



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 01:43 PM UTC

PDB ID : 8YVG / pdb_00008yvg
EMDB ID : EMD-39600
Title : canine immunoproteasome 20S subunit in complex with compound 1
Authors : Kashima, A.; Arai, Y.
Deposited on : 2024-03-28
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

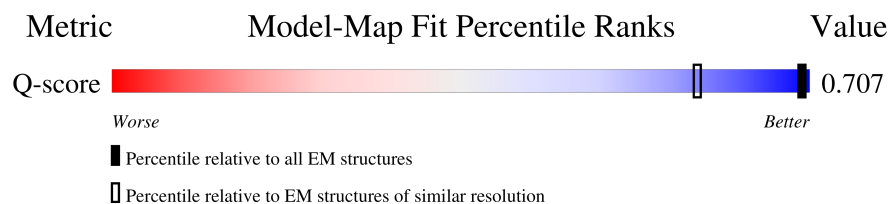
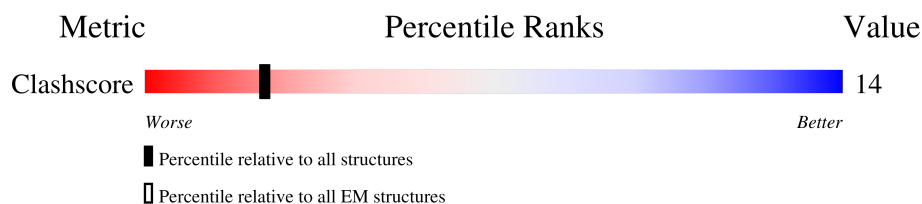
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

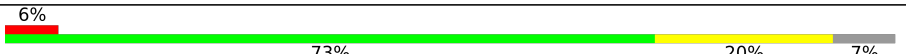
The reported resolution of this entry is 2.00 Å.

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



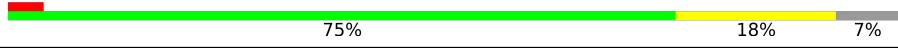
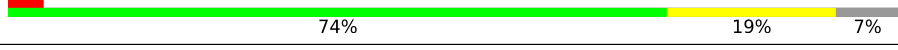
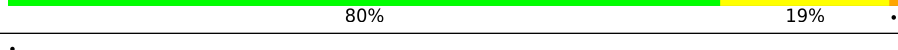
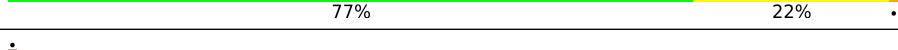
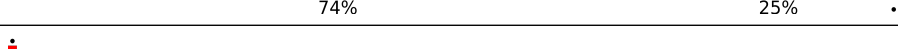
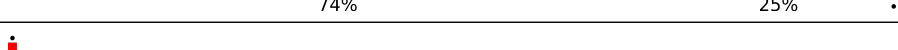
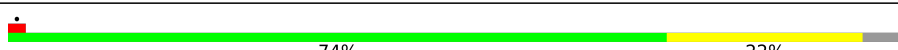
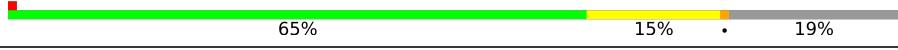
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Q-score	-	25397	1659 (1.50 - 2.50)

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

Mol	Chain	Length	Quality of chain
1	H	241	 72% 22% 7%
1	M	241	 72% 22% 7%
2	I	248	 24% 62% 31% 7%
2	N	248	 24% 62% 31% 7%
3	O	261	 6% 72% 20% 7%
3	Z	261	 6% 73% 20% 7%

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Mol	Chain	Length	Quality of chain
4	P	234	
4	b	234	
5	J	255	
5	Q	255	
6	T	201	
6	V	201	
7	U	205	
7	Y	205	
8	C	204	
8	D	204	
9	S	241	
9	X	241	
10	G	263	
10	L	263	
11	K	246	
11	R	246	
12	A	199	
12	F	199	
13	B	273	
13	E	273	
14	W	264	
14	a	264	

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 47844 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	M	225	Total	C	N	O	S	0	0
			1720	1083	286	340	11		
1	H	225	Total	C	N	O	S	0	0
			1720	1083	286	340	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	N	231	Total	C	N	O	S	0	0
			1815	1144	321	345	5		
2	I	231	Total	C	N	O	S	0	0
			1815	1144	321	345	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	O	242	Total	C	N	O	S	0	0
			1904	1204	326	364	10		
3	Z	242	Total	C	N	O	S	0	0
			1904	1204	326	364	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	P	226	Total	C	N	O	S	0	0
			1769	1132	298	333	6		
4	b	226	Total	C	N	O	S	0	0
			1769	1132	298	333	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Q	238	Total	C	N	O	S	0	0
			1866	1185	318	352	11		
5	J	238	Total	C	N	O	S	0	0
			1866	1185	318	352	11		

- Molecule 6 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	T	196	Total	C	N	O	S	0	0
			1567	1004	264	290	9		
6	V	196	Total	C	N	O	S	0	0
			1567	1004	264	290	9		

- Molecule 7 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	U	204	Total	C	N	O	S	0	0
			1593	1014	265	295	19		
7	Y	204	Total	C	N	O	S	0	0
			1593	1014	265	295	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	201	Total	C	N	O	S	0	0
			1568	980	269	306	13		
8	D	201	Total	C	N	O	S	0	0
			1568	980	269	306	13		

- Molecule 9 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	S	212	Total	C	N	O	S	0	0
			1644	1041	280	313	10		
9	X	212	Total	C	N	O	S	0	0
			1644	1041	280	313	10		

- Molecule 10 is a protein called Proteasome subunit alpha type.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	234	Total	C	N	O	S	0	0
			1832	1148	329	344	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	234	Total	C	N	O	S	0	0
			1832	1148	329	344	11		

- Molecule 11 is a protein called Proteasome subunit alpha type.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	236	Total	C	N	O	S	0	0
			1817	1153	302	349	13		
11	R	236	Total	C	N	O	S	0	0
			1817	1153	302	349	13		

- Molecule 12 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	199	Total	C	N	O	S	0	0
			1488	934	254	290	10		
12	A	199	Total	C	N	O	S	0	0
			1488	934	254	290	10		

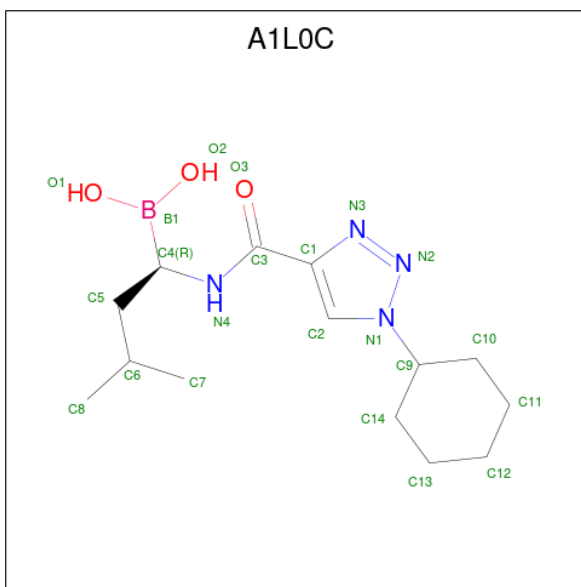
- Molecule 13 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	E	219	Total	C	N	O	S	0	0
			1622	1014	286	313	9		
13	B	219	Total	C	N	O	S	0	0
			1622	1014	286	313	9		

- Molecule 14 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	W	214	Total	C	N	O	S	0	0
			1673	1056	288	317	12		
14	a	214	Total	C	N	O	S	0	0
			1673	1056	288	317	12		

- Molecule 15 is [(1R)-1-[(1-cyclohexyl-1,2,3-triazol-4-yl)carbonylamino]-3-methyl-butyl]boronic acid (CCD ID: A1L0C) (formula: C₁₄H₂₅BN₄O₃) (labeled as "Ligand of Interest" by depositor).

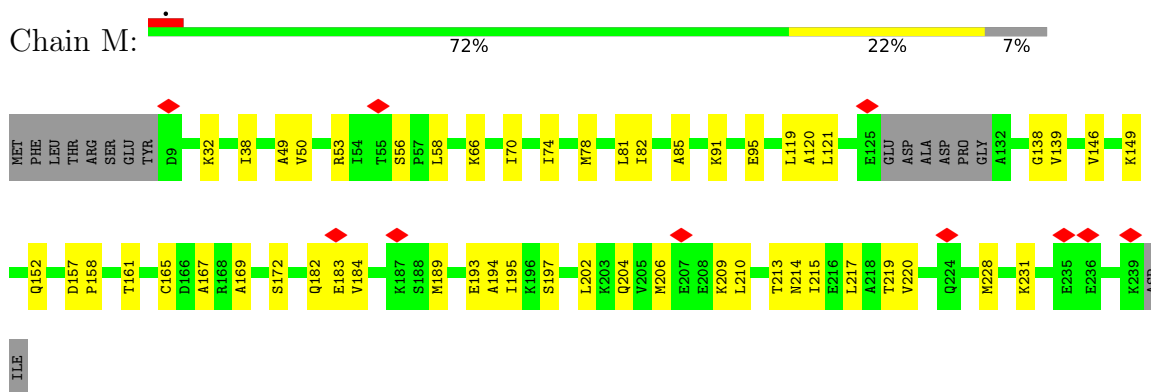


Mol	Chain	Residues	Atoms					AltConf
15	C	1	Total	B	C	N	O	0
			22	1	14	4	3	
15	F	1	Total	B	C	N	O	0
			22	1	14	4	3	
15	A	1	Total	B	C	N	O	0
			22	1	14	4	3	
15	D	1	Total	B	C	N	O	0
			22	1	14	4	3	

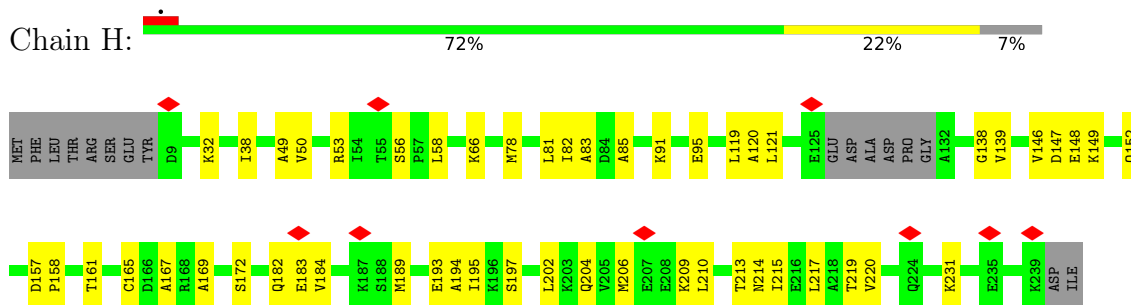
3 Residue-property plots

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

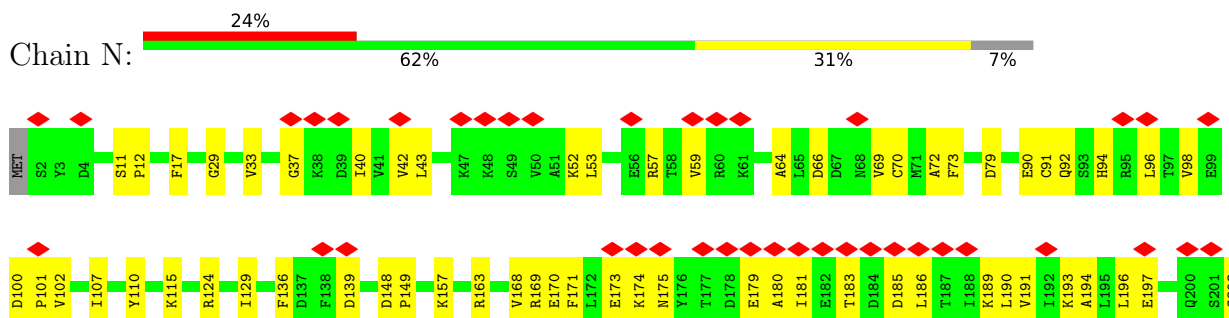
- Molecule 1: Proteasome subunit alpha type



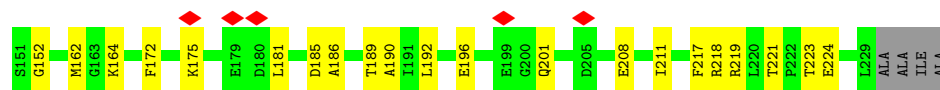
- Molecule 1: Proteasome subunit alpha type



- Molecule 2: Proteasome subunit alpha type







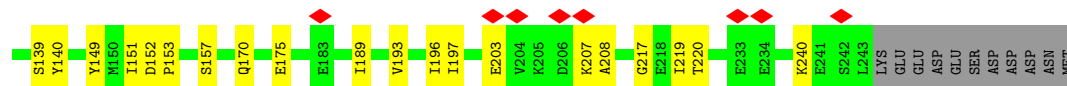
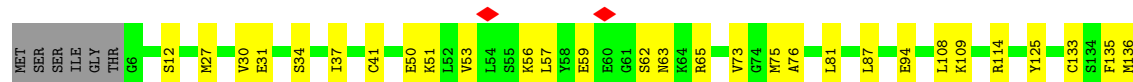
• Molecule 4: Proteasome subunit alpha type

Chain b: 74% 22%



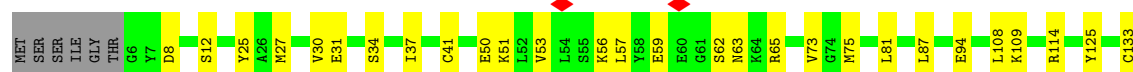
• Molecule 5: Proteasome subunit alpha type

Chain Q: 74% 19% 7%



• Molecule 5: Proteasome subunit alpha type

Chain J: 75% 18% 7%



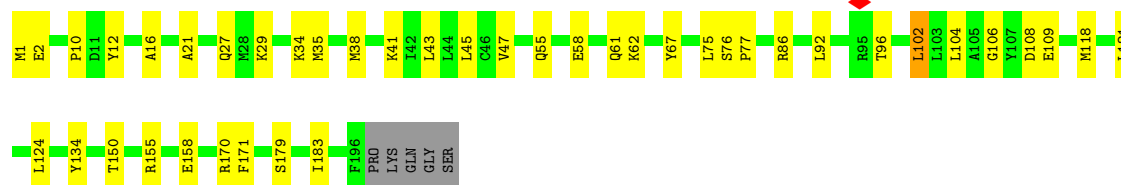
• Molecule 6: Proteasome subunit beta

Chain T: 77% 20%



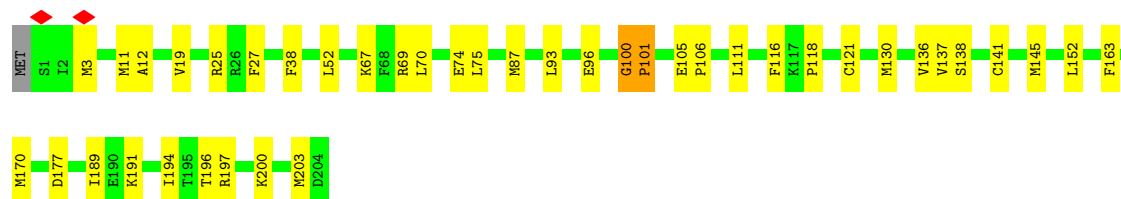
• Molecule 6: Proteasome subunit beta

Chain V:  77% 20%



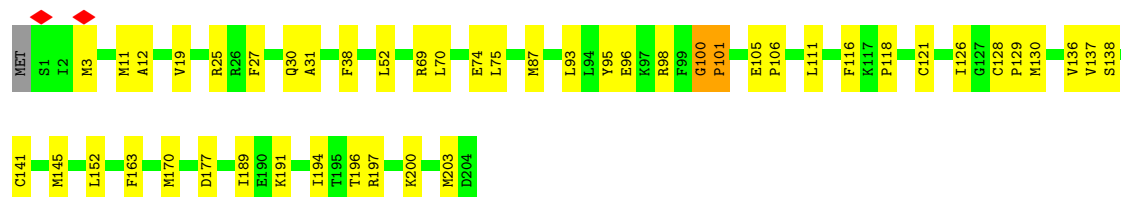
- Molecule 7: Proteasome subunit beta

Chain U:  80% 19%



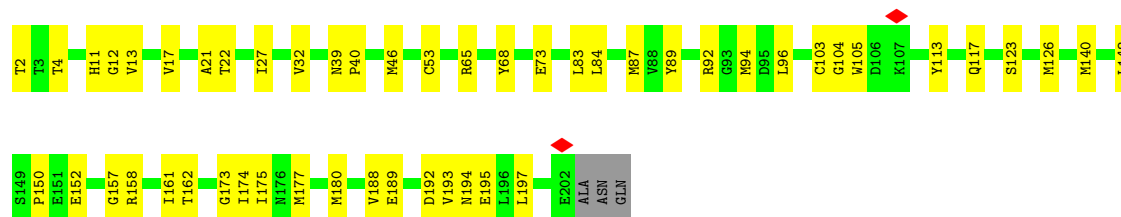
- Molecule 7: Proteasome subunit beta

Chain Y:  77% 22%



- Molecule 8: Proteasome subunit beta type-8

Chain C:  74% 25%



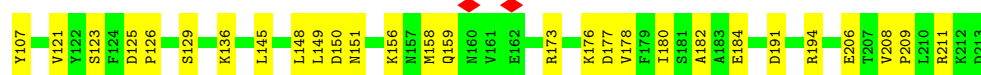
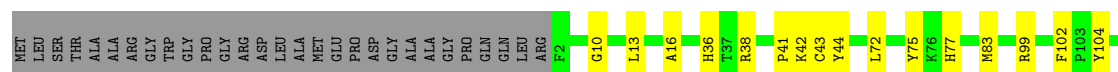
- Molecule 8: Proteasome subunit beta type-8

Chain D:  74% 25%

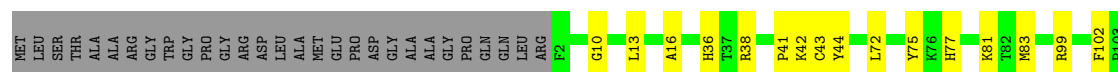




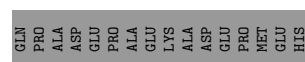
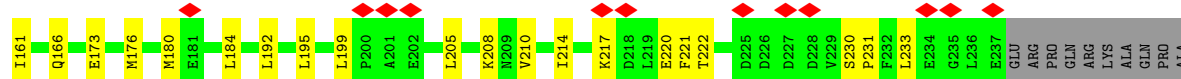
- Molecule 9: Proteasome subunit beta



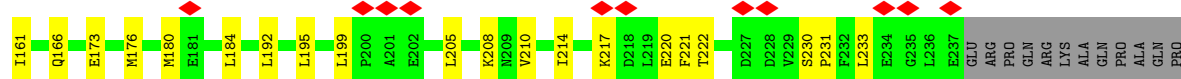
- Molecule 9: Proteasome subunit beta



- Molecule 10: Proteasome subunit alpha type



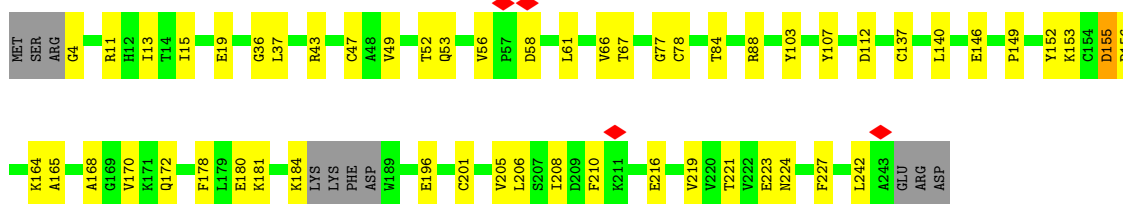
- Molecule 10: Proteasome subunit alpha type



ALA
ASP
GLU
PRO
GLU
ALA
LYS
ASP
GLU
PRO
MET
GLU
HIS

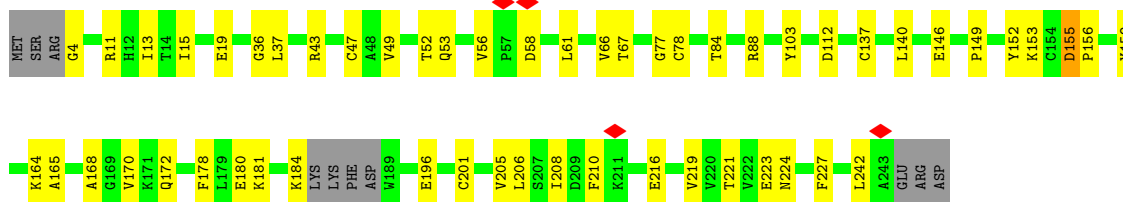
• Molecule 11: Proteasome subunit alpha type

Chain K:  74% 22%



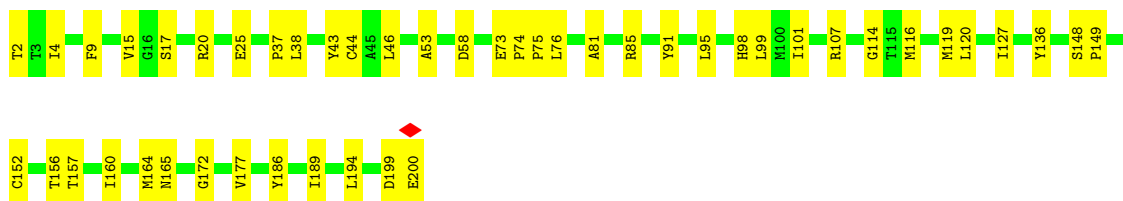
• Molecule 11: Proteasome subunit alpha type

Chain R:  74% 22%



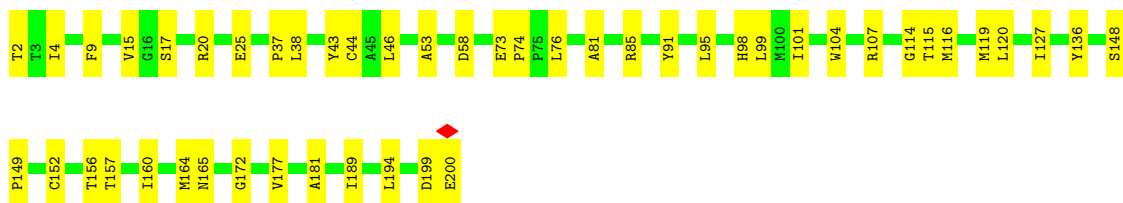
• Molecule 12: Proteasome subunit beta

Chain F:  76% 24%



• Molecule 12: Proteasome subunit beta

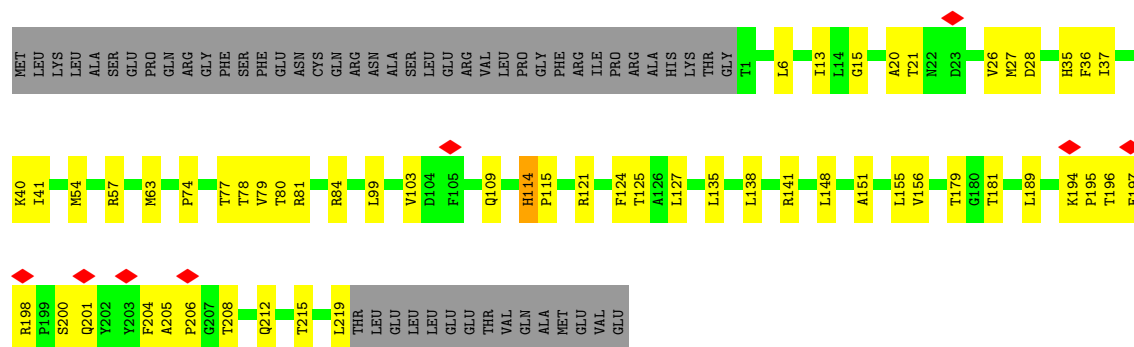
Chain A:  76% 24%



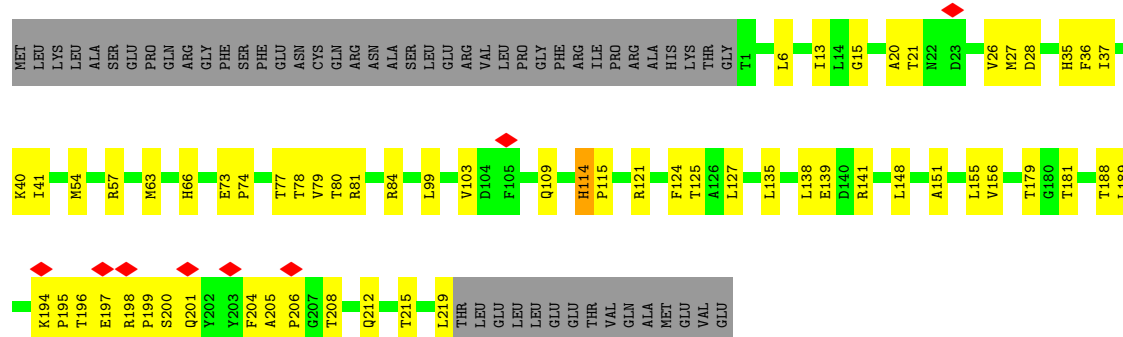
• Molecule 13: Proteasome subunit beta

Chain E:  60% 20% 20%

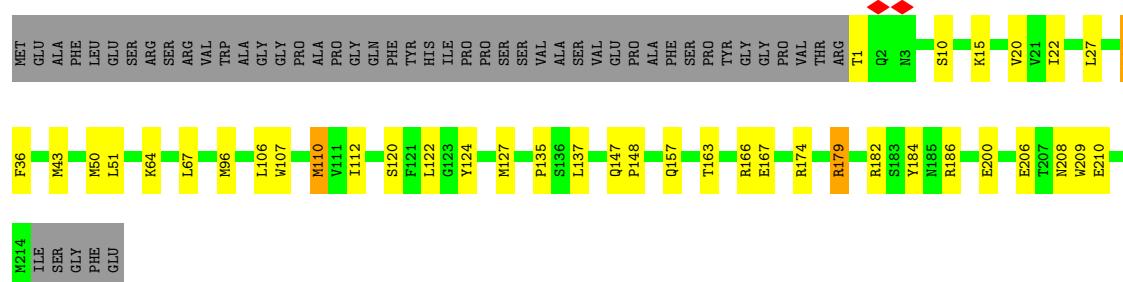




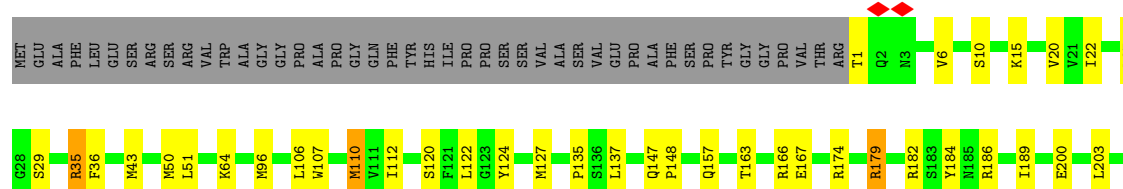
• Molecule 13: Proteasome subunit beta



• Molecule 14: Proteasome subunit beta



• Molecule 14: Proteasome subunit beta



E206	E207	N208	W209	E210	W214	ILE	SER	GLY	PHE	GLU
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	896501	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	91.875	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.208	Depositor
Minimum map value	-0.104	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0247	Depositor
Map size (Å)	292.16, 292.16, 292.16	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: A1L0C

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	H	0.42	0/1745	0.81	3/2354 (0.1%)
1	M	0.42	0/1745	0.81	5/2354 (0.2%)
2	I	0.38	0/1842	0.83	1/2489 (0.0%)
2	N	0.38	0/1842	0.83	1/2489 (0.0%)
3	O	0.43	0/1934	0.79	2/2608 (0.1%)
3	Z	0.43	0/1934	0.79	2/2608 (0.1%)
4	P	0.45	0/1808	0.83	3/2449 (0.1%)
4	b	0.45	0/1808	0.83	3/2449 (0.1%)
5	J	0.45	0/1901	0.83	1/2559 (0.0%)
5	Q	0.46	0/1901	0.83	1/2559 (0.0%)
6	T	0.47	0/1599	0.83	1/2163 (0.0%)
6	V	0.47	0/1599	0.83	1/2163 (0.0%)
7	U	0.49	0/1622	0.84	3/2186 (0.1%)
7	Y	0.49	0/1622	0.84	3/2186 (0.1%)
8	C	0.83	0/1600	1.06	0/2160
8	D	0.83	0/1600	1.06	0/2160
9	S	0.87	1/1675 (0.1%)	1.13	2/2258 (0.1%)
9	X	0.87	1/1675 (0.1%)	1.13	2/2258 (0.1%)
10	G	0.43	0/1866	0.89	3/2522 (0.1%)
10	L	0.43	0/1866	0.89	3/2522 (0.1%)
11	K	0.45	0/1849	0.84	5/2503 (0.2%)
11	R	0.45	0/1849	0.84	5/2503 (0.2%)
12	A	0.49	0/1517	0.84	2/2058 (0.1%)
12	F	0.49	0/1517	0.84	2/2058 (0.1%)
13	B	0.92	3/1650 (0.2%)	1.16	1/2242 (0.0%)
13	E	0.92	3/1650 (0.2%)	1.16	1/2242 (0.0%)
14	W	0.49	0/1706	0.87	7/2308 (0.3%)
14	a	0.48	0/1706	0.87	7/2308 (0.3%)
All	All	0.56	8/48628 (0.0%)	0.90	70/65718 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	E	114	HIS	CE1-NE2	9.55	1.42	1.32
13	B	114	HIS	CE1-NE2	9.55	1.42	1.32
9	S	36	HIS	CE1-NE2	6.60	1.39	1.32
9	X	36	HIS	CE1-NE2	6.60	1.39	1.32
13	E	114	HIS	ND1-CE1	6.30	1.38	1.32
13	B	114	HIS	ND1-CE1	6.30	1.38	1.32
13	E	35	HIS	CG-ND1	5.07	1.43	1.38
13	B	35	HIS	CG-ND1	5.07	1.43	1.38

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	37	ILE	N-CA-C	-8.60	104.17	111.56
13	E	37	ILE	N-CA-C	-8.59	104.18	111.56
7	Y	100	GLY	CA-C-N	7.37	127.33	120.03
7	Y	100	GLY	C-N-CA	7.37	127.33	120.03
7	U	100	GLY	CA-C-N	7.36	127.31	120.03
7	U	100	GLY	C-N-CA	7.36	127.31	120.03
10	L	148	CYS	CA-C-N	7.26	126.89	119.56
10	L	148	CYS	C-N-CA	7.26	126.89	119.56
10	G	148	CYS	CA-C-N	7.19	126.82	119.56
10	G	148	CYS	C-N-CA	7.19	126.82	119.56
4	P	67	ILE	N-CA-C	-6.96	105.82	111.81
4	b	67	ILE	N-CA-C	-6.91	105.87	111.81
14	a	35	ARG	N-CA-C	6.52	118.18	111.14
14	W	35	ARG	N-CA-C	6.52	118.18	111.14
14	a	10	SER	N-CA-C	6.52	118.71	110.24
14	W	10	SER	N-CA-C	6.51	118.70	110.24
3	Z	151	ASP	CA-C-N	6.15	126.60	119.47
3	Z	151	ASP	C-N-CA	6.15	126.60	119.47
3	O	151	ASP	CA-C-N	6.12	126.57	119.47
3	O	151	ASP	C-N-CA	6.12	126.57	119.47
5	J	73	VAL	N-CA-C	5.99	116.50	108.11
5	Q	73	VAL	N-CA-C	5.98	116.48	108.11
11	K	210	PHE	N-CA-C	5.98	118.01	110.24
11	R	210	PHE	N-CA-C	5.97	118.00	110.24
4	b	19	VAL	N-CA-C	5.95	117.40	110.62
4	P	19	VAL	N-CA-C	5.92	117.37	110.62
1	M	70	ILE	N-CA-C	-5.77	106.85	111.81
11	K	164	LYS	N-CA-C	-5.74	104.47	112.45
11	R	164	LYS	N-CA-C	-5.72	104.49	112.45
12	F	101	ILE	N-CA-C	5.65	116.08	108.17
12	A	101	ILE	N-CA-C	5.64	116.07	108.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	124	GLY	N-CA-C	5.63	119.20	111.54
4	b	124	GLY	N-CA-C	5.63	119.19	111.54
14	W	157	GLN	CA-C-N	5.56	125.66	119.32
14	W	157	GLN	C-N-CA	5.56	125.66	119.32
14	a	157	GLN	CA-C-N	5.54	125.63	119.32
14	a	157	GLN	C-N-CA	5.54	125.63	119.32
6	T	102	LEU	N-CA-C	5.43	117.05	108.96
6	V	102	LEU	N-CA-C	5.42	117.03	108.96
14	W	106	LEU	N-CA-C	-5.39	99.73	108.41
14	a	106	LEU	N-CA-C	-5.39	99.73	108.41
12	F	20	ARG	N-CA-C	5.37	118.00	109.24
12	A	20	ARG	N-CA-C	5.36	117.97	109.24
14	a	110	MET	N-CA-C	5.33	118.25	109.72
11	R	84	THR	N-CA-C	5.33	116.78	111.07
11	K	84	THR	N-CA-C	5.33	116.77	111.07
14	W	110	MET	N-CA-C	5.30	118.20	109.72
2	I	157	LYS	N-CA-C	-5.30	104.41	112.04
2	N	157	LYS	N-CA-C	-5.27	104.45	112.04
11	R	155	ASP	CA-C-N	5.27	125.08	119.28
11	R	155	ASP	C-N-CA	5.27	125.08	119.28
11	K	155	ASP	CA-C-N	5.27	125.08	119.28
11	K	155	ASP	C-N-CA	5.27	125.08	119.28
9	S	102	PHE	CA-C-N	5.25	125.19	119.78
9	S	102	PHE	C-N-CA	5.25	125.19	119.78
9	X	102	PHE	CA-C-N	5.25	125.19	119.78
9	X	102	PHE	C-N-CA	5.25	125.19	119.78
14	W	179	ARG	N-CA-C	5.18	120.46	113.72
7	Y	101	PRO	N-CA-C	5.18	119.17	111.41
14	a	179	ARG	N-CA-C	5.17	120.45	113.72
7	U	101	PRO	N-CA-C	5.14	119.12	111.41
1	M	56	SER	CA-C-N	5.13	124.75	119.56
1	M	56	SER	C-N-CA	5.13	124.75	119.56
1	H	56	SER	CA-C-N	5.11	124.72	119.56
1	H	56	SER	C-N-CA	5.11	124.72	119.56
1	M	120	ALA	N-CA-C	5.10	116.64	111.14
1	H	120	ALA	N-CA-C	5.09	116.64	111.14
10	L	70	ILE	N-CA-C	5.07	115.41	108.12
10	G	70	ILE	N-CA-C	5.06	115.40	108.12
1	M	74	ILE	N-CA-C	5.01	115.34	108.12

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1720	0	1719	60	0
1	M	1720	0	1719	61	0
2	I	1815	0	1845	96	0
2	N	1815	0	1845	96	0
3	O	1904	0	1918	48	0
3	Z	1904	0	1918	47	0
4	P	1769	0	1761	56	0
4	b	1769	0	1761	52	0
5	J	1866	0	1855	43	0
5	Q	1866	0	1855	48	0
6	T	1567	0	1567	38	0
6	V	1567	0	1567	39	0
7	U	1593	0	1614	32	0
7	Y	1593	0	1614	34	0
8	C	1568	0	1510	49	0
8	D	1568	0	1510	50	0
9	S	1644	0	1638	44	0
9	X	1644	0	1638	42	0
10	G	1832	0	1823	62	0
10	L	1832	0	1823	65	0
11	K	1817	0	1808	50	0
11	R	1817	0	1808	48	0
12	A	1488	0	1441	48	0
12	F	1488	0	1441	46	0
13	B	1622	0	1634	83	0
13	E	1622	0	1634	76	0
14	W	1673	0	1650	33	0
14	a	1673	0	1650	37	0
15	A	22	0	0	1	0
15	C	22	0	0	1	0
15	D	22	0	0	1	0
15	F	22	0	0	1	0
All	All	47844	0	47566	1314	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 14.

All (1314) 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)
10:G:79:ALA:CB	1:H:121:LEU:HD12	1.38	1.53
2:I:42:VAL:CG1	2:I:191:VAL:HG21	1.37	1.52
2:N:42:VAL:CG1	2:N:191:VAL:HG21	1.37	1.51
1:M:121:LEU:HD12	10:L:79:ALA:CB	1.39	1.46
2:N:42:VAL:HG11	2:N:191:VAL:CG2	1.67	1.25
13:B:205:ALA:HB1	13:B:206:PRO:CD	1.68	1.24
2:I:42:VAL:HG11	2:I:191:VAL:CG2	1.67	1.23
5:Q:41:CYS:HB3	5:Q:189:ILE:CD1	1.68	1.22
5:J:41:CYS:HB3	5:J:189:ILE:CD1	1.68	1.22
10:G:57:ALA:HB2	1:H:165:CYS:SG	1.81	1.21
13:B:205:ALA:CB	13:B:206:PRO:HD2	1.71	1.20
13:E:205:ALA:HB1	13:E:206:PRO:CD	1.68	1.20
6:T:96:THR:HB	8:D:92:ARG:NH2	1.57	1.19
13:E:205:ALA:CB	13:E:206:PRO:HD2	1.71	1.19
10:G:79:ALA:HB3	1:H:121:LEU:CD1	1.72	1.18
8:C:92:ARG:NH2	6:V:96:THR:HB	1.58	1.17
1:M:121:LEU:CD1	10:L:79:ALA:CB	2.24	1.16
1:M:121:LEU:CD1	10:L:79:ALA:HB3	1.74	1.14
1:M:165:CYS:SG	10:L:57:ALA:HB2	1.86	1.14
10:G:79:ALA:CB	1:H:121:LEU:CD1	2.24	1.14
10:G:57:ALA:CB	1:H:165:CYS:SG	2.35	1.12
1:M:121:LEU:HD12	10:L:79:ALA:HB3	1.14	1.10
1:M:165:CYS:SG	10:L:57:ALA:CB	2.40	1.10
2:I:42:VAL:HG12	2:I:191:VAL:HG21	1.34	1.09
1:M:121:LEU:HD12	10:L:79:ALA:HB1	1.31	1.09
1:M:161:THR:OG1	10:L:78:THR:HG21	1.52	1.08
10:G:78:THR:HG21	1:H:161:THR:OG1	1.52	1.08
10:G:79:ALA:HB3	1:H:121:LEU:HD12	1.11	1.07
10:G:79:ALA:HB1	1:H:121:LEU:HD12	1.33	1.07
13:E:200:SER:OG	9:X:173:ARG:HD2	1.55	1.07
9:S:173:ARG:HD2	13:B:200:SER:OG	1.54	1.07
2:N:42:VAL:HG12	2:N:191:VAL:HG21	1.34	1.07
8:C:65:ARG:NH1	8:C:68:TYR:CD2	2.23	1.06
8:D:65:ARG:NH1	8:D:68:TYR:CD2	2.23	1.05
10:G:47:VAL:HG12	10:G:195:LEU:HD22	1.37	1.04
10:L:47:VAL:HG12	10:L:195:LEU:HD22	1.37	1.02
9:S:148:LEU:HD23	9:S:178:VAL:HG12	1.37	1.02
2:N:42:VAL:CG1	2:N:191:VAL:CG2	2.28	1.01
9:X:148:LEU:HD23	9:X:178:VAL:HG12	1.37	1.01
2:N:169:ARG:HB2	2:N:169:ARG:HH11	1.24	1.01
12:A:15:VAL:HG13	12:A:177:VAL:HG22	1.43	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:F:15:VAL:HG13	12:F:177:VAL:HG22	1.43	0.99
2:I:169:ARG:HH11	2:I:169:ARG:HB2	1.24	0.98
2:I:42:VAL:CG1	2:I:191:VAL:CG2	2.28	0.98
5:J:41:CYS:CB	5:J:189:ILE:CD1	2.43	0.97
9:S:173:ARG:HB3	13:B:200:SER:HB2	1.46	0.96
5:Q:41:CYS:CB	5:Q:189:ILE:CD1	2.42	0.96
4:b:59:ARG:NH1	4:b:59:ARG:HB2	1.81	0.96
4:P:59:ARG:HH11	4:P:59:ARG:HB2	1.31	0.96
6:T:96:THR:HB	8:D:92:ARG:HH21	1.27	0.96
13:E:200:SER:HB2	9:X:173:ARG:HB3	1.47	0.96
2:N:196:LEU:HD11	2:N:202:GLY:HA3	1.48	0.95
7:Y:25:ARG:HG2	7:Y:25:ARG:HH11	1.31	0.95
2:N:42:VAL:HG11	2:N:191:VAL:HG21	0.95	0.95
4:P:59:ARG:HB2	4:P:59:ARG:NH1	1.80	0.95
2:N:40:ILE:HD12	2:N:212:ARG:HG3	1.47	0.95
3:Z:174:MET:CE	3:Z:195:LYS:HG2	1.97	0.95
5:J:41:CYS:HB3	5:J:189:ILE:HD13	1.47	0.95
2:I:40:ILE:HD12	2:I:212:ARG:HG3	1.47	0.94
2:I:42:VAL:HG11	2:I:191:VAL:HG21	0.95	0.94
2:N:64:ALA:HB2	2:N:217:LEU:HD22	1.47	0.94
2:I:64:ALA:HB2	2:I:217:LEU:HD22	1.47	0.94
4:b:59:ARG:HB2	4:b:59:ARG:HH11	1.31	0.94
3:O:174:MET:HE2	3:O:195:LYS:HG2	1.50	0.94
7:U:25:ARG:HG2	7:U:25:ARG:HH11	1.31	0.94
10:G:47:VAL:CG1	10:G:195:LEU:HD22	1.98	0.94
3:O:174:MET:CE	3:O:195:LYS:HG2	1.97	0.93
13:E:63:MET:HE2	13:E:74:PRO:HB3	1.50	0.93
5:Q:41:CYS:HB3	5:Q:189:ILE:HD13	1.47	0.93
3:Z:151:ASP:HB2	3:Z:152:PRO:HD2	1.50	0.93
2:I:196:LEU:HD11	2:I:202:GLY:HA3	1.48	0.93
10:L:47:VAL:CG1	10:L:195:LEU:HD22	1.98	0.93
3:Z:174:MET:HE2	3:Z:195:LYS:HG2	1.50	0.92
13:E:204:PHE:HE1	9:X:158:MET:HE2	1.32	0.92
13:B:205:ALA:HB1	13:B:206:PRO:HD2	0.94	0.92
9:S:158:MET:HE2	13:B:204:PHE:HE1	1.31	0.91
3:O:151:ASP:HB2	3:O:152:PRO:HD2	1.50	0.91
13:B:63:MET:HE2	13:B:74:PRO:HB3	1.50	0.91
8:C:92:ARG:HH21	6:V:96:THR:HB	1.29	0.91
11:K:196:GLU:HG3	11:K:242:LEU:HD21	1.52	0.91
13:E:205:ALA:HB1	13:E:206:PRO:HD2	0.94	0.91
11:R:196:GLU:HG3	11:R:242:LEU:HD21	1.52	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:88:ARG:HH21	4:P:88:ARG:HG2	1.36	0.89
2:N:100:ASP:OD1	2:N:101:PRO:HD2	1.72	0.89
10:G:56:LEU:HD13	1:H:167:ALA:HB3	1.53	0.89
11:K:155:ASP:HB2	11:K:156:PRO:CD	2.03	0.89
6:V:102:LEU:HD11	6:V:118:MET:HE3	1.54	0.89
11:R:155:ASP:HB2	11:R:156:PRO:CD	2.03	0.89
3:O:151:ASP:HB2	3:O:152:PRO:CD	2.04	0.88
3:Z:151:ASP:HB2	3:Z:152:PRO:CD	2.03	0.88
11:R:49:VAL:HG22	11:R:219:VAL:HG12	1.56	0.88
4:b:88:ARG:HG2	4:b:88:ARG:HH21	1.37	0.87
2:I:100:ASP:OD1	2:I:101:PRO:HD2	1.73	0.87
2:I:183:THR:HG22	2:I:186:LEU:HB2	1.57	0.87
10:G:166:GLN:O	10:G:166:GLN:NE2	2.08	0.87
11:K:49:VAL:HG22	11:K:219:VAL:HG12	1.56	0.87
2:N:183:THR:HG22	2:N:186:LEU:HB2	1.57	0.87
13:B:109:GLN:HG3	13:B:121:ARG:HH11	1.40	0.87
11:R:155:ASP:HB2	11:R:156:PRO:HD2	1.56	0.87
11:K:155:ASP:HB2	11:K:156:PRO:HD2	1.56	0.86
6:T:102:LEU:HD11	6:T:118:MET:HE3	1.54	0.86
2:N:169:ARG:HH11	2:N:169:ARG:CB	1.88	0.86
13:E:109:GLN:HG3	13:E:121:ARG:HH11	1.40	0.86
2:I:169:ARG:HH11	2:I:169:ARG:CB	1.88	0.86
10:L:166:GLN:O	10:L:166:GLN:NE2	2.08	0.85
8:C:65:ARG:NH1	8:C:68:TYR:HD2	1.71	0.85
4:b:53:SER:HB2	11:K:180:GLU:OE2	1.76	0.85
11:R:196:GLU:HG3	11:R:242:LEU:CD2	2.06	0.85
12:A:116:MET:SD	12:A:116:MET:N	2.50	0.84
11:K:196:GLU:HG3	11:K:242:LEU:CD2	2.06	0.84
2:I:29:GLY:O	2:I:163:ARG:HG2	1.78	0.84
11:K:88:ARG:HH21	11:K:88:ARG:HG2	1.42	0.84
12:F:116:MET:SD	12:F:116:MET:N	2.50	0.84
2:N:29:GLY:O	2:N:163:ARG:HG2	1.78	0.84
10:G:78:THR:CG2	1:H:161:THR:OG1	2.26	0.83
11:R:88:ARG:HG2	11:R:88:ARG:HH21	1.42	0.83
6:T:96:THR:CB	8:D:92:ARG:NH2	2.40	0.83
1:H:49:ALA:HB2	1:H:217:LEU:HD12	1.61	0.83
4:P:53:SER:HB2	11:R:180:GLU:OE2	1.78	0.83
8:D:65:ARG:NH1	8:D:68:TYR:HD2	1.71	0.83
1:M:167:ALA:HB3	10:L:56:LEU:HD13	1.58	0.82
12:A:15:VAL:HG13	12:A:177:VAL:CG2	2.09	0.82
1:M:49:ALA:HB2	1:M:217:LEU:HD12	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:100:GLY:H	7:U:101:PRO:HD3	1.42	0.82
12:F:15:VAL:CG1	12:F:177:VAL:CG2	2.58	0.82
12:F:15:VAL:HG13	12:F:177:VAL:CG2	2.09	0.82
1:M:161:THR:OG1	10:L:78:THR:CG2	2.26	0.82
12:A:15:VAL:CG1	12:A:177:VAL:CG2	2.57	0.82
7:Y:100:GLY:H	7:Y:101:PRO:HD3	1.42	0.81
14:a:174:ARG:HD2	14:a:206:GLU:O	1.81	0.81
7:Y:70:LEU:O	7:Y:74:GLU:HG2	1.81	0.80
3:O:174:MET:HE3	3:O:195:LYS:NZ	1.97	0.80
9:S:158:MET:HE2	13:B:204:PHE:CE1	2.17	0.80
13:E:204:PHE:CE1	9:X:158:MET:HE2	2.17	0.80
6:T:1:MET:HG2	6:T:134:TYR:H	1.47	0.79
3:Z:174:MET:HE3	3:Z:195:LYS:NZ	1.97	0.79
8:C:104:GLY:HA2	8:C:180:MET:HE3	1.64	0.79
14:W:174:ARG:HD2	14:W:206:GLU:O	1.81	0.79
8:D:104:GLY:HA2	8:D:180:MET:HE3	1.64	0.78
7:U:70:LEU:O	7:U:74:GLU:HG2	1.81	0.78
8:C:92:ARG:NH2	6:V:96:THR:CB	2.42	0.78
9:S:173:ARG:CB	13:B:200:SER:HB2	2.13	0.78
14:a:174:ARG:CD	14:a:206:GLU:O	2.32	0.78
6:V:1:MET:HG2	6:V:134:TYR:H	1.47	0.78
13:E:200:SER:HB2	9:X:173:ARG:CB	2.14	0.78
5:Q:152:ASP:HB2	5:Q:153:PRO:HD2	1.66	0.77
1:H:50:VAL:HG11	1:H:66:LYS:HB2	1.67	0.77
13:E:194:LYS:HG3	13:E:195:PRO:HD2	1.66	0.77
2:N:139:ASP:OD1	2:N:139:ASP:N	2.17	0.77
14:W:174:ARG:CD	14:W:206:GLU:O	2.32	0.77
12:A:38:LEU:HD11	12:A:44:CYS:HB3	1.66	0.77
5:J:152:ASP:HB2	5:J:153:PRO:HD2	1.66	0.77
13:E:200:SER:CB	9:X:173:ARG:HD2	2.14	0.77
9:X:184:GLU:OE2	9:X:211:ARG:HD2	1.85	0.77
9:S:148:LEU:HD23	9:S:178:VAL:CG1	2.15	0.77
11:K:196:GLU:HG3	11:K:242:LEU:CG	2.15	0.77
11:R:196:GLU:HG3	11:R:242:LEU:CG	2.15	0.76
2:I:175:ASN:O	2:I:190:LEU:HD21	1.84	0.76
2:N:175:ASN:O	2:N:190:LEU:HD21	1.84	0.76
9:S:173:ARG:HD2	13:B:200:SER:CB	2.14	0.76
9:S:184:GLU:OE2	9:S:211:ARG:HD2	1.85	0.76
13:B:194:LYS:HG3	13:B:195:PRO:HD2	1.66	0.76
12:F:38:LEU:HD11	12:F:44:CYS:HB3	1.66	0.76
4:P:88:ARG:HG2	4:P:88:ARG:NH2	1.98	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:92:ARG:HH22	6:V:96:THR:HB	1.51	0.76
9:X:148:LEU:HD23	9:X:178:VAL:CG1	2.15	0.76
6:T:2:GLU:HG2	6:T:34:LYS:HE2	1.68	0.76
1:M:50:VAL:HG11	1:M:66:LYS:HB2	1.66	0.75
2:N:196:LEU:CD1	2:N:202:GLY:HA3	2.16	0.75
2:I:196:LEU:CD1	2:I:202:GLY:HA3	2.16	0.75
9:X:148:LEU:CD2	9:X:178:VAL:HG12	2.17	0.75
6:V:2:GLU:HG2	6:V:34:LYS:HE2	1.68	0.75
2:N:90:GLU:HG2	2:N:110:TYR:CD1	2.22	0.74
12:A:189:ILE:HG22	12:A:194:LEU:HD23	1.69	0.74
2:I:90:GLU:HG2	2:I:110:TYR:CD1	2.23	0.74
4:P:149:ASP:HB2	4:P:150:PRO:HD2	1.68	0.74
12:F:189:ILE:HG22	12:F:194:LEU:HD23	1.69	0.74
6:T:96:THR:HB	8:D:92:ARG:HH22	1.50	0.74
9:S:148:LEU:CD2	9:S:178:VAL:HG12	2.17	0.74
11:R:196:GLU:CG	11:R:242:LEU:HD21	2.18	0.74
3:Z:35:LEU:HD23	3:Z:197:LEU:HD13	1.70	0.74
11:K:196:GLU:CG	11:K:242:LEU:HD21	2.18	0.73
12:A:15:VAL:CG1	12:A:177:VAL:HG22	2.19	0.73
8:C:162:THR:HG22	8:C:197:LEU:HD13	1.70	0.73
4:b:149:ASP:HB2	4:b:150:PRO:HD2	1.68	0.73
5:J:170:GLN:HA	5:J:170:GLN:NE2	2.04	0.73
2:N:66:ASP:OD2	2:N:91:CYS:HB3	1.89	0.73
13:E:6:LEU:HD12	13:E:6:LEU:C	2.14	0.73
5:Q:41:CYS:HB3	5:Q:189:ILE:HD11	1.68	0.73
8:D:162:THR:HG22	8:D:197:LEU:HD13	1.70	0.73
3:O:35:LEU:HD23	3:O:197:LEU:HD13	1.70	0.72
5:Q:175:GLU:HB3	5:Q:196:ILE:HG12	1.71	0.72
2:I:66:ASP:OD2	2:I:91:CYS:HB3	1.89	0.72
8:C:158:ARG:NH2	8:C:189:GLU:OE2	2.21	0.72
2:I:139:ASP:OD1	2:I:139:ASP:N	2.17	0.72
5:Q:170:GLN:HA	5:Q:170:GLN:NE2	2.04	0.72
4:P:185:ASP:O	4:P:189:THR:HG22	1.89	0.72
13:B:6:LEU:C	13:B:6:LEU:HD12	2.14	0.72
7:Y:25:ARG:HG2	7:Y:25:ARG:NH1	2.05	0.71
13:E:40:LYS:CD	13:E:40:LYS:H	2.02	0.71
6:V:62:LYS:HD3	2:I:96:LEU:HD22	1.73	0.71
13:B:156:VAL:HG21	13:B:189:LEU:HD11	1.73	0.71
4:b:149:ASP:HB2	4:b:150:PRO:CD	2.21	0.71
13:E:156:VAL:HG21	13:E:189:LEU:HD11	1.73	0.71
14:a:179:ARG:HG3	13:B:135:LEU:CD1	2.21	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:b:185:ASP:O	4:b:189:THR:HG22	1.89	0.71
5:J:175:GLU:HB3	5:J:196:ILE:HG12	1.71	0.71
5:J:41:CYS:HB3	5:J:189:ILE:HD11	1.68	0.71
2:I:70:CYS:HB3	2:I:211:MET:SD	2.31	0.71
2:N:70:CYS:HB3	2:N:211:MET:SD	2.31	0.70
4:P:149:ASP:HB2	4:P:150:PRO:CD	2.21	0.70
2:I:180:ALA:HB1	2:I:190:LEU:CD2	2.21	0.70
8:D:157:GLY:HA3	8:D:177:MET:CE	2.22	0.70
13:B:40:LYS:H	13:B:40:LYS:CD	2.02	0.70
2:N:96:LEU:HD22	6:T:62:LYS:HD3	1.74	0.70
7:U:25:ARG:HG2	7:U:25:ARG:NH1	2.05	0.70
12:F:15:VAL:CG1	12:F:177:VAL:HG22	2.19	0.70
13:B:141:ARG:HG3	13:B:141:ARG:HH11	1.56	0.70
8:C:157:GLY:HA3	8:C:177:MET:CE	2.22	0.70
13:E:141:ARG:HH11	13:E:141:ARG:HG3	1.56	0.70
8:D:158:ARG:NH2	8:D:189:GLU:OE2	2.21	0.70
5:Q:152:ASP:HB2	5:Q:153:PRO:CD	2.21	0.69
12:F:91:TYR:HB2	12:F:95:LEU:HD12	1.74	0.69
13:E:198:ARG:O	13:E:198:ARG:HG2	1.90	0.69
11:K:103:TYR:O	13:B:81:ARG:HD3	1.92	0.69
12:F:76:LEU:HD21	12:F:107:ARG:HG3	1.74	0.69
13:E:135:LEU:CD1	14:W:179:ARG:HG3	2.22	0.69
12:A:76:LEU:CD2	12:A:107:ARG:HG3	2.22	0.69
12:A:76:LEU:HD21	12:A:107:ARG:HG3	1.74	0.69
12:A:91:TYR:HB2	12:A:95:LEU:HD12	1.74	0.69
10:G:56:LEU:CD1	1:H:167:ALA:HB3	2.22	0.69
8:C:158:ARG:HD3	8:C:189:GLU:OE2	1.91	0.69
7:Y:100:GLY:H	7:Y:101:PRO:CD	2.06	0.69
3:Z:201:MET:HE1	3:Z:210:LYS:HB3	1.74	0.69
2:N:180:ALA:HB1	2:N:190:LEU:CD2	2.21	0.69
7:U:116:PHE:CE2	7:U:191:LYS:HE3	2.28	0.69
8:C:192:ASP:HB3	8:C:195:GLU:HG3	1.74	0.69
13:B:198:ARG:O	13:B:198:ARG:HG2	1.90	0.69
11:K:181:LYS:HA	11:K:184:LYS:HE2	1.75	0.69
8:D:158:ARG:HD3	8:D:189:GLU:OE2	1.91	0.69
1:H:213:THR:HG22	1:H:231:LYS:HE3	1.75	0.69
5:J:152:ASP:HB2	5:J:153:PRO:CD	2.21	0.69
7:Y:116:PHE:CE2	7:Y:191:LYS:HE3	2.28	0.68
5:J:41:CYS:CB	5:J:189:ILE:HD12	2.23	0.68
10:L:50:LYS:HB3	10:L:59:HIS:HB3	1.75	0.68
8:D:192:ASP:HB3	8:D:195:GLU:HG3	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:W:96:MET:HE3	14:W:127:MET:HA	1.75	0.68
11:R:181:LYS:HA	11:R:184:LYS:HE2	1.75	0.68
12:F:76:LEU:CD2	12:F:107:ARG:HG3	2.22	0.68
5:Q:41:CYS:CB	5:Q:189:ILE:HD12	2.23	0.68
1:M:213:THR:HG22	1:M:231:LYS:HE3	1.75	0.68
3:O:201:MET:HE1	3:O:210:LYS:HB3	1.74	0.68
7:U:100:GLY:H	7:U:101:PRO:CD	2.06	0.68
1:M:165:CYS:SG	10:L:57:ALA:HB1	2.33	0.68
10:G:35:THR:HG23	10:G:133:LEU:HD12	1.76	0.68
5:Q:59:GLU:OE2	10:L:157:ARG:HG2	1.94	0.67
10:G:50:LYS:HB3	10:G:59:HIS:HB3	1.75	0.67
5:J:41:CYS:CB	5:J:189:ILE:HD11	2.24	0.67
10:G:57:ALA:HB1	1:H:165:CYS:SG	2.30	0.67
14:a:96:MET:HE3	14:a:127:MET:HA	1.75	0.67
13:B:109:GLN:HG3	13:B:121:ARG:NH1	2.08	0.67
13:B:141:ARG:HG3	13:B:141:ARG:NH1	2.08	0.67
4:P:175:LYS:O	4:P:175:LYS:HG2	1.95	0.67
13:E:109:GLN:HG3	13:E:121:ARG:NH1	2.08	0.67
10:L:35:THR:HG23	10:L:133:LEU:HD12	1.76	0.67
13:E:141:ARG:HG3	13:E:141:ARG:NH1	2.08	0.67
4:b:175:LYS:O	4:b:175:LYS:HG2	1.95	0.66
13:E:81:ARG:HD3	11:R:103:TYR:O	1.95	0.66
1:M:206:MET:HE1	1:M:214:ASN:ND2	2.11	0.66
2:I:221:ASN:HB2	2:I:222:PRO:HD2	1.78	0.66
3:O:174:MET:HE3	3:O:195:LYS:HZ1	1.59	0.66
4:P:74:VAL:CG1	4:P:134:LEU:HB2	2.26	0.66
8:D:73:GLU:O	8:D:73:GLU:HG2	1.96	0.66
10:G:157:ARG:HG2	5:J:59:GLU:OE2	1.95	0.66
4:b:88:ARG:HG2	4:b:88:ARG:NH2	1.98	0.66
3:O:35:LEU:C	3:O:35:LEU:HD12	2.21	0.65
10:G:65:HIS:HD2	9:X:77:HIS:NE2	1.95	0.65
3:Z:35:LEU:HD12	3:Z:35:LEU:C	2.21	0.65
4:b:53:SER:CB	11:K:180:GLU:OE2	2.44	0.65
4:b:74:VAL:CG1	4:b:134:LEU:HB2	2.26	0.65
8:D:126:MET:SD	8:D:140:MET:HE3	2.37	0.65
9:X:43:CYS:SG	9:X:194:ARG:NH2	2.69	0.65
13:B:54:MET:HA	13:B:54:MET:HE2	1.79	0.65
3:O:196:VAL:O	3:O:200:THR:HG23	1.96	0.65
4:b:88:ARG:HH21	4:b:88:ARG:CG	2.09	0.65
2:N:221:ASN:HB2	2:N:222:PRO:HD2	1.78	0.65
13:E:54:MET:HE2	13:E:54:MET:HA	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:70:CYS:HB2	2:N:217:LEU:HD11	1.78	0.65
3:Z:196:VAL:O	3:Z:200:THR:HG23	1.96	0.65
11:K:88:ARG:HG2	11:K:88:ARG:NH2	2.12	0.65
12:A:119:MET:O	12:A:119:MET:HG3	1.97	0.65
9:S:43:CYS:SG	9:S:194:ARG:NH2	2.69	0.65
12:F:116:MET:HE2	14:a:36:PHE:HZ	1.62	0.65
10:L:192:LEU:HD13	10:L:233:LEU:HD23	1.79	0.65
4:P:53:SER:CB	11:R:180:GLU:OE2	2.45	0.64
7:Y:19:VAL:HG23	7:Y:189:ILE:HB	1.79	0.64
2:N:96:LEU:CD1	6:T:58:GLU:HB3	2.27	0.64
4:P:88:ARG:HH21	4:P:88:ARG:CG	2.09	0.64
2:I:70:CYS:HB2	2:I:217:LEU:HD11	1.78	0.64
8:C:73:GLU:O	8:C:73:GLU:HG2	1.96	0.64
10:G:192:LEU:HD13	10:G:233:LEU:HD23	1.79	0.64
12:F:43:TYR:HH	12:F:186:TYR:HE2	1.45	0.64
9:X:176:LYS:NZ	9:X:206:GLU:OE2	2.21	0.64
2:N:170:GLU:OE1	2:N:170:GLU:HA	1.98	0.64
13:E:135:LEU:HD11	14:W:179:ARG:HG3	1.80	0.64
13:E:200:SER:OG	9:X:173:ARG:NH2	2.30	0.64
2:I:170:GLU:OE1	2:I:170:GLU:HA	1.98	0.64
3:O:57:ASP:OD2	4:P:38:LYS:HE2	1.98	0.64
4:P:172:PHE:CD2	4:P:196:GLU:OE1	2.51	0.64
12:F:119:MET:O	12:F:119:MET:HG3	1.97	0.64
13:E:6:LEU:HD11	13:E:151:ALA:HB1	1.80	0.64
14:a:179:ARG:HG3	13:B:135:LEU:HD11	1.80	0.64
13:B:6:LEU:HD11	13:B:151:ALA:HB1	1.80	0.64
9:S:173:ARG:NH2	13:B:200:SER:OG	2.30	0.64
7:U:19:VAL:HG23	7:U:189:ILE:HB	1.79	0.64
9:S:99:ARG:HG3	9:S:104:TYR:CE2	2.33	0.64
1:H:206:MET:HE1	1:H:214:ASN:ND2	2.11	0.64
9:X:99:ARG:HG3	9:X:104:TYR:CE2	2.33	0.64
9:S:145:LEU:HD21	9:S:182:ALA:HB2	1.79	0.64
11:R:88:ARG:HG2	11:R:88:ARG:NH2	2.12	0.64
6:V:58:GLU:HB3	2:I:96:LEU:CD1	2.28	0.63
1:M:167:ALA:HB3	10:L:56:LEU:CD1	2.27	0.63
8:C:126:MET:SD	8:C:140:MET:HE3	2.37	0.63
13:E:40:LYS:NZ	13:E:103:VAL:O	2.32	0.63
9:X:145:LEU:HD21	9:X:182:ALA:HB2	1.79	0.63
13:B:81:ARG:NH2	13:B:84:ARG:HH12	1.96	0.63
1:M:165:CYS:HG	10:L:57:ALA:HB2	1.63	0.63
4:b:172:PHE:CD2	4:b:196:GLU:OE1	2.51	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:W:36:PHE:HZ	12:A:116:MET:HE2	1.61	0.63
11:R:196:GLU:HG3	11:R:242:LEU:HG	1.80	0.63
13:B:40:LYS:NZ	13:B:103:VAL:O	2.32	0.63
13:B:205:ALA:CB	13:B:206:PRO:CD	2.44	0.63
13:E:148:LEU:C	13:E:148:LEU:HD23	2.24	0.63
12:A:200:GLU:HB3	14:a:186:ARG:NH1	2.14	0.63
14:a:208:ASN:HD21	14:a:210:GLU:HB2	1.64	0.63
13:B:148:LEU:HD23	13:B:148:LEU:C	2.24	0.63
11:K:196:GLU:HG3	11:K:242:LEU:HG	1.80	0.63
12:F:200:GLU:HB3	14:W:186:ARG:NH1	2.14	0.63
8:D:65:ARG:HD2	8:D:65:ARG:O	2.00	0.62
13:E:81:ARG:NH2	13:E:84:ARG:HH12	1.96	0.62
5:J:151:ILE:HG12	5:J:157:SER:HB2	1.81	0.62
13:E:13:ILE:CD1	13:E:151:ALA:HB3	2.29	0.62
7:Y:200:LYS:HA	13:B:212:GLN:NE2	2.15	0.62
2:I:169:ARG:HH11	2:I:169:ARG:CG	2.13	0.62
2:I:185:ASP:N	2:I:185:ASP:OD1	2.32	0.62
13:B:13:ILE:CD1	13:B:151:ALA:HB3	2.30	0.62
6:T:171:PHE:O	6:V:27:GLN:NE2	2.32	0.62
14:W:208:ASN:HD21	14:W:210:GLU:HB2	1.64	0.62
5:Q:151:ILE:HG12	5:Q:157:SER:HB2	1.81	0.62
7:U:200:LYS:HA	13:E:212:GLN:NE2	2.14	0.62
1:H:184:VAL:O	1:H:184:VAL:HG22	2.00	0.62
12:A:157:THR:HG23	12:A:189:ILE:HD12	1.82	0.62
9:S:77:HIS:NE2	10:L:65:HIS:HD2	1.97	0.61
3:Z:57:ASP:OD2	4:b:38:LYS:HE2	1.99	0.61
5:J:170:GLN:HA	5:J:170:GLN:HE21	1.65	0.61
7:Y:93:LEU:C	7:Y:93:LEU:HD23	2.25	0.61
13:E:40:LYS:H	13:E:40:LYS:HD3	1.65	0.61
4:P:54:ILE:CD1	11:R:184:LYS:HB3	2.30	0.61
1:H:91:LYS:HE2	1:H:119:LEU:HD11	1.82	0.61
2:N:185:ASP:N	2:N:185:ASP:OD1	2.32	0.61
4:b:54:ILE:CD1	11:K:184:LYS:HB3	2.30	0.61
10:L:72:ILE:HG22	10:L:134:ILE:HG12	1.83	0.61
10:G:72:ILE:HG22	10:G:134:ILE:HG12	1.82	0.61
9:X:43:CYS:O	9:X:194:ARG:NH2	2.33	0.61
9:S:43:CYS:O	9:S:194:ARG:NH2	2.33	0.61
2:I:40:ILE:CD1	2:I:212:ARG:HG3	2.24	0.61
1:M:184:VAL:HG22	1:M:184:VAL:O	2.00	0.61
2:N:90:GLU:OE1	2:N:90:GLU:HA	2.01	0.61
6:T:27:GLN:NE2	6:V:171:PHE:O	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:R:58:ASP:HB3	11:R:61:LEU:HD12	1.83	0.61
8:D:39:ASN:HB2	8:D:40:PRO:CD	2.31	0.61
8:C:39:ASN:HB2	8:C:40:PRO:CD	2.31	0.61
8:C:65:ARG:HD2	8:C:65:ARG:O	1.99	0.61
5:J:53:VAL:HG23	5:J:53:VAL:O	2.01	0.61
1:M:91:LYS:HE2	1:M:119:LEU:HD11	1.82	0.61
2:N:57:ARG:HH11	2:N:57:ARG:CG	2.14	0.61
8:C:46:MET:HG2	8:C:53:CYS:HB3	1.82	0.61
2:I:96:LEU:O	2:I:96:LEU:HG	2.00	0.61
2:N:40:ILE:CD1	2:N:212:ARG:HG3	2.24	0.60
10:G:79:ALA:HB3	1:H:121:LEU:HD11	1.79	0.60
11:K:58:ASP:HB3	11:K:61:LEU:HD12	1.83	0.60
2:I:57:ARG:HH11	2:I:57:ARG:CG	2.14	0.60
8:C:117:GLN:H	8:C:117:GLN:HE21	1.47	0.60
12:A:165:ASN:ND2	12:A:199:ASP:OD1	2.34	0.60
12:F:157:THR:HG23	12:F:189:ILE:HD12	1.82	0.60
8:D:117:GLN:H	8:D:117:GLN:HE21	1.47	0.60
5:Q:63:ASN:OD1	10:L:154:PHE:CD2	2.54	0.60
4:b:106:THR:OG1	4:b:139:ASN:ND2	2.30	0.60
13:E:109:GLN:CG	13:E:121:ARG:HH11	2.14	0.60
1:H:78:MET:HG3	1:H:82:ILE:HD12	1.83	0.60
12:F:165:ASN:ND2	12:F:199:ASP:OD1	2.34	0.60
8:D:46:MET:HG2	8:D:53:CYS:HB3	1.82	0.60
5:Q:53:VAL:HG23	5:Q:53:VAL:O	2.01	0.60
5:Q:170:GLN:HA	5:Q:170:GLN:HE21	1.65	0.60
8:C:157:GLY:HA3	8:C:177:MET:HE1	1.83	0.60
12:A:85:ARG:HB2	12:A:120:LEU:HD13	1.84	0.60
10:L:49:LEU:HD21	10:L:199:LEU:CD2	2.32	0.60
2:N:169:ARG:HH11	2:N:169:ARG:CG	2.13	0.60
2:N:96:LEU:O	2:N:96:LEU:HG	2.00	0.60
7:U:93:LEU:C	7:U:93:LEU:HD23	2.25	0.60
1:M:78:MET:HG3	1:M:82:ILE:HD12	1.83	0.60
13:B:6:LEU:HD12	13:B:6:LEU:O	2.02	0.60
3:Z:174:MET:HE3	3:Z:195:LYS:HZ2	1.65	0.59
13:E:6:LEU:HD12	13:E:6:LEU:O	2.02	0.59
11:R:11:ARG:HG2	11:R:11:ARG:HH11	1.68	0.59
13:B:109:GLN:CG	13:B:121:ARG:HH11	2.14	0.59
5:Q:41:CYS:CB	5:Q:189:ILE:HD11	2.24	0.59
1:M:189:MET:HE2	1:M:194:ALA:HA	1.85	0.59
4:b:75:TYR:HB3	4:b:82:TYR:CD1	2.37	0.59
12:F:85:ARG:HB2	12:F:120:LEU:HD13	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:169:ARG:HB2	2:I:169:ARG:NH1	2.08	0.59
8:D:157:GLY:HA3	8:D:177:MET:HE1	1.83	0.59
4:P:75:TYR:HB3	4:P:82:TYR:CD1	2.37	0.59
11:R:56:VAL:HG12	11:R:56:VAL:O	2.03	0.59
1:H:148:GLU:OE2	9:X:81:LYS:NZ	2.32	0.59
13:B:40:LYS:H	13:B:40:LYS:HD3	1.65	0.59
1:M:91:LYS:HG2	1:M:119:LEU:HD11	1.85	0.59
8:D:13:VAL:HG11	8:D:103:CYS:SG	2.43	0.59
5:Q:27:MET:O	5:Q:31:GLU:HG3	2.03	0.59
10:G:57:ALA:CA	1:H:165:CYS:SG	2.91	0.59
2:I:90:GLU:OE1	2:I:90:GLU:HA	2.01	0.59
13:B:13:ILE:HD12	13:B:151:ALA:HB1	1.84	0.59
1:H:189:MET:HE2	1:H:194:ALA:HA	1.85	0.58
5:J:27:MET:O	5:J:31:GLU:HG3	2.03	0.58
12:F:81:ALA:HB1	12:F:120:LEU:HD11	1.84	0.58
2:N:220:LEU:HD13	2:N:224:GLU:HG2	1.85	0.58
9:S:75:TYR:CD1	9:S:83:MET:HG3	2.39	0.58
13:B:13:ILE:HD12	13:B:151:ALA:CB	2.33	0.58
3:Z:49:ARG:NH1	3:Z:212:GLU:OE2	2.37	0.58
3:Z:161:ALA:HB3	2:I:53:LEU:HD22	1.85	0.58
13:E:13:ILE:HD12	13:E:151:ALA:HB1	1.84	0.58
11:R:43:ARG:HD2	11:R:149:PRO:O	2.03	0.58
1:H:157:ASP:HB2	1:H:158:PRO:CD	2.34	0.58
3:Z:174:MET:HE3	3:Z:195:LYS:HZ1	1.68	0.58
12:A:81:ALA:HB1	12:A:120:LEU:HD11	1.84	0.58
1:M:53:ARG:O	1:M:53:ARG:HG2	2.03	0.58
10:G:49:LEU:HD21	10:G:199:LEU:HD21	1.85	0.58
10:G:49:LEU:HD21	10:G:199:LEU:CD2	2.32	0.58
13:B:81:ARG:HH21	13:B:84:ARG:HH12	1.50	0.58
13:B:63:MET:HE1	13:B:78:THR:HG21	1.85	0.58
1:H:91:LYS:HG2	1:H:119:LEU:HD11	1.84	0.58
12:F:172:GLY:HA2	14:W:209:TRP:CH2	2.39	0.58
13:E:13:ILE:HD12	13:E:151:ALA:CB	2.33	0.58
10:G:154:PHE:CD2	5:J:63:ASN:OD1	2.57	0.58
11:K:11:ARG:HH11	11:K:11:ARG:HG2	1.68	0.58
3:O:171:ALA:HB2	3:O:200:THR:HG21	1.86	0.57
8:C:13:VAL:HG11	8:C:103:CYS:SG	2.43	0.57
9:S:159:GLN:HG2	13:B:208:THR:O	2.04	0.57
13:E:63:MET:HE1	13:E:78:THR:HG21	1.85	0.57
9:X:123:SER:HB3	9:X:136:LYS:HG2	1.85	0.57
3:Z:58:GLU:CD	3:Z:58:GLU:H	2.13	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:X:75:TYR:CD1	9:X:83:MET:HG3	2.39	0.57
9:S:123:SER:HB3	9:S:136:LYS:HG2	1.85	0.57
13:E:81:ARG:HH21	13:E:84:ARG:HH12	1.50	0.57
9:S:176:LYS:NZ	9:S:206:GLU:OE2	2.21	0.57
11:K:56:VAL:HG12	11:K:56:VAL:O	2.03	0.57
13:E:208:THR:O	9:X:159:GLN:HG2	2.04	0.57
2:N:11:SER:OG	2:N:12:PRO:HD2	2.05	0.57
1:H:53:ARG:O	1:H:53:ARG:HG2	2.03	0.57
11:K:43:ARG:HD2	11:K:149:PRO:O	2.03	0.57
2:I:42:VAL:HG12	2:I:191:VAL:CG2	2.14	0.57
1:M:157:ASP:HB2	1:M:158:PRO:CD	2.34	0.57
3:O:49:ARG:NH1	3:O:212:GLU:OE2	2.37	0.57
10:L:49:LEU:HD21	10:L:199:LEU:HD21	1.85	0.57
1:M:121:LEU:HD11	10:L:79:ALA:HB3	1.79	0.57
3:Z:171:ALA:HB2	3:Z:200:THR:HG21	1.86	0.57
2:I:220:LEU:HD13	2:I:224:GLU:HG2	1.85	0.57
9:X:41:PRO:HB3	9:X:194:ARG:HD2	1.86	0.57
2:I:11:SER:OG	2:I:12:PRO:HD2	2.05	0.57
2:I:42:VAL:HG11	2:I:191:VAL:HG23	1.78	0.57
11:K:37:LEU:HD22	11:K:53:GLN:HB3	1.87	0.56
6:V:67:TYR:CD1	6:V:75:LEU:HG	2.40	0.56
10:L:59:HIS:CD2	10:L:208:LYS:O	2.58	0.56
1:M:91:LYS:HG2	1:M:119:LEU:CD1	2.35	0.56
5:Q:53:VAL:HG22	5:Q:208:ALA:O	2.06	0.56
10:G:59:HIS:CD2	10:G:208:LYS:O	2.58	0.56
1:H:91:LYS:HG2	1:H:119:LEU:CD1	2.35	0.56
4:b:54:ILE:HD13	11:K:184:LYS:HB3	1.87	0.56
11:K:56:VAL:HG22	11:K:66:VAL:HG11	1.87	0.56
12:F:148:SER:HB2	12:F:149:PRO:HD2	1.87	0.56
12:A:172:GLY:HA2	14:a:209:TRP:CH2	2.40	0.56
12:A:189:ILE:CG2	12:A:194:LEU:HD23	2.35	0.56
10:L:230:SER:HB2	10:L:231:PRO:HD3	1.88	0.56
10:G:230:SER:HB2	10:G:231:PRO:HD3	1.88	0.56
12:A:148:SER:HB2	12:A:149:PRO:HD2	1.87	0.56
2:N:148:ASP:HB2	2:N:149:PRO:HD2	1.87	0.56
6:T:67:TYR:CD1	6:T:75:LEU:HG	2.40	0.56
13:E:20:ALA:HB3	13:E:28:ASP:HB3	1.88	0.56
11:R:78:CYS:HB2	11:R:140:LEU:HD23	1.86	0.56
13:B:40:LYS:CD	13:B:40:LYS:N	2.69	0.56
8:C:161:ILE:HB	8:C:175:ILE:HD12	1.87	0.56
9:S:41:PRO:HB3	9:S:194:ARG:HD2	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:R:37:LEU:HD22	11:R:53:GLN:HB3	1.87	0.56
8:D:113:TYR:CE2	8:D:123:SER:HB2	2.41	0.56
8:D:161:ILE:HB	8:D:175:ILE:HD12	1.87	0.56
14:W:174:ARG:HD3	14:W:206:GLU:O	2.05	0.56
11:K:78:CYS:HB2	11:K:140:LEU:HD23	1.86	0.56
9:X:43:CYS:SG	9:X:194:ARG:HD3	2.46	0.56
9:S:10:GLY:HA3	9:S:42:LYS:HE2	1.87	0.55
13:B:20:ALA:HB3	13:B:28:ASP:HB3	1.88	0.55
3:O:58:GLU:H	3:O:58:GLU:CD	2.13	0.55
9:S:43:CYS:SG	9:S:194:ARG:HD3	2.46	0.55
11:R:223:GLU:OE2	11:R:223:GLU:HA	2.06	0.55
5:J:53:VAL:HG22	5:J:208:ALA:O	2.06	0.55
11:R:56:VAL:HG22	11:R:66:VAL:HG11	1.87	0.55
11:R:201:CYS:O	11:R:205:VAL:HG13	2.07	0.55
9:X:10:GLY:HA3	9:X:42:LYS:HE2	1.87	0.55
8:C:113:TYR:CE2	8:C:123:SER:HB2	2.41	0.55
12:F:189:ILE:CG2	12:F:194:LEU:HD23	2.35	0.55
13:E:201:GLN:H	13:E:201:GLN:NE2	2.05	0.55
2:I:148:ASP:HB2	2:I:149:PRO:HD2	1.88	0.55
2:N:148:ASP:HB2	2:N:149:PRO:CD	2.37	0.55
6:V:2:GLU:HG2	6:V:34:LYS:CE	2.37	0.55
12:A:58:ASP:OD2	13:B:84:ARG:NH1	2.33	0.55
13:E:13:ILE:CD1	13:E:151:ALA:CB	2.85	0.55
4:P:106:THR:OG1	4:P:139:ASN:ND2	2.30	0.55
6:T:43:LEU:HB2	6:T:183:ILE:HD11	1.89	0.55
8:C:65:ARG:NH1	8:C:68:TYR:CE2	2.66	0.55
3:Z:34:CYS:HB2	3:Z:164:ILE:HG13	1.89	0.55
2:I:183:THR:CG2	2:I:186:LEU:HB2	2.34	0.55
2:N:40:ILE:CA	2:N:136:PHE:HZ	2.20	0.55
2:N:42:VAL:HG12	2:N:191:VAL:CG2	2.14	0.55
2:N:218:LYS:C	2:N:218:LYS:HD3	2.32	0.55
2:N:227:LYS:O	2:N:231:GLU:HG2	2.07	0.55
6:V:43:LEU:HB2	6:V:183:ILE:HD11	1.89	0.55
11:R:137:CYS:SG	11:R:153:LYS:HD2	2.47	0.55
13:B:201:GLN:H	13:B:201:GLN:NE2	2.05	0.55
2:N:171:PHE:CD1	2:N:171:PHE:C	2.85	0.54
11:K:201:CYS:O	11:K:205:VAL:HG13	2.07	0.54
1:M:165:CYS:SG	10:L:57:ALA:CA	2.95	0.54
2:I:227:LYS:O	2:I:231:GLU:HG2	2.07	0.54
4:b:181:LEU:HD21	4:b:186:ALA:HA	1.89	0.54
11:K:77:GLY:HA3	11:K:227:PHE:CD1	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:137:CYS:SG	11:K:153:LYS:HD2	2.47	0.54
12:F:58:ASP:OD2	13:E:84:ARG:NH1	2.33	0.54
4:P:74:VAL:HG12	4:P:134:LEU:HB2	1.90	0.54
10:G:220:GLU:O	10:G:222:THR:HG23	2.08	0.54
4:b:51:GLN:HA	4:b:51:GLN:NE2	2.23	0.54
12:F:15:VAL:HG12	12:F:177:VAL:HG23	1.90	0.54
2:I:148:ASP:HB2	2:I:149:PRO:CD	2.37	0.54
13:B:13:ILE:CD1	13:B:151:ALA:CB	2.85	0.54
13:B:15:GLY:HA3	13:B:155:LEU:HD11	1.90	0.54
4:P:181:LEU:HD21	4:P:186:ALA:HA	1.89	0.54
5:Q:34:SER:CB	5:Q:65:ARG:HH12	2.21	0.54
12:F:127:ILE:HD11	12:F:136:TYR:CE1	2.43	0.54
2:I:40:ILE:CA	2:I:136:PHE:HZ	2.20	0.54
9:X:151:ASN:ND2	9:X:158:MET:HE3	2.23	0.54
4:P:51:GLN:HA	4:P:51:GLN:NE2	2.23	0.54
10:G:199:LEU:HD11	10:G:205:LEU:HD23	1.90	0.54
3:Z:44:LEU:C	3:Z:44:LEU:HD12	2.32	0.54
2:I:171:PHE:CD1	2:I:171:PHE:C	2.85	0.54
11:R:77:GLY:HA3	11:R:227:PHE:CD1	2.43	0.54
4:b:74:VAL:HG12	4:b:134:LEU:HB2	1.90	0.54
5:J:41:CYS:SG	5:J:189:ILE:HD12	2.48	0.54
3:O:44:LEU:HD12	3:O:44:LEU:C	2.32	0.53
7:U:137:VAL:HG11	7:U:145:MET:HB3	1.90	0.53
1:H:32:LYS:O	1:H:172:SER:HA	2.09	0.53
5:J:34:SER:CB	5:J:65:ARG:HH12	2.21	0.53
10:L:220:GLU:O	10:L:222:THR:HG23	2.08	0.53
8:D:162:THR:HG22	8:D:197:LEU:CD1	2.38	0.53
5:Q:41:CYS:SG	5:Q:189:ILE:HD12	2.48	0.53
7:Y:137:VAL:HG11	7:Y:145:MET:HB3	1.90	0.53
13:E:15:GLY:HA3	13:E:155:LEU:HD11	1.90	0.53
3:O:34:CYS:HB2	3:O:164:ILE:HG13	1.89	0.53
14:a:174:ARG:HD3	14:a:206:GLU:O	2.05	0.53
5:J:75:MET:HE3	5:J:135:PHE:CG	2.44	0.53
11:K:78:CYS:CB	11:K:140:LEU:HD23	2.38	0.53
12:A:73:GLU:HB2	12:A:74:PRO:HD2	1.91	0.53
8:C:162:THR:HG22	8:C:197:LEU:CD1	2.38	0.53
12:A:15:VAL:HG12	12:A:177:VAL:HG23	1.90	0.53
12:A:127:ILE:HD11	12:A:136:TYR:CE1	2.43	0.53
8:D:21:ALA:HB2	8:D:32:VAL:HG21	1.91	0.53
2:N:208:LEU:HB2	2:N:225:ILE:HD11	1.90	0.53
12:F:46:LEU:CD2	12:F:99:LEU:HD11	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:38:LEU:HD21	12:A:44:CYS:SG	2.49	0.53
11:R:4:GLY:N	11:R:19:GLU:OE2	2.41	0.53
4:P:76:SER:HB2	4:P:162:MET:HE3	1.90	0.53
9:S:151:ASN:ND2	9:S:158:MET:HE3	2.23	0.53
11:K:4:GLY:N	11:K:19:GLU:OE2	2.41	0.53
1:M:32:LYS:O	1:M:172:SER:HA	2.09	0.53
4:P:54:ILE:HD13	11:R:184:LYS:HB3	1.90	0.53
10:G:41:LYS:HD3	10:G:180:MET:HB3	1.90	0.53
1:H:91:LYS:CE	1:H:119:LEU:HD11	2.38	0.53
10:L:199:LEU:HD11	10:L:205:LEU:HD23	1.90	0.53
11:R:78:CYS:CB	11:R:140:LEU:HD23	2.38	0.53
5:Q:75:MET:HE3	5:Q:135:PHE:CG	2.44	0.53
13:E:63:MET:CE	13:E:74:PRO:HB3	2.31	0.53
2:I:218:LYS:HD3	2:I:218:LYS:C	2.32	0.53
8:D:65:ARG:HH11	8:D:68:TYR:HD2	1.43	0.53
1:M:91:LYS:CE	1:M:119:LEU:HD11	2.38	0.52
2:N:183:THR:CG2	2:N:186:LEU:HB2	2.34	0.52
4:P:149:ASP:CB	4:P:150:PRO:CD	2.86	0.52
8:C:21:ALA:HB2	8:C:32:VAL:HG21	1.91	0.52
4:b:76:SER:HB2	4:b:162:MET:HE3	1.90	0.52
12:A:46:LEU:CD2	12:A:99:LEU:HD11	2.39	0.52
2:I:136:PHE:HE1	2:I:211:MET:O	1.92	0.52
3:Z:51:ASN:HB3	3:Z:56:LEU:HD13	1.91	0.52
7:Y:69:ARG:NH2	7:Y:96:GLU:OE2	2.40	0.52
13:B:99:LEU:HD22	13:B:125:THR:OG1	2.10	0.52
13:B:189:LEU:HD13	13:B:189:LEU:C	2.33	0.52
1:M:91:LYS:CD	1:M:119:LEU:HD11	2.40	0.52
2:N:40:ILE:N	2:N:136:PHE:HZ	2.08	0.52
3:O:51:ASN:HB3	3:O:56:LEU:HD13	1.91	0.52
1:H:91:LYS:CD	1:H:119:LEU:HD11	2.40	0.52
11:K:223:GLU:HA	11:K:223:GLU:OE2	2.06	0.52
13:E:189:LEU:C	13:E:189:LEU:HD13	2.33	0.52
5:Q:56:LYS:HB2	10:L:176:MET:HE1	1.92	0.52
6:V:58:GLU:HB3	2:I:96:LEU:HD13	1.92	0.52
12:F:38:LEU:HD21	12:F:44:CYS:SG	2.49	0.52
11:R:88:ARG:NH2	11:R:88:ARG:CG	2.73	0.52
6:T:35:MET:HG2	6:T:45:LEU:HG	1.91	0.52
8:C:65:ARG:HH11	8:C:68:TYR:HD2	1.43	0.52
2:I:208:LEU:HB2	2:I:225:ILE:HD11	1.90	0.52
1:H:204:GLN:O	1:H:204:GLN:HG2	2.10	0.52
5:J:175:GLU:OE2	5:J:175:GLU:HA	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q:51:LYS:HE2	5:Q:62:SER:O	2.10	0.52
2:N:57:ARG:CG	2:N:57:ARG:NH1	2.73	0.52
8:C:174:ILE:HG22	8:C:192:ASP:HA	1.92	0.52
10:G:74:ILE:HG22	10:G:132:LEU:CD2	2.40	0.52
4:b:149:ASP:CB	4:b:150:PRO:CD	2.86	0.52
13:E:99:LEU:HD22	13:E:125:THR:OG1	2.10	0.52
14:a:1:THR:O	14:a:107:TRP:HE3	1.93	0.52
10:L:41:LYS:HD3	10:L:180:MET:HB3	1.91	0.52
2:N:136:PHE:HE1	2:N:211:MET:O	1.92	0.52
12:F:157:THR:CG2	12:F:189:ILE:HD12	2.40	0.52
13:B:99:LEU:HG	13:B:127:LEU:HD12	1.92	0.52
6:T:96:THR:CG2	8:D:92:ARG:NH2	2.73	0.51
12:F:156:THR:O	12:F:160:ILE:HG13	2.10	0.51
13:E:6:LEU:C	13:E:6:LEU:CD1	2.83	0.51
3:Z:61:PHE:CZ	3:Z:227:VAL:CG2	2.93	0.51
4:b:59:ARG:HH11	4:b:59:ARG:CB	2.14	0.51
12:F:73:GLU:HB2	12:F:74:PRO:HD2	1.91	0.51
13:E:179:THR:HG23	13:E:181:THR:H	1.75	0.51
2:I:40:ILE:N	2:I:136:PHE:HZ	2.08	0.51
2:I:57:ARG:CG	2:I:57:ARG:NH1	2.73	0.51
2:N:79:ASP:OD1	3:O:119:GLN:NE2	2.43	0.51
3:O:174:MET:HE3	3:O:195:LYS:HZ2	1.74	0.51
2:I:180:ALA:HB1	2:I:190:LEU:HD23	1.92	0.51
8:D:174:ILE:HG22	8:D:192:ASP:HA	1.92	0.51
3:O:61:PHE:CZ	3:O:227:VAL:CG2	2.93	0.51
6:V:35:MET:HG2	6:V:45:LEU:HG	1.91	0.51
12:F:114:GLY:HA3	12:F:116:MET:HE1	1.93	0.51
14:W:1:THR:O	14:W:107:TRP:HE3	1.93	0.51
2:N:42:VAL:HG11	2:N:191:VAL:HG23	1.78	0.51
2:N:169:ARG:HB2	2:N:169:ARG:NH1	2.08	0.51
6:T:86:ARG:O	6:T:86:ARG:HD3	2.11	0.51
10:G:210:VAL:HG12	10:G:210:VAL:O	2.10	0.51
12:A:156:THR:O	12:A:160:ILE:HG13	2.10	0.51
12:A:157:THR:CG2	12:A:189:ILE:HD12	2.40	0.51
8:D:96:LEU:O	8:D:117:GLN:HG3	2.11	0.51
7:U:69:ARG:NH2	7:U:96:GLU:OE2	2.40	0.51
1:H:206:MET:HE1	1:H:214:ASN:HD21	1.76	0.51
10:L:74:ILE:HG22	10:L:132:LEU:CD2	2.40	0.51
11:R:88:ARG:HH21	11:R:88:ARG:CG	2.16	0.51
2:N:180:ALA:HB1	2:N:190:LEU:HD23	1.92	0.51
10:G:71:GLY:HA3	10:G:221:PHE:CZ	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:51:LYS:HE2	5:J:62:SER:O	2.10	0.51
6:V:155:ARG:NE	6:V:158:GLU:OE2	2.36	0.51
13:E:21:THR:HG22	13:E:26:VAL:HA	1.93	0.51
8:C:4:THR:HG22	8:C:17:VAL:HG12	1.93	0.51
13:E:99:LEU:HG	13:E:127:LEU:HD12	1.92	0.51
6:T:16:ALA:HA	6:T:179:SER:O	2.11	0.51
11:R:53:GLN:CD	11:R:206:LEU:HD21	2.35	0.51
9:X:16:ALA:HB2	9:X:121:VAL:HG23	1.93	0.51
1:M:204:GLN:O	1:M:204:GLN:HG2	2.09	0.51
10:G:166:GLN:HE21	10:G:166:GLN:C	2.15	0.51
6:V:86:ARG:O	6:V:86:ARG:HD3	2.11	0.51
13:E:205:ALA:CB	13:E:206:PRO:CD	2.44	0.51
12:A:114:GLY:HA3	12:A:116:MET:HE1	1.93	0.51
10:L:210:VAL:HG12	10:L:210:VAL:O	2.10	0.51
4:P:221:THR:HG23	4:P:223:THR:H	1.77	0.50
5:J:34:SER:HB2	5:J:65:ARG:HH12	1.76	0.50
5:Q:175:GLU:OE2	5:Q:175:GLU:HA	2.10	0.50
11:K:53:GLN:CD	11:K:206:LEU:HD21	2.35	0.50
1:M:206:MET:HE1	1:M:214:ASN:HD21	1.76	0.50
2:N:92:GLN:OE1	2:N:92:GLN:HA	2.10	0.50
4:P:208:GLU:OE2	4:P:219:ARG:HD2	2.12	0.50
8:C:96:LEU:O	8:C:117:GLN:HG3	2.11	0.50
9:S:16:ALA:HB2	9:S:121:VAL:HG23	1.93	0.50
10:G:57:ALA:HA	1:H:165:CYS:SG	2.51	0.50
1:H:157:ASP:HB2	1:H:158:PRO:HD2	1.94	0.50
6:T:2:GLU:HG2	6:T:34:LYS:CE	2.37	0.50
13:E:156:VAL:HG21	13:E:189:LEU:CD1	2.41	0.50
11:R:13:ILE:HG13	11:R:15:ILE:HG12	1.92	0.50
7:U:27:PHE:HB2	7:U:38:PHE:HB2	1.94	0.50
3:Z:49:ARG:HD3	3:Z:209:GLU:O	2.12	0.50
7:Y:116:PHE:CD2	7:Y:191:LYS:HE3	2.47	0.50
13:B:179:THR:HG23	13:B:181:THR:H	1.75	0.50
7:Y:27:PHE:HB2	7:Y:38:PHE:HB2	1.94	0.50
13:B:21:THR:HG22	13:B:26:VAL:HA	1.93	0.50
6:T:155:ARG:NE	6:T:158:GLU:OE2	2.36	0.50
6:V:34:LYS:HD3	6:V:47:VAL:HG12	1.94	0.50
2:I:92:GLN:OE1	2:I:92:GLN:HA	2.10	0.50
13:B:63:MET:CE	13:B:74:PRO:HB3	2.31	0.50
5:Q:34:SER:HB2	5:Q:65:ARG:HH12	1.76	0.50
5:Q:56:LYS:HD2	10:L:173:GLU:HG2	1.93	0.50
11:K:196:GLU:CG	11:K:242:LEU:CD2	2.82	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:W:147:GLN:HB3	14:W:148:PRO:HD3	1.94	0.50
8:C:92:ARG:NH2	6:V:96:THR:CG2	2.75	0.50
9:S:38:ARG:NH1	9:S:191:ASP:OD1	2.38	0.50
9:S:177:ASP:OD1	13:B:198:ARG:HB2	2.12	0.50
1:H:183:GLU:O	1:H:183:GLU:HG3	2.12	0.50
13:E:201:GLN:NE2	13:E:201:GLN:N	2.60	0.50
10:L:71:GLY:HA3	10:L:221:PHE:CZ	2.46	0.50
1:M:183:GLU:O	1:M:183:GLU:HG3	2.12	0.49
2:N:73:PHE:CD1	2:N:73:PHE:C	2.90	0.49
5:Q:37:ILE:HD11	5:Q:193:VAL:HG13	1.94	0.49
11:K:36:GLY:HA2	11:K:170:VAL:HG21	1.94	0.49
14:a:147:GLN:HB3	14:a:148:PRO:HD3	1.94	0.49
2:I:69:VAL:HG11	2:I:107:ILE:HG21	1.94	0.49
2:N:180:ALA:HB1	2:N:190:LEU:HD22	1.93	0.49
3:Z:119:GLN:NE2	2:I:79:ASP:OD1	2.44	0.49
4:b:74:VAL:HG13	4:b:134:LEU:HB2	1.94	0.49
4:b:221:THR:HG23	4:b:223:THR:H	1.76	0.49
12:A:98:HIS:CE1	12:A:116:MET:HE3	2.48	0.49
2:I:218:LYS:C	2:I:218:LYS:CD	2.85	0.49
13:B:6:LEU:C	13:B:6:LEU:CD1	2.83	0.49
7:U:116:PHE:CD2	7:U:191:LYS:HE3	2.47	0.49
4:b:208:GLU:OE2	4:b:219:ARG:HD2	2.12	0.49
6:V:16:ALA:HA	6:V:179:SER:O	2.11	0.49
7:Y:152:LEU:HD13	13:B:204:PHE:HE2	1.78	0.49
11:R:196:GLU:CG	11:R:242:LEU:CD2	2.82	0.49
8:D:4:THR:HG22	8:D:17:VAL:HG12	1.93	0.49
6:V:118:MET:HE2	6:V:124:LEU:HD13	1.95	0.49
10:L:69:HIS:O	10:L:136:GLY:HA2	2.13	0.49
8:D:84:LEU:HA	8:D:87:MET:HE3	1.93	0.49
3:O:49:ARG:HD3	3:O:209:GLU:O	2.12	0.49
1:H:58:LEU:HD21	2:I:173:GLU:HA	1.94	0.49
3:Z:206:LEU:HB3	3:Z:237:ILE:HD13	1.94	0.49
13:E:198:ARG:HB2	9:X:177:ASP:OD1	2.12	0.49
12:A:91:TYR:HB2	12:A:95:LEU:CD1	2.42	0.49
2:I:73:PHE:CD1	2:I:73:PHE:C	2.90	0.49
13:B:201:GLN:NE2	13:B:201:GLN:N	2.60	0.49
2:N:218:LYS:C	2:N:218:LYS:CD	2.85	0.49
11:K:13:ILE:HG13	11:K:15:ILE:HG12	1.92	0.49
12:F:25:GLU:HG2	14:W:182:ARG:HG2	1.94	0.49
13:B:36:PHE:C	13:B:36:PHE:CD1	2.91	0.49
13:B:141:ARG:HH11	13:B:141:ARG:CG	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:179:GLU:H	2:N:179:GLU:CD	2.21	0.49
8:C:84:LEU:HA	8:C:87:MET:HE3	1.93	0.49
4:P:74:VAL:HG13	4:P:134:LEU:HB2	1.94	0.49
6:T:86:ARG:HD3	6:T:86:ARG:C	2.38	0.49
10:G:69:HIS:O	10:G:136:GLY:HA2	2.13	0.49
5:J:37:ILE:HD11	5:J:193:VAL:HG13	1.94	0.49
11:K:88:ARG:NH2	11:K:88:ARG:CG	2.73	0.49
8:D:83:LEU:HD22	8:D:87:MET:HE2	1.95	0.49
1:M:206:MET:CE	1:M:214:ASN:ND2	2.76	0.49
6:T:34:LYS:HD3	6:T:47:VAL:HG12	1.94	0.49
1:M:157:ASP:HB2	1:M:158:PRO:HD2	1.94	0.49
2:N:69:VAL:HG11	2:N:107:ILE:HG21	1.94	0.49
7:U:100:GLY:N	7:U:101:PRO:CD	2.69	0.49
6:V:77:PRO:HD2	6:V:108:ASP:HB2	1.95	0.49
1:M:195:ILE:HD11	1:M:219:THR:HG21	1.95	0.48
3:O:206:LEU:HB3	3:O:237:ILE:HD13	1.95	0.48
7:U:152:LEU:HD13	13:E:204:PHE:HE2	1.77	0.48
8:C:83:LEU:HD22	8:C:87:MET:HE2	1.95	0.48
13:E:36:PHE:CD1	13:E:36:PHE:C	2.91	0.48
2:N:179:GLU:O	2:N:186:LEU:HD13	2.14	0.48
1:H:209:LYS:O	1:H:214:ASN:ND2	2.47	0.48
5:J:219:ILE:HG23	5:J:220:THR:HG23	1.95	0.48
2:I:179:GLU:H	2:I:179:GLU:CD	2.21	0.48
4:P:50:LYS:NZ	4:P:50:LYS:HB3	2.28	0.48
9:S:44:TYR:N	9:S:44:TYR:CD1	2.81	0.48
13:B:156:VAL:HG21	13:B:189:LEU:CD1	2.41	0.48
1:M:165:CYS:SG	10:L:57:ALA:HA	2.54	0.48
6:T:118:MET:HE2	6:T:124:LEU:HD13	1.94	0.48
1:H:85:ALA:HB2	1:H:139:VAL:HG21	1.96	0.48
2:I:221:ASN:ND2	2:I:224:GLU:HB2	2.28	0.48
2:N:96:LEU:HD13	6:T:58:GLU:HB3	1.93	0.48
6:T:41:LYS:O	6:T:106:GLY:HA2	2.13	0.48
12:A:46:LEU:HD22	12:A:53:ALA:HB1	1.96	0.48
9:X:125:ASP:HB2	9:X:126:PRO:CD	2.44	0.48
2:N:221:ASN:ND2	2:N:224:GLU:HB2	2.28	0.48
13:E:135:LEU:HD11	14:W:179:ARG:CG	2.44	0.48
11:R:36:GLY:HA2	11:R:170:VAL:HG21	1.94	0.48
4:P:37:ILE:HD12	4:P:190:ALA:HB2	1.96	0.48
9:S:125:ASP:HB2	9:S:126:PRO:CD	2.44	0.48
1:H:202:LEU:HA	1:H:202:LEU:HD23	1.74	0.48
12:F:98:HIS:CE1	12:F:116:MET:HE3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:a:15:LYS:HD2	14:a:135:PRO:HA	1.96	0.48
2:I:169:ARG:CG	2:I:169:ARG:NH1	2.73	0.48
9:X:13:LEU:HD11	9:X:149:LEU:HD11	1.95	0.48
13:B:81:ARG:NH2	13:B:84:ARG:NH1	2.62	0.48
5:Q:219:ILE:HG23	5:Q:220:THR:HG23	1.96	0.48
4:b:50:LYS:NZ	4:b:50:LYS:HB3	2.28	0.48
12:F:46:LEU:HD22	12:F:53:ALA:HB1	1.96	0.48
14:a:179:ARG:CG	13:B:135:LEU:HD11	2.43	0.48
2:I:220:LEU:N	2:I:220:LEU:HD23	2.29	0.48
9:X:75:TYR:CG	9:X:83:MET:HG3	2.48	0.48
9:X:125:ASP:OD2	9:X:129:SER:HB3	2.14	0.48
9:S:180:ILE:CD1	13:B:196:THR:HB	2.44	0.48
10:G:176:MET:HE1	5:J:56:LYS:HB2	1.95	0.48
2:N:220:LEU:N	2:N:220:LEU:HD23	2.29	0.48
1:H:206:MET:CE	1:H:214:ASN:ND2	2.76	0.48
12:A:15:VAL:CG1	12:A:177:VAL:HG23	2.42	0.48
14:a:122:LEU:HG	14:a:137:LEU:HD12	1.96	0.48
1:M:157:ASP:CB	1:M:158:PRO:CD	2.91	0.47
2:N:189:LYS:HG3	2:N:193:LYS:HE3	1.96	0.47
7:U:105:GLU:HB2	7:U:138:SER:OG	2.14	0.47
8:C:22:THR:HG22	8:C:27:ILE:HA	1.96	0.47
9:S:13:LEU:HD11	9:S:149:LEU:HD11	1.95	0.47
9:S:75:TYR:CG	9:S:83:MET:HG3	2.48	0.47
1:H:195:ILE:HD11	1:H:219:THR:HG21	1.95	0.47
6:V:41:LYS:O	6:V:106:GLY:HA2	2.14	0.47
6:V:86:ARG:HD3	6:V:86:ARG:C	2.38	0.47
14:W:36:PHE:CZ	12:A:116:MET:HE2	2.47	0.47
10:L:166:GLN:HE21	10:L:166:GLN:C	2.15	0.47
2:I:189:LYS:HG3	2:I:193:LYS:HE3	1.96	0.47
2:N:179:GLU:OE1	2:N:179:GLU:N	2.38	0.47
7:Y:105:GLU:HB2	7:Y:138:SER:OG	2.14	0.47
13:E:196:THR:HB	9:X:180:ILE:CD1	2.44	0.47
14:W:15:LYS:HD2	14:W:135:PRO:HA	1.96	0.47
2:I:197:GLU:OE1	2:I:197:GLU:HA	2.14	0.47
8:D:22:THR:HG22	8:D:27:ILE:HA	1.96	0.47
1:M:209:LYS:O	1:M:214:ASN:ND2	2.47	0.47
9:S:13:LEU:CD1	9:S:149:LEU:HD11	2.44	0.47
4:b:37:ILE:HD12	4:b:190:ALA:HB2	1.96	0.47
14:W:122:LEU:HG	14:W:137:LEU:HD12	1.96	0.47
12:A:15:VAL:HG12	12:A:177:VAL:CG2	2.41	0.47
10:L:184:LEU:HD11	10:L:214:ILE:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:179:GLU:O	2:I:186:LEU:HD13	2.14	0.47
9:X:184:GLU:OE2	9:X:211:ARG:CD	2.61	0.47
1:M:85:ALA:HB2	1:M:139:VAL:HG21	1.96	0.47
1:M:182:GLN:HA	10:L:56:LEU:HD11	1.97	0.47
4:P:59:ARG:HH11	4:P:59:ARG:CB	2.14	0.47
4:P:221:THR:HG22	4:P:224:GLU:H	1.79	0.47
8:C:83:LEU:CD2	8:C:87:MET:HE2	2.45	0.47
10:G:184:LEU:HD11	10:G:214:ILE:HG21	1.96	0.47
1:H:213:THR:HG22	1:H:231:LYS:CE	2.44	0.47
13:E:135:LEU:HD12	14:W:179:ARG:HG3	1.96	0.47
9:S:125:ASP:OD2	9:S:129:SER:HB3	2.14	0.47
10:G:49:LEU:CD2	10:G:199:LEU:HD21	2.45	0.47
14:a:35:ARG:HG2	14:a:36:PHE:CE2	2.50	0.47
2:I:180:ALA:HB1	2:I:190:LEU:HD22	1.93	0.47
11:R:178:PHE:CD1	11:R:178:PHE:C	2.93	0.47
8:D:11:HIS:CD2	8:D:150:PRO:HD3	2.50	0.47
6:T:77:PRO:HD2	6:T:108:ASP:HB2	1.95	0.47
8:C:92:ARG:HH22	6:V:96:THR:CB	2.20	0.47
13:E:81:ARG:NH2	13:E:84:ARG:NH1	2.62	0.47
5:Q:151:ILE:HG12	5:Q:157:SER:CB	2.45	0.47
5:Q:203:GLU:CD	5:Q:203:GLU:N	2.72	0.47
7:U:25:ARG:NH1	7:U:25:ARG:CG	2.73	0.47
8:C:13:VAL:HB	8:C:180:MET:HB3	1.97	0.47
1:H:157:ASP:CB	1:H:158:PRO:CD	2.91	0.47
3:Z:240:HIS:HA	3:Z:243:GLU:HB2	1.97	0.47
5:J:108:LEU:HD22	5:J:139:SER:HB3	1.97	0.47
6:V:76:SER:HB2	6:V:108:ASP:OD2	2.15	0.47
9:X:13:LEU:CD1	9:X:149:LEU:HD11	2.44	0.47
9:X:44:TYR:N	9:X:44:TYR:CD1	2.81	0.47
2:N:169:ARG:CG	2:N:169:ARG:NH1	2.73	0.47
4:P:49:LYS:HB2	4:P:49:LYS:HE2	1.51	0.47
6:T:10:PRO:HG3	6:T:150:THR:HA	1.97	0.47
4:b:55:LEU:HD22	11:K:165:ALA:HB3	1.97	0.47
11:K:178:PHE:CD1	11:K:178:PHE:C	2.93	0.47
7:Y:100:GLY:N	7:Y:101:PRO:CD	2.69	0.47
10:L:49:LEU:CD2	10:L:199:LEU:HD21	2.45	0.47
2:I:64:ALA:HB2	2:I:217:LEU:CD2	2.33	0.47
13:B:40:LYS:HD3	13:B:40:LYS:N	2.27	0.47
1:M:213:THR:HG22	1:M:231:LYS:CE	2.44	0.47
14:W:35:ARG:HG2	14:W:36:PHE:CE2	2.50	0.47
2:I:98:VAL:HG12	2:I:98:VAL:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:13:VAL:HB	8:D:180:MET:HB3	1.97	0.47
2:N:98:VAL:HG12	2:N:98:VAL:O	2.15	0.47
5:J:203:GLU:CD	5:J:203:GLU:N	2.73	0.47
14:W:43:MET:HG3	14:W:64:LYS:HD2	1.97	0.47
2:N:197:GLU:OE1	2:N:197:GLU:HA	2.14	0.46
5:Q:108:LEU:HD22	5:Q:139:SER:HB3	1.97	0.46
11:K:155:ASP:CB	11:K:156:PRO:CD	2.78	0.46
13:E:197:GLU:OE1	13:E:197:GLU:HA	2.16	0.46
10:L:74:ILE:HG22	10:L:132:LEU:HD22	1.96	0.46
2:N:52:LYS:HB2	2:N:52:LYS:HE2	1.35	0.46
2:N:94:HIS:CG	2:N:102:VAL:HG12	2.50	0.46
8:C:11:HIS:CD2	8:C:150:PRO:HD3	2.50	0.46
4:b:221:THR:HG22	4:b:224:GLU:H	1.79	0.46
6:V:10:PRO:HG3	6:V:150:THR:HA	1.97	0.46
14:a:112:ILE:HD12	14:a:112:ILE:N	2.30	0.46
12:F:91:TYR:HB2	12:F:95:LEU:CD1	2.42	0.46
14:a:43:MET:HG3	14:a:64:LYS:HD2	1.97	0.46
2:I:90:GLU:HG2	2:I:110:TYR:CE1	2.51	0.46
6:T:12:TYR:CD1	6:T:12:TYR:C	2.93	0.46
12:F:116:MET:HE2	14:a:36:PHE:CZ	2.47	0.46
14:W:112:ILE:HD12	14:W:112:ILE:N	2.30	0.46
10:L:35:THR:HG23	10:L:133:LEU:CD1	2.46	0.46
2:I:174:LYS:H	2:I:174:LYS:HG2	1.45	0.46
9:X:38:ARG:NH1	9:X:191:ASP:OD1	2.38	0.46
3:O:240:HIS:HA	3:O:243:GLU:HB2	1.97	0.46
10:G:137:TYR:CZ	10:G:217:LYS:HA	2.51	0.46
5:J:50:GLU:HG2	5:J:50:GLU:O	2.14	0.46
7:Y:52:LEU:HD23	7:Y:106:PRO:HB3	1.97	0.46
7:Y:203:MET:H	8:D:194:ASN:ND2	2.14	0.46
10:L:71:GLY:HA3	10:L:221:PHE:CE1	2.51	0.46
8:D:83:LEU:CD2	8:D:87:MET:HE2	2.45	0.46
2:N:90:GLU:HG2	2:N:110:TYR:CE1	2.51	0.46
3:Z:178:ASP:OD2	3:Z:195:LYS:HE2	2.15	0.46
4:b:164:LYS:HB3	4:b:164:LYS:HE2	1.55	0.46
6:V:109:GLU:H	6:V:109:GLU:HG2	1.56	0.46
13:E:54:MET:HE1	13:E:57:ARG:NH1	2.31	0.46
14:W:27:LEU:HD22	14:W:184:TYR:HB2	1.98	0.46
5:Q:50:GLU:O	5:Q:50:GLU:HG2	2.14	0.46
5:Q:56:LYS:CB	10:L:176:MET:HE1	2.46	0.46
12:A:25:GLU:HG2	14:a:182:ARG:HG2	1.96	0.46
13:B:124:PHE:HB2	13:B:138:LEU:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:124:ARG:HB3	3:O:124:PHE:HB3	1.98	0.46
6:V:12:TYR:CD1	6:V:12:TYR:C	2.93	0.46
14:W:51:LEU:C	14:W:51:LEU:HD23	2.41	0.46
8:D:65:ARG:NH1	8:D:68:TYR:CE2	2.66	0.46
1:M:58:LEU:HD21	2:N:173:GLU:HA	1.98	0.46
3:O:178:ASP:OD2	3:O:195:LYS:HE2	2.15	0.46
4:b:134:LEU:HD23	4:b:134:LEU:HA	1.85	0.46
12:A:98:HIS:CD2	12:A:98:HIS:C	2.94	0.46
10:L:118:ILE:N	10:L:119:PRO:HD2	2.31	0.46
2:I:94:HIS:CG	2:I:102:VAL:HG12	2.50	0.46
2:N:64:ALA:HB2	2:N:217:LEU:CD2	2.33	0.46
6:T:76:SER:HB2	6:T:108:ASP:OD2	2.15	0.46
7:U:12:ALA:HB3	7:U:136:VAL:CG2	2.46	0.46
7:U:196:THR:HB	13:E:215:THR:HG23	1.98	0.46
4:b:59:ARG:H	4:b:59:ARG:HG3	1.56	0.46
6:V:102:LEU:HD11	6:V:118:MET:CE	2.37	0.46
6:V:104:LEU:C	6:V:104:LEU:HD23	2.41	0.46
14:W:22:ILE:HG12	14:W:50:MET:HE3	1.97	0.46
14:a:51:LEU:C	14:a:51:LEU:HD23	2.41	0.46
10:L:137:TYR:CZ	10:L:217:LYS:HA	2.51	0.46
13:B:54:MET:HE1	13:B:57:ARG:NH1	2.31	0.46
3:O:59:VAL:HG13	4:P:142:ARG:NH2	2.30	0.45
4:P:164:LYS:HB3	4:P:164:LYS:HE2	1.55	0.45
10:G:74:ILE:HG22	10:G:132:LEU:HD22	1.96	0.45
2:I:52:LYS:HE2	2:I:52:LYS:HB2	1.35	0.45
2:I:196:LEU:HD13	2:I:196:LEU:HA	1.72	0.45
8:C:173:GLY:O	8:C:193:VAL:HG22	2.17	0.45
10:G:35:THR:HG22	10:G:161:ILE:HG13	1.99	0.45
10:G:230:SER:CB	10:G:231:PRO:HD3	2.46	0.45
1:H:83:ALA:HB1	2:I:116:GLN:HG3	1.98	0.45
5:J:8:ASP:OD2	5:J:25:TYR:OH	2.30	0.45
11:K:67:THR:OG1	11:K:216:GLU:OE2	2.22	0.45
12:A:2:THR:CB	15:A:301:A1L0C:O2	2.64	0.45
14:a:179:ARG:HG3	13:B:135:LEU:HD12	1.96	0.45
13:B:197:GLU:OE1	13:B:197:GLU:HA	2.16	0.45
3:O:59:VAL:CG1	4:P:142:ARG:NH2	2.79	0.45
3:O:205:LYS:HB2	3:O:205:LYS:HE2	1.38	0.45
7:U:3:MET:CE	7:U:105:GLU:HG3	2.47	0.45
10:G:35:THR:HG23	10:G:133:LEU:CD1	2.46	0.45
5:J:12:SER:HB3	5:J:125:TYR:HA	1.99	0.45
13:E:124:PHE:HB2	13:E:138:LEU:HD13	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:W:96:MET:HE2	14:W:110:MET:HE1	1.99	0.45
2:I:37:GLY:HA2	2:I:181:ILE:HD12	1.99	0.45
2:N:37:GLY:HA2	2:N:181:ILE:HD12	1.98	0.45
2:N:174:LYS:H	2:N:174:LYS:HG2	1.45	0.45
5:Q:57:LEU:HB3	10:L:158:ALA:O	2.17	0.45
10:G:57:ALA:HA	1:H:165:CYS:HA	1.98	0.45
3:Z:59:VAL:HG13	4:b:142:ARG:NH2	2.32	0.45
3:Z:59:VAL:CG1	4:b:142:ARG:NH2	2.80	0.45
5:J:151:ILE:HG12	5:J:157:SER:CB	2.45	0.45
7:Y:12:ALA:HB3	7:Y:136:VAL:CG2	2.46	0.45
9:X:107:TYR:CE1	9:X:126:PRO:HD3	2.51	0.45
3:O:50:ARG:HD3	3:O:50:ARG:HA	1.80	0.45
3:O:197:LEU:HD12	3:O:197:LEU:HA	1.65	0.45
10:G:118:ILE:N	10:G:119:PRO:HD2	2.31	0.45
1:H:193:GLU:O	1:H:197:SER:HB2	2.17	0.45
12:A:4:ILE:HG22	12:A:17:SER:HB3	1.99	0.45
13:B:135:LEU:C	13:B:135:LEU:HD13	2.41	0.45
10:G:71:GLY:HA3	10:G:221:PHE:CE1	2.51	0.45
3:Z:151:ASP:CB	3:Z:152:PRO:CD	2.77	0.45
7:Y:30:GLN:HB3	7:Y:31:ALA:H	1.65	0.45
12:F:98:HIS:CD2	12:F:98:HIS:C	2.94	0.45
14:a:96:MET:HE2	14:a:110:MET:HE1	1.99	0.45
11:R:52:THR:CG2	11:R:216:GLU:HB2	2.47	0.45
7:U:52:LEU:HD23	7:U:106:PRO:HB3	1.97	0.45
9:S:208:VAL:HA	9:S:209:PRO:HD3	1.84	0.45
14:a:27:LEU:HD22	14:a:184:TYR:HB2	1.98	0.45
10:L:148:CYS:HB3	10:L:149:PRO:HD2	1.99	0.45
10:L:230:SER:CB	10:L:231:PRO:HD3	2.46	0.45
11:R:168:ALA:HA	11:R:172:GLN:HG3	1.99	0.45
8:D:173:GLY:O	8:D:193:VAL:HG22	2.17	0.45
4:P:58:GLU:CD	4:P:58:GLU:H	2.24	0.45
5:Q:30:VAL:HG22	5:Q:133:CYS:HA	1.99	0.45
5:Q:109:LYS:HG3	5:Q:149:TYR:OH	2.17	0.45
6:T:104:LEU:C	6:T:104:LEU:HD23	2.41	0.45
9:S:107:TYR:CE1	9:S:126:PRO:HD3	2.51	0.45
9:S:184:GLU:OE2	9:S:211:ARG:CD	2.61	0.45
10:G:173:GLU:HG2	5:J:56:LYS:HD2	1.99	0.45
1:H:78:MET:HE2	1:H:78:MET:HB3	1.72	0.45
4:b:49:LYS:HG3	4:b:49:LYS:O	2.17	0.45
11:K:112:ASP:HB3	11:K:152:TYR:CZ	2.52	0.45
7:U:203:MET:H	8:C:194:ASN:ND2	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:89:TYR:CZ	6:V:55:GLN:HG3	2.51	0.45
10:G:154:PHE:HD2	5:J:63:ASN:OD1	1.99	0.45
3:Z:50:ARG:HD3	3:Z:50:ARG:HA	1.80	0.45
5:J:30:VAL:HG22	5:J:133:CYS:HA	1.99	0.45
2:N:204:LYS:HB2	2:N:204:LYS:HE3	1.60	0.45
6:T:21:ALA:HB3	6:T:29:LYS:HB3	1.99	0.45
5:J:109:LYS:HG3	5:J:149:TYR:OH	2.17	0.45
7:Y:3:MET:CE	7:Y:105:GLU:HG3	2.47	0.45
12:A:4:ILE:HG22	12:A:17:SER:CB	2.47	0.45
11:R:112:ASP:HB3	11:R:152:TYR:CZ	2.52	0.45
2:N:59:VAL:O	2:N:59:VAL:HG23	2.17	0.44
2:N:220:LEU:N	2:N:220:LEU:CD2	2.80	0.44
8:C:46:MET:CG	8:C:53:CYS:HB3	2.47	0.44
11:K:52:THR:CG2	11:K:216:GLU:HB2	2.47	0.44
12:F:2:THR:CB	15:F:301:A1L0C:O2	2.64	0.44
12:A:9:PHE:HB3	12:A:152:CYS:SG	2.58	0.44
14:a:22:ILE:HG12	14:a:50:MET:HE3	1.97	0.44
4:P:72:GLY:HA3	4:P:217:PHE:CE1	2.52	0.44
3:Z:238:LYS:HB2	3:Z:238:LYS:HE2	1.26	0.44
8:D:157:GLY:CA	8:D:177:MET:HE1	2.47	0.44
4:P:51:GLN:HA	4:P:51:GLN:HE21	1.82	0.44
5:Q:12:SER:HB3	5:Q:125:TYR:HA	1.99	0.44
12:F:46:LEU:HD22	12:F:99:LEU:HD11	1.99	0.44
14:a:43:MET:HE3	14:a:64:LYS:HG3	2.00	0.44
2:I:40:ILE:HA	2:I:136:PHE:HZ	1.82	0.44
1:M:49:ALA:CB	1:M:217:LEU:HD12	2.40	0.44
4:P:54:ILE:HD11	11:R:184:LYS:HB3	1.98	0.44
4:P:62:HIS:HB3	4:P:208:GLU:OE2	2.17	0.44
10:G:148:CYS:HB3	10:G:149:PRO:HD2	1.99	0.44
5:J:63:ASN:HD22	5:J:81:LEU:HD23	1.83	0.44
11:K:224:ASN:C	11:K:224:ASN:HD22	2.24	0.44
6:V:21:ALA:HB3	6:V:29:LYS:HB3	1.99	0.44
13:E:135:LEU:C	13:E:135:LEU:HD13	2.41	0.44
10:L:35:THR:HG22	10:L:161:ILE:HG13	1.99	0.44
1:M:193:GLU:O	1:M:197:SER:HB2	2.17	0.44
4:P:59:ARG:H	4:P:59:ARG:HG3	1.56	0.44
4:P:114:ALA:HB1	4:P:152:GLY:O	2.18	0.44
4:b:62:HIS:HB3	4:b:208:GLU:OE2	2.17	0.44
6:V:38:MET:HE1	6:V:61:GLN:HB2	1.99	0.44
7:Y:196:THR:HB	13:B:215:THR:HG23	1.98	0.44
14:a:179:ARG:NH2	13:B:139:GLU:OE2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:148:ASP:CB	2:N:149:PRO:CD	2.96	0.44
2:N:211:MET:HE3	2:N:211:MET:HB3	1.78	0.44
4:P:142:ARG:HG2	4:P:143:PRO:HD2	1.99	0.44
5:Q:41:CYS:HB2	5:Q:189:ILE:HD11	2.00	0.44
5:Q:63:ASN:OD1	10:L:154:PHE:HD2	1.96	0.44
5:Q:63:ASN:HD22	5:Q:81:LEU:HD23	1.83	0.44
6:T:55:GLN:HG3	8:D:89:TYR:CZ	2.52	0.44
6:T:67:TYR:CG	6:T:75:LEU:HG	2.53	0.44
12:F:9:PHE:HB3	12:F:152:CYS:SG	2.58	0.44
13:E:41:ILE:HD13	13:E:79:VAL:HG21	2.00	0.44
2:I:59:VAL:O	2:I:59:VAL:HG23	2.17	0.44
2:N:40:ILE:HA	2:N:136:PHE:HZ	1.83	0.44
2:N:53:LEU:HD22	3:O:161:ALA:HB3	2.00	0.44
12:F:4:ILE:HG22	12:F:17:SER:CB	2.47	0.44
12:F:4:ILE:HG22	12:F:17:SER:HB3	1.99	0.44
12:A:46:LEU:HD22	12:A:99:LEU:HD11	1.99	0.44
7:U:130:MET:HG3	13:E:27:MET:SD	2.58	0.44
4:b:58:GLU:H	4:b:58:GLU:CD	2.24	0.44
4:b:72:GLY:HA3	4:b:217:PHE:CE1	2.52	0.44
6:V:67:TYR:CG	6:V:75:LEU:HG	2.53	0.44
13:E:196:THR:HB	9:X:180:ILE:HD13	1.99	0.44
12:A:98:HIS:CG	12:A:116:MET:HB3	2.53	0.44
11:R:224:ASN:C	11:R:224:ASN:HD22	2.24	0.44
13:B:41:ILE:HD13	13:B:79:VAL:HG21	2.00	0.44
1:M:91:LYS:CG	1:M:119:LEU:HD11	2.47	0.44
1:H:146:VAL:HG23	1:H:220:VAL:HG22	1.99	0.44
13:E:77:THR:O	13:E:80:THR:HG22	2.18	0.44
13:B:77:THR:O	13:B:80:THR:HG22	2.18	0.44
3:O:238:LYS:HE2	3:O:238:LYS:HB2	1.26	0.43
1:H:38:ILE:HD13	1:H:169:ALA:HB2	2.00	0.43
4:b:114:ALA:HB1	4:b:152:GLY:O	2.18	0.43
4:b:142:ARG:HG2	4:b:143:PRO:HD2	1.99	0.43
7:Y:130:MET:HG3	13:B:27:MET:SD	2.57	0.43
2:I:179:GLU:CD	2:I:179:GLU:N	2.76	0.43
13:B:198:ARG:HA	13:B:199:PRO:HD3	1.83	0.43
3:O:58:GLU:CD	3:O:58:GLU:N	2.76	0.43
7:U:11:MET:HG2	7:U:170:MET:SD	2.58	0.43
9:S:173:ARG:HD2	13:B:200:SER:HB2	1.98	0.43
11:K:168:ALA:HA	11:K:172:GLN:HG3	1.99	0.43
1:M:78:MET:HE2	1:M:78:MET:HB3	1.72	0.43
3:O:151:ASP:CB	3:O:152:PRO:CD	2.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:221:THR:HG23	4:P:223:THR:N	2.33	0.43
5:Q:87:LEU:HD23	5:Q:87:LEU:HA	1.86	0.43
7:U:19:VAL:HG13	7:U:118:PRO:HB3	2.00	0.43
9:S:180:ILE:HD13	13:B:196:THR:HB	1.99	0.43
3:Z:35:LEU:HG	3:Z:46:ALA:HB3	2.00	0.43
3:Z:197:LEU:HD12	3:Z:197:LEU:HA	1.65	0.43
12:F:98:HIS:CG	12:F:116:MET:HB3	2.53	0.43
14:W:43:MET:HE3	14:W:64:LYS:HG3	2.00	0.43
2:N:179:GLU:CD	2:N:179:GLU:N	2.76	0.43
14:W:51:LEU:HD21	14:W:110:MET:HG2	2.01	0.43
2:I:148:ASP:CB	2:I:149:PRO:CD	2.96	0.43
2:I:179:GLU:N	2:I:179:GLU:OE1	2.38	0.43
3:O:91:ARG:HG2	7:U:75:LEU:HD13	2.01	0.43
8:C:89:TYR:CE2	6:V:55:GLN:HG3	2.53	0.43
7:Y:11:MET:HG2	7:Y:170:MET:SD	2.58	0.43
2:I:65:LEU:HD23	2:I:65:LEU:HA	1.83	0.43
1:M:38:ILE:HD13	1:M:169:ALA:HB2	2.00	0.43
1:M:189:MET:HE2	1:M:194:ALA:CA	2.47	0.43
4:b:221:THR:HG23	4:b:223:THR:N	2.33	0.43
5:J:140:TYR:CG	5:J:217:GLY:HA2	2.54	0.43
2:I:220:LEU:N	2:I:220:LEU:CD2	2.80	0.43
2:N:215:GLN:HE21	2:N:215:GLN:HB2	1.61	0.43
5:J:87:LEU:HD23	5:J:87:LEU:HA	1.86	0.43
14:W:124:TYR:CD1	14:W:124:TYR:C	2.97	0.43
2:I:70:CYS:CB	2:I:217:LEU:HD11	2.48	0.43
4:P:49:LYS:O	4:P:49:LYS:HG3	2.17	0.43
6:T:38:MET:HE1	6:T:61:GLN:HB2	1.99	0.43
10:G:84:LEU:HD23	10:G:84:LEU:HA	1.86	0.43
1:H:49:ALA:CB	1:H:217:LEU:HD12	2.40	0.43
1:H:91:LYS:CG	1:H:119:LEU:HD11	2.47	0.43
1:H:189:MET:HE2	1:H:194:ALA:CA	2.47	0.43
10:L:49:LEU:HD21	10:L:199:LEU:HD23	2.01	0.43
2:I:204:LYS:HB2	2:I:204:LYS:HE3	1.60	0.43
8:D:39:ASN:HB2	8:D:40:PRO:HD3	2.01	0.43
1:M:202:LEU:HA	1:M:202:LEU:HD23	1.74	0.43
2:N:43:LEU:HD13	2:N:72:ALA:HB2	2.01	0.43
4:P:104:ILE:HA	4:P:105:PRO:HD3	1.94	0.43
8:C:94:MET:HE2	8:C:94:MET:HB3	1.94	0.43
14:a:51:LEU:HD21	14:a:110:MET:HG2	2.01	0.43
1:M:149:LYS:HB2	1:M:152:GLN:HE22	1.84	0.43
5:Q:41:CYS:HB3	5:Q:189:ILE:HD12	1.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:194:ILE:HG12	13:E:219:LEU:HD21	2.01	0.43
1:H:49:ALA:HB2	1:H:217:LEU:CD1	2.42	0.43
4:b:49:LYS:HB2	4:b:49:LYS:HE2	1.52	0.43
11:K:206:LEU:HB3	11:K:208:ILE:HD12	2.00	0.43
7:Y:141:CYS:HB3	7:Y:177:ASP:HB2	2.00	0.43
12:F:127:ILE:HD11	12:F:136:TYR:CD1	2.54	0.43
14:a:166:ARG:NH2	14:a:200:GLU:OE2	2.45	0.43
8:D:46:MET:CG	8:D:53:CYS:HB3	2.47	0.43
1:M:146:VAL:HG23	1:M:220:VAL:HG22	1.99	0.42
3:O:174:MET:SD	3:O:199:LYS:HD2	2.58	0.42
1:H:149:LYS:HB2	1:H:152:GLN:HE22	1.84	0.42
11:K:181:LYS:H	11:K:181:LYS:HG3	1.65	0.42
2:I:223:GLU:HA	2:I:226:GLU:HB2	2.01	0.42
10:G:52:ALA:HB2	10:G:59:HIS:CE1	2.54	0.42
7:Y:111:LEU:HD23	7:Y:118:PRO:HA	2.00	0.42
7:Y:128:CYS:HA	7:Y:129:PRO:HD3	1.83	0.42
14:W:163:THR:O	14:W:167:GLU:HG3	2.19	0.42
8:D:188:VAL:HG12	8:D:189:GLU:CG	2.49	0.42
1:M:81:LEU:HD12	1:M:138:GLY:HA3	2.02	0.42
11:K:178:PHE:HA	11:K:181:LYS:HZ2	1.84	0.42
10:L:4:ASN:C	10:L:4:ASN:HD22	2.27	0.42
2:I:174:LYS:HZ3	2:I:174:LYS:HG3	1.74	0.42
2:N:40:ILE:HA	2:N:136:PHE:CZ	2.55	0.42
3:O:222:LYS:NZ	3:O:224:VAL:HG22	2.35	0.42
4:P:134:LEU:HD23	4:P:134:LEU:HA	1.85	0.42
8:C:148:LEU:HD22	8:C:152:GLU:HB3	2.02	0.42
8:C:188:VAL:HG12	8:C:189:GLU:CG	2.49	0.42
3:Z:174:MET:SD	3:Z:199:LYS:HD2	2.58	0.42
6:V:92:LEU:HD11	6:V:121:LEU:HD23	2.01	0.42
7:Y:19:VAL:HG13	7:Y:118:PRO:HB3	2.00	0.42
12:A:160:ILE:HG22	12:A:164:MET:SD	2.59	0.42
14:a:124:TYR:CD1	14:a:124:TYR:C	2.97	0.42
3:O:35:LEU:HG	3:O:46:ALA:HB3	2.01	0.42
9:S:150:ASP:HB3	9:S:156:LYS:HD2	2.01	0.42
11:K:107:TYR:OH	13:B:66:HIS:HE1	2.02	0.42
10:L:52:ALA:HB2	10:L:59:HIS:CE1	2.54	0.42
1:M:49:ALA:HB2	1:M:217:LEU:CD1	2.42	0.42
1:M:210:LEU:HD12	1:M:215:ILE:HG21	2.02	0.42
3:O:35:LEU:HD12	3:O:35:LEU:O	2.19	0.42
5:Q:175:GLU:CB	5:Q:196:ILE:HG12	2.46	0.42
9:S:75:TYR:CD1	9:S:75:TYR:C	2.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:128:ARG:HD3	4:b:10:THR:O	2.19	0.42
4:b:189:THR:HA	4:b:192:LEU:HD12	2.02	0.42
12:F:160:ILE:HG22	12:F:164:MET:SD	2.59	0.42
2:I:40:ILE:HG13	2:I:211:MET:O	2.20	0.42
2:I:43:LEU:HD23	2:I:43:LEU:HA	1.87	0.42
7:U:141:CYS:HB3	7:U:177:ASP:HB2	2.00	0.42
8:C:2:THR:CB	15:C:301:A1L0C:O2	2.68	0.42
3:Z:137:ILE:O	3:Z:137:ILE:HG13	2.20	0.42
11:K:146:GLU:H	11:K:146:GLU:HG3	1.66	0.42
7:Y:194:ILE:HG12	13:B:219:LEU:HD21	2.02	0.42
2:I:43:LEU:HD13	2:I:72:ALA:HB2	2.01	0.42
9:X:75:TYR:CD1	9:X:75:TYR:C	2.97	0.42
5:Q:94:GLU:OE2	5:Q:114:ARG:CZ	2.68	0.42
5:Q:207:LYS:HB2	5:Q:207:LYS:HE3	1.49	0.42
9:S:123:SER:CB	9:S:136:LYS:HG2	2.50	0.42
10:G:56:LEU:HD11	1:H:182:GLN:HA	2.02	0.42
10:G:88:MET:HG2	10:G:112:ILE:HD11	2.02	0.42
3:Z:222:LYS:NZ	3:Z:224:VAL:HG22	2.35	0.42
4:b:51:GLN:HA	4:b:51:GLN:HE21	1.82	0.42
4:b:73:LEU:HD11	4:b:135:ILE:HG13	2.02	0.42
11:K:178:PHE:HA	11:K:181:LYS:NZ	2.35	0.42
12:A:37:PRO:HB3	12:A:43:TYR:CE1	2.55	0.42
11:R:206:LEU:HB3	11:R:208:ILE:HD12	2.00	0.42
8:D:12:GLY:HA2	8:D:105:TRP:HZ3	1.84	0.42
2:N:231:GLU:HG2	2:N:231:GLU:H	1.62	0.42
7:U:67:LYS:HD3	7:U:67:LYS:HA	1.81	0.42
7:U:111:LEU:HD23	7:U:118:PRO:HA	2.00	0.42
3:Z:79:ILE:HB	3:Z:82:ASP:HB2	2.02	0.42
7:Y:87:MET:HG3	7:Y:121:CYS:SG	2.60	0.42
1:M:228:MET:HB2	1:M:228:MET:HE2	1.82	0.42
2:N:43:LEU:HD23	2:N:43:LEU:HA	1.87	0.42
2:N:57:ARG:HH11	2:N:57:ARG:HG3	1.84	0.42
3:O:79:ILE:HB	3:O:82:ASP:HB2	2.02	0.42
4:P:56:TYR:HE2	11:R:159:TYR:OH	2.02	0.42
5:Q:240:LYS:HE3	5:Q:240:LYS:HB2	1.91	0.42
7:U:163:PHE:CE1	7:U:197:ARG:HD2	2.55	0.42
10:G:158:ALA:O	5:J:57:LEU:HB3	2.20	0.42
3:Z:27:ALA:HB2	4:b:16:GLY:O	2.19	0.42
4:b:54:ILE:HD11	11:K:184:LYS:HB3	1.99	0.42
5:J:94:GLU:OE2	5:J:114:ARG:CZ	2.68	0.42
12:A:127:ILE:HD11	12:A:136:TYR:CD1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:83:LEU:HD23	10:L:83:LEU:HA	1.88	0.42
2:N:40:ILE:HG13	2:N:211:MET:O	2.20	0.41
2:N:223:GLU:HA	2:N:226:GLU:HB2	2.01	0.41
5:Q:140:TYR:CG	5:Q:217:GLY:HA2	2.54	0.41
6:T:92:LEU:HD11	6:T:121:LEU:HD23	2.02	0.41
8:C:39:ASN:CB	8:C:40:PRO:CD	2.96	0.41
9:S:72:LEU:HD22	9:S:83:MET:SD	2.60	0.41
14:W:166:ARG:NH2	14:W:200:GLU:OE2	2.45	0.41
2:I:40:ILE:HA	2:I:136:PHE:CZ	2.55	0.41
4:P:32:ALA:HA	4:P:33:PRO:HD3	1.87	0.41
4:P:52:LYS:H	4:P:52:LYS:HG2	1.49	0.41
4:P:73:LEU:HD11	4:P:135:ILE:HG13	2.02	0.41
7:U:87:MET:HG3	7:U:121:CYS:SG	2.60	0.41
10:G:49:LEU:HD21	10:G:199:LEU:HD23	2.01	0.41
10:G:176:MET:HE1	5:J:56:LYS:CB	2.50	0.41
3:Z:35:LEU:HD12	3:Z:35:LEU:O	2.20	0.41
3:Z:205:LYS:HB2	3:Z:205:LYS:HE2	1.38	0.41
7:Y:163:PHE:CE1	7:Y:197:ARG:HD2	2.55	0.41
13:E:40:LYS:HD3	13:E:40:LYS:N	2.27	0.41
13:E:114:HIS:HB3	13:E:115:PRO:HD2	2.02	0.41
10:L:88:MET:HG2	10:L:112:ILE:HD11	2.02	0.41
11:R:47:CYS:HB2	11:R:221:THR:HG22	2.02	0.41
11:R:178:PHE:HA	11:R:181:LYS:NZ	2.35	0.41
9:X:150:ASP:HB3	9:X:156:LYS:HD2	2.02	0.41
1:M:50:VAL:CG1	1:M:66:LYS:HB2	2.45	0.41
2:N:227:LYS:HB3	2:N:227:LYS:HE3	1.51	0.41
6:T:96:THR:CB	8:D:92:ARG:HH22	2.18	0.41
10:G:4:ASN:C	10:G:4:ASN:HD22	2.27	0.41
14:a:1:THR:O	14:a:107:TRP:CE3	2.73	0.41
10:L:50:LYS:HB2	10:L:50:LYS:HE2	1.98	0.41
2:I:168:VAL:HG13	2:I:194:ALA:HB1	2.02	0.41
2:I:173:GLU:H	2:I:173:GLU:HG2	1.54	0.41
11:R:67:THR:OG1	11:R:216:GLU:OE2	2.22	0.41
9:X:123:SER:CB	9:X:136:LYS:HG2	2.50	0.41
13:B:201:GLN:C	13:B:201:GLN:CD	2.88	0.41
1:H:204:GLN:HE21	1:H:204:GLN:HB3	1.60	0.41
3:Z:45:LEU:HD13	3:Z:75:SER:HB2	2.03	0.41
13:E:201:GLN:C	13:E:201:GLN:CD	2.88	0.41
14:a:163:THR:O	14:a:167:GLU:HG3	2.20	0.41
14:a:179:ARG:CD	13:B:135:LEU:HD11	2.49	0.41
8:D:148:LEU:HD22	8:D:152:GLU:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:55:GLN:HG3	8:D:89:TYR:CE2	2.55	0.41
12:F:74:PRO:HA	12:F:75:PRO:HD3	1.86	0.41
14:W:67:LEU:HD12	14:W:67:LEU:HA	1.92	0.41
1:M:204:GLN:HE21	1:M:204:GLN:HB3	1.60	0.41
3:O:27:ALA:HB2	4:P:16:GLY:O	2.20	0.41
6:T:170:ARG:HA	6:T:170:ARG:HD3	1.51	0.41
10:L:230:SER:N	10:L:231:PRO:CD	2.83	0.41
2:I:57:ARG:HH11	2:I:57:ARG:HG3	1.84	0.41
2:N:53:LEU:HD11	3:O:176:LYS:HG2	2.03	0.41
3:O:66:TYR:CD1	3:O:66:TYR:N	2.89	0.41
3:O:137:ILE:O	3:O:137:ILE:HG13	2.20	0.41
4:P:189:THR:HA	4:P:192:LEU:HD12	2.02	0.41
1:H:210:LEU:HD12	1:H:215:ILE:HG21	2.02	0.41
12:F:37:PRO:HB3	12:F:43:TYR:CE1	2.55	0.41
10:L:69:HIS:HB2	10:L:137:TYR:O	2.21	0.41
11:R:146:GLU:H	11:R:146:GLU:HG3	1.65	0.41
8:D:39:ASN:CB	8:D:40:PRO:CD	2.96	0.41
1:H:81:LEU:HD12	1:H:138:GLY:HA3	2.02	0.41
7:Y:126:ILE:H	7:Y:126:ILE:HG13	1.60	0.41
2:I:33:VAL:CG2	2:I:168:VAL:HG11	2.51	0.41
13:B:73:GLU:HA	13:B:74:PRO:HD3	1.88	0.41
3:O:180:LYS:HG2	3:O:184:MET:HE1	2.02	0.41
5:Q:76:ALA:HB3	5:Q:136:MET:HE3	2.03	0.41
8:C:12:GLY:HA2	8:C:105:TRP:HZ3	1.84	0.41
9:S:125:ASP:HB2	9:S:126:PRO:HD2	2.02	0.41
3:Z:91:ARG:HG2	7:Y:75:LEU:HD13	2.02	0.41
11:K:47:CYS:HB2	11:K:221:THR:HG22	2.02	0.41
6:V:170:ARG:HD3	6:V:170:ARG:HA	1.51	0.41
13:E:135:LEU:HD11	14:W:179:ARG:CD	2.51	0.41
13:E:155:LEU:HD13	13:E:155:LEU:C	2.45	0.41
12:A:104:TRP:CZ2	12:A:181:ALA:HB2	2.56	0.41
14:a:110:MET:HB2	14:a:110:MET:HE3	1.81	0.41
14:a:189:ILE:HD12	14:a:203:LEU:HD13	2.03	0.41
10:L:34:ALA:HA	10:L:161:ILE:O	2.21	0.41
8:D:2:THR:CB	15:D:301:A1L0C:O2	2.68	0.41
13:B:114:HIS:HB3	13:B:115:PRO:HD2	2.02	0.41
2:N:168:VAL:HG13	2:N:194:ALA:HB1	2.02	0.41
4:P:201:GLN:NE2	4:P:201:GLN:HA	2.36	0.41
4:P:211:ILE:HD11	4:P:218:ARG:HG2	2.03	0.41
3:Z:66:TYR:CD1	3:Z:66:TYR:N	2.89	0.41
4:b:211:ILE:HD11	4:b:218:ARG:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:W:20:VAL:HG23	14:W:120:SER:HB2	2.03	0.41
12:A:115:THR:O	12:A:115:THR:OG1	2.38	0.41
2:I:90:GLU:HG2	2:I:110:TYR:CG	2.55	0.41
9:X:72:LEU:HD22	9:X:83:MET:SD	2.60	0.41
1:M:91:LYS:O	1:M:95:GLU:HG2	2.21	0.40
2:N:33:VAL:CG2	2:N:168:VAL:HG11	2.51	0.40
10:G:34:ALA:HA	10:G:161:ILE:O	2.21	0.40
1:H:91:LYS:O	1:H:95:GLU:HG2	2.22	0.40
3:Z:241:GLU:N	3:Z:241:GLU:OE1	2.55	0.40
8:D:10:GLN:HG3	8:D:11:HIS:CD2	2.56	0.40
13:B:155:LEU:C	13:B:155:LEU:HD13	2.45	0.40
13:B:188:THR:O	13:B:188:THR:CG2	2.70	0.40
1:M:152:GLN:HE21	1:M:152:GLN:HB2	1.73	0.40
1:M:182:GLN:HE21	1:M:182:GLN:HB3	1.70	0.40
2:N:70:CYS:CB	2:N:217:LEU:HD11	2.48	0.40
2:N:90:GLU:HG2	2:N:110:TYR:CG	2.55	0.40
3:O:230:GLN:HE21	3:O:230:GLN:HB2	1.65	0.40
10:G:230:SER:N	10:G:231:PRO:CD	2.83	0.40
4:b:75:TYR:HB3	4:b:82:TYR:CE1	2.57	0.40
5:J:240:LYS:HE3	5:J:240:LYS:HB2	1.91	0.40
13:E:109:GLN:HE21	13:E:109:GLN:HB2	1.78	0.40
14:a:6:VAL:HA	14:a:29:SER:O	2.21	0.40
10:L:74:ILE:O	10:L:74:ILE:HG12	2.22	0.40
2:I:62:ILE:HD13	2:I:209:ALA:HB3	2.04	0.40
2:I:65:LEU:HD11	2:I:71:MET:SD	2.62	0.40
3:O:45:LEU:HD13	3:O:75:SER:HB2	2.03	0.40
3:O:229:LYS:O	3:O:233:VAL:HG23	2.21	0.40
6:T:102:LEU:HD11	6:T:118:MET:CE	2.37	0.40
10:G:69:HIS:HB2	10:G:137:TYR:O	2.21	0.40
1:H:147:ASP:HB2	1:H:148:GLU:H	1.72	0.40
3:Z:180:LYS:HG2	3:Z:184:MET:HE1	2.02	0.40
14:a:20:VAL:HG23	14:a:120:SER:HB2	2.03	0.40
4:P:55:LEU:HD22	11:R:165:ALA:HB3	2.03	0.40
3:Z:21:VAL:HG11	3:Z:153:SER:HB3	2.03	0.40
3:Z:35:LEU:C	3:Z:35:LEU:CD1	2.93	0.40
2:I:211:MET:HE3	2:I:211:MET:HB3	1.79	0.40
2:N:17:PHE:HD1	2:N:17:PHE:HA	1.80	0.40
2:N:115:LYS:HE2	2:N:129:ILE:HD12	2.04	0.40
4:P:221:THR:CG2	4:P:224:GLU:H	2.35	0.40
5:Q:50:GLU:HB2	5:Q:197:ILE:HG23	2.03	0.40
8:C:157:GLY:CA	8:C:177:MET:HE1	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Y:95:TYR:CE1	7:Y:98:ARG:HD3	2.57	0.40
10:L:166:GLN:NE2	10:L:166:GLN:C	2.77	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	A1L0C	F	301	12	19,23,23	0.45	0	25,31,31	0.76	0
15	A1L0C	D	301	8	19,23,23	0.63	0	25,31,31	1.18	3 (12%)
15	A1L0C	C	301	8	19,23,23	0.63	0	25,31,31	1.18	3 (12%)
15	A1L0C	A	301	12	19,23,23	0.44	0	25,31,31	0.77	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	A1L0C	F	301	12	-	3/15/28/28	0/2/2/2
15	A1L0C	D	301	8	-	4/15/28/28	0/2/2/2
15	A1L0C	C	301	8	-	4/15/28/28	0/2/2/2
15	A1L0C	A	301	12	-	3/15/28/28	0/2/2/2

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	C	301	A1L0C	C1-N3-N2	3.17	111.53	108.84
15	D	301	A1L0C	C1-N3-N2	3.17	111.53	108.84
15	C	301	A1L0C	B1-C4-C5	-3.15	106.36	112.31
15	D	301	A1L0C	B1-C4-C5	-3.15	106.36	112.31
15	C	301	A1L0C	C1-C3-N4	2.08	118.18	115.22
15	D	301	A1L0C	C1-C3-N4	2.08	118.18	115.22

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	C	301	A1L0C	C2-C1-C3-N4
15	C	301	A1L0C	C2-C1-C3-O3
15	C	301	A1L0C	N3-C1-C3-N4
15	D	301	A1L0C	C2-C1-C3-N4
15	D	301	A1L0C	C2-C1-C3-O3
15	D	301	A1L0C	N3-C1-C3-N4
15	C	301	A1L0C	N3-C1-C3-O3
15	D	301	A1L0C	N3-C1-C3-O3
15	F	301	A1L0C	O3-C3-N4-C4

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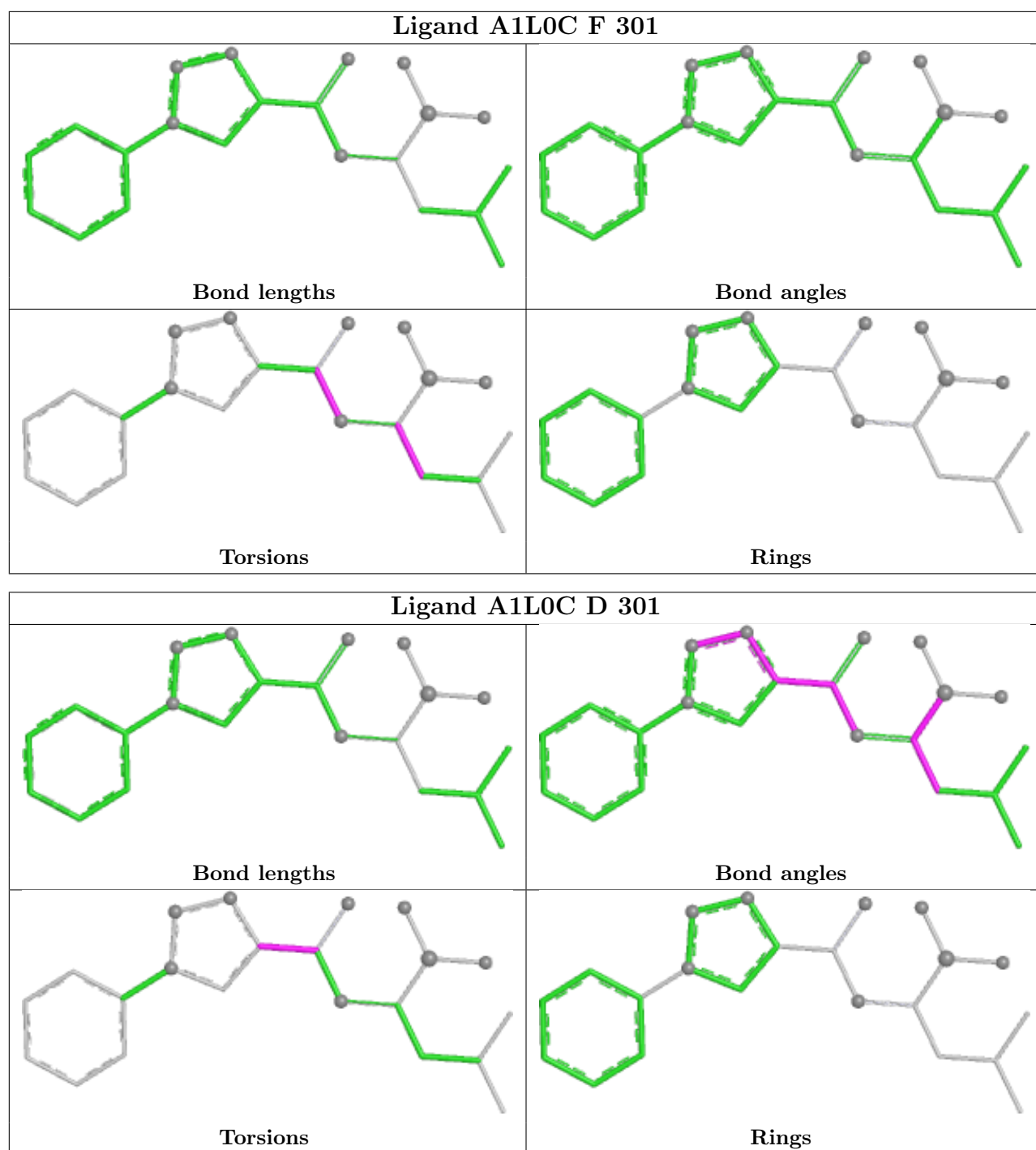
Mol	Chain	Res	Type	Atoms
15	A	301	A1L0C	O3-C3-N4-C4
15	F	301	A1L0C	N4-C4-C5-C6
15	A	301	A1L0C	N4-C4-C5-C6
15	F	301	A1L0C	C1-C3-N4-C4
15	A	301	A1L0C	C1-C3-N4-C4

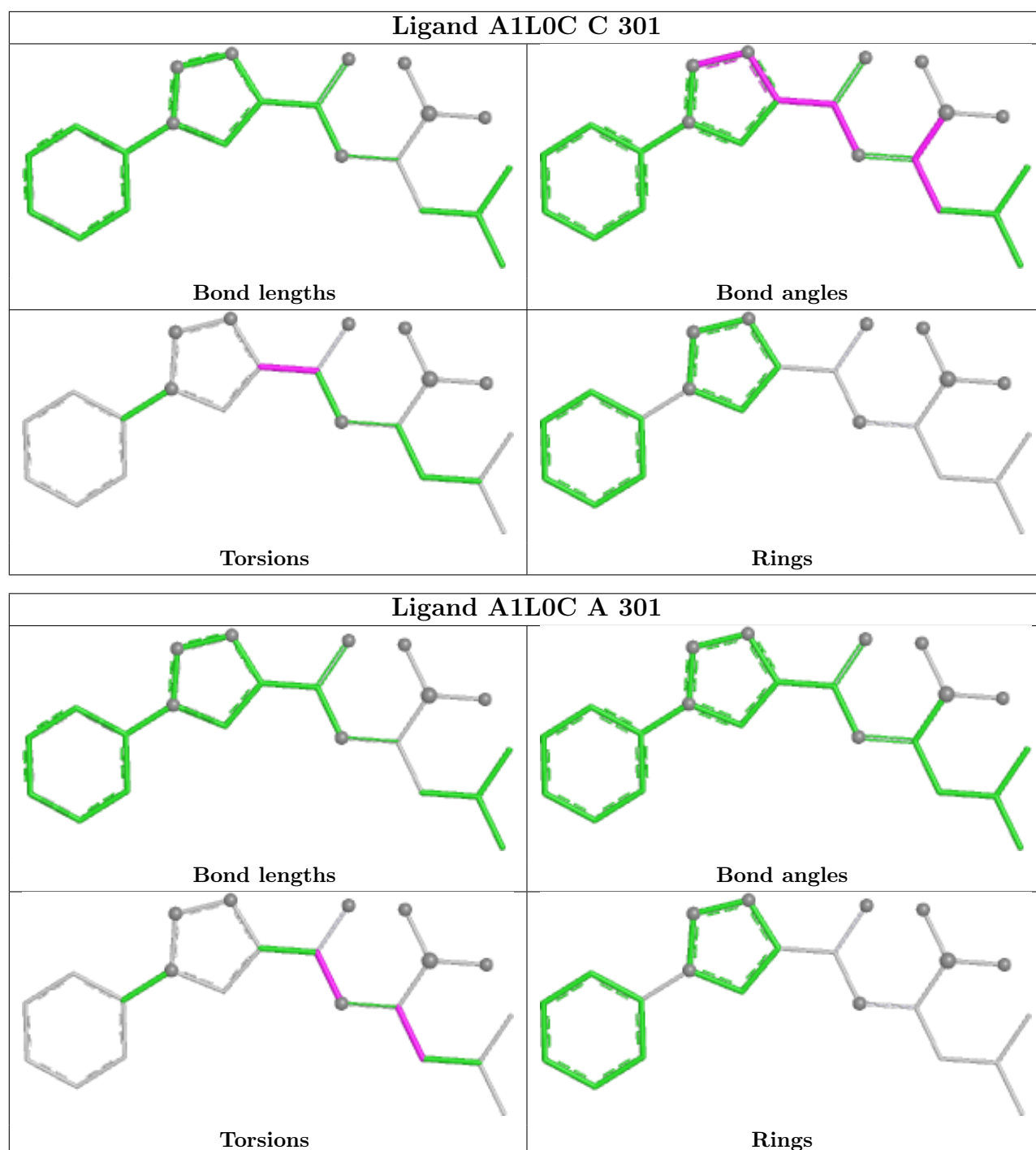
There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	F	301	A1L0C	1	0
15	D	301	A1L0C	1	0
15	C	301	A1L0C	1	0
15	A	301	A1L0C	1	0

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





5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

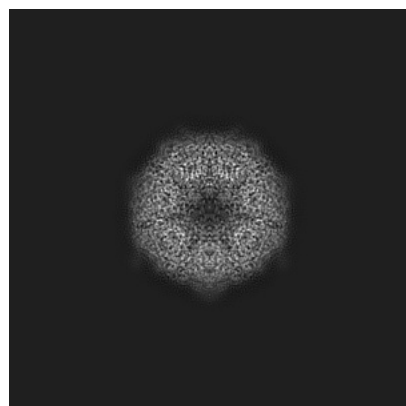
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39600. These allow visual inspection of the internal detail of the map and identification of artifacts.

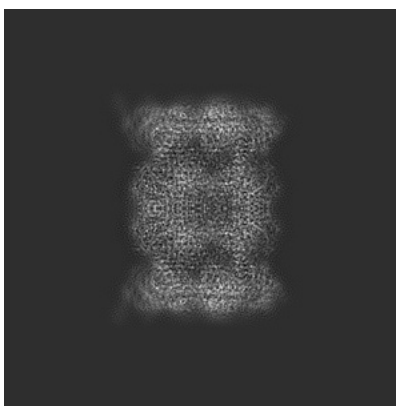
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

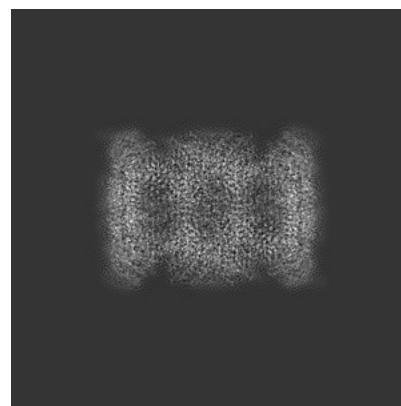
6.1.1 Primary map



X

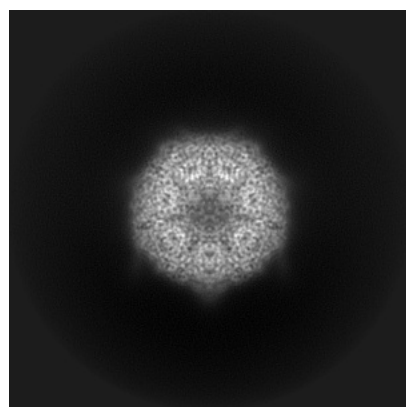


Y

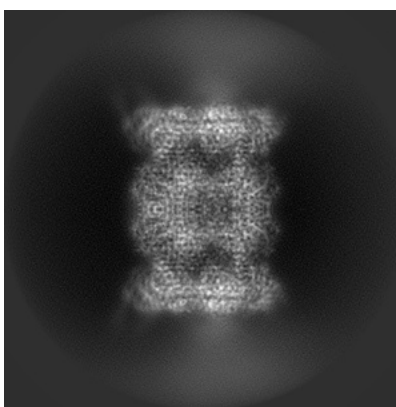


Z

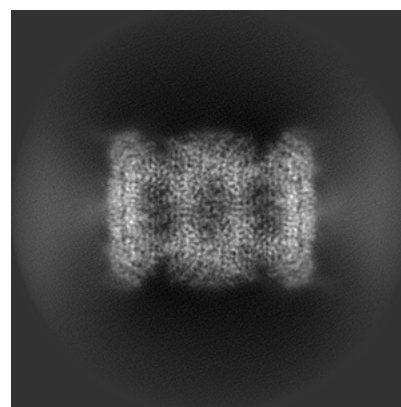
6.1.2 Raw map



X



Y

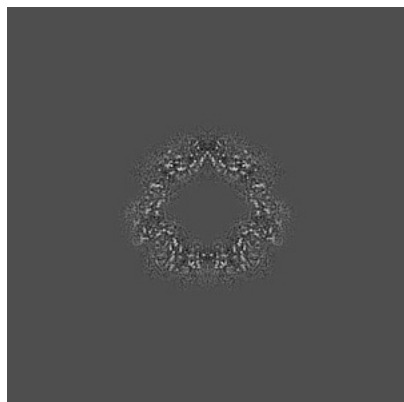


Z

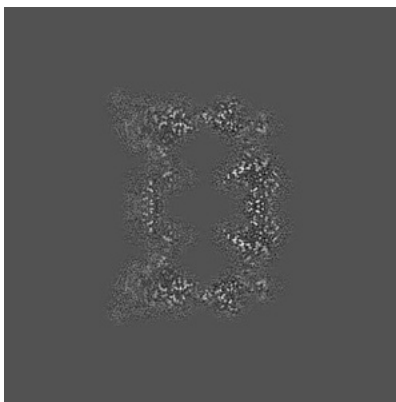
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 176

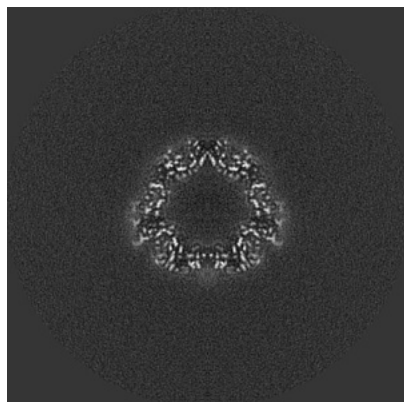


Y Index: 176

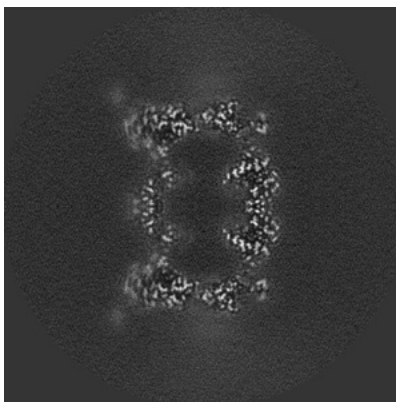


Z Index: 176

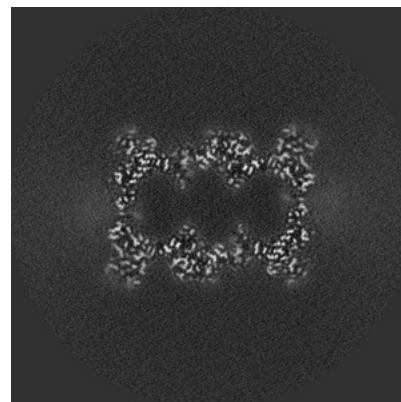
6.2.2 Raw map



X Index: 176



Y Index: 176

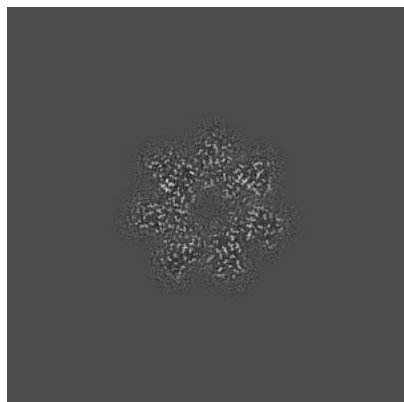


Z Index: 176

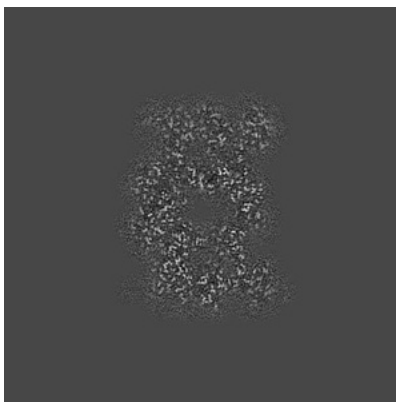
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

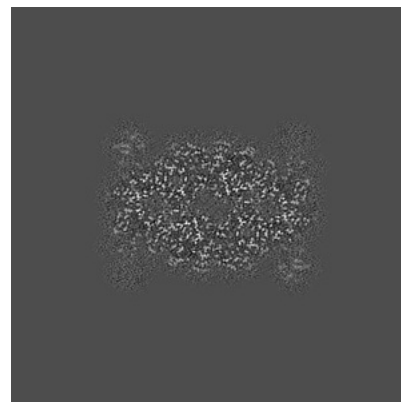
6.3.1 Primary map



X Index: 154

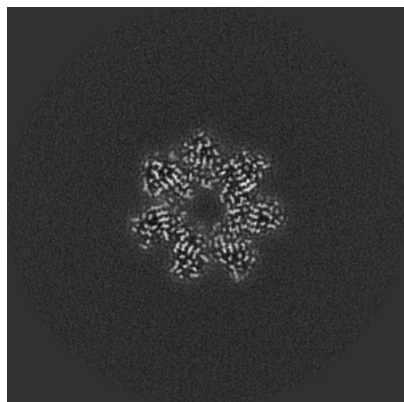


Y Index: 204

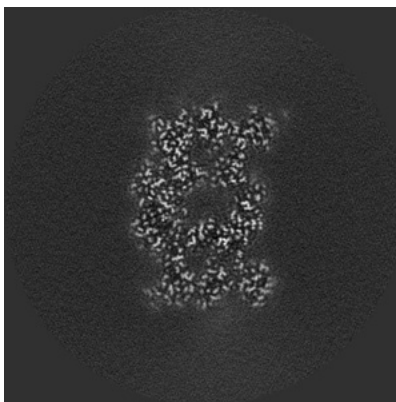


Z Index: 206

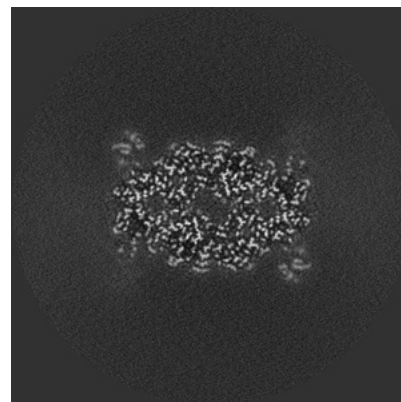
6.3.2 Raw map



X Index: 198



Y Index: 148

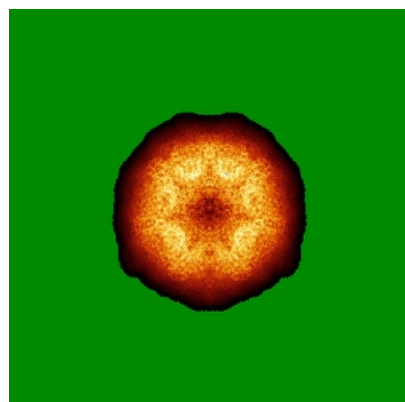


Z Index: 206

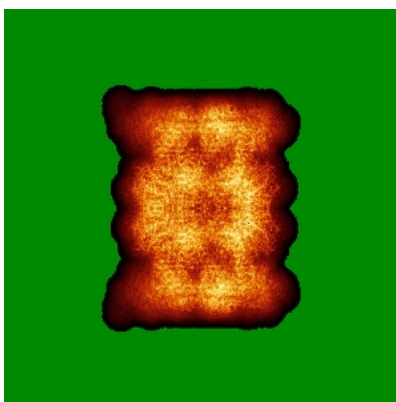
The images above show the largest variance slices of the map in three orthogonal directions.

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

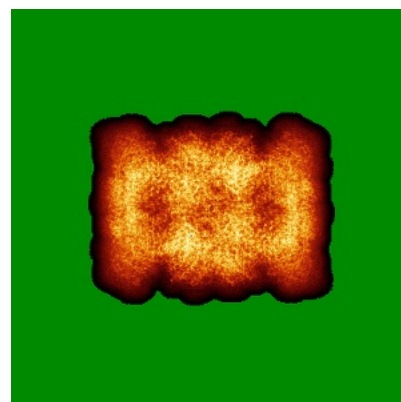
6.4.1 Primary map



X

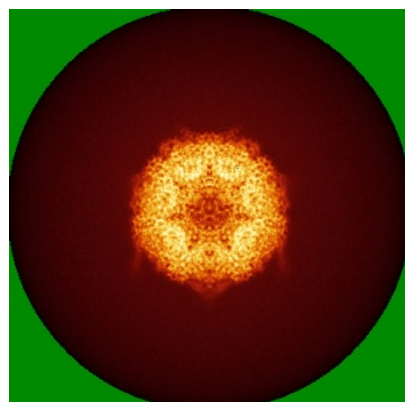


Y

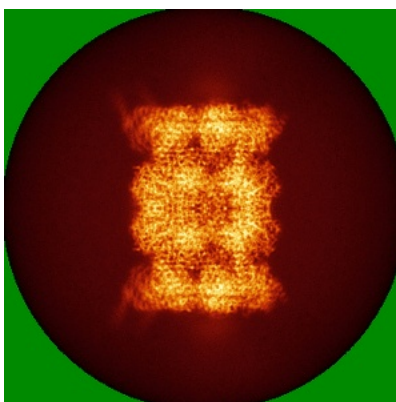


Z

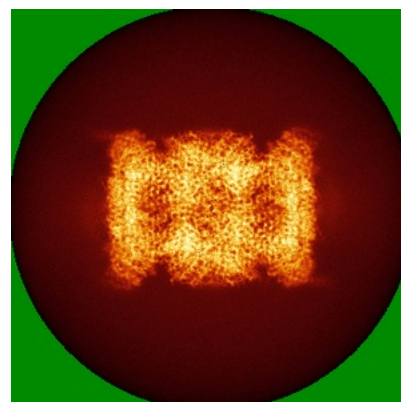
6.4.2 Raw map



X



Y

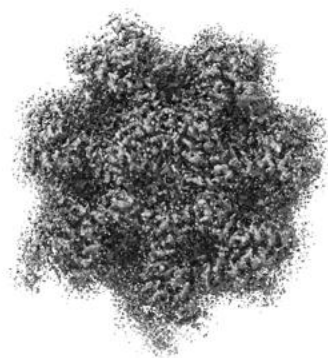


Z

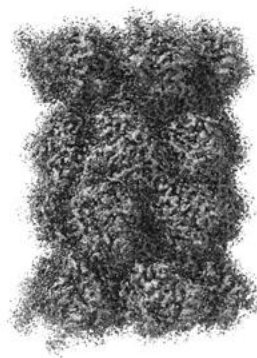
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

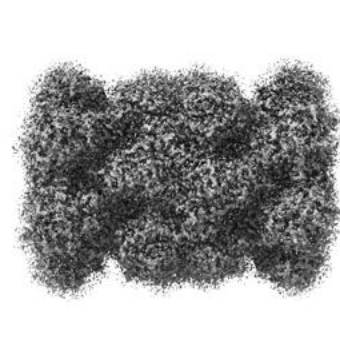
6.5.1 Primary map



X



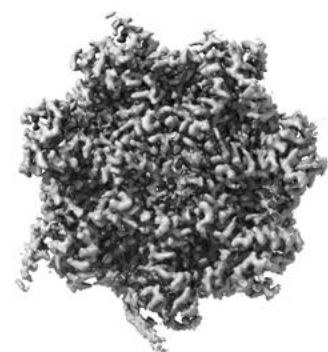
Y



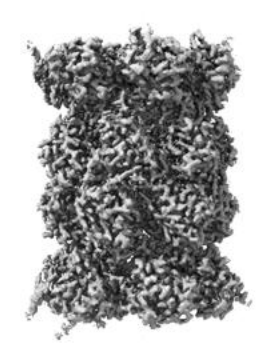
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0247. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

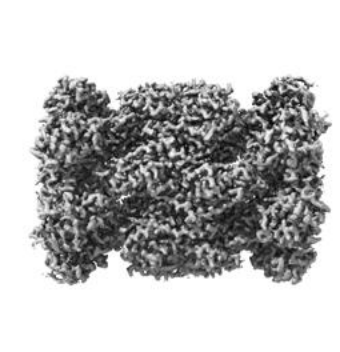
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

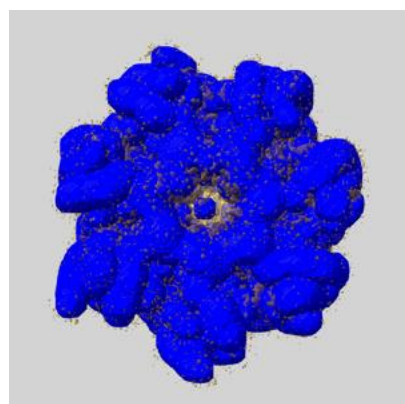
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

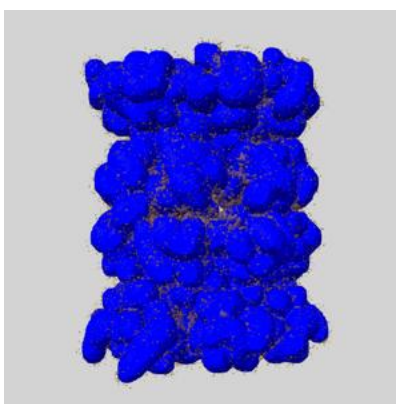
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

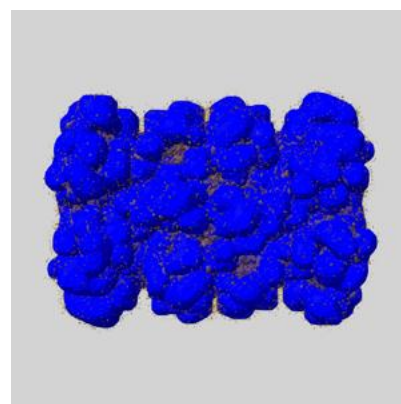
6.6.1 emd_39600_msk_1.map [i](#)



X



Y

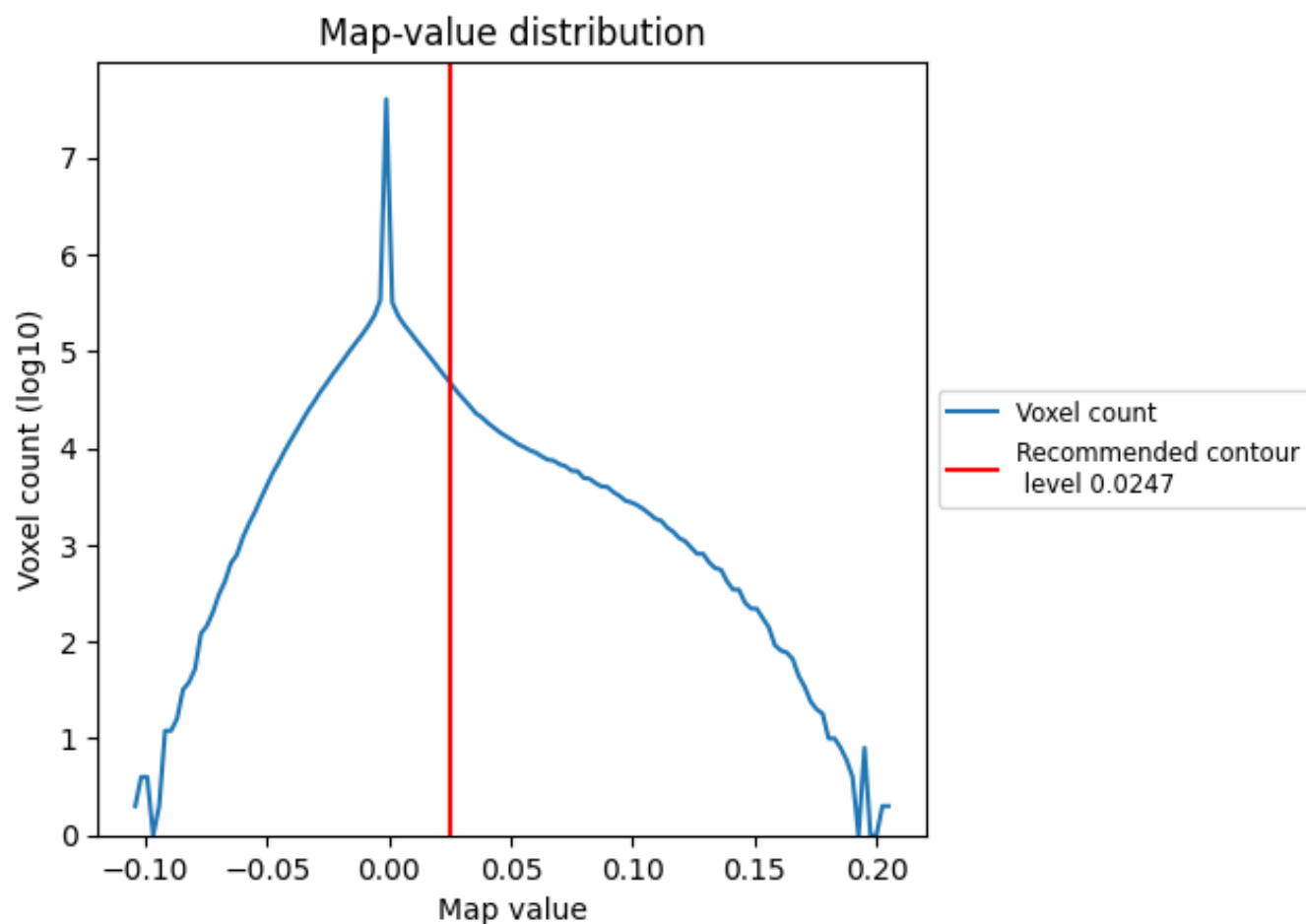


Z

7 Map analysis [i](#)

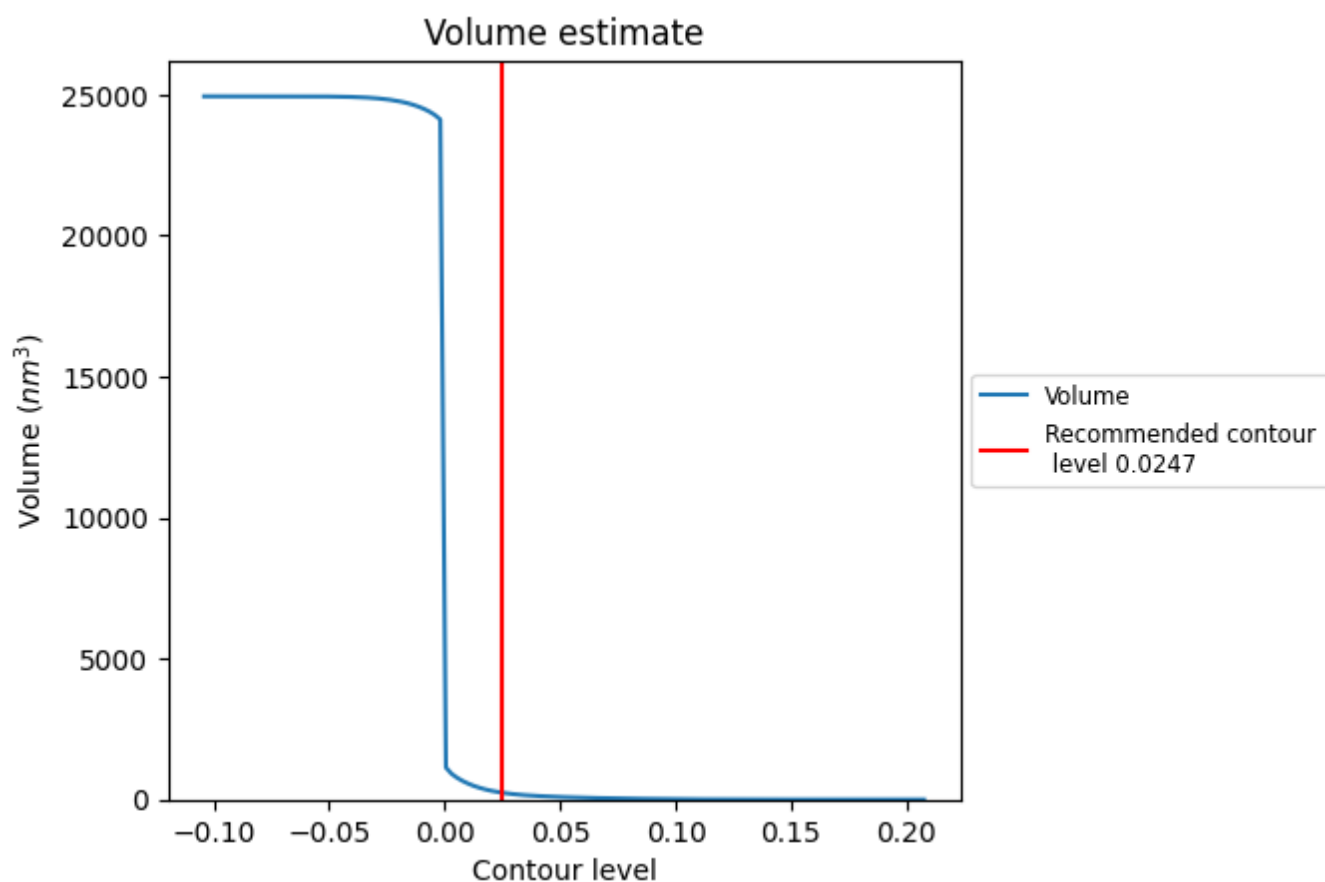
This section contains the results of statistical analysis of the map.

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.

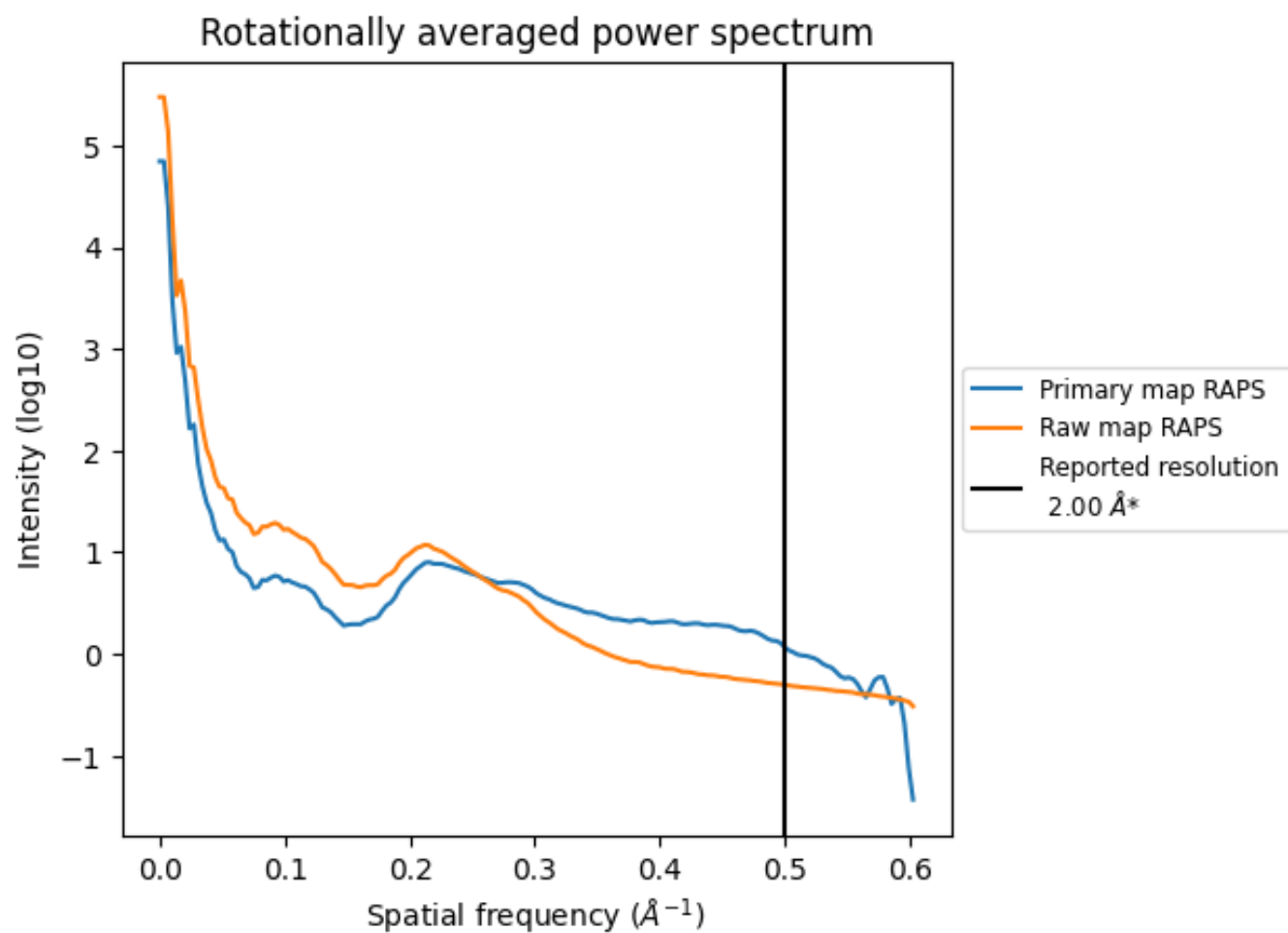
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 245 nm³; this corresponds to an approximate mass of 221 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 ⓘ

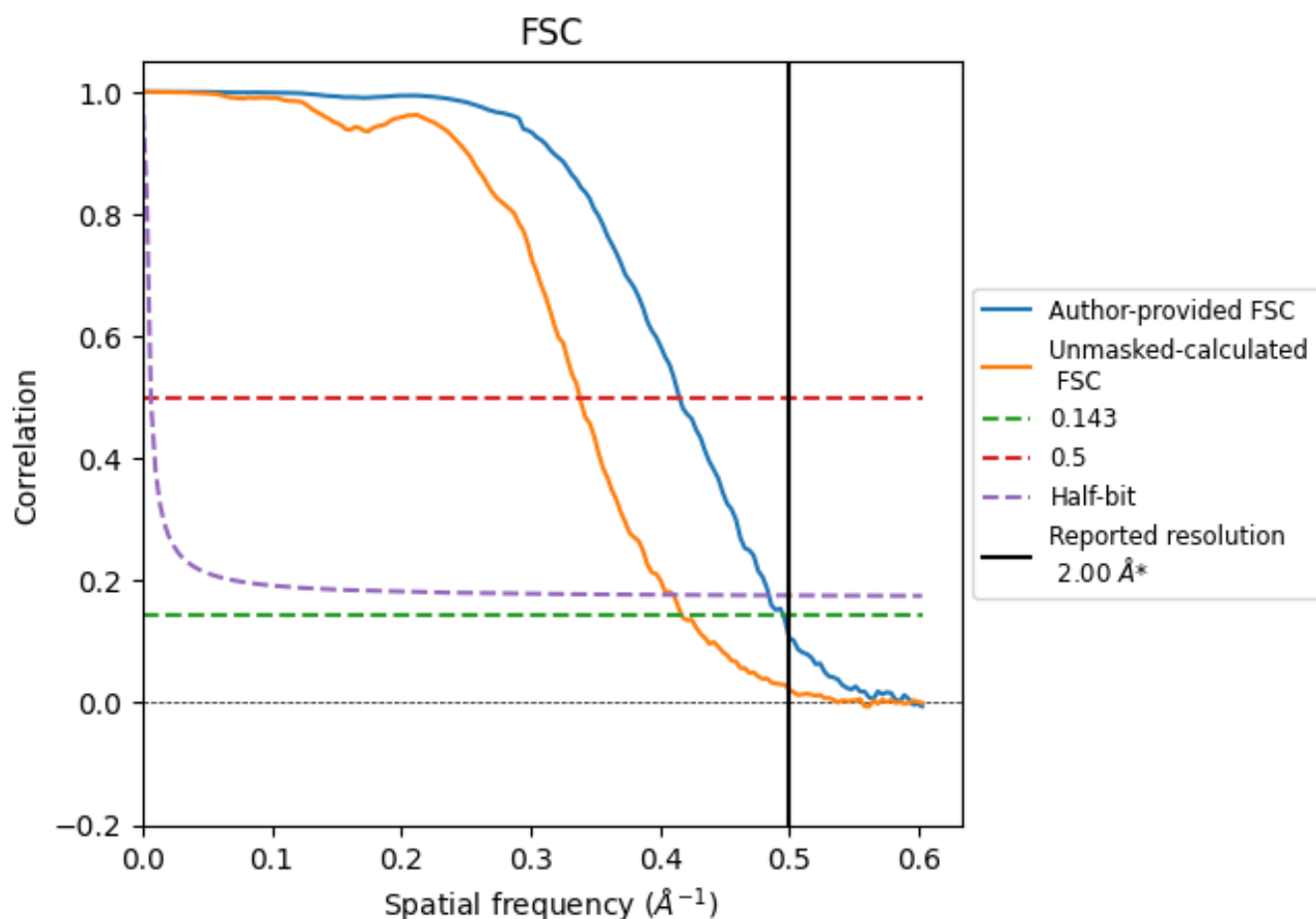


*Reported resolution corresponds to spatial frequency of 0.500 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.500 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

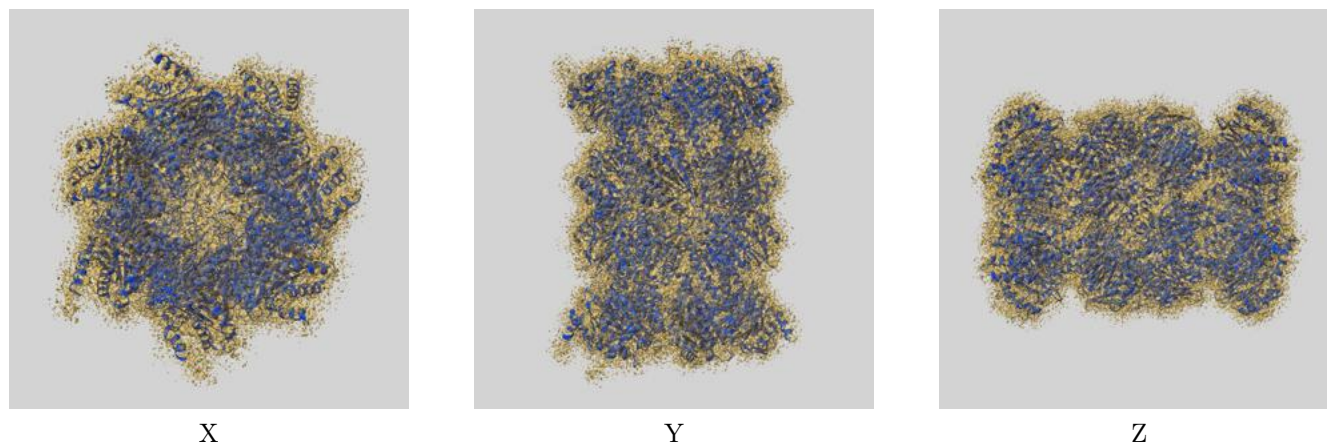
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.00	-	-
Author-provided FSC curve	2.02	2.41	2.07
Unmasked-calculated*	2.40	2.96	2.44

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.40 differs from the reported value 2.0 by more than 10 %

9 Map-model fit [i](#)

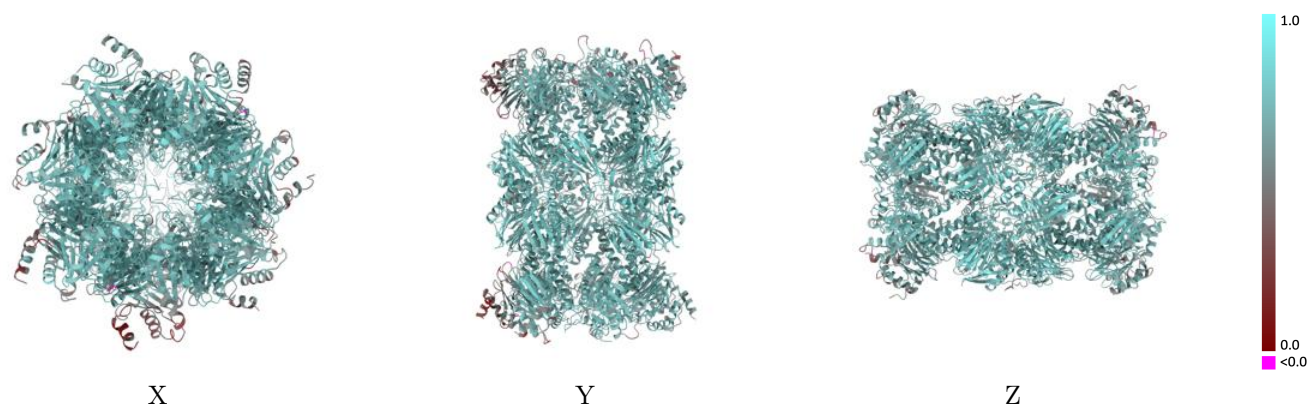
This section contains information regarding the fit between EMDB map EMD-39600 and PDB model 8YVG. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



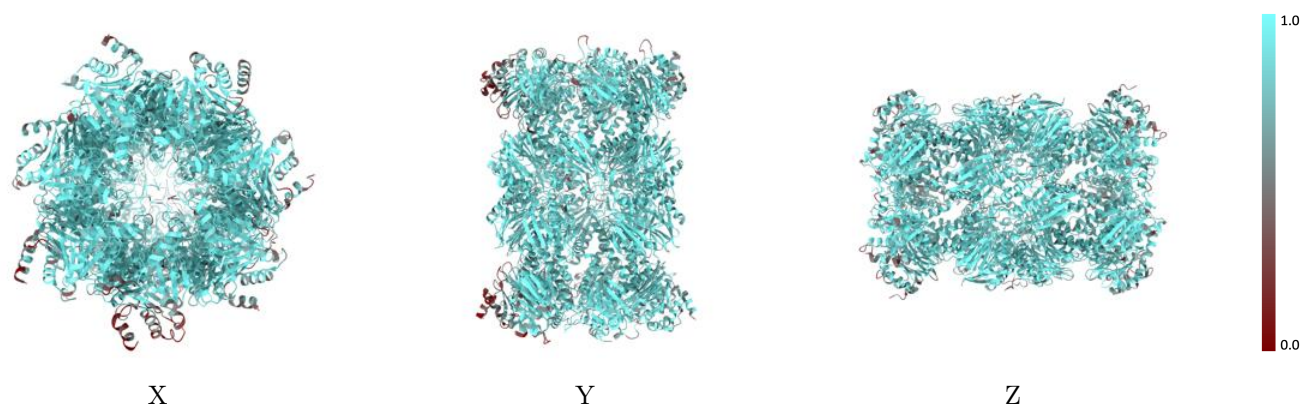
The images above show the 3D surface view of the map at the recommended contour level 0.0247 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



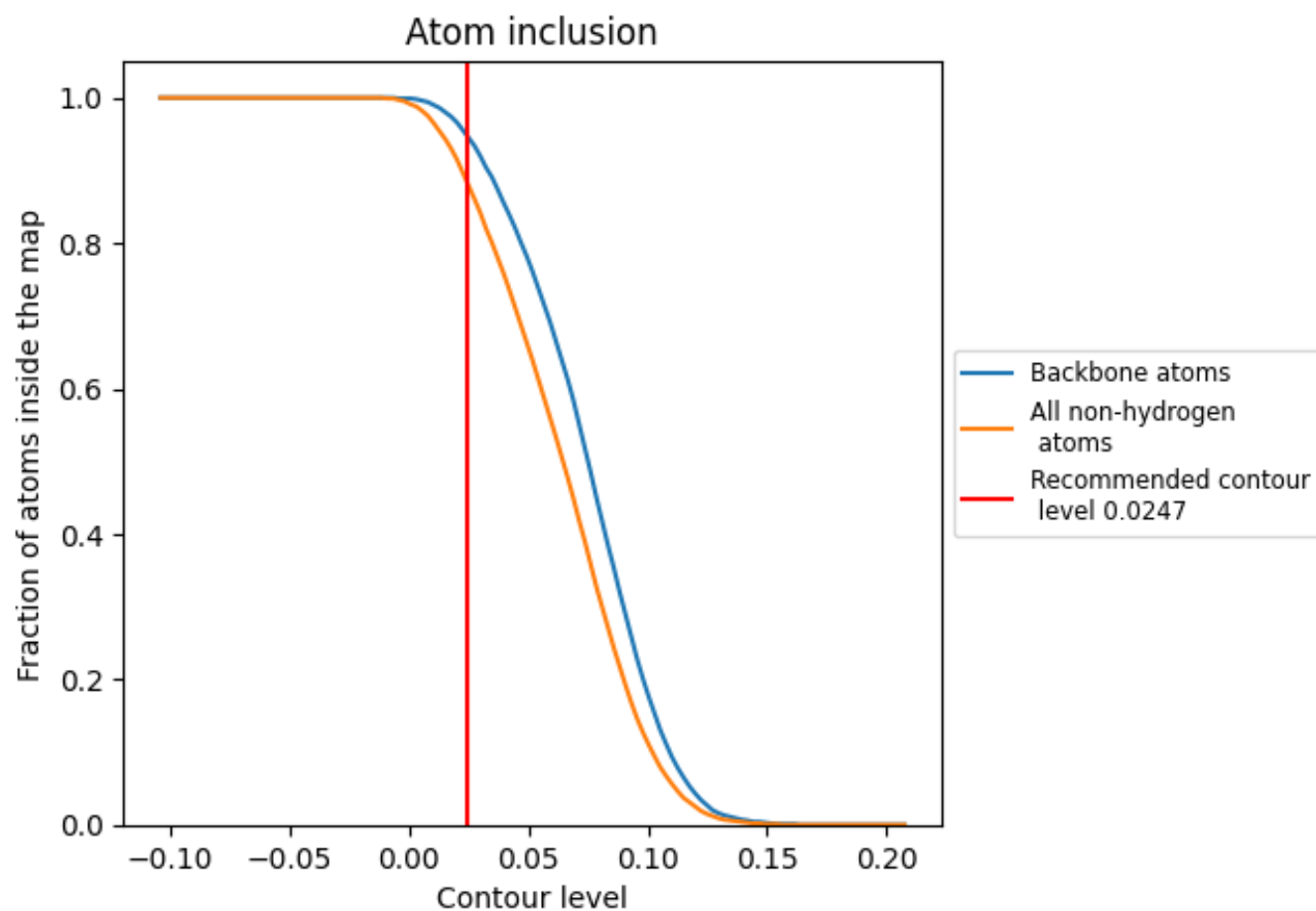
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0247).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0247) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8810	 0.7070
A	 0.9300	 0.7450
B	 0.8910	 0.7200
C	 0.9320	 0.7430
D	 0.9320	 0.7420
E	 0.8920	 0.7200
F	 0.9300	 0.7440
G	 0.8470	 0.6690
H	 0.8530	 0.6760
I	 0.6600	 0.5580
J	 0.8660	 0.6920
K	 0.8980	 0.7110
L	 0.8450	 0.6730
M	 0.8490	 0.6770
N	 0.6640	 0.5600
O	 0.8530	 0.6870
P	 0.8900	 0.6990
Q	 0.8650	 0.6880
R	 0.8990	 0.7110
S	 0.9290	 0.7610
T	 0.9430	 0.7510
U	 0.9400	 0.7590
V	 0.9420	 0.7530
W	 0.9400	 0.7670
X	 0.9290	 0.7590
Y	 0.9390	 0.7590
Z	 0.8540	 0.6880
a	 0.9400	 0.7650
b	 0.8890	 0.7000

