13:M:121:CYS:HB2	13:M:158:TYR:HD2	1.82	0.44
14:N:27:ARG:HG2	14:N:225:GLN:OE1	2.18	0.44
3:Q:13:SER:HB3	3:Q:17:ARG:N	2.32	0.44
5:S:50:SER:O	5:S:217:VAL:HA	2.16	0.44
13:a:121:CYS:HB2	13:a:158:TYR:CD2	2.52	0.44
3:C:35:ILE:HG12	3:C:196:LEU:HD12	2.00	0.44
10:J:59:ALA:HB3	11:K:123:ASN:OD1	2.17	0.44
11:Y:184:TYR:CG	11:Y:185:ASP:N	2.86	0.44
6:F:7:ASP:HA	6:F:12:ILE:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:68:ASP:O	6:F:219:PRO:HB2	2.17	0.44
6:F:70:ILE:HA	6:F:136:ALA:CB	2.48	0.44
11:K:13:VAL:HB	11:K:183:MET:HG3	2.00	0.44
11:K:184:TYR:CG	11:K:185:ASP:N	2.86	0.44
13:M:120:LEU:HA	13:M:120:LEU:HD23	1.69	0.44
2:P:86:LEU:HD12	2:P:132:LEU:HD11	1.99	0.44
9:W:66:HIS:ND1	9:W:78:MET:HE1	2.33	0.44
10:X:59:ALA:HB3	11:Y:123:ASN:OD1	2.17	0.44
13:a:194:ASN:OD1	13:a:195:LEU:N	2.51	0.44
2:B:111:VAL:HG22	2:B:136:ILE:HD12	2.00	0.44
5:E:152:GLY:HA2	5:E:153:PRO:HD3	1.79	0.44
6:F:145:GLU:HB3	6:F:155:TYR:CE1	2.53	0.44
6:F:223:ILE:O	6:F:228:LEU:HD22	2.17	0.44
8:H:1:THR:O	8:H:183:GLY:HA3	2.18	0.44
8:H:49:SER:O	8:H:53:GLN:HG3	2.17	0.44
3:Q:193:LEU:HD23	3:Q:196:LEU:HD22	1.99	0.44
6:T:145:GLU:HB3	6:T:155:TYR:CE1	2.53	0.44
7:U:50:CYS:C	7:U:51:ILE:HD12	2.43	0.44
11:Y:62:ARG:HE	11:Y:63:LYS:NZ	2.16	0.44
11:Y:151:LEU:HG	11:Y:152:THR:O	2.18	0.44
12:Z:33:LYS:HZ1	12:Z:45:MET:HE2	1.71	0.44
13:a:118:ARG:O	13:a:122:VAL:HG23	2.18	0.44
14:b:54:PHE:HB3	14:b:113:ILE:HG12	1.99	0.44
4:D:156:TRP:HA	5:E:59:ILE:HA	2.00	0.44
5:E:79:SER:OG	5:E:172:ILE:HB	2.17	0.44
6:F:10:ASN:HB3	6:F:21:GLN:CB	2.46	0.44
6:F:69:TYR:CD1	6:F:219:PRO:HA	2.52	0.44
6:F:93:LEU:HD13	13:M:102:LEU:HB2	1.98	0.44
9:I:42:TRP:CZ3	9:I:185:HIS:ND1	2.85	0.44
9:I:136:ALA:HA	14:b:212:ILE:HG21	1.99	0.44
11:K:18:ASP:HA	11:K:178:TYR:CD1	2.52	0.44
11:K:151:LEU:HG	11:K:152:THR:O	2.18	0.44
13:M:57:LEU:HG	13:M:64:TYR:HD2	1.83	0.44
1:O:73:THR:OG1	1:O:75:ILE:HG22	2.18	0.44
5:S:101:PHE:HD1	12:Z:61:LYS:HD3	1.83	0.44
6:T:69:TYR:CD1	6:T:219:PRO:HA	2.52	0.44
11:Y:108:ASP:CG	11:Y:111:ASP:H	2.25	0.44
14:b:16:LYS:HB2	14:b:159:LEU:HD23	2.00	0.44
1:A:73:THR:OG1	1:A:75:ILE:HG22	2.18	0.44
4:D:9:VAL:HG23	5:E:23:GLN:OE1	2.18	0.44
5:E:101:PHE:HD1	12:L:61:LYS:HD3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:13:VAL:HG23	11:K:113:TYR:CD1	2.53	0.44
12:L:35:ILE:HD12	12:L:56:GLU:HG3	2.00	0.44
13:M:127:ARG:O	13:M:127:ARG:HG2	2.18	0.44
5:S:226:ASP:C	5:S:228:THR:N	2.76	0.44
7:U:122:ILE:HD12	7:U:154:ILE:HG21	2.00	0.44
11:Y:27:LYS:NZ	12:Z:133:THR:HG22	2.33	0.44
13:a:85:MET:N	13:a:133:TYR:HD2	2.14	0.44
2:B:68:ILE:HG21	2:B:110:LEU:HD21	1.99	0.43
13:M:121:CYS:HB2	13:M:158:TYR:CD2	2.52	0.43
13:M:194:ASN:OD1	13:M:195:LEU:N	2.51	0.43
1:O:65:LYS:HB2	1:O:67:LEU:HG	1.99	0.43
2:P:111:VAL:HG22	2:P:136:ILE:HD12	2.00	0.43
4:R:156:TRP:HA	5:S:59:ILE:HA	2.00	0.43
11:Y:148:HIS:CD2	11:Y:151:LEU:HD13	2.53	0.43
6:F:35:ALA:O	6:F:159:SER:HA	2.18	0.43
7:G:233:HIS:HB3	7:G:236:ILE:CG1	2.48	0.43
8:H:189:ILE:HG21	8:H:213:CYS:HB3	1.99	0.43
9:I:177:VAL:HG13	9:I:184:GLN:HB2	2.00	0.43
15:I:300:7F1:C29	10:J:138:ASP:OD2	2.65	0.43
12:L:100:ILE:HG12	12:L:113:TYR:HD1	1.83	0.43
13:M:206:ILE:HG21	13:M:220:THR:HG21	2.00	0.43
14:N:75:ASN:OD1	14:N:75:ASN:N	2.51	0.43
2:P:71:HIS:HD2	2:P:139:VAL:HB	1.83	0.43
3:Q:35:ILE:HG12	3:Q:196:LEU:HD12	2.00	0.43
5:S:79:SER:OG	5:S:172:ILE:HB	2.17	0.43
12:Z:35:ILE:HD12	12:Z:56:GLU:HG3	2.00	0.43
2:B:162:CYS:SG	2:B:174:LEU:HD11	2.59	0.43
3:C:35:ILE:O	3:C:45:LEU:HG	2.19	0.43
5:E:213:SER:O	5:E:217:VAL:HG22	2.18	0.43
7:G:171:ASN:HB3	7:G:175:PHE:HE2	1.83	0.43
9:I:66:HIS:ND1	9:I:78:MET:HE1	2.33	0.43
9:I:84:THR:HG21	9:I:119:SER:HB2	2.00	0.43
12:L:33:LYS:HE3	12:L:45:MET:HG3	2.00	0.43
14:N:103:LYS:HA	14:N:108:PRO:HG3	2.00	0.43
1:O:77:ASN:HA	1:O:83:GLY:HA2	2.00	0.43
1:O:125:CYS:SG	1:O:165:PHE:N	2.91	0.43
5:S:152:GLY:HA2	5:S:153:PRO:HD3	1.79	0.43
5:S:213:SER:O	5:S:217:VAL:HG22	2.18	0.43
8:V:1:THR:O	8:V:183:GLY:HA3	2.18	0.43
14:b:75:ASN:OD1	14:b:75:ASN:N	2.51	0.43
2:B:70:GLU:O	2:B:218:PRO:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:24:ALA:O	3:C:28:ILE:HG23	2.18	0.43
6:F:26:SER:O	6:F:30:LYS:HG2	2.19	0.43
10:J:60:THR:HG22	11:K:123:ASN:N	2.32	0.43
11:K:27:LYS:NZ	12:L:133:THR:HG22	2.33	0.43
12:L:184:TYR:HD2	12:L:185:ASP:O	2.02	0.43
14:N:165:ASP:N	14:N:169:THR:O	2.50	0.43
3:Q:24:ALA:O	3:Q:28:ILE:HG23	2.18	0.43
8:V:38:ASN:HB3	8:V:40:ASN:OD1	2.18	0.43
11:Y:13:VAL:HB	11:Y:183:MET:HG3	2.00	0.43
12:Z:3:THR:HG22	12:Z:16:VAL:HG23	2.00	0.43
13:a:49:VAL:HG12	13:a:225:ILE:HB	2.00	0.43
7:U:138:ILE:HG22	7:U:140:ILE:HG13	2.00	0.43
1:A:160:PHE:HA	1:A:165:PHE:O	2.19	0.43
2:B:71:HIS:HD2	2:B:139:VAL:HB	1.83	0.43
9:I:1:THR:N	15:I:300:7F1:O01	2.50	0.43
11:K:62:ARG:HE	11:K:63:LYS:NZ	2.16	0.43
11:K:108:ASP:CG	11:K:111:ASP:H	2.25	0.43
12:L:3:THR:HG22	12:L:16:VAL:HG23	2.00	0.43
14:N:54:PHE:CD2	14:N:61:ALA:HB1	2.53	0.43
2:P:161:THR:OG1	2:P:162:CYS:N	2.52	0.43
4:R:9:VAL:HG23	5:S:23:GLN:OE1	2.18	0.43
7:U:75:ASN:OD1	7:U:76:ILE:N	2.52	0.43
7:U:233:HIS:HB3	7:U:236:ILE:CG1	2.48	0.43
8:V:189:ILE:HG21	8:V:213:CYS:HB3	1.99	0.43
11:Y:118:CYS:O	11:Y:132:HIS:HE1	2.02	0.43
13:a:48:TYR:OH	13:a:193:PHE:HB3	2.19	0.43
14:b:103:LYS:HA	14:b:108:PRO:HG3	2.00	0.43
1:A:231:VAL:O	1:A:243:GLN:HG3	2.18	0.43
2:B:161:THR:OG1	2:B:162:CYS:N	2.52	0.43
11:K:118:CYS:O	11:K:132:HIS:HE1	2.02	0.43
11:K:148:HIS:CD2	11:K:151:LEU:HD13	2.53	0.43
13:M:44:THR:OG1	13:M:147:GLY:O	2.26	0.43
1:O:234:VAL:HA	1:O:241:PHE:HA	1.99	0.43
2:P:70:GLU:O	2:P:218:PRO:HA	2.18	0.43
2:P:162:CYS:SG	2:P:174:LEU:HD11	2.59	0.43
7:U:175:PHE:CE1	7:U:200:ILE:HA	2.49	0.43
8:V:20:THR:HG1	8:V:33:LYS:HZ1	1.60	0.43
1:A:77:ASN:HA	1:A:83:GLY:HA2	2.00	0.43
3:C:158:GLY:O	4:D:56:PRO:HA	2.19	0.43
6:F:213:VAL:HG12	6:F:218:HIS:NE2	2.34	0.43
7:G:50:CYS:SG	7:G:68:ARG:HB3	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:4:LEU:HD22	12:L:160:ILE:HG13	2.01	0.43
13:M:215:TYR:CD1	9:W:167:LEU:HD13	2.54	0.43
3:Q:35:ILE:O	3:Q:45:LEU:HG	2.19	0.43
4:R:164:ASN:O	4:R:167:ILE:HG22	2.19	0.43
1:A:36:ASN:HA	1:A:176:ASN:CB	2.49	0.43
4:D:107:ILE:HD12	4:D:107:ILE:HA	1.87	0.43
7:G:122:ILE:HD12	7:G:154:ILE:HG21	2.00	0.43
9:I:77:SER:OG	9:I:111:TYR:OH	2.30	0.43
3:Q:155:ASN:ND2	4:R:77:ASN:HB3	2.34	0.43
6:T:35:ALA:O	6:T:159:SER:HA	2.18	0.43
13:a:57:LEU:HG	13:a:64:TYR:HD2	1.83	0.43
14:b:27:ARG:HG2	14:b:225:GLN:OE1	2.18	0.43
6:F:25:ALA:O	6:F:28:ALA:HB3	2.19	0.43
7:G:72:VAL:O	7:G:73:ASN:ND2	2.52	0.43
1:O:15:ILE:HG22	1:O:16:PHE:N	2.34	0.43
1:O:36:ASN:HA	1:O:176:ASN:CB	2.49	0.43
3:Q:158:GLY:O	4:R:56:PRO:HA	2.19	0.43
7:U:171:ASN:HB3	7:U:175:PHE:HE2	1.83	0.43
12:Z:184:TYR:HD2	12:Z:185:ASP:O	2.02	0.43
14:b:21:ILE:HG23	14:b:229:VAL:HB	2.01	0.43
1:A:15:ILE:HG22	1:A:16:PHE:N	2.34	0.42
2:B:20:VAL:HG12	2:B:24:TYR:CZ	2.54	0.42
2:B:89:ARG:O	2:B:93:GLU:HG2	2.19	0.42
7:G:175:PHE:CE1	7:G:200:ILE:HG23	2.54	0.42
8:H:38:ASN:HB3	8:H:40:ASN:OD1	2.18	0.42
11:K:101:ASN:HB3	11:K:132:HIS:ND1	2.34	0.42
11:K:171:PHE:HA	11:Y:27:LYS:HB2	2.01	0.42
1:O:160:PHE:HA	1:O:165:PHE:O	2.19	0.42
15:W:300:7F1:C24	10:X:140:ILE:CB	2.92	0.42
11:Y:13:VAL:HG23	11:Y:113:TYR:CD1	2.53	0.42
12:Z:100:ILE:HG12	12:Z:113:TYR:HD1	1.83	0.42
13:a:91:THR:HG21	14:b:100:TYR:CE2	2.54	0.42
14:b:54:PHE:CD2	14:b:61:ALA:HB1	2.53	0.42
14:b:211:ARG:HA	14:b:214:TYR:CE2	2.54	0.42
3:C:139:TYR:HB2	3:C:145:TYR:CD1	2.54	0.42
7:G:50:CYS:C	7:G:51:ILE:HD12	2.43	0.42
7:G:154:ILE:HG13	7:G:160:CYS:CB	2.49	0.42
11:K:27:LYS:HB2	11:Y:171:PHE:HA	2.01	0.42
11:K:180:LEU:HD12	11:K:180:LEU:O	2.19	0.42
14:N:16:LYS:HB2	14:N:159:LEU:HD23	2.00	0.42
14:N:27:ARG:O	14:N:40:VAL:N	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:90:PRO:CG	7:U:159:ALA:HB2	2.50	0.42
1:O:231:VAL:O	1:O:243:GLN:HG3	2.18	0.42
2:P:19:LEU:HD23	2:P:19:LEU:HA	1.88	0.42
2:P:20:VAL:HG12	2:P:24:TYR:CZ	2.54	0.42
3:Q:102:ASN:HB2	11:Y:83:PHE:CG	2.55	0.42
3:Q:105:GLN:HA	3:Q:106:PRO:HD3	1.90	0.42
10:X:61:ASP:OD2	10:X:104:PRO:HA	2.20	0.42
12:Z:33:LYS:HZ2	12:Z:45:MET:CE	2.26	0.42
12:Z:147:LEU:HB3	12:Z:148:ASN:H	1.62	0.42
14:b:21:ILE:HB	14:b:159:LEU:HD23	2.01	0.42
1:A:90:PRO:CG	7:G:159:ALA:HB2	2.50	0.42
2:B:147:TYR:CD1	2:B:157:ASN:HA	2.53	0.42
3:C:102:ASN:HB2	11:K:83:PHE:CG	2.55	0.42
8:H:26:ILE:HD12	14:b:215:PHE:O	2.20	0.42
7:U:129:TRP:CE3	7:U:129:TRP:N	2.80	0.42
11:Y:37:TYR:O	11:Y:39:ILE:HG12	2.19	0.42
11:Y:59:GLU:O	11:Y:63:LYS:HD3	2.19	0.42
11:Y:172:LEU:O	11:Y:174:THR:OG1	2.34	0.42
4:D:145:TYR:HD1	4:D:155:ALA:HA	1.84	0.42
4:D:164:ASN:O	4:D:167:ILE:HG22	2.19	0.42
5:E:88:LEU:HA	5:E:88:LEU:HD23	1.84	0.42
8:H:230:ILE:HB	8:H:241:PHE:CD2	2.54	0.42
9:I:41:ILE:HD12	9:I:76:VAL:HG13	2.02	0.42
13:M:48:TYR:OH	13:M:193:PHE:HB3	2.19	0.42
2:P:32:SER:O	2:P:165:LYS:N	2.51	0.42
4:R:33:VAL:HG13	4:R:193:ILE:HD11	2.01	0.42
6:T:77:ILE:HD11	6:T:80:ASP:OD2	2.19	0.42
7:U:72:VAL:O	7:U:73:ASN:ND2	2.52	0.42
7:U:113:ILE:HD11	8:V:70:ASN:CB	2.50	0.42
9:W:177:VAL:HG13	9:W:184:GLN:HB2	2.00	0.42
12:Z:4:LEU:HD22	12:Z:160:ILE:HG13	2.01	0.42
3:C:175:LEU:HG	3:C:195:THR:HG21	2.02	0.42
6:F:77:ILE:HD11	6:F:80:ASP:OD2	2.19	0.42
10:J:174:ASN:O	10:J:177:PHE:HB3	2.19	0.42
13:M:48:TYR:HB3	13:M:226:ASP:OD1	2.19	0.42
13:M:49:VAL:HG12	13:M:225:ILE:HB	2.00	0.42
13:M:91:THR:HG21	14:N:100:TYR:CE2	2.54	0.42
7:U:154:ILE:HG13	7:U:160:CYS:CB	2.49	0.42
7:U:223:LYS:HA	7:U:227:TYR:CE1	2.55	0.42
11:Y:5:ILE:HD13	11:Y:5:ILE:HG21	1.84	0.42
12:Z:33:LYS:HE3	12:Z:45:MET:HG3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:THR:OG1	1:A:135:ALA:HA	2.20	0.42
12:L:9:LYS:CD	12:L:146:ASN:HB3	2.50	0.42
12:L:149:LEU:HD11	12:L:178:HIS:CD2	2.55	0.42
13:M:118:ARG:O	13:M:122:VAL:HG23	2.18	0.42
14:N:21:ILE:HG23	14:N:229:VAL:HB	2.01	0.42
14:N:211:ARG:HA	14:N:214:TYR:CE2	2.54	0.42
14:N:215:PHE:O	8:V:26:ILE:HD12	2.20	0.42
6:T:25:ALA:O	6:T:28:ALA:HB3	2.19	0.42
8:V:230:ILE:HB	8:V:241:PHE:CD2	2.54	0.42
5:E:226:ASP:C	5:E:228:THR:N	2.76	0.42
7:G:173:GLU:OE1	7:G:176:LYS:HD2	2.20	0.42
13:M:38:GLY:O	13:M:39:THR:C	2.63	0.42
14:N:21:ILE:HB	14:N:159:LEU:HD23	2.01	0.42
3:Q:105:GLN:HE21	3:Q:109:GLN:CB	2.33	0.42
7:U:175:PHE:CE1	7:U:200:ILE:HG23	2.54	0.42
9:W:41:ILE:HD12	9:W:76:VAL:HG13	2.02	0.42
9:W:47:GLY:O	15:W:300:7F1:N01	2.53	0.42
10:X:174:ASN:O	10:X:177:PHE:HB3	2.19	0.42
11:Y:101:ASN:HB3	11:Y:132:HIS:ND1	2.34	0.42
13:a:33:TYR:HA	13:a:85:MET:SD	2.60	0.42
13:a:206:ILE:HG21	13:a:220:THR:HG21	2.00	0.42
3:C:155:ASN:ND2	4:D:77:ASN:HB3	2.34	0.42
5:E:12:VAL:HG13	5:E:23:GLN:HG2	2.02	0.42
5:E:42:VAL:HG13	5:E:44:ASP:H	1.84	0.42
7:G:11:SER:HB3	7:G:14:THR:HB	2.01	0.42
7:G:113:ILE:HD11	8:H:70:ASN:CB	2.50	0.42
7:G:223:LYS:HA	7:G:227:TYR:CE1	2.55	0.42
9:I:47:GLY:O	15:I:300:7F1:N01	2.53	0.42
9:I:167:LEU:HD13	13:a:215:TYR:CD1	2.54	0.42
2:P:147:TYR:CD1	2:P:157:ASN:HA	2.53	0.42
7:U:50:CYS:SG	7:U:68:ARG:HB3	2.59	0.42
8:V:19:ARG:NH1	8:V:26:ILE:HD13	2.35	0.42
10:X:50:ASN:O	10:X:113:GLY:HA3	2.20	0.42
7:G:75:ASN:OD1	7:G:76:ILE:N	2.52	0.42
12:L:7:LYS:HG3	12:L:11:GLY:C	2.45	0.42
4:R:63:ILE:HG23	4:R:88:ARG:NH2	2.35	0.42
7:U:51:ILE:HG13	7:U:216:VAL:HG12	2.01	0.42
7:U:171:ASN:HB3	7:U:175:PHE:CE2	2.55	0.42
11:Y:180:LEU:HD12	11:Y:180:LEU:O	2.19	0.42
12:Z:149:LEU:HD11	12:Z:178:HIS:CD2	2.55	0.42
3:C:105:GLN:HE21	3:C:109:GLN:CB	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:33:VAL:HG13	4:D:193:ILE:HD11	2.01	0.42
10:J:61:ASP:OD2	10:J:104:PRO:HA	2.20	0.42
11:K:59:GLU:O	11:K:63:LYS:HD3	2.19	0.42
5:S:42:VAL:HG13	5:S:44:ASP:H	1.84	0.42
6:T:10:ASN:HB3	6:T:21:GLN:CB	2.46	0.42
6:T:213:VAL:HG12	6:T:218:HIS:NE2	2.34	0.42
11:Y:5:ILE:HD11	11:Y:139:VAL:HG11	2.02	0.42
4:D:63:ILE:HG23	4:D:88:ARG:NH2	2.35	0.41
7:G:47:ILE:HG22	7:G:219:SER:O	2.20	0.41
6:T:26:SER:O	6:T:30:LYS:HG2	2.19	0.41
6:T:97:PHE:CB	13:a:98:LYS:HD2	2.50	0.41
7:U:34:ASN:OD1	7:U:82:GLY:HA2	2.20	0.41
9:W:12:VAL:HG23	9:W:108:PRO:HB3	2.02	0.41
12:Z:9:LYS:CD	12:Z:146:ASN:HB3	2.50	0.41
13:a:48:TYR:HB3	13:a:226:ASP:OD1	2.19	0.41
5:E:36:THR:HA	5:E:173:GLY:HA3	2.02	0.41
6:F:145:GLU:HG3	6:F:158:LEU:HD21	2.02	0.41
8:H:19:ARG:HD2	8:H:26:ILE:HG12	2.02	0.41
3:Q:139:TYR:HB2	3:Q:145:TYR:CD1	2.54	0.41
6:T:70:ILE:HA	6:T:136:ALA:CB	2.48	0.41
7:U:47:ILE:HG22	7:U:219:SER:O	2.20	0.41
10:X:27:LEU:HD23	10:X:27:LEU:HA	1.86	0.41
10:X:67:GLU:HG3	11:Y:83:PHE:HZ	1.85	0.41
10:X:136:ALA:HB2	10:X:150:VAL:HG11	2.02	0.41
14:b:189:LEU:HB2	14:b:209:CYS:SG	2.60	0.41
7:G:51:ILE:HG13	7:G:216:VAL:HG12	2.01	0.41
7:G:193:ILE:HG23	7:G:218:PHE:CD2	2.56	0.41
15:I:300:7F1:C14	15:I:300:7F1:C03	2.98	0.41
10:J:136:ALA:HB2	10:J:150:VAL:HG11	2.02	0.41
11:K:172:LEU:O	11:K:174:THR:OG1	2.34	0.41
12:L:113:TYR:CE1	12:L:128:CYS:HB3	2.56	0.41
13:M:120:LEU:HD13	13:M:152:TYR:OH	2.21	0.41
14:N:189:LEU:HB2	14:N:209:CYS:SG	2.60	0.41
1:O:14:THR:OG1	1:O:135:ALA:HA	2.20	0.41
4:R:145:TYR:HD1	4:R:155:ALA:HA	1.84	0.41
8:V:21:SER:HA	8:V:26:ILE:HA	2.02	0.41
12:Z:7:LYS:HG3	12:Z:11:GLY:C	2.45	0.41
3:C:109:GLN:CD	11:K:72:ASN:HD22	2.28	0.41
8:H:189:ILE:CG1	8:H:217:ALA:HB2	2.49	0.41
11:K:37:TYR:O	11:K:39:ILE:HG12	2.19	0.41
12:L:33:LYS:O	12:L:45:MET:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:107:ILE:HD12	4:R:107:ILE:HA	1.87	0.41
7:U:71:HIS:HB2	7:U:73:ASN:O	2.21	0.41
8:V:189:ILE:CG1	8:V:217:ALA:HB2	2.49	0.41
12:Z:113:TYR:CE1	12:Z:128:CYS:HB3	2.56	0.41
12:Z:173:LYS:HE2	12:Z:173:LYS:HB2	1.89	0.41
14:b:112:ASN:HB3	14:b:163:PHE:CE1	2.55	0.41
5:E:103:TYR:HB3	13:M:118:ARG:CB	2.50	0.41
7:G:49:CYS:HB2	7:G:218:PHE:HD1	1.85	0.41
8:H:21:SER:HA	8:H:26:ILE:HA	2.02	0.41
13:M:119:LEU:O	13:M:123:ILE:HG13	2.21	0.41
1:O:78:ILE:O	1:O:79:THR:HG23	2.21	0.41
1:O:87:VAL:N	1:O:143:SER:O	2.46	0.41
7:U:11:SER:HB3	7:U:14:THR:HB	2.01	0.41
8:V:17:ASP:HB3	8:V:228:ILE:HG22	2.02	0.41
13:a:119:LEU:O	13:a:123:ILE:HG13	2.21	0.41
5:E:32:LYS:O	5:E:174:SER:HB2	2.20	0.41
9:I:12:VAL:HG23	9:I:108:PRO:HB3	2.02	0.41
14:N:112:ASN:HB3	14:N:163:PHE:CE1	2.55	0.41
2:P:8:PHE:O	2:P:126:GLY:N	2.50	0.41
4:R:70:CYS:CB	4:R:214:LEU:HD13	2.51	0.41
6:T:145:GLU:HG3	6:T:158:LEU:HD21	2.02	0.41
7:U:16:SER:OG	7:U:20:ARG:N	2.53	0.41
7:U:75:ASN:HD21	7:U:108:ASN:ND2	2.18	0.41
7:U:173:GLU:OE1	7:U:176:LYS:HD2	2.20	0.41
1:A:78:ILE:O	1:A:79:THR:HG23	2.21	0.41
2:B:223:THR:HG23	2:B:226:GLU:H	1.86	0.41
5:E:42:VAL:HG21	5:E:196:ALA:HB2	2.02	0.41
6:F:97:PHE:CB	13:M:98:LYS:HD2	2.50	0.41
6:F:219:PRO:HB2	6:F:220:TRP:H	1.69	0.41
7:G:71:HIS:HB2	7:G:73:ASN:O	2.21	0.41
7:G:77:ILE:HG22	7:G:141:SER:O	2.21	0.41
9:I:151:GLY:O	9:I:155:VAL:HG12	2.20	0.41
11:K:4:LEU:HD11	11:K:48:GLY:HA3	2.03	0.41
12:L:8:PHE:HE2	12:L:10:ASP:HB2	1.86	0.41
13:M:33:TYR:HA	13:M:85:MET:SD	2.60	0.41
13:M:41:ILE:O	13:M:51:LEU:HD12	2.20	0.41
1:O:14:THR:O	1:O:15:ILE:HD13	2.21	0.41
2:P:40:ALA:HB1	2:P:182:ILE:O	2.21	0.41
5:S:12:VAL:HG13	5:S:23:GLN:HG2	2.02	0.41
5:S:36:THR:HA	5:S:173:GLY:HA3	2.02	0.41
7:U:49:CYS:HB2	7:U:218:PHE:HD1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:151:GLY:O	9:W:155:VAL:HG12	2.20	0.41
15:W:300:7F1:C14	15:W:300:7F1:C03	2.98	0.41
2:B:8:PHE:O	2:B:126:GLY:N	2.50	0.41
3:C:86:LEU:HD23	3:C:86:LEU:HA	1.86	0.41
4:D:70:CYS:CB	4:D:214:LEU:HD13	2.51	0.41
5:E:71:ASP:HB2	5:E:74:ILE:HD12	2.03	0.41
7:G:16:SER:OG	7:G:20:ARG:N	2.53	0.41
7:G:34:ASN:OD1	7:G:82:GLY:HA2	2.20	0.41
8:H:17:ASP:HB3	8:H:228:ILE:HG22	2.02	0.41
14:N:12:VAL:HG23	14:N:55:SER:HB2	2.02	0.41
2:P:89:ARG:O	2:P:93:GLU:HG2	2.19	0.41
3:Q:76:VAL:HA	3:Q:134:PHE:CB	2.50	0.41
3:Q:175:LEU:HG	3:Q:195:THR:HG21	2.02	0.41
5:S:32:LYS:O	5:S:174:SER:HB2	2.20	0.41
5:S:191:MET:HE1	5:S:199:LEU:HD13	2.03	0.41
7:U:193:ILE:HG23	7:U:218:PHE:CD2	2.56	0.41
12:Z:33:LYS:O	12:Z:45:MET:HG2	2.20	0.41
12:Z:51:ASP:O	12:Z:55:TRP:CD1	2.74	0.41
13:a:38:GLY:O	13:a:39:THR:C	2.63	0.41
2:B:40:ALA:HB1	2:B:182:ILE:O	2.21	0.41
3:C:76:VAL:HA	3:C:134:PHE:CB	2.50	0.41
4:D:96:LEU:HB2	11:K:63:LYS:HG2	2.02	0.41
5:E:191:MET:HE1	5:E:199:LEU:HD13	2.03	0.41
7:G:171:ASN:HB3	7:G:175:PHE:CE2	2.55	0.41
10:J:67:GLU:HG3	11:K:83:PHE:HZ	1.85	0.41
12:L:42:LEU:C	12:L:42:LEU:HD12	2.46	0.41
13:M:89:ILE:HG23	13:M:93:HIS:CE1	2.56	0.41
14:N:42:ARG:H	14:N:225:GLN:NE2	1.97	0.41
14:N:227:VAL:HG22	14:N:236:TYR:HA	2.03	0.41
4:R:118:PHE:N	4:R:118:PHE:CD1	2.89	0.41
8:V:19:ARG:HD2	8:V:26:ILE:HG12	2.02	0.41
11:Y:4:LEU:HD11	11:Y:48:GLY:HA3	2.03	0.41
12:Z:15:ALA:HB2	12:Z:176:VAL:HG12	2.02	0.41
13:a:89:ILE:HG23	13:a:93:HIS:CE1	2.56	0.41
13:a:120:LEU:HD13	13:a:152:TYR:OH	2.21	0.41
2:B:119:GLN:HG2	3:C:85:ILE:CG1	2.51	0.41
4:D:145:TYR:HE1	4:D:155:ALA:HB2	1.85	0.41
4:D:181:GLU:HB2	4:D:184:ASP:CB	2.48	0.41
6:F:9:ASP:OD1	6:F:12:ILE:HG12	2.21	0.41
7:G:12:VAL:HG11	7:G:133:PRO:HD3	2.03	0.41
10:J:59:ALA:O	10:J:63:GLN:OE1	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:105:ILE:HG13	2:P:106:LEU:O	2.21	0.41
3:Q:38:ILE:HG12	3:Q:43:VAL:HG22	2.03	0.41
4:R:145:TYR:HE1	4:R:155:ALA:HB2	1.85	0.41
5:S:88:LEU:HD23	5:S:88:LEU:HA	1.84	0.41
9:W:52:LEU:O	9:W:56:THR:OG1	2.35	0.41
10:X:59:ALA:O	10:X:63:GLN:OE1	2.39	0.41
11:Y:7:LEU:HD11	11:Y:147:TYR:CD1	2.56	0.41
11:Y:171:PHE:CE2	11:Y:172:LEU:HB3	2.57	0.41
13:a:34:ILE:HG12	13:a:85:MET:HE3	2.03	0.41
1:A:23:TYR:O	1:A:26:GLU:N	2.50	0.40
3:C:76:VAL:HG11	3:C:83:ALA:HB1	2.03	0.40
3:C:105:GLN:HA	3:C:106:PRO:HD3	1.90	0.40
10:J:50:ASN:O	10:J:113:GLY:HA3	2.20	0.40
1:O:232:ALA:HA	1:O:243:GLN:HA	2.04	0.40
3:Q:109:GLN:CD	11:Y:72:ASN:HD22	2.28	0.40
5:S:103:TYR:HB3	13:a:118:ARG:CB	2.50	0.40
6:T:225:SER:O	6:T:228:LEU:HB3	2.22	0.40
14:b:186:LEU:HD21	14:b:190:ARG:NH2	2.36	0.40
2:B:19:LEU:HD23	2:B:19:LEU:HA	1.88	0.40
2:B:111:VAL:HG13	2:B:149:ILE:HD11	2.03	0.40
6:F:42:ASP:C	6:F:141:PRO:HG2	2.47	0.40
8:H:19:ARG:NH1	8:H:26:ILE:HD13	2.35	0.40
12:L:15:ALA:HB2	12:L:176:VAL:HG12	2.02	0.40
14:N:186:LEU:HD21	14:N:190:ARG:NH2	2.36	0.40
14:N:216:ARG:HD3	14:N:216:ARG:HA	1.92	0.40
4:R:96:LEU:HB2	11:Y:63:LYS:HG2	2.02	0.40
6:T:42:ASP:C	6:T:141:PRO:HG2	2.47	0.40
9:W:104:ASP:HB2	9:W:105:VAL:H	1.72	0.40
11:Y:65:VAL:HG21	11:Y:81:PHE:CE1	2.57	0.40
14:b:199:GLU:HB3	14:b:203:ARG:NH2	2.37	0.40
1:A:87:VAL:N	1:A:143:SER:O	2.46	0.40
8:H:76:PHE:CD2	8:H:157:ASP:HB2	2.57	0.40
11:K:21:SER:OG	11:K:30:ASN:O	2.33	0.40
11:K:40:HIS:CD2	11:K:69:GLN:NE2	2.80	0.40
11:K:178:TYR:N	11:K:194:THR:O	2.43	0.40
12:L:51:ASP:O	12:L:55:TRP:CD1	2.74	0.40
14:N:42:ARG:N	14:N:225:GLN:HE22	1.97	0.40
14:N:60:ASP:HB2	14:N:111:ASN:HD21	1.87	0.40
14:N:99:PHE:CD2	14:N:164:VAL:HG11	2.57	0.40
2:P:128:ARG:HA	2:P:129:PRO:HD3	1.97	0.40
14:b:103:LYS:HA	14:b:108:PRO:CG	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ILE:HD11	1:A:241:PHE:HZ	1.87	0.40
3:C:38:ILE:HG12	3:C:43:VAL:HG22	2.03	0.40
3:C:160:PHE:HB3	3:C:179:TRP:CZ2	2.57	0.40
7:G:129:TRP:CZ2	7:G:130:HIS:CD2	3.09	0.40
7:G:180:GLU:C	7:G:182:LYS:H	2.30	0.40
10:J:63:GLN:O	10:J:67:GLU:HB2	2.21	0.40
10:J:159:LEU:HD23	10:J:159:LEU:HA	1.88	0.40
11:K:5:ILE:HD11	11:K:139:VAL:HG11	2.02	0.40
11:K:173:LEU:HG	11:Y:173:LEU:HG	2.02	0.40
11:K:178:TYR:O	11:K:194:THR:HB	2.22	0.40
13:M:119:LEU:O	13:M:122:VAL:HB	2.21	0.40
1:O:154:LYS:HA	1:O:155:PRO:HD2	1.95	0.40
7:U:12:VAL:HG11	7:U:133:PRO:HD3	2.03	0.40
12:Z:59:LEU:HD22	12:Z:83:LEU:HD11	2.04	0.40
14:b:12:VAL:HG23	14:b:55:SER:HB2	2.02	0.40
1:A:14:THR:O	1:A:15:ILE:HD13	2.21	0.40
4:D:65:LEU:HD13	4:D:87:THR:CG2	2.49	0.40
6:F:84:LEU:HD21	6:F:128:PHE:CE2	2.56	0.40
11:K:7:LEU:HD11	11:K:147:TYR:CD1	2.56	0.40
11:K:46:LEU:O	11:K:102:CYS:HA	2.22	0.40
13:M:156:GLY:O	13:M:158:TYR:N	2.54	0.40
2:P:119:GLN:HG2	3:Q:85:ILE:CG1	2.51	0.40
3:Q:160:PHE:HB3	3:Q:179:TRP:CZ2	2.57	0.40
4:R:50:ILE:HA	4:R:51:PRO:HD3	1.92	0.40
7:U:76:ILE:HG22	7:U:77:ILE:N	2.37	0.40
7:U:77:ILE:HG22	7:U:141:SER:O	2.21	0.40
12:Z:160:ILE:HG21	12:Z:160:ILE:HD13	1.84	0.40
13:a:156:GLY:O	13:a:158:TYR:N	2.54	0.40
14:b:60:ASP:HB2	14:b:111:ASN:HD21	1.87	0.40
14:b:61:ALA:HB2	14:b:111:ASN:OD1	2.22	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	211/260 (81%)	202 (96%)	7 (3%)	2 (1%)	14	46
1	O	211/260 (81%)	202 (96%)	7 (3%)	2 (1%)	14	46
2	B	206/235 (88%)	200 (97%)	5 (2%)	1 (0%)	24	57
2	P	206/235 (88%)	200 (97%)	5 (2%)	1 (0%)	24	57
3	C	216/246 (88%)	202 (94%)	12 (6%)	2 (1%)	14	46
3	Q	216/246 (88%)	202 (94%)	12 (6%)	2 (1%)	14	46
4	D	209/241 (87%)	200 (96%)	7 (3%)	2 (1%)	12	45
4	R	209/241 (87%)	200 (96%)	7 (3%)	2 (1%)	12	45
5	E	213/256 (83%)	201 (94%)	8 (4%)	4 (2%)	6	33
5	S	213/256 (83%)	201 (94%)	8 (4%)	4 (2%)	6	33
6	F	215/254 (85%)	196 (91%)	16 (7%)	3 (1%)	9	38
6	T	215/254 (85%)	196 (91%)	16 (7%)	3 (1%)	9	38
7	G	213/252 (84%)	200 (94%)	12 (6%)	1 (0%)	24	57
7	U	213/252 (84%)	200 (94%)	12 (6%)	1 (0%)	24	57
8	H	187/252 (74%)	170 (91%)	14 (8%)	3 (2%)	7	36
8	V	187/252 (74%)	170 (91%)	14 (8%)	3 (2%)	7	36
9	I	182/229 (80%)	164 (90%)	14 (8%)	4 (2%)	5	30
9	W	182/229 (80%)	164 (90%)	14 (8%)	4 (2%)	5	30
10	J	187/218 (86%)	178 (95%)	7 (4%)	2 (1%)	11	43
10	X	187/218 (86%)	178 (95%)	7 (4%)	2 (1%)	11	43
11	K	192/195 (98%)	181 (94%)	8 (4%)	3 (2%)	7	36
11	Y	192/195 (98%)	181 (94%)	8 (4%)	3 (2%)	7	36
12	L	185/211 (88%)	174 (94%)	9 (5%)	2 (1%)	11	43
12	Z	185/211 (88%)	174 (94%)	9 (5%)	2 (1%)	11	43
13	M	193/240 (80%)	176 (91%)	15 (8%)	2 (1%)	12	45
13	a	193/240 (80%)	176 (91%)	15 (8%)	2 (1%)	12	45
14	N	179/265 (68%)	171 (96%)	8 (4%)	0	100	100
14	b	179/265 (68%)	171 (96%)	8 (4%)	0	100	100
All	All	5576/6708 (83%)	5230 (94%)	284 (5%)	62 (1%)	14	43

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	38	SER
5	E	151	ASN
9	I	24	PRO
9	I	188	PRO
13	M	64	TYR
4	R	38	SER
5	S	151	ASN
9	W	24	PRO
9	W	188	PRO
13	a	64	TYR
3	C	217	ASN
8	H	233	ILE
8	H	237	PHE
3	Q	217	ASN
8	V	233	ILE
8	V	237	PHE
2	B	180	LYS
4	D	178	GLU
6	F	219	PRO
7	G	66	TYR
11	K	71	GLN
11	K	172	LEU
12	L	182	ASN
2	P	180	LYS
4	R	178	GLU
6	T	219	PRO
7	U	66	TYR
11	Y	71	GLN
11	Y	172	LEU
12	Z	182	ASN
1	A	236	THR
3	C	123	GLN
5	E	121	LEU
5	E	227	GLN
9	I	10	ASN
10	J	71	TYR
13	M	59	LEU
1	O	236	THR
3	Q	123	GLN
5	S	121	LEU
5	S	227	GLN
9	W	10	ASN
10	X	71	TYR

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Mol	Chain	Res	Type
13	a	59	LEU
1	A	136	TYR
6	F	139	ASN
6	F	162	ALA
10	J	104	PRO
1	O	136	TYR
6	T	139	ASN
6	T	162	ALA
10	X	104	PRO
5	E	22	PHE
8	H	236	SER
11	K	96	ASN
5	S	22	PHE
8	V	236	SER
11	Y	96	ASN
12	L	37	ILE
12	Z	37	ILE
9	I	108	PRO
9	W	108	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	118/231 (51%)	118 (100%)	0	100	100
1	O	118/231 (51%)	118 (100%)	0	100	100
2	B	111/205 (54%)	110 (99%)	1 (1%)	70	76
2	P	111/205 (54%)	110 (99%)	1 (1%)	70	76
3	C	129/213 (61%)	129 (100%)	0	100	100
3	Q	129/213 (61%)	129 (100%)	0	100	100
4	D	107/207 (52%)	107 (100%)	0	100	100
4	R	107/207 (52%)	107 (100%)	0	100	100
5	E	126/223 (56%)	126 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	S	126/223 (56%)	126 (100%)	0	100	100
6	F	127/227 (56%)	127 (100%)	0	100	100
6	T	127/227 (56%)	127 (100%)	0	100	100
7	G	140/229 (61%)	139 (99%)	1 (1%)	76	78
7	U	140/229 (61%)	139 (99%)	1 (1%)	76	78
8	H	118/231 (51%)	117 (99%)	1 (1%)	73	77
8	V	118/231 (51%)	117 (99%)	1 (1%)	73	77
9	I	117/194 (60%)	117 (100%)	0	100	100
9	W	117/194 (60%)	117 (100%)	0	100	100
10	J	118/191 (62%)	118 (100%)	0	100	100
10	X	118/191 (62%)	118 (100%)	0	100	100
11	K	138/174 (79%)	138 (100%)	0	100	100
11	Y	138/174 (79%)	138 (100%)	0	100	100
12	L	127/176 (72%)	127 (100%)	0	100	100
12	Z	127/176 (72%)	127 (100%)	0	100	100
13	M	139/216 (64%)	138 (99%)	1 (1%)	76	78
13	a	139/216 (64%)	138 (99%)	1 (1%)	76	78
14	N	122/239 (51%)	121 (99%)	1 (1%)	73	77
14	b	122/239 (51%)	121 (99%)	1 (1%)	73	77
All	All	3474/5912 (59%)	3464 (100%)	10 (0%)	84	83

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	163	VAL
7	G	51	ILE
8	H	89	ASP
13	M	234	THR
14	N	75	ASN
2	P	163	VAL
7	U	51	ILE
8	V	89	ASP
13	a	234	THR
14	b	75	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	71	HIS
2	B	119	GLN
2	B	189	HIS
3	C	20	GLN
3	C	109	GLN
3	C	113	GLN
3	C	119	GLN
3	C	149	HIS
4	D	69	ASN
4	D	92	GLN
4	D	116	GLN
4	D	175	ASN
5	E	97	ASN
6	F	189	HIS
7	G	108	ASN
7	G	123	HIS
7	G	130	HIS
8	H	194	GLN
8	H	219	HIS
8	H	232	ASN
8	H	245	ASN
9	I	114	HIS
9	I	145	ASN
9	I	184	GLN
11	K	64	ASN
11	K	69	GLN
11	K	88	ASN
11	K	114	GLN
11	K	148	HIS
12	L	182	ASN
13	M	107	HIS
14	N	65	HIS
14	N	196	ASN
14	N	222	ASN
1	O	12	HIS
2	P	71	HIS
2	P	119	GLN
3	Q	20	GLN
3	Q	80	ASN
3	Q	113	GLN
3	Q	119	GLN

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Mol	Chain	Res	Type
3	Q	149	HIS
4	R	69	ASN
4	R	92	GLN
4	R	116	GLN
4	R	175	ASN
5	S	97	ASN
6	T	189	HIS
7	U	108	ASN
7	U	123	HIS
7	U	130	HIS
8	V	194	GLN
8	V	219	HIS
8	V	232	ASN
8	V	245	ASN
9	W	114	HIS
9	W	145	ASN
9	W	184	GLN
11	Y	42	ASN
11	Y	64	ASN
11	Y	69	GLN
11	Y	88	ASN
11	Y	114	GLN
11	Y	148	HIS
12	Z	106	HIS
12	Z	182	ASN
13	a	107	HIS
13	a	179	ASN
13	a	192	ASN
14	b	65	HIS
14	b	196	ASN
14	b	222	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
15	7F1	W	300	9	52,53,53	3.53	19 (36%)	70,74,74	2.58	21 (30%)
15	7F1	I	300	9	52,53,53	3.53	19 (36%)	70,74,74	2.58	21 (30%)

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
15	7F1	W	300	9	-	17/41/50/50	0/5/5/5
15	7F1	I	300	9	-	17/41/50/50	0/5/5/5

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	I	300	7F1	C03-C02	15.04	1.55	1.31
15	W	300	7F1	C03-C02	15.04	1.55	1.31
15	I	300	7F1	C14-N01	7.32	1.49	1.34
15	W	300	7F1	C14-N01	7.32	1.49	1.34
15	I	300	7F1	C20-N03	7.02	1.49	1.34
15	W	300	7F1	C20-N03	7.02	1.49	1.34
15	I	300	7F1	C29-N04	6.83	1.48	1.34
15	W	300	7F1	C29-N04	6.83	1.48	1.34
15	I	300	7F1	C28-N05	-6.51	1.32	1.47
15	W	300	7F1	C28-N05	-6.51	1.32	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	I	300	7F1	C03-S01	5.28	1.84	1.75
15	W	300	7F1	C03-S01	5.28	1.84	1.75
15	I	300	7F1	C27-N05	-5.03	1.33	1.46
15	W	300	7F1	C27-N05	-5.03	1.33	1.46
15	I	300	7F1	C26-N05	-4.73	1.34	1.46
15	W	300	7F1	C26-N05	-4.73	1.34	1.46
15	I	300	7F1	C31-N06	4.64	1.45	1.37
15	W	300	7F1	C31-N06	4.64	1.45	1.37
15	I	300	7F1	C08-N02	4.33	1.44	1.37
15	W	300	7F1	C08-N02	4.33	1.44	1.37
15	I	300	7F1	C22-C23	3.96	1.57	1.50
15	W	300	7F1	C22-C23	3.96	1.57	1.50
15	I	300	7F1	C05-C06	3.57	1.57	1.50
15	W	300	7F1	C05-C06	3.57	1.57	1.50
15	I	300	7F1	C07-C08	2.98	1.45	1.41
15	W	300	7F1	C07-C08	2.98	1.45	1.41
15	I	300	7F1	O04-C20	-2.72	1.18	1.23
15	W	300	7F1	O04-C20	-2.72	1.18	1.23
15	I	300	7F1	C30-C31	2.44	1.44	1.41
15	W	300	7F1	C30-C31	2.44	1.44	1.41
15	I	300	7F1	C10-C07	-2.35	1.36	1.39
15	W	300	7F1	C10-C07	-2.35	1.36	1.39
15	I	300	7F1	C07-C06	2.30	1.47	1.44
15	W	300	7F1	C07-C06	2.30	1.47	1.44
15	I	300	7F1	O03-C14	-2.27	1.19	1.23
15	W	300	7F1	O03-C14	-2.27	1.19	1.23
15	I	300	7F1	O06-C29	-2.23	1.18	1.23
15	W	300	7F1	O06-C29	-2.23	1.18	1.23

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	I	300	7F1	C07-C06-C09	7.39	113.72	106.16
15	W	300	7F1	C07-C06-C09	7.39	113.72	106.16
15	I	300	7F1	C30-C23-C32	7.37	113.70	106.16
15	W	300	7F1	C30-C23-C32	7.37	113.70	106.16
15	I	300	7F1	C08-N02-C09	5.98	114.40	109.08
15	W	300	7F1	C08-N02-C09	5.98	114.40	109.08
15	I	300	7F1	C06-C09-N02	-5.85	103.88	110.31
15	W	300	7F1	C06-C09-N02	-5.85	103.88	110.31
15	I	300	7F1	C23-C32-N06	-5.44	104.33	110.31
15	W	300	7F1	C23-C32-N06	-5.44	104.33	110.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	I	300	7F1	C02-C03-S01	-5.01	109.64	121.89
15	W	300	7F1	C02-C03-S01	-5.01	109.64	121.89
15	I	300	7F1	C31-N06-C32	4.61	113.17	109.08
15	W	300	7F1	C31-N06-C32	4.61	113.17	109.08
15	I	300	7F1	C07-C08-N02	-4.27	103.96	107.52
15	W	300	7F1	C07-C08-N02	-4.27	103.96	107.52
15	I	300	7F1	C13-C08-N02	4.12	137.33	130.74
15	W	300	7F1	C13-C08-N02	4.12	137.33	130.74
15	I	300	7F1	C30-C31-N06	-3.68	104.45	107.52
15	W	300	7F1	C30-C31-N06	-3.68	104.45	107.52
15	I	300	7F1	C27-N05-C26	3.67	116.76	108.84
15	W	300	7F1	C27-N05-C26	3.67	116.76	108.84
15	I	300	7F1	C36-C31-N06	3.67	136.61	130.74
15	W	300	7F1	C36-C31-N06	3.67	136.61	130.74
15	I	300	7F1	C13-C08-C07	-3.60	118.70	122.19
15	W	300	7F1	C13-C08-C07	-3.60	118.70	122.19
15	I	300	7F1	C36-C31-C30	-3.36	118.94	122.19
15	W	300	7F1	C36-C31-C30	-3.36	118.94	122.19
15	I	300	7F1	C25-O05-C24	3.20	120.23	109.88
15	W	300	7F1	C25-O05-C24	3.20	120.23	109.88
15	I	300	7F1	C08-C07-C06	-3.10	104.03	107.17
15	W	300	7F1	C08-C07-C06	-3.10	104.03	107.17
15	I	300	7F1	C31-C30-C23	-2.80	104.34	107.17
15	W	300	7F1	C31-C30-C23	-2.80	104.34	107.17
15	I	300	7F1	C33-C30-C31	2.73	121.67	118.84
15	W	300	7F1	C33-C30-C31	2.73	121.67	118.84
15	I	300	7F1	C10-C07-C08	2.59	121.52	118.84
15	W	300	7F1	C10-C07-C08	2.59	121.52	118.84
15	I	300	7F1	C01-C02-C03	-2.52	113.04	125.91
15	W	300	7F1	C01-C02-C03	-2.52	113.04	125.91
15	I	300	7F1	C17-C16-C15	-2.20	109.50	115.40
15	W	300	7F1	C17-C16-C15	-2.20	109.50	115.40

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	I	300	7F1	N01-C01-C02-C03
15	I	300	7F1	C05-C01-C02-C03
15	I	300	7F1	C02-C03-S01-O01
15	I	300	7F1	C01-C02-C03-S01
15	W	300	7F1	N01-C01-C02-C03

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Mol	Chain	Res	Type	Atoms
15	W	300	7F1	C05-C01-C02-C03
15	W	300	7F1	C02-C03-S01-O01
15	W	300	7F1	C01-C02-C03-S01
15	I	300	7F1	N03-C15-C16-C17
15	W	300	7F1	N03-C15-C16-C17
15	I	300	7F1	C14-C15-C16-C17
15	W	300	7F1	C14-C15-C16-C17
15	I	300	7F1	C15-C16-C17-C19
15	W	300	7F1	C15-C16-C17-C19
15	I	300	7F1	C15-C16-C17-C18
15	W	300	7F1	C15-C16-C17-C18
15	I	300	7F1	N05-C28-C29-N04
15	W	300	7F1	N05-C28-C29-N04
15	I	300	7F1	C29-C28-N05-C26
15	W	300	7F1	C29-C28-N05-C26
15	I	300	7F1	C02-C03-S01-O02
15	W	300	7F1	C02-C03-S01-O02
15	I	300	7F1	C29-C28-N05-C27
15	W	300	7F1	C29-C28-N05-C27
15	I	300	7F1	C20-C21-N04-C29
15	W	300	7F1	C20-C21-N04-C29
15	I	300	7F1	N05-C28-C29-O06
15	W	300	7F1	N05-C28-C29-O06
15	I	300	7F1	C01-C05-C06-C09
15	I	300	7F1	C21-C22-C23-C32
15	W	300	7F1	C01-C05-C06-C09
15	W	300	7F1	C21-C22-C23-C32
15	I	300	7F1	C01-C05-C06-C07
15	W	300	7F1	C01-C05-C06-C07

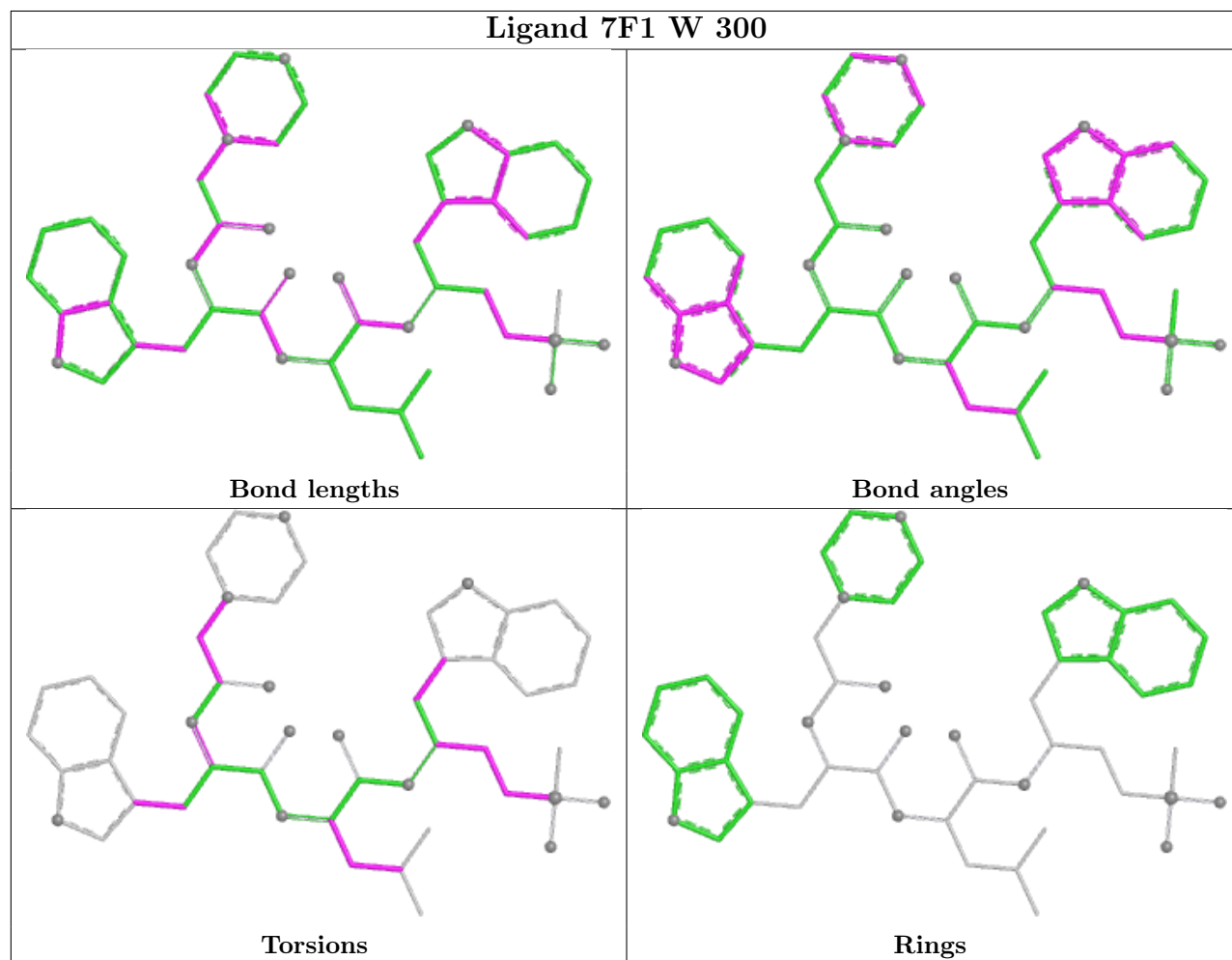
There are no ring outliers.

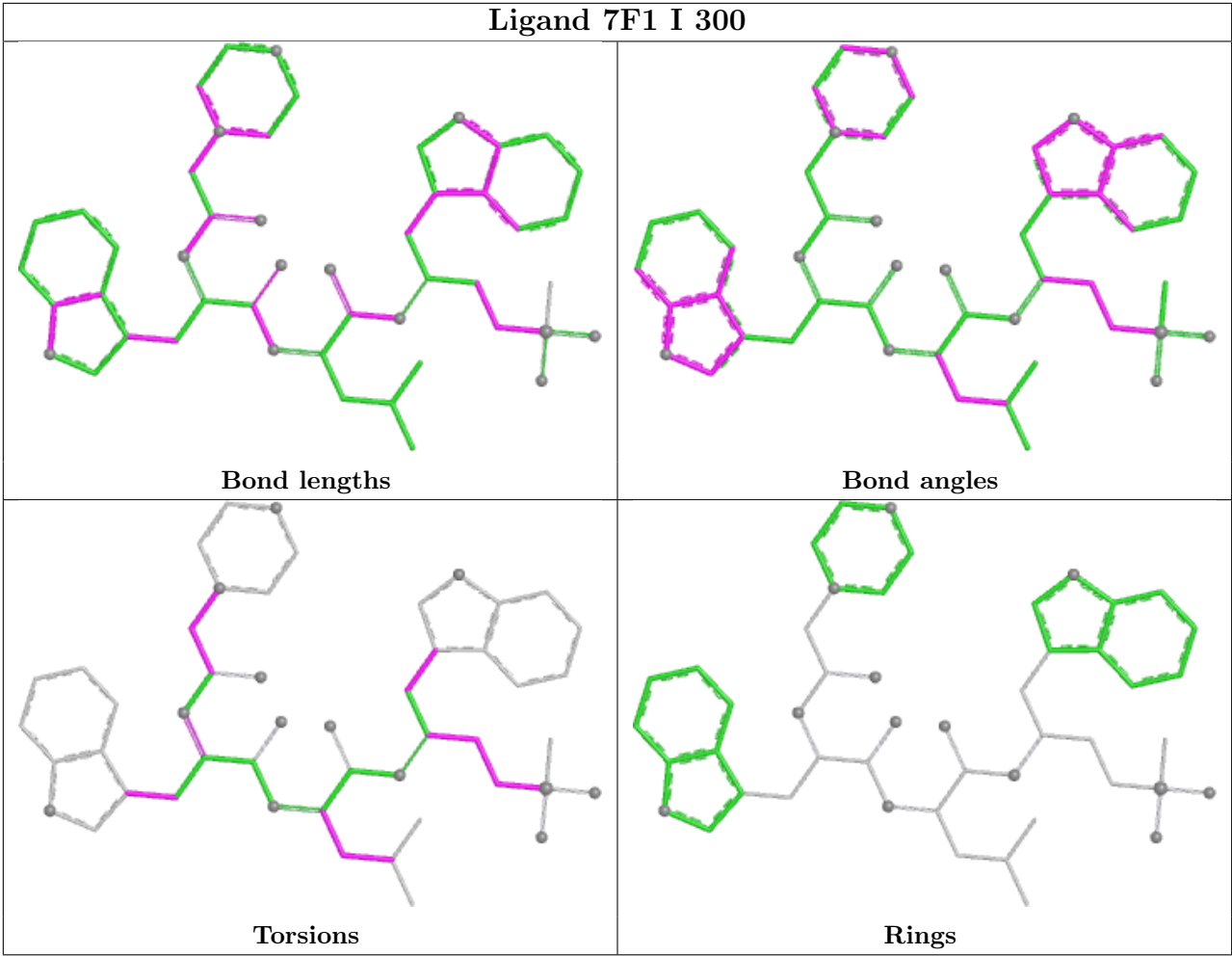
2 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	W	300	7F1	17	0
15	I	300	7F1	18	0

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

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





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
9	I	1
9	W	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	1:THR	C	2:THR	N	1.69
1	W	1:THR	C	2:THR	N	1.69

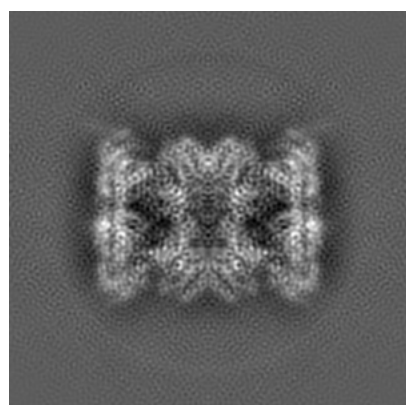
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3231. These allow visual inspection of the internal detail of the map and identification of artifacts.

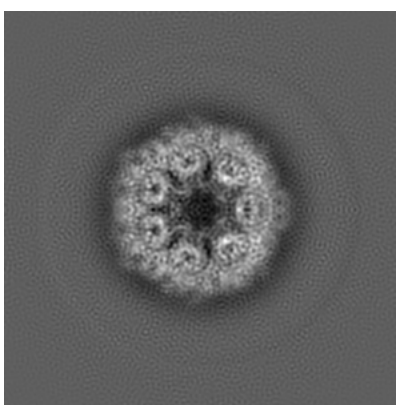
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

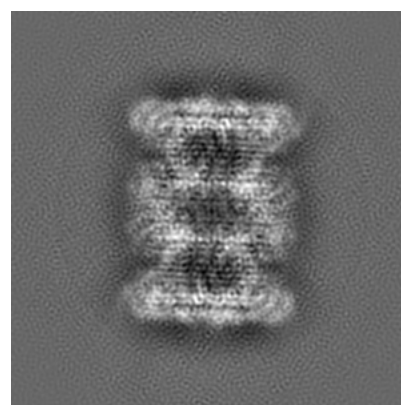
6.1.1 Primary map



X



Y

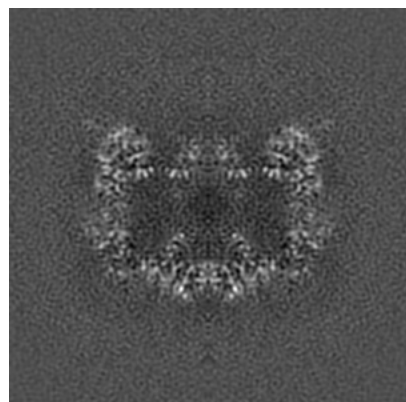


Z

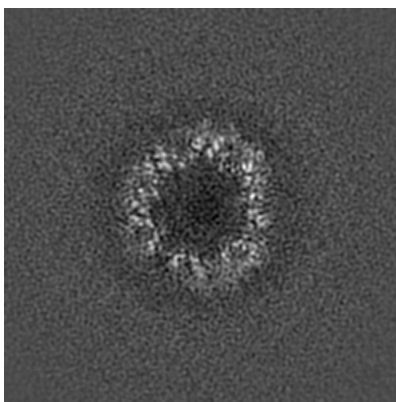
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

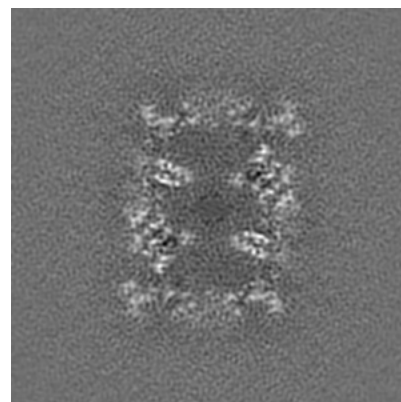
6.2.1 Primary map



X Index: 128



Y Index: 128

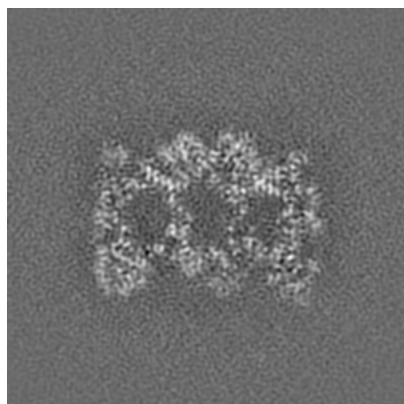


Z Index: 128

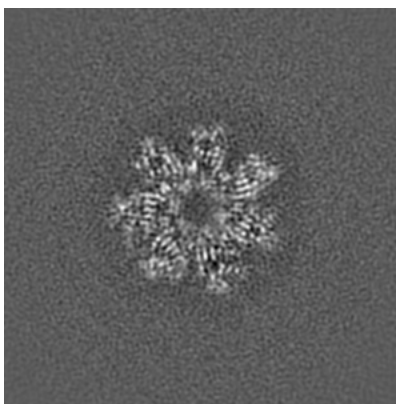
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

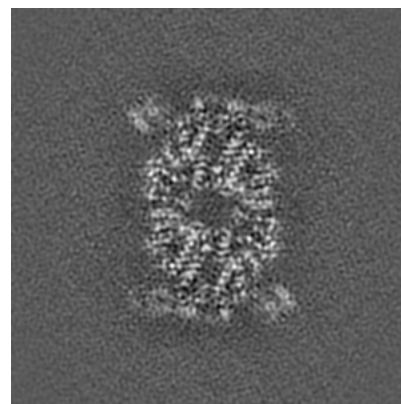
6.3.1 Primary map



X Index: 109



Y Index: 145

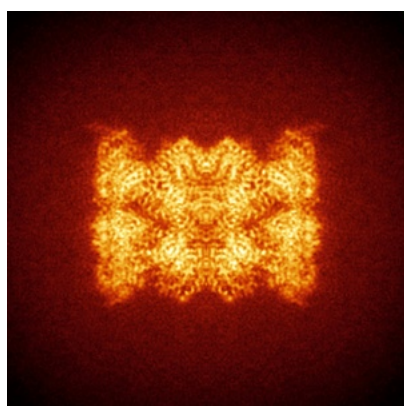


Z Index: 101

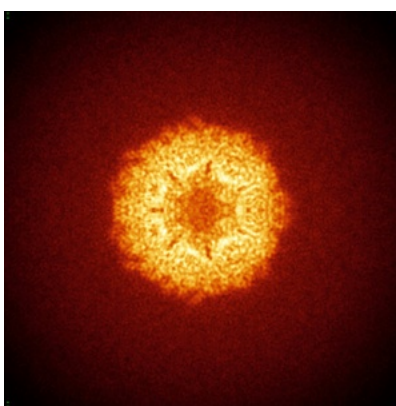
The images above show the largest variance slices of the map in three orthogonal directions.

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

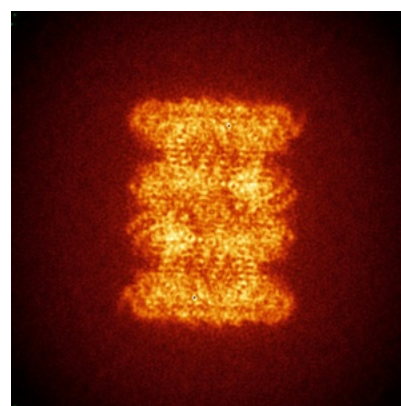
6.4.1 Primary map



X



Y

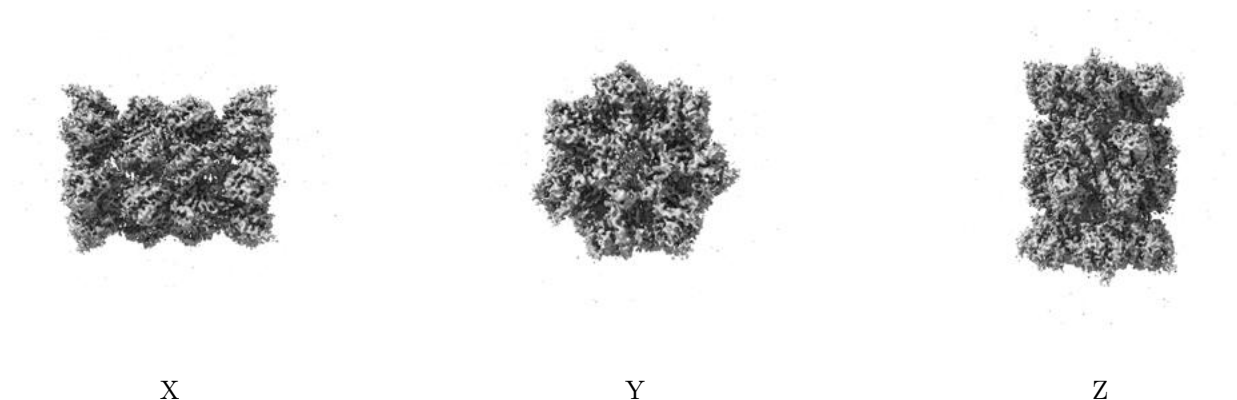


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

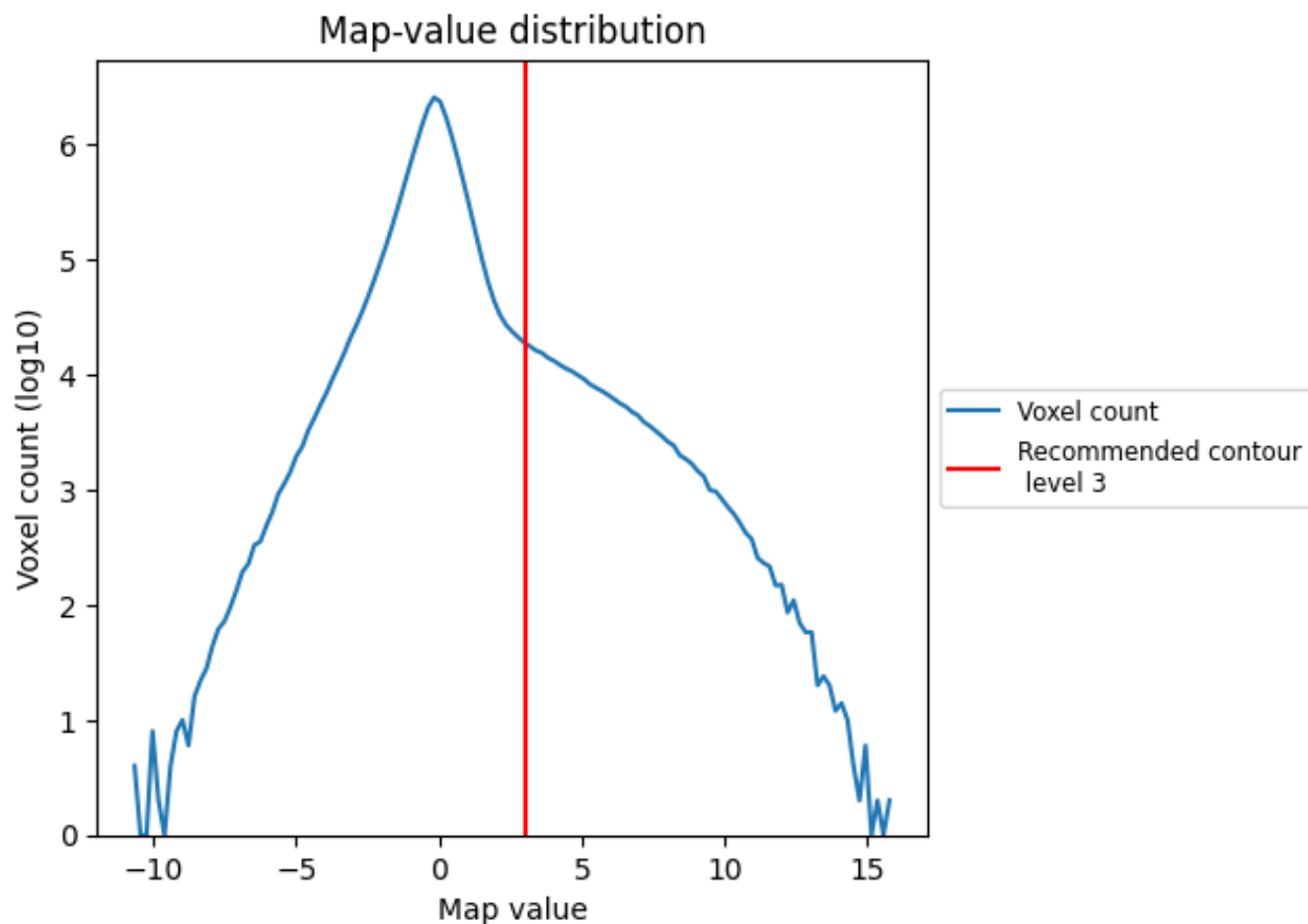
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

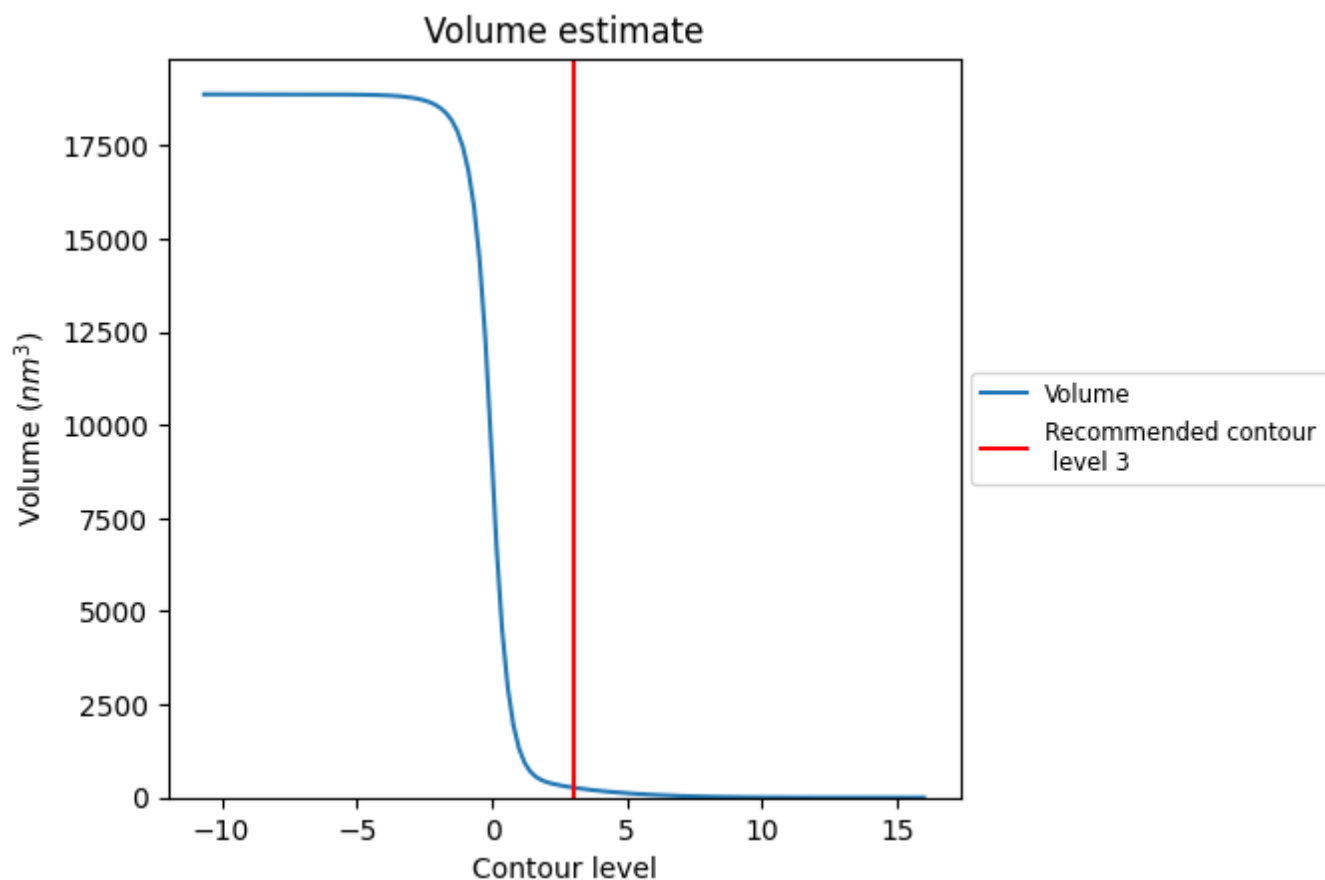
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

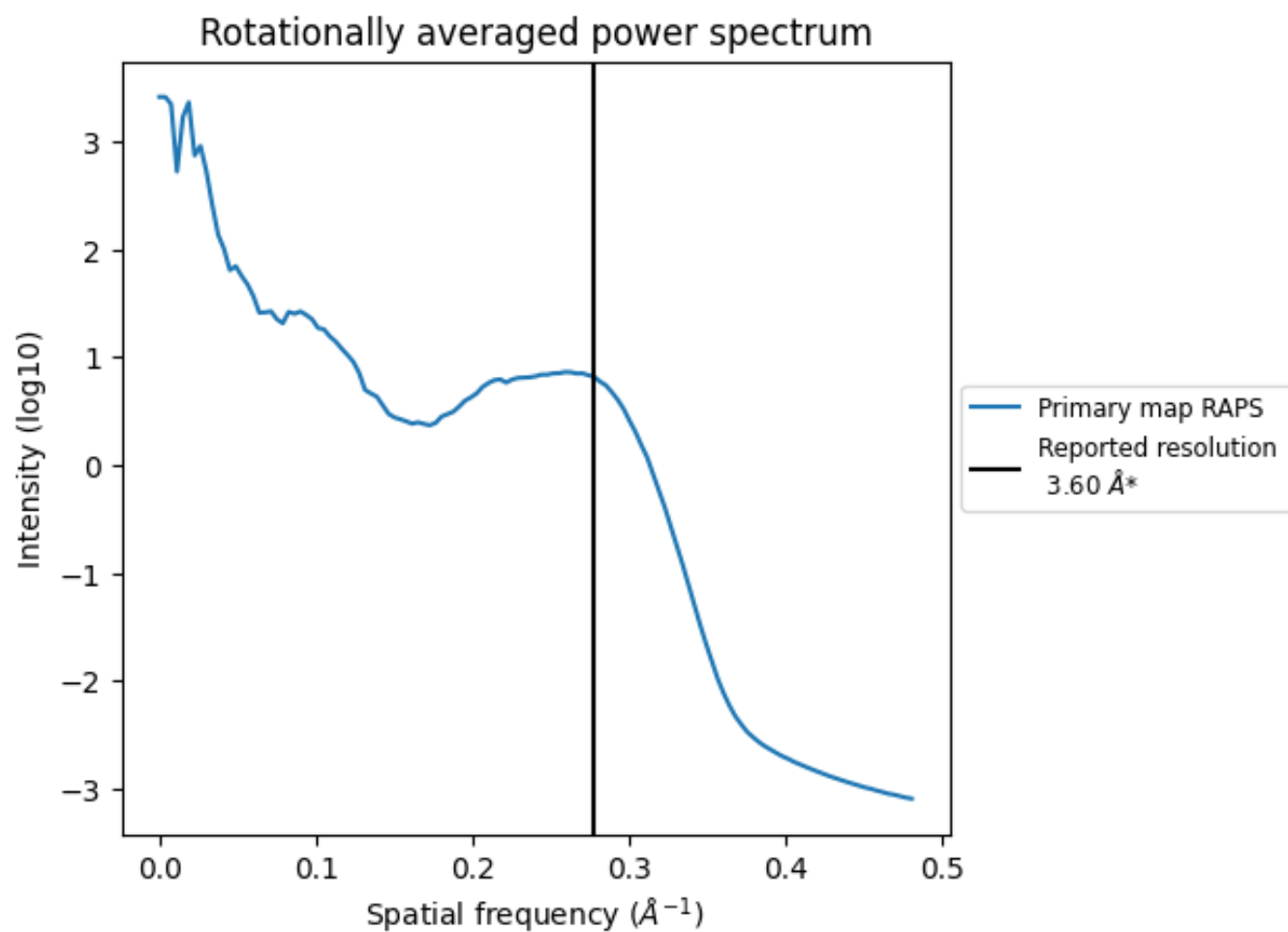
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 268 nm³; this corresponds to an approximate mass of 242 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

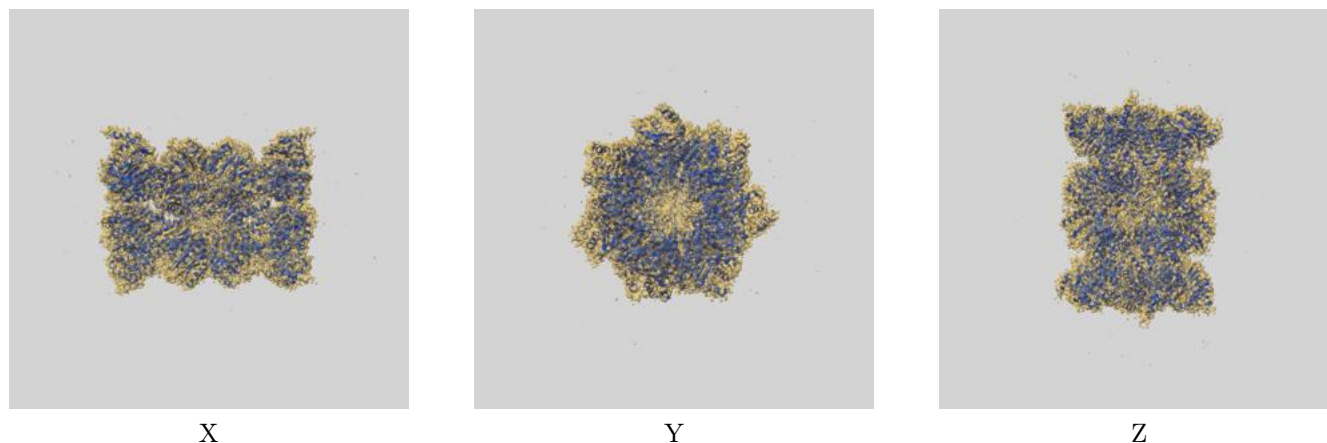
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

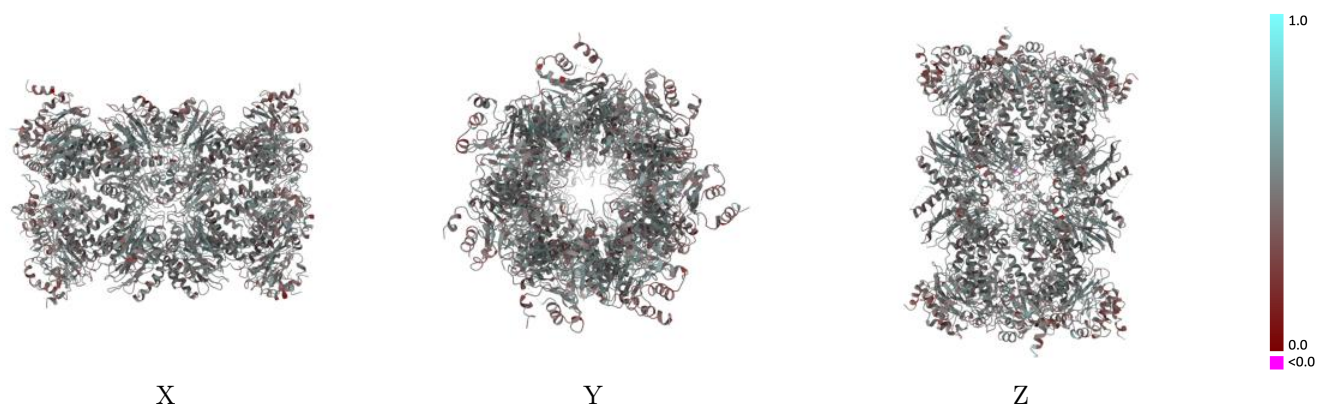
This section contains information regarding the fit between EMDB map EMD-3231 and PDB model 5FMG. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

9.1 Map-model overlay [i](#)



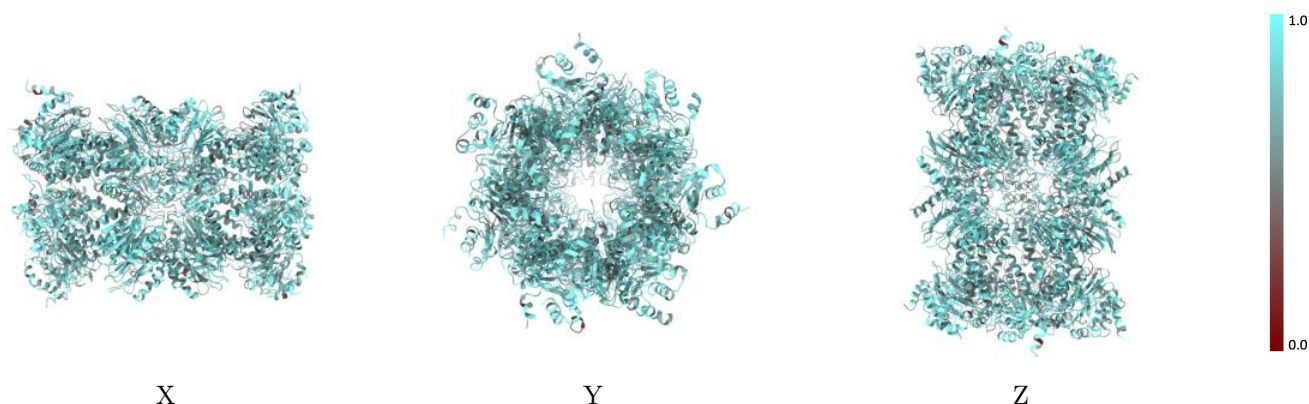
The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



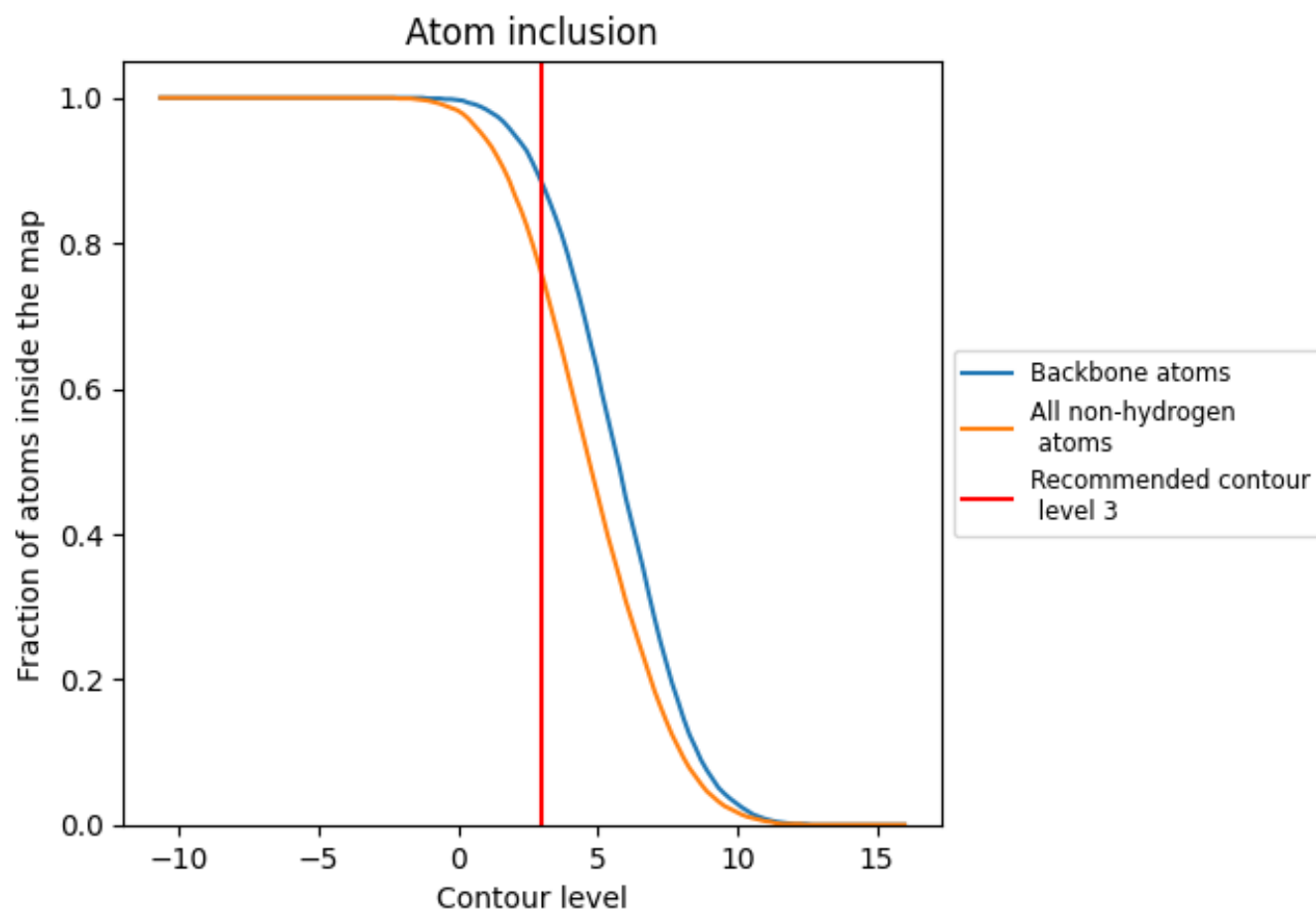
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7570	 0.4700
A	 0.7360	 0.4620
B	 0.7640	 0.4720
C	 0.7840	 0.4600
D	 0.7350	 0.4640
E	 0.7710	 0.4570
F	 0.7550	 0.4710
G	 0.7470	 0.4590
H	 0.7520	 0.4790
I	 0.7880	 0.4880
J	 0.7130	 0.4780
K	 0.7360	 0.4600
L	 0.7890	 0.4720
M	 0.7650	 0.4800
N	 0.7560	 0.4840
O	 0.7370	 0.4610
P	 0.7670	 0.4720
Q	 0.7880	 0.4600
R	 0.7360	 0.4630
S	 0.7740	 0.4580
T	 0.7510	 0.4730
U	 0.7490	 0.4600
V	 0.7570	 0.4790
W	 0.7810	 0.4850
X	 0.7100	 0.4780
Y	 0.7360	 0.4590
Z	 0.7900	 0.4730
a	 0.7630	 0.4800
b	 0.7540	 0.4860

