



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 01:01 AM UTC

PDB ID : 8YIZ / pdb_00008yiz
EMDB ID : EMD-39334
Title : Cryo-EM structure of human proteasome assembly intermediate preholo-2
Authors : Han, Y.; Han, Q.; Tang, Q.; Zhang, Y.; Liu, K.
Deposited on : 2024-02-29
Resolution : 3.79 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:

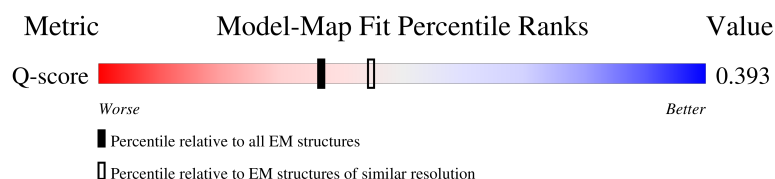
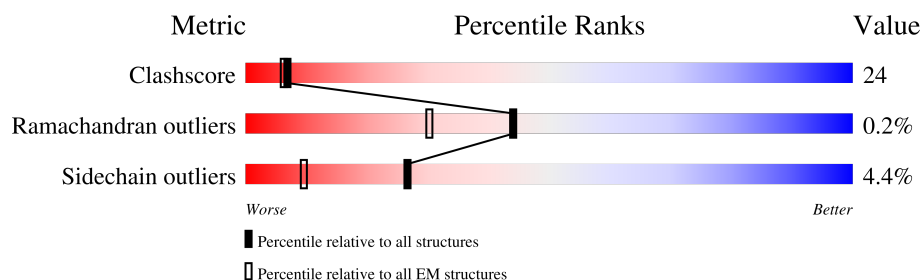
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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

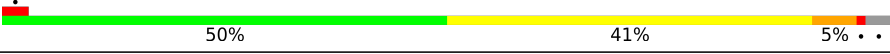
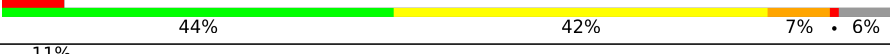
The reported resolution of this entry is 3.79 Å.

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



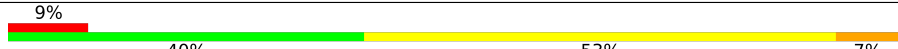
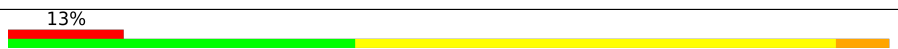
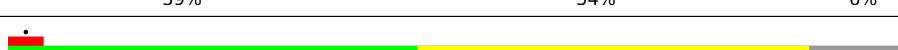
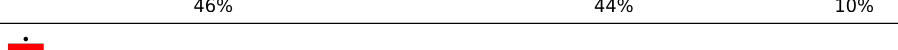
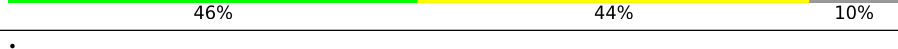
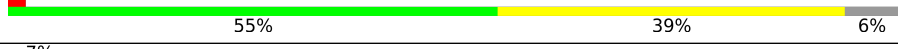
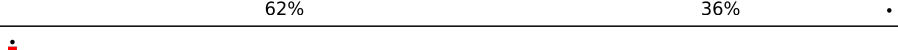
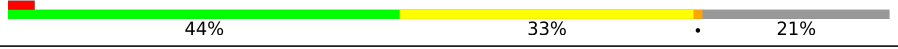
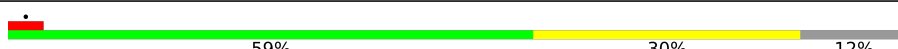
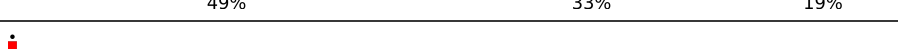
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10018 (3.29 - 4.29)

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

Mol	Chain	Length	Quality of chain
1	A	234	
1	O	234	
2	B	261	
2	P	261	

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Mol	Chain	Length	Quality of chain
3	C	248	
3	Q	248	
4	D	241	
4	R	241	
5	E	263	
5	S	263	
6	F	255	
6	T	255	
7	G	246	
7	U	246	
8	H	277	
8	V	277	
9	I	205	
9	W	205	
10	J	201	
10	X	201	
11	K	263	
11	Y	263	
12	L	241	
12	Z	241	
13	M	253	
13	a	253	
14	N	239	
14	b	239	
15	f	288	

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Mol	Chain	Length	Quality of chain
16	g	264	49% 57% 42%

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 52599 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-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	O	228	Total	C	N	O	S	0	0
			1760	1124	296	334	6		
1	A	228	Total	C	N	O	S	0	0
			1760	1124	296	334	6		

- Molecule 2 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	245	Total	C	N	O	S	0	0
			1894	1196	321	367	10		
2	B	245	Total	C	N	O	S	0	0
			1894	1196	321	367	10		

- Molecule 3 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Q	239	Total	C	N	O	S	0	0
			1849	1159	325	360	5		
3	C	239	Total	C	N	O	S	0	0
			1849	1159	325	360	5		

- Molecule 4 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	R	241	Total	C	N	O	S	0	0
			1840	1159	305	364	12		
4	D	241	Total	C	N	O	S	0	0
			1840	1159	305	364	12		

- Molecule 5 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	S	238	Total	C	N	O	S	1	0
			1859	1165	335	348	11		
5	E	238	Total	C	N	O	S	1	0
			1859	1165	335	348	11		

- Molecule 6 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	T	239	Total	C	N	O	S	1	0
			1858	1180	318	348	12		
6	F	239	Total	C	N	O	S	1	0
			1858	1180	318	348	12		

- Molecule 7 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	U	245	Total	C	N	O	S	0	0
			1893	1201	317	361	14		
7	G	245	Total	C	N	O	S	0	0
			1893	1201	317	361	14		

- Molecule 8 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	V	220	Total	C	N	O	S	2	0
			1655	1042	278	322	13		
8	H	220	Total	C	N	O	S	2	0
			1655	1042	278	322	13		

- Molecule 9 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	W	200	Total	C	N	O	S	2	0
			1576	1004	265	289	18		
9	I	200	Total	C	N	O	S	2	0
			1576	1004	265	289	18		

- Molecule 10 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	196	Total	C	N	O	S	2	0
			1581	1013	269	289	10		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	196	Total	C	N	O	S	2	0
			1581	1013	269	289	10		

- Molecule 11 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Y	208	Total	C	N	O	S	3	0
			1631	1030	286	304	11		
11	K	208	Total	C	N	O	S	3	0
			1631	1030	286	304	11		

- Molecule 12 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Z	213	Total	C	N	O	S	1	0
			1644	1043	281	309	11		
12	L	213	Total	C	N	O	S	1	0
			1644	1043	281	309	11		

- Molecule 13 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	a	206	Total	C	N	O	S	1	0
			1605	1012	277	305	11		
13	M	206	Total	C	N	O	S	1	0
			1605	1012	277	305	11		

- Molecule 14 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	b	200	Total	C	N	O	S	1	0
			1504	943	256	292	13		
14	N	200	Total	C	N	O	S	1	0
			1504	943	256	292	13		

- Molecule 15 is a protein called Proteasome assembly chaperone 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	f	281	Total	C	N	O	S	0	0
			2239	1426	375	419	19		

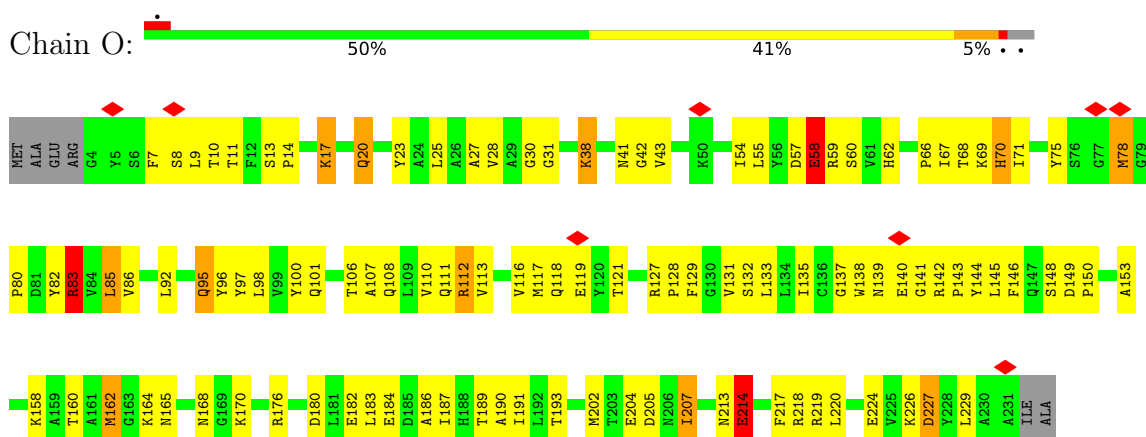
- Molecule 16 is a protein called Proteasome assembly chaperone 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	g	264	Total	C	N	O	S	0	0
			2062	1323	336	388	15		

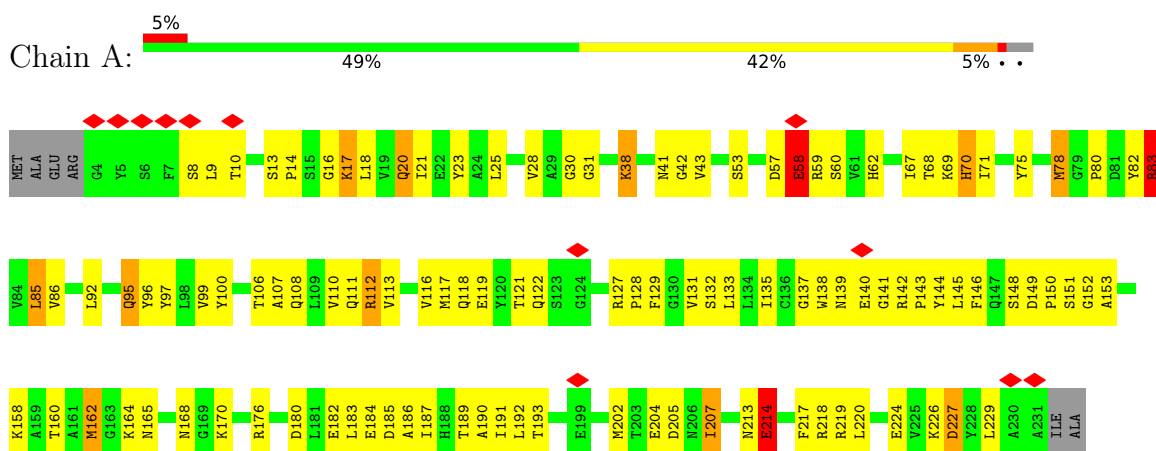
3 Residue-property plots

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.

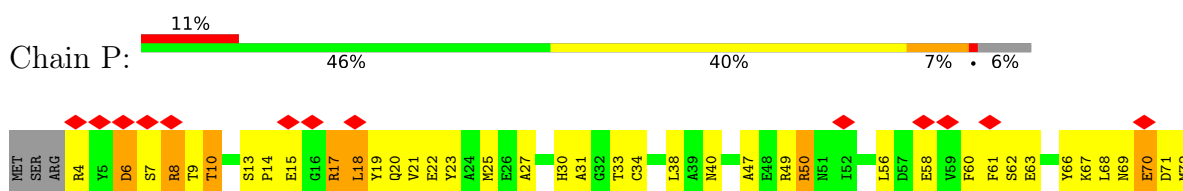
- Molecule 1: Proteasome subunit alpha type-2

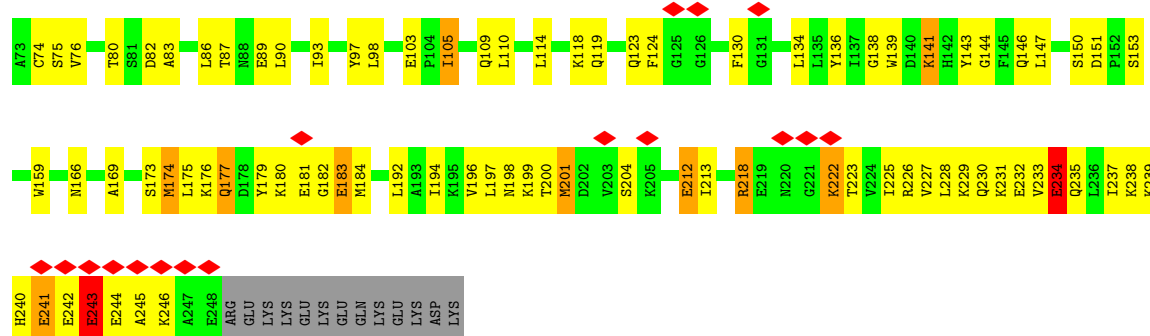


- Molecule 1: Proteasome subunit alpha type-2

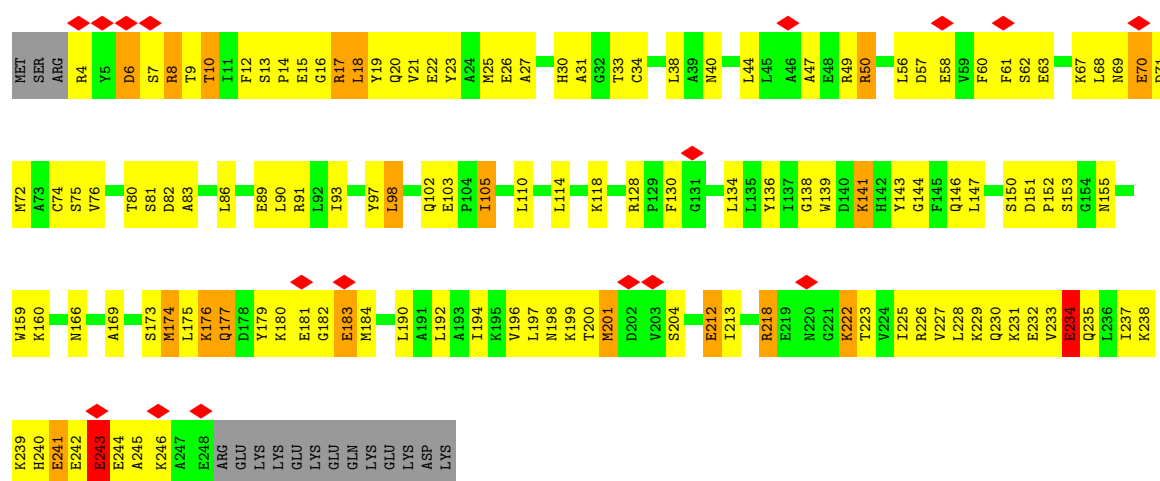
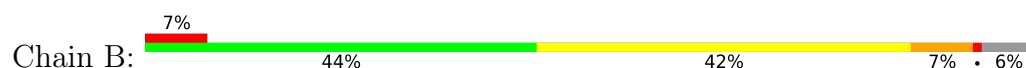


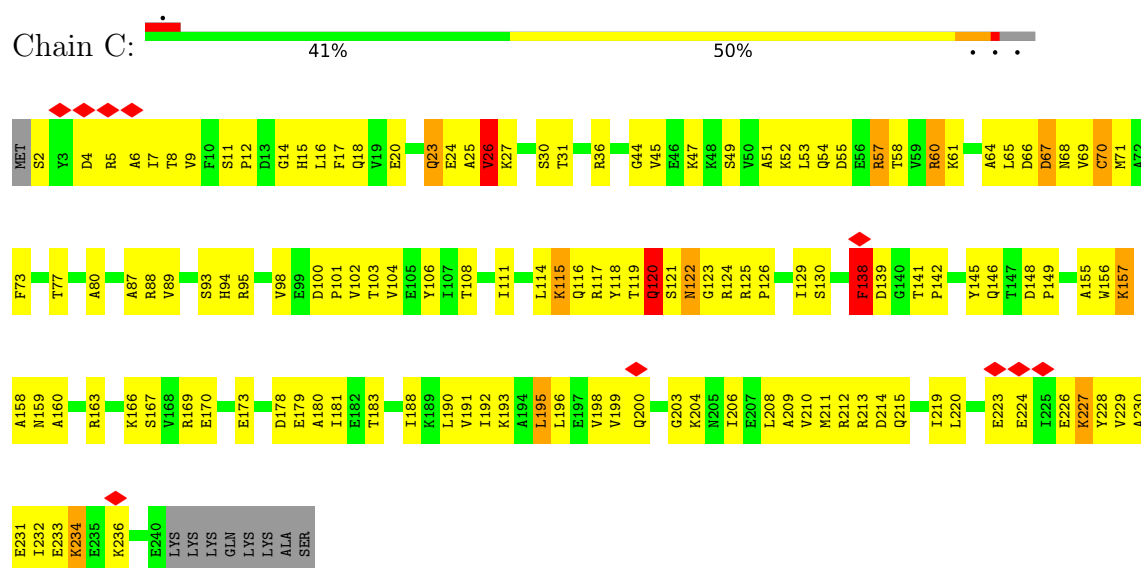
- Molecule 2: Proteasome subunit alpha type-4





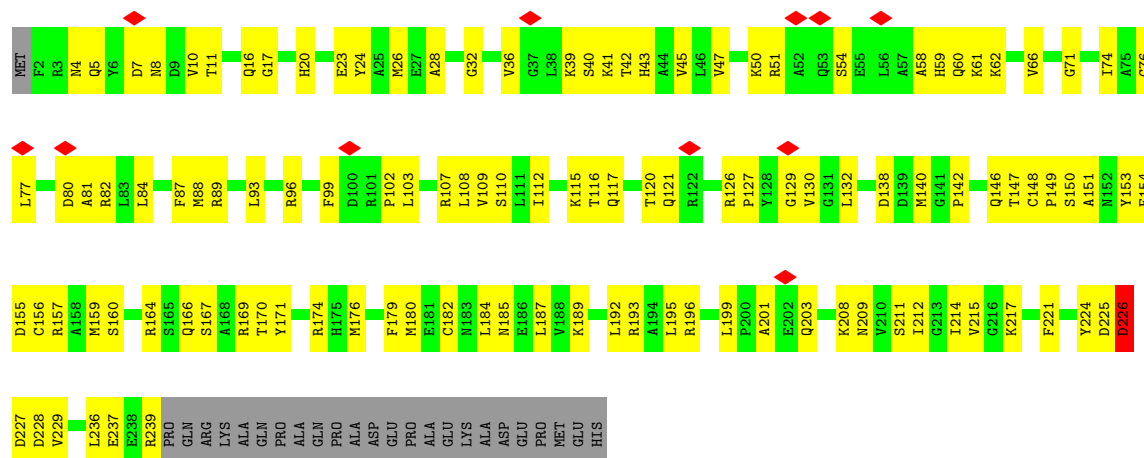
• Molecule 2: Proteasome subunit alpha type-4



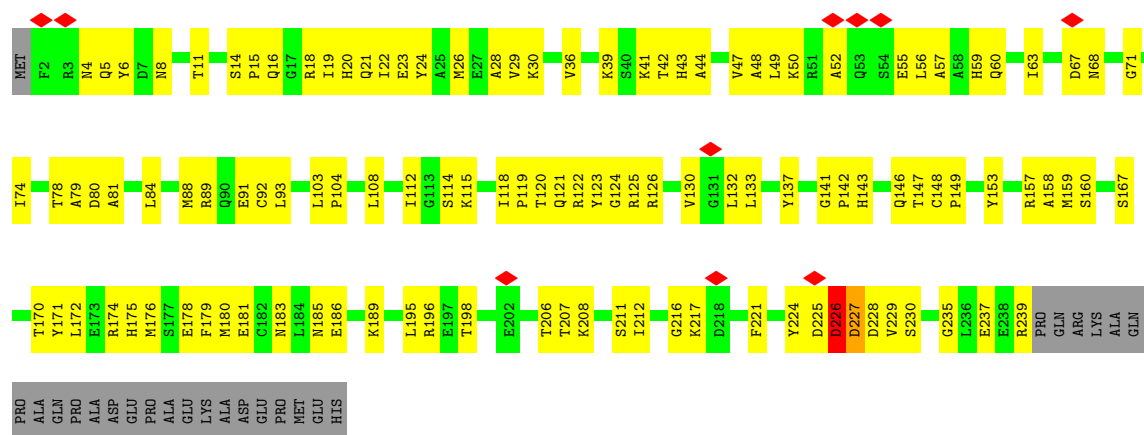




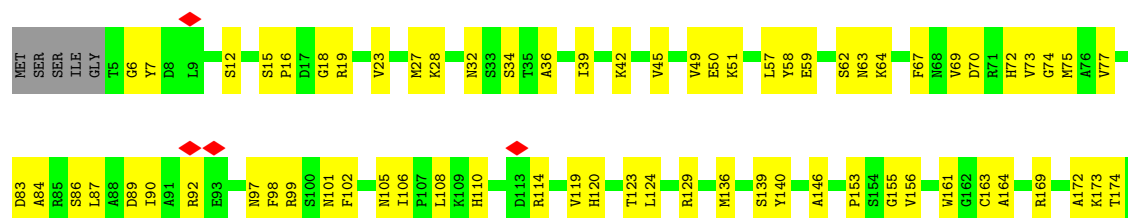
• Molecule 5: Proteasome subunit alpha type-1

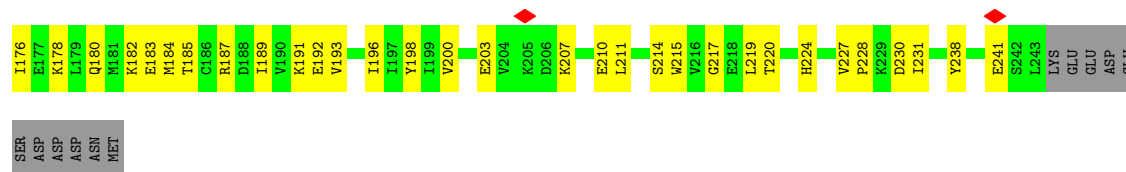


• Molecule 5: Proteasome subunit alpha type-1



• Molecule 6: Proteasome subunit alpha type-3

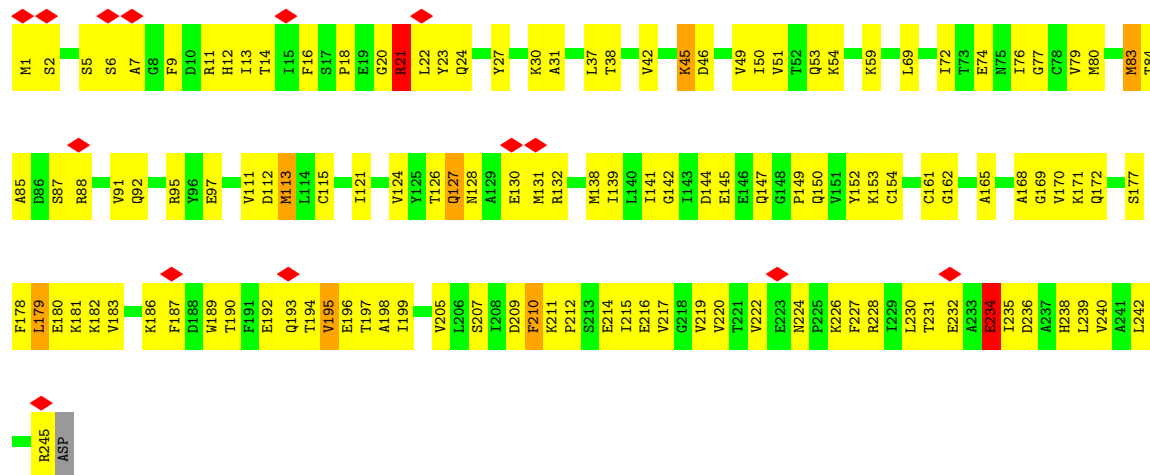




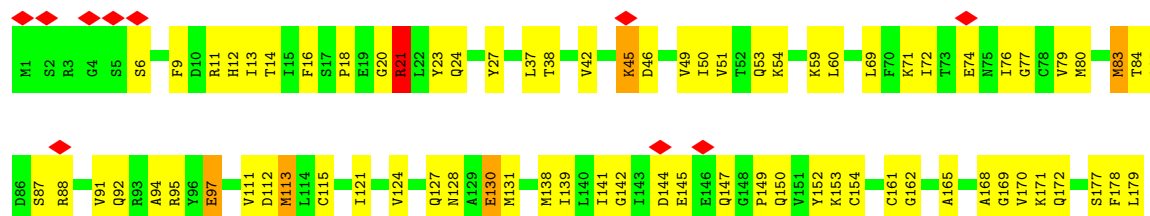
• Molecule 6: Proteasome subunit alpha type-3

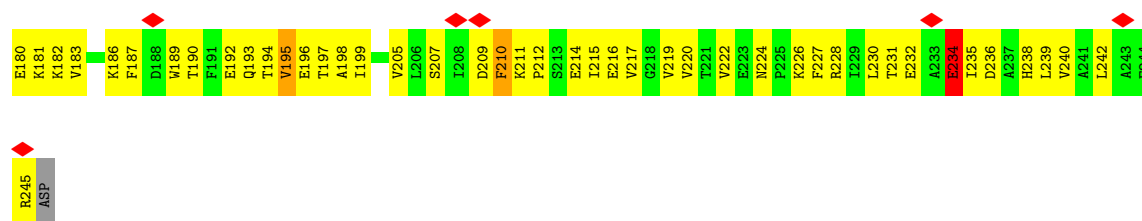


• Molecule 7: Proteasome subunit alpha type-6

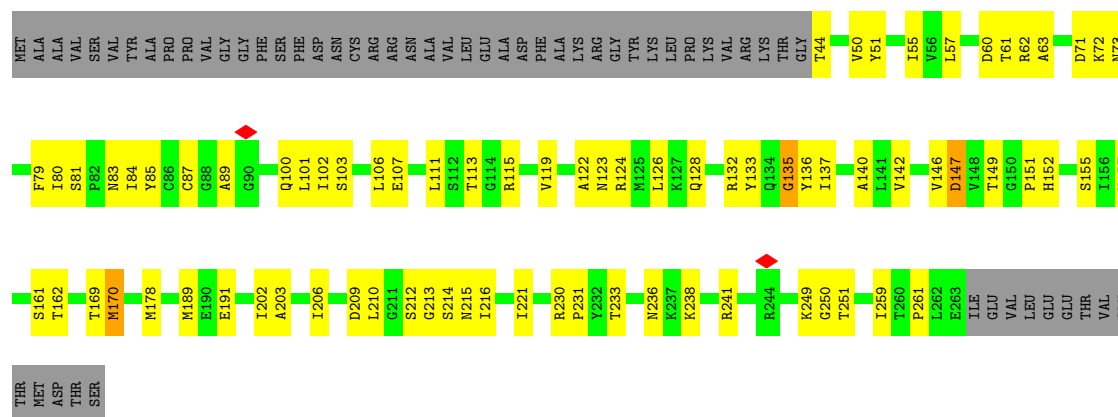


• Molecule 7: Proteasome subunit alpha type-6

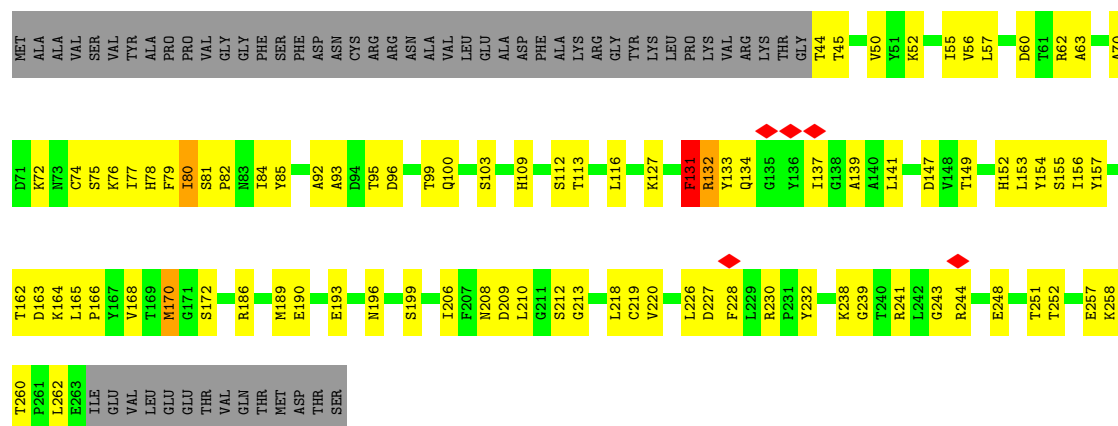




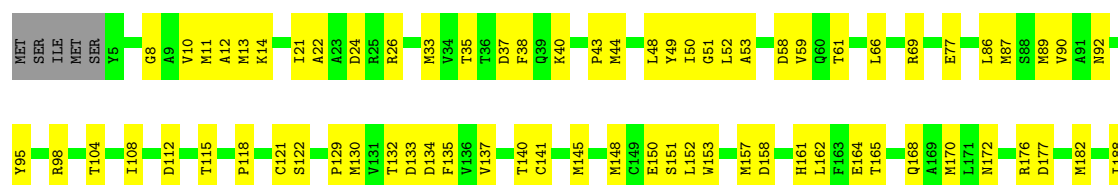
• Molecule 8: Proteasome subunit beta type-7

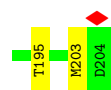


• Molecule 8: Proteasome subunit beta type-7

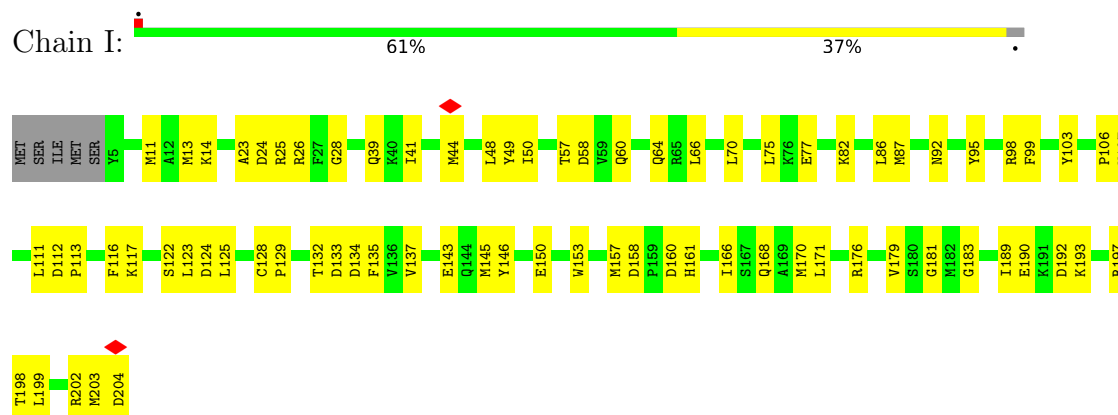


• Molecule 9: Proteasome subunit beta type-3





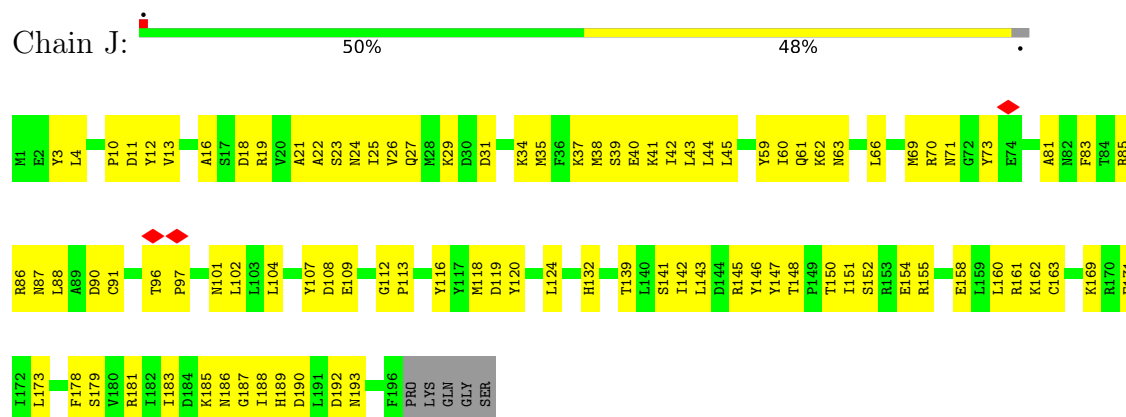
• Molecule 9: Proteasome subunit beta type-3



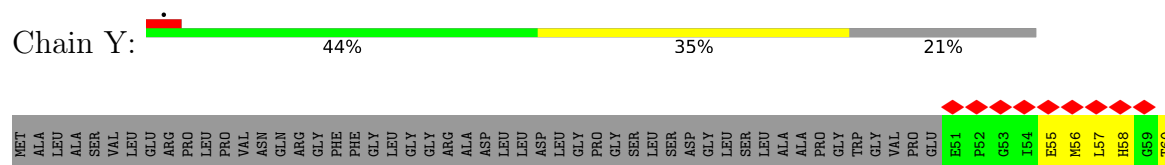
• Molecule 10: Proteasome subunit beta type-2

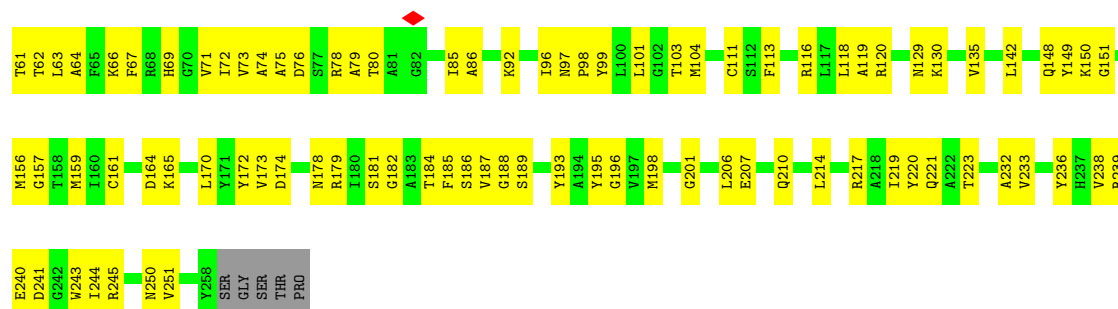


• Molecule 10: Proteasome subunit beta type-2



• Molecule 11: Proteasome subunit beta type-5

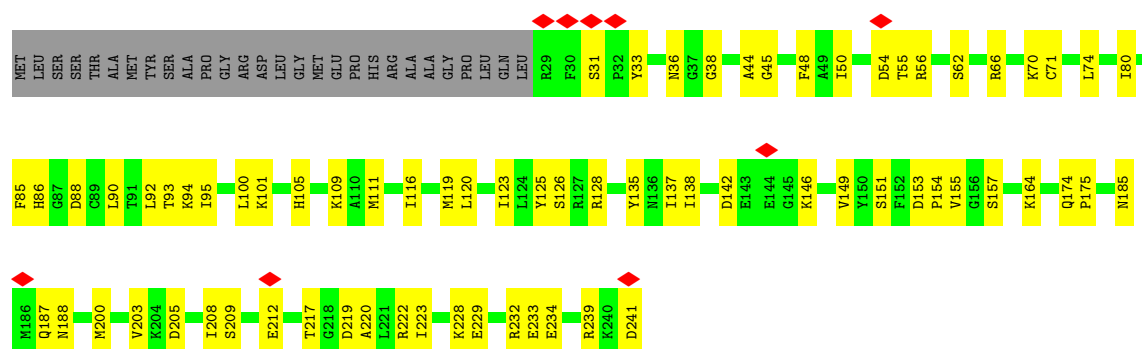




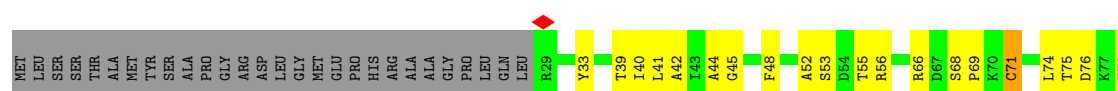
• Molecule 11: Proteasome subunit beta type-5

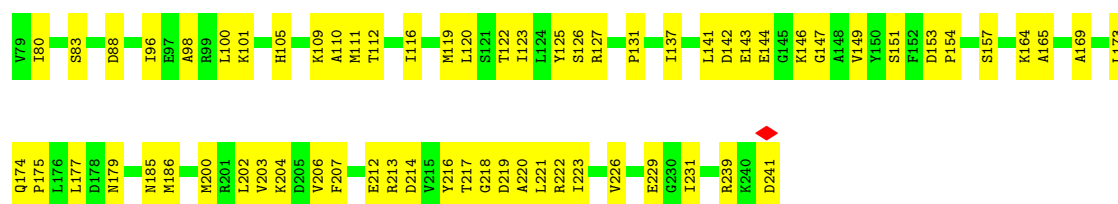


• Molecule 12: Proteasome subunit beta type-1

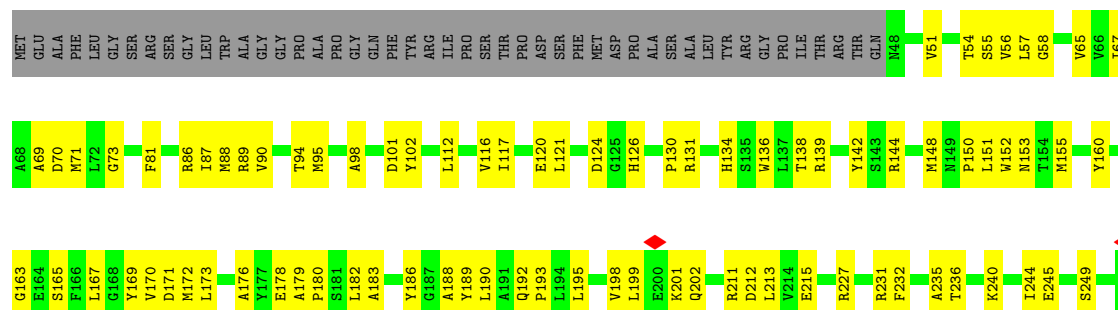


• Molecule 12: Proteasome subunit beta type-1

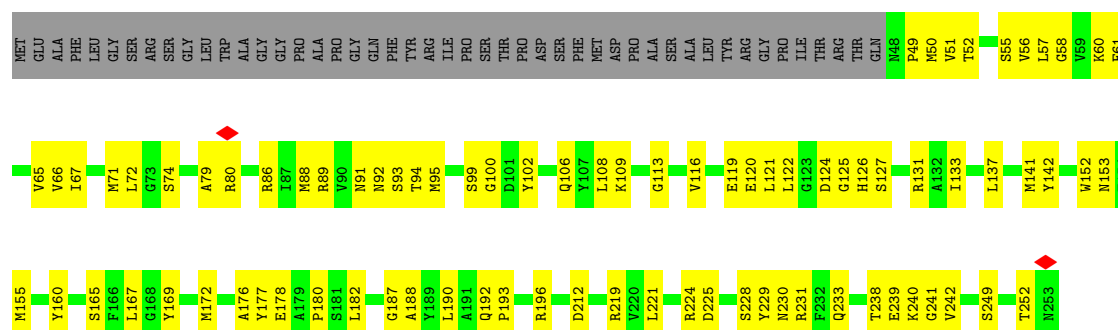




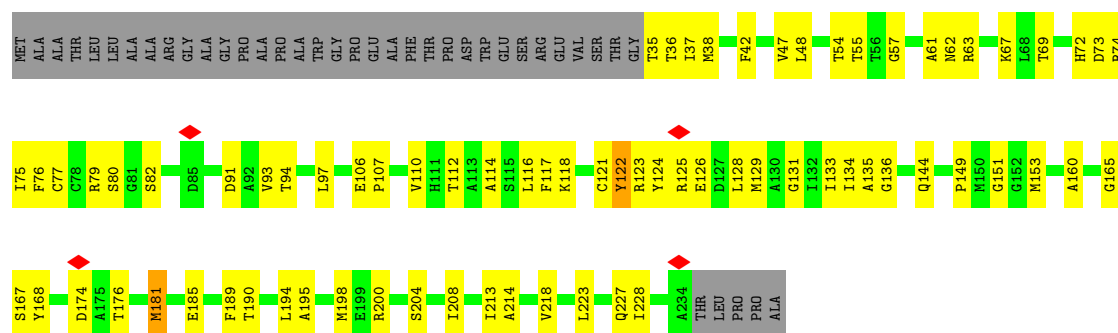
• Molecule 13: Proteasome subunit beta type-4



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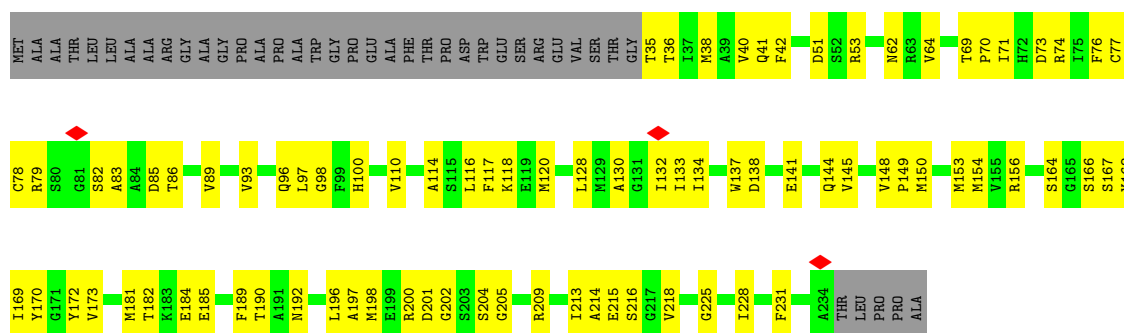


• Molecule 14: Proteasome subunit beta type-6



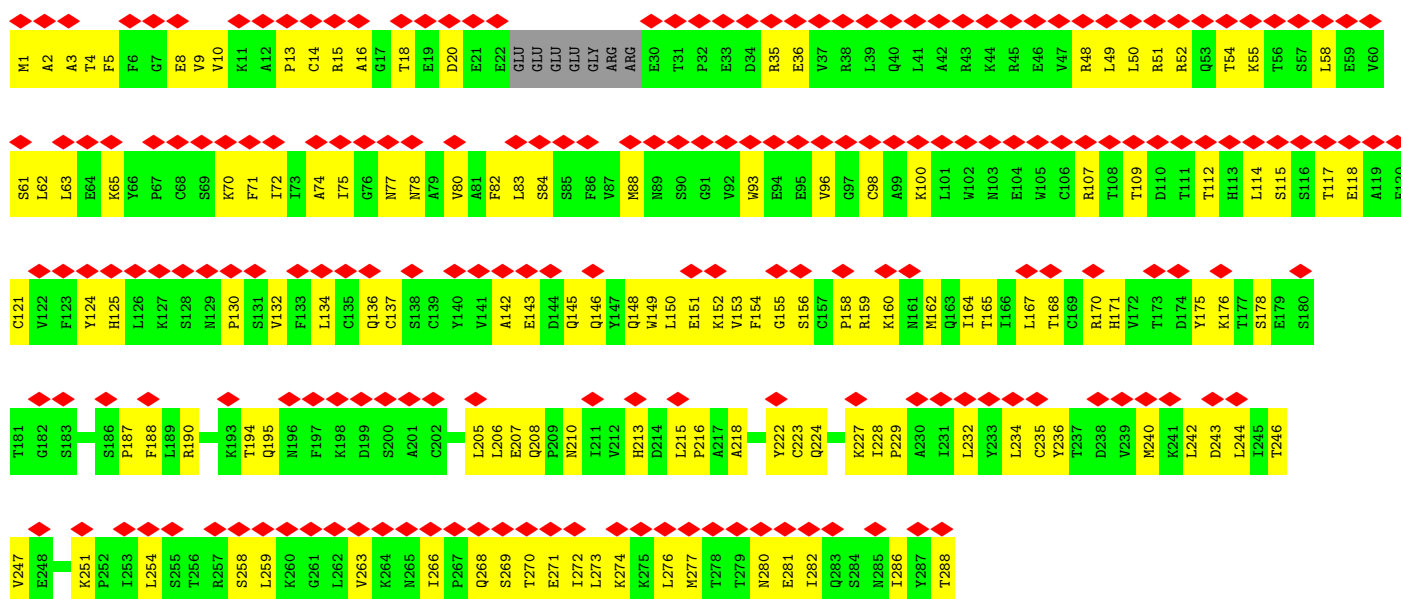
• Molecule 14: Proteasome subunit beta type-6

Chain N: 

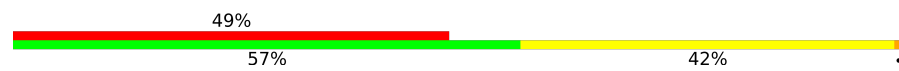


• Molecule 15: Proteasome assembly chaperone 1

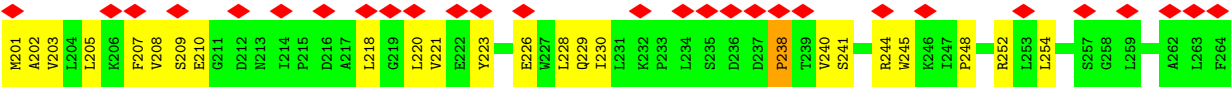
Chain f: 



• Molecule 16: Proteasome assembly chaperone 2

Chain g: 





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	4605	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI 12	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49.41	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.243	Depositor
Minimum map value	-0.612	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.074	Depositor
Recommended contour level	0.328	Depositor
Map size (Å)	316.49997, 316.49997, 316.49997	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.055, 1.055, 1.055	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.31	0/1799	0.66	3/2442 (0.1%)
1	O	0.31	0/1799	0.66	3/2442 (0.1%)
2	B	0.34	0/1924	0.76	7/2602 (0.3%)
2	P	0.34	0/1924	0.76	7/2602 (0.3%)
3	C	0.35	0/1875	0.76	3/2540 (0.1%)
3	Q	0.35	0/1875	0.76	3/2540 (0.1%)
4	D	0.31	0/1869	0.67	2/2523 (0.1%)
4	R	0.31	0/1869	0.68	2/2523 (0.1%)
5	E	0.28	0/1896	0.49	0/2563
5	S	0.28	0/1896	0.50	0/2563
6	F	0.24	0/1896	0.41	0/2556
6	T	0.27	0/1896	0.54	0/2556
7	G	0.28	0/1927	0.64	5/2606 (0.2%)
7	U	0.28	0/1927	0.64	5/2606 (0.2%)
8	H	0.30	0/1688	0.63	2/2288 (0.1%)
8	V	0.28	0/1688	0.51	0/2288
9	I	0.30	0/1608	0.52	0/2168
9	W	0.29	0/1608	0.46	0/2168
10	J	0.31	0/1620	0.46	0/2191
10	X	0.31	0/1620	0.48	0/2191
11	K	0.32	0/1673	0.51	0/2258
11	Y	0.32	0/1673	0.50	0/2258
12	L	0.29	0/1677	0.48	0/2260
12	Z	0.28	0/1677	0.45	0/2260
13	M	0.28	0/1638	0.47	0/2216
13	a	0.31	0/1638	0.53	0/2216
14	N	0.31	0/1533	0.56	0/2074
14	b	0.30	0/1533	0.51	1/2074 (0.0%)
15	f	0.20	0/2285	0.55	0/3097
16	g	0.20	0/2108	0.51	1/2858 (0.0%)
All	All	0.30	0/53639	0.58	44/72529 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected

by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	O	0	1
2	B	0	1
2	P	0	1
3	C	0	3
3	Q	0	3
4	D	0	3
4	R	0	3
5	E	0	1
5	S	0	1
6	F	0	1
8	H	0	1
8	V	0	1
10	X	0	1
11	K	0	1
All	All	0	23

There are no bond length outliers.

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	U	21	ARG	CG-CD-NE	8.91	131.61	112.00
7	G	21	ARG	CG-CD-NE	8.89	131.56	112.00
2	P	234	GLU	CA-CB-CG	8.63	131.37	114.10
2	B	234	GLU	CA-CB-CG	8.63	131.35	114.10
2	P	243	GLU	CA-C-N	-8.15	105.69	121.58
2	P	243	GLU	C-N-CA	-8.15	105.69	121.58
2	B	243	GLU	CA-C-N	-8.14	105.71	121.58
2	B	243	GLU	C-N-CA	-8.14	105.71	121.58
3	Q	120	GLN	CA-CB-CG	7.04	128.18	114.10
3	C	120	GLN	CA-CB-CG	7.04	128.17	114.10
7	G	210	PHE	CA-C-N	-6.69	98.93	122.15
7	G	210	PHE	C-N-CA	-6.69	98.93	122.15
7	U	210	PHE	CA-C-N	-6.69	98.95	122.15
7	U	210	PHE	C-N-CA	-6.69	98.95	122.15
1	O	83	ARG	CG-CD-NE	6.45	126.18	112.00
1	A	83	ARG	CG-CD-NE	6.41	126.11	112.00
1	A	214	GLU	CA-CB-CG	6.37	126.84	114.10
1	O	214	GLU	CA-CB-CG	6.36	126.81	114.10
2	B	17	ARG	NE-CZ-NH1	-6.15	115.35	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	17	ARG	NE-CZ-NH1	-6.12	115.39	121.50
4	D	168	ARG	CB-CG-CD	5.98	125.06	111.30
4	R	168	ARG	CB-CG-CD	5.97	125.04	111.30
3	Q	138	PHE	N-CA-CB	-5.71	100.83	110.49
3	C	138	PHE	N-CA-CB	-5.68	100.89	110.49
8	H	79	PHE	CA-C-N	5.64	132.12	121.97
8	H	79	PHE	C-N-CA	5.64	132.12	121.97
7	U	21	ARG	CB-CG-CD	5.53	124.03	111.30
7	G	21	ARG	CB-CG-CD	5.53	124.02	111.30
2	P	234	GLU	N-CA-CB	5.39	118.64	110.28
2	B	234	GLU	N-CA-CB	5.39	118.63	110.28
7	G	234	GLU	CA-CB-CG	5.37	124.85	114.10
16	g	167	ARG	CA-CB-CG	5.37	124.84	114.10
7	U	234	GLU	CA-CB-CG	5.35	124.81	114.10
2	B	243	GLU	CA-CB-CG	5.25	124.60	114.10
2	P	243	GLU	CA-CB-CG	5.25	124.59	114.10
1	O	59	ARG	N-CA-CB	-5.14	102.73	111.27
14	b	122	TYR	N-CA-C	-5.14	107.30	113.21
4	D	192	LYS	CB-CG-CD	-5.13	99.50	111.30
4	R	192	LYS	CB-CG-CD	-5.12	99.52	111.30
1	A	59	ARG	N-CA-CB	-5.09	102.83	111.27
2	B	17	ARG	NE-CZ-NH2	5.04	123.73	119.20
3	Q	138	PHE	CB-CA-C	5.03	120.43	110.42
2	P	17	ARG	NE-CZ-NH2	5.02	123.72	119.20
3	C	138	PHE	CB-CA-C	5.02	120.42	110.42

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	58	GLU	Peptide
2	B	212	GLU	Peptide
3	C	120	GLN	Peptide
3	C	122	ASN	Peptide
3	C	26	VAL	Peptide
4	D	132	ALA	Peptide
4	D	148	GLU	Peptide
4	D	29	GLU	Peptide
5	E	226	ASP	Peptide
6	F	22	GLN	Peptide
8	H	131	PHE	Peptide
11	K	57	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	O	58	GLU	Peptide
2	P	212	GLU	Peptide
3	Q	120	GLN	Peptide
3	Q	122	ASN	Peptide
3	Q	26	VAL	Peptide
4	R	132	ALA	Peptide
4	R	148	GLU	Peptide
4	R	29	GLU	Peptide
5	S	226	ASP	Peptide
8	V	135	GLY	Peptide
10	X	97	PRO	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1760	0	1723	97	0
1	O	1760	0	1723	93	0
2	B	1894	0	1863	128	0
2	P	1894	0	1863	120	0
3	C	1849	0	1819	145	0
3	Q	1849	0	1819	150	0
4	D	1840	0	1828	131	0
4	R	1840	0	1828	133	0
5	E	1859	0	1842	103	0
5	S	1859	0	1842	114	0
6	F	1858	0	1834	85	0
6	T	1858	0	1834	93	0
7	G	1893	0	1893	105	0
7	U	1893	0	1893	117	0
8	H	1655	0	1658	77	0
8	V	1655	0	1658	74	0
9	I	1576	0	1593	68	0
9	W	1576	0	1593	60	0
10	J	1581	0	1585	81	0
10	X	1581	0	1585	70	0
11	K	1631	0	1599	74	0
11	Y	1631	0	1599	86	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	L	1644	0	1641	73	0
12	Z	1644	0	1641	62	0
13	M	1605	0	1586	67	0
13	a	1605	0	1586	70	0
14	N	1504	0	1475	75	0
14	b	1504	0	1475	54	0
15	f	2239	0	2256	163	0
16	g	2062	0	2092	111	0
All	All	52599	0	52226	2546	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 24.

All (2546) 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)
4:R:4:THR:HB	15:f:15:ARG:HG3	1.37	1.05
4:R:167:ALA:HB1	4:R:181:LEU:HD21	1.45	0.98
4:D:167:ALA:HB1	4:D:181:LEU:HD21	1.45	0.97
3:C:120:GLN:HB3	4:D:133:MET:HA	1.44	0.97
7:U:189:TRP:HB3	7:U:194:THR:HG23	1.48	0.96
7:G:189:TRP:HB3	7:G:194:THR:HG23	1.48	0.96
2:B:34:CYS:HG	2:B:75:SER:HG	1.14	0.96
14:N:79:ARG:HB2	14:N:86:THR:HB	1.48	0.95
5:S:41:LYS:HG2	5:S:180:MET:HE3	1.48	0.94
2:P:50:ARG:HH11	2:P:50:ARG:HG3	1.32	0.94
3:C:5:ARG:HH11	4:D:10:ARG:HB3	1.30	0.94
2:B:50:ARG:HH11	2:B:50:ARG:HG3	1.32	0.93
1:O:214:GLU:OE1	1:O:214:GLU:N	2.03	0.90
1:A:214:GLU:OE1	1:A:214:GLU:N	2.03	0.90
10:J:19:ARG:NH1	10:J:31:ASP:OD1	2.05	0.90
1:A:106:THR:HG21	1:A:137:GLY:HA3	1.55	0.89
3:Q:5:ARG:HG2	15:f:1:MET:HA	1.53	0.89
15:f:121:CYS:H	15:f:137:CYS:HB3	1.38	0.89
14:N:93:VAL:HG21	14:N:117:PHE:HD1	1.34	0.89
4:R:5:ARG:H	15:f:15:ARG:HA	1.36	0.88
2:P:34:CYS:HG	2:P:75:SER:HG	1.20	0.88
9:W:157:MET:HE3	9:W:162:LEU:HA	1.56	0.88
7:G:21:ARG:HH11	7:G:21:ARG:HB2	1.37	0.87
3:Q:92:GLN:NE2	10:X:65:GLN:OE1	2.07	0.87
1:O:106:THR:HG21	1:O:137:GLY:HA3	1.55	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:9:ASP:HB3	4:R:22:PHE:HD2	1.40	0.87
4:D:9:ASP:HB3	4:D:22:PHE:HD2	1.40	0.86
7:U:21:ARG:HB2	7:U:21:ARG:HH11	1.37	0.86
13:a:150:PRO:HG2	13:a:152:TRP:HE1	1.42	0.85
1:O:83:ARG:HB3	1:O:83:ARG:HH21	1.41	0.85
9:I:13:MET:HG2	9:I:135:PHE:HB3	1.58	0.84
1:A:83:ARG:HB3	1:A:83:ARG:HH21	1.41	0.84
3:C:120:GLN:OE1	3:C:120:GLN:N	2.09	0.84
3:Q:120:GLN:OE1	3:Q:120:GLN:N	2.09	0.84
2:P:49:ARG:HG3	2:P:212:GLU:OE2	1.78	0.83
8:H:127:LYS:NZ	8:H:162:THR:OG1	2.09	0.83
3:Q:5:ARG:NE	15:f:2:ALA:O	2.10	0.83
8:V:44:THR:N	8:V:212:SER:HG	1.75	0.83
15:f:213:HIS:CD2	16:g:55:MET:HB3	2.14	0.83
14:b:149:PRO:HG2	14:b:153:MET:HE3	1.58	0.83
9:W:188:ILE:HB	9:W:195:THR:HB	1.60	0.82
6:F:9:LEU:HD23	7:G:11:ARG:HH22	1.44	0.82
3:Q:120:GLN:HB3	4:R:133:MET:HA	1.61	0.82
5:S:26:MET:HE1	5:S:148:CYS:HB3	1.60	0.82
2:B:234:GLU:OE1	2:B:234:GLU:N	2.13	0.82
2:B:49:ARG:HG3	2:B:212:GLU:OE2	1.78	0.82
2:P:234:GLU:OE1	2:P:234:GLU:N	2.13	0.82
15:f:115:SER:HB3	15:f:118:GLU:HB2	1.59	0.82
3:C:9:VAL:HG13	4:D:23:GLN:HE22	1.43	0.81
2:B:103:GLU:OE1	2:B:141:LYS:NZ	2.13	0.81
5:E:6:TYR:CD2	5:E:15:PRO:HD3	2.16	0.81
7:U:178:PHE:HA	7:U:181:LYS:HE2	1.63	0.81
1:O:10:THR:HG21	15:f:5:PHE:HZ	1.46	0.81
8:V:238:LYS:NZ	9:W:150:GLU:OE1	2.13	0.81
7:G:178:PHE:HA	7:G:181:LYS:HE2	1.63	0.81
2:P:103:GLU:OE1	2:P:141:LYS:NZ	2.13	0.80
7:U:21:ARG:HD2	7:U:23:TYR:HE1	1.46	0.80
12:Z:209:SER:HB3	9:I:150:GLU:HG3	1.64	0.80
1:O:158:LYS:NZ	2:P:56:LEU:O	2.14	0.80
16:g:179:ILE:HG23	16:g:188:LYS:HE2	1.64	0.80
7:G:21:ARG:HD2	7:G:23:TYR:HE1	1.46	0.80
5:S:51:ARG:H	5:S:60:GLN:HE22	1.29	0.79
4:R:5:ARG:N	15:f:15:ARG:HA	1.96	0.79
4:R:9:ASP:OD1	4:R:10:ARG:NH2	2.16	0.79
4:D:9:ASP:OD1	4:D:10:ARG:NH2	2.16	0.79
5:E:146:GLN:NE2	5:E:148:CYS:SG	2.56	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:66:LYS:NZ	11:Y:182:GLY:O	2.15	0.79
3:C:12:PRO:HA	4:D:26:TYR:CE2	2.17	0.78
5:S:226:ASP:O	5:S:228:ASP:N	2.17	0.78
3:C:20:GLU:HA	3:C:23:GLN:HB2	1.66	0.78
7:G:212:PRO:HD3	7:G:239:LEU:HD21	1.66	0.78
11:K:78:ARG:HE	11:K:230:GLY:HA3	1.46	0.78
8:V:124:ARG:HG3	8:V:128:GLN:HE22	1.49	0.77
1:O:127:ARG:NE	7:U:126:THR:O	2.17	0.77
12:L:40:ILE:HD12	12:L:137:ILE:HG12	1.66	0.77
7:U:5:SER:N	15:f:8:GLU:O	2.16	0.77
15:f:254:LEU:HA	15:f:259:LEU:HD22	1.65	0.77
7:G:113:MET:SD	8:H:113:THR:HA	2.24	0.77
1:O:70:HIS:HA	1:O:217:PHE:H	1.50	0.77
3:Q:229:VAL:HA	3:Q:232:ILE:HB	1.67	0.77
13:a:153:ASN:HB3	13:a:155:MET:HE3	1.63	0.77
7:G:189:TRP:HD1	7:G:194:THR:HA	1.50	0.77
12:Z:200:MET:HE1	12:Z:223:ILE:HG21	1.66	0.77
7:G:50:ILE:HD12	7:G:79:VAL:HB	1.66	0.77
1:O:101:GLN:OE1	8:V:100:GLN:NE2	2.18	0.77
7:U:50:ILE:HD12	7:U:79:VAL:HB	1.66	0.77
7:U:69:LEU:HD12	7:U:216:GLU:HG2	1.67	0.77
15:f:277:MET:HA	15:f:280:ASN:HB3	1.65	0.76
3:Q:20:GLU:HA	3:Q:23:GLN:HB2	1.66	0.76
7:U:212:PRO:HD3	7:U:239:LEU:HD21	1.66	0.76
1:A:70:HIS:HA	1:A:217:PHE:H	1.50	0.76
7:G:69:LEU:HD12	7:G:216:GLU:HG2	1.67	0.76
8:H:131:PHE:O	8:H:133:TYR:N	2.19	0.76
2:B:4:ARG:NE	3:C:2:SER:O	2.17	0.76
3:C:119:THR:O	4:D:135:ARG:NH1	2.18	0.76
5:E:6:TYR:HD2	5:E:15:PRO:HD3	1.50	0.76
8:V:84:ILE:HD13	8:V:119:VAL:HG22	1.67	0.75
1:O:83:ARG:HB3	1:O:83:ARG:NH2	2.01	0.75
8:H:57:LEU:HB2	8:H:219:CYS:HB3	1.66	0.75
10:J:183:ILE:HG12	10:J:188:ILE:HG22	1.68	0.75
14:b:37:ILE:HD12	14:b:133:ILE:HG12	1.69	0.75
6:T:34:SER:OG	6:T:50:GLU:OE2	2.03	0.75
12:L:53:SER:HG	12:L:71[A]:CYS:HG	1.30	0.75
1:A:106:THR:H	1:A:139:ASN:HD21	1.35	0.75
1:A:83:ARG:HB3	1:A:83:ARG:NH2	2.01	0.75
10:J:41:LYS:NZ	10:J:185:LYS:O	2.19	0.75
3:Q:5:ARG:NE	15:f:2:ALA:H	1.85	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:144:GLN:OE1	14:N:156:ARG:NH2	2.15	0.74
12:L:41:LEU:HB3	12:L:52:ALA:HB3	1.69	0.74
7:U:189:TRP:HD1	7:U:194:THR:HA	1.50	0.74
11:Y:80:THR:HG22	11:Y:85:ILE:HG22	1.67	0.74
12:Z:187:GLN:NE2	12:Z:188:ASN:OD1	2.21	0.74
13:a:131:ARG:NH1	13:a:178:GLU:OE2	2.20	0.74
6:F:156:VAL:HG22	7:G:84:THR:HB	1.70	0.74
9:W:35:THR:HG22	9:W:37:ASP:H	1.53	0.74
2:P:6:ASP:OD1	2:P:6:ASP:N	2.21	0.74
10:X:18:ASP:O	10:X:34:LYS:NZ	2.20	0.74
5:E:67:ASP:OD1	5:E:68:ASN:N	2.20	0.74
3:Q:3:TYR:CD2	15:f:1:MET:HE3	2.23	0.74
1:A:16:GLY:HA3	2:B:26:GLU:HB2	1.69	0.74
6:F:80:LEU:HG	6:F:83:ASP:H	1.53	0.74
8:H:141:LEU:HB2	8:H:156:ILE:HB	1.68	0.74
3:C:229:VAL:HA	3:C:232:ILE:HB	1.67	0.74
12:L:88:ASP:OD1	13:M:142:TYR:OH	2.04	0.74
2:P:8:ARG:HH11	15:f:8:GLU:HG2	1.52	0.73
11:Y:219:ILE:HG21	11:Y:233:VAL:HG21	1.69	0.73
10:J:85:ARG:HA	10:J:118:MET:HE1	1.69	0.73
1:O:106:THR:H	1:O:139:ASN:HD21	1.35	0.73
7:U:23:TYR:OH	16:g:131:ASP:OD1	2.06	0.73
5:E:26:MET:HE1	5:E:148:CYS:HB3	1.70	0.73
7:G:194:THR:HG22	7:G:195:VAL:H	1.53	0.73
4:D:101:PHE:CE1	11:K:120:ARG:HD2	2.24	0.73
6:F:229:LYS:HE3	6:F:232:ARG:HH21	1.53	0.73
14:N:132:ILE:HG23	14:N:148:VAL:O	1.87	0.73
13:M:60:LYS:HA	13:M:65:VAL:HG22	1.69	0.73
9:W:26:ARG:HH12	11:K:227:ALA:HB2	1.54	0.73
5:E:226:ASP:O	5:E:228:ASP:N	2.22	0.73
5:S:146:GLN:NE2	5:S:148:CYS:SG	2.61	0.73
10:J:44:LEU:HD11	10:J:102:LEU:HD12	1.70	0.73
7:U:194:THR:HG22	7:U:195:VAL:H	1.53	0.72
2:B:136:TYR:HE1	2:B:150:SER:HB2	1.54	0.72
6:F:69:VAL:HG23	6:F:73:VAL:HG13	1.69	0.72
4:D:71:ASP:OD1	4:D:72:ALA:N	2.21	0.72
4:R:71:ASP:OD1	4:R:72:ALA:N	2.21	0.72
10:X:181:ARG:HG3	10:X:190:ASP:HA	1.72	0.72
3:C:14:GLY:HA3	4:D:30:ALA:HB2	1.70	0.72
1:O:165:ASN:OD1	1:O:168:ASN:ND2	2.23	0.72
6:F:191:LYS:NZ	6:F:234:GLU:OE1	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:66:ASP:HA	10:X:69:MET:HE3	1.70	0.72
6:T:98:PHE:CD2	6:T:106:ILE:HG13	2.24	0.72
8:V:73:ASN:OD1	8:V:230:ARG:NH2	2.22	0.72
1:A:165:ASN:OD1	1:A:168:ASN:ND2	2.23	0.72
2:B:6:ASP:N	2:B:6:ASP:OD1	2.21	0.72
15:f:51:ARG:HG3	15:f:54:THR:HB	1.72	0.72
3:C:36:ARG:HG3	3:C:142:PRO:HB2	1.72	0.72
2:P:136:TYR:HE1	2:P:150:SER:HB2	1.54	0.71
6:F:175:GLU:HB3	6:F:196:ILE:HD12	1.69	0.71
6:T:70:ASP:OD1	6:T:73:VAL:N	2.20	0.71
4:D:5:ARG:HD2	5:E:5:GLN:OE1	1.91	0.71
6:F:93:GLU:O	6:F:97:ASN:ND2	2.22	0.71
5:S:132:LEU:HB2	5:S:147:THR:HB	1.72	0.71
6:T:51:LYS:NZ	6:T:63:ASN:O	2.22	0.71
12:L:74:LEU:HD11	12:L:80:ILE:HB	1.72	0.71
3:Q:5:ARG:HH22	15:f:10:VAL:HG13	1.54	0.71
6:T:64:LYS:HG3	6:T:67:PHE:HE1	1.55	0.71
15:f:52:ARG:NH2	15:f:98:CYS:SG	2.63	0.71
3:C:117:ARG:HA	3:C:120:GLN:HE22	1.55	0.71
13:a:244:ILE:H	13:a:244:ILE:HD12	1.54	0.71
5:E:50:LYS:HB3	5:E:59:HIS:HB2	1.73	0.71
3:C:233:GLU:HA	3:C:236:LYS:HG2	1.73	0.71
4:D:9:ASP:HB3	4:D:22:PHE:CD2	2.25	0.71
8:H:206:ILE:HG12	8:H:213:GLY:HA2	1.73	0.71
2:P:90:LEU:HD21	2:P:114:LEU:HB2	1.73	0.71
13:M:72:LEU:HD12	13:M:229:TYR:HB2	1.73	0.71
15:f:61:SER:O	15:f:65:LYS:N	2.23	0.70
4:R:29:GLU:O	15:f:107:ARG:NH2	2.18	0.70
8:V:215:ASN:HD21	8:V:231:PRO:HB3	1.55	0.70
14:b:114:ALA:HA	14:b:134:ILE:HD11	1.70	0.70
15:f:195:GLN:NE2	16:g:70:GLU:OE1	2.24	0.70
3:Q:117:ARG:HA	3:Q:120:GLN:HE22	1.54	0.70
2:B:160:LYS:NZ	3:C:54:GLN:O	2.24	0.70
3:C:9:VAL:HG13	4:D:23:GLN:NE2	2.04	0.70
6:F:35:THR:HA	6:F:166:GLY:HA3	1.72	0.70
10:X:39:SER:OG	10:X:40:GLU:OE1	2.10	0.70
16:g:142:LEU:HD21	16:g:163:MET:HE2	1.74	0.70
3:C:209:ALA:HA	3:C:220:LEU:HD23	1.73	0.70
3:Q:209:ALA:HA	3:Q:220:LEU:HD23	1.73	0.70
3:Q:226:GLU:HB3	3:Q:229:VAL:HG22	1.74	0.70
15:f:286:ILE:HG23	15:f:288:THR:H	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:36:ARG:HG3	3:Q:142:PRO:HB2	1.72	0.70
7:U:80:MET:HG3	7:U:87:SER:HB2	1.74	0.70
8:V:81:SER:HB3	8:V:84:ILE:HG22	1.73	0.70
13:M:131:ARG:NH1	13:M:178:GLU:OE2	2.24	0.70
14:N:198:MET:HE2	14:N:198:MET:HA	1.74	0.70
2:P:13:SER:OG	2:P:17:ARG:NH1	2.25	0.70
4:R:147:ASP:O	4:R:150:GLY:N	2.25	0.70
5:S:50:LYS:NZ	5:S:60:GLN:O	2.21	0.70
6:T:69:VAL:HG13	6:T:73:VAL:HG23	1.73	0.70
3:C:66:ASP:HA	10:J:69:MET:HE3	1.74	0.70
2:B:50:ARG:HG3	2:B:50:ARG:NH1	2.05	0.69
4:R:10:ARG:NH1	15:f:1:MET:SD	2.65	0.69
14:N:97:LEU:HA	14:N:100:HIS:HB3	1.74	0.69
14:b:97:LEU:HD21	14:b:116:LEU:HD13	1.75	0.69
2:B:13:SER:OG	2:B:17:ARG:NH1	2.25	0.69
2:P:8:ARG:NE	15:f:8:GLU:OE2	2.25	0.69
3:Q:233:GLU:HA	3:Q:236:LYS:HG2	1.73	0.69
5:S:121:GLN:NE2	6:T:129:ARG:O	2.25	0.69
13:a:90:VAL:HG13	13:a:112:LEU:HD21	1.74	0.69
14:b:74:ARG:NH1	14:b:214:ALA:O	2.26	0.69
10:J:119:ASP:OD1	10:J:120:TYR:N	2.25	0.69
4:R:5:ARG:HG3	15:f:14:CYS:C	2.17	0.69
5:S:164:ARG:NH2	15:f:243:ASP:OD2	2.25	0.69
2:B:90:LEU:HD21	2:B:114:LEU:HB2	1.73	0.69
8:V:50:VAL:HG12	8:V:55:ILE:HG22	1.73	0.69
16:g:33:ASP:OD1	16:g:89:GLN:NE2	2.24	0.69
4:D:147:ASP:O	4:D:150:GLY:N	2.25	0.69
10:J:43:LEU:HB2	10:J:183:ILE:HD11	1.75	0.69
10:X:2:GLU:OE1	10:X:34:LYS:HE2	1.92	0.69
15:f:190:ARG:NH1	15:f:205:LEU:O	2.25	0.69
2:P:69:ASN:OD1	2:P:72:MET:N	2.18	0.69
14:b:38:MET:HE1	14:b:190:THR:HG23	1.74	0.69
1:A:108:GLN:NE2	9:I:77:GLU:HG3	2.08	0.69
13:M:137:LEU:HD21	13:M:155:MET:HE2	1.73	0.69
3:Q:45:VAL:HG11	3:Q:61:LYS:HB3	1.75	0.69
11:Y:62:THR:HG23	11:Y:75:ALA:HB2	1.74	0.69
12:L:39:THR:HG21	12:L:169:ALA:HB3	1.75	0.69
2:B:69:ASN:OD1	2:B:72:MET:N	2.18	0.68
3:C:226:GLU:HB3	3:C:229:VAL:HG22	1.74	0.68
12:Z:44:ALA:HB2	12:Z:149:VAL:HG23	1.74	0.68
12:L:123:ILE:O	12:L:126:SER:OG	2.10	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:42:VAL:HG12	7:G:165:ALA:HB1	1.75	0.68
7:G:194:THR:HG22	7:G:195:VAL:HG13	1.75	0.68
8:H:241:ARG:NH1	9:I:153:TRP:O	2.23	0.68
9:I:202:ARG:NH2	9:I:204:ASP:OD2	2.26	0.68
14:N:166:SER:HA	14:N:169:ILE:HG22	1.76	0.68
3:C:45:VAL:HG11	3:C:61:LYS:HB3	1.75	0.68
7:G:80:MET:HG3	7:G:87:SER:HB2	1.74	0.68
4:R:9:ASP:HB3	4:R:22:PHE:CD2	2.25	0.68
15:f:121:CYS:N	15:f:137:CYS:HB3	2.09	0.68
4:D:162:PHE:O	5:E:60:GLN:NE2	2.20	0.68
14:N:93:VAL:HG21	14:N:117:PHE:CD1	2.23	0.68
15:f:254:LEU:HD22	15:f:263:VAL:HG11	1.75	0.68
4:D:10:ARG:HB2	5:E:8:ASN:HD21	1.59	0.68
7:U:194:THR:HG22	7:U:195:VAL:HG13	1.75	0.68
2:B:8:ARG:NH2	3:C:4:ASP:OD2	2.27	0.68
2:P:8:ARG:NH2	3:Q:4:ASP:OD2	2.27	0.68
7:U:42:VAL:HG12	7:U:165:ALA:HB1	1.75	0.68
9:W:158:ASP:OD1	9:W:161:HIS:ND1	2.26	0.68
4:R:168:ARG:NH1	15:f:282:ILE:HG12	2.09	0.67
4:D:220:VAL:HG12	4:D:226:PHE:HA	1.76	0.67
10:X:169:LYS:O	10:J:27:GLN:NE2	2.27	0.67
8:H:95:THR:HG22	8:H:139:ALA:HB1	1.75	0.67
9:I:26:ARG:NE	9:I:179:VAL:O	2.23	0.67
2:P:124:PHE:HB3	3:Q:124:ARG:HA	1.76	0.67
3:Q:210:VAL:HG22	3:Q:220:LEU:HD21	1.76	0.67
4:R:220:VAL:HG12	4:R:226:PHE:HA	1.76	0.67
10:X:153:ARG:NH1	10:X:184:ASP:OD2	2.28	0.67
10:X:170:ARG:NH2	11:K:199:ASP:OD1	2.27	0.67
15:f:271:GLU:O	15:f:274:LYS:HG3	1.94	0.67
5:S:36:VAL:HB	5:S:47:VAL:HB	1.77	0.67
9:W:33:MET:O	11:K:225:ARG:NH1	2.26	0.67
4:D:99:HIS:ND1	4:D:107:MET:HG3	2.09	0.67
5:E:50:LYS:HE2	5:E:211:SER:HB3	1.76	0.67
7:G:21:ARG:HH11	7:G:21:ARG:CB	2.06	0.67
16:g:165:LYS:HE3	16:g:177:PHE:HD2	1.58	0.67
3:C:57:ARG:HD3	3:C:58:THR:HG23	1.77	0.67
3:C:210:VAL:HG22	3:C:220:LEU:HD21	1.76	0.67
8:H:156:ILE:HA	8:H:162:THR:HG22	1.77	0.67
2:P:58:GLU:HG3	2:P:60:PHE:HD1	1.60	0.67
16:g:228:LEU:HB3	16:g:230:ILE:HG23	1.76	0.67
7:G:171:LYS:NZ	7:G:205:VAL:O	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:11:ASP:O	10:J:185:LYS:NZ	2.22	0.67
10:J:83:PHE:O	10:J:87:ASN:ND2	2.27	0.67
2:B:58:GLU:HG3	2:B:60:PHE:HD1	1.60	0.67
13:M:152:TRP:CD2	13:M:172:MET:HE1	2.30	0.67
9:W:168:GLN:NE2	12:L:186:MET:SD	2.68	0.67
6:F:152:ASP:OD1	6:F:156:VAL:N	2.28	0.67
7:U:171:LYS:NZ	7:U:205:VAL:O	2.27	0.67
10:X:161:ARG:HH12	10:X:194:ILE:HD12	1.60	0.67
16:g:37:SER:HB2	16:g:248:PRO:HG3	1.77	0.67
14:N:213:ILE:HG13	14:N:218:VAL:HG12	1.77	0.67
15:f:160:LYS:NZ	15:f:227:LYS:O	2.29	0.66
3:C:138:PHE:HD1	3:C:139:ASP:N	1.94	0.66
4:D:13:ASN:HB3	5:E:126:ARG:HB3	1.77	0.66
10:X:148:THR:OG1	10:X:150:THR:O	2.12	0.66
11:Y:142:LEU:HD21	11:Y:156[B]:MET:HE1	1.77	0.66
4:R:99:HIS:ND1	4:R:107:MET:HG3	2.09	0.66
4:R:77:ALA:HB3	4:R:142:LEU:HB2	1.77	0.66
7:G:42:VAL:HG23	7:G:195:VAL:HG12	1.78	0.66
2:P:230:GLN:O	2:P:233:VAL:N	2.29	0.66
3:Q:138:PHE:HD1	3:Q:138:PHE:C	2.04	0.66
7:U:49:VAL:HG22	7:U:219:VAL:HG12	1.77	0.66
2:B:230:GLN:O	2:B:233:VAL:N	2.29	0.66
10:J:41:LYS:HZ3	10:J:187:GLY:H	1.41	0.66
10:J:81:ALA:HB1	10:J:124:LEU:HD11	1.77	0.66
16:g:1:MET:N	16:g:48:TYR:O	2.28	0.66
7:G:21:ARG:HD2	7:G:23:TYR:CE1	2.30	0.66
8:H:257:GLU:HG3	9:I:197:ARG:HD2	1.77	0.66
14:N:169:ILE:HG13	14:N:173:VAL:HG23	1.78	0.66
7:U:21:ARG:HD2	7:U:23:TYR:CE1	2.30	0.66
10:J:18:ASP:O	10:J:34:LYS:NZ	2.28	0.66
3:Q:57:ARG:HD3	3:Q:58:THR:HG23	1.77	0.66
4:D:69:GLU:HA	4:D:75:GLY:HA2	1.77	0.66
4:D:77:ALA:HB3	4:D:142:LEU:HB2	1.77	0.66
6:F:8:ASP:O	6:F:22:GLN:NE2	2.29	0.66
14:N:117:PHE:CE2	14:N:132:ILE:HB	2.31	0.66
3:Q:138:PHE:HD1	3:Q:139:ASP:N	1.94	0.65
5:S:203:GLN:O	5:S:239:ARG:NH1	2.28	0.65
14:b:82:SER:OG	14:b:129:MET:O	2.11	0.65
15:f:176:LYS:NZ	16:g:254:LEU:O	2.29	0.65
8:H:209:ASP:OD1	8:H:210:LEU:N	2.29	0.65
7:U:21:ARG:HH11	7:U:21:ARG:CB	2.06	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:f:51:ARG:NH1	15:f:52:ARG:O	2.29	0.65
16:g:241:SER:HA	16:g:244:ARG:HB3	1.78	0.65
7:G:224:ASN:HB3	7:G:228:ARG:NH2	2.11	0.65
7:U:42:VAL:HG23	7:U:195:VAL:HG12	1.78	0.65
7:U:224:ASN:HB3	7:U:228:ARG:NH2	2.11	0.65
7:G:49:VAL:HG22	7:G:219:VAL:HG12	1.77	0.65
12:Z:123:ILE:O	12:Z:126:SER:OG	2.15	0.65
4:R:13:ASN:HB3	5:S:126:ARG:HD3	1.78	0.65
4:R:88:LEU:HD23	4:R:119:LEU:HD23	1.79	0.65
2:B:155:ASN:OD1	3:C:77:THR:OG1	2.13	0.65
3:C:11:SER:HB3	3:C:15:HIS:H	1.61	0.65
3:C:138:PHE:HD1	3:C:138:PHE:C	2.04	0.65
4:D:24:VAL:O	4:D:28:ILE:HG12	1.96	0.65
8:H:257:GLU:OE1	9:I:197:ARG:NH1	2.29	0.65
4:R:35:SER:HB2	4:R:51:GLU:HG3	1.79	0.65
2:B:176:LYS:HB2	3:C:53:LEU:HD23	1.77	0.65
12:L:200:MET:HE1	12:L:223:ILE:HG21	1.77	0.65
3:Q:193:LYS:HA	3:Q:196:LEU:HD12	1.79	0.65
15:f:149:TRP:HZ3	15:f:215:LEU:HD21	1.62	0.65
3:C:115:LYS:HZ2	3:C:149:PRO:HA	1.60	0.65
7:G:189:TRP:HE1	7:G:197:THR:HG21	1.62	0.65
4:R:24:VAL:O	4:R:28:ILE:HG12	1.96	0.65
7:G:189:TRP:CD1	7:G:194:THR:HA	2.32	0.65
10:J:4:LEU:HD13	10:J:45:LEU:HB3	1.77	0.65
3:Q:11:SER:HB3	3:Q:15:HIS:N	2.12	0.65
3:C:103:THR:HG23	3:C:106:TYR:H	1.62	0.65
2:P:30:HIS:O	2:P:50:ARG:NH2	2.30	0.64
6:T:108:LEU:HD21	6:T:139:SER:HB3	1.78	0.64
2:B:30:HIS:O	2:B:50:ARG:NH2	2.30	0.64
6:T:156:VAL:HG22	7:U:84:THR:HB	1.77	0.64
9:I:190:GLU:HG3	9:I:192:ASP:H	1.62	0.64
4:R:69:GLU:HA	4:R:75:GLY:HA2	1.77	0.64
6:F:50:GLU:OE2	6:F:201:HIS:ND1	2.30	0.64
7:U:196:GLU:HB3	7:U:242:LEU:HD21	1.80	0.64
9:I:132:THR:HG22	9:I:134:ASP:H	1.62	0.64
3:Q:11:SER:HB3	3:Q:15:HIS:H	1.61	0.64
4:D:88:LEU:HD23	4:D:119:LEU:HD23	1.79	0.64
14:N:169:ILE:HD11	14:N:172:TYR:HD2	1.63	0.64
2:P:72:MET:HG2	2:P:138:GLY:HA3	1.79	0.64
6:T:73:VAL:HG12	6:T:139:SER:HB2	1.79	0.64
3:C:11:SER:HB3	3:C:15:HIS:N	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:189:TRP:HE1	7:U:197:THR:HG21	1.62	0.64
9:W:89:MET:O	9:W:92:ASN:ND2	2.30	0.64
8:H:44:THR:N	8:H:212:SER:HG	1.96	0.64
10:J:86:ARG:HH22	10:J:90:ASP:HB3	1.63	0.64
4:R:146:VAL:HG21	4:R:222:PRO:HA	1.80	0.64
3:C:119:THR:C	4:D:135:ARG:HH12	2.06	0.64
4:D:35:SER:HB2	4:D:51:GLU:HG3	1.79	0.64
11:K:239:ARG:HE	11:K:244:ILE:HG13	1.62	0.64
13:M:219:ARG:HH11	13:M:252:THR:HG21	1.61	0.64
5:S:76:GLY:HA3	5:S:130:VAL:HA	1.79	0.64
3:C:66:ASP:OD1	3:C:95:ARG:NH2	2.31	0.64
12:L:142:ASP:OD1	12:L:146:LYS:N	2.31	0.64
3:Q:195:LEU:O	3:Q:199:VAL:N	2.31	0.64
6:T:45:VAL:HG23	6:T:146:ALA:HB1	1.80	0.64
11:Y:193:TYR:HB3	10:J:141:SER:HB3	1.79	0.64
1:A:85:LEU:HD21	1:A:129:PHE:CE2	2.32	0.64
3:C:18:GLN:HB3	3:C:126:PRO:HG3	1.80	0.64
3:C:193:LYS:HA	3:C:196:LEU:HD12	1.79	0.64
6:F:89:ASP:HA	6:F:92:ARG:HD2	1.80	0.64
3:Q:103:THR:HG23	3:Q:106:TYR:H	1.62	0.63
4:R:236:GLU:HA	4:R:239:LYS:HE3	1.80	0.63
1:O:92:LEU:HD12	1:O:112:ARG:HG3	1.80	0.63
6:T:215:TRP:CE3	6:T:227:VAL:HG22	2.33	0.63
3:C:31:THR:OG1	3:C:163:ARG:O	2.16	0.63
12:L:212:GLU:OE2	12:L:213:ARG:HG2	1.97	0.63
1:O:85:LEU:HD21	1:O:129:PHE:CE2	2.32	0.63
3:Q:115:LYS:NZ	3:Q:149:PRO:HA	2.13	0.63
1:A:92:LEU:HD12	1:A:112:ARG:HG3	1.80	0.63
4:D:99:HIS:HD2	4:D:103:TYR:HB2	1.62	0.63
14:N:182:THR:N	14:N:185:GLU:OE2	2.26	0.63
9:W:14:LYS:HD2	9:W:118:PRO:HB2	1.81	0.63
11:Y:104:MET:HG3	11:Y:111:CYS:HB2	1.81	0.63
4:R:99:HIS:HD2	4:R:103:TYR:HB2	1.62	0.63
15:f:74:ALA:HB2	15:f:83:LEU:HD22	1.80	0.63
14:N:148:VAL:HG23	14:N:153:MET:HG2	1.78	0.63
2:P:143:TYR:HH	10:X:73:TYR:HD2	1.44	0.63
9:I:57:THR:O	10:J:85:ARG:NH2	2.31	0.63
2:P:50:ARG:HG3	2:P:50:ARG:NH1	2.05	0.63
4:R:91:LYS:NZ	4:R:119:LEU:HD13	2.13	0.63
6:T:15:SER:OG	6:T:19:ARG:N	2.32	0.63
2:B:33:THR:OG1	2:B:166:ASN:OD1	2.16	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:91:LYS:NZ	4:D:119:LEU:HD13	2.13	0.63
5:E:157:ARG:HD2	5:E:176:MET:HE3	1.80	0.63
10:J:96:THR:HB	10:J:97:PRO:HD3	1.80	0.63
1:O:10:THR:HG21	15:f:5:PHE:CZ	2.31	0.63
3:C:170:GLU:HA	3:C:173:GLU:OE1	1.99	0.63
6:F:16:PRO:HA	7:G:27:TYR:CE1	2.34	0.63
12:L:56:ARG:HH21	12:L:218:GLY:HA3	1.64	0.63
6:F:15:SER:OG	6:F:19:ARG:N	2.31	0.63
7:U:189:TRP:CD1	7:U:194:THR:HA	2.32	0.62
11:Y:60:THR:OG1	11:Y:189:SER:N	2.31	0.62
13:a:116:VAL:O	13:a:120:GLU:HG2	1.99	0.62
14:b:72:HIS:ND1	14:b:73:ASP:OD1	2.26	0.62
3:C:115:LYS:NZ	3:C:149:PRO:HA	2.13	0.62
3:C:138:PHE:C	3:C:138:PHE:CD1	2.77	0.62
4:D:99:HIS:CD2	4:D:103:TYR:HB2	2.33	0.62
4:D:236:GLU:HA	4:D:239:LYS:HE3	1.81	0.62
11:K:140:LYS:O	11:K:144:ASN:ND2	2.23	0.62
3:Q:31:THR:OG1	3:Q:163:ARG:O	2.16	0.62
4:R:97:GLN:HB3	11:Y:120:ARG:HG2	1.80	0.62
4:R:99:HIS:CD2	4:R:103:TYR:HB2	2.33	0.62
13:a:150:PRO:HG2	13:a:152:TRP:NE1	2.14	0.62
1:A:80:PRO:HA	1:A:83:ARG:NH2	2.14	0.62
2:B:72:MET:HG2	2:B:138:GLY:HA3	1.79	0.62
4:D:146:VAL:HG21	4:D:222:PRO:HA	1.80	0.62
14:N:117:PHE:HE2	14:N:132:ILE:HB	1.64	0.62
14:N:173:VAL:HG13	14:N:189:PHE:HZ	1.63	0.62
3:Q:3:TYR:HD2	15:f:1:MET:HG3	1.64	0.62
15:f:51:ARG:O	15:f:55:LYS:N	2.18	0.62
3:C:195:LEU:O	3:C:199:VAL:N	2.31	0.62
16:g:2:PHE:HE1	16:g:77:VAL:HG21	1.63	0.62
3:Q:66:ASP:OD1	3:Q:95:ARG:NH2	2.31	0.62
15:f:273:LEU:HD12	15:f:277:MET:HE1	1.81	0.62
7:G:196:GLU:HB3	7:G:242:LEU:HD21	1.80	0.62
14:N:148:VAL:HG21	14:N:153:MET:N	2.15	0.62
2:P:7:SER:HB3	2:P:8:ARG:HD2	1.82	0.62
8:V:83:ASN:ND2	8:V:146:VAL:O	2.33	0.62
5:E:20:HIS:HB3	5:E:24:TYR:CE2	2.35	0.62
6:F:83:ASP:OD2	6:F:132:GLY:N	2.33	0.62
6:F:136:MET:HE1	6:F:150:MET:HG2	1.81	0.62
8:V:62:ARG:HE	8:V:212:SER:C	2.08	0.62
8:V:123:ASN:ND2	8:V:162:THR:OG1	2.23	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:26:VAL:HG21	11:Y:195:TYR:CD2	2.34	0.62
13:a:183:ALA:HB3	13:a:192:GLN:HB2	1.82	0.62
16:g:32:MET:HE2	16:g:87:ALA:HB1	1.81	0.62
5:S:117:GLN:NE2	6:T:83:ASP:OD1	2.31	0.62
3:Q:170:GLU:HA	3:Q:173:GLU:OE1	1.99	0.61
15:f:170:ARG:HB2	15:f:236:TYR:CE1	2.34	0.61
5:E:49:LEU:HB2	5:E:195:LEU:HD21	1.82	0.61
8:H:252:THR:OG1	9:I:168:GLN:OE1	2.18	0.61
13:M:152:TRP:O	13:M:153:ASN:ND2	2.33	0.61
3:Q:18:GLN:HB3	3:Q:126:PRO:HG3	1.80	0.61
3:Q:114:LEU:HA	3:Q:117:ARG:HG2	1.82	0.61
4:R:36:THR:HA	4:R:171:GLY:HA3	1.82	0.61
4:R:73:HIS:CE1	4:R:106:THR:HB	2.36	0.61
8:V:236:ASN:O	12:L:239:ARG:NH1	2.34	0.61
13:a:198:VAL:HG11	13:a:213:LEU:HD21	1.80	0.61
1:O:20:GLN:OE1	1:O:20:GLN:HA	2.00	0.61
2:P:33:THR:OG1	2:P:166:ASN:OD1	2.16	0.61
5:E:195:LEU:O	5:E:198:THR:OG1	2.18	0.61
8:H:155:SER:OG	8:H:163:ASP:OD1	2.17	0.61
7:U:1:MET:H2	15:f:3:ALA:HA	1.65	0.61
1:O:80:PRO:HA	1:O:83:ARG:NH2	2.14	0.61
5:S:189:LYS:NZ	5:S:237:GLU:OE1	2.31	0.61
9:W:13:MET:HG2	9:W:135:PHE:HB3	1.83	0.61
16:g:78:TYR:O	16:g:87:ALA:N	2.29	0.61
1:A:20:GLN:HA	1:A:20:GLN:OE1	2.00	0.61
9:I:160:ASP:OD1	9:I:161:HIS:N	2.31	0.61
10:J:86:ARG:HH12	10:J:90:ASP:HB3	1.65	0.61
3:Q:138:PHE:C	3:Q:138:PHE:CD1	2.78	0.61
8:V:80:ILE:HB	8:V:84:ILE:HG23	1.82	0.61
8:V:147[B]:ASP:OD1	8:V:149:THR:OG1	2.14	0.61
16:g:79:SER:HA	16:g:86:VAL:HA	1.83	0.61
5:E:39:LYS:NZ	5:E:142:PRO:O	2.25	0.61
2:P:38:LEU:O	2:P:179:TYR:OH	2.19	0.61
4:R:15:PHE:HE1	5:S:126:ARG:HB2	1.65	0.61
6:T:198:TYR:HE1	6:T:211:LEU:HD22	1.64	0.61
2:B:38:LEU:O	2:B:179:TYR:OH	2.19	0.61
4:D:157:ASP:OD1	4:D:159:SER:OG	2.16	0.61
10:J:90:ASP:OD1	10:J:91:CYS:N	2.33	0.61
10:J:161:ARG:HH21	10:J:162:LYS:HG2	1.66	0.61
1:O:38:LYS:HA	1:O:43:VAL:HG22	1.83	0.61
4:R:8:TYR:HB3	4:R:22:PHE:HE2	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:60:GLU:OE2	4:R:63:SER:OG	2.14	0.61
5:S:208:LYS:O	5:S:208:LYS:NZ	2.24	0.61
1:A:38:LYS:HA	1:A:43:VAL:HG22	1.83	0.61
2:B:213:ILE:HG22	2:B:228:LEU:HD13	1.83	0.61
15:f:71:PHE:HB3	15:f:164:ILE:HG12	1.83	0.61
12:L:179:ASN:OD1	12:L:186:MET:HE2	1.99	0.61
3:Q:180:ALA:HB1	3:Q:190:LEU:HD11	1.83	0.61
1:A:158:LYS:HG3	2:B:57:ASP:HB3	1.83	0.61
2:B:7:SER:HB3	2:B:8:ARG:HD2	1.82	0.61
11:K:219:ILE:HG21	11:K:233:VAL:HG11	1.83	0.61
1:O:138:TRP:NE1	1:O:141:GLY:HA2	2.16	0.60
4:R:16:SER:HB3	4:R:20:ARG:HG3	1.83	0.60
1:A:58:GLU:OE2	1:A:205:ASP:HB3	2.01	0.60
1:A:138:TRP:NE1	1:A:141:GLY:HA2	2.16	0.60
14:N:117:PHE:CD2	14:N:132:ILE:HD12	2.36	0.60
11:Y:76:ASP:OD1	11:Y:92:LYS:NZ	2.34	0.60
12:Z:212:GLU:HB3	8:H:72:LYS:HE2	1.82	0.60
5:E:80:ASP:OD1	5:E:126:ARG:NH2	2.33	0.60
3:Q:200:GLN:NE2	3:Q:204:LYS:O	2.34	0.60
10:X:102:LEU:HB2	10:X:118:MET:HB2	1.82	0.60
11:Y:71:VAL:HG11	11:Y:161:CYS:HB2	1.82	0.60
6:F:37:ILE:HD11	6:F:193:VAL:HG13	1.82	0.60
5:S:156:CYS:SG	5:S:157:ARG:N	2.75	0.60
5:S:157:ARG:NH2	6:T:59:GLU:OE2	2.34	0.60
6:T:70:ASP:CG	6:T:73:VAL:HG22	2.26	0.60
11:Y:58:HIS:NE2	11:Y:80:THR:O	2.34	0.60
16:g:59:ASN:ND2	16:g:67:ASN:O	2.34	0.60
4:R:83:ALA:HA	4:R:86:LYS:HZ1	1.64	0.60
5:S:155:ASP:HB3	6:T:62:SER:HB2	1.84	0.60
15:f:78:ASN:ND2	15:f:246:THR:HB	2.16	0.60
7:G:190:THR:H	7:G:193:GLN:NE2	1.98	0.60
7:U:190:THR:H	7:U:193:GLN:NE2	1.98	0.60
13:a:56:VAL:HG12	13:a:69:ALA:HB2	1.84	0.60
15:f:195:GLN:H	15:f:224:GLN:HG2	1.66	0.60
1:A:69:LYS:O	1:A:217:PHE:N	2.35	0.60
4:D:8:TYR:HB3	4:D:22:PHE:HE2	1.66	0.60
5:E:121:GLN:OE1	6:F:129:ARG:NH2	2.35	0.60
15:f:148:GLN:O	15:f:152:LYS:HG2	2.00	0.60
4:D:36:THR:HA	4:D:171:GLY:HA3	1.82	0.60
8:V:73:ASN:O	8:V:230:ARG:NH2	2.35	0.60
16:g:43:LYS:HD2	16:g:76:GLU:HG2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:47:ALA:HB3	2:P:212:GLU:HG3	1.84	0.60
7:U:38:THR:OG1	7:U:170:VAL:N	2.35	0.60
3:C:200:GLN:NE2	3:C:204:LYS:O	2.34	0.60
5:E:44:ALA:HB2	5:E:142:PRO:HB3	1.83	0.60
1:O:69:LYS:O	1:O:217:PHE:N	2.35	0.60
9:W:61:THR:HG23	10:X:86:ARG:HH12	1.66	0.60
4:D:73:HIS:CE1	4:D:106:THR:HB	2.36	0.60
4:D:83:ALA:HA	4:D:86:LYS:HZ1	1.67	0.60
11:K:79:ALA:HB3	11:K:86:ALA:HB3	1.84	0.60
1:O:135:ILE:HB	1:O:146:PHE:HB2	1.84	0.59
6:T:99:ARG:NH2	6:T:105:ASN:OD1	2.30	0.59
7:U:54:LYS:N	7:U:214:GLU:O	2.35	0.59
3:C:155:ALA:HB3	4:D:63:SER:OG	2.02	0.59
8:H:248:GLU:O	8:H:251:THR:OG1	2.18	0.59
10:J:154:GLU:O	10:J:158:GLU:HG2	2.02	0.59
4:R:4:THR:HA	15:f:15:ARG:O	2.01	0.59
4:R:101:PHE:HA	11:Y:116:ARG:HH21	1.67	0.59
5:S:157:ARG:HD2	5:S:176:MET:SD	2.42	0.59
10:X:38:MET:HE1	10:X:61:GLN:HA	1.83	0.59
12:Z:85:PHE:HZ	13:a:173:LEU:HB3	1.67	0.59
15:f:170:ARG:HB2	15:f:236:TYR:HE1	1.67	0.59
2:P:213:ILE:HG22	2:P:228:LEU:HD13	1.83	0.59
11:Y:186:SER:HB3	11:Y:195:TYR:CE1	2.37	0.59
15:f:93:TRP:HB3	15:f:124:TYR:HB3	1.83	0.59
16:g:238:PRO:C	16:g:240:VAL:H	2.10	0.59
2:B:47:ALA:HB3	2:B:212:GLU:HG3	1.83	0.59
2:B:139:TRP:CD2	2:B:218:ARG:NH1	2.71	0.59
3:C:114:LEU:HA	3:C:117:ARG:HG2	1.82	0.59
4:D:165:CYS:HA	5:E:57:ALA:HA	1.84	0.59
5:S:47:VAL:HG12	5:S:195:LEU:HD22	1.83	0.59
15:f:2:ALA:HB2	15:f:9:VAL:O	2.03	0.59
3:C:104:VAL:HG12	3:C:145:TYR:HD2	1.66	0.59
5:S:71:GLY:HA3	5:S:221:PHE:CE2	2.38	0.59
12:Z:212:GLU:OE2	8:H:238:LYS:HG3	2.03	0.59
16:g:100:LYS:HG3	16:g:189:THR:HG21	1.84	0.59
4:D:60:GLU:OE2	4:D:63:SER:OG	2.14	0.59
6:F:70:ASP:OD1	6:F:71:ARG:N	2.34	0.59
7:G:49:VAL:HG21	7:G:195:VAL:HG21	1.84	0.59
3:Q:104:VAL:HG12	3:Q:145:TYR:HD2	1.66	0.59
5:S:41:LYS:HG3	5:S:180:MET:O	2.03	0.59
7:U:38:THR:HA	7:U:169:GLY:HA3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:49:VAL:HG21	7:U:195:VAL:HG21	1.84	0.59
12:Z:119:MET:O	12:Z:119:MET:HE3	2.02	0.59
12:Z:142:ASP:OD1	12:Z:146:LYS:N	2.35	0.59
15:f:266:ILE:O	15:f:269:SER:OG	2.16	0.59
4:D:16:SER:HB3	4:D:20:ARG:HG3	1.83	0.59
7:G:16:PHE:HB3	7:G:20:GLY:HA2	1.85	0.59
8:H:244:ARG:HD2	8:H:244:ARG:O	2.03	0.59
1:O:108:GLN:NE2	9:W:77:GLU:HG2	2.18	0.59
6:T:74:GLY:HA3	6:T:224:HIS:CE1	2.38	0.59
7:U:51:VAL:HG22	7:U:217:VAL:HG22	1.85	0.59
7:U:207:SER:HB2	7:U:210:PHE:HE1	1.68	0.59
11:Y:66:LYS:HZ1	11:Y:170:LEU:HB3	1.67	0.59
13:a:88:MET:HE1	13:a:112:LEU:HD13	1.83	0.59
16:g:73:ILE:N	16:g:76:GLU:OE2	2.24	0.59
2:B:16:GLY:HA3	3:C:25:ALA:HB2	1.85	0.59
7:G:38:THR:OG1	7:G:170:VAL:N	2.35	0.59
9:I:41:ILE:HD11	9:I:49:TYR:HB3	1.85	0.59
9:I:143:GLU:OE1	9:I:143:GLU:N	2.36	0.59
1:O:58:GLU:OE2	1:O:205:ASP:HB3	2.01	0.59
1:A:67:ILE:HD11	1:A:86:VAL:HG13	1.85	0.59
3:C:180:ALA:HB1	3:C:190:LEU:HD11	1.83	0.59
9:I:11:MET:HB2	9:I:145:MET:HE1	1.84	0.59
13:M:119:GLU:HA	13:M:122:LEU:HD12	1.85	0.59
14:N:132:ILE:HG13	14:N:134:ILE:HG13	1.84	0.59
16:g:83:ARG:NH1	16:g:229:GLN:O	2.36	0.58
8:H:56:VAL:HG13	8:H:220:VAL:HG22	1.85	0.58
8:H:186:ARG:CZ	8:H:189:MET:HE1	2.32	0.58
2:P:197:LEU:O	2:P:201:MET:HB2	2.03	0.58
8:V:62:ARG:NH1	8:V:213:GLY:O	2.35	0.58
2:B:234:GLU:HA	2:B:237:ILE:HG22	1.85	0.58
6:F:141:SER:O	6:F:145:GLY:N	2.36	0.58
7:G:54:LYS:N	7:G:214:GLU:O	2.35	0.58
8:H:96:ASP:O	8:H:99:THR:OG1	2.20	0.58
9:I:44:MET:HE3	9:I:44:MET:HA	1.84	0.58
2:P:10:THR:HG22	3:Q:125:ARG:HB3	1.85	0.58
2:P:76:VAL:HG21	2:P:83:ALA:CB	2.33	0.58
2:P:143:TYR:CG	3:Q:57:ARG:NH2	2.71	0.58
3:Q:45:VAL:HG21	3:Q:61:LYS:HG2	1.86	0.58
15:f:80:VAL:HG23	15:f:136:GLN:HB3	1.85	0.58
7:G:207:SER:HB2	7:G:210:PHE:HE1	1.68	0.58
10:J:88:LEU:HD23	10:J:118:MET:HE3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:200:MET:SD	12:L:204:LYS:HE3	2.43	0.58
7:U:16:PHE:HB3	7:U:20:GLY:HA2	1.85	0.58
11:Y:142:LEU:HD22	11:Y:173:VAL:HG11	1.83	0.58
13:a:117:ILE:O	13:a:121:LEU:HG	2.02	0.58
1:A:135:ILE:HB	1:A:146:PHE:HB2	1.84	0.58
11:Y:67:PHE:CE1	11:Y:72:ILE:HD11	2.38	0.58
15:f:14:CYS:SG	15:f:18:THR:HB	2.43	0.58
2:B:76:VAL:HG21	2:B:83:ALA:CB	2.33	0.58
4:D:23:GLN:HB3	4:D:136:PRO:HG3	1.86	0.58
7:G:38:THR:HA	7:G:169:GLY:HA3	1.85	0.58
10:J:139:THR:HB	10:J:163:CYS:SG	2.43	0.58
2:P:8:ARG:HH11	15:f:8:GLU:CG	2.14	0.58
2:P:139:TRP:CD2	2:P:218:ARG:NH1	2.71	0.58
2:P:234:GLU:HA	2:P:237:ILE:HG22	1.85	0.58
14:b:176:THR:HB	14:b:189:PHE:HE1	1.68	0.58
15:f:62:LEU:N	15:f:153:VAL:O	2.36	0.58
1:A:97:TYR:O	1:A:97:TYR:HD1	1.87	0.58
2:B:12:PHE:CE1	3:C:125:ARG:HD2	2.37	0.58
2:B:197:LEU:O	2:B:201:MET:HB2	2.03	0.58
6:T:140:TYR:HD1	6:T:146:ALA:HB2	1.69	0.58
10:J:39:SER:OG	10:J:40:GLU:N	2.36	0.58
1:O:75:TYR:HB3	1:O:82:TYR:CD1	2.39	0.58
5:S:215:VAL:HB	5:S:221:PHE:HD1	1.69	0.58
6:T:51:LYS:O	6:T:210:GLU:N	2.35	0.58
9:W:48:LEU:HD21	9:W:86:LEU:HD13	1.85	0.58
12:Z:222:ARG:NH1	12:Z:233:GLU:OE2	2.37	0.58
12:Z:228:LYS:HG3	12:Z:229:GLU:OE2	2.04	0.58
15:f:35:ARG:NH1	15:f:36:GLU:HG2	2.18	0.58
1:A:53:SER:OG	7:G:180:GLU:OE1	2.17	0.58
7:U:1:MET:H3	15:f:5:PHE:C	2.12	0.58
13:a:87:ILE:HD12	13:a:235:ALA:HB2	1.86	0.58
1:O:67:ILE:HD11	1:O:86:VAL:HG13	1.85	0.58
3:Q:208:LEU:HG	3:Q:228:TYR:HE1	1.69	0.58
5:S:109:VAL:HA	5:S:112:ILE:HD12	1.86	0.58
11:Y:67:PHE:HE1	11:Y:72:ILE:HD11	1.69	0.58
11:K:110:ASP:OD1	12:L:125:TYR:OH	2.14	0.58
5:S:88:MET:SD	5:S:108:LEU:HD21	2.44	0.57
9:W:121:CYS:SG	9:W:122:SER:N	2.77	0.57
10:X:35:MET:HG2	10:X:45:LEU:HD23	1.85	0.57
7:G:51:VAL:HG22	7:G:217:VAL:HG22	1.85	0.57
11:K:77:SER:HA	11:K:92:LYS:HZ1	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:44:ALA:HB2	12:L:149:VAL:HG23	1.86	0.57
12:L:153:ASP:OD1	12:L:157:SER:N	2.36	0.57
15:f:48:ARG:NH2	15:f:55:LYS:O	2.37	0.57
15:f:49:LEU:HG	15:f:58:LEU:HD13	1.86	0.57
1:A:75:TYR:HB3	1:A:82:TYR:CD1	2.39	0.57
3:C:208:LEU:HG	3:C:228:TYR:HE1	1.68	0.57
13:M:169:TYR:HB2	13:M:182:LEU:HD13	1.85	0.57
11:Y:71:VAL:HG21	11:Y:170:LEU:HD12	1.86	0.57
15:f:78:ASN:HD21	15:f:246:THR:HB	1.68	0.57
1:A:122:GLN:HE22	2:B:130:PHE:HE1	1.49	0.57
4:D:5:ARG:HB2	5:E:4:ASN:HB2	1.86	0.57
7:G:80:MET:HE1	7:G:138:MET:HB2	1.86	0.57
10:J:19:ARG:HD2	10:J:179:SER:HB3	1.86	0.57
13:M:72:LEU:HD21	13:M:74:SER:OG	2.04	0.57
14:N:35:THR:N	14:N:51:ASP:OD2	2.37	0.57
5:S:156:CYS:HB3	5:S:159:MET:HG2	1.86	0.57
7:U:141:ILE:HD12	7:U:220:VAL:HG22	1.86	0.57
3:C:12:PRO:HA	4:D:26:TYR:HE2	1.67	0.57
7:G:21:ARG:HB2	7:G:21:ARG:NH1	2.16	0.57
10:J:71:ASN:HB3	10:J:73:TYR:CZ	2.39	0.57
11:K:236:TYR:CE2	11:K:245[B]:ARG:HG3	2.39	0.57
3:Q:5:ARG:CZ	15:f:2:ALA:H	2.17	0.57
4:R:23:GLN:HB3	4:R:136:PRO:HG3	1.86	0.57
8:V:215:ASN:ND2	8:V:231:PRO:HB3	2.18	0.57
11:Y:62:THR:HG21	11:Y:103:THR:HB	1.85	0.57
3:C:120:GLN:HG3	4:D:133:MET:SD	2.44	0.57
3:C:157:LYS:HZ2	4:D:58:LEU:HA	1.70	0.57
5:E:74:ILE:HG21	5:E:81:ALA:HB1	1.86	0.57
14:N:41:GLN:HB2	14:N:145:VAL:HG22	1.86	0.57
15:f:50:LEU:HB2	15:f:55:LYS:HD2	1.87	0.57
16:g:119:ILE:HD13	16:g:228:LEU:HD21	1.87	0.57
12:L:41:LEU:O	12:L:52:ALA:N	2.37	0.57
7:U:80:MET:HE1	7:U:138:MET:HB2	1.86	0.57
8:V:89:ALA:O	8:V:140:ALA:N	2.35	0.57
8:V:206:ILE:HG13	8:V:213:GLY:HA2	1.87	0.57
14:b:75:ILE:HD13	14:b:136:GLY:HA3	1.85	0.57
16:g:126:SER:HG	16:g:129:ARG:HH21	1.52	0.57
10:J:148:THR:H	10:J:151:ILE:HD11	1.69	0.57
11:K:156[A]:MET:H	11:K:175:SER:HB3	1.69	0.57
2:P:15:GLU:O	3:Q:28:LYS:NZ	2.27	0.57
3:Q:6:ALA:O	3:Q:9:VAL:HG23	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:61:THR:H	11:Y:188:GLY:HA3	1.69	0.57
15:f:16:ALA:HB3	15:f:18:THR:OG1	2.04	0.57
16:g:55:MET:HG3	16:g:74:ASN:HB3	1.87	0.57
2:B:229:LYS:N	2:B:232:GLU:OE2	2.38	0.57
4:D:5:ARG:CB	5:E:4:ASN:HB2	2.35	0.57
14:N:196:LEU:HD21	14:N:231:PHE:HD2	1.70	0.57
2:P:58:GLU:HG3	2:P:60:PHE:CD1	2.40	0.57
12:Z:92:LEU:HA	12:Z:95:ILE:HG22	1.86	0.57
15:f:277:MET:O	15:f:280:ASN:ND2	2.29	0.57
1:A:122:GLN:HB2	2:B:128:ARG:CZ	2.34	0.57
3:C:57:ARG:HG2	3:C:58:THR:N	2.10	0.57
3:C:188:ILE:O	3:C:192:ILE:HG12	2.05	0.57
6:F:70:ASP:HA	13:M:121:LEU:HD21	1.87	0.57
11:K:156[B]:MET:H	11:K:175:SER:HB3	1.69	0.57
11:K:181:SER:OG	11:K:182:GLY:N	2.37	0.57
2:P:229:LYS:N	2:P:232:GLU:OE2	2.38	0.57
4:R:22:PHE:O	4:R:26:TYR:HD1	1.88	0.57
4:R:44:GLU:OE2	4:R:191:LEU:N	2.38	0.57
5:S:138:ASP:OD2	13:a:126:HIS:NE2	2.37	0.57
7:U:144:ASP:HB3	7:U:150:GLN:HE22	1.70	0.57
15:f:251:LYS:HG3	15:f:254:LEU:HD12	1.87	0.57
4:D:22:PHE:O	4:D:26:TYR:HD1	1.88	0.57
4:D:231:LYS:O	4:D:234:LEU:N	2.38	0.57
8:V:133:TYR:HD2	8:V:137:ILE:HD11	1.69	0.56
3:C:87:ALA:HB2	3:C:111:ILE:HD11	1.86	0.56
8:H:45:THR:N	8:H:60:ASP:OD2	2.38	0.56
9:I:124:ASP:OD1	9:I:125:LEU:N	2.36	0.56
3:Q:195:LEU:HA	3:Q:198:VAL:HG12	1.86	0.56
15:f:4:THR:OG1	15:f:8:GLU:OE2	2.23	0.56
1:A:190:ALA:O	1:A:193:THR:OG1	2.20	0.56
3:C:45:VAL:HG21	3:C:61:LYS:HG2	1.86	0.56
4:D:98:ASN:HA	4:D:101:PHE:CE1	2.39	0.56
6:F:192:GLU:O	6:F:196:ILE:HG12	2.05	0.56
8:H:193:GLU:OE1	8:H:193:GLU:N	2.38	0.56
2:P:17:ARG:H	2:P:17:ARG:HD3	1.71	0.56
4:R:98:ASN:HA	4:R:101:PHE:CE1	2.39	0.56
8:V:202:ILE:O	8:V:206:ILE:HD12	2.05	0.56
16:g:8:SER:OG	16:g:9:ALA:N	2.38	0.56
2:B:40:ASN:HD21	2:B:182:GLY:C	2.13	0.56
2:B:58:GLU:HG3	2:B:60:PHE:CD1	2.40	0.56
3:C:117:ARG:HA	3:C:120:GLN:NE2	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:195:LEU:HA	3:C:198:VAL:HG12	1.86	0.56
5:E:5:GLN:HE21	6:F:9:LEU:HD11	1.70	0.56
8:H:157:TYR:HB2	8:H:161:SER:HB2	1.86	0.56
10:J:37:LYS:NZ	10:J:39:SER:O	2.39	0.56
14:N:148:VAL:HG21	14:N:153:MET:H	1.70	0.56
1:O:97:TYR:O	1:O:97:TYR:HD1	1.87	0.56
2:P:143:TYR:CD1	3:Q:57:ARG:NH2	2.73	0.56
3:Q:57:ARG:HG2	3:Q:58:THR:N	2.10	0.56
3:Q:117:ARG:HA	3:Q:120:GLN:NE2	2.20	0.56
5:E:18:ARG:HE	5:E:23:GLU:CD	2.14	0.56
1:O:149:ASP:HB3	1:O:153:ALA:HB3	1.88	0.56
3:Q:155:ALA:HB3	4:R:63:SER:OG	2.05	0.56
13:a:101:ASP:OD1	13:a:102:TYR:N	2.38	0.56
2:B:49:ARG:HD3	2:B:63:GLU:OE2	2.06	0.56
4:D:216:GLU:HB2	4:D:228:MET:HE1	1.87	0.56
3:Q:139:ASP:OD1	3:Q:141:THR:HG22	2.06	0.56
3:Q:188:ILE:O	3:Q:192:ILE:HG12	2.05	0.56
5:S:51:ARG:N	5:S:60:GLN:HE22	1.99	0.56
12:Z:239:ARG:HB3	12:Z:241:ASP:OD1	2.04	0.56
16:g:61:TYR:OH	16:g:89:GLN:NE2	2.35	0.56
1:A:132:SER:HB2	1:A:150:PRO:HD3	1.87	0.56
2:B:17:ARG:H	2:B:17:ARG:HD3	1.71	0.56
4:D:44:GLU:OE2	4:D:191:LEU:N	2.38	0.56
3:Q:87:ALA:HB2	3:Q:111:ILE:HD11	1.86	0.56
8:V:71:ASP:OD1	8:V:72:LYS:N	2.38	0.56
13:a:65:VAL:HG11	13:a:167:LEU:HD13	1.87	0.56
14:b:208:ILE:HB	14:b:223:LEU:HB2	1.87	0.56
15:f:268:GLN:O	15:f:271:GLU:HG3	2.06	0.56
3:C:6:ALA:O	3:C:9:VAL:HG23	2.05	0.56
3:C:118:TYR:CE1	3:C:124:ARG:HD3	2.41	0.56
4:R:28:ILE:O	4:R:31:ILE:HB	2.06	0.56
4:R:41:GLN:HA	4:R:46:VAL:HG12	1.86	0.56
4:R:157:ASP:OD1	4:R:159:SER:OG	2.16	0.56
5:S:140:MET:O	5:S:140:MET:HE3	2.05	0.56
10:X:38:MET:HA	10:X:38:MET:HE3	1.88	0.56
10:X:101:ASN:HB3	10:X:132:HIS:CD2	2.40	0.56
2:B:17:ARG:NH1	2:B:19:TYR:HE1	2.04	0.56
4:R:231:LYS:O	4:R:234:LEU:N	2.38	0.56
13:a:155:MET:N	13:a:170:VAL:O	2.37	0.56
14:b:167:SER:O	14:N:168:TYR:HA	2.05	0.56
15:f:208:GLN:NE2	16:g:58:ASN:O	2.33	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:ASP:HB3	1:A:153:ALA:HB3	1.88	0.56
5:E:137:TYR:CE1	5:E:141:GLY:HA2	2.40	0.56
7:G:141:ILE:HD12	7:G:220:VAL:HG22	1.86	0.56
2:P:118:LYS:NZ	2:P:150:SER:OG	2.39	0.56
4:R:216:GLU:HB2	4:R:228:MET:HE1	1.87	0.56
5:S:159:MET:HE3	5:S:160:SER:H	1.69	0.56
14:b:35:THR:HA	14:b:67:LYS:HZ2	1.72	0.56
1:A:189:THR:O	1:A:193:THR:HG23	2.06	0.56
10:J:148:THR:OG1	10:J:150:THR:O	2.24	0.56
13:M:65:VAL:HG23	13:M:165:SER:HB3	1.88	0.56
2:P:49:ARG:HD3	2:P:63:GLU:OE2	2.06	0.55
5:S:26:MET:HE3	5:S:150:SER:HB3	1.88	0.55
11:Y:67:PHE:CE2	11:Y:69:HIS:HB2	2.40	0.55
14:b:93:VAL:HG11	14:b:117:PHE:CZ	2.42	0.55
6:F:92:ARG:HH12	13:M:121:LEU:HB3	1.72	0.55
7:G:144:ASP:HB3	7:G:150:GLN:HE22	1.70	0.55
3:Q:118:TYR:CE1	3:Q:124:ARG:HD3	2.41	0.55
4:R:4:THR:OG1	5:S:4:ASN:OD1	2.24	0.55
5:S:80:ASP:OD2	5:S:129:GLY:N	2.39	0.55
16:g:152:GLN:N	16:g:152:GLN:OE1	2.38	0.55
5:E:206:THR:HG23	5:E:208:LYS:H	1.71	0.55
2:B:118:LYS:NZ	2:B:150:SER:OG	2.39	0.55
3:C:139:ASP:OD1	3:C:141:THR:HG22	2.06	0.55
10:J:181:ARG:NE	10:J:190:ASP:OD1	2.39	0.55
1:A:30:GLY:O	1:A:164:LYS:NZ	2.38	0.55
4:D:28:ILE:O	4:D:31:ILE:HB	2.06	0.55
2:P:17:ARG:NH1	2:P:19:TYR:HE1	2.04	0.55
11:Y:73:VAL:O	11:Y:236:TYR:N	2.35	0.55
4:D:41:GLN:HA	4:D:46:VAL:HG12	1.86	0.55
5:E:20:HIS:HB3	5:E:24:TYR:HE2	1.69	0.55
1:O:189:THR:O	1:O:193:THR:HG23	2.06	0.55
8:V:55:ILE:HD11	8:V:221:ILE:HD12	1.87	0.55
1:A:62:HIS:CE1	1:A:219:ARG:HH12	2.25	0.55
3:C:26:VAL:O	3:C:27:LYS:HD3	2.07	0.55
3:C:71:MET:HE1	3:C:73:PHE:HB3	1.89	0.55
3:C:116:GLN:O	3:C:119:THR:OG1	2.21	0.55
14:N:148:VAL:HG22	14:N:149:PRO:O	2.06	0.55
3:Q:230:ALA:O	3:Q:233:GLU:HG3	2.07	0.55
5:S:93:LEU:HD11	12:Z:101:LYS:HB2	1.89	0.55
16:g:41:MET:HG3	16:g:80:LEU:HB2	1.88	0.55
5:E:26:MET:HB3	5:E:30:LYS:HZ1	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:172:LEU:HB3	6:F:57:LEU:HD11	1.89	0.55
10:X:170:ARG:HD2	10:J:26:VAL:HG13	1.89	0.55
3:C:61:LYS:HE3	3:C:73:PHE:O	2.07	0.55
3:C:192:ILE:O	3:C:196:LEU:HG	2.07	0.55
4:D:72:ALA:O	4:D:226:PHE:N	2.39	0.55
1:O:62:HIS:CE1	1:O:219:ARG:HH12	2.25	0.55
2:P:21:VAL:HG22	2:P:25:MET:HE1	1.89	0.55
16:g:139:PHE:O	16:g:140:ARG:NH2	2.34	0.55
16:g:160:TRP:NE1	16:g:226:GLU:OE2	2.40	0.55
5:E:104:PRO:HB3	13:M:126:HIS:CE1	2.42	0.55
6:F:31:GLU:OE2	6:F:169:ARG:NH1	2.40	0.55
9:I:82:LYS:HZ3	9:I:113:PRO:HD2	1.72	0.55
3:Q:61:LYS:HE3	3:Q:73:PHE:O	2.07	0.54
3:Q:159:ASN:OD1	3:Q:160:ALA:N	2.39	0.54
15:f:121:CYS:H	15:f:137:CYS:CB	2.17	0.54
8:H:132:ARG:HG3	8:H:133:TYR:N	2.21	0.54
2:P:40:ASN:HD21	2:P:182:GLY:C	2.13	0.54
7:U:85:ALA:O	7:U:88:ARG:HB2	2.06	0.54
7:U:147:GLN:OE1	7:U:147:GLN:N	2.41	0.54
9:W:13:MET:SD	9:W:153:TRP:HD1	2.30	0.54
10:X:37:LYS:HZ1	10:X:181:ARG:HH12	1.55	0.54
3:C:23:GLN:OE1	3:C:23:GLN:HA	2.07	0.54
13:M:102:TYR:HE2	13:M:106:GLN:HE21	1.55	0.54
3:Q:26:VAL:O	3:Q:27:LYS:HD3	2.07	0.54
5:S:10:VAL:HG21	5:S:127:PRO:HD3	1.90	0.54
6:T:7:TYR:HD2	6:T:16:PRO:HD3	1.72	0.54
9:W:86:LEU:O	9:W:90:VAL:HG23	2.07	0.54
13:a:155:MET:HB2	13:a:170:VAL:HB	1.89	0.54
13:a:201:LYS:HD2	13:a:202:GLN:HB2	1.89	0.54
13:a:231:ARG:HG2	13:a:249:SER:HB3	1.89	0.54
16:g:111:LYS:HD3	16:g:199:ILE:HD11	1.90	0.54
6:F:140:TYR:HD1	6:F:146:ALA:HB2	1.71	0.54
8:H:137:ILE:HG13	9:I:98:ARG:NH2	2.22	0.54
1:O:30:GLY:O	1:O:164:LYS:NZ	2.38	0.54
1:O:132:SER:HB2	1:O:150:PRO:HD3	1.88	0.54
1:O:176:ARG:NH1	1:O:176:ARG:HB2	2.23	0.54
1:O:190:ALA:O	1:O:193:THR:OG1	2.20	0.54
3:Q:231:GLU:O	3:Q:234:LYS:HB2	2.08	0.54
4:R:146:VAL:HG23	4:R:150:GLY:HA2	1.89	0.54
5:S:50:LYS:NZ	5:S:59:HIS:HB2	2.22	0.54
6:T:192:GLU:O	6:T:196:ILE:HG12	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:g:226:GLU:O	16:g:229:GLN:NE2	2.40	0.54
2:B:21:VAL:HG22	2:B:25:MET:HE1	1.89	0.54
2:B:86:LEU:HD21	2:B:130:PHE:CD2	2.43	0.54
3:C:230:ALA:O	3:C:233:GLU:HG3	2.07	0.54
4:D:7:GLU:OE1	4:D:7:GLU:N	2.41	0.54
7:G:195:VAL:O	7:G:198:ALA:N	2.40	0.54
12:L:55:THR:OG1	12:L:66:ARG:O	2.19	0.54
14:N:41:GLN:NE2	14:N:42:PHE:O	2.40	0.54
3:Q:5:ARG:HH21	15:f:2:ALA:HB3	1.72	0.54
3:Q:23:GLN:OE1	3:Q:23:GLN:HA	2.07	0.54
3:Q:232:ILE:O	3:Q:236:LYS:HG2	2.07	0.54
5:S:109:VAL:HG22	5:S:153:TYR:CD2	2.43	0.54
5:S:225:ASP:O	5:S:229:VAL:HG13	2.07	0.54
3:C:191:VAL:O	3:C:195:LEU:HG	2.08	0.54
6:F:80:LEU:HD23	6:F:83:ASP:HB2	1.90	0.54
1:O:132:SER:OG	1:O:148:SER:O	2.26	0.54
6:T:120:HIS:O	6:T:123:THR:HG22	2.08	0.54
16:g:129:ARG:HD3	16:g:207:PHE:CG	2.43	0.54
16:g:167:ARG:NE	16:g:175:SER:O	2.41	0.54
2:B:50:ARG:HH11	2:B:50:ARG:CG	2.14	0.54
2:B:143:TYR:CG	3:C:57:ARG:NH2	2.75	0.54
5:E:167:SER:O	5:E:170:THR:OG1	2.23	0.54
7:G:85:ALA:O	7:G:88:ARG:HB2	2.07	0.54
12:L:221:LEU:HD12	12:L:222:ARG:N	2.23	0.54
1:O:55:LEU:HB3	7:U:165:ALA:O	2.08	0.54
2:P:17:ARG:NH1	2:P:19:TYR:CE1	2.76	0.54
2:P:238:LYS:HA	2:P:241:GLU:HG2	1.90	0.54
10:X:39:SER:OG	10:X:40:GLU:N	2.40	0.54
15:f:84:SER:O	15:f:88:MET:HB3	2.08	0.54
9:I:137:VAL:HG11	9:I:145:MET:HB3	1.88	0.54
12:L:55:THR:HG22	12:L:69:PRO:HA	1.90	0.54
14:N:117:PHE:HD2	14:N:132:ILE:HD12	1.72	0.54
1:O:55:LEU:HD11	7:U:179:LEU:HB3	1.90	0.54
2:P:9:THR:HA	2:P:20:GLN:HG3	1.90	0.54
3:Q:191:VAL:O	3:Q:195:LEU:HG	2.08	0.54
3:Q:192:ILE:O	3:Q:196:LEU:HG	2.07	0.54
4:R:7:GLU:OE1	4:R:7:GLU:N	2.41	0.54
11:Y:57:LEU:HD13	12:Z:153:ASP:HB3	1.88	0.54
12:Z:55:THR:OG1	12:Z:220:ALA:HB3	2.07	0.54
16:g:35:ILE:HG22	16:g:41:MET:HE1	1.88	0.54
2:B:9:THR:HA	2:B:20:GLN:HG3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:65:ARG:NH2	6:F:78:ALA:HA	2.23	0.54
6:F:126:SER:H	7:G:130:GLU:HB2	1.72	0.54
10:J:10:PRO:HD3	10:J:151:ILE:H	1.73	0.54
3:Q:71:MET:HE1	3:Q:73:PHE:HB3	1.89	0.54
3:Q:88:ARG:HD3	10:X:70:ARG:HG2	1.89	0.54
6:T:139:SER:OG	6:T:140:TYR:N	2.40	0.54
7:U:195:VAL:O	7:U:198:ALA:N	2.40	0.54
3:C:231:GLU:O	3:C:234:LYS:HB2	2.08	0.54
7:G:147:GLN:OE1	7:G:147:GLN:N	2.41	0.54
3:Q:16:LEU:HD12	3:Q:16:LEU:H	1.73	0.53
4:R:109:VAL:HG21	4:R:145:GLY:HA3	1.90	0.53
12:Z:200:MET:HA	12:Z:200:MET:HE3	1.90	0.53
13:a:58:GLY:HA3	13:a:67:ILE:HG22	1.90	0.53
14:b:194:LEU:O	14:b:198:MET:HG2	2.07	0.53
3:C:16:LEU:HD12	3:C:16:LEU:H	1.73	0.53
4:D:10:ARG:HB2	5:E:8:ASN:ND2	2.23	0.53
5:E:6:TYR:CE2	5:E:15:PRO:HD3	2.42	0.53
10:J:16:ALA:HB2	10:J:160:LEU:HD21	1.89	0.53
4:R:202:LEU:O	4:R:206:MET:HG3	2.08	0.53
9:W:172:ASN:ND2	12:L:185:ASN:OD1	2.41	0.53
12:Z:50:ILE:HG21	12:Z:203:VAL:HG21	1.88	0.53
12:Z:151:SER:HB2	12:Z:164:LYS:HD2	1.90	0.53
14:b:223:LEU:HD12	14:b:227:GLN:HB3	1.90	0.53
2:B:139:TRP:NE1	2:B:144:GLY:HA2	2.23	0.53
9:I:11:MET:HB2	9:I:145:MET:CE	2.39	0.53
1:O:182:GLU:OE1	1:O:184:GLU:N	2.38	0.53
1:O:214:GLU:H	1:O:214:GLU:CD	2.10	0.53
3:Q:92:GLN:HB3	10:X:62:LYS:HG3	1.89	0.53
5:S:50:LYS:HZ2	5:S:59:HIS:HB2	1.73	0.53
12:Z:232:ARG:NH1	12:Z:234:GLU:OE2	2.41	0.53
4:D:202:LEU:O	4:D:206:MET:HG3	2.08	0.53
10:J:35:MET:HB2	10:J:45:LEU:HD13	1.90	0.53
14:N:85:ASP:HB2	14:N:128:LEU:HD22	1.90	0.53
14:N:130:ALA:HB3	14:N:150:MET:HA	1.89	0.53
2:P:4:ARG:NE	3:Q:2:SER:O	2.37	0.53
2:P:86:LEU:HD21	2:P:130:PHE:CD2	2.43	0.53
7:U:21:ARG:HB2	7:U:21:ARG:NH1	2.16	0.53
7:U:139:ILE:HG12	7:U:153:LYS:HG3	1.91	0.53
16:g:64:THR:H	16:g:67:ASN:HD21	1.57	0.53
3:C:7:ILE:N	3:C:122:ASN:OD1	2.38	0.53
3:C:159:ASN:OD1	3:C:160:ALA:N	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:111:CYS:O	11:K:115:GLU:HG2	2.08	0.53
14:N:110:VAL:HG23	14:N:138:ASP:HB3	1.90	0.53
5:S:42:THR:HB	5:S:217:LYS:HZ1	1.72	0.53
13:a:167:LEU:HG	13:a:182:LEU:HD12	1.91	0.53
15:f:162:MET:HE1	15:f:164:ILE:HD11	1.91	0.53
2:B:17:ARG:NH1	2:B:19:TYR:CE1	2.76	0.53
3:C:230:ALA:O	3:C:234:LYS:HE2	2.09	0.53
13:M:124:ASP:OD1	13:M:125:GLY:N	2.42	0.53
2:P:139:TRP:NE1	2:P:144:GLY:HA2	2.23	0.53
9:W:98:ARG:O	9:W:98:ARG:NH1	2.30	0.53
13:a:73:GLY:N	13:a:81:PHE:O	2.39	0.53
2:B:238:LYS:HA	2:B:241:GLU:HG2	1.90	0.53
3:C:12:PRO:HA	4:D:26:TYR:CD2	2.44	0.53
13:M:55:SER:O	13:M:86:ARG:NH2	2.33	0.53
14:N:164:SER:OG	14:N:201:ASP:OD2	2.21	0.53
3:Q:233:GLU:HA	3:Q:236:LYS:CG	2.39	0.53
1:A:176:ARG:HB2	1:A:176:ARG:NH1	2.23	0.53
3:C:68:ASN:HA	3:C:211:MET:HE1	1.90	0.53
3:C:232:ILE:O	3:C:236:LYS:HG2	2.07	0.53
6:F:8:ASP:HB3	6:F:21:PHE:HD2	1.73	0.53
6:T:39:ILE:HD12	6:T:193:VAL:HG22	1.91	0.53
14:b:121:CYS:C	14:b:123:ARG:H	2.16	0.53
15:f:160:LYS:NZ	15:f:229:PRO:HD3	2.22	0.53
15:f:190:ARG:NH2	15:f:207:GLU:OE2	2.42	0.53
16:g:33:ASP:OD1	16:g:61:TYR:OH	2.19	0.53
11:K:140:LYS:HD3	11:K:179:ARG:NE	2.23	0.53
1:O:204:GLU:OE1	1:O:226:LYS:N	2.42	0.53
3:Q:208:LEU:O	3:Q:220:LEU:HB2	2.09	0.53
4:R:76:CYS:SG	4:R:141:LEU:HD12	2.49	0.53
13:a:86:ARG:NH1	13:a:98:ALA:O	2.42	0.53
13:a:180:PRO:HB2	13:a:199:LEU:HD21	1.91	0.53
16:g:4:PRO:HA	16:g:45:GLY:HA3	1.90	0.53
1:A:118:GLN:O	1:A:121:THR:OG1	2.21	0.53
3:C:226:GLU:O	3:C:229:VAL:N	2.42	0.53
4:D:35:SER:O	4:D:79:SER:OG	2.20	0.53
4:D:146:VAL:HG23	4:D:150:GLY:HA2	1.89	0.53
5:E:115:LYS:O	5:E:119:PRO:HD3	2.09	0.53
14:N:69:THR:OG1	14:N:79:ARG:NH1	2.41	0.53
14:N:149:PRO:HD2	14:N:153:MET:HE2	1.91	0.53
14:N:201:ASP:OD1	14:N:202:GLY:N	2.42	0.53
3:Q:230:ALA:O	3:Q:234:LYS:HE2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:185:THR:O	6:T:189:ILE:HG12	2.09	0.53
7:U:121:ILE:O	7:U:124:VAL:HG12	2.09	0.53
11:Y:56:MET:HG2	12:Z:155:VAL:HG21	1.90	0.53
15:f:63:LEU:O	15:f:159:ARG:NH2	2.41	0.53
15:f:242:LEU:HD12	15:f:280:ASN:HB2	1.90	0.53
1:A:99:VAL:HG13	9:I:92:ASN:HD22	1.74	0.53
4:D:76:CYS:SG	4:D:141:LEU:HD12	2.49	0.53
10:J:41:LYS:NZ	10:J:187:GLY:H	2.07	0.53
11:K:78:ARG:NE	11:K:230:GLY:HA3	2.19	0.53
13:M:58:GLY:HA2	13:M:67:ILE:HG22	1.90	0.53
3:Q:5:ARG:HB3	15:f:2:ALA:O	2.08	0.52
3:Q:226:GLU:O	3:Q:229:VAL:N	2.42	0.52
6:T:72:HIS:CE1	6:T:105:ASN:HB3	2.44	0.52
16:g:167:ARG:HD3	16:g:175:SER:OG	2.09	0.52
2:B:68:LEU:HD11	2:B:74:CYS:SG	2.49	0.52
3:C:5:ARG:HD2	4:D:10:ARG:HB3	1.90	0.52
4:D:48:LEU:HD23	4:D:77:ALA:HB2	1.90	0.52
6:F:34:SER:OG	6:F:50:GLU:O	2.16	0.52
6:F:35:THR:HG22	6:F:168:ALA:H	1.74	0.52
10:J:102:LEU:HB2	10:J:118:MET:HB3	1.91	0.52
10:J:192:ASP:N	10:J:192:ASP:OD1	2.42	0.52
2:P:8:ARG:NH1	15:f:8:GLU:HG2	2.22	0.52
5:S:103:LEU:HD23	5:S:108:LEU:HD12	1.90	0.52
8:V:249:LYS:HD2	8:V:250:GLY:N	2.25	0.52
10:X:165:GLU:OE2	11:K:200[B]:ARG:NH1	2.41	0.52
16:g:126:SER:OG	16:g:129:ARG:NH2	2.37	0.52
2:P:34:CYS:SG	2:P:75:SER:OG	2.49	0.52
7:U:187:PHE:HA	7:U:189:TRP:CZ3	2.45	0.52
15:f:14:CYS:SG	15:f:15:ARG:N	2.83	0.52
6:F:75:MET:HE3	6:F:135:PHE:CD1	2.44	0.52
6:F:230:ASP:N	6:F:230:ASP:OD1	2.42	0.52
10:J:145:ARG:HG3	10:J:146:TYR:CD1	2.43	0.52
11:K:251:VAL:HA	11:K:254:LEU:HD12	1.90	0.52
4:R:48:LEU:HD23	4:R:77:ALA:HB2	1.90	0.52
1:A:133:LEU:HB2	1:A:148:SER:HB3	1.91	0.52
4:D:109:VAL:HG21	4:D:145:GLY:HA3	1.91	0.52
8:H:186:ARG:O	8:H:189:MET:HE3	2.09	0.52
8:H:258:LYS:NZ	8:H:260:THR:OG1	2.26	0.52
2:P:169:ALA:O	2:P:173:SER:OG	2.24	0.52
7:U:2:SER:O	15:f:3:ALA:HB2	2.09	0.52
9:W:203:MET:HE2	9:W:203:MET:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:f:175:TYR:OH	15:f:207:GLU:OE1	2.25	0.52
16:g:73:ILE:HG13	16:g:75:ALA:H	1.74	0.52
11:K:62:THR:OG1	11:K:187:VAL:N	2.30	0.52
11:K:66:LYS:HD3	11:K:183:ALA:HA	1.92	0.52
6:T:119:VAL:HG13	6:T:155:GLY:HA2	1.90	0.52
13:a:169:TYR:HB2	13:a:182:LEU:HD13	1.92	0.52
16:g:241:SER:HB2	16:g:245:TRP:HE1	1.74	0.52
2:B:136:TYR:CE1	2:B:150:SER:HB2	2.42	0.52
5:E:42:THR:HA	5:E:217:LYS:HE2	1.91	0.52
7:G:187:PHE:HA	7:G:189:TRP:CZ3	2.45	0.52
8:H:92:ALA:O	8:H:95:THR:OG1	2.22	0.52
8:H:149:THR:OG1	8:H:152:HIS:NE2	2.39	0.52
11:K:56:MET:SD	11:K:109:ALA:HB3	2.49	0.52
12:L:214:ASP:OD2	12:L:216:TYR:N	2.42	0.52
2:P:68:LEU:HD11	2:P:74:CYS:SG	2.49	0.52
3:Q:51:ALA:O	3:Q:54:GLN:HG2	2.10	0.52
14:b:80:SER:OG	14:b:131:GLY:O	2.26	0.52
16:g:34:LEU:HD23	16:g:221:VAL:HG21	1.92	0.52
1:A:38:LYS:HD3	1:A:158:LYS:HA	1.92	0.52
1:A:83:ARG:HH21	1:A:83:ARG:CB	2.18	0.52
7:G:139:ILE:HG12	7:G:153:LYS:HG3	1.91	0.52
9:I:11:MET:HE3	9:I:166:ILE:HG13	1.92	0.52
1:O:133:LEU:HB2	1:O:148:SER:HB3	1.91	0.52
1:O:213:ASN:HB2	1:O:214:GLU:OE1	2.10	0.52
2:P:19:TYR:HB3	2:P:23:TYR:CE2	2.45	0.52
6:T:120:HIS:HA	6:T:123:THR:HG22	1.92	0.52
9:W:87:MET:SD	9:W:129:PRO:HB3	2.50	0.52
9:W:122:SER:HB3	9:W:130:MET:HE3	1.91	0.52
11:Y:129:ASN:O	11:Y:130:LYS:HG3	2.10	0.52
3:C:108:THR:HG21	3:C:145:TYR:HB3	1.92	0.52
9:I:58:ASP:OD2	9:I:103:TYR:N	2.36	0.52
1:O:83:ARG:HH21	1:O:83:ARG:CB	2.18	0.52
6:T:98:PHE:HD2	6:T:106:ILE:HG13	1.72	0.52
8:V:113:THR:HG22	8:V:115:ARG:HG2	1.91	0.52
9:W:176:ARG:NH2	11:K:85:ILE:O	2.37	0.52
16:g:167:ARG:CB	16:g:170:PRO:HA	2.40	0.52
7:G:115:CYS:SG	7:G:152:TYR:HB3	2.50	0.52
10:J:66:LEU:HD21	10:J:70:ARG:HH22	1.74	0.52
12:L:52:ALA:HB1	12:L:207:PHE:CE2	2.45	0.52
4:R:105:GLU:CD	4:R:105:GLU:N	2.68	0.52
9:W:141:CYS:HB2	9:W:145:MET:HE2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:152:LEU:HB3	9:W:165:THR:HG23	1.92	0.52
15:f:176:LYS:HB2	15:f:210:ASN:OD1	2.10	0.52
1:A:204:GLU:OE1	1:A:226:LYS:N	2.42	0.52
4:D:105:GLU:CD	4:D:105:GLU:N	2.68	0.52
5:E:103:LEU:HD12	5:E:104:PRO:HD2	1.92	0.52
3:Q:68:ASN:HA	3:Q:211:MET:HE1	1.91	0.51
10:X:142:ILE:HD11	11:K:196:GLY:C	2.34	0.51
11:Y:118:LEU:HD13	11:Y:142:LEU:HD12	1.90	0.51
11:Y:219:ILE:HD13	11:Y:233:VAL:HG23	1.91	0.51
1:A:95:GLN:OE1	1:A:95:GLN:N	2.43	0.51
2:B:19:TYR:HB3	2:B:23:TYR:CE2	2.45	0.51
3:C:196:LEU:HA	3:C:199:VAL:HG12	1.91	0.51
12:L:151:SER:HB2	12:L:164:LYS:HG2	1.92	0.51
13:M:152:TRP:HA	13:M:172:MET:HE3	1.92	0.51
1:O:27:ALA:HB2	7:U:20:GLY:HA3	1.91	0.51
1:O:38:LYS:HD3	1:O:158:LYS:HA	1.92	0.51
1:O:132:SER:HB3	1:O:162:MET:HE1	1.93	0.51
10:X:2:GLU:HB2	10:X:47:VAL:HG21	1.92	0.51
1:A:127:ARG:HD2	7:G:16:PHE:CE1	2.45	0.51
2:B:143:TYR:HB2	2:B:146:GLN:NE2	2.25	0.51
6:F:19:ARG:HH21	6:F:21:PHE:HE1	1.57	0.51
7:G:186:LYS:HZ3	7:G:189:TRP:H	1.58	0.51
10:J:101:ASN:HB3	10:J:132:HIS:CD2	2.44	0.51
1:O:95:GLN:OE1	1:O:95:GLN:N	2.43	0.51
3:Q:5:ARG:HH11	4:R:10:ARG:HB3	1.75	0.51
4:R:32:LYS:HB2	15:f:107:ARG:NH2	2.24	0.51
7:U:115:CYS:SG	7:U:152:TYR:HB3	2.50	0.51
11:Y:217:ARG:HD2	10:J:145:ARG:HD3	1.91	0.51
15:f:190:ARG:HD2	15:f:206:LEU:HA	1.91	0.51
16:g:2:PHE:CE1	16:g:77:VAL:HG21	2.43	0.51
1:A:213:ASN:HB2	1:A:214:GLU:OE1	2.10	0.51
5:E:48:ALA:HB3	5:E:63:ILE:HD11	1.92	0.51
8:H:81:SER:HB2	8:H:82:PRO:HD2	1.91	0.51
3:Q:173:GLU:OE1	4:R:58:LEU:HD11	2.10	0.51
3:Q:212:ARG:HB2	3:Q:215:GLN:NE2	2.26	0.51
5:S:77:LEU:HG	5:S:129:GLY:O	2.10	0.51
10:X:45:LEU:HD12	10:X:103:LEU:HB2	1.93	0.51
11:Y:55:GLU:HB2	12:Z:154:PRO:HG2	1.93	0.51
16:g:147:MET:HB2	16:g:200:GLN:HB3	1.93	0.51
3:C:51:ALA:O	3:C:54:GLN:HG2	2.10	0.51
3:C:208:LEU:O	3:C:220:LEU:HB2	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:121:ILE:O	7:G:124:VAL:HG12	2.09	0.51
12:L:55:THR:HB	12:L:68:SER:N	2.25	0.51
2:P:97:TYR:CG	2:P:105:ILE:HD12	2.46	0.51
5:S:74:ILE:HG21	5:S:81:ALA:HB1	1.92	0.51
16:g:181:ILE:HG22	16:g:188:LYS:HB2	1.92	0.51
8:H:85:TYR:CE2	8:H:226:LEU:HD11	2.46	0.51
10:J:101:ASN:OD1	10:J:120:TYR:N	2.42	0.51
12:L:214:ASP:OD2	12:L:217:THR:HG23	2.10	0.51
2:P:234:GLU:O	2:P:238:LYS:HG2	2.11	0.51
3:Q:116:GLN:O	3:Q:119:THR:OG1	2.21	0.51
5:S:50:LYS:HB3	5:S:209:ASN:HA	1.93	0.51
6:T:106:ILE:HD12	6:T:106:ILE:H	1.75	0.51
3:C:220:LEU:HD13	3:C:227:LYS:HE3	1.92	0.51
10:J:86:ARG:O	10:J:86:ARG:NH2	2.44	0.51
11:K:51:GLU:OE2	11:K:55:GLU:N	2.44	0.51
3:Q:108:THR:HG21	3:Q:145:TYR:HB3	1.92	0.51
4:R:190:THR:OG1	4:R:193:GLU:HB2	2.11	0.51
11:Y:172:TYR:HB2	11:Y:185:PHE:CD2	2.46	0.51
11:Y:186:SER:O	11:Y:195:TYR:OH	2.24	0.51
12:Z:56:ARG:NH2	12:Z:241:ASP:OXT	2.33	0.51
15:f:109:THR:O	15:f:112:THR:HG23	2.11	0.51
16:g:59:ASN:H	16:g:72:SER:HB3	1.75	0.51
1:A:122:GLN:HG3	2:B:128:ARG:HG2	1.93	0.51
2:B:230:GLN:O	2:B:234:GLU:OE1	2.28	0.51
10:J:38:MET:HE3	10:J:44:LEU:HB3	1.92	0.51
2:P:50:ARG:HH11	2:P:50:ARG:CG	2.14	0.51
3:Q:196:LEU:HA	3:Q:199:VAL:HG12	1.91	0.51
4:R:15:PHE:CE1	5:S:126:ARG:HB2	2.44	0.51
4:R:118:ASN:OD1	5:S:82:ARG:HD3	2.11	0.51
16:g:167:ARG:NH2	16:g:177:PHE:HB3	2.26	0.51
3:C:67:ASP:C	3:C:67:ASP:OD1	2.54	0.51
3:C:98:VAL:O	3:C:98:VAL:HG12	2.11	0.51
3:C:223:GLU:HG2	3:C:224:GLU:N	2.26	0.51
4:D:17:PRO:HA	5:E:24:TYR:CD1	2.46	0.51
11:K:51:GLU:HG3	11:K:55:GLU:HG2	1.93	0.51
1:O:54:ILE:N	7:U:180:GLU:OE1	2.44	0.51
2:P:143:TYR:HB2	2:P:146:GLN:NE2	2.25	0.51
2:P:230:GLN:O	2:P:234:GLU:OE1	2.28	0.51
3:Q:220:LEU:HD13	3:Q:227:LYS:HE3	1.92	0.51
4:R:35:SER:O	4:R:79:SER:OG	2.20	0.51
7:U:5:SER:O	15:f:9:VAL:HA	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:81:SER:O	8:V:83:ASN:N	2.44	0.51
16:g:164:GLU:OE1	16:g:164:GLU:N	2.44	0.51
1:A:132:SER:OG	1:A:148:SER:O	2.26	0.51
7:G:12:HIS:CE1	7:G:13:ILE:HG22	2.46	0.51
5:S:156:CYS:SG	6:T:57:LEU:HB3	2.51	0.51
7:U:5:SER:O	15:f:10:VAL:N	2.35	0.51
3:C:233:GLU:HA	3:C:236:LYS:CG	2.38	0.51
5:E:29:VAL:HG21	5:E:149:PRO:HD3	1.93	0.51
1:O:118:GLN:O	1:O:121:THR:OG1	2.21	0.50
3:Q:100:ASP:OD1	3:Q:101:PRO:HD2	2.11	0.50
3:Q:223:GLU:HG2	3:Q:224:GLU:N	2.26	0.50
6:T:203:GLU:O	6:T:207:LYS:HG3	2.11	0.50
7:U:77:GLY:HA3	7:U:227:PHE:CD2	2.46	0.50
9:W:24:ASP:OD1	9:W:24:ASP:N	2.44	0.50
14:b:198:MET:SD	14:b:204:SER:HB3	2.52	0.50
7:G:80:MET:HE3	7:G:80:MET:HA	1.93	0.50
12:L:239:ARG:NH2	12:L:241:ASP:OD2	2.44	0.50
14:N:53:ARG:CZ	14:N:205:GLY:HA3	2.41	0.50
3:C:120:GLN:CB	4:D:133:MET:HA	2.29	0.50
4:D:190:THR:OG1	4:D:193:GLU:HB2	2.10	0.50
7:G:77:GLY:HA3	7:G:227:PHE:CD2	2.46	0.50
8:H:155:SER:HB3	8:H:168:VAL:HG11	1.91	0.50
4:R:101:PHE:HA	11:Y:116:ARG:NH2	2.26	0.50
10:X:137:PHE:HB3	11:K:192:VAL:HG21	1.94	0.50
4:D:97:GLN:NE2	11:K:123:ARG:HG2	2.26	0.50
6:F:215:TRP:CE3	6:F:227:VAL:HG22	2.46	0.50
5:S:45:VAL:HG12	5:S:214:ILE:HG23	1.93	0.50
6:T:140:TYR:HB3	6:T:217:GLY:HA2	1.94	0.50
3:C:67:ASP:HB3	3:C:95:ARG:HH22	1.76	0.50
5:E:41:LYS:HG3	5:E:180:MET:HG3	1.92	0.50
5:E:189:LYS:HZ1	5:E:235:GLY:C	2.20	0.50
9:I:158:ASP:OD1	9:I:161:HIS:ND1	2.40	0.50
6:T:230:ASP:OD1	6:T:231:ILE:HD12	2.11	0.50
9:W:148:MET:HG2	12:L:175:PRO:HB2	1.93	0.50
11:Y:79:ALA:O	11:Y:86:ALA:N	2.43	0.50
13:a:71:MET:N	13:a:71:MET:SD	2.85	0.50
2:B:97:TYR:CG	2:B:105:ILE:HD12	2.46	0.50
5:E:183:ASN:OD1	5:E:186:GLU:N	2.24	0.50
5:E:227:ASP:OD1	5:E:230:SER:OG	2.29	0.50
8:H:228:PHE:HA	8:H:230:ARG:CZ	2.42	0.50
12:L:143:GLU:OE1	12:L:143:GLU:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:174:MET:HE1	2:P:199:LYS:CB	2.41	0.50
3:Q:67:ASP:C	3:Q:67:ASP:OD1	2.54	0.50
3:Q:80:ALA:HB2	3:Q:129:ILE:HG21	1.94	0.50
6:T:230:ASP:OD1	6:T:230:ASP:N	2.43	0.50
7:U:12:HIS:CE1	7:U:13:ILE:HG22	2.46	0.50
7:U:79:VAL:HG12	7:U:139:ILE:HB	1.94	0.50
7:U:80:MET:HA	7:U:80:MET:HE3	1.93	0.50
7:U:230:LEU:HD22	7:U:234:GLU:HG3	1.94	0.50
8:V:155:SER:HB2	8:V:170[A]:MET:HE2	1.92	0.50
15:f:75:ILE:HA	15:f:137:CYS:O	2.11	0.50
1:A:132:SER:HB3	1:A:162:MET:HE1	1.93	0.50
3:C:23:GLN:HE22	3:C:148:ASP:HB3	1.77	0.50
6:F:202:ASP:OD2	6:F:205:LYS:HB2	2.12	0.50
7:G:38:THR:HG1	7:G:170:VAL:H	1.57	0.50
2:P:8:ARG:HE	15:f:8:GLU:CD	2.16	0.50
2:P:240:HIS:HA	2:P:243:GLU:CD	2.37	0.50
3:Q:7:ILE:N	3:Q:122:ASN:OD1	2.38	0.50
3:Q:23:GLN:HE22	3:Q:148:ASP:HB3	1.77	0.50
4:R:5:ARG:HH22	16:g:210:GLU:CG	2.24	0.50
9:W:8:GLY:HA2	9:W:24:ASP:OD2	2.12	0.50
9:W:22:ALA:C	9:W:170:MET:HE1	2.37	0.50
9:W:137:VAL:HG11	9:W:145:MET:HB3	1.94	0.50
11:Y:101:LEU:HD21	11:Y:243:TRP:CZ2	2.47	0.50
11:Y:217:ARG:O	11:Y:221:GLN:HG2	2.12	0.50
12:Z:90:LEU:O	12:Z:94:LYS:HG2	2.11	0.50
12:Z:94:LYS:HD3	13:a:139:ARG:NH1	2.27	0.50
1:A:14:PRO:HA	2:B:23:TYR:CD1	2.47	0.50
2:B:174:MET:O	2:B:177:GLN:HG3	2.11	0.50
2:B:174:MET:HE1	2:B:199:LYS:CB	2.41	0.50
2:B:234:GLU:O	2:B:238:LYS:HG2	2.11	0.50
3:C:80:ALA:HB2	3:C:129:ILE:HG21	1.94	0.50
3:C:145:TYR:CE1	3:C:155:ALA:HB2	2.47	0.50
3:C:212:ARG:HB2	3:C:215:GLN:NE2	2.26	0.50
12:L:203:VAL:HA	12:L:206:VAL:HG22	1.92	0.50
3:Q:98:VAL:HG12	3:Q:98:VAL:O	2.11	0.50
3:Q:156:TRP:CZ3	4:R:59:MET:HG3	2.47	0.50
10:X:91:CYS:HG	10:X:98:TYR:HD2	1.56	0.50
13:a:124:ASP:OD2	13:a:126:HIS:ND1	2.45	0.50
3:C:145:TYR:CD1	3:C:155:ALA:HB2	2.46	0.50
12:L:33:TYR:OH	12:L:131:PRO:O	2.28	0.50
14:N:35:THR:N	14:N:204:SER:HG	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:113:VAL:HA	1:O:116:VAL:HG12	1.94	0.50
2:P:174:MET:O	2:P:177:GLN:HG3	2.11	0.50
6:T:110:HIS:O	6:T:114:ARG:HG2	2.12	0.50
6:T:180:GLN:HB2	6:T:184:MET:HE3	1.92	0.50
8:V:209:ASP:OD1	8:V:210:LEU:N	2.45	0.50
11:Y:101:LEU:HB2	11:Y:161:CYS:SG	2.52	0.50
11:Y:150:LYS:HD3	11:Y:151:GLY:N	2.26	0.50
15:f:160:LYS:HZ1	15:f:229:PRO:HD3	1.77	0.50
1:A:182:GLU:OE1	1:A:184:GLU:N	2.38	0.50
2:B:12:PHE:HZ	3:C:125:ARG:NH1	2.10	0.50
4:D:70:ILE:N	4:D:74:ILE:O	2.45	0.50
7:G:161:CYS:SG	7:G:162:GLY:N	2.85	0.50
9:I:137:VAL:HG22	9:I:146:TYR:CE1	2.47	0.50
4:R:19:GLY:HA3	5:S:28:ALA:HB2	1.94	0.49
4:R:96:THR:HA	4:R:107:MET:SD	2.52	0.49
10:X:64:VAL:HG13	10:X:75:LEU:HD12	1.93	0.49
13:a:211:ARG:NH2	13:a:245:GLU:OE1	2.44	0.49
15:f:50:LEU:HD22	15:f:100:LYS:HB2	1.94	0.49
15:f:82:PHE:HD2	15:f:83:LEU:HD12	1.77	0.49
16:g:2:PHE:HE2	16:g:10:PRO:HG2	1.77	0.49
1:A:42:GLY:HA3	1:A:183:LEU:HD22	1.93	0.49
2:B:231:LYS:HA	2:B:234:GLU:OE2	2.12	0.49
2:B:240:HIS:HA	2:B:243:GLU:CD	2.37	0.49
3:C:64:ALA:HA	3:C:70:CYS:HA	1.94	0.49
5:E:89:ARG:HG2	12:L:105:HIS:CE1	2.47	0.49
2:P:76:VAL:HG21	2:P:83:ALA:HB2	1.94	0.49
2:P:136:TYR:CE1	2:P:150:SER:HB2	2.42	0.49
2:P:175:LEU:HD13	2:P:196:VAL:HG21	1.94	0.49
3:Q:145:TYR:CE1	3:Q:155:ALA:HB2	2.47	0.49
8:V:83:ASN:ND2	8:V:147[A]:ASP:OD1	2.45	0.49
8:V:142:VAL:HG23	8:V:170[B]:MET:HG3	1.92	0.49
12:Z:185:ASN:CG	9:I:171:LEU:HB3	2.37	0.49
13:a:240:LYS:N	13:a:240:LYS:HD2	2.27	0.49
15:f:16:ALA:HB1	16:g:22:VAL:HG12	1.93	0.49
15:f:18:THR:O	15:f:20:ASP:N	2.42	0.49
15:f:70:LYS:HB2	15:f:132:VAL:HG22	1.94	0.49
2:B:175:LEU:HD13	2:B:196:VAL:HG21	1.94	0.49
3:C:6:ALA:O	3:C:8:THR:N	2.45	0.49
5:E:19:ILE:HG23	5:E:22:ILE:HB	1.93	0.49
6:F:118:TYR:CZ	6:F:122:TYR:HE2	2.30	0.49
7:G:192:GLU:C	7:G:194:THR:H	2.19	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:63:ALA:O	8:H:70:ALA:N	2.42	0.49
9:I:111:LEU:HB3	9:I:116:PHE:HA	1.94	0.49
12:L:42:ALA:HB2	12:L:137:ILE:HD12	1.94	0.49
4:R:70:ILE:N	4:R:74:ILE:O	2.45	0.49
8:V:72:LYS:HG3	8:V:72:LYS:O	2.12	0.49
13:a:65:VAL:HG23	13:a:165:SER:HB3	1.94	0.49
13:a:134:HIS:O	13:a:138:THR:HG23	2.13	0.49
13:a:152:TRP:HA	13:a:172:MET:HE1	1.93	0.49
15:f:125:HIS:ND1	15:f:130:PRO:HB3	2.27	0.49
1:A:113:VAL:HA	1:A:116:VAL:HG12	1.94	0.49
3:C:100:ASP:OD1	3:C:101:PRO:HD2	2.11	0.49
7:G:79:VAL:HG12	7:G:139:ILE:HB	1.94	0.49
8:H:52:LYS:HG3	8:H:189:MET:O	2.13	0.49
11:K:68:ARG:NE	11:K:205:ASP:OD1	2.45	0.49
14:N:96:GLN:C	14:N:98:GLY:H	2.21	0.49
3:Q:115:LYS:HZ1	3:Q:149:PRO:HA	1.77	0.49
3:Q:145:TYR:CD1	3:Q:155:ALA:HB2	2.46	0.49
6:T:69:VAL:CG1	6:T:73:VAL:HG23	2.41	0.49
7:U:192:GLU:C	7:U:194:THR:H	2.18	0.49
9:W:14:LYS:HE2	9:W:133:ASP:HA	1.93	0.49
10:X:52:ASP:OD2	10:X:98:TYR:HA	2.13	0.49
2:B:105:ILE:HG12	2:B:110:LEU:HB2	1.93	0.49
2:B:201:MET:HE1	2:B:204:SER:OG	2.12	0.49
12:L:66:ARG:HH21	13:M:196:ARG:HD2	1.76	0.49
13:M:160:TYR:OH	13:M:239:GLU:OE2	2.23	0.49
4:R:5:ARG:HH22	16:g:210:GLU:HG2	1.77	0.49
5:S:192:LEU:HD21	5:S:212:ILE:HD11	1.94	0.49
7:U:161:CYS:SG	7:U:162:GLY:N	2.85	0.49
10:X:68:LYS:C	10:X:68:LYS:HD3	2.38	0.49
11:Y:207:GLU:HB2	11:Y:210:GLN:CD	2.38	0.49
11:Y:250:ASN:OD1	11:Y:251:VAL:N	2.46	0.49
14:b:125:ARG:HB2	14:b:128:LEU:HG	1.95	0.49
3:C:24:GLU:HA	3:C:27:LYS:HE2	1.95	0.49
3:C:158:ALA:O	4:D:58:LEU:HD22	2.13	0.49
5:E:181:GLU:HG2	5:E:181:GLU:O	2.12	0.49
8:H:93:ALA:HB2	9:I:128:CYS:HB2	1.95	0.49
9:I:49:TYR:HD1	9:I:189:ILE:HD11	1.77	0.49
1:O:202:MET:HE1	1:O:207:ILE:HD11	1.94	0.49
2:P:105:ILE:HG12	2:P:110:LEU:HB2	1.93	0.49
3:Q:5:ARG:HD2	4:R:10:ARG:HB3	1.93	0.49
3:Q:6:ALA:O	3:Q:8:THR:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:44:MET:N	9:W:44:MET:SD	2.85	0.49
11:Y:62:THR:O	11:Y:186:SER:OG	2.20	0.49
11:Y:66:LYS:NZ	11:Y:170:LEU:HB3	2.26	0.49
15:f:112:THR:C	15:f:114:LEU:H	2.20	0.49
1:A:214:GLU:H	1:A:214:GLU:CD	2.10	0.49
10:J:146:TYR:CD2	10:J:162:LYS:HE2	2.47	0.49
13:M:49:PRO:HB3	13:M:152:TRP:CD1	2.48	0.49
1:O:42:GLY:HA3	1:O:183:LEU:HD22	1.93	0.49
11:Y:148:GLN:O	11:Y:149:TYR:HB2	2.13	0.49
15:f:194:THR:HA	16:g:71:LEU:HD22	1.93	0.49
4:D:96:THR:HA	4:D:107:MET:SD	2.52	0.49
4:D:146:VAL:HA	4:D:150:GLY:O	2.13	0.49
7:G:230:LEU:HD22	7:G:234:GLU:HG3	1.94	0.49
5:S:61:LYS:NZ	5:S:211:SER:OG	2.46	0.49
2:B:169:ALA:O	2:B:173:SER:OG	2.24	0.49
8:H:55:ILE:HG22	8:H:57:LEU:HD12	1.95	0.49
2:P:231:LYS:HA	2:P:234:GLU:OE2	2.12	0.49
3:Q:67:ASP:HB3	3:Q:95:ARG:HH22	1.76	0.49
6:T:97:ASN:O	6:T:101:ASN:ND2	2.45	0.49
8:V:236:ASN:ND2	12:L:241:ASP:OD2	2.44	0.49
10:X:99[B]:HIS:HA	10:X:120:TYR:HB2	1.95	0.49
11:Y:135:VAL:HG23	11:Y:164:ASP:HB3	1.93	0.49
12:Z:153:ASP:OD1	12:Z:157:SER:N	2.45	0.49
15:f:266:ILE:O	15:f:270:THR:HG23	2.13	0.49
11:K:66:LYS:HB3	11:K:71:VAL:HG22	1.94	0.49
11:K:67:PHE:CE2	11:K:69:HIS:HB2	2.48	0.49
11:K:94:ILE:HG13	11:K:115:GLU:OE2	2.13	0.49
12:L:40:ILE:HG23	12:L:83:SER:HB2	1.95	0.49
5:S:51:ARG:O	5:S:59:HIS:CD2	2.66	0.49
13:a:70:ASP:HA	13:a:232:PHE:HA	1.94	0.49
16:g:240:VAL:O	16:g:244:ARG:N	2.46	0.49
2:B:242:GLU:O	2:B:245:ALA:HB3	2.13	0.49
4:D:97:GLN:HB3	11:K:120:ARG:HG3	1.95	0.49
8:H:109:HIS:O	8:H:113:THR:HG23	2.13	0.49
2:P:201:MET:HE1	2:P:204:SER:OG	2.12	0.48
2:P:242:GLU:O	2:P:245:ALA:HB3	2.13	0.48
3:Q:14:GLY:O	3:Q:15:HIS:ND1	2.46	0.48
4:R:18:GLU:HG3	15:f:171:HIS:CE1	2.48	0.48
4:R:72:ALA:O	4:R:226:PHE:N	2.38	0.48
8:V:133:TYR:CD2	8:V:137:ILE:HD11	2.48	0.48
10:X:99[A]:HIS:HA	10:X:120:TYR:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:208:ILE:HG12	8:H:239:GLY:HA3	1.94	0.48
12:L:120:LEU:HA	12:L:123:ILE:HG22	1.95	0.48
13:M:225:ASP:HB3	13:M:228:SER:HB3	1.94	0.48
13:a:54:THR:HG23	13:a:55:SER:N	2.28	0.48
13:a:70:ASP:OD1	13:a:86:ARG:NH2	2.41	0.48
13:a:212[A]:ASP:HA	13:a:215:GLU:CD	2.38	0.48
14:b:79:ARG:HH21	14:b:79:ARG:HG3	1.78	0.48
15:f:16:ALA:HB2	16:g:23:SER:O	2.13	0.48
1:A:23:TYR:CE1	7:G:18:PRO:HA	2.48	0.48
6:F:215:TRP:HE1	6:F:220:THR:HG23	1.78	0.48
11:K:77:SER:CA	11:K:92:LYS:HZ1	2.26	0.48
12:L:45:GLY:HA3	12:L:48:PHE:CE1	2.46	0.48
3:Q:3:TYR:HB2	15:f:1:MET:SD	2.53	0.48
5:S:20:HIS:ND1	5:S:23:GLU:OE2	2.46	0.48
5:S:42:THR:HB	5:S:217:LYS:NZ	2.28	0.48
5:S:154:PHE:HB3	6:T:58:TYR:CE1	2.48	0.48
6:T:203:GLU:O	6:T:207:LYS:N	2.46	0.48
11:Y:85:ILE:HG13	11:Y:85:ILE:O	2.12	0.48
1:A:122:GLN:HB2	2:B:128:ARG:NH2	2.29	0.48
2:B:235:GLN:HA	2:B:238:LYS:NZ	2.28	0.48
3:C:94:HIS:ND1	3:C:102:VAL:HG12	2.28	0.48
7:U:230:LEU:HD22	7:U:234:GLU:CG	2.44	0.48
13:a:54:THR:HB	13:a:227:ARG:O	2.13	0.48
14:b:62:ASN:OD1	14:b:63:ARG:N	2.46	0.48
7:G:194:THR:O	7:G:196:GLU:N	2.47	0.48
10:J:186:ASN:O	10:J:189:HIS:NE2	2.47	0.48
11:K:97:ASN:O	11:K:243:TRP:NE1	2.43	0.48
12:L:109:LYS:NZ	12:L:110:ALA:O	2.39	0.48
2:P:228:LEU:HD23	2:P:232:GLU:HG3	1.94	0.48
2:P:235:GLN:HA	2:P:238:LYS:NZ	2.29	0.48
7:U:194:THR:O	7:U:196:GLU:N	2.46	0.48
13:a:190:LEU:C	13:a:193:PRO:HD2	2.38	0.48
14:b:124:TYR:HB3	14:b:125:ARG:NH2	2.28	0.48
1:A:202:MET:HE1	1:A:207:ILE:HD11	1.94	0.48
4:D:211:ASN:OD1	4:D:214:ASN:N	2.42	0.48
10:J:3:TYR:HD2	10:J:178:PHE:HE2	1.61	0.48
4:R:146:VAL:HA	4:R:150:GLY:O	2.13	0.48
10:X:165:GLU:OE2	11:K:200[A]:ARG:NH1	2.46	0.48
11:Y:98:PRO:HA	11:Y:243:TRP:HE1	1.77	0.48
11:Y:98:PRO:HA	11:Y:243:TRP:NE1	2.28	0.48
14:b:38:MET:HG2	14:b:160:ALA:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:b:93:VAL:O	14:b:97:LEU:HD23	2.13	0.48
16:g:21:ALA:HB3	16:g:122:SER:HA	1.95	0.48
16:g:73:ILE:O	16:g:91:ARG:NE	2.44	0.48
8:H:262:LEU:HB2	9:I:192:ASP:O	2.12	0.48
11:K:226:ASP:CG	11:K:228:TYR:H	2.22	0.48
1:O:66:PRO:HG2	8:V:111:LEU:HD11	1.96	0.48
1:O:186:ALA:HA	1:O:189:THR:HG22	1.95	0.48
5:S:156:CYS:HB2	6:T:58:TYR:CD1	2.48	0.48
6:T:6:GLY:HA3	16:g:209:SER:HB2	1.96	0.48
6:T:215:TRP:CZ3	6:T:227:VAL:HG22	2.48	0.48
8:V:103:SER:O	8:V:107:GLU:HG2	2.14	0.48
8:V:259:ILE:HG22	8:V:261:PRO:HD3	1.96	0.48
9:W:44:MET:HE2	9:W:66:LEU:HD22	1.96	0.48
1:A:158:LYS:NZ	2:B:56:LEU:O	2.38	0.48
1:A:186:ALA:HA	1:A:189:THR:HG22	1.95	0.48
2:B:228:LEU:HD23	2:B:232:GLU:HG3	1.94	0.48
3:C:14:GLY:O	3:C:15:HIS:ND1	2.46	0.48
6:F:141:SER:HB3	6:F:144:ASP:OD1	2.14	0.48
7:G:242:LEU:HA	7:G:245:ARG:HH12	1.79	0.48
9:I:11:MET:CE	9:I:166:ILE:HG13	2.44	0.48
9:I:24:ASP:N	9:I:170:MET:HE1	2.28	0.48
10:J:19:ARG:NH2	10:J:193:ASN:HD22	2.12	0.48
11:K:148:GLN:HA	11:K:148:GLN:OE1	2.13	0.48
12:L:56:ARG:HE	12:L:217:THR:C	2.21	0.48
3:Q:115:LYS:HZ2	3:Q:149:PRO:HA	1.78	0.48
6:T:16:PRO:O	7:U:30:LYS:HE2	2.14	0.48
6:T:64:LYS:HG3	6:T:67:PHE:CE1	2.42	0.48
11:Y:182:GLY:HA3	11:Y:185:PHE:CE1	2.49	0.48
12:Z:85:PHE:HD2	12:Z:88:ASP:H	1.60	0.48
13:a:134:HIS:NE2	13:a:176:ALA:HB1	2.29	0.48
14:b:69:THR:HB	14:b:77:CYS:SG	2.54	0.48
1:A:41:ASN:OD1	1:A:183:LEU:HB2	2.14	0.48
2:B:76:VAL:HG21	2:B:83:ALA:HB2	1.94	0.48
3:C:11:SER:O	4:D:26:TYR:HD2	1.97	0.48
5:E:181:GLU:OE1	5:E:181:GLU:N	2.46	0.48
7:G:112:ASP:OD1	7:G:113:MET:N	2.47	0.48
8:V:241:ARG:NH2	9:W:151:SER:HA	2.28	0.48
10:X:95:ARG:HA	10:X:95:ARG:NE	2.29	0.48
11:Y:172:TYR:HB2	11:Y:185:PHE:CE2	2.48	0.48
12:Z:66:ARG:HB3	12:Z:219:ASP:HB3	1.96	0.48
14:b:123:ARG:HB3	14:b:126:GLU:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:239:LYS:O	2:B:242:GLU:HG3	2.14	0.48
7:G:196:GLU:HB3	7:G:242:LEU:HD11	1.96	0.48
8:H:72:LYS:NZ	9:I:150:GLU:OE2	2.45	0.48
1:O:23:TYR:CE1	7:U:18:PRO:HA	2.49	0.48
3:Q:94:HIS:ND1	3:Q:102:VAL:HG12	2.28	0.48
7:U:196:GLU:HB3	7:U:242:LEU:HD11	1.96	0.48
9:W:10:VAL:HG23	9:W:53:ALA:HB2	1.95	0.48
14:b:36:THR:HG22	14:b:165:GLY:HA3	1.95	0.48
16:g:141:TYR:HB3	16:g:223:TYR:OH	2.14	0.48
6:F:7:TYR:HA	7:G:11:ARG:NH2	2.29	0.48
6:F:70:ASP:HB3	6:F:73:VAL:HG12	1.96	0.48
6:F:72:HIS:CE1	6:F:105:ASN:HB3	2.49	0.48
11:K:201:GLY:HA3	11:K:214:LEU:HD13	1.95	0.48
13:M:238:THR:OG1	13:M:239:GLU:OE1	2.32	0.48
2:P:143:TYR:CD2	3:Q:57:ARG:NH2	2.82	0.47
4:R:175:GLU:OE1	15:f:117:THR:OG1	2.31	0.47
15:f:143:GLU:OE1	15:f:143:GLU:N	2.44	0.47
16:g:141:TYR:O	16:g:142:LEU:HD22	2.14	0.47
16:g:165:LYS:HE3	16:g:177:PHE:CD2	2.44	0.47
1:A:16:GLY:O	2:B:27:ALA:HB2	2.14	0.47
4:D:41:GLN:HE21	4:D:151:PRO:C	2.22	0.47
5:E:185:ASN:O	5:E:189:LYS:HG3	2.13	0.47
8:H:132:ARG:C	8:H:134:GLN:H	2.22	0.47
11:K:98:PRO:HA	11:K:243:TRP:NE1	2.28	0.47
14:N:148:VAL:CG2	14:N:153:MET:HG2	2.44	0.47
2:P:239:LYS:O	2:P:242:GLU:HG3	2.14	0.47
3:Q:24:GLU:HA	3:Q:27:LYS:HE2	1.95	0.47
4:R:16:SER:HB2	4:R:22:PHE:HE1	1.80	0.47
4:R:35:SER:HA	4:R:53:ARG:HH11	1.79	0.47
4:R:125:GLU:O	4:R:128:ALA:N	2.46	0.47
5:S:51:ARG:O	5:S:59:HIS:HD2	1.98	0.47
7:U:5:SER:C	15:f:10:VAL:HG23	2.40	0.47
16:g:79:SER:HB3	16:g:86:VAL:HG23	1.95	0.47
3:C:157:LYS:NZ	4:D:58:LEU:HA	2.29	0.47
8:H:96:ASP:O	8:H:100:GLN:HG3	2.14	0.47
8:H:154:TYR:CE1	8:H:164:LYS:HB2	2.49	0.47
3:Q:64:ALA:HA	3:Q:70:CYS:HA	1.94	0.47
4:R:42:THR:HG21	4:R:189:MET:HB3	1.96	0.47
5:S:99:PHE:HE1	13:a:136:TRP:HD1	1.61	0.47
7:U:91:VAL:O	7:U:95:ARG:HG3	2.14	0.47
1:A:152:GLY:C	2:B:81:SER:HB3	2.38	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:171:TYR:HA	5:E:174:ARG:HG2	1.97	0.47
9:I:60:GLN:O	9:I:64:GLN:HG3	2.14	0.47
10:J:171:PHE:CE2	10:J:173:LEU:HB2	2.49	0.47
13:M:169:TYR:O	13:M:176:ALA:HA	2.15	0.47
12:Z:174:GLN:HE22	9:I:176:ARG:NH2	2.12	0.47
15:f:77:ASN:OD1	15:f:78:ASN:N	2.48	0.47
15:f:218:ALA:HB2	16:g:54:PRO:HG3	1.96	0.47
16:g:74:ASN:OD1	16:g:75:ALA:N	2.47	0.47
1:A:80:PRO:HA	1:A:83:ARG:HH21	1.79	0.47
2:B:76:VAL:HG21	2:B:83:ALA:HB1	1.95	0.47
2:B:91:ARG:NH1	9:I:75:LEU:O	2.47	0.47
2:B:222:LYS:HA	2:B:222:LYS:HD2	1.53	0.47
4:D:35:SER:HA	4:D:53:ARG:HH11	1.79	0.47
6:F:6:GLY:O	7:G:11:ARG:NH1	2.47	0.47
6:F:83:ASP:OD2	6:F:131:PHE:HB3	2.14	0.47
11:K:67:PHE:HE1	11:K:72:ILE:HG23	1.80	0.47
11:K:150:LYS:HZ2	11:K:176:GLU:HB2	1.79	0.47
13:M:61:PHE:HE2	13:M:66:VAL:HG13	1.78	0.47
14:N:38:MET:HE1	14:N:190:THR:HA	1.97	0.47
2:P:143:TYR:OH	10:X:73:TYR:HD2	1.97	0.47
2:P:222:LYS:HD2	2:P:223:THR:H	1.79	0.47
4:R:88:LEU:HD22	4:R:116:VAL:HG13	1.97	0.47
6:T:108:LEU:HD21	6:T:139:SER:CB	2.43	0.47
9:W:134:ASP:OD1	9:W:135:PHE:N	2.45	0.47
13:a:212[B]:ASP:HA	13:a:215:GLU:CD	2.38	0.47
16:g:55:MET:SD	16:g:91:ARG:HD2	2.54	0.47
2:B:222:LYS:HD2	2:B:223:THR:H	1.79	0.47
5:E:5:GLN:HB3	6:F:9:LEU:HD11	1.96	0.47
10:J:42:ILE:HG23	10:J:104:LEU:HD11	1.96	0.47
11:K:61:THR:HG22	11:K:219:ILE:HD12	1.96	0.47
14:N:35:THR:HG22	14:N:164:SER:H	1.80	0.47
1:O:143:PRO:O	1:O:144:TYR:HD1	1.98	0.47
6:T:6:GLY:HA2	16:g:210:GLU:H	1.79	0.47
15:f:171:HIS:NE2	15:f:240:MET:HG2	2.28	0.47
5:E:89:ARG:NH1	12:L:105:HIS:HB3	2.30	0.47
5:E:185:ASN:OD1	5:E:186:GLU:N	2.47	0.47
9:I:23:ALA:C	9:I:170:MET:HE1	2.39	0.47
11:K:56:MET:HE1	11:K:110:ASP:OD2	2.14	0.47
13:M:67:ILE:HG12	13:M:95:MET:HE1	1.95	0.47
13:M:89:ARG:HG3	13:M:242:VAL:HB	1.95	0.47
3:Q:206:ILE:O	3:Q:206:ILE:HG13	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:5:ARG:HG3	15:f:14:CYS:CA	2.43	0.47
5:S:47:VAL:HG22	5:S:212:ILE:HD12	1.97	0.47
5:S:88:MET:HA	5:S:88:MET:HE2	1.96	0.47
5:S:237:GLU:OE1	5:S:237:GLU:N	2.41	0.47
6:T:87:LEU:HD23	6:T:90:ILE:HD12	1.96	0.47
6:T:172:ALA:HA	6:T:200:VAL:HG11	1.97	0.47
7:U:242:LEU:HA	7:U:245:ARG:HH12	1.79	0.47
8:V:57:LEU:HD23	8:V:87:CYS:SG	2.54	0.47
8:V:189:MET:HA	8:V:189:MET:HE3	1.97	0.47
11:Y:174:ASP:OD1	11:Y:178:ASN:N	2.45	0.47
11:Y:201:GLY:HA3	11:Y:214:LEU:HD13	1.96	0.47
14:b:133:ILE:O	14:b:133:ILE:HG13	2.14	0.47
15:f:2:ALA:O	15:f:3:ALA:HB3	2.15	0.47
15:f:244:LEU:O	15:f:247:VAL:HB	2.15	0.47
16:g:167:ARG:HH21	16:g:177:PHE:N	2.13	0.47
2:B:241:GLU:HA	2:B:244:GLU:OE1	2.15	0.47
3:C:44:GLY:HA2	3:C:208:LEU:HB3	1.97	0.47
3:C:206:ILE:O	3:C:206:ILE:HG13	2.15	0.47
4:D:88:LEU:HD22	4:D:116:VAL:HG13	1.97	0.47
5:E:196:ARG:HG2	5:E:239:ARG:NH2	2.29	0.47
7:G:91:VAL:O	7:G:95:ARG:HG3	2.14	0.47
9:I:26:ARG:HB2	9:I:181:GLY:O	2.15	0.47
10:J:38:MET:HA	10:J:61:GLN:OE1	2.14	0.47
11:K:56:MET:O	11:K:57:LEU:HG	2.15	0.47
12:L:144:GLU:N	12:L:144:GLU:OE2	2.48	0.47
12:L:212:GLU:CD	12:L:213:ARG:HG2	2.40	0.47
1:O:41:ASN:OD1	1:O:183:LEU:HB2	2.14	0.47
4:R:143:PHE:O	4:R:153:LEU:HA	2.15	0.47
7:U:112:ASP:OD1	7:U:113:MET:N	2.47	0.47
10:X:172:ILE:HG23	10:X:173:LEU:HD22	1.96	0.47
14:b:106:GLU:HG2	14:b:107:PRO:HD2	1.97	0.47
2:B:70:GLU:HA	2:B:70:GLU:OE2	2.14	0.47
2:B:151:ASP:OD2	2:B:153:SER:OG	2.33	0.47
5:E:55:GLU:OE1	5:E:55:GLU:N	2.48	0.47
2:P:18:LEU:O	2:P:22:GLU:HG3	2.15	0.47
4:R:41:GLN:HE21	4:R:151:PRO:C	2.22	0.47
7:U:77:GLY:HA3	7:U:227:PHE:CE2	2.49	0.47
9:W:95:TYR:CE1	9:W:98:ARG:HD3	2.50	0.47
11:Y:220:TYR:HD2	11:Y:221:GLN:OE1	1.98	0.47
13:a:71:MET:HE2	13:a:71:MET:HB2	1.62	0.47
15:f:134:LEU:HB3	15:f:136:GLN:HE21	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:119:GLU:CD	13:M:127:SER:HA	2.40	0.47
14:N:117:PHE:CD2	14:N:134:ILE:HD11	2.49	0.47
3:Q:14:GLY:HA3	4:R:30:ALA:HB2	1.95	0.47
3:Q:65:LEU:HD13	3:Q:88:ARG:HG3	1.97	0.47
5:S:112:ILE:O	5:S:116:THR:HG23	2.15	0.47
6:T:169:ARG:HG3	6:T:173:LYS:NZ	2.30	0.47
11:Y:181:SER:OG	11:Y:182:GLY:N	2.48	0.47
12:Z:120:LEU:HA	12:Z:123:ILE:HG22	1.97	0.47
15:f:72:ILE:HG23	15:f:165:THR:HB	1.96	0.47
16:g:20:PRO:HB2	16:g:29:GLN:NE2	2.29	0.47
3:C:15:HIS:O	3:C:16:LEU:C	2.58	0.47
3:C:118:TYR:CD1	3:C:124:ARG:HD3	2.50	0.47
4:D:42:THR:HG21	4:D:189:MET:HB3	1.96	0.47
7:G:77:GLY:HA3	7:G:227:PHE:CE2	2.49	0.47
7:G:210:PHE:CD2	7:G:215:ILE:HD11	2.49	0.47
7:G:230:LEU:HD22	7:G:234:GLU:CG	2.44	0.47
8:H:76:LYS:HB3	8:H:78:HIS:CE1	2.50	0.47
11:K:150:LYS:NZ	11:K:176:GLU:HB2	2.30	0.47
12:L:127:ARG:HH11	12:L:127:ARG:HG3	1.80	0.47
13:M:80:ARG:HG3	14:N:170:TYR:OH	2.15	0.47
14:N:96:GLN:HB3	14:N:116:LEU:HD21	1.97	0.47
14:N:138:ASP:OD2	14:N:141:GLU:HG2	2.15	0.47
2:P:76:VAL:HG21	2:P:83:ALA:HB1	1.95	0.46
8:V:124:ARG:HD3	8:V:128:GLN:OE1	2.15	0.46
11:Y:239:ARG:HH21	11:Y:244:ILE:HG23	1.79	0.46
12:Z:100:LEU:HA	12:Z:111:MET:HE3	1.96	0.46
4:D:16:SER:HB2	4:D:22:PHE:HE1	1.80	0.46
7:G:45:LYS:H	7:G:45:LYS:HG3	1.37	0.46
7:G:189:TRP:NE1	7:G:197:THR:HG21	2.29	0.46
11:K:118:LEU:HD12	11:K:142:LEU:HB2	1.97	0.46
2:P:70:GLU:HA	2:P:70:GLU:OE2	2.14	0.46
3:Q:118:TYR:CD1	3:Q:124:ARG:HD3	2.50	0.46
5:S:43:HIS:ND1	5:S:184:LEU:HD13	2.30	0.46
9:W:52:LEU:HB3	9:W:59:VAL:HG22	1.97	0.46
11:Y:219:ILE:O	11:Y:223:THR:HG22	2.16	0.46
2:B:71:ASP:O	2:B:225:ILE:HD11	2.16	0.46
13:M:52:THR:HA	13:M:100:GLY:O	2.15	0.46
14:N:225:GLY:O	14:N:228:ILE:HG12	2.15	0.46
1:O:80:PRO:HA	1:O:83:ARG:HH21	1.79	0.46
2:P:119:GLN:NE2	3:Q:79:ASP:OD1	2.34	0.46
3:Q:5:ARG:NH2	15:f:2:ALA:HB3	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:f:121:CYS:CA	15:f:137:CYS:HB3	2.44	0.46
1:A:31:GLY:O	1:A:164:LYS:HG2	2.15	0.46
4:D:232:GLU:OE1	4:D:232:GLU:N	2.43	0.46
5:E:207:THR:HG21	5:E:227:ASP:HA	1.97	0.46
8:H:153:LEU:HD21	8:H:168:VAL:HG22	1.96	0.46
13:M:167:LEU:HG	13:M:182:LEU:HD12	1.96	0.46
13:M:229:TYR:CE2	13:M:231:ARG:HG3	2.50	0.46
3:Q:156:TRP:CE3	4:R:59:MET:HG3	2.50	0.46
6:T:187:ARG:NH1	6:T:219:LEU:HD22	2.31	0.46
6:T:191:LYS:HB3	6:T:238:TYR:CD2	2.50	0.46
7:U:231:THR:O	7:U:235:ILE:N	2.32	0.46
15:f:83:LEU:HD11	15:f:167:LEU:HD13	1.98	0.46
15:f:176:LYS:H	15:f:210:ASN:ND2	2.13	0.46
15:f:178:SER:HB3	16:g:252:ARG:HH22	1.79	0.46
4:D:200:ILE:HD11	4:D:241:ILE:OXT	2.16	0.46
6:F:161:TRP:HB2	7:G:60:LEU:O	2.16	0.46
7:G:113:MET:HA	7:G:113:MET:CE	2.46	0.46
14:N:70:PRO:HB3	14:N:76:PHE:CZ	2.49	0.46
3:Q:44:GLY:HA2	3:Q:208:LEU:HB3	1.96	0.46
4:R:5:ARG:O	5:S:4:ASN:CG	2.58	0.46
4:R:108:THR:O	4:R:112:VAL:HG23	2.15	0.46
5:S:61:LYS:HA	5:S:61:LYS:HD2	1.63	0.46
7:U:210:PHE:CD2	7:U:215:ILE:HD11	2.49	0.46
1:A:143:PRO:O	1:A:144:TYR:HD1	1.98	0.46
4:D:125:GLU:O	4:D:128:ALA:N	2.47	0.46
5:E:146:GLN:HG2	5:E:147:THR:N	2.30	0.46
5:E:176:MET:HA	5:E:179:PHE:CD2	2.51	0.46
7:G:6:SER:HB3	7:G:11:ARG:HD2	1.98	0.46
10:J:23:SER:OG	10:J:24:ASN:N	2.48	0.46
1:O:60:SER:HB2	7:U:152:TYR:OH	2.14	0.46
2:P:60:PHE:O	2:P:62:SER:N	2.45	0.46
2:P:71:ASP:O	2:P:225:ILE:HD11	2.16	0.46
4:R:209:LYS:HG2	4:R:210:LEU:H	1.81	0.46
5:S:39:LYS:HD2	5:S:142:PRO:HB2	1.97	0.46
5:S:110:SER:HA	5:S:153:TYR:HE2	1.80	0.46
6:T:23:VAL:O	6:T:27:MET:HG2	2.16	0.46
6:T:101:ASN:OD1	6:T:102:PHE:N	2.48	0.46
7:U:113:MET:HA	7:U:113:MET:CE	2.46	0.46
8:V:62:ARG:HG2	8:V:63:ALA:N	2.30	0.46
10:X:2:GLU:HB2	10:X:47:VAL:CG2	2.46	0.46
3:C:65:LEU:HD13	3:C:88:ARG:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:166:ASP:O	5:E:56:LEU:HB3	2.16	0.46
5:E:67:ASP:OD2	5:E:92:CYS:HB3	2.16	0.46
5:E:114:SER:O	5:E:118:ILE:HG12	2.15	0.46
8:H:186:ARG:NH1	8:H:189:MET:HE1	2.30	0.46
12:L:56:ARG:HD2	12:L:216:TYR:C	2.41	0.46
13:M:91:ASN:OD1	13:M:94:THR:HB	2.16	0.46
2:P:90:LEU:HD11	2:P:114:LEU:HD22	1.98	0.46
3:Q:226:GLU:CB	3:Q:229:VAL:HG22	2.45	0.46
4:R:147:ASP:C	4:R:150:GLY:H	2.23	0.46
7:U:6:SER:HB3	7:U:11:ARG:HD2	1.98	0.46
13:a:89:ARG:HB2	13:a:244:ILE:HD11	1.96	0.46
4:D:73:HIS:HB2	4:D:146:VAL:HG12	1.98	0.46
14:N:36:THR:HG21	14:N:197:ALA:CB	2.46	0.46
14:N:132:ILE:CG2	14:N:148:VAL:HG13	2.46	0.46
1:O:226:LYS:HE2	1:O:226:LYS:HA	1.98	0.46
2:P:241:GLU:HA	2:P:244:GLU:OE1	2.15	0.46
3:Q:15:HIS:O	3:Q:16:LEU:C	2.58	0.46
5:S:50:LYS:HG3	5:S:62:LYS:NZ	2.31	0.46
13:a:153:ASN:HD22	13:a:155:MET:HE3	1.81	0.46
15:f:151:GLU:HA	15:f:155:GLY:H	1.81	0.46
4:D:209:LYS:HG2	4:D:210:LEU:H	1.81	0.46
7:G:194:THR:HG22	7:G:195:VAL:N	2.26	0.46
9:I:92:ASN:O	9:I:95:TYR:N	2.43	0.46
12:L:111:MET:HE1	12:L:119:MET:SD	2.56	0.46
13:M:65:VAL:HG11	13:M:167:LEU:HD13	1.97	0.46
1:O:31:GLY:O	1:O:164:LYS:HG2	2.15	0.46
4:R:73:HIS:O	4:R:145:GLY:HA2	2.16	0.46
5:S:62:LYS:HE2	5:S:62:LYS:HB2	1.78	0.46
5:S:189:LYS:HE2	5:S:236:LEU:HA	1.98	0.46
7:U:242:LEU:HA	7:U:245:ARG:NH1	2.31	0.46
15:f:18:THR:O	15:f:18:THR:HG22	2.16	0.46
15:f:273:LEU:HB3	15:f:277:MET:HE1	1.97	0.46
16:g:36:ILE:HA	16:g:41:MET:HE2	1.97	0.46
4:D:163:VAL:HG23	4:D:165:CYS:HB3	1.98	0.46
6:F:40:ARG:HA	6:F:45:VAL:HG12	1.97	0.46
6:F:51:LYS:HD2	6:F:212:GLU:CD	2.40	0.46
13:M:60:LYS:N	13:M:180:PRO:O	2.39	0.46
14:N:198:MET:SD	14:N:205:GLY:HA2	2.56	0.46
1:O:83:ARG:NH2	1:O:83:ARG:CB	2.76	0.46
5:S:16:GLN:HA	6:T:28:LYS:NZ	2.31	0.46
5:S:171:TYR:HA	5:S:174:ARG:NH2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:194:THR:HG22	7:U:195:VAL:N	2.26	0.46
8:V:157:TYR:HB2	8:V:161:SER:OG	2.16	0.46
10:X:25:ILE:HB	10:J:171:PHE:HE1	1.81	0.46
5:E:147:THR:HG22	5:E:153:TYR:HB3	1.97	0.46
10:J:146:TYR:CE2	10:J:162:LYS:HE2	2.51	0.46
11:K:59:GLY:O	11:K:189:SER:N	2.40	0.46
1:O:98:LEU:HD23	8:V:100:GLN:HG2	1.98	0.45
3:Q:47:LYS:O	3:Q:49:SER:N	2.44	0.45
4:R:200:ILE:HD11	4:R:241:ILE:OXT	2.16	0.45
5:S:17:GLY:O	6:T:32:ASN:ND2	2.49	0.45
5:S:89:ARG:CZ	12:Z:105:HIS:HB3	2.45	0.45
6:T:172:ALA:O	6:T:176:ILE:HG13	2.17	0.45
14:b:174:ASP:OD2	14:N:200:ARG:NE	2.31	0.45
1:A:14:PRO:HA	2:B:23:TYR:CE1	2.52	0.45
3:C:68:ASN:ND2	3:C:102:VAL:O	2.50	0.45
4:D:143:PHE:O	4:D:153:LEU:HA	2.15	0.45
7:G:37:LEU:HA	7:G:53:GLN:OE1	2.17	0.45
12:L:41:LEU:HD13	12:L:165:ALA:HB2	1.98	0.45
5:S:107:ARG:NH2	13:a:126:HIS:HB2	2.30	0.45
7:U:189:TRP:NE1	7:U:197:THR:HG21	2.29	0.45
7:U:212:PRO:HB3	7:U:235:ILE:HG22	1.98	0.45
9:W:176:ARG:HD2	9:W:176:ARG:HA	1.69	0.45
10:X:66:LEU:O	10:X:70:ARG:HG3	2.16	0.45
11:Y:174:ASP:CG	11:Y:178:ASN:HB2	2.42	0.45
1:A:226:LYS:HE2	1:A:226:LYS:HA	1.98	0.45
2:B:18:LEU:O	2:B:22:GLU:HG3	2.15	0.45
2:B:27:ALA:O	2:B:31:ALA:N	2.49	0.45
4:D:108:THR:O	4:D:112:VAL:HG23	2.15	0.45
7:G:242:LEU:HA	7:G:245:ARG:NH1	2.31	0.45
11:K:53:GLY:HA2	12:L:154:PRO:HG2	1.98	0.45
11:K:79:ALA:CB	11:K:86:ALA:HB3	2.46	0.45
14:N:82:SER:O	14:N:86:THR:OG1	2.25	0.45
3:Q:166:LYS:O	3:Q:169:ARG:N	2.50	0.45
4:R:166:ASP:N	4:R:166:ASP:OD1	2.49	0.45
7:U:18:PRO:HD2	16:g:131:ASP:CG	2.41	0.45
12:Z:109:LYS:HZ2	12:Z:111:MET:HA	1.81	0.45
13:a:57:LEU:HD12	13:a:195:LEU:HD11	1.98	0.45
14:b:123:ARG:NE	14:b:151:GLY:O	2.50	0.45
6:F:108:LEU:HD23	6:F:147:GLN:HB2	1.98	0.45
8:H:161:SER:OG	14:N:83:ALA:HB3	2.17	0.45
11:K:97:ASN:C	11:K:99:TYR:H	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:125:GLU:HB2	4:R:128:ALA:HB3	1.97	0.45
5:S:99:PHE:HE1	13:a:136:TRP:CD1	2.35	0.45
10:X:45:LEU:HB2	10:X:103:LEU:HB2	1.97	0.45
12:Z:125:TYR:O	12:Z:128:ARG:N	2.50	0.45
2:B:134:LEU:O	2:B:150:SER:N	2.46	0.45
14:N:74:ARG:NH1	14:N:214:ALA:O	2.48	0.45
14:N:184:GLU:HG3	14:N:185:GLU:N	2.30	0.45
1:O:224:GLU:HA	1:O:227:ASP:HB2	1.99	0.45
2:P:27:ALA:O	2:P:31:ALA:N	2.49	0.45
2:P:97:TYR:CE2	2:P:105:ILE:HA	2.52	0.45
3:Q:68:ASN:ND2	3:Q:102:VAL:O	2.50	0.45
3:Q:92:GLN:HG3	10:X:66:LEU:HB2	1.98	0.45
5:S:166:GLN:OE1	5:S:169:ARG:NH2	2.40	0.45
6:T:83:ASP:OD2	6:T:129:ARG:NH2	2.49	0.45
9:W:11:MET:N	9:W:22:ALA:O	2.40	0.45
10:X:53:THR:HG22	10:X:100:VAL:HG12	1.98	0.45
15:f:16:ALA:HB1	16:g:22:VAL:CG1	2.46	0.45
16:g:110:VAL:O	16:g:114:GLY:N	2.30	0.45
1:A:28:VAL:HG22	1:A:131:VAL:HA	1.99	0.45
1:A:28:VAL:HG21	1:A:150:PRO:HG2	1.99	0.45
4:D:73:HIS:O	4:D:145:GLY:HA2	2.16	0.45
4:D:107:MET:HE2	4:D:112:VAL:HA	1.98	0.45
6:F:114:ARG:O	6:F:117:MET:HG3	2.17	0.45
2:P:241:GLU:HA	2:P:244:GLU:CD	2.41	0.45
4:R:31:ILE:O	4:R:34:GLY:N	2.29	0.45
5:S:208:LYS:HA	5:S:208:LYS:HD2	1.66	0.45
6:T:12:SER:HA	7:U:132:ARG:HB2	1.99	0.45
9:W:89:MET:HA	9:W:92:ASN:ND2	2.32	0.45
10:X:38:MET:HB2	10:X:42:ILE:HB	1.98	0.45
2:B:91:ARG:HD3	9:I:75:LEU:HB3	1.98	0.45
3:C:166:LYS:O	3:C:169:ARG:N	2.50	0.45
5:E:52:ALA:HA	5:E:59:HIS:CE1	2.52	0.45
10:J:116:TYR:HD2	10:J:124:LEU:HD21	1.82	0.45
13:M:56:VAL:HG23	13:M:99:SER:HB3	1.99	0.45
13:M:88:MET:SD	13:M:109:LYS:HG3	2.57	0.45
4:R:107:MET:HE2	4:R:112:VAL:HA	1.98	0.45
1:A:68:THR:OG1	1:A:70:HIS:ND1	2.50	0.45
1:A:224:GLU:HA	1:A:227:ASP:HB2	1.99	0.45
2:B:198:ASN:HD22	2:B:240:HIS:CE1	2.35	0.45
4:D:125:GLU:HB2	4:D:128:ALA:HB3	1.98	0.45
4:D:166:ASP:N	4:D:166:ASP:OD1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:171:ALA:O	6:F:174:THR:OG1	2.31	0.45
7:G:144:ASP:OD1	7:G:144:ASP:N	2.45	0.45
7:G:231:THR:O	7:G:235:ILE:N	2.32	0.45
8:H:56:VAL:HG22	8:H:220:VAL:HG13	1.98	0.45
8:H:132:ARG:HG3	8:H:133:TYR:H	1.81	0.45
11:K:59:GLY:HA2	11:K:106:GLY:H	1.82	0.45
13:M:116:VAL:O	13:M:120:GLU:HG2	2.17	0.45
2:P:139:TRP:CE2	2:P:218:ARG:NH1	2.85	0.45
6:T:98:PHE:O	6:T:102:PHE:HB2	2.17	0.45
7:U:76:ILE:HD12	7:U:111:VAL:HG22	1.99	0.45
7:U:186:LYS:NZ	7:U:189:TRP:H	2.15	0.45
13:a:95:MET:HE1	13:a:236:THR:C	2.42	0.45
15:f:80:VAL:CG2	15:f:136:GLN:HB3	2.46	0.45
15:f:150:LEU:HD12	15:f:222:TYR:HD2	1.81	0.45
15:f:243:ASP:O	15:f:247:VAL:HG23	2.17	0.45
2:B:90:LEU:HD11	2:B:114:LEU:HD22	1.98	0.45
2:B:97:TYR:CE2	2:B:105:ILE:HA	2.52	0.45
2:B:139:TRP:CE2	2:B:218:ARG:NH1	2.85	0.45
2:B:241:GLU:HA	2:B:244:GLU:CD	2.41	0.45
4:D:91:LYS:HZ2	4:D:119:LEU:HD13	1.81	0.45
4:D:224:GLN:OE1	4:D:225:ASN:N	2.50	0.45
5:E:133:LEU:HD23	5:E:133:LEU:HA	1.79	0.45
6:F:6:GLY:O	7:G:11:ARG:NH2	2.50	0.45
6:F:228:PRO:HG2	6:F:231:ILE:HD12	1.97	0.45
11:K:162:GLY:O	11:K:169:GLY:N	2.50	0.45
4:R:7:GLU:N	5:S:8:ASN:HD22	2.15	0.45
4:R:41:GLN:NE2	4:R:151:PRO:O	2.48	0.45
4:R:85:ALA:O	4:R:89:ILE:HG12	2.17	0.45
6:T:214:SER:HA	6:T:227:VAL:HG23	1.99	0.45
6:T:238:TYR:HA	6:T:241:GLU:HG2	1.97	0.45
10:X:26:VAL:HG11	11:Y:195:TYR:HE2	1.82	0.45
1:A:60:SER:HB2	7:G:152:TYR:OH	2.17	0.45
4:D:85:ALA:O	4:D:89:ILE:HG12	2.17	0.45
4:D:147:ASP:C	4:D:150:GLY:H	2.23	0.45
5:E:71:GLY:HA3	5:E:221:PHE:CZ	2.52	0.45
5:E:88:MET:SD	5:E:112:ILE:HD11	2.56	0.45
5:E:174:ARG:HE	5:E:175:HIS:CE1	2.34	0.45
8:H:155:SER:HB2	8:H:170[A]:MET:HE2	1.99	0.45
9:I:14:LYS:HD3	9:I:133:ASP:O	2.17	0.45
11:K:172:TYR:O	11:K:179:ARG:HA	2.17	0.45
14:N:141:GLU:HG3	14:N:144:GLN:NE2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:149:ASP:OD1	1:O:150:PRO:HD2	2.17	0.45
6:T:196:ILE:O	6:T:200:VAL:HG22	2.16	0.45
7:U:45:LYS:H	7:U:45:LYS:HG3	1.37	0.45
8:V:102:ILE:O	8:V:106:LEU:HD23	2.17	0.45
9:W:132:THR:HG21	9:W:135:PHE:O	2.17	0.45
15:f:216:PRO:HB2	15:f:232:LEU:HD11	1.98	0.45
3:C:111:ILE:O	3:C:115:LYS:HG3	2.16	0.45
7:G:183:VAL:HA	7:G:189:TRP:HH2	1.82	0.45
12:L:229:GLU:OE1	12:L:229:GLU:N	2.49	0.45
4:R:224:GLN:OE1	4:R:225:ASN:N	2.50	0.44
6:T:215:TRP:CH2	6:T:228:PRO:HD2	2.52	0.44
7:U:24:GLN:HA	7:U:27:TYR:HD2	1.82	0.44
7:U:142:GLY:O	7:U:149:PRO:HA	2.17	0.44
7:U:238:HIS:O	7:U:242:LEU:HD23	2.17	0.44
2:B:238:LYS:O	2:B:241:GLU:HG3	2.17	0.44
5:E:43:HIS:CD2	5:E:216:GLY:HA3	2.52	0.44
6:F:118:TYR:CE2	6:F:122:TYR:HE2	2.35	0.44
6:F:140:TYR:HA	6:F:146:ALA:HA	1.99	0.44
10:J:4:LEU:HD22	10:J:45:LEU:HD12	1.98	0.44
10:J:22:ALA:HA	10:J:26:VAL:O	2.16	0.44
10:J:60:ILE:HA	10:J:63:ASN:HD22	1.82	0.44
14:N:89:VAL:HG12	14:N:117:PHE:CE1	2.52	0.44
1:O:78:MET:HE3	1:O:78:MET:HB2	1.76	0.44
4:R:15:PHE:CE1	5:S:126:ARG:HD2	2.52	0.44
8:V:170[B]:MET:HB3	8:V:170[B]:MET:HE2	1.66	0.44
9:W:11:MET:HG3	9:W:12:ALA:N	2.31	0.44
10:X:88:LEU:HA	10:X:91:CYS:SG	2.57	0.44
13:a:179:ALA:HB3	13:a:182:LEU:HD21	2.00	0.44
13:a:186:TYR:HA	13:a:189:TYR:HD2	1.82	0.44
15:f:171:HIS:CD2	15:f:240:MET:HE2	2.53	0.44
16:g:119:ILE:HG12	16:g:202:ALA:HB3	1.99	0.44
1:A:70:HIS:HD1	1:A:71:ILE:HG12	1.81	0.44
1:A:149:ASP:OD1	1:A:150:PRO:HD2	2.17	0.44
2:B:180:LYS:HB3	2:B:183:GLU:OE1	2.17	0.44
4:D:161:THR:HG22	5:E:78:THR:HB	1.99	0.44
7:G:24:GLN:HA	7:G:27:TYR:HD2	1.82	0.44
7:G:142:GLY:O	7:G:149:PRO:HA	2.17	0.44
10:J:116:TYR:CD2	10:J:124:LEU:HD21	2.52	0.44
11:K:65:PHE:CD1	11:K:198:MET:HE3	2.53	0.44
12:Z:54:ASP:OD1	12:Z:54:ASP:N	2.49	0.44
14:b:55:THR:OG1	14:b:57:GLY:O	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:b:200:ARG:NH1	13:M:79:ALA:O	2.45	0.44
2:B:60:PHE:O	2:B:62:SER:N	2.45	0.44
5:E:158:ALA:O	5:E:159:MET:HB2	2.18	0.44
7:G:212:PRO:HB3	7:G:235:ILE:HG22	1.98	0.44
7:G:238:HIS:O	7:G:242:LEU:HD23	2.17	0.44
10:J:169:LYS:HD2	10:J:169:LYS:O	2.17	0.44
11:K:186:SER:HB3	11:K:195:TYR:CE1	2.52	0.44
1:O:70:HIS:HD1	1:O:71:ILE:HG12	1.81	0.44
2:P:198:ASN:HD22	2:P:240:HIS:CE1	2.35	0.44
4:R:191:LEU:HD12	4:R:191:LEU:HA	1.80	0.44
6:T:70:ASP:OD1	6:T:73:VAL:HG22	2.16	0.44
11:Y:96:ILE:HG23	11:Y:119:ALA:HB2	1.99	0.44
12:Z:31:SER:HB3	12:Z:33:TYR:CD2	2.52	0.44
14:b:112:THR:O	14:b:116:LEU:HD12	2.17	0.44
3:C:116:GLN:HB2	4:D:83:ALA:HB1	1.98	0.44
5:E:120:THR:HG22	6:F:129:ARG:HH21	1.83	0.44
5:E:207:THR:CG2	5:E:227:ASP:HA	2.48	0.44
6:F:51:LYS:HD2	6:F:212:GLU:OE1	2.17	0.44
6:F:215:TRP:CZ3	6:F:227:VAL:HG22	2.53	0.44
11:K:219:ILE:HG21	11:K:233:VAL:CG1	2.46	0.44
1:O:9:LEU:HD22	1:O:128:PRO:HD3	2.00	0.44
1:O:68:THR:OG1	1:O:70:HIS:ND1	2.50	0.44
3:Q:51:ALA:O	3:Q:53:LEU:N	2.51	0.44
3:Q:55:ASP:OD1	3:Q:57:ARG:HB3	2.18	0.44
3:Q:138:PHE:CD1	3:Q:139:ASP:N	2.80	0.44
5:S:196:ARG:O	5:S:239:ARG:NH2	2.51	0.44
7:U:21:ARG:CB	7:U:21:ARG:NH1	2.78	0.44
7:U:128:ASN:HB2	7:U:131:MET:HG2	2.00	0.44
7:U:183:VAL:HA	7:U:189:TRP:HH2	1.82	0.44
11:Y:184:THR:HB	11:Y:198:MET:SD	2.58	0.44
15:f:286:ILE:HG23	15:f:288:THR:N	2.26	0.44
2:B:8:ARG:O	2:B:10:THR:OG1	2.36	0.44
6:F:35:THR:HG21	6:F:168:ALA:HB3	1.99	0.44
2:P:109:GLN:HE21	10:X:71:ASN:CG	2.26	0.44
2:P:134:LEU:HB2	2:P:150:SER:HB3	2.00	0.44
2:P:180:LYS:HB3	2:P:183:GLU:OE1	2.17	0.44
6:T:203:GLU:N	6:T:203:GLU:OE1	2.51	0.44
7:U:37:LEU:HA	7:U:53:GLN:OE1	2.17	0.44
12:Z:74:LEU:N	12:Z:74:LEU:HD12	2.33	0.44
12:Z:205:ASP:OD2	8:H:243:GLY:N	2.51	0.44
16:g:218:LEU:HA	16:g:221:VAL:HG22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:ARG:HD2	7:G:16:PHE:HE1	1.83	0.44
4:D:41:GLN:NE2	4:D:151:PRO:O	2.48	0.44
5:E:71:GLY:HA3	5:E:221:PHE:CE1	2.53	0.44
6:F:54:LEU:HB2	6:F:58:TYR:HE2	1.82	0.44
8:H:220:VAL:HB	8:H:227:ASP:OD2	2.17	0.44
13:M:169:TYR:HD2	13:M:177:TYR:CE2	2.36	0.44
13:M:187:GLY:HA2	13:M:221:LEU:HD21	2.00	0.44
3:Q:88:ARG:CZ	10:X:70:ARG:HA	2.47	0.44
4:R:4:THR:HB	15:f:15:ARG:CG	2.28	0.44
4:R:73:HIS:HB2	4:R:146:VAL:HG12	1.98	0.44
4:R:123:PHE:CZ	4:R:136:PRO:HB3	2.53	0.44
5:S:66:VAL:O	12:Z:105:HIS:NE2	2.51	0.44
6:T:77:VAL:HG11	6:T:84:ALA:HB1	2.00	0.44
11:Y:64:ALA:HB3	11:Y:159:MET:HE3	2.00	0.44
15:f:15:ARG:HB3	16:g:25:GLY:H	1.83	0.44
15:f:176:LYS:O	15:f:210:ASN:ND2	2.41	0.44
1:A:182:GLU:OE2	1:A:185:ASP:N	2.41	0.44
2:B:86:LEU:HD21	2:B:130:PHE:CG	2.53	0.44
10:J:12:TYR:N	10:J:113:PRO:HG3	2.33	0.44
14:N:89:VAL:HG12	14:N:117:PHE:HE1	1.83	0.44
14:N:114:ALA:C	14:N:154:MET:HE1	2.42	0.44
1:O:187:ILE:O	1:O:191:ILE:HG12	2.17	0.44
3:Q:111:ILE:O	3:Q:115:LYS:HG3	2.16	0.44
4:R:211:ASN:OD1	4:R:214:ASN:N	2.42	0.44
5:S:40:SER:HB3	5:S:187:LEU:HD22	1.99	0.44
5:S:51:ARG:H	5:S:60:GLN:NE2	2.06	0.44
7:U:212:PRO:HG3	7:U:236:ASP:HB2	2.00	0.44
9:W:50:ILE:CD1	9:W:108:ILE:HG13	2.48	0.44
1:A:10:THR:HA	2:B:128:ARG:HB3	2.00	0.44
2:B:12:PHE:HE1	3:C:125:ARG:HD2	1.82	0.44
4:D:7:GLU:OE2	5:E:5:GLN:NE2	2.50	0.44
5:E:178:GLU:OE1	5:E:178:GLU:N	2.45	0.44
7:G:186:LYS:NZ	7:G:189:TRP:H	2.15	0.44
8:H:80:ILE:HG22	8:H:103:SER:HB3	1.99	0.44
9:I:25[B]:ARG:HG3	9:I:183:GLY:C	2.43	0.44
12:L:39:THR:HG22	12:L:169:ALA:H	1.83	0.44
13:M:50:MET:HE2	13:M:50:MET:HB3	1.75	0.44
1:O:28:VAL:HG22	1:O:131:VAL:HA	1.98	0.44
1:O:28:VAL:HG21	1:O:150:PRO:HG2	1.99	0.44
2:P:8:ARG:O	2:P:10:THR:OG1	2.36	0.44
2:P:238:LYS:O	2:P:241:GLU:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:36:VAL:HG23	5:S:195:LEU:HD13	2.00	0.44
11:Y:76:ASP:OD1	11:Y:76:ASP:C	2.61	0.44
12:Z:80:ILE:HD12	12:Z:137:ILE:O	2.18	0.44
13:a:51:VAL:O	13:a:101:ASP:HA	2.17	0.44
4:D:233:GLU:HA	4:D:236:GLU:HG3	1.99	0.44
6:F:36:ALA:N	6:F:165:ILE:O	2.51	0.44
6:F:86:SER:O	6:F:90:ILE:HG12	2.17	0.44
7:G:46:ASP:O	7:G:222:VAL:N	2.49	0.44
9:I:70:LEU:HD12	9:I:86:LEU:HD13	2.00	0.44
9:I:87:MET:SD	9:I:129:PRO:HB3	2.58	0.44
2:P:86:LEU:HD21	2:P:130:PHE:CG	2.53	0.43
4:R:163:VAL:HG23	4:R:165:CYS:HB3	1.98	0.43
7:U:196:GLU:H	7:U:196:GLU:CD	2.24	0.43
8:V:124:ARG:HG3	8:V:128:GLN:NE2	2.26	0.43
10:X:35:MET:HE3	10:X:43:LEU:HD13	1.99	0.43
12:Z:109:LYS:HB3	12:Z:109:LYS:HE3	1.81	0.43
13:a:169:TYR:CE1	13:a:171:ASP:HB3	2.53	0.43
15:f:50:LEU:HD23	15:f:50:LEU:H	1.82	0.43
15:f:72:ILE:O	15:f:134:LEU:HA	2.18	0.43
16:g:41:MET:HB3	16:g:78:TYR:HB3	1.99	0.43
2:B:13:SER:C	2:B:15:GLU:H	2.25	0.43
3:C:51:ALA:O	3:C:53:LEU:N	2.51	0.43
3:C:125:ARG:NH1	3:C:126:PRO:O	2.51	0.43
3:C:220:LEU:CD1	3:C:227:LYS:HE3	2.49	0.43
6:F:9:LEU:HD23	7:G:11:ARG:NH2	2.23	0.43
6:F:65:ARG:NH2	6:F:77:VAL:O	2.49	0.43
1:O:14:PRO:HA	2:P:23:TYR:CE1	2.53	0.43
3:Q:17:PHE:HD1	3:Q:20:GLU:OE2	2.01	0.43
4:R:91:LYS:HZ2	4:R:119:LEU:HD13	1.82	0.43
5:S:96:ARG:HH22	5:S:102:PRO:HG3	1.83	0.43
6:T:6:GLY:CA	16:g:210:GLU:H	2.31	0.43
6:T:86:SER:O	6:T:90:ILE:HG13	2.18	0.43
9:W:150:GLU:HG2	12:L:212:GLU:OE2	2.18	0.43
14:b:91:ASP:O	14:b:94:THR:HG22	2.18	0.43
15:f:63:LEU:HD11	15:f:154:PHE:HD2	1.83	0.43
15:f:208:GLN:NE2	16:g:59:ASN:O	2.51	0.43
1:A:187:ILE:O	1:A:191:ILE:HG12	2.17	0.43
4:D:88:LEU:HD23	4:D:88:LEU:HA	1.87	0.43
5:E:36:VAL:HG12	5:E:160:SER:HB2	2.01	0.43
5:E:123:TYR:CG	5:E:124:GLY:N	2.86	0.43
5:E:189:LYS:NZ	5:E:235:GLY:O	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:217:LYS:N	5:E:217:LYS:HD3	2.32	0.43
5:E:237:GLU:OE1	5:E:237:GLU:N	2.49	0.43
9:I:204:ASP:OD1	9:I:204:ASP:N	2.49	0.43
10:J:21:ALA:O	10:J:27:GLN:HA	2.17	0.43
10:J:152:SER:H	10:J:155:ARG:NH2	2.16	0.43
11:K:54:ILE:HG23	11:K:54:ILE:O	2.19	0.43
1:O:13:SER:HB3	1:O:17:LYS:O	2.18	0.43
3:Q:220:LEU:CD1	3:Q:227:LYS:HE3	2.48	0.43
4:R:164:GLN:O	5:S:58:ALA:HB3	2.19	0.43
5:S:5:GLN:HG3	15:f:15:ARG:NH1	2.34	0.43
5:S:54:SER:HA	15:f:282:ILE:HD12	2.00	0.43
5:S:164:ARG:NH1	15:f:187:PRO:HD3	2.33	0.43
6:T:27:MET:HE1	6:T:153:PRO:HD2	2.00	0.43
6:T:70:ASP:OD1	6:T:72:HIS:N	2.51	0.43
8:V:241:ARG:HH12	9:W:151:SER:HB3	1.83	0.43
9:W:11:MET:O	9:W:21:ILE:HG13	2.18	0.43
11:Y:80:THR:HA	11:Y:85:ILE:HA	2.01	0.43
14:b:123:ARG:HB3	14:b:126:GLU:CB	2.48	0.43
16:g:120:VAL:N	16:g:202:ALA:O	2.50	0.43
16:g:201:MET:SD	16:g:203:VAL:HG23	2.59	0.43
2:B:213:ILE:HD13	2:B:213:ILE:HA	1.86	0.43
4:D:102:THR:HG23	12:L:122:THR:HG21	2.00	0.43
10:J:107:TYR:CE1	10:J:112:GLY:HA2	2.53	0.43
14:N:71:ILE:HD11	14:N:77:CYS:SG	2.58	0.43
14:N:196:LEU:HD21	14:N:231:PHE:CD2	2.51	0.43
3:Q:172:LEU:HB3	4:R:58:LEU:HD21	2.00	0.43
4:R:13:ASN:HB3	5:S:126:ARG:CD	2.48	0.43
5:S:214:ILE:HD12	5:S:224:TYR:CE1	2.54	0.43
6:T:215:TRP:HE1	6:T:220:THR:HG23	1.83	0.43
7:U:23:TYR:CE2	16:g:134:LEU:HD13	2.54	0.43
7:U:192:GLU:C	7:U:194:THR:N	2.76	0.43
8:V:73:ASN:OD1	8:V:73:ASN:O	2.37	0.43
9:W:43:PRO:HB3	9:W:49:TYR:CE2	2.54	0.43
10:X:4:LEU:HD13	10:X:45:LEU:HB3	1.99	0.43
12:Z:54:ASP:HB3	12:Z:217:THR:HG23	2.00	0.43
14:b:149:PRO:HD2	14:b:153:MET:HB2	2.01	0.43
14:b:213:ILE:HD13	14:b:218:VAL:HG13	1.99	0.43
16:g:141:TYR:C	16:g:142:LEU:HD22	2.43	0.43
3:C:88:ARG:HE	10:J:69:MET:HG3	1.84	0.43
4:D:121:LEU:HD13	5:E:79:ALA:HB1	2.00	0.43
5:E:224:TYR:HB3	5:E:229:VAL:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:9:PHE:CE1	7:G:18:PRO:HD3	2.53	0.43
9:I:106:PRO:HD2	9:I:123:LEU:HB2	2.00	0.43
11:K:104:MET:HE3	11:K:104:MET:HB2	1.77	0.43
11:K:184:THR:HB	11:K:198:MET:HE2	2.00	0.43
12:L:53:SER:OG	12:L:71[A]:CYS:SG	2.54	0.43
12:L:112:THR:O	12:L:116:ILE:HG12	2.19	0.43
2:P:13:SER:C	2:P:15:GLU:H	2.25	0.43
3:Q:125:ARG:NH1	3:Q:126:PRO:O	2.51	0.43
3:Q:146:GLN:OE1	3:Q:156:TRP:NE1	2.49	0.43
4:R:137:PHE:O	4:R:158:PRO:HB3	2.18	0.43
4:R:233:GLU:HA	4:R:236:GLU:HG3	1.99	0.43
10:X:180:VAL:C	10:X:181:ARG:HD3	2.43	0.43
12:Z:153:ASP:OD2	12:Z:157:SER:HB3	2.19	0.43
15:f:2:ALA:CB	15:f:10:VAL:HA	2.48	0.43
15:f:187:PRO:HB2	15:f:235:CYS:SG	2.58	0.43
1:A:9:LEU:HD22	1:A:128:PRO:HD3	2.00	0.43
3:C:115:LYS:HB3	3:C:115:LYS:HE3	1.72	0.43
4:D:137:PHE:O	4:D:158:PRO:HB3	2.18	0.43
11:K:85:ILE:HG21	11:K:88:GLN:OE1	2.18	0.43
1:O:57:ASP:OD2	1:O:60:SER:N	2.52	0.43
7:U:5:SER:O	15:f:10:VAL:HG23	2.18	0.43
8:V:71:ASP:CG	8:V:73:ASN:H	2.27	0.43
11:Y:97:ASN:C	11:Y:99:TYR:H	2.25	0.43
14:b:54:THR:O	14:b:61:ALA:N	2.51	0.43
16:g:167:ARG:HB2	16:g:170:PRO:HA	2.01	0.43
2:B:240:HIS:O	2:B:244:GLU:OE1	2.37	0.43
4:D:56:SER:OG	4:D:58:LEU:HD12	2.18	0.43
4:D:123:PHE:CZ	4:D:136:PRO:HB3	2.53	0.43
6:F:65:ARG:HH21	6:F:78:ALA:HA	1.82	0.43
6:F:186:CYS:O	6:F:190:VAL:HG23	2.18	0.43
6:F:186:CYS:HA	6:F:189:ILE:HG22	2.01	0.43
7:G:212:PRO:HG3	7:G:236:ASP:HB2	2.00	0.43
8:H:165:LEU:HD11	14:N:62:ASN:OD1	2.19	0.43
9:I:122:SER:C	9:I:123:LEU:HD12	2.43	0.43
13:M:88:MET:SD	13:M:109:LYS:HA	2.59	0.43
1:O:71:ILE:CD1	1:O:106:THR:HG22	2.49	0.43
4:R:56:SER:OG	4:R:58:LEU:HD12	2.17	0.43
6:T:174:THR:O	6:T:178:LYS:HE3	2.19	0.43
8:V:178:MET:HE3	13:M:224:ARG:CZ	2.49	0.43
11:Y:157:GLY:O	11:Y:187:VAL:HG11	2.19	0.43
13:a:198:VAL:O	13:a:201:LYS:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:f:96:VAL:HG13	15:f:125:HIS:CD2	2.54	0.43
16:g:129:ARG:NH1	16:g:134:LEU:HD23	2.34	0.43
16:g:252:ARG:O	16:g:254:LEU:HG	2.18	0.43
1:A:142:ARG:NH1	1:A:144:TYR:HE1	2.17	0.43
5:E:23:GLU:O	5:E:26:MET:HB2	2.19	0.43
7:G:84:THR:O	7:G:87:SER:OG	2.32	0.43
8:H:50:VAL:O	8:H:50:VAL:HG13	2.18	0.43
8:H:164:LYS:C	8:H:165:LEU:HD22	2.44	0.43
13:M:192:GLN:NE2	13:M:196:ARG:HH12	2.17	0.43
4:R:199:LEU:HD23	4:R:210:LEU:HD21	2.01	0.43
6:T:7:TYR:HE2	6:T:16:PRO:HG3	1.82	0.43
11:Y:120:ARG:HD2	11:Y:120:ARG:C	2.44	0.43
12:Z:36:ASN:OD1	12:Z:86:HIS:N	2.28	0.43
13:a:102:TYR:HD2	14:b:153:MET:SD	2.42	0.43
14:b:195:ALA:O	14:b:198:MET:HB2	2.19	0.43
2:B:134:LEU:HB2	2:B:150:SER:HB3	2.00	0.43
5:E:84:LEU:HD12	5:E:130:VAL:HG11	2.01	0.43
7:G:192:GLU:C	7:G:194:THR:N	2.76	0.43
9:I:39:GLN:OE1	9:I:39:GLN:HA	2.18	0.43
11:K:65:PHE:HD1	11:K:198:MET:HE3	1.84	0.43
13:M:190:LEU:O	13:M:193:PRO:HD2	2.19	0.43
13:M:238:THR:HG23	13:M:240:LYS:H	1.84	0.43
2:P:240:HIS:O	2:P:244:GLU:OE1	2.37	0.43
7:U:9:PHE:CE1	7:U:18:PRO:HD3	2.53	0.43
7:U:46:ASP:O	7:U:222:VAL:N	2.49	0.43
8:V:230:ARG:HG2	8:V:230:ARG:HH11	1.83	0.43
12:Z:125:TYR:CE1	12:Z:128:ARG:HB2	2.53	0.43
13:a:148:MET:HE2	13:a:148:MET:HB2	1.80	0.43
14:b:118:LYS:O	14:b:122:TYR:HB2	2.19	0.43
15:f:150:LEU:HD12	15:f:222:TYR:CD2	2.54	0.43
5:E:6:TYR:CD2	5:E:14:SER:HA	2.53	0.43
7:G:128:ASN:HB2	7:G:131:MET:HG2	2.00	0.43
5:S:41:LYS:CG	5:S:180:MET:HE3	2.34	0.43
5:S:84:LEU:HA	5:S:84:LEU:HD23	1.72	0.43
7:U:1:MET:N	15:f:5:PHE:O	2.52	0.43
13:a:69:ALA:O	13:a:232:PHE:HB2	2.19	0.43
13:a:193:PRO:HA	8:H:208:ASN:OD1	2.18	0.43
14:b:168:TYR:HA	14:N:167:SER:O	2.19	0.43
15:f:259:LEU:O	15:f:259:LEU:HD23	2.19	0.43
3:C:47:LYS:O	3:C:49:SER:N	2.44	0.43
4:D:82:ILE:O	4:D:86:LYS:NZ	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:76:ILE:HD12	7:G:111:VAL:HG22	1.99	0.43
7:G:83:MET:HE2	7:G:83:MET:HB2	1.71	0.43
10:J:29:LYS:HG2	10:J:31:ASP:H	1.84	0.43
13:M:238:THR:OG1	13:M:239:GLU:N	2.51	0.43
14:N:74:ARG:NH2	14:N:216:SER:O	2.44	0.43
1:O:11:THR:HG22	2:P:8:ARG:H	1.84	0.42
6:T:73:VAL:HG12	6:T:139:SER:CB	2.47	0.42
8:V:119:VAL:HG23	8:V:147[A]:ASP:OD2	2.19	0.42
9:W:182:MET:HE1	9:W:203:MET:O	2.19	0.42
11:Y:60:THR:H	11:Y:92:LYS:NZ	2.17	0.42
14:b:42:PHE:CD2	14:b:47:VAL:HG23	2.54	0.42
2:B:143:TYR:CD1	3:C:57:ARG:NH2	2.87	0.42
4:D:47:CYS:C	4:D:48:LEU:HD12	2.44	0.42
5:E:14:SER:C	5:E:16:GLN:H	2.26	0.42
8:H:75:SER:O	8:H:77:ILE:HD13	2.19	0.42
9:I:48:LEU:HD21	9:I:86:LEU:HD22	2.00	0.42
11:K:91:LYS:HE3	11:K:91:LYS:HB3	1.74	0.42
12:L:111:MET:SD	12:L:116:ILE:HD13	2.59	0.42
2:P:86:LEU:HD12	2:P:114:LEU:HD21	2.01	0.42
7:U:168:ALA:HA	7:U:172:GLN:CD	2.44	0.42
8:V:51:TYR:OH	8:V:191:GLU:OE2	2.25	0.42
8:V:61:THR:H	8:V:214:SER:HB2	1.84	0.42
10:X:161:ARG:O	10:X:165:GLU:HG3	2.19	0.42
12:Z:74:LEU:HD11	12:Z:80:ILE:HG22	2.02	0.42
13:a:54:THR:HG23	13:a:55:SER:H	1.84	0.42
16:g:153:ASN:OD1	16:g:154:LYS:N	2.52	0.42
3:C:5:ARG:NH1	4:D:10:ARG:HB3	2.13	0.42
3:C:55:ASP:OD1	3:C:57:ARG:HB3	2.18	0.42
5:E:47:VAL:HG12	5:E:195:LEU:HD22	2.01	0.42
5:E:91:GLU:OE1	5:E:91:GLU:HA	2.18	0.42
6:F:197:ILE:HG21	6:F:211:LEU:HD13	2.00	0.42
7:G:21:ARG:CB	7:G:21:ARG:NH1	2.78	0.42
7:G:178:PHE:CZ	7:G:182:LYS:HE3	2.55	0.42
1:O:107:ALA:O	1:O:110:VAL:HG12	2.19	0.42
1:O:142:ARG:NH1	1:O:144:TYR:HE1	2.17	0.42
2:P:60:PHE:C	2:P:62:SER:H	2.27	0.42
3:Q:166:LYS:O	3:Q:170:GLU:OE1	2.37	0.42
4:R:15:PHE:CE2	5:S:77:LEU:HD11	2.54	0.42
4:R:47:CYS:C	4:R:48:LEU:HD12	2.44	0.42
5:S:179:PHE:HA	5:S:182:CYS:SG	2.59	0.42
6:T:18:GLY:HA3	7:U:31:ALA:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:74:GLU:OE2	7:U:74:GLU:N	2.53	0.42
9:W:26:ARG:HG2	9:W:182:MET:HG3	2.01	0.42
11:Y:113:PHE:CD1	12:Z:125:TYR:HE2	2.36	0.42
13:a:144:ARG:NE	13:a:151:LEU:HG	2.34	0.42
16:g:89:GLN:OE1	16:g:90:LEU:N	2.53	0.42
2:B:6:ASP:O	2:B:7:SER:OG	2.37	0.42
3:C:226:GLU:CB	3:C:229:VAL:HG22	2.45	0.42
9:I:50:ILE:HG13	9:I:107:VAL:O	2.18	0.42
9:I:124:ASP:OD1	9:I:125:LEU:HD23	2.20	0.42
10:J:25:ILE:HG13	10:J:26:VAL:HG23	2.01	0.42
12:L:174:GLN:HA	12:L:177:LEU:HD12	2.01	0.42
2:P:47:ALA:HB3	2:P:212:GLU:CG	2.50	0.42
2:P:68:LEU:HD21	2:P:90:LEU:HD13	2.01	0.42
5:S:120:THR:HG22	6:T:129:ARG:HH21	1.84	0.42
15:f:286:ILE:C	15:f:288:THR:H	2.27	0.42
16:g:106:LEU:O	16:g:110:VAL:HG23	2.20	0.42
1:A:13:SER:HB3	1:A:17:LYS:O	2.18	0.42
1:A:71:ILE:CD1	1:A:106:THR:HG22	2.49	0.42
4:D:199:LEU:HD23	4:D:210:LEU:HD21	2.01	0.42
5:E:93:LEU:HD12	12:L:98:ALA:HA	2.02	0.42
7:G:74:GLU:N	7:G:74:GLU:OE2	2.53	0.42
8:H:76:LYS:HZ3	8:H:230:ARG:HB3	1.84	0.42
13:M:133:ILE:H	13:M:133:ILE:HD12	1.83	0.42
14:N:169:ILE:HG13	14:N:169:ILE:O	2.19	0.42
2:P:134:LEU:O	2:P:150:SER:N	2.46	0.42
5:S:71:GLY:HA3	5:S:221:PHE:CZ	2.55	0.42
5:S:199:LEU:HD23	5:S:203:GLN:HB3	2.01	0.42
13:a:188:ALA:O	13:a:193:PRO:HD3	2.20	0.42
16:g:58:ASN:HD21	16:g:69:THR:HA	1.84	0.42
5:E:137:TYR:HE1	5:E:217:LYS:HZ2	1.66	0.42
6:F:161:TRP:CZ2	6:F:182:LYS:HE3	2.55	0.42
7:G:226:LYS:HB2	7:G:228:ARG:HE	1.85	0.42
13:M:57:LEU:O	13:M:67:ILE:HB	2.19	0.42
13:M:233:GLN:HA	13:M:233:GLN:OE1	2.19	0.42
1:O:96:TYR:CZ	1:O:100:TYR:HD2	2.38	0.42
2:P:114:LEU:HD12	2:P:114:LEU:HA	1.86	0.42
8:V:135:GLY:C	8:V:136:TYR:CD1	2.97	0.42
10:X:148:THR:H	10:X:151:ILE:HD11	1.84	0.42
11:Y:63:LEU:HD11	11:Y:74:ALA:HB3	2.00	0.42
15:f:121:CYS:HA	15:f:137:CYS:HB3	2.01	0.42
16:g:118:VAL:O	16:g:201:MET:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:TYR:CZ	1:A:100:TYR:HD2	2.38	0.42
2:B:147:LEU:HB3	2:B:159:TRP:O	2.20	0.42
3:C:68:ASN:OD1	3:C:68:ASN:N	2.53	0.42
3:C:200:GLN:HG2	3:C:200:GLN:O	2.19	0.42
5:E:88:MET:HE1	5:E:108:LEU:HD21	2.01	0.42
7:G:168:ALA:HA	7:G:172:GLN:CD	2.44	0.42
13:M:152:TRP:CE3	13:M:172:MET:HE1	2.55	0.42
2:P:230:GLN:O	2:P:233:VAL:HB	2.19	0.42
4:R:82:ILE:O	4:R:86:LYS:NZ	2.51	0.42
6:T:36:ALA:HB1	6:T:49:VAL:HG22	2.02	0.42
10:X:91:CYS:SG	10:X:98:TYR:CE2	3.11	0.42
10:X:98:TYR:O	10:X:100:VAL:HG13	2.19	0.42
11:Y:96:ILE:H	11:Y:96:ILE:HD12	1.85	0.42
12:Z:116:ILE:HG22	12:Z:138:ILE:HD13	2.02	0.42
15:f:48:ARG:NH1	15:f:49:LEU:O	2.52	0.42
16:g:64:THR:H	16:g:67:ASN:ND2	2.17	0.42
16:g:181:ILE:HD12	16:g:205:LEU:HD22	2.02	0.42
1:A:18:LEU:HA	1:A:18:LEU:HD23	1.78	0.42
1:A:158:LYS:CG	2:B:57:ASP:HB3	2.50	0.42
2:B:60:PHE:C	2:B:62:SER:H	2.27	0.42
3:C:7:ILE:HD11	3:C:124:ARG:O	2.20	0.42
3:C:166:LYS:HG3	3:C:167:SER:H	1.84	0.42
3:C:178:ASP:OD1	3:C:179:GLU:N	2.53	0.42
4:D:52:LYS:C	4:D:53:ARG:HG2	2.44	0.42
6:F:45:VAL:HG13	6:F:146:ALA:HB1	2.01	0.42
7:G:212:PRO:CD	7:G:239:LEU:HD21	2.43	0.42
9:I:87:MET:HE3	9:I:87:MET:HB3	1.92	0.42
12:L:141:LEU:HD23	12:L:147:GLY:HA2	2.01	0.42
13:M:108:LEU:HD23	13:M:108:LEU:HA	1.93	0.42
2:P:147:LEU:HB3	2:P:159:TRP:O	2.20	0.42
3:Q:115:LYS:HE3	3:Q:115:LYS:HB3	1.72	0.42
4:R:180:SER:O	4:R:183:GLU:HG2	2.20	0.42
5:S:32:GLY:O	5:S:51:ARG:NH2	2.50	0.42
5:S:201:ALA:HA	5:S:239:ARG:CZ	2.49	0.42
8:V:241:ARG:HH22	9:W:151:SER:HA	1.85	0.42
10:X:35:MET:HB2	10:X:181:ARG:HH21	1.85	0.42
11:Y:63:LEU:HA	11:Y:186:SER:HA	2.00	0.42
11:Y:232:ALA:HA	11:Y:250:ASN:HA	2.02	0.42
14:b:79:ARG:HG3	14:b:79:ARG:NH2	2.35	0.42
1:A:57:ASP:OD2	1:A:60:SER:N	2.52	0.42
1:A:107:ALA:O	1:A:110:VAL:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:17:PHE:HD1	3:C:20:GLU:OE2	2.01	0.42
9:I:198:THR:C	9:I:199:LEU:HD12	2.44	0.42
11:K:78:ARG:NH2	11:K:229:SER:O	2.52	0.42
2:P:139:TRP:CG	2:P:218:ARG:NH1	2.88	0.42
2:P:213:ILE:HD13	2:P:213:ILE:HA	1.86	0.42
3:Q:88:ARG:NH2	10:X:69:MET:O	2.53	0.42
3:Q:200:GLN:HG2	3:Q:200:GLN:O	2.19	0.42
4:R:140:ALA:C	4:R:141:LEU:HD22	2.45	0.42
5:S:149:PRO:C	5:S:151:ALA:H	2.28	0.42
5:S:167:SER:O	5:S:170:THR:OG1	2.33	0.42
5:S:193:ARG:HG3	5:S:196:ARG:NH2	2.35	0.42
6:T:89:ASP:HA	6:T:92:ARG:HG2	2.01	0.42
10:X:108:ASP:OD2	10:X:111:GLU:HB2	2.20	0.42
11:Y:156[B]:MET:HE2	11:Y:156[B]:MET:HB3	1.78	0.42
15:f:281:GLU:HG3	15:f:282:ILE:N	2.35	0.42
2:B:230:GLN:O	2:B:233:VAL:HB	2.19	0.42
4:D:168:ARG:NH1	4:D:178:GLN:CD	2.78	0.42
5:E:93:LEU:HD11	12:L:101:LYS:HB2	2.02	0.42
6:F:136:MET:HE1	6:F:150:MET:CG	2.48	0.42
7:G:12:HIS:CD2	7:G:14:THR:H	2.38	0.42
9:I:66:LEU:HD11	9:I:86:LEU:HD11	2.02	0.42
14:N:38:MET:SD	14:N:40:VAL:HG23	2.60	0.42
14:N:73:ASP:OD1	14:N:74:ARG:N	2.53	0.42
4:R:52:LYS:C	4:R:53:ARG:HG2	2.44	0.42
5:S:185:ASN:OD1	5:S:185:ASN:N	2.52	0.42
6:T:75:MET:HG2	6:T:136:MET:O	2.20	0.42
6:T:120:HIS:ND1	7:U:85:ALA:HB1	2.35	0.42
7:U:178:PHE:CZ	7:U:182:LYS:HE3	2.55	0.42
8:V:60:ASP:OD1	8:V:60:ASP:N	2.51	0.42
8:V:151:PRO:O	8:V:152:HIS:ND1	2.53	0.42
9:W:33:MET:HG3	9:W:182:MET:SD	2.60	0.42
10:X:40:GLU:HG2	10:X:41:LYS:HG3	2.02	0.42
12:Z:90:LEU:HA	12:Z:93:THR:HG22	2.01	0.42
14:b:123:ARG:HG2	14:b:126:GLU:HA	2.02	0.42
16:g:3:VAL:HG23	16:g:46:TYR:HB2	2.01	0.42
2:B:61:PHE:O	2:B:227:VAL:HG21	2.20	0.42
6:F:73:VAL:HG23	6:F:139:SER:HB3	2.02	0.42
6:F:218:GLU:OE1	6:F:218:GLU:N	2.51	0.42
13:M:113:GLY:HA2	13:M:116:VAL:HG12	2.02	0.42
13:M:124:ASP:CG	13:M:126:HIS:HD1	2.28	0.42
13:M:188:ALA:O	13:M:192:GLN:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:64:VAL:O	14:N:209:ARG:NH2	2.45	0.42
14:N:117:PHE:HD2	14:N:134:ILE:HD11	1.85	0.42
1:O:8:SER:O	1:O:9:LEU:HB3	2.20	0.41
1:O:127:ARG:NH1	7:U:127:GLN:HE22	2.18	0.41
4:R:168:ARG:NH1	4:R:178:GLN:CD	2.78	0.41
5:S:40:SER:OG	5:S:43:HIS:N	2.47	0.41
5:S:156:CYS:HA	6:T:58:TYR:HA	2.00	0.41
6:T:18:GLY:CA	7:U:31:ALA:HB2	2.50	0.41
7:U:83:MET:HE2	7:U:83:MET:HB2	1.71	0.41
8:V:62:ARG:HB2	8:V:214:SER:OG	2.20	0.41
11:Y:104:MET:HG3	11:Y:111:CYS:CB	2.50	0.41
12:Z:45:GLY:HA3	12:Z:48:PHE:CE1	2.55	0.41
16:g:220:LEU:HD12	16:g:220:LEU:HA	1.86	0.41
1:A:116:VAL:O	1:A:119:GLU:HG2	2.20	0.41
2:B:159:TRP:CE3	3:C:54:GLN:OE1	2.73	0.41
8:H:190:GLU:HB2	8:H:193:GLU:OE1	2.20	0.41
8:H:218:LEU:HD23	8:H:232:TYR:HB3	2.02	0.41
10:J:143:LEU:O	10:J:147:TYR:HB2	2.20	0.41
12:L:41:LEU:N	12:L:52:ALA:O	2.41	0.41
13:M:167:LEU:HD12	13:M:167:LEU:HA	1.90	0.41
14:N:83:ALA:O	14:N:86:THR:OG1	2.38	0.41
1:O:7:PHE:HD2	7:U:7:ALA:HB1	1.84	0.41
1:O:97:TYR:CD1	1:O:97:TYR:C	2.99	0.41
3:Q:202:GLY:O	3:Q:204:LYS:N	2.49	0.41
4:R:16:SER:HB2	4:R:22:PHE:CE1	2.55	0.41
4:R:21:LEU:HD23	4:R:22:PHE:N	2.35	0.41
8:V:132:ARG:HH11	8:V:132:ARG:HG2	1.85	0.41
10:X:167:LEU:HD23	10:X:167:LEU:HA	1.95	0.41
14:b:181[B]:MET:HE3	14:b:181[B]:MET:HB3	1.92	0.41
16:g:20:PRO:HD3	16:g:32:MET:SD	2.60	0.41
1:A:8:SER:O	1:A:9:LEU:HB3	2.20	0.41
1:A:97:TYR:CD1	1:A:97:TYR:C	2.99	0.41
3:C:7:ILE:HG23	3:C:122:ASN:OD1	2.20	0.41
4:D:21:LEU:HD23	4:D:22:PHE:N	2.35	0.41
4:D:206:MET:HE1	4:D:210:LEU:HD13	2.02	0.41
5:E:212:ILE:H	5:E:212:ILE:HD12	1.85	0.41
9:I:112:ASP:HB3	9:I:116:PHE:N	2.35	0.41
13:M:91:ASN:ND2	13:M:93:SER:H	2.18	0.41
3:Q:47:LYS:C	3:Q:49:SER:H	2.28	0.41
3:Q:166:LYS:HG3	3:Q:167:SER:H	1.84	0.41
7:U:12:HIS:CD2	7:U:14:THR:H	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:89:ALA:N	8:V:140:ALA:O	2.52	0.41
8:V:102:ILE:HG13	8:V:126:LEU:HD22	2.01	0.41
10:X:88:LEU:HG	10:X:122:ALA:HB2	2.02	0.41
11:Y:174:ASP:OD2	11:Y:178:ASN:HB2	2.20	0.41
1:A:99:VAL:HG13	9:I:92:ASN:ND2	2.34	0.41
2:B:68:LEU:HD21	2:B:90:LEU:HD13	2.01	0.41
3:C:89:VAL:HG22	10:J:66:LEU:HD21	2.02	0.41
4:D:140:ALA:C	4:D:141:LEU:HD22	2.45	0.41
4:D:180:SER:O	4:D:183:GLU:HG2	2.20	0.41
5:E:11:THR:C	6:F:129:ARG:HB3	2.45	0.41
5:E:122:ARG:HB2	5:E:125:ARG:HD3	2.02	0.41
6:F:34:SER:HB3	6:F:65:ARG:HH12	1.86	0.41
6:F:65:ARG:C	6:F:66:LEU:HD22	2.44	0.41
7:G:144:ASP:CG	7:G:145:GLU:H	2.28	0.41
9:I:41:ILE:HD12	9:I:50:ILE:O	2.20	0.41
9:I:77:GLU:OE1	9:I:77:GLU:N	2.52	0.41
9:I:190:GLU:HG2	9:I:193:LYS:O	2.20	0.41
11:K:240:GLU:O	11:K:241:ASP:C	2.63	0.41
14:N:137:TRP:NE1	14:N:215:GLU:OE2	2.54	0.41
1:O:55:LEU:HD22	7:U:165:ALA:HB3	2.02	0.41
1:O:97:TYR:HD1	1:O:97:TYR:C	2.28	0.41
2:P:61:PHE:O	2:P:227:VAL:HG21	2.20	0.41
3:Q:7:ILE:HG23	3:Q:122:ASN:OD1	2.20	0.41
3:Q:24:GLU:HA	3:Q:27:LYS:NZ	2.35	0.41
4:R:35:SER:HA	4:R:53:ARG:NH1	2.35	0.41
6:T:42:LYS:HD3	6:T:183:GLU:HA	2.01	0.41
8:V:249:LYS:HD2	8:V:250:GLY:H	1.84	0.41
9:W:69:ARG:HB3	9:W:89:MET:HE2	2.02	0.41
11:Y:165:LYS:HB2	11:Y:165:LYS:HE2	1.84	0.41
11:Y:240:GLU:O	11:Y:241:ASP:C	2.64	0.41
15:f:50:LEU:HD21	15:f:98:CYS:SG	2.60	0.41
15:f:70:LYS:NZ	15:f:258:SER:O	2.40	0.41
2:B:139:TRP:CG	2:B:218:ARG:NH1	2.88	0.41
3:C:24:GLU:HA	3:C:27:LYS:NZ	2.35	0.41
3:C:146:GLN:OE1	3:C:156:TRP:NE1	2.49	0.41
3:C:166:LYS:O	3:C:170:GLU:OE1	2.37	0.41
4:D:85:ALA:HB2	4:D:139:VAL:HG21	2.01	0.41
6:F:173:LYS:O	6:F:177:GLU:HG3	2.20	0.41
8:H:196:ASN:O	8:H:199:SER:N	2.53	0.41
12:L:66:ARG:HB3	12:L:219:ASP:HB3	2.02	0.41
14:N:192:ASN:O	14:N:196:LEU:HD23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:113:VAL:O	1:O:116:VAL:HG12	2.20	0.41
2:P:151:ASP:OD2	2:P:153:SER:OG	2.33	0.41
4:R:85:ALA:HB2	4:R:139:VAL:HG21	2.01	0.41
9:W:58:ASP:HB3	9:W:104:THR:HG23	2.03	0.41
10:X:35:MET:HE2	10:X:181:ARG:NH2	2.36	0.41
10:X:45:LEU:HD12	10:X:103:LEU:CB	2.51	0.41
15:f:168:THR:O	15:f:234:LEU:HD12	2.20	0.41
15:f:171:HIS:HE2	15:f:240:MET:HG2	1.85	0.41
1:A:97:TYR:HD1	1:A:97:TYR:C	2.28	0.41
2:B:20:GLN:HA	2:B:23:TYR:HD2	1.85	0.41
3:C:57:ARG:O	3:C:60:ARG:HG2	2.21	0.41
3:C:138:PHE:CD1	3:C:139:ASP:N	2.79	0.41
4:D:35:SER:HA	4:D:53:ARG:NH1	2.35	0.41
4:D:51:GLU:HA	4:D:215:ILE:HG22	2.03	0.41
5:E:225:ASP:O	5:E:229:VAL:HG13	2.19	0.41
6:F:191:LYS:HB3	6:F:238:TYR:CE2	2.56	0.41
9:I:98:ARG:HG3	9:I:99:PHE:CD1	2.55	0.41
10:J:19:ARG:HH22	10:J:193:ASN:HD22	1.69	0.41
12:L:75:THR:HG22	12:L:76:ASP:H	1.84	0.41
12:L:96:ILE:O	12:L:100:LEU:HD23	2.21	0.41
3:Q:7:ILE:HD11	3:Q:124:ARG:O	2.20	0.41
5:S:11:THR:O	5:S:11:THR:HG22	2.20	0.41
5:S:87:PHE:CD2	5:S:115:LYS:HE3	2.55	0.41
6:T:124:LEU:HD23	6:T:124:LEU:O	2.21	0.41
7:U:18:PRO:HD2	16:g:131:ASP:OD1	2.19	0.41
9:W:182:MET:HE1	9:W:203:MET:C	2.46	0.41
10:X:26:VAL:HG21	11:Y:195:TYR:HD2	1.80	0.41
14:b:63:ARG:HG2	13:M:224:ARG:NH2	2.36	0.41
2:B:86:LEU:HD12	2:B:114:LEU:HD21	2.01	0.41
2:B:98:LEU:O	2:B:102:GLN:N	2.43	0.41
3:C:203:GLY:C	3:C:204:LYS:HE2	2.46	0.41
6:F:139:SER:HA	6:F:216:VAL:HG11	2.03	0.41
8:H:63:ALA:HB2	8:H:74:CYS:SG	2.60	0.41
14:N:78:CYS:HB2	14:N:133:ILE:HG12	2.01	0.41
1:O:131:VAL:O	1:O:150:PRO:HG3	2.21	0.41
4:R:22:PHE:C	4:R:26:TYR:HD1	2.28	0.41
4:R:31:ILE:HD13	4:R:31:ILE:HA	1.90	0.41
4:R:123:PHE:O	4:R:134:SER:HA	2.21	0.41
5:S:7:ASP:HB2	5:S:24:TYR:CE2	2.56	0.41
6:T:163:CYS:SG	6:T:164:ALA:N	2.94	0.41
7:U:186:LYS:HZ3	7:U:189:TRP:H	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:236:ASN:HD22	12:L:241:ASP:CG	2.29	0.41
14:b:110:VAL:HB	14:b:144:GLN:OE1	2.20	0.41
15:f:272:ILE:O	15:f:276:LEU:HD23	2.21	0.41
16:g:61:TYR:HH	16:g:89:GLN:HE21	1.63	0.41
16:g:80:LEU:N	16:g:85:LEU:O	2.33	0.41
16:g:131:ASP:HA	16:g:134:LEU:HB2	2.03	0.41
4:D:22:PHE:C	4:D:26:TYR:HD1	2.28	0.41
5:E:18:ARG:NE	5:E:23:GLU:OE2	2.47	0.41
8:H:44:THR:O	8:H:172:SER:N	2.40	0.41
9:I:112:ASP:HB3	9:I:117:LYS:H	1.86	0.41
10:J:10:PRO:CD	10:J:151:ILE:H	2.33	0.41
10:J:59:TYR:O	10:J:62:LYS:HG2	2.21	0.41
10:J:145:ARG:HG3	10:J:146:TYR:CE1	2.55	0.41
11:K:185:PHE:H	11:K:198:MET:HE1	1.86	0.41
2:P:20:GLN:HA	2:P:23:TYR:HD2	1.85	0.41
3:Q:119:THR:O	4:R:135:ARG:NH1	2.54	0.41
3:Q:121:SER:O	3:Q:122:ASN:C	2.64	0.41
3:Q:173:GLU:HB3	4:R:58:LEU:HG	2.02	0.41
3:Q:181:ILE:O	3:Q:181:ILE:HG22	2.21	0.41
7:U:12:HIS:CG	7:U:13:ILE:N	2.89	0.41
8:V:203:ALA:HA	8:V:206:ILE:HD13	2.03	0.41
9:W:140:THR:OG1	9:W:177:ASP:OD2	2.32	0.41
13:a:160:TYR:CZ	13:a:163:GLY:HA2	2.56	0.41
14:b:181[B]:MET:HB3	14:b:185:GLU:HG3	2.03	0.41
15:f:188:PHE:HE2	15:f:190:ARG:HE	1.69	0.41
15:f:223:CYS:O	15:f:228:ILE:N	2.54	0.41
15:f:269:SER:O	15:f:273:LEU:HD23	2.21	0.41
3:C:181:ILE:HG22	3:C:181:ILE:O	2.21	0.41
4:D:171:GLY:O	4:D:174:SER:HB3	2.21	0.41
6:F:41:CYS:HA	6:F:181:MET:O	2.21	0.41
7:G:71:LYS:HA	7:G:227:PHE:CD2	2.56	0.41
10:J:13:VAL:HG12	10:J:183:ILE:HB	2.03	0.41
11:K:95:GLU:OE1	11:K:95:GLU:N	2.45	0.41
12:L:55:THR:OG1	12:L:220:ALA:HB3	2.21	0.41
14:N:117:PHE:HB3	14:N:134:ILE:HD11	2.03	0.41
1:O:98:LEU:O	8:V:100:GLN:NE2	2.53	0.41
1:O:116:VAL:O	1:O:119:GLU:HG2	2.20	0.41
1:O:135:ILE:O	1:O:145:LEU:HD12	2.21	0.41
1:O:138:TRP:NE1	1:O:214:GLU:HA	2.35	0.41
2:P:4:ARG:N	2:P:14:PRO:HD3	2.36	0.41
2:P:80:THR:O	2:P:83:ALA:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:57:ARG:O	3:Q:60:ARG:HG2	2.20	0.41
3:Q:203:GLY:C	3:Q:204:LYS:HE2	2.46	0.41
4:R:51:GLU:HA	4:R:215:ILE:HG22	2.03	0.41
4:R:206:MET:HE1	4:R:210:LEU:HD13	2.02	0.41
5:S:159:MET:HE3	5:S:159:MET:HA	2.03	0.41
10:X:35:MET:CE	10:X:43:LEU:HD13	2.51	0.41
10:X:170:ARG:NE	11:K:195:TYR:HD2	2.18	0.41
11:Y:71:VAL:HG12	11:Y:238:VAL:HB	2.02	0.41
11:Y:113:PHE:CD2	12:Z:125:TYR:HD2	2.38	0.41
12:Z:174:GLN:N	12:Z:175:PRO:HD2	2.36	0.41
13:a:94:THR:OG1	13:a:130:PRO:HG3	2.21	0.41
14:b:48:LEU:HD21	14:b:135:ALA:HB3	2.02	0.41
16:g:21:ALA:N	16:g:121:LEU:O	2.47	0.41
16:g:238:PRO:C	16:g:240:VAL:N	2.77	0.41
16:g:241:SER:HB2	16:g:245:TRP:NE1	2.35	0.41
1:A:113:VAL:O	1:A:116:VAL:HG12	2.20	0.41
1:A:135:ILE:O	1:A:145:LEU:HD12	2.21	0.41
1:A:160:THR:OG1	1:A:170:LYS:HE2	2.21	0.41
2:B:47:ALA:O	2:B:212:GLU:HG2	2.21	0.41
3:C:57:ARG:HH11	3:C:57:ARG:HD2	1.78	0.41
3:C:121:SER:O	3:C:122:ASN:C	2.64	0.41
4:D:16:SER:HB2	4:D:22:PHE:CE1	2.55	0.41
4:D:22:PHE:O	4:D:23:GLN:C	2.64	0.41
4:D:31:ILE:O	4:D:34:GLY:N	2.29	0.41
4:D:103:TYR:CD1	12:L:111:MET:HE3	2.56	0.41
8:H:50:VAL:HG12	8:H:166:PRO:HA	2.03	0.41
8:H:85:TYR:HD2	8:H:219:CYS:SG	2.44	0.41
9:I:157:MET:HE2	9:I:157:MET:HB3	1.93	0.41
10:J:35:MET:HE3	10:J:181:ARG:HD2	2.03	0.41
12:L:100:LEU:HD11	12:L:116:ILE:HD11	2.02	0.41
12:L:202:LEU:O	12:L:206:VAL:HG13	2.20	0.41
1:O:98:LEU:HD21	8:V:101:LEU:HA	2.02	0.41
1:O:160:THR:OG1	1:O:170:LYS:HE2	2.21	0.41
1:O:219:ARG:O	1:O:220:LEU:HD23	2.21	0.41
2:P:58:GLU:C	2:P:60:PHE:H	2.28	0.41
4:R:171:GLY:O	4:R:174:SER:HB3	2.21	0.41
7:U:22:LEU:HA	7:U:22:LEU:HD23	1.72	0.41
8:V:122:ALA:O	8:V:126:LEU:HD23	2.21	0.41
9:W:51:GLY:C	9:W:52:LEU:HD22	2.46	0.41
11:Y:172:TYR:O	11:Y:179:ARG:HA	2.20	0.41
12:Z:85:PHE:HE2	13:a:142:TYR:OH	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:f:62:LEU:HD23	15:f:153:VAL:HG13	2.03	0.41
1:A:83:ARG:NH2	1:A:83:ARG:CB	2.76	0.41
2:B:151:ASP:OD1	2:B:152:PRO:HD2	2.21	0.41
2:B:176:LYS:HB2	3:C:53:LEU:CD2	2.47	0.41
4:D:6:SER:HA	5:E:4:ASN:O	2.21	0.41
8:H:81:SER:O	8:H:84:ILE:HG12	2.20	0.41
11:K:57:LEU:HD12	11:K:107:GLY:N	2.37	0.41
11:K:171:TYR:CE2	11:K:181:SER:HB2	2.56	0.41
12:L:169:ALA:O	12:L:173:LEU:HD23	2.21	0.41
13:M:141:MET:HE2	13:M:141:MET:HB2	1.77	0.41
13:M:230:ASN:O	13:M:249:SER:HA	2.21	0.41
2:P:123:GLN:OE1	3:Q:125:ARG:NH2	2.54	0.40
3:Q:5:ARG:NH1	4:R:10:ARG:HB3	2.36	0.40
8:V:216:ILE:HD13	8:V:233:THR:HB	2.03	0.40
8:V:251:THR:HB	9:W:164:GLU:OE2	2.21	0.40
10:X:164:LEU:HD22	10:X:178:PHE:CE2	2.56	0.40
11:Y:196:GLY:CA	10:J:142:ILE:HD11	2.51	0.40
12:Z:66:ARG:HG2	12:Z:219:ASP:OD2	2.20	0.40
13:a:124:ASP:OD1	13:a:124:ASP:N	2.48	0.40
1:A:138:TRP:NE1	1:A:214:GLU:HA	2.35	0.40
2:B:174:MET:SD	2:B:196:VAL:HG22	2.62	0.40
6:F:203:GLU:H	6:F:203:GLU:CD	2.28	0.40
9:I:26:ARG:NH1	9:I:28:GLY:HA3	2.35	0.40
10:J:86:ARG:NH1	10:J:90:ASP:HB3	2.34	0.40
2:P:34:CYS:SG	2:P:47:ALA:HB2	2.62	0.40
2:P:47:ALA:O	2:P:212:GLU:HG2	2.21	0.40
3:Q:3:TYR:HB2	15:f:1:MET:CG	2.51	0.40
3:Q:68:ASN:OD1	3:Q:68:ASN:N	2.53	0.40
6:T:161:TRP:CE2	6:T:182:LYS:HE3	2.56	0.40
7:U:224:ASN:O	7:U:228:ARG:NH2	2.54	0.40
7:U:226:LYS:HB2	7:U:228:ARG:HE	1.85	0.40
9:W:38:PHE:HD2	9:W:40:LYS:HE2	1.86	0.40
10:X:39:SER:HG	10:X:40:GLU:H	1.67	0.40
11:Y:55:GLU:HG3	12:Z:135:TYR:OH	2.21	0.40
12:Z:62:SER:N	8:H:210:LEU:HD23	2.36	0.40
14:b:228:ILE:H	14:b:228:ILE:HD12	1.86	0.40
15:f:146:GLN:HG3	15:f:215:LEU:HD13	2.03	0.40
15:f:156:SER:O	15:f:158:PRO:HD3	2.22	0.40
16:g:143:LEU:HD12	16:g:148:GLN:OE1	2.20	0.40
6:F:63:ASN:O	6:F:65:ARG:HG3	2.22	0.40
8:H:116:LEU:HD23	8:H:116:LEU:HA	1.96	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:60:GLN:HB2	10:J:85:ARG:NH2	2.37	0.40
12:L:226:VAL:HG22	12:L:231:ILE:HG12	2.03	0.40
2:P:66:TYR:CD2	2:P:87:THR:HG21	2.56	0.40
5:S:156:CYS:HA	6:T:59:GLU:H	1.87	0.40
8:V:146:VAL:HA	8:V:151:PRO:HA	2.03	0.40
9:W:112:ASP:OD1	9:W:115:THR:N	2.38	0.40
11:Y:245[A]:ARG:HE	11:Y:245[A]:ARG:HB2	1.59	0.40
13:a:151:LEU:HA	13:a:151:LEU:HD23	1.78	0.40
14:b:76:PHE:CE2	14:b:213:ILE:HD11	2.55	0.40
15:f:142:ALA:N	15:f:145:GLN:HB2	2.36	0.40
16:g:27:VAL:HG21	16:g:208:VAL:HG11	2.04	0.40
16:g:167:ARG:HH21	16:g:177:PHE:H	1.68	0.40
1:A:21:ILE:HG21	1:A:151:SER:HB3	2.03	0.40
2:B:4:ARG:N	2:B:14:PRO:HD3	2.36	0.40
3:C:213:ARG:HG2	3:C:214:ASP:CG	2.46	0.40
5:E:21:GLN:HA	5:E:24:TYR:HD2	1.86	0.40
8:H:62:ARG:HE	8:H:212:SER:C	2.29	0.40
8:H:127:LYS:HE2	8:H:127:LYS:HB2	1.75	0.40
11:K:103:THR:O	11:K:158:THR:HG22	2.22	0.40
13:M:71:MET:HE1	13:M:233:GLN:CD	2.46	0.40
2:P:222:LYS:HD2	2:P:222:LYS:HA	1.52	0.40
8:V:79:PHE:HA	8:V:85:TYR:CE1	2.55	0.40
11:Y:60:THR:H	11:Y:92:LYS:HZ3	1.69	0.40
11:Y:206:LEU:HD12	11:Y:210:GLN:HE21	1.85	0.40
12:Z:38:GLY:HA3	12:Z:70:LYS:HE3	2.03	0.40
13:a:89:ARG:HB2	13:a:244:ILE:CD1	2.52	0.40
16:g:167:ARG:HB3	16:g:170:PRO:HA	2.04	0.40
1:A:131:VAL:O	1:A:150:PRO:HG3	2.21	0.40
1:A:189:THR:HA	1:A:192:LEU:HD12	2.04	0.40
1:A:219:ARG:O	1:A:220:LEU:HD23	2.21	0.40
2:B:80:THR:O	2:B:83:ALA:HB3	2.21	0.40
2:B:240:HIS:HA	2:B:243:GLU:OE2	2.22	0.40
5:E:142:PRO:O	5:E:143:HIS:ND1	2.54	0.40
8:H:218:LEU:HD13	8:H:218:LEU:HA	1.96	0.40
9:I:111:LEU:HA	9:I:117:LYS:O	2.22	0.40
9:I:203:MET:HA	9:I:203:MET:HE2	2.02	0.40
12:L:74:LEU:HD12	12:L:78:THR:HG22	2.04	0.40
13:M:92:ASN:O	13:M:241:GLY:HA2	2.21	0.40
13:M:190:LEU:C	13:M:193:PRO:HD2	2.46	0.40
14:N:89:VAL:HG13	14:N:120:MET:HG2	2.03	0.40
3:Q:71:MET:HB3	3:Q:133:ILE:HD13	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:215:TRP:CZ2	6:T:219:LEU:HD23	2.57	0.40
7:U:144:ASP:CG	7:U:145:GLU:H	2.28	0.40
8:V:169:THR:C	8:V:170[B]:MET:HG2	2.46	0.40
12:Z:151:SER:CB	12:Z:164:LYS:HD2	2.51	0.40
12:Z:187:GLN:HB3	8:H:251:THR:O	2.21	0.40
13:a:71:MET:HE1	13:a:231:ARG:HB3	2.03	0.40
15:f:188:PHE:CE1	15:f:236:TYR:HB2	2.57	0.40
1:A:78:MET:HE3	1:A:78:MET:HB2	1.76	0.40
2:B:44:LEU:HD22	2:B:190:LEU:HD23	2.04	0.40
2:B:58:GLU:C	2:B:60:PHE:H	2.28	0.40
3:C:65:LEU:HB2	3:C:69:VAL:HG12	2.04	0.40
4:D:19:GLY:HA3	5:E:28:ALA:N	2.36	0.40
7:G:94:ALA:HA	7:G:97:GLU:HB2	2.04	0.40
8:H:109:HIS:O	8:H:112:SER:OG	2.25	0.40
10:J:108:ASP:OD1	10:J:109:GLU:N	2.54	0.40
11:K:223:THR:OG1	11:K:230:GLY:HA2	2.20	0.40
13:M:51:VAL:HA	13:M:74:SER:O	2.21	0.40
14:N:118:LYS:HD3	14:N:154:MET:HG2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	226/234 (97%)	206 (91%)	20 (9%)	0	100	100
1	O	226/234 (97%)	207 (92%)	19 (8%)	0	100	100
2	B	243/261 (93%)	223 (92%)	20 (8%)	0	100	100
2	P	243/261 (93%)	223 (92%)	20 (8%)	0	100	100
3	C	237/248 (96%)	198 (84%)	37 (16%)	2 (1%)	16	48
3	Q	237/248 (96%)	198 (84%)	37 (16%)	2 (1%)	16	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	239/241 (99%)	206 (86%)	33 (14%)	0	100	100
4	R	239/241 (99%)	206 (86%)	33 (14%)	0	100	100
5	E	237/263 (90%)	215 (91%)	20 (8%)	2 (1%)	16	48
5	S	237/263 (90%)	215 (91%)	20 (8%)	2 (1%)	16	48
6	F	238/255 (93%)	226 (95%)	12 (5%)	0	100	100
6	T	238/255 (93%)	225 (94%)	13 (6%)	0	100	100
7	G	243/246 (99%)	218 (90%)	24 (10%)	1 (0%)	30	62
7	U	243/246 (99%)	218 (90%)	24 (10%)	1 (0%)	30	62
8	H	220/277 (79%)	190 (86%)	27 (12%)	3 (1%)	9	37
8	V	220/277 (79%)	202 (92%)	18 (8%)	0	100	100
9	I	200/205 (98%)	186 (93%)	14 (7%)	0	100	100
9	W	200/205 (98%)	185 (92%)	15 (8%)	0	100	100
10	J	196/201 (98%)	185 (94%)	11 (6%)	0	100	100
10	X	196/201 (98%)	183 (93%)	13 (7%)	0	100	100
11	K	209/263 (80%)	181 (87%)	27 (13%)	1 (0%)	24	57
11	Y	209/263 (80%)	188 (90%)	21 (10%)	0	100	100
12	L	212/241 (88%)	202 (95%)	10 (5%)	0	100	100
12	Z	212/241 (88%)	198 (93%)	14 (7%)	0	100	100
13	M	205/253 (81%)	195 (95%)	10 (5%)	0	100	100
13	a	205/253 (81%)	192 (94%)	13 (6%)	0	100	100
14	N	199/239 (83%)	179 (90%)	20 (10%)	0	100	100
14	b	199/239 (83%)	181 (91%)	18 (9%)	0	100	100
15	f	277/288 (96%)	245 (88%)	31 (11%)	1 (0%)	30	62
16	g	262/264 (99%)	233 (89%)	28 (11%)	1 (0%)	30	62
All	All	6747/7406 (91%)	6109 (90%)	622 (9%)	16 (0%)	44	73

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	S	227	ASP
5	E	227	ASP
8	H	80	ILE
8	H	132	ARG
3	Q	138	PHE

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Mol	Chain	Res	Type
5	S	226	ASP
3	C	138	PHE
5	E	226	ASP
8	H	131	PHE
11	K	81	ALA
15	f	13	PRO
7	U	195	VAL
16	g	238	PRO
7	G	195	VAL
3	Q	123	GLY
3	C	123	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	182/191 (95%)	161 (88%)	21 (12%)	5	23
1	O	182/191 (95%)	161 (88%)	21 (12%)	5	23
2	B	197/221 (89%)	167 (85%)	30 (15%)	3	16
2	P	197/221 (89%)	167 (85%)	30 (15%)	3	16
3	C	193/211 (92%)	174 (90%)	19 (10%)	7	29
3	Q	193/211 (92%)	174 (90%)	19 (10%)	7	29
4	D	200/203 (98%)	174 (87%)	26 (13%)	4	20
4	R	200/203 (98%)	174 (87%)	26 (13%)	4	20
5	E	200/224 (89%)	200 (100%)	0	100	100
5	S	200/224 (89%)	200 (100%)	0	100	100
6	F	193/212 (91%)	193 (100%)	0	100	100
6	T	193/212 (91%)	193 (100%)	0	100	100
7	G	205/210 (98%)	186 (91%)	19 (9%)	8	30
7	U	205/210 (98%)	186 (91%)	19 (9%)	8	30
8	H	180/228 (79%)	176 (98%)	4 (2%)	45	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	V	180/228 (79%)	176 (98%)	4 (2%)	45	63
9	I	170/174 (98%)	170 (100%)	0	100	100
9	W	170/174 (98%)	170 (100%)	0	100	100
10	J	169/171 (99%)	169 (100%)	0	100	100
10	X	169/171 (99%)	169 (100%)	0	100	100
11	K	164/202 (81%)	160 (98%)	4 (2%)	43	62
11	Y	164/202 (81%)	163 (99%)	1 (1%)	78	79
12	L	176/199 (88%)	174 (99%)	2 (1%)	65	73
12	Z	176/199 (88%)	174 (99%)	2 (1%)	65	73
13	M	170/206 (82%)	168 (99%)	2 (1%)	63	72
13	a	170/206 (82%)	170 (100%)	0	100	100
14	N	156/181 (86%)	154 (99%)	2 (1%)	61	71
14	b	156/181 (86%)	154 (99%)	2 (1%)	61	71
15	f	256/262 (98%)	256 (100%)	0	100	100
16	g	237/237 (100%)	237 (100%)	0	100	100
All	All	5603/6165 (91%)	5350 (96%)	253 (4%)	27	48

All (253) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	17	LYS
1	O	20	GLN
1	O	25	LEU
1	O	38	LYS
1	O	58	GLU
1	O	70	HIS
1	O	78	MET
1	O	83	ARG
1	O	85	LEU
1	O	95	GLN
1	O	111	GLN
1	O	112	ARG
1	O	117	MET
1	O	140	GLU
1	O	162	MET
1	O	180	ASP
1	O	207	ILE

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Mol	Chain	Res	Type
1	O	214	GLU
1	O	218	ARG
1	O	227	ASP
1	O	229	LEU
2	P	6	ASP
2	P	8	ARG
2	P	10	THR
2	P	18	LEU
2	P	50	ARG
2	P	67	LYS
2	P	70	GLU
2	P	82	ASP
2	P	89	GLU
2	P	93	ILE
2	P	98	LEU
2	P	105	ILE
2	P	141	LYS
2	P	174	MET
2	P	176	LYS
2	P	177	GLN
2	P	181	GLU
2	P	183	GLU
2	P	184	MET
2	P	192	LEU
2	P	194	ILE
2	P	200	THR
2	P	201	MET
2	P	218	ARG
2	P	222	LYS
2	P	226	ARG
2	P	234	GLU
2	P	241	GLU
2	P	243	GLU
2	P	246	LYS
3	Q	23	GLN
3	Q	26	VAL
3	Q	30	SER
3	Q	52	LYS
3	Q	57	ARG
3	Q	60	ARG
3	Q	67	ASP
3	Q	70	CYS

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Mol	Chain	Res	Type
3	Q	93	SER
3	Q	115	LYS
3	Q	120	GLN
3	Q	130	SER
3	Q	138	PHE
3	Q	157	LYS
3	Q	183	THR
3	Q	195	LEU
3	Q	219	ILE
3	Q	227	LYS
3	Q	234	LYS
4	R	1	MET
4	R	3	LEU
4	R	20	ARG
4	R	23	GLN
4	R	29	GLU
4	R	52	LYS
4	R	60	GLU
4	R	69	GLU
4	R	87	THR
4	R	91	LYS
4	R	105	GLU
4	R	110	GLU
4	R	111	SER
4	R	113	THR
4	R	114	GLN
4	R	148	GLU
4	R	149	LYS
4	R	153	LEU
4	R	156	MET
4	R	184	VAL
4	R	189	MET
4	R	192	LYS
4	R	197	SER
4	R	199	LEU
4	R	206	MET
4	R	239	LYS
7	U	21	ARG
7	U	45	LYS
7	U	59	LYS
7	U	72	ILE
7	U	83	MET

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Mol	Chain	Res	Type
7	U	92	GLN
7	U	97	GLU
7	U	113	MET
7	U	127	GLN
7	U	130	GLU
7	U	154	CYS
7	U	177	SER
7	U	179	LEU
7	U	199	ILE
7	U	209	ASP
7	U	211	LYS
7	U	232	GLU
7	U	234	GLU
7	U	240	VAL
8	V	147[A]	ASP
8	V	147[B]	ASP
8	V	170[A]	MET
8	V	170[B]	MET
11	Y	78	ARG
12	Z	71[A]	CYS
12	Z	71[B]	CYS
14	b	181[A]	MET
14	b	181[B]	MET
1	A	17	LYS
1	A	20	GLN
1	A	25	LEU
1	A	38	LYS
1	A	58	GLU
1	A	70	HIS
1	A	78	MET
1	A	83	ARG
1	A	85	LEU
1	A	95	GLN
1	A	111	GLN
1	A	112	ARG
1	A	117	MET
1	A	140	GLU
1	A	162	MET
1	A	180	ASP
1	A	207	ILE
1	A	214	GLU
1	A	218	ARG

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Mol	Chain	Res	Type
1	A	227	ASP
1	A	229	LEU
2	B	6	ASP
2	B	8	ARG
2	B	10	THR
2	B	18	LEU
2	B	50	ARG
2	B	67	LYS
2	B	70	GLU
2	B	82	ASP
2	B	89	GLU
2	B	93	ILE
2	B	98	LEU
2	B	105	ILE
2	B	141	LYS
2	B	174	MET
2	B	176	LYS
2	B	177	GLN
2	B	181	GLU
2	B	183	GLU
2	B	184	MET
2	B	192	LEU
2	B	194	ILE
2	B	200	THR
2	B	201	MET
2	B	218	ARG
2	B	222	LYS
2	B	226	ARG
2	B	234	GLU
2	B	241	GLU
2	B	243	GLU
2	B	246	LYS
3	C	23	GLN
3	C	26	VAL
3	C	30	SER
3	C	52	LYS
3	C	57	ARG
3	C	60	ARG
3	C	67	ASP
3	C	70	CYS
3	C	93	SER
3	C	115	LYS

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Mol	Chain	Res	Type
3	C	120	GLN
3	C	130	SER
3	C	138	PHE
3	C	157	LYS
3	C	183	THR
3	C	195	LEU
3	C	219	ILE
3	C	227	LYS
3	C	234	LYS
4	D	1	MET
4	D	3	LEU
4	D	20	ARG
4	D	23	GLN
4	D	29	GLU
4	D	52	LYS
4	D	60	GLU
4	D	69	GLU
4	D	87	THR
4	D	91	LYS
4	D	105	GLU
4	D	110	GLU
4	D	111	SER
4	D	113	THR
4	D	114	GLN
4	D	148	GLU
4	D	149	LYS
4	D	153	LEU
4	D	156	MET
4	D	184	VAL
4	D	189	MET
4	D	192	LYS
4	D	197	SER
4	D	199	LEU
4	D	206	MET
4	D	239	LYS
7	G	21	ARG
7	G	45	LYS
7	G	59	LYS
7	G	72	ILE
7	G	83	MET
7	G	92	GLN
7	G	97	GLU

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Mol	Chain	Res	Type
7	G	113	MET
7	G	127	GLN
7	G	130	GLU
7	G	154	CYS
7	G	177	SER
7	G	179	LEU
7	G	199	ILE
7	G	209	ASP
7	G	211	LYS
7	G	232	GLU
7	G	234	GLU
7	G	240	VAL
8	H	147[A]	ASP
8	H	147[B]	ASP
8	H	170[A]	MET
8	H	170[B]	MET
11	K	78	ARG
11	K	80	THR
11	K	156[A]	MET
11	K	156[B]	MET
12	L	71[A]	CYS
12	L	71[B]	CYS
13	M	212[A]	ASP
13	M	212[B]	ASP
14	N	181[A]	MET
14	N	181[B]	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	101	GLN
1	O	165	ASN
1	O	168	ASN
2	P	51	ASN
2	P	109	GLN
2	P	149	GLN
2	P	198	ASN
3	Q	23	GLN
3	Q	154	HIS
4	R	97	GLN
4	R	99	HIS
5	S	146	GLN

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Mol	Chain	Res	Type
8	V	100	GLN
9	W	92	ASN
9	W	168	GLN
10	X	32	HIS
10	X	61	GLN
10	X	71	ASN
11	Y	210	GLN
12	Z	180	GLN
12	Z	185	ASN
15	f	171	HIS
1	A	101	GLN
1	A	165	ASN
1	A	168	ASN
2	B	51	ASN
2	B	109	GLN
2	B	149	GLN
2	B	198	ASN
3	C	23	GLN
4	D	97	GLN
4	D	99	HIS
5	E	5	GLN
5	E	8	ASN
5	E	65	HIS
5	E	146	GLN
6	F	63	ASN
7	G	127	GLN
8	H	100	GLN
8	H	208	ASN
8	H	236	ASN
9	I	92	ASN
10	J	27	GLN
10	J	63	ASN
10	J	65	GLN
10	J	71	ASN
10	J	110	HIS
11	K	255	HIS
13	M	91	ASN
13	M	192	GLN
14	N	87	GLN
14	N	157	GLN

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](#)

There are no ligands in this entry.

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.

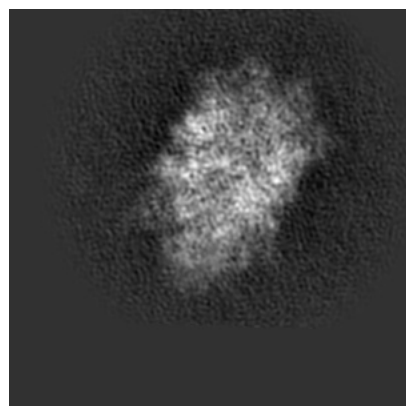
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39334. These allow visual inspection of the internal detail of the map and identification of artifacts.

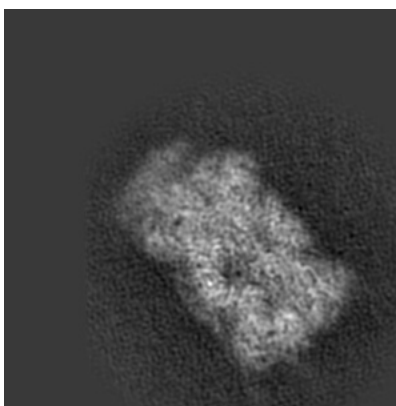
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

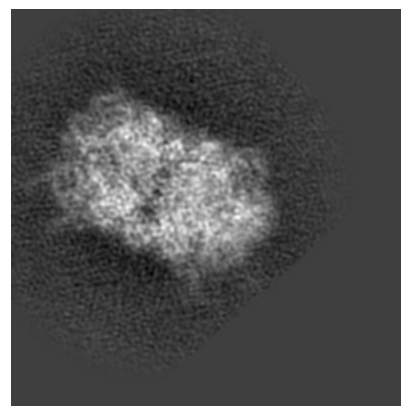
6.1.1 Primary map



X

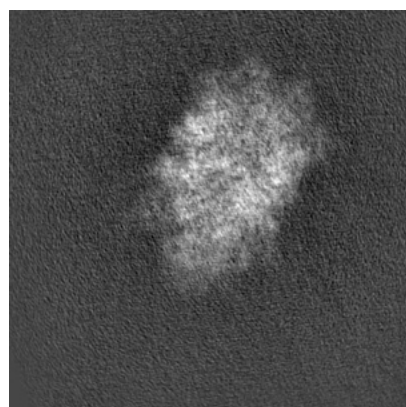


Y

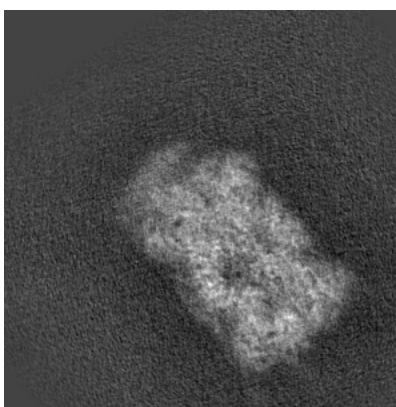


Z

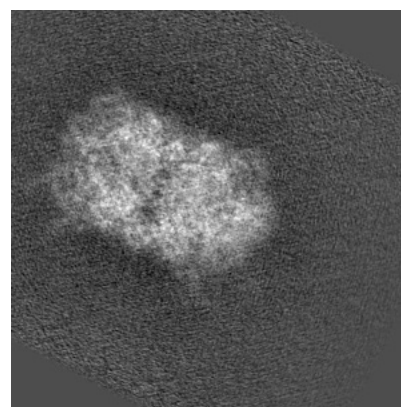
6.1.2 Raw map



X



Y

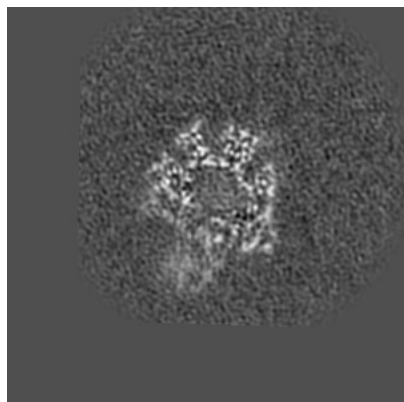


Z

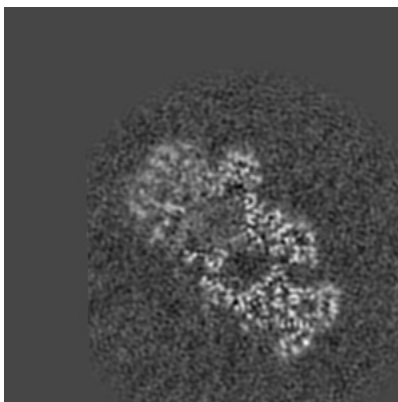
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

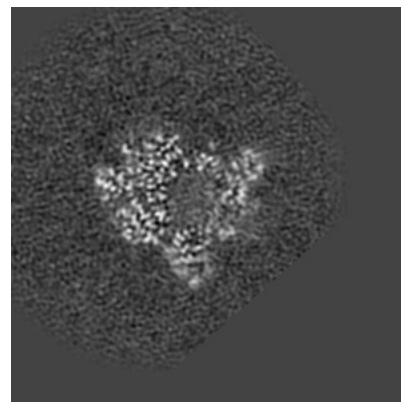
6.2.1 Primary map



X Index: 150

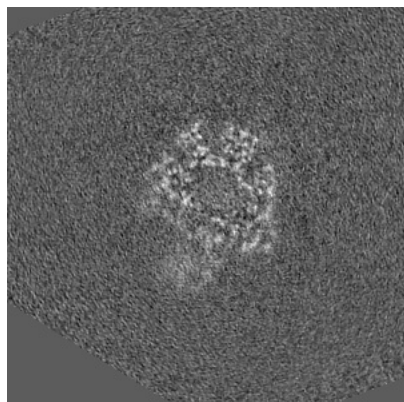


Y Index: 150

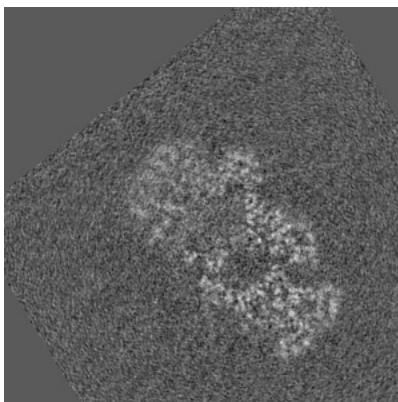


Z Index: 150

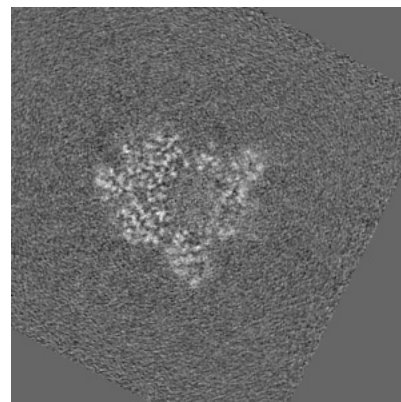
6.2.2 Raw map



X Index: 150



Y Index: 150

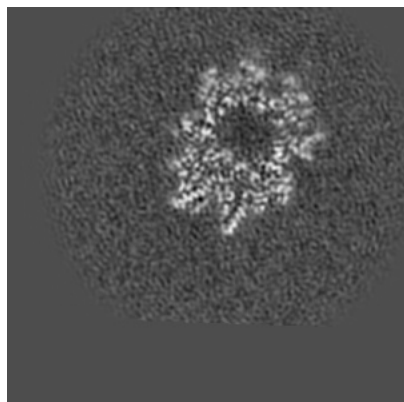


Z Index: 150

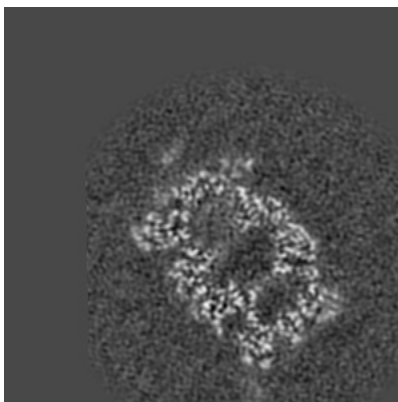
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

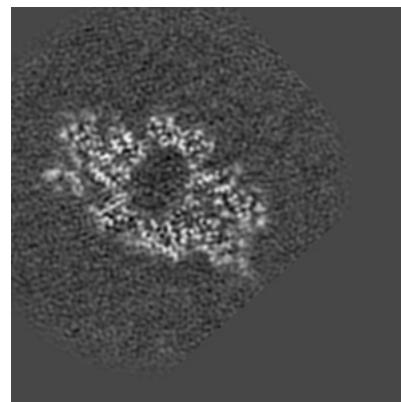
6.3.1 Primary map



X Index: 87

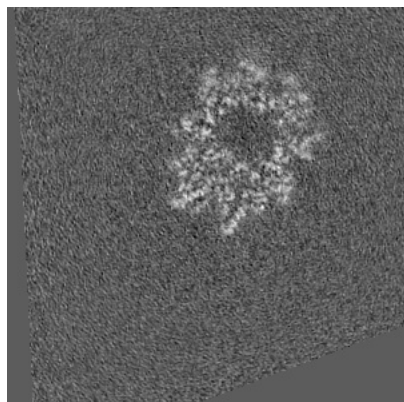


Y Index: 164

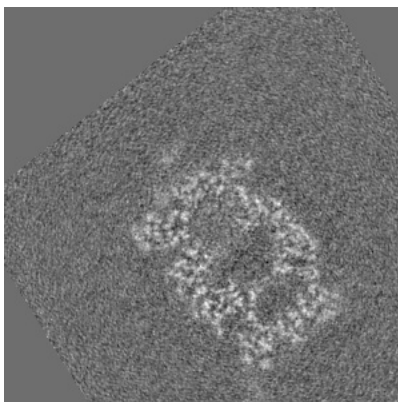


Z Index: 179

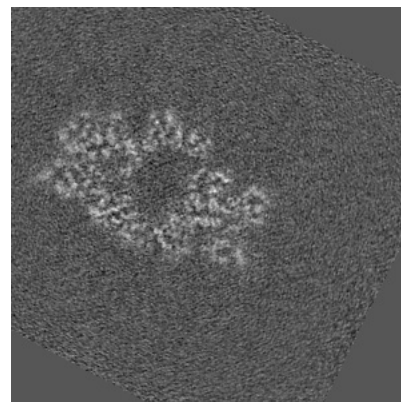
6.3.2 Raw map



X Index: 87



Y Index: 164

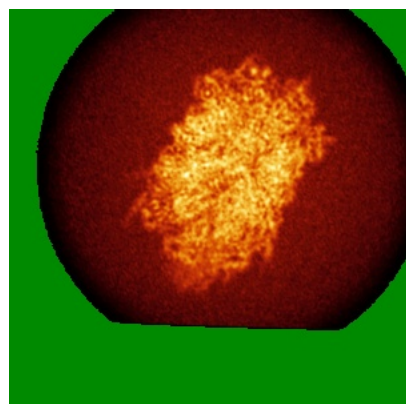


Z Index: 182

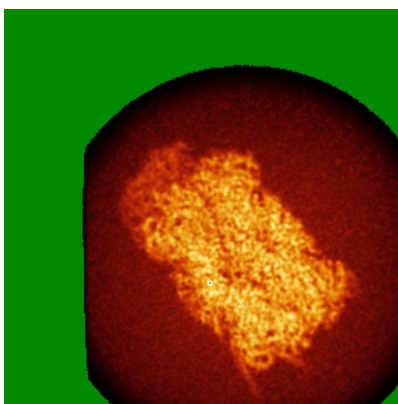
The images above show the largest variance slices of the map in three orthogonal directions.

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

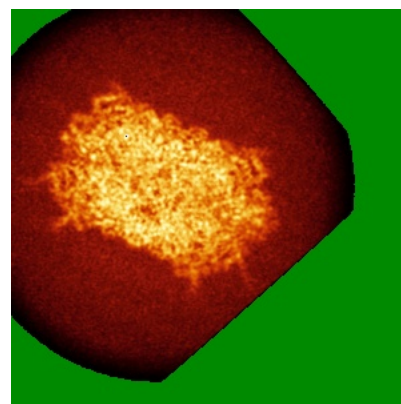
6.4.1 Primary map



X

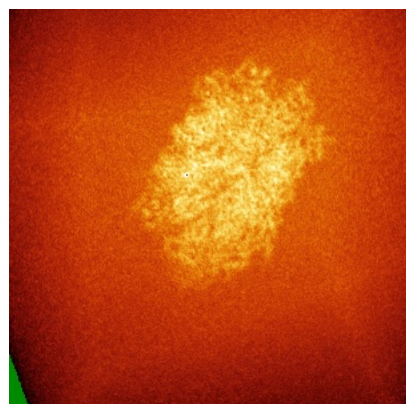


Y

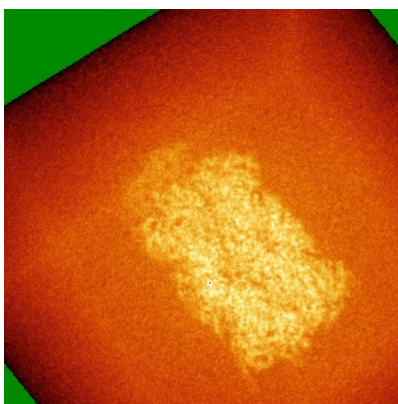


Z

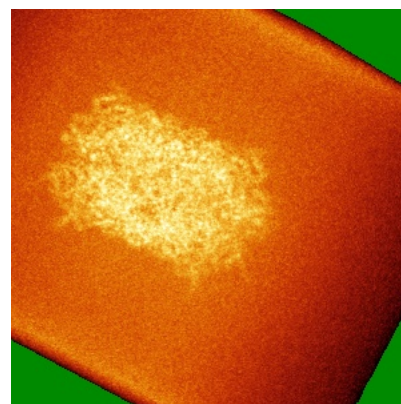
6.4.2 Raw map



X



Y

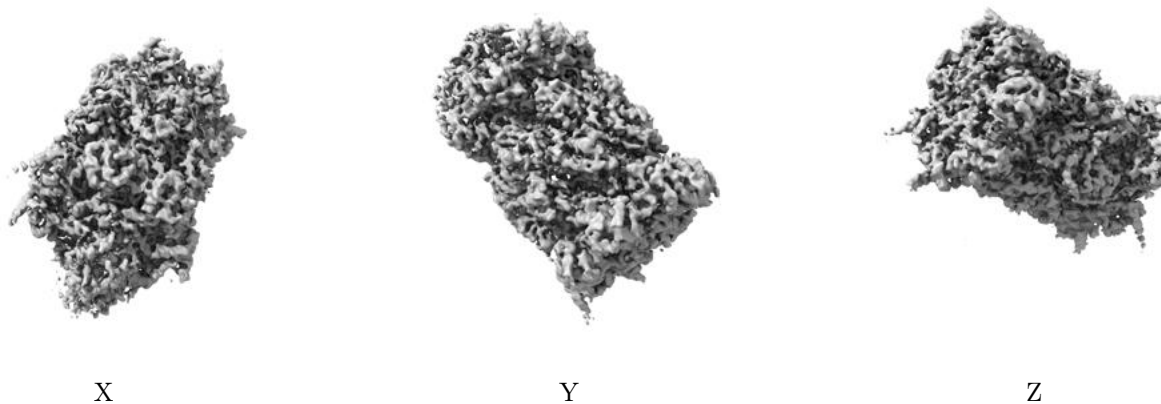


Z

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.

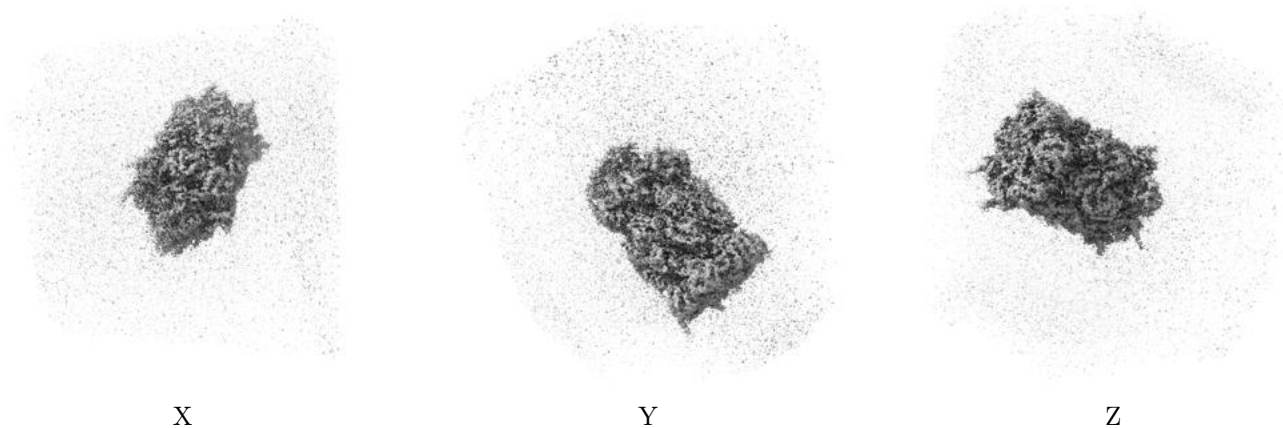
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.328. 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



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.

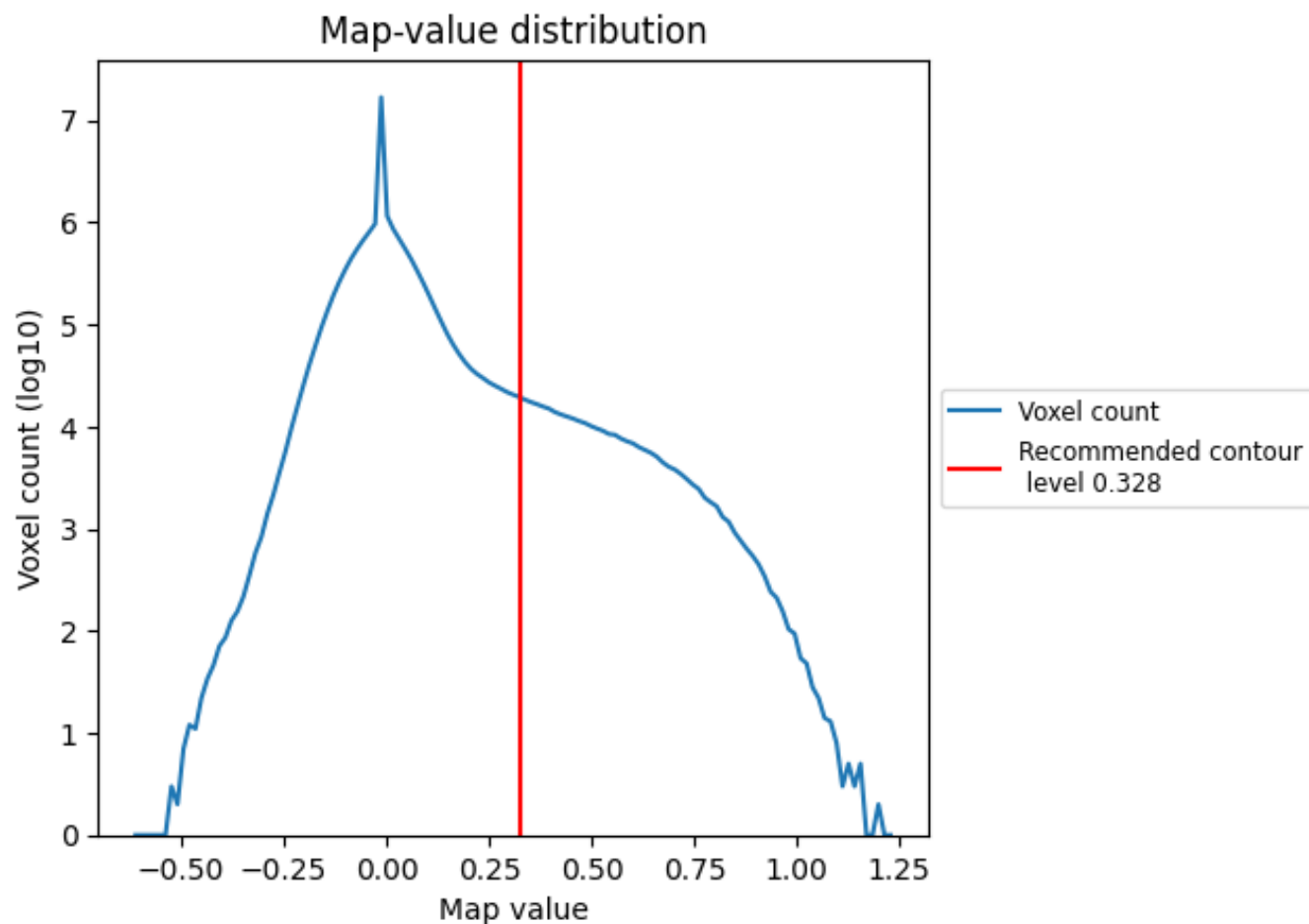
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

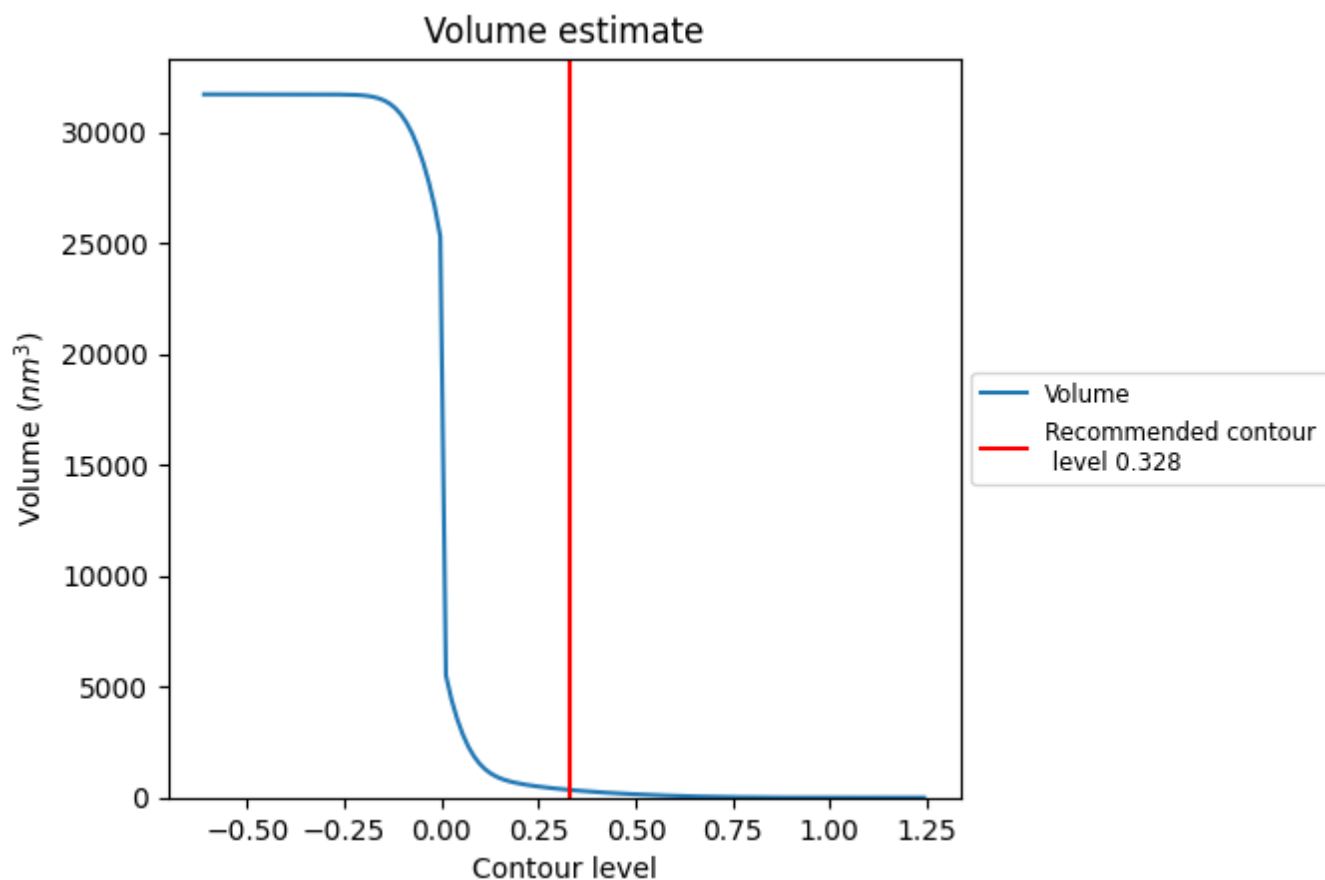
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

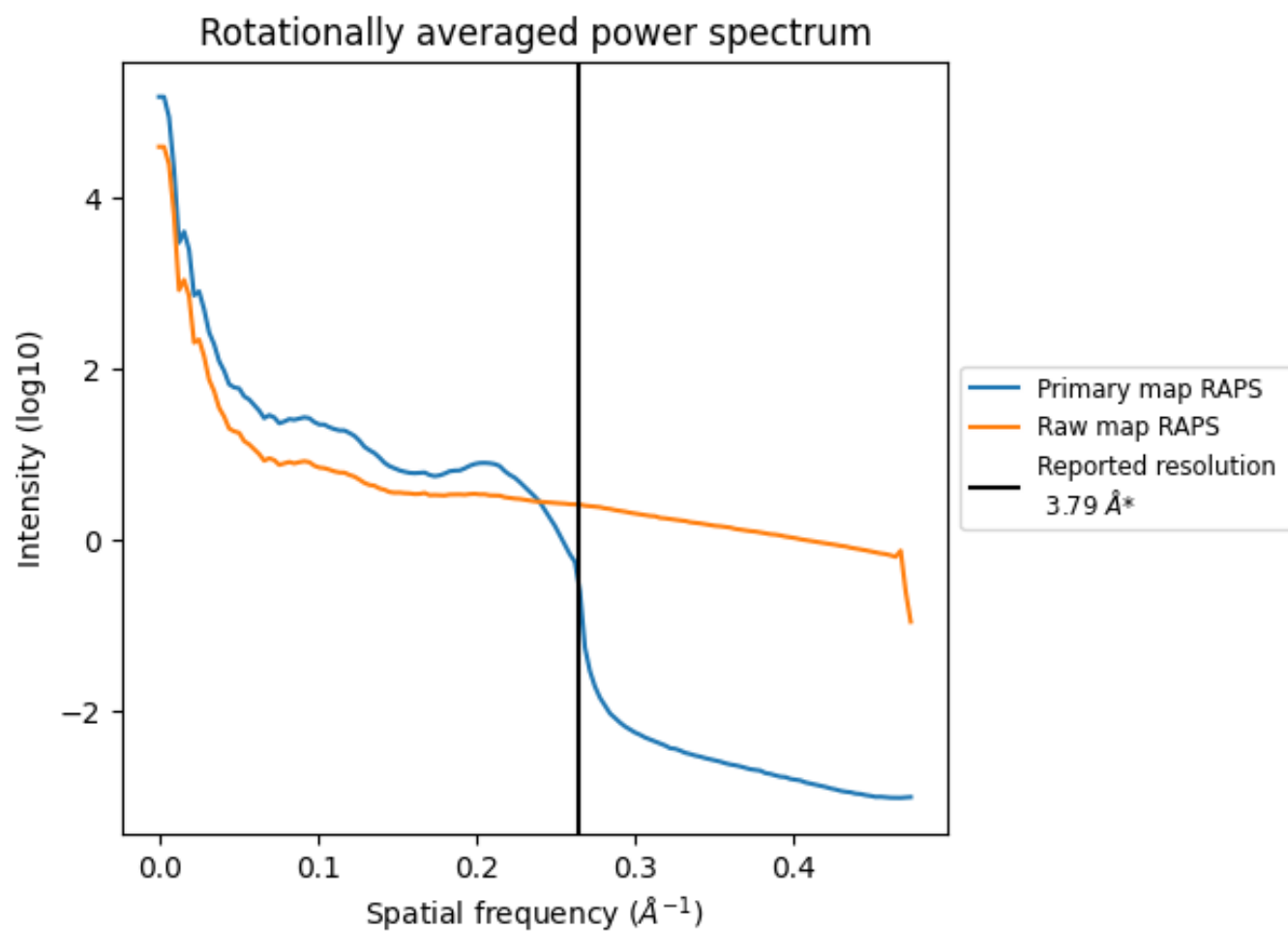
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 349 nm³; this corresponds to an approximate mass of 315 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 ⓘ

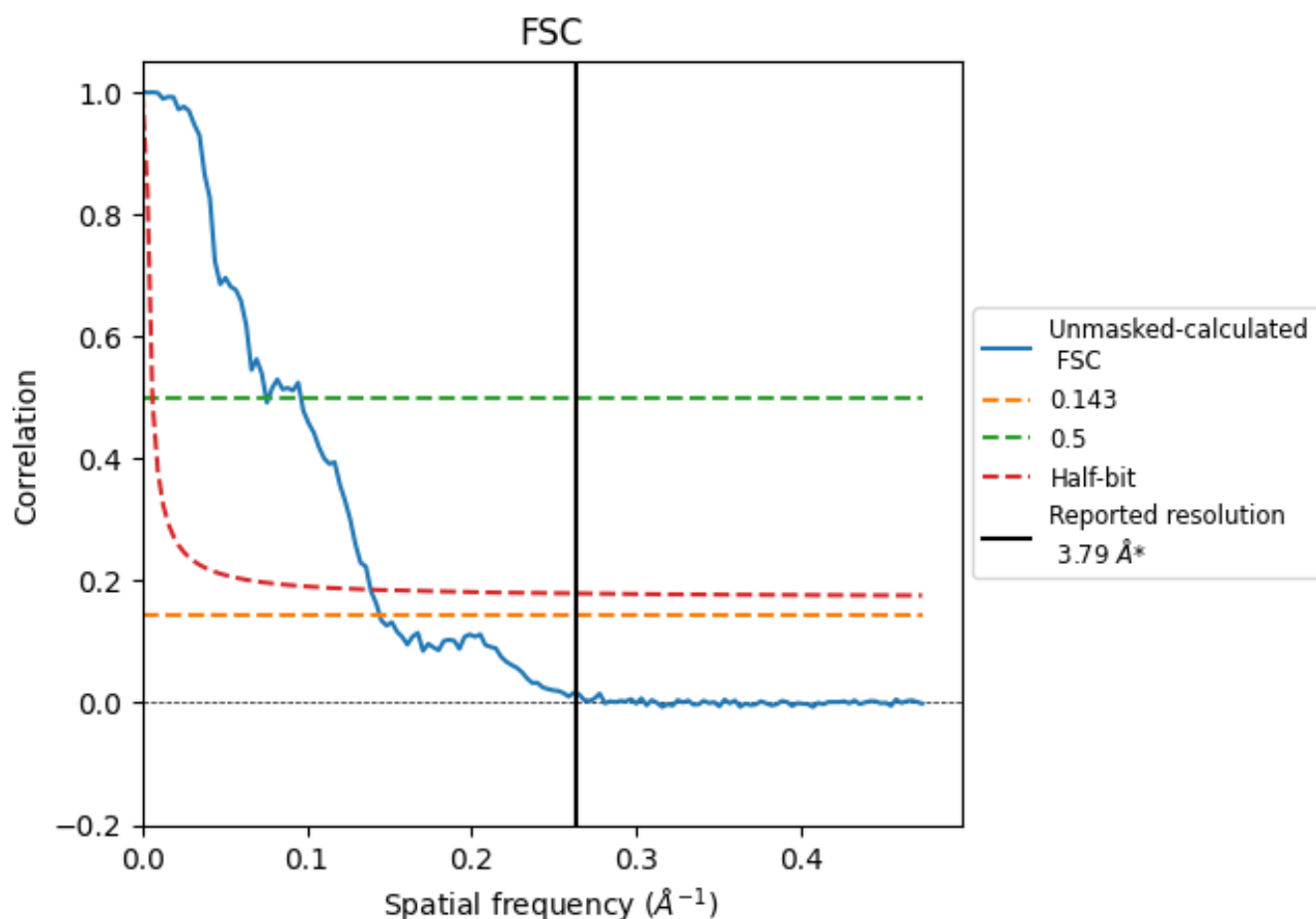


*Reported resolution corresponds to spatial frequency of 0.264 Å⁻¹

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 $0.264 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

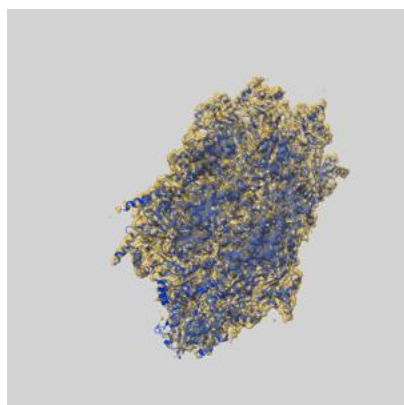
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.79	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.93	13.30	7.20

*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 6.93 differs from the reported value 3.79 by more than 10 %

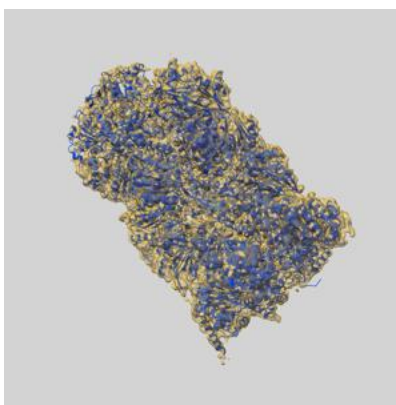
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-39334 and PDB model 8YIZ. Per-residue inclusion information can be found in section [3](#) on page [9](#).

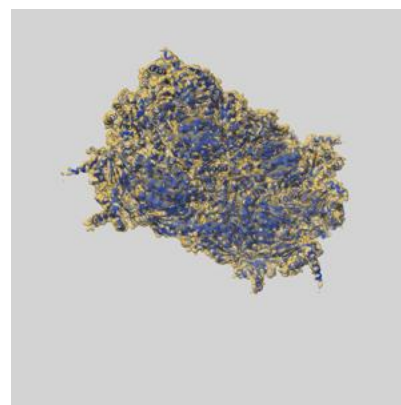
9.1 Map-model overlay [i](#)



X



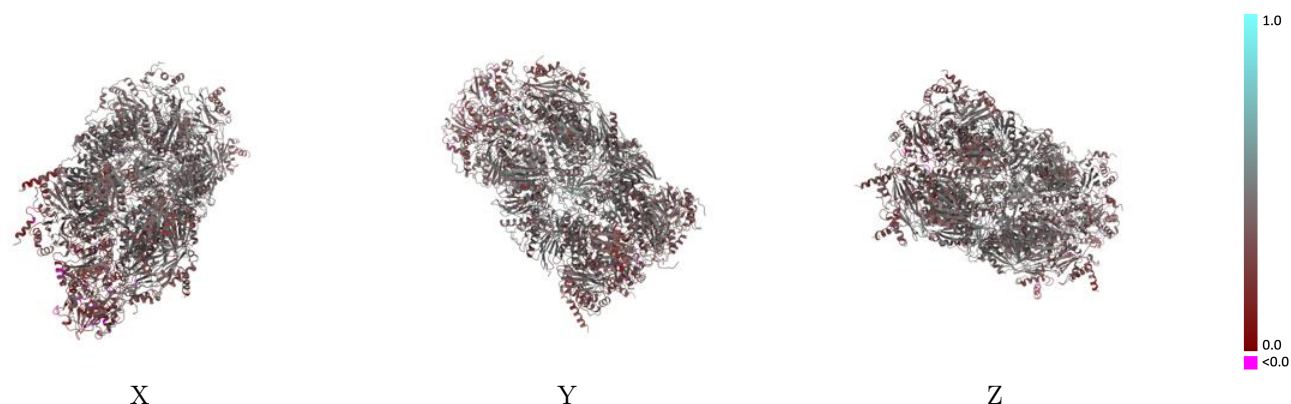
Y



Z

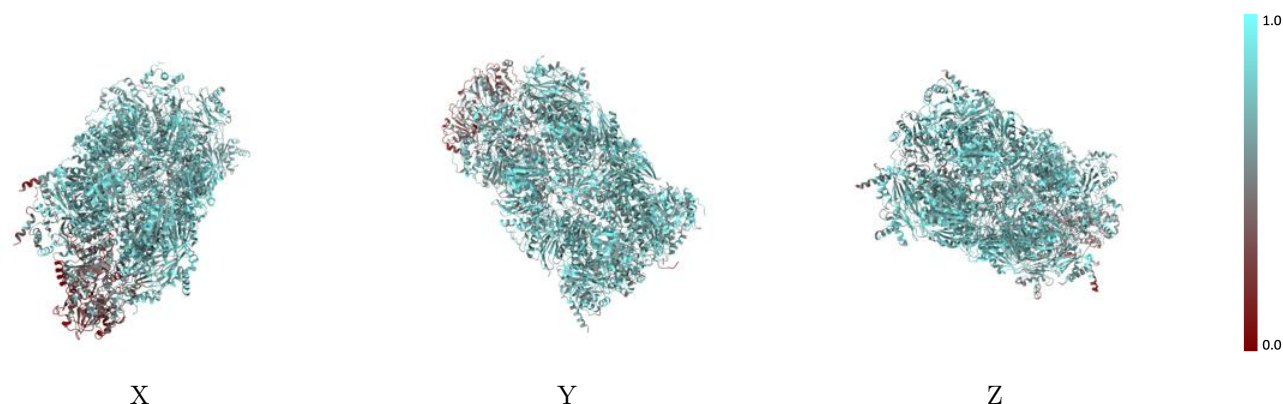
The images above show the 3D surface view of the map at the recommended contour level 0.328 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



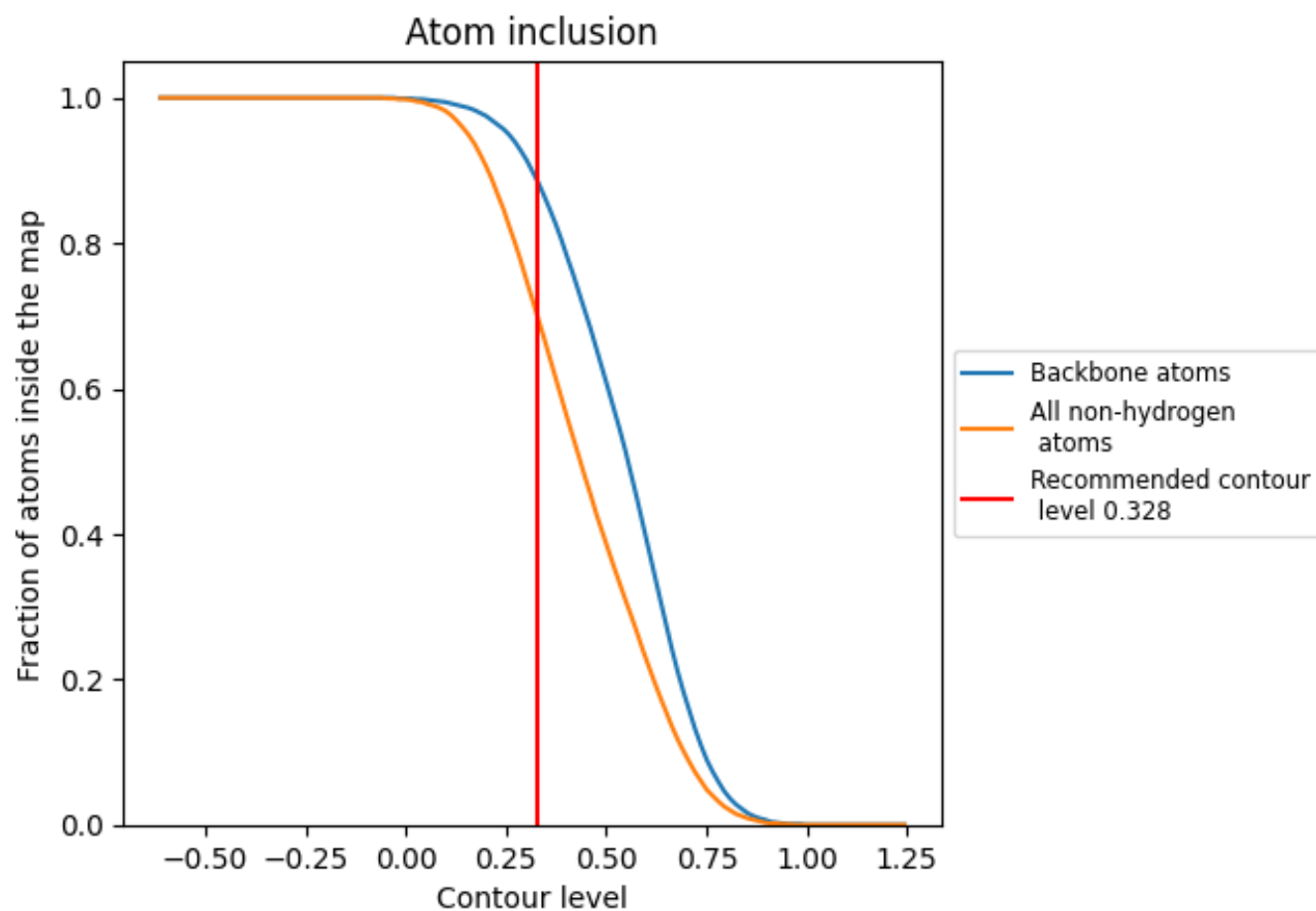
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.328).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 70% 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 (0.328) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7000	 0.3930
A	 0.7280	 0.3640
B	 0.7100	 0.3790
C	 0.7220	 0.3740
D	 0.6860	 0.3760
E	 0.7540	 0.3960
F	 0.7480	 0.4080
G	 0.7240	 0.3440
H	 0.7740	 0.4240
I	 0.7590	 0.4400
J	 0.7740	 0.4330
K	 0.7750	 0.4300
L	 0.7590	 0.4350
M	 0.7830	 0.4370
N	 0.7720	 0.4350
O	 0.7300	 0.3860
P	 0.6590	 0.3500
Q	 0.6270	 0.3200
R	 0.6190	 0.3380
S	 0.7140	 0.4020
T	 0.7470	 0.3940
U	 0.7160	 0.3810
V	 0.7580	 0.4260
W	 0.7630	 0.4480
X	 0.7650	 0.4430
Y	 0.7540	 0.4260
Z	 0.7560	 0.4310
a	 0.7760	 0.4310
b	 0.7680	 0.4350
f	 0.2570	 0.2910
g	 0.3890	 0.3150

