



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 09:40 AM UTC

PDB ID : 6WM3 / pdb_00006wm3
EMDB ID : EMD-21848
Title : Human V-ATPase in state 2 with SidK and ADP
Authors : Wang, L.; Wu, H.; Fu, T.M.
Deposited on : 2020-04-20
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

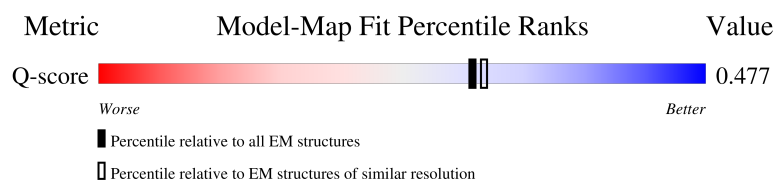
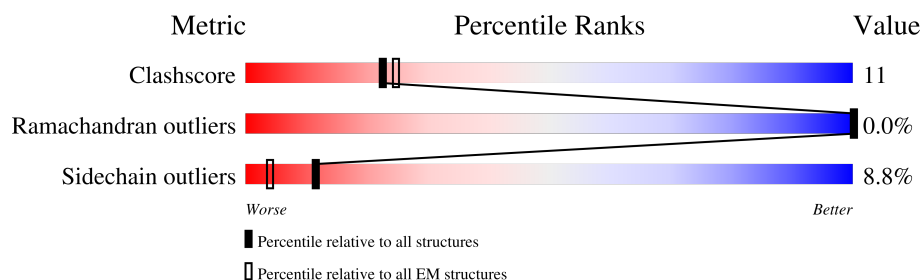
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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	14717 (2.90 - 3.90)

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	R	837	
2	O	382	
3	H	226	
3	I	226	

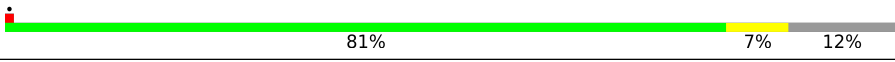
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Mol	Chain	Length	Quality of chain
3	J	226	
4	K	118	
4	L	118	
4	M	118	
5	S	81	
6	T	137	
7	U	470	
8	V	350	
9	0	205	
10	1	155	
10	2	155	
10	3	155	
10	4	155	
10	5	155	
10	6	155	
10	7	155	
10	8	155	
10	9	155	
11	Q	351	
12	A	617	
12	B	617	
12	C	617	
13	D	511	
13	E	511	
13	F	511	

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Mol	Chain	Length	Quality of chain
14	X	573	
14	Y	573	
14	Z	573	
15	G	247	
16	N	119	
17	P	483	

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 69755 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 V-type proton ATPase 116 kDa subunit a isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	753	Total	C	N	O	S	0	0
			6147	4016	1023	1068	40		

- Molecule 2 is a protein called V-type proton ATPase subunit C 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	O	375	Total	C	N	O	0	0
			1864	1114	375	375		

- Molecule 3 is a protein called V-type proton ATPase subunit E 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	225	Total	C	N	O	S	0	0
			1822	1143	322	347	10		
3	I	225	Total	C	N	O	S	0	0
			1822	1143	322	347	10		
3	H	225	Total	C	N	O	S	0	0
			1822	1143	322	347	10		

- Molecule 4 is a protein called V-type proton ATPase subunit G 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	114	Total	C	N	O	S	0	0
			938	573	179	183	3		
4	L	114	Total	C	N	O	S	0	0
			938	573	179	183	3		
4	K	114	Total	C	N	O	S	0	0
			938	573	179	183	3		

- Molecule 5 is a protein called V-type proton ATPase subunit e 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	S	77	Total	C	N	O	S	0	0
			631	436	97	93	5		

- Molecule 6 is a protein called Ribonuclease kappa.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	T	85	Total	C	N	O	S	0	0
			658	434	102	115	7		

- Molecule 7 is a protein called V-type proton ATPase subunit S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	U	204	Total	C	N	O	S	0	0
			1662	1086	267	299	10		

- Molecule 8 is a protein called Renin receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	V	49	Total	C	N	O	S	0	0
			411	280	57	71	3		

- Molecule 9 is a protein called V-type proton ATPase 21 kDa proteolipid subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	0	204	Total	C	N	O	S	0	0
			1498	990	238	259	11		

- Molecule 10 is a protein called V-type proton ATPase 16 kDa proteolipid subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	1	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
10	2	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
10	3	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
10	4	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
10	5	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
10	6	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	7	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
10	8	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
10	9	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		

- Molecule 11 is a protein called V-type proton ATPase subunit d 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Q	351	Total	C	N	O	S	0	0
			2844	1834	463	532	15		

- Molecule 12 is a protein called V-type proton ATPase catalytic subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	C	600	Total	C	N	O	S	0	0
			4656	2952	786	890	28		
12	A	600	Total	C	N	O	S	0	0
			4656	2952	786	890	28		
12	B	600	Total	C	N	O	S	0	0
			4656	2952	786	890	28		

- Molecule 13 is a protein called V-type proton ATPase subunit B, brain isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	F	468	Total	C	N	O	S	0	0
			3666	2325	625	696	20		
13	D	468	Total	C	N	O	S	0	0
			3666	2325	625	696	20		
13	E	468	Total	C	N	O	S	0	0
			3666	2325	625	696	20		

- Molecule 14 is a protein called SidK.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Z	262	Total	C	N	O	S	0	0
			2110	1339	353	408	10		
14	X	267	Total	C	N	O	S	0	0
			2136	1355	359	411	11		
14	Y	262	Total	C	N	O	S	0	0
			2111	1339	354	408	10		

- Molecule 15 is a protein called V-type proton ATPase subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	G	213	Total	C	N	O	S	0	0
			1717	1090	310	312	5		

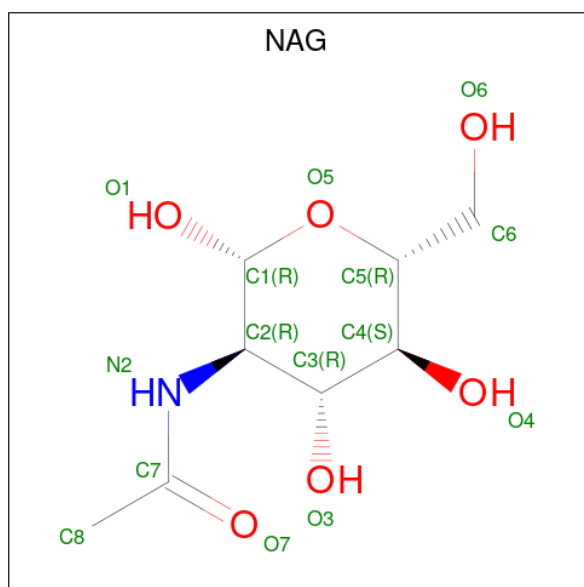
- Molecule 16 is a protein called V-type proton ATPase subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	N	110	Total	C	N	O	S	0	0
			875	552	157	164	2		

- Molecule 17 is a protein called V-type proton ATPase subunit H.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	427	Total	C	N	O		0	0
			2121	1267	427	427			

- Molecule 18 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



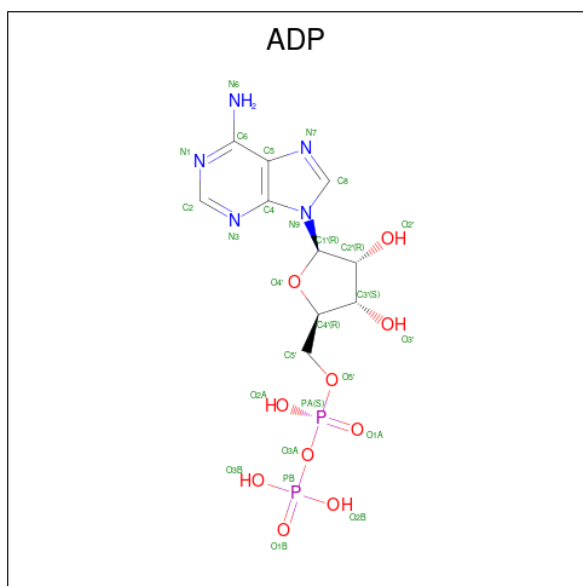
Mol	Chain	Residues	Atoms					AltConf
18	R	1	Total	C	N	O		0
			14	8	1	5		
18	S	1	Total	C	N	O		0
			14	8	1	5		
18	U	1	Total	C	N	O		0
			14	8	1	5		

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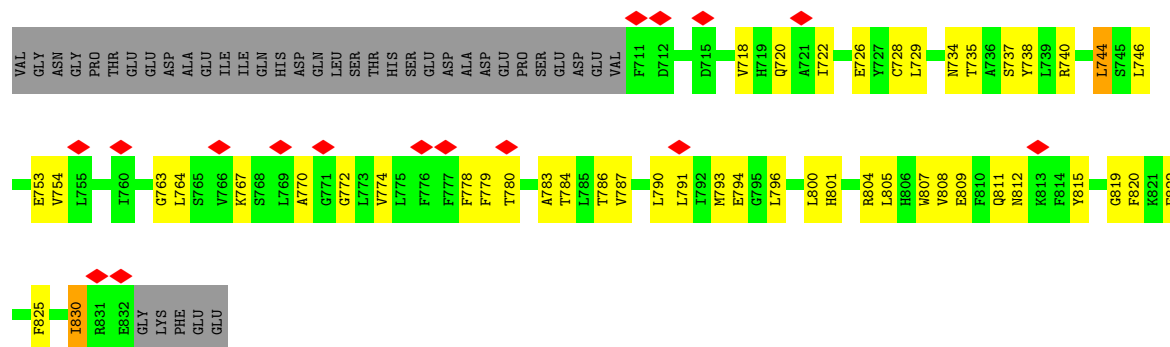
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Mol	Chain	Residues	Atoms				AltConf
18	U	1	Total	C	N	O	0
			14	8	1	5	
18	U	1	Total	C	N	O	0
			14	8	1	5	
18	U	1	Total	C	N	O	0
			14	8	1	5	
18	U	1	Total	C	N	O	0
			14	8	1	5	
18	U	1	Total	C	N	O	0
			14	8	1	5	

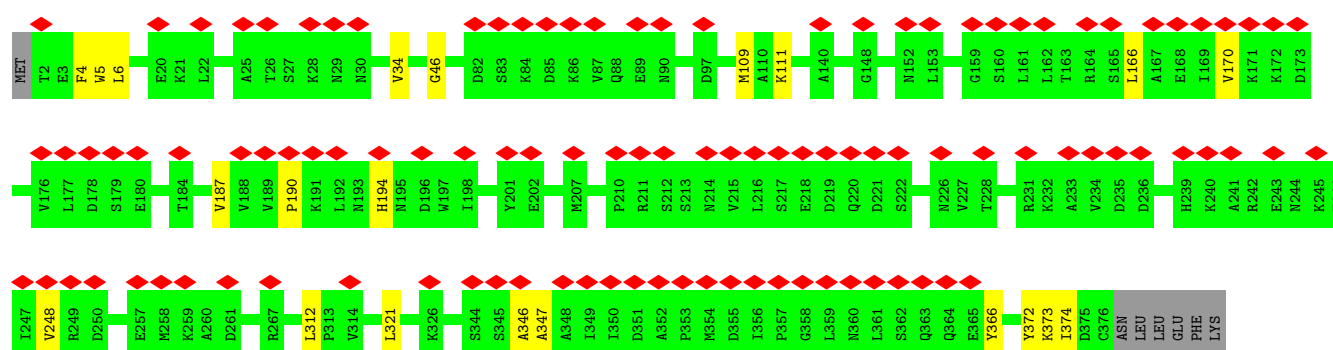
- Molecule 19 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



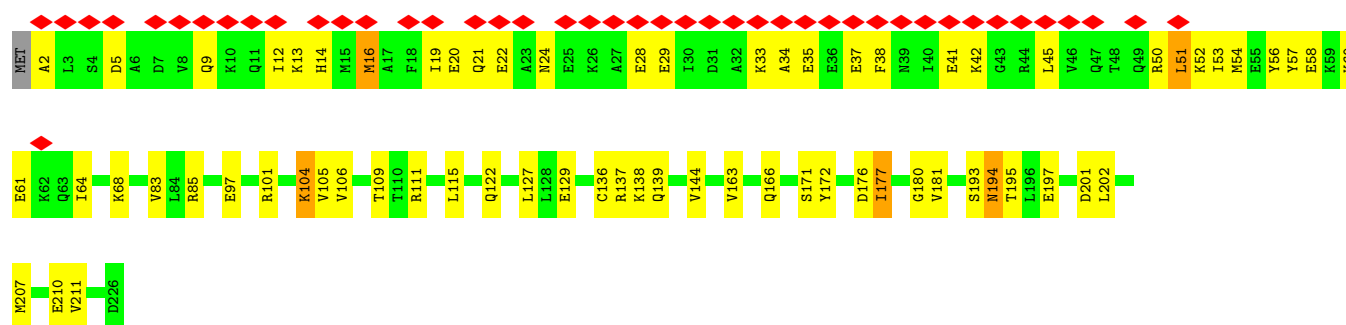
Mol	Chain	Residues	Atoms					AltConf
19	B	1	Total	C	N	O	P	0
			27	10	5	10	2	



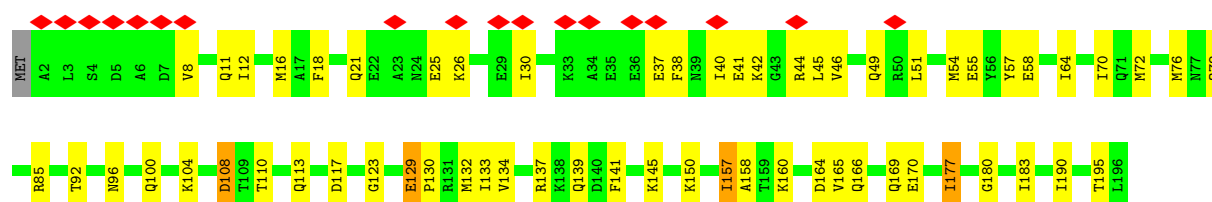
• Molecule 2: V-type proton ATPase subunit C 1



• Molecule 3: V-type proton ATPase subunit E 1

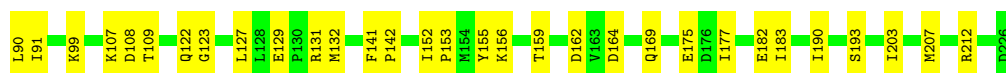
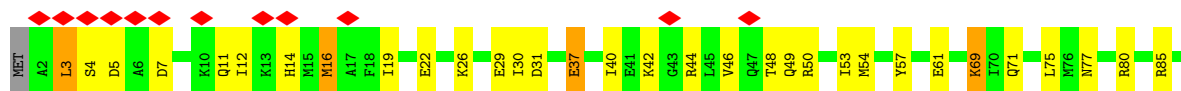


• Molecule 3: V-type proton ATPase subunit E 1

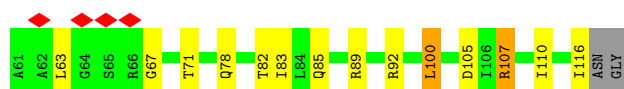
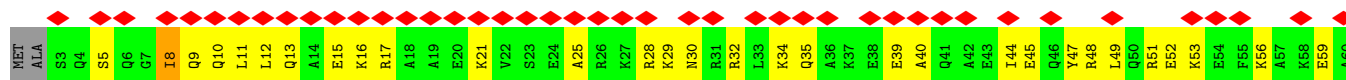
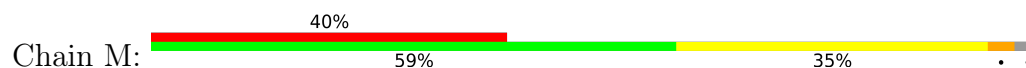




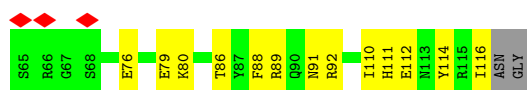
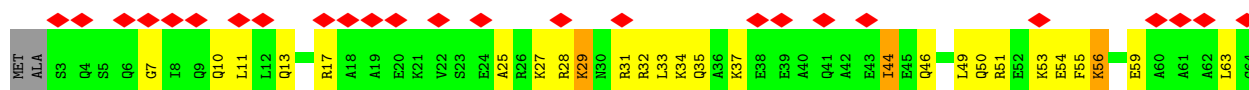
- Molecule 3: V-type proton ATPase subunit E 1



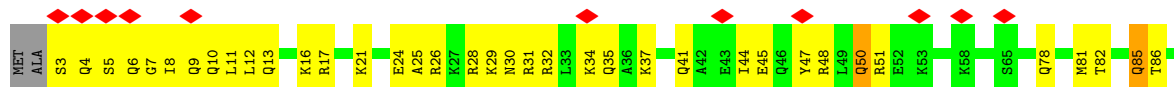
- Molecule 4: V-type proton ATPase subunit G 1



- Molecule 4: V-type proton ATPase subunit G 1



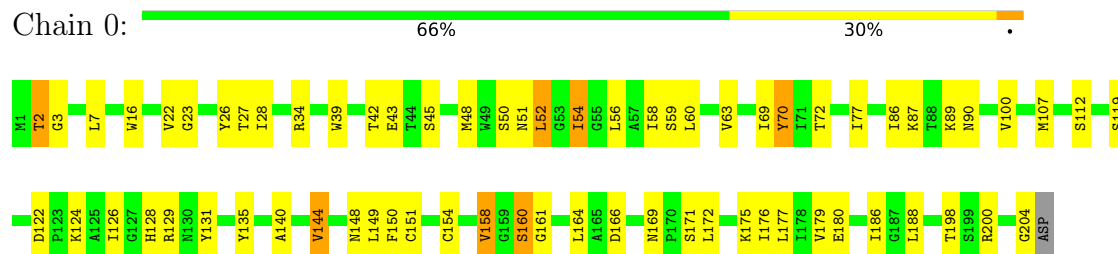
- Molecule 4: V-type proton ATPase subunit G 1



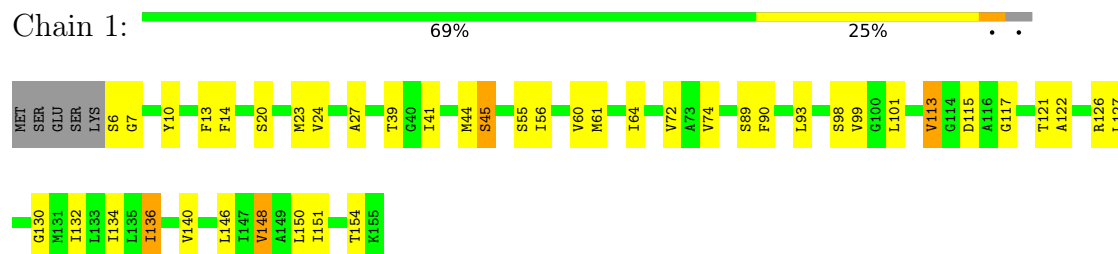
- Molecule 5: V-type proton ATPase subunit e 1



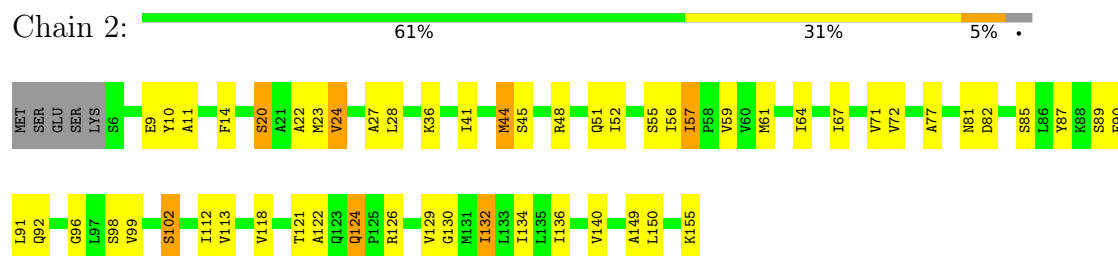
- Molecule 9: V-type proton ATPase 21 kDa proteolipid subunit



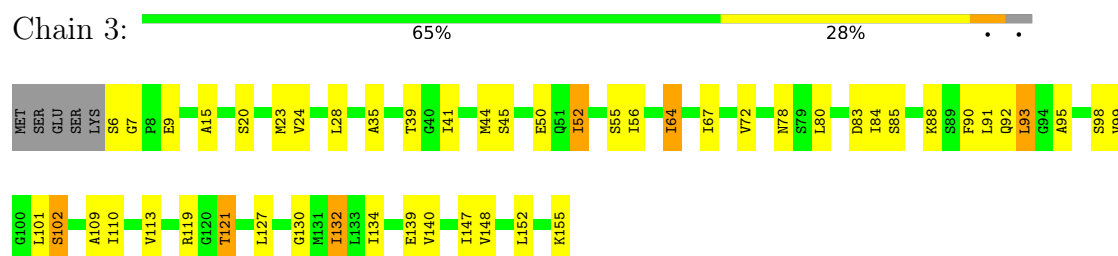
- Molecule 10: V-type proton ATPase 16 kDa proteolipid subunit



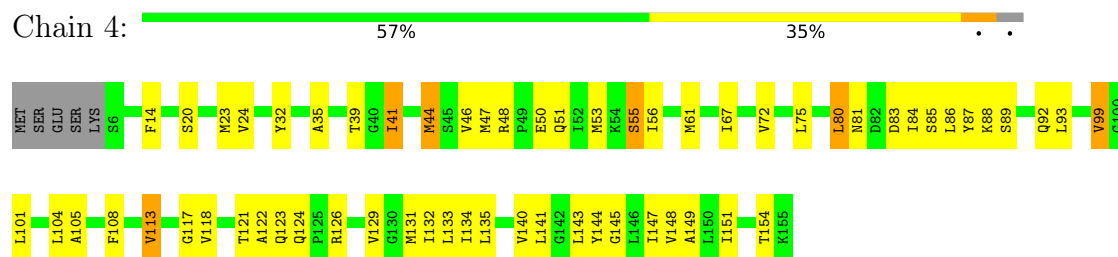
- Molecule 10: V-type proton ATPase 16 kDa proteolipid subunit



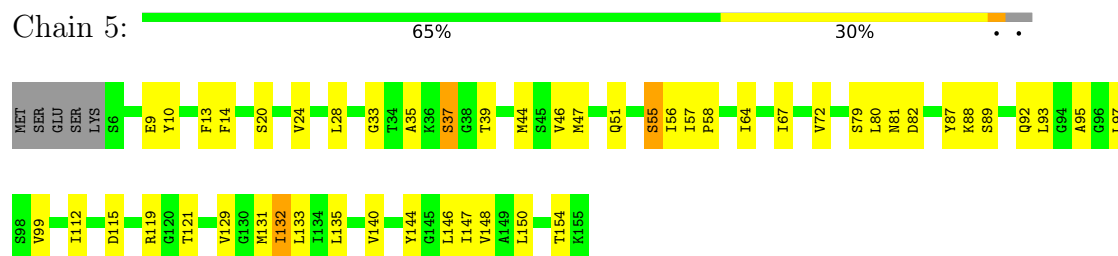
- Molecule 10: V-type proton ATPase 16 kDa proteolipid subunit



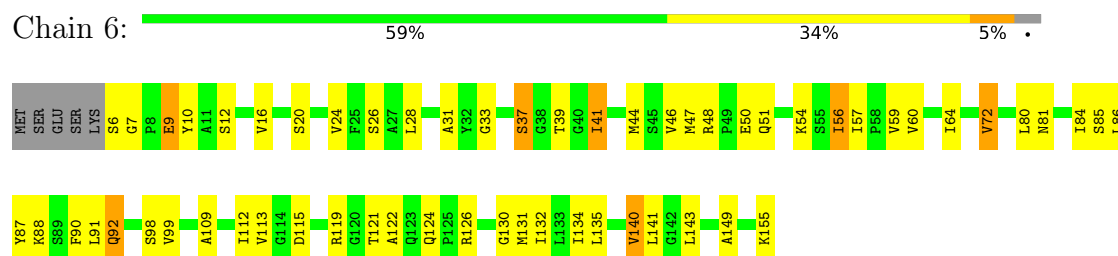
- Molecule 10: V-type proton ATPase 16 kDa proteolipid subunit



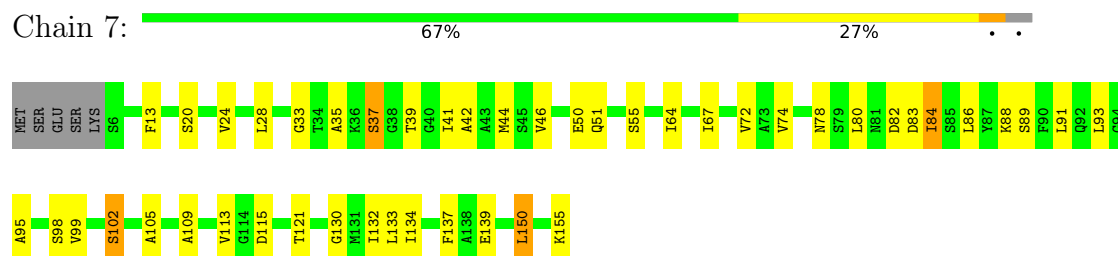
- Molecule 10: V-type proton ATPase 16 kDa proteolipid subunit



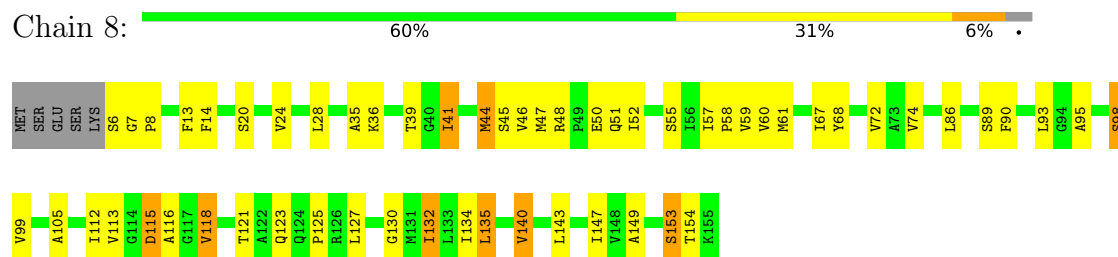
- Molecule 10: V-type proton ATPase 16 kDa proteolipid subunit



- Molecule 10: V-type proton ATPase 16 kDa proteolipid subunit

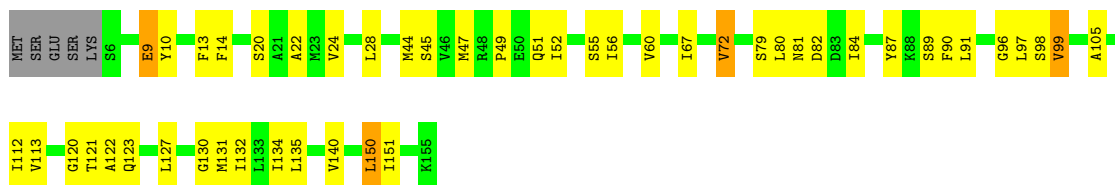


- Molecule 10: V-type proton ATPase 16 kDa proteolipid subunit



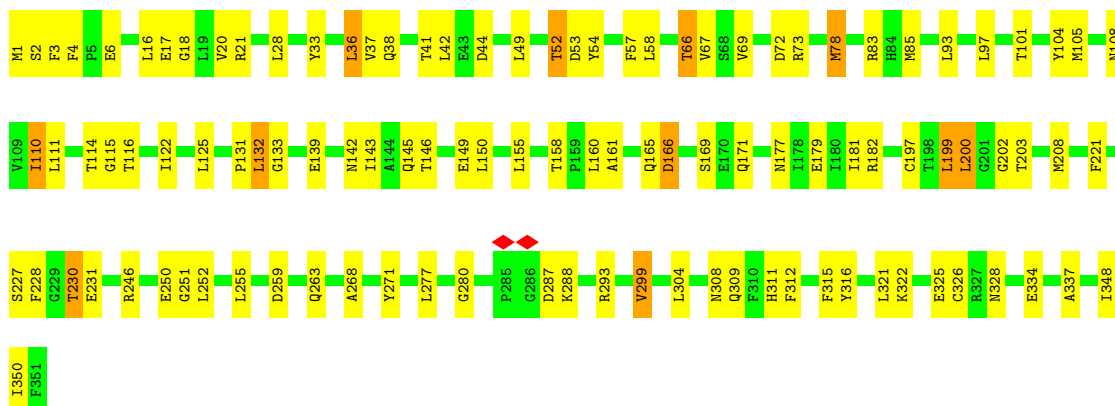
- Molecule 10: V-type proton ATPase 16 kDa proteolipid subunit

Chain 9: 



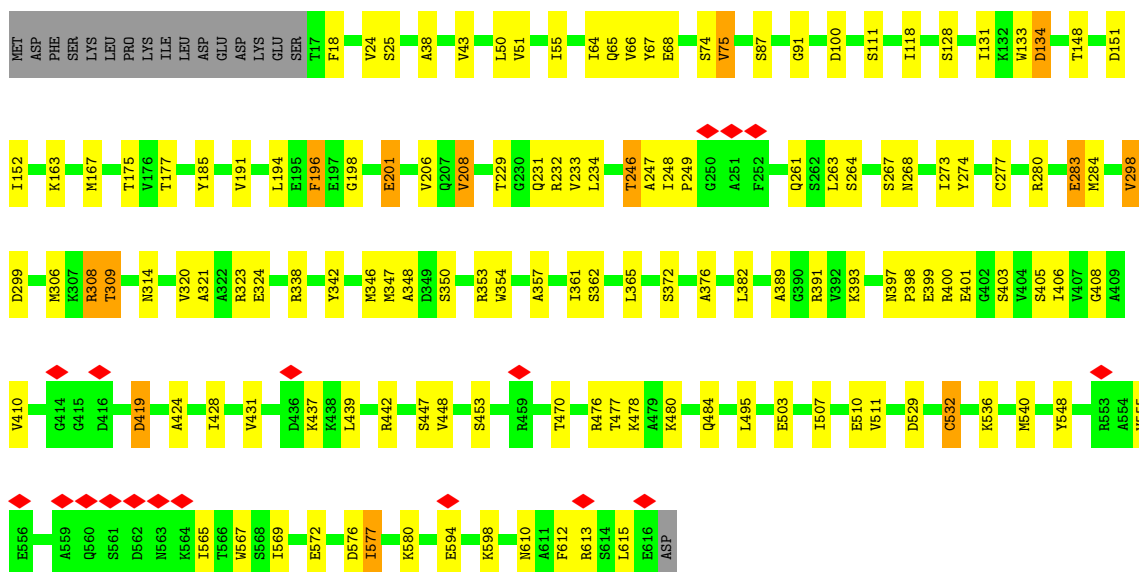
- Molecule 11: V-type proton ATPase subunit d 1

Chain Q: 



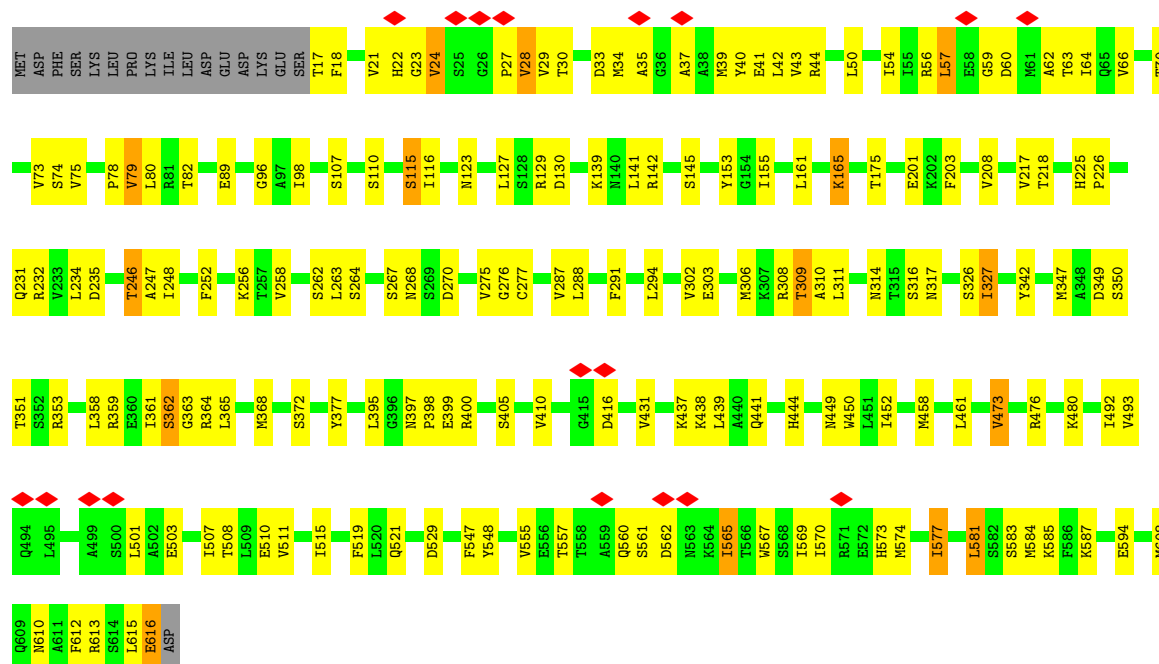
- Molecule 12: V-type proton ATPase catalytic subunit A

Chain C: 



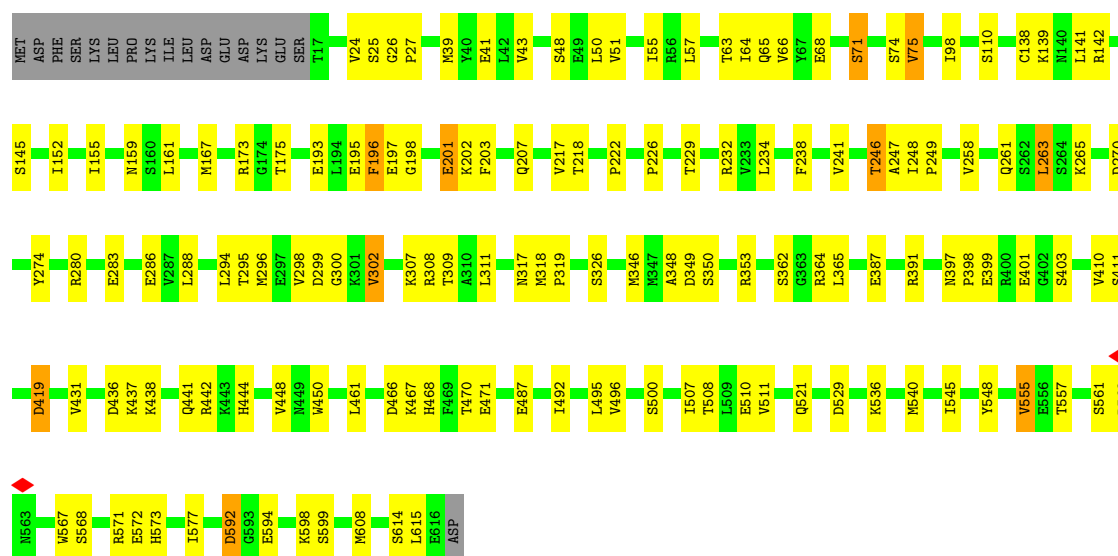
- Molecule 12: V-type proton ATPase catalytic subunit A

Chain A: 



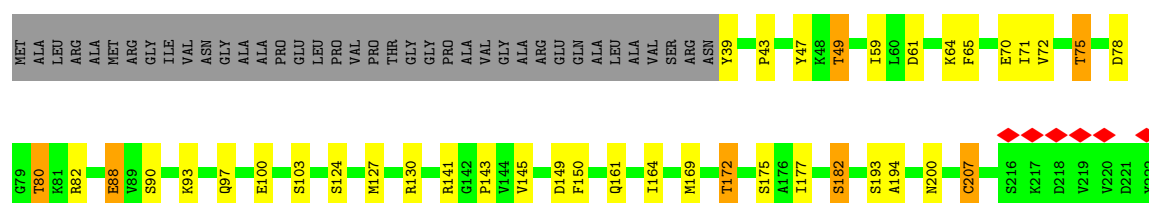
• Molecule 12: V-type proton ATPase catalytic subunit A

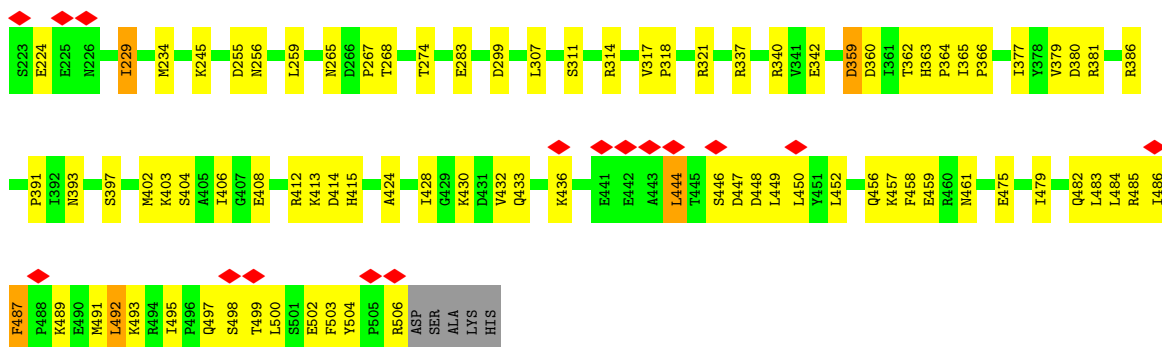
Chain B: 74% 22%



• Molecule 13: V-type proton ATPase subunit B, brain isoform

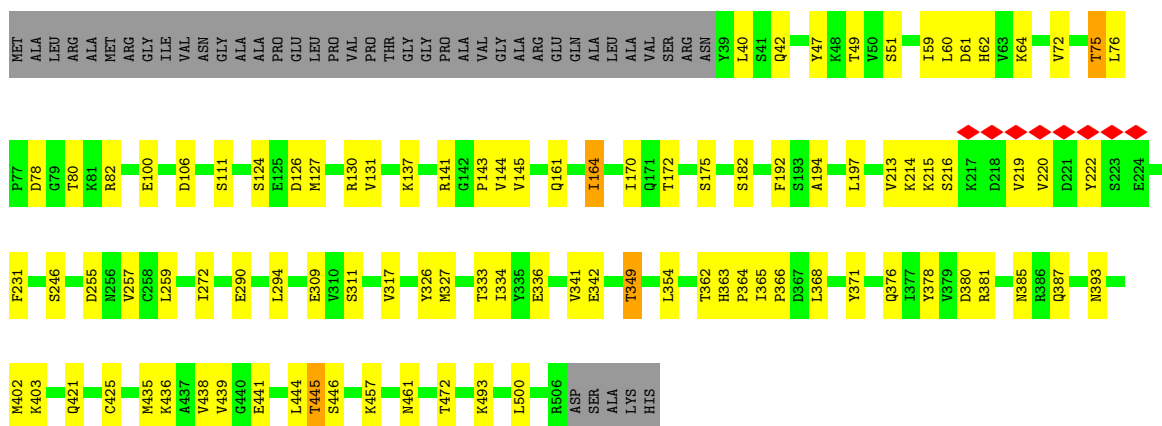
Chain F: 67% 22% 8%





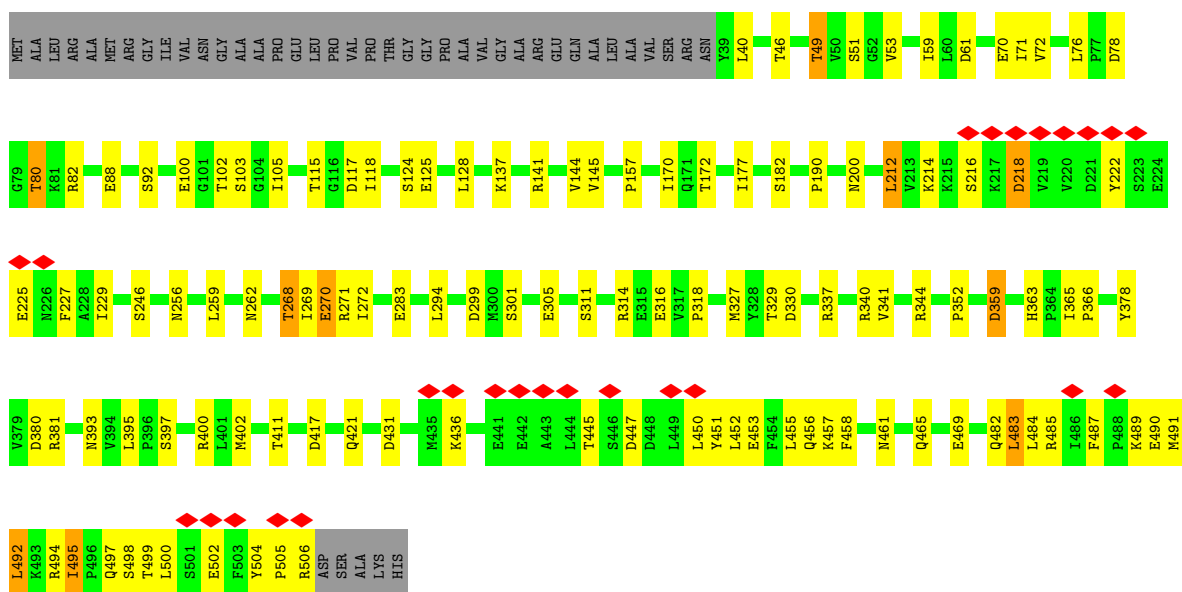
- Molecule 13: V-type proton ATPase subunit B, brain isoform

Chain D: 73% 18% 8%



- Molecule 13: V-type proton ATPase subunit B, brain isoform

Chain E: 5% 68% 22% 8%



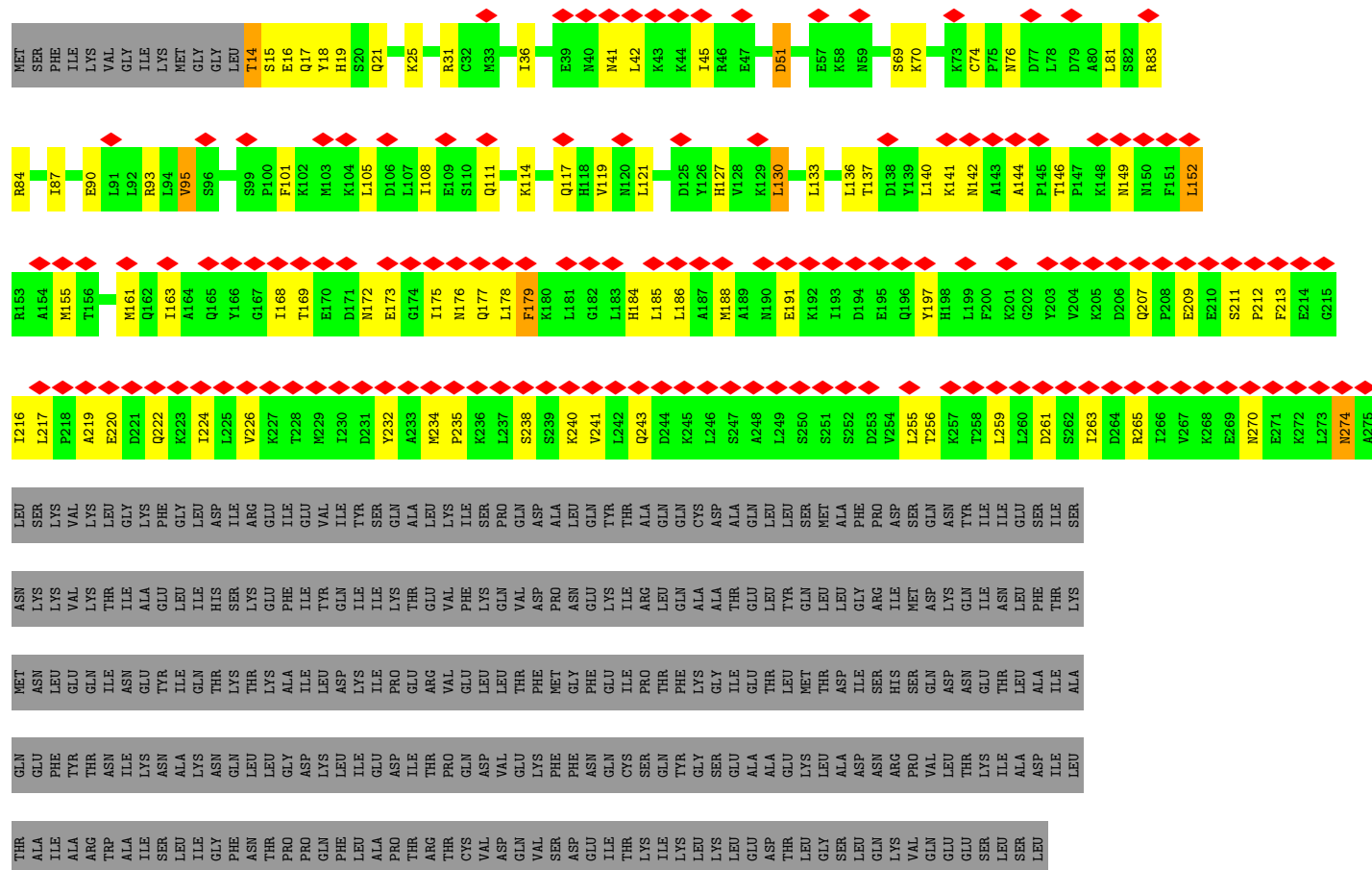
- Molecule 14: SidK



ILE
THR
LYS
ILE
LYS
LYS
LEU
LYS
LEU
GLY
ASP
MET
THR
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GLY
SER
LEU
GLN
LYS
VAL
GLN
GLU
SER
SER
LEU

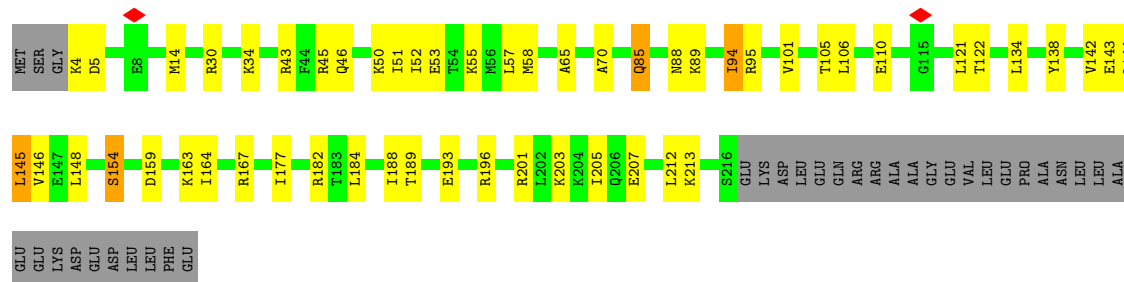
• Molecule 14: SidK

Chain Y: 25% 30% 14% 54%



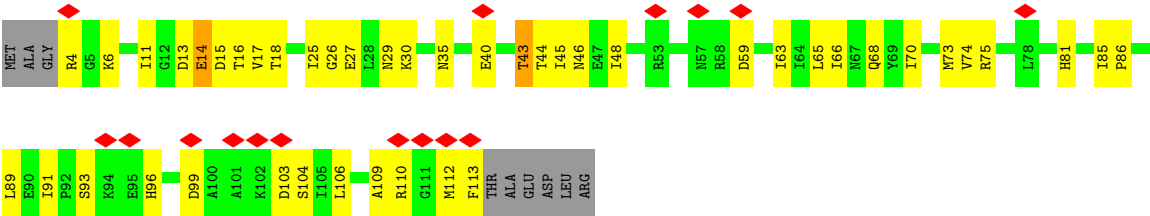
• Molecule 15: V-type proton ATPase subunit D

Chain G: 64% 20% 14%

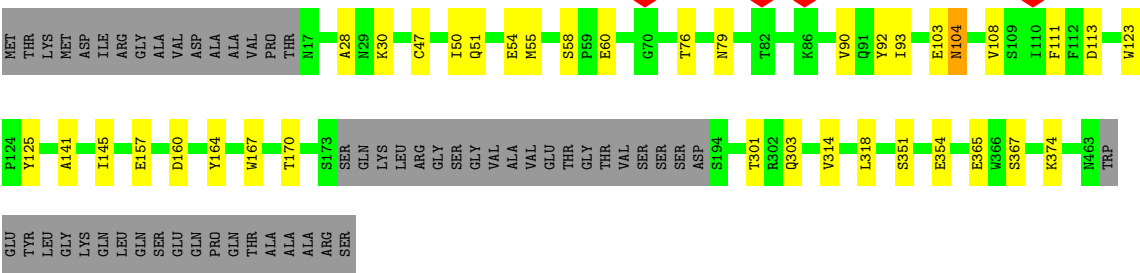
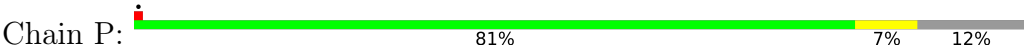


• Molecule 16: V-type proton ATPase subunit F

Chain N: 13% 55% 36% 8%



• Molecule 17: V-type proton ATPase subunit H



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1000000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.1	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	28.244	Depositor
Minimum map value	-15.673	Depositor
Average map value	0.016	Depositor
Map value standard deviation	1.165	Depositor
Recommended contour level	3.5	Depositor
Map size ($\text{\AA}$)	388.80002, 388.80002, 388.80002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

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

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	R	0.16	0/6306	0.35	0/8534
2	O	0.13	0/1863	0.33	0/2600
3	H	0.26	0/1839	0.36	0/2462
3	I	0.28	0/1839	0.46	0/2462
3	J	0.25	0/1839	0.41	0/2462
4	K	0.23	0/945	0.41	0/1258
4	L	0.29	0/945	0.44	0/1258
4	M	0.22	0/945	0.38	0/1258
5	S	0.16	0/657	0.37	0/902
6	T	0.14	0/674	0.37	0/915
7	U	0.29	0/1716	0.46	0/2333
8	V	0.32	0/425	0.46	0/582
9	0	0.36	0/1532	0.50	0/2082
10	1	0.37	0/1080	0.49	0/1461
10	2	0.36	0/1080	0.48	0/1461
10	3	0.35	0/1080	0.47	0/1461
10	4	0.34	0/1080	0.48	0/1461
10	5	0.32	0/1080	0.43	0/1461
10	6	0.30	0/1080	0.42	0/1461
10	7	0.31	0/1080	0.45	0/1461
10	8	0.33	0/1080	0.46	0/1461
10	9	0.35	0/1080	0.45	0/1461
11	Q	0.34	0/2910	0.46	0/3940
12	A	0.38	0/4752	0.46	1/6435 (0.0%)
12	B	0.41	0/4752	0.43	0/6435
12	C	0.37	0/4752	0.42	0/6435
13	D	0.43	0/3739	0.43	0/5067
13	E	0.42	0/3739	0.47	0/5067
13	F	0.40	0/3739	0.48	0/5067
14	X	0.23	0/2170	0.36	0/2926
14	Y	0.16	0/2145	0.34	0/2893
14	Z	0.20	0/2143	0.34	0/2888

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
15	G	0.26	0/1735	0.38	0/2320
16	N	0.16	0/889	0.32	0/1200
17	P	0.24	0/2119	0.56	0/2955
All	All	0.32	0/70829	0.43	1/95885 (0.0%)

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
3	I	0	1
12	A	0	2
13	E	0	1
13	F	0	1
17	P	0	1
All	All	0	6

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	287	VAL	N-CA-C	-6.92	106.75	113.53

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	A	23	GLY	Peptide
12	A	33	ASP	Peptide
13	E	451	TYR	Peptide
13	F	487	PHE	Peptide
3	I	224	PHE	Peptide
17	P	164	TYR	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	R	6147	0	6172	250	0
2	O	1864	0	830	12	0
3	H	1822	0	1886	54	0
3	I	1822	0	1886	42	0
3	J	1822	0	1886	52	0
4	K	938	0	947	43	0
4	L	938	0	947	28	0
4	M	938	0	947	34	0
5	S	631	0	646	20	0
6	T	658	0	652	16	0
7	U	1662	0	1583	46	0
8	V	411	0	401	12	0
9	0	1498	0	1544	48	0
10	1	1065	0	1131	23	0
10	2	1065	0	1131	30	0
10	3	1065	0	1131	32	0
10	4	1065	0	1131	33	0
10	5	1065	0	1131	29	0
10	6	1065	0	1131	44	0
10	7	1065	0	1131	31	0
10	8	1065	0	1131	37	0
10	9	1065	0	1131	33	0
11	Q	2844	0	2782	81	0
12	A	4656	0	4642	104	0
12	B	4656	0	4642	80	0
12	C	4656	0	4642	78	0
13	D	3666	0	3665	55	0
13	E	3666	0	3665	73	0
13	F	3666	0	3665	70	0
14	X	2136	0	2158	45	0
14	Y	2111	0	2134	55	0
14	Z	2110	0	2132	51	0
15	G	1717	0	1829	36	0
16	N	875	0	878	32	0
17	P	2121	0	941	21	0
18	R	14	0	13	1	0
18	S	14	0	13	0	0
18	U	84	0	78	1	0
19	B	27	0	12	2	0
All	All	69755	0	68397	1563	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 11.

All (1563) 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)
13:F:446:SER:O	13:F:450:LEU:HB2	1.73	0.88
14:Z:19:HIS:HD1	14:Z:69:SER:HG	1.21	0.88
9:0:77:ILE:HG21	10:1:117:GLY:HA2	1.60	0.84
3:H:22:GLU:HG3	4:K:17:ARG:HH11	1.41	0.84
12:C:314:ASN:HD21	12:C:323:ARG:HG2	1.41	0.83
1:R:734:ASN:HD22	1:R:809:GLU:HG3	1.45	0.81
7:U:401:GLN:HE22	8:V:296:ALA:H	1.28	0.81
9:0:54:ILE:HD12	9:0:112:SER:HB2	1.63	0.81
10:2:72:VAL:HG11	10:2:99:VAL:HG11	1.64	0.80
12:B:442:ARG:NH2	13:E:431:ASP:OD2	2.15	0.80
1:R:176:ASN:H	1:R:241:ARG:HH12	1.29	0.80
17:P:90:VAL:O	17:P:93:ILE:N	2.12	0.80
10:7:28:LEU:HD12	10:8:105:ALA:HB2	1.64	0.80
10:6:140:VAL:HA	10:6:143:LEU:HD12	1.64	0.79
12:A:24:VAL:HB	12:A:29:VAL:HA	1.63	0.79
1:R:482:ARG:HG2	5:S:77:LYS:HA	1.65	0.79
1:R:132:LEU:HD11	1:R:254:ARG:HE	1.48	0.78
12:A:24:VAL:HG11	12:A:70:THR:HG21	1.63	0.78
3:J:50:ARG:NH2	3:J:54:MET:SD	2.56	0.78
3:J:54:MET:HA	4:M:51:ARG:HH22	1.48	0.77
10:8:113:VAL:HG21	10:8:134:ILE:HG21	1.64	0.77
13:F:491:MET:O	13:F:493:LYS:NZ	2.17	0.77
14:Y:172:ASN:HB3	14:Y:175:ILE:HG12	1.67	0.77
5:S:69:LYS:HG2	5:S:72:THR:HG22	1.66	0.77
16:N:26:GLY:HA2	16:N:35:ASN:HD21	1.50	0.77
1:R:49:ARG:NH2	1:R:308:ASN:O	2.17	0.76
12:C:50:LEU:HD23	12:C:68:GLU:HB2	1.67	0.76
1:R:173:GLY:H	1:R:221:ILE:HG21	1.52	0.75
10:7:98:SER:O	10:7:102:SER:OG	2.05	0.75
12:C:25:SER:HB2	13:F:88:GLU:HG2	1.68	0.75
1:R:385:THR:HG22	1:R:388:GLU:HB2	1.67	0.75
10:4:84:ILE:HG22	10:4:86:LEU:H	1.52	0.75
14:X:192:LYS:O	14:X:196:GLN:NE2	2.20	0.75
1:R:397:ILE:HD11	5:S:40:MET:HG3	1.68	0.74
9:0:107:MET:HG3	9:0:144:VAL:HG11	1.68	0.74
12:C:263:LEU:O	12:C:267:SER:OG	2.03	0.74
1:R:18:GLN:O	1:R:22:ALA:N	2.19	0.74
12:B:592:ASP:OD1	12:B:592:ASP:N	2.18	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:257:PRO:HB3	7:U:270:TRP:HB2	1.70	0.74
1:R:188:TRP:HD1	1:R:222:ILE:HD11	1.52	0.73
14:Z:226:VAL:HA	14:Z:229:MET:HE2	1.69	0.73
13:E:498:SER:OG	13:E:502:GLU:OE2	2.06	0.73
10:3:113:VAL:HG21	10:3:134:ILE:HG21	1.68	0.73
10:1:6:SER:OG	10:1:7:GLY:N	2.21	0.73
1:R:389:ILE:HG21	1:R:554:LEU:HD11	1.70	0.72
7:U:314:GLU:HA	7:U:320:THR:HA	1.71	0.72
1:R:177:ARG:HD3	1:R:218:SER:HB3	1.71	0.72
17:P:51:GLN:HA	17:P:55:MET:H	1.53	0.72
10:7:72:VAL:HG11	10:7:99:VAL:HG11	1.71	0.72
10:8:44:MET:HG2	10:8:118:VAL:HG13	1.70	0.72
11:Q:114:THR:OG1	15:G:85:GLN:NE2	2.22	0.72
11:Q:143:ILE:HG13	11:Q:145:GLN:H	1.54	0.72
4:L:34:LYS:HA	4:L:37:LYS:HD2	1.72	0.72
1:R:262:ASN:HA	1:R:265:ILE:HD12	1.71	0.72
12:B:419:ASP:OD1	12:B:419:ASP:N	2.23	0.72
13:F:444:LEU:HB3	13:F:449:LEU:HB2	1.70	0.72
3:I:85:ARG:NH1	13:E:141:ARG:O	2.23	0.71
3:H:129:GLU:H	3:H:132:MET:HE2	1.54	0.71
12:C:511:VAL:HG11	12:C:548:TYR:HB2	1.72	0.71
9:0:51:ASN:HD22	10:1:90:PHE:HB3	1.53	0.71
10:5:64:ILE:HA	10:5:67:ILE:HD12	1.73	0.71
10:6:57:ILE:HD13	10:6:132:ILE:HD11	1.71	0.71
10:3:28:LEU:HD12	10:4:105:ALA:HB2	1.73	0.71
13:E:262:ASN:ND2	13:E:270:GLU:OE1	2.24	0.71
19:B:701:ADP:O3B	13:E:400:ARG:NH1	2.23	0.70
10:6:113:VAL:HG21	10:6:134:ILE:HG21	1.71	0.70
11:Q:166:ASP:N	11:Q:166:ASP:OD1	2.24	0.70
1:R:191:CYS:SG	1:R:194:ASN:ND2	2.65	0.70
1:R:304:TYR:O	1:R:308:ASN:N	2.21	0.70
7:U:392:PRO:O	7:U:394:GLN:NE2	2.25	0.70
10:6:72:VAL:HG11	10:6:99:VAL:HG11	1.73	0.69
1:R:737:SER:O	1:R:740:ARG:NH1	2.25	0.69
10:2:113:VAL:HG21	10:2:134:ILE:HG21	1.73	0.69
15:G:193:GLU:OE1	15:G:196:ARG:NH1	2.25	0.69
12:C:419:ASP:OD2	12:C:419:ASP:N	2.25	0.69
10:5:144:TYR:HA	10:5:147:ILE:HD12	1.75	0.69
10:5:51:GLN:O	10:5:55:SER:OG	2.11	0.69
7:U:411:GLN:HG2	8:V:293:TYR:HA	1.74	0.69
9:0:126:ILE:HG13	9:0:131:TYR:HE2	1.55	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:25:PRO:HA	5:S:28:ILE:HG12	1.75	0.69
12:C:264:SER:O	12:C:308:ARG:NH2	2.26	0.69
10:6:44:MET:HE2	10:6:122:ALA:HB1	1.74	0.68
10:7:51:GLN:O	10:7:55:SER:OG	2.10	0.68
14:Y:270:ASN:O	14:Y:274:ASN:ND2	2.26	0.68
10:9:120:GLY:HA2	10:9:123:GLN:HE21	1.58	0.68
14:X:98:ILE:HA	14:X:160:GLN:HE21	1.56	0.68
1:R:804:ARG:NH1	1:R:809:GLU:OE1	2.26	0.68
3:H:108:ASP:OD1	3:H:109:THR:N	2.26	0.68
10:4:84:ILE:HG21	10:4:89:SER:HB2	1.76	0.68
16:N:68:GLN:HE22	16:N:99:ASP:H	1.42	0.68
13:E:436:LYS:HD2	13:E:452:LEU:HD12	1.74	0.68
1:R:12:LEU:HD23	1:R:357:THR:HG21	1.75	0.68
14:Z:229:MET:HE1	14:Z:255:LEU:HD13	1.76	0.68
17:P:50:ILE:O	17:P:54:GLU:N	2.26	0.68
10:8:72:VAL:HG11	10:8:99:VAL:HG11	1.76	0.68
13:F:318:PRO:HG2	15:G:201:ARG:HD2	1.77	0.67
17:P:314:VAL:O	17:P:318:LEU:N	2.27	0.67
14:Z:144:ALA:O	14:Z:149:ASN:ND2	2.20	0.67
12:B:444:HIS:ND1	12:B:521:GLN:OE1	2.26	0.67
12:A:232:ARG:NH1	12:A:519:PHE:O	2.27	0.67
13:E:489:LYS:HB3	13:E:500:LEU:HD13	1.76	0.67
3:I:92:THR:O	3:I:96:ASN:ND2	2.26	0.67
10:2:14:PHE:HB2	10:2:89:SER:HB3	1.77	0.67
10:5:88:LYS:O	10:5:92:GLN:NE2	2.24	0.67
10:3:23:MET:HG2	10:4:148:VAL:HG11	1.76	0.66
1:R:179:ARG:HD2	1:R:241:ARG:HB3	1.77	0.66
1:R:473:ASN:ND2	1:R:475:PHE:O	2.29	0.66
13:F:49:THR:O	13:F:49:THR:OG1	2.14	0.66
12:B:274:TYR:HB3	12:B:311:LEU:HD23	1.77	0.66
1:R:270:MET:HG2	1:R:274:GLN:HE22	1.61	0.66
7:U:387:ARG:HH12	18:U:505:NAG:H5	1.60	0.66
12:B:43:VAL:HG21	12:B:64:ILE:HD13	1.77	0.66
13:F:88:GLU:HG3	13:F:314:ARG:HH12	1.60	0.66
13:E:268:THR:O	13:E:271:ARG:N	2.28	0.66
14:Z:172:ASN:OD1	14:Z:173:GLU:N	2.28	0.66
14:X:242:LEU:HA	14:X:245:LYS:HD3	1.77	0.66
10:3:72:VAL:HG11	10:3:99:VAL:HG11	1.77	0.66
13:D:219:VAL:HA	13:D:222:TYR:HB2	1.76	0.66
15:G:43:ARG:NH1	15:G:46:GLN:OE1	2.29	0.66
1:R:804:ARG:NH1	1:R:804:ARG:O	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:F:47:TYR:HB3	13:F:49:THR:HG23	1.78	0.65
13:F:457:LYS:O	13:F:461:ASN:HB2	1.96	0.65
14:X:207:GLN:HG2	14:X:212:PRO:HG3	1.77	0.65
10:2:23:MET:HG2	10:3:148:VAL:HG21	1.78	0.65
1:R:469:SER:OG	1:R:753:GLU:OE1	2.14	0.65
13:F:485:ARG:NH2	13:F:503:PHE:O	2.29	0.65
7:U:357:ASN:HB2	7:U:385:VAL:HG22	1.78	0.65
1:R:192:ARG:HB2	2:O:346:ALA:HA	1.79	0.65
9:O:164:LEU:HD21	11:Q:18:GLY:HA2	1.77	0.65
13:D:214:LYS:HD2	13:D:220:VAL:HG13	1.79	0.65
14:Y:101:PHE:HZ	14:Y:216:ILE:HG23	1.63	0.64
14:Z:172:ASN:HB3	14:Z:175:ILE:HG12	1.79	0.64
1:R:178:GLU:OE1	1:R:241:ARG:NH1	2.30	0.64
1:R:349:PRO:HG2	3:H:11:GLN:HG2	1.79	0.64
12:B:577:ILE:HG21	12:B:608:MET:HG3	1.78	0.64
10:2:44:MET:HG3	10:2:122:ALA:HB2	1.79	0.64
13:D:445:THR:OG1	13:D:446:SER:N	2.29	0.64
13:E:421:GLN:HB2	13:E:495:ILE:HD11	1.79	0.64
1:R:310:CYS:HB3	1:R:319:LEU:HD21	1.78	0.64
12:B:391:ARG:NH1	12:B:401:GLU:OE2	2.31	0.64
10:3:98:SER:O	10:3:102:SER:OG	2.16	0.64
11:Q:328:ASN:ND2	11:Q:348:ILE:O	2.24	0.64
13:F:492:LEU:HD13	13:F:495:ILE:HD13	1.78	0.64
2:O:187:VAL:HA	2:O:248:VAL:HA	1.78	0.64
7:U:413:SER:HA	8:V:294:ASN:HD22	1.61	0.64
10:5:72:VAL:HG21	10:5:99:VAL:HG11	1.80	0.63
10:9:84:ILE:HG21	10:9:89:SER:HB2	1.80	0.63
10:9:130:GLY:O	10:9:134:ILE:HG12	1.98	0.63
12:C:134:ASP:N	12:C:134:ASP:OD1	2.30	0.63
12:C:594:GLU:HG2	12:C:598:LYS:HD2	1.78	0.63
1:R:281:ARG:HA	1:R:284:GLN:HE21	1.63	0.63
1:R:657:VAL:HA	1:R:660:ARG:HB2	1.80	0.63
3:H:30:ILE:HG21	4:K:25:ALA:HA	1.81	0.63
17:P:47:CYS:O	17:P:51:GLN:N	2.31	0.63
1:R:110:GLU:OE1	1:R:114:ASN:ND2	2.31	0.63
1:R:424:VAL:HA	1:R:427:GLU:HG3	1.79	0.63
10:4:113:VAL:HG21	10:4:134:ILE:HG21	1.79	0.63
13:D:438:VAL:HG13	13:D:439:VAL:HG13	1.81	0.63
3:I:180:GLY:HA3	3:I:195:THR:HA	1.80	0.63
12:A:107:SER:OG	13:D:161:GLN:NE2	2.32	0.63
12:A:364:ARG:HD3	13:D:326:TYR:HD2	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:426:ARG:HD2	1:R:429:ARG:HD2	1.79	0.62
4:K:17:ARG:HH22	4:K:21:LYS:HB2	1.63	0.62
1:R:17:LEU:O	1:R:319:LEU:N	2.33	0.62
12:B:436:ASP:OD1	12:B:437:LYS:N	2.32	0.62
17:P:111:PHE:C	17:P:113:ASP:H	2.07	0.62
1:R:120:ARG:NH1	1:R:121:ASN:OD1	2.31	0.62
12:C:277:CYS:O	12:C:314:ASN:ND2	2.32	0.62
1:R:194:ASN:O	3:I:11:GLN:NE2	2.33	0.62
3:H:49:GLN:HG3	4:K:44:ILE:HG12	1.81	0.62
9:O:160:SER:OG	11:Q:309:GLN:NE2	2.33	0.62
1:R:68:VAL:O	1:R:72:ILE:HG13	2.00	0.62
1:R:96:ASP:OD1	1:R:96:ASP:N	2.33	0.62
1:R:34:LYS:NZ	1:R:329:ASP:OD2	2.32	0.61
1:R:297:VAL:O	1:R:301:LYS:N	2.27	0.61
3:H:85:ARG:NH1	13:D:141:ARG:O	2.34	0.61
7:U:357:ASN:N	7:U:385:VAL:O	2.33	0.61
10:8:57:ILE:HD13	10:8:132:ILE:HD11	1.80	0.61
13:F:458:PHE:HA	13:F:483:LEU:HD21	1.82	0.61
14:X:148:LYS:NZ	14:X:188:MET:O	2.28	0.61
14:X:209:GLU:OE1	14:X:211:SER:N	2.30	0.61
10:9:9:GLU:OE2	10:9:10:TYR:N	2.33	0.61
12:B:399:GLU:OE2	14:Y:25:LYS:NZ	2.33	0.61
17:P:108:VAL:O	17:P:111:PHE:N	2.24	0.61
3:J:9:GLN:O	3:J:13:LYS:HB2	2.00	0.61
12:A:29:VAL:HB	12:A:66:VAL:HB	1.83	0.61
9:O:171:SER:O	9:O:175:LYS:NZ	2.33	0.61
12:B:196:PHE:O	12:B:198:GLY:N	2.33	0.61
14:Z:83:ARG:NH2	14:Z:118:HIS:O	2.33	0.61
1:R:288:LYS:HA	1:R:291:ARG:HE	1.66	0.61
10:8:28:LEU:HD12	10:9:105:ALA:HB2	1.83	0.61
13:F:130:ARG:NH2	13:F:143:PRO:O	2.29	0.61
10:8:58:PRO:HG3	10:8:135:LEU:HD21	1.83	0.61
12:B:55:ILE:HD12	12:B:365:LEU:HD11	1.82	0.61
13:F:386:ARG:NH2	13:F:459:GLU:OE1	2.34	0.61
7:U:374:VAL:HG23	7:U:397:LEU:HB2	1.82	0.61
10:4:51:GLN:O	10:4:55:SER:OG	2.18	0.61
14:Z:140:LEU:HD21	14:Z:152:LEU:HB3	1.82	0.61
7:U:341:THR:OG1	7:U:342:MET:N	2.34	0.61
10:4:88:LYS:O	10:4:92:GLN:NE2	2.32	0.61
12:A:246:THR:OG1	12:A:247:ALA:N	2.33	0.61
12:B:63:THR:HG21	12:B:365:LEU:HD21	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Y:36:ILE:HG13	14:Y:95:VAL:HG11	1.83	0.61
1:R:335:PHE:HB3	1:R:339:ARG:HH22	1.66	0.60
15:G:148:LEU:HD23	16:N:89:LEU:HD23	1.83	0.60
1:R:737:SER:HB3	1:R:740:ARG:HH22	1.66	0.60
12:A:37:ALA:HB1	12:A:54:ILE:HG21	1.81	0.60
14:Y:152:LEU:HG	14:Y:185:LEU:HD23	1.84	0.60
10:2:23:MET:HE3	10:2:27:ALA:HB2	1.82	0.60
13:F:100:GLU:N	13:F:100:GLU:OE1	2.34	0.60
13:E:490:GLU:OE1	13:E:497:GLN:NE2	2.33	0.60
7:U:416:SER:O	9:O:34:ARG:NH2	2.31	0.60
12:C:503:GLU:OE1	12:C:567:TRP:N	2.31	0.60
12:A:246:THR:HB	12:A:431:VAL:HB	1.82	0.60
13:F:363:HIS:HB3	13:F:366:PRO:HD2	1.83	0.60
14:Y:42:LEU:HD12	14:Y:105:LEU:HD23	1.83	0.60
9:O:60:LEU:HA	9:O:63:VAL:HG12	1.83	0.60
14:Z:201:LYS:HD2	14:Z:260:LEU:HD12	1.84	0.60
12:B:246:THR:HB	12:B:431:VAL:HB	1.84	0.60
1:R:175:ILE:HG12	1:R:180:ILE:HD13	1.82	0.60
8:V:338:ILE:O	11:Q:165:GLN:NE2	2.35	0.60
12:A:560:GLN:OE1	12:A:560:GLN:N	2.32	0.60
13:F:447:ASP:OD1	13:F:448:ASP:N	2.34	0.60
13:D:327:MET:HE1	13:D:365:ILE:HG12	1.84	0.60
14:X:209:GLU:OE1	14:X:210:GLU:N	2.35	0.60
15:G:45:ARG:HG2	16:N:112:MET:HE1	1.84	0.60
3:H:156:LYS:HE2	3:H:162:ASP:HA	1.82	0.60
10:5:81:ASN:OD1	10:5:82:ASP:N	2.33	0.60
10:5:80:LEU:HB3	10:6:155:LYS:HE3	1.83	0.59
7:U:295:LEU:HD21	7:U:311:LEU:HD23	1.84	0.59
12:C:151:ASP:OD2	12:C:397:ASN:ND2	2.34	0.59
13:E:88:GLU:OE1	13:E:314:ARG:NH2	2.35	0.59
1:R:118:LEU:HD22	1:R:272:LEU:HD13	1.84	0.59
12:C:477:THR:HG23	13:D:387:GLN:HG3	1.84	0.59
14:Y:222:GLN:HB3	14:Y:255:LEU:HD23	1.84	0.59
10:6:33:GLY:O	10:6:37:SER:OG	2.18	0.59
10:3:130:GLY:O	10:3:134:ILE:HG12	2.03	0.59
10:5:14:PHE:HB2	10:5:89:SER:OG	2.03	0.59
7:U:375:SER:OG	7:U:396:MET:SD	2.58	0.59
12:A:56:ARG:NH1	12:A:57:LEU:O	2.36	0.59
12:A:350:SER:HB2	12:A:353:ARG:HG2	1.84	0.59
13:F:61:ASP:OD2	13:F:93:LYS:NZ	2.35	0.59
17:P:141:ALA:O	17:P:145:ILE:N	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:49:ARG:NH2	1:R:310:CYS:O	2.34	0.59
3:I:49:GLN:HB3	4:L:44:ILE:HD11	1.84	0.59
3:H:155:TYR:O	3:H:159:THR:HG22	2.03	0.59
7:U:417:ASP:O	9:O:34:ARG:NH2	2.34	0.59
11:Q:110:ILE:HG13	11:Q:182:ARG:HB2	1.85	0.59
13:D:61:ASP:OD1	13:D:62:HIS:N	2.35	0.59
14:X:217:LEU:HD12	14:X:221:ASP:HB2	1.84	0.59
10:9:51:GLN:HE22	10:9:121:THR:HG22	1.68	0.59
12:A:510:GLU:HG2	12:A:567:TRP:CZ2	2.36	0.59
13:F:430:LYS:O	13:F:433:GLN:HG3	2.03	0.59
5:S:70:ASN:N	5:S:70:ASN:OD1	2.35	0.59
12:B:229:THR:HG22	12:B:263:LEU:HG	1.85	0.59
1:R:593:LYS:NZ	1:R:606:PRO:O	2.34	0.58
12:B:161:LEU:HD13	12:B:307:LYS:HB2	1.84	0.58
14:Y:140:LEU:HD11	14:Y:152:LEU:HB3	1.85	0.58
1:R:767:LYS:HB3	1:R:770:ALA:HB3	1.85	0.58
4:K:17:ARG:NH2	4:K:21:LYS:HB2	2.18	0.58
10:8:130:GLY:O	10:8:134:ILE:HG12	2.03	0.58
10:8:6:SER:OG	10:8:7:GLY:N	2.32	0.58
12:A:252:PHE:O	12:A:437:LYS:NZ	2.27	0.58
10:7:130:GLY:O	10:7:134:ILE:HG12	2.04	0.58
3:J:20:GLU:O	4:M:21:LYS:NZ	2.37	0.58
10:2:36:LYS:HE2	10:2:112:ILE:HD13	1.85	0.58
12:A:43:VAL:HG21	12:A:64:ILE:HD13	1.86	0.58
1:R:627:MET:HE3	1:R:632:GLN:HB3	1.84	0.58
11:Q:208:MET:HE1	11:Q:316:TYR:CD1	2.38	0.58
13:E:190:PRO:HB3	13:E:352:PRO:HG2	1.85	0.58
13:E:421:GLN:HE21	13:E:495:ILE:HD11	1.68	0.58
3:J:5:ASP:O	3:J:9:GLN:HB2	2.02	0.58
4:L:29:LYS:O	4:L:33:LEU:HG	2.03	0.58
10:5:95:ALA:O	10:5:99:VAL:HG12	2.04	0.58
10:6:131:MET:O	10:6:135:LEU:HG	2.03	0.58
11:Q:227:SER:O	11:Q:227:SER:OG	2.19	0.58
1:R:188:TRP:HB3	1:R:192:ARG:HB3	1.85	0.57
1:R:227:ASP:O	1:R:231:ASN:ND2	2.37	0.57
3:I:129:GLU:HG3	3:I:130:PRO:HD2	1.85	0.57
13:E:417:ASP:HB3	13:E:495:ILE:HG23	1.86	0.57
10:3:6:SER:N	10:3:83:ASP:OD2	2.37	0.57
12:C:232:ARG:NH2	12:C:529:ASP:OD2	2.37	0.57
13:E:49:THR:O	13:E:49:THR:OG1	2.20	0.57
10:2:20:SER:O	10:2:24:VAL:HG13	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:2:52:ILE:O	10:2:55:SER:N	2.33	0.57
12:C:91:GLY:HA3	12:C:206:VAL:HG12	1.87	0.57
13:E:76:LEU:HD21	13:E:82:ARG:HH21	1.69	0.57
14:Z:48:ASP:OD2	14:Z:116:LYS:NZ	2.32	0.57
4:K:8:ILE:O	4:K:12:LEU:HG	2.04	0.57
12:B:317:ASN:HB3	13:E:157:PRO:HB3	1.86	0.57
14:Z:268:LYS:HA	14:Z:271:GLU:HG2	1.86	0.57
10:4:48:ARG:NE	10:4:122:ALA:O	2.38	0.57
10:6:85:SER:OG	10:6:88:LYS:NZ	2.24	0.57
10:7:20:SER:O	10:7:24:VAL:HG12	2.04	0.57
11:Q:122:ILE:H	11:Q:145:GLN:HE22	1.52	0.57
1:R:14:GLN:HB3	1:R:320:ILE:HD11	1.86	0.57
4:K:115:ARG:CZ	12:A:18:PHE:HD1	2.17	0.57
7:U:365:SER:O	7:U:406:ASN:ND2	2.36	0.57
12:A:115:SER:OG	12:A:116:ILE:N	2.36	0.57
12:B:74:SER:OG	12:B:75:VAL:N	2.33	0.57
13:E:71:ILE:O	13:E:115:THR:OG1	2.22	0.57
13:E:365:ILE:HB	13:E:366:PRO:HD3	1.86	0.57
1:R:14:GLN:OE1	4:K:3:SER:N	2.38	0.57
15:G:95:ARG:NH2	15:G:110:GLU:OE2	2.38	0.57
3:H:22:GLU:HG3	4:K:17:ARG:NH1	2.13	0.57
10:7:88:LYS:HA	10:7:91:LEU:HD12	1.86	0.57
12:B:145:SER:OG	14:Y:31:ARG:NH1	2.38	0.57
14:Y:261:ASP:O	14:Y:265:ARG:HG2	2.05	0.57
2:O:46:GLY:O	3:I:21:GLN:NE2	2.37	0.57
11:Q:161:ALA:O	11:Q:165:GLN:HG2	2.05	0.57
14:X:19:HIS:CD2	14:X:70:LYS:HG2	2.40	0.57
14:X:134:ASN:HA	14:X:137:THR:HG22	1.86	0.57
14:Y:240:LYS:HG3	14:Y:243:GLN:HE21	1.70	0.56
16:N:75:ARG:NH1	16:N:104:SER:OG	2.38	0.56
13:F:380:ASP:OD1	13:F:381:ARG:N	2.37	0.56
13:F:498:SER:O	13:F:502:GLU:HB2	2.05	0.56
1:R:754:VAL:HG11	10:8:147:ILE:HG12	1.86	0.56
3:H:26:LYS:O	3:H:29:GLU:HG3	2.05	0.56
13:D:231:PHE:HB3	13:D:259:LEU:HD12	1.86	0.56
13:E:301:SER:O	13:E:305:GLU:HG3	2.06	0.56
14:X:146:THR:O	14:X:150:ASN:ND2	2.39	0.56
16:N:11:ILE:HB	16:N:66:ILE:HG12	1.87	0.56
12:B:568:SER:O	12:B:572:GLU:HG2	2.06	0.56
13:E:227:PHE:HE2	13:E:294:LEU:HD12	1.70	0.56
1:R:122:PHE:O	1:R:126:THR:HG23	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:50:ARG:HH11	3:J:51:LEU:HD12	1.69	0.56
3:J:176:ASP:OD1	3:J:176:ASP:N	2.35	0.56
1:R:481:VAL:HB	5:S:76:LEU:HD22	1.86	0.56
1:R:609:LEU:HD23	1:R:610:ILE:HD13	1.86	0.56
14:Z:98:ILE:HG23	14:Z:160:GLN:HB3	1.88	0.56
1:R:11:THR:N	1:R:325:CYS:O	2.30	0.56
14:X:222:GLN:O	14:X:226:VAL:HG23	2.06	0.56
14:X:242:LEU:HD23	14:X:245:LYS:HD3	1.88	0.56
1:R:437:ASN:OD1	1:R:437:ASN:N	2.33	0.56
4:L:25:ALA:O	4:L:29:LYS:HG2	2.06	0.56
9:O:2:THR:OG1	9:O:3:GLY:N	2.37	0.56
10:4:20:SER:O	10:4:24:VAL:HG12	2.05	0.56
10:5:35:ALA:O	10:5:39:THR:HG23	2.06	0.56
12:B:226:PRO:HG3	12:B:461:LEU:HD22	1.86	0.56
14:Y:238:SER:OG	14:Y:270:ASN:OD1	2.19	0.56
10:3:41:ILE:HD11	10:3:55:SER:O	2.06	0.56
1:R:654:LYS:HA	1:R:657:VAL:HG22	1.88	0.56
10:4:14:PHE:HB2	10:4:89:SER:OG	2.06	0.56
1:R:4:LEU:HD12	1:R:6:ARG:HH21	1.70	0.55
1:R:132:LEU:HD12	1:R:255:LYS:HG2	1.88	0.55
1:R:184:GLU:HA	1:R:187:LEU:HD12	1.87	0.55
3:I:54:MET:O	3:I:58:GLU:HG2	2.05	0.55
8:V:335:TYR:HD1	8:V:337:SER:H	1.54	0.55
10:1:23:MET:HE3	10:1:27:ALA:HB2	1.89	0.55
10:1:45:SER:O	10:1:45:SER:OG	2.16	0.55
10:6:91:LEU:HD13	10:6:155:LYS:HB3	1.89	0.55
11:Q:259:ASP:HB2	11:Q:263:GLN:HE22	1.69	0.55
12:C:246:THR:HB	12:C:431:VAL:HB	1.88	0.55
12:A:201:GLU:OE2	12:A:203:PHE:HB2	2.05	0.55
13:F:489:LYS:NZ	13:F:504:TYR:HB2	2.21	0.55
1:R:421:VAL:HA	1:R:424:VAL:HG22	1.89	0.55
11:Q:54:TYR:OH	11:Q:325:GLU:OE1	2.23	0.55
13:E:421:GLN:HE22	13:E:494:ARG:HG3	1.71	0.55
14:Z:14:THR:OG1	14:Z:15:SER:N	2.35	0.55
1:R:179:ARG:HD3	1:R:240:PHE:HD1	1.72	0.55
1:R:484:MET:HB3	1:R:489:TRP:HD1	1.72	0.55
7:U:262:ASP:OD1	7:U:263:THR:N	2.39	0.55
8:V:334:GLY:O	10:3:119:ARG:NH2	2.36	0.55
11:Q:200:LEU:O	11:Q:202:GLY:N	2.34	0.55
12:A:362:SER:OG	12:A:363:GLY:N	2.39	0.55
14:Y:19:HIS:CD2	14:Y:70:LYS:HG2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:5:SER:O	4:M:9:GLN:HG2	2.07	0.55
4:L:86:THR:HA	4:L:89:ARG:HD2	1.89	0.55
12:B:350:SER:HB2	12:B:353:ARG:HG2	1.88	0.55
1:R:93:ASP:O	1:R:97:LEU:HG	2.05	0.55
13:D:130:ARG:NH2	13:D:143:PRO:O	2.36	0.55
14:Z:90:GLU:OE2	14:Z:93:ARG:NH1	2.39	0.55
10:3:7:GLY:HA3	10:3:85:SER:HA	1.87	0.55
11:Q:1:MET:HG3	11:Q:2:SER:H	1.72	0.55
1:R:229:LEU:HD12	1:R:229:LEU:H	1.71	0.55
4:K:32:ARG:HA	4:K:35:GLN:HG3	1.88	0.55
12:C:66:VAL:HG12	12:C:68:GLU:H	1.72	0.55
13:E:212:LEU:HB3	13:E:214:LYS:HG3	1.89	0.55
14:Z:220:GLU:O	14:Z:224:ILE:HG12	2.06	0.55
13:E:283:GLU:OE2	13:E:337:ARG:NH2	2.38	0.55
14:X:195:GLU:OE1	14:X:195:GLU:N	2.40	0.55
4:L:50:GLN:HA	4:L:53:LYS:HE2	1.88	0.55
9:0:129:ARG:NH2	9:0:204:GLY:O	2.40	0.55
10:6:59:VAL:HG21	10:7:134:ILE:HD12	1.88	0.55
10:8:50:GLU:OE2	10:8:50:GLU:N	2.36	0.55
12:B:238:PHE:HZ	12:B:450:TRP:HA	1.71	0.55
3:J:85:ARG:NH1	13:F:141:ARG:O	2.40	0.54
3:H:212:ARG:NH2	13:D:126:ASP:OD2	2.40	0.54
12:A:398:PRO:HD2	12:A:400:ARG:HH11	1.71	0.54
17:P:58:SER:C	17:P:60:GLU:H	2.15	0.54
12:A:145:SER:OG	14:X:31:ARG:NH1	2.40	0.54
13:E:447:ASP:HA	13:E:450:LEU:HB2	1.89	0.54
15:G:203:LYS:O	15:G:207:GLU:HG2	2.06	0.54
1:R:201:GLU:HG2	1:R:218:SER:HA	1.90	0.54
3:J:38:PHE:HB2	4:M:32:ARG:NE	2.23	0.54
3:J:129:GLU:OE2	13:F:64:LYS:NZ	2.31	0.54
3:H:175:GLU:OE2	3:H:175:GLU:N	2.38	0.54
10:4:144:TYR:HA	10:4:147:ILE:HD12	1.88	0.54
1:R:15:LEU:HG	1:R:17:LEU:HD21	1.89	0.54
1:R:65:LEU:HB2	1:R:290:ILE:HD11	1.88	0.54
12:C:594:GLU:OE2	12:C:598:LYS:NZ	2.35	0.54
16:N:59:ASP:OD1	16:N:59:ASP:N	2.41	0.54
1:R:585:TYR:CZ	1:R:589:LEU:HD21	2.42	0.54
3:H:182:GLU:HG2	3:H:193:SER:HA	1.89	0.54
4:K:26:ARG:O	4:K:30:ASN:ND2	2.39	0.54
4:K:31:ARG:NH2	4:K:35:GLN:HG2	2.23	0.54
6:T:95:GLN:OE1	6:T:99:ASN:ND2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Q:17:GLU:OE2	11:Q:21:ARG:NE	2.40	0.54
14:X:144:ALA:O	14:X:149:ASN:ND2	2.35	0.54
15:G:145:LEU:HD12	16:N:65:LEU:HD21	1.90	0.54
16:N:85:ILE:HB	16:N:86:PRO:HD3	1.89	0.54
1:R:300:MET:HA	1:R:303:ILE:HG22	1.88	0.54
10:6:48:ARG:HH11	10:6:51:GLN:HE22	1.54	0.54
13:F:255:ASP:N	13:F:255:ASP:OD1	2.40	0.54
1:R:64:LYS:HG3	1:R:102:GLU:HG2	1.87	0.54
10:6:48:ARG:NE	10:6:122:ALA:O	2.41	0.54
11:Q:115:GLY:HA3	11:Q:125:LEU:HD11	1.90	0.54
4:M:40:ALA:O	4:M:44:ILE:HG13	2.06	0.54
13:D:182:SER:HB2	13:D:402:MET:HG3	1.90	0.54
2:O:166:LEU:O	2:O:170:VAL:N	2.29	0.54
13:F:450:LEU:HD12	13:F:487:PHE:CE1	2.43	0.54
10:9:131:MET:O	10:9:135:LEU:HG	2.08	0.54
11:Q:20:VAL:HG21	11:Q:315:PHE:CD2	2.43	0.54
12:C:246:THR:OG1	12:C:247:ALA:N	2.40	0.54
12:A:270:ASP:HB2	12:A:342:TYR:HB3	1.90	0.54
13:F:504:TYR:O	13:F:506:ARG:N	2.40	0.54
11:Q:231:GLU:CD	11:Q:231:GLU:H	2.16	0.53
12:B:397:ASN:O	12:B:399:GLU:N	2.41	0.53
1:R:14:GLN:OE1	1:R:353:ASN:ND2	2.41	0.53
1:R:123:LEU:HD12	1:R:207:GLU:HG2	1.90	0.53
3:H:3:LEU:HD13	3:H:7:ASP:HB2	1.89	0.53
3:H:26:LYS:HG3	4:K:17:ARG:HH12	1.72	0.53
3:H:57:TYR:O	3:H:61:GLU:HG3	2.08	0.53
12:A:263:LEU:O	12:A:267:SER:OG	2.23	0.53
12:A:610:ASN:OD1	12:A:613:ARG:NH1	2.40	0.53
14:X:241:VAL:O	14:X:245:LYS:HG3	2.07	0.53
14:Y:220:GLU:O	14:Y:224:ILE:HG13	2.08	0.53
3:J:180:GLY:HA3	3:J:195:THR:HA	1.91	0.53
4:K:13:GLN:HE21	4:K:16:LYS:HD3	1.72	0.53
10:1:130:GLY:O	10:1:134:ILE:HG12	2.09	0.53
10:8:20:SER:O	10:8:24:VAL:HG13	2.09	0.53
12:C:51:VAL:HG23	12:C:67:TYR:HB2	1.90	0.53
12:B:298:VAL:O	12:B:300:GLY:N	2.41	0.53
1:R:614:ASN:ND2	1:R:619:SER:OG	2.41	0.53
3:J:38:PHE:HB2	4:M:32:ARG:CZ	2.39	0.53
4:K:4:GLN:HG2	4:K:5:SER:H	1.73	0.53
6:T:51:ALA:HB1	6:T:126:VAL:HB	1.90	0.53
12:A:264:SER:O	12:A:308:ARG:NH2	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:45:LEU:HD12	3:I:46:VAL:N	2.22	0.53
12:A:60:ASP:O	12:A:62:ALA:N	2.42	0.53
13:D:436:LYS:HB2	13:D:444:LEU:HD11	1.91	0.53
14:Z:133:LEU:O	14:Z:137:THR:HG23	2.08	0.53
6:T:66:ILE:O	6:T:70:ILE:HG12	2.08	0.53
12:C:280:ARG:HB2	12:C:283:GLU:HG2	1.91	0.53
12:C:610:ASN:OD1	12:C:613:ARG:NH1	2.42	0.53
12:A:57:LEU:HD23	12:A:59:GLY:O	2.08	0.53
12:B:346:MET:HE2	12:B:348:ALA:HB2	1.90	0.53
13:F:70:GLU:HG2	13:F:71:ILE:H	1.74	0.53
14:Y:259:LEU:O	14:Y:263:ILE:HG13	2.09	0.53
3:J:54:MET:O	3:J:58:GLU:HG2	2.09	0.53
3:H:123:GLY:HA3	3:H:183:ILE:HD13	1.89	0.53
12:B:234:LEU:HD21	12:B:448:VAL:HG11	1.91	0.53
10:2:81:ASN:OD1	10:2:82:ASP:N	2.42	0.53
10:6:20:SER:O	10:6:24:VAL:HG13	2.07	0.53
13:F:444:LEU:HD23	13:F:449:LEU:HG	1.91	0.53
17:P:157:GLU:O	17:P:160:ASP:N	2.42	0.53
1:R:728:CYS:SG	1:R:729:LEU:N	2.82	0.53
1:R:793:MET:HG3	10:8:140:VAL:HG21	1.91	0.53
4:M:35:GLN:O	4:M:39:GLU:HG2	2.09	0.53
4:M:85:GLN:O	4:M:89:ARG:HG2	2.08	0.53
3:I:51:LEU:O	3:I:55:GLU:HG2	2.09	0.53
3:H:152:ILE:HG23	3:H:153:PRO:HD3	1.91	0.53
9:O:140:ALA:O	9:O:144:VAL:HG22	2.09	0.53
1:R:121:ASN:O	1:R:125:LEU:HG	2.09	0.53
12:A:24:VAL:CG1	12:A:70:THR:HG21	2.35	0.53
14:Y:18:TYR:OH	14:Y:76:ASN:O	2.19	0.53
14:Y:155:MET:HG2	14:Y:178:LEU:HD11	1.91	0.53
14:Y:213:PHE:O	14:Y:222:GLN:NE2	2.42	0.53
15:G:55:LYS:HE2	15:G:148:LEU:HD21	1.91	0.53
3:J:105:VAL:HG13	3:J:111:ARG:HH21	1.75	0.52
11:Q:158:THR:HG22	11:Q:160:LEU:H	1.74	0.52
12:C:196:PHE:O	12:C:198:GLY:N	2.41	0.52
1:R:188:TRP:CD1	1:R:222:ILE:HD11	2.40	0.52
10:5:20:SER:O	10:5:24:VAL:HG12	2.09	0.52
11:Q:179:GLU:HG2	11:Q:182:ARG:NH1	2.24	0.52
12:A:573:HIS:CD2	12:A:615:LEU:HD13	2.44	0.52
13:E:102:THR:HA	13:E:105:ILE:HD12	1.91	0.52
13:E:458:PHE:HA	13:E:483:LEU:HD11	1.92	0.52
14:X:194:ASP:OD2	14:X:232:TYR:OH	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:X:229:MET:HG3	14:X:255:LEU:HD11	1.91	0.52
1:R:129:LYS:HG3	1:R:265:ILE:HD13	1.90	0.52
10:1:20:SER:O	10:1:24:VAL:HG13	2.09	0.52
1:R:180:ILE:HG12	1:R:219:VAL:HA	1.92	0.52
10:1:61:MET:HA	10:1:64:ILE:HD12	1.91	0.52
10:6:51:GLN:HA	10:6:54:LYS:HZ3	1.74	0.52
16:N:93:SER:OG	16:N:96:HIS:N	2.36	0.52
4:M:17:ARG:HG3	4:M:21:LYS:HE3	1.91	0.52
12:A:17:THR:OG1	12:A:79:VAL:O	2.28	0.52
13:E:218:ASP:OD1	13:E:218:ASP:N	2.31	0.52
1:R:531:PHE:HB2	5:S:64:PHE:HE1	1.74	0.52
14:Z:225:LEU:O	14:Z:229:MET:HG3	2.10	0.52
14:X:200:PHE:O	14:X:204:VAL:HG23	2.10	0.52
14:X:207:GLN:NE2	14:X:212:PRO:HB3	2.25	0.52
14:Y:207:GLN:NE2	14:Y:209:GLU:O	2.43	0.52
1:R:351:ILE:HG22	3:H:3:LEU:HD21	1.90	0.52
3:J:37:GLU:O	3:J:41:GLU:HG3	2.10	0.52
3:I:21:GLN:O	3:I:25:GLU:HG2	2.10	0.52
10:2:41:ILE:HD11	10:2:55:SER:O	2.10	0.52
12:A:96:GLY:HA2	12:A:306:MET:HE3	1.92	0.52
13:E:500:LEU:HD23	13:E:504:TYR:CE2	2.45	0.52
4:M:8:ILE:O	4:M:12:LEU:HG	2.10	0.52
4:L:7:GLY:O	4:L:11:LEU:HG	2.10	0.52
4:K:24:GLU:O	4:K:28:ARG:HG2	2.10	0.52
11:Q:41:THR:HB	11:Q:44:ASP:HB2	1.92	0.52
12:A:397:ASN:O	12:A:399:GLU:N	2.41	0.52
13:F:489:LYS:HE3	13:F:500:LEU:O	2.10	0.52
13:D:76:LEU:HD21	13:D:82:ARG:HH21	1.75	0.52
14:Z:148:LYS:NZ	14:Z:188:MET:O	2.40	0.52
1:R:465:ASN:O	1:R:471:SER:OG	2.20	0.52
13:D:255:ASP:OD1	13:D:255:ASP:N	2.43	0.52
3:J:35:GLU:OE1	4:M:32:ARG:NH1	2.43	0.52
10:6:109:ALA:O	10:6:113:VAL:HG12	2.10	0.52
12:A:44:ARG:NH2	12:A:123:ASN:OD1	2.43	0.52
13:F:379:VAL:HG13	13:F:391:PRO:HG2	1.92	0.52
13:F:424:ALA:O	13:F:428:ILE:HG12	2.10	0.52
3:J:57:TYR:HA	3:J:60:LYS:HD2	1.91	0.51
9:O:87:LYS:NZ	10:1:126:ARG:O	2.31	0.51
13:E:141:ARG:HA	14:X:9:LYS:HD2	1.93	0.51
1:R:175:ILE:H	1:R:219:VAL:HG11	1.75	0.51
3:I:57:TYR:CD1	4:L:51:ARG:HB3	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:0:128:HIS:ND1	10:9:9:GLU:OE1	2.43	0.51
1:R:57:ARG:HB3	1:R:61:MET:HE3	1.92	0.51
1:R:58:CYS:HA	1:R:61:MET:SD	2.50	0.51
3:H:44:ARG:O	3:H:48:THR:HG23	2.10	0.51
10:2:48:ARG:HB3	10:2:51:GLN:HG3	1.92	0.51
10:2:124:GLN:O	10:2:126:ARG:N	2.43	0.51
10:6:81:ASN:H	10:6:84:ILE:HD11	1.75	0.51
12:C:507:ILE:HD11	12:C:555:VAL:HG21	1.91	0.51
14:Z:52:VAL:HG12	14:Z:75:PRO:HG2	1.92	0.51
3:J:35:GLU:O	3:J:38:PHE:HB3	2.11	0.51
12:A:268:ASN:OD1	12:A:268:ASN:N	2.40	0.51
12:A:359:ARG:NH1	12:A:372:SER:O	2.43	0.51
12:B:436:ASP:OD2	12:B:438:LYS:NZ	2.33	0.51
13:F:182:SER:OG	13:F:402:MET:SD	2.68	0.51
14:Z:43:LYS:O	14:Z:47:GLU:HG2	2.10	0.51
1:R:764:LEU:HD22	6:T:82:ASP:OD1	2.10	0.51
10:3:20:SER:O	10:3:24:VAL:HG12	2.10	0.51
10:4:53:MET:N	10:4:53:MET:SD	2.84	0.51
10:7:33:GLY:O	10:7:37:SER:OG	2.22	0.51
12:B:280:ARG:NH1	12:B:283:GLU:OE1	2.43	0.51
14:Y:184:HIS:O	14:Y:188:MET:HG2	2.10	0.51
1:R:801:HIS:O	1:R:805:LEU:N	2.44	0.51
10:8:115:ASP:OD1	10:8:116:ALA:N	2.44	0.51
13:F:283:GLU:OE2	13:F:337:ARG:NH2	2.35	0.51
14:Z:148:LYS:NZ	14:Z:186:LEU:O	2.40	0.51
1:R:648:PRO:HA	1:R:651:LEU:HB3	1.92	0.51
10:5:44:MET:HG2	10:5:119:ARG:HG2	1.92	0.51
11:Q:108:ASN:ND2	11:Q:133:GLY:O	2.44	0.51
13:F:365:ILE:HB	13:F:366:PRO:HD3	1.92	0.51
3:J:24:ASN:O	3:J:28:GLU:HG2	2.10	0.51
3:J:138:LYS:HD3	3:J:172:TYR:CZ	2.45	0.51
4:K:7:GLY:O	4:K:11:LEU:HG	2.10	0.51
10:2:98:SER:O	10:2:102:SER:OG	2.28	0.51
10:3:35:ALA:O	10:3:39:THR:HG23	2.10	0.51
10:3:64:ILE:HA	10:3:67:ILE:HD12	1.91	0.51
10:8:68:TYR:CZ	10:8:143:LEU:HD13	2.46	0.51
14:Z:143:ALA:HB1	14:Z:149:ASN:ND2	2.25	0.51
1:R:409:ASP:OD1	1:R:412:HIS:ND1	2.38	0.51
1:R:763:GLY:HA2	1:R:778:PHE:HD2	1.76	0.51
4:L:28:ARG:O	4:L:32:ARG:HG2	2.11	0.51
10:1:72:VAL:HG11	10:1:99:VAL:HG11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Q:83:ARG:NH2	11:Q:131:PRO:O	2.43	0.51
12:A:30:THR:HG23	12:A:63:THR:HB	1.92	0.51
12:B:152:ILE:HG12	12:B:167:MET:HG2	1.93	0.51
13:F:482:GLN:O	13:F:486:ILE:HG12	2.11	0.51
13:D:131:VAL:HG13	13:D:259:LEU:HD23	1.93	0.51
13:E:380:ASP:HB2	13:E:393:ASN:HB2	1.93	0.51
1:R:383:ILE:O	1:R:819:GLY:N	2.29	0.51
10:8:45:SER:HB2	10:8:52:ILE:HG22	1.92	0.51
10:9:44:MET:HG3	10:9:122:ALA:HB2	1.92	0.51
1:R:174:VAL:HB	1:R:243:SER:HB3	1.93	0.50
1:R:190:VAL:HG13	1:R:191:CYS:H	1.76	0.50
3:I:113:GLN:NE2	3:I:117:ASP:OD1	2.45	0.50
12:C:268:ASN:OD1	12:C:268:ASN:N	2.44	0.50
14:X:243:GLN:O	14:X:247:SER:OG	2.24	0.50
4:K:47:TYR:O	4:K:50:GLN:HB3	2.12	0.50
10:4:61:MET:SD	10:4:135:LEU:HB3	2.51	0.50
10:6:6:SER:OG	10:6:7:GLY:N	2.44	0.50
11:Q:20:VAL:HG22	11:Q:85:MET:SD	2.51	0.50
12:A:565:ILE:HB	12:A:569:ILE:HG21	1.92	0.50
14:Z:211:SER:O	14:Z:211:SER:OG	2.30	0.50
1:R:202:ILE:HB	1:R:217:LYS:HB2	1.92	0.50
3:H:46:VAL:O	3:H:50:ARG:HB2	2.10	0.50
12:A:364:ARG:HD3	13:D:326:TYR:CD2	2.44	0.50
12:A:444:HIS:ND1	12:A:521:GLN:OE1	2.38	0.50
1:R:484:MET:HB3	1:R:489:TRP:CD1	2.46	0.50
2:O:6:LEU:N	2:O:372:TYR:O	2.42	0.50
13:F:377:ILE:O	13:F:397:SER:OG	2.29	0.50
1:R:808:VAL:O	1:R:812:ASN:ND2	2.33	0.50
4:M:44:ILE:HG22	4:M:48:ARG:HD3	1.93	0.50
3:I:16:MET:HE3	4:L:10:GLN:CD	2.37	0.50
9:0:89:LYS:NZ	9:0:166:ASP:OD2	2.26	0.50
12:C:43:VAL:HG21	12:C:64:ILE:HD13	1.91	0.50
12:C:274:TYR:HD2	12:C:347:MET:HE3	1.76	0.50
13:E:100:GLU:OE1	13:E:100:GLU:N	2.44	0.50
1:R:38:ARG:NH2	1:R:359:GLN:OE1	2.34	0.50
1:R:246:PRO:HB2	1:R:254:ARG:HH12	1.76	0.50
3:J:12:ILE:O	3:J:16:MET:HB2	2.12	0.50
3:J:137:ARG:NH1	3:J:177:ILE:O	2.44	0.50
9:0:50:SER:O	9:0:54:ILE:HG22	2.11	0.50
10:8:95:ALA:O	10:8:99:VAL:HG12	2.12	0.50
12:C:249:PRO:HB3	12:C:410:VAL:HB	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:371:THR:HB	1:R:396:ILE:HD11	1.94	0.50
1:R:570:PHE:HB2	1:R:654:LYS:HB2	1.94	0.50
1:R:772:GLY:HA2	6:T:107:ASN:HB3	1.93	0.50
12:C:346:MET:HE2	12:C:348:ALA:HB2	1.93	0.50
12:B:511:VAL:HG11	12:B:548:TYR:HB2	1.93	0.50
14:Z:263:ILE:O	14:Z:267:VAL:HG23	2.12	0.50
1:R:490:THR:OG1	1:R:491:GLU:N	2.45	0.50
3:H:77:ASN:OD1	3:H:80:ARG:NH2	2.44	0.50
9:O:172:LEU:O	9:O:176:ILE:HG13	2.12	0.50
10:1:150:LEU:O	10:1:154:THR:OG1	2.25	0.50
10:8:61:MET:SD	10:8:135:LEU:HB3	2.52	0.50
12:C:397:ASN:O	12:C:399:GLU:N	2.45	0.50
1:R:580:THR:HA	1:R:584:GLY:HA3	1.94	0.50
14:Y:133:LEU:O	14:Y:137:THR:HG23	2.11	0.50
16:N:6:LYS:NZ	16:N:59:ASP:O	2.35	0.50
9:O:150:PHE:CD1	10:9:28:LEU:HB2	2.47	0.49
10:6:44:MET:HE1	10:6:47:MET:SD	2.52	0.49
10:6:72:VAL:HG11	10:6:99:VAL:CG1	2.42	0.49
12:B:232:ARG:NH2	12:B:529:ASP:OD2	2.45	0.49
1:R:41:ASN:HD21	1:R:311:ASN:HA	1.77	0.49
1:R:737:SER:HB3	1:R:740:ARG:NH2	2.28	0.49
10:8:123:GLN:O	10:8:125:PRO:HD3	2.11	0.49
11:Q:69:VAL:O	11:Q:73:ARG:HG2	2.12	0.49
11:Q:280:GLY:C	11:Q:293:ARG:HE	2.20	0.49
12:C:232:ARG:NE	12:C:532:CYS:SG	2.84	0.49
13:D:124:SER:O	13:D:127:MET:HG2	2.11	0.49
13:E:457:LYS:O	13:E:461:ASN:HB2	2.12	0.49
13:E:487:PHE:HB3	13:E:491:MET:HE2	1.94	0.49
14:X:211:SER:O	14:X:211:SER:OG	2.27	0.49
7:U:261:ASN:HB3	7:U:265:PRO:HB3	1.94	0.49
7:U:335:SER:O	7:U:337:ARG:N	2.45	0.49
10:7:35:ALA:O	10:7:39:THR:HG23	2.12	0.49
11:Q:2:SER:C	11:Q:4:PHE:H	2.19	0.49
12:C:391:ARG:NH1	12:C:401:GLU:OE2	2.45	0.49
1:R:131:ILE:HG13	1:R:246:PRO:HG3	1.94	0.49
3:H:12:ILE:HG23	3:H:16:MET:HE2	1.94	0.49
11:Q:28:LEU:HG	11:Q:325:GLU:OE2	2.13	0.49
15:G:50:LYS:O	15:G:53:GLU:HG3	2.12	0.49
1:R:316:GLN:HE22	3:H:19:ILE:HG12	1.78	0.49
1:R:628:LEU:N	1:R:632:GLN:OE1	2.43	0.49
12:C:476:ARG:O	12:C:480:LYS:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:439:MET:HG3	1:R:440:PHE:N	2.26	0.49
9:O:150:PHE:CE1	10:9:28:LEU:HB2	2.47	0.49
10:6:9:GLU:OE2	10:6:10:TYR:N	2.40	0.49
1:R:170:PHE:HD2	1:R:223:PHE:HB3	1.78	0.49
1:R:171:VAL:HG22	1:R:248:PRO:HD2	1.94	0.49
4:L:13:GLN:O	4:L:17:ARG:HG3	2.12	0.49
4:L:46:GLN:O	4:L:49:LEU:HG	2.12	0.49
4:L:88:PHE:O	4:L:89:ARG:C	2.56	0.49
10:4:117:GLY:HA3	10:4:131:MET:HG3	1.95	0.49
10:6:28:LEU:HD12	10:7:105:ALA:HB2	1.95	0.49
10:9:45:SER:OG	10:9:52:ILE:HD11	2.13	0.49
12:C:55:ILE:HD12	12:C:365:LEU:HD11	1.94	0.49
12:A:256:LYS:NZ	12:A:349:ASP:OD2	2.46	0.49
12:B:173:ARG:NH2	14:Y:16:GLU:OE2	2.43	0.49
17:P:90:VAL:O	17:P:92:TYR:N	2.46	0.49
1:R:536:LYS:O	1:R:540:SER:OG	2.31	0.49
1:R:809:GLU:OE1	1:R:809:GLU:N	2.46	0.49
4:K:81:MET:O	4:K:85:GLN:NE2	2.45	0.49
6:T:75:HIS:NE2	6:T:98:TYR:HB3	2.28	0.49
6:T:79:LEU:HD22	6:T:79:LEU:H	1.77	0.49
9:O:169:ASN:OD1	9:O:171:SER:OG	2.27	0.49
12:C:231:GLN:HB2	12:C:233:VAL:O	2.13	0.49
13:F:207:CYS:SG	13:F:229:ILE:HD12	2.52	0.49
13:D:100:GLU:OE1	13:D:100:GLU:N	2.46	0.49
3:I:108:ASP:O	3:I:110:THR:HG23	2.12	0.49
12:C:64:ILE:HG22	12:C:65:GLN:O	2.12	0.49
12:A:28:VAL:HG22	12:A:364:ARG:HB3	1.94	0.49
12:A:39:MET:HE3	12:A:40:TYR:HE2	1.78	0.49
12:A:511:VAL:HG11	12:A:548:TYR:HB2	1.94	0.49
1:R:276:GLU:O	1:R:280:GLN:N	2.44	0.49
1:R:362:PRO:HA	1:R:820:PHE:HB2	1.94	0.49
3:I:12:ILE:HG22	3:I:16:MET:HE1	1.94	0.49
7:U:373:TYR:CE2	7:U:380:LYS:HD2	2.48	0.49
12:C:306:MET:HA	12:C:309:THR:HG22	1.93	0.49
12:C:338:ARG:HG3	12:C:403:SER:N	2.27	0.49
12:B:349:ASP:O	12:B:350:SER:OG	2.28	0.49
17:P:28:ALA:O	17:P:30:LYS:N	2.46	0.49
17:P:167:TRP:O	17:P:170:THR:N	2.46	0.49
1:R:79:ILE:HG22	1:R:287:ALA:HB1	1.95	0.48
10:6:60:VAL:O	10:6:64:ILE:HG12	2.13	0.48
10:9:55:SER:O	10:9:55:SER:OG	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:B:318:MET:HB3	12:B:319:PRO:HD2	1.95	0.48
12:B:510:GLU:HG3	12:B:567:TRP:CE2	2.48	0.48
13:F:360:ASP:OD2	13:F:362:THR:OG1	2.27	0.48
15:G:65:ALA:HB1	15:G:138:TYR:CE2	2.47	0.48
1:R:787:VAL:HA	1:R:791:LEU:HB2	1.96	0.48
11:Q:246:ARG:HH21	11:Q:271:TYR:HD2	1.58	0.48
14:Y:87:ILE:HD13	14:Y:121:LEU:HD22	1.94	0.48
1:R:60:GLU:O	1:R:64:LYS:HG2	2.13	0.48
1:R:398:THR:HG21	1:R:547:HIS:CE1	2.48	0.48
1:R:555:SER:OG	1:R:559:HIS:NE2	2.46	0.48
1:R:718:VAL:O	1:R:722:ILE:HG12	2.12	0.48
3:J:29:GLU:O	3:J:33:LYS:HG2	2.13	0.48
10:5:57:ILE:HD13	10:5:132:ILE:HD11	1.95	0.48
10:7:82:ASP:OD1	10:7:83:ASP:N	2.47	0.48
11:Q:52:THR:OG1	11:Q:53:ASP:N	2.43	0.48
11:Q:122:ILE:O	11:Q:125:LEU:N	2.46	0.48
12:B:66:VAL:HG12	12:B:68:GLU:H	1.78	0.48
13:D:363:HIS:HB3	13:D:366:PRO:HD2	1.95	0.48
16:N:14:GLU:O	16:N:18:THR:HG23	2.14	0.48
1:R:26:VAL:HG13	1:R:303:ILE:HD11	1.95	0.48
3:H:4:SER:OG	3:H:5:ASP:N	2.46	0.48
4:K:45:GLU:HA	4:K:48:ARG:NH2	2.29	0.48
12:B:594:GLU:O	12:B:598:LYS:HG3	2.13	0.48
13:D:365:ILE:HB	13:D:366:PRO:HD3	1.96	0.48
1:R:641:VAL:O	1:R:645:LEU:HG	2.14	0.48
3:I:18:PHE:O	3:I:21:GLN:HG3	2.13	0.48
4:L:110:ILE:HD11	4:L:114:TYR:CD2	2.49	0.48
5:S:30:LYS:HD2	5:S:34:ARG:HD3	1.94	0.48
11:Q:221:PHE:CZ	11:Q:268:ALA:HB2	2.49	0.48
12:A:583:SER:O	12:A:583:SER:OG	2.31	0.48
13:D:376:GLN:HG3	13:D:378:TYR:CD2	2.49	0.48
1:R:230:LYS:O	1:R:234:LYS:HG2	2.13	0.48
9:0:160:SER:OG	9:0:161:GLY:N	2.45	0.48
10:9:98:SER:OG	10:9:99:VAL:N	2.45	0.48
11:Q:171:GLN:N	11:Q:171:GLN:OE1	2.46	0.48
12:C:376:ALA:HB1	13:D:309:GLU:HA	1.96	0.48
12:A:145:SER:HG	14:X:31:ARG:HH11	1.61	0.48
12:A:439:LEU:HD12	12:A:444:HIS:CD2	2.48	0.48
14:Z:217:LEU:HD12	14:Z:218:PRO:HD2	1.94	0.48
14:X:224:ILE:O	14:X:228:THR:HG23	2.13	0.48
1:R:47:PHE:HA	1:R:52:VAL:HB	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:226:GLY:HA3	1:R:229:LEU:HD13	1.95	0.48
1:R:800:LEU:O	1:R:804:ARG:N	2.35	0.48
10:1:14:PHE:HB2	10:1:89:SER:OG	2.14	0.48
10:6:31:ALA:HB1	10:7:109:ALA:HB2	1.96	0.48
10:6:56:ILE:HD13	10:7:133:LEU:HD13	1.96	0.48
12:A:22:HIS:HB3	12:A:30:THR:O	2.14	0.48
12:A:561:SER:OG	12:A:562:ASP:N	2.46	0.48
12:B:496:VAL:O	15:G:167:ARG:HD3	2.13	0.48
14:Z:246:LEU:HA	14:Z:249:LEU:HD12	1.95	0.48
1:R:296:LYS:O	1:R:300:MET:N	2.39	0.48
6:T:52:ALA:HA	6:T:55:ILE:HD12	1.96	0.48
15:G:143:GLU:O	15:G:146:VAL:HG12	2.14	0.48
14:X:56:ALA:O	14:X:58:LYS:HD2	2.14	0.48
16:N:29:ASN:OD1	16:N:30:LYS:N	2.45	0.48
4:M:67:GLY:O	4:M:71:THR:HG23	2.14	0.47
9:0:48:MET:O	9:0:52:LEU:HB2	2.14	0.47
10:1:61:MET:HE1	10:1:136:ILE:HD13	1.95	0.47
10:4:81:ASN:ND2	10:4:83:ASP:H	2.12	0.47
10:8:127:LEU:HD12	10:8:127:LEU:HA	1.75	0.47
10:8:149:ALA:O	10:8:153:SER:OG	2.31	0.47
11:Q:20:VAL:HG21	11:Q:315:PHE:CE2	2.49	0.47
11:Q:110:ILE:HD11	11:Q:181:ILE:HG22	1.96	0.47
12:B:561:SER:OG	12:B:562:ASP:N	2.47	0.47
1:R:69:GLU:HG3	1:R:290:ILE:HG12	1.96	0.47
1:R:123:LEU:O	1:R:126:THR:OG1	2.26	0.47
1:R:578:PHE:O	1:R:581:SER:OG	2.31	0.47
1:R:779:PHE:O	1:R:783:ALA:N	2.36	0.47
3:J:42:LYS:HZ2	4:M:40:ALA:HA	1.79	0.47
3:J:53:ILE:HG13	3:J:54:MET:N	2.29	0.47
12:A:275:VAL:HG11	12:A:327:ILE:HD13	1.96	0.47
13:F:193:SER:OG	13:F:194:ALA:N	2.46	0.47
9:0:51:ASN:ND2	10:1:90:PHE:HB3	2.26	0.47
10:2:99:VAL:HB	10:2:149:ALA:HB2	1.95	0.47
10:8:13:PHE:HB2	10:9:90:PHE:CE2	2.50	0.47
11:Q:93:LEU:HD13	11:Q:312:PHE:CD1	2.50	0.47
11:Q:334:GLU:HG2	15:G:70:ALA:HB1	1.95	0.47
12:A:24:VAL:HG11	12:A:29:VAL:HG13	1.96	0.47
12:B:265:LYS:HG2	12:B:294:LEU:HD13	1.97	0.47
14:X:23:VAL:HG13	14:X:65:ILE:HD13	1.96	0.47
15:G:55:LYS:NZ	16:N:103:ASP:OD2	2.36	0.47
3:J:50:ARG:NH1	3:J:51:LEU:HD12	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:52:GLU:O	4:M:56:LYS:HG2	2.14	0.47
4:K:5:SER:O	4:K:9:GLN:HG2	2.14	0.47
9:0:23:GLY:O	9:0:27:THR:HG22	2.14	0.47
9:0:42:THR:HA	9:0:131:TYR:HE1	1.80	0.47
12:A:248:ILE:O	12:A:248:ILE:HG13	2.15	0.47
3:I:8:VAL:O	3:I:12:ILE:HG13	2.14	0.47
10:8:35:ALA:O	10:8:39:THR:HG23	2.15	0.47
12:A:449:ASN:HD22	12:A:452:ILE:HG12	1.79	0.47
13:F:380:ASP:HB2	13:F:393:ASN:HB2	1.96	0.47
14:Z:177:GLN:HE21	14:Z:181:LEU:HD23	1.80	0.47
14:X:36:ILE:HD11	14:X:91:LEU:HG	1.96	0.47
14:Y:219:ALA:HA	14:Y:222:GLN:OE1	2.14	0.47
1:R:253:GLU:HA	1:R:256:GLU:HB2	1.97	0.47
11:Q:250:GLU:HG3	11:Q:251:GLY:H	1.80	0.47
13:E:500:LEU:O	13:E:504:TYR:HB2	2.14	0.47
14:Y:133:LEU:HB2	14:Y:179:PHE:CZ	2.50	0.47
1:R:132:LEU:HD11	1:R:254:ARG:NE	2.23	0.47
1:R:270:MET:HE3	1:R:270:MET:HB3	1.76	0.47
1:R:373:GLY:HA3	1:R:449:ILE:HD11	1.96	0.47
4:M:78:GLN:O	4:M:82:THR:HG23	2.14	0.47
3:I:206:GLN:HE22	13:E:40:LEU:HB2	1.80	0.47
4:L:32:ARG:O	4:L:35:GLN:HG3	2.14	0.47
4:K:6:GLN:O	4:K:10:GLN:HG2	2.14	0.47
7:U:360:GLN:HB2	7:U:383:LEU:HD22	1.97	0.47
9:0:58:ILE:HG21	10:1:148:VAL:HG11	1.95	0.47
10:8:59:VAL:HG21	10:9:134:ILE:HD12	1.95	0.47
10:8:132:ILE:HD13	10:8:132:ILE:HA	1.74	0.47
12:B:25:SER:O	12:B:25:SER:OG	2.31	0.47
12:B:138:CYS:HB3	12:B:141:LEU:HD12	1.96	0.47
12:B:246:THR:OG1	12:B:247:ALA:N	2.48	0.47
12:B:261:GLN:NE2	12:B:286:GLU:OE2	2.37	0.47
13:F:359:ASP:OD1	13:F:359:ASP:N	2.44	0.47
13:F:484:LEU:HD22	13:F:492:LEU:HD22	1.97	0.47
13:D:457:LYS:O	13:D:461:ASN:HB2	2.15	0.47
13:E:124:SER:OG	13:E:125:GLU:N	2.47	0.47
16:N:13:ASP:O	16:N:17:VAL:HG23	2.14	0.47
1:R:89:PRO:O	1:R:94:MET:HE1	2.14	0.47
1:R:297:VAL:HA	1:R:300:MET:HB2	1.96	0.47
1:R:374:PHE:CZ	1:R:449:ILE:HG13	2.49	0.47
1:R:440:PHE:HA	1:R:443:VAL:HG22	1.95	0.47
1:R:487:TYR:HB3	18:R:901:NAG:HN2	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:786:THR:O	1:R:790:LEU:HB2	2.14	0.47
4:L:55:PHE:HB3	4:L:56:LYS:HZ3	1.79	0.47
4:L:55:PHE:O	4:L:59:GLU:HG2	2.15	0.47
10:4:50:GLU:CD	10:4:50:GLU:H	2.23	0.47
10:4:80:LEU:HD23	10:4:81:ASN:H	1.80	0.47
11:Q:122:ILE:H	11:Q:145:GLN:NE2	2.13	0.47
11:Q:230:THR:OG1	11:Q:231:GLU:N	2.48	0.47
10:8:51:GLN:O	10:8:55:SER:OG	2.20	0.47
10:9:22:ALA:HB2	10:9:96:GLY:HA2	1.97	0.47
11:Q:199:LEU:HD23	11:Q:199:LEU:HA	1.72	0.47
12:C:100:ASP:OD1	12:C:100:ASP:N	2.48	0.47
1:R:98:GLU:HA	1:R:101:PHE:HB3	1.97	0.47
3:J:210:GLU:OE1	13:F:39:TYR:OH	2.31	0.47
3:H:50:ARG:O	3:H:54:MET:HG2	2.15	0.47
10:2:9:GLU:O	10:2:11:ALA:N	2.47	0.47
10:4:32:TYR:CD2	10:4:108:PHE:HD1	2.32	0.47
10:6:88:LYS:O	10:6:92:GLN:NE2	2.46	0.47
10:8:47:MET:C	10:8:48:ARG:HD2	2.40	0.47
12:B:265:LYS:HE3	12:B:294:LEU:HD11	1.97	0.47
12:B:299:ASP:HB2	14:Y:186:LEU:HG	1.97	0.47
14:X:213:PHE:HB3	14:X:217:LEU:HD21	1.97	0.47
14:Y:90:GLU:OE2	14:Y:127:HIS:ND1	2.27	0.47
1:R:97:LEU:O	1:R:100:ASN:ND2	2.38	0.46
3:H:12:ILE:HD11	4:K:6:GLN:HB3	1.96	0.46
10:1:60:VAL:O	10:1:64:ILE:HG13	2.15	0.46
10:4:35:ALA:O	10:4:39:THR:HG23	2.15	0.46
11:Q:97:LEU:O	11:Q:101:THR:HG23	2.15	0.46
12:A:458:MET:HE1	12:A:480:LYS:HE3	1.97	0.46
12:B:397:ASN:HB2	12:B:398:PRO:HD3	1.97	0.46
13:F:485:ARG:C	13:F:487:PHE:H	2.22	0.46
14:X:136:LEU:HD23	14:X:186:LEU:HD22	1.96	0.46
16:N:40:GLU:OE2	16:N:40:GLU:N	2.48	0.46
1:R:305:HIS:HA	1:R:308:ASN:HB3	1.96	0.46
10:9:113:VAL:HG21	10:9:134:ILE:HG21	1.97	0.46
12:C:50:LEU:HD12	12:C:50:LEU:H	1.81	0.46
12:C:65:GLN:NE2	12:C:321:ALA:HB2	2.30	0.46
12:C:75:VAL:HG22	13:F:65:PHE:HA	1.98	0.46
12:A:276:GLY:O	12:A:314:ASN:HB2	2.15	0.46
13:D:49:THR:O	13:D:49:THR:OG1	2.29	0.46
14:Z:207:GLN:HA	14:Z:207:GLN:OE1	2.15	0.46
4:M:11:LEU:O	4:M:15:GLU:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:41:GLU:OE2	3:I:42:LYS:HG2	2.15	0.46
3:H:122:GLN:NE2	13:D:42:GLN:HA	2.31	0.46
4:K:34:LYS:HA	4:K:34:LYS:HD3	1.69	0.46
10:5:150:LEU:O	10:5:154:THR:OG1	2.18	0.46
12:C:74:SER:OG	12:C:75:VAL:N	2.47	0.46
12:A:142:ARG:CZ	12:A:142:ARG:HB2	2.45	0.46
12:A:507:ILE:O	12:A:511:VAL:HG23	2.14	0.46
13:F:452:LEU:O	13:F:456:GLN:HG2	2.14	0.46
13:D:376:GLN:HG3	13:D:378:TYR:CE2	2.50	0.46
13:D:380:ASP:HB2	13:D:393:ASN:HB2	1.97	0.46
13:E:78:ASP:OD2	13:E:80:THR:OG1	2.33	0.46
10:1:44:MET:HE2	10:1:122:ALA:HB2	1.97	0.46
12:C:133:TRP:N	12:C:185:TYR:O	2.41	0.46
14:Y:141:LYS:HD3	14:Y:142:ASN:ND2	2.30	0.46
1:R:195:VAL:HG11	1:R:224:PHE:HA	1.97	0.46
1:R:764:LEU:HD13	6:T:84:PRO:HG3	1.97	0.46
2:O:347:ALA:HB1	2:O:366:TYR:HA	1.98	0.46
3:H:69:LYS:HB3	3:H:69:LYS:HE3	1.69	0.46
10:5:87:TYR:HD2	10:5:88:LYS:HE3	1.80	0.46
14:Y:144:ALA:O	14:Y:149:ASN:ND2	2.48	0.46
1:R:49:ARG:HH22	1:R:310:CYS:H	1.61	0.46
1:R:337:LEU:O	1:R:341:THR:HG23	2.15	0.46
1:R:517:GLY:H	5:S:56:ILE:HD11	1.78	0.46
3:I:215:LEU:HA	4:L:91:ASN:HB2	1.97	0.46
4:L:59:GLU:O	4:L:63:LEU:HG	2.16	0.46
3:H:129:GLU:OE2	13:D:64:LYS:NZ	2.40	0.46
12:C:536:LYS:O	12:C:540:MET:HG3	2.16	0.46
12:A:29:VAL:CG1	12:A:66:VAL:HB	2.45	0.46
13:E:216:SER:OG	13:E:218:ASP:OD1	2.31	0.46
14:X:172:ASN:OD1	14:X:173:GLU:N	2.48	0.46
1:R:226:GLY:O	1:R:230:LYS:HB2	2.15	0.46
7:U:362:THR:HG22	7:U:363:GLY:H	1.80	0.46
9:O:177:LEU:HA	9:O:180:GLU:OE1	2.15	0.46
10:2:130:GLY:O	10:2:134:ILE:HG12	2.16	0.46
11:Q:78:MET:HE2	11:Q:78:MET:HB3	1.83	0.46
3:I:164:ASP:OD2	3:I:166:GLN:NE2	2.48	0.46
10:2:85:SER:C	10:2:87:TYR:H	2.23	0.46
10:8:14:PHE:HB2	10:8:89:SER:HB2	1.98	0.46
12:C:354:TRP:HZ3	12:C:382:LEU:HD23	1.79	0.46
14:Z:148:LYS:HD2	14:Z:196:GLN:NE2	2.31	0.46
14:X:52:VAL:HG12	14:X:75:PRO:HG3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:22:ALA:O	1:R:26:VAL:HG12	2.16	0.46
10:2:91:LEU:HD13	10:2:155:LYS:HB3	1.97	0.46
12:C:234:LEU:HD21	12:C:448:VAL:HG21	1.98	0.46
13:F:78:ASP:OD1	13:F:80:THR:HG22	2.16	0.46
13:E:82:ARG:HD3	13:E:100:GLU:HB2	1.97	0.46
1:R:289:ASN:HB3	1:R:293:TRP:CD1	2.51	0.46
1:R:744:LEU:HD13	10:7:67:ILE:HD13	1.97	0.46
4:L:111:HIS:HD2	4:L:112:GLU:N	2.14	0.46
3:H:19:ILE:HG23	4:K:17:ARG:HB2	1.98	0.46
3:H:49:GLN:O	3:H:53:ILE:HG12	2.16	0.46
9:0:70:TYR:CD1	9:0:70:TYR:C	2.95	0.46
11:Q:66:THR:HG22	11:Q:67:VAL:H	1.80	0.46
11:Q:179:GLU:OE2	15:G:122:THR:HA	2.15	0.46
12:C:442:ARG:HG2	13:F:428:ILE:HD11	1.97	0.46
12:B:573:HIS:CD2	12:B:615:LEU:HD13	2.51	0.46
13:E:359:ASP:OD1	13:E:359:ASP:N	2.45	0.46
1:R:184:GLU:HB3	1:R:220:PHE:HB2	1.98	0.45
1:R:530:THR:HB	10:7:78:ASN:HD21	1.80	0.45
3:J:21:GLN:HA	4:M:21:LYS:HZ1	1.81	0.45
4:K:78:GLN:O	4:K:82:THR:HG23	2.16	0.45
10:4:99:VAL:HB	10:4:149:ALA:HB2	1.98	0.45
12:A:368:MET:HE1	13:E:318:PRO:HG3	1.99	0.45
12:B:50:LEU:HD23	12:B:68:GLU:HB2	1.97	0.45
13:F:486:ILE:HB	13:F:487:PHE:CE2	2.50	0.45
13:E:341:VAL:HG23	13:E:344:ARG:HG3	1.98	0.45
15:G:95:ARG:HG3	16:N:4:ARG:HB3	1.98	0.45
1:R:570:PHE:CE2	1:R:657:VAL:HG21	2.51	0.45
3:I:141:PHE:CZ	3:I:145:LYS:HD3	2.51	0.45
5:S:79:HIS:HE1	6:T:75:HIS:O	1.99	0.45
9:0:124:LYS:HD3	9:0:124:LYS:HA	1.79	0.45
10:3:45:SER:OG	10:3:52:ILE:HD11	2.16	0.45
10:3:109:ALA:O	10:3:113:VAL:HG12	2.15	0.45
11:Q:299:VAL:HG11	11:Q:350:ILE:HG22	1.97	0.45
12:A:226:PRO:HG3	12:A:461:LEU:HD22	1.98	0.45
12:B:298:VAL:HG22	12:B:299:ASP:H	1.81	0.45
14:Z:50:GLN:HE21	14:Z:54:ILE:HB	1.81	0.45
16:N:40:GLU:N	16:N:43:THR:OG1	2.47	0.45
1:R:203:GLU:CD	1:R:203:GLU:H	2.23	0.45
1:R:611:HIS:CE1	1:R:627:MET:HA	2.52	0.45
3:J:13:LYS:HA	3:J:16:MET:HB3	1.97	0.45
4:M:25:ALA:HA	4:M:28:ARG:HH11	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:16:MET:HG3	4:K:13:GLN:HG2	1.98	0.45
7:U:292:VAL:C	7:U:294:GLU:H	2.24	0.45
10:2:59:VAL:HG21	10:3:134:ILE:HD12	1.98	0.45
12:B:71:SER:O	12:B:71:SER:OG	2.33	0.45
14:Z:58:LYS:NZ	14:Z:59:ASN:O	2.43	0.45
17:P:111:PHE:C	17:P:113:ASP:N	2.71	0.45
1:R:179:ARG:HD3	1:R:240:PHE:CD1	2.49	0.45
1:R:446:GLY:HA2	1:R:449:ILE:HD13	1.98	0.45
3:I:49:GLN:CB	4:L:44:ILE:HD11	2.46	0.45
7:U:271:ALA:HA	7:U:399:ASP:O	2.16	0.45
10:5:9:GLU:HG3	10:5:10:TYR:H	1.81	0.45
11:Q:177:ASN:HD22	15:G:121:LEU:HD12	1.81	0.45
12:A:42:LEU:O	12:A:82:THR:OG1	2.31	0.45
12:A:277:CYS:HB3	12:A:326:SER:OG	2.16	0.45
13:E:455:LEU:HD23	13:E:455:LEU:HA	1.70	0.45
14:X:106:ASP:OD1	14:X:106:ASP:N	2.49	0.45
14:Y:163:ILE:HD12	14:Y:168:ILE:HD13	1.99	0.45
1:R:375:GLN:O	1:R:375:GLN:NE2	2.49	0.45
1:R:807:TRP:HA	1:R:811:GLN:HG3	1.98	0.45
3:J:61:GLU:O	3:J:64:ILE:HG13	2.17	0.45
10:4:88:LYS:H	10:4:88:LYS:HD2	1.82	0.45
12:A:317:ASN:HB2	13:D:336:GLU:HG2	1.97	0.45
12:A:581:LEU:HD22	12:A:584:MET:HE2	1.98	0.45
12:B:500:SER:O	12:B:500:SER:OG	2.33	0.45
15:G:184:LEU:HA	15:G:184:LEU:HD23	1.78	0.45
2:O:5:TRP:HA	2:O:373:LYS:HA	1.98	0.45
3:J:19:ILE:HA	3:J:22:GLU:HB3	1.98	0.45
10:5:131:MET:O	10:5:135:LEU:HG	2.17	0.45
10:6:85:SER:HG	10:6:88:LYS:HZ2	1.53	0.45
13:E:457:LYS:HA	13:E:457:LYS:HD3	1.81	0.45
14:Y:42:LEU:HD23	14:Y:45:ILE:HG13	1.97	0.45
16:N:109:ALA:HB1	16:N:112:MET:HB2	1.99	0.45
1:R:410:PHE:HD2	1:R:467:CYS:HB2	1.82	0.45
3:J:57:TYR:O	3:J:61:GLU:HG3	2.17	0.45
3:J:197:GLU:OE2	3:J:197:GLU:N	2.48	0.45
7:U:369:PHE:O	7:U:401:GLN:HA	2.17	0.45
10:4:141:LEU:HD23	10:4:141:LEU:HA	1.83	0.45
10:4:143:LEU:HD12	10:4:143:LEU:HA	1.69	0.45
10:9:20:SER:O	10:9:24:VAL:HG12	2.17	0.45
10:9:87:TYR:O	10:9:91:LEU:HG	2.16	0.45
12:C:372:SER:O	12:C:372:SER:OG	2.26	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:B:241:VAL:HG12	12:B:461:LEU:HD21	1.99	0.45
13:D:435:MET:O	13:D:439:VAL:HG22	2.16	0.45
14:X:172:ASN:OD1	14:X:174:GLY:N	2.50	0.45
14:X:267:VAL:O	14:X:271:GLU:HG2	2.16	0.45
14:Y:101:PHE:CZ	14:Y:216:ILE:HG23	2.47	0.45
16:N:68:GLN:NE2	16:N:99:ASP:H	2.10	0.45
1:R:72:ILE:HG12	1:R:283:LEU:HD13	1.99	0.45
1:R:448:TYR:O	1:R:452:LEU:HD12	2.17	0.45
6:T:45:CYS:N	6:T:125:GLN:HG2	2.32	0.45
7:U:340:PHE:N	7:U:365:SER:OG	2.50	0.45
7:U:377:LEU:HB2	7:U:379:LYS:O	2.17	0.45
7:U:410:GLU:OE2	7:U:411:GLN:NE2	2.50	0.45
10:4:124:GLN:OE1	10:4:126:ARG:N	2.49	0.45
10:7:50:GLU:N	10:7:50:GLU:OE2	2.50	0.45
11:Q:57:PHE:CE1	11:Q:58:LEU:HG	2.52	0.45
12:C:152:ILE:HG12	12:C:167:MET:HG2	1.98	0.45
12:C:510:GLU:HG3	12:C:567:TRP:NE1	2.31	0.45
12:A:24:VAL:CB	12:A:29:VAL:HA	2.40	0.45
12:A:309:THR:OG1	12:A:310:ALA:N	2.50	0.45
13:E:117:ASP:OD1	13:E:118:ILE:N	2.50	0.45
14:Z:134:ASN:O	14:Z:138:ASP:HB2	2.16	0.45
14:Z:242:LEU:HD22	14:Z:266:ILE:HG23	1.99	0.45
14:Y:41:ASN:HB3	14:Y:105:LEU:HD21	1.99	0.45
10:3:50:GLU:H	10:3:50:GLU:CD	2.24	0.45
12:C:510:GLU:HG3	12:C:567:TRP:CE2	2.51	0.45
12:A:288:LEU:HD23	12:A:288:LEU:HA	1.75	0.45
1:R:175:ILE:H	1:R:219:VAL:CG1	2.29	0.45
1:R:611:HIS:HE1	1:R:627:MET:HA	1.82	0.45
3:I:26:LYS:O	3:I:30:ILE:HG12	2.16	0.45
4:K:112:GLU:H	4:K:112:GLU:HG3	1.34	0.45
8:V:338:ILE:HG13	8:V:339:ILE:HD12	1.98	0.45
13:D:164:ILE:HD11	13:D:342:GLU:HA	1.98	0.45
1:R:12:LEU:HD13	1:R:324:TRP:CD2	2.52	0.44
1:R:85:ASN:HD21	1:R:830:ILE:HG21	1.81	0.44
1:R:234:LYS:HA	1:R:237:CYS:SG	2.58	0.44
4:M:100:LEU:HD13	4:M:100:LEU:HA	1.78	0.44
9:O:161:GLY:N	11:Q:309:GLN:HE22	2.15	0.44
12:C:87:SER:HB2	12:C:208:VAL:HG12	1.99	0.44
12:C:298:VAL:HG23	12:C:299:ASP:H	1.82	0.44
1:R:61:MET:HG2	1:R:98:GLU:CG	2.46	0.44
1:R:374:PHE:CD2	1:R:396:ILE:HG12	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:403:PHE:CD1	1:R:453:MET:HG2	2.53	0.44
1:R:647:VAL:HB	1:R:648:PRO:HD3	1.98	0.44
3:J:136:CYS:HB3	3:J:144:VAL:HG21	1.97	0.44
3:J:207:MET:HE2	3:J:207:MET:HB3	1.85	0.44
5:S:68:LEU:HD12	5:S:72:THR:HG21	1.98	0.44
7:U:313:TYR:O	7:U:321:VAL:N	2.39	0.44
9:O:39:TRP:CE2	9:O:43:GLU:HG3	2.52	0.44
10:8:61:MET:HB3	10:8:61:MET:HE2	1.76	0.44
11:Q:322:LYS:NZ	11:Q:326:CYS:SG	2.76	0.44
13:F:492:LEU:H	13:F:492:LEU:HG	1.57	0.44
13:F:497:GLN:N	13:F:497:GLN:OE1	2.50	0.44
13:E:141:ARG:HA	14:X:9:LYS:HZ3	1.81	0.44
13:E:484:LEU:HD13	13:E:492:LEU:HD22	1.98	0.44
14:Z:152:LEU:HD23	14:Z:152:LEU:HA	1.79	0.44
1:R:428:SER:O	1:R:432:SER:OG	2.34	0.44
4:K:103:VAL:HG12	4:K:103:VAL:O	2.17	0.44
7:U:278:TYR:O	7:U:392:PRO:HB2	2.17	0.44
10:3:95:ALA:O	10:3:99:VAL:HG12	2.17	0.44
10:7:109:ALA:O	10:7:113:VAL:HG12	2.17	0.44
11:Q:78:MET:HG3	11:Q:322:LYS:HD2	1.99	0.44
12:C:398:PRO:HD2	12:C:400:ARG:HH11	1.82	0.44
12:A:24:VAL:HB	12:A:28:VAL:O	2.18	0.44
12:A:547:PHE:HB2	12:A:608:MET:SD	2.57	0.44
13:D:137:LYS:HB3	13:D:137:LYS:HE2	1.66	0.44
1:R:289:ASN:HD22	1:R:293:TRP:HE1	1.64	0.44
3:J:21:GLN:NE2	3:J:24:ASN:HB3	2.32	0.44
10:6:98:SER:OG	10:6:99:VAL:N	2.50	0.44
12:C:194:LEU:HD23	12:C:201:GLU:HB3	1.99	0.44
12:B:296:MET:HE2	12:B:296:MET:HB3	1.80	0.44
12:B:567:TRP:HE1	12:B:571:ARG:HH21	1.65	0.44
13:F:412:ARG:HH21	13:F:414:ASP:CG	2.24	0.44
14:Y:217:LEU:HD23	14:Y:217:LEU:H	1.82	0.44
2:O:4:PHE:O	2:O:374:ILE:N	2.42	0.44
3:H:57:TYR:CE1	4:K:51:ARG:HB2	2.52	0.44
5:S:30:LYS:HD2	5:S:30:LYS:HA	1.74	0.44
10:6:72:VAL:HG21	10:6:99:VAL:HG11	1.99	0.44
11:Q:146:THR:HB	11:Q:149:GLU:HB2	2.00	0.44
12:C:163:LYS:O	12:C:342:TYR:OH	2.23	0.44
12:A:56:ARG:HG2	12:A:57:LEU:H	1.82	0.44
13:F:363:HIS:CG	13:F:364:PRO:HD2	2.51	0.44
13:E:200:ASN:OD1	13:E:200:ASN:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:X:196:GLN:H	14:X:196:GLN:HG2	1.50	0.44
14:Y:226:VAL:HB	14:Y:255:LEU:HD21	1.99	0.44
15:G:106:LEU:HD13	15:G:154:SER:HB2	1.99	0.44
3:J:127:LEU:HD23	3:J:127:LEU:HA	1.84	0.44
3:I:214:ALA:O	4:L:91:ASN:ND2	2.44	0.44
3:H:53:ILE:CD1	4:K:47:TYR:HB3	2.47	0.44
7:U:369:PHE:O	7:U:401:GLN:HG3	2.18	0.44
7:U:370:HIS:C	7:U:370:HIS:CD2	2.95	0.44
9:0:200:ARG:NH2	10:9:80:LEU:O	2.46	0.44
10:1:10:TYR:HA	10:2:90:PHE:HE2	1.82	0.44
10:3:15:ALA:HB3	10:3:80:LEU:HD21	1.98	0.44
10:3:72:VAL:HG21	10:3:99:VAL:HG11	2.00	0.44
10:3:121:THR:OG1	10:3:127:LEU:HB3	2.17	0.44
10:4:48:ARG:NH1	10:4:51:GLN:OE1	2.50	0.44
12:C:393:LYS:HE3	12:C:393:LYS:HB2	1.77	0.44
12:C:576:ASP:O	12:C:580:LYS:HG2	2.17	0.44
14:Z:34:GLN:O	14:Z:34:GLN:NE2	2.51	0.44
14:Z:87:ILE:HD13	14:Z:116:LYS:HA	2.00	0.44
14:Y:69:SER:HA	14:Y:74:CYS:SG	2.57	0.44
4:L:27:LYS:HD2	4:L:27:LYS:HA	1.72	0.44
3:H:99:LYS:HE3	3:H:99:LYS:HB2	1.85	0.44
3:H:190:ILE:HG12	13:D:47:TYR:CD2	2.52	0.44
9:0:158:VAL:HG11	9:0:179:VAL:HG23	1.99	0.44
10:8:98:SER:OG	10:8:99:VAL:N	2.51	0.44
12:C:577:ILE:HD12	12:C:577:ILE:HA	1.76	0.44
12:A:34:MET:HE3	12:A:35:ALA:H	1.81	0.44
12:A:34:MET:HE3	12:A:35:ALA:N	2.33	0.44
12:B:145:SER:OG	14:Y:31:ARG:HD3	2.17	0.44
12:B:159:ASN:ND2	12:B:307:LYS:HB3	2.33	0.44
13:F:172:THR:O	13:F:172:THR:OG1	2.34	0.44
15:G:95:ARG:HD3	16:N:4:ARG:HE	1.81	0.44
3:J:24:ASN:HB2	4:M:21:LYS:HZ3	1.82	0.44
11:Q:203:THR:HB	11:Q:311:HIS:HB3	1.98	0.44
13:D:78:ASP:OD1	13:D:80:THR:HG23	2.18	0.44
13:D:216:SER:O	13:D:220:VAL:HG23	2.18	0.44
15:G:58:MET:HG3	15:G:145:LEU:HD21	2.00	0.44
1:R:12:LEU:HD22	1:R:324:TRP:CH2	2.53	0.44
1:R:384:GLY:N	1:R:815:TYR:OH	2.51	0.44
1:R:801:HIS:CD2	10:7:64:ILE:HD11	2.53	0.44
3:I:158:ALA:C	3:I:160:LYS:H	2.26	0.44
3:H:127:LEU:HA	3:H:127:LEU:HD23	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:66:ILE:HG13	6:T:67:MET:N	2.32	0.44
12:B:536:LYS:O	12:B:540:MET:HG3	2.17	0.44
1:R:61:MET:HG2	1:R:98:GLU:HG3	2.00	0.43
1:R:526:THR:OG1	5:S:67:GLN:O	2.36	0.43
1:R:612:PHE:O	1:R:615:MET:HG3	2.18	0.43
4:M:17:ARG:O	4:M:21:LYS:HG2	2.18	0.43
4:K:111:HIS:HD2	4:K:112:GLU:H	1.64	0.43
10:6:115:ASP:O	10:6:119:ARG:HG3	2.18	0.43
10:8:8:PRO:HG2	10:8:86:LEU:HD22	2.00	0.43
11:Q:142:ASN:O	11:Q:142:ASN:ND2	2.51	0.43
12:B:466:ASP:O	12:B:470:THR:HG22	2.18	0.43
13:F:124:SER:O	13:F:127:MET:HG2	2.18	0.43
13:F:408:GLU:OE1	13:F:413:LYS:HB3	2.18	0.43
13:E:487:PHE:HB3	13:E:491:MET:CE	2.48	0.43
14:Y:234:MET:HB3	14:Y:235:PRO:HD3	2.00	0.43
1:R:55:VAL:O	1:R:59:GLU:HG2	2.18	0.43
1:R:185:ARG:HG2	1:R:188:TRP:CZ3	2.54	0.43
1:R:211:THR:HG23	1:R:213:ASP:H	1.83	0.43
1:R:512:GLY:HA3	5:S:4:HIS:HB2	2.00	0.43
4:L:91:ASN:N	4:L:91:ASN:OD1	2.51	0.43
10:7:95:ALA:O	10:7:99:VAL:HG12	2.18	0.43
11:Q:3:PHE:O	11:Q:3:PHE:CG	2.71	0.43
11:Q:139:GLU:O	11:Q:143:ILE:HG22	2.18	0.43
11:Q:251:GLY:O	11:Q:255:LEU:N	2.50	0.43
12:C:261:GLN:O	12:C:264:SER:OG	2.24	0.43
12:C:324:GLU:HA	12:C:354:TRP:CD1	2.53	0.43
12:C:511:VAL:HG21	12:C:548:TYR:HD1	1.82	0.43
12:A:232:ARG:NH2	12:A:529:ASP:OD1	2.50	0.43
12:A:573:HIS:HD2	12:A:574:MET:HG2	1.83	0.43
13:F:489:LYS:HZ2	13:F:504:TYR:HB2	1.83	0.43
1:R:574:PRO:HB2	1:R:650:MET:HG3	2.00	0.43
7:U:355:TYR:HB2	7:U:387:ARG:HB2	1.99	0.43
10:4:99:VAL:HG23	10:4:145:GLY:C	2.43	0.43
12:C:194:LEU:CD2	12:C:201:GLU:HB3	2.48	0.43
12:B:507:ILE:HD11	12:B:555:VAL:HG21	1.99	0.43
13:E:269:ILE:HD12	13:E:269:ILE:H	1.83	0.43
14:Z:139:TYR:HD2	14:Z:140:LEU:HD22	1.83	0.43
14:X:256:THR:OG1	14:X:257:LYS:N	2.51	0.43
1:R:129:LYS:HB3	1:R:133:ARG:HH22	1.82	0.43
1:R:418:LEU:HA	1:R:421:VAL:HB	1.99	0.43
1:R:553:SER:HA	1:R:572:PHE:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:650:MET:O	1:R:720:GLN:NE2	2.36	0.43
7:U:366:ILE:HG22	7:U:406:ASN:HD22	1.83	0.43
7:U:372:GLU:OE1	8:V:301:PHE:N	2.52	0.43
10:2:22:ALA:HB2	10:2:96:GLY:HA2	2.00	0.43
10:3:132:ILE:HD13	10:3:132:ILE:HA	1.75	0.43
10:7:150:LEU:HD13	10:7:150:LEU:HA	1.86	0.43
11:Q:321:LEU:HD22	11:Q:350:ILE:HD12	2.00	0.43
12:A:57:LEU:HB2	13:E:53:VAL:O	2.18	0.43
12:A:397:ASN:HD22	12:A:397:ASN:HA	1.62	0.43
13:F:75:THR:O	13:F:75:THR:OG1	2.32	0.43
14:Z:262:SER:O	14:Z:265:ARG:HG2	2.18	0.43
15:G:5:ASP:OD2	15:G:182:ARG:NE	2.51	0.43
15:G:57:LEU:HD23	15:G:144:LEU:HD11	1.99	0.43
15:G:89:LYS:HA	16:N:27:GLU:HB2	2.00	0.43
4:M:45:GLU:O	4:M:49:LEU:HG	2.17	0.43
5:S:38:ILE:HG13	5:S:39:THR:N	2.33	0.43
10:4:85:SER:C	10:4:87:TYR:H	2.27	0.43
11:Q:287:ASP:OD1	11:Q:288:LYS:N	2.44	0.43
12:C:167:MET:HE3	12:C:167:MET:HB2	1.83	0.43
12:B:238:PHE:CZ	12:B:450:TRP:HA	2.53	0.43
13:E:70:GLU:HG2	13:E:71:ILE:H	1.83	0.43
13:E:465:GLN:NE2	13:E:469:GLU:O	2.50	0.43
13:E:500:LEU:HD23	13:E:504:TYR:CZ	2.54	0.43
14:X:130:LEU:HA	14:X:130:LEU:HD23	1.73	0.43
1:R:35:VAL:HB	1:R:323:VAL:HG21	2.01	0.43
1:R:65:LEU:HA	1:R:101:PHE:HZ	1.84	0.43
3:I:64:ILE:HD12	3:I:64:ILE:HA	1.91	0.43
3:I:211:VAL:O	3:I:215:LEU:HB2	2.19	0.43
3:H:141:PHE:HB3	3:H:142:PRO:HD3	2.01	0.43
10:2:57:ILE:HD12	10:2:132:ILE:HD11	2.01	0.43
13:D:380:ASP:OD2	13:D:381:ARG:N	2.50	0.43
17:P:365:GLU:O	17:P:367:SER:N	2.50	0.43
1:R:91:PRO:HD2	1:R:94:MET:HE3	2.00	0.43
1:R:294:PHE:HE2	1:R:298:ARG:HH11	1.65	0.43
1:R:572:PHE:HE2	1:R:576:ILE:HD13	1.82	0.43
4:M:13:GLN:O	4:M:16:LYS:HG3	2.18	0.43
4:K:4:GLN:HG2	4:K:5:SER:N	2.34	0.43
7:U:274:PHE:N	7:U:286:THR:OG1	2.28	0.43
9:0:135:TYR:CD2	10:9:13:PHE:HB2	2.53	0.43
10:5:97:LEU:HD23	10:5:97:LEU:HA	1.88	0.43
12:C:38:ALA:HA	13:D:106:ASP:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:C:247:ALA:HA	12:C:408:GLY:O	2.19	0.43
12:A:28:VAL:CG2	12:A:364:ARG:HB3	2.48	0.43
14:Y:14:THR:HG22	14:Y:15:SER:H	1.82	0.43
14:Y:173:GLU:O	14:Y:177:GLN:HG2	2.19	0.43
15:G:4:LYS:HB2	15:G:5:ASP:H	1.62	0.43
1:R:183:PHE:CE1	1:R:187:LEU:HD11	2.54	0.43
3:I:137:ARG:HD3	3:I:177:ILE:HG22	2.01	0.43
3:I:210:GLU:OE1	3:I:210:GLU:N	2.51	0.43
6:T:52:ALA:O	6:T:56:VAL:HG22	2.18	0.43
9:O:126:ILE:HG13	9:O:131:TYR:CE2	2.45	0.43
10:1:132:ILE:HD13	10:1:132:ILE:HA	1.77	0.43
14:Z:125:ASP:N	14:Z:125:ASP:OD1	2.51	0.43
14:X:72:GLY:HA2	14:X:76:ASN:HD21	1.84	0.43
1:R:556:LEU:HB3	1:R:572:PHE:CD1	2.54	0.43
3:H:107:LYS:HD3	3:H:107:LYS:HA	1.88	0.43
7:U:323:PHE:HB3	7:U:345:LEU:HD11	2.00	0.43
8:V:302:GLU:N	8:V:302:GLU:OE2	2.52	0.43
10:2:9:GLU:C	10:2:11:ALA:H	2.27	0.43
12:A:155:ILE:HD11	12:A:165:LYS:HD3	2.01	0.43
14:Y:197:TYR:CZ	14:Y:232:TYR:HB2	2.54	0.43
1:R:207:GLU:HB2	1:R:212:GLY:HA2	2.01	0.43
1:R:542:ILE:HD12	1:R:587:VAL:HG13	1.99	0.43
3:H:42:LYS:O	3:H:46:VAL:HG13	2.19	0.43
4:K:31:ARG:HH21	4:K:35:GLN:HG2	1.84	0.43
11:Q:2:SER:C	11:Q:4:PHE:N	2.77	0.43
11:Q:277:LEU:HD22	11:Q:293:ARG:HB3	2.01	0.43
14:Y:51:ASP:OD1	14:Y:84:ARG:NH2	2.39	0.43
1:R:257:MET:HE3	1:R:257:MET:HB3	1.74	0.42
3:J:97:GLU:OE1	4:M:92:ARG:NH1	2.52	0.42
4:M:30:ASN:O	4:M:34:LYS:HE3	2.19	0.42
8:V:316:ALA:O	8:V:319:LEU:HG	2.18	0.42
9:O:86:ILE:HB	9:O:90:ASN:OD1	2.18	0.42
10:3:88:LYS:O	10:3:92:GLN:HG2	2.19	0.42
10:6:130:GLY:O	10:6:134:ILE:HG12	2.19	0.42
10:8:57:ILE:HG22	10:8:135:LEU:HD23	1.99	0.42
12:C:128:SER:OG	12:C:131:ILE:HG13	2.19	0.42
12:B:64:ILE:HG22	12:B:65:GLN:O	2.18	0.42
14:Z:267:VAL:O	14:Z:271:GLU:HG2	2.19	0.42
1:R:780:THR:O	1:R:784:THR:N	2.51	0.42
2:O:190:PRO:O	2:O:194:HIS:N	2.52	0.42
3:J:115:LEU:HD12	3:J:115:LEU:HA	1.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:59:GLU:O	4:M:63:LEU:HG	2.20	0.42
4:K:99:LEU:O	4:K:103:VAL:HG23	2.19	0.42
6:T:123:PHE:HA	6:T:126:VAL:HG12	2.00	0.42
10:6:50:GLU:OE1	10:6:51:GLN:NE2	2.51	0.42
10:9:97:LEU:HD23	10:9:97:LEU:HA	1.83	0.42
11:Q:208:MET:HE1	11:Q:316:TYR:CG	2.54	0.42
12:A:56:ARG:O	12:A:57:LEU:HD12	2.19	0.42
14:Y:191:GLU:OE2	14:Y:191:GLU:N	2.47	0.42
16:N:15:ASP:OD1	16:N:16:THR:N	2.53	0.42
16:N:70:ILE:O	16:N:74:VAL:HG22	2.19	0.42
17:P:58:SER:C	17:P:60:GLU:N	2.74	0.42
1:R:576:ILE:O	1:R:580:THR:HG23	2.19	0.42
3:J:41:GLU:OE1	3:J:42:LYS:HG2	2.19	0.42
12:B:26:GLY:HA3	12:B:364:ARG:NH1	2.35	0.42
12:B:545:ILE:HD13	12:B:545:ILE:HA	1.81	0.42
13:F:475:GLU:O	13:F:479:ILE:HG13	2.20	0.42
14:Y:81:LEU:HD12	14:Y:81:LEU:HA	1.70	0.42
1:R:362:PRO:HG2	1:R:822:PHE:HD1	1.85	0.42
1:R:556:LEU:HD23	1:R:572:PHE:HE1	1.82	0.42
3:J:16:MET:HG2	4:M:10:GLN:HE21	1.84	0.42
4:L:55:PHE:HB3	4:L:56:LYS:NZ	2.35	0.42
3:H:91:ILE:HD13	3:H:91:ILE:HA	1.89	0.42
3:H:131:ARG:NH1	3:H:164:ASP:OD1	2.52	0.42
11:Q:252:LEU:HD23	11:Q:252:LEU:HA	1.78	0.42
12:C:350:SER:HB2	12:C:353:ARG:HG2	2.01	0.42
12:A:437:LYS:O	12:A:441:GLN:HG2	2.19	0.42
13:F:414:ASP:OD1	13:F:414:ASP:N	2.53	0.42
13:D:194:ALA:H	13:D:197:LEU:HD12	1.84	0.42
13:D:403:LYS:HE3	13:D:403:LYS:HB2	1.87	0.42
13:E:395:LEU:HD23	13:E:395:LEU:HA	1.84	0.42
14:X:143:ALA:HB1	14:X:149:ASN:ND2	2.34	0.42
15:G:94:ILE:HA	15:G:94:ILE:HD13	1.73	0.42
16:N:110:ARG:HD3	16:N:113:PHE:HE2	1.83	0.42
17:P:123:TRP:O	17:P:125:TYR:N	2.47	0.42
1:R:195:VAL:HG22	1:R:196:PHE:H	1.85	0.42
1:R:293:TRP:O	1:R:297:VAL:HG22	2.20	0.42
2:O:312:LEU:H	3:I:18:PHE:HZ	1.68	0.42
3:I:123:GLY:HA3	3:I:183:ILE:HD13	2.02	0.42
10:2:136:ILE:HD13	10:2:136:ILE:HA	1.82	0.42
10:3:95:ALA:HB2	10:3:152:LEU:HB2	2.02	0.42
10:4:131:MET:HE2	10:4:131:MET:HB3	1.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:9:47:MET:O	10:9:49:PRO:HD3	2.20	0.42
12:A:153:TYR:HH	12:A:203:PHE:HD2	1.64	0.42
12:A:612:PHE:O	12:A:616:GLU:HB2	2.19	0.42
12:B:201:GLU:HG2	12:B:202:LYS:N	2.33	0.42
13:E:137:LYS:HE2	13:E:137:LYS:HB3	1.82	0.42
14:Z:249:LEU:HD22	14:Z:259:LEU:HD12	2.01	0.42
14:Y:17:GLN:O	14:Y:21:GLN:HG2	2.18	0.42
16:N:26:GLY:HA2	16:N:35:ASN:ND2	2.26	0.42
17:P:103:GLU:O	17:P:104:ASN:C	2.62	0.42
1:R:521:ILE:O	1:R:524:ILE:HG12	2.20	0.42
3:J:14:HIS:O	3:J:19:ILE:HG23	2.20	0.42
3:J:194:ASN:HD22	3:J:194:ASN:HA	1.64	0.42
3:I:96:ASN:O	3:I:100:GLN:HG2	2.19	0.42
10:5:144:TYR:O	10:5:148:VAL:HG22	2.20	0.42
11:Q:42:LEU:HD11	11:Q:337:ALA:HB2	2.02	0.42
11:Q:67:VAL:HG11	11:Q:334:GLU:OE2	2.20	0.42
12:C:437:LYS:HD2	12:C:437:LYS:HA	1.69	0.42
15:G:146:VAL:HG23	16:N:63:ILE:HD11	2.01	0.42
1:R:740:ARG:HD3	1:R:801:HIS:HB3	2.00	0.42
3:H:141:PHE:HE1	3:H:169:GLN:HG2	1.83	0.42
10:6:41:ILE:HD11	10:6:56:ILE:HA	2.01	0.42
10:7:41:ILE:HD11	10:7:55:SER:O	2.19	0.42
10:7:80:LEU:HA	10:7:80:LEU:HD23	1.81	0.42
10:9:120:GLY:HA2	10:9:123:GLN:NE2	2.29	0.42
10:9:121:THR:OG1	10:9:127:LEU:HB3	2.19	0.42
12:C:507:ILE:O	12:C:511:VAL:HG23	2.20	0.42
12:A:317:ASN:ND2	13:D:336:GLU:HB3	2.34	0.42
13:F:169:MET:HE1	13:F:415:HIS:HE1	1.85	0.42
1:R:175:ILE:HG13	1:R:177:ARG:H	1.85	0.42
1:R:196:PHE:CE1	3:I:12:ILE:HG12	2.55	0.42
1:R:292:VAL:HA	1:R:295:ILE:HD12	2.01	0.42
1:R:547:HIS:HD2	1:R:738:TYR:OH	2.03	0.42
7:U:428:MET:HG2	9:0:48:MET:SD	2.60	0.42
10:5:150:LEU:HD23	10:5:150:LEU:HA	1.85	0.42
10:7:13:PHE:HB2	10:8:90:PHE:CE2	2.54	0.42
12:A:225:HIS:HA	12:A:226:PRO:HD3	1.93	0.42
13:E:227:PHE:CE2	13:E:294:LEU:HD12	2.52	0.42
14:Y:111:GLN:NE2	14:Y:169:THR:OG1	2.51	0.42
16:N:45:ILE:HG22	16:N:73:MET:SD	2.60	0.42
1:R:35:VAL:HG23	1:R:825:PHE:HB3	2.01	0.42
1:R:180:ILE:HD11	1:R:220:PHE:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:484:MET:SD	1:R:506:LEU:HD12	2.60	0.42
3:I:132:MET:O	3:I:165:VAL:HA	2.20	0.42
9:0:119:SER:O	9:0:119:SER:OG	2.34	0.42
10:9:9:GLU:CD	10:9:10:TYR:H	2.25	0.42
10:9:151:ILE:HD13	10:9:151:ILE:HA	1.85	0.42
11:Q:304:LEU:HD12	11:Q:304:LEU:HA	1.80	0.42
12:A:231:GLN:O	12:A:235:ASP:HB2	2.20	0.42
12:A:310:ALA:O	12:A:311:LEU:HD23	2.20	0.42
12:B:387:GLU:HG2	13:F:265:ASN:HB3	2.01	0.42
15:G:159:ASP:OD1	15:G:163:LYS:NZ	2.53	0.42
3:H:31:ASP:OD1	4:K:28:ARG:NH2	2.53	0.42
9:0:59:SER:OG	10:1:101:LEU:HD23	2.19	0.42
10:5:82:ASP:HA	10:6:87:TYR:CE1	2.55	0.42
11:Q:271:TYR:CD1	11:Q:271:TYR:N	2.86	0.42
12:C:478:LYS:HD2	12:C:478:LYS:HA	1.92	0.42
12:A:28:VAL:HG21	12:A:364:ARG:HE	1.85	0.42
12:B:139:LYS:HE3	12:B:139:LYS:HB3	1.84	0.42
12:B:270:ASP:OD1	12:B:270:ASP:N	2.53	0.42
12:B:467:LYS:HG2	12:B:468:HIS:CD2	2.55	0.42
13:F:149:ASP:OD1	13:F:150:PHE:N	2.53	0.42
13:D:192:PHE:HE1	13:D:354:LEU:HD22	1.85	0.42
14:Y:101:PHE:CE1	14:Y:161:MET:HB3	2.55	0.42
14:Y:175:ILE:HG13	14:Y:176:ASN:N	2.34	0.42
17:P:76:THR:O	17:P:79:ASN:N	2.52	0.42
1:R:236:ILE:O	1:R:240:PHE:HB2	2.19	0.41
1:R:804:ARG:NH2	1:R:809:GLU:OE2	2.53	0.41
4:M:53:LYS:HE2	4:M:53:LYS:HB3	1.89	0.41
4:K:29:LYS:HA	4:K:29:LYS:HD3	1.84	0.41
7:U:435:PHE:CE2	9:0:56:LEU:HD21	2.55	0.41
10:6:80:LEU:O	10:7:155:LYS:NZ	2.28	0.41
13:D:364:PRO:O	13:D:368:LEU:HG	2.20	0.41
13:E:222:TYR:HA	13:E:225:GLU:HG2	2.01	0.41
14:Z:234:MET:HB3	14:Z:235:PRO:HD3	2.01	0.41
16:N:14:GLU:OE2	16:N:15:ASP:N	2.53	0.41
3:I:117:ASP:OD2	3:I:150:LYS:NZ	2.43	0.41
7:U:261:ASN:HA	7:U:265:PRO:HA	2.01	0.41
10:4:46:VAL:HG23	10:4:47:MET:HG2	2.02	0.41
10:6:48:ARG:NH1	10:6:51:GLN:HE22	2.18	0.41
10:9:81:ASN:O	10:9:84:ILE:HG12	2.19	0.41
11:Q:308:ASN:HB2	11:Q:311:HIS:CE1	2.55	0.41
12:A:577:ILE:HD12	12:A:577:ILE:HA	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:B:295:THR:HB	12:B:302:VAL:HG13	2.01	0.41
13:E:92:SER:O	13:E:92:SER:OG	2.33	0.41
14:Z:245:LYS:HB3	14:Z:245:LYS:HE2	1.86	0.41
14:X:71:SER:O	14:X:73:LYS:NZ	2.53	0.41
14:Y:114:LYS:O	14:Y:117:GLN:NE2	2.35	0.41
15:G:88:ASN:OD1	15:G:89:LYS:N	2.53	0.41
1:R:193:GLY:O	3:I:11:GLN:NE2	2.52	0.41
1:R:483:PRO:O	1:R:486:THR:HG22	2.21	0.41
1:R:790:LEU:O	1:R:794:GLU:HB2	2.20	0.41
3:J:101:ARG:O	3:J:104:LYS:NZ	2.47	0.41
3:I:42:LYS:HB3	3:I:42:LYS:HE3	1.88	0.41
4:K:45:GLU:CD	4:K:48:ARG:HH22	2.28	0.41
10:5:44:MET:CG	10:5:119:ARG:HG2	2.50	0.41
10:5:79:SER:O	10:5:79:SER:OG	2.32	0.41
10:9:14:PHE:HB2	10:9:89:SER:OG	2.21	0.41
12:C:389:ALA:HB2	12:C:406:ILE:HG13	2.01	0.41
12:A:473:VAL:HG13	12:A:476:ARG:NH2	2.34	0.41
13:E:450:LEU:O	13:E:453:GLU:HB3	2.21	0.41
13:E:482:GLN:HA	13:E:485:ARG:CB	2.50	0.41
13:E:504:TYR:N	13:E:505:PRO:HD2	2.36	0.41
14:X:116:LYS:HB3	14:X:116:LYS:HE2	1.71	0.41
14:Y:130:LEU:HA	14:Y:130:LEU:HD13	1.77	0.41
16:N:44:THR:OG1	16:N:46:ASN:OD1	2.37	0.41
17:P:301:THR:C	17:P:303:GLN:H	2.27	0.41
1:R:35:VAL:O	1:R:825:PHE:N	2.33	0.41
1:R:72:ILE:HD13	1:R:287:ALA:HB2	2.02	0.41
1:R:517:GLY:N	5:S:56:ILE:HD11	2.35	0.41
2:O:109:MET:C	2:O:111:LYS:H	2.28	0.41
3:J:68:LYS:HE3	3:J:68:LYS:HB2	1.86	0.41
3:I:40:ILE:O	3:I:44:ARG:HG3	2.20	0.41
4:L:31:ARG:HA	4:L:34:LYS:HE2	2.03	0.41
3:H:16:MET:O	3:H:19:ILE:HB	2.20	0.41
7:U:434:LEU:HD13	7:U:434:LEU:HA	1.85	0.41
9:O:42:THR:HA	9:O:131:TYR:CE1	2.55	0.41
10:2:132:ILE:HD13	10:2:132:ILE:HA	1.73	0.41
10:5:13:PHE:HB2	10:6:90:PHE:CE2	2.56	0.41
10:8:41:ILE:HD11	10:8:55:SER:O	2.20	0.41
11:Q:104:TYR:CE1	11:Q:132:LEU:HD12	2.56	0.41
12:A:34:MET:O	12:A:62:ALA:HB2	2.21	0.41
13:D:170:ILE:HG13	13:D:349:THR:HG21	2.02	0.41
13:E:327:MET:HE1	13:E:365:ILE:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Y:133:LEU:HB2	14:Y:179:PHE:HZ	1.85	0.41
1:R:36:GLN:H	1:R:323:VAL:HG23	1.84	0.41
1:R:91:PRO:HB2	1:R:93:ASP:OD1	2.19	0.41
1:R:111:ILE:HD13	1:R:111:ILE:HA	1.84	0.41
1:R:423:MET:HE3	1:R:423:MET:HB2	1.84	0.41
1:R:770:ALA:O	1:R:774:VAL:HG22	2.21	0.41
3:J:24:ASN:HB2	4:M:21:LYS:NZ	2.36	0.41
3:J:35:GLU:CD	4:M:32:ARG:HH11	2.29	0.41
3:H:190:ILE:HG12	13:D:47:TYR:HD2	1.85	0.41
4:K:41:GLN:O	4:K:45:GLU:HG2	2.20	0.41
9:0:70:TYR:HA	10:1:113:VAL:CG1	2.50	0.41
10:4:23:MET:HG2	10:5:148:VAL:HG21	2.02	0.41
10:5:57:ILE:HB	10:5:58:PRO:HD3	2.02	0.41
10:5:72:VAL:HG21	10:5:99:VAL:CG1	2.49	0.41
10:9:150:LEU:HD12	10:9:150:LEU:HA	1.89	0.41
11:Q:33:TYR:O	11:Q:36:LEU:N	2.53	0.41
12:A:27:PRO:HG2	12:A:364:ARG:HG3	2.02	0.41
12:B:39:MET:HE3	12:B:39:MET:HB2	1.75	0.41
12:B:258:VAL:HG11	19:B:701:ADP:C5	2.56	0.41
13:E:182:SER:HB2	13:E:402:MET:HG3	2.02	0.41
14:Z:16:GLU:HG2	14:Z:17:GLN:N	2.34	0.41
14:Z:37:ASP:OD2	14:Z:42:LEU:N	2.53	0.41
1:R:180:ILE:HG22	1:R:181:PRO:HD3	2.01	0.41
1:R:400:PRO:HA	1:R:453:MET:HG3	2.01	0.41
1:R:454:GLY:O	1:R:458:MET:HG3	2.20	0.41
3:I:157:ILE:HD13	3:I:157:ILE:HA	1.86	0.41
7:U:274:PHE:H	7:U:286:THR:HG1	1.61	0.41
9:0:16:TRP:HA	9:0:16:TRP:CE3	2.56	0.41
10:3:91:LEU:HA	10:3:91:LEU:HD23	1.81	0.41
11:Q:143:ILE:HD13	11:Q:150:LEU:HB2	2.02	0.41
11:Q:277:LEU:HD23	11:Q:277:LEU:HA	1.88	0.41
12:C:357:ALA:O	12:C:361:ILE:HG12	2.20	0.41
12:A:21:VAL:HG21	12:A:73:VAL:HG12	2.03	0.41
12:A:116:ILE:HD12	13:D:341:VAL:HG11	2.03	0.41
12:A:450:TRP:CD1	12:A:450:TRP:C	2.99	0.41
12:B:203:PHE:HZ	12:B:207:GLN:HB3	1.85	0.41
12:B:249:PRO:HA	12:B:410:VAL:O	2.21	0.41
13:D:421:GLN:NE2	13:D:425:CYS:SG	2.86	0.41
13:E:378:TYR:HD2	13:E:393:ASN:HB3	1.86	0.41
13:E:421:GLN:NE2	13:E:494:ARG:HG3	2.33	0.41
14:Z:217:LEU:HD21	14:Z:221:ASP:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:X:268:LYS:HA	14:X:271:GLU:HG2	2.02	0.41
3:H:156:LYS:HE3	3:H:156:LYS:HB2	1.76	0.41
6:T:98:TYR:O	6:T:102:GLU:HG3	2.19	0.41
7:U:303:ASN:HB2	7:U:306:PHE:HB3	2.03	0.41
9:O:164:LEU:HD23	9:O:164:LEU:HA	1.78	0.41
10:3:101:LEU:HD23	10:3:101:LEU:HA	1.85	0.41
10:5:33:GLY:O	10:5:37:SER:OG	2.32	0.41
10:6:124:GLN:OE1	10:6:126:ARG:N	2.48	0.41
10:8:99:VAL:HB	10:8:149:ALA:HB2	2.03	0.41
10:9:72:VAL:HG11	10:9:99:VAL:HG11	2.02	0.41
10:9:112:ILE:HD11	11:Q:3:PHE:HZ	1.85	0.41
13:F:100:GLU:O	13:F:267:PRO:HB3	2.21	0.41
14:Z:256:THR:OG1	14:Z:258:THR:OG1	2.32	0.41
1:R:244:LEU:HD12	1:R:244:LEU:HA	1.87	0.41
3:J:2:ALA:HB1	3:J:5:ASP:HB3	2.02	0.41
3:J:122:GLN:NE2	13:F:43:PRO:HD3	2.35	0.41
3:H:75:LEU:HD23	3:H:75:LEU:HA	1.89	0.41
5:S:39:THR:O	5:S:43:THR:HG23	2.21	0.41
8:V:313:ILE:HD11	10:3:93:LEU:HD11	2.02	0.41
10:4:41:ILE:HD11	10:4:55:SER:O	2.21	0.41
12:A:18:PHE:CD2	12:A:78:PRO:HA	2.56	0.41
12:A:39:MET:HB3	12:A:40:TYR:HD2	1.86	0.41
12:A:493:VAL:HG22	12:A:501:LEU:HD11	2.03	0.41
13:F:164:ILE:HD11	13:F:342:GLU:HA	2.03	0.41
13:D:192:PHE:CE1	13:D:354:LEU:HD22	2.55	0.41
13:E:363:HIS:HB3	13:E:366:PRO:HD2	2.03	0.41
15:G:213:LYS:HE2	15:G:213:LYS:HB3	1.76	0.41
16:N:66:ILE:O	16:N:91:ILE:HD12	2.21	0.41
1:R:18:GLN:OE1	1:R:21:ALA:N	2.43	0.41
1:R:46:VAL:O	1:R:52:VAL:HB	2.20	0.41
1:R:100:ASN:O	1:R:104:ILE:HG12	2.20	0.41
1:R:250:THR:HG23	1:R:251:PRO:HD3	2.03	0.41
1:R:583:PHE:CE1	1:R:735:THR:HG21	2.56	0.41
1:R:791:LEU:HA	1:R:791:LEU:HD23	1.84	0.41
1:R:830:ILE:H	1:R:830:ILE:HG13	1.68	0.41
3:H:16:MET:N	3:H:16:MET:SD	2.93	0.41
3:H:90:LEU:HD23	3:H:90:LEU:HA	1.96	0.41
7:U:283:GLU:HG2	7:U:316:LEU:HD12	2.03	0.41
7:U:286:THR:N	7:U:287:PRO:HD2	2.36	0.41
8:V:297:TYR:HB3	8:V:299:TYR:CE2	2.55	0.41
10:1:41:ILE:HD11	10:1:55:SER:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:2:10:TYR:HA	10:3:90:PHE:HE2	1.86	0.41
10:6:9:GLU:CD	10:6:10:TYR:H	2.27	0.41
10:6:99:VAL:HB	10:6:149:ALA:HB2	2.03	0.41
11:Q:1:MET:HG3	11:Q:2:SER:N	2.36	0.41
11:Q:1:MET:C	11:Q:3:PHE:H	2.28	0.41
12:C:540:MET:HE2	12:C:540:MET:HB3	1.82	0.41
12:A:153:TYR:OH	12:A:203:PHE:HD2	2.03	0.41
12:B:27:PRO:HD2	12:B:364:ARG:HH11	1.86	0.41
12:B:138:CYS:O	12:B:139:LYS:HB3	2.21	0.41
13:F:307:LEU:HD12	13:F:307:LEU:HA	1.88	0.41
13:E:482:GLN:HA	13:E:485:ARG:HB3	2.03	0.41
14:Z:83:ARG:O	14:Z:87:ILE:HG13	2.21	0.41
14:Z:130:LEU:HA	14:Z:130:LEU:HD23	1.88	0.41
16:N:106:LEU:O	16:N:110:ARG:NH2	2.54	0.41
1:R:64:LYS:HB2	1:R:101:PHE:HE2	1.86	0.41
3:J:34:ALA:HB2	4:M:29:LYS:HE2	2.03	0.41
4:L:76:GLU:O	4:L:79:GLU:HG2	2.20	0.41
4:K:37:LYS:HE3	4:K:37:LYS:HB3	1.87	0.41
4:K:86:THR:O	4:K:90:GLN:HG2	2.20	0.41
10:2:77:ALA:O	10:3:155:LYS:HE2	2.21	0.41
10:4:101:LEU:HD23	10:4:101:LEU:HA	1.94	0.41
10:7:113:VAL:HG21	10:7:134:ILE:CG2	2.51	0.41
11:Q:37:VAL:HG23	11:Q:38:GLN:HG2	2.03	0.41
11:Q:105:MET:HE3	11:Q:105:MET:HB2	1.88	0.41
12:C:484:GLN:HG3	13:D:385:ASN:HB3	2.02	0.41
12:A:364:ARG:NE	12:A:364:ARG:HA	2.36	0.41
12:B:387:GLU:O	12:B:387:GLU:HG3	2.20	0.41
13:E:49:THR:OG1	13:E:61:ASP:O	2.38	0.41
14:Z:63:GLU:O	14:Z:67:GLU:HG2	2.21	0.41
15:G:14:MET:HE2	15:G:14:MET:HB3	1.99	0.41
1:R:801:HIS:HA	1:R:804:ARG:HB3	2.03	0.40
4:M:105:ASP:OD1	4:M:107:ARG:NH1	2.55	0.40
4:L:31:ARG:HA	4:L:31:ARG:HD2	1.85	0.40
3:H:26:LYS:HG3	4:K:17:ARG:NH1	2.34	0.40
5:S:78:TYR:CD1	6:T:94:PRO:HD3	2.55	0.40
7:U:453:MET:SD	7:U:453:MET:N	2.92	0.40
10:1:13:PHE:HB2	10:2:90:PHE:CE2	2.57	0.40
10:5:46:VAL:O	10:5:47:MET:HE2	2.21	0.40
11:Q:49:LEU:O	11:Q:52:THR:HG23	2.21	0.40
12:A:139:LYS:HG2	12:A:139:LYS:O	2.21	0.40
15:G:30:ARG:NH1	15:G:30:ARG:HB3	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:175:ILE:HD12	1:R:241:ARG:NH1	2.36	0.40
1:R:401:PHE:CE2	5:S:47:CYS:HB2	2.56	0.40
4:M:32:ARG:CZ	4:M:32:ARG:HA	2.50	0.40
3:I:72:MET:HB2	3:I:72:MET:HE2	1.84	0.40
5:S:38:ILE:HG13	5:S:39:THR:H	1.86	0.40
10:6:12:SER:O	10:6:16:VAL:HG23	2.21	0.40
10:6:24:VAL:CG1	10:7:98:SER:HA	2.52	0.40
10:6:60:VAL:HG12	10:7:137:PHE:CZ	2.56	0.40
11:Q:16:LEU:HD23	11:Q:16:LEU:HA	1.93	0.40
12:C:424:ALA:O	12:C:428:ILE:HD12	2.21	0.40
12:A:349:ASP:O	12:A:350:SER:OG	2.35	0.40
13:F:485:ARG:C	13:F:487:PHE:N	2.78	0.40
13:D:75:THR:O	13:D:75:THR:OG1	2.39	0.40
13:D:493:LYS:HE2	13:D:493:LYS:HB2	1.82	0.40
13:E:128:LEU:HD22	13:E:256:ASN:O	2.21	0.40
14:Y:83:ARG:O	14:Y:87:ILE:HG12	2.21	0.40
14:Y:211:SER:HB2	14:Y:256:THR:HA	2.03	0.40
14:Y:212:PRO:O	14:Y:216:ILE:HD13	2.20	0.40
9:0:188:LEU:HD23	9:0:188:LEU:HA	1.61	0.40
10:2:72:VAL:HG11	10:2:99:VAL:CG1	2.43	0.40
10:3:80:LEU:HD23	10:3:80:LEU:HA	1.88	0.40
10:4:44:MET:HB2	10:4:122:ALA:HB2	2.04	0.40
10:7:42:ALA:HA	10:8:127:LEU:HD21	2.02	0.40
12:A:127:LEU:O	12:A:129:ARG:NH1	2.54	0.40
12:B:193:GLU:HG3	12:B:202:LYS:HG2	2.02	0.40
12:B:222:PRO:O	12:B:391:ARG:NH2	2.55	0.40
13:F:321:ARG:O	13:F:321:ARG:HG3	2.21	0.40
13:D:441:GLU:H	13:D:441:GLU:HG3	1.76	0.40
3:H:37:GLU:O	3:H:40:ILE:HG22	2.21	0.40
4:K:45:GLU:HA	4:K:48:ARG:HH22	1.84	0.40
9:0:100:VAL:HG13	9:0:148:ASN:HB3	2.03	0.40
10:3:72:VAL:HG11	10:3:99:VAL:CG1	2.48	0.40
10:7:86:LEU:HA	10:7:89:SER:OG	2.21	0.40
12:A:27:PRO:HD3	13:D:326:TYR:CB	2.51	0.40
12:A:362:SER:O	12:A:365:LEU:N	2.49	0.40
13:E:452:LEU:O	13:E:456:GLN:HG3	2.21	0.40
14:Z:188:MET:HE3	14:Z:188:MET:HB2	2.00	0.40
15:G:134:LEU:HA	15:G:134:LEU:HD12	1.77	0.40
17:P:351:SER:O	17:P:354:GLU:N	2.55	0.40
1:R:74:LYS:HE3	1:R:74:LYS:HB3	1.62	0.40
1:R:128:LEU:HD23	1:R:128:LEU:HA	1.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:34:VAL:O	2:O:321:LEU:HA	2.21	0.40
3:J:50:ARG:HA	3:J:53:ILE:HG12	2.03	0.40
10:6:47:MET:HE2	10:6:47:MET:HB3	1.90	0.40
10:7:84:ILE:HG21	10:7:89:SER:HB3	2.04	0.40
10:8:47:MET:HE2	10:8:47:MET:HB3	1.90	0.40
12:A:29:VAL:CB	12:A:66:VAL:HB	2.48	0.40
13:E:380:ASP:OD1	13:E:381:ARG:N	2.55	0.40
15:G:101:VAL:HG13	15:G:101:VAL:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	R	747/837 (89%)	701 (94%)	46 (6%)	0	100	100
2	O	373/382 (98%)	348 (93%)	25 (7%)	0	100	100
3	H	223/226 (99%)	217 (97%)	6 (3%)	0	100	100
3	I	223/226 (99%)	208 (93%)	15 (7%)	0	100	100
3	J	223/226 (99%)	212 (95%)	10 (4%)	1 (0%)	30	59
4	K	112/118 (95%)	110 (98%)	2 (2%)	0	100	100
4	L	112/118 (95%)	107 (96%)	5 (4%)	0	100	100
4	M	112/118 (95%)	110 (98%)	2 (2%)	0	100	100
5	S	75/81 (93%)	73 (97%)	2 (3%)	0	100	100
6	T	83/137 (61%)	75 (90%)	8 (10%)	0	100	100
7	U	202/470 (43%)	163 (81%)	39 (19%)	0	100	100
8	V	47/350 (13%)	42 (89%)	5 (11%)	0	100	100
9	0	202/205 (98%)	183 (91%)	19 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	1	148/155 (96%)	138 (93%)	10 (7%)	0	100	100
10	2	148/155 (96%)	138 (93%)	10 (7%)	0	100	100
10	3	148/155 (96%)	137 (93%)	11 (7%)	0	100	100
10	4	148/155 (96%)	140 (95%)	8 (5%)	0	100	100
10	5	148/155 (96%)	137 (93%)	11 (7%)	0	100	100
10	6	148/155 (96%)	142 (96%)	6 (4%)	0	100	100
10	7	148/155 (96%)	142 (96%)	6 (4%)	0	100	100
10	8	148/155 (96%)	143 (97%)	5 (3%)	0	100	100
10	9	148/155 (96%)	139 (94%)	9 (6%)	0	100	100
11	Q	349/351 (99%)	312 (89%)	37 (11%)	0	100	100
12	A	598/617 (97%)	537 (90%)	61 (10%)	0	100	100
12	B	598/617 (97%)	542 (91%)	56 (9%)	0	100	100
12	C	598/617 (97%)	542 (91%)	56 (9%)	0	100	100
13	D	466/511 (91%)	431 (92%)	35 (8%)	0	100	100
13	E	466/511 (91%)	433 (93%)	33 (7%)	0	100	100
13	F	466/511 (91%)	432 (93%)	34 (7%)	0	100	100
14	X	265/573 (46%)	250 (94%)	15 (6%)	0	100	100
14	Y	260/573 (45%)	252 (97%)	8 (3%)	0	100	100
14	Z	258/573 (45%)	248 (96%)	10 (4%)	0	100	100
15	G	211/247 (85%)	205 (97%)	6 (3%)	0	100	100
16	N	108/119 (91%)	101 (94%)	7 (6%)	0	100	100
17	P	423/483 (88%)	328 (78%)	93 (22%)	2 (0%)	24	54
All	All	9132/11192 (82%)	8418 (92%)	711 (8%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	J	16	MET
17	P	104	ASN
17	P	374	LYS

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	R	674/746 (90%)	631 (94%)	43 (6%)	16	42
3	H	198/199 (100%)	189 (96%)	9 (4%)	24	51
3	I	198/199 (100%)	181 (91%)	17 (9%)	10	33
3	J	198/199 (100%)	179 (90%)	19 (10%)	8	28
4	K	99/101 (98%)	93 (94%)	6 (6%)	17	43
4	L	99/101 (98%)	92 (93%)	7 (7%)	13	39
4	M	99/101 (98%)	92 (93%)	7 (7%)	13	39
5	S	69/72 (96%)	65 (94%)	4 (6%)	18	45
6	T	71/116 (61%)	67 (94%)	4 (6%)	19	46
7	U	182/397 (46%)	158 (87%)	24 (13%)	4	16
8	V	44/308 (14%)	39 (89%)	5 (11%)	5	21
9	0	154/155 (99%)	134 (87%)	20 (13%)	4	16
10	1	107/112 (96%)	92 (86%)	15 (14%)	3	13
10	2	107/112 (96%)	87 (81%)	20 (19%)	1	6
10	3	107/112 (96%)	92 (86%)	15 (14%)	3	13
10	4	107/112 (96%)	86 (80%)	21 (20%)	1	5
10	5	107/112 (96%)	94 (88%)	13 (12%)	5	19
10	6	107/112 (96%)	93 (87%)	14 (13%)	4	16
10	7	107/112 (96%)	95 (89%)	12 (11%)	6	21
10	8	107/112 (96%)	89 (83%)	18 (17%)	2	9
10	9	107/112 (96%)	96 (90%)	11 (10%)	7	24
11	Q	306/306 (100%)	287 (94%)	19 (6%)	16	43
12	A	508/525 (97%)	450 (89%)	58 (11%)	5	21
12	B	508/525 (97%)	467 (92%)	41 (8%)	11	36
12	C	508/525 (97%)	470 (92%)	38 (8%)	12	38
13	D	401/430 (93%)	372 (93%)	29 (7%)	13	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	E	401/430 (93%)	366 (91%)	35 (9%)	9	32
13	F	401/430 (93%)	362 (90%)	39 (10%)	8	28
14	X	239/519 (46%)	223 (93%)	16 (7%)	15	41
14	Y	238/519 (46%)	225 (94%)	13 (6%)	19	46
14	Z	237/519 (46%)	224 (94%)	13 (6%)	19	46
15	G	184/212 (87%)	169 (92%)	15 (8%)	10	35
16	N	94/100 (94%)	89 (95%)	5 (5%)	20	47
All	All	7073/8742 (81%)	6448 (91%)	625 (9%)	11	31

All (625) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	R	47	PHE
1	R	52	VAL
1	R	74	LYS
1	R	80	MET
1	R	93	ASP
1	R	96	ASP
1	R	100	ASN
1	R	175	ILE
1	R	190	VAL
1	R	192	ARG
1	R	250	THR
1	R	283	LEU
1	R	300	MET
1	R	308	ASN
1	R	312	ILE
1	R	323	VAL
1	R	325	CYS
1	R	363	THR
1	R	368	ASN
1	R	371	THR
1	R	385	THR
1	R	396	ILE
1	R	437	ASN
1	R	471	SER
1	R	490	THR
1	R	492	GLU
1	R	503	ASN
1	R	535	PHE

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Mol	Chain	Res	Type
1	R	549	LEU
1	R	552	VAL
1	R	568	ILE
1	R	573	ILE
1	R	581	SER
1	R	582	LEU
1	R	598	ASP
1	R	607	SER
1	R	613	ILE
1	R	644	LEU
1	R	726	GLU
1	R	744	LEU
1	R	746	LEU
1	R	796	LEU
1	R	830	ILE
3	J	45	LEU
3	J	51	LEU
3	J	52	LYS
3	J	56	TYR
3	J	83	VAL
3	J	104	LYS
3	J	106	VAL
3	J	109	THR
3	J	139	GLN
3	J	163	VAL
3	J	166	GLN
3	J	171	SER
3	J	177	ILE
3	J	181	VAL
3	J	193	SER
3	J	194	ASN
3	J	201	ASP
3	J	202	LEU
3	J	211	VAL
4	M	8	ILE
4	M	47	TYR
4	M	83	ILE
4	M	100	LEU
4	M	107	ARG
4	M	110	ILE
4	M	116	ILE
3	I	37	GLU

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Mol	Chain	Res	Type
3	I	38	PHE
3	I	70	ILE
3	I	76	MET
3	I	78	GLN
3	I	104	LYS
3	I	108	ASP
3	I	129	GLU
3	I	133	ILE
3	I	134	VAL
3	I	139	GLN
3	I	157	ILE
3	I	169	GLN
3	I	170	GLU
3	I	177	ILE
3	I	190	ILE
3	I	208	MET
4	L	29	LYS
4	L	44	ILE
4	L	54	GLU
4	L	56	LYS
4	L	80	LYS
4	L	92	ARG
4	L	116	ILE
3	H	3	LEU
3	H	14	HIS
3	H	16	MET
3	H	37	GLU
3	H	69	LYS
3	H	71	GLN
3	H	177	ILE
3	H	203	ILE
3	H	207	MET
4	K	50	GLN
4	K	85	GLN
4	K	92	ARG
4	K	100	LEU
4	K	112	GLU
4	K	116	ILE
5	S	11	ILE
5	S	36	VAL
5	S	39	THR
5	S	68	LEU

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Mol	Chain	Res	Type
6	T	79	LEU
6	T	96	ASN
6	T	116	LEU
6	T	128	LEU
7	U	258	VAL
7	U	266	ARG
7	U	297	LEU
7	U	310	SER
7	U	311	LEU
7	U	320	THR
7	U	326	ILE
7	U	334	VAL
7	U	340	PHE
7	U	341	THR
7	U	347	VAL
7	U	365	SER
7	U	374	VAL
7	U	385	VAL
7	U	398	GLN
7	U	407	VAL
7	U	423	SER
7	U	427	TRP
7	U	430	LEU
7	U	434	LEU
7	U	447	ILE
7	U	453	MET
7	U	455	ARG
7	U	458	ASP
8	V	306	VAL
8	V	309	MET
8	V	313	ILE
8	V	315	ILE
8	V	338	ILE
9	0	2	THR
9	0	7	LEU
9	0	22	VAL
9	0	26	TYR
9	0	28	ILE
9	0	45	SER
9	0	52	LEU
9	0	54	ILE
9	0	69	ILE

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Mol	Chain	Res	Type
9	0	70	TYR
9	0	72	THR
9	0	122	ASP
9	0	144	VAL
9	0	149	LEU
9	0	151	CYS
9	0	154	CYS
9	0	158	VAL
9	0	160	SER
9	0	186	ILE
9	0	198	THR
10	1	39	THR
10	1	45	SER
10	1	56	ILE
10	1	74	VAL
10	1	93	LEU
10	1	98	SER
10	1	113	VAL
10	1	115	ASP
10	1	121	THR
10	1	127	LEU
10	1	136	ILE
10	1	140	VAL
10	1	146	LEU
10	1	148	VAL
10	1	151	ILE
10	2	20	SER
10	2	24	VAL
10	2	28	LEU
10	2	44	MET
10	2	45	SER
10	2	56	ILE
10	2	57	ILE
10	2	61	MET
10	2	64	ILE
10	2	67	ILE
10	2	71	VAL
10	2	92	GLN
10	2	102	SER
10	2	118	VAL
10	2	121	THR
10	2	124	GLN

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Mol	Chain	Res	Type
10	2	129	VAL
10	2	132	ILE
10	2	140	VAL
10	2	150	LEU
10	3	9	GLU
10	3	44	MET
10	3	52	ILE
10	3	56	ILE
10	3	64	ILE
10	3	78	ASN
10	3	84	ILE
10	3	93	LEU
10	3	102	SER
10	3	110	ILE
10	3	121	THR
10	3	132	ILE
10	3	139	GLU
10	3	140	VAL
10	3	147	ILE
10	4	41	ILE
10	4	44	MET
10	4	55	SER
10	4	56	ILE
10	4	67	ILE
10	4	72	VAL
10	4	75	LEU
10	4	80	LEU
10	4	93	LEU
10	4	99	VAL
10	4	104	LEU
10	4	113	VAL
10	4	118	VAL
10	4	121	THR
10	4	123	GLN
10	4	129	VAL
10	4	132	ILE
10	4	133	LEU
10	4	140	VAL
10	4	151	ILE
10	4	154	THR
10	5	28	LEU
10	5	37	SER

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Mol	Chain	Res	Type
10	5	55	SER
10	5	56	ILE
10	5	93	LEU
10	5	112	ILE
10	5	115	ASP
10	5	121	THR
10	5	129	VAL
10	5	132	ILE
10	5	133	LEU
10	5	140	VAL
10	5	146	LEU
10	6	9	GLU
10	6	26	SER
10	6	37	SER
10	6	39	THR
10	6	41	ILE
10	6	46	VAL
10	6	56	ILE
10	6	72	VAL
10	6	86	LEU
10	6	92	GLN
10	6	112	ILE
10	6	121	THR
10	6	140	VAL
10	6	141	LEU
10	7	37	SER
10	7	44	MET
10	7	46	VAL
10	7	74	VAL
10	7	84	ILE
10	7	93	LEU
10	7	102	SER
10	7	115	ASP
10	7	121	THR
10	7	132	ILE
10	7	139	GLU
10	7	150	LEU
10	8	36	LYS
10	8	41	ILE
10	8	44	MET
10	8	46	VAL
10	8	60	VAL

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Mol	Chain	Res	Type
10	8	67	ILE
10	8	74	VAL
10	8	93	LEU
10	8	98	SER
10	8	112	ILE
10	8	115	ASP
10	8	118	VAL
10	8	121	THR
10	8	132	ILE
10	8	135	LEU
10	8	140	VAL
10	8	153	SER
10	8	154	THR
10	9	9	GLU
10	9	56	ILE
10	9	60	VAL
10	9	67	ILE
10	9	72	VAL
10	9	79	SER
10	9	82	ASP
10	9	99	VAL
10	9	132	ILE
10	9	140	VAL
10	9	150	LEU
11	Q	6	GLU
11	Q	36	LEU
11	Q	52	THR
11	Q	66	THR
11	Q	72	ASP
11	Q	78	MET
11	Q	110	ILE
11	Q	111	LEU
11	Q	116	THR
11	Q	132	LEU
11	Q	155	LEU
11	Q	166	ASP
11	Q	169	SER
11	Q	197	CYS
11	Q	199	LEU
11	Q	200	LEU
11	Q	228	PHE
11	Q	230	THR

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Mol	Chain	Res	Type
11	Q	299	VAL
12	C	18	PHE
12	C	24	VAL
12	C	75	VAL
12	C	111	SER
12	C	118	ILE
12	C	134	ASP
12	C	148	THR
12	C	175	THR
12	C	177	THR
12	C	191	VAL
12	C	196	PHE
12	C	201	GLU
12	C	208	VAL
12	C	229	THR
12	C	246	THR
12	C	248	ILE
12	C	273	ILE
12	C	283	GLU
12	C	284	MET
12	C	298	VAL
12	C	308	ARG
12	C	309	THR
12	C	320	VAL
12	C	362	SER
12	C	405	SER
12	C	419	ASP
12	C	439	LEU
12	C	447	SER
12	C	453	SER
12	C	470	THR
12	C	495	LEU
12	C	532	CYS
12	C	565	ILE
12	C	569	ILE
12	C	572	GLU
12	C	577	ILE
12	C	612	PHE
12	C	615	LEU
12	A	24	VAL
12	A	28	VAL
12	A	41	GLU

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Mol	Chain	Res	Type
12	A	50	LEU
12	A	57	LEU
12	A	74	SER
12	A	75	VAL
12	A	79	VAL
12	A	80	LEU
12	A	89	GLU
12	A	98	ILE
12	A	110	SER
12	A	115	SER
12	A	130	ASP
12	A	141	LEU
12	A	161	LEU
12	A	165	LYS
12	A	175	THR
12	A	208	VAL
12	A	217	VAL
12	A	218	THR
12	A	234	LEU
12	A	246	THR
12	A	258	VAL
12	A	262	SER
12	A	291	PHE
12	A	294	LEU
12	A	302	VAL
12	A	303	GLU
12	A	309	THR
12	A	316	SER
12	A	327	ILE
12	A	347	MET
12	A	351	THR
12	A	358	LEU
12	A	361	ILE
12	A	362	SER
12	A	377	TYR
12	A	395	LEU
12	A	405	SER
12	A	410	VAL
12	A	416	ASP
12	A	438	LYS
12	A	473	VAL
12	A	492	ILE

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Mol	Chain	Res	Type
12	A	503	GLU
12	A	508	THR
12	A	515	ILE
12	A	555	VAL
12	A	557	THR
12	A	565	ILE
12	A	570	ILE
12	A	577	ILE
12	A	581	LEU
12	A	585	LYS
12	A	587	LYS
12	A	594	GLU
12	A	616	GLU
12	B	24	VAL
12	B	41	GLU
12	B	48	SER
12	B	51	VAL
12	B	57	LEU
12	B	71	SER
12	B	75	VAL
12	B	98	ILE
12	B	110	SER
12	B	142	ARG
12	B	155	ILE
12	B	175	THR
12	B	195	GLU
12	B	196	PHE
12	B	197	GLU
12	B	201	GLU
12	B	217	VAL
12	B	218	THR
12	B	246	THR
12	B	248	ILE
12	B	263	LEU
12	B	288	LEU
12	B	302	VAL
12	B	308	ARG
12	B	309	THR
12	B	326	SER
12	B	362	SER
12	B	403	SER
12	B	411	SER

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Mol	Chain	Res	Type
12	B	419	ASP
12	B	441	GLN
12	B	471	GLU
12	B	487	GLU
12	B	492	ILE
12	B	495	LEU
12	B	508	THR
12	B	555	VAL
12	B	557	THR
12	B	592	ASP
12	B	599	SER
12	B	614	SER
13	F	49	THR
13	F	59	ILE
13	F	72	VAL
13	F	75	THR
13	F	80	THR
13	F	82	ARG
13	F	88	GLU
13	F	90	SER
13	F	97	GLN
13	F	103	SER
13	F	145	VAL
13	F	161	GLN
13	F	172	THR
13	F	175	SER
13	F	177	ILE
13	F	182	SER
13	F	200	ASN
13	F	207	CYS
13	F	224	GLU
13	F	229	ILE
13	F	234	MET
13	F	245	LYS
13	F	256	ASN
13	F	259	LEU
13	F	268	THR
13	F	274	THR
13	F	299	ASP
13	F	311	SER
13	F	317	VAL
13	F	340	ARG

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Mol	Chain	Res	Type
13	F	359	ASP
13	F	403	LYS
13	F	404	SER
13	F	406	ILE
13	F	432	VAL
13	F	436	LYS
13	F	444	LEU
13	F	492	LEU
13	F	499	THR
13	D	40	LEU
13	D	51	SER
13	D	59	ILE
13	D	60	LEU
13	D	72	VAL
13	D	75	THR
13	D	111	SER
13	D	144	VAL
13	D	145	VAL
13	D	164	ILE
13	D	172	THR
13	D	175	SER
13	D	213	VAL
13	D	215	LYS
13	D	246	SER
13	D	257	VAL
13	D	272	ILE
13	D	290	GLU
13	D	294	LEU
13	D	311	SER
13	D	317	VAL
13	D	333	THR
13	D	334	ILE
13	D	349	THR
13	D	362	THR
13	D	371	TYR
13	D	445	THR
13	D	472	THR
13	D	500	LEU
13	E	46	THR
13	E	49	THR
13	E	51	SER
13	E	59	ILE

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Mol	Chain	Res	Type
13	E	72	VAL
13	E	80	THR
13	E	103	SER
13	E	144	VAL
13	E	145	VAL
13	E	170	ILE
13	E	172	THR
13	E	177	ILE
13	E	212	LEU
13	E	218	ASP
13	E	229	ILE
13	E	246	SER
13	E	259	LEU
13	E	268	THR
13	E	270	GLU
13	E	272	ILE
13	E	299	ASP
13	E	311	SER
13	E	316	GLU
13	E	329	THR
13	E	330	ASP
13	E	340	ARG
13	E	359	ASP
13	E	397	SER
13	E	411	THR
13	E	445	THR
13	E	483	LEU
13	E	492	LEU
13	E	495	ILE
13	E	499	THR
13	E	506	ARG
14	Z	14	THR
14	Z	15	SER
14	Z	35	THR
14	Z	59	ASN
14	Z	60	TYR
14	Z	99	SER
14	Z	125	ASP
14	Z	146	THR
14	Z	181	LEU
14	Z	216	ILE
14	Z	241	VAL

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Mol	Chain	Res	Type
14	Z	260	LEU
14	Z	273	LEU
14	X	17	GLN
14	X	35	THR
14	X	36	ILE
14	X	52	VAL
14	X	74	CYS
14	X	119	VAL
14	X	126	TYR
14	X	163	ILE
14	X	196	GLN
14	X	199	LEU
14	X	217	LEU
14	X	221	ASP
14	X	247	SER
14	X	256	THR
14	X	260	LEU
14	X	267	VAL
14	Y	14	THR
14	Y	51	ASP
14	Y	93	ARG
14	Y	95	VAL
14	Y	108	ILE
14	Y	119	VAL
14	Y	130	LEU
14	Y	136	LEU
14	Y	146	THR
14	Y	152	LEU
14	Y	179	PHE
14	Y	241	VAL
14	Y	274	ASN
15	G	34	LYS
15	G	51	ILE
15	G	52	ILE
15	G	85	GLN
15	G	94	ILE
15	G	105	THR
15	G	142	VAL
15	G	145	LEU
15	G	154	SER
15	G	164	ILE
15	G	177	ILE

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Mol	Chain	Res	Type
15	G	188	ILE
15	G	189	THR
15	G	205	ILE
15	G	212	LEU
16	N	14	GLU
16	N	25	ILE
16	N	43	THR
16	N	48	ILE
16	N	81	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (127) such sidechains are listed below:

Mol	Chain	Res	Type
1	R	76	ASN
1	R	85	ASN
1	R	194	ASN
1	R	231	ASN
1	R	252	GLN
1	R	289	ASN
1	R	316	GLN
1	R	353	ASN
1	R	473	ASN
1	R	523	ASN
1	R	547	HIS
1	R	723	HIS
1	R	734	ASN
1	R	748	HIS
3	J	21	GLN
3	J	39	ASN
3	J	66	GLN
3	J	78	GLN
3	J	126	GLN
3	J	139	GLN
3	J	194	ASN
3	J	206	GLN
3	J	221	ASN
4	M	10	GLN
4	M	78	GLN
4	M	90	GLN
3	I	11	GLN
3	I	122	GLN
3	I	161	ASN

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Mol	Chain	Res	Type
3	I	169	GLN
3	I	206	GLN
4	L	41	GLN
3	H	9	GLN
3	H	49	GLN
3	H	122	GLN
3	H	161	ASN
4	K	35	GLN
4	K	111	HIS
5	S	59	GLN
5	S	67	GLN
7	U	329	ASN
7	U	338	HIS
7	U	370	HIS
7	U	389	GLN
7	U	394	GLN
7	U	398	GLN
7	U	401	GLN
7	U	403	GLN
7	U	406	ASN
8	V	294	ASN
8	V	327	ASN
8	V	330	ASN
9	0	51	ASN
9	0	132	HIS
9	0	148	ASN
10	2	51	GLN
10	4	81	ASN
10	4	123	GLN
10	7	78	ASN
10	8	51	GLN
10	9	51	GLN
10	9	92	GLN
10	9	123	GLN
11	Q	50	GLN
11	Q	88	HIS
11	Q	142	ASN
11	Q	145	GLN
11	Q	297	HIS
11	Q	308	ASN
11	Q	309	GLN
11	Q	311	HIS

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Mol	Chain	Res	Type
11	Q	338	GLN
12	C	22	HIS
12	C	65	GLN
12	C	123	ASN
12	C	231	GLN
12	C	261	GLN
12	C	314	ASN
12	A	317	ASN
12	A	397	ASN
12	A	573	HIS
12	B	123	ASN
12	B	164	HIS
12	B	172	ASN
12	B	184	ASN
12	B	207	GLN
12	B	231	GLN
12	B	261	GLN
12	B	397	ASN
12	B	468	HIS
12	B	560	GLN
12	B	573	HIS
13	F	199	HIS
13	F	209	GLN
13	F	237	ASN
13	F	256	ASN
13	F	415	HIS
13	D	161	GLN
13	D	187	GLN
13	D	199	HIS
13	E	54	ASN
13	E	73	HIS
13	E	199	HIS
13	E	251	ASN
13	E	256	ASN
13	E	265	ASN
13	E	358	ASN
13	E	421	GLN
14	Z	34	GLN
14	Z	50	GLN
14	Z	134	ASN
14	Z	176	ASN
14	Z	177	GLN

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Mol	Chain	Res	Type
14	Z	222	GLN
14	X	19	HIS
14	X	160	GLN
14	X	207	GLN
14	Y	19	HIS
14	Y	76	ASN
14	Y	135	GLN
14	Y	142	ASN
14	Y	150	ASN
14	Y	243	GLN
15	G	31	ASN
15	G	85	GLN
15	G	100	ASN
16	N	54	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](#)

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	ADP	B	701	-	28,29,29	1.41	5 (17%)	43,45,45	1.80	9 (20%)
18	NAG	U	504	7	14,14,15	0.31	0	17,19,21	0.61	0
18	NAG	U	503	7	14,14,15	0.19	0	17,19,21	0.47	0
18	NAG	U	502	7	14,14,15	0.29	0	17,19,21	0.57	0
18	NAG	S	101	5	14,14,15	0.27	0	17,19,21	0.55	0
18	NAG	U	501	7	14,14,15	0.33	0	17,19,21	0.57	0
18	NAG	R	901	1	14,14,15	0.52	0	17,19,21	0.59	0
18	NAG	U	505	7	14,14,15	0.20	0	17,19,21	0.39	0
18	NAG	U	506	7	14,14,15	0.25	0	17,19,21	0.52	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	ADP	B	701	-	-	1/16/32/32	0/3/3/3
18	NAG	U	504	7	-	4/6/23/26	0/1/1/1
18	NAG	U	503	7	-	1/6/23/26	0/1/1/1
18	NAG	U	502	7	-	2/6/23/26	0/1/1/1
18	NAG	S	101	5	-	0/6/23/26	0/1/1/1
18	NAG	U	501	7	-	2/6/23/26	0/1/1/1
18	NAG	R	901	1	-	3/6/23/26	0/1/1/1
18	NAG	U	505	7	-	4/6/23/26	0/1/1/1
18	NAG	U	506	7	-	4/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	701	ADP	C5-C4	4.26	1.46	1.39
19	B	701	ADP	C5-N7	-2.84	1.33	1.39
19	B	701	ADP	C4-N9	-2.25	1.33	1.37
19	B	701	ADP	C5-C6	2.22	1.47	1.41
19	B	701	ADP	C8-N7	2.10	1.35	1.31

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	701	ADP	C5-C4-N3	-5.87	118.64	126.72
19	B	701	ADP	N3-C4-N9	4.52	134.86	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	701	ADP	C2-N3-C4	3.53	120.44	111.83
19	B	701	ADP	C4-C5-N7	-3.30	106.81	110.58
19	B	701	ADP	N3-C2-N1	-2.98	124.06	128.58
19	B	701	ADP	C3'-C2'-C1'	2.33	105.87	101.46
19	B	701	ADP	C5-N7-C8	2.30	107.07	103.45
19	B	701	ADP	C4-N9-C8	2.25	108.11	105.74
19	B	701	ADP	C2'-C3'-C4'	2.04	106.54	102.61

There are no chirality outliers.

All (21) torsion outliers are listed below:

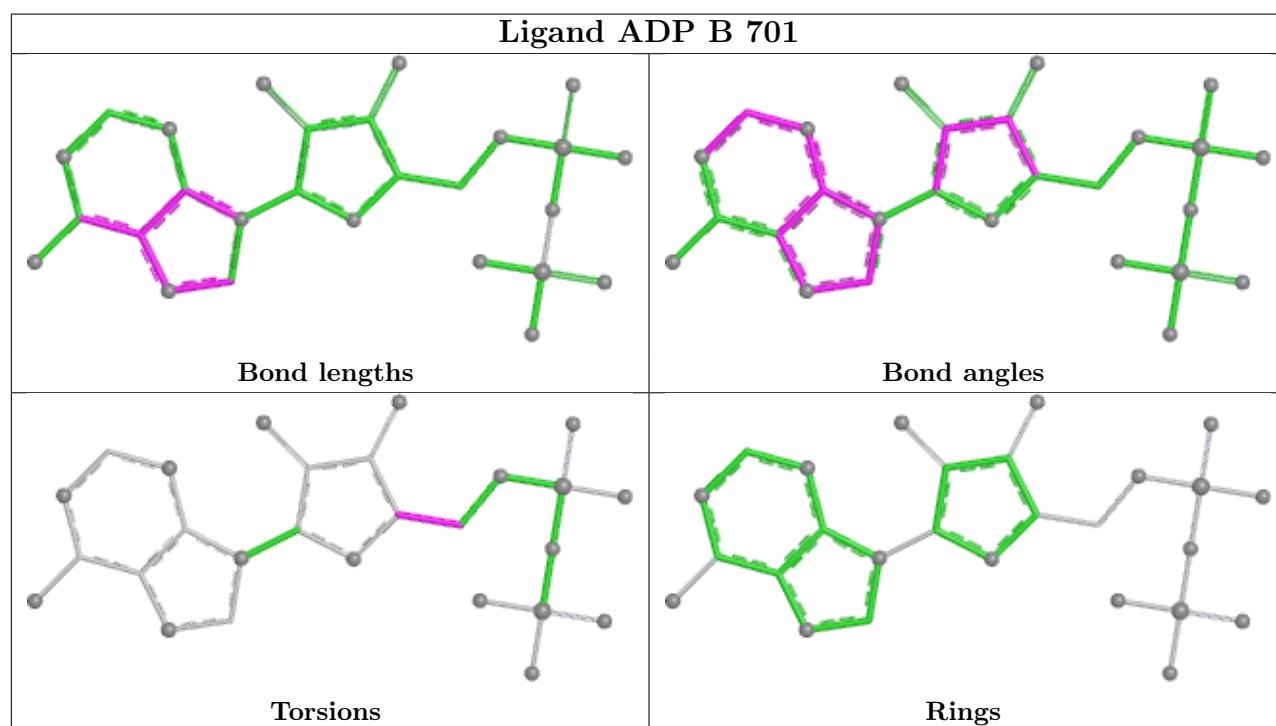
Mol	Chain	Res	Type	Atoms
18	U	501	NAG	C4-C5-C6-O6
18	U	505	NAG	O5-C5-C6-O6
18	U	506	NAG	O5-C5-C6-O6
18	U	502	NAG	O5-C5-C6-O6
18	U	501	NAG	O5-C5-C6-O6
18	U	504	NAG	O5-C5-C6-O6
18	U	505	NAG	C4-C5-C6-O6
18	U	504	NAG	C4-C5-C6-O6
18	U	506	NAG	C4-C5-C6-O6
18	U	505	NAG	C8-C7-N2-C2
18	U	505	NAG	O7-C7-N2-C2
18	U	503	NAG	O5-C5-C6-O6
18	R	901	NAG	O5-C5-C6-O6
18	U	502	NAG	C4-C5-C6-O6
19	B	701	ADP	O4'-C4'-C5'-O5'
18	R	901	NAG	C3-C2-N2-C7
18	U	504	NAG	C3-C2-N2-C7
18	U	506	NAG	C3-C2-N2-C7
18	R	901	NAG	C1-C2-N2-C7
18	U	504	NAG	C1-C2-N2-C7
18	U	506	NAG	C1-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B	701	ADP	2	0
18	R	901	NAG	1	0
18	U	505	NAG	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

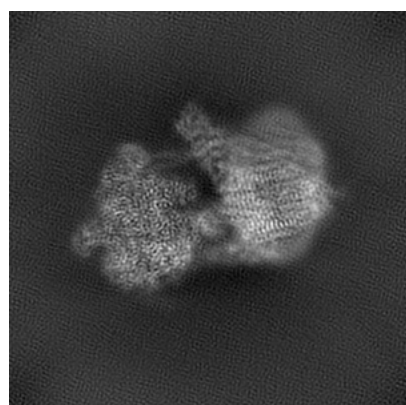
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21848. These allow visual inspection of the internal detail of the map and identification of artifacts.

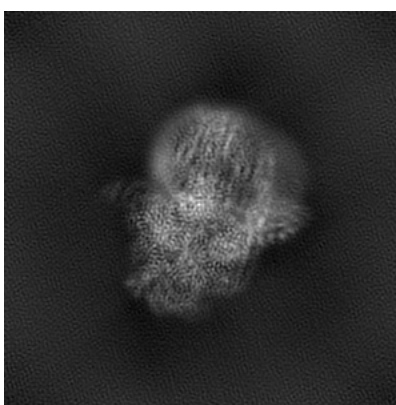
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

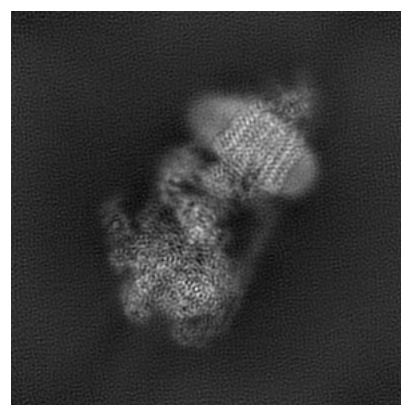
6.1.1 Primary map



X



Y

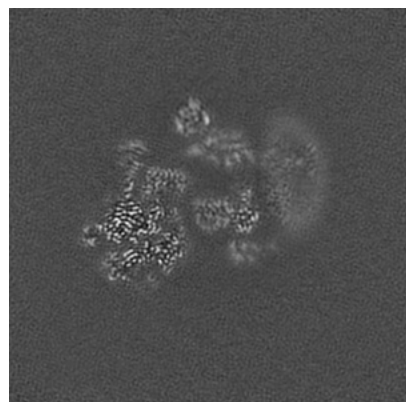


Z

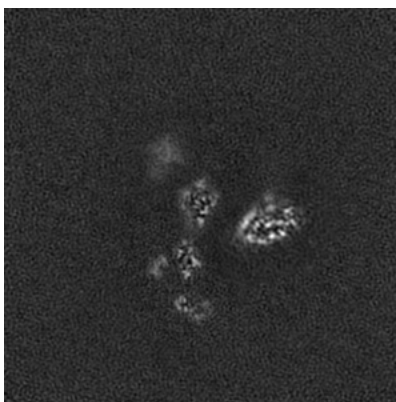
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

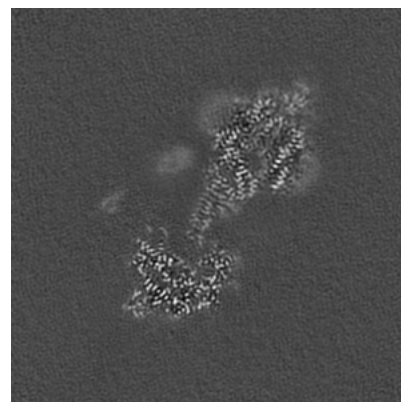
6.2.1 Primary map



X Index: 180



Y Index: 180

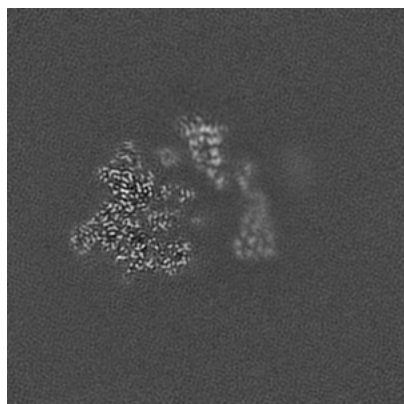


Z Index: 180

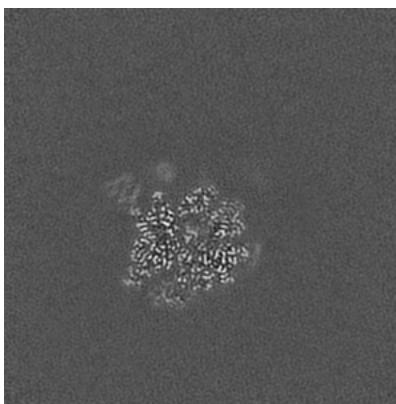
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

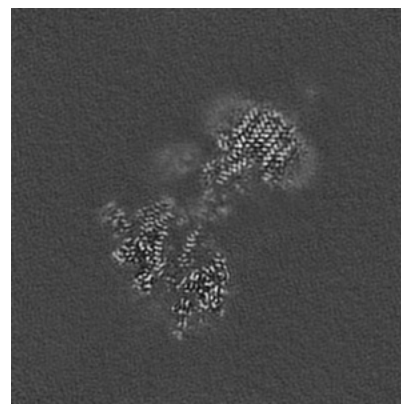
6.3.1 Primary map



X Index: 157



Y Index: 128

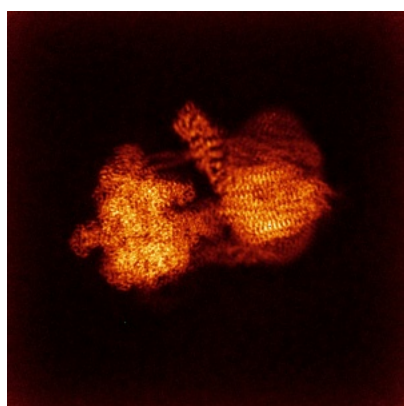


Z Index: 167

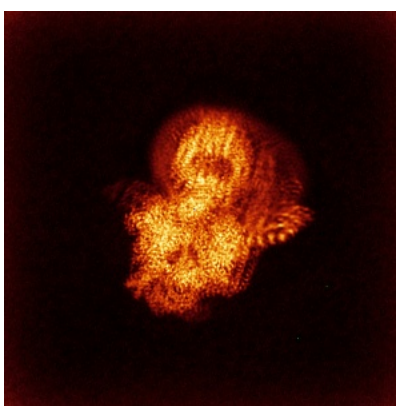
The images above show the largest variance slices of the map in three orthogonal directions.

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

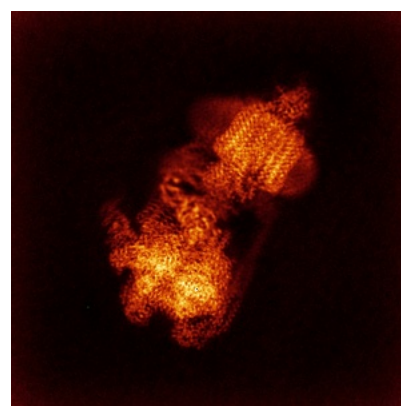
6.4.1 Primary map



X



Y

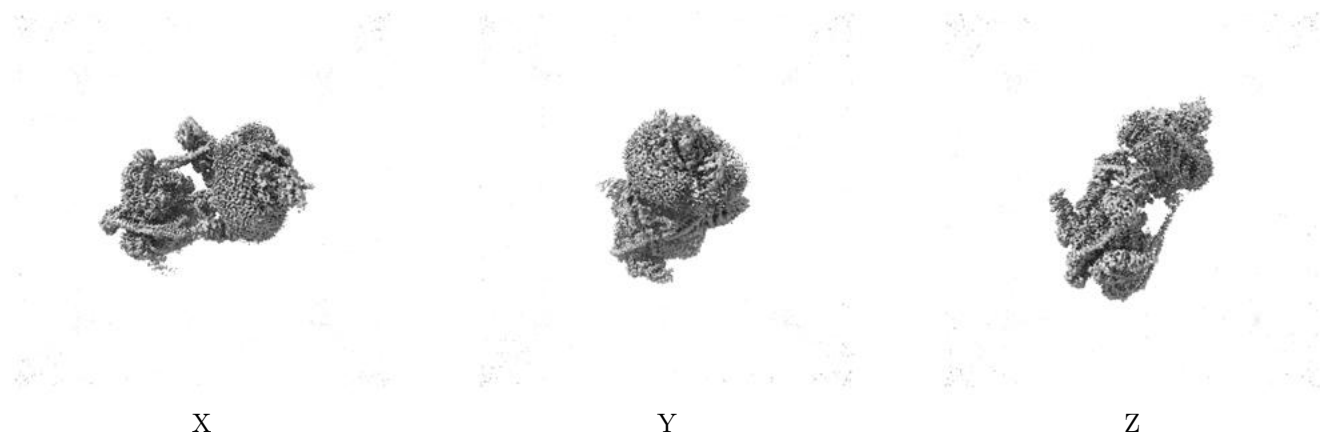


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

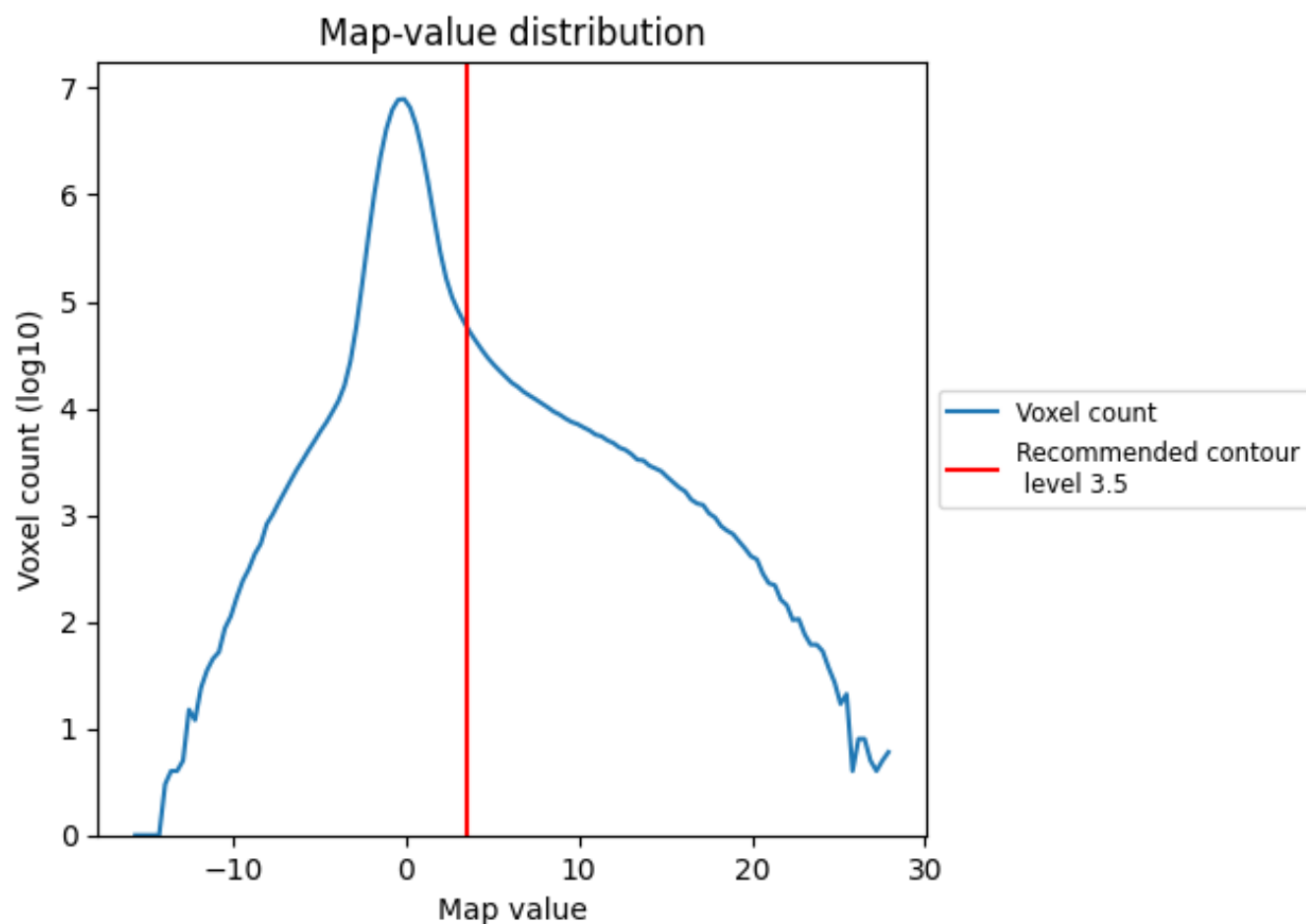
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

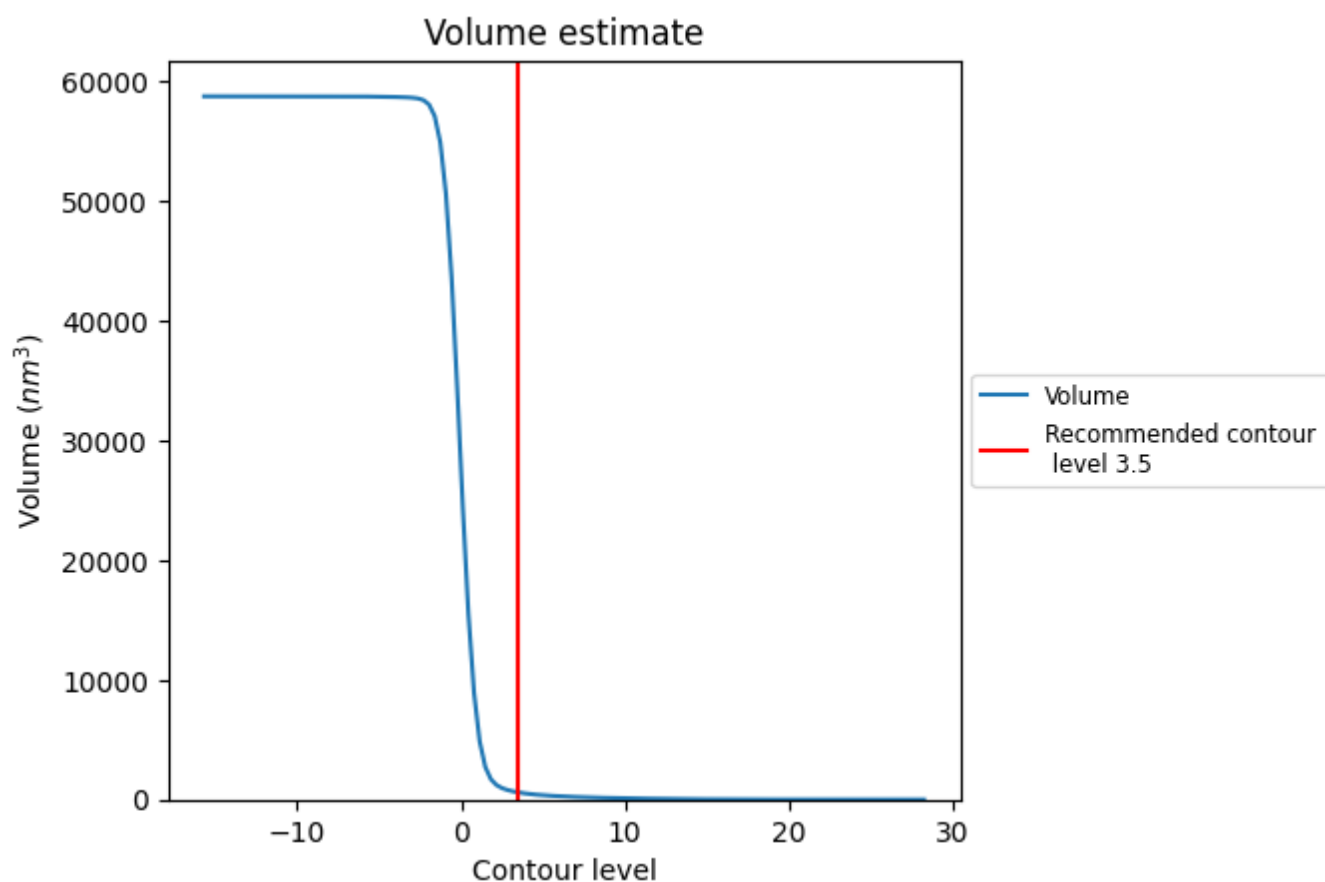
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

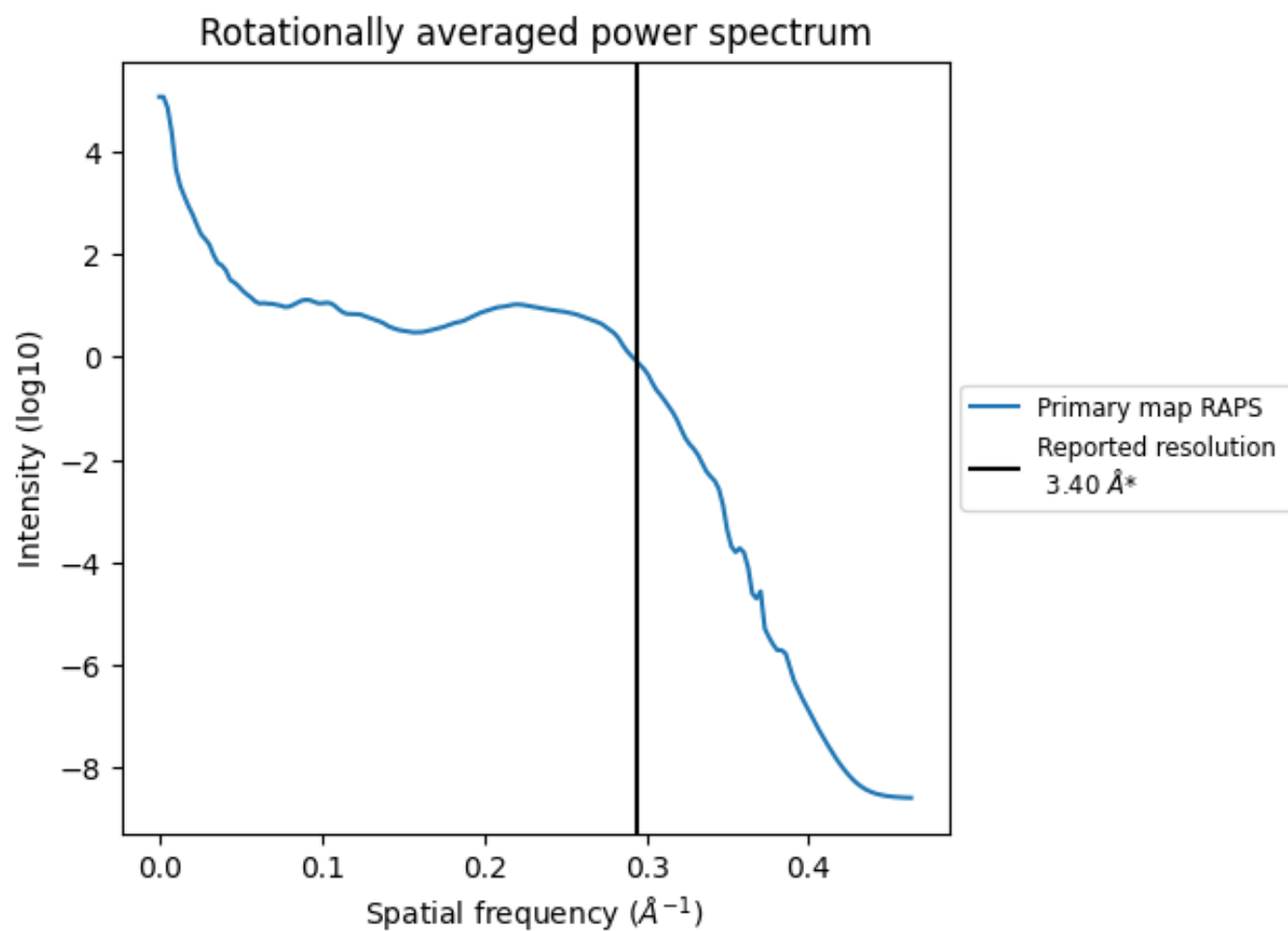
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 599 nm³; this corresponds to an approximate mass of 541 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 0.294 Å⁻¹

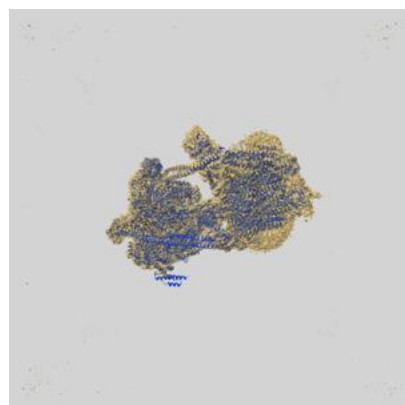
8 Fourier-Shell correlation ⓘ

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

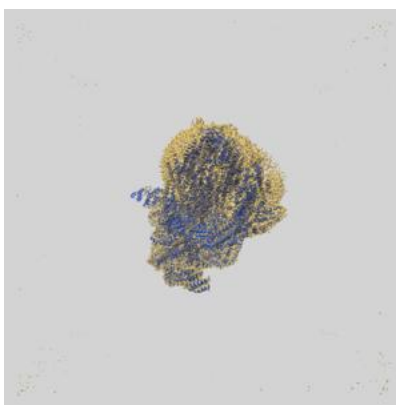
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21848 and PDB model 6WM3. Per-residue inclusion information can be found in section [3](#) on page [10](#).

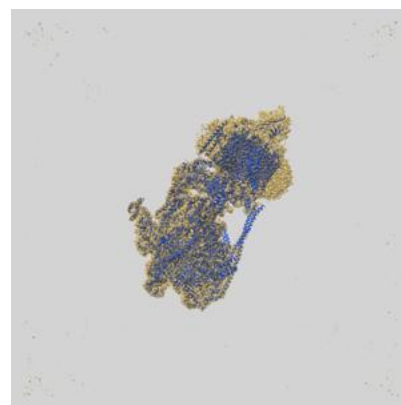
9.1 Map-model overlay [i](#)



X



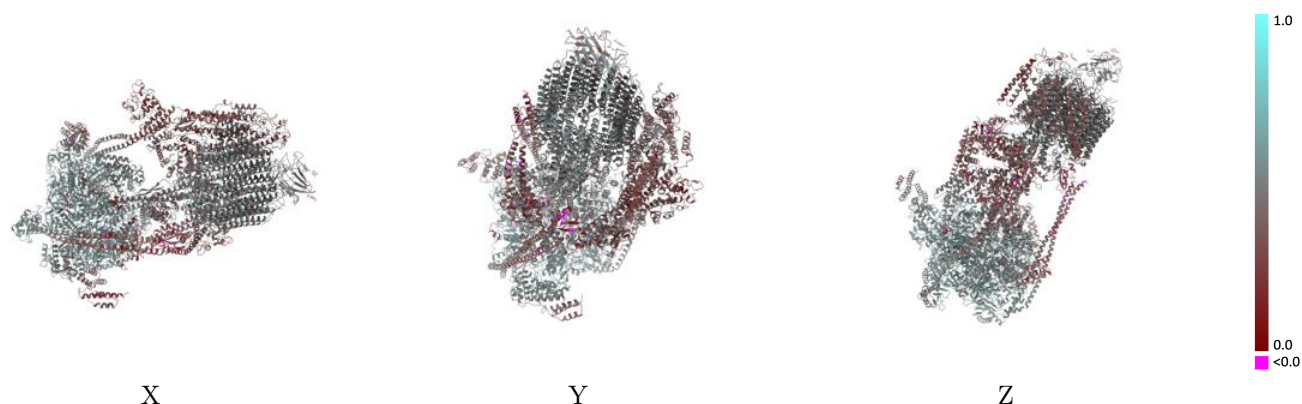
Y



Z

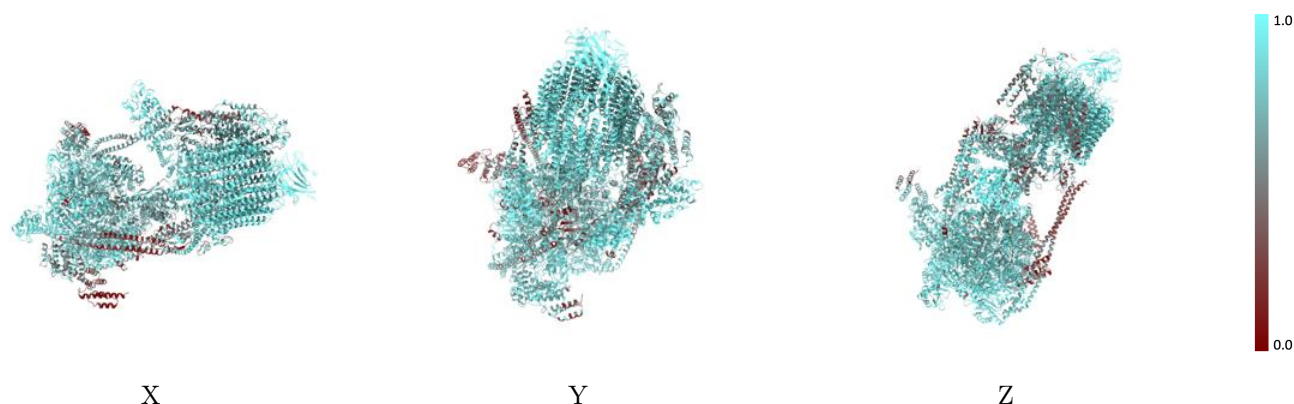
The images above show the 3D surface view of the map at the recommended contour level 3.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



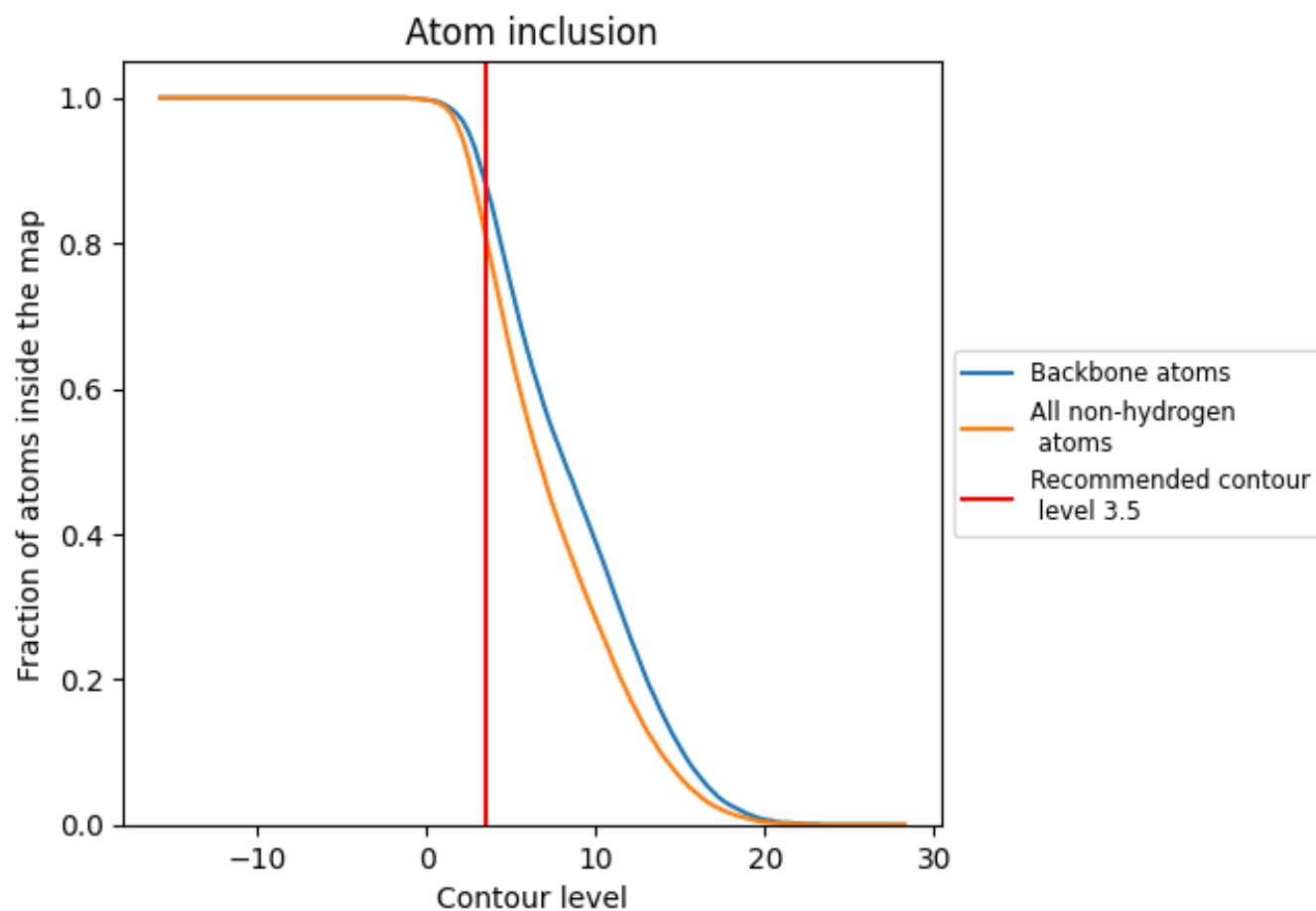
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (3.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8110	 0.4770
0	 0.9280	 0.5020
1	 0.9210	 0.4950
2	 0.9240	 0.4830
3	 0.9200	 0.4790
4	 0.9140	 0.4720
5	 0.9150	 0.4730
6	 0.8800	 0.4650
7	 0.8620	 0.4730
8	 0.8740	 0.4820
9	 0.9040	 0.4930
A	 0.8780	 0.5390
B	 0.9180	 0.5680
C	 0.8760	 0.5490
D	 0.9100	 0.5700
E	 0.8720	 0.5420
F	 0.8870	 0.5480
G	 0.8120	 0.5050
H	 0.8170	 0.4710
I	 0.7800	 0.4820
J	 0.7170	 0.4680
K	 0.7250	 0.4150
L	 0.6340	 0.3970
M	 0.5280	 0.3870
N	 0.6800	 0.4170
O	 0.6870	 0.2830
P	 0.9700	 0.3510
Q	 0.8860	 0.4970
R	 0.6060	 0.3440
S	 0.7100	 0.3930
T	 0.5990	 0.3230
U	 0.9350	 0.4690
V	 0.9300	 0.4860
X	 0.7490	 0.4880
Y	 0.3920	 0.4180
Z	 0.6880	 0.4610

