Full wwPDB EM Validation Report

Oct 27, 2024 – 12:45 AM EDT

PDB ID	:	6WM4
EMDB ID	:	EMD-21849
Title	:	Human V-ATPase in state 3 with SidK and ADP
Authors	:	Wang, L.; Wu, H.; Fu, T.M.
Deposited on	:	2020-04-20
Resolution	:	3.60 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:

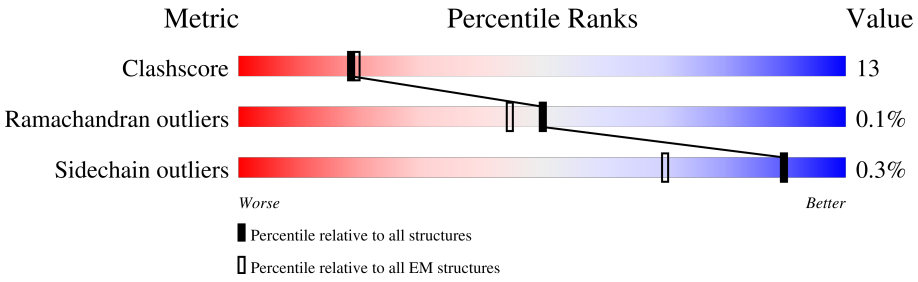
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 <=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	15% 53% 37% 10%
2	O	382	29% 48% 50% .
3	H	226	. 75% 24% .
3	I	226	5% 71% 29%
3	J	226	18% 81% 18%
4	K	118	7% 57% 40% .
4	L	118	19% 64% 32% . .
4	M	118	41% 63% 34% .

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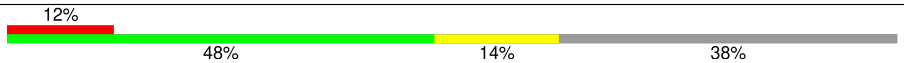
Mol	Chain	Length	Quality of chain
5	S	81	
6	T	137	
7	A	617	
7	B	617	
7	C	617	
8	D	511	
8	E	511	
8	F	511	
9	X	573	
9	Y	573	
9	Z	573	
10	G	247	
11	N	119	
12	U	470	
13	V	350	
14	0	205	
15	1	155	
15	2	155	
15	3	155	
15	4	155	
15	5	155	
15	6	155	
15	7	155	
15	8	155	
15	9	155	

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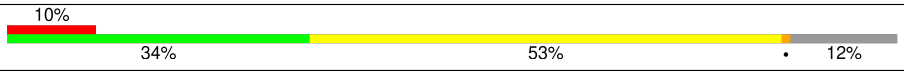
Mol	Chain	Length	Quality of chain
16	Q	351	
17	P	483	

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 72308 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	S	0	0
			3035	1944	512	569	10		

- 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	224	Total	C	N	O	S	0	0
			1817	1140	321	346	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 catalytic subunit A.

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

- Molecule 8 is a protein called V-type proton ATPase subunit B, brain isoform.

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

- Molecule 9 is a protein called SidK.

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

- Molecule 10 is a protein called V-type proton ATPase subunit D.

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

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

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

- Molecule 12 is a protein called V-type proton ATPase subunit S1.

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

- Molecule 13 is a protein called Renin receptor.

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

- Molecule 14 is a protein called V-type proton ATPase 21 kDa proteolipid subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	0	204	Total	C	N	O	S	0	0
			1498	990	238	259	11		

- Molecule 15 is a protein called V-type proton ATPase 16 kDa proteolipid subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	1	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
15	2	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
15	3	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
15	4	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
15	5	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
15	6	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
15	7	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
15	8	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
15	9	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		

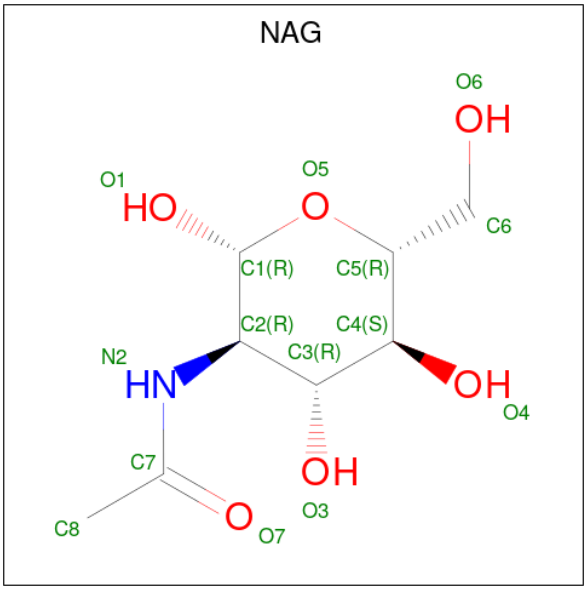
- Molecule 16 is a protein called V-type proton ATPase subunit d 1.

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

- 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	S	0	0
			3508	2228	605	648	27		

- Molecule 18 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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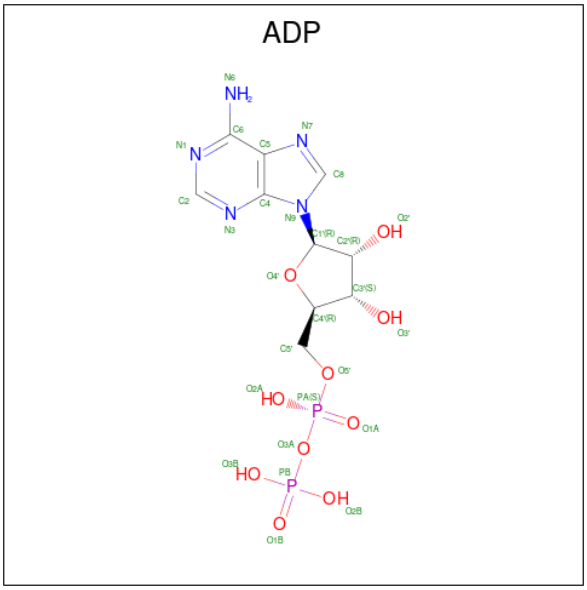
Mol	Chain	Residues	Atoms				AltConf
18	R	1	Total	C	N	O	0
			14	8	1	5	
18	U	1	Total	C	N	O	0
			14	8	1	5	
18	U	1	Total	C	N	O	0
			14	8	1	5	
18	U	1	Total	C	N	O	0
			14	8	1	5	
18	U	1	Total	C	N	O	0
			14	8	1	5	
18	U	1	Total	C	N	O	0
			14	8	1	5	
18	U	1	Total	C	N	O	0
			14	8	1	5	

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



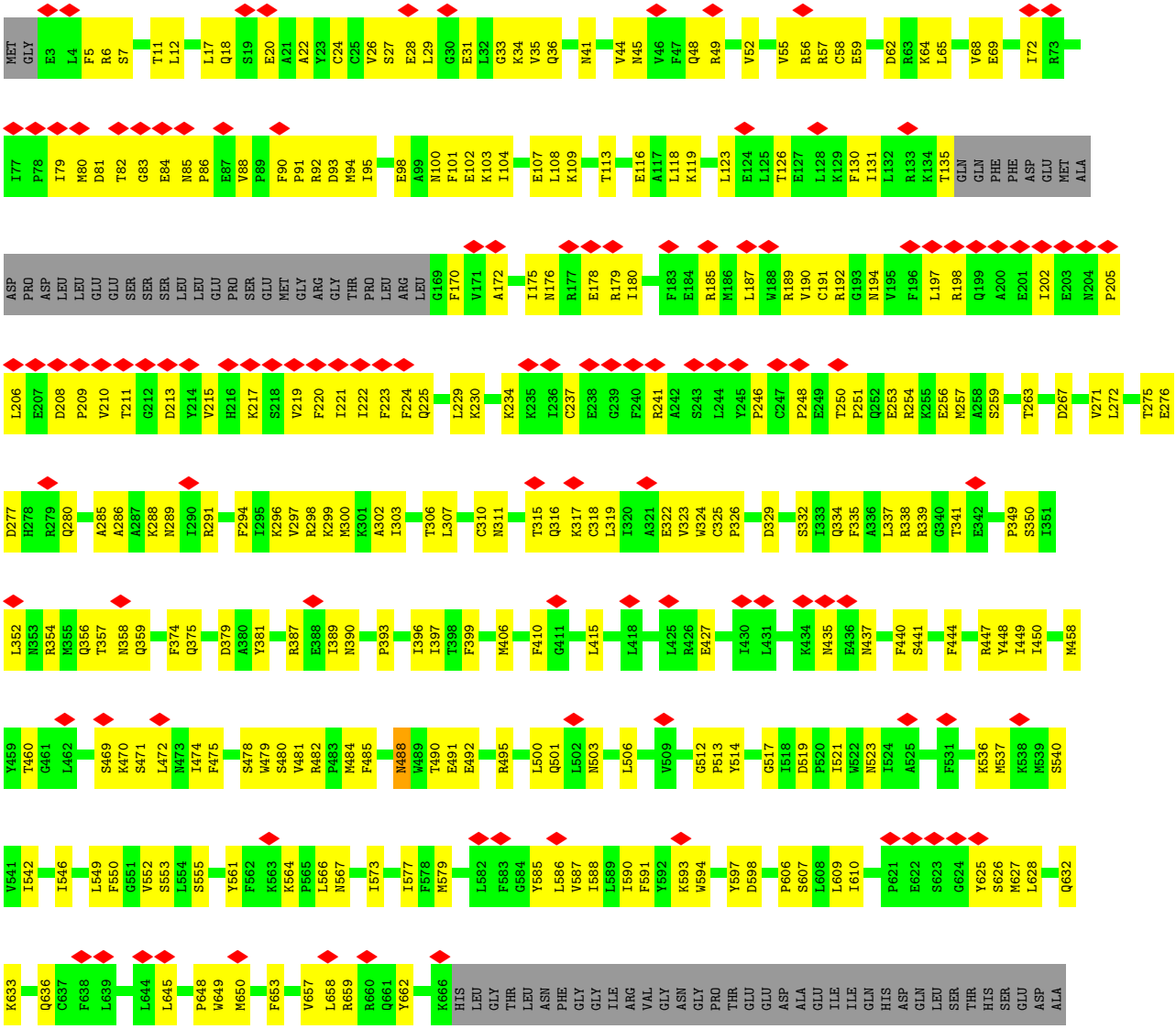
Mol	Chain	Residues	Atoms					AltConf
19	A	1	Total	C	N	O	P	0
			27	10	5	10	2	

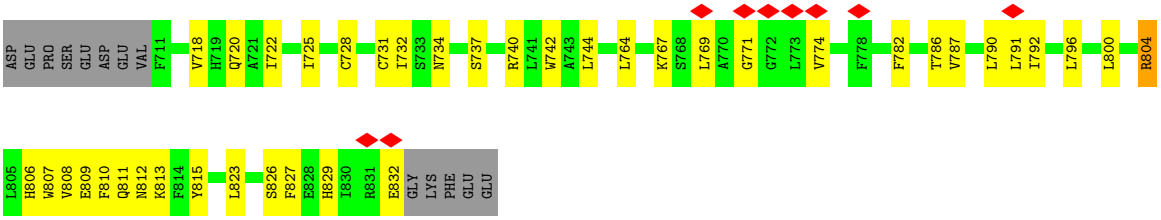
3 Residue-property plots (i)

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

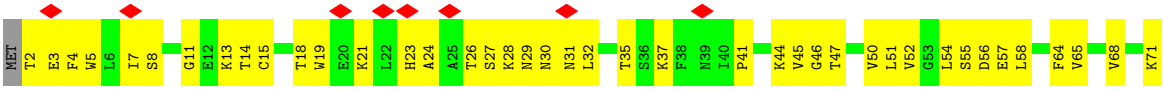
• Molecule 1: V-type proton ATPase 116 kDa subunit a isoform 1

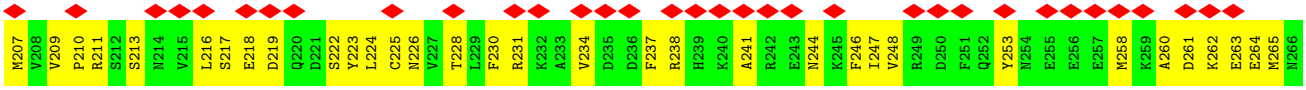
Chain R:

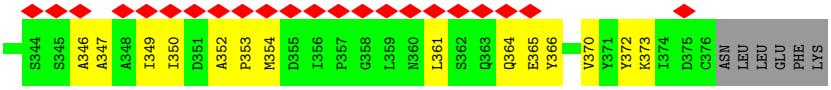




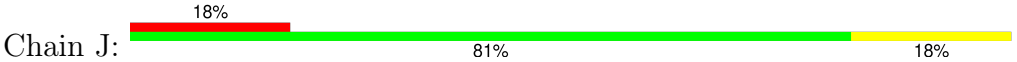
• Molecule 2: V-type proton ATPase subunit C 1

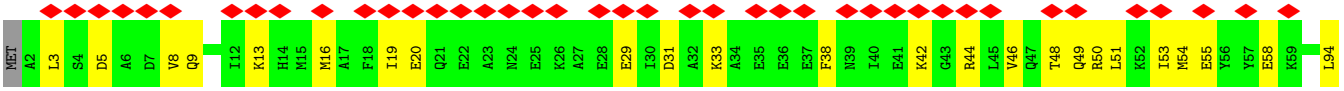


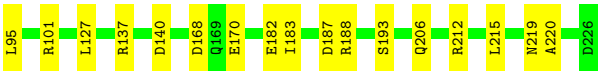




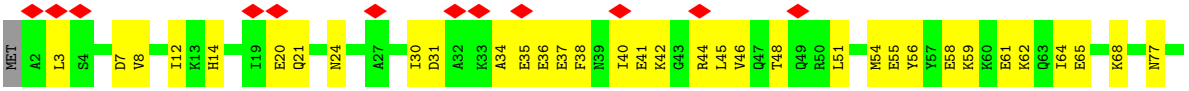
• Molecule 3: V-type proton ATPase subunit E 1





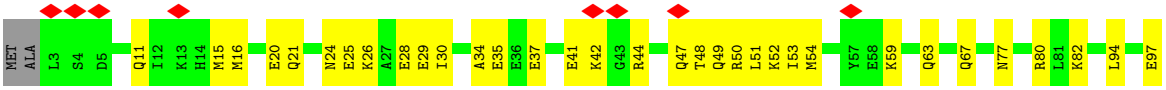


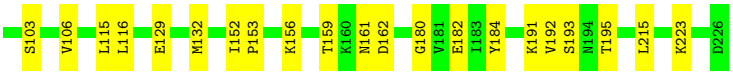
• Molecule 3: V-type proton ATPase subunit E 1



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

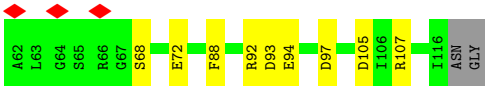
Chain H:





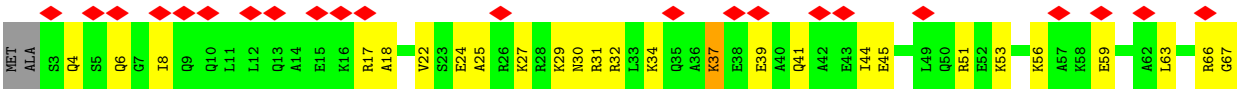
• Molecule 4: V-type proton ATPase subunit G 1

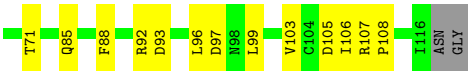
Chain M:



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

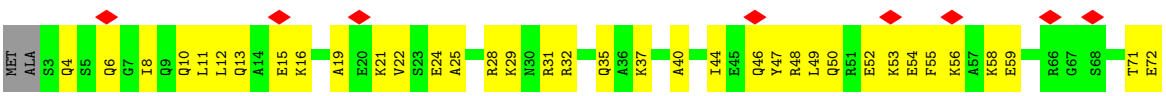
Chain L:





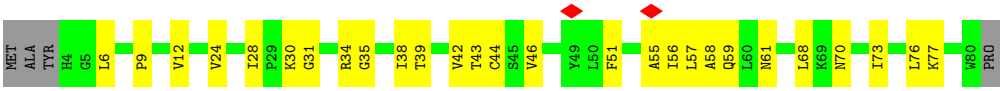
• Molecule 4: V-type proton ATPase subunit G 1

Chain K:



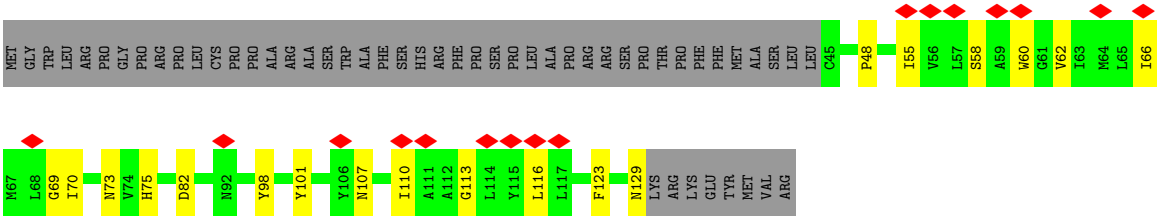
• Molecule 5: V-type proton ATPase subunit e 1

Chain S:



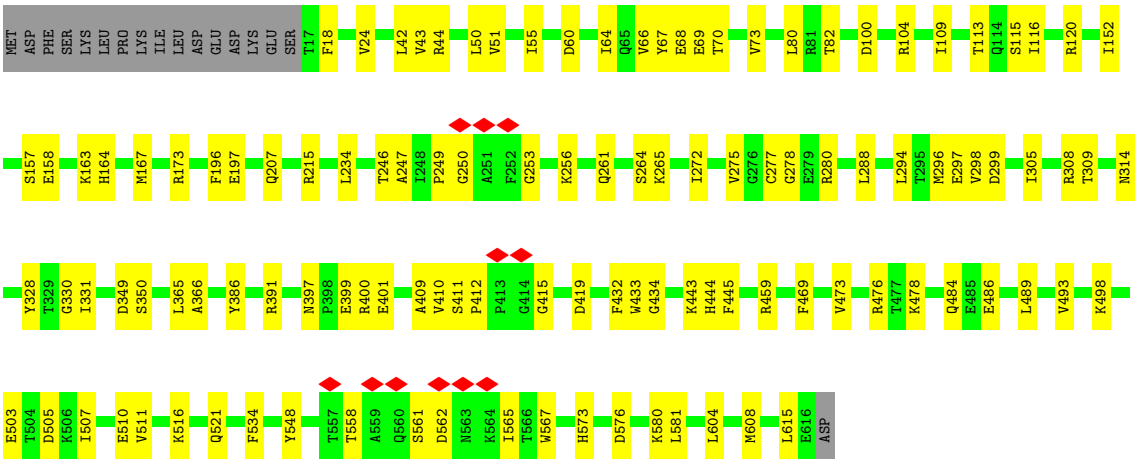
• Molecule 6: Ribonuclease kappa

Chain T:



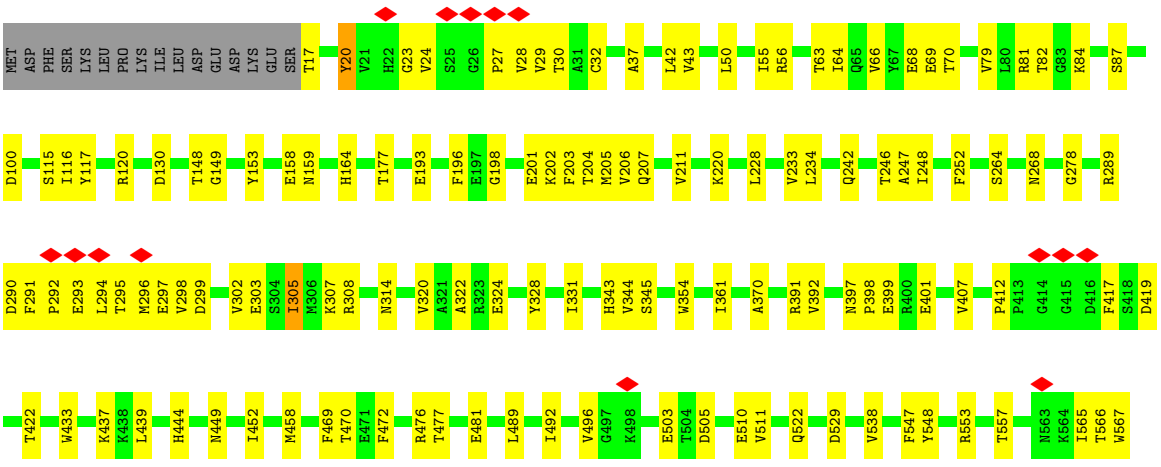
• Molecule 7: V-type proton ATPase catalytic subunit A

Chain B:



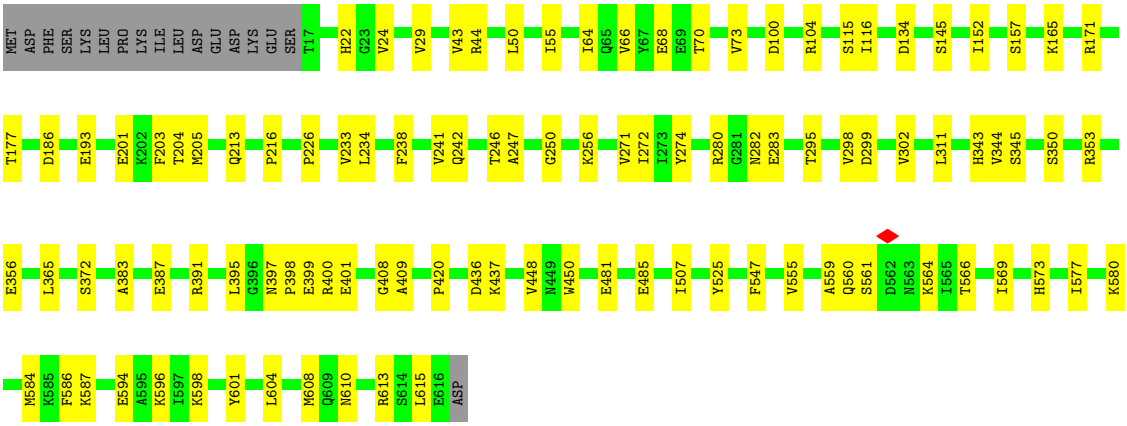
• Molecule 7: V-type proton ATPase catalytic subunit A

Chain C:



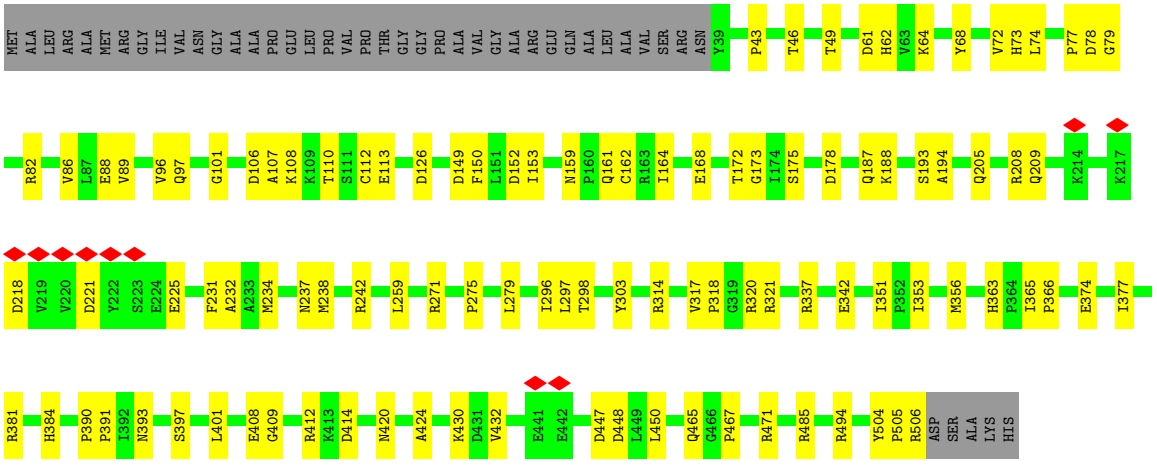
• Molecule 7: V-type proton ATPase catalytic subunit A

Chain A:



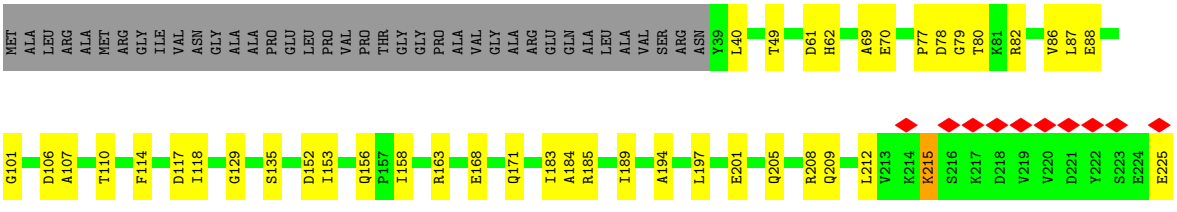
• Molecule 8: V-type proton ATPase subunit B, brain isoform

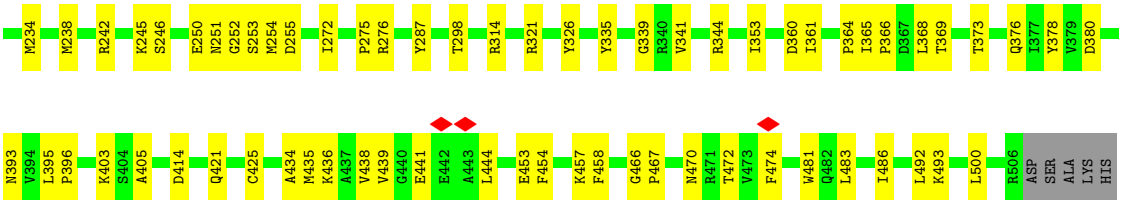
Chain E:



• Molecule 8: V-type proton ATPase subunit B, brain isoform

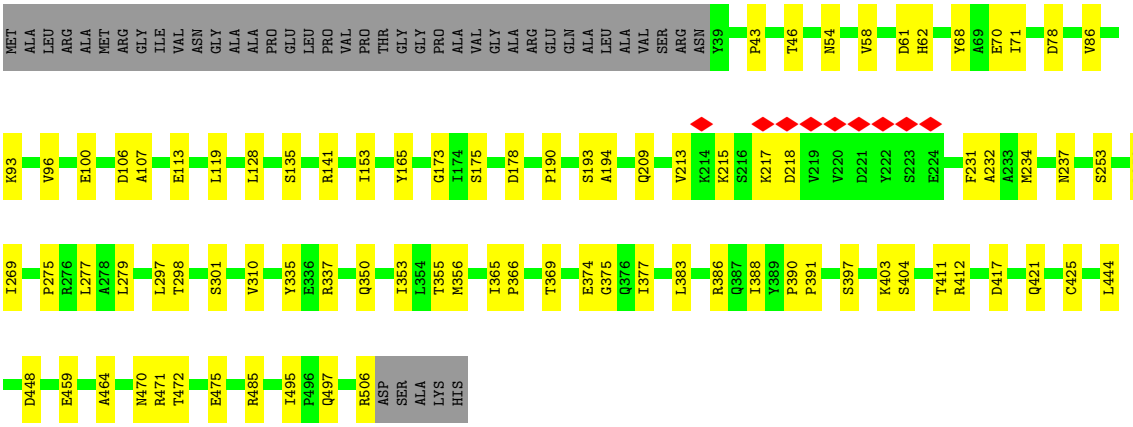
Chain F:





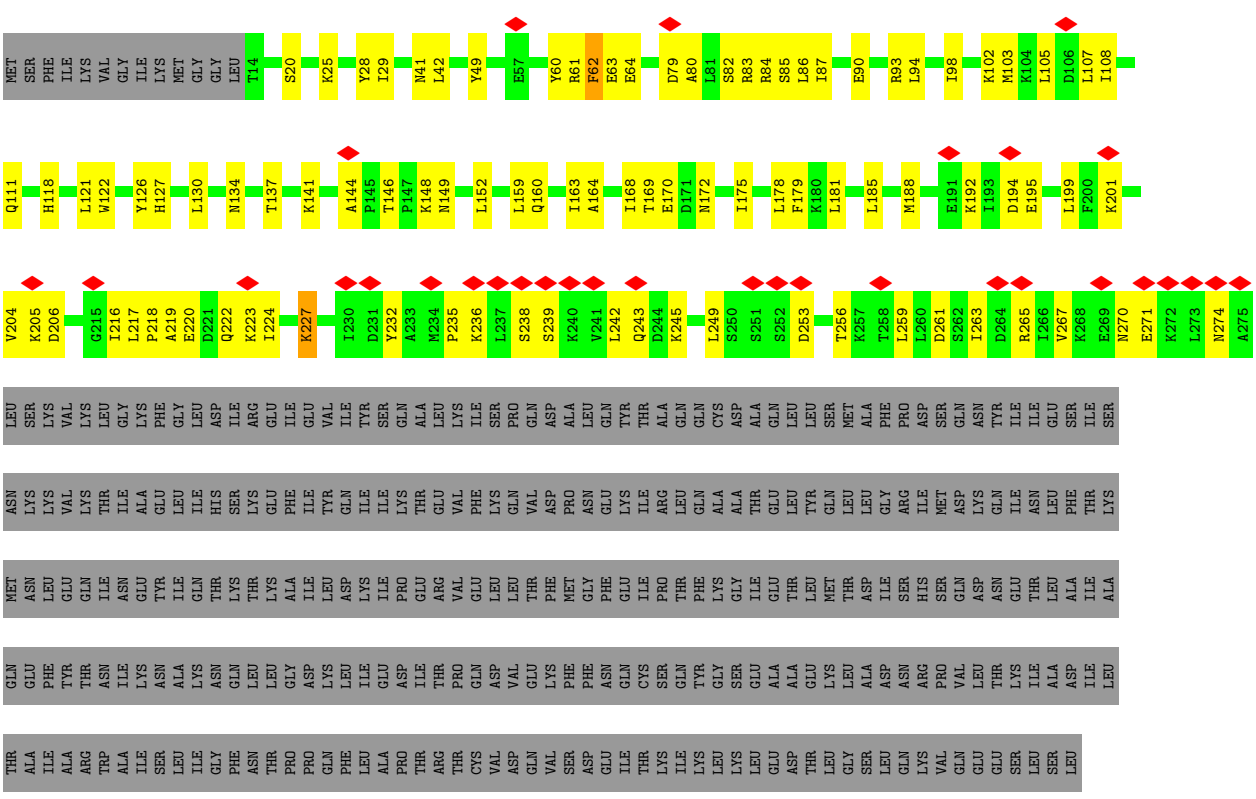
• Molecule 8: V-type proton ATPase subunit B, brain isoform

Chain D:



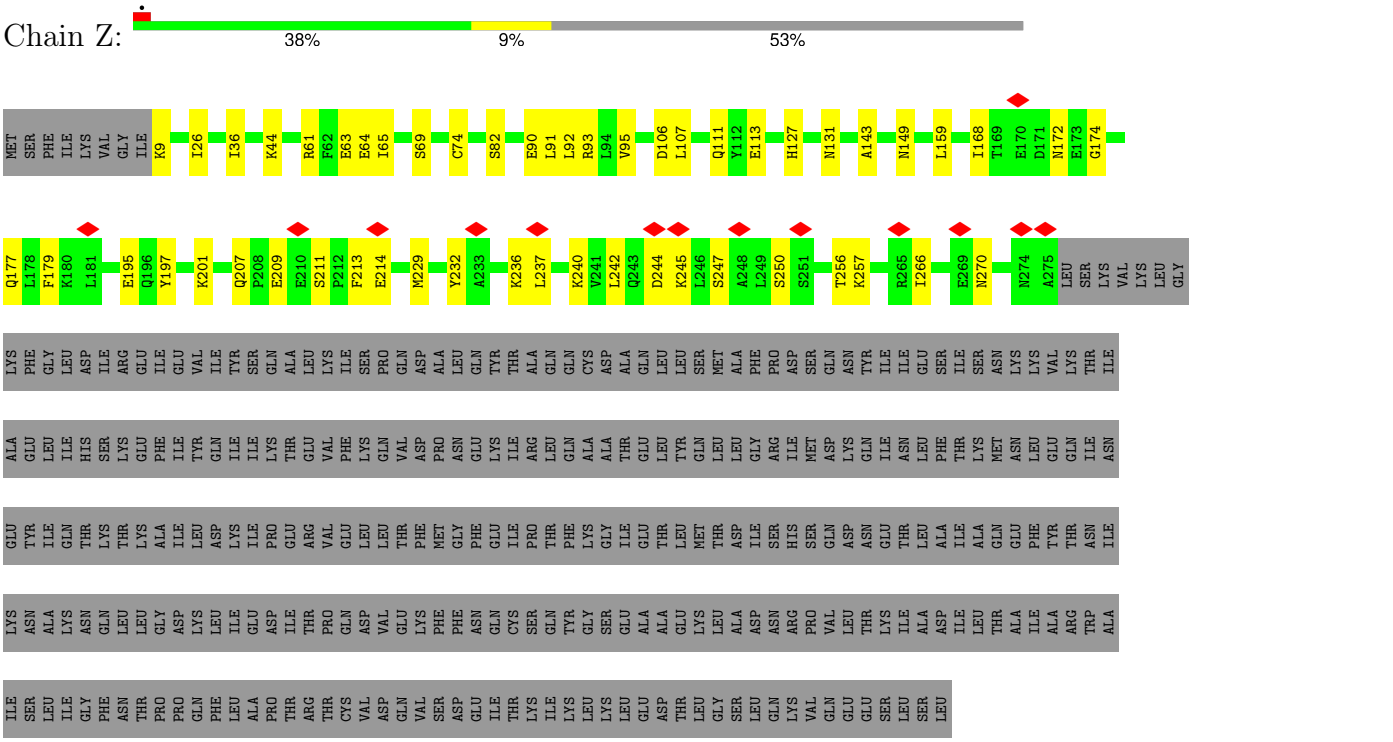
• Molecule 9: SidK

Chain Y:



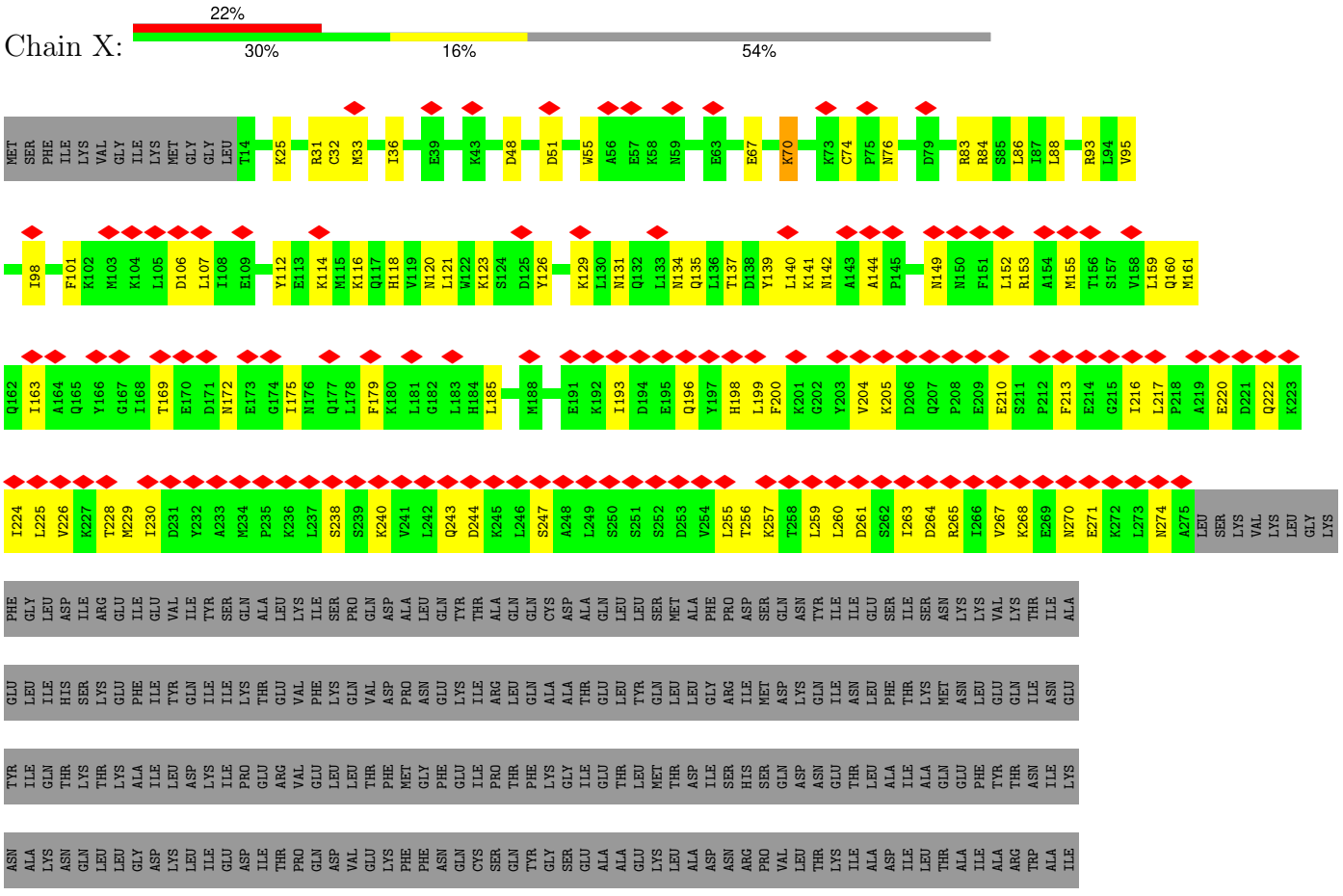
• Molecule 9: SidK

Chain Z:



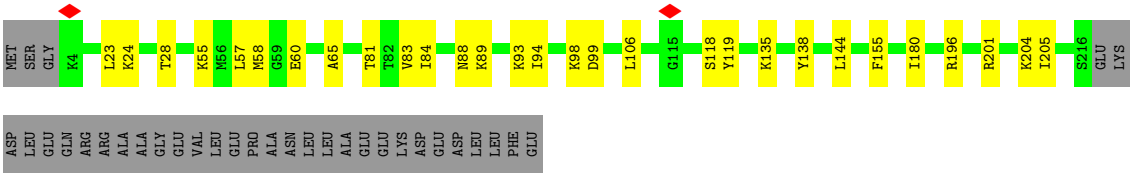
• Molecule 9: SidK

Chain X:



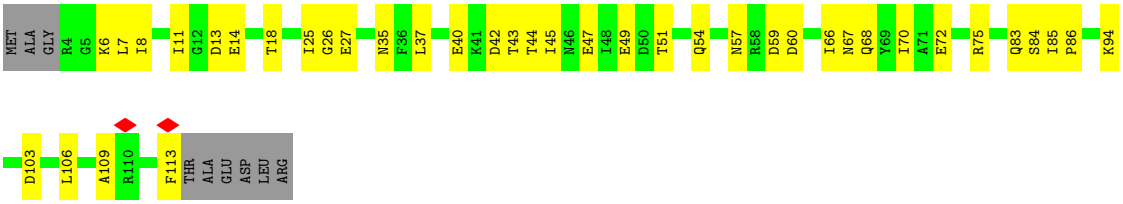
• Molecule 10: V-type proton ATPase subunit D

Chain G:



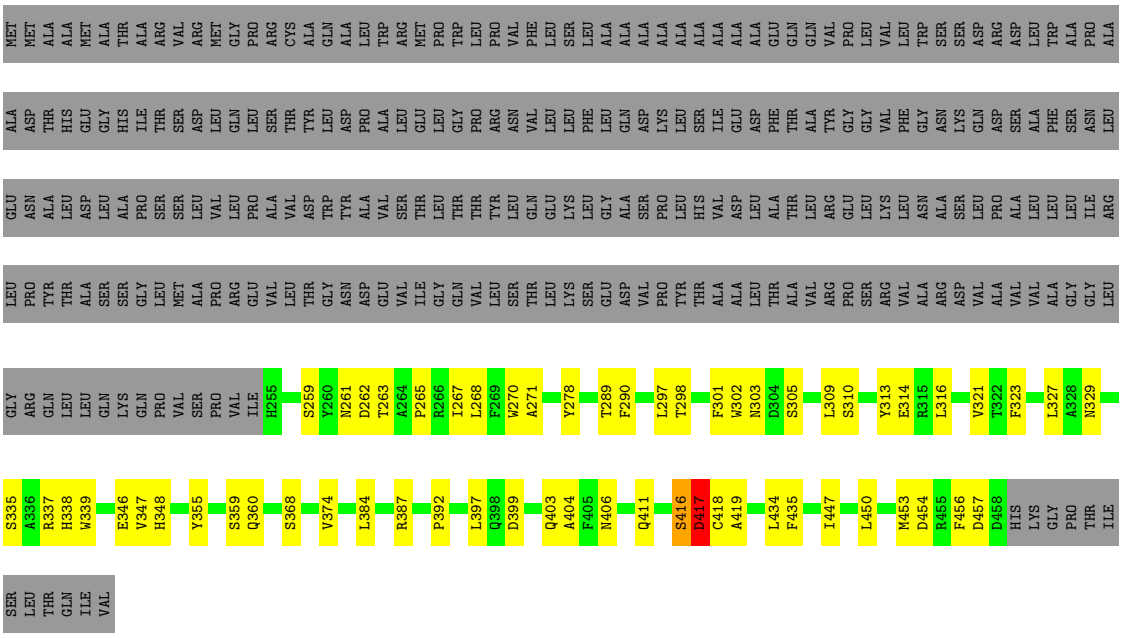
• Molecule 11: V-type proton ATPase subunit F

Chain N:



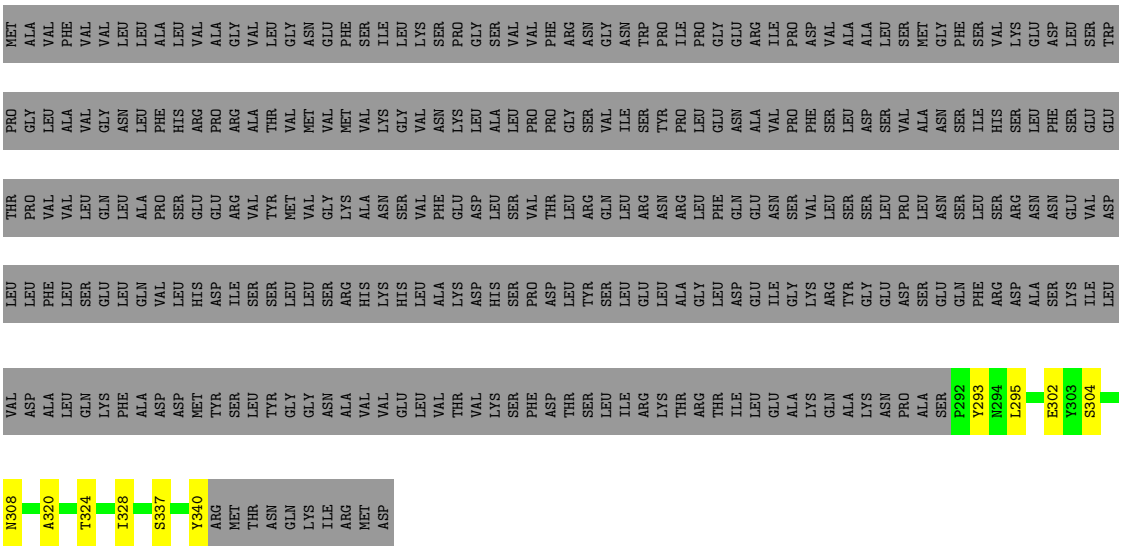
• Molecule 12: V-type proton ATPase subunit S1

Chain U:



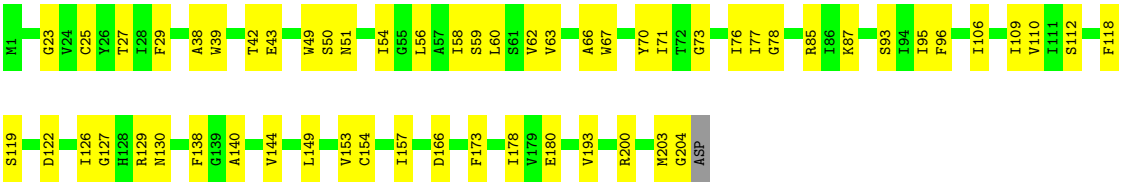
• Molecule 13: Renin receptor

Chain V:



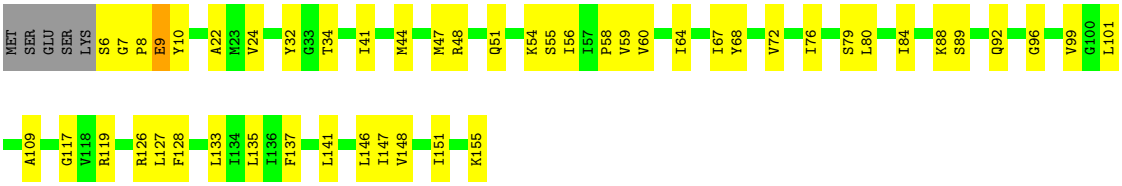
• Molecule 14: V-type proton ATPase 21 kDa proteolipid subunit

Chain 0:



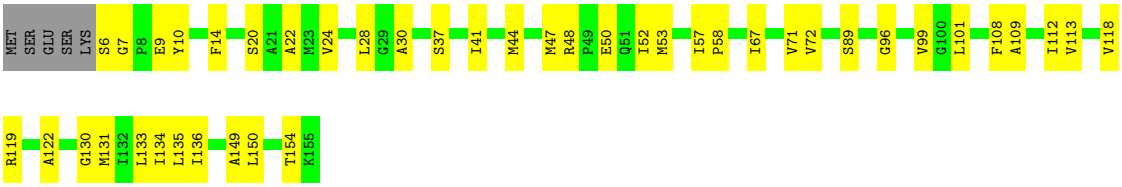
• Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit

Chain 1:



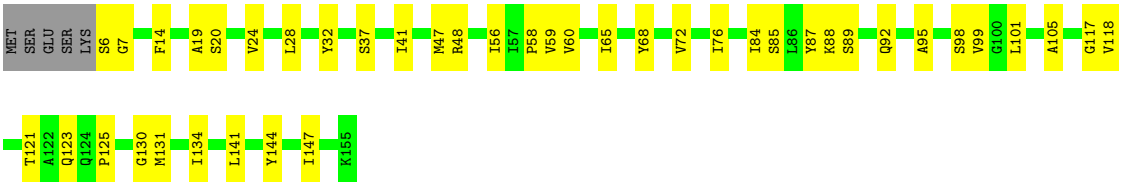
• Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit

Chain 2:



• Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit

Chain 3:

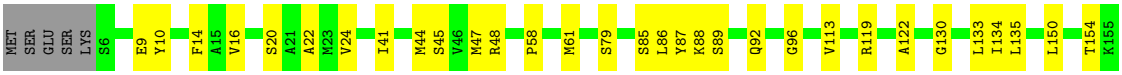


• Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit

Chain 4:

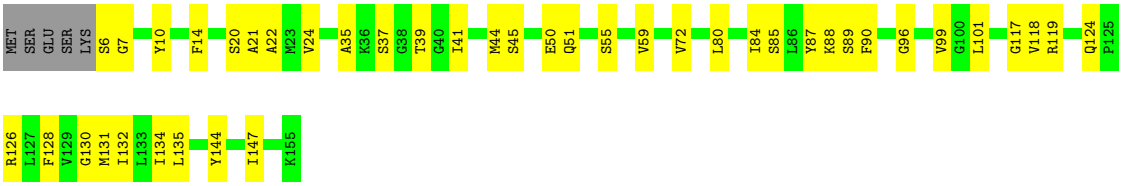
• Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit

Chain 5:



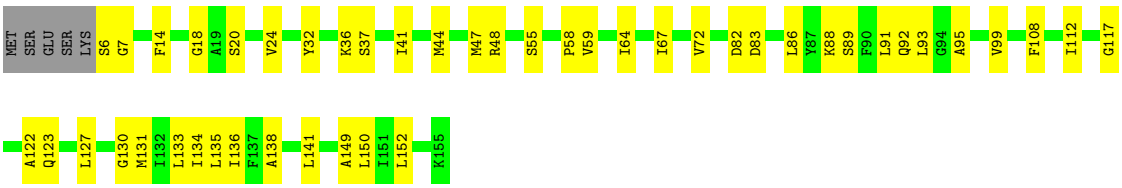
• Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit

Chain 6:



• Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit

Chain 7:

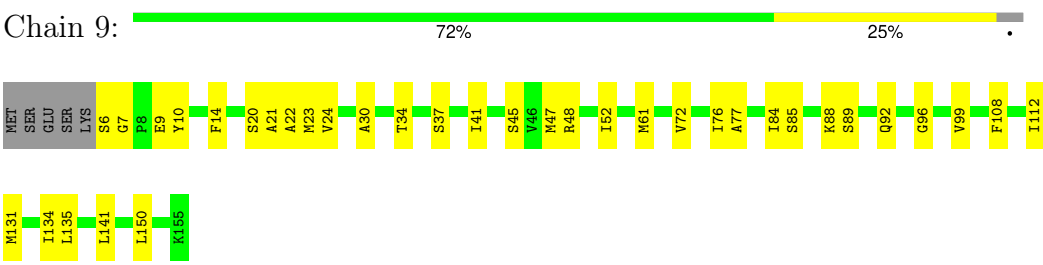


• Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit

Chain 8:

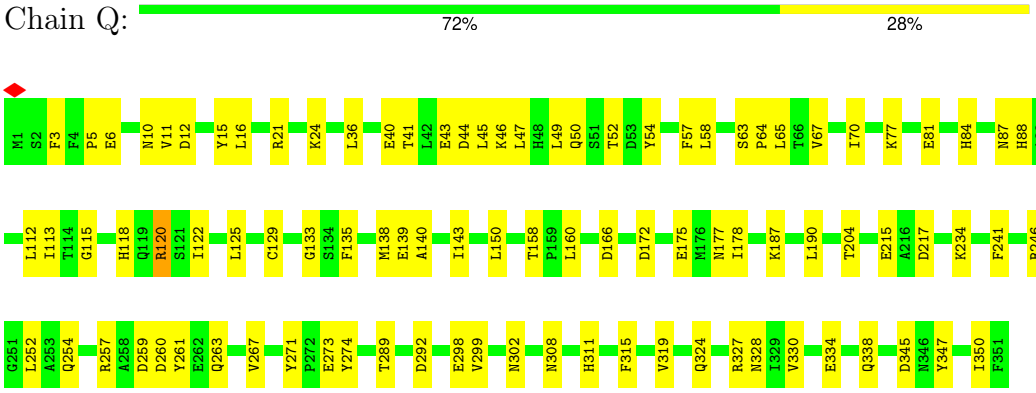
• Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit

Chain 9:



• Molecule 16: V-type proton ATPase subunit d 1

Chain Q:



• Molecule 17: V-type proton ATPase subunit H

Chain P:


D403
P404
Q405
A408
V409
D413
Y417
V418
R419
R423
G424
K425
R426
V427
I428
E429
Q430
L431
G432
G433
K434
Q435
L436
V437
M438
N439
H440
M441
D445
V448
R449
Y450
N451
A452
L453
V456
Q457
K458
L459
M460
N463
TRP
GLU
TYR
LEU
GLY
LYS
GLN
LEU
GLN
SER
GLU
GLN
PRO
GLN
THR
ALA
ALA
ALA
ARG
SER

4 Experimental information (i)

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 ($e^-/Å^2$)	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	27.492	Depositor
Minimum map value	-13.678	Depositor
Average map value	0.017	Depositor
Map value standard deviation	1.157	Depositor
Recommended contour level	3.7	Depositor
Map size (Å)	388.80002, 388.80002, 388.80002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: NAG, ADP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	R	0.27	0/6306	0.42	0/8534
2	O	0.27	0/3092	0.47	0/4182
3	H	0.34	0/1834	0.46	0/2455
3	I	0.32	0/1839	0.45	0/2462
3	J	0.32	0/1839	0.44	0/2462
4	K	0.30	0/945	0.45	0/1258
4	L	0.28	0/945	0.41	0/1258
4	M	0.28	0/945	0.41	0/1258
5	S	0.28	0/657	0.44	0/902
6	T	0.28	0/674	0.45	0/915
7	A	0.44	0/4752	0.47	0/6435
7	B	0.40	0/4752	0.47	0/6435
7	C	0.40	0/4752	0.51	0/6435
8	D	0.44	0/3739	0.48	0/5067
8	E	0.44	0/3739	0.49	0/5067
8	F	0.41	0/3739	0.48	0/5067
9	X	0.27	0/2145	0.43	0/2893
9	Y	0.28	0/2143	0.41	0/2888
9	Z	0.31	0/2170	0.45	0/2926
10	G	0.35	0/1735	0.45	0/2320
11	N	0.28	0/889	0.43	0/1200
12	U	0.36	0/1716	0.48	0/2333
13	V	0.43	0/425	0.45	0/582
14	0	0.41	0/1532	0.51	0/2082
15	1	0.39	0/1080	0.51	0/1461
15	2	0.39	0/1080	0.49	0/1461
15	3	0.40	0/1080	0.50	0/1461
15	4	0.40	0/1080	0.52	0/1461
15	5	0.40	0/1080	0.49	0/1461
15	6	0.40	0/1080	0.48	0/1461
15	7	0.40	0/1080	0.48	0/1461
15	8	0.39	0/1080	0.51	0/1461

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
15	9	0.40	0/1080	0.51	0/1461
16	Q	0.43	0/2910	0.52	0/3940
17	P	0.39	1/3576 (0.0%)	0.53	1/4819 (0.0%)
All	All	0.37	1/73510 (0.0%)	0.47	1/99324 (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
2	O	0	1
7	C	0	2
12	U	0	1
15	1	0	1
17	P	0	1
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	P	151	TRP	CB-CG	15.72	1.78	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	P	151	TRP	CA-CB-CG	11.73	135.99	113.70

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	1	9	GLU	Peptide
7	C	20	TYR	Peptide
7	C	305	ILE	Peptide
2	O	312	LEU	Peptide
17	P	150	ALA	Peptide
12	U	417	ASP	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	6147	0	6172	233	0
2	O	3035	0	3077	154	0
3	H	1817	0	1881	43	0
3	I	1822	0	1886	54	0
3	J	1822	0	1886	32	0
4	K	938	0	947	43	0
4	L	938	0	947	35	0
4	M	938	0	947	34	0
5	S	631	0	647	24	0
6	T	658	0	652	15	0
7	A	4656	0	4642	65	0
7	B	4656	0	4642	85	0
7	C	4656	0	4642	115	0
8	D	3666	0	3665	57	0
8	E	3666	0	3665	78	0
8	F	3666	0	3665	70	0
9	X	2111	0	2134	59	0
9	Y	2110	0	2132	61	0
9	Z	2136	0	2158	40	0
10	G	1717	0	1829	23	0
11	N	875	0	878	28	0
12	U	1662	0	1583	49	0
13	V	411	0	401	8	0
14	0	1498	0	1544	49	0
15	1	1065	0	1131	39	0
15	2	1065	0	1131	33	0
15	3	1065	0	1131	31	0
15	4	1065	0	1131	27	0
15	5	1065	0	1131	25	0
15	6	1065	0	1131	28	0
15	7	1065	0	1131	32	0
15	8	1065	0	1131	17	0
15	9	1065	0	1131	29	0
16	Q	2844	0	2782	72	0
17	P	3508	0	3483	242	0
18	R	28	0	26	2	0
18	U	84	0	78	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	A	27	0	12	1	0
All	All	72308	0	73182	1855	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 13.

All (1855) 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)
17:P:151:TRP:CB	17:P:151:TRP:CG	1.78	1.66
17:P:148:LEU:H	17:P:151:TRP:HD1	0.99	0.93
17:P:149:ALA:C	17:P:151:TRP:HB2	1.92	0.90
17:P:150:ALA:N	17:P:151:TRP:HB2	1.88	0.88
7:C:296:MET:HG2	7:C:305:ILE:HD13	1.56	0.87
7:C:24:VAL:HG11	7:C:70:THR:HG21	1.58	0.85
7:B:391:ARG:NH1	7:B:401:GLU:OE2	2.10	0.84
1:R:123:LEU:HG	1:R:209:PRO:HA	1.62	0.82
3:H:97:GLU:OE1	4:K:92:ARG:NH2	2.13	0.82
1:R:800:LEU:HD21	15:1:133:LEU:HD12	1.63	0.80
17:P:147:LYS:HA	17:P:151:TRP:HA	1.61	0.80
3:I:30:ILE:HG21	4:L:25:ALA:HB1	1.64	0.80
9:Y:144:ALA:O	9:Y:149:ASN:ND2	2.13	0.80
4:K:53:LYS:HA	4:K:56:LYS:HD2	1.64	0.78
17:P:148:LEU:N	17:P:151:TRP:HB3	1.99	0.78
7:B:459:ARG:NH2	8:F:201:GLU:OE1	2.17	0.77
7:A:234:LEU:HD21	7:A:448:VAL:HG11	1.64	0.77
8:F:82:ARG:NH1	8:F:101:GLY:O	2.18	0.77
17:P:61:GLU:HA	17:P:64:GLU:HG3	1.67	0.76
17:P:273:LEU:HB2	17:P:285:ILE:HD13	1.67	0.76
1:R:210:VAL:HG23	1:R:211:THR:HG23	1.67	0.76
7:B:264:SER:O	7:B:308:ARG:NH2	2.16	0.76
7:B:350:SER:H	7:B:409:ALA:HB3	1.49	0.76
8:E:298:THR:HG23	8:E:353:ILE:HD11	1.67	0.76
2:O:211:ARG:HG3	4:M:4:GLN:HG2	1.67	0.76
6:T:113:GLY:HA2	6:T:116:LEU:HD12	1.67	0.76
7:B:296:MET:HG3	7:B:305:ILE:HG22	1.66	0.76
17:P:256:MET:HA	17:P:259:HIS:CD2	2.21	0.75
8:F:238:MET:SD	8:F:242:ARG:NH2	2.60	0.75
3:J:20:GLU:HA	4:M:17:ARG:HH12	1.50	0.75
3:I:38:PHE:HB2	4:L:32:ARG:HG3	1.67	0.75
17:P:148:LEU:N	17:P:151:TRP:HD1	1.81	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:385:GLU:HG3	17:P:390:LEU:HG	1.66	0.75
3:H:44:ARG:HE	4:K:37:LYS:HE2	1.51	0.75
9:Y:61:ARG:O	9:Y:64:GLU:N	2.19	0.75
2:O:190:PRO:HA	2:O:222:SER:HA	1.66	0.74
17:P:215:ARG:NH1	17:P:249:LEU:O	2.20	0.74
2:O:92:LEU:HD22	2:O:97:ASP:HA	1.69	0.74
9:Z:211:SER:HB2	9:Z:214:GLU:HG3	1.70	0.74
12:U:453:MET:SD	15:1:119:ARG:NH2	2.61	0.74
1:R:316:GLN:HG3	1:R:318:CYS:H	1.53	0.74
7:B:50:LEU:HD23	7:B:68:GLU:HB2	1.71	0.73
7:A:391:ARG:NH1	7:A:401:GLU:OE2	2.20	0.73
17:P:146:ALA:O	17:P:151:TRP:CG	2.42	0.72
1:R:191:CYS:HB2	1:R:229:LEU:HD21	1.72	0.72
7:C:290:ASP:HA	7:C:293:GLU:HG3	1.72	0.72
9:Z:201:LYS:NZ	9:Z:229:MET:SD	2.63	0.72
17:P:293:LEU:HD21	17:P:341:LYS:HD2	1.70	0.72
7:B:265:LYS:HE3	7:B:294:LEU:HD21	1.70	0.72
7:B:278:GLY:H	7:B:314:ASN:HD22	1.36	0.72
2:O:21:LYS:HD2	2:O:37:LYS:HG3	1.70	0.72
9:X:172:ASN:HB3	9:X:175:ILE:HG12	1.71	0.71
1:R:12:LEU:HD11	1:R:322:GLU:HB3	1.72	0.71
9:Z:207:GLN:HE22	9:Z:209:GLU:HB2	1.54	0.71
3:H:30:ILE:HG23	4:K:25:ALA:HB2	1.72	0.71
2:O:210:PRO:HD2	3:J:8:VAL:HG23	1.70	0.71
3:I:182:GLU:HG2	3:I:193:SER:HA	1.73	0.71
9:Y:90:GLU:OE2	9:Y:127:HIS:ND1	2.19	0.71
17:P:229:GLY:O	17:P:233:ASN:ND2	2.24	0.71
3:I:65:GLU:HG2	3:I:68:LYS:HE2	1.73	0.71
9:Y:25:LYS:HE2	9:Y:82:SER:HA	1.73	0.71
17:P:283:ARG:HA	17:P:331:ILE:HD11	1.72	0.71
17:P:148:LEU:N	17:P:151:TRP:CD1	2.54	0.70
1:R:176:ASN:HA	1:R:217:LYS:HA	1.74	0.70
14:0:87:LYS:NZ	15:1:126:ARG:O	2.24	0.70
7:C:503:GLU:OE2	7:C:567:TRP:N	2.25	0.70
1:R:198:ARG:HH22	1:R:248:PRO:HG2	1.55	0.70
8:F:421:GLN:NE2	8:F:425:CYS:SG	2.62	0.70
16:Q:298:GLU:OE2	16:Q:302:ASN:ND2	2.24	0.70
7:C:264:SER:O	7:C:308:ARG:NH2	2.24	0.70
9:X:36:ILE:HG13	9:X:95:VAL:HG21	1.71	0.70
9:X:140:LEU:HD12	9:X:153:ARG:HE	1.56	0.70
17:P:307:LEU:HD22	17:P:311:GLN:HE21	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:183:ILE:HD12	8:F:189:ILE:HG21	1.74	0.70
15:1:59:VAL:HG21	15:2:134:ILE:HD12	1.73	0.70
2:O:100:THR:OG1	2:O:104:ARG:NH2	2.19	0.69
7:A:436:ASP:OD1	7:A:437:LYS:N	2.25	0.69
1:R:481:VAL:HG11	5:S:76:LEU:HD13	1.74	0.69
8:E:82:ARG:NH1	8:E:101:GLY:O	2.24	0.69
8:F:414:ASP:OD2	8:F:481:TRP:NE1	2.21	0.69
9:X:210:GLU:HA	9:X:257:LYS:HE2	1.73	0.69
7:A:560:GLN:NE2	7:A:561:SER:OG	2.26	0.69
1:R:90:PHE:O	1:R:92:ARG:NH2	2.26	0.69
1:R:490:THR:HG22	1:R:491:GLU:H	1.56	0.69
1:R:585:TYR:HA	1:R:588:ILE:HD12	1.74	0.69
9:X:205:LYS:HD3	9:X:260:LEU:HD11	1.72	0.69
2:O:30:ASN:OD1	2:O:330:LYS:NZ	2.26	0.69
14:0:71:ILE:HG21	14:0:157:ILE:HD13	1.75	0.69
9:Y:87:ILE:HD13	9:Y:121:LEU:HD22	1.74	0.68
15:3:117:GLY:HA3	15:3:131:MET:HG3	1.75	0.68
7:B:558:THR:HG21	7:B:565:ILE:HG13	1.74	0.68
12:U:298:THR:O	12:U:310:SER:OG	2.11	0.68
2:O:99:VAL:HA	2:O:102:ILE:HD12	1.76	0.68
17:P:108:VAL:O	17:P:110:ILE:N	2.26	0.68
17:P:256:MET:HA	17:P:259:HIS:HD2	1.56	0.68
15:3:59:VAL:HG21	15:4:134:ILE:HD12	1.74	0.68
1:R:734:ASN:ND2	1:R:809:GLU:OE2	2.27	0.68
7:C:29:VAL:HG12	7:C:30:THR:H	1.58	0.68
8:E:88:GLU:OE1	8:E:314:ARG:NH2	2.26	0.68
8:D:175:SER:OG	8:D:471:ARG:NH1	2.27	0.68
17:P:136:PHE:O	17:P:140:MET:N	2.25	0.68
1:R:18:GLN:HE22	1:R:20:GLU:HG3	1.59	0.68
1:R:91:PRO:HG2	1:R:94:MET:HG2	1.76	0.68
7:C:43:VAL:HG21	7:C:64:ILE:HD13	1.76	0.68
17:P:227:ILE:HA	17:P:230:VAL:HG12	1.75	0.68
14:0:122:ASP:HB2	14:0:126:ILE:HD13	1.74	0.67
7:C:50:LEU:HD23	7:C:68:GLU:HB2	1.76	0.67
7:A:395:LEU:O	7:A:400:ARG:NH2	2.27	0.67
14:0:59:SER:HB3	15:1:101:LEU:HD23	1.74	0.67
16:Q:324:GLN:OE1	16:Q:327:ARG:NH1	2.27	0.67
17:P:38:GLN:OE1	17:P:40:GLN:NE2	2.27	0.67
3:H:44:ARG:NH2	3:H:48:THR:OG1	2.28	0.67
7:B:443:LYS:HB2	8:E:494:ARG:CZ	2.23	0.67
2:O:23:HIS:O	2:O:27:SER:N	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:50:GLN:HA	4:K:53:LYS:HE2	1.76	0.67
9:X:120:ASN:HB3	9:X:123:LYS:HE2	1.76	0.67
17:P:52:ARG:HH22	17:P:68:THR:HG22	1.58	0.67
1:R:444:PHE:O	1:R:447:ARG:NH1	2.28	0.67
1:R:650:MET:O	1:R:720:GLN:NE2	2.28	0.67
11:N:11:ILE:HB	11:N:66:ILE:HG12	1.76	0.67
14:0:112:SER:O	15:1:155:LYS:NZ	2.27	0.67
17:P:150:ALA:N	17:P:151:TRP:CB	2.58	0.67
17:P:151:TRP:CG	17:P:151:TRP:HB2	2.21	0.67
7:C:20:TYR:HB3	7:C:32:CYS:HB2	1.76	0.66
8:F:298:THR:HG23	8:F:353:ILE:HD11	1.76	0.66
2:O:35:THR:HB	2:O:321:LEU:HD13	1.75	0.66
2:O:350:ILE:HG22	2:O:352:ALA:H	1.61	0.66
17:P:124:PRO:HA	17:P:127:LEU:HD13	1.78	0.66
10:G:119:TYR:O	10:G:135:LYS:NZ	2.28	0.66
15:9:117:GLY:HA3	15:9:131:MET:HG3	1.77	0.66
1:R:35:VAL:HB	1:R:323:VAL:HB	1.78	0.66
17:P:102:GLN:HG3	17:P:143:ARG:HE	1.61	0.66
3:H:37:GLU:HG3	4:K:29:LYS:HG2	1.78	0.66
15:4:6:SER:N	15:4:83:ASP:OD2	2.28	0.66
3:H:77:ASN:OD1	3:H:80:ARG:NH2	2.28	0.66
8:F:441:GLU:HG2	8:F:444:LEU:HD12	1.77	0.66
1:R:7:SER:O	1:R:387:ARG:NH1	2.28	0.66
2:O:11:GLY:O	2:O:315:ASN:ND2	2.29	0.66
16:Q:108:ASN:ND2	16:Q:133:GLY:O	2.29	0.66
9:Y:205:LYS:NZ	9:Y:206:ASP:OD1	2.28	0.66
3:J:31:ASP:OD2	4:M:28:ARG:NH1	2.29	0.65
8:F:106:ASP:OD1	8:F:107:ALA:N	2.26	0.65
9:Y:270:ASN:O	9:Y:274:ASN:N	2.25	0.65
7:B:43:VAL:HG21	7:B:64:ILE:HD13	1.78	0.65
17:P:103:GLU:HG3	17:P:104:ASN:H	1.62	0.65
8:F:369:THR:O	8:F:373:THR:OG1	2.14	0.65
8:D:46:THR:HG22	8:D:113:GLU:HB2	1.77	0.65
1:R:131:ILE:HG13	1:R:246:PRO:HG3	1.78	0.65
8:D:141:ARG:HA	9:Z:9:LYS:HD2	1.77	0.65
12:U:267:ILE:HG22	12:U:404:ALA:HA	1.78	0.65
16:Q:158:THR:HG22	16:Q:160:LEU:H	1.60	0.65
7:C:242:GLN:NE2	7:C:268:ASN:OD1	2.27	0.65
15:6:117:GLY:HA3	15:6:131:MET:HG3	1.77	0.65
12:U:355:TYR:HB2	12:U:387:ARG:HG3	1.79	0.65
14:0:109:ILE:HD13	15:1:151:ILE:HD13	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:5:88:LYS:O	15:5:92:GLN:HG2	1.97	0.65
15:4:47:MET:HG3	15:4:48:ARG:HG2	1.78	0.64
3:I:42:LYS:NZ	4:L:39:GLU:OE1	2.31	0.64
1:R:598:ASP:HA	5:S:61:ASN:HB3	1.79	0.64
1:R:809:GLU:O	1:R:813:LYS:NZ	2.30	0.64
9:Z:242:LEU:HD23	9:Z:266:ILE:HG23	1.79	0.64
15:2:113:VAL:HG21	15:2:134:ILE:HG21	1.79	0.64
2:O:336:HIS:HB2	2:O:349:ILE:HD11	1.79	0.64
16:Q:259:ASP:N	16:Q:263:GLN:OE1	2.27	0.64
2:O:218:GLU:HA	2:O:223:TYR:HA	1.79	0.64
4:K:32:ARG:HA	4:K:35:GLN:HE21	1.62	0.64
7:C:278:GLY:N	7:C:314:ASN:O	2.25	0.64
7:A:171:ARG:NH2	7:A:213:GLN:OE1	2.31	0.64
7:A:350:SER:H	7:A:409:ALA:HB3	1.63	0.64
8:E:86:VAL:HG12	8:E:96:VAL:HG22	1.80	0.64
17:P:133:GLN:HG2	17:P:138:VAL:HG11	1.80	0.64
2:O:312:LEU:H	3:I:14:HIS:CE1	2.16	0.64
17:P:130:LEU:HA	17:P:138:VAL:HG12	1.78	0.64
3:H:50:ARG:HD3	4:K:44:ILE:HD11	1.80	0.64
1:R:786:THR:HA	1:R:790:LEU:HD13	1.80	0.64
3:H:16:MET:O	3:H:20:GLU:HG2	1.97	0.64
1:R:315:THR:HB	4:K:11:LEU:HD12	1.79	0.63
7:A:282:ASN:ND2	8:D:374:GLU:OE2	2.29	0.63
15:2:47:MET:HG3	15:2:48:ARG:HG2	1.80	0.63
8:F:201:GLU:OE2	8:F:201:GLU:N	2.28	0.63
15:7:47:MET:HG3	15:7:48:ARG:HG2	1.80	0.63
17:P:293:LEU:O	17:P:296:SER:OG	2.16	0.63
2:O:322:GLN:NE2	2:O:324:ASN:OD1	2.30	0.63
7:C:115:SER:OG	7:C:116:ILE:N	2.32	0.63
1:R:192:ARG:HD3	2:O:309:ARG:HA	1.79	0.63
5:S:73:ILE:HA	5:S:76:LEU:HG	1.80	0.63
17:P:114:TYR:HD2	17:P:119:LYS:HZ1	1.46	0.63
3:I:3:LEU:HD13	3:I:7:ASP:HB3	1.81	0.63
7:C:295:THR:HB	7:C:303:GLU:C	2.19	0.63
1:R:64:LYS:HG2	1:R:102:GLU:HG2	1.79	0.63
10:G:55:LYS:NZ	11:N:103:ASP:OD2	2.25	0.63
17:P:266:ILE:HG23	17:P:267:PRO:HD3	1.80	0.63
4:K:48:ARG:O	4:K:52:GLU:HG2	1.99	0.63
6:T:55:ILE:HD11	6:T:123:PHE:HB2	1.80	0.63
8:E:106:ASP:OD1	8:E:107:ALA:N	2.32	0.63
1:R:44:VAL:HG13	1:R:48:GLN:HB2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Y:256:THR:HG23	9:Y:259:LEU:H	1.62	0.63
2:O:219:ASP:OD1	2:O:222:SER:N	2.33	0.62
9:Y:111:GLN:OE1	9:Y:168:ILE:N	2.32	0.62
15:3:47:MET:HG2	15:3:48:ARG:HG2	1.82	0.62
15:7:72:VAL:HG11	15:7:99:VAL:HG11	1.81	0.62
17:P:204:CYS:O	17:P:208:MET:HG2	1.98	0.62
1:R:334:GLN:HG2	1:R:337:LEU:HD12	1.80	0.62
18:R:902:NAG:O6	5:S:70:ASN:ND2	2.33	0.62
15:4:44:MET:HB2	15:4:122:ALA:HB2	1.81	0.62
15:7:130:GLY:O	15:7:134:ILE:HG12	1.98	0.62
1:R:28:GLU:HB3	1:R:339:ARG:HH11	1.65	0.62
9:Z:36:ILE:HG13	9:Z:95:VAL:HG11	1.81	0.62
9:Z:61:ARG:NH2	9:Z:63:GLU:OE2	2.31	0.62
2:O:194:HIS:CD2	2:O:223:TYR:HB2	2.35	0.62
8:F:272:ILE:O	8:F:276:ARG:NH1	2.32	0.62
17:P:215:ARG:HD3	17:P:250:LEU:HA	1.79	0.62
3:J:168:ASP:OD2	3:J:188:ARG:NH2	2.33	0.62
11:N:26:GLY:HA2	11:N:35:ASN:HD21	1.63	0.62
12:U:374:VAL:HG23	12:U:397:LEU:HB2	1.82	0.62
1:R:208:ASP:HB2	1:R:213:ASP:H	1.64	0.62
9:Z:44:LYS:NZ	9:Z:113:GLU:OE2	2.33	0.62
2:O:52:VAL:O	2:O:55:SER:OG	2.13	0.61
4:L:30:ASN:OD1	4:L:31:ARG:NH1	2.33	0.61
9:Y:267:VAL:O	9:Y:271:GLU:HG2	2.00	0.61
1:R:45:ASN:HB2	1:R:48:GLN:HE22	1.65	0.61
1:R:722:ILE:HA	1:R:725:ILE:HG22	1.83	0.61
3:I:101:ARG:NH2	4:L:97:ASP:OD1	2.32	0.61
4:K:54:GLU:HG3	4:K:58:LYS:HE2	1.81	0.61
7:A:610:ASN:OD1	7:A:613:ARG:NH2	2.33	0.61
2:O:139:ARG:NH2	2:O:275:GLN:OE1	2.32	0.61
3:H:159:THR:O	3:H:161:ASN:ND2	2.33	0.61
2:O:241:ALA:HB1	2:O:246:PHE:HB2	1.82	0.61
3:J:42:LYS:HA	4:M:40:ALA:HB2	1.81	0.61
9:Z:232:TYR:O	9:Z:236:LYS:NZ	2.27	0.61
17:P:49:PHE:HB3	17:P:52:ARG:HH21	1.66	0.61
2:O:13:LYS:NZ	2:O:15:CYS:SG	2.69	0.61
9:Y:29:ILE:HD11	9:Y:85:SER:HA	1.81	0.61
11:N:94:LYS:HD2	16:Q:338:GLN:HE21	1.65	0.61
13:V:328:ILE:HG12	15:3:32:TYR:HD1	1.64	0.61
15:6:72:VAL:HG11	15:6:99:VAL:HG11	1.83	0.61
3:I:30:ILE:O	4:L:29:LYS:NZ	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:185:LEU:HD11	2:O:234:VAL:HG13	1.83	0.61
7:B:399:GLU:HG2	9:Y:86:LEU:HD13	1.82	0.61
14:0:129:ARG:HH22	14:0:204:GLY:HA3	1.65	0.61
7:C:391:ARG:NH1	7:C:401:GLU:OE2	2.33	0.61
8:D:485:ARG:HH12	8:D:506:ARG:HH21	1.49	0.61
9:X:270:ASN:HD22	9:X:274:ASN:HD21	1.48	0.61
15:5:113:VAL:HG21	15:5:134:ILE:HG21	1.82	0.61
17:P:364:LEU:O	17:P:405:GLN:NE2	2.31	0.61
12:U:359:SER:OG	12:U:360:GLN:OE1	2.14	0.61
15:2:28:LEU:HD12	15:3:105:ALA:HB2	1.82	0.61
15:7:6:SER:OG	15:7:7:GLY:N	2.33	0.61
16:Q:308:ASN:HB2	16:Q:311:HIS:CD2	2.35	0.61
2:O:231:ARG:O	2:O:231:ARG:NH2	2.29	0.60
3:H:49:GLN:HA	3:H:52:LYS:HE2	1.83	0.60
15:1:88:LYS:O	15:1:92:GLN:NE2	2.33	0.60
7:C:566:THR:H	7:C:569:ILE:HD12	1.65	0.60
14:0:60:LEU:HA	14:0:63:VAL:HG12	1.84	0.60
17:P:155:LEU:HD21	17:P:214:TYR:HB3	1.84	0.60
17:P:209:LEU:HD12	17:P:246:SER:HB2	1.83	0.60
8:E:238:MET:SD	8:E:242:ARG:NH2	2.75	0.60
16:Q:217:ASP:OD2	16:Q:274:TYR:OH	2.12	0.60
16:Q:246:ARG:NH1	16:Q:273:GLU:OE1	2.32	0.60
17:P:146:ALA:C	17:P:151:TRP:CG	2.74	0.60
17:P:234:LYS:NZ	17:P:235:CYS:O	2.34	0.60
16:Q:254:GLN:HG3	16:Q:267:VAL:HG22	1.81	0.60
1:R:782:PHE:O	1:R:786:THR:OG1	2.16	0.60
17:P:17:ASN:OD1	17:P:18:ILE:HD12	2.01	0.60
1:R:170:PHE:O	1:R:198:ARG:NH2	2.35	0.60
4:M:28:ARG:O	4:M:32:ARG:N	2.34	0.60
8:D:217:LYS:HG2	8:D:218:ASP:H	1.66	0.60
9:Y:259:LEU:O	9:Y:263:ILE:HG12	2.00	0.60
17:P:151:TRP:CG	17:P:151:TRP:HB3	2.21	0.60
9:X:48:ASP:OD2	9:X:116:LYS:NZ	2.34	0.60
12:U:454:ASP:OD1	12:U:454:ASP:N	2.34	0.60
14:0:71:ILE:HG23	16:Q:10:ASN:HD22	1.66	0.60
1:R:517:GLY:O	5:S:59:GLN:NE2	2.31	0.60
15:2:6:SER:OG	15:2:7:GLY:N	2.35	0.60
3:I:61:GLU:HA	3:I:64:ILE:HG12	1.83	0.59
7:C:567:TRP:HE1	7:C:571:ARG:HH21	1.48	0.59
8:F:208:ARG:NH2	8:F:467:PRO:O	2.34	0.59
14:0:193:VAL:HG11	15:9:23:MET:HG2	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:325:LYS:HG3	2:O:326:LYS:HG2	1.82	0.59
8:F:360:ASP:OD1	8:F:361:ILE:N	2.34	0.59
8:F:436:LYS:HG3	8:F:444:LEU:HD11	1.84	0.59
15:6:44:MET:HG3	15:6:119:ARG:HA	1.84	0.59
9:X:259:LEU:O	9:X:263:ILE:HG13	2.01	0.59
12:U:416:SER:O	12:U:417:ASP:HB2	2.02	0.59
17:P:108:VAL:C	17:P:110:ILE:H	2.05	0.59
3:H:35:GLU:OE2	17:P:210:ARG:NH2	2.35	0.59
8:E:318:PRO:HG3	10:G:201:ARG:HD2	1.85	0.59
16:Q:177:ASN:OD1	16:Q:178:ILE:N	2.32	0.59
1:R:190:VAL:HG13	1:R:191:CYS:H	1.68	0.59
6:T:66:ILE:O	6:T:70:ILE:HG12	2.02	0.59
11:N:6:LYS:NZ	11:N:59:ASP:O	2.35	0.59
17:P:304:GLU:O	17:P:308:ALA:HB2	2.03	0.59
1:R:607:SER:HB3	1:R:610:ILE:HG22	1.83	0.59
4:K:8:ILE:O	4:K:12:LEU:HG	2.03	0.59
8:E:175:SER:OG	8:E:471:ARG:NH1	2.36	0.59
12:U:403:GLN:NE2	12:U:406:ASN:O	2.34	0.59
14:0:39:TRP:NE1	14:0:43:GLU:OE1	2.35	0.59
15:6:59:VAL:HG21	15:7:134:ILE:HD12	1.84	0.59
7:A:100:ASP:OD1	7:A:104:ARG:N	2.27	0.59
8:E:106:ASP:OD1	8:E:108:LYS:N	2.34	0.59
15:5:150:LEU:O	15:5:154:THR:HG22	2.03	0.59
17:P:87:GLU:HA	17:P:90:VAL:HG12	1.85	0.59
7:B:246:THR:OG1	7:B:247:ALA:N	2.34	0.59
9:X:213:PHE:O	9:X:222:GLN:NE2	2.36	0.59
12:U:368:SER:HB3	12:U:403:GLN:HB2	1.85	0.59
15:5:48:ARG:NH1	15:5:122:ALA:O	2.36	0.59
17:P:103:GLU:O	17:P:105:HIS:ND1	2.35	0.59
1:R:329:ASP:HB2	1:R:332:SER:HB3	1.85	0.59
9:Y:98:ILE:HG22	9:Y:160:GLN:HG2	1.84	0.59
17:P:244:ILE:HG13	17:P:284:ILE:HG13	1.84	0.59
17:P:283:ARG:HG2	17:P:331:ILE:HD11	1.85	0.59
17:P:329:GLU:O	17:P:332:SER:OG	2.17	0.59
3:J:206:GLN:HE22	8:F:40:LEU:HB2	1.67	0.58
11:N:8:ILE:HB	11:N:25:ILE:HG12	1.85	0.58
14:0:200:ARG:NH2	15:9:77:ALA:O	2.36	0.58
1:R:286:ALA:HA	1:R:289:ASN:HD22	1.68	0.58
7:B:109:ILE:O	7:B:113:THR:OG1	2.20	0.58
9:Y:146:THR:HG23	9:Y:149:ASN:H	1.66	0.58
9:Z:61:ARG:NH1	9:Z:64:GLU:OE2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Z:90:GLU:OE2	9:Z:127:HIS:ND1	2.32	0.58
10:G:93:LYS:HE2	11:N:7:LEU:HD21	1.85	0.58
15:1:34:THR:HG23	15:1:59:VAL:HG13	1.84	0.58
17:P:76:THR:O	17:P:80:LEU:HB2	2.03	0.58
1:R:17:LEU:HD13	1:R:22:ALA:HA	1.84	0.58
3:J:16:MET:HE1	4:M:11:LEU:HA	1.85	0.58
7:B:296:MET:SD	7:B:308:ARG:NH2	2.75	0.58
8:F:194:ALA:HB3	8:F:197:LEU:HD12	1.85	0.58
16:Q:46:LYS:O	16:Q:50:GLN:HG3	2.03	0.58
1:R:170:PHE:HE1	1:R:225:GLN:HG2	1.68	0.58
7:C:177:THR:OG1	7:C:193:GLU:O	2.21	0.58
7:C:298:VAL:HG23	7:C:299:ASP:H	1.67	0.58
7:A:274:TYR:HB3	7:A:311:LEU:HD23	1.85	0.58
8:E:231:PHE:HB3	8:E:259:LEU:HD23	1.86	0.58
12:U:329:ASN:ND2	12:U:339:TRP:O	2.33	0.58
15:1:9:GLU:O	15:1:10:TYR:HB2	2.02	0.58
1:R:296:LYS:O	1:R:300:MET:N	2.36	0.58
1:R:597:TYR:OH	1:R:627:MET:O	2.21	0.58
1:R:787:VAL:HA	1:R:791:LEU:HD12	1.86	0.58
2:O:68:VAL:O	2:O:72:VAL:HG23	2.02	0.58
7:A:24:VAL:HG12	7:A:29:VAL:HG13	1.84	0.58
14:0:154:CYS:HG	15:9:34:THR:HG1	1.49	0.58
17:P:149:ALA:N	17:P:151:TRP:CG	2.71	0.58
3:J:46:VAL:HG23	4:M:44:ILE:HG13	1.85	0.58
7:C:592:ASP:HB3	7:C:596:LYS:HD2	1.85	0.58
7:A:226:PRO:HA	7:A:241:VAL:HA	1.85	0.58
17:P:433:GLY:HA2	17:P:436:LEU:HD13	1.85	0.58
1:R:118:LEU:HD22	1:R:272:LEU:HD13	1.85	0.58
2:O:263:GLU:OE2	2:O:267:ARG:NH1	2.37	0.58
17:P:80:LEU:HA	17:P:83:HIS:HB2	1.86	0.58
15:2:109:ALA:O	15:2:113:VAL:HG12	2.04	0.58
1:R:18:GLN:O	1:R:22:ALA:N	2.24	0.58
9:Y:217:LEU:HD12	9:Y:218:PRO:HD2	1.84	0.58
8:E:208:ARG:NH2	8:E:467:PRO:O	2.37	0.58
8:D:298:THR:HG23	8:D:353:ILE:HD11	1.86	0.58
15:1:76:ILE:HD12	15:1:92:GLN:HG3	1.85	0.58
15:6:10:TYR:CZ	15:7:86:LEU:HD21	2.39	0.58
2:O:332:ARG:HD2	2:O:354:MET:HB3	1.86	0.57
17:P:441:MET:HE1	17:P:456:VAL:HG11	1.85	0.57
7:A:559:ALA:HA	7:A:564:LYS:HG3	1.85	0.57
8:F:365:ILE:HB	8:F:366:PRO:HD3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:61:ASP:OD2	8:D:93:LYS:NZ	2.36	0.57
17:P:259:HIS:O	17:P:262:ARG:NH1	2.36	0.57
1:R:45:ASN:H	1:R:48:GLN:NE2	2.02	0.57
17:P:313:LYS:HG3	17:P:316:LYS:HD3	1.86	0.57
1:R:65:LEU:HA	1:R:68:VAL:HG12	1.86	0.57
1:R:88:VAL:HA	1:R:299:LYS:HE2	1.85	0.57
15:7:138:ALA:HA	15:7:141:LEU:HD23	1.86	0.57
15:8:9:GLU:HG3	15:8:10:TYR:H	1.68	0.57
3:H:182:GLU:HG2	3:H:193:SER:HA	1.86	0.57
8:E:447:ASP:HA	8:E:450:LEU:HD12	1.86	0.57
1:R:500:LEU:HD23	5:S:73:ILE:HD12	1.86	0.57
2:O:2:THR:HG22	2:O:3:GLU:H	1.68	0.57
3:H:34:ALA:O	4:K:32:ARG:NH1	2.37	0.57
7:C:37:ALA:HB2	7:C:81:ARG:HD3	1.87	0.57
7:C:242:GLN:OE1	7:C:343:HIS:ND1	2.38	0.57
7:C:291:PHE:CG	7:C:305:ILE:HG13	2.39	0.57
7:A:201:GLU:OE2	7:A:203:PHE:HB2	2.05	0.57
11:N:72:GLU:OE2	11:N:75:ARG:NH2	2.35	0.57
15:2:130:GLY:O	15:2:134:ILE:HG12	2.04	0.57
17:P:261:ARG:NH1	17:P:301:THR:O	2.38	0.57
17:P:445:ASP:HB3	17:P:448:VAL:HG22	1.86	0.57
9:X:106:ASP:OD1	9:X:107:LEU:N	2.37	0.57
9:X:261:ASP:O	9:X:265:ARG:HG2	2.03	0.57
1:R:28:GLU:HG2	1:R:339:ARG:HE	1.69	0.57
1:R:480:SER:HA	1:R:482:ARG:HH11	1.70	0.57
15:5:9:GLU:O	15:5:10:TYR:HB2	2.05	0.57
7:B:51:VAL:HG23	7:B:67:TYR:HB2	1.86	0.57
7:B:69:GLU:OE1	7:B:120:ARG:NH2	2.38	0.57
12:U:289:THR:HG22	12:U:290:PHE:H	1.70	0.57
3:I:93:ASP:OD2	4:L:92:ARG:NH2	2.38	0.56
8:F:152:ASP:OD1	8:F:153:ILE:N	2.37	0.56
7:C:290:ASP:OD1	7:C:291:PHE:N	2.38	0.56
8:D:377:ILE:O	8:D:397:SER:OG	2.23	0.56
15:2:20:SER:O	15:2:24:VAL:HG12	2.05	0.56
15:6:51:GLN:O	15:6:55:SER:OG	2.15	0.56
17:P:147:LYS:HA	17:P:151:TRP:CA	2.34	0.56
1:R:41:ASN:HB2	1:R:44:VAL:HB	1.85	0.56
1:R:178:GLU:O	1:R:179:ARG:NH2	2.34	0.56
1:R:435:ASN:HD22	1:R:441:SER:HA	1.70	0.56
4:L:105:ASP:OD2	4:L:107:ARG:NH1	2.33	0.56
9:Y:94:LEU:HA	9:Y:130:LEU:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:0:38:ALA:O	14:0:42:THR:HG23	2.05	0.56
15:5:9:GLU:HG3	15:5:10:TYR:H	1.69	0.56
15:8:59:VAL:HG21	15:9:134:ILE:HD12	1.87	0.56
17:P:224:VAL:O	17:P:228:MET:HG3	2.04	0.56
9:Y:126:TYR:HE1	9:Y:169:THR:HA	1.70	0.56
17:P:148:LEU:HD11	17:P:155:LEU:HB3	1.88	0.56
17:P:356:SER:HA	17:P:359:LEU:HD12	1.87	0.56
17:P:150:ALA:CB	17:P:151:TRP:HE3	2.19	0.56
1:R:44:VAL:HG11	1:R:49:ARG:HE	1.70	0.56
1:R:57:ARG:HD3	1:R:95:ILE:HG21	1.88	0.56
2:O:101:TYR:HE1	2:O:295:ILE:HG21	1.70	0.56
3:J:38:PHE:HE1	4:M:35:GLN:HG3	1.70	0.56
8:E:205:GLN:O	8:E:209:GLN:HG2	2.06	0.56
1:R:288:LYS:O	1:R:291:ARG:NE	2.34	0.56
2:O:28:LYS:HD2	2:O:28:LYS:N	2.21	0.56
2:O:29:ASN:HD22	2:O:324:ASN:HD22	1.53	0.56
2:O:64:PHE:O	2:O:68:VAL:HG23	2.06	0.56
2:O:303:PHE:O	2:O:307:VAL:HG23	2.05	0.56
3:I:21:GLN:HA	3:I:24:ASN:HD21	1.69	0.56
7:C:295:THR:HG21	7:C:302:VAL:HG13	1.87	0.56
8:E:279:LEU:HB3	8:E:337:ARG:HD2	1.86	0.56
9:Y:159:LEU:HD21	9:Y:179:PHE:CE1	2.40	0.56
14:0:42:THR:HA	15:9:10:TYR:OH	2.06	0.56
2:O:13:LYS:HG3	2:O:15:CYS:H	1.69	0.56
7:C:449:ASN:HD22	7:C:452:ILE:HG12	1.70	0.56
15:8:72:VAL:HG11	15:8:99:VAL:HG11	1.86	0.56
17:P:215:ARG:O	17:P:219:VAL:HG23	2.06	0.56
17:P:392:LYS:O	17:P:396:LYS:NZ	2.39	0.56
4:K:11:LEU:O	4:K:15:GLU:HG3	2.06	0.56
8:F:438:VAL:HG23	8:F:439:VAL:HG23	1.87	0.56
15:5:14:PHE:HB2	15:5:89:SER:OG	2.06	0.56
17:P:119:LYS:HA	17:P:153:LYS:HZ1	1.71	0.56
17:P:149:ALA:N	17:P:151:TRP:CB	2.69	0.56
7:C:296:MET:HG2	7:C:305:ILE:HG21	1.88	0.55
1:R:93:ASP:N	1:R:93:ASP:OD1	2.38	0.55
1:R:299:LYS:HG2	1:R:827:PHE:CE2	2.41	0.55
2:O:19:TRP:O	2:O:26:THR:HG23	2.06	0.55
4:K:31:ARG:HH11	4:K:32:ARG:HB3	1.71	0.55
8:D:70:GLU:H	8:D:86:VAL:HG22	1.72	0.55
15:7:72:VAL:HG21	15:7:99:VAL:HG21	1.89	0.55
3:I:51:LEU:O	3:I:55:GLU:HG2	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:11:GLN:O	3:H:15:MET:HG2	2.06	0.55
7:C:303:GLU:OE2	7:C:307:LYS:NZ	2.35	0.55
15:1:58:PRO:HG3	15:1:135:LEU:HD11	1.88	0.55
15:4:84:ILE:HG21	15:4:89:SER:HB2	1.89	0.55
15:7:58:PRO:HG3	15:7:135:LEU:HD11	1.88	0.55
17:P:111:PHE:CD1	17:P:152:GLY:HA3	2.40	0.55
8:E:363:HIS:HB3	8:E:366:PRO:HD2	1.88	0.55
8:F:492:LEU:HD12	8:F:500:LEU:HD21	1.89	0.55
12:U:261:ASN:HB2	12:U:265:PRO:HB3	1.87	0.55
15:3:56:ILE:HD12	15:4:134:ILE:HD11	1.89	0.55
15:6:144:TYR:HA	15:6:147:ILE:HD12	1.88	0.55
15:7:82:ASP:OD1	15:7:83:ASP:N	2.40	0.55
12:U:261:ASN:HB3	18:U:503:NAG:HN2	1.72	0.55
2:O:50:VAL:O	2:O:54:LEU:HG	2.07	0.55
4:K:21:LYS:HE2	4:K:28:ARG:HH12	1.72	0.55
7:C:116:ILE:HD13	8:F:341:VAL:HG11	1.89	0.55
9:X:240:LYS:HA	9:X:243:GLN:HB2	1.89	0.55
9:X:244:ASP:HA	9:X:247:SER:HB3	1.88	0.55
15:6:124:GLN:OE1	15:6:126:ARG:N	2.40	0.55
17:P:19:ILE:N	17:P:196:GLN:OE1	2.40	0.55
2:O:350:ILE:HG13	2:O:361:LEU:HB2	1.87	0.55
4:M:41:GLN:HA	4:M:44:ILE:HD12	1.88	0.55
3:I:189:LYS:HD2	8:E:49:THR:HG22	1.89	0.55
4:K:46:GLN:HA	4:K:49:LEU:HB2	1.88	0.55
1:R:564:LYS:HB3	1:R:567:ASN:HD22	1.71	0.55
15:2:9:GLU:HG3	15:2:10:TYR:H	1.72	0.55
4:K:44:ILE:HA	4:K:47:TYR:HB3	1.88	0.55
9:X:220:GLU:O	9:X:224:ILE:HG13	2.07	0.55
17:P:252:PHE:O	17:P:295:LYS:NZ	2.39	0.55
2:O:5:TRP:CD1	2:O:323:PRO:HG3	2.42	0.54
3:J:137:ARG:NE	3:J:140:ASP:OD2	2.36	0.54
14:0:58:ILE:HG12	15:1:148:VAL:HG21	1.89	0.54
16:Q:63:SER:HB2	16:Q:64:PRO:HD3	1.89	0.54
1:R:55:VAL:HA	1:R:58:CYS:SG	2.48	0.54
1:R:180:ILE:HD11	1:R:220:PHE:H	1.72	0.54
2:O:13:LYS:NZ	2:O:14:THR:OG1	2.40	0.54
7:C:291:PHE:HB2	7:C:292:PRO:HD3	1.88	0.54
11:N:37:LEU:HD22	11:N:51:THR:HG21	1.88	0.54
13:V:302:GLU:N	13:V:302:GLU:OE1	2.40	0.54
8:F:454:PHE:HB2	8:F:486:ILE:HD11	1.89	0.54
9:Z:111:GLN:OE1	9:Z:168:ILE:N	2.35	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:119:ARG:HH12	16:Q:90:TYR:HE1	1.55	0.54
15:7:47:MET:SD	16:Q:250:GLU:HB3	2.47	0.54
15:9:47:MET:HG3	15:9:48:ARG:HG2	1.90	0.54
17:P:399:GLU:HG2	17:P:436:LEU:HD23	1.89	0.54
1:R:109:LYS:O	1:R:113:THR:HG23	2.07	0.54
1:R:593:LYS:HE3	1:R:606:PRO:HD2	1.90	0.54
3:I:51:LEU:HA	3:I:54:MET:HG2	1.89	0.54
7:C:17:THR:OG1	7:C:79:VAL:O	2.23	0.54
12:U:270:TRP:NE1	12:U:399:ASP:OD2	2.38	0.54
14:0:77:ILE:HG21	15:1:117:GLY:HA2	1.89	0.54
1:R:397:ILE:HG21	5:S:43:THR:HB	1.88	0.54
7:C:412:PRO:HG3	7:C:417:PHE:HE1	1.72	0.54
7:A:242:GLN:OE1	7:A:343:HIS:ND1	2.40	0.54
8:E:298:THR:HA	8:E:353:ILE:HG12	1.89	0.54
9:X:134:ASN:HA	9:X:137:THR:HG22	1.89	0.54
15:3:123:GLN:O	15:3:125:PRO:HD3	2.08	0.54
16:Q:271:TYR:HD2	16:Q:274:TYR:HD2	1.56	0.54
3:J:44:ARG:O	3:J:48:THR:HG23	2.07	0.54
7:A:280:ARG:HG3	7:A:283:GLU:HG2	1.90	0.54
8:F:78:ASP:OD1	8:F:79:GLY:N	2.40	0.54
17:P:84:ILE:HG21	17:P:93:ILE:HD13	1.89	0.54
17:P:423:ARG:O	17:P:427:VAL:HG23	2.08	0.54
1:R:294:PHE:HE1	1:R:298:ARG:HH11	1.55	0.54
7:C:477:THR:O	7:C:481:GLU:HG2	2.08	0.54
8:F:129:GLY:HA2	8:F:254:MET:O	2.08	0.54
8:F:215:LYS:NZ	8:F:474:PHE:HB2	2.22	0.54
9:Z:172:ASN:OD1	9:Z:174:GLY:N	2.41	0.54
15:4:56:ILE:HD13	15:5:133:LEU:HD22	1.88	0.54
15:7:64:ILE:HA	15:7:67:ILE:HD12	1.90	0.54
15:8:14:PHE:HB2	15:8:89:SER:OG	2.08	0.54
1:R:317:LYS:NZ	17:P:327:ASP:OD2	2.40	0.54
1:R:549:LEU:HD21	1:R:579:MET:HG2	1.89	0.54
1:R:829:HIS:HB3	1:R:832:GLU:HB3	1.88	0.54
2:O:120:ASN:O	2:O:124:ILE:HG13	2.07	0.54
7:B:419:ASP:OD1	7:B:419:ASP:N	2.38	0.54
1:R:427:GLU:OE2	1:R:447:ARG:NE	2.34	0.54
2:O:193:ASN:O	2:O:197:TRP:N	2.41	0.54
7:B:196:PHE:CD2	7:B:197:GLU:HG2	2.42	0.54
8:D:232:ALA:HB3	8:D:297:LEU:HD23	1.90	0.54
9:Y:181:LEU:HD12	9:Y:199:LEU:HD11	1.90	0.54
17:P:148:LEU:C	17:P:151:TRP:HB3	2.28	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:58:CYS:HB2	1:R:297:VAL:HG23	1.90	0.54
2:O:194:HIS:HA	2:O:197:TRP:HB3	1.89	0.54
7:B:493:VAL:HB	7:B:498:LYS:HG3	1.88	0.54
7:C:69:GLU:HB3	7:C:120:ARG:NH1	2.23	0.54
8:F:209:GLN:HE22	8:F:470:ASN:HA	1.73	0.54
8:D:234:MET:SD	8:D:275:PRO:HG3	2.48	0.54
16:Q:299:VAL:HG11	16:Q:350:ILE:HG22	1.89	0.54
17:P:380:ALA:HA	17:P:383:LEU:HD23	1.90	0.54
11:N:7:LEU:N	11:N:60:ASP:O	2.39	0.53
1:R:22:ALA:O	1:R:26:VAL:HG22	2.08	0.53
1:R:36:GLN:OE1	1:R:823:LEU:N	2.40	0.53
1:R:478:SER:OG	1:R:512:GLY:O	2.25	0.53
1:R:566:LEU:HD22	1:R:658:LEU:HD11	1.90	0.53
2:O:211:ARG:O	2:O:211:ARG:NH2	2.31	0.53
7:A:383:ALA:O	7:A:387:GLU:HG2	2.08	0.53
8:E:173:GLY:O	8:E:465:GLN:NE2	2.38	0.53
8:F:287:TYR:OH	8:F:339:GLY:O	2.21	0.53
9:X:33:MET:HG2	9:X:88:LEU:HD21	1.90	0.53
12:U:329:ASN:HD21	12:U:338:HIS:HB3	1.72	0.53
15:3:72:VAL:HG11	15:3:99:VAL:HG11	1.90	0.53
15:4:72:VAL:HG11	15:4:99:VAL:HG11	1.90	0.53
17:P:90:VAL:O	17:P:94:LEU:HB3	2.09	0.53
17:P:228:MET:SD	17:P:265:ILE:HD11	2.49	0.53
9:X:67:GLU:HG2	9:X:70:LYS:HE3	1.90	0.53
17:P:33:TRP:CE3	17:P:47:CYS:HB3	2.44	0.53
17:P:167:TRP:O	17:P:171:GLN:N	2.42	0.53
1:R:208:ASP:H	1:R:213:ASP:N	2.07	0.53
3:I:135:ARG:NH2	3:I:168:ASP:OD2	2.42	0.53
3:J:101:ARG:NH2	4:M:97:ASP:OD1	2.41	0.53
9:Y:98:ILE:HD12	9:Y:164:ALA:HB2	1.89	0.53
9:X:131:ASN:O	9:X:135:GLN:HG3	2.07	0.53
12:U:259:SER:HB3	12:U:268:LEU:HD23	1.88	0.53
14:0:96:PHE:HD2	14:0:180:GLU:HG2	1.73	0.53
15:5:20:SER:O	15:5:24:VAL:HG12	2.07	0.53
1:R:130:PHE:HB3	1:R:202:ILE:HG12	1.90	0.53
1:R:194:ASN:H	1:R:224:PHE:HE2	1.56	0.53
4:L:106:ILE:HG23	4:L:108:PRO:HD3	1.91	0.53
7:A:100:ASP:OD1	7:A:100:ASP:N	2.41	0.53
15:3:28:LEU:HD12	15:4:105:ALA:HB2	1.90	0.53
15:8:41:ILE:HD13	15:8:118:VAL:HG21	1.91	0.53
15:9:72:VAL:HG11	15:9:99:VAL:HG11	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:175:ILE:HD11	1:R:179:ARG:H	1.74	0.53
2:O:217:SER:O	2:O:224:LEU:N	2.37	0.53
3:H:94:LEU:HD13	3:H:215:LEU:HD11	1.89	0.53
7:C:370:ALA:O	10:G:196:ARG:NH2	2.42	0.53
15:8:20:SER:O	15:8:24:VAL:HG12	2.09	0.53
17:P:215:ARG:HH12	17:P:252:PHE:HB2	1.74	0.53
17:P:290:ARG:NH1	17:P:334:ASP:HA	2.23	0.53
3:H:25:GLU:OE2	17:P:283:ARG:NH2	2.41	0.53
5:S:30:LYS:NZ	5:S:31:GLY:O	2.29	0.53
8:F:246:SER:O	8:F:250:GLU:HG2	2.08	0.53
14:0:73:GLY:HA2	14:0:76:ILE:HG22	1.91	0.53
14:0:126:ILE:HG22	14:0:126:ILE:O	2.08	0.53
15:1:56:ILE:HD12	15:2:134:ILE:HD11	1.91	0.53
15:6:50:GLU:N	15:6:50:GLU:OE1	2.41	0.53
7:C:397:ASN:O	7:C:399:GLU:N	2.42	0.53
15:2:150:LEU:O	15:2:154:THR:HG22	2.08	0.53
1:R:329:ASP:OD2	1:R:329:ASP:N	2.42	0.53
1:R:811:GLN:HB3	1:R:815:TYR:HB3	1.91	0.53
7:C:24:VAL:HG11	7:C:29:VAL:HG13	1.91	0.53
15:2:108:PHE:O	15:2:112:ILE:HG22	2.08	0.53
15:7:99:VAL:HB	15:7:149:ALA:HB2	1.91	0.53
17:P:34:GLN:O	17:P:37:LEU:HG	2.09	0.53
9:Y:83:ARG:NH2	9:Y:118:HIS:O	2.42	0.52
15:9:84:ILE:HG22	15:9:85:SER:H	1.73	0.52
17:P:22:LYS:NZ	17:P:134:ASP:O	2.38	0.52
17:P:84:ILE:HD11	17:P:89:THR:HG22	1.91	0.52
17:P:150:ALA:N	17:P:151:TRP:CE3	2.71	0.52
2:O:198:ILE:HG23	2:O:199:LYS:HD3	1.91	0.52
8:E:365:ILE:HB	8:E:366:PRO:HD3	1.91	0.52
8:D:165:TYR:OH	8:D:403:LYS:NZ	2.41	0.52
8:D:209:GLN:HB2	8:D:470:ASN:HD22	1.75	0.52
12:U:447:ILE:O	12:U:450:LEU:HG	2.10	0.52
12:U:450:LEU:HD23	15:1:32:TYR:CE1	2.45	0.52
4:M:30:ASN:HA	4:M:33:LEU:HG	1.91	0.52
8:E:377:ILE:O	8:E:397:SER:OG	2.27	0.52
8:F:69:ALA:H	8:F:86:VAL:HG13	1.74	0.52
9:X:226:VAL:O	9:X:230:ILE:HG12	2.09	0.52
2:O:72:VAL:HA	2:O:75:TYR:HD2	1.75	0.52
2:O:298:LYS:O	2:O:302:VAL:HG23	2.09	0.52
3:J:38:PHE:HB2	4:M:32:ARG:HG3	1.92	0.52
8:F:61:ASP:OD1	8:F:62:HIS:N	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:804:ARG:HH21	14:0:95:ILE:HD12	1.75	0.52
7:B:158:GLU:HG3	7:B:164:HIS:HB2	1.91	0.52
8:D:365:ILE:HB	8:D:366:PRO:HD3	1.92	0.52
15:7:59:VAL:HG21	15:8:134:ILE:HD12	1.91	0.52
17:P:74:ALA:HA	17:P:77:PHE:HD2	1.75	0.52
17:P:304:GLU:O	17:P:308:ALA:CB	2.58	0.52
8:D:106:ASP:OD1	8:D:107:ALA:N	2.35	0.52
9:Z:236:LYS:O	9:Z:270:ASN:ND2	2.42	0.52
16:Q:172:ASP:HA	16:Q:175:GLU:HG2	1.91	0.52
17:P:160:ASP:HA	17:P:164:TYR:CE1	2.44	0.52
17:P:248:TRP:HD1	17:P:288:ALA:HA	1.75	0.52
17:P:340:GLU:O	17:P:344:GLU:HG2	2.09	0.52
2:O:8:SER:HB2	2:O:370:VAL:HB	1.92	0.52
2:O:41:PRO:HB3	2:O:107:TRP:CD1	2.44	0.52
2:O:260:ALA:O	2:O:263:GLU:HG2	2.09	0.52
7:A:353:ARG:NH1	7:A:356:GLU:OE2	2.42	0.52
2:O:112:TYR:HB3	2:O:121:ILE:HD12	1.92	0.52
2:O:149:ASN:HB3	2:O:268:LEU:HD21	1.91	0.52
3:H:21:GLN:NE2	17:P:238:GLN:OE1	2.43	0.52
5:S:9:PRO:HA	5:S:12:VAL:HG12	1.91	0.52
9:X:140:LEU:HD21	9:X:152:LEU:HB3	1.92	0.52
9:X:256:THR:H	9:X:259:LEU:HD13	1.75	0.52
15:8:50:GLU:OE1	15:8:50:GLU:N	2.29	0.52
17:P:86:LYS:O	17:P:90:VAL:N	2.33	0.52
7:C:29:VAL:HG12	7:C:30:THR:N	2.23	0.52
8:F:205:GLN:O	8:F:209:GLN:HB2	2.10	0.52
15:5:24:VAL:HG21	15:6:101:LEU:HD13	1.91	0.52
17:P:408:ALA:HB1	17:P:451:ASN:HD21	1.75	0.52
1:R:390:ASN:O	1:R:393:PRO:HD2	2.10	0.52
1:R:787:VAL:HA	1:R:791:LEU:HB2	1.91	0.52
8:F:185:ARG:NH2	8:F:212:LEU:HD23	2.25	0.52
15:3:24:VAL:HG21	15:4:101:LEU:HD13	1.92	0.52
16:Q:5:PRO:O	16:Q:6:GLU:HG2	2.10	0.52
17:P:168:ILE:HA	17:P:171:GLN:HB2	1.91	0.52
17:P:213:GLU:HG3	17:P:214:TYR:H	1.73	0.52
17:P:213:GLU:HG3	17:P:214:TYR:HD1	1.75	0.52
17:P:120:ASN:O	17:P:124:PRO:HG2	2.11	0.51
1:R:460:THR:HG23	5:S:51:PHE:CE2	2.45	0.51
2:O:328:LEU:HD12	2:O:328:LEU:H	1.74	0.51
6:T:82:ASP:N	6:T:82:ASP:OD1	2.44	0.51
8:E:61:ASP:OD1	8:E:62:HIS:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:9:37:SER:O	15:9:41:ILE:HG12	2.09	0.51
17:P:132:ARG:HA	17:P:132:ARG:CZ	2.40	0.51
1:R:80:MET:SD	1:R:291:ARG:NH2	2.83	0.51
1:R:202:ILE:HB	1:R:217:LYS:HB2	1.92	0.51
1:R:469:SER:OG	1:R:470:LYS:NZ	2.43	0.51
7:B:288:LEU:HD21	8:E:161:GLN:HG2	1.93	0.51
7:A:584:MET:O	7:A:601:TYR:OH	2.27	0.51
9:Z:36:ILE:HD11	9:Z:91:LEU:HG	1.92	0.51
12:U:289:THR:OG1	12:U:313:TYR:OH	2.28	0.51
12:U:417:ASP:OD1	12:U:418:CYS:N	2.44	0.51
16:Q:108:ASN:ND2	16:Q:129:CYS:HB2	2.25	0.51
17:P:387:ASN:O	17:P:392:LYS:HG3	2.11	0.51
1:R:5:PHE:HE1	5:S:35:GLY:HA3	1.75	0.51
2:O:293:ALA:O	2:O:297:VAL:HG23	2.10	0.51
3:H:44:ARG:HG2	3:H:47:GLN:HE21	1.76	0.51
7:B:115:SER:OG	7:B:116:ILE:N	2.44	0.51
7:C:399:GLU:OE2	9:Z:82:SER:OG	2.26	0.51
8:D:173:GLY:HA3	8:D:209:GLN:HE21	1.74	0.51
9:X:144:ALA:H	9:X:149:ASN:HD22	1.58	0.51
16:Q:115:GLY:HA3	16:Q:125:LEU:HD11	1.92	0.51
7:B:249:PRO:HG3	7:B:432:PHE:CE1	2.45	0.51
7:A:238:PHE:CZ	7:A:450:TRP:HA	2.45	0.51
14:0:112:SER:OG	15:1:155:LYS:NZ	2.34	0.51
17:P:141:ALA:HA	17:P:144:ILE:HB	1.93	0.51
1:R:250:THR:HG23	1:R:251:PRO:HD3	1.93	0.51
1:R:272:LEU:O	1:R:276:GLU:HG2	2.11	0.51
1:R:737:SER:HB2	1:R:740:ARG:HH12	1.74	0.51
3:I:101:ARG:HH11	4:L:96:LEU:HD23	1.76	0.51
12:U:297:LEU:HD11	12:U:309:LEU:HD11	1.92	0.51
15:5:41:ILE:O	15:5:45:SER:HB2	2.10	0.51
3:I:20:GLU:HA	4:L:17:ARG:HH12	1.76	0.51
3:H:44:ARG:NE	4:K:37:LYS:HE2	2.20	0.51
7:C:193:GLU:HG2	7:C:202:LYS:HG2	1.93	0.51
7:C:472:PHE:HD1	7:C:538:VAL:HG23	1.76	0.51
15:2:22:ALA:HB2	15:2:96:GLY:HA2	1.91	0.51
17:P:315:LEU:O	17:P:319:GLU:HG3	2.11	0.51
10:G:81:THR:HA	10:G:84:ILE:HG22	1.92	0.51
10:G:155:PHE:HZ	11:N:109:ALA:HB2	1.76	0.51
17:P:257:CYS:SG	17:P:258:GLU:N	2.83	0.51
11:N:83:GLN:HG2	11:N:84:SER:H	1.76	0.51
1:R:100:ASN:O	1:R:104:ILE:HG12	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:282:TRP:O	2:O:286:ASN:ND2	2.44	0.50
8:E:232:ALA:HB3	8:E:297:LEU:HD23	1.94	0.50
4:M:88:PHE:CE1	4:M:92:ARG:HD2	2.46	0.50
8:D:100:GLU:OE1	8:D:100:GLU:N	2.44	0.50
17:P:31:VAL:HG11	17:P:96:MET:SD	2.51	0.50
1:R:332:SER:HA	1:R:335:PHE:HD2	1.76	0.50
4:M:105:ASP:OD2	4:M:107:ARG:NH1	2.36	0.50
3:I:30:ILE:HG23	4:L:29:LYS:HE2	1.94	0.50
8:E:424:ALA:HB2	8:E:494:ARG:CZ	2.42	0.50
10:G:99:ASP:O	10:G:106:LEU:N	2.44	0.50
12:U:261:ASN:HB3	18:U:503:NAG:N2	2.25	0.50
15:9:14:PHE:HB2	15:9:89:SER:OG	2.11	0.50
15:9:45:SER:HA	15:9:52:ILE:HD11	1.94	0.50
1:R:80:MET:SD	1:R:80:MET:N	2.84	0.50
7:B:158:GLU:OE2	7:B:164:HIS:ND1	2.45	0.50
7:C:100:ASP:OD1	7:C:100:ASP:N	2.43	0.50
7:C:458:MET:HG2	7:C:476:ARG:NH1	2.26	0.50
7:A:580:LYS:HE3	7:A:604:LEU:HD13	1.93	0.50
9:Y:49:TYR:HE1	9:Y:84:ARG:HB3	1.76	0.50
9:X:155:MET:HE1	9:X:185:LEU:HD13	1.93	0.50
15:1:6:SER:OG	15:1:7:GLY:N	2.44	0.50
15:1:72:VAL:HG11	15:1:99:VAL:HG11	1.94	0.50
17:P:151:TRP:O	17:P:153:LYS:N	2.45	0.50
1:R:649:TRP:O	1:R:650:MET:HG2	2.11	0.50
7:B:66:VAL:HG12	7:B:68:GLU:H	1.76	0.50
7:B:173:ARG:HD3	9:Y:20:SER:OG	2.10	0.50
7:C:553:ARG:O	7:C:557:THR:HG23	2.12	0.50
8:E:187:GLN:HG3	8:E:401:LEU:HD12	1.93	0.50
15:4:14:PHE:HB2	15:4:89:SER:OG	2.11	0.50
15:7:20:SER:O	15:7:24:VAL:HG12	2.12	0.50
1:R:427:GLU:OE2	1:R:448:TYR:OH	2.23	0.50
8:E:77:PRO:HD3	8:E:110:THR:HG22	1.92	0.50
12:U:335:SER:O	12:U:337:ARG:N	2.42	0.50
15:7:44:MET:HB2	15:7:122:ALA:HB2	1.93	0.50
1:R:277:ASP:O	1:R:280:GLN:NE2	2.45	0.50
1:R:297:VAL:HA	1:R:300:MET:HB2	1.94	0.50
4:M:45:GLU:OE1	4:M:48:ARG:NH1	2.33	0.50
4:L:27:LYS:O	4:L:31:ARG:HG2	2.12	0.50
4:L:93:ASP:N	4:L:93:ASP:OD1	2.44	0.50
6:T:107:ASN:HA	6:T:110:ILE:HG22	1.94	0.50
9:Y:148:LYS:NZ	9:Y:188:MET:O	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:U:346:GLU:OE1	12:U:348:HIS:NE2	2.37	0.50
16:Q:16:LEU:HD11	16:Q:88:HIS:O	2.11	0.50
1:R:11:THR:HA	1:R:356:GLN:HE22	1.77	0.50
7:B:298:VAL:HG23	7:B:299:ASP:H	1.75	0.50
7:B:366:ALA:HA	8:E:317:VAL:HG21	1.92	0.50
7:B:581:LEU:HD21	7:B:608:MET:HE1	1.94	0.50
8:D:335:TYR:CE2	8:D:369:THR:HG23	2.47	0.50
9:Y:261:ASP:OD1	9:Y:265:ARG:NH1	2.45	0.50
9:X:139:TYR:HD2	9:X:140:LEU:HD22	1.76	0.50
12:U:327:LEU:HD22	12:U:404:ALA:HB2	1.93	0.50
14:0:77:ILE:HG23	15:1:127:LEU:HD23	1.91	0.50
15:8:118:VAL:HA	15:8:121:THR:HG22	1.93	0.50
17:P:40:GLN:NE2	17:P:41:MET:HG2	2.27	0.50
17:P:121:THR:HA	17:P:124:PRO:HB2	1.93	0.50
2:O:112:TYR:HB3	2:O:121:ILE:HG23	1.93	0.50
2:O:347:ALA:HA	2:O:366:TYR:HB3	1.93	0.50
9:Z:195:GLU:N	9:Z:195:GLU:OE1	2.43	0.50
16:Q:247:LEU:HD13	16:Q:271:TYR:HE2	1.76	0.50
1:R:271:VAL:O	1:R:275:THR:HG23	2.10	0.49
2:O:121:ILE:HD13	2:O:124:ILE:HD12	1.94	0.49
2:O:202:GLU:HG3	3:J:3:LEU:HD13	1.93	0.49
3:J:51:LEU:O	3:J:55:GLU:HG2	2.11	0.49
3:J:182:GLU:HG2	3:J:193:SER:HA	1.94	0.49
7:C:153:TYR:HH	7:C:203:PHE:HD2	1.60	0.49
8:E:420:ASN:O	8:E:494:ARG:NH1	2.45	0.49
15:1:79:SER:O	15:1:79:SER:OG	2.25	0.49
17:P:68:THR:HB	17:P:73:CYS:HB2	1.94	0.49
17:P:299:ARG:HG3	17:P:302:ARG:HH21	1.76	0.49
1:R:628:LEU:N	1:R:632:GLN:OE1	2.37	0.49
7:B:401:GLU:OE1	9:Y:122:TRP:NE1	2.45	0.49
7:A:55:ILE:HD12	7:A:365:LEU:HD11	1.93	0.49
7:A:399:GLU:OE2	9:X:25:LYS:NZ	2.43	0.49
12:U:262:ASP:OD1	12:U:263:THR:N	2.39	0.49
12:U:303:ASN:HB3	12:U:305:SER:H	1.76	0.49
17:P:43:SER:O	17:P:47:CYS:HB2	2.12	0.49
17:P:150:ALA:HB3	17:P:151:TRP:HE3	1.75	0.49
17:P:244:ILE:HA	17:P:247:ILE:HG22	1.94	0.49
17:P:430:GLN:HE22	17:P:431:LEU:HD23	1.76	0.49
1:R:36:GLN:HB3	1:R:324:TRP:HB2	1.93	0.49
1:R:98:GLU:HA	1:R:101:PHE:HB3	1.94	0.49
2:O:149:ASN:O	2:O:153:LEU:HG	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:24:VAL:HB	7:C:29:VAL:HA	1.93	0.49
9:Y:219:ALA:HA	9:Y:222:GLN:HG3	1.93	0.49
14:0:39:TRP:O	14:0:42:THR:OG1	2.24	0.49
15:6:37:SER:O	15:6:41:ILE:HG12	2.12	0.49
7:B:100:ASP:OD2	7:B:104:ARG:NH2	2.37	0.49
7:B:253:GLY:HA3	7:B:256:LYS:HE2	1.93	0.49
7:A:586:PHE:HD2	8:D:497:GLN:HE22	1.61	0.49
9:Y:93:ARG:NH2	9:Y:134:ASN:OD1	2.30	0.49
15:2:67:ILE:O	15:2:71:VAL:HG23	2.13	0.49
15:5:16:VAL:HG11	15:6:90:PHE:O	2.12	0.49
2:O:5:TRP:HE3	2:O:7:ILE:HD11	1.77	0.49
4:K:4:GLN:O	4:K:8:ILE:HG12	2.12	0.49
8:F:171:GLN:HE22	8:F:472:THR:HG22	1.76	0.49
14:0:153:VAL:O	14:0:157:ILE:HG12	2.12	0.49
15:2:131:MET:O	15:2:135:LEU:HG	2.13	0.49
17:P:399:GLU:OE1	17:P:440:HIS:NE2	2.45	0.49
1:R:387:ARG:NE	1:R:561:TYR:OH	2.34	0.49
1:R:495:ARG:NH2	18:R:902:NAG:O4	2.36	0.49
3:I:175:GLU:OE1	3:I:175:GLU:N	2.36	0.49
7:B:207:GLN:HE22	7:B:215:ARG:HH22	1.59	0.49
7:B:443:LYS:HG3	7:B:445:PHE:CZ	2.47	0.49
10:G:88:ASN:OD1	10:G:118:SER:OG	2.22	0.49
15:3:65:ILE:O	15:3:68:TYR:HB2	2.11	0.49
15:6:128:PHE:O	15:6:132:ILE:HG12	2.12	0.49
17:P:397:LEU:HA	17:P:400:VAL:HB	1.93	0.49
2:O:75:TYR:O	2:O:79:VAL:HG23	2.12	0.49
2:O:298:LYS:NZ	2:O:373:LYS:O	2.45	0.49
5:S:34:ARG:O	5:S:38:ILE:HG12	2.11	0.49
7:B:44:ARG:HB2	7:B:80:LEU:HB3	1.94	0.49
7:B:275:VAL:HG21	7:B:330:GLY:HA3	1.94	0.49
7:C:570:ILE:HG23	7:C:574:MET:HE3	1.95	0.49
8:E:485:ARG:NE	8:E:504:TYR:O	2.38	0.49
9:Y:185:LEU:HD12	9:Y:199:LEU:HD23	1.95	0.49
9:X:144:ALA:H	9:X:149:ASN:ND2	2.10	0.49
1:R:410:PHE:HE1	1:R:458:MET:HG3	1.77	0.49
1:R:804:ARG:HG3	15:1:137:PHE:CZ	2.48	0.49
2:O:187:VAL:HG22	2:O:248:VAL:HG12	1.95	0.49
3:I:56:TYR:HA	3:I:59:LYS:HE3	1.93	0.49
3:I:219:ASN:OD1	3:I:220:ALA:N	2.46	0.49
8:F:376:GLN:HG3	8:F:378:TYR:CE2	2.48	0.49
9:X:159:LEU:O	9:X:163:ILE:HG12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:72:VAL:HG21	15:1:99:VAL:HG21	1.95	0.49
2:O:29:ASN:HD22	2:O:324:ASN:ND2	2.11	0.49
2:O:202:GLU:CD	2:O:210:PRO:HG3	2.33	0.49
7:B:173:ARG:HD2	9:Y:62:PHE:HE1	1.77	0.49
7:A:250:GLY:O	7:A:256:LYS:NZ	2.40	0.49
8:D:61:ASP:OD1	8:D:62:HIS:N	2.46	0.49
9:Z:256:THR:OG1	9:Z:257:LYS:N	2.45	0.49
14:0:54:ILE:HD11	14:0:112:SER:HB2	1.95	0.49
15:7:41:ILE:HD12	15:7:55:SER:HB3	1.95	0.49
17:P:52:ARG:HH12	17:P:68:THR:HG22	1.77	0.49
17:P:244:ILE:HD13	17:P:269:LEU:HD11	1.93	0.49
1:R:62:ASP:HA	1:R:65:LEU:HG	1.94	0.49
4:M:41:GLN:HA	4:M:44:ILE:HB	1.94	0.49
5:S:43:THR:HA	5:S:46:VAL:HG12	1.94	0.49
7:B:484:GLN:O	7:B:484:GLN:NE2	2.46	0.49
8:F:168:GLU:OE2	8:F:185:ARG:NH1	2.46	0.49
8:F:458:PHE:HA	8:F:483:LEU:HD21	1.95	0.49
15:9:41:ILE:HD13	15:9:118:VAL:HG21	1.95	0.49
17:P:147:LYS:C	17:P:151:TRP:HB3	2.33	0.49
1:R:69:GLU:HA	1:R:72:ILE:HD12	1.94	0.48
1:R:79:ILE:H	1:R:79:ILE:HD12	1.78	0.48
1:R:185:ARG:O	1:R:189:ARG:N	2.43	0.48
1:R:475:PHE:HB2	1:R:514:TYR:CZ	2.48	0.48
2:O:166:LEU:O	2:O:170:VAL:HG22	2.13	0.48
8:D:386:ARG:NH2	8:D:459:GLU:OE1	2.34	0.48
17:P:225:ASN:OD1	17:P:226:CYS:N	2.45	0.48
1:R:381:TYR:HB2	1:R:807:TRP:CD2	2.48	0.48
2:O:107:TRP:HE1	2:O:114:ILE:HG12	1.78	0.48
2:O:331:LEU:O	2:O:335:LEU:HG	2.13	0.48
3:I:31:ASP:O	3:I:35:GLU:HG2	2.14	0.48
4:K:25:ALA:HA	4:K:28:ARG:HE	1.78	0.48
4:K:99:LEU:O	4:K:103:VAL:HG23	2.13	0.48
8:E:193:SER:OG	8:E:194:ALA:N	2.46	0.48
10:G:24:LYS:O	10:G:28:THR:HG23	2.13	0.48
17:P:314:VAL:O	17:P:318:LEU:HG	2.13	0.48
1:R:542:ILE:HD13	1:R:587:VAL:HG22	1.95	0.48
4:M:29:LYS:O	4:M:33:LEU:N	2.37	0.48
7:B:503:GLU:O	7:B:507:ILE:HG12	2.13	0.48
7:C:419:ASP:N	7:C:419:ASP:OD1	2.44	0.48
15:3:88:LYS:O	15:3:92:GLN:HG2	2.13	0.48
15:9:6:SER:OG	15:9:7:GLY:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:43:GLU:OE1	16:Q:43:GLU:N	2.47	0.48
16:Q:234:LYS:NZ	16:Q:257:ARG:O	2.45	0.48
17:P:208:MET:HB3	17:P:214:TYR:HE2	1.79	0.48
17:P:240:GLN:O	17:P:244:ILE:HG22	2.13	0.48
17:P:398:LEU:HD21	17:P:437:VAL:HG23	1.95	0.48
2:O:198:ILE:HG13	2:O:213:SER:HB2	1.94	0.48
8:E:152:ASP:OD1	8:E:153:ILE:N	2.45	0.48
9:Z:211:SER:O	9:Z:214:GLU:N	2.46	0.48
17:P:97:VAL:O	17:P:100:MET:HG3	2.13	0.48
1:R:33:GLY:HA3	1:R:826:SER:OG	2.14	0.48
4:M:11:LEU:O	4:M:15:GLU:HG3	2.13	0.48
7:C:120:ARG:HH11	7:C:120:ARG:HG3	1.78	0.48
7:A:295:THR:HB	7:A:302:VAL:HG22	1.94	0.48
11:N:44:THR:HG23	11:N:47:GLU:H	1.78	0.48
15:9:61:MET:SD	15:9:135:LEU:HB3	2.54	0.48
1:R:26:VAL:HA	1:R:29:LEU:HB2	1.96	0.48
1:R:546:ILE:H	1:R:546:ILE:HD12	1.78	0.48
1:R:633:LYS:HA	1:R:636:GLN:HE21	1.78	0.48
3:I:37:GLU:O	3:I:41:GLU:HG3	2.13	0.48
3:H:53:ILE:HD13	4:K:48:ARG:HD2	1.96	0.48
4:K:52:GLU:HA	4:K:55:PHE:HB3	1.96	0.48
7:B:576:ASP:OD1	7:B:576:ASP:N	2.47	0.48
7:C:211:VAL:HG12	7:C:328:TYR:HB3	1.95	0.48
7:C:510:GLU:HG3	7:C:567:TRP:CE2	2.48	0.48
8:E:237:ASN:OD1	8:E:237:ASN:N	2.44	0.48
8:E:408:GLU:OE2	8:E:409:GLY:N	2.46	0.48
8:E:424:ALA:HB2	8:E:494:ARG:NH2	2.28	0.48
17:P:359:LEU:HA	17:P:364:LEU:HD21	1.95	0.48
1:R:593:LYS:HD3	1:R:628:LEU:HG	1.96	0.48
2:O:45:VAL:HG13	2:O:46:GLY:H	1.78	0.48
7:C:234:LEU:HD22	7:C:433:TRP:CG	2.49	0.48
8:D:135:SER:O	8:D:135:SER:OG	2.32	0.48
14:0:78:GLY:HA3	16:Q:15:TYR:HA	1.96	0.48
16:Q:54:TYR:HB3	16:Q:57:PHE:CE1	2.49	0.48
17:P:452:ALA:O	17:P:456:VAL:HG23	2.14	0.48
3:I:48:THR:O	3:I:51:LEU:HG	2.13	0.48
4:L:67:GLY:O	4:L:71:THR:HG23	2.14	0.48
7:B:573:HIS:CD2	7:B:615:LEU:HB2	2.48	0.48
7:A:66:VAL:HG12	7:A:68:GLU:H	1.77	0.48
8:F:135:SER:O	8:F:135:SER:OG	2.30	0.48
12:U:314:GLU:OE2	12:U:314:GLU:N	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:3:6:SER:OG	15:3:7:GLY:N	2.47	0.48
16:Q:113:ILE:HG22	16:Q:150:LEU:HD23	1.95	0.48
17:P:74:ALA:HA	17:P:77:PHE:HB2	1.95	0.48
17:P:196:GLN:HG3	17:P:197:TYR:N	2.27	0.48
2:O:47:THR:OG1	2:O:50:VAL:HG22	2.13	0.48
7:B:157:SER:OG	7:B:163:LYS:NZ	2.42	0.48
12:U:457:ASP:HA	16:Q:87:ASN:ND2	2.29	0.48
17:P:77:PHE:HA	17:P:80:LEU:HB2	1.96	0.48
17:P:151:TRP:CZ2	17:P:207:LEU:HD13	2.49	0.48
17:P:353:ASP:OD1	17:P:354:GLU:N	2.46	0.48
2:O:128:GLY:O	2:O:131:GLN:HG2	2.13	0.48
2:O:187:VAL:HG21	2:O:197:TRP:CH2	2.49	0.48
3:J:54:MET:O	3:J:58:GLU:HG2	2.14	0.48
4:K:71:THR:OG1	4:K:72:GLU:N	2.47	0.48
5:S:39:THR:HA	5:S:42:VAL:HG12	1.95	0.48
7:B:250:GLY:C	7:B:412:PRO:HD2	2.34	0.48
7:B:511:VAL:HG11	7:B:548:TYR:HB2	1.96	0.48
7:B:561:SER:OG	7:B:562:ASP:N	2.46	0.48
7:C:576:ASP:OD1	7:C:577:ILE:N	2.47	0.48
9:Y:159:LEU:HD13	9:Y:178:LEU:HB3	1.96	0.48
11:N:45:ILE:O	11:N:49:GLU:HG2	2.14	0.48
17:P:62:LYS:HG2	17:P:107:ARG:HD3	1.96	0.48
1:R:609:LEU:HD21	14:0:110:VAL:HG22	1.95	0.47
3:H:24:ASN:O	3:H:28:GLU:HG2	2.14	0.47
8:D:86:VAL:HG12	8:D:96:VAL:HG22	1.96	0.47
9:X:98:ILE:HA	9:X:160:GLN:HE21	1.79	0.47
12:U:417:ASP:HB3	12:U:419:ALA:H	1.78	0.47
12:U:457:ASP:OD1	16:Q:87:ASN:ND2	2.38	0.47
14:0:93:SER:HA	14:0:180:GLU:OE2	2.14	0.47
15:7:95:ALA:HB2	15:7:152:LEU:HB3	1.96	0.47
2:O:167:ALA:HB1	2:O:258:MET:HA	1.96	0.47
4:L:18:ALA:O	4:L:22:VAL:HG13	2.13	0.47
7:B:42:LEU:O	7:B:82:THR:OG1	2.30	0.47
16:Q:58:LEU:HD11	16:Q:70:ILE:HG12	1.95	0.47
17:P:151:TRP:HZ2	17:P:207:LEU:HB3	1.78	0.47
17:P:197:TYR:O	17:P:201:VAL:HG22	2.13	0.47
17:P:424:GLY:O	17:P:428:ILE:HG12	2.13	0.47
2:O:128:GLY:O	2:O:132:ILE:HG13	2.14	0.47
7:B:280:ARG:HD3	8:E:374:GLU:HG2	1.95	0.47
7:B:489:LEU:HD21	7:B:505:ASP:HB3	1.95	0.47
7:A:525:TYR:CZ	8:D:403:LYS:HD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:47:MET:HG3	15:1:48:ARG:HG2	1.96	0.47
17:P:291:ASN:O	17:P:295:LYS:HG2	2.14	0.47
17:P:332:SER:O	17:P:336:LYS:HG3	2.14	0.47
1:R:83:GLY:O	1:R:84:GLU:HG2	2.15	0.47
1:R:259:SER:O	1:R:263:THR:HG23	2.14	0.47
1:R:485:PHE:CE2	5:S:77:LYS:HD2	2.49	0.47
2:O:209:VAL:HB	2:O:228:THR:HG23	1.96	0.47
3:J:50:ARG:O	3:J:54:MET:HB2	2.14	0.47
3:H:184:TYR:CD2	3:H:191:LYS:HB3	2.49	0.47
7:C:439:LEU:HD12	7:C:444:HIS:CD2	2.49	0.47
7:A:115:SER:OG	7:A:116:ILE:N	2.47	0.47
15:6:85:SER:C	15:6:87:TYR:H	2.17	0.47
17:P:103:GLU:O	17:P:105:HIS:N	2.48	0.47
2:O:184:THR:HA	2:O:228:THR:HA	1.95	0.47
4:K:31:ARG:NH1	4:K:32:ARG:HB3	2.29	0.47
8:E:168:GLU:OE1	8:E:168:GLU:N	2.45	0.47
8:F:298:THR:HA	8:F:353:ILE:HG12	1.97	0.47
15:7:37:SER:O	15:7:41:ILE:HG12	2.14	0.47
17:P:98:ASP:O	17:P:102:GLN:HB2	2.15	0.47
17:P:298:GLU:O	17:P:301:THR:OG1	2.21	0.47
1:R:34:LYS:HE3	1:R:326:PRO:HG2	1.96	0.47
1:R:91:PRO:HG2	1:R:94:MET:CG	2.43	0.47
1:R:189:ARG:HE	2:O:346:ALA:HA	1.80	0.47
1:R:447:ARG:HA	1:R:450:ILE:HG22	1.96	0.47
2:O:189:VAL:HG13	2:O:194:HIS:CD2	2.50	0.47
9:X:226:VAL:HA	9:X:229:MET:HG3	1.96	0.47
9:X:238:SER:HB2	9:X:270:ASN:HD21	1.80	0.47
13:V:304:SER:O	13:V:308:ASN:ND2	2.46	0.47
17:P:162:ASN:HA	17:P:167:TRP:CZ2	2.48	0.47
1:R:116:GLU:O	1:R:119:LYS:HG2	2.15	0.47
1:R:500:LEU:N	5:S:68:LEU:O	2.37	0.47
1:R:537:MET:O	1:R:540:SER:OG	2.24	0.47
1:R:566:LEU:HD13	1:R:658:LEU:HD21	1.96	0.47
1:R:591:PHE:HD1	5:S:57:LEU:HD23	1.80	0.47
1:R:718:VAL:O	1:R:722:ILE:HG12	2.15	0.47
2:O:32:LEU:O	2:O:324:ASN:ND2	2.47	0.47
2:O:143:TYR:HA	2:O:146:LEU:HD12	1.96	0.47
2:O:332:ARG:HG3	2:O:354:MET:HG3	1.96	0.47
3:J:16:MET:HE2	3:J:19:ILE:HB	1.97	0.47
4:M:26:ARG:O	4:M:29:LYS:HB2	2.15	0.47
4:L:6:GLN:OE1	4:L:6:GLN:N	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:6:GLN:O	4:K:10:GLN:HG2	2.14	0.47
6:T:98:TYR:HA	6:T:101:TYR:HD2	1.79	0.47
7:B:261:GLN:O	7:B:264:SER:OG	2.27	0.47
7:B:277:CYS:O	7:B:350:SER:OG	2.30	0.47
7:C:29:VAL:HG21	7:C:66:VAL:HB	1.97	0.47
7:C:252:PHE:O	7:C:437:LYS:NZ	2.47	0.47
7:A:238:PHE:HZ	7:A:450:TRP:HA	1.78	0.47
7:A:547:PHE:HB2	7:A:608:MET:SD	2.54	0.47
8:E:46:THR:HA	8:E:113:GLU:HA	1.97	0.47
8:D:421:GLN:NE2	8:D:425:CYS:SG	2.87	0.47
13:V:293:TYR:O	13:V:295:LEU:N	2.45	0.47
13:V:320:ALA:O	13:V:324:THR:HG22	2.15	0.47
13:V:337:SER:O	13:V:340:TYR:OH	2.19	0.47
15:1:84:ILE:HG21	15:1:89:SER:HB2	1.95	0.47
15:2:44:MET:HB2	15:2:122:ALA:HB2	1.97	0.47
15:4:20:SER:O	15:4:24:VAL:HG12	2.15	0.47
15:7:123:GLN:NE2	16:Q:249:PRO:O	2.48	0.47
16:Q:109:VAL:HG21	16:Q:160:LEU:HD12	1.97	0.47
17:P:290:ARG:HH12	17:P:337:PHE:HB3	1.78	0.47
1:R:357:THR:HG23	1:R:359:GLN:H	1.80	0.47
2:O:213:SER:HA	2:O:226:ASN:O	2.15	0.47
7:B:294:LEU:HD23	7:B:305:ILE:HD13	1.96	0.47
7:B:444:HIS:CE1	7:B:521:GLN:HB2	2.50	0.47
7:A:246:THR:OG1	7:A:247:ALA:N	2.47	0.47
15:1:64:ILE:HA	15:1:67:ILE:HD12	1.95	0.47
15:6:84:ILE:HG23	15:6:88:LYS:HB2	1.96	0.47
16:Q:41:THR:HG23	16:Q:44:ASP:H	1.80	0.47
16:Q:190:LEU:HD11	16:Q:215:GLU:HG3	1.96	0.47
17:P:104:ASN:HA	17:P:107:ARG:HB2	1.95	0.47
17:P:376:TRP:CH2	17:P:413:ASP:HB2	2.49	0.47
1:R:374:PHE:CD1	1:R:396:ILE:HA	2.50	0.47
1:R:550:PHE:O	1:R:553:SER:OG	2.32	0.47
2:O:280:VAL:HG23	2:O:281:ARG:H	1.80	0.47
7:C:248:ILE:HD11	7:C:433:TRP:HE3	1.79	0.47
8:E:61:ASP:OD1	8:E:62:HIS:ND1	2.48	0.47
8:D:253:SER:O	8:D:253:SER:OG	2.25	0.47
15:2:41:ILE:HD13	15:2:118:VAL:HG21	1.96	0.47
17:P:64:GLU:O	17:P:68:THR:HG23	2.14	0.47
3:J:94:LEU:HD13	3:J:215:LEU:HD11	1.96	0.47
3:I:46:VAL:HA	4:L:44:ILE:HD11	1.97	0.47
3:H:129:GLU:H	3:H:132:MET:HE2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:148:THR:OG1	7:C:149:GLY:N	2.47	0.47
8:E:172:THR:OG1	8:E:178:ASP:OD1	2.30	0.47
8:D:301:SER:OG	8:D:355:THR:O	2.28	0.47
9:Y:107:LEU:O	9:Y:111:GLN:HG3	2.16	0.47
16:Q:21:ARG:NH2	16:Q:308:ASN:O	2.48	0.47
17:P:91:GLN:NE2	17:P:135:PRO:O	2.48	0.47
1:R:7:SER:HB3	1:R:387:ARG:H	1.79	0.46
3:I:8:VAL:O	3:I:12:ILE:HG13	2.15	0.46
7:B:250:GLY:N	7:B:410:VAL:O	2.47	0.46
7:C:29:VAL:HB	7:C:66:VAL:H	1.81	0.46
7:C:314:ASN:ND2	7:C:322:ALA:O	2.48	0.46
7:C:492:ILE:O	7:C:496:VAL:HG22	2.14	0.46
9:Z:159:LEU:HD21	9:Z:179:PHE:HE1	1.81	0.46
9:X:129:LYS:HD3	9:X:179:PHE:HE2	1.80	0.46
11:N:68:GLN:O	11:N:72:GLU:HG2	2.15	0.46
15:4:51:GLN:HG2	15:4:54:LYS:HD2	1.97	0.46
17:P:293:LEU:HD13	17:P:338:LEU:HD13	1.97	0.46
1:R:229:LEU:HD11	2:O:52:VAL:HG11	1.98	0.46
1:R:594:TRP:CD1	5:S:58:ALA:HA	2.51	0.46
2:O:333:GLU:O	2:O:337:GLU:HG2	2.15	0.46
7:B:397:ASN:HB3	9:Y:28:TYR:CG	2.50	0.46
9:Y:42:LEU:HD21	9:Y:108:ILE:HG21	1.96	0.46
9:Y:218:PRO:HB2	9:Y:220:GLU:OE1	2.15	0.46
9:X:141:LYS:HD3	9:X:142:ASN:OD1	2.15	0.46
15:2:37:SER:O	15:2:41:ILE:HG12	2.16	0.46
15:5:58:PRO:HG3	15:5:135:LEU:HD11	1.96	0.46
17:P:210:ARG:HA	17:P:249:LEU:HD12	1.97	0.46
2:O:350:ILE:HG13	2:O:361:LEU:HD12	1.98	0.46
3:I:35:GLU:O	3:I:38:PHE:HB3	2.15	0.46
7:B:55:ILE:HD12	7:B:365:LEU:HD11	1.97	0.46
9:Y:102:LYS:O	9:Y:164:ALA:HB1	2.14	0.46
9:X:55:TRP:CD1	9:X:74:CYS:HB3	2.51	0.46
9:X:268:LYS:HA	9:X:271:GLU:HG2	1.98	0.46
10:G:94:ILE:HB	11:N:6:LYS:HB2	1.98	0.46
12:U:316:LEU:HD23	12:U:321:VAL:HG21	1.96	0.46
15:5:130:GLY:O	15:5:134:ILE:HG12	2.15	0.46
17:P:333:GLU:HA	17:P:336:LYS:NZ	2.30	0.46
2:O:18:THR:O	2:O:23:HIS:HB2	2.15	0.46
8:F:168:GLU:N	8:F:168:GLU:OE1	2.49	0.46
8:F:321:ARG:HD2	8:F:364:PRO:HD3	1.98	0.46
9:X:126:TYR:HE1	9:X:169:THR:HA	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:U:314:GLU:H	12:U:314:GLU:CD	2.18	0.46
16:Q:187:LYS:NZ	16:Q:241:PHE:O	2.46	0.46
17:P:39:GLY:H	17:P:44:ALA:HB2	1.80	0.46
17:P:115:ALA:HB1	17:P:118:SER:HB2	1.97	0.46
17:P:449:ARG:O	17:P:453:LEU:HG	2.16	0.46
1:R:81:ASP:OD2	1:R:291:ARG:HB2	2.15	0.46
1:R:277:ASP:HA	1:R:280:GLN:HE21	1.80	0.46
2:O:56:ASP:OD2	2:O:57:GLU:N	2.48	0.46
8:F:255:ASP:OD1	8:F:255:ASP:N	2.43	0.46
15:4:30:ALA:O	15:4:34:THR:HG23	2.15	0.46
15:6:35:ALA:O	15:6:39:THR:HG23	2.16	0.46
17:P:146:ALA:O	17:P:151:TRP:CA	2.63	0.46
1:R:56:ARG:O	1:R:59:GLU:HG3	2.15	0.46
1:R:170:PHE:HB3	1:R:223:PHE:HB3	1.96	0.46
1:R:302:ALA:O	1:R:306:THR:OG1	2.21	0.46
8:F:245:LYS:HE2	8:F:245:LYS:HB3	1.68	0.46
8:D:71:ILE:HD11	8:D:119:LEU:HB2	1.97	0.46
11:N:106:LEU:HB3	11:N:113:PHE:HZ	1.81	0.46
15:1:24:VAL:HG13	15:2:101:LEU:HB3	1.98	0.46
15:2:14:PHE:HB2	15:2:89:SER:HB2	1.97	0.46
17:P:150:ALA:H	17:P:151:TRP:HE3	1.53	0.46
17:P:373:GLU:OE1	17:P:377:ARG:NH2	2.36	0.46
1:R:91:PRO:HB2	1:R:93:ASP:OD1	2.16	0.46
1:R:104:ILE:O	1:R:108:LEU:HG	2.15	0.46
1:R:513:PRO:HB2	5:S:56:ILE:HD11	1.98	0.46
1:R:625:TYR:HD2	1:R:627:MET:HG2	1.80	0.46
7:C:397:ASN:HB2	7:C:398:PRO:HD3	1.96	0.46
9:X:86:LEU:HG	9:X:121:LEU:HD23	1.97	0.46
9:X:198:HIS:HD2	9:X:199:LEU:HD22	1.81	0.46
15:3:37:SER:O	15:3:41:ILE:HG13	2.16	0.46
15:4:88:LYS:O	15:4:92:GLN:HG2	2.16	0.46
15:6:20:SER:O	15:6:24:VAL:HG12	2.16	0.46
15:6:130:GLY:O	15:6:134:ILE:HG13	2.14	0.46
17:P:49:PHE:HB3	17:P:52:ARG:NH2	2.30	0.46
17:P:53:PHE:HA	17:P:61:GLU:HB3	1.98	0.46
17:P:235:CYS:HB3	17:P:239:LEU:HD23	1.97	0.46
3:H:48:THR:O	3:H:51:LEU:HG	2.15	0.46
7:C:87:SER:HA	7:C:211:VAL:HG23	1.97	0.46
7:C:196:PHE:O	7:C:198:GLY:N	2.47	0.46
7:C:204:THR:OG1	7:C:205:MET:N	2.49	0.46
15:4:76:ILE:HD12	15:4:92:GLN:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:7:133:LEU:O	15:7:136:ILE:HG22	2.16	0.46
17:P:52:ARG:NH2	17:P:68:THR:HG22	2.27	0.46
17:P:419:ARG:HD2	17:P:458:LYS:HD2	1.98	0.46
4:L:4:GLN:O	4:L:8:ILE:HG12	2.16	0.46
8:D:231:PHE:HB3	8:D:259:LEU:HD23	1.97	0.46
9:Y:220:GLU:O	9:Y:224:ILE:HG12	2.16	0.46
9:Z:211:SER:HA	9:Z:256:THR:HA	1.98	0.46
11:N:66:ILE:HG22	11:N:67:ASN:O	2.16	0.46
16:Q:77:LYS:NZ	16:Q:81:GLU:OE2	2.39	0.46
1:R:399:PHE:HD1	1:R:806:HIS:HD2	1.63	0.46
1:R:740:ARG:HB3	1:R:744:LEU:HD23	1.98	0.46
4:L:63:LEU:HB3	4:L:66:ARG:HH11	1.80	0.46
7:C:573:HIS:CD2	7:C:615:LEU:HD12	2.50	0.46
9:X:225:LEU:HG	9:X:255:LEU:HD21	1.98	0.46
10:G:204:LYS:HE2	10:G:204:LYS:HB2	1.71	0.46
12:U:411:GLN:N	12:U:411:GLN:OE1	2.49	0.46
15:5:85:SER:C	15:5:87:TYR:H	2.19	0.46
15:9:88:LYS:O	15:9:92:GLN:HG2	2.16	0.46
17:P:149:ALA:CA	17:P:151:TRP:HB2	2.45	0.46
2:O:195:ASN:OD1	2:O:199:LYS:NZ	2.49	0.45
3:I:44:ARG:NH1	3:I:45:LEU:HB3	2.31	0.45
7:C:565:ILE:HA	7:C:569:ILE:HD12	1.98	0.45
7:A:43:VAL:HG21	7:A:64:ILE:HD13	1.98	0.45
8:E:412:ARG:HH21	8:E:414:ASP:CG	2.19	0.45
9:X:193:ILE:HA	9:X:196:GLN:HE21	1.80	0.45
17:P:150:ALA:O	17:P:152:GLY:N	2.49	0.45
1:R:130:PHE:HZ	1:R:206:LEU:H	1.64	0.45
1:R:722:ILE:HG13	14:0:178:ILE:HD12	1.98	0.45
3:H:48:THR:HG22	3:H:52:LYS:NZ	2.31	0.45
7:B:152:ILE:HG12	7:B:167:MET:HG2	1.97	0.45
7:B:349:ASP:O	7:B:350:SER:OG	2.34	0.45
8:E:320:ARG:HH21	8:E:321:ARG:HE	1.64	0.45
8:E:381:ARG:O	8:E:384:HIS:N	2.44	0.45
9:X:83:ARG:NH2	9:X:118:HIS:O	2.48	0.45
11:N:67:ASN:HB2	11:N:70:ILE:HD13	1.97	0.45
15:4:38:GLY:HA3	15:5:113:VAL:HG23	1.98	0.45
15:5:44:MET:HG2	15:5:119:ARG:HA	1.98	0.45
16:Q:328:ASN:ND2	16:Q:347:TYR:HB2	2.32	0.45
16:Q:345:ASP:OD1	16:Q:345:ASP:N	2.49	0.45
17:P:132:ARG:C	17:P:135:PRO:HD2	2.36	0.45
17:P:146:ALA:O	17:P:151:TRP:CB	2.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:355:TYR:CE2	17:P:359:LEU:HD11	2.52	0.45
1:R:256:GLU:O	1:R:259:SER:OG	2.26	0.45
8:F:395:LEU:HB2	8:F:396:PRO:HD3	1.98	0.45
8:D:269:ILE:HD12	8:D:310:VAL:HG22	1.98	0.45
10:G:65:ALA:HB1	10:G:138:TYR:CE1	2.51	0.45
15:1:41:ILE:O	15:1:44:MET:HG3	2.17	0.45
15:6:14:PHE:HB2	15:6:89:SER:HB3	1.97	0.45
15:8:84:ILE:HG22	15:8:85:SER:H	1.81	0.45
4:K:13:GLN:O	4:K:16:LYS:HG2	2.17	0.45
6:T:62:VAL:O	6:T:66:ILE:HG12	2.17	0.45
9:Y:235:PRO:O	9:Y:236:LYS:HB2	2.16	0.45
10:G:23:LEU:HB2	10:G:180:ILE:HG21	1.97	0.45
17:P:299:ARG:HG3	17:P:302:ARG:HE	1.81	0.45
2:O:201:TYR:OH	2:O:211:ARG:N	2.47	0.45
2:O:201:TYR:HB2	2:O:237:PHE:HZ	1.81	0.45
4:M:68:SER:O	4:M:72:GLU:HG2	2.17	0.45
3:I:180:GLY:HA3	3:I:195:THR:HA	1.99	0.45
4:L:25:ALA:O	4:L:29:LYS:HG2	2.16	0.45
3:H:26:LYS:O	3:H:29:GLU:HG3	2.16	0.45
7:C:576:ASP:O	7:C:580:LYS:HG2	2.16	0.45
9:Y:79:ASP:OD2	9:Y:80:ALA:N	2.50	0.45
11:N:94:LYS:HD2	16:Q:338:GLN:NE2	2.29	0.45
12:U:270:TRP:CE2	13:V:295:LEU:HD21	2.51	0.45
16:Q:289:THR:HG23	16:Q:292:ASP:H	1.81	0.45
17:P:344:GLU:HA	17:P:347:GLN:HE21	1.82	0.45
1:R:81:ASP:HA	1:R:291:ARG:HD2	1.98	0.45
1:R:119:LYS:O	1:R:123:LEU:HB2	2.17	0.45
1:R:490:THR:HB	1:R:492:GLU:OE1	2.16	0.45
1:R:503:ASN:HB3	1:R:506:LEU:HD12	1.99	0.45
2:O:193:ASN:HB3	2:O:196:ASP:HB3	1.98	0.45
7:B:412:PRO:HG2	7:B:415:GLY:HA2	1.98	0.45
7:B:486:GLU:OE1	7:B:516:LYS:NZ	2.36	0.45
7:C:228:LEU:H	7:C:268:ASN:ND2	2.14	0.45
7:C:291:PHE:HB3	7:C:305:ILE:H	1.81	0.45
7:C:297:GLU:H	7:C:297:GLU:CD	2.19	0.45
9:Z:92:LEU:HA	9:Z:95:VAL:HG12	1.98	0.45
9:Z:257:LYS:HE3	9:Z:257:LYS:HB2	1.62	0.45
11:N:40:GLU:O	11:N:43:THR:OG1	2.35	0.45
15:2:30:ALA:HB3	15:3:141:LEU:HD11	1.99	0.45
15:3:20:SER:O	15:3:24:VAL:HG12	2.17	0.45
17:P:146:ALA:O	17:P:151:TRP:CD2	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:175:ILE:HG21	1:R:180:ILE:HD13	1.98	0.45
2:O:164:ARG:HH11	2:O:168:GLU:HB2	1.81	0.45
4:M:8:ILE:HA	4:M:11:LEU:HG	1.99	0.45
3:I:58:GLU:O	3:I:62:LYS:HG2	2.17	0.45
4:K:76:GLU:HG3	4:K:80:LYS:HE3	1.99	0.45
7:C:27:PRO:HD3	8:F:326:TYR:CB	2.46	0.45
7:C:320:VAL:HG13	7:C:361:ILE:HD11	1.99	0.45
7:C:324:GLU:O	7:C:354:TRP:NE1	2.44	0.45
8:F:234:MET:SD	8:F:275:PRO:HG3	2.57	0.45
9:X:32:CYS:SG	9:X:88:LEU:HG	2.56	0.45
9:X:217:LEU:HD23	9:X:217:LEU:H	1.81	0.45
15:1:68:TYR:HB3	15:1:146:LEU:HD21	1.99	0.45
17:P:390:LEU:O	17:P:394:LEU:HG	2.17	0.45
1:R:35:VAL:HG12	1:R:325:CYS:HB3	1.98	0.45
2:O:197:TRP:NE1	2:O:225:CYS:SG	2.90	0.45
7:A:24:VAL:HG21	8:D:68:TYR:HB2	1.98	0.45
8:E:234:MET:SD	8:E:275:PRO:HG3	2.56	0.45
16:Q:260:ASP:OD1	16:Q:261:TYR:N	2.49	0.45
17:P:140:MET:SD	17:P:144:ILE:HG13	2.57	0.45
17:P:157:GLU:O	17:P:160:ASP:N	2.46	0.45
17:P:249:LEU:HA	17:P:252:PHE:HD2	1.82	0.45
1:R:374:PHE:CZ	1:R:449:ILE:HG13	2.51	0.45
7:C:56:ARG:HD2	8:D:54:ASN:ND2	2.32	0.45
8:E:393:ASN:O	8:E:397:SER:OG	2.25	0.45
8:F:158:ILE:HB	8:F:163:ARG:HH21	1.82	0.45
9:Y:239:SER:O	9:Y:243:GLN:HG3	2.17	0.45
15:7:108:PHE:O	15:7:112:ILE:HG22	2.17	0.45
16:Q:138:MET:HE3	16:Q:139:GLU:H	1.81	0.45
17:P:435:GLN:HA	17:P:438:MET:SD	2.57	0.45
1:R:90:PHE:N	1:R:91:PRO:HD3	2.31	0.45
1:R:253:GLU:O	1:R:257:MET:HG2	2.16	0.45
1:R:352:LEU:O	1:R:354:ARG:NH2	2.49	0.45
2:O:206:GLU:HG2	2:O:207:MET:H	1.82	0.45
7:B:234:LEU:HG	7:B:433:TRP:CE2	2.52	0.45
7:C:469:PHE:O	7:C:470:THR:OG1	2.32	0.45
7:A:566:THR:H	7:A:569:ILE:HD12	1.82	0.45
8:E:159:ASN:HB3	8:E:162:CYS:SG	2.57	0.45
8:D:141:ARG:HG2	9:Z:9:LYS:HG3	1.99	0.45
9:Y:201:LYS:HA	9:Y:204:VAL:HG12	1.98	0.45
9:X:120:ASN:HD22	9:X:123:LYS:HG2	1.82	0.45
15:4:21:ALA:HA	15:4:24:VAL:HG12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:145:ILE:C	17:P:147:LYS:H	2.20	0.45
2:O:4:PHE:HA	2:O:323:PRO:HD2	1.99	0.44
2:O:201:TYR:HA	2:O:204:LEU:HD12	1.98	0.44
3:I:184:TYR:CD1	3:I:191:LYS:HB3	2.51	0.44
7:C:289:ARG:C	7:C:292:PRO:HD2	2.37	0.44
7:C:344:VAL:HG12	7:C:345:SER:N	2.32	0.44
7:C:522:GLN:HG3	7:C:529:ASP:HB3	1.98	0.44
7:A:233:VAL:HG22	7:A:234:LEU:H	1.81	0.44
8:D:193:SER:OG	8:D:194:ALA:N	2.50	0.44
11:N:40:GLU:HB2	11:N:42:ASP:OD1	2.17	0.44
15:2:52:ILE:HG23	15:2:53:MET:H	1.80	0.44
15:3:60:VAL:HG22	15:4:137:PHE:HE2	1.81	0.44
16:Q:315:PHE:O	16:Q:319:VAL:HG23	2.17	0.44
1:R:202:ILE:HG22	1:R:205:PRO:HG3	1.98	0.44
1:R:205:PRO:HG2	1:R:215:VAL:O	2.17	0.44
1:R:806:HIS:O	1:R:810:PHE:HB3	2.17	0.44
3:I:65:GLU:O	3:I:68:LYS:HG2	2.17	0.44
3:H:63:GLN:O	3:H:67:GLN:HG2	2.18	0.44
5:S:6:LEU:HD23	5:S:6:LEU:H	1.81	0.44
8:F:335:TYR:HE2	8:F:369:THR:HG22	1.82	0.44
15:5:24:VAL:HG23	15:6:101:LEU:HB3	1.99	0.44
17:P:54:GLU:O	17:P:56:LYS:HD2	2.17	0.44
1:R:406:MET:HB3	1:R:744:LEU:HB3	2.00	0.44
4:M:27:LYS:HE2	4:M:31:ARG:HH21	1.82	0.44
7:C:511:VAL:HG21	7:C:548:TYR:HB2	1.98	0.44
8:E:430:LYS:HA	8:E:430:LYS:HD3	1.83	0.44
14:0:140:ALA:O	14:0:144:VAL:HG12	2.17	0.44
15:7:14:PHE:HB2	15:7:89:SER:OG	2.17	0.44
16:Q:11:VAL:HG12	16:Q:12:ASP:OD1	2.17	0.44
16:Q:122:ILE:HG13	16:Q:143:ILE:HD13	1.99	0.44
17:P:64:GLU:HA	17:P:67:GLN:OE1	2.16	0.44
1:R:24:CYS:HB2	1:R:90:PHE:CZ	2.53	0.44
1:R:267:ASP:O	1:R:271:VAL:HG22	2.16	0.44
1:R:767:LYS:HG2	1:R:769:LEU:H	1.83	0.44
2:O:152:ASN:HB3	2:O:156:LYS:NZ	2.33	0.44
2:O:174:ASP:CG	2:O:216:LEU:HB2	2.38	0.44
4:L:34:LYS:HA	4:L:37:LYS:HG3	2.00	0.44
6:T:58:SER:O	6:T:62:VAL:HG13	2.17	0.44
6:T:75:HIS:O	6:T:75:HIS:ND1	2.50	0.44
12:U:384:LEU:HD23	12:U:384:LEU:HA	1.79	0.44
15:6:45:SER:HB2	15:7:127:LEU:HD21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:40:GLU:N	16:Q:40:GLU:OE1	2.50	0.44
16:Q:112:LEU:HD22	16:Q:122:ILE:HD12	1.99	0.44
16:Q:328:ASN:HD21	16:Q:347:TYR:HB2	1.83	0.44
17:P:426:ARG:O	17:P:429:GLU:HG2	2.18	0.44
2:O:161:LEU:HD13	2:O:224:LEU:HD22	2.00	0.44
2:O:313:PRO:HD3	3:I:14:HIS:HE1	1.83	0.44
3:J:127:LEU:HD22	3:J:183:ILE:HG22	2.00	0.44
7:C:246:THR:OG1	7:C:247:ALA:N	2.50	0.44
7:C:246:THR:HG23	7:C:407:VAL:HA	1.99	0.44
7:A:134:ASP:OD2	7:A:157:SER:OG	2.35	0.44
7:A:594:GLU:O	7:A:598:LYS:HG3	2.17	0.44
8:E:296:ILE:HD13	8:E:351:ILE:HB	2.00	0.44
8:D:153:ILE:HD11	8:D:277:LEU:HG	2.00	0.44
15:3:130:GLY:O	15:3:134:ILE:HG13	2.18	0.44
15:9:150:LEU:HD23	15:9:150:LEU:HA	1.80	0.44
1:R:808:VAL:O	1:R:812:ASN:HB2	2.17	0.44
2:O:312:LEU:HD22	3:I:21:GLN:HE22	1.82	0.44
2:O:364:GLN:HG2	2:O:365:GLU:OE1	2.17	0.44
3:I:155:TYR:O	3:I:159:THR:HG22	2.18	0.44
9:Y:223:LYS:HE2	9:Y:253:ASP:OD1	2.17	0.44
14:0:166:ASP:OD2	14:0:173:PHE:HB2	2.17	0.44
15:2:99:VAL:HB	15:2:149:ALA:HB2	1.99	0.44
15:8:57:ILE:O	15:8:60:VAL:HG22	2.18	0.44
17:P:119:LYS:HD3	17:P:153:LYS:HE3	1.99	0.44
17:P:320:ASN:OD1	17:P:321:LEU:N	2.51	0.44
17:P:429:GLU:HA	17:P:434:LYS:HG2	2.00	0.44
1:R:472:LEU:HB3	1:R:474:ILE:HG12	1.98	0.44
1:R:725:ILE:HA	1:R:728:CYS:SG	2.57	0.44
2:O:175:PHE:CD2	2:O:253:TYR:HB2	2.52	0.44
7:B:510:GLU:HG3	7:B:567:TRP:CE2	2.52	0.44
7:C:23:GLY:H	8:F:88:GLU:HB2	1.83	0.44
7:C:24:VAL:O	8:F:314:ARG:NH1	2.50	0.44
7:A:44:ARG:HA	7:A:50:LEU:O	2.17	0.44
7:A:233:VAL:HG13	7:A:234:LEU:HG	2.00	0.44
8:E:46:THR:O	8:E:46:THR:OG1	2.33	0.44
8:E:164:ILE:HD11	8:E:342:GLU:HA	2.00	0.44
8:F:87:LEU:HD22	8:F:314:ARG:HD3	2.00	0.44
8:F:209:GLN:NE2	8:F:470:ASN:HA	2.33	0.44
9:Z:143:ALA:HB1	9:Z:149:ASN:ND2	2.33	0.44
9:X:159:LEU:HD21	9:X:179:PHE:CE1	2.53	0.44
9:X:200:PHE:O	9:X:204:VAL:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:5:47:MET:H	15:5:47:MET:HG2	1.69	0.44
15:7:24:VAL:HG21	15:8:101:LEU:HD13	1.99	0.44
15:8:9:GLU:O	15:8:10:TYR:HB2	2.18	0.44
17:P:213:GLU:HG3	17:P:214:TYR:N	2.32	0.44
17:P:296:SER:HB3	17:P:302:ARG:HD3	1.99	0.44
17:P:392:LYS:HB3	17:P:392:LYS:HE3	1.75	0.44
1:R:189:ARG:NH1	2:O:346:ALA:O	2.51	0.44
2:O:71:LYS:HG3	2:O:75:TYR:CE2	2.53	0.44
4:M:52:GLU:O	4:M:56:LYS:HG2	2.18	0.44
3:I:94:LEU:HD13	3:I:215:LEU:HD11	2.00	0.44
3:I:176:ASP:OD1	3:I:176:ASP:N	2.50	0.44
7:C:233:VAL:HG13	7:C:234:LEU:HG	2.00	0.44
15:1:60:VAL:O	15:1:64:ILE:HG13	2.18	0.44
15:9:20:SER:O	15:9:24:VAL:HG12	2.18	0.44
16:Q:166:ASP:OD1	16:Q:166:ASP:N	2.50	0.44
16:Q:247:LEU:O	16:Q:252:LEU:HG	2.18	0.44
7:A:216:PRO:HB2	7:A:395:LEU:HD11	2.00	0.44
9:Z:69:SER:HA	9:Z:74:CYS:HB2	2.00	0.44
15:9:22:ALA:HB2	15:9:96:GLY:HA2	1.99	0.44
16:Q:36:LEU:HD22	16:Q:45:LEU:HD12	1.99	0.44
17:P:260:LEU:HA	17:P:262:ARG:NH1	2.33	0.44
17:P:302:ARG:NH1	17:P:305:TYR:OH	2.51	0.44
1:R:471:SER:HB2	1:R:523:ASN:HD22	1.83	0.43
2:O:312:LEU:HG	3:I:14:HIS:ND1	2.32	0.43
4:M:54:GLU:O	4:M:58:LYS:HG2	2.19	0.43
7:B:60:ASP:OD1	7:B:60:ASP:N	2.51	0.43
7:B:558:THR:OG1	7:B:562:ASP:O	2.35	0.43
7:C:547:PHE:HB2	7:C:608:MET:SD	2.58	0.43
9:Z:209:GLU:OE1	9:Z:209:GLU:N	2.51	0.43
9:Z:240:LYS:NZ	9:Z:244:ASP:OD1	2.38	0.43
9:X:216:ILE:HG13	9:X:217:LEU:N	2.33	0.43
15:1:54:LYS:HB3	15:1:128:PHE:CE2	2.53	0.43
15:5:9:GLU:HG3	15:5:10:TYR:N	2.33	0.43
17:P:31:VAL:HB	17:P:92:TYR:HE2	1.83	0.43
17:P:47:CYS:SG	17:P:50:ILE:HD12	2.57	0.43
17:P:121:THR:HA	17:P:124:PRO:HG2	1.99	0.43
17:P:243:MET:O	17:P:246:SER:OG	2.31	0.43
2:O:325:LYS:HE2	2:O:326:LYS:HD3	2.00	0.43
4:K:40:ALA:O	4:K:44:ILE:HG22	2.18	0.43
7:B:70:THR:O	7:B:73:VAL:HG12	2.17	0.43
8:F:251:ASN:O	8:F:253:SER:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:173:GLY:N	8:D:178:ASP:OD2	2.52	0.43
12:U:323:PHE:CD2	12:U:347:VAL:HG12	2.54	0.43
14:0:127:GLY:HA2	14:0:130:ASN:H	1.83	0.43
17:P:365:GLU:OE2	17:P:366:TRP:N	2.51	0.43
1:R:478:SER:HB3	1:R:519:ASP:OD2	2.17	0.43
2:O:207:MET:HB3	2:O:230:PHE:HB2	2.00	0.43
7:C:159:ASN:ND2	7:C:307:LYS:HB3	2.33	0.43
8:D:190:PRO:HD2	8:D:375:GLY:O	2.18	0.43
11:N:13:ASP:N	11:N:13:ASP:OD1	2.50	0.43
12:U:301:PHE:CG	12:U:302:TRP:N	2.86	0.43
16:Q:190:LEU:HA	16:Q:190:LEU:HD23	1.71	0.43
16:Q:330:VAL:O	16:Q:334:GLU:HG2	2.19	0.43
1:R:375:GLN:NE2	1:R:379:ASP:OD1	2.51	0.43
3:I:136:CYS:SG	3:I:144:VAL:HG11	2.58	0.43
6:T:98:TYR:HA	6:T:101:TYR:CD2	2.53	0.43
7:C:55:ILE:HG22	7:C:63:THR:OG1	2.18	0.43
8:E:317:VAL:HG22	10:G:205:ILE:HD13	2.00	0.43
9:Z:174:GLY:O	9:Z:177:GLN:HG2	2.18	0.43
10:G:58:MET:HB2	10:G:144:LEU:HD21	2.00	0.43
14:0:85:ARG:H	14:0:85:ARG:HG3	1.67	0.43
15:3:14:PHE:HB2	15:3:89:SER:OG	2.18	0.43
15:3:24:VAL:HG23	15:4:101:LEU:HB3	1.99	0.43
15:6:131:MET:O	15:6:135:LEU:HG	2.18	0.43
3:I:55:GLU:O	3:I:59:LYS:HG2	2.19	0.43
5:S:55:ALA:O	5:S:59:GLN:NE2	2.48	0.43
6:T:48:PRO:HA	6:T:129:ASN:ND2	2.34	0.43
7:B:234:LEU:HG	7:B:433:TRP:CD2	2.54	0.43
8:E:320:ARG:HE	8:E:320:ARG:HB3	1.69	0.43
8:E:485:ARG:HH12	8:E:506:ARG:HH21	1.65	0.43
8:D:279:LEU:HB3	8:D:337:ARG:HD2	1.99	0.43
9:Y:41:ASN:ND2	9:Y:105:LEU:HD21	2.33	0.43
9:Y:134:ASN:HA	9:Y:137:THR:HG22	1.99	0.43
14:0:49:TRP:HB3	14:0:138:PHE:HB2	2.01	0.43
15:9:141:LEU:HD23	15:9:141:LEU:HA	1.63	0.43
17:P:163:TYR:O	17:P:168:ILE:HG13	2.19	0.43
17:P:293:LEU:HD21	17:P:341:LYS:CD	2.46	0.43
3:J:5:ASP:HA	3:J:8:VAL:HG12	2.00	0.43
3:H:115:LEU:HD12	3:H:115:LEU:HA	1.87	0.43
4:K:75:LYS:HG2	4:K:79:GLU:OE1	2.18	0.43
7:B:253:GLY:HA3	7:B:256:LYS:HG3	2.01	0.43
7:B:510:GLU:HG3	7:B:567:TRP:NE1	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:331:ILE:HA	7:C:331:ILE:HD12	1.84	0.43
8:E:193:SER:O	8:E:356:MET:HG2	2.19	0.43
8:E:271:ARG:O	8:E:303:TYR:HD1	2.02	0.43
8:D:279:LEU:HD21	8:D:350:GLN:HE21	1.83	0.43
9:X:159:LEU:HD21	9:X:179:PHE:CD1	2.54	0.43
15:3:37:SER:OG	15:3:58:PRO:HB2	2.19	0.43
15:4:32:TYR:CD2	15:4:108:PHE:HD1	2.37	0.43
16:Q:58:LEU:HD13	16:Q:65:LEU:HD11	1.99	0.43
17:P:368:PRO:O	17:P:372:SER:N	2.52	0.43
1:R:357:THR:OG1	1:R:358:ASN:N	2.52	0.43
1:R:397:ILE:HD11	5:S:44:CYS:HB2	2.01	0.43
2:O:167:ALA:O	2:O:258:MET:HB3	2.19	0.43
3:J:9:GLN:O	3:J:13:LYS:HG2	2.18	0.43
4:M:18:ALA:O	4:M:22:VAL:HG23	2.19	0.43
3:I:36:GLU:O	3:I:40:ILE:HG13	2.18	0.43
3:I:97:GLU:HG2	4:L:96:LEU:HD21	2.00	0.43
4:K:103:VAL:O	4:K:103:VAL:HG12	2.18	0.43
7:B:443:LYS:HB2	8:E:494:ARG:NE	2.33	0.43
7:B:489:LEU:O	7:B:493:VAL:HG13	2.18	0.43
7:A:152:ILE:HD13	7:A:165:LYS:HD3	2.01	0.43
7:A:272:ILE:HD13	7:A:345:SER:HB3	2.00	0.43
7:A:569:ILE:HG22	7:A:615:LEU:HD21	1.99	0.43
8:E:188:LYS:HG3	8:E:188:LYS:O	2.19	0.43
8:F:49:THR:O	8:F:49:THR:OG1	2.29	0.43
8:D:411:THR:OG1	8:D:412:ARG:N	2.52	0.43
8:D:444:LEU:HB3	8:D:448:ASP:HB2	2.00	0.43
14:0:23:GLY:O	14:0:27:THR:HG22	2.19	0.43
15:6:21:ALA:HA	15:6:24:VAL:HG12	2.00	0.43
16:Q:271:TYR:HD2	16:Q:274:TYR:CD2	2.35	0.43
1:R:503:ASN:OD1	1:R:506:LEU:N	2.51	0.43
2:O:51:LEU:HD12	2:O:54:LEU:HD12	2.01	0.43
3:I:111:ARG:HA	3:I:114:VAL:HG12	2.01	0.43
3:I:129:GLU:OE2	8:E:64:LYS:NZ	2.35	0.43
7:A:145:SER:OG	9:X:31:ARG:HD3	2.19	0.43
7:A:397:ASN:HB2	7:A:398:PRO:HD3	1.99	0.43
9:Y:61:ARG:O	9:Y:63:GLU:N	2.52	0.43
12:U:453:MET:O	15:2:119:ARG:NH1	2.52	0.43
15:2:72:VAL:HG11	15:2:99:VAL:HG11	2.01	0.43
15:6:22:ALA:HB2	15:6:96:GLY:HA2	2.00	0.43
15:9:135:LEU:HD23	15:9:135:LEU:HA	1.85	0.43
16:Q:84:HIS:HE1	16:Q:88:HIS:CE1	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:39:GLY:HA3	17:P:44:ALA:N	2.33	0.43
1:R:6:ARG:HG2	1:R:389:ILE:HA	2.00	0.43
1:R:172:ALA:HB2	1:R:198:ARG:HB3	2.01	0.43
1:R:645:LEU:O	1:R:648:PRO:HD2	2.19	0.43
2:O:336:HIS:NE2	2:O:349:ILE:O	2.51	0.43
3:J:38:PHE:HA	4:M:36:ALA:HB2	2.01	0.43
4:L:53:LYS:HA	4:L:53:LYS:HD3	1.65	0.43
3:H:44:ARG:HG2	3:H:47:GLN:NE2	2.34	0.43
7:A:587:LYS:HA	7:A:587:LYS:HD3	1.60	0.43
10:G:98:LYS:HD3	10:G:98:LYS:HA	1.80	0.43
15:8:77:ALA:O	15:8:80:LEU:HB2	2.19	0.43
17:P:24:ALA:HA	17:P:27:ARG:HB3	2.00	0.43
17:P:293:LEU:HG	17:P:305:TYR:HE1	1.84	0.43
1:R:85:ASN:HB2	1:R:86:PRO:HD3	2.00	0.43
2:O:7:ILE:HA	2:O:370:VAL:O	2.19	0.43
2:O:97:ASP:HB3	2:O:100:THR:HG22	2.01	0.43
2:O:167:ALA:HA	2:O:258:MET:HG2	2.00	0.43
2:O:260:ALA:O	2:O:264:GLU:HG2	2.18	0.43
4:K:54:GLU:O	4:K:58:LYS:HG2	2.19	0.43
6:T:98:TYR:HA	6:T:101:TYR:HB2	2.01	0.43
7:C:228:LEU:HB2	7:C:268:ASN:HD22	1.83	0.43
8:E:78:ASP:OD1	8:E:79:GLY:N	2.52	0.43
9:Z:93:ARG:NH2	9:Z:131:ASN:OD1	2.52	0.43
12:U:289:THR:HG22	12:U:290:PHE:N	2.33	0.43
14:0:62:VAL:HG13	15:1:141:LEU:HB3	2.01	0.43
15:3:118:VAL:HA	15:3:121:THR:HG22	2.00	0.43
15:4:128:PHE:O	15:4:132:ILE:HG12	2.19	0.43
15:9:47:MET:O	15:9:48:ARG:HD2	2.18	0.43
16:Q:118:HIS:HB2	16:Q:120:ARG:HE	1.84	0.43
1:R:552:VAL:O	1:R:555:SER:OG	2.28	0.42
2:O:188:VAL:N	2:O:247:ILE:O	2.51	0.42
3:H:28:GLU:HB3	17:P:245:PHE:CZ	2.54	0.42
3:H:41:GLU:OE2	3:H:42:LYS:HE3	2.19	0.42
3:H:103:SER:O	3:H:106:VAL:HG22	2.19	0.42
3:H:116:LEU:HD23	3:H:116:LEU:HA	1.82	0.42
7:C:130:ASP:OD1	7:C:130:ASP:N	2.47	0.42
7:C:439:LEU:HD12	7:C:444:HIS:CG	2.54	0.42
7:C:610:ASN:OD1	7:C:613:ARG:NH1	2.52	0.42
7:A:204:THR:OG1	7:A:205:MET:N	2.51	0.42
8:F:215:LYS:HZ3	8:F:474:PHE:HB2	1.81	0.42
9:Y:194:ASP:OD1	9:Y:232:TYR:OH	2.30	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:X:93:ARG:NH2	9:X:134:ASN:HD22	2.17	0.42
9:X:101:PHE:CE1	9:X:161:MET:HB3	2.54	0.42
9:X:112:TYR:CZ	9:X:116:LYS:HD2	2.54	0.42
15:2:57:ILE:HB	15:2:58:PRO:HD3	2.00	0.42
15:9:9:GLU:HG2	15:9:10:TYR:CE2	2.54	0.42
17:P:74:ALA:HA	17:P:77:PHE:CD2	2.53	0.42
17:P:268:VAL:O	17:P:272:ILE:HG12	2.19	0.42
1:R:792:ILE:O	1:R:796:LEU:N	2.46	0.42
2:O:58:LEU:HD21	2:O:304:VAL:HG11	2.00	0.42
4:L:32:ARG:HD3	4:L:32:ARG:HA	1.68	0.42
3:H:53:ILE:HD11	4:K:48:ARG:HH21	1.84	0.42
7:B:250:GLY:O	7:B:411:SER:HA	2.19	0.42
7:A:271:VAL:HG12	7:A:272:ILE:N	2.34	0.42
19:A:701:ADP:H8	19:A:701:ADP:H5'1	1.84	0.42
8:E:72:VAL:HG21	8:E:96:VAL:HG11	2.01	0.42
15:7:91:LEU:HD23	15:7:91:LEU:HA	1.80	0.42
17:P:264:ASN:OD1	17:P:267:PRO:HG2	2.19	0.42
17:P:403:ASP:OD2	17:P:405:GLN:HG3	2.19	0.42
1:R:82:THR:OG1	1:R:83:GLY:N	2.53	0.42
1:R:303:ILE:HG22	1:R:307:LEU:HD23	2.02	0.42
1:R:310:CYS:SG	1:R:311:ASN:N	2.92	0.42
1:R:771:GLY:O	1:R:774:VAL:HG22	2.20	0.42
2:O:262:LYS:HA	2:O:265:MET:HE2	2.01	0.42
4:K:24:GLU:OE1	4:K:28:ARG:NH2	2.46	0.42
7:C:24:VAL:CG1	7:C:29:VAL:HG13	2.50	0.42
7:C:201:GLU:OE2	7:C:203:PHE:HB2	2.19	0.42
9:Y:249:LEU:HD13	9:Y:263:ILE:HD13	2.01	0.42
9:Z:247:SER:O	9:Z:250:SER:OG	2.37	0.42
14:0:66:ALA:HB1	15:1:109:ALA:HB2	2.01	0.42
14:0:67:TRP:HA	14:0:70:TYR:CE1	2.54	0.42
15:9:72:VAL:O	15:9:76:ILE:HG12	2.20	0.42
17:P:395:THR:HB	17:P:396:LYS:NZ	2.35	0.42
1:R:338:ARG:HA	1:R:341:THR:HG22	2.01	0.42
7:B:473:VAL:HG13	7:B:476:ARG:NH2	2.35	0.42
7:A:177:THR:OG1	7:A:193:GLU:O	2.31	0.42
8:E:49:THR:OG1	8:E:49:THR:O	2.36	0.42
8:E:221:ASP:O	8:E:225:GLU:HG2	2.19	0.42
10:G:83:VAL:HG21	11:N:18:THR:HG23	2.00	0.42
12:U:261:ASN:HA	12:U:265:PRO:HA	2.01	0.42
16:Q:140:ALA:O	16:Q:143:ILE:HD11	2.19	0.42
16:Q:150:LEU:HA	16:Q:150:LEU:HD12	1.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:199:GLN:O	17:P:242:GLN:NE2	2.42	0.42
1:R:479:TRP:CD1	1:R:521:ILE:HG21	2.54	0.42
1:R:606:PRO:HG3	1:R:626:SER:HB3	2.00	0.42
2:O:150:LEU:O	2:O:154:GLU:HG2	2.19	0.42
7:C:294:LEU:HD23	7:C:294:LEU:HA	1.84	0.42
7:A:604:LEU:HD12	7:A:604:LEU:HA	1.83	0.42
8:E:74:LEU:HG	8:E:112:CYS:SG	2.60	0.42
8:D:356:MET:HB3	8:D:366:PRO:HG3	2.02	0.42
12:U:456:PHE:CE2	15:2:119:ARG:HB3	2.55	0.42
14:0:51:ASN:HA	14:0:54:ILE:HG22	2.01	0.42
14:0:63:VAL:HG13	14:0:149:LEU:HD13	2.00	0.42
15:1:7:GLY:HA2	15:1:8:PRO:HD3	1.95	0.42
17:P:91:GLN:HE21	17:P:95:THR:HG1	1.68	0.42
17:P:314:VAL:O	17:P:318:LEU:N	2.49	0.42
1:R:135:THR:O	1:R:135:THR:OG1	2.29	0.42
2:O:150:LEU:HD22	2:O:269:SER:HA	2.01	0.42
3:I:21:GLN:HA	3:I:24:ASN:ND2	2.33	0.42
4:L:51:ARG:HE	4:L:51:ARG:HB3	1.68	0.42
3:H:159:THR:HG22	3:H:161:ASN:ND2	2.35	0.42
7:B:24:VAL:HG22	8:E:89:VAL:HG22	2.02	0.42
7:C:291:PHE:O	7:C:295:THR:HG22	2.20	0.42
7:A:481:GLU:O	7:A:485:GLU:HG2	2.19	0.42
8:F:493:LYS:HE2	8:F:493:LYS:HB3	1.87	0.42
8:D:237:ASN:OD1	8:D:237:ASN:N	2.48	0.42
9:Y:152:LEU:HD23	9:Y:152:LEU:HA	1.80	0.42
9:Y:170:GLU:OE2	9:Y:172:ASN:HB2	2.20	0.42
9:Z:207:GLN:NE2	9:Z:209:GLU:HB2	2.29	0.42
10:G:94:ILE:HD13	10:G:94:ILE:HA	1.90	0.42
15:2:50:GLU:H	15:2:50:GLU:CD	2.23	0.42
17:P:194:SER:OG	17:P:195:SER:N	2.52	0.42
1:R:28:GLU:HA	1:R:31:GLU:HB2	2.00	0.42
1:R:187:LEU:HD23	1:R:222:ILE:H	1.84	0.42
2:O:65:VAL:HG13	2:O:294:TRP:HD1	1.85	0.42
2:O:125:ILE:O	2:O:129:VAL:HG22	2.20	0.42
8:F:117:ASP:OD1	8:F:118:ILE:N	2.53	0.42
8:D:388:ILE:HG23	8:D:464:ALA:HB2	2.02	0.42
9:Y:172:ASN:HB3	9:Y:175:ILE:HG12	2.02	0.42
9:Y:216:ILE:HG13	9:Y:217:LEU:N	2.34	0.42
9:Z:211:SER:O	9:Z:213:PHE:N	2.52	0.42
15:4:150:LEU:HD23	15:4:150:LEU:HA	1.76	0.42
15:5:61:MET:SD	15:5:135:LEU:HB3	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:126:PHE:HA	17:P:129:MET:HB2	2.02	0.42
1:R:176:ASN:OD1	1:R:241:ARG:NH1	2.52	0.42
1:R:598:ASP:OD1	1:R:598:ASP:N	2.51	0.42
4:L:41:GLN:O	4:L:45:GLU:HG2	2.19	0.42
4:L:99:LEU:O	4:L:103:VAL:HG23	2.19	0.42
3:H:223:LYS:HA	3:H:223:LYS:HD3	1.89	0.42
7:C:24:VAL:HB	7:C:28:VAL:O	2.20	0.42
7:C:42:LEU:O	7:C:82:THR:OG1	2.19	0.42
7:A:372:SER:HB2	7:A:420:PRO:HG2	2.01	0.42
15:7:18:GLY:HA3	15:7:93:LEU:HA	2.01	0.42
17:P:119:LYS:HZ2	17:P:153:LYS:HE3	1.84	0.42
17:P:280:LYS:HE2	17:P:280:LYS:HB3	1.94	0.42
17:P:356:SER:O	17:P:360:LYS:HG2	2.20	0.42
17:P:399:GLU:HG2	17:P:436:LEU:CD2	2.48	0.42
1:R:123:LEU:O	1:R:126:THR:HG22	2.20	0.42
1:R:190:VAL:HG13	1:R:191:CYS:N	2.33	0.42
2:O:97:ASP:OD1	2:O:98:LEU:N	2.53	0.42
2:O:170:VAL:HG12	2:O:224:LEU:HD21	2.01	0.42
2:O:238:ARG:HB3	2:O:248:VAL:HG21	2.01	0.42
4:M:34:LYS:HA	4:M:37:LYS:HG2	2.01	0.42
3:H:50:ARG:O	3:H:54:MET:HG2	2.20	0.42
7:C:158:GLU:OE2	7:C:164:HIS:ND1	2.53	0.42
8:E:390:PRO:HA	8:E:391:PRO:HD3	1.89	0.42
8:F:466:GLY:HA2	8:F:467:PRO:HD3	1.79	0.42
8:D:128:LEU:HD23	8:D:128:LEU:HA	1.91	0.42
9:X:114:LYS:HD3	9:X:114:LYS:HA	1.91	0.42
10:G:65:ALA:HB1	10:G:138:TYR:CZ	2.55	0.42
17:P:124:PRO:O	17:P:127:LEU:HB2	2.20	0.42
17:P:397:LEU:HB3	17:P:401:SER:OG	2.20	0.42
17:P:428:ILE:O	17:P:432:GLY:N	2.53	0.42
1:R:116:GLU:HA	1:R:119:LYS:HD3	2.02	0.42
1:R:349:PRO:O	1:R:350:SER:OG	2.35	0.42
2:O:24:ALA:HB2	2:O:31:ASN:HD22	1.85	0.42
2:O:136:LEU:HD11	2:O:286:ASN:ND2	2.35	0.42
2:O:180:GLU:OE1	4:M:11:LEU:HB3	2.20	0.42
9:Z:143:ALA:HB1	9:Z:149:ASN:HD22	1.84	0.42
10:G:57:LEU:O	10:G:60:GLU:HG3	2.20	0.42
12:U:456:PHE:O	16:Q:87:ASN:HB3	2.20	0.42
15:3:101:LEU:HD23	15:3:101:LEU:HA	1.85	0.42
15:6:6:SER:OG	15:6:7:GLY:N	2.51	0.42
17:P:89:THR:O	17:P:93:ILE:HG22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:234:LYS:HA	1:R:237:CYS:SG	2.60	0.41
4:M:31:ARG:HH11	4:M:34:LYS:HG3	1.84	0.41
4:L:106:ILE:HG23	4:L:107:ARG:N	2.35	0.41
4:K:19:ALA:HA	4:K:22:VAL:HG12	2.01	0.41
7:B:207:GLN:HE21	7:B:215:ARG:HH12	1.68	0.41
7:B:573:HIS:CG	7:B:615:LEU:HD13	2.55	0.41
7:B:580:LYS:CB	7:B:604:LEU:HD11	2.50	0.41
7:A:298:VAL:HG13	7:A:299:ASP:H	1.83	0.41
8:E:97:GLN:HG3	8:E:97:GLN:O	2.20	0.41
8:F:184:ALA:HB2	8:F:405:ALA:HB2	2.01	0.41
9:X:33:MET:HA	9:X:36:ILE:HG22	2.01	0.41
15:4:50:GLU:O	15:4:54:LYS:HE3	2.20	0.41
15:6:41:ILE:HD12	15:6:55:SER:HB3	2.02	0.41
16:Q:16:LEU:HD23	16:Q:16:LEU:HA	1.86	0.41
17:P:80:LEU:HD12	17:P:83:HIS:ND1	2.34	0.41
17:P:365:GLU:HA	17:P:405:GLN:OE1	2.20	0.41
17:P:387:ASN:HB3	17:P:389:GLU:HG2	2.02	0.41
17:P:456:VAL:O	17:P:460:MET:HG2	2.20	0.41
1:R:285:ALA:HA	1:R:288:LYS:HZ3	1.85	0.41
1:R:500:LEU:HD12	1:R:501:GLN:H	1.85	0.41
1:R:659:ARG:HA	1:R:662:TYR:HB3	2.02	0.41
1:R:764:LEU:HD22	6:T:82:ASP:HA	2.01	0.41
2:O:244:ASN:HB3	2:O:246:PHE:CE2	2.55	0.41
3:J:219:ASN:OD1	3:J:220:ALA:N	2.53	0.41
5:S:73:ILE:HA	5:S:76:LEU:CG	2.49	0.41
7:B:297:GLU:N	7:B:297:GLU:OE1	2.52	0.41
7:B:478:LYS:HE2	7:B:478:LYS:HB2	1.87	0.41
9:X:224:ILE:O	9:X:228:THR:HG23	2.20	0.41
12:U:435:PHE:CZ	14:0:56:LEU:HD21	2.54	0.41
15:7:95:ALA:O	15:7:99:VAL:HG12	2.20	0.41
15:8:95:ALA:O	15:8:99:VAL:HG12	2.19	0.41
16:Q:109:VAL:HG23	16:Q:135:PHE:HZ	1.85	0.41
1:R:118:LEU:HD11	1:R:271:VAL:HG23	2.01	0.41
2:O:333:GLU:HG3	2:O:354:MET:SD	2.61	0.41
3:J:29:GLU:O	3:J:33:LYS:HG3	2.20	0.41
3:H:180:GLY:HA3	3:H:195:THR:HA	2.02	0.41
7:C:233:VAL:HG22	7:C:234:LEU:H	1.85	0.41
7:C:290:ASP:O	7:C:294:LEU:N	2.45	0.41
8:F:453:GLU:OE2	8:F:457:LYS:HE3	2.20	0.41
9:Y:103:MET:HE2	9:Y:103:MET:HB3	1.72	0.41
11:N:54:GLN:HA	11:N:57:ASN:HD22	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:3:76:ILE:HD12	15:3:92:GLN:HB3	2.01	0.41
17:P:281:VAL:O	17:P:285:ILE:HG22	2.20	0.41
1:R:437:ASN:HB3	1:R:440:PHE:HB3	2.01	0.41
1:R:488:ASN:N	1:R:488:ASN:ND2	2.68	0.41
1:R:800:LEU:O	1:R:804:ARG:N	2.45	0.41
2:O:136:LEU:HD11	2:O:286:ASN:CG	2.41	0.41
2:O:280:VAL:HB	2:O:284:LYS:HE3	2.03	0.41
3:I:118:GLY:HA3	4:L:106:ILE:HG21	2.02	0.41
3:H:15:MET:HB3	4:K:10:GLN:HG3	2.01	0.41
7:B:249:PRO:HG2	7:B:434:GLY:HA2	2.01	0.41
8:E:46:THR:HG22	8:E:113:GLU:HB2	2.02	0.41
15:1:147:ILE:HD13	15:1:147:ILE:HA	1.85	0.41
15:3:98:SER:OG	15:3:99:VAL:N	2.54	0.41
15:4:80:LEU:HD23	15:4:80:LEU:HA	1.92	0.41
17:P:123:TRP:CH2	17:P:153:LYS:HG2	2.55	0.41
17:P:129:MET:O	17:P:130:LEU:HB2	2.20	0.41
17:P:367:SER:OG	17:P:369:VAL:HG12	2.20	0.41
1:R:725:ILE:HA	1:R:728:CYS:HG	1.85	0.41
2:O:51:LEU:HA	2:O:54:LEU:HD12	2.02	0.41
4:L:56:LYS:HA	4:L:56:LYS:HD3	1.87	0.41
3:H:82:LYS:NZ	4:K:74:GLU:OE2	2.54	0.41
7:C:295:THR:OG1	7:C:302:VAL:HG13	2.19	0.41
7:C:295:THR:CG2	7:C:302:VAL:HG13	2.50	0.41
7:C:489:LEU:HD11	7:C:505:ASP:HB3	2.01	0.41
8:F:434:ALA:O	8:F:438:VAL:HG22	2.20	0.41
8:D:472:THR:OG1	8:D:475:GLU:HG3	2.19	0.41
9:Y:146:THR:HG22	9:Y:149:ASN:ND2	2.35	0.41
14:0:106:ILE:HD13	14:0:106:ILE:HA	1.91	0.41
15:3:19:ALA:HB2	15:3:76:ILE:HG21	2.02	0.41
1:R:24:CYS:O	1:R:27:SER:OG	2.30	0.41
2:O:134:ASN:HA	2:O:137:LYS:HE3	2.02	0.41
2:O:261:ASP:O	2:O:265:MET:HG3	2.21	0.41
2:O:325:LYS:HD2	2:O:325:LYS:HA	1.78	0.41
3:I:90:LEU:HD23	3:I:90:LEU:HA	1.85	0.41
3:H:156:LYS:HE2	3:H:162:ASP:HA	2.02	0.41
7:C:587:LYS:HD3	7:C:587:LYS:HA	1.79	0.41
8:E:73:HIS:HB2	8:E:113:GLU:HG2	2.02	0.41
8:E:432:VAL:HG21	8:E:448:ASP:HB3	2.02	0.41
8:F:380:ASP:OD2	8:F:393:ASN:ND2	2.53	0.41
8:D:485:ARG:HH12	8:D:506:ARG:NH2	2.18	0.41
9:X:267:VAL:O	9:X:271:GLU:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:V:302:GLU:OE2	15:2:10:TYR:OH	2.37	0.41
16:Q:47:LEU:HA	16:Q:50:GLN:CD	2.41	0.41
1:R:495:ARG:HA	1:R:495:ARG:HD3	1.83	0.41
2:O:305:GLU:CD	2:O:370:VAL:HG13	2.40	0.41
3:J:187:ASP:OD1	3:J:187:ASP:N	2.39	0.41
7:C:116:ILE:HD11	8:F:344:ARG:CZ	2.50	0.41
8:F:77:PRO:HD3	8:F:110:THR:HG22	2.02	0.41
8:F:435:MET:HA	8:F:438:VAL:HG22	2.03	0.41
9:Y:238:SER:HB3	9:Y:274:ASN:HD21	1.84	0.41
12:U:278:TYR:O	12:U:392:PRO:HB2	2.20	0.41
14:0:118:PHE:O	14:0:119:SER:OG	2.34	0.41
15:2:133:LEU:O	15:2:136:ILE:HG22	2.20	0.41
16:Q:204:THR:HA	16:Q:311:HIS:HB2	2.02	0.41
1:R:197:LEU:HD23	1:R:197:LEU:HA	1.94	0.41
1:R:573:ILE:O	1:R:577:ILE:HG12	2.20	0.41
1:R:653:PHE:O	1:R:657:VAL:N	2.41	0.41
2:O:92:LEU:HB3	2:O:96:VAL:O	2.20	0.41
4:M:93:ASP:OD1	4:M:94:GLU:N	2.54	0.41
3:I:77:ASN:OD1	3:I:80:ARG:NH2	2.54	0.41
3:I:87:ARG:NH2	8:E:126:ASP:OD2	2.54	0.41
7:B:272:ILE:O	7:B:309:THR:HA	2.21	0.41
7:B:328:TYR:HA	7:B:331:ILE:HG22	2.03	0.41
7:A:344:VAL:HG12	7:A:345:SER:N	2.35	0.41
8:D:58:VAL:N	8:D:96:VAL:O	2.51	0.41
8:D:213:VAL:O	8:D:215:LYS:N	2.51	0.41
15:3:41:ILE:HD13	15:3:56:ILE:HD13	2.03	0.41
17:P:99:ASP:HA	17:P:102:GLN:HB3	2.03	0.41
1:R:219:VAL:HB	1:R:221:ILE:HD11	2.03	0.41
1:R:482:ARG:O	1:R:484:MET:HG2	2.21	0.41
2:O:301:ARG:HB3	2:O:372:TYR:CZ	2.56	0.41
2:O:364:GLN:OE1	2:O:364:GLN:N	2.49	0.41
3:J:16:MET:CE	4:M:11:LEU:HA	2.49	0.41
4:M:6:GLN:HA	4:M:9:GLN:HB3	2.03	0.41
3:I:42:LYS:O	3:I:46:VAL:HG12	2.21	0.41
4:L:96:LEU:HD12	4:L:96:LEU:HA	1.89	0.41
4:K:12:LEU:HA	4:K:15:GLU:OE1	2.20	0.41
4:K:56:LYS:HA	4:K:59:GLU:OE1	2.21	0.41
7:C:204:THR:HG23	7:C:206:VAL:H	1.84	0.41
7:C:220:LYS:HG2	7:C:392:VAL:HG12	2.03	0.41
7:C:417:PHE:HD1	7:C:422:THR:HG21	1.85	0.41
7:A:22:HIS:O	7:A:22:HIS:CG	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:507:ILE:HD11	7:A:555:VAL:HG21	2.02	0.41
7:A:596:LYS:HE2	7:A:596:LYS:HB2	1.87	0.41
8:E:218:ASP:HB3	8:E:221:ASP:HB2	2.03	0.41
8:E:317:VAL:HA	10:G:205:ILE:HD11	2.03	0.41
8:F:364:PRO:O	8:F:368:LEU:HG	2.20	0.41
8:D:404:SER:O	8:D:404:SER:OG	2.29	0.41
9:Y:192:LYS:HB3	9:Y:195:GLU:HB2	2.02	0.41
9:Y:224:ILE:O	9:Y:227:LYS:HG3	2.20	0.41
11:N:85:ILE:HB	11:N:86:PRO:HD3	2.03	0.41
14:0:42:THR:HG22	15:9:10:TYR:OH	2.21	0.41
15:1:22:ALA:HB2	15:1:96:GLY:HA2	2.03	0.41
15:1:51:GLN:O	15:1:55:SER:OG	2.25	0.41
15:3:7:GLY:HA3	15:3:84:ILE:O	2.21	0.41
15:9:21:ALA:HA	15:9:24:VAL:HG12	2.02	0.41
16:Q:49:LEU:O	16:Q:52:THR:OG1	2.34	0.41
16:Q:328:ASN:OD1	16:Q:347:TYR:HB2	2.21	0.41
17:P:114:TYR:HD2	17:P:119:LYS:NZ	2.17	0.41
17:P:277:VAL:O	17:P:277:VAL:HG23	2.21	0.41
17:P:316:LYS:HA	17:P:319:GLU:OE2	2.20	0.41
17:P:366:TRP:CE2	17:P:409:VAL:HG12	2.56	0.41
1:R:310:CYS:SG	1:R:319:LEU:HD12	2.61	0.41
2:O:195:ASN:O	2:O:198:ILE:HG22	2.21	0.41
3:J:20:GLU:HA	4:M:17:ARG:NH1	2.27	0.41
3:J:95:LEU:HD23	3:J:95:LEU:HA	1.89	0.41
4:L:24:GLU:HA	4:L:27:LYS:HD2	2.03	0.41
4:K:114:TYR:CE2	4:K:116:ILE:HG22	2.56	0.41
7:B:24:VAL:HG21	8:E:68:TYR:HB2	2.03	0.41
7:C:228:LEU:H	7:C:268:ASN:HD21	1.69	0.41
7:C:573:HIS:CG	7:C:615:LEU:HD12	2.56	0.41
7:A:247:ALA:HA	7:A:408:GLY:O	2.21	0.41
7:A:573:HIS:CG	7:A:615:LEU:HD13	2.56	0.41
8:D:279:LEU:HA	8:D:279:LEU:HD23	1.78	0.41
9:Y:141:LYS:HE3	9:Y:141:LYS:HB3	1.96	0.41
15:3:95:ALA:O	15:3:99:VAL:HG12	2.21	0.41
15:5:79:SER:O	15:5:79:SER:OG	2.23	0.41
16:Q:143:ILE:H	16:Q:143:ILE:HD12	1.85	0.41
17:P:62:LYS:HA	17:P:107:ARG:NH1	2.36	0.41
17:P:162:ASN:HA	17:P:167:TRP:HZ2	1.84	0.41
3:I:150:LYS:HB2	3:I:150:LYS:HE3	1.87	0.40
3:H:152:ILE:N	3:H:153:PRO:HD2	2.36	0.40
3:H:192:VAL:HG13	8:D:43:PRO:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:31:ARG:HE	4:K:32:ARG:HB3	1.86	0.40
7:A:70:THR:O	7:A:73:VAL:HG22	2.22	0.40
7:A:577:ILE:HG21	7:A:608:MET:HG3	2.03	0.40
8:D:390:PRO:HA	8:D:391:PRO:HD3	1.90	0.40
9:Y:242:LEU:HA	9:Y:245:LYS:HD3	2.03	0.40
9:Z:242:LEU:HA	9:Z:245:LYS:HD2	2.02	0.40
14:0:50:SER:OG	14:0:51:ASN:N	2.54	0.40
15:3:85:SER:C	15:3:87:TYR:H	2.23	0.40
15:4:136:ILE:HD13	15:4:136:ILE:HA	1.97	0.40
16:Q:67:VAL:HG21	16:Q:334:GLU:CD	2.41	0.40
1:R:223:PHE:CZ	1:R:230:LYS:HE3	2.56	0.40
1:R:633:LYS:HA	1:R:636:GLN:NE2	2.36	0.40
1:R:731:CYS:SG	1:R:732:ILE:N	2.94	0.40
2:O:117:SER:HB3	2:O:120:ASN:OD1	2.21	0.40
3:J:49:GLN:O	3:J:53:ILE:HG22	2.20	0.40
4:M:56:LYS:O	4:M:59:GLU:HG3	2.21	0.40
3:I:122:GLN:NE2	8:E:43:PRO:HD3	2.36	0.40
4:K:56:LYS:HA	4:K:59:GLU:CD	2.42	0.40
5:S:24:VAL:HG13	5:S:28:ILE:HG12	2.03	0.40
7:B:104:ARG:HE	7:B:104:ARG:HB2	1.78	0.40
7:B:469:PHE:CZ	7:B:534:PHE:HD2	2.39	0.40
7:C:84:LYS:HD2	7:C:87:SER:OG	2.21	0.40
7:C:117:TYR:HB3	8:F:156:GLN:HB2	2.03	0.40
8:E:420:ASN:HB3	8:E:494:ARG:HH11	1.87	0.40
8:F:212:LEU:HD13	8:F:225:GLU:HB2	2.01	0.40
8:D:78:ASP:OD1	8:D:78:ASP:N	2.54	0.40
9:Z:106:ASP:OD1	9:Z:107:LEU:N	2.54	0.40
9:Z:168:ILE:HD12	9:Z:168:ILE:HA	1.92	0.40
10:G:89:LYS:HA	11:N:27:GLU:HB2	2.04	0.40
11:N:14:GLU:OE2	11:N:18:THR:OG1	2.33	0.40
12:U:271:ALA:HA	12:U:399:ASP:O	2.21	0.40
14:0:42:THR:HA	15:9:10:TYR:CZ	2.56	0.40
15:2:41:ILE:O	15:2:44:MET:HG3	2.22	0.40
15:4:101:LEU:HD23	15:4:101:LEU:HA	1.86	0.40
15:6:41:ILE:CD1	15:6:118:VAL:HG21	2.51	0.40
17:P:46:ASP:O	17:P:50:ILE:HG13	2.21	0.40
17:P:309:MET:SD	17:P:310:ILE:HG13	2.61	0.40
17:P:438:MET:HA	17:P:441:MET:HG3	2.04	0.40
1:R:415:LEU:HD11	6:T:60:TRP:CE2	2.57	0.40
1:R:586:LEU:O	1:R:590:ILE:HG13	2.22	0.40
1:R:731:CYS:SG	1:R:732:ILE:HD12	2.62	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:352:ALA:HB1	2:O:353:PRO:HD2	2.04	0.40
3:I:34:ALA:O	3:I:37:GLU:HG3	2.21	0.40
7:C:203:PHE:HZ	7:C:207:GLN:HB3	1.86	0.40
7:C:417:PHE:CD1	7:C:422:THR:HG21	2.56	0.40
7:A:186:ASP:OD1	7:A:186:ASP:N	2.55	0.40
8:E:149:ASP:OD1	8:E:150:PHE:N	2.54	0.40
8:F:70:GLU:OE2	8:F:114:PHE:HD2	2.05	0.40
8:F:78:ASP:OD1	8:F:80:THR:HG22	2.21	0.40
8:D:383:LEU:HD22	8:D:388:ILE:HD12	2.02	0.40
8:D:417:ASP:HB3	8:D:495:ILE:HG23	2.03	0.40
9:Y:163:ILE:HD13	9:Y:163:ILE:HA	1.94	0.40
9:Z:26:ILE:HG21	9:Z:65:ILE:HD11	2.03	0.40
9:Z:197:TYR:CE2	9:Z:201:LYS:HE2	2.56	0.40
12:U:434:LEU:HD23	12:U:434:LEU:HA	1.88	0.40
14:0:118:PHE:HE1	14:0:203:MET:HG2	1.86	0.40
15:7:32:TYR:OH	15:7:36:LYS:HE3	2.21	0.40
15:7:88:LYS:O	15:7:92:GLN:HG2	2.22	0.40
15:9:30:ALA:O	15:9:34:THR:HG23	2.21	0.40
16:Q:3:PHE:O	16:Q:3:PHE:CG	2.74	0.40
17:P:141:ALA:O	17:P:145:ILE:HG12	2.21	0.40
17:P:249:LEU:HA	17:P:252:PHE:CD2	2.55	0.40
17:P:408:ALA:HB2	17:P:448:VAL:HG12	2.02	0.40
1:R:179:ARG:HA	1:R:179:ARG:HD3	1.90	0.40
2:O:71:LYS:HD2	2:O:71:LYS:HA	1.82	0.40
2:O:79:VAL:O	2:O:81:GLU:HG2	2.21	0.40
2:O:92:LEU:O	2:O:288:SER:OG	2.37	0.40
2:O:119:LYS:O	2:O:122:SER:OG	2.31	0.40
3:J:170:GLU:N	3:J:170:GLU:OE2	2.55	0.40
4:L:59:GLU:O	4:L:63:LEU:HG	2.21	0.40
4:L:85:GLN:HA	4:L:88:PHE:HD1	1.86	0.40
9:Y:60:TYR:HD1	9:Y:60:TYR:HA	1.79	0.40
12:U:450:LEU:HD13	15:2:112:ILE:HD12	2.03	0.40
15:3:144:TYR:HA	15:3:147:ILE:HD12	2.02	0.40
15:6:80:LEU:HD23	15:6:80:LEU:HA	1.80	0.40
15:7:117:GLY:HA3	15:7:131:MET:HG3	2.03	0.40
15:8:150:LEU:HA	15:8:150:LEU:HD23	1.88	0.40
15:9:108:PHE:O	15:9:112:ILE:HG22	2.21	0.40
17:P:119:LYS:HA	17:P:122:ALA:HB2	2.04	0.40
1:R:52:VAL:HA	1:R:55:VAL:HG22	2.02	0.40
1:R:103:LYS:O	1:R:107:GLU:HG3	2.22	0.40
1:R:536:LYS:HB3	1:R:742:TRP:HD1	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:628:LEU:HD13	1:R:632:GLN:HE22	1.86	0.40
2:O:45:VAL:HG13	2:O:46:GLY:N	2.36	0.40
2:O:325:LYS:O	2:O:327:THR:HG23	2.21	0.40
6:T:69:GLY:O	6:T:73:ASN:ND2	2.54	0.40
7:B:443:LYS:HD3	8:E:494:ARG:NH2	2.37	0.40
8:E:504:TYR:HB3	8:E:505:PRO:HD3	2.03	0.40
9:Z:237:LEU:HD23	9:Z:237:LEU:HA	1.86	0.40
9:X:51:ASP:OD1	9:X:84:ARG:NH2	2.40	0.40
9:X:74:CYS:O	9:X:76:ASN:N	2.55	0.40
9:X:264:ASP:O	9:X:267:VAL:HG12	2.21	0.40
14:0:25:CYS:HB3	14:0:29:PHE:CE2	2.56	0.40
15:1:80:LEU:HA	15:1:80:LEU:HD23	1.80	0.40
15:2:52:ILE:HG23	15:2:53:MET:N	2.35	0.40
15:5:22:ALA:HB2	15:5:96:GLY:CA	2.51	0.40
15:5:22:ALA:HB2	15:5:96:GLY:HA2	2.03	0.40
15:5:85:SER:O	15:5:86:LEU:HB3	2.22	0.40
15:7:150:LEU:HD23	15:7:150:LEU:HA	1.85	0.40
15:8:54:LYS:HB3	15:8:54:LYS:HE3	1.85	0.40
17:P:384:ASN:ND2	17:P:417:TYR:OH	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	R	747/837 (89%)	682 (91%)	65 (9%)	0	100	100
2	O	373/382 (98%)	331 (89%)	42 (11%)	0	100	100
3	H	222/226 (98%)	215 (97%)	7 (3%)	0	100	100
3	I	223/226 (99%)	218 (98%)	5 (2%)	0	100	100
3	J	223/226 (99%)	218 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	K	112/118 (95%)	101 (90%)	11 (10%)	0	100	100
4	L	112/118 (95%)	111 (99%)	1 (1%)	0	100	100
4	M	112/118 (95%)	110 (98%)	2 (2%)	0	100	100
5	S	75/81 (93%)	71 (95%)	4 (5%)	0	100	100
6	T	83/137 (61%)	77 (93%)	6 (7%)	0	100	100
7	A	598/617 (97%)	546 (91%)	52 (9%)	0	100	100
7	B	598/617 (97%)	544 (91%)	54 (9%)	0	100	100
7	C	598/617 (97%)	540 (90%)	58 (10%)	0	100	100
8	D	466/511 (91%)	428 (92%)	38 (8%)	0	100	100
8	E	466/511 (91%)	429 (92%)	37 (8%)	0	100	100
8	F	466/511 (91%)	427 (92%)	38 (8%)	1 (0%)	44	73
9	X	260/573 (45%)	247 (95%)	13 (5%)	0	100	100
9	Y	258/573 (45%)	248 (96%)	9 (4%)	1 (0%)	30	63
9	Z	265/573 (46%)	250 (94%)	15 (6%)	0	100	100
10	G	211/247 (85%)	205 (97%)	6 (3%)	0	100	100
11	N	108/119 (91%)	104 (96%)	4 (4%)	0	100	100
12	U	202/470 (43%)	172 (85%)	28 (14%)	2 (1%)	13	46
13	V	47/350 (13%)	44 (94%)	3 (6%)	0	100	100
14	0	202/205 (98%)	191 (95%)	11 (5%)	0	100	100
15	1	148/155 (96%)	143 (97%)	5 (3%)	0	100	100
15	2	148/155 (96%)	144 (97%)	4 (3%)	0	100	100
15	3	148/155 (96%)	141 (95%)	7 (5%)	0	100	100
15	4	148/155 (96%)	142 (96%)	6 (4%)	0	100	100
15	5	148/155 (96%)	144 (97%)	4 (3%)	0	100	100
15	6	148/155 (96%)	141 (95%)	7 (5%)	0	100	100
15	7	148/155 (96%)	139 (94%)	9 (6%)	0	100	100
15	8	148/155 (96%)	140 (95%)	8 (5%)	0	100	100
15	9	148/155 (96%)	141 (95%)	7 (5%)	0	100	100
16	Q	349/351 (99%)	309 (88%)	40 (12%)	0	100	100
17	P	423/483 (88%)	367 (87%)	54 (13%)	2 (0%)	25	59
All	All	9131/11192 (82%)	8460 (93%)	665 (7%)	6 (0%)	50	79

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
17	P	109	SER
12	U	416	SER
12	U	417	ASP
17	P	104	ASN
9	Y	62	PHE
8	F	252	GLY

5.3.2 Protein sidechains (i)

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%)	671 (100%)	3 (0%)	89 95
2	O	337/344 (98%)	336 (100%)	1 (0%)	91 96
3	H	198/199 (100%)	197 (100%)	1 (0%)	86 93
3	I	198/199 (100%)	198 (100%)	0	100 100
3	J	198/199 (100%)	197 (100%)	1 (0%)	86 93
4	K	99/101 (98%)	98 (99%)	1 (1%)	73 85
4	L	99/101 (98%)	98 (99%)	1 (1%)	73 85
4	M	99/101 (98%)	99 (100%)	0	100 100
5	S	69/72 (96%)	69 (100%)	0	100 100
6	T	71/116 (61%)	71 (100%)	0	100 100
7	A	508/525 (97%)	508 (100%)	0	100 100
7	B	508/525 (97%)	505 (99%)	3 (1%)	84 92
7	C	508/525 (97%)	508 (100%)	0	100 100
8	D	401/430 (93%)	401 (100%)	0	100 100
8	E	401/430 (93%)	401 (100%)	0	100 100
8	F	401/430 (93%)	399 (100%)	2 (0%)	86 93
9	X	238/519 (46%)	237 (100%)	1 (0%)	89 95
9	Y	237/519 (46%)	236 (100%)	1 (0%)	89 95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	Z	239/519 (46%)	239 (100%)	0	100	100
10	G	184/212 (87%)	184 (100%)	0	100	100
11	N	94/100 (94%)	94 (100%)	0	100	100
12	U	182/397 (46%)	182 (100%)	0	100	100
13	V	44/308 (14%)	44 (100%)	0	100	100
14	0	154/155 (99%)	154 (100%)	0	100	100
15	1	107/112 (96%)	107 (100%)	0	100	100
15	2	107/112 (96%)	107 (100%)	0	100	100
15	3	107/112 (96%)	107 (100%)	0	100	100
15	4	107/112 (96%)	107 (100%)	0	100	100
15	5	107/112 (96%)	107 (100%)	0	100	100
15	6	107/112 (96%)	107 (100%)	0	100	100
15	7	107/112 (96%)	107 (100%)	0	100	100
15	8	107/112 (96%)	107 (100%)	0	100	100
15	9	107/112 (96%)	107 (100%)	0	100	100
16	Q	306/306 (100%)	304 (99%)	2 (1%)	81	90
17	P	385/429 (90%)	382 (99%)	3 (1%)	79	88
All	All	7795/9515 (82%)	7775 (100%)	20 (0%)	90	96

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	R	254	ARG
1	R	488	ASN
1	R	804	ARG
2	O	44	LYS
3	J	212	ARG
4	L	37	LYS
3	H	59	LYS
4	K	115	ARG
7	B	18	PHE
7	B	386	TYR
7	B	400	ARG
8	F	215	LYS
8	F	403	LYS
9	Y	227	LYS

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Mol	Chain	Res	Type
9	X	70	LYS
16	Q	24	LYS
16	Q	120	ARG
17	P	116	ARG
17	P	259	HIS
17	P	434	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (102) such sidechains are listed below:

Mol	Chain	Res	Type
1	R	48	GLN
1	R	194	ASN
1	R	273	ASN
1	R	280	GLN
1	R	289	ASN
1	R	343	HIS
1	R	365	ASN
1	R	435	ASN
1	R	473	ASN
1	R	523	ASN
1	R	547	HIS
1	R	600	HIS
1	R	734	ASN
1	R	806	HIS
1	R	811	GLN
2	O	31	ASN
2	O	94	ASN
2	O	286	ASN
2	O	322	GLN
2	O	324	ASN
3	J	14	HIS
3	J	206	GLN
3	I	9	GLN
3	I	11	GLN
3	I	14	HIS
3	I	113	GLN
3	I	206	GLN
4	L	10	GLN
3	H	21	GLN
3	H	24	ASN
3	H	126	GLN
3	H	161	ASN

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Mol	Chain	Res	Type
4	K	91	ASN
5	S	61	ASN
5	S	67	GLN
6	T	73	ASN
6	T	129	ASN
7	B	146	HIS
7	B	207	GLN
7	B	314	ASN
7	B	430	GLN
7	B	444	HIS
7	C	397	ASN
7	C	449	ASN
7	C	468	HIS
7	C	484	GLN
7	C	573	HIS
7	A	397	ASN
7	A	444	HIS
7	A	468	HIS
7	A	560	GLN
8	E	262	ASN
8	F	171	GLN
8	F	363	HIS
8	F	421	GLN
8	D	42	GLN
8	D	421	GLN
8	D	470	ASN
8	D	497	GLN
9	Y	17	GLN
9	Y	59	ASN
9	Y	76	ASN
9	Y	198	HIS
9	Y	274	ASN
9	Z	19	HIS
9	Z	190	ASN
9	X	21	GLN
9	X	120	ASN
9	X	134	ASN
9	X	150	ASN
9	X	160	GLN
9	X	198	HIS
9	X	270	ASN
9	X	274	ASN

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Mol	Chain	Res	Type
10	G	130	GLN
10	G	174	HIS
11	N	29	ASN
11	N	33	HIS
11	N	57	ASN
11	N	81	HIS
12	U	329	ASN
12	U	398	GLN
12	U	445	HIS
14	0	132	HIS
15	1	92	GLN
16	Q	10	ASN
16	Q	84	HIS
16	Q	88	HIS
16	Q	137	GLN
16	Q	309	GLN
16	Q	338	GLN
16	Q	340	HIS
17	P	32	ASN
17	P	72	GLN
17	P	79	ASN
17	P	206	GLN
17	P	238	GLN
17	P	274	GLN
17	P	291	ASN
17	P	311	GLN
17	P	384	ASN
17	P	430	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	A	701	-	24,29,29	0.79	0	29,45,45	1.26	3 (10%)
18	NAG	U	505	12	14,14,15	0.16	0	17,19,21	0.42	0
18	NAG	R	902	-	14,14,15	0.21	0	17,19,21	0.45	0
18	NAG	U	501	12	14,14,15	0.36	0	17,19,21	0.64	1 (5%)
18	NAG	U	502	12	14,14,15	0.27	0	17,19,21	0.45	0
18	NAG	R	901	1	14,14,15	0.23	0	17,19,21	0.42	0
18	NAG	U	506	12	14,14,15	0.23	0	17,19,21	0.41	0
18	NAG	U	504	12	14,14,15	0.49	0	17,19,21	0.72	1 (5%)
18	NAG	U	503	12	14,14,15	0.51	0	17,19,21	0.65	1 (5%)

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	A	701	-	-	1/12/32/32	0/3/3/3
18	NAG	U	505	12	-	4/6/23/26	0/1/1/1
18	NAG	R	902	-	-	2/6/23/26	0/1/1/1
18	NAG	U	501	12	-	2/6/23/26	0/1/1/1
18	NAG	U	502	12	-	2/6/23/26	0/1/1/1
18	NAG	R	901	1	-	2/6/23/26	0/1/1/1
18	NAG	U	506	12	-	1/6/23/26	0/1/1/1
18	NAG	U	504	12	-	4/6/23/26	0/1/1/1
18	NAG	U	503	12	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A	701	ADP	N3-C2-N1	-3.66	123.71	128.67
19	A	701	ADP	C4-C5-N7	-2.29	106.92	109.34
18	U	504	NAG	C1-O5-C5	2.20	115.14	112.19
18	U	501	NAG	C1-O5-C5	2.18	115.11	112.19
18	U	503	NAG	C1-O5-C5	2.14	115.05	112.19
19	A	701	ADP	C4'-O4'-C1'	2.02	111.78	109.92

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	U	505	NAG	C4-C5-C6-O6
18	U	505	NAG	O5-C5-C6-O6
18	U	501	NAG	C4-C5-C6-O6
18	R	901	NAG	O5-C5-C6-O6
18	U	503	NAG	C4-C5-C6-O6
18	U	502	NAG	O5-C5-C6-O6
18	R	901	NAG	C4-C5-C6-O6
18	U	501	NAG	O5-C5-C6-O6
18	R	902	NAG	O5-C5-C6-O6
18	U	504	NAG	O5-C5-C6-O6
18	U	505	NAG	C8-C7-N2-C2
18	U	505	NAG	O7-C7-N2-C2
18	R	902	NAG	C4-C5-C6-O6
18	U	503	NAG	O5-C5-C6-O6
18	U	502	NAG	C4-C5-C6-O6
18	U	504	NAG	C4-C5-C6-O6
18	U	506	NAG	O5-C5-C6-O6
18	U	504	NAG	C3-C2-N2-C7
18	U	504	NAG	C1-C2-N2-C7
19	A	701	ADP	O4'-C4'-C5'-O5'

There are no ring outliers.

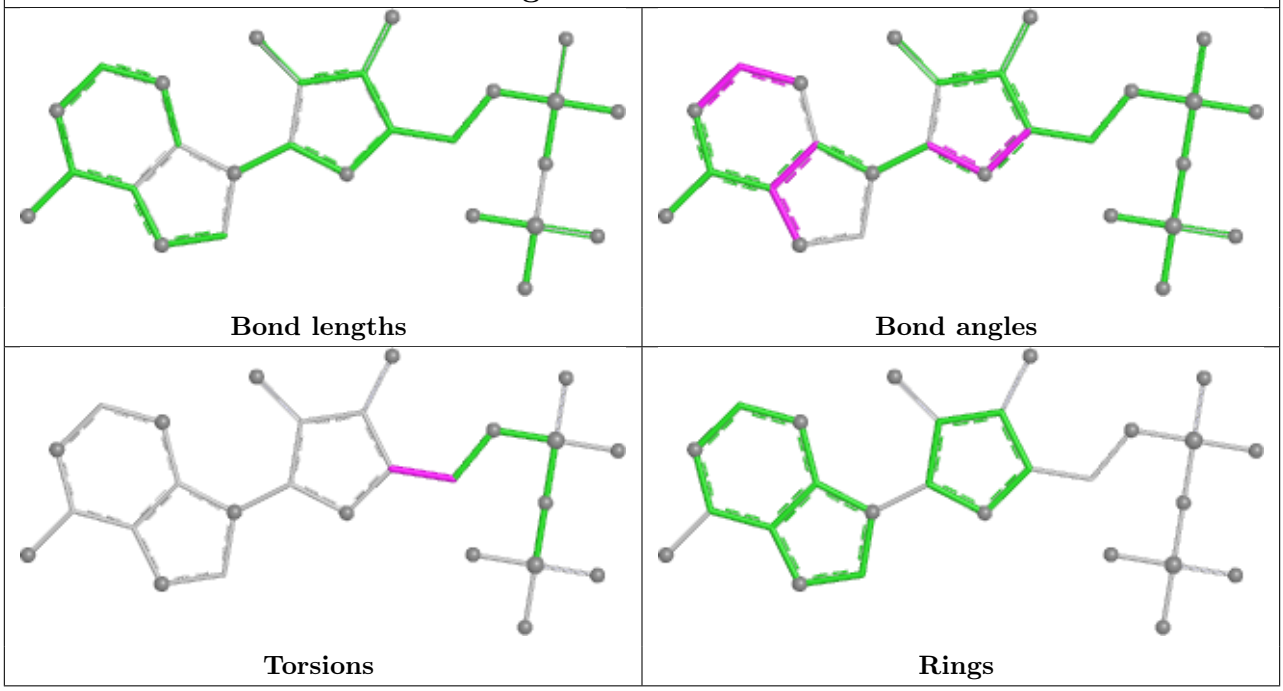
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	701	ADP	1	0
18	R	902	NAG	2	0
18	U	503	NAG	2	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 then 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.

Ligand ADP A 701



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.

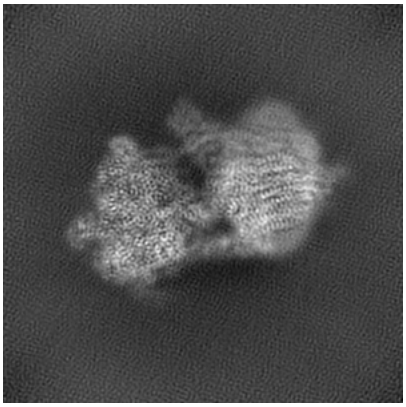
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-21849. These allow visual inspection of the internal detail of the map and identification of artifacts.

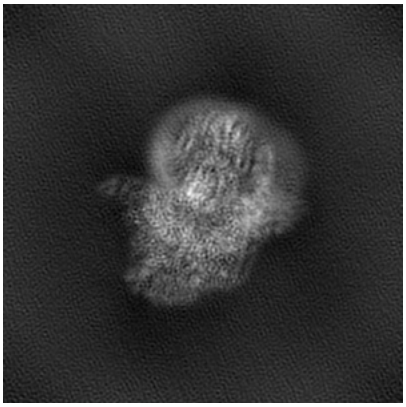
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

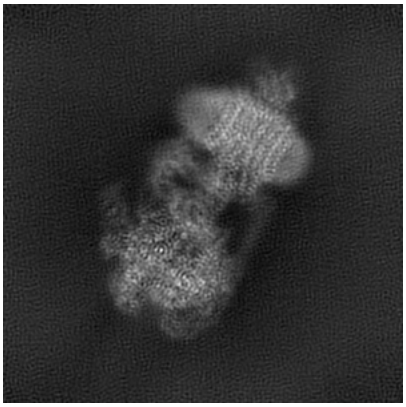
6.1.1 Primary map



X



Y

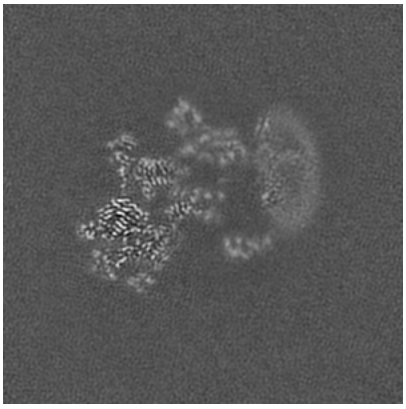


Z

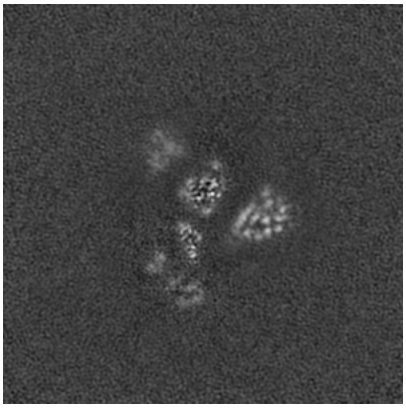
The images above show the map projected in three orthogonal directions.

6.2 Central slices

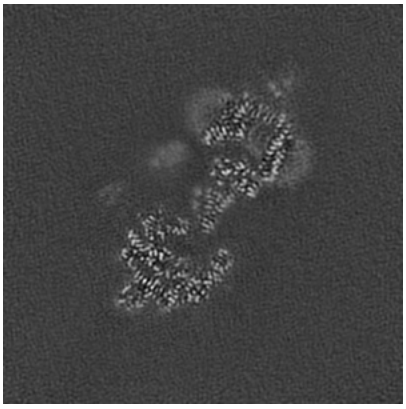
6.2.1 Primary map



X Index: 180



Y Index: 180

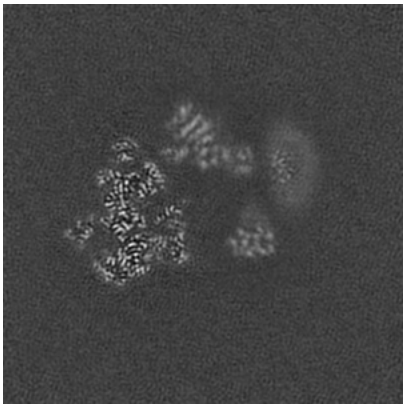


Z Index: 180

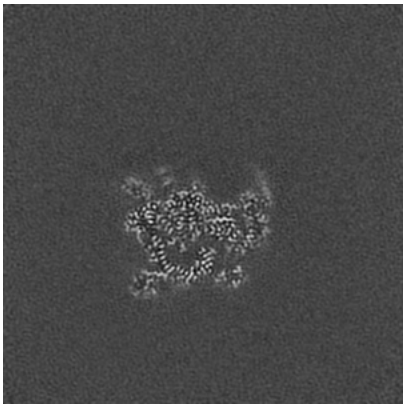
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

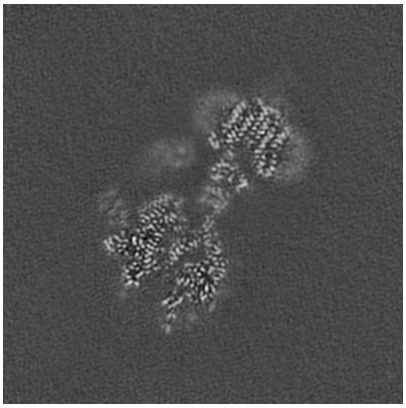
6.3.1 Primary map



X Index: 167



Y Index: 110

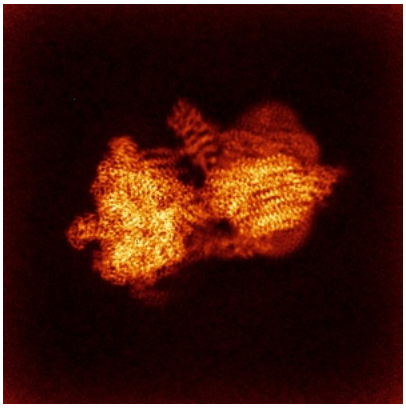


Z Index: 168

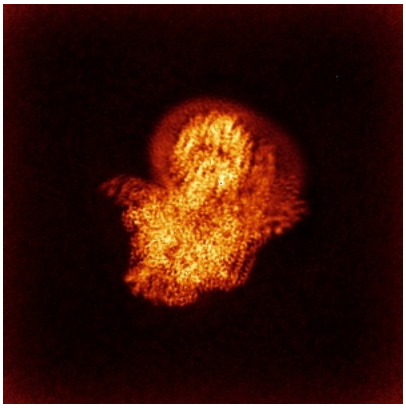
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

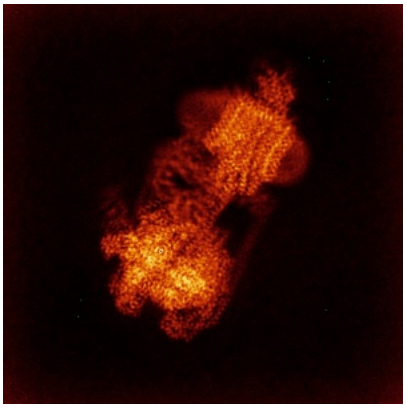
6.4.1 Primary map



X



Y

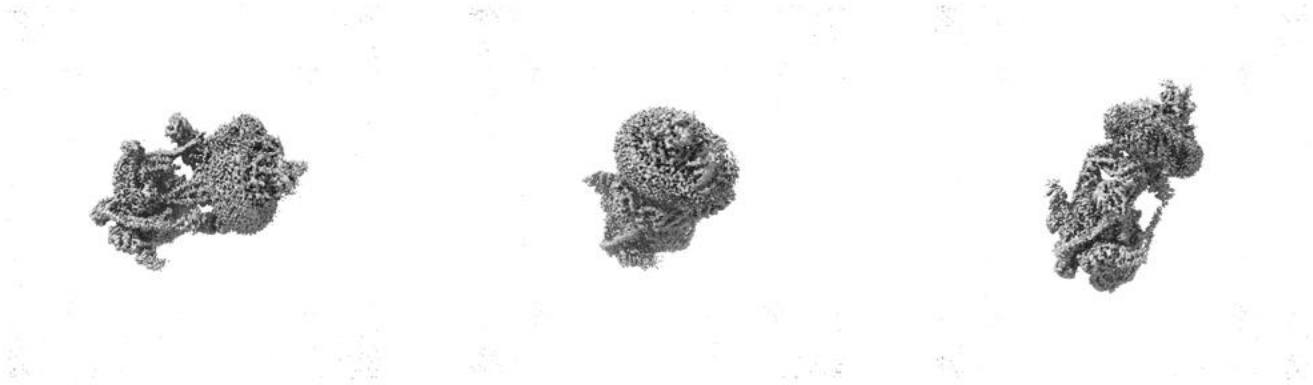


Z

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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 3.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

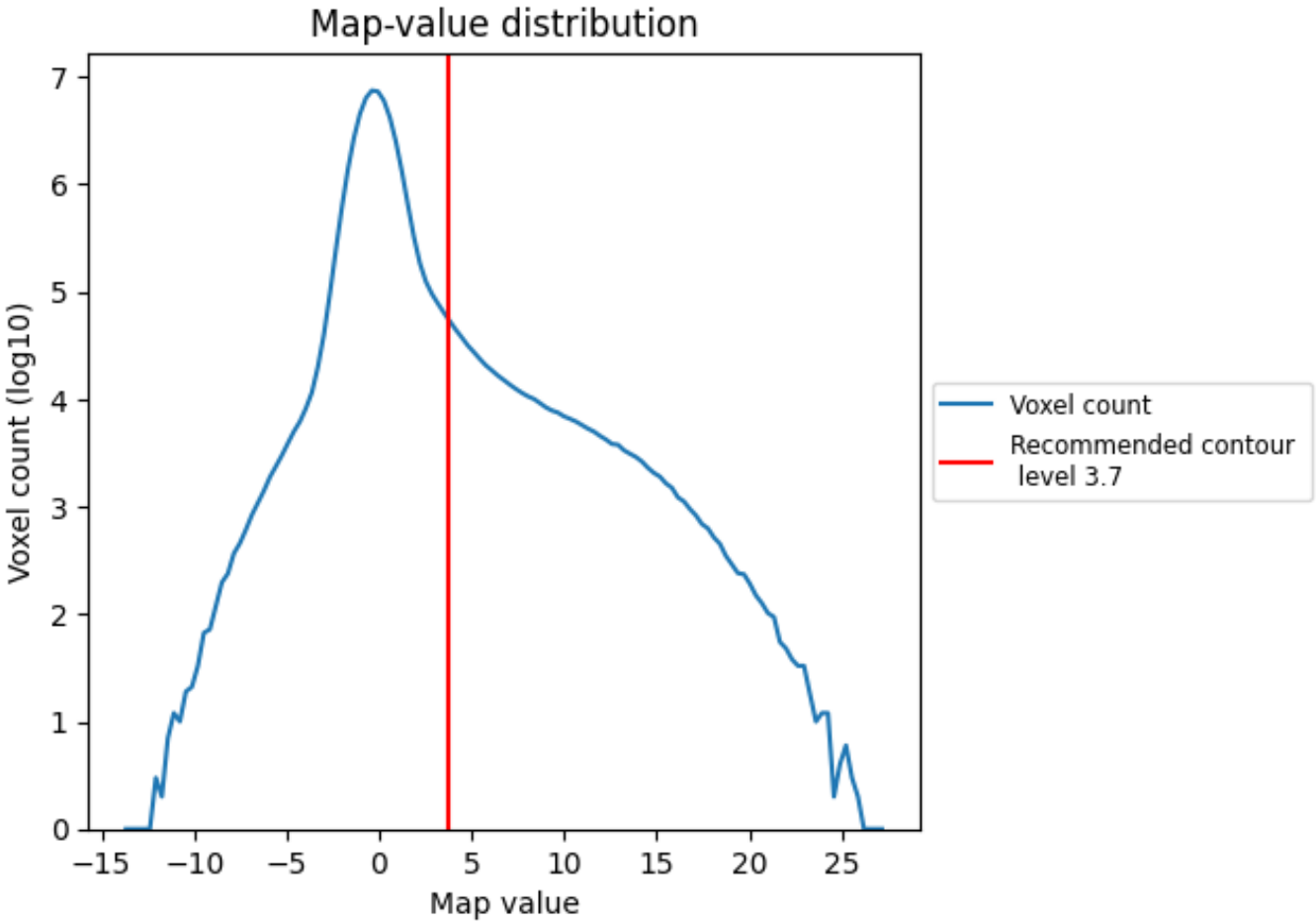
6.6 Mask visualisation (i)

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

7 Map analysis

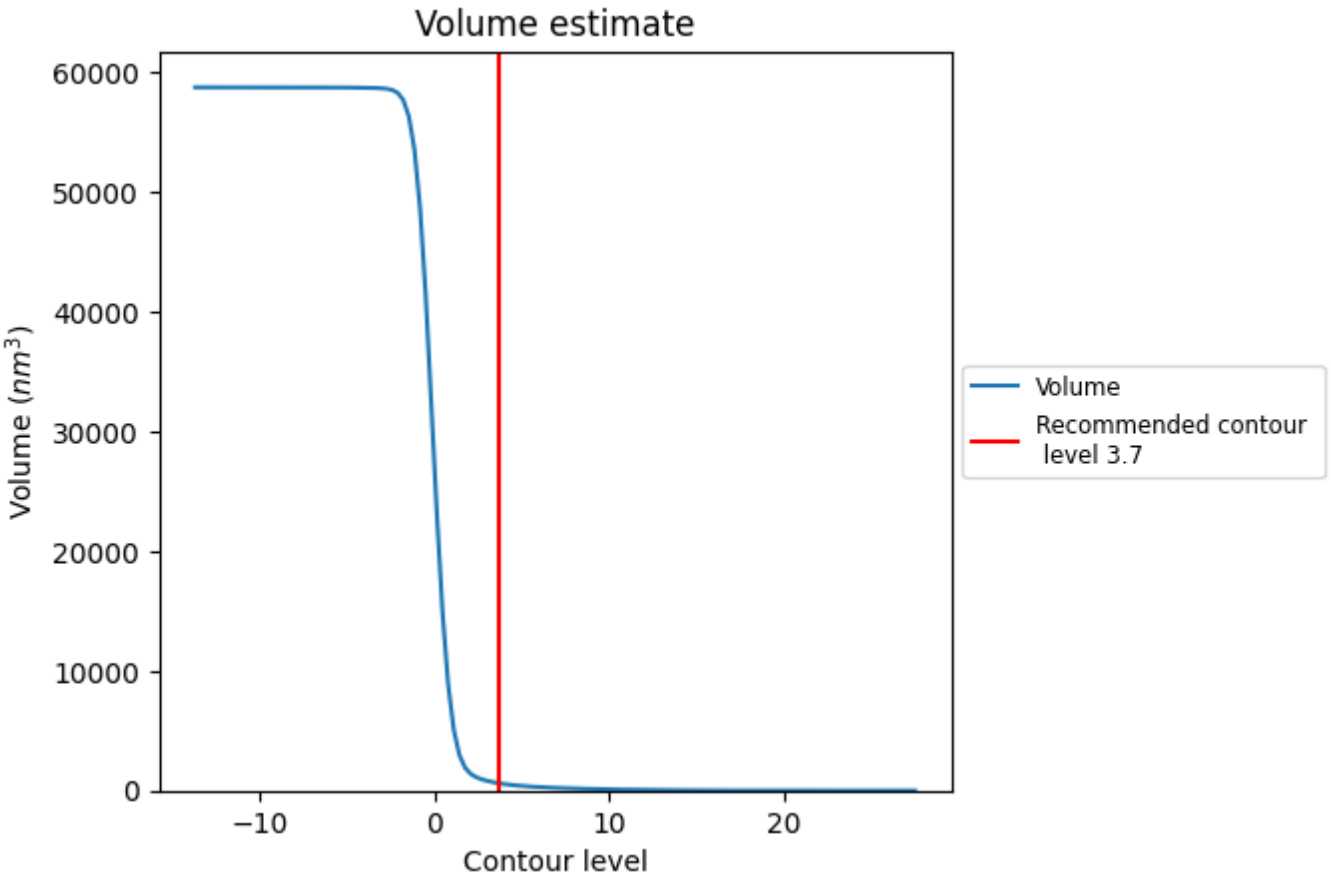
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

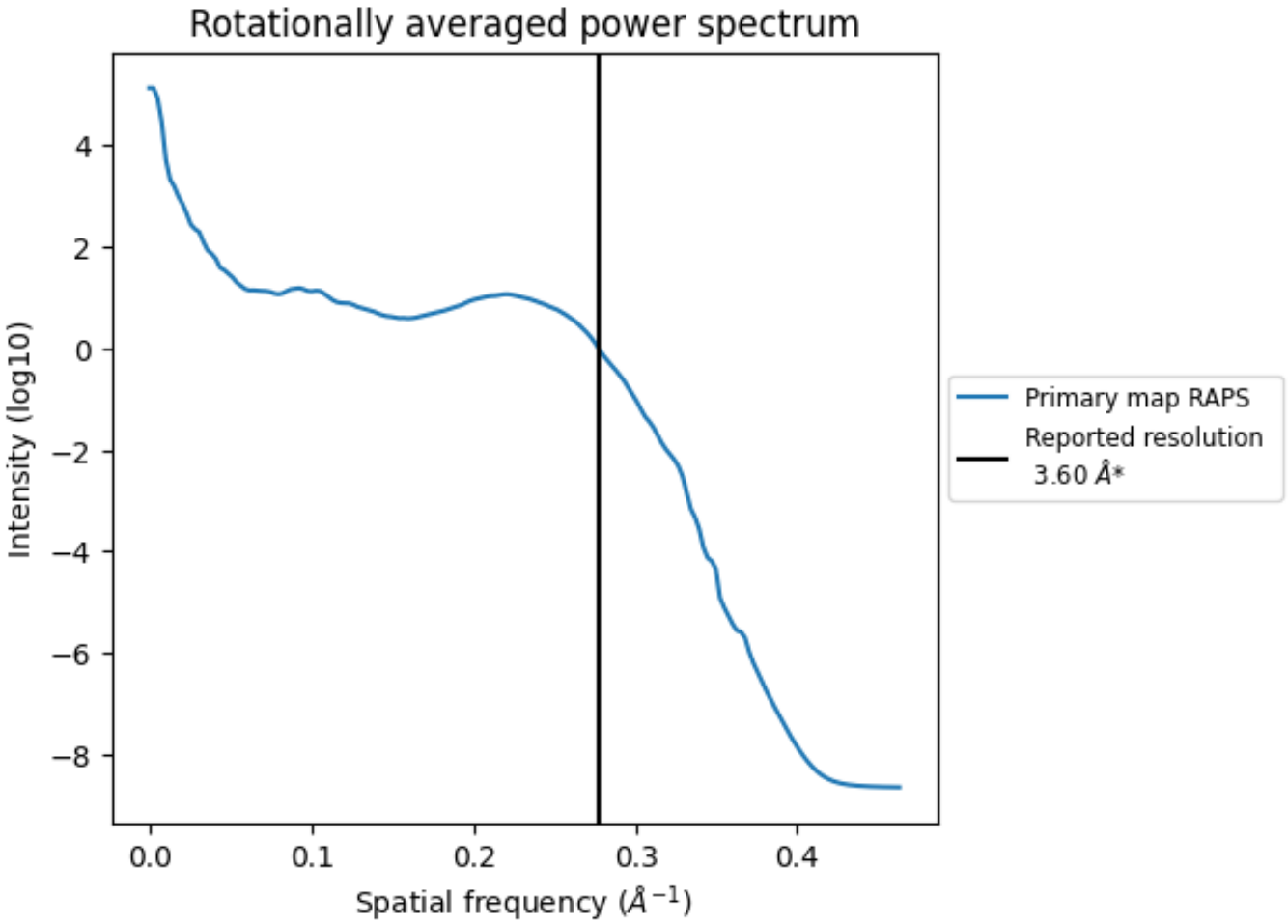
7.2 Volume estimate



The volume at the recommended contour level is 610 nm^3; this corresponds to an approximate mass of 551 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 (i)



*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

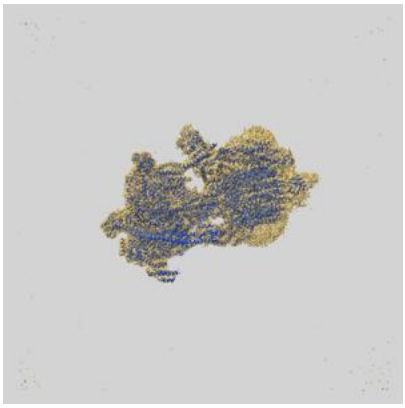
8 Fourier-Shell correlation (i)

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

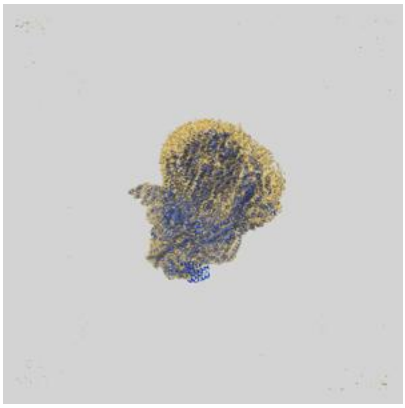
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-21849 and PDB model 6WM4. Per-residue inclusion information can be found in section 3 on page 10.

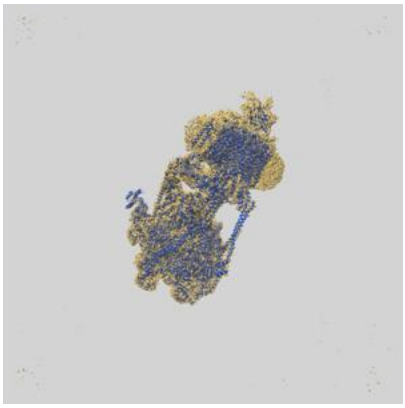
9.1 Map-model overlay



X



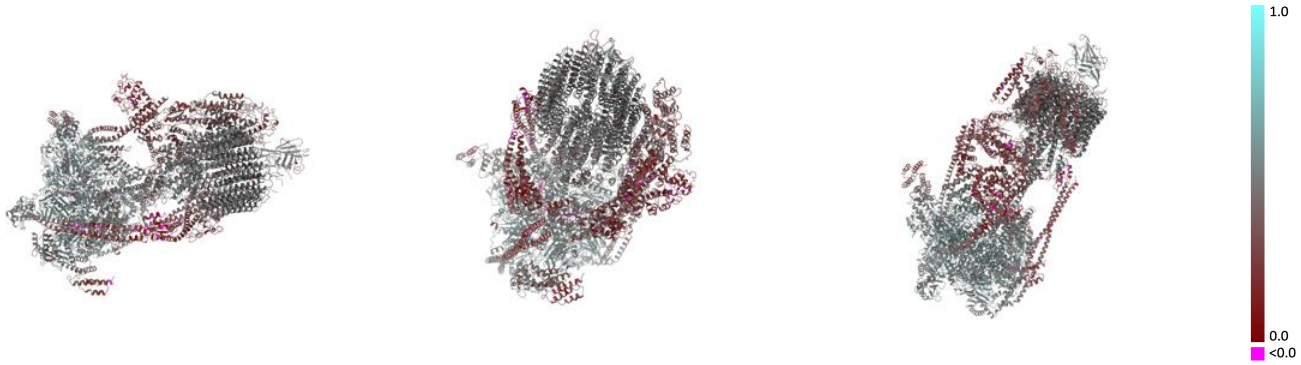
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.7 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.

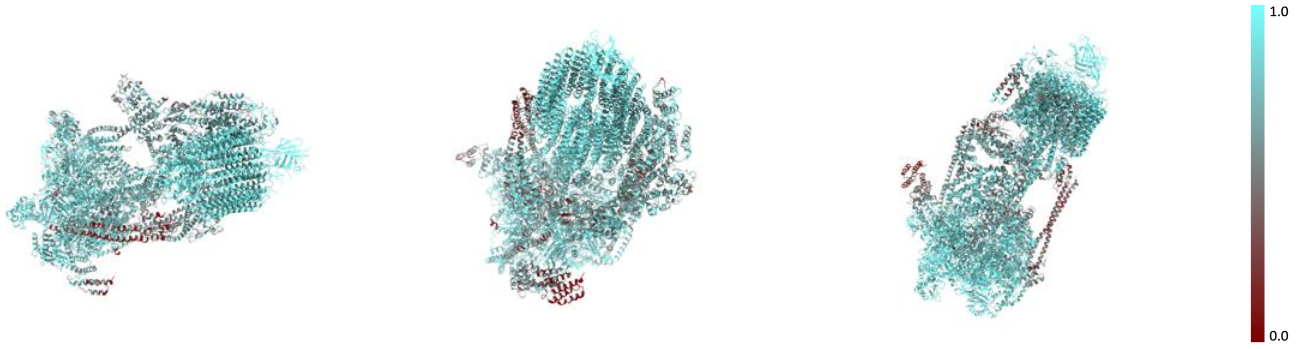
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

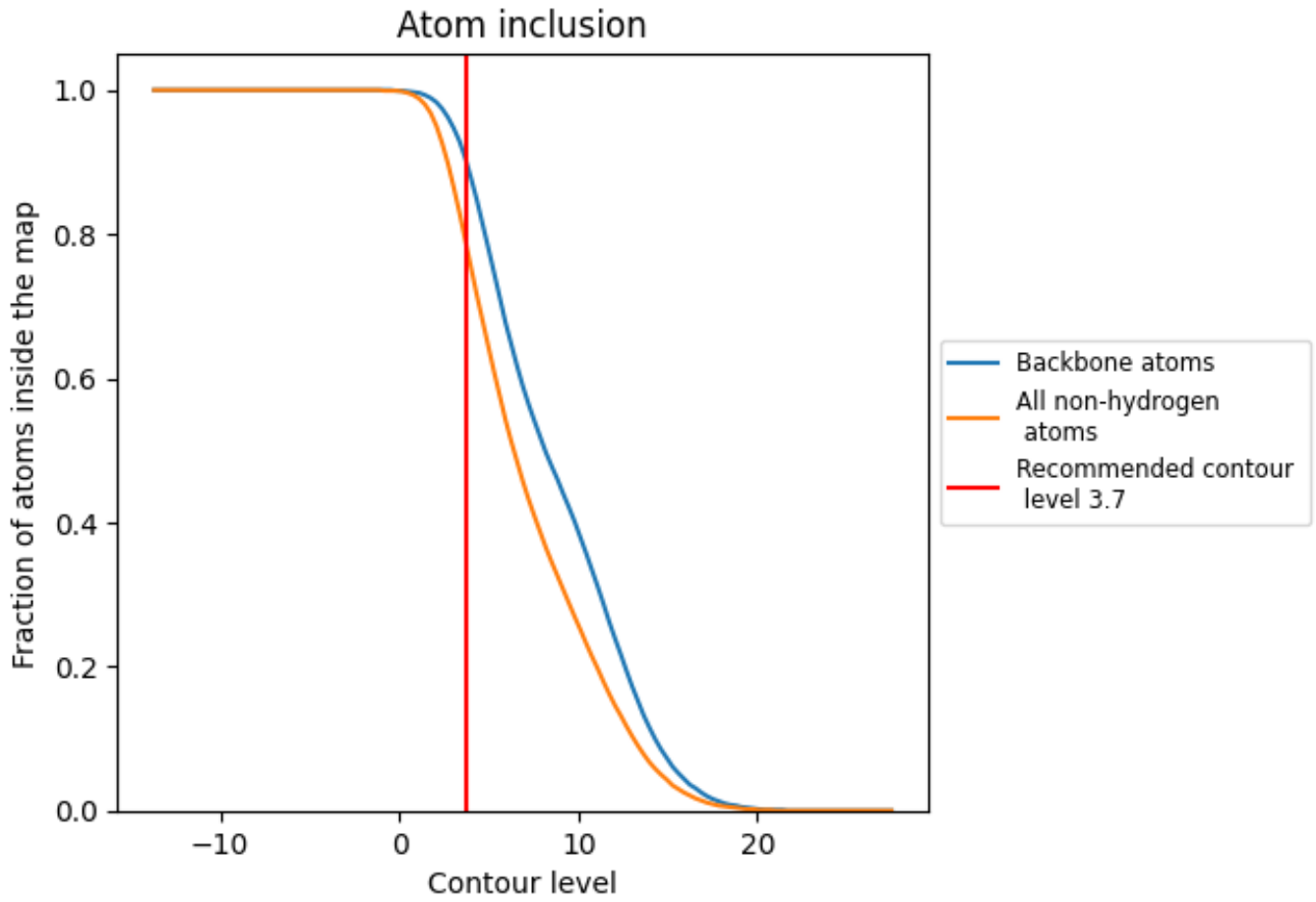
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (3.7).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 79% 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 (3.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7910	0.4420
0	0.8870	0.4770
1	0.8620	0.4750
2	0.8900	0.4680
3	0.8910	0.4610
4	0.8900	0.4610
5	0.9160	0.4630
6	0.8880	0.4550
7	0.9180	0.4610
8	0.8930	0.4690
9	0.8970	0.4700
A	0.9020	0.5430
B	0.8670	0.5220
C	0.8620	0.5110
D	0.9010	0.5500
E	0.8940	0.5400
F	0.8770	0.5290
G	0.8250	0.4950
H	0.8150	0.4440
I	0.7830	0.4210
J	0.7230	0.4190
K	0.7080	0.3680
L	0.6370	0.3600
M	0.4840	0.3280
N	0.7500	0.4380
O	0.5310	0.2150
P	0.6650	0.2330
Q	0.8890	0.4850
R	0.6270	0.3220
S	0.7360	0.3480
T	0.6390	0.2880
U	0.9350	0.4670
V	0.9200	0.4730
X	0.4230	0.3990
Y	0.6830	0.4170
Z	0.7790	0.4620