Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 06:00 pm GMT

PDB ID	:	3ZQ0
EMDB ID	:	EMD-2326
Title	:	Visualizing GroEL-ES in the Act of Encapsulating a Non-Native Substrate Protein
Authors	:	Chen, D.-H.; Madan, D.; Weaver, J.; Lin, Z.; Schroder, G.F.; Chiu, W.; Rye, H.S.
Deposited on	:	2013-03-04
Resolution	:	9.20 Å(reported)
Based on initial model	:	1AON

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:

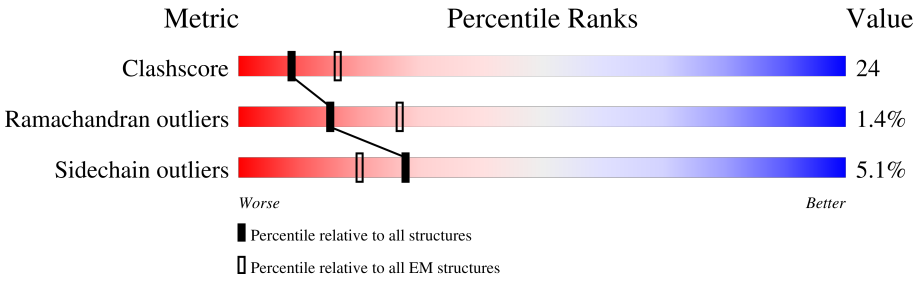
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 9.20 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	A	524	26% 58% 39% ·
1	B	524	36% 55% 41% ·
1	C	524	34% 56% 40% ·
1	D	524	34% 60% 37% ·
1	E	524	29% 55% 40% 5%
1	F	524	31% 57% 40% ·
1	G	524	33% 55% 42% · ·
1	H	524	38% 62% 36% ·

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Mol	Chain	Length	Quality of chain
1	I	524	38% 62% 36%
1	J	524	38% 63% 34%
1	K	524	34% 58% 40%
1	L	524	38% 60% 38%
1	M	524	34% 57% 41%
1	N	524	39% 61% 37%
2	O	97	52% 51% 39% 9%
2	P	97	60% 47% 43% 9%
2	Q	97	53% 63% 30% 6%
2	R	97	54% 56% 37% 7%
2	S	97	55% 39% 52% 9%
2	T	97	51% 52% 37% 11%
2	U	97	55% 53% 40% 6%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 59276 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 60 KDA CHAPERONIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	524	Total	C	N	O	S	0	0
			3856	2397	665	774	20		
1	B	524	Total	C	N	O	S	0	0
			3856	2397	665	774	20		
1	C	524	Total	C	N	O	S	0	0
			3856	2397	665	774	20		
1	D	524	Total	C	N	O	S	0	0
			3856	2397	665	774	20		
1	E	524	Total	C	N	O	S	0	0
			3856	2397	665	774	20		
1	F	524	Total	C	N	O	S	0	0
			3856	2397	665	774	20		
1	G	524	Total	C	N	O	S	0	0
			3856	2397	665	774	20		
1	H	524	Total	C	N	O	S	0	0
			3856	2397	665	774	20		
1	I	524	Total	C	N	O	S	0	0
			3856	2397	665	774	20		
1	J	524	Total	C	N	O	S	0	0
			3856	2397	665	774	20		
1	K	524	Total	C	N	O	S	0	0
			3856	2397	665	774	20		
1	L	524	Total	C	N	O	S	0	0
			3856	2397	665	774	20		
1	M	524	Total	C	N	O	S	0	0
			3856	2397	665	774	20		
1	N	524	Total	C	N	O	S	0	0
			3856	2397	665	774	20		

- Molecule 2 is a protein called 10 KDA CHAPERONIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	O	97	Total	C	N	O	S	0	0
			728	454	127	145	2		

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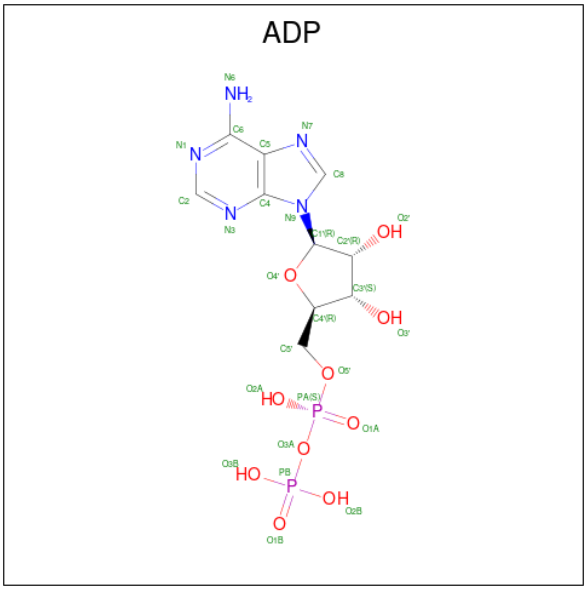
Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	97	Total	C	N	O	S	0	0
			728	454	127	145	2		
2	Q	97	Total	C	N	O	S	0	0
			728	454	127	145	2		
2	R	97	Total	C	N	O	S	0	0
			728	454	127	145	2		
2	S	97	Total	C	N	O	S	0	0
			728	454	127	145	2		
2	T	97	Total	C	N	O	S	0	0
			728	454	127	145	2		
2	U	97	Total	C	N	O	S	0	0
			728	454	127	145	2		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	E	1	Total	C	N	O	P	0
			27	10	5	10	2	

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Mol	Chain	Residues	Atoms					AltConf
3	F	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	G	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

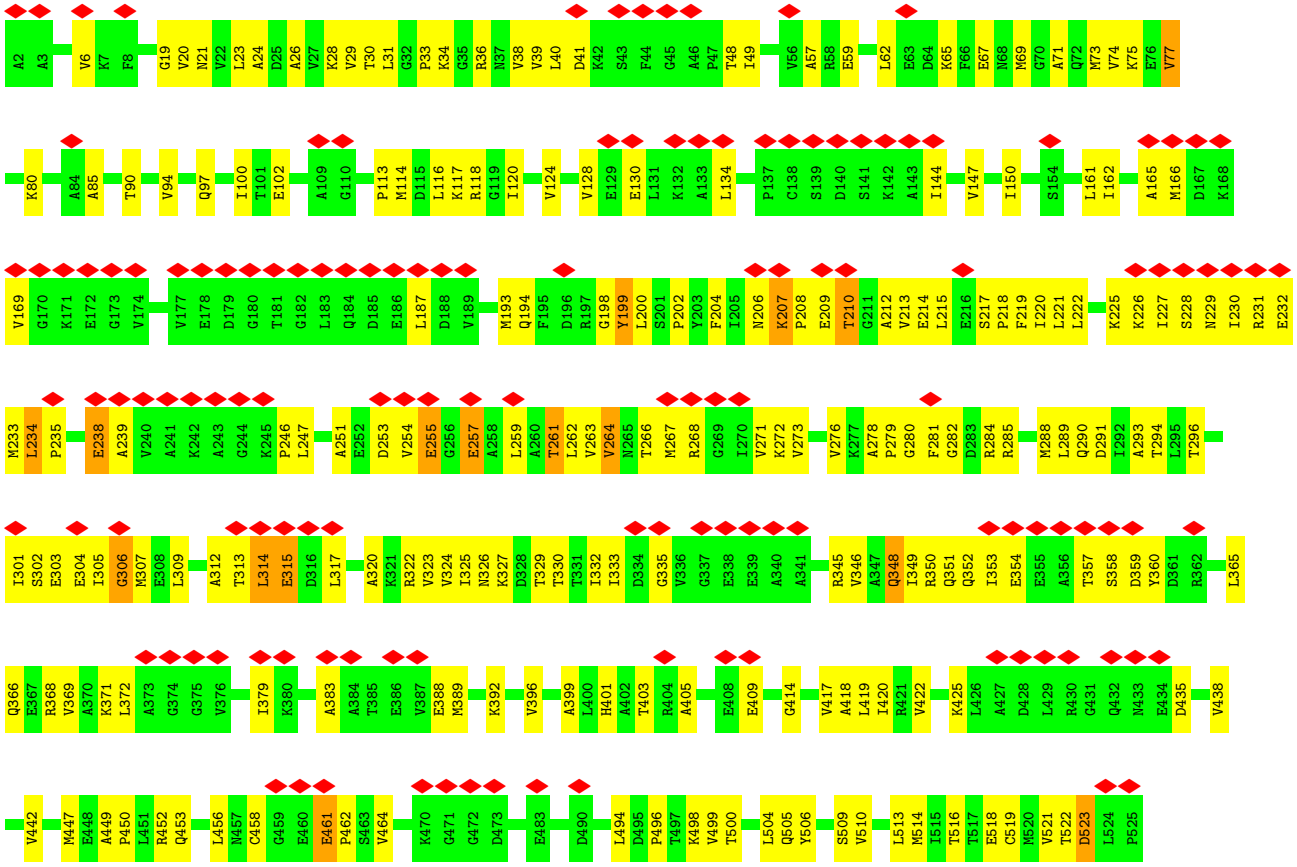
Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Mg	0
			1	1	
4	B	1	Total	Mg	0
			1	1	
4	C	1	Total	Mg	0
			1	1	
4	D	1	Total	Mg	0
			1	1	
4	E	1	Total	Mg	0
			1	1	
4	F	1	Total	Mg	0
			1	1	
4	G	1	Total	Mg	0
			1	1	

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.

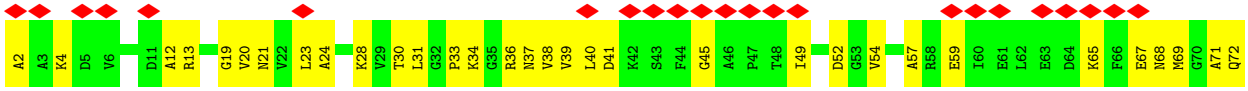
• Molecule 1: 60 KDA CHAPERONIN

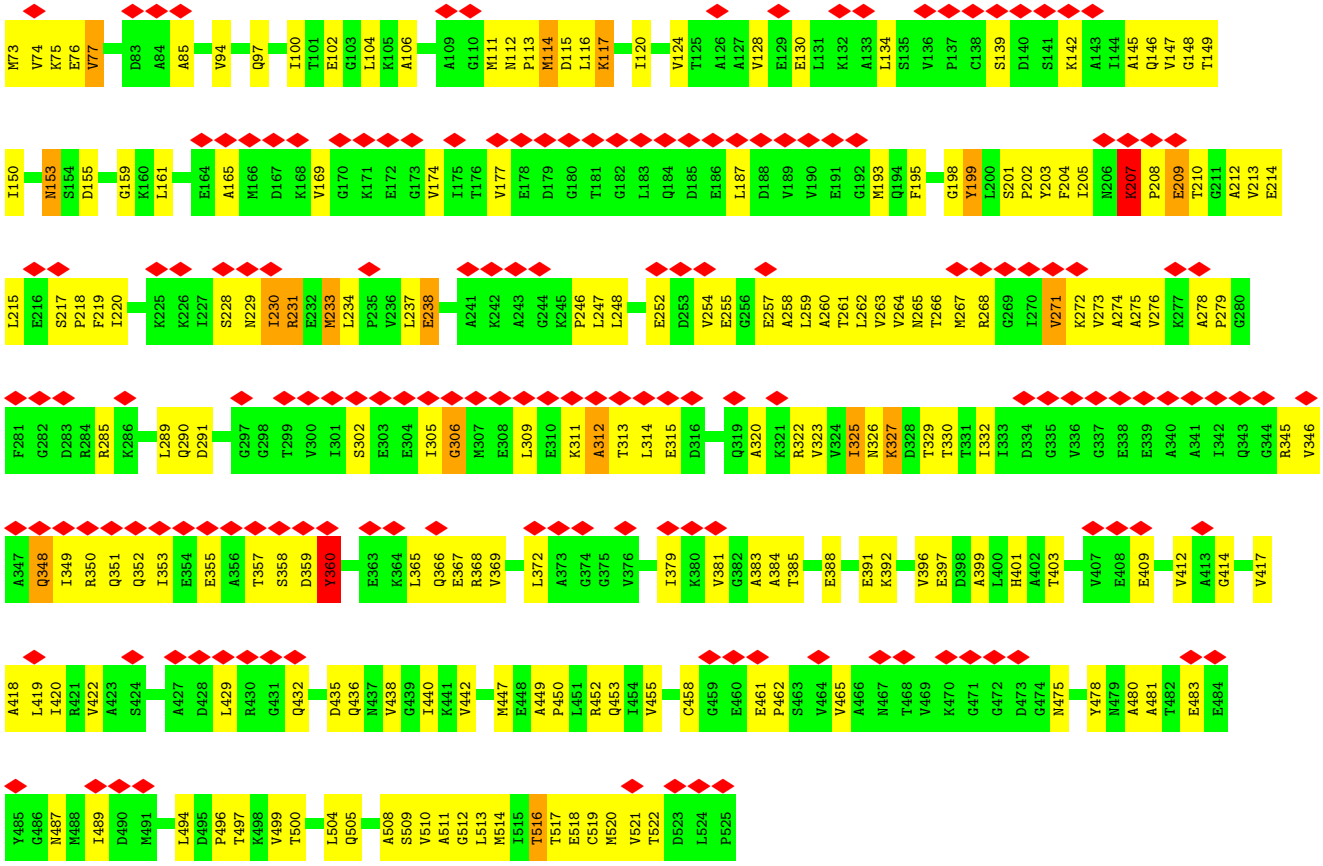
Chain A:



• Molecule 1: 60 KDA CHAPERONIN

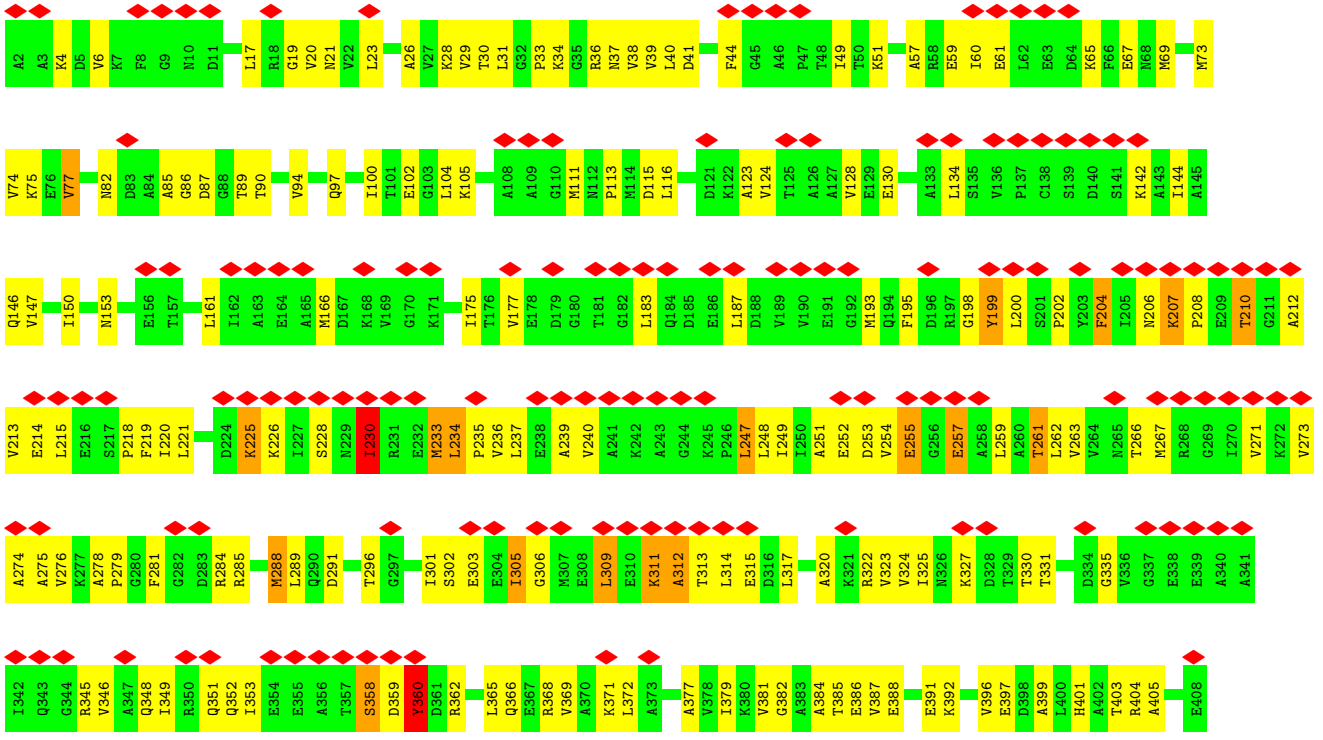
Chain B:

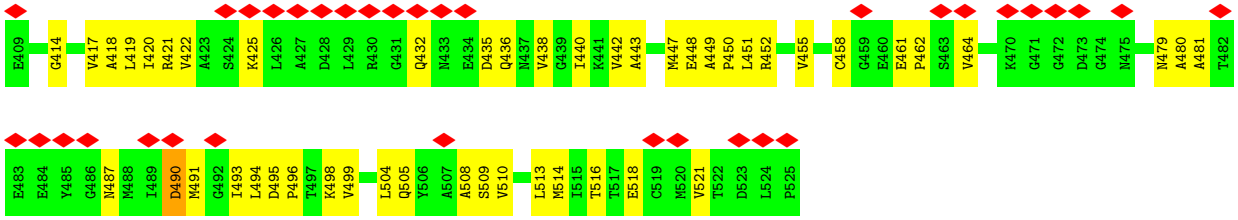




• Molecule 1: 60 KDA CHAPERONIN

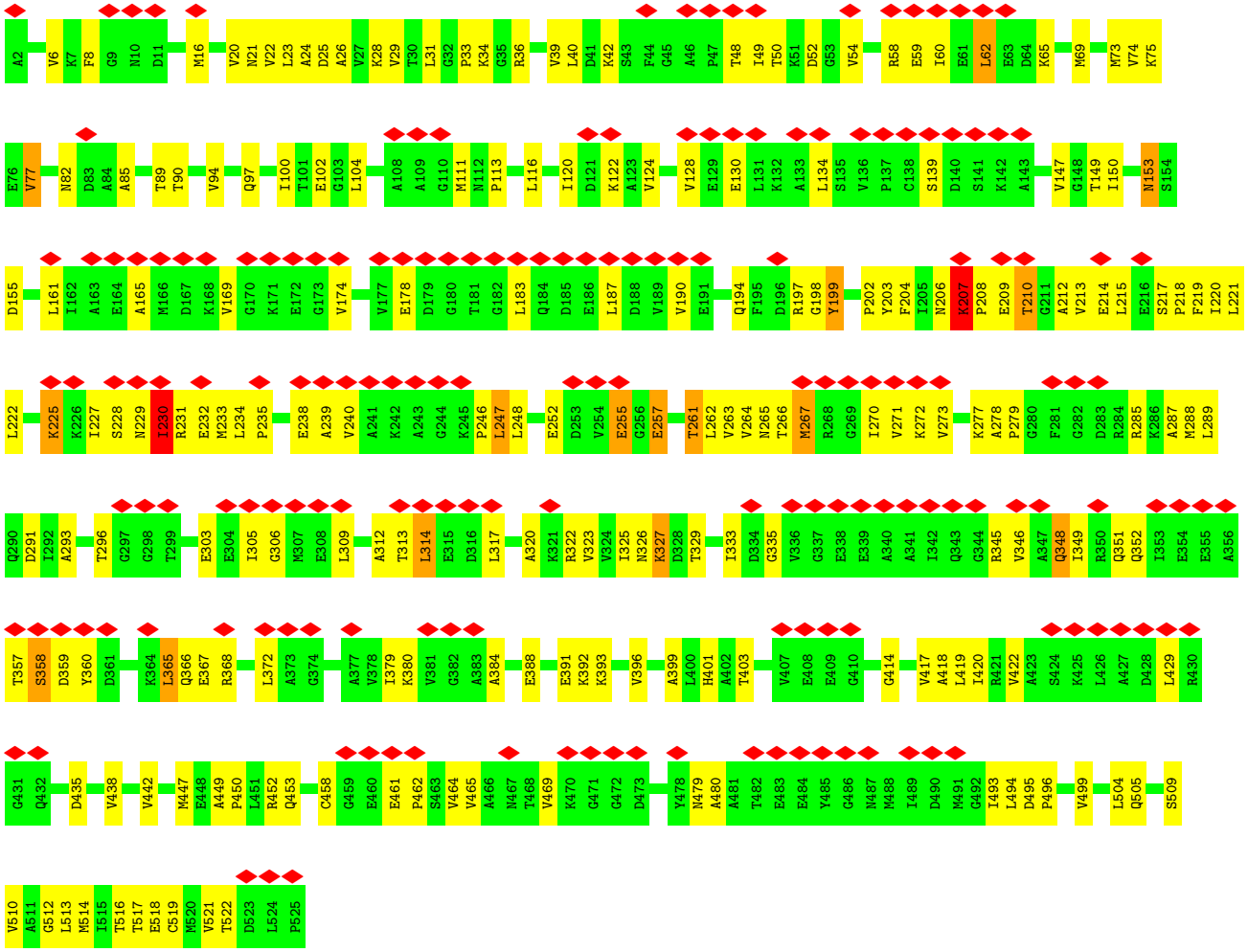
Chain C:





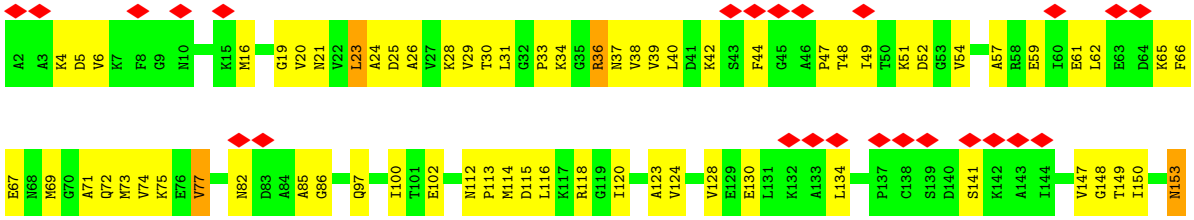
• Molecule 1: 60 KDA CHAPERONIN

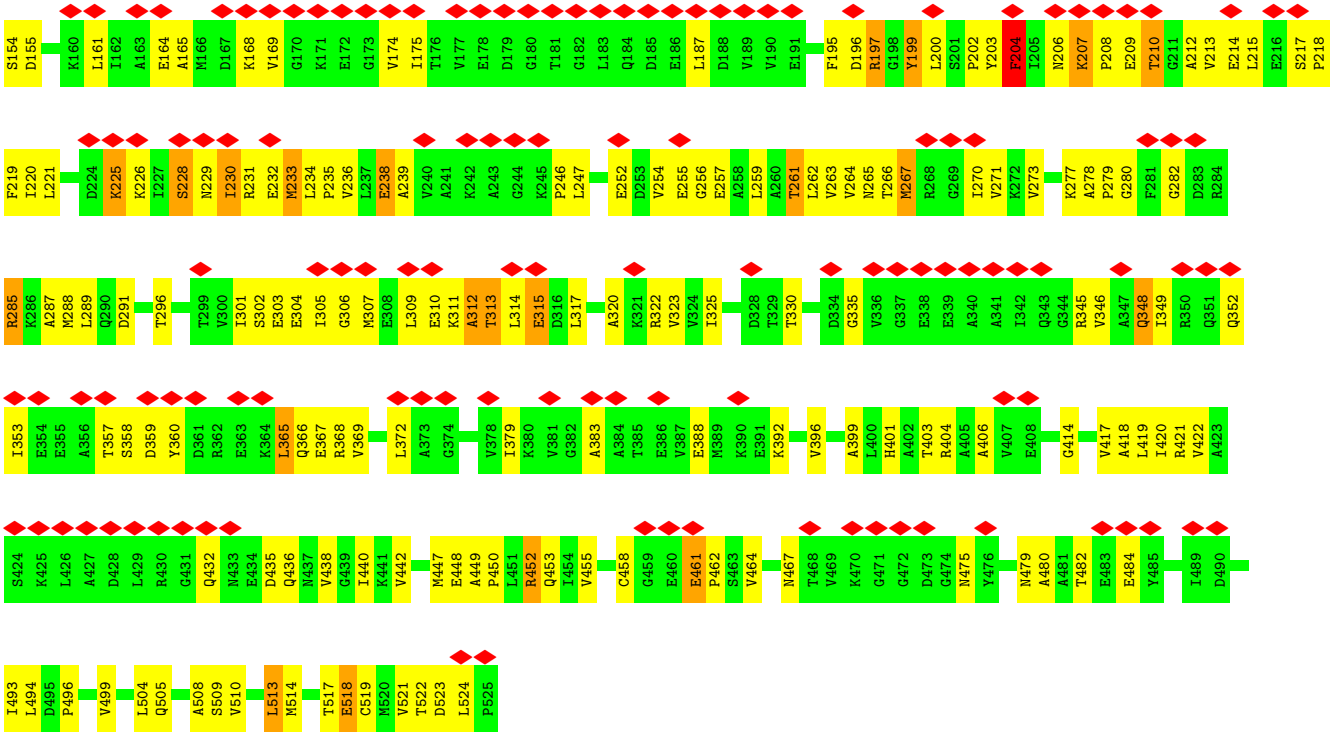
Chain D:



• Molecule 1: 60 KDA CHAPERONIN

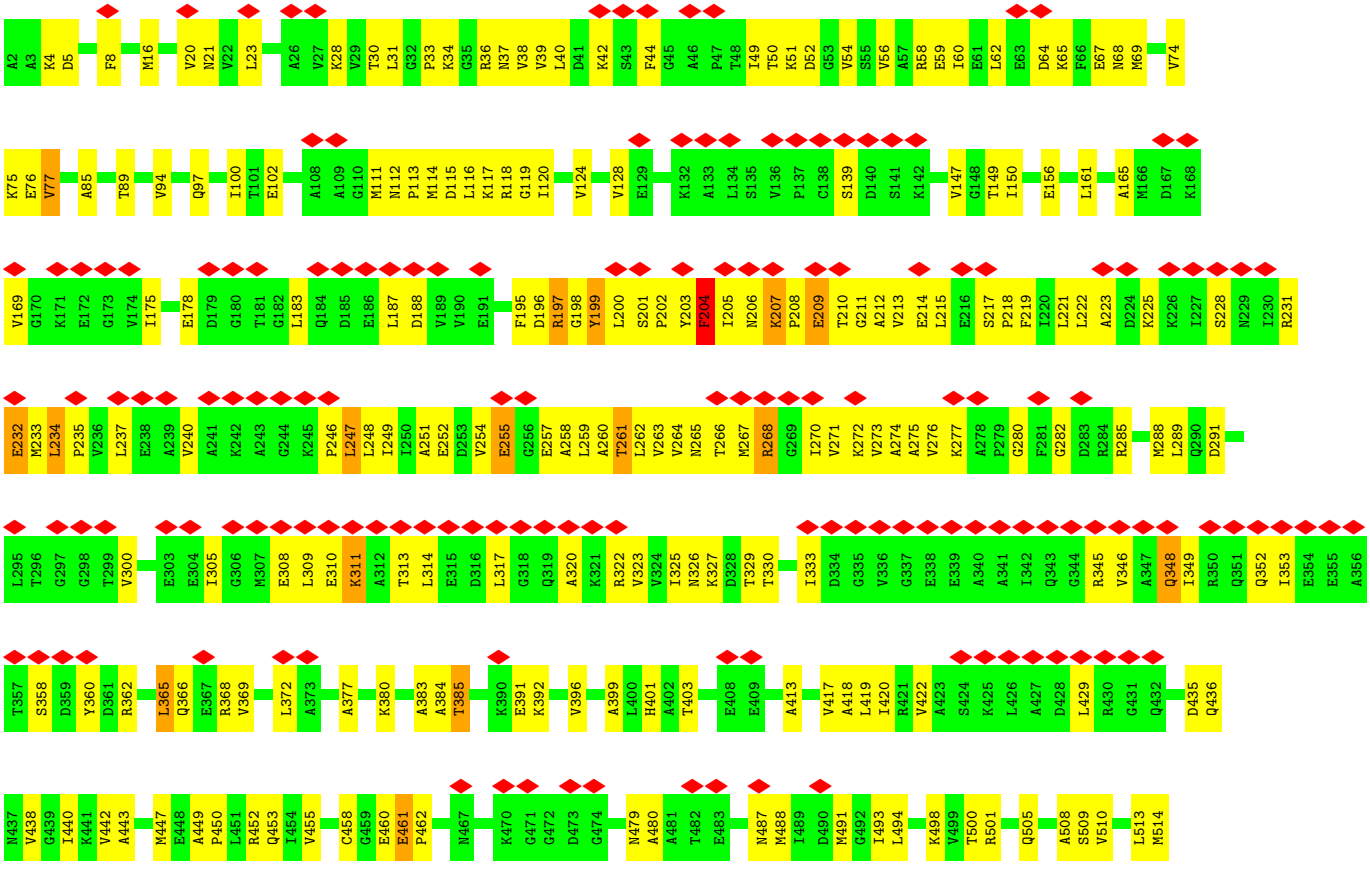
Chain E:

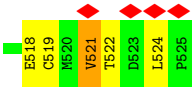




• Molecule 1: 60 KDA CHAPERONIN

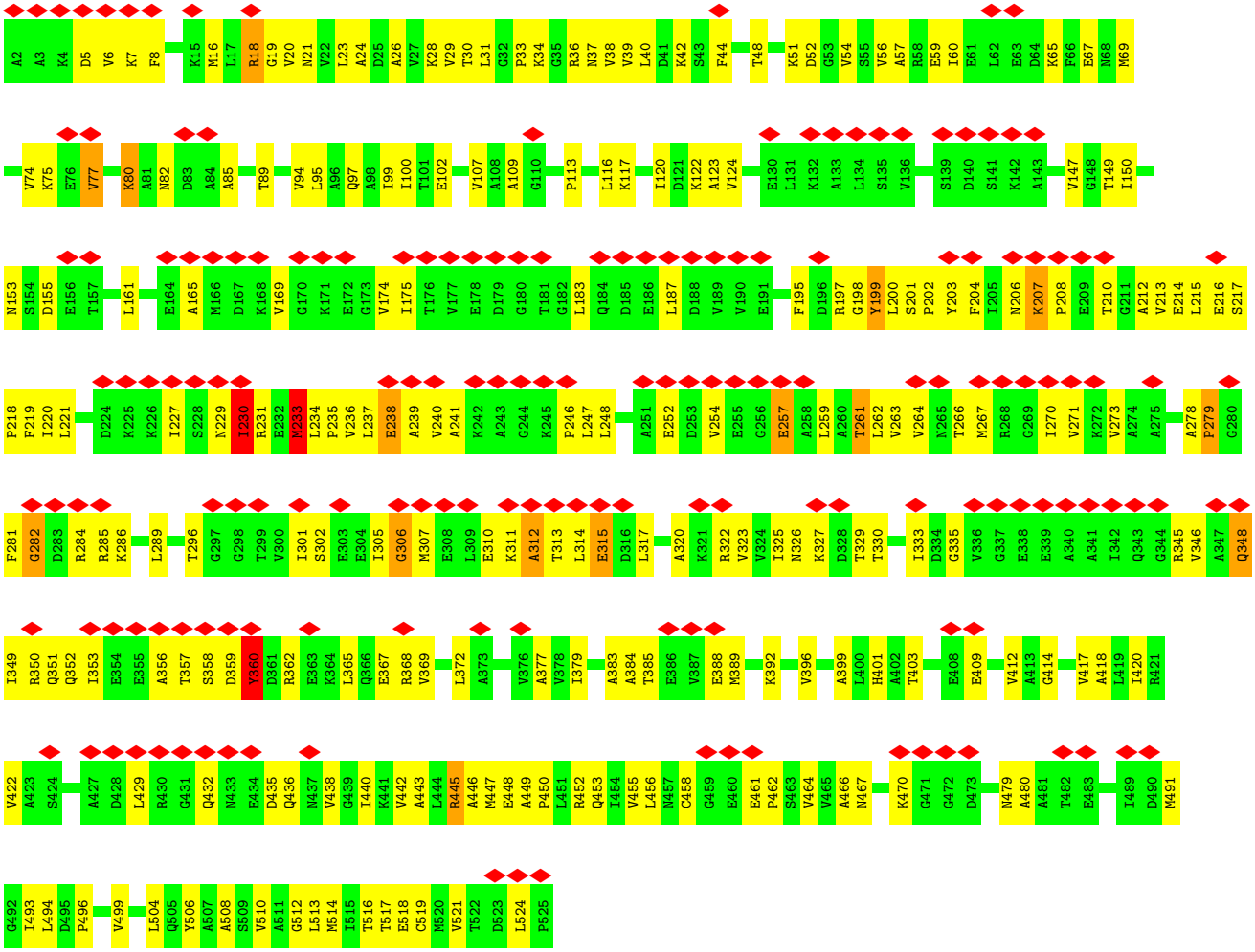
Chain F:





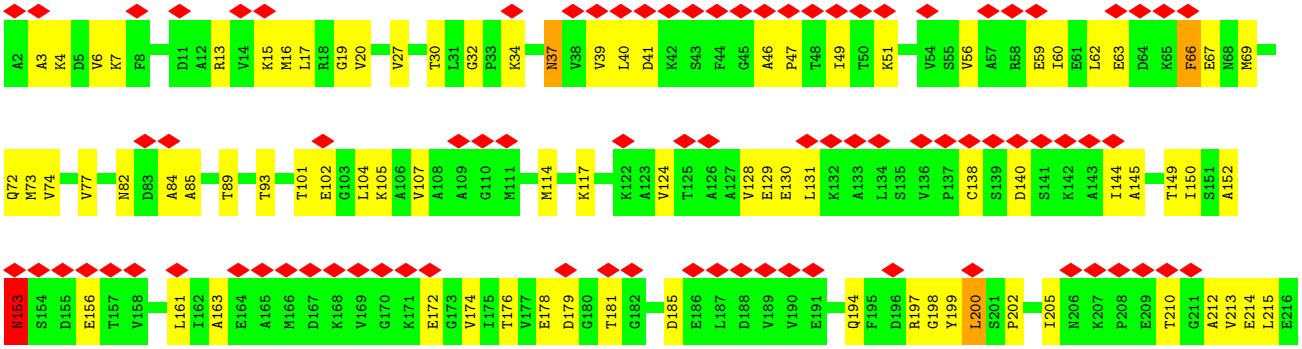
• Molecule 1: 60 KDA CHAPERONIN

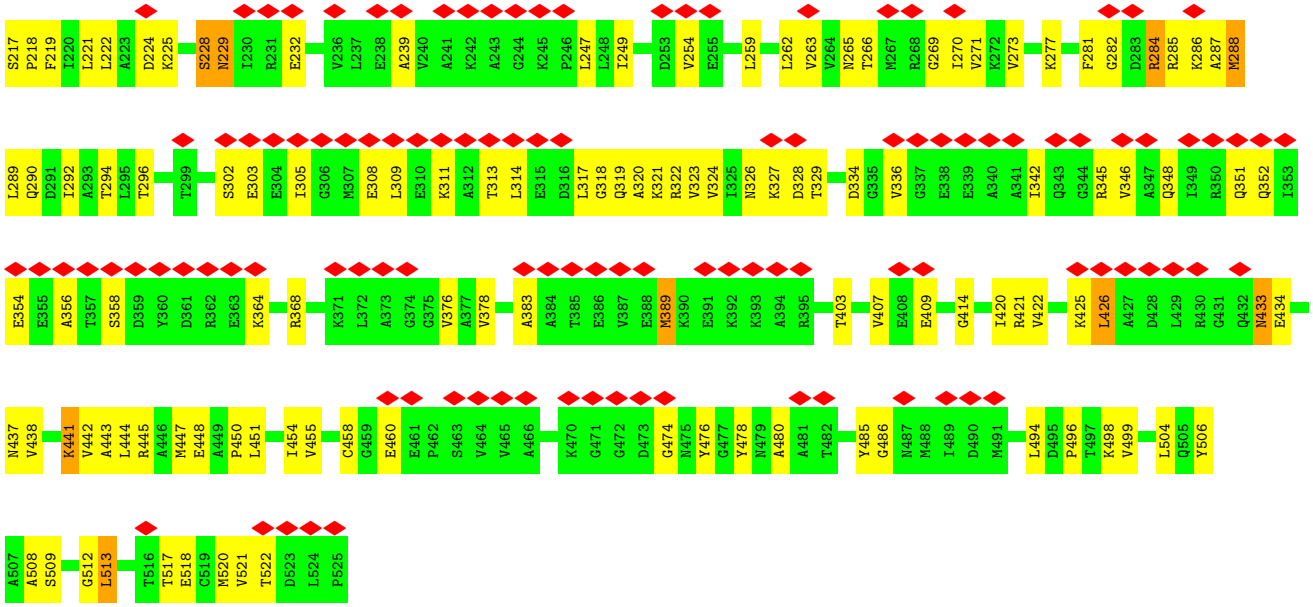
Chain G:



• Molecule 1: 60 KDA CHAPERONIN

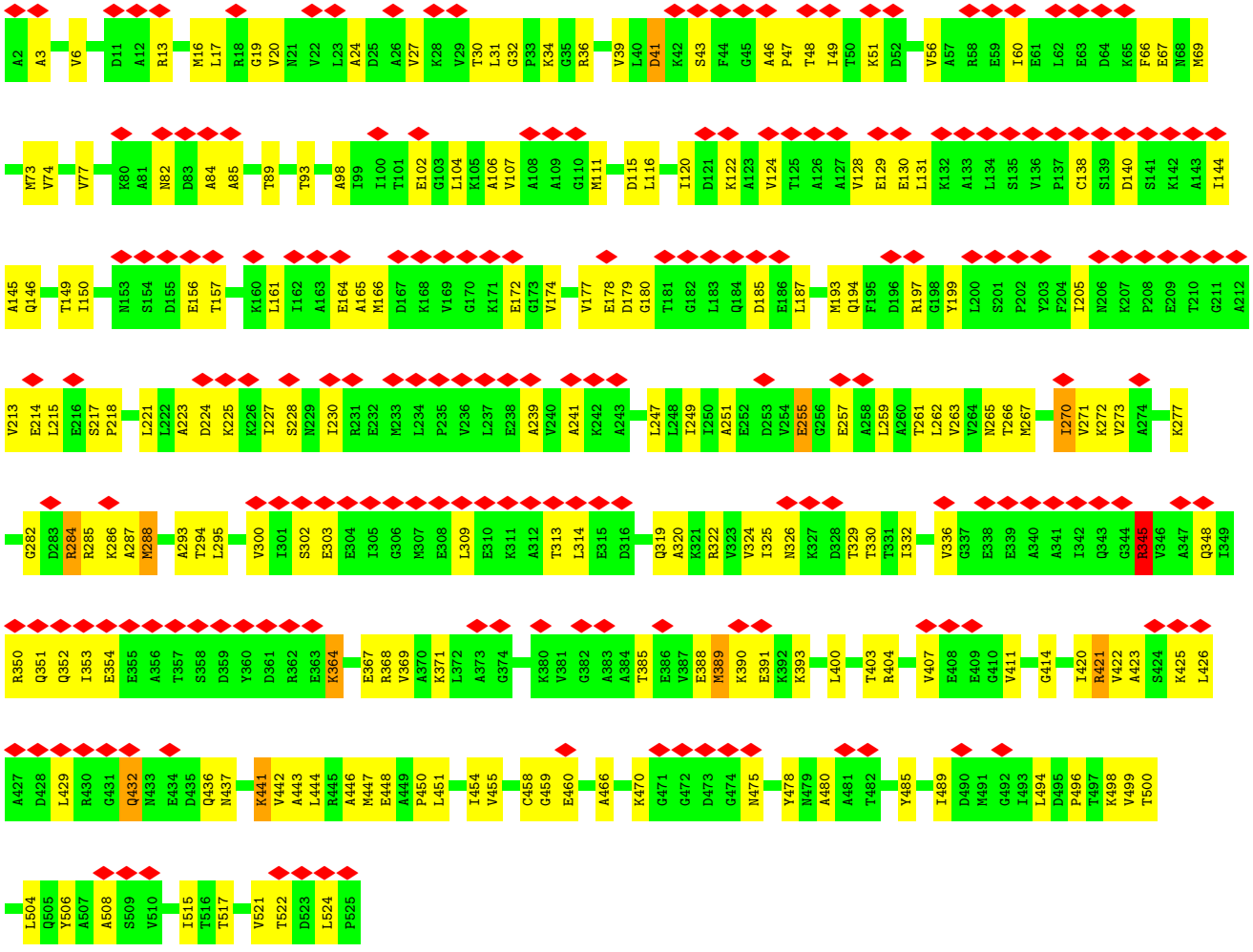
Chain H:





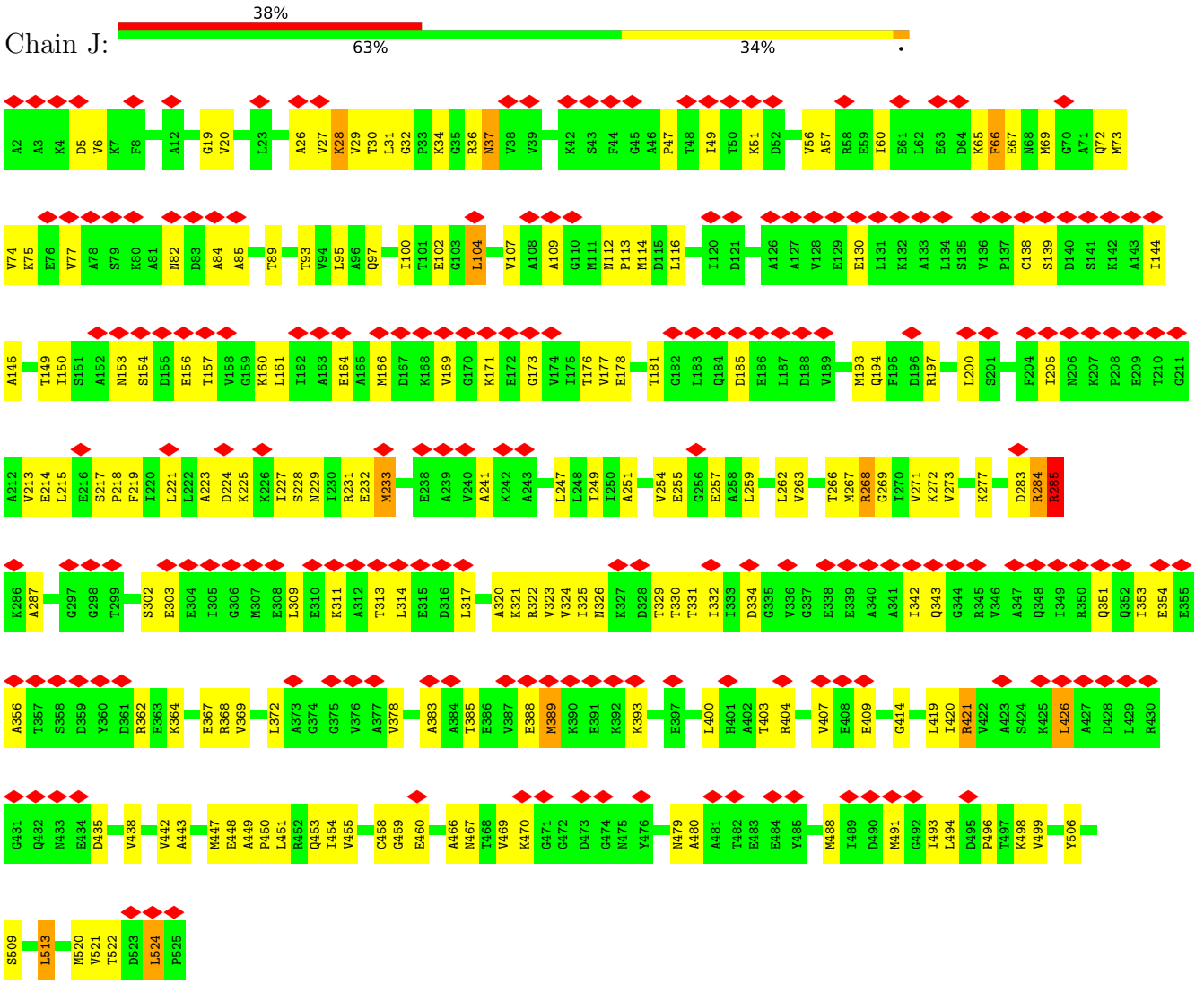
• Molecule 1: 60 KDA CHAPERONIN

Chain I:



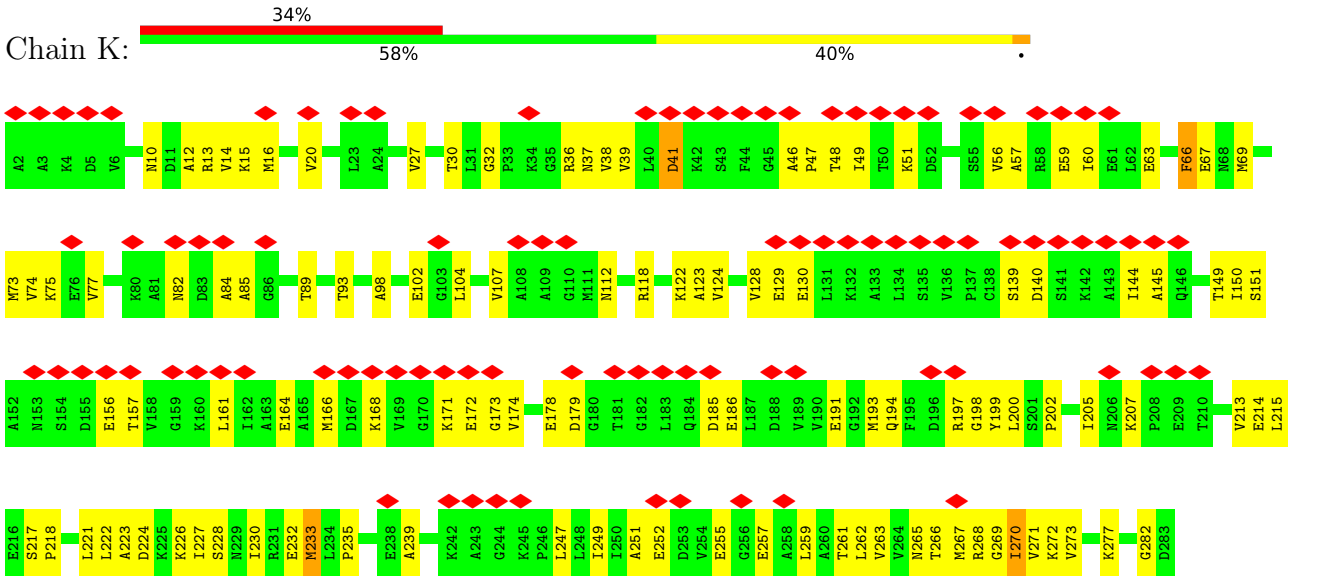
• Molecule 1: 60 KDA CHAPERONIN

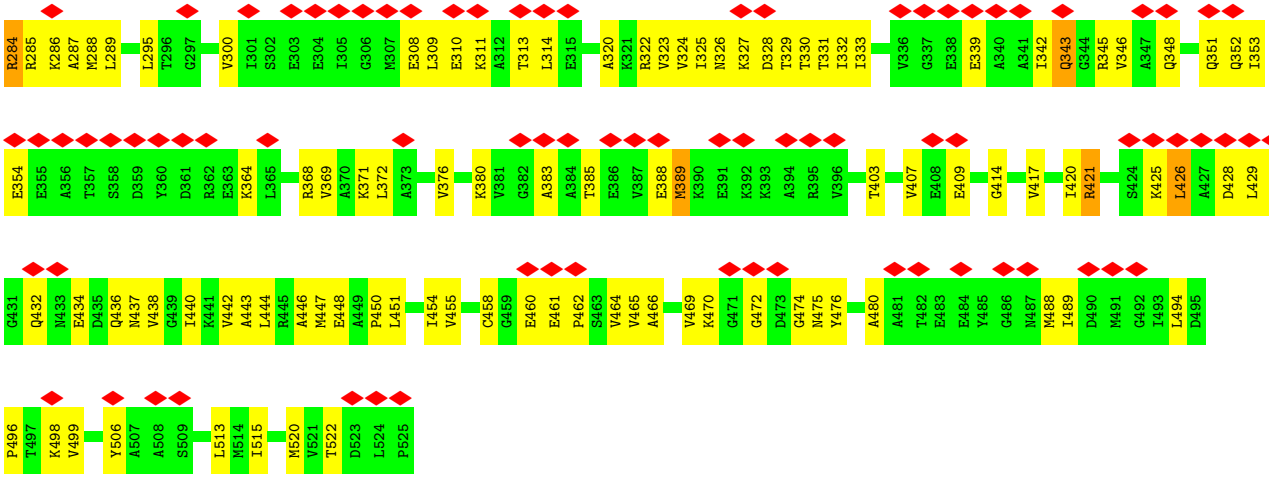
Chain J:



• Molecule 1: 60 KDA CHAPERONIN

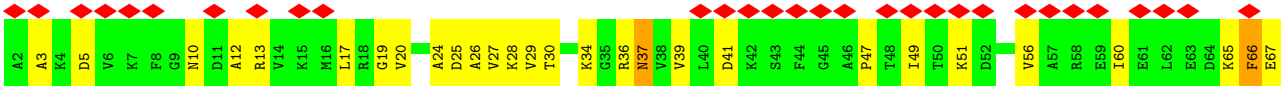
Chain K:

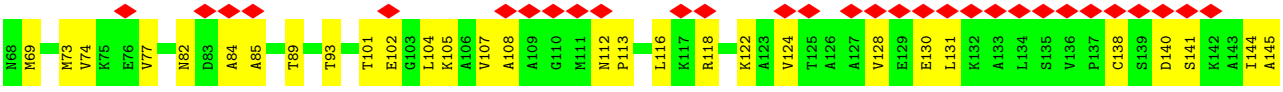


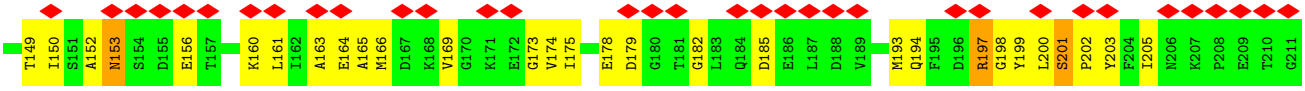


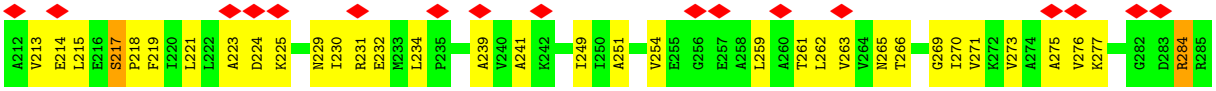
• Molecule 1: 60 KDA CHAPERONIN

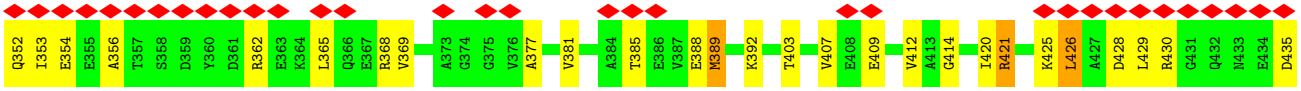
Chain L:

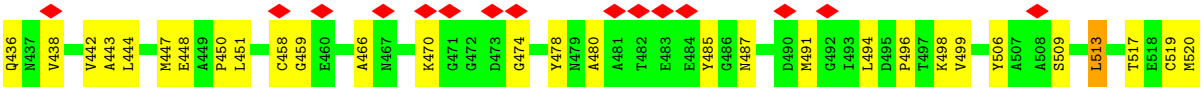


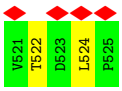






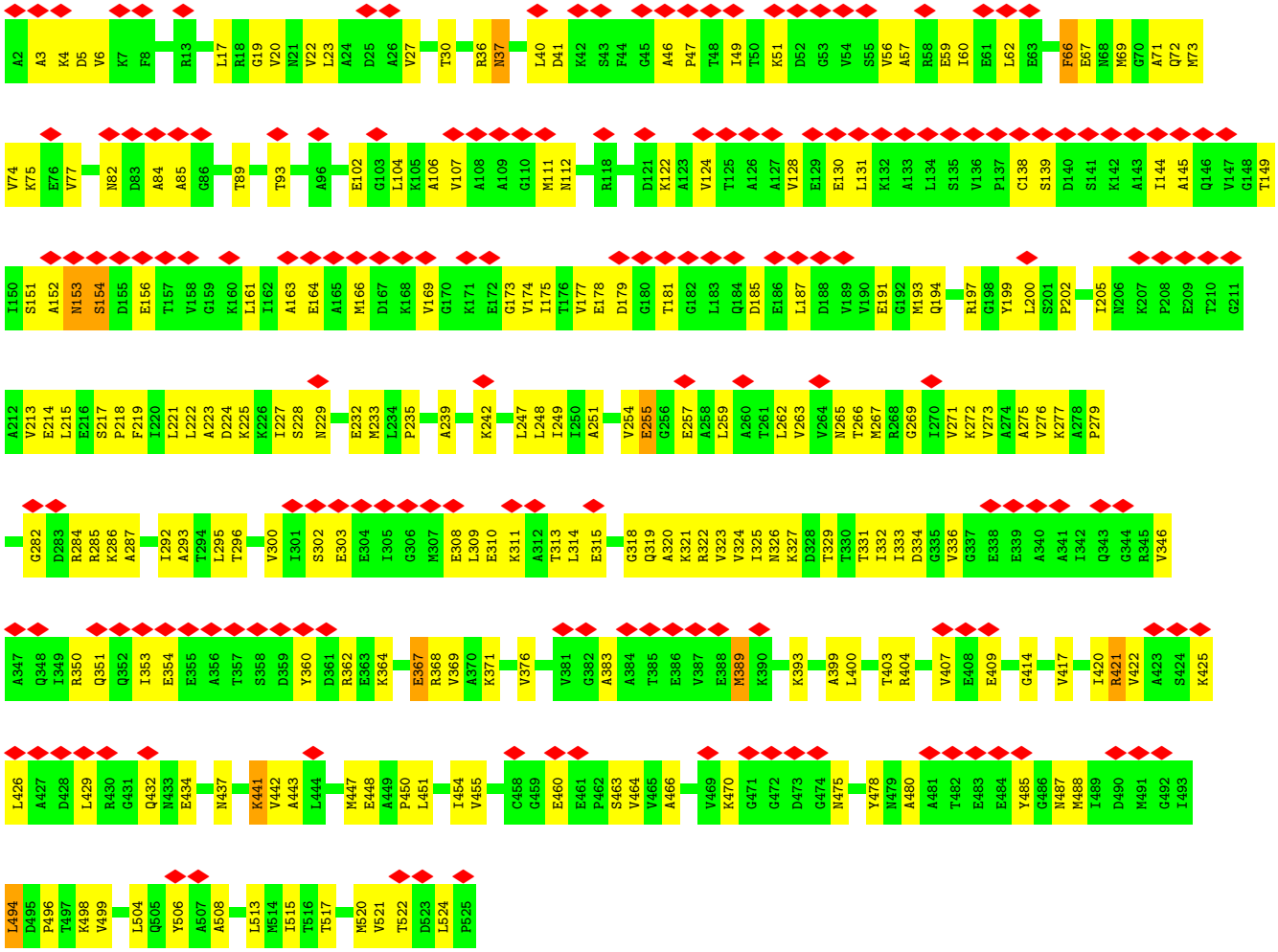






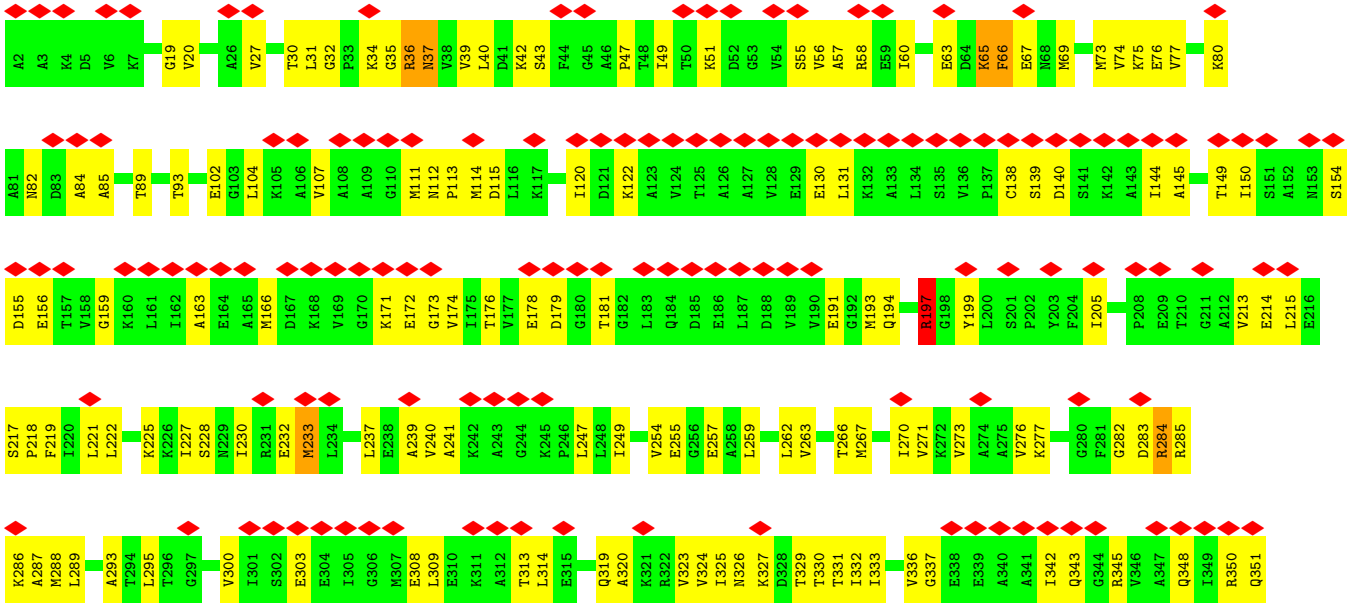
• Molecule 1: 60 KDA CHAPERONIN

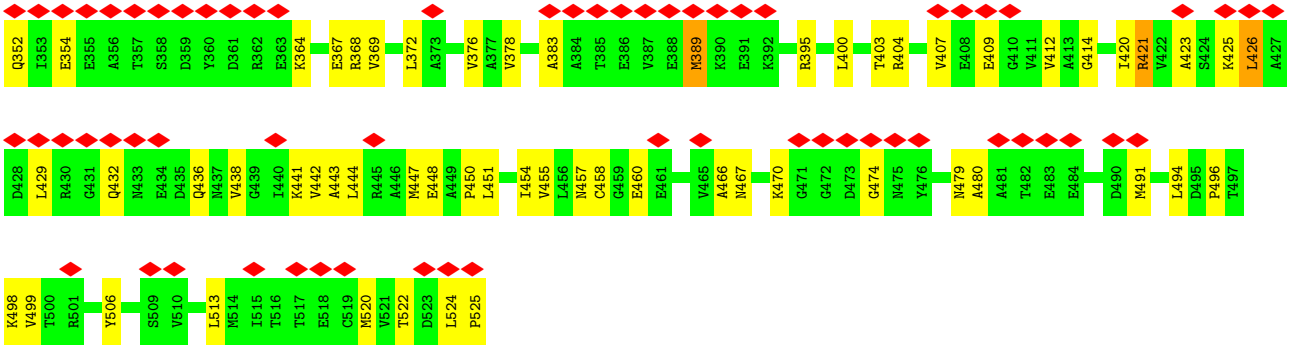
Chain M:



• Molecule 1: 60 KDA CHAPERONIN

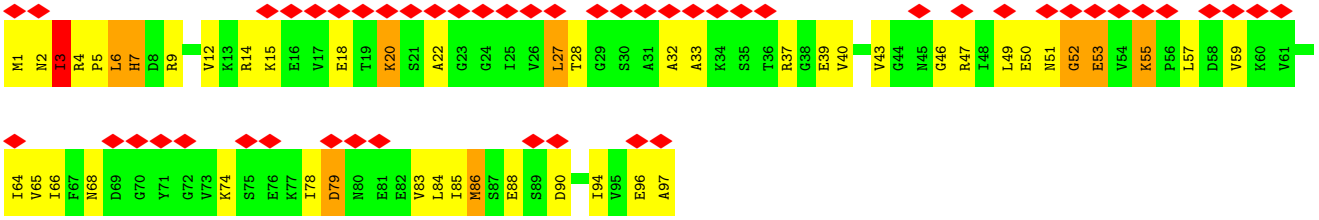
Chain N:





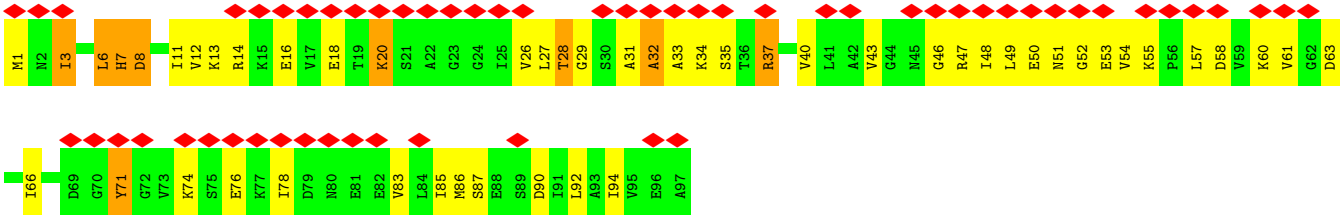
• Molecule 2: 10 KDA CHAPERONIN

Chain O:



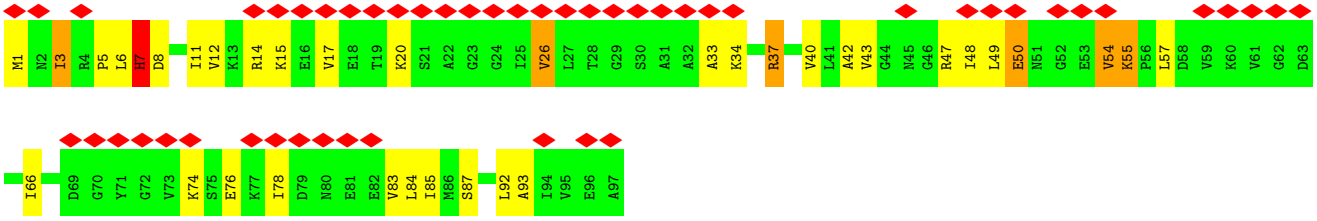
• Molecule 2: 10 KDA CHAPERONIN

Chain P:



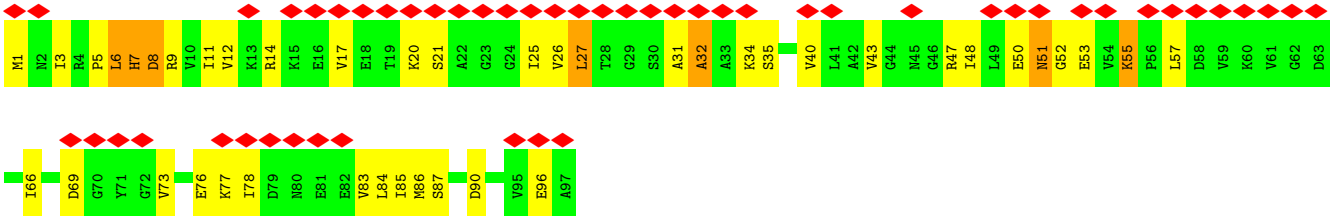
• Molecule 2: 10 KDA CHAPERONIN

Chain Q:



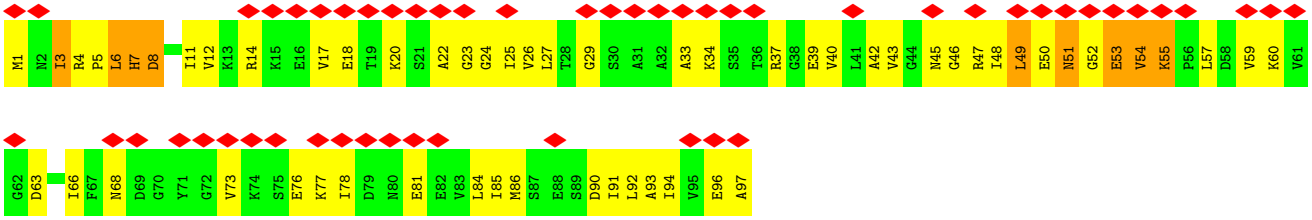
• Molecule 2: 10 KDA CHAPERONIN

Chain R:



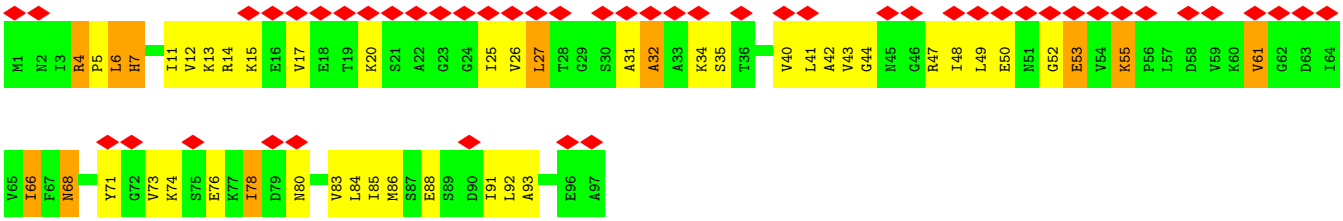
• Molecule 2: 10 KDA CHAPERONIN

Chain S:



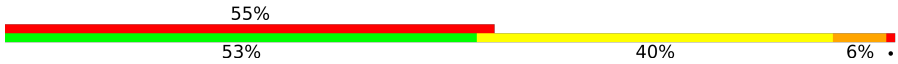
• Molecule 2: 10 KDA CHAPERONIN

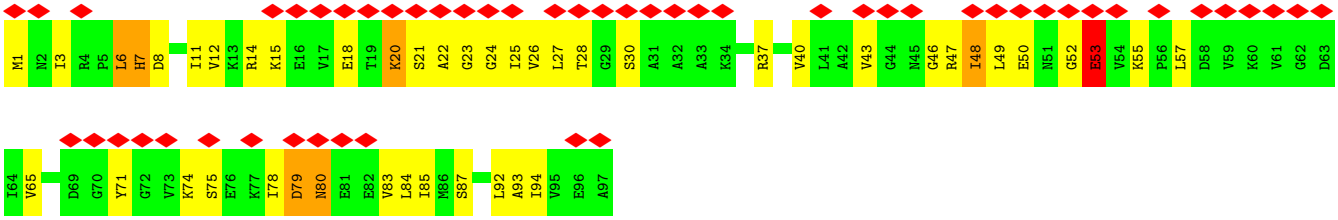
Chain T:



• Molecule 2: 10 KDA CHAPERONIN

Chain U:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	17611	Depositor
Resolution determination method	Not provided	
CTF correction method	EACH FRAME	Depositor
Microscope	JEOL KYOTO-3000SFF	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	30	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4700	Depositor
Magnification	73530	Depositor
Image detector	GENERIC GATAN	Depositor
Maximum map value	2.286	Depositor
Minimum map value	-0.472	Depositor
Average map value	0.043	Depositor
Map value standard deviation	0.209	Depositor
Recommended contour level	1.2	Depositor
Map size (Å)	367.19998, 367.19998, 367.19998	wwPDB
Map dimensions	180, 180, 180	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.04, 2.04, 2.04	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	A	0.37	0/3884	0.60	0/5243
1	B	0.37	0/3884	0.62	1/5243 (0.0%)
1	C	0.37	0/3884	0.62	0/5243
1	D	0.36	0/3884	0.61	0/5243
1	E	0.45	4/3884 (0.1%)	1.85	7/5243 (0.1%)
1	F	0.37	0/3884	0.61	0/5243
1	G	0.37	0/3884	0.63	0/5243
1	H	0.35	0/3884	0.60	0/5243
1	I	0.36	0/3884	0.62	1/5243 (0.0%)
1	J	0.36	0/3884	0.61	1/5243 (0.0%)
1	K	0.35	0/3884	0.60	0/5243
1	L	0.36	0/3884	0.60	0/5243
1	M	0.36	0/3884	0.61	0/5243
1	N	0.35	0/3884	0.60	0/5243
2	O	0.45	0/732	0.76	0/983
2	P	0.39	0/732	0.75	0/983
2	Q	0.40	0/732	0.69	0/983
2	R	0.45	0/732	0.74	0/983
2	S	0.43	0/732	0.73	0/983
2	T	0.42	0/732	0.75	2/983 (0.2%)
2	U	0.43	0/732	0.73	0/983
All	All	0.37	4/59500 (0.0%)	0.77	12/80283 (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
1	E	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	204	PHE	CB-CG	10.07	1.68	1.51
1	E	204	PHE	CG-CD1	7.69	1.50	1.38
1	E	204	PHE	CE1-CZ	5.70	1.48	1.37
1	E	204	PHE	CD1-CE1	-5.55	1.28	1.39

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	204	PHE	CD1-CE1-CZ	-75.38	29.65	120.10
1	E	204	PHE	CG-CD1-CE1	-61.55	53.10	120.80
1	E	204	PHE	CD1-CG-CD2	-40.88	65.15	118.30
1	E	204	PHE	CB-CG-CD1	38.19	147.53	120.80
1	E	204	PHE	CZ-CE2-CD2	-37.45	75.16	120.10
1	E	204	PHE	CG-CD2-CE2	-32.88	84.64	120.80
1	E	204	PHE	CE1-CZ-CE2	-28.45	68.80	120.00
1	I	345	ARG	NE-CZ-NH1	6.47	123.54	120.30
2	T	71	TYR	CB-CG-CD1	-5.96	117.42	121.00
1	J	285	ARG	NE-CZ-NH1	5.70	123.15	120.30
2	T	71	TYR	CB-CG-CD2	5.28	124.17	121.00
1	B	117	LYS	CB-CA-C	-5.09	100.22	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	204	PHE	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3856	0	3976	201	0
1	B	3856	0	3976	250	0
1	C	3856	0	3976	231	0
1	D	3856	0	3976	209	0
1	E	3856	0	3976	242	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3856	0	3976	232	0
1	G	3856	0	3976	236	0
1	H	3856	0	3976	165	0
1	I	3856	0	3976	178	0
1	J	3856	0	3976	157	0
1	K	3856	0	3976	178	0
1	L	3856	0	3976	180	0
1	M	3856	0	3976	179	0
1	N	3856	0	3976	166	0
2	O	728	0	762	41	0
2	P	728	0	762	46	0
2	Q	728	0	762	39	0
2	R	728	0	762	40	0
2	S	728	0	762	61	0
2	T	728	0	762	52	0
2	U	728	0	762	59	0
3	A	27	0	12	4	0
3	B	27	0	12	5	0
3	C	27	0	12	7	0
3	D	27	0	12	3	0
3	E	27	0	12	7	0
3	F	27	0	12	4	0
3	G	27	0	12	3	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
All	All	59276	0	61082	2844	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

All (2844) 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)
1:G:237:LEU:HD22	2:U:26:VAL:HG22	1.23	1.14
1:A:352:GLN:HB3	1:A:365:LEU:HD11	1.33	1.08
1:D:322:ARG:HB3	1:D:333:ILE:HD12	1.37	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:306:GLY:HA3	1:D:264:VAL:HG21	1.45	0.98
1:C:352:GLN:HB3	1:C:365:LEU:HD11	1.45	0.98
1:M:85:ALA:HB1	1:M:499:VAL:HG12	1.47	0.97
1:B:262:LEU:HD11	1:B:273:VAL:HB	1.48	0.95
1:C:513:LEU:HD11	1:D:388:GLU:HA	1.44	0.94
1:A:322:ARG:HB3	1:A:333:ILE:HD12	1.49	0.94
1:C:161:LEU:HD11	1:C:187:LEU:HB2	1.50	0.94
1:J:85:ALA:HB1	1:J:499:VAL:HG12	1.51	0.93
1:B:199:TYR:HB3	1:B:325:ILE:HG21	1.52	0.91
1:B:161:LEU:HD11	1:B:187:LEU:HB2	1.50	0.91
1:L:85:ALA:HB1	1:L:499:VAL:HG12	1.53	0.91
1:E:161:LEU:HD11	1:E:187:LEU:HB2	1.51	0.90
1:H:205:ILE:HA	1:H:213:VAL:HG22	1.53	0.90
1:L:49:ILE:HD11	1:M:73:MET:HE3	1.51	0.89
1:G:161:LEU:HD11	1:G:187:LEU:HB2	1.56	0.88
1:C:305:ILE:HG22	1:C:306:GLY:H	1.39	0.88
1:D:39:VAL:HG22	1:D:49:ILE:HG12	1.55	0.88
1:K:205:ILE:HA	1:K:213:VAL:HG22	1.52	0.88
1:I:205:ILE:HA	1:I:213:VAL:HG22	1.53	0.88
1:J:205:ILE:HA	1:J:213:VAL:HG22	1.54	0.87
1:D:262:LEU:HD11	1:D:273:VAL:HB	1.57	0.86
1:M:46:ALA:HB1	1:M:47:PRO:HD2	1.55	0.86
1:I:85:ALA:HB1	1:I:499:VAL:HG12	1.58	0.86
1:F:204:PHE:CE1	1:F:213:VAL:HG11	2.12	0.85
1:C:509:SER:HB2	1:D:384:ALA:HB3	1.59	0.85
1:G:262:LEU:HD11	1:G:273:VAL:HB	1.59	0.85
1:L:13:ARG:HB3	1:L:104:LEU:HD11	1.59	0.85
1:H:39:VAL:HG22	1:H:49:ILE:HG12	1.57	0.85
1:H:85:ALA:HB1	1:H:499:VAL:HG12	1.59	0.84
1:B:39:VAL:HG22	1:B:49:ILE:HG12	1.58	0.84
1:E:291:ASP:HB2	1:E:372:LEU:HD21	1.59	0.84
1:N:524:LEU:HD22	1:N:525:PRO:HD2	1.58	0.83
1:A:230:ILE:HD12	1:A:309:LEU:HD21	1.61	0.83
1:N:205:ILE:HA	1:N:213:VAL:HG22	1.59	0.83
1:I:77:VAL:HG22	1:I:506:TYR:HB3	1.60	0.83
1:N:85:ALA:HB1	1:N:499:VAL:HG12	1.61	0.83
1:G:322:ARG:HB3	1:G:333:ILE:HD12	1.60	0.83
2:P:3:ILE:HG12	2:P:78:ILE:HD13	1.60	0.83
1:G:467:ASN:HD21	1:M:464:VAL:HG22	1.43	0.82
1:L:205:ILE:HA	1:L:213:VAL:HG22	1.59	0.82
1:M:364:LYS:HA	1:M:367:GLU:OE2	1.79	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:GLN:HB3	1:B:365:LEU:HD11	1.61	0.82
1:A:262:LEU:HD11	1:A:273:VAL:HB	1.62	0.81
1:D:346:VAL:HA	1:D:349:ILE:HD12	1.62	0.81
1:K:85:ALA:HB1	1:K:499:VAL:HG12	1.62	0.81
1:E:73:MET:SD	1:F:49:ILE:HD11	2.19	0.81
1:H:69:MET:HE3	1:H:522:THR:HB	1.62	0.81
1:A:212:ALA:HA	1:A:325:ILE:O	1.81	0.81
1:C:346:VAL:HA	1:C:349:ILE:HD12	1.62	0.81
1:G:212:ALA:HA	1:G:325:ILE:O	1.80	0.81
1:I:122:LYS:HE2	1:I:429:LEU:HD11	1.60	0.81
1:C:266:THR:HA	1:C:271:VAL:O	1.81	0.81
1:J:458:CYS:SG	1:J:480:ALA:HB1	2.21	0.81
1:B:302:SER:HB3	1:B:305:ILE:HD12	1.63	0.80
1:E:195:PHE:CE1	1:E:330:THR:HB	2.16	0.80
1:F:509:SER:HB2	1:G:384:ALA:HB3	1.63	0.80
1:I:270:ILE:HG22	1:I:271:VAL:HG23	1.61	0.80
1:L:69:MET:HE3	1:L:522:THR:HB	1.63	0.80
1:E:265:ASN:HD21	2:S:26:VAL:HG13	1.45	0.80
1:I:13:ARG:HB3	1:I:104:LEU:HD11	1.61	0.80
1:F:346:VAL:HA	1:F:349:ILE:HD12	1.62	0.79
2:T:66:ILE:HB	2:T:93:ALA:HB3	1.63	0.79
1:L:270:ILE:HG22	1:L:271:VAL:HG23	1.63	0.79
1:E:6:VAL:HG12	1:E:521:VAL:HG22	1.65	0.78
1:F:39:VAL:HG22	1:F:49:ILE:HG12	1.65	0.78
1:L:82:ASN:HB2	1:L:89:THR:OG1	1.82	0.78
2:O:59:VAL:HG12	2:O:94:ILE:HD11	1.65	0.78
1:E:195:PHE:CD1	1:E:197:ARG:HD3	2.19	0.78
1:H:351:GLN:O	1:H:354:GLU:HG2	1.83	0.78
1:K:239:ALA:HB1	1:K:314:LEU:HD11	1.65	0.78
1:B:201:SER:HB3	1:B:259:LEU:HD22	1.66	0.77
1:I:239:ALA:HB1	1:I:314:LEU:HD11	1.66	0.77
1:D:252:GLU:HA	1:D:285:ARG:NH1	2.00	0.77
1:H:131:LEU:HD12	1:H:422:VAL:HG11	1.65	0.77
1:L:122:LYS:HE2	1:L:429:LEU:HD11	1.66	0.77
1:A:305:ILE:HD11	1:B:203:TYR:CD1	2.20	0.77
1:K:39:VAL:HG22	1:K:49:ILE:CD1	2.15	0.77
1:M:82:ASN:HB2	1:M:89:THR:OG1	1.84	0.77
1:C:77:VAL:HG12	1:C:510:VAL:HG21	1.67	0.77
1:G:34:LYS:HD2	1:G:458:CYS:SG	2.24	0.77
1:J:82:ASN:HB2	1:J:89:THR:OG1	1.85	0.76
1:F:161:LEU:HD11	1:F:187:LEU:HB2	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:20:LYS:CB	2:P:27:LEU:HG	2.16	0.76
1:B:193:MET:HB3	1:B:332:ILE:HG22	1.67	0.76
1:D:198:GLY:HA3	1:D:327:LYS:O	1.86	0.76
1:K:353:ILE:HD11	1:K:369:VAL:HG21	1.68	0.76
1:E:226:LYS:O	1:E:230:ILE:HD11	1.86	0.76
1:L:77:VAL:HG22	1:L:506:TYR:HB3	1.67	0.76
1:M:420:ILE:HG13	1:M:451:LEU:HD22	1.68	0.76
1:N:82:ASN:HB2	1:N:89:THR:OG1	1.85	0.76
1:E:349:ILE:HG23	1:E:365:LEU:HD21	1.68	0.75
1:L:214:GLU:HG2	1:L:324:VAL:HG12	1.69	0.75
1:B:263:VAL:O	1:B:267:MET:HG2	1.85	0.75
1:H:13:ARG:HB3	1:H:104:LEU:HD11	1.65	0.75
1:K:214:GLU:HG2	1:K:324:VAL:HG12	1.68	0.75
1:E:197:ARG:HG2	1:E:277:LYS:O	1.86	0.75
1:C:263:VAL:O	1:C:267:MET:HG2	1.86	0.75
1:H:102:GLU:HB2	1:H:442:VAL:HG13	1.68	0.75
1:F:212:ALA:HA	1:F:325:ILE:O	1.87	0.74
1:K:82:ASN:HB2	1:K:89:THR:OG1	1.87	0.74
2:S:52:GLY:O	2:S:53:GLU:HB2	1.87	0.74
1:F:208:PRO:HB2	1:F:212:ALA:HB3	1.69	0.74
1:H:214:GLU:HG2	1:H:324:VAL:HG12	1.68	0.74
1:I:49:ILE:HD11	1:J:73:MET:HE2	1.68	0.74
1:N:214:GLU:HG2	1:N:324:VAL:HG12	1.68	0.74
1:M:205:ILE:HA	1:M:213:VAL:HG22	1.69	0.74
1:B:40:LEU:HD13	1:B:59:GLU:HG3	1.68	0.74
1:C:204:PHE:CE1	1:C:213:VAL:HG11	2.23	0.74
1:K:420:ILE:HD13	1:K:448:GLU:HA	1.70	0.74
1:A:34:LYS:HD2	1:A:458:CYS:SG	2.28	0.73
1:G:6:VAL:HG12	1:G:521:VAL:HG22	1.69	0.73
1:I:161:LEU:HD21	1:I:185:ASP:HB3	1.69	0.73
1:C:240:VAL:HG21	1:C:247:LEU:HD23	1.70	0.73
1:A:510:VAL:HG13	1:B:385:THR:HG21	1.68	0.73
1:F:249:ILE:HB	1:F:275:ALA:HB2	1.70	0.73
1:B:265:ASN:OD1	2:P:27:LEU:HB3	1.89	0.73
1:B:513:LEU:HD11	1:C:388:GLU:HA	1.71	0.73
1:F:231:ARG:O	1:F:233:MET:HG2	1.87	0.73
1:G:40:LEU:HD22	1:G:59:GLU:HG3	1.71	0.73
1:H:82:ASN:HB2	1:H:89:THR:OG1	1.88	0.73
1:D:77:VAL:CG1	1:D:510:VAL:HG21	2.18	0.73
1:L:221:LEU:HD12	1:L:249:ILE:HG23	1.69	0.73
1:N:228:SER:O	1:N:257:GLU:HB2	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:214:GLU:HG2	1:J:324:VAL:HG12	1.71	0.73
1:F:199:TYR:CZ	1:F:202:PRO:HA	2.24	0.72
1:H:433:ASN:HD22	1:H:434:GLU:H	1.36	0.72
1:L:230:ILE:HD11	1:L:261:THR:HG21	1.71	0.72
1:A:39:VAL:HG22	1:A:49:ILE:HG12	1.71	0.72
1:K:421:ARG:O	1:K:425:LYS:HG2	1.89	0.72
2:T:12:VAL:HG12	2:T:40:VAL:HA	1.71	0.72
1:F:247:LEU:HB3	1:F:273:VAL:HG13	1.71	0.72
1:B:305:ILE:HG22	1:B:306:GLY:H	1.54	0.72
1:F:231:ARG:HH21	1:F:237:LEU:HD12	1.54	0.72
1:F:349:ILE:HG23	1:F:365:LEU:HD21	1.72	0.72
1:A:198:GLY:HA3	1:A:327:LYS:O	1.88	0.71
1:J:420:ILE:HD13	1:J:448:GLU:HA	1.72	0.71
1:B:12:ALA:HB1	1:B:520:MET:HG2	1.72	0.71
1:E:31:LEU:HD12	3:E:1:ADP:H5'1	1.71	0.71
1:F:124:VAL:HG21	1:F:508:ALA:HB1	1.71	0.71
2:R:12:VAL:HG12	2:R:40:VAL:HA	1.71	0.71
1:D:161:LEU:HD11	1:D:187:LEU:HB2	1.71	0.71
1:H:458:CYS:SG	1:H:480:ALA:HB1	2.30	0.71
1:N:458:CYS:SG	1:N:480:ALA:HB1	2.30	0.71
1:J:221:LEU:HD12	1:J:249:ILE:HG23	1.71	0.71
1:D:266:THR:HA	1:D:271:VAL:O	1.91	0.71
1:L:326:ASN:OD1	1:L:329:THR:HB	1.89	0.71
1:C:479:ASN:HB2	1:C:491:MET:SD	2.30	0.71
1:G:231:ARG:O	1:G:233:MET:HG3	1.91	0.71
1:H:450:PRO:O	1:H:454:ILE:HG12	1.91	0.71
1:L:241:ALA:HB2	1:L:271:VAL:HG21	1.72	0.71
1:E:510:VAL:HG13	1:F:385:THR:HG21	1.72	0.71
1:G:40:LEU:HD21	1:G:56:VAL:HA	1.71	0.70
1:D:212:ALA:HA	1:D:325:ILE:O	1.90	0.70
1:F:34:LYS:HD2	1:F:458:CYS:SG	2.31	0.70
1:K:420:ILE:HG13	1:K:451:LEU:HD22	1.71	0.70
1:L:12:ALA:HB1	1:L:520:MET:HG2	1.74	0.70
1:I:241:ALA:HB2	1:I:271:VAL:HG21	1.74	0.70
1:B:174:VAL:HG21	1:B:367:GLU:HA	1.72	0.70
1:B:212:ALA:HA	1:B:325:ILE:O	1.91	0.70
1:D:74:VAL:O	1:D:77:VAL:HG13	1.92	0.70
1:F:518:GLU:HB2	1:G:36:ARG:HB2	1.71	0.70
1:G:234:LEU:HD22	2:U:26:VAL:HG11	1.72	0.70
1:C:204:PHE:CZ	1:C:213:VAL:HG11	2.27	0.70
1:G:359:ASP:O	1:G:360:TYR:HB2	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:VAL:HG12	1:A:510:VAL:HG21	1.74	0.70
1:C:266:THR:HG22	1:C:273:VAL:H	1.55	0.70
1:F:147:VAL:HG23	1:F:403:THR:HG22	1.73	0.70
1:F:266:THR:HG22	1:F:273:VAL:H	1.57	0.69
1:E:262:LEU:HD11	1:E:273:VAL:HB	1.74	0.69
1:H:420:ILE:HG13	1:H:451:LEU:HD22	1.74	0.69
2:P:12:VAL:HG12	2:P:40:VAL:HA	1.74	0.69
1:H:228:SER:O	1:H:229:ASN:HB2	1.90	0.69
1:N:420:ILE:HG13	1:N:451:LEU:HD22	1.73	0.69
1:I:450:PRO:O	1:I:454:ILE:HG12	1.93	0.69
2:R:14:ARG:CZ	2:R:34:LYS:HE3	2.23	0.69
1:A:263:VAL:O	1:A:267:MET:HG2	1.93	0.69
1:C:207:LYS:HB3	1:C:208:PRO:HD3	1.73	0.69
1:F:509:SER:CB	1:G:384:ALA:HB3	2.23	0.69
1:J:56:VAL:O	1:J:60:ILE:HG12	1.92	0.69
1:F:240:VAL:HG21	1:F:247:LEU:HD23	1.74	0.69
2:S:68:ASN:ND2	2:T:74:LYS:HE2	2.08	0.69
1:A:100:ILE:HD13	1:A:514:MET:SD	2.33	0.69
1:B:518:GLU:HB2	1:C:36:ARG:CB	2.22	0.69
1:B:518:GLU:HB2	1:C:36:ARG:HB2	1.75	0.69
1:C:57:ALA:O	1:C:75:LYS:HE2	1.93	0.69
1:D:42:LYS:HE2	1:D:48:THR:OG1	1.92	0.69
1:D:458:CYS:SG	1:D:480:ALA:HB1	2.32	0.69
1:K:450:PRO:O	1:K:454:ILE:HG12	1.93	0.69
1:F:513:LEU:CD1	1:G:388:GLU:HA	2.22	0.68
1:G:31:LEU:HD23	1:G:453:GLN:HB3	1.75	0.68
1:H:37:ASN:ND2	1:I:517:THR:HA	2.07	0.68
1:C:305:ILE:HG22	1:C:306:GLY:N	2.08	0.68
1:A:351:GLN:HG2	1:B:210:THR:HG23	1.75	0.68
1:B:77:VAL:CG1	1:B:510:VAL:HG21	2.23	0.68
1:F:119:GLY:O	1:F:440:ILE:HD13	1.93	0.68
1:J:414:GLY:N	1:J:494:LEU:HA	2.08	0.68
1:G:57:ALA:O	1:G:75:LYS:HE2	1.93	0.68
1:G:215:LEU:O	1:G:322:ARG:HA	1.93	0.68
1:I:82:ASN:HB2	1:I:89:THR:OG1	1.94	0.68
1:N:450:PRO:O	1:N:454:ILE:HG12	1.93	0.68
2:S:7:HIS:HB2	2:S:46:GLY:O	1.92	0.68
1:A:266:THR:HA	1:A:271:VAL:O	1.94	0.68
1:F:252:GLU:HA	1:F:285:ARG:NH1	2.09	0.68
1:C:239:ALA:HB1	1:C:314:LEU:HD23	1.76	0.68
1:H:239:ALA:HB1	1:H:314:LEU:HD11	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:179:ASP:HA	1:M:389:MET:HE3	1.75	0.68
1:A:161:LEU:HD11	1:A:187:LEU:HB2	1.75	0.68
1:E:77:VAL:CG1	1:E:510:VAL:HG21	2.24	0.68
1:I:32:GLY:HA2	1:I:454:ILE:HD12	1.76	0.68
1:D:285:ARG:O	1:D:289:LEU:HG	1.94	0.67
1:I:266:THR:HG22	1:I:273:VAL:H	1.57	0.67
1:J:77:VAL:HG22	1:J:506:TYR:HB3	1.76	0.67
1:B:230:ILE:HG23	1:B:309:LEU:CD2	2.24	0.67
1:H:138:CYS:SG	1:H:144:ILE:HD13	2.34	0.67
1:L:232:GLU:HB3	1:L:309:LEU:HB2	1.75	0.67
1:D:247:LEU:HD21	1:D:317:LEU:HD13	1.77	0.67
1:G:266:THR:HG22	1:G:273:VAL:H	1.59	0.67
1:G:479:ASN:HB2	1:G:491:MET:SD	2.34	0.67
1:H:414:GLY:N	1:H:494:LEU:HA	2.09	0.67
1:E:34:LYS:HD2	1:E:458:CYS:SG	2.34	0.67
1:H:30:THR:HB	1:H:51:LYS:O	1.94	0.67
1:F:74:VAL:O	1:F:77:VAL:HG13	1.94	0.67
1:J:450:PRO:O	1:J:454:ILE:HG12	1.94	0.67
2:R:8:ASP:HB2	2:R:47:ARG:HA	1.77	0.67
2:U:78:ILE:HD12	2:U:83:VAL:HG21	1.76	0.67
1:A:85:ALA:O	1:A:401:HIS:HB3	1.95	0.67
1:M:217:SER:N	1:M:218:PRO:HD3	2.10	0.67
2:P:3:ILE:HG12	2:P:78:ILE:CD1	2.24	0.67
1:D:65:LYS:O	1:D:69:MET:HG3	1.95	0.67
1:D:85:ALA:O	1:D:401:HIS:HB3	1.94	0.67
1:H:441:LYS:O	1:H:445:ARG:HG2	1.94	0.67
1:F:262:LEU:HD21	1:F:274:ALA:HA	1.76	0.67
1:H:77:VAL:HG22	1:H:506:TYR:HB3	1.76	0.67
1:J:351:GLN:O	1:J:354:GLU:HG2	1.94	0.67
1:H:433:ASN:HD22	1:H:434:GLU:N	1.91	0.67
1:B:257:GLU:O	1:B:261:THR:HG22	1.96	0.66
1:K:218:PRO:HG2	1:K:323:VAL:HG12	1.77	0.66
1:N:266:THR:HG22	1:N:273:VAL:H	1.58	0.66
1:C:285:ARG:O	1:C:289:LEU:HG	1.94	0.66
1:F:458:CYS:SG	1:F:480:ALA:HB1	2.35	0.66
1:D:345:ARG:O	1:D:348:GLN:HG3	1.95	0.66
1:E:74:VAL:O	1:E:77:VAL:HG13	1.95	0.66
1:L:284:ARG:HD3	1:L:284:ARG:N	2.10	0.66
1:N:138:CYS:SG	1:N:144:ILE:HD13	2.34	0.66
2:Q:12:VAL:HG12	2:Q:40:VAL:HA	1.75	0.66
1:F:204:PHE:CD1	1:F:274:ALA:HB3	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:420:ILE:HD13	1:H:448:GLU:HA	1.78	0.66
2:P:20:LYS:HB3	2:P:27:LEU:HG	1.75	0.66
1:B:368:ARG:O	1:B:372:LEU:HG	1.96	0.66
1:I:458:CYS:SG	1:I:480:ALA:HB1	2.36	0.66
1:L:414:GLY:N	1:L:494:LEU:HA	2.10	0.66
1:A:31:LEU:HD23	1:A:453:GLN:HB3	1.77	0.66
1:F:201:SER:HB3	1:F:259:LEU:HD22	1.78	0.66
1:G:458:CYS:SG	1:G:480:ALA:HB1	2.36	0.66
1:N:239:ALA:HB1	1:N:314:LEU:HD11	1.78	0.66
1:A:345:ARG:O	1:A:349:ILE:HG13	1.96	0.66
1:B:113:PRO:HA	1:B:116:LEU:HD12	1.78	0.66
1:E:285:ARG:O	1:E:289:LEU:HG	1.96	0.66
1:G:204:PHE:CD1	1:G:266:THR:HB	2.31	0.66
1:H:326:ASN:OD1	1:H:329:THR:HB	1.96	0.66
1:I:414:GLY:N	1:I:494:LEU:HA	2.11	0.66
1:L:420:ILE:HD13	1:L:448:GLU:HA	1.78	0.66
1:N:414:GLY:N	1:N:494:LEU:HA	2.10	0.66
1:F:311:LYS:HG3	1:F:311:LYS:O	1.94	0.65
1:H:161:LEU:HD21	1:H:185:ASP:HB3	1.78	0.65
2:T:5:PRO:HD3	2:T:42:ALA:HB1	1.78	0.65
1:E:265:ASN:ND2	2:S:26:VAL:HG13	2.11	0.65
1:J:145:ALA:O	1:J:149:THR:HG23	1.97	0.65
1:D:34:LYS:HD2	1:D:458:CYS:SG	2.36	0.65
1:I:284:ARG:HD3	1:I:364:LYS:HG2	1.77	0.65
1:J:197:ARG:HG2	1:J:277:LYS:O	1.96	0.65
1:E:325:ILE:HG12	1:E:330:THR:HG23	1.79	0.65
1:J:326:ASN:OD1	1:J:329:THR:HB	1.97	0.65
2:O:78:ILE:HG22	2:O:79:ASP:OD1	1.97	0.65
1:D:417:VAL:HA	1:D:420:ILE:HG22	1.78	0.65
1:J:69:MET:O	1:J:73:MET:HG3	1.97	0.65
2:O:7:HIS:HB2	2:O:46:GLY:O	1.96	0.65
1:A:304:GLU:O	1:B:260:ALA:HA	1.97	0.65
1:B:266:THR:HG22	1:B:273:VAL:H	1.62	0.65
1:G:31:LEU:HD12	3:G:1:ADP:H5'1	1.79	0.65
1:G:220:ILE:HD13	1:G:296:THR:HG21	1.78	0.65
1:I:217:SER:N	1:I:218:PRO:HD3	2.12	0.65
1:M:450:PRO:O	1:M:454:ILE:HG12	1.97	0.65
1:C:65:LYS:O	1:C:69:MET:HG3	1.97	0.65
1:E:31:LEU:CD1	3:E:1:ADP:H5'1	2.27	0.65
1:E:212:ALA:HA	1:E:325:ILE:O	1.96	0.65
1:M:69:MET:HE1	1:M:522:THR:HB	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:122:LYS:HE2	1:N:429:LEU:HD11	1.78	0.65
1:E:305:ILE:HD11	1:F:203:TYR:CD1	2.31	0.65
1:E:510:VAL:CG1	1:F:385:THR:HG21	2.26	0.65
1:F:479:ASN:HB2	1:F:491:MET:SD	2.37	0.65
2:T:11:ILE:CD1	2:T:85:ILE:HG12	2.27	0.65
1:A:352:GLN:CB	1:A:365:LEU:HD11	2.21	0.65
1:C:417:VAL:HA	1:C:420:ILE:HG22	1.79	0.65
1:N:313:THR:HG22	1:N:314:LEU:H	1.61	0.65
1:N:351:GLN:O	1:N:354:GLU:HG2	1.96	0.65
2:U:43:VAL:HG13	2:U:57:LEU:HD12	1.79	0.65
1:F:65:LYS:O	1:F:69:MET:HG3	1.97	0.65
1:H:197:ARG:HG2	1:H:277:LYS:O	1.96	0.65
1:B:519:CYS:HB3	1:C:38:VAL:HG22	1.78	0.64
1:I:345:ARG:HG2	1:I:345:ARG:HH11	1.63	0.64
1:J:266:THR:HG22	1:J:273:VAL:H	1.62	0.64
1:K:313:THR:HG22	1:K:314:LEU:H	1.62	0.64
1:L:39:VAL:HB	1:M:520:MET:HG2	1.78	0.64
1:L:197:ARG:HG2	1:L:277:LYS:O	1.96	0.64
1:N:77:VAL:HG22	1:N:506:TYR:HB3	1.78	0.64
1:H:84:ALA:O	1:H:498:LYS:HE2	1.97	0.64
1:J:342:ILE:HG23	1:J:372:LEU:HD11	1.80	0.64
1:L:145:ALA:O	1:L:149:THR:HG23	1.96	0.64
2:Q:47:ARG:HB3	2:Q:55:LYS:CG	2.27	0.64
1:B:285:ARG:O	1:B:289:LEU:HG	1.97	0.64
1:K:414:GLY:N	1:K:494:LEU:HA	2.12	0.64
1:L:217:SER:N	1:L:218:PRO:HD3	2.12	0.64
1:L:420:ILE:HG13	1:L:451:LEU:HD22	1.80	0.64
2:P:47:ARG:HD2	2:P:49:LEU:HD12	1.78	0.64
1:A:368:ARG:O	1:A:372:LEU:HG	1.96	0.64
1:M:197:ARG:HG2	1:M:277:LYS:O	1.97	0.64
1:H:69:MET:O	1:H:73:MET:HG3	1.97	0.64
1:A:65:LYS:O	1:A:69:MET:HG3	1.97	0.64
1:B:199:TYR:CZ	1:B:202:PRO:HA	2.32	0.64
1:C:34:LYS:HD2	1:C:458:CYS:SG	2.38	0.64
1:C:249:ILE:HB	1:C:275:ALA:HB2	1.80	0.64
1:D:220:ILE:HG23	1:D:248:LEU:HD12	1.80	0.64
1:G:207:LYS:HB3	1:G:208:PRO:HD3	1.79	0.64
1:I:420:ILE:HG13	1:I:451:LEU:HD22	1.79	0.64
1:B:213:VAL:HB	1:B:325:ILE:HB	1.79	0.64
2:T:5:PRO:HG3	2:T:11:ILE:HG12	1.79	0.64
1:A:57:ALA:O	1:A:75:LYS:HE2	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:365:LEU:HD22	1:D:366:GLN:NE2	2.13	0.64
1:D:518:GLU:HB2	1:E:36:ARG:HG3	1.80	0.64
1:B:353:ILE:HG12	1:B:366:GLN:NE2	2.13	0.63
1:G:285:ARG:O	1:G:289:LEU:HG	1.98	0.63
1:G:346:VAL:HA	1:G:349:ILE:HD12	1.80	0.63
1:J:30:THR:HB	1:J:51:LYS:O	1.98	0.63
1:J:228:SER:O	1:J:257:GLU:HB3	1.98	0.63
2:U:3:ILE:HD13	2:U:11:ILE:HG13	1.80	0.63
1:A:218:PRO:HD2	1:A:320:ALA:O	1.98	0.63
1:B:262:LEU:O	1:B:266:THR:HG23	1.98	0.63
1:F:263:VAL:O	1:F:267:MET:HG2	1.98	0.63
1:L:69:MET:O	1:L:73:MET:HG3	1.99	0.63
1:M:266:THR:HG22	1:M:273:VAL:H	1.63	0.63
2:U:6:LEU:HD13	2:U:7:HIS:NE2	2.14	0.63
1:A:452:ARG:HB2	1:A:462:PRO:HB3	1.81	0.63
1:B:261:THR:HB	2:P:29:GLY:H	1.63	0.63
1:D:346:VAL:O	1:D:349:ILE:HB	1.97	0.63
1:E:207:LYS:HB3	1:E:208:PRO:HD3	1.80	0.63
1:J:161:LEU:HD21	1:J:185:ASP:HB3	1.81	0.63
2:O:18:GLU:OE1	2:O:33:ALA:HB3	1.98	0.63
1:B:31:LEU:HD12	3:B:1:ADP:H5'1	1.81	0.63
1:J:20:VAL:HG23	1:J:74:VAL:HG21	1.79	0.63
2:S:66:ILE:HG23	2:T:76:GLU:OE2	1.98	0.63
1:C:198:GLY:HA3	1:C:327:LYS:O	1.97	0.63
1:E:200:LEU:HD22	1:E:254:VAL:HB	1.79	0.63
1:E:247:LEU:HD21	1:E:317:LEU:HD13	1.81	0.63
1:N:69:MET:O	1:N:73:MET:HG3	1.98	0.63
1:H:63:GLU:HA	1:I:3:ALA:CB	2.28	0.63
1:M:84:ALA:O	1:M:498:LYS:HE2	1.99	0.63
1:N:20:VAL:HG23	1:N:74:VAL:HG21	1.80	0.63
1:B:74:VAL:O	1:B:77:VAL:HG13	1.98	0.63
1:B:218:PRO:HD2	1:B:320:ALA:O	1.98	0.63
1:C:353:ILE:HG12	1:C:366:GLN:NE2	2.13	0.63
1:F:207:LYS:HB3	1:F:208:PRO:HD3	1.81	0.63
1:M:69:MET:O	1:M:73:MET:HG3	1.98	0.63
1:M:214:GLU:HG2	1:M:324:VAL:HG12	1.81	0.63
1:B:215:LEU:O	1:B:322:ARG:HA	1.98	0.63
1:C:218:PRO:HD2	1:C:320:ALA:O	1.99	0.63
1:C:452:ARG:HB2	1:C:462:PRO:HB3	1.81	0.63
1:I:345:ARG:HH11	1:I:345:ARG:CG	2.12	0.63
1:J:420:ILE:CD1	1:J:448:GLU:HA	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:174:VAL:HG21	1:N:194:GLN:HB3	1.80	0.63
1:E:266:THR:HA	1:E:271:VAL:O	1.98	0.62
1:F:204:PHE:CE1	1:F:274:ALA:HB3	2.34	0.62
1:L:85:ALA:HB1	1:L:499:VAL:CG1	2.28	0.62
1:A:204:PHE:CD1	1:A:266:THR:HB	2.34	0.62
1:F:266:THR:HA	1:F:271:VAL:O	1.98	0.62
1:G:77:VAL:CG1	1:G:510:VAL:HG21	2.29	0.62
1:G:221:LEU:HD11	1:G:301:ILE:HD11	1.81	0.62
1:K:403:THR:O	1:K:407:VAL:HG23	1.99	0.62
1:M:239:ALA:HB1	1:M:314:LEU:HD11	1.81	0.62
1:N:199:TYR:CE2	1:N:327:LYS:HA	2.33	0.62
1:N:420:ILE:HD13	1:N:448:GLU:HA	1.80	0.62
1:E:438:VAL:O	1:E:442:VAL:HG23	1.99	0.62
1:G:200:LEU:HD22	1:G:254:VAL:HB	1.81	0.62
1:G:238:GLU:HG3	1:G:239:ALA:N	2.13	0.62
1:H:455:VAL:HG13	1:H:460:GLU:HB2	1.81	0.62
1:I:284:ARG:HD3	1:I:364:LYS:HE3	1.80	0.62
1:C:349:ILE:HG22	1:C:353:ILE:HG13	1.81	0.62
1:D:77:VAL:HG12	1:D:510:VAL:HG21	1.80	0.62
1:M:161:LEU:HD21	1:M:185:ASP:HB3	1.82	0.62
1:B:352:GLN:HB3	1:B:365:LEU:CD1	2.30	0.62
1:G:161:LEU:HD21	1:G:379:ILE:HG23	1.80	0.62
1:I:247:LEU:H	1:I:273:VAL:HG12	1.63	0.62
1:J:130:GLU:HG3	1:J:426:LEU:CD2	2.28	0.62
1:K:197:ARG:HG2	1:K:277:LYS:O	1.98	0.62
2:S:18:GLU:OE1	2:S:33:ALA:HB3	2.00	0.62
1:G:74:VAL:O	1:G:77:VAL:HG13	1.98	0.62
1:J:229:ASN:HD21	1:J:231:ARG:NH1	1.98	0.62
1:K:102:GLU:HB2	1:K:442:VAL:HG13	1.80	0.62
2:R:47:ARG:HB3	2:R:55:LYS:CG	2.29	0.62
1:C:77:VAL:CG1	1:C:510:VAL:HG21	2.28	0.62
1:B:359:ASP:O	1:B:360:TYR:HB2	2.00	0.62
1:G:229:ASN:C	1:G:231:ARG:H	2.03	0.62
1:K:27:VAL:HG11	1:K:93:THR:HG21	1.82	0.62
2:O:2:ASN:C	2:O:3:ILE:HG13	2.20	0.62
1:A:150:ILE:HG21	1:A:494:LEU:O	1.98	0.62
1:C:74:VAL:O	1:C:77:VAL:HG13	1.99	0.62
1:E:77:VAL:HG12	1:E:510:VAL:HG21	1.82	0.62
1:F:518:GLU:HB2	1:G:36:ARG:CB	2.29	0.62
1:H:266:THR:HG22	1:H:273:VAL:H	1.65	0.62
1:J:32:GLY:HA2	1:J:454:ILE:HD12	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:150:ILE:HG21	1:J:494:LEU:HD21	1.82	0.62
2:U:7:HIS:CE1	2:U:48:ILE:HD11	2.35	0.62
2:S:78:ILE:O	2:S:81:GLU:HG2	1.99	0.62
1:E:102:GLU:HB3	1:E:442:VAL:HG13	1.81	0.61
1:E:345:ARG:O	1:E:348:GLN:HG3	1.99	0.61
1:F:228:SER:CB	1:F:255:GLU:HG2	2.30	0.61
1:M:30:THR:HB	1:M:51:LYS:O	2.00	0.61
1:E:305:ILE:HG23	1:F:263:VAL:HG12	1.82	0.61
1:L:26:ALA:O	1:L:29:VAL:HG22	2.00	0.61
1:M:77:VAL:HG22	1:M:506:TYR:HB3	1.82	0.61
1:N:166:MET:HE2	1:N:171:LYS:HA	1.82	0.61
1:A:74:VAL:O	1:A:77:VAL:HG13	2.00	0.61
1:F:519:CYS:SG	1:G:29:VAL:HG21	2.40	0.61
1:J:421:ARG:HA	1:J:421:ARG:HE	1.65	0.61
1:M:313:THR:HG22	1:M:314:LEU:H	1.65	0.61
1:B:111:MET:HE1	1:B:438:VAL:HG11	1.83	0.61
1:C:359:ASP:O	1:C:360:TYR:HB2	1.98	0.61
1:E:61:GLU:HG2	1:E:72:GLN:OE1	1.99	0.61
1:F:368:ARG:O	1:F:372:LEU:HG	2.00	0.61
1:K:263:VAL:O	1:K:267:MET:HG2	2.00	0.61
1:A:206:ASN:HB3	1:A:214:GLU:H	1.66	0.61
1:E:232:GLU:HB3	1:E:310:GLU:OE2	2.00	0.61
1:G:174:VAL:HG21	1:G:367:GLU:HA	1.81	0.61
1:N:217:SER:N	1:N:218:PRO:HD3	2.15	0.61
2:O:66:ILE:HG23	2:P:76:GLU:OE2	1.99	0.61
1:H:518:GLU:HG3	1:N:36:ARG:HG3	1.80	0.61
1:K:458:CYS:SG	1:K:480:ALA:HB1	2.41	0.61
1:D:232:GLU:HA	1:D:234:LEU:HD12	1.80	0.61
1:F:4:LYS:HG3	1:G:59:GLU:O	2.01	0.61
1:M:145:ALA:O	1:M:149:THR:HG23	2.00	0.61
2:S:6:LEU:HD13	2:S:7:HIS:CD2	2.35	0.61
1:A:226:LYS:O	1:A:230:ILE:HD11	2.01	0.61
1:J:181:THR:O	1:K:282:GLY:HA3	2.00	0.61
1:L:165:ALA:HB1	1:L:175:ILE:HD12	1.81	0.61
1:B:346:VAL:HA	1:B:349:ILE:HD12	1.82	0.61
1:J:219:PHE:HB3	1:J:317:LEU:HD23	1.82	0.61
1:J:420:ILE:HG13	1:J:451:LEU:HD22	1.83	0.61
1:L:30:THR:HB	1:L:51:LYS:O	2.01	0.61
1:M:200:LEU:HB3	1:M:259:LEU:HD11	1.81	0.61
1:B:513:LEU:CD1	1:C:388:GLU:HA	2.30	0.61
1:D:231:ARG:NE	1:D:261:THR:HG21	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:199:TYR:CZ	1:G:202:PRO:HA	2.36	0.61
1:H:46:ALA:HB1	1:H:47:PRO:HD2	1.83	0.61
1:I:84:ALA:O	1:I:498:LYS:HE2	2.00	0.61
1:I:197:ARG:HG2	1:I:277:LYS:O	1.99	0.61
1:J:217:SER:N	1:J:218:PRO:HD3	2.16	0.61
1:M:326:ASN:OD1	1:M:329:THR:HB	2.00	0.61
2:O:78:ILE:HD13	2:O:83:VAL:CG2	2.31	0.61
1:J:84:ALA:O	1:J:498:LYS:HE2	2.01	0.60
1:L:20:VAL:HG23	1:L:74:VAL:HG21	1.81	0.60
1:L:459:GLY:HA3	1:M:112:ASN:HD21	1.65	0.60
1:E:239:ALA:HB1	1:E:314:LEU:HD22	1.82	0.60
1:G:183:LEU:CD2	1:G:384:ALA:HA	2.30	0.60
2:T:5:PRO:HB2	2:T:44:GLY:CA	2.31	0.60
1:A:29:VAL:HB	1:G:518:GLU:HG2	1.84	0.60
1:B:19:GLY:HA3	1:B:67:GLU:O	2.02	0.60
1:G:229:ASN:HA	1:G:257:GLU:OE2	2.00	0.60
1:H:176:THR:OG1	1:H:378:VAL:HG12	2.01	0.60
1:I:263:VAL:O	1:I:267:MET:HG2	2.01	0.60
2:O:43:VAL:HG13	2:O:57:LEU:HD12	1.83	0.60
2:P:92:LEU:HB3	2:Q:85:ILE:HG21	1.84	0.60
1:A:383:ALA:HB3	1:A:389:MET:HE2	1.83	0.60
1:D:215:LEU:O	1:D:322:ARG:HA	2.01	0.60
1:G:204:PHE:CE1	1:G:266:THR:HB	2.35	0.60
1:I:69:MET:O	1:I:73:MET:HG3	2.02	0.60
1:L:266:THR:HG22	1:L:273:VAL:H	1.66	0.60
1:A:77:VAL:CG1	1:A:510:VAL:HG21	2.31	0.60
1:D:227:ILE:HA	1:D:230:ILE:HG23	1.83	0.60
1:D:509:SER:HB3	1:E:388:GLU:OE1	2.01	0.60
1:H:19:GLY:HA3	1:H:67:GLU:O	2.02	0.60
1:I:20:VAL:HG23	1:I:74:VAL:HG21	1.83	0.60
1:K:259:LEU:O	1:K:263:VAL:HG23	2.02	0.60
1:L:102:GLU:HB2	1:L:442:VAL:HG13	1.82	0.60
2:U:20:LYS:HG2	2:U:27:LEU:HG	1.81	0.60
1:M:420:ILE:HD13	1:M:448:GLU:HA	1.84	0.60
1:A:31:LEU:HD12	3:A:1:ADP:H5'1	1.84	0.60
1:H:56:VAL:O	1:H:60:ILE:HG12	2.02	0.60
1:I:104:LEU:O	1:I:107:VAL:HG22	2.02	0.60
1:M:122:LYS:HE3	1:M:429:LEU:HD11	1.82	0.60
1:E:4:LYS:HE3	1:F:59:GLU:OE1	2.02	0.60
1:E:199:TYR:CZ	1:E:202:PRO:HA	2.36	0.60
1:E:247:LEU:HB3	1:E:273:VAL:HG13	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:270:ILE:HG23	2:S:25:ILE:HB	1.82	0.60
1:E:348:GLN:HB2	1:F:209:GLU:HG2	1.83	0.60
1:G:201:SER:HB3	1:G:259:LEU:HD22	1.84	0.60
1:I:145:ALA:O	1:I:149:THR:HG23	2.00	0.60
1:I:313:THR:HG22	1:I:314:LEU:H	1.66	0.60
1:K:30:THR:HB	1:K:51:LYS:O	2.01	0.60
1:A:285:ARG:O	1:A:289:LEU:HG	2.02	0.60
1:J:285:ARG:HG2	1:J:285:ARG:HH11	1.67	0.60
1:B:349:ILE:HG21	1:B:369:VAL:CG2	2.32	0.59
1:C:195:PHE:CE1	1:C:330:THR:HB	2.37	0.59
1:C:352:GLN:HB3	1:C:365:LEU:CD1	2.26	0.59
1:F:285:ARG:O	1:F:289:LEU:HG	2.02	0.59
1:G:123:ALA:HB2	1:G:440:ILE:HG23	1.84	0.59
1:H:63:GLU:HG2	1:I:524:LEU:HD11	1.84	0.59
1:K:145:ALA:O	1:K:149:THR:HG23	2.02	0.59
1:K:217:SER:N	1:K:218:PRO:HD3	2.17	0.59
1:A:215:LEU:O	1:A:322:ARG:HA	2.02	0.59
1:F:178:GLU:O	1:F:380:LYS:HA	2.03	0.59
1:H:218:PRO:HG2	1:H:323:VAL:HG12	1.84	0.59
1:K:179:ASP:HA	1:K:389:MET:CE	2.32	0.59
1:A:214:GLU:HA	1:A:323:VAL:O	2.02	0.59
1:E:225:LYS:HE2	1:E:309:LEU:HG	1.85	0.59
1:E:266:THR:HG22	1:E:273:VAL:H	1.66	0.59
1:G:206:ASN:HD22	1:G:215:LEU:HD23	1.66	0.59
1:G:417:VAL:HA	1:G:420:ILE:HG22	1.84	0.59
1:H:271:VAL:HG12	1:H:273:VAL:HG13	1.84	0.59
1:A:30:THR:HG22	1:A:36:ARG:O	2.02	0.59
1:A:302:SER:OG	1:A:305:ILE:HB	2.03	0.59
1:B:193:MET:HB3	1:B:332:ILE:CG2	2.31	0.59
1:B:252:GLU:HA	1:B:285:ARG:NH1	2.17	0.59
1:D:230:ILE:HG13	1:D:309:LEU:HD23	1.84	0.59
1:F:305:ILE:HG12	1:G:263:VAL:HG11	1.84	0.59
1:K:287:ALA:HB1	1:K:368:ARG:CZ	2.32	0.59
1:B:323:VAL:HG12	1:B:332:ILE:HG13	1.85	0.59
1:J:19:GLY:HA3	1:J:67:GLU:O	2.02	0.59
1:D:77:VAL:HG11	1:D:510:VAL:HG21	1.84	0.59
1:G:452:ARG:HB2	1:G:462:PRO:HB3	1.84	0.59
1:L:56:VAL:O	1:L:60:ILE:HG12	2.01	0.59
1:C:39:VAL:HG22	1:C:49:ILE:HG12	1.83	0.59
1:D:207:LYS:HG2	1:D:208:PRO:HD3	1.85	0.59
1:E:509:SER:CB	1:F:384:ALA:HB3	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:77:VAL:CG1	1:F:510:VAL:HG21	2.32	0.59
1:H:145:ALA:O	1:H:149:THR:HG23	2.03	0.59
1:I:466:ALA:O	1:I:470:LYS:HG2	2.01	0.59
1:M:254:VAL:HG12	1:M:259:LEU:HB2	1.85	0.59
2:Q:47:ARG:HH22	2:R:48:ILE:HG13	1.67	0.59
1:A:518:GLU:HB2	1:B:36:ARG:CB	2.32	0.59
1:D:518:GLU:HG2	1:E:29:VAL:HB	1.82	0.59
1:L:138:CYS:SG	1:L:144:ILE:HD13	2.43	0.59
1:L:287:ALA:HB1	1:L:368:ARG:NH2	2.17	0.59
1:A:449:ALA:HA	1:A:452:ARG:HG2	1.85	0.59
1:H:104:LEU:O	1:H:107:VAL:HG22	2.03	0.59
1:I:19:GLY:HA3	1:I:67:GLU:O	2.03	0.59
1:I:34:LYS:HB2	1:I:458:CYS:SG	2.42	0.59
1:I:325:ILE:CD1	1:I:330:THR:HG23	2.33	0.59
1:L:29:VAL:HB	1:L:36:ARG:HB2	1.85	0.59
1:M:56:VAL:O	1:M:60:ILE:HG12	2.03	0.59
1:D:231:ARG:HB2	1:D:257:GLU:OE1	2.03	0.59
1:G:77:VAL:HG12	1:G:510:VAL:HG21	1.83	0.59
1:I:107:VAL:HG11	1:I:515:ILE:HG23	1.83	0.59
1:I:262:LEU:O	1:I:266:THR:HG23	2.02	0.59
1:J:69:MET:HE3	1:J:522:THR:HB	1.83	0.59
1:J:262:LEU:O	1:J:266:THR:HG23	2.03	0.59
1:M:49:ILE:HD13	1:N:513:LEU:HD21	1.85	0.59
1:A:349:ILE:HG21	1:A:369:VAL:HG22	1.84	0.58
1:D:20:VAL:HG13	1:D:74:VAL:HG11	1.83	0.58
1:G:235:PRO:HA	1:G:238:GLU:HG2	1.85	0.58
1:H:217:SER:N	1:H:218:PRO:HD3	2.18	0.58
1:J:169:VAL:HG13	1:J:173:GLY:HA3	1.85	0.58
1:J:285:ARG:HH11	1:J:285:ARG:CG	2.16	0.58
1:N:36:ARG:HD3	1:N:457:ASN:HA	1.85	0.58
2:T:5:PRO:HB2	2:T:44:GLY:HA2	1.84	0.58
1:C:215:LEU:O	1:C:322:ARG:HA	2.03	0.58
1:C:438:VAL:O	1:C:442:VAL:HG23	2.03	0.58
1:D:263:VAL:O	1:D:267:MET:HB2	2.03	0.58
1:F:349:ILE:HG21	1:F:369:VAL:HG22	1.84	0.58
1:H:414:GLY:H	1:H:494:LEU:HA	1.67	0.58
1:I:420:ILE:HD13	1:I:448:GLU:HA	1.83	0.58
1:A:346:VAL:HA	1:A:349:ILE:HD12	1.83	0.58
1:B:349:ILE:O	1:B:352:GLN:HB2	2.03	0.58
1:F:249:ILE:HB	1:F:275:ALA:CB	2.32	0.58
1:G:345:ARG:O	1:G:349:ILE:HG13	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:266:THR:HG22	1:K:273:VAL:H	1.68	0.58
1:M:232:GLU:HB3	1:M:309:LEU:HB2	1.85	0.58
1:N:218:PRO:HG2	1:N:323:VAL:HG12	1.85	0.58
1:N:364:LYS:O	1:N:367:GLU:HG2	2.03	0.58
1:B:31:LEU:CD1	3:B:1:ADP:H5'1	2.34	0.58
1:B:77:VAL:HG12	1:B:510:VAL:HG21	1.85	0.58
1:C:204:PHE:CZ	1:C:274:ALA:HB3	2.38	0.58
1:E:252:GLU:HA	1:E:285:ARG:HH12	1.66	0.58
1:G:266:THR:HA	1:G:271:VAL:O	2.03	0.58
1:L:149:THR:CG2	1:L:156:GLU:HA	2.34	0.58
1:M:262:LEU:O	1:M:266:THR:HG23	2.03	0.58
1:A:306:GLY:HA3	1:B:264:VAL:HG21	1.86	0.58
1:D:218:PRO:HD2	1:D:320:ALA:O	2.04	0.58
1:H:313:THR:HG22	1:H:314:LEU:H	1.67	0.58
1:K:179:ASP:HA	1:K:389:MET:HE3	1.84	0.58
1:K:199:TYR:CE2	1:K:327:LYS:HA	2.38	0.58
1:C:73:MET:SD	1:D:49:ILE:HD11	2.44	0.58
1:F:519:CYS:O	1:G:38:VAL:HA	2.04	0.58
1:H:20:VAL:HG23	1:H:74:VAL:HG21	1.84	0.58
1:K:221:LEU:HD12	1:K:249:ILE:HG23	1.86	0.58
1:A:259:LEU:O	1:A:263:VAL:HG23	2.03	0.58
1:C:247:LEU:HB3	1:C:273:VAL:HG13	1.86	0.58
1:F:31:LEU:HD12	3:F:1:ADP:H5'1	1.85	0.58
1:H:200:LEU:HD23	1:H:254:VAL:HB	1.86	0.58
1:K:84:ALA:O	1:K:498:LYS:HE2	2.03	0.58
1:K:161:LEU:HD21	1:K:185:ASP:HB3	1.84	0.58
1:L:47:PRO:HD3	1:M:72:GLN:HG2	1.86	0.58
1:M:228:SER:O	1:M:257:GLU:HB3	2.03	0.58
2:S:20:LYS:NZ	2:S:27:LEU:HD11	2.19	0.58
1:B:57:ALA:O	1:B:75:LYS:HE2	2.03	0.58
1:C:252:GLU:HG3	1:C:285:ARG:HH11	1.67	0.58
1:E:102:GLU:CB	1:E:442:VAL:HG13	2.33	0.58
1:L:84:ALA:O	1:L:498:LYS:HE2	2.04	0.58
1:M:225:LYS:HD3	1:M:303:GLU:CG	2.32	0.58
1:M:403:THR:O	1:M:407:VAL:HG23	2.04	0.58
2:P:58:ASP:HB3	2:Q:6:LEU:HD21	1.86	0.58
2:R:78:ILE:HD13	2:R:83:VAL:HG21	1.85	0.58
1:E:57:ALA:O	1:E:75:LYS:HE2	2.03	0.58
1:E:85:ALA:O	1:E:401:HIS:HB3	2.03	0.58
1:E:206:ASN:HB3	1:E:214:GLU:H	1.68	0.58
1:E:213:VAL:HB	1:E:325:ILE:HB	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:85:ALA:O	1:F:401:HIS:HB3	2.04	0.58
1:G:231:ARG:HB2	1:G:257:GLU:OE1	2.04	0.58
1:H:63:GLU:HA	1:I:3:ALA:HB1	1.85	0.58
1:I:199:TYR:HB3	1:I:325:ILE:HG21	1.86	0.58
1:K:197:ARG:HE	1:K:277:LYS:CB	2.17	0.58
1:K:466:ALA:O	1:K:470:LYS:HG2	2.03	0.58
2:P:20:LYS:HG3	2:P:28:THR:O	2.03	0.58
2:R:66:ILE:HG23	2:S:76:GLU:OE1	2.04	0.58
2:S:5:PRO:HD3	2:S:42:ALA:HB1	1.86	0.58
2:S:14:ARG:CD	2:S:34:LYS:HE2	2.33	0.58
1:F:349:ILE:HG21	1:F:369:VAL:CG2	2.34	0.58
1:H:348:GLN:O	1:H:352:GLN:HG3	2.03	0.58
1:I:164:GLU:HG3	1:I:187:LEU:HD13	1.86	0.58
1:I:230:ILE:HD11	1:I:261:THR:HG21	1.86	0.58
1:J:217:SER:HA	1:J:320:ALA:O	2.04	0.58
2:R:20:LYS:HD2	2:R:27:LEU:HD23	1.86	0.58
2:T:20:LYS:HD2	2:T:27:LEU:HG	1.86	0.58
1:B:452:ARG:HB2	1:B:462:PRO:HB3	1.86	0.57
1:C:252:GLU:HG3	1:C:285:ARG:NH1	2.18	0.57
1:D:368:ARG:O	1:D:372:LEU:HG	2.03	0.57
1:F:102:GLU:CB	1:F:442:VAL:HG13	2.34	0.57
1:H:217:SER:HA	1:H:320:ALA:O	2.04	0.57
1:J:385:THR:HG23	1:J:388:GLU:H	1.69	0.57
2:O:65:VAL:HG12	2:O:94:ILE:HG12	1.85	0.57
2:Q:3:ILE:HD13	2:Q:11:ILE:HG21	1.84	0.57
1:A:231:ARG:HB3	1:A:257:GLU:OE1	2.04	0.57
1:F:20:VAL:HG13	1:F:74:VAL:HG11	1.86	0.57
1:H:518:GLU:CG	1:N:36:ARG:HG3	2.34	0.57
2:R:78:ILE:HD13	2:R:83:VAL:CG2	2.34	0.57
1:C:302:SER:HB3	1:C:305:ILE:CD1	2.34	0.57
1:E:100:ILE:HD13	1:E:514:MET:SD	2.44	0.57
1:F:247:LEU:HD12	1:F:249:ILE:HG13	1.85	0.57
1:N:270:ILE:HG22	1:N:271:VAL:HG23	1.86	0.57
1:A:102:GLU:HB2	1:A:442:VAL:HG13	1.85	0.57
1:F:247:LEU:HD21	1:F:317:LEU:HD13	1.85	0.57
1:I:69:MET:HE3	1:I:522:THR:HB	1.85	0.57
1:H:49:ILE:HD11	1:I:73:MET:HE3	1.87	0.57
1:H:420:ILE:CD1	1:H:448:GLU:HA	2.34	0.57
1:I:31:LEU:HG	1:I:454:ILE:HD11	1.87	0.57
1:M:131:LEU:HD12	1:M:422:VAL:HG11	1.84	0.57
1:M:421:ARG:HA	1:M:421:ARG:NE	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:LYS:CB	1:A:208:PRO:HD3	2.35	0.57
1:C:509:SER:CB	1:D:384:ALA:HB3	2.32	0.57
1:E:4:LYS:HG2	1:E:523:ASP:OD1	2.03	0.57
1:J:149:THR:CG2	1:J:156:GLU:HA	2.34	0.57
1:M:30:THR:HG22	1:M:36:ARG:O	2.04	0.57
1:M:138:CYS:SG	1:M:144:ILE:HD13	2.45	0.57
1:B:204:PHE:CE1	1:B:266:THR:HB	2.40	0.57
1:I:414:GLY:H	1:I:494:LEU:HA	1.69	0.57
1:K:228:SER:O	1:K:257:GLU:HB3	2.04	0.57
1:N:217:SER:HA	1:N:320:ALA:O	2.05	0.57
1:A:266:THR:HG22	1:A:273:VAL:H	1.70	0.57
1:H:282:GLY:HA3	1:N:181:THR:O	2.05	0.57
1:J:509:SER:O	1:J:513:LEU:HD13	2.04	0.57
1:K:178:GLU:OE2	1:K:333:ILE:HG21	2.05	0.57
2:P:60:LYS:O	2:P:63:ASP:HB2	2.04	0.57
2:R:14:ARG:NH2	2:R:84:LEU:HD21	2.20	0.57
1:C:147:VAL:HG23	1:C:403:THR:HG22	1.85	0.57
1:C:193:MET:SD	1:C:371:LYS:HB3	2.45	0.57
1:D:58:ARG:HA	1:D:75:LYS:HD2	1.87	0.57
1:H:130:GLU:HG3	1:H:426:LEU:CD2	2.34	0.57
1:N:271:VAL:HG12	1:N:273:VAL:HG13	1.86	0.57
1:N:420:ILE:CD1	1:N:448:GLU:HA	2.35	0.57
2:S:37:ARG:HH21	2:T:78:ILE:HD12	1.70	0.57
1:A:199:TYR:CZ	1:A:202:PRO:HA	2.40	0.57
1:B:237:LEU:HD22	2:P:26:VAL:CG2	2.35	0.57
1:D:73:MET:CE	1:E:49:ILE:HD11	2.35	0.57
1:E:150:ILE:HG21	1:E:494:LEU:O	2.03	0.57
1:J:403:THR:O	1:J:407:VAL:HG23	2.05	0.57
1:K:472:GLY:HA3	1:K:476:TYR:CD2	2.39	0.57
1:B:117:LYS:HG2	1:B:512:GLY:O	2.04	0.56
1:G:95:LEU:O	1:G:99:ILE:HG12	2.05	0.56
2:T:17:VAL:HG13	2:T:34:LYS:HA	1.87	0.56
2:T:92:LEU:HB3	2:U:85:ILE:HG21	1.85	0.56
1:A:193:MET:SD	1:A:371:LYS:HG2	2.45	0.56
1:A:419:LEU:HD11	1:A:500:THR:HG23	1.87	0.56
1:D:519:CYS:O	1:E:38:VAL:HA	2.05	0.56
1:F:100:ILE:HD13	1:F:514:MET:SD	2.45	0.56
1:H:150:ILE:HG21	1:H:494:LEU:CD2	2.35	0.56
1:H:447:MET:O	1:H:450:PRO:HD2	2.04	0.56
1:J:414:GLY:H	1:J:494:LEU:HA	1.68	0.56
1:M:466:ALA:O	1:M:470:LYS:HG2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:11:ILE:HD12	2:T:85:ILE:HG12	1.86	0.56
1:A:209:GLU:HB2	1:G:351:GLN:HG3	1.87	0.56
1:A:305:ILE:O	1:A:307:MET:N	2.36	0.56
1:B:76:GLU:OE1	1:C:386:GLU:HB3	2.06	0.56
1:B:228:SER:HA	1:B:255:GLU:HB2	1.87	0.56
1:E:225:LYS:HB3	1:E:303:GLU:OE1	2.05	0.56
1:F:519:CYS:HB2	1:G:38:VAL:HG22	1.85	0.56
1:G:239:ALA:HB1	1:G:314:LEU:HD23	1.87	0.56
1:I:420:ILE:CD1	1:I:448:GLU:HA	2.36	0.56
1:K:414:GLY:H	1:K:494:LEU:HA	1.71	0.56
1:L:49:ILE:HD11	1:M:73:MET:CE	2.31	0.56
1:L:262:LEU:O	1:L:266:THR:HG23	2.05	0.56
1:N:282:GLY:O	1:N:285:ARG:HG2	2.05	0.56
2:R:17:VAL:HG22	2:R:35:SER:H	1.71	0.56
1:A:349:ILE:HG21	1:A:369:VAL:CG2	2.35	0.56
1:B:65:LYS:O	1:B:69:MET:HG3	2.05	0.56
1:D:305:ILE:HD11	1:E:203:TYR:CD1	2.40	0.56
1:F:518:GLU:HB2	1:G:36:ARG:HD2	1.88	0.56
1:I:30:THR:HB	1:I:51:LYS:O	2.05	0.56
1:K:41:ASP:HB2	1:L:69:MET:HE1	1.86	0.56
1:K:326:ASN:OD1	1:K:329:THR:HB	2.05	0.56
1:L:130:GLU:HG3	1:L:426:LEU:CD2	2.36	0.56
1:N:287:ALA:HB1	1:N:368:ARG:CZ	2.35	0.56
1:A:36:ARG:CG	1:G:518:GLU:HB2	2.36	0.56
1:E:206:ASN:HD22	1:E:215:LEU:HD23	1.70	0.56
1:F:198:GLY:HA3	1:F:327:LYS:O	2.06	0.56
1:G:80:LYS:HD2	1:G:506:TYR:CE1	2.41	0.56
1:K:69:MET:O	1:K:73:MET:HG3	2.06	0.56
1:L:239:ALA:HB1	1:L:314:LEU:HD11	1.87	0.56
2:Q:5:PRO:HD3	2:Q:42:ALA:HB1	1.87	0.56
1:A:227:ILE:O	1:A:255:GLU:HG2	2.06	0.56
1:C:368:ARG:O	1:C:372:LEU:HG	2.06	0.56
1:F:510:VAL:HG13	1:G:385:THR:HG21	1.87	0.56
1:G:150:ILE:HG21	1:G:494:LEU:O	2.06	0.56
1:G:195:PHE:CE1	1:G:330:THR:HB	2.40	0.56
1:G:368:ARG:O	1:G:372:LEU:HG	2.06	0.56
1:J:241:ALA:HB2	1:J:271:VAL:HG22	1.87	0.56
1:L:426:LEU:HD12	1:L:444:LEU:HD21	1.87	0.56
1:M:247:LEU:HB3	1:M:273:VAL:HG11	1.88	0.56
1:E:197:ARG:HH21	1:E:279:PRO:HD3	1.71	0.56
1:E:217:SER:HA	1:E:320:ALA:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:112:ASN:CG	1:G:34:LYS:HG2	2.26	0.56
1:F:346:VAL:O	1:F:349:ILE:HB	2.05	0.56
1:F:449:ALA:HA	1:F:452:ARG:HG2	1.87	0.56
1:H:3:ALA:HB1	1:N:63:GLU:HA	1.86	0.56
1:I:131:LEU:HD12	1:I:422:VAL:HG11	1.88	0.56
1:I:214:GLU:HG2	1:I:324:VAL:HG12	1.87	0.56
1:K:232:GLU:HB3	1:K:309:LEU:HB2	1.87	0.56
1:N:414:GLY:H	1:N:494:LEU:HA	1.70	0.56
1:B:114:MET:HA	1:B:117:LYS:HE3	1.87	0.56
1:B:120:ILE:O	1:B:124:VAL:HG23	2.06	0.56
1:C:4:LYS:HG3	1:D:59:GLU:O	2.05	0.56
1:E:279:PRO:HD2	1:E:285:ARG:HB2	1.88	0.56
1:I:421:ARG:NE	1:I:421:ARG:HA	2.20	0.56
1:M:437:ASN:O	1:M:441:LYS:HD3	2.06	0.56
1:B:77:VAL:HG11	1:B:510:VAL:HG21	1.88	0.56
1:B:112:ASN:ND2	1:C:34:LYS:HG2	2.21	0.56
1:B:113:PRO:HB2	1:B:516:THR:HA	1.88	0.56
1:C:102:GLU:CB	1:C:442:VAL:HG13	2.35	0.56
1:F:65:LYS:HB3	1:F:522:THR:OG1	2.06	0.56
1:F:345:ARG:O	1:F:348:GLN:HG3	2.04	0.56
1:J:213:VAL:O	1:J:324:VAL:HA	2.06	0.56
1:J:225:LYS:HD3	1:J:303:GLU:CG	2.35	0.56
2:Q:55:LYS:HD3	2:R:51:ASN:CB	2.36	0.56
1:D:266:THR:CG2	1:D:273:VAL:H	2.19	0.56
1:C:225:LYS:HB3	1:C:303:GLU:OE1	2.06	0.55
1:D:305:ILE:HD11	1:E:203:TYR:CE1	2.41	0.55
1:E:21:ASN:HD22	1:E:97:GLN:HE22	1.53	0.55
1:E:305:ILE:HG12	1:F:263:VAL:HG11	1.87	0.55
1:H:69:MET:CE	1:H:522:THR:HB	2.34	0.55
1:I:288:MET:HA	1:I:288:MET:HE3	1.87	0.55
1:N:466:ALA:O	1:N:470:LYS:HG2	2.06	0.55
2:Q:15:LYS:HE2	2:Q:37:ARG:HB3	1.87	0.55
2:U:52:GLY:C	2:U:53:GLU:HG3	2.27	0.55
1:A:6:VAL:HG12	1:A:521:VAL:HG22	1.87	0.55
1:D:306:GLY:HA3	1:E:264:VAL:HG21	1.88	0.55
1:E:147:VAL:HG23	1:E:403:THR:HG22	1.87	0.55
1:G:31:LEU:CD1	3:G:1:ADP:H5'1	2.37	0.55
1:N:241:ALA:HB2	1:N:271:VAL:CG2	2.36	0.55
2:O:12:VAL:HG12	2:O:40:VAL:HA	1.87	0.55
2:U:3:ILE:CG1	2:U:78:ILE:HD13	2.35	0.55
1:B:252:GLU:HG3	1:B:285:ARG:HH11	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:349:ILE:O	1:C:352:GLN:HB2	2.06	0.55
1:K:157:THR:O	1:K:161:LEU:HD12	2.06	0.55
1:L:104:LEU:O	1:L:107:VAL:HG22	2.07	0.55
1:L:178:GLU:OE2	1:L:322:ARG:HD3	2.06	0.55
2:O:2:ASN:O	2:O:3:ILE:HG13	2.06	0.55
1:C:213:VAL:HB	1:C:325:ILE:HB	1.88	0.55
1:E:270:ILE:HD13	2:S:25:ILE:O	2.07	0.55
1:F:228:SER:CA	1:F:255:GLU:HG2	2.37	0.55
1:G:234:LEU:N	1:G:235:PRO:HD2	2.22	0.55
1:N:313:THR:HG22	1:N:314:LEU:N	2.21	0.55
1:D:265:ASN:O	1:D:270:ILE:HB	2.07	0.55
1:E:262:LEU:O	1:E:266:THR:HG23	2.06	0.55
1:F:452:ARG:HB2	1:F:462:PRO:HB3	1.89	0.55
1:H:232:GLU:HB3	1:H:309:LEU:HB2	1.88	0.55
1:L:414:GLY:H	1:L:494:LEU:HA	1.72	0.55
1:N:232:GLU:HB3	1:N:309:LEU:HB2	1.88	0.55
1:D:288:MET:HA	1:D:291:ASP:OD1	2.07	0.55
1:E:518:GLU:HG3	1:F:36:ARG:HB2	1.89	0.55
1:H:199:TYR:CE2	1:H:327:LYS:HA	2.41	0.55
1:I:17:LEU:HB2	1:I:104:LEU:CD2	2.36	0.55
1:J:269:GLY:O	1:K:257:GLU:HG3	2.07	0.55
2:S:73:VAL:HG11	2:S:84:LEU:HD23	1.89	0.55
2:U:7:HIS:CG	2:U:48:ILE:HD11	2.41	0.55
1:A:513:LEU:HD11	1:B:388:GLU:CA	2.37	0.55
1:A:521:VAL:O	1:B:41:ASP:HB2	2.06	0.55
1:B:31:LEU:HD22	1:B:94:VAL:HG21	1.89	0.55
1:C:111:MET:CE	1:C:438:VAL:HG21	2.37	0.55
1:D:231:ARG:HE	1:D:261:THR:HG21	1.70	0.55
1:E:215:LEU:O	1:E:322:ARG:HA	2.07	0.55
1:F:112:ASN:ND2	1:G:34:LYS:HG2	2.21	0.55
1:G:19:GLY:HA3	1:G:67:GLU:O	2.06	0.55
1:G:442:VAL:HA	1:G:445:ARG:NE	2.21	0.55
1:I:49:ILE:HD11	1:J:73:MET:CE	2.35	0.55
1:J:28:LYS:HD3	1:J:453:GLN:OE1	2.06	0.55
1:L:420:ILE:CD1	1:L:448:GLU:HA	2.35	0.55
1:N:30:THR:HB	1:N:51:LYS:O	2.06	0.55
1:C:493:ILE:HD13	3:C:1:ADP:C2	2.42	0.55
1:E:349:ILE:HG21	1:E:369:VAL:HG22	1.89	0.55
1:H:221:LEU:HD12	1:H:249:ILE:HG23	1.87	0.55
1:J:31:LEU:HG	1:J:454:ILE:HD11	1.88	0.55
1:L:381:VAL:HB	1:L:389:MET:CE	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:197:ARG:HG2	1:N:277:LYS:O	2.07	0.55
1:B:2:ALA:O	1:C:61:GLU:HB3	2.07	0.55
1:C:40:LEU:HD13	1:C:59:GLU:HG3	1.89	0.55
1:H:229:ASN:HB3	1:H:232:GLU:OE1	2.06	0.55
2:O:20:LYS:HD3	2:O:28:THR:O	2.06	0.55
1:A:522:THR:HA	1:B:41:ASP:CB	2.37	0.55
1:C:85:ALA:O	1:C:401:HIS:HB3	2.08	0.55
1:D:111:MET:CE	1:D:438:VAL:HG21	2.37	0.55
1:F:165:ALA:O	1:F:169:VAL:HG22	2.07	0.55
1:F:438:VAL:O	1:F:442:VAL:HG23	2.07	0.55
1:G:449:ALA:HA	1:G:452:ARG:HG2	1.88	0.55
1:K:39:VAL:HG22	1:K:49:ILE:HD13	1.89	0.55
1:B:264:VAL:HG13	1:B:268:ARG:HH11	1.73	0.54
1:B:517:THR:HG21	1:B:520:MET:SD	2.47	0.54
1:C:345:ARG:O	1:C:349:ILE:HG13	2.06	0.54
1:E:234:LEU:HD23	2:S:22:ALA:HB1	1.88	0.54
1:F:124:VAL:HG21	1:F:508:ALA:CB	2.38	0.54
1:J:215:LEU:HB3	1:J:218:PRO:HG3	1.88	0.54
1:N:259:LEU:O	1:N:263:VAL:HG23	2.07	0.54
1:A:213:VAL:HB	1:A:325:ILE:HB	1.89	0.54
1:B:198:GLY:HA3	1:B:327:LYS:O	2.07	0.54
1:B:234:LEU:O	1:B:238:GLU:HB3	2.06	0.54
1:C:102:GLU:HB2	1:C:442:VAL:HG13	1.88	0.54
1:F:521:VAL:HG21	1:G:40:LEU:HD23	1.88	0.54
1:L:284:ARG:HH11	1:L:284:ARG:H	1.55	0.54
1:M:23:LEU:HB2	1:M:71:ALA:HB1	1.89	0.54
1:M:282:GLY:O	1:M:285:ARG:HG2	2.06	0.54
1:N:155:ASP:HB2	1:N:395:ARG:NH2	2.22	0.54
1:N:237:LEU:O	1:N:240:VAL:HG22	2.07	0.54
2:O:74:LYS:HB2	2:O:85:ILE:HB	1.89	0.54
1:A:234:LEU:N	1:A:235:PRO:HD2	2.23	0.54
1:A:326:ASN:OD1	1:A:329:THR:HB	2.08	0.54
1:A:518:GLU:HB2	1:B:36:ARG:HB3	1.88	0.54
1:C:228:SER:HA	1:C:255:GLU:HB2	1.89	0.54
1:E:348:GLN:CB	1:F:209:GLU:HG2	2.37	0.54
1:E:458:CYS:SG	1:E:480:ALA:HB1	2.47	0.54
1:H:214:GLU:HG2	1:H:324:VAL:CG1	2.37	0.54
1:N:150:ILE:HG21	1:N:494:LEU:CD2	2.37	0.54
1:N:166:MET:CE	1:N:407:VAL:HG21	2.37	0.54
1:A:209:GLU:O	1:A:210:THR:HB	2.08	0.54
1:A:509:SER:HB2	1:B:384:ALA:HB3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:PHE:O	1:B:329:THR:HG23	2.07	0.54
1:C:183:LEU:O	1:C:382:GLY:HA3	2.06	0.54
1:F:37:ASN:OD1	1:F:51:LYS:HB2	2.07	0.54
1:K:455:VAL:HG13	1:K:460:GLU:HB2	1.89	0.54
1:D:102:GLU:CB	1:D:442:VAL:HG13	2.37	0.54
1:F:69:MET:SD	1:F:522:THR:HB	2.47	0.54
1:G:7:LYS:O	1:G:519:CYS:HA	2.07	0.54
1:G:65:LYS:O	1:G:69:MET:HG3	2.07	0.54
1:G:213:VAL:HB	1:G:325:ILE:HB	1.89	0.54
1:L:381:VAL:O	1:L:389:MET:HE2	2.08	0.54
1:M:27:VAL:HG11	1:M:93:THR:HG21	1.88	0.54
1:M:215:LEU:HB3	1:M:218:PRO:HG3	1.88	0.54
1:B:419:LEU:HD11	1:B:500:THR:HG23	1.87	0.54
1:C:262:LEU:HD11	1:C:273:VAL:HB	1.90	0.54
1:D:40:LEU:HD13	1:D:59:GLU:HG3	1.89	0.54
1:D:265:ASN:HA	1:D:270:ILE:HD12	1.89	0.54
1:D:414:GLY:O	1:D:417:VAL:HG12	2.07	0.54
1:E:4:LYS:HE2	1:F:59:GLU:O	2.07	0.54
1:K:426:LEU:HD12	1:K:444:LEU:HD21	1.90	0.54
1:N:174:VAL:CG2	1:N:194:GLN:HB3	2.37	0.54
2:Q:5:PRO:HG3	2:Q:42:ALA:HB1	1.89	0.54
2:R:53:GLU:HB3	2:S:51:ASN:HD22	1.72	0.54
1:A:199:TYR:CE1	1:A:202:PRO:HA	2.42	0.54
1:A:264:VAL:CG1	1:G:306:GLY:H	2.20	0.54
1:D:187:LEU:HD13	1:D:379:ILE:HG12	1.89	0.54
1:D:207:LYS:CG	1:D:208:PRO:HD3	2.37	0.54
1:F:237:LEU:HD22	2:T:26:VAL:HG11	1.89	0.54
1:F:305:ILE:HG23	1:G:263:VAL:HG12	1.89	0.54
1:G:302:SER:OG	1:G:305:ILE:HB	2.07	0.54
1:H:3:ALA:CB	1:N:63:GLU:HA	2.38	0.54
1:K:421:ARG:HD2	1:K:474:GLY:O	2.08	0.54
1:L:215:LEU:HB3	1:L:218:PRO:HG3	1.88	0.54
1:M:197:ARG:HE	1:M:277:LYS:HZ3	1.54	0.54
2:T:17:VAL:HG22	2:T:35:SER:H	1.73	0.54
1:A:19:GLY:HA3	1:A:67:GLU:O	2.07	0.54
1:A:264:VAL:HG13	1:G:306:GLY:H	1.72	0.54
1:C:230:ILE:HG23	1:C:309:LEU:HD21	1.90	0.54
1:F:206:ASN:HB2	1:F:213:VAL:HG13	1.89	0.54
1:F:252:GLU:HA	1:F:285:ARG:HH11	1.72	0.54
1:G:198:GLY:HA3	1:G:327:LYS:O	2.07	0.54
1:L:102:GLU:HA	1:L:102:GLU:OE1	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:313:THR:HG22	1:L:314:LEU:H	1.72	0.54
1:L:421:ARG:HD2	1:L:474:GLY:O	2.06	0.54
1:A:36:ARG:HG2	1:G:518:GLU:HB2	1.88	0.54
1:A:80:LYS:HD2	1:A:506:TYR:CZ	2.43	0.54
1:D:235:PRO:HA	1:D:238:GLU:HG2	1.90	0.54
1:D:262:LEU:O	1:D:266:THR:HG23	2.08	0.54
1:D:345:ARG:O	1:D:349:ILE:HG13	2.07	0.54
1:E:19:GLY:HA3	1:E:67:GLU:O	2.08	0.54
1:E:220:ILE:HD13	1:E:296:THR:HG21	1.90	0.54
1:F:102:GLU:HB3	1:F:442:VAL:HG13	1.89	0.54
1:G:383:ALA:HB3	1:G:389:MET:HB2	1.90	0.54
1:J:267:MET:C	1:J:268:ARG:HG2	2.27	0.54
1:L:265:ASN:O	1:L:269:GLY:HA3	2.08	0.54
1:M:199:TYR:CE1	1:M:202:PRO:HA	2.42	0.54
1:M:218:PRO:HG2	1:M:323:VAL:HG12	1.89	0.54
2:S:48:ILE:O	2:S:48:ILE:HG22	2.08	0.54
1:B:291:ASP:HB2	1:B:372:LEU:HD21	1.89	0.54
1:E:114:MET:HG3	1:E:118:ARG:NH1	2.23	0.54
1:E:238:GLU:HB2	2:S:24:GLY:N	2.22	0.54
1:G:218:PRO:HD2	1:G:320:ALA:O	2.08	0.54
1:H:287:ALA:HB1	1:H:368:ARG:CZ	2.38	0.54
1:L:254:VAL:HG12	1:L:259:LEU:HB2	1.90	0.54
1:L:381:VAL:HB	1:L:389:MET:HE1	1.89	0.54
1:M:247:LEU:HB3	1:M:273:VAL:CG1	2.38	0.54
1:D:21:ASN:HD22	1:D:97:GLN:HE22	1.56	0.53
1:D:207:LYS:HG2	1:D:208:PRO:CD	2.37	0.53
1:E:252:GLU:HG3	1:E:285:ARG:HH11	1.72	0.53
1:H:49:ILE:HD11	1:I:73:MET:CE	2.38	0.53
1:I:46:ALA:CB	1:J:72:GLN:HB3	2.38	0.53
1:I:271:VAL:HG12	1:I:273:VAL:HG13	1.90	0.53
1:K:194:GLN:HG3	1:K:331:THR:HB	1.90	0.53
1:L:496:PRO:HB2	1:L:499:VAL:HG13	1.90	0.53
1:M:151:SER:OG	1:M:399:ALA:HA	2.07	0.53
2:Q:47:ARG:HG2	2:Q:49:LEU:H	1.72	0.53
2:S:8:ASP:HA	2:S:57:LEU:HD21	1.90	0.53
1:B:33:PRO:HA	1:B:153:ASN:ND2	2.23	0.53
1:C:206:ASN:HB3	1:C:214:GLU:H	1.73	0.53
1:G:231:ARG:NE	1:G:234:LEU:HD21	2.23	0.53
1:I:217:SER:HA	1:I:320:ALA:O	2.08	0.53
1:J:225:LYS:HD3	1:J:303:GLU:CD	2.29	0.53
1:K:342:ILE:HG23	1:K:372:LEU:HD11	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:LYS:HE3	1:A:513:LEU:HD23	1.90	0.53
1:A:208:PRO:HB2	1:A:212:ALA:HB3	1.89	0.53
1:D:227:ILE:HA	1:D:230:ILE:CG2	2.38	0.53
1:F:114:MET:HG3	1:F:118:ARG:NH1	2.23	0.53
1:G:195:PHE:CE1	1:G:197:ARG:HB2	2.44	0.53
1:H:265:ASN:O	1:H:269:GLY:HA3	2.09	0.53
1:J:254:VAL:HG12	1:J:259:LEU:HB2	1.91	0.53
1:K:383:ALA:HB3	1:K:389:MET:HB2	1.90	0.53
1:N:262:LEU:O	1:N:266:THR:HG23	2.09	0.53
1:N:403:THR:O	1:N:407:VAL:HG23	2.09	0.53
1:D:238:GLU:HG3	1:D:239:ALA:N	2.23	0.53
1:F:150:ILE:HG21	1:F:494:LEU:O	2.08	0.53
1:F:199:TYR:O	1:F:199:TYR:HD1	1.91	0.53
1:G:252:GLU:HG3	1:G:285:ARG:HH11	1.73	0.53
1:H:294:THR:HG21	1:H:345:ARG:HB2	1.91	0.53
1:I:403:THR:O	1:I:407:VAL:HG23	2.09	0.53
1:K:10:ASN:O	1:K:14:VAL:HG22	2.08	0.53
1:L:179:ASP:HA	1:L:389:MET:SD	2.48	0.53
1:A:513:LEU:HD11	1:B:388:GLU:HA	1.90	0.53
1:C:249:ILE:HB	1:C:275:ALA:CB	2.37	0.53
1:E:124:VAL:HG13	1:E:504:LEU:CD1	2.38	0.53
1:E:175:ILE:H	1:E:404:ARG:HH22	1.56	0.53
1:E:349:ILE:HG21	1:E:369:VAL:CG2	2.39	0.53
1:E:461:GLU:HB2	1:E:464:VAL:HB	1.91	0.53
1:I:34:LYS:HD3	1:J:114:MET:SD	2.48	0.53
1:I:199:TYR:HB3	1:I:325:ILE:CG2	2.38	0.53
1:L:175:ILE:CD1	1:L:377:ALA:HB3	2.39	0.53
1:A:222:LEU:HD13	1:A:293:ALA:HB2	1.91	0.53
1:C:262:LEU:O	1:C:266:THR:HG23	2.08	0.53
1:C:262:LEU:HD21	1:C:274:ALA:HA	1.90	0.53
1:F:276:VAL:HG21	1:F:330:THR:HG21	1.89	0.53
1:G:39:VAL:O	1:G:40:LEU:HB2	2.08	0.53
1:H:219:PHE:HB3	1:H:317:LEU:HD23	1.91	0.53
1:H:437:ASN:O	1:H:441:LYS:HD2	2.09	0.53
1:J:353:ILE:HD11	1:J:369:VAL:HG21	1.90	0.53
1:J:443:ALA:O	1:J:447:MET:HG3	2.09	0.53
1:L:175:ILE:HD13	1:L:377:ALA:HB3	1.90	0.53
1:L:225:LYS:HD3	1:L:303:GLU:CG	2.39	0.53
1:M:400:LEU:HD21	1:M:404:ARG:HE	1.74	0.53
2:S:17:VAL:HG13	2:S:34:LYS:HA	1.90	0.53
1:B:521:VAL:HB	1:C:40:LEU:HD23	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:ARG:HG2	1:D:277:LYS:O	2.09	0.53
1:F:147:VAL:HG12	1:F:494:LEU:HB2	1.91	0.53
1:F:493:ILE:HD13	3:F:1:ADP:C2	2.43	0.53
1:G:206:ASN:HB3	1:G:214:GLU:H	1.73	0.53
1:I:161:LEU:HA	1:I:164:GLU:HG2	1.91	0.53
1:L:389:MET:SD	1:L:389:MET:C	2.87	0.53
2:P:3:ILE:CG1	2:P:78:ILE:HD13	2.37	0.53
1:A:305:ILE:HG12	1:B:263:VAL:HG11	1.90	0.53
1:B:230:ILE:HG23	1:B:309:LEU:HD23	1.91	0.53
1:E:261:THR:HG22	2:S:29:GLY:H	1.74	0.53
1:E:305:ILE:HG23	1:F:263:VAL:CG1	2.38	0.53
1:F:228:SER:HA	1:F:255:GLU:HG2	1.89	0.53
1:L:200:LEU:HD11	1:L:277:LYS:HG3	1.91	0.53
1:L:293:ALA:HB2	1:L:300:VAL:HG13	1.90	0.53
1:M:66:PHE:CZ	1:M:522:THR:HG22	2.44	0.53
1:A:65:LYS:HB3	1:A:522:THR:OG1	2.09	0.53
1:A:210:THR:O	1:A:210:THR:HG22	2.08	0.53
1:C:111:MET:SD	1:C:438:VAL:HG11	2.49	0.53
2:U:11:ILE:HD12	2:U:85:ILE:HG12	1.91	0.53
1:B:345:ARG:O	1:B:348:GLN:HG3	2.09	0.53
1:C:100:ILE:HD11	1:C:514:MET:HE3	1.91	0.53
1:E:232:GLU:HA	1:E:234:LEU:HD13	1.90	0.53
1:F:219:PHE:HB2	1:F:247:LEU:HD22	1.91	0.53
1:I:39:VAL:CG1	1:I:47:PRO:HB2	2.38	0.53
1:I:46:ALA:HB2	1:J:72:GLN:HB3	1.91	0.53
1:I:295:LEU:HD23	1:I:332:ILE:HD11	1.91	0.53
1:K:227:ILE:CD1	1:K:309:LEU:HD11	2.39	0.53
1:M:17:LEU:HB2	1:M:104:LEU:HD23	1.91	0.53
2:Q:47:ARG:HB3	2:Q:55:LYS:HG3	1.90	0.53
2:R:6:LEU:HD13	2:R:7:HIS:ND1	2.24	0.53
2:R:43:VAL:HG13	2:R:57:LEU:HD12	1.90	0.53
2:S:37:ARG:NH2	2:T:78:ILE:HA	2.24	0.53
1:B:4:LYS:HD2	1:B:521:VAL:HG12	1.91	0.52
1:C:199:TYR:O	1:C:199:TYR:HD1	1.92	0.52
1:C:461:GLU:O	1:C:464:VAL:HG12	2.09	0.52
1:E:128:VAL:HG21	1:E:505:GLN:HE21	1.74	0.52
1:H:517:THR:HA	1:N:37:ASN:HD22	1.74	0.52
1:K:199:TYR:CE2	1:K:205:ILE:HD11	2.45	0.52
1:M:421:ARG:O	1:M:425:LYS:HG2	2.09	0.52
2:U:3:ILE:HG12	2:U:78:ILE:HD13	1.92	0.52
1:A:238:GLU:HG3	1:A:239:ALA:N	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:106:ALA:HB1	1:I:111:MET:SD	2.49	0.52
1:K:140:ASP:O	1:K:144:ILE:HG12	2.09	0.52
1:K:447:MET:O	1:K:450:PRO:HD2	2.09	0.52
1:M:447:MET:O	1:M:450:PRO:HD2	2.09	0.52
2:O:6:LEU:HD12	2:O:6:LEU:O	2.08	0.52
2:P:58:ASP:OD2	2:Q:7:HIS:HB3	2.10	0.52
2:U:65:VAL:HG12	2:U:94:ILE:HG12	1.90	0.52
1:A:36:ARG:HB3	1:G:518:GLU:HB2	1.90	0.52
1:A:417:VAL:HA	1:A:420:ILE:HG22	1.90	0.52
1:B:350:ARG:HD3	1:B:353:ILE:HD12	1.91	0.52
1:E:455:VAL:O	1:E:458:CYS:HB2	2.09	0.52
1:I:215:LEU:HB3	1:I:218:PRO:HG3	1.90	0.52
1:J:69:MET:CE	1:J:522:THR:HB	2.38	0.52
1:M:20:VAL:CG2	1:M:74:VAL:HG21	2.39	0.52
1:M:149:THR:CG2	1:M:156:GLU:HA	2.39	0.52
1:M:232:GLU:HA	1:M:310:GLU:HG3	1.90	0.52
1:A:353:ILE:HG12	1:A:366:GLN:NE2	2.24	0.52
1:C:247:LEU:HD12	1:C:249:ILE:HG13	1.92	0.52
1:C:458:CYS:SG	1:C:480:ALA:HB1	2.48	0.52
1:E:234:LEU:HB3	2:S:23:GLY:HA2	1.90	0.52
1:E:432:GLN:HB2	1:E:436:GLN:OE1	2.08	0.52
1:F:207:LYS:CB	1:F:208:PRO:HD3	2.38	0.52
1:F:218:PRO:HD2	1:F:320:ALA:O	2.09	0.52
1:K:227:ILE:HD12	1:K:309:LEU:HD11	1.91	0.52
1:K:230:ILE:CD1	1:K:261:THR:HG21	2.40	0.52
1:K:262:LEU:O	1:K:266:THR:HG23	2.09	0.52
1:M:69:MET:CE	1:M:522:THR:HB	2.39	0.52
2:S:53:GLU:O	2:S:54:VAL:HG23	2.09	0.52
1:A:226:LYS:HA	1:A:253:ASP:O	2.10	0.52
1:B:114:MET:CE	1:B:117:LYS:HE2	2.40	0.52
1:B:254:VAL:HG21	1:B:275:ALA:HB1	1.90	0.52
1:D:28:LYS:HD2	1:D:453:GLN:CD	2.30	0.52
1:D:40:LEU:HD22	1:D:59:GLU:HG3	1.91	0.52
1:E:115:ASP:O	1:E:436:GLN:HG2	2.09	0.52
1:F:77:VAL:HG11	1:F:510:VAL:HG21	1.92	0.52
1:G:116:LEU:HD23	1:G:435:ASP:O	2.09	0.52
1:I:41:ASP:OD1	1:I:47:PRO:HB3	2.09	0.52
1:K:63:GLU:HB2	1:L:3:ALA:HB1	1.91	0.52
1:K:420:ILE:CD1	1:K:448:GLU:HA	2.39	0.52
1:L:447:MET:O	1:L:450:PRO:HD2	2.10	0.52
1:N:69:MET:HE1	1:N:522:THR:HB	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:3:ILE:HD13	2:P:11:ILE:HD13	1.92	0.52
1:E:207:LYS:CB	1:E:208:PRO:HD3	2.38	0.52
1:E:349:ILE:HG22	1:E:353:ILE:HG13	1.92	0.52
1:F:204:PHE:CD1	1:F:274:ALA:CB	2.93	0.52
1:F:265:ASN:HB3	1:F:271:VAL:HG22	1.91	0.52
1:F:518:GLU:CB	1:G:36:ARG:HB2	2.39	0.52
1:I:102:GLU:HA	1:I:102:GLU:OE1	2.09	0.52
1:K:271:VAL:HG12	1:K:273:VAL:HG13	1.91	0.52
1:K:348:GLN:O	1:K:352:GLN:HG3	2.09	0.52
1:N:267:MET:HG3	1:N:267:MET:O	2.09	0.52
2:T:20:LYS:HB3	2:T:27:LEU:HG	1.92	0.52
1:A:230:ILE:HD12	1:A:309:LEU:CD2	2.36	0.52
1:C:207:LYS:CB	1:C:208:PRO:HD3	2.38	0.52
1:D:147:VAL:HG23	1:D:403:THR:HG22	1.90	0.52
1:F:262:LEU:O	1:F:266:THR:HG23	2.10	0.52
1:H:247:LEU:H	1:H:273:VAL:HG12	1.73	0.52
1:I:69:MET:CE	1:I:522:THR:HB	2.40	0.52
1:K:351:GLN:O	1:K:354:GLU:HG2	2.10	0.52
1:L:286:LYS:HE2	1:L:286:LYS:HA	1.92	0.52
1:M:102:GLU:HB2	1:M:442:VAL:HG13	1.91	0.52
1:M:266:THR:HG22	1:M:272:LYS:HA	1.92	0.52
1:N:421:ARG:HD2	1:N:474:GLY:O	2.10	0.52
2:U:18:GLU:OE1	2:U:30:SER:HA	2.10	0.52
1:N:348:GLN:O	1:N:352:GLN:HG3	2.10	0.52
1:A:38:VAL:HG22	1:G:519:CYS:HB3	1.92	0.52
1:A:461:GLU:HB2	1:A:464:VAL:HG12	1.92	0.52
1:B:458:CYS:SG	1:B:480:ALA:HB1	2.50	0.52
1:C:247:LEU:HD13	1:C:248:LEU:N	2.25	0.52
1:F:56:VAL:O	1:F:60:ILE:HG12	2.09	0.52
1:G:40:LEU:HD22	1:G:59:GLU:CG	2.37	0.52
1:H:443:ALA:O	1:H:447:MET:HG3	2.10	0.52
1:L:144:ILE:HG21	1:L:163:ALA:HA	1.91	0.52
1:L:288:MET:HA	1:L:288:MET:HE3	1.90	0.52
1:A:204:PHE:CE1	1:A:266:THR:HB	2.45	0.52
1:B:220:ILE:HD13	1:B:248:LEU:HB3	1.92	0.52
1:C:28:LYS:HG2	1:C:94:VAL:HG22	1.92	0.52
1:D:221:LEU:HD13	1:D:317:LEU:HD21	1.91	0.52
1:E:419:LEU:HA	1:E:422:VAL:HG22	1.92	0.52
1:E:513:LEU:O	1:E:513:LEU:HD22	2.10	0.52
1:G:33:PRO:HA	1:G:153:ASN:ND2	2.25	0.52
1:G:234:LEU:HD13	2:U:22:ALA:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:409:GLU:OE1	1:L:498:LYS:HA	2.10	0.52
1:M:181:THR:O	1:N:282:GLY:HA3	2.10	0.52
2:O:12:VAL:HA	2:O:39:GLU:O	2.10	0.52
2:O:15:LYS:HD3	2:O:37:ARG:CB	2.40	0.52
2:T:50:GLU:HG2	2:T:50:GLU:O	2.10	0.52
1:A:213:VAL:O	1:A:324:VAL:HA	2.10	0.51
1:C:26:ALA:O	1:C:29:VAL:HG22	2.10	0.51
1:F:120:ILE:O	1:F:124:VAL:HG23	2.09	0.51
1:F:231:ARG:O	1:F:233:MET:N	2.43	0.51
1:I:230:ILE:CD1	1:I:261:THR:HG21	2.39	0.51
1:I:313:THR:HG22	1:I:314:LEU:N	2.24	0.51
1:J:102:GLU:HB2	1:J:442:VAL:HG13	1.91	0.51
1:B:351:GLN:HG2	1:C:210:THR:OG1	2.10	0.51
1:C:20:VAL:HG13	1:C:74:VAL:HG11	1.92	0.51
1:C:124:VAL:HG13	1:C:504:LEU:CD1	2.41	0.51
1:D:124:VAL:HG13	1:D:504:LEU:CD1	2.39	0.51
1:E:219:PHE:HB2	1:E:247:LEU:CD2	2.40	0.51
1:E:349:ILE:O	1:E:352:GLN:HB2	2.08	0.51
1:I:389:MET:HG3	1:I:390:LYS:N	2.24	0.51
1:J:400:LEU:HD21	1:J:404:ARG:HE	1.75	0.51
1:K:284:ARG:HG2	1:K:364:LYS:HE3	1.92	0.51
1:N:400:LEU:HD21	1:N:404:ARG:HE	1.75	0.51
2:Q:49:LEU:O	2:Q:50:GLU:HB2	2.09	0.51
2:T:47:ARG:O	2:T:55:LYS:HE2	2.09	0.51
1:D:204:PHE:CE1	1:D:266:THR:HB	2.45	0.51
1:D:287:ALA:HB1	1:D:368:ARG:HH22	1.75	0.51
1:E:493:ILE:HD13	3:E:1:ADP:C2	2.45	0.51
1:F:58:ARG:HA	1:F:75:LYS:HE3	1.92	0.51
1:G:33:PRO:HD3	3:G:1:ADP:C5	2.45	0.51
1:H:117:LYS:NZ	1:H:512:GLY:HA3	2.26	0.51
1:I:166:MET:CE	1:I:407:VAL:HG21	2.40	0.51
1:J:95:LEU:HD21	1:J:419:LEU:HD13	1.92	0.51
1:K:30:THR:HG22	1:K:36:ARG:O	2.10	0.51
1:A:165:ALA:O	1:A:169:VAL:HG22	2.10	0.51
1:B:115:ASP:O	1:B:436:GLN:HG2	2.11	0.51
1:B:355:GLU:HG3	1:B:357:THR:H	1.75	0.51
1:D:296:THR:HG22	1:D:335:GLY:HA3	1.91	0.51
1:D:349:ILE:O	1:D:352:GLN:HB2	2.10	0.51
1:E:509:SER:HB2	1:F:384:ALA:HB3	1.92	0.51
1:F:76:GLU:OE1	1:G:385:THR:HB	2.10	0.51
1:G:165:ALA:O	1:G:169:VAL:HG22	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:56:VAL:O	1:K:60:ILE:HG12	2.11	0.51
1:L:230:ILE:CD1	1:L:261:THR:HG21	2.39	0.51
1:L:313:THR:HG22	1:L:314:LEU:N	2.26	0.51
2:P:43:VAL:HG13	2:P:57:LEU:HD12	1.93	0.51
2:T:68:ASN:HB2	2:T:92:LEU:HD11	1.91	0.51
2:U:14:ARG:NH2	2:U:84:LEU:HD21	2.26	0.51
1:C:518:GLU:HB2	1:D:36:ARG:HD3	1.93	0.51
1:E:302:SER:OG	1:E:305:ILE:HB	2.10	0.51
1:F:417:VAL:HA	1:F:420:ILE:HG22	1.92	0.51
1:G:447:MET:O	1:G:450:PRO:HD2	2.10	0.51
1:H:215:LEU:HB3	1:H:218:PRO:HG3	1.91	0.51
1:J:166:MET:HE2	1:J:171:LYS:HA	1.93	0.51
1:K:285:ARG:HG2	1:K:285:ARG:HH11	1.74	0.51
1:A:296:THR:HG22	1:A:335:GLY:HA3	1.91	0.51
1:B:21:ASN:HA	1:B:97:GLN:HE22	1.76	0.51
1:B:165:ALA:O	1:B:169:VAL:HG22	2.10	0.51
1:B:230:ILE:HG23	1:B:309:LEU:HD21	1.91	0.51
1:G:221:LEU:HD11	1:G:301:ILE:CD1	2.41	0.51
1:H:140:ASP:O	1:H:144:ILE:HG12	2.09	0.51
1:H:421:ARG:HE	1:H:474:GLY:N	2.07	0.51
1:K:224:ASP:O	1:K:252:GLU:HG2	2.09	0.51
1:L:403:THR:O	1:L:407:VAL:HG23	2.11	0.51
1:L:421:ARG:O	1:L:425:LYS:HG2	2.10	0.51
1:M:219:PHE:CZ	1:M:314:LEU:HD23	2.45	0.51
1:M:247:LEU:H	1:M:273:VAL:HG12	1.76	0.51
1:N:215:LEU:HB3	1:N:218:PRO:HG3	1.91	0.51
2:P:31:ALA:O	2:P:32:ALA:HB2	2.10	0.51
2:R:25:ILE:O	2:R:25:ILE:HG22	2.11	0.51
1:A:438:VAL:O	1:A:442:VAL:HG23	2.10	0.51
1:E:399:ALA:O	1:E:403:THR:HG23	2.10	0.51
1:H:16:MET:HG3	1:H:520:MET:SD	2.49	0.51
1:L:19:GLY:HA3	1:L:67:GLU:O	2.10	0.51
1:M:235:PRO:CG	1:M:310:GLU:HA	2.40	0.51
1:D:199:TYR:CZ	1:D:202:PRO:HA	2.45	0.51
1:I:411:VAL:HG21	1:I:494:LEU:HD12	1.93	0.51
1:J:27:VAL:HG11	1:J:93:THR:HG21	1.93	0.51
1:K:313:THR:HG22	1:K:314:LEU:N	2.23	0.51
1:M:475:ASN:HB2	1:M:487:ASN:HD21	1.76	0.51
1:N:174:VAL:HG12	1:N:376:VAL:HG13	1.93	0.51
1:B:187:LEU:HD13	1:B:379:ILE:HG12	1.93	0.51
1:C:225:LYS:O	1:C:251:ALA:HB1	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:278:ALA:HB1	1:D:285:ARG:HB2	1.91	0.51
1:L:12:ALA:HB1	1:L:520:MET:CG	2.41	0.51
1:L:118:ARG:HD2	1:L:436:GLN:OE1	2.11	0.51
1:L:466:ALA:O	1:L:470:LYS:HG2	2.10	0.51
1:M:414:GLY:N	1:M:494:LEU:HA	2.25	0.51
2:P:7:HIS:O	2:P:8:ASP:HB3	2.09	0.51
1:B:349:ILE:HG21	1:B:369:VAL:HG22	1.93	0.51
1:E:218:PRO:HD2	1:E:320:ALA:O	2.09	0.51
1:G:438:VAL:O	1:G:442:VAL:HG23	2.11	0.51
1:J:30:THR:HG22	1:J:36:ARG:O	2.11	0.51
1:K:149:THR:CG2	1:K:156:GLU:HA	2.40	0.51
1:K:432:GLN:NE2	1:K:436:GLN:HE22	2.09	0.51
2:O:52:GLY:O	2:O:53:GLU:HB2	2.11	0.51
2:O:78:ILE:HD13	2:O:83:VAL:HG21	1.93	0.51
2:T:25:ILE:HG22	2:T:25:ILE:O	2.10	0.51
1:B:207:LYS:HB3	1:B:208:PRO:HD3	1.92	0.50
1:E:221:LEU:HD13	1:E:317:LEU:HD21	1.92	0.50
1:G:230:ILE:HG23	1:G:230:ILE:O	2.11	0.50
1:L:27:VAL:HG11	1:L:93:THR:HG21	1.92	0.50
1:M:350:ARG:HE	1:M:369:VAL:HG11	1.76	0.50
1:M:475:ASN:HB2	1:M:487:ASN:ND2	2.26	0.50
1:N:447:MET:O	1:N:450:PRO:HD2	2.11	0.50
2:O:86:MET:HB2	2:O:90:ASP:OD2	2.11	0.50
2:P:20:LYS:HB3	2:P:27:LEU:HA	1.91	0.50
2:U:11:ILE:CD1	2:U:85:ILE:HG12	2.41	0.50
1:A:247:LEU:HD21	1:A:317:LEU:HD13	1.92	0.50
1:B:350:ARG:HA	1:B:353:ILE:HD12	1.93	0.50
1:B:438:VAL:O	1:B:442:VAL:HG23	2.10	0.50
1:C:147:VAL:HG12	1:C:494:LEU:HB2	1.92	0.50
1:C:259:LEU:O	1:C:263:VAL:HG23	2.11	0.50
1:C:305:ILE:HD11	1:D:203:TYR:CZ	2.46	0.50
1:C:306:GLY:HA3	1:D:264:VAL:CG2	2.31	0.50
1:D:150:ILE:HG21	1:D:494:LEU:O	2.11	0.50
1:D:352:GLN:C	1:D:365:LEU:HD11	2.31	0.50
1:A:31:LEU:HD22	1:A:94:VAL:HG21	1.93	0.50
1:B:28:LYS:HD2	1:B:453:GLN:CD	2.32	0.50
1:B:229:ASN:HA	1:B:257:GLU:OE1	2.10	0.50
1:C:82:ASN:HB2	1:C:89:THR:HG21	1.92	0.50
1:D:213:VAL:HB	1:D:325:ILE:HB	1.92	0.50
1:D:438:VAL:O	1:D:442:VAL:HG23	2.11	0.50
1:E:33:PRO:HD3	3:E:1:ADP:C5	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:313:THR:HB	1:E:315:GLU:HG3	1.92	0.50
1:F:308:GLU:HB2	1:F:311:LYS:HB3	1.93	0.50
1:K:150:ILE:HG21	1:K:494:LEU:CD2	2.41	0.50
1:K:222:LEU:HB3	1:K:289:LEU:HD11	1.93	0.50
2:R:55:LYS:HB3	2:S:51:ASN:OD1	2.11	0.50
1:B:349:ILE:HD13	1:B:369:VAL:HG22	1.92	0.50
1:C:204:PHE:CE1	1:C:274:ALA:HB3	2.47	0.50
1:E:33:PRO:HA	1:E:153:ASN:ND2	2.26	0.50
1:E:165:ALA:O	1:E:169:VAL:HG22	2.12	0.50
1:F:231:ARG:NH2	1:F:237:LEU:HD12	2.25	0.50
1:G:442:VAL:O	1:G:445:ARG:HD2	2.11	0.50
1:J:259:LEU:O	1:J:263:VAL:HG23	2.12	0.50
1:L:351:GLN:O	1:L:354:GLU:HG2	2.12	0.50
1:N:179:ASP:HA	1:N:389:MET:CE	2.41	0.50
1:N:241:ALA:HB2	1:N:271:VAL:HG21	1.92	0.50
2:O:57:LEU:HD22	2:O:88:GLU:HB2	1.93	0.50
1:A:351:GLN:HG2	1:B:210:THR:CG2	2.40	0.50
1:B:409:GLU:O	1:B:409:GLU:HG2	2.12	0.50
1:C:134:LEU:HD11	1:C:425:LYS:HE2	1.93	0.50
1:F:518:GLU:HG2	1:G:29:VAL:HB	1.93	0.50
1:G:56:VAL:O	1:G:60:ILE:HG12	2.11	0.50
1:I:149:THR:CG2	1:I:156:GLU:HA	2.42	0.50
1:J:313:THR:HG22	1:J:314:LEU:N	2.27	0.50
1:K:41:ASP:OD1	1:L:69:MET:HG2	2.11	0.50
1:L:150:ILE:HG21	1:L:494:LEU:CD2	2.41	0.50
1:N:131:LEU:HD11	1:N:412:VAL:HG11	1.94	0.50
1:N:150:ILE:HG21	1:N:494:LEU:HD21	1.94	0.50
1:N:227:ILE:HD12	1:N:309:LEU:CD1	2.42	0.50
1:C:237:LEU:HD22	2:Q:26:VAL:HG11	1.94	0.50
1:E:66:PHE:HA	1:E:69:MET:HE3	1.94	0.50
1:E:230:ILE:HD12	1:E:309:LEU:HD21	1.93	0.50
1:G:443:ALA:O	1:G:447:MET:HG3	2.12	0.50
1:H:40:LEU:CD2	1:I:521:VAL:HB	2.42	0.50
2:O:78:ILE:HD13	2:O:83:VAL:HG22	1.94	0.50
2:R:86:MET:HB2	2:R:90:ASP:OD2	2.12	0.50
1:A:257:GLU:O	1:A:261:THR:HG22	2.11	0.50
1:A:278:ALA:HB1	1:A:279:PRO:HD2	1.93	0.50
1:B:111:MET:SD	1:B:438:VAL:HG21	2.51	0.50
1:B:519:CYS:O	1:C:38:VAL:HA	2.12	0.50
1:D:22:VAL:HG11	1:D:62:LEU:HD11	1.94	0.50
1:D:266:THR:HG22	1:D:273:VAL:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:296:THR:HG22	1:E:335:GLY:HA3	1.93	0.50
1:F:215:LEU:O	1:F:322:ARG:HA	2.11	0.50
1:F:352:GLN:HB3	1:F:365:LEU:HG	1.92	0.50
1:H:259:LEU:O	1:H:263:VAL:HG23	2.12	0.50
1:K:20:VAL:HG23	1:K:74:VAL:HG21	1.92	0.50
1:K:130:GLU:HG3	1:K:426:LEU:CD2	2.42	0.50
1:K:227:ILE:HD12	1:K:309:LEU:CD1	2.42	0.50
1:K:266:THR:O	1:K:272:LYS:HD3	2.11	0.50
1:L:365:LEU:O	1:L:369:VAL:HG23	2.12	0.50
1:N:383:ALA:HB3	1:N:389:MET:HB2	1.94	0.50
1:B:100:ILE:HD13	1:B:514:MET:SD	2.51	0.50
1:B:124:VAL:HG21	1:B:508:ALA:CB	2.42	0.50
1:B:237:LEU:HD22	2:P:26:VAL:HG22	1.93	0.50
1:B:346:VAL:O	1:B:349:ILE:HB	2.12	0.50
1:E:20:VAL:HG13	1:E:74:VAL:HG11	1.93	0.50
1:J:66:PHE:O	1:J:69:MET:HB2	2.12	0.50
1:K:197:ARG:HE	1:K:277:LYS:HB2	1.76	0.50
1:M:420:ILE:CD1	1:M:448:GLU:HA	2.41	0.50
2:T:68:ASN:OD1	2:U:74:LYS:HD2	2.12	0.50
1:L:319:GLN:O	1:L:336:VAL:HG23	2.12	0.50
1:M:174:VAL:HG12	1:M:376:VAL:HG13	1.93	0.50
1:N:166:MET:HE1	1:N:407:VAL:HG21	1.94	0.50
2:S:93:ALA:HA	2:T:6:LEU:N	2.26	0.50
2:U:8:ASP:HB2	2:U:47:ARG:HA	1.93	0.50
2:U:15:LYS:HE2	2:U:37:ARG:HB3	1.94	0.50
1:A:349:ILE:O	1:A:352:GLN:HB2	2.12	0.49
1:B:518:GLU:HB2	1:C:36:ARG:HB3	1.92	0.49
1:C:284:ARG:O	1:C:288:MET:HB2	2.12	0.49
1:C:518:GLU:HB2	1:D:36:ARG:CB	2.42	0.49
1:E:5:ASP:HB2	1:E:524:LEU:HG	1.93	0.49
1:F:5:ASP:HB2	1:F:524:LEU:HD23	1.94	0.49
1:G:345:ARG:O	1:G:348:GLN:HG3	2.11	0.49
1:G:352:GLN:HB3	1:G:365:LEU:CD1	2.42	0.49
1:H:17:LEU:HB2	1:H:104:LEU:CD2	2.42	0.49
1:H:421:ARG:HH11	1:H:421:ARG:HA	1.77	0.49
1:M:271:VAL:HG12	1:M:273:VAL:HG13	1.92	0.49
2:S:43:VAL:HG13	2:S:57:LEU:HD12	1.93	0.49
1:B:12:ALA:HB1	1:B:520:MET:CG	2.40	0.49
1:B:199:TYR:HB3	1:B:325:ILE:CG2	2.35	0.49
1:D:234:LEU:N	1:D:235:PRO:HD2	2.26	0.49
1:E:25:ASP:OD1	1:E:28:LYS:HE2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:37:ASN:OD1	1:E:51:LYS:HB2	2.12	0.49
1:H:181:THR:O	1:I:282:GLY:HA3	2.11	0.49
1:K:235:PRO:HG3	1:K:310:GLU:HA	1.94	0.49
1:M:6:VAL:HG22	1:M:521:VAL:HG22	1.93	0.49
1:M:193:MET:H	1:M:332:ILE:HG13	1.76	0.49
1:M:193:MET:HG3	1:M:371:LYS:HB3	1.94	0.49
1:N:145:ALA:O	1:N:149:THR:HG23	2.12	0.49
2:R:7:HIS:HB3	2:R:48:ILE:HB	1.93	0.49
1:B:220:ILE:CD1	1:B:248:LEU:HB3	2.42	0.49
1:C:254:VAL:HG21	1:C:275:ALA:CB	2.42	0.49
1:E:346:VAL:HA	1:E:349:ILE:HD12	1.94	0.49
1:F:77:VAL:HG12	1:F:510:VAL:HG21	1.94	0.49
1:F:221:LEU:HD13	1:F:317:LEU:HD21	1.94	0.49
1:H:409:GLU:OE1	1:H:498:LYS:HA	2.11	0.49
1:I:39:VAL:HB	1:J:520:MET:HG2	1.92	0.49
1:L:174:VAL:HG11	1:L:194:GLN:HB2	1.94	0.49
1:M:223:ALA:HB3	1:M:251:ALA:HB2	1.94	0.49
1:N:227:ILE:HD12	1:N:309:LEU:HD11	1.95	0.49
2:O:20:LYS:HB3	2:O:27:LEU:HG	1.92	0.49
1:F:33:PRO:HD3	3:F:1:ADP:C5	2.48	0.49
1:G:220:ILE:HG23	1:G:248:LEU:HD12	1.94	0.49
1:J:20:VAL:CG2	1:J:74:VAL:HG21	2.42	0.49
1:J:49:ILE:HD13	1:K:513:LEU:HD21	1.95	0.49
1:J:116:LEU:HD23	1:J:435:ASP:O	2.11	0.49
1:K:32:GLY:HA2	1:K:454:ILE:HD12	1.94	0.49
1:K:443:ALA:O	1:K:447:MET:HG3	2.12	0.49
1:L:49:ILE:CD1	1:M:73:MET:HE3	2.33	0.49
1:M:106:ALA:O	1:M:111:MET:HB2	2.11	0.49
2:Q:47:ARG:O	2:Q:55:LYS:HE2	2.12	0.49
1:A:102:GLU:CB	1:A:442:VAL:HG13	2.43	0.49
1:B:102:GLU:HB2	1:B:442:VAL:HG13	1.94	0.49
1:B:417:VAL:HA	1:B:420:ILE:HG22	1.94	0.49
1:B:518:GLU:HG2	1:C:29:VAL:HB	1.93	0.49
1:C:175:ILE:HG12	1:C:377:ALA:HB3	1.94	0.49
1:C:305:ILE:HG22	1:D:264:VAL:HG23	1.95	0.49
1:F:447:MET:O	1:F:450:PRO:HD2	2.11	0.49
1:F:513:LEU:HD11	1:G:388:GLU:HA	1.94	0.49
1:G:24:ALA:O	1:G:28:LYS:HG3	2.13	0.49
1:I:447:MET:O	1:I:450:PRO:HD2	2.11	0.49
1:K:63:GLU:HB2	1:L:3:ALA:CB	2.43	0.49
1:K:268:ARG:HA	1:K:268:ARG:HE	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:46:ALA:HB1	1:M:47:PRO:CD	2.36	0.49
2:S:11:ILE:HG12	2:S:85:ILE:HG12	1.95	0.49
2:T:14:ARG:NH2	2:T:84:LEU:HD21	2.27	0.49
2:U:8:ASP:O	2:U:87:SER:HA	2.12	0.49
1:F:40:LEU:HD13	1:F:59:GLU:HG3	1.95	0.49
1:H:509:SER:O	1:H:513:LEU:HD13	2.12	0.49
1:L:41:ASP:HB2	1:M:69:MET:HE2	1.93	0.49
1:M:383:ALA:HB3	1:M:389:MET:HB2	1.95	0.49
1:N:66:PHE:CZ	1:N:522:THR:HG22	2.48	0.49
2:P:20:LYS:CG	2:P:27:LEU:HG	2.43	0.49
1:D:165:ALA:O	1:D:169:VAL:HG22	2.13	0.49
1:D:206:ASN:CB	1:D:214:GLU:H	2.26	0.49
1:D:247:LEU:HB3	1:D:273:VAL:HG13	1.94	0.49
1:F:228:SER:HB2	1:F:255:GLU:HG2	1.94	0.49
1:F:257:GLU:O	1:F:261:THR:HG22	2.12	0.49
1:G:238:GLU:HB2	2:U:25:ILE:H	1.78	0.49
1:I:459:GLY:HA3	1:J:112:ASN:HD21	1.77	0.49
1:J:356:ALA:HB1	1:J:362:ARG:NH2	2.28	0.49
1:J:383:ALA:HB3	1:J:389:MET:HB2	1.94	0.49
1:L:276:VAL:CG1	1:L:325:ILE:HD13	2.43	0.49
2:O:15:LYS:HD3	2:O:37:ARG:HB2	1.95	0.49
1:A:120:ILE:O	1:A:124:VAL:HG23	2.12	0.49
1:C:116:LEU:HD23	1:C:435:ASP:O	2.13	0.49
1:C:124:VAL:HG21	1:C:508:ALA:CB	2.42	0.49
1:G:102:GLU:CB	1:G:442:VAL:HG13	2.42	0.49
1:G:102:GLU:HB3	1:G:442:VAL:HG13	1.95	0.49
1:I:20:VAL:CG2	1:I:74:VAL:HG21	2.43	0.49
1:I:180:GLY:H	1:I:389:MET:HE1	1.78	0.49
1:I:265:ASN:ND2	1:I:270:ILE:HB	2.28	0.49
1:J:218:PRO:HG2	1:J:323:VAL:HG12	1.94	0.49
1:L:232:GLU:HA	1:L:310:GLU:HG3	1.94	0.49
1:L:509:SER:O	1:L:513:LEU:HD13	2.13	0.49
1:M:221:LEU:HD12	1:M:249:ILE:HG23	1.94	0.49
1:A:194:GLN:O	1:A:371:LYS:HD3	2.12	0.49
1:A:217:SER:HA	1:A:320:ALA:O	2.13	0.49
1:C:324:VAL:HB	1:C:331:THR:HB	1.94	0.49
1:C:346:VAL:O	1:C:349:ILE:HB	2.13	0.49
1:D:207:LYS:CD	1:D:208:PRO:HD3	2.43	0.49
1:D:278:ALA:HB1	1:D:279:PRO:HD2	1.95	0.49
1:G:464:VAL:HG23	1:M:463:SER:OG	2.13	0.49
1:I:124:VAL:HG13	1:I:504:LEU:CD1	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:351:GLN:O	1:I:354:GLU:HG2	2.13	0.49
1:J:247:LEU:H	1:J:273:VAL:HG12	1.77	0.49
1:K:265:ASN:O	1:K:269:GLY:HA3	2.13	0.49
1:L:39:VAL:HG22	1:L:49:ILE:HG12	1.94	0.49
1:M:179:ASP:HA	1:M:389:MET:CE	2.43	0.49
2:Q:55:LYS:HD3	2:R:51:ASN:CG	2.32	0.49
2:R:7:HIS:CG	2:R:48:ILE:HD13	2.47	0.49
1:A:453:GLN:NE2	1:A:456:LEU:HD23	2.26	0.49
1:D:206:ASN:O	1:D:207:LYS:HB3	2.12	0.49
1:F:288:MET:HG2	1:F:368:ARG:HE	1.78	0.49
1:G:452:ARG:HB2	1:G:462:PRO:CB	2.43	0.49
1:I:478:TYR:HB2	1:I:485:TYR:CE2	2.48	0.49
1:K:150:ILE:HG21	1:K:494:LEU:HD21	1.95	0.49
1:K:214:GLU:HG2	1:K:324:VAL:CG1	2.41	0.49
1:K:230:ILE:HD11	1:K:261:THR:HG21	1.94	0.49
1:L:325:ILE:HG12	1:L:330:THR:HG23	1.94	0.49
2:R:8:ASP:CB	2:R:47:ARG:HA	2.43	0.49
1:A:221:LEU:HD13	1:A:317:LEU:HD21	1.95	0.48
1:B:102:GLU:CB	1:B:442:VAL:HG13	2.43	0.48
1:C:175:ILE:H	1:C:404:ARG:NH2	2.10	0.48
1:C:220:ILE:HD12	1:C:296:THR:HG21	1.95	0.48
1:F:247:LEU:HD13	1:F:248:LEU:N	2.28	0.48
1:I:106:ALA:O	1:I:111:MET:HB2	2.13	0.48
1:I:348:GLN:O	1:I:352:GLN:HG3	2.13	0.48
1:J:225:LYS:HD3	1:J:303:GLU:HG3	1.95	0.48
1:L:287:ALA:HB1	1:L:368:ARG:CZ	2.43	0.48
1:M:224:ASP:HB3	1:M:302:SER:HA	1.95	0.48
1:N:326:ASN:OD1	1:N:329:THR:HB	2.12	0.48
2:T:6:LEU:HD12	2:T:7:HIS:CD2	2.48	0.48
2:U:7:HIS:CD2	2:U:48:ILE:HD11	2.48	0.48
1:B:147:VAL:HG12	1:B:494:LEU:HB2	1.95	0.48
1:C:19:GLY:HA3	1:C:67:GLU:O	2.13	0.48
1:C:455:VAL:O	1:C:458:CYS:HB2	2.12	0.48
1:G:100:ILE:HD13	1:G:514:MET:HG2	1.94	0.48
1:G:240:VAL:HG21	1:G:247:LEU:HD23	1.93	0.48
1:I:17:LEU:HB2	1:I:104:LEU:HD23	1.95	0.48
1:I:177:VAL:CG1	1:I:393:LYS:HG3	2.43	0.48
1:L:217:SER:HA	1:L:320:ALA:O	2.13	0.48
1:L:385:THR:HG23	1:L:388:GLU:H	1.77	0.48
1:L:459:GLY:HA3	1:M:112:ASN:ND2	2.27	0.48
1:M:259:LEU:O	1:M:263:VAL:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:130:GLU:HG3	1:N:426:LEU:CD2	2.42	0.48
1:N:319:GLN:HB2	1:N:336:VAL:HG21	1.95	0.48
2:R:11:ILE:HG12	2:R:85:ILE:HG12	1.95	0.48
1:A:26:ALA:HA	1:G:8:PHE:CE2	2.48	0.48
1:B:149:THR:HG23	1:B:155:ASP:C	2.34	0.48
1:B:381:VAL:CG1	1:B:392:LYS:HG3	2.43	0.48
1:B:475:ASN:HB2	1:B:487:ASN:ND2	2.28	0.48
1:C:6:VAL:HG12	1:C:521:VAL:HG22	1.95	0.48
1:C:21:ASN:HA	1:C:97:GLN:HE22	1.78	0.48
1:C:31:LEU:HD12	3:C:1:ADP:H5'1	1.95	0.48
1:C:204:PHE:CE2	1:C:213:VAL:HG21	2.48	0.48
1:E:52:ASP:OD1	1:E:54:VAL:HG12	2.13	0.48
1:F:418:ALA:O	1:F:422:VAL:HG13	2.14	0.48
1:F:513:LEU:HD12	1:G:388:GLU:HA	1.94	0.48
1:G:414:GLY:O	1:G:417:VAL:HG12	2.14	0.48
1:I:30:THR:HG22	1:I:36:ARG:O	2.12	0.48
1:L:241:ALA:CB	1:L:271:VAL:HG21	2.41	0.48
2:R:43:VAL:CG1	2:R:57:LEU:HD12	2.43	0.48
1:B:124:VAL:HG21	1:B:508:ALA:HB1	1.94	0.48
1:C:309:LEU:H	1:C:309:LEU:HD12	1.78	0.48
1:C:358:SER:HA	1:C:362:ARG:HG3	1.95	0.48
1:D:25:ASP:HA	1:D:28:LYS:HE2	1.95	0.48
1:D:102:GLU:HB2	1:D:442:VAL:HG13	1.94	0.48
1:D:214:GLU:HA	1:D:323:VAL:O	2.14	0.48
1:E:23:LEU:HG	1:E:74:VAL:HG23	1.96	0.48
1:E:124:VAL:HG21	1:E:508:ALA:CB	2.44	0.48
1:E:365:LEU:HD13	1:E:366:GLN:HE22	1.78	0.48
1:H:149:THR:CG2	1:H:156:GLU:HA	2.43	0.48
1:I:400:LEU:HD21	1:I:404:ARG:HE	1.77	0.48
1:L:356:ALA:HB1	1:L:362:ARG:NH2	2.29	0.48
1:A:40:LEU:HD13	1:A:59:GLU:HG3	1.94	0.48
1:C:199:TYR:CZ	1:C:202:PRO:HA	2.48	0.48
1:G:237:LEU:HD22	2:U:26:VAL:CG2	2.16	0.48
1:H:403:THR:O	1:H:407:VAL:HG23	2.13	0.48
1:I:293:ALA:HB2	1:I:300:VAL:HG13	1.93	0.48
1:J:488:MET:HA	1:J:491:MET:HG2	1.96	0.48
1:L:152:ALA:O	1:L:153:ASN:HB2	2.13	0.48
1:A:21:ASN:HD22	1:A:97:GLN:HE22	1.62	0.48
1:A:288:MET:HG2	1:A:368:ARG:HE	1.78	0.48
1:B:34:LYS:HE3	1:B:481:ALA:HA	1.96	0.48
1:B:228:SER:HB3	1:B:255:GLU:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:ASN:C	1:B:231:ARG:H	2.16	0.48
1:E:148:GLY:HA2	1:E:399:ALA:HB1	1.94	0.48
1:G:221:LEU:HD13	1:G:317:LEU:HD21	1.95	0.48
1:I:27:VAL:HG11	1:I:93:THR:HG21	1.96	0.48
1:I:455:VAL:HG13	1:I:460:GLU:HB2	1.96	0.48
1:K:123:ALA:HB2	1:K:440:ILE:HG23	1.94	0.48
1:K:227:ILE:HG21	1:K:233:MET:SD	2.53	0.48
1:K:270:ILE:HG22	1:K:271:VAL:HG23	1.96	0.48
1:L:229:ASN:ND2	1:L:231:ARG:HH12	2.12	0.48
1:L:294:THR:HG21	1:L:345:ARG:HB2	1.96	0.48
2:O:74:LYS:HG3	2:U:92:LEU:CD1	2.44	0.48
1:A:31:LEU:CD1	3:A:1:ADP:H5'1	2.42	0.48
1:B:20:VAL:HG13	1:B:74:VAL:HG11	1.96	0.48
1:C:204:PHE:CG	1:C:204:PHE:O	2.66	0.48
1:D:228:SER:N	1:D:230:ILE:HG23	2.28	0.48
1:D:262:LEU:HD11	1:D:273:VAL:CB	2.38	0.48
1:D:278:ALA:HB3	1:D:285:ARG:NH1	2.29	0.48
1:E:261:THR:CG2	2:S:29:GLY:H	2.26	0.48
1:E:288:MET:HG2	1:E:368:ARG:HE	1.79	0.48
1:E:418:ALA:O	1:E:422:VAL:HG13	2.14	0.48
1:F:197:ARG:HG2	1:F:277:LYS:O	2.13	0.48
1:G:350:ARG:HD3	1:G:353:ILE:HD12	1.95	0.48
1:H:63:GLU:CA	1:I:3:ALA:HB1	2.43	0.48
1:H:124:VAL:HG13	1:H:504:LEU:CD1	2.44	0.48
1:H:222:LEU:HD22	1:H:289:LEU:HD11	1.96	0.48
1:I:131:LEU:HD21	1:I:500:THR:HG22	1.95	0.48
1:J:284:ARG:HG2	1:J:364:LYS:HE2	1.95	0.48
1:J:455:VAL:HG13	1:J:460:GLU:HB2	1.96	0.48
1:K:69:MET:SD	1:K:520:MET:HE2	2.54	0.48
1:L:161:LEU:HD21	1:L:185:ASP:HB3	1.95	0.48
1:A:65:LYS:NZ	1:A:523:ASP:HB2	2.28	0.48
1:B:33:PRO:HD3	3:B:1:ADP:C5	2.49	0.48
1:C:420:ILE:HG13	1:C:448:GLU:HG2	1.95	0.48
1:G:30:THR:HG22	1:G:36:ARG:O	2.14	0.48
1:H:517:THR:HG21	1:N:39:VAL:HG23	1.94	0.48
1:I:496:PRO:HD2	1:I:499:VAL:HG21	1.95	0.48
1:K:325:ILE:HG12	1:K:330:THR:HG23	1.96	0.48
1:M:20:VAL:HG23	1:M:74:VAL:HG21	1.96	0.48
1:M:199:TYR:CE2	1:M:327:LYS:HA	2.48	0.48
2:Q:8:ASP:O	2:Q:87:SER:HA	2.12	0.48
1:B:146:GLN:HE21	1:B:494:LEU:HD11	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:VAL:HG21	1:C:505:GLN:HE21	1.79	0.48
1:D:252:GLU:HA	1:D:285:ARG:HH11	1.78	0.48
1:E:263:VAL:O	1:E:267:MET:HB2	2.13	0.48
1:F:117:LYS:HE3	1:F:513:LEU:CD2	2.43	0.48
1:F:147:VAL:O	1:F:150:ILE:HG22	2.13	0.48
1:F:183:LEU:CD2	1:F:384:ALA:HA	2.44	0.48
1:F:204:PHE:CG	1:F:204:PHE:O	2.67	0.48
1:I:437:ASN:O	1:I:441:LYS:HD2	2.14	0.48
1:K:57:ALA:O	1:K:75:LYS:HE3	2.14	0.48
1:N:233:MET:CE	1:N:309:LEU:HD13	2.44	0.48
2:P:58:ASP:HB2	2:Q:6:LEU:HD11	1.96	0.48
2:Q:47:ARG:O	2:Q:55:LYS:HG2	2.14	0.48
1:A:73:MET:SD	1:B:49:ILE:HD11	2.53	0.48
1:A:272:LYS:HB2	1:A:272:LYS:NZ	2.29	0.48
1:C:451:LEU:HD23	1:C:451:LEU:C	2.34	0.48
1:K:287:ALA:HB1	1:K:368:ARG:NH2	2.28	0.48
1:M:321:LYS:HD2	1:M:334:ASP:OD2	2.12	0.48
2:Q:66:ILE:HG23	2:R:76:GLU:OE2	2.14	0.48
1:B:207:LYS:CB	1:B:208:PRO:HD3	2.44	0.47
1:B:449:ALA:HA	1:B:452:ARG:HG2	1.96	0.47
1:D:6:VAL:HG12	1:D:521:VAL:HG22	1.95	0.47
1:E:147:VAL:O	1:E:150:ILE:HG22	2.14	0.47
1:E:309:LEU:HD12	1:E:309:LEU:H	1.78	0.47
1:E:348:GLN:HA	1:F:209:GLU:HG2	1.94	0.47
1:F:147:VAL:CG2	1:F:403:THR:HG22	2.44	0.47
1:G:262:LEU:O	1:G:266:THR:HG23	2.14	0.47
1:I:39:VAL:HA	1:I:48:THR:O	2.13	0.47
2:R:31:ALA:O	2:R:32:ALA:HB2	2.14	0.47
1:A:509:SER:CB	1:B:384:ALA:HB3	2.44	0.47
1:D:85:ALA:HB3	1:D:499:VAL:HG12	1.97	0.47
1:E:210:THR:HG22	1:E:210:THR:O	2.14	0.47
1:E:467:ASN:HD21	1:K:464:VAL:HG22	1.79	0.47
1:E:496:PRO:O	1:E:499:VAL:HG22	2.14	0.47
1:H:290:GLN:HG3	1:H:345:ARG:HE	1.79	0.47
1:J:150:ILE:HG21	1:J:494:LEU:CD2	2.44	0.47
1:J:176:THR:OG1	1:J:378:VAL:HG12	2.14	0.47
1:K:496:PRO:HD2	1:K:499:VAL:HG21	1.96	0.47
1:L:276:VAL:HG13	1:L:325:ILE:HD13	1.96	0.47
1:L:319:GLN:HB2	1:L:336:VAL:HG21	1.97	0.47
1:N:56:VAL:O	1:N:60:ILE:HG12	2.14	0.47
1:N:131:LEU:CD1	1:N:412:VAL:HG11	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:266:THR:HG21	1:N:273:VAL:O	2.15	0.47
1:N:455:VAL:HG12	1:N:460:GLU:O	2.14	0.47
2:U:7:HIS:HB2	2:U:46:GLY:O	2.13	0.47
1:B:230:ILE:O	1:B:230:ILE:HG22	2.13	0.47
1:C:17:LEU:HD13	1:C:104:LEU:HD12	1.96	0.47
1:C:31:LEU:CD1	3:C:1:ADP:H5'1	2.45	0.47
1:C:230:ILE:O	1:C:230:ILE:CG2	2.62	0.47
1:D:272:LYS:HB2	1:D:272:LYS:NZ	2.28	0.47
1:D:512:GLY:O	1:D:516:THR:HG23	2.14	0.47
1:E:219:PHE:HB2	1:E:247:LEU:HD22	1.95	0.47
1:E:519:CYS:HB3	1:F:38:VAL:HG22	1.97	0.47
1:F:50:THR:HA	1:F:391:GLU:OE1	2.14	0.47
1:H:34:LYS:HB2	1:H:458:CYS:SG	2.54	0.47
1:H:225:LYS:HD3	1:H:303:GLU:CD	2.34	0.47
1:J:233:MET:CE	1:J:309:LEU:HD13	2.44	0.47
1:L:5:ASP:HB2	1:L:524:LEU:HD23	1.96	0.47
1:C:351:GLN:HG2	1:D:210:THR:HG23	1.97	0.47
1:E:124:VAL:O	1:E:128:VAL:HG23	2.14	0.47
1:E:195:PHE:CE1	1:E:197:ARG:NH1	2.83	0.47
1:G:234:LEU:HB3	2:U:23:GLY:HA3	1.96	0.47
1:G:326:ASN:OD1	1:G:329:THR:HB	2.15	0.47
1:I:150:ILE:HG21	1:I:494:LEU:CD2	2.44	0.47
1:I:166:MET:HE1	1:I:407:VAL:HG21	1.97	0.47
1:I:287:ALA:HB1	1:I:368:ARG:CZ	2.44	0.47
1:J:479:ASN:OD1	1:J:493:ILE:HG13	2.15	0.47
2:O:14:ARG:NH2	2:O:84:LEU:HD21	2.29	0.47
1:A:116:LEU:HD23	1:A:435:ASP:O	2.14	0.47
1:B:257:GLU:HG3	2:P:31:ALA:HB2	1.96	0.47
1:C:230:ILE:O	1:C:230:ILE:HG22	2.14	0.47
1:C:418:ALA:O	1:C:422:VAL:HG13	2.14	0.47
1:F:252:GLU:HG3	1:F:285:ARG:HH11	1.79	0.47
1:H:37:ASN:HD22	1:I:517:THR:HA	1.78	0.47
1:I:31:LEU:HG	1:I:454:ILE:CD1	2.45	0.47
1:I:228:SER:O	1:I:257:GLU:HB3	2.15	0.47
1:K:107:VAL:HG11	1:K:515:ILE:HG23	1.96	0.47
1:L:49:ILE:HD12	1:M:513:LEU:HD21	1.97	0.47
1:L:199:TYR:HA	1:L:276:VAL:HG12	1.96	0.47
1:M:104:LEU:HA	1:M:107:VAL:HG22	1.97	0.47
1:M:177:VAL:CG1	1:M:393:LYS:HG3	2.44	0.47
1:N:228:SER:HA	1:N:255:GLU:HB2	1.96	0.47
2:T:48:ILE:HG22	2:T:48:ILE:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:MET:SD	1:C:49:ILE:HD11	2.55	0.47
1:B:106:ALA:HB1	1:B:111:MET:HE3	1.96	0.47
1:D:147:VAL:O	1:D:150:ILE:HG22	2.15	0.47
1:E:164:GLU:O	1:E:168:LYS:HB2	2.14	0.47
1:E:345:ARG:O	1:E:349:ILE:HG13	2.14	0.47
1:F:247:LEU:HB3	1:F:273:VAL:CG1	2.42	0.47
1:G:418:ALA:O	1:G:422:VAL:HG13	2.14	0.47
1:I:41:ASP:HB2	1:J:521:VAL:O	2.14	0.47
1:I:179:ASP:HA	1:I:389:MET:CE	2.44	0.47
1:I:285:ARG:HG3	1:I:286:LYS:N	2.29	0.47
1:J:325:ILE:HG12	1:J:330:THR:HG23	1.97	0.47
1:M:313:THR:HG22	1:M:314:LEU:N	2.30	0.47
1:N:227:ILE:CD1	1:N:309:LEU:HD11	2.45	0.47
2:S:3:ILE:HD13	2:S:11:ILE:HG21	1.96	0.47
1:A:128:VAL:HG21	1:A:505:GLN:HE21	1.80	0.47
1:A:262:LEU:O	1:A:266:THR:HG23	2.14	0.47
1:B:147:VAL:HG23	1:B:403:THR:HG22	1.97	0.47
1:B:259:LEU:O	1:B:263:VAL:HG23	2.15	0.47
1:B:326:ASN:OD1	1:B:329:THR:HB	2.15	0.47
1:C:100:ILE:HD11	1:C:514:MET:CE	2.45	0.47
1:C:447:MET:O	1:C:450:PRO:HD2	2.14	0.47
1:D:42:LYS:HE2	1:D:48:THR:HG1	1.79	0.47
1:E:346:VAL:O	1:E:349:ILE:HB	2.15	0.47
1:E:359:ASP:O	1:E:360:TYR:HB3	2.15	0.47
1:F:291:ASP:HB2	1:F:372:LEU:HD21	1.96	0.47
1:G:21:ASN:HD22	1:G:97:GLN:HE22	1.63	0.47
1:G:238:GLU:CB	2:U:24:GLY:HA3	2.44	0.47
1:K:174:VAL:HG13	1:K:194:GLN:OE1	2.14	0.47
1:L:37:ASN:HD22	1:M:517:THR:HA	1.80	0.47
1:L:39:VAL:HG23	1:M:517:THR:HG21	1.95	0.47
1:L:174:VAL:HG21	1:L:194:GLN:HB3	1.96	0.47
1:L:223:ALA:HB3	1:L:251:ALA:HB2	1.97	0.47
1:L:348:GLN:O	1:L:352:GLN:HG3	2.13	0.47
2:P:78:ILE:HD12	2:P:83:VAL:HG21	1.96	0.47
2:Q:66:ILE:HD12	2:Q:93:ALA:HB3	1.97	0.47
1:A:147:VAL:O	1:A:150:ILE:HG22	2.15	0.47
1:A:447:MET:O	1:A:450:PRO:HD2	2.15	0.47
1:E:174:VAL:HG21	1:E:367:GLU:HA	1.97	0.47
1:H:114:MET:SD	1:N:34:LYS:HB3	2.54	0.47
1:J:241:ALA:HB2	1:J:271:VAL:CG2	2.44	0.47
1:J:459:GLY:HA3	1:K:112:ASN:HD21	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:73:VAL:HG11	2:T:84:LEU:HD23	1.96	0.47
2:U:3:ILE:HG13	2:U:78:ILE:HD13	1.97	0.47
1:A:65:LYS:HZ2	1:A:523:ASP:HB2	1.80	0.47
1:B:111:MET:HG2	1:B:435:ASP:OD1	2.14	0.47
1:D:452:ARG:HB2	1:D:462:PRO:HB3	1.97	0.47
1:E:39:VAL:HG22	1:E:49:ILE:HG12	1.97	0.47
1:G:302:SER:O	1:G:307:MET:HB2	2.15	0.47
1:H:478:TYR:HB2	1:H:485:TYR:CE2	2.50	0.47
1:I:223:ALA:HB3	1:I:251:ALA:HB2	1.96	0.47
1:I:326:ASN:HD21	1:I:329:THR:HB	1.79	0.47
1:J:37:ASN:OD1	1:K:513:LEU:HD12	2.15	0.47
1:J:104:LEU:O	1:J:107:VAL:HG22	2.15	0.47
2:P:7:HIS:HB2	2:P:46:GLY:O	2.15	0.47
2:Q:14:ARG:NH2	2:Q:84:LEU:HD21	2.29	0.47
2:Q:48:ILE:HG22	2:Q:48:ILE:O	2.15	0.47
1:A:288:MET:HA	1:A:291:ASP:OD1	2.15	0.47
1:A:522:THR:HA	1:B:41:ASP:HB2	1.96	0.47
1:B:85:ALA:O	1:B:401:HIS:HB3	2.15	0.47
1:D:210:THR:O	1:D:210:THR:HG22	2.15	0.47
1:D:417:VAL:O	1:D:420:ILE:HG22	2.14	0.47
1:E:306:GLY:HA3	1:F:264:VAL:HG21	1.97	0.47
1:E:392:LYS:O	1:E:396:VAL:HG23	2.15	0.47
1:F:222:LEU:HD22	1:F:300:VAL:HG22	1.97	0.47
1:F:237:LEU:C	1:F:237:LEU:HD23	2.35	0.47
1:I:157:THR:O	1:I:161:LEU:HD13	2.14	0.47
1:L:478:TYR:HB2	1:L:485:TYR:CE2	2.50	0.47
1:N:319:GLN:HB2	1:N:336:VAL:CG2	2.44	0.47
2:O:14:ARG:HG2	2:O:15:LYS:O	2.15	0.47
2:T:13:LYS:HB3	2:T:41:LEU:HD11	1.96	0.47
1:A:114:MET:HG3	1:A:118:ARG:NH1	2.31	0.46
1:B:266:THR:HA	1:B:271:VAL:O	2.14	0.46
1:B:349:ILE:HG23	1:B:365:LEU:HD21	1.96	0.46
1:C:419:LEU:HA	1:C:422:VAL:HG22	1.97	0.46
1:C:443:ALA:O	1:C:447:MET:HG3	2.16	0.46
1:E:306:GLY:HA3	1:F:264:VAL:CG2	2.45	0.46
1:E:452:ARG:HB2	1:E:462:PRO:HB2	1.96	0.46
1:F:113:PRO:HA	1:F:116:LEU:HD12	1.97	0.46
1:G:100:ILE:CD1	1:G:514:MET:HG2	2.45	0.46
1:G:227:ILE:HA	1:G:230:ILE:HG22	1.95	0.46
1:H:41:ASP:HB2	1:I:69:MET:CE	2.45	0.46
1:H:199:TYR:CE1	1:H:202:PRO:HA	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:266:THR:HG22	1:I:272:LYS:HA	1.98	0.46
1:K:197:ARG:HE	1:K:277:LYS:HB3	1.80	0.46
1:N:277:LYS:HB2	1:N:277:LYS:NZ	2.30	0.46
2:S:14:ARG:NH2	2:S:84:LEU:HD21	2.30	0.46
1:A:215:LEU:HB3	1:A:246:PRO:HB2	1.96	0.46
1:A:228:SER:HA	1:A:255:GLU:HG2	1.97	0.46
1:A:281:PHE:HB3	1:A:284:ARG:HE	1.80	0.46
1:B:247:LEU:HB3	1:B:273:VAL:HG13	1.98	0.46
1:C:302:SER:HB3	1:C:305:ILE:HD13	1.97	0.46
1:D:215:LEU:HB3	1:D:246:PRO:HB2	1.98	0.46
1:E:149:THR:HG23	1:E:155:ASP:C	2.35	0.46
1:F:270:ILE:HG21	2:T:26:VAL:HA	1.98	0.46
1:F:349:ILE:O	1:F:352:GLN:HB2	2.15	0.46
1:G:102:GLU:HG3	1:G:445:ARG:HD3	1.96	0.46
1:I:46:ALA:CA	1:J:72:GLN:HB3	2.46	0.46
1:I:224:ASP:HB3	1:I:302:SER:HA	1.97	0.46
1:I:319:GLN:HB2	1:I:336:VAL:HG21	1.96	0.46
1:J:194:GLN:HG3	1:J:331:THR:HB	1.97	0.46
1:L:443:ALA:O	1:L:447:MET:HG3	2.15	0.46
1:N:191:GLU:OE1	1:N:342:ILE:HG21	2.15	0.46
2:U:50:GLU:HG2	2:U:50:GLU:O	2.15	0.46
1:B:209:GLU:O	1:B:210:THR:HB	2.16	0.46
1:C:161:LEU:HD21	1:C:379:ILE:HG23	1.97	0.46
1:C:236:VAL:HG22	1:C:312:ALA:O	2.14	0.46
1:C:348:GLN:HA	1:D:209:GLU:HG2	1.96	0.46
1:D:102:GLU:HB3	1:D:442:VAL:HG13	1.97	0.46
1:D:217:SER:N	1:D:218:PRO:HD3	2.31	0.46
1:E:77:VAL:HG11	1:E:510:VAL:HG21	1.94	0.46
1:G:124:VAL:HG21	1:G:508:ALA:HB1	1.96	0.46
1:G:281:PHE:O	1:G:284:ARG:HB3	2.15	0.46
1:G:365:LEU:O	1:G:369:VAL:HG23	2.15	0.46
1:J:5:ASP:HB2	1:J:524:LEU:CD2	2.45	0.46
1:J:138:CYS:SG	1:J:144:ILE:HD13	2.55	0.46
1:J:287:ALA:HB1	1:J:368:ARG:CZ	2.45	0.46
1:K:186:GLU:HB2	1:K:380:LYS:HB2	1.96	0.46
1:L:25:ASP:HA	1:L:28:LYS:HE2	1.97	0.46
1:L:101:THR:O	1:L:105:LYS:HG3	2.14	0.46
1:L:116:LEU:HD23	1:L:435:ASP:O	2.15	0.46
1:M:124:VAL:HG13	1:M:504:LEU:CD1	2.45	0.46
1:M:225:LYS:HD3	1:M:303:GLU:CD	2.35	0.46
1:M:229:ASN:HB3	1:M:232:GLU:OE1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:94:ILE:HB	2:T:4:ARG:HG3	1.98	0.46
2:T:68:ASN:CG	2:U:74:LYS:HD2	2.36	0.46
1:A:36:ARG:HD2	1:G:113:PRO:HG2	1.97	0.46
1:C:215:LEU:O	1:C:322:ARG:HG3	2.16	0.46
1:D:31:LEU:HD12	3:D:1:ADP:H5'1	1.97	0.46
1:D:392:LYS:O	1:D:396:VAL:HG23	2.16	0.46
1:E:120:ILE:O	1:E:124:VAL:HG23	2.16	0.46
1:H:287:ALA:HB1	1:H:368:ARG:NH2	2.31	0.46
1:J:6:VAL:HG22	1:J:521:VAL:HG22	1.98	0.46
1:K:191:GLU:HB3	1:K:295:LEU:CD1	2.45	0.46
1:L:17:LEU:HB2	1:L:104:LEU:CD2	2.45	0.46
1:M:284:ARG:HG2	1:M:364:LYS:HE2	1.98	0.46
1:N:221:LEU:HD12	1:N:249:ILE:HG23	1.98	0.46
1:N:225:LYS:HD3	1:N:303:GLU:HG3	1.98	0.46
1:N:423:ALA:HA	1:N:444:LEU:HD22	1.95	0.46
2:P:58:ASP:CB	2:Q:6:LEU:HD21	2.45	0.46
1:A:33:PRO:HD3	3:A:1:ADP:C5	2.50	0.46
1:B:291:ASP:HB2	1:B:372:LEU:CD2	2.45	0.46
1:B:309:LEU:CD1	1:B:309:LEU:H	2.29	0.46
1:C:33:PRO:HA	1:C:153:ASN:ND2	2.30	0.46
1:C:208:PRO:HB2	1:C:212:ALA:HB3	1.98	0.46
1:D:73:MET:HE3	1:E:49:ILE:HD11	1.97	0.46
1:D:465:VAL:O	1:D:469:VAL:HG23	2.16	0.46
1:E:238:GLU:HB2	2:S:24:GLY:CA	2.45	0.46
1:E:449:ALA:HA	1:E:452:ARG:CD	2.45	0.46
1:G:85:ALA:O	1:G:401:HIS:HB3	2.16	0.46
1:G:282:GLY:O	1:G:286:LYS:HG2	2.16	0.46
1:I:193:MET:HG3	1:I:371:LYS:HB3	1.97	0.46
1:K:104:LEU:HA	1:K:107:VAL:HG22	1.96	0.46
1:K:178:GLU:OE2	1:K:322:ARG:HD3	2.15	0.46
1:L:221:LEU:HD13	1:L:221:LEU:C	2.36	0.46
1:N:19:GLY:HA3	1:N:67:GLU:O	2.15	0.46
2:R:77:LYS:C	2:R:78:ILE:HD12	2.35	0.46
1:A:313:THR:HB	1:A:315:GLU:HG3	1.97	0.46
1:D:206:ASN:HB3	1:D:214:GLU:H	1.80	0.46
1:D:519:CYS:HB3	1:E:38:VAL:HG22	1.97	0.46
1:E:291:ASP:HB2	1:E:372:LEU:CD2	2.39	0.46
1:F:21:ASN:HA	1:F:97:GLN:HE22	1.80	0.46
1:F:246:PRO:HA	1:F:272:LYS:O	2.15	0.46
1:G:147:VAL:HG23	1:G:403:THR:HG22	1.97	0.46
1:H:224:ASP:HB3	1:H:302:SER:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:478:TYR:CE2	1:I:480:ALA:HA	2.50	0.46
1:K:77:VAL:HG22	1:K:506:TYR:HB3	1.97	0.46
1:K:205:ILE:HD12	1:K:205:ILE:N	2.31	0.46
1:L:166:MET:CE	1:L:407:VAL:HG21	2.46	0.46
1:L:345:ARG:HH22	1:L:368:ARG:HH22	1.62	0.46
1:N:102:GLU:HB2	1:N:442:VAL:HG13	1.97	0.46
1:N:225:LYS:HD3	1:N:303:GLU:CG	2.45	0.46
2:O:66:ILE:HD11	2:P:3:ILE:HG21	1.97	0.46
2:R:84:LEU:HB3	2:R:86:MET:HE3	1.97	0.46
1:B:204:PHE:CD2	1:B:274:ALA:HB2	2.50	0.46
1:B:258:ALA:O	1:B:262:LEU:HB2	2.15	0.46
1:B:455:VAL:HG21	1:B:465:VAL:HG11	1.96	0.46
1:C:123:ALA:HB2	1:C:440:ILE:HG23	1.98	0.46
1:D:100:ILE:HD13	1:D:514:MET:SD	2.55	0.46
1:D:230:ILE:O	1:D:230:ILE:CG1	2.64	0.46
1:E:252:GLU:HG3	1:E:285:ARG:NH1	2.30	0.46
1:F:202:PRO:O	1:F:205:ILE:HG13	2.15	0.46
1:F:217:SER:N	1:F:218:PRO:HD3	2.30	0.46
1:G:281:PHE:H	1:G:284:ARG:HD2	1.81	0.46
1:G:399:ALA:O	1:G:403:THR:HG23	2.16	0.46
1:H:284:ARG:HG2	1:H:364:LYS:HE2	1.98	0.46
1:K:39:VAL:HG23	1:L:517:THR:HG21	1.96	0.46
1:K:215:LEU:HB3	1:K:218:PRO:HG3	1.97	0.46
1:K:282:GLY:O	1:K:285:ARG:HG2	2.16	0.46
1:L:338:GLU:HA	1:L:338:GLU:OE1	2.16	0.46
1:M:351:GLN:O	1:M:354:GLU:HG2	2.16	0.46
2:O:12:VAL:HG23	2:O:84:LEU:HB2	1.98	0.46
2:R:6:LEU:HD12	2:R:6:LEU:O	2.16	0.46
1:A:351:GLN:HG2	1:B:210:THR:CB	2.45	0.46
1:B:447:MET:O	1:B:450:PRO:HD2	2.15	0.46
1:C:496:PRO:HG2	1:C:499:VAL:HG22	1.97	0.46
1:E:265:ASN:HB3	1:E:271:VAL:HG22	1.97	0.46
1:E:288:MET:HA	1:E:291:ASP:OD1	2.15	0.46
1:F:23:LEU:HD13	1:F:23:LEU:C	2.36	0.46
1:F:128:VAL:HG21	1:F:505:GLN:HE21	1.80	0.46
1:H:426:LEU:HD12	1:H:444:LEU:HD21	1.97	0.46
1:J:57:ALA:O	1:J:75:LYS:HE3	2.16	0.46
1:J:223:ALA:HB3	1:J:251:ALA:HB2	1.98	0.46
1:J:266:THR:HG21	1:J:273:VAL:O	2.15	0.46
1:K:12:ALA:HB1	1:K:520:MET:HG3	1.97	0.46
1:L:350:ARG:HA	1:L:353:ILE:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:84:ALA:O	1:N:498:LYS:HE2	2.16	0.46
1:N:284:ARG:HG2	1:N:364:LYS:HE3	1.96	0.46
2:Q:43:VAL:HG13	2:Q:57:LEU:HD12	1.97	0.46
1:B:204:PHE:CD1	1:B:266:THR:HB	2.51	0.46
1:B:418:ALA:O	1:B:422:VAL:HG13	2.16	0.46
1:C:230:ILE:HG23	1:C:309:LEU:CD2	2.46	0.46
1:D:447:MET:O	1:D:450:PRO:HD2	2.15	0.46
1:F:322:ARG:O	1:F:333:ILE:HG12	2.16	0.46
1:F:345:ARG:O	1:F:349:ILE:HG13	2.16	0.46
1:H:420:ILE:HG13	1:H:451:LEU:CD2	2.42	0.46
1:I:138:CYS:SG	1:I:144:ILE:HD13	2.56	0.46
1:J:284:ARG:HD2	1:J:364:LYS:HG2	1.98	0.46
1:K:122:LYS:HE2	1:K:429:LEU:HD11	1.98	0.46
1:K:428:ASP:O	1:K:430:ARG:HG2	2.15	0.46
1:L:65:LYS:HD3	1:L:522:THR:OG1	2.16	0.46
1:M:227:ILE:HD12	1:M:309:LEU:HD11	1.98	0.46
1:N:308:GLU:HG2	1:N:309:LEU:N	2.31	0.46
1:N:496:PRO:HD2	1:N:499:VAL:HG21	1.97	0.46
2:O:47:ARG:HB3	2:O:55:LYS:CG	2.46	0.46
2:S:12:VAL:HG12	2:S:40:VAL:HA	1.97	0.46
2:T:52:GLY:C	2:T:53:GLU:HG2	2.36	0.46
2:U:12:VAL:HG12	2:U:40:VAL:HA	1.98	0.46
1:D:122:LYS:HE2	1:D:429:LEU:HD11	1.97	0.46
1:E:123:ALA:HB2	1:E:440:ILE:HG23	1.98	0.46
1:E:215:LEU:HB3	1:E:246:PRO:HB2	1.97	0.46
1:E:348:GLN:CA	1:F:209:GLU:HG2	2.45	0.46
1:I:46:ALA:HA	1:J:72:GLN:HB3	1.98	0.46
1:K:20:VAL:CG2	1:K:74:VAL:HG21	2.46	0.46
1:M:265:ASN:O	1:M:269:GLY:HA3	2.15	0.46
1:N:218:PRO:HG2	1:N:323:VAL:CG1	2.45	0.46
1:A:345:ARG:O	1:A:348:GLN:HG3	2.17	0.45
1:B:195:PHE:CE1	1:B:330:THR:HB	2.51	0.45
1:D:228:SER:HA	1:D:255:GLU:CG	2.46	0.45
1:E:234:LEU:O	1:E:238:GLU:HB3	2.16	0.45
1:F:28:LYS:HD2	1:F:453:GLN:NE2	2.32	0.45
1:F:199:TYR:CE1	1:F:202:PRO:HA	2.51	0.45
1:F:225:LYS:HZ3	1:F:309:LEU:HA	1.81	0.45
1:G:199:TYR:HD1	1:G:199:TYR:H	1.63	0.45
1:H:296:THR:HB	1:H:318:GLY:HA3	1.99	0.45
1:J:228:SER:HA	1:J:255:GLU:HB2	1.97	0.45
1:K:139:SER:HA	1:K:171:LYS:NZ	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:247:LEU:H	1:N:273:VAL:HG12	1.80	0.45
1:A:262:LEU:HD11	1:A:273:VAL:CB	2.41	0.45
1:B:23:LEU:C	1:B:23:LEU:HD13	2.37	0.45
1:D:149:THR:HG23	1:D:155:ASP:C	2.37	0.45
1:D:174:VAL:HG21	1:D:367:GLU:HA	1.96	0.45
1:E:214:GLU:HA	1:E:323:VAL:O	2.16	0.45
1:G:261:THR:HB	2:U:28:THR:HA	1.97	0.45
1:J:200:LEU:HB3	1:J:259:LEU:HD11	1.99	0.45
1:L:140:ASP:O	1:L:144:ILE:HG12	2.16	0.45
1:N:286:LYS:HA	1:N:286:LYS:HE2	1.98	0.45
1:A:199:TYR:O	1:A:199:TYR:HD1	1.99	0.45
1:A:350:ARG:HD3	1:A:353:ILE:HD12	1.98	0.45
1:A:388:GLU:HA	1:G:513:LEU:HD11	1.97	0.45
1:C:21:ASN:HD22	1:C:97:GLN:HE22	1.63	0.45
1:D:69:MET:SD	1:D:522:THR:HB	2.56	0.45
1:D:128:VAL:HG21	1:D:505:GLN:HE21	1.81	0.45
1:E:448:GLU:O	1:E:452:ARG:HD2	2.16	0.45
1:F:204:PHE:CG	1:F:274:ALA:CB	3.00	0.45
1:G:124:VAL:HG21	1:G:508:ALA:CB	2.46	0.45
1:G:124:VAL:HG13	1:G:504:LEU:CD1	2.46	0.45
1:H:41:ASP:HB2	1:I:69:MET:HE2	1.97	0.45
1:I:266:THR:HG21	1:I:273:VAL:O	2.17	0.45
1:I:345:ARG:CG	1:I:345:ARG:NH1	2.77	0.45
1:I:385:THR:HG23	1:I:388:GLU:H	1.80	0.45
1:L:478:TYR:CE2	1:L:480:ALA:HA	2.50	0.45
1:M:276:VAL:HG13	1:M:325:ILE:HD13	1.99	0.45
1:M:287:ALA:HB1	1:M:368:ARG:NH2	2.31	0.45
1:C:175:ILE:HA	1:C:377:ALA:O	2.17	0.45
1:D:199:TYR:CE1	1:D:202:PRO:HA	2.51	0.45
1:D:418:ALA:O	1:D:422:VAL:HG13	2.16	0.45
1:E:256:GLY:HA2	1:E:259:LEU:HB2	1.98	0.45
1:F:234:LEU:N	1:F:235:PRO:HD2	2.31	0.45
1:G:217:SER:N	1:G:218:PRO:HD3	2.30	0.45
1:J:215:LEU:HB2	1:J:323:VAL:CG1	2.47	0.45
1:K:98:ALA:HB1	1:K:446:ALA:HA	1.98	0.45
1:K:247:LEU:H	1:K:273:VAL:HG12	1.81	0.45
1:K:417:VAL:HG21	1:K:488:MET:HG3	1.98	0.45
1:M:161:LEU:HA	1:M:164:GLU:HG2	1.99	0.45
2:T:14:ARG:HG2	2:T:15:LYS:O	2.16	0.45
2:U:3:ILE:HD11	2:U:11:ILE:HG21	1.97	0.45
1:A:290:GLN:O	1:A:294:THR:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:THR:O	1:A:359:ASP:N	2.49	0.45
1:C:392:LYS:O	1:C:396:VAL:HG23	2.16	0.45
1:D:116:LEU:HD23	1:D:435:ASP:O	2.16	0.45
1:D:240:VAL:HG21	1:D:247:LEU:HD23	1.97	0.45
1:E:147:VAL:HA	1:E:150:ILE:HG22	1.98	0.45
1:E:496:PRO:HG2	1:E:499:VAL:CG2	2.47	0.45
1:F:205:ILE:HG12	1:F:211:GLY:HA2	1.99	0.45
1:F:362:ARG:O	1:F:366:GLN:HB2	2.17	0.45
1:G:42:LYS:HE2	1:G:48:THR:OG1	2.17	0.45
1:G:414:GLY:HA3	1:G:493:ILE:HG22	1.98	0.45
1:I:388:GLU:O	1:I:391:GLU:HB3	2.17	0.45
1:K:475:ASN:ND2	1:K:489:ILE:HD12	2.31	0.45
1:L:169:VAL:HG13	1:L:173:GLY:HA3	1.99	0.45
1:M:313:THR:HB	1:M:315:GLU:HG2	1.98	0.45
2:T:68:ASN:HD22	2:T:92:LEU:HD12	1.80	0.45
2:U:7:HIS:ND1	2:U:48:ILE:HD11	2.31	0.45
1:C:115:ASP:O	1:C:436:GLN:HG2	2.17	0.45
1:D:199:TYR:O	1:D:199:TYR:HD1	1.99	0.45
1:E:449:ALA:O	1:E:452:ARG:HG2	2.16	0.45
1:F:111:MET:CE	1:F:438:VAL:HG21	2.46	0.45
1:H:321:LYS:HD2	1:H:334:ASP:OD2	2.16	0.45
1:H:496:PRO:HD2	1:H:499:VAL:HG21	1.99	0.45
1:I:294:THR:OG1	1:I:345:ARG:HD2	2.17	0.45
1:J:28:LYS:CE	1:J:97:GLN:HE22	2.29	0.45
1:L:30:THR:HG22	1:L:36:ARG:O	2.16	0.45
1:M:3:ALA:HB3	1:M:524:LEU:HD12	1.99	0.45
1:N:34:LYS:HD2	1:N:458:CYS:SG	2.57	0.45
2:S:46:GLY:HA3	2:S:55:LYS:O	2.16	0.45
2:S:49:LEU:O	2:S:50:GLU:HB3	2.16	0.45
2:S:68:ASN:HB2	2:S:92:LEU:HD11	1.98	0.45
1:A:23:LEU:HD13	1:A:23:LEU:C	2.37	0.45
1:A:496:PRO:HG2	1:A:499:VAL:HG22	1.99	0.45
1:B:305:ILE:HG22	1:B:306:GLY:N	2.29	0.45
1:D:246:PRO:HA	1:D:272:LYS:O	2.16	0.45
1:F:64:ASP:HB3	1:F:67:GLU:HB2	1.99	0.45
1:F:288:MET:HA	1:F:291:ASP:OD1	2.17	0.45
1:G:26:ALA:O	1:G:29:VAL:HG22	2.16	0.45
1:G:432:GLN:HE21	1:G:436:GLN:HE22	1.64	0.45
1:G:496:PRO:HG2	1:G:499:VAL:HG22	1.98	0.45
1:K:235:PRO:CG	1:K:310:GLU:HA	2.46	0.45
1:M:311:LYS:N	1:M:311:LYS:HD2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:314:LEU:H	1:M:314:LEU:HD12	1.82	0.45
2:Q:11:ILE:HG12	2:Q:85:ILE:HG12	1.99	0.45
2:T:91:ILE:O	2:U:6:LEU:HB3	2.17	0.45
1:C:320:ALA:HA	1:C:335:GLY:HA2	1.99	0.45
1:D:190:VAL:HG11	1:D:194:GLN:OE1	2.15	0.45
1:E:175:ILE:H	1:E:404:ARG:NH2	2.14	0.45
1:E:414:GLY:O	1:E:417:VAL:HG12	2.16	0.45
1:F:271:VAL:HB	1:F:273:VAL:HG23	1.98	0.45
1:G:241:ALA:CB	2:U:25:ILE:HB	2.46	0.45
1:H:17:LEU:HB2	1:H:104:LEU:HD23	1.99	0.45
1:M:178:GLU:OE2	1:M:322:ARG:HD3	2.17	0.45
1:M:308:GLU:HG2	1:M:309:LEU:N	2.32	0.45
1:N:57:ALA:O	1:N:75:LYS:HE3	2.17	0.45
1:N:174:VAL:HG11	1:N:194:GLN:HB2	1.99	0.45
1:N:479:ASN:CB	1:N:491:MET:HE1	2.47	0.45
2:Q:5:PRO:CD	2:Q:42:ALA:HB1	2.46	0.45
1:A:207:LYS:HB2	1:A:208:PRO:HD3	1.98	0.45
1:B:116:LEU:HD23	1:B:435:ASP:O	2.17	0.45
1:B:352:GLN:OE1	1:B:365:LEU:HD11	2.17	0.45
1:C:87:ASP:HB3	1:C:499:VAL:HG11	1.99	0.45
1:C:399:ALA:O	1:C:403:THR:HG23	2.17	0.45
1:D:16:MET:O	1:D:20:VAL:HG23	2.17	0.45
1:E:24:ALA:O	1:E:28:LYS:HG3	2.16	0.45
1:E:195:PHE:HD1	1:E:197:ARG:HD3	1.78	0.45
1:E:278:ALA:HB1	1:E:279:PRO:HD2	1.98	0.45
1:F:102:GLU:HB2	1:F:442:VAL:HG13	1.98	0.45
1:F:326:ASN:OD1	1:F:329:THR:HB	2.17	0.45
1:G:99:ILE:HD13	1:G:446:ALA:CB	2.46	0.45
1:G:234:LEU:CB	2:U:23:GLY:HA3	2.46	0.45
1:G:392:LYS:O	1:G:396:VAL:HG23	2.17	0.45
1:H:124:VAL:O	1:H:128:VAL:HG23	2.17	0.45
1:H:124:VAL:HG21	1:H:508:ALA:CB	2.47	0.45
1:J:229:ASN:HD21	1:J:231:ARG:HH12	1.63	0.45
1:J:313:THR:HG22	1:J:314:LEU:H	1.82	0.45
1:K:385:THR:HG23	1:K:388:GLU:H	1.82	0.45
1:M:496:PRO:HD2	1:M:499:VAL:HG21	1.98	0.45
1:N:32:GLY:HA2	1:N:454:ILE:HD12	1.99	0.45
1:A:187:LEU:HD13	1:A:379:ILE:HG12	1.97	0.45
1:B:262:LEU:HD11	1:B:273:VAL:CB	2.31	0.45
1:C:102:GLU:HB3	1:C:442:VAL:HG13	1.99	0.45
1:D:270:ILE:HG22	1:D:271:VAL:HG13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:479:ASN:CG	1:D:493:ILE:HD11	2.37	0.45
1:E:252:GLU:HA	1:E:285:ARG:NH1	2.32	0.45
1:E:264:VAL:HG11	2:S:27:LEU:HD22	1.99	0.45
1:F:206:ASN:HB3	1:F:214:GLU:H	1.82	0.45
1:F:487:ASN:O	1:F:491:MET:HG3	2.16	0.45
1:G:28:LYS:HG2	1:G:94:VAL:HG22	1.99	0.45
1:G:82:ASN:HB2	1:G:89:THR:HG21	1.99	0.45
1:H:27:VAL:HG11	1:H:93:THR:HG21	1.99	0.45
1:K:218:PRO:HG2	1:K:323:VAL:CG1	2.46	0.45
2:P:50:GLU:O	2:P:50:GLU:HG2	2.17	0.45
2:P:86:MET:HB2	2:P:90:ASP:OD2	2.17	0.45
2:Q:3:ILE:HG12	2:Q:78:ILE:HG13	1.98	0.45
1:A:36:ARG:HB3	1:G:518:GLU:CB	2.47	0.44
1:A:313:THR:HG22	1:A:314:LEU:H	1.83	0.44
1:C:33:PRO:HD3	3:C:1:ADP:C5	2.52	0.44
1:C:113:PRO:CB	1:C:516:THR:HA	2.48	0.44
1:D:50:THR:HA	1:D:391:GLU:OE2	2.17	0.44
1:D:351:GLN:HG2	1:E:210:THR:OG1	2.16	0.44
1:E:5:ASP:O	1:E:521:VAL:HA	2.16	0.44
1:E:301:ILE:HA	1:E:307:MET:SD	2.58	0.44
1:E:517:THR:CG2	1:F:39:VAL:HG23	2.47	0.44
1:F:461:GLU:H	1:F:461:GLU:HG2	1.64	0.44
1:G:215:LEU:O	1:G:322:ARG:HG3	2.17	0.44
1:J:66:PHE:CZ	1:J:522:THR:HG22	2.52	0.44
1:K:164:GLU:O	1:K:168:LYS:HG2	2.17	0.44
1:K:193:MET:H	1:K:332:ILE:HG13	1.81	0.44
1:K:228:SER:HA	1:K:255:GLU:HB2	1.99	0.44
2:S:11:ILE:HB	2:S:42:ALA:HB3	1.99	0.44
1:A:41:ASP:HB2	1:G:69:MET:SD	2.57	0.44
1:B:217:SER:N	1:B:218:PRO:HD3	2.32	0.44
1:C:221:LEU:HD11	1:C:301:ILE:HD11	1.99	0.44
1:C:237:LEU:C	1:C:237:LEU:HD23	2.37	0.44
1:D:496:PRO:O	1:D:499:VAL:HG22	2.18	0.44
1:E:287:ALA:HB1	1:E:368:ARG:HH22	1.82	0.44
1:G:39:VAL:HG13	1:G:48:THR:O	2.17	0.44
1:I:56:VAL:O	1:I:60:ILE:HG12	2.18	0.44
1:K:66:PHE:O	1:K:69:MET:HB2	2.17	0.44
1:M:191:GLU:HB3	1:M:295:LEU:CD1	2.48	0.44
1:M:235:PRO:HG2	1:M:310:GLU:HA	1.98	0.44
1:M:319:GLN:HE21	1:M:336:VAL:HG21	1.83	0.44
1:N:42:LYS:HG2	1:N:43:SER:H	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:71:TYR:O	2:P:74:LYS:HE2	2.17	0.44
2:S:7:HIS:HB3	2:S:45:ASN:HB2	1.99	0.44
2:S:60:LYS:HG2	2:S:63:ASP:OD2	2.17	0.44
1:A:113:PRO:HB2	1:A:516:THR:HG23	1.98	0.44
1:B:85:ALA:CB	1:B:499:VAL:HG12	2.47	0.44
1:B:261:THR:CB	2:P:29:GLY:H	2.29	0.44
1:C:31:LEU:HD22	1:C:94:VAL:HG21	1.99	0.44
1:C:105:LYS:HG3	1:J:109:ALA:O	2.17	0.44
1:C:449:ALA:HA	1:C:452:ARG:HG2	1.99	0.44
1:E:365:LEU:HD13	1:E:366:GLN:NE2	2.32	0.44
1:E:406:ALA:HB2	1:E:496:PRO:HB3	1.98	0.44
1:G:23:LEU:HD13	1:G:23:LEU:C	2.37	0.44
1:G:350:ARG:HA	1:G:353:ILE:HD12	1.99	0.44
1:H:383:ALA:HB3	1:H:389:MET:HB2	1.97	0.44
1:I:228:SER:HA	1:I:255:GLU:HB2	1.99	0.44
1:K:199:TYR:CZ	1:K:205:ILE:HD11	2.52	0.44
1:L:124:VAL:O	1:L:128:VAL:HG23	2.17	0.44
1:M:228:SER:HA	1:M:255:GLU:HG2	2.00	0.44
1:M:296:THR:HB	1:M:318:GLY:HA3	1.99	0.44
1:N:179:ASP:HA	1:N:389:MET:HE3	1.99	0.44
1:A:162:ILE:HG21	1:A:403:THR:HG21	2.00	0.44
1:C:30:THR:CG2	1:C:38:VAL:HG23	2.48	0.44
1:C:142:LYS:O	1:C:146:GLN:HG3	2.17	0.44
1:C:254:VAL:HG12	1:C:259:LEU:HG	2.00	0.44
1:C:257:GLU:O	1:C:261:THR:HG22	2.18	0.44
1:C:452:ARG:HB2	1:C:462:PRO:CB	2.45	0.44
1:D:31:LEU:HD22	1:D:94:VAL:HG21	2.00	0.44
1:D:513:LEU:HD11	1:E:388:GLU:HG3	1.99	0.44
1:E:447:MET:O	1:E:450:PRO:HD2	2.18	0.44
1:G:204:PHE:CD1	1:G:266:THR:CB	3.00	0.44
1:G:296:THR:HG22	1:G:335:GLY:HA3	1.99	0.44
1:G:349:ILE:O	1:G:352:GLN:HB2	2.17	0.44
1:I:350:ARG:HE	1:I:369:VAL:HG11	1.82	0.44
1:J:409:GLU:OE1	1:J:498:LYS:HA	2.18	0.44
1:M:249:ILE:HB	1:M:275:ALA:CB	2.47	0.44
1:M:478:TYR:CE2	1:M:480:ALA:HA	2.53	0.44
1:N:214:GLU:HG2	1:N:324:VAL:CG1	2.41	0.44
2:P:37:ARG:HA	2:P:37:ARG:HD2	1.92	0.44
2:R:50:GLU:O	2:R:52:GLY:N	2.51	0.44
2:S:20:LYS:HZ3	2:S:27:LEU:HD11	1.82	0.44
1:B:414:GLY:O	1:B:417:VAL:HG12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:510:VAL:HG13	1:C:385:THR:HG21	1.98	0.44
1:C:33:PRO:HA	1:C:153:ASN:HD21	1.83	0.44
1:C:214:GLU:HA	1:C:323:VAL:O	2.17	0.44
1:C:281:PHE:O	1:C:284:ARG:HG2	2.18	0.44
1:C:487:ASN:HB3	1:C:490:ASP:HB2	1.99	0.44
1:D:113:PRO:HA	1:D:116:LEU:HD12	1.99	0.44
1:D:183:LEU:HD21	1:D:384:ALA:HB2	2.00	0.44
1:D:217:SER:N	1:D:218:PRO:CD	2.80	0.44
1:E:118:ARG:HD2	1:E:436:GLN:HE21	1.83	0.44
1:F:429:LEU:O	1:F:440:ILE:HG21	2.18	0.44
1:G:147:VAL:O	1:G:150:ILE:HG22	2.18	0.44
1:H:266:THR:HG21	1:H:273:VAL:O	2.18	0.44
1:N:40:LEU:HD22	1:N:40:LEU:N	2.33	0.44
1:N:120:ILE:HG23	1:N:443:ALA:HB2	1.99	0.44
2:S:86:MET:HB2	2:S:90:ASP:OD2	2.17	0.44
1:B:85:ALA:HB3	1:B:499:VAL:HG12	2.00	0.44
1:B:278:ALA:HB1	1:B:285:ARG:HB2	1.99	0.44
1:C:414:GLY:HA2	1:C:495:ASP:OD2	2.17	0.44
1:F:8:PHE:CD2	1:F:519:CYS:SG	3.06	0.44
1:F:268:ARG:HA	1:F:268:ARG:HE	1.82	0.44
1:F:443:ALA:O	1:F:447:MET:HG3	2.18	0.44
1:G:16:MET:O	1:G:20:VAL:HG23	2.17	0.44
1:G:175:ILE:HA	1:G:377:ALA:O	2.17	0.44
1:G:301:ILE:HA	1:G:307:MET:CE	2.47	0.44
1:H:144:ILE:HG21	1:H:163:ALA:HA	1.99	0.44
1:H:277:LYS:NZ	1:H:277:LYS:HB2	2.32	0.44
1:I:345:ARG:O	1:I:348:GLN:HB2	2.18	0.44
1:J:100:ILE:HG23	1:J:104:LEU:CD2	2.47	0.44
1:K:124:VAL:O	1:K:128:VAL:HG23	2.16	0.44
1:K:178:GLU:O	1:K:380:LYS:HA	2.18	0.44
1:L:487:ASN:O	1:L:491:MET:HG3	2.17	0.44
2:U:78:ILE:O	2:U:79:ASP:HB2	2.18	0.44
1:A:239:ALA:HB1	1:A:314:LEU:HD23	2.00	0.44
1:B:214:GLU:HA	1:B:323:VAL:O	2.18	0.44
1:B:231:ARG:HB2	1:B:257:GLU:OE1	2.17	0.44
1:B:496:PRO:O	1:B:499:VAL:HG22	2.16	0.44
1:C:166:MET:SD	1:C:403:THR:HB	2.58	0.44
1:C:199:TYR:HB3	1:C:325:ILE:HG21	1.99	0.44
1:C:221:LEU:HD11	1:C:301:ILE:CD1	2.48	0.44
1:C:247:LEU:HB3	1:C:273:VAL:CG1	2.48	0.44
1:C:345:ARG:O	1:C:348:GLN:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4:LYS:HB3	1:E:521:VAL:HG12	2.00	0.44
1:E:461:GLU:H	1:E:461:GLU:HG2	1.60	0.44
1:G:147:VAL:HG12	1:G:494:LEU:HB2	1.98	0.44
1:H:198:GLY:CA	1:H:328:ASP:HA	2.48	0.44
1:I:6:VAL:HG22	1:I:521:VAL:HG22	1.99	0.44
1:J:193:MET:H	1:J:332:ILE:HG13	1.83	0.44
1:J:227:ILE:HG21	1:J:233:MET:SD	2.57	0.44
1:J:284:ARG:CG	1:J:364:LYS:HE2	2.48	0.44
1:L:295:LEU:HD23	1:L:332:ILE:HD11	1.99	0.44
1:M:166:MET:CE	1:M:407:VAL:HG21	2.48	0.44
2:O:68:ASN:ND2	2:P:74:LYS:HE3	2.33	0.44
1:B:24:ALA:O	1:B:28:LYS:HG3	2.18	0.44
1:C:221:LEU:HD13	1:C:317:LEU:HD21	1.99	0.44
1:C:496:PRO:HG2	1:C:499:VAL:CG2	2.48	0.44
1:E:30:THR:CG2	1:E:38:VAL:HG23	2.47	0.44
1:E:33:PRO:HG3	3:E:1:ADP:C6	2.53	0.44
1:G:77:VAL:HG11	1:G:510:VAL:HG21	1.98	0.44
1:G:219:PHE:O	1:G:247:LEU:HD22	2.18	0.44
1:H:40:LEU:HD23	1:I:521:VAL:HB	2.00	0.44
1:H:179:ASP:HA	1:H:389:MET:CE	2.48	0.44
1:H:476:TYR:HA	1:H:486:GLY:O	2.17	0.44
1:I:47:PRO:HG3	1:J:69:MET:HB3	1.98	0.44
1:J:29:VAL:HB	1:J:36:ARG:HB2	2.00	0.44
1:L:494:LEU:N	1:L:494:LEU:HD23	2.33	0.44
1:M:285:ARG:CG	1:M:286:LYS:N	2.80	0.44
1:N:55:SER:HA	1:N:58:ARG:NH1	2.33	0.44
2:P:6:LEU:HD12	2:P:6:LEU:HA	1.75	0.44
2:Q:48:ILE:HG12	2:Q:54:VAL:CG1	2.48	0.44
1:A:200:LEU:HD22	1:A:254:VAL:HB	1.99	0.44
1:A:215:LEU:O	1:A:322:ARG:HG3	2.17	0.44
1:B:199:TYR:H	1:B:199:TYR:HD1	1.66	0.44
1:B:202:PRO:O	1:B:205:ILE:HG13	2.18	0.44
1:B:325:ILE:CD1	1:B:330:THR:HG23	2.48	0.44
1:B:399:ALA:O	1:B:403:THR:HG23	2.17	0.44
1:C:161:LEU:CD1	1:C:187:LEU:HB2	2.35	0.44
1:C:513:LEU:HD11	1:D:388:GLU:CA	2.32	0.44
1:D:120:ILE:O	1:D:124:VAL:HG23	2.17	0.44
1:H:284:ARG:HG2	1:H:364:LYS:HZ1	1.82	0.44
1:H:302:SER:HB2	1:H:305:ILE:HD12	2.00	0.44
1:I:174:VAL:HG21	1:I:194:GLN:HB3	2.00	0.44
1:I:496:PRO:O	1:I:499:VAL:HG22	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:178:GLU:OE2	1:J:322:ARG:HD3	2.17	0.44
1:J:232:GLU:HB3	1:J:309:LEU:HB2	1.99	0.44
1:M:222:LEU:HD13	1:M:293:ALA:HB2	2.00	0.44
1:M:287:ALA:HB1	1:M:368:ARG:CZ	2.47	0.44
1:N:144:ILE:HG21	1:N:163:ALA:HA	2.00	0.44
2:S:3:ILE:HD13	2:S:11:ILE:HD13	1.99	0.44
1:D:229:ASN:C	1:D:231:ARG:H	2.21	0.43
1:F:199:TYR:O	1:F:199:TYR:CD1	2.71	0.43
1:G:107:VAL:HG22	1:G:113:PRO:HG3	1.99	0.43
1:G:122:LYS:HE2	1:G:429:LEU:HD11	2.00	0.43
1:G:233:MET:O	1:G:236:VAL:HB	2.18	0.43
1:G:237:LEU:HD23	1:G:237:LEU:C	2.38	0.43
1:H:63:GLU:HA	1:I:3:ALA:HB2	2.00	0.43
1:H:72:GLN:HB3	1:N:47:PRO:HD2	2.00	0.43
1:I:432:GLN:H	1:I:436:GLN:NE2	2.16	0.43
1:L:288:MET:HA	1:L:288:MET:CE	2.48	0.43
1:M:37:ASN:OD1	1:N:513:LEU:HD12	2.17	0.43
1:N:222:LEU:HB3	1:N:289:LEU:HD11	2.00	0.43
2:P:14:ARG:CD	2:P:34:LYS:HE2	2.47	0.43
2:P:66:ILE:HG21	2:Q:76:GLU:HG3	1.99	0.43
2:S:48:ILE:HG12	2:S:54:VAL:HG22	2.00	0.43
1:A:264:VAL:HG13	1:G:305:ILE:HG23	2.00	0.43
1:A:519:CYS:HB3	1:B:38:VAL:HG22	1.99	0.43
1:B:4:LYS:HG3	1:C:60:ILE:HA	2.00	0.43
1:B:150:ILE:HD11	3:B:1:ADP:C5	2.53	0.43
1:B:254:VAL:HG21	1:B:275:ALA:CB	2.47	0.43
1:B:345:ARG:O	1:B:349:ILE:HG13	2.17	0.43
1:C:150:ILE:HD11	3:C:1:ADP:C5	2.53	0.43
1:D:449:ALA:HA	1:D:452:ARG:HG2	1.99	0.43
1:E:280:GLY:HA2	1:E:285:ARG:HH21	1.83	0.43
1:F:188:ASP:OD2	1:F:380:LYS:HE3	2.18	0.43
1:H:20:VAL:CG2	1:H:74:VAL:HG21	2.47	0.43
1:H:517:THR:HA	1:N:37:ASN:ND2	2.33	0.43
1:I:259:LEU:O	1:I:263:VAL:HG23	2.18	0.43
1:J:466:ALA:O	1:J:470:LYS:HG2	2.17	0.43
1:L:225:LYS:HD3	1:L:303:GLU:CD	2.39	0.43
1:M:149:THR:HG22	1:M:156:GLU:HA	1.99	0.43
1:M:194:GLN:HG3	1:M:331:THR:HB	1.99	0.43
1:N:409:GLU:OE1	1:N:498:LYS:HA	2.18	0.43
1:A:100:ILE:CD1	1:A:514:MET:SD	3.05	0.43
1:C:233:MET:O	1:C:236:VAL:HB	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:207:LYS:HB3	1:D:207:LYS:NZ	2.32	0.43
1:D:225:LYS:HD3	1:D:225:LYS:N	2.33	0.43
1:D:248:LEU:C	1:D:248:LEU:HD13	2.39	0.43
1:E:116:LEU:HD23	1:E:435:ASP:O	2.18	0.43
1:F:31:LEU:CD1	3:F:1:ADP:H5'1	2.49	0.43
1:F:498:LYS:HG3	1:F:501:ARG:NH2	2.34	0.43
1:G:234:LEU:HD22	2:U:26:VAL:HG21	1.99	0.43
1:G:311:LYS:O	1:G:312:ALA:HB2	2.18	0.43
1:G:346:VAL:O	1:G:349:ILE:HB	2.17	0.43
1:I:102:GLU:HB2	1:I:442:VAL:HG13	2.00	0.43
1:M:57:ALA:O	1:M:75:LYS:HE3	2.18	0.43
1:M:295:LEU:HD23	1:M:332:ILE:HD11	2.00	0.43
1:M:443:ALA:O	1:M:447:MET:HG3	2.18	0.43
1:N:295:LEU:HD23	1:N:332:ILE:HD11	2.01	0.43
2:U:43:VAL:CG1	2:U:57:LEU:HD12	2.46	0.43
2:U:74:LYS:HB2	2:U:85:ILE:HB	2.00	0.43
1:A:276:VAL:HG21	1:A:330:THR:HG21	2.01	0.43
1:C:124:VAL:HG21	1:C:508:ALA:HB1	2.01	0.43
1:D:100:ILE:O	1:D:104:LEU:HG	2.17	0.43
1:E:65:LYS:HB3	1:E:522:THR:OG1	2.18	0.43
1:F:21:ASN:HD22	1:F:97:GLN:HE22	1.66	0.43
1:F:54:VAL:HB	1:F:89:THR:HG21	1.99	0.43
1:F:270:ILE:CD1	2:T:27:LEU:HB2	2.48	0.43
1:G:39:VAL:O	1:G:40:LEU:CB	2.66	0.43
1:G:52:ASP:OD1	1:G:54:VAL:HG12	2.18	0.43
1:G:231:ARG:HH21	2:U:26:VAL:CG1	2.32	0.43
1:H:6:VAL:HG22	1:H:521:VAL:HG22	2.01	0.43
1:I:420:ILE:HG13	1:I:451:LEU:CD2	2.45	0.43
1:J:47:PRO:HG3	1:K:69:MET:HA	2.00	0.43
1:J:449:ALA:HB3	1:J:450:PRO:HD3	2.00	0.43
1:K:223:ALA:O	1:K:251:ALA:HA	2.17	0.43
1:K:308:GLU:HB3	1:K:311:LYS:HD3	1.99	0.43
1:L:69:MET:CE	1:L:522:THR:HB	2.40	0.43
1:L:131:LEU:CD1	1:L:412:VAL:HG11	2.48	0.43
2:P:63:ASP:OD1	2:P:94:ILE:HG23	2.19	0.43
2:Q:55:LYS:HD3	2:R:51:ASN:HB2	2.00	0.43
2:R:6:LEU:C	2:R:6:LEU:CD1	2.87	0.43
2:R:6:LEU:HD22	2:R:7:HIS:CE1	2.52	0.43
2:S:96:GLU:OE2	2:T:4:ARG:HG2	2.18	0.43
1:B:124:VAL:O	1:B:128:VAL:HG23	2.18	0.43
1:B:246:PRO:HA	1:B:272:LYS:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:392:LYS:O	1:B:396:VAL:HG23	2.18	0.43
1:C:23:LEU:C	1:C:23:LEU:HD13	2.39	0.43
1:E:40:LEU:HD13	1:E:59:GLU:HG3	1.99	0.43
1:F:30:THR:CG2	1:F:38:VAL:HG23	2.48	0.43
1:F:200:LEU:O	1:F:202:PRO:HD3	2.18	0.43
1:F:349:ILE:HD13	1:F:369:VAL:HG22	2.01	0.43
1:G:117:LYS:HE3	1:G:513:LEU:CD2	2.49	0.43
1:H:152:ALA:O	1:H:153:ASN:HB2	2.19	0.43
1:I:225:LYS:HD3	1:I:303:GLU:CD	2.38	0.43
1:K:494:LEU:N	1:K:494:LEU:HD23	2.34	0.43
1:L:34:LYS:HB2	1:L:458:CYS:SG	2.59	0.43
1:L:266:THR:HG21	1:L:273:VAL:O	2.18	0.43
1:L:428:ASP:O	1:L:430:ARG:HG2	2.19	0.43
1:M:152:ALA:O	1:M:153:ASN:CB	2.66	0.43
1:N:20:VAL:CG2	1:N:74:VAL:HG21	2.48	0.43
1:N:277:LYS:HB2	1:N:277:LYS:HZ3	1.84	0.43
2:P:43:VAL:HG23	2:P:61:VAL:HG22	2.00	0.43
2:S:25:ILE:O	2:S:25:ILE:HG22	2.18	0.43
2:U:3:ILE:O	2:U:3:ILE:HD12	2.18	0.43
1:A:365:LEU:O	1:A:369:VAL:HG23	2.18	0.43
1:B:150:ILE:HG21	1:B:494:LEU:O	2.19	0.43
1:C:147:VAL:O	1:C:150:ILE:HG22	2.17	0.43
1:C:349:ILE:HD13	1:C:369:VAL:HG22	2.00	0.43
1:D:23:LEU:HD13	1:D:23:LEU:C	2.39	0.43
1:D:52:ASP:OD1	1:D:54:VAL:HG12	2.19	0.43
1:D:222:LEU:HD22	1:D:293:ALA:HB2	2.00	0.43
1:E:197:ARG:NH2	1:E:279:PRO:HD3	2.33	0.43
1:E:262:LEU:CD1	1:E:273:VAL:HB	2.45	0.43
1:F:124:VAL:O	1:F:128:VAL:HG23	2.17	0.43
1:F:213:VAL:HB	1:F:325:ILE:HB	2.00	0.43
1:F:413:ALA:HB1	1:F:488:MET:HB2	2.01	0.43
1:G:313:THR:HB	1:G:315:GLU:HG3	1.99	0.43
1:H:66:PHE:CZ	1:H:522:THR:HG22	2.54	0.43
1:H:319:GLN:O	1:H:336:VAL:HG23	2.19	0.43
1:H:421:ARG:O	1:H:425:LYS:HG2	2.18	0.43
1:I:131:LEU:CD1	1:I:422:VAL:HG11	2.48	0.43
1:I:423:ALA:HA	1:I:444:LEU:HD22	2.01	0.43
1:J:66:PHE:HA	1:J:69:MET:SD	2.59	0.43
1:J:130:GLU:HG3	1:J:426:LEU:HD22	2.00	0.43
1:K:39:VAL:HG23	1:L:517:THR:CG2	2.49	0.43
1:K:345:ARG:HH22	1:K:368:ARG:HH22	1.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:381:VAL:CG1	1:L:392:LYS:HD3	2.49	0.43
1:M:124:VAL:HG21	1:M:508:ALA:CB	2.47	0.43
1:M:200:LEU:HB3	1:M:259:LEU:CD1	2.48	0.43
1:M:434:GLU:HA	1:M:437:ASN:HD22	1.83	0.43
1:N:104:LEU:O	1:N:107:VAL:HG22	2.19	0.43
1:N:479:ASN:HB3	1:N:491:MET:HE1	2.00	0.43
2:O:96:GLU:O	2:O:97:ALA:HB3	2.19	0.43
2:S:5:PRO:HG3	2:S:42:ALA:HB1	2.00	0.43
2:S:91:ILE:O	2:T:6:LEU:HG	2.19	0.43
1:D:230:ILE:O	1:D:230:ILE:HG12	2.19	0.43
1:D:449:ALA:O	1:D:452:ARG:HG2	2.19	0.43
1:F:116:LEU:HD23	1:F:435:ASP:O	2.19	0.43
1:F:231:ARG:HH11	1:F:258:ALA:HB1	1.83	0.43
1:F:247:LEU:HD12	1:F:249:ILE:CG1	2.48	0.43
1:G:33:PRO:HA	1:G:153:ASN:HD21	1.82	0.43
1:G:149:THR:HG23	1:G:155:ASP:C	2.39	0.43
1:G:248:LEU:C	1:G:248:LEU:HD13	2.39	0.43
1:H:131:LEU:CD1	1:H:422:VAL:HG11	2.44	0.43
1:H:174:VAL:HG12	1:H:376:VAL:HG13	2.01	0.43
1:I:98:ALA:HB1	1:I:446:ALA:HA	2.01	0.43
1:I:215:LEU:HB3	1:I:218:PRO:CG	2.47	0.43
1:K:38:VAL:HG22	1:L:519:CYS:HB3	2.01	0.43
1:N:111:MET:SD	1:N:438:VAL:HG21	2.59	0.43
2:S:12:VAL:CG2	2:S:86:MET:HE1	2.48	0.43
1:A:24:ALA:O	1:A:28:LYS:HG3	2.19	0.43
1:A:418:ALA:O	1:A:422:VAL:HG13	2.19	0.43
1:B:37:ASN:HB3	1:B:49:ILE:CG2	2.48	0.43
1:B:100:ILE:O	1:B:104:LEU:HG	2.18	0.43
1:B:124:VAL:HG13	1:B:504:LEU:CD1	2.48	0.43
1:C:150:ILE:HG21	1:C:494:LEU:O	2.19	0.43
1:C:349:ILE:HG21	1:C:369:VAL:CG2	2.48	0.43
1:E:39:VAL:HA	1:E:48:THR:O	2.18	0.43
1:E:124:VAL:HG21	1:E:508:ALA:HB1	2.00	0.43
1:E:496:PRO:HG2	1:E:499:VAL:HG22	2.00	0.43
1:F:30:THR:HG22	1:F:36:ARG:O	2.18	0.43
1:F:232:GLU:O	1:F:310:GLU:HG3	2.19	0.43
1:G:147:VAL:HA	1:G:150:ILE:HG22	2.01	0.43
1:H:32:GLY:HA2	1:H:454:ILE:HD12	2.00	0.43
1:J:421:ARG:NH2	1:J:469:VAL:O	2.51	0.43
1:K:364:LYS:O	1:K:368:ARG:HG3	2.19	0.43
1:N:342:ILE:HG23	1:N:372:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:11:ILE:HA	2:S:84:LEU:O	2.18	0.43
1:A:365:LEU:HD22	1:A:366:GLN:HE22	1.83	0.43
1:B:145:ALA:O	1:B:159:GLY:HA3	2.18	0.43
1:D:21:ASN:ND2	1:D:97:GLN:HE22	2.17	0.43
1:D:113:PRO:CB	1:D:516:THR:HA	2.49	0.43
1:D:313:THR:HG22	1:D:314:LEU:H	1.84	0.43
1:D:464:VAL:HG22	1:J:467:ASN:CG	2.39	0.43
1:E:311:LYS:O	1:E:312:ALA:HB2	2.19	0.43
1:F:52:ASP:OD1	1:F:54:VAL:HG12	2.18	0.43
1:G:219:PHE:HB2	1:G:247:LEU:CD2	2.48	0.43
1:H:262:LEU:O	1:H:266:THR:HG23	2.18	0.43
1:I:146:GLN:HE21	1:I:150:ILE:HD11	1.84	0.43
1:I:325:ILE:HD11	1:I:330:THR:HG23	2.01	0.43
1:L:112:ASN:HA	1:L:113:PRO:HD3	1.93	0.43
1:L:198:GLY:HA3	1:L:327:LYS:O	2.18	0.43
2:R:47:ARG:HB3	2:R:55:LYS:CD	2.49	0.43
1:A:496:PRO:HG2	1:A:499:VAL:CG2	2.49	0.43
1:B:69:MET:SD	1:B:522:THR:HB	2.58	0.43
1:B:231:ARG:O	1:B:233:MET:HG2	2.19	0.43
1:C:239:ALA:HB1	1:C:314:LEU:CD2	2.46	0.43
1:D:113:PRO:HG2	1:E:36:ARG:HD3	2.01	0.43
1:E:28:LYS:HD2	1:E:453:GLN:CD	2.39	0.43
1:F:254:VAL:HG12	1:F:259:LEU:HG	2.01	0.43
1:K:217:SER:HA	1:K:320:ALA:O	2.18	0.43
1:L:150:ILE:HG21	1:L:494:LEU:HD21	2.00	0.43
1:L:438:VAL:O	1:L:442:VAL:HG23	2.19	0.43
1:M:178:GLU:OE2	1:M:333:ILE:HG21	2.19	0.43
1:A:220:ILE:HD13	1:A:296:THR:HG21	2.00	0.42
1:B:509:SER:HB2	1:C:384:ALA:HB3	2.01	0.42
1:C:305:ILE:HD11	1:D:203:TYR:CE1	2.54	0.42
1:D:393:LYS:NZ	1:D:393:LYS:HB3	2.34	0.42
1:E:33:PRO:CG	1:E:480:ALA:HB3	2.49	0.42
1:E:37:ASN:HB3	1:E:49:ILE:CG2	2.49	0.42
1:E:150:ILE:HD11	3:E:1:ADP:C5	2.54	0.42
1:E:517:THR:HG21	1:F:39:VAL:HG23	2.00	0.42
1:F:288:MET:HG3	1:F:368:ARG:HH21	1.83	0.42
1:G:40:LEU:HD22	1:G:59:GLU:CB	2.49	0.42
1:H:438:VAL:O	1:H:442:VAL:HG23	2.18	0.42
1:H:478:TYR:CE2	1:H:480:ALA:HA	2.54	0.42
1:K:46:ALA:HB1	1:K:47:PRO:HD2	2.01	0.42
1:L:224:ASP:HB3	1:L:302:SER:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:20:LYS:HB3	2:T:27:LEU:CD1	2.49	0.42
2:U:48:ILE:O	2:U:49:LEU:HD23	2.19	0.42
1:A:134:LEU:HD11	1:A:425:LYS:NZ	2.34	0.42
1:A:302:SER:CB	1:A:305:ILE:HB	2.50	0.42
1:A:409:GLU:HG2	1:A:409:GLU:O	2.19	0.42
1:B:76:GLU:OE2	1:C:387:VAL:HG13	2.19	0.42
1:B:266:THR:CG2	1:B:273:VAL:H	2.30	0.42
1:D:219:PHE:O	1:D:247:LEU:HD22	2.19	0.42
1:E:16:MET:O	1:E:20:VAL:HG23	2.18	0.42
1:E:25:ASP:HA	1:E:28:LYS:CE	2.49	0.42
1:E:228:SER:HB2	1:E:229:ASN:H	1.67	0.42
1:E:236:VAL:HG22	1:E:312:ALA:O	2.19	0.42
1:G:175:ILE:HG12	1:G:377:ALA:HB3	2.00	0.42
1:I:221:LEU:HD12	1:I:249:ILE:HG23	2.00	0.42
1:J:214:GLU:HG2	1:J:324:VAL:CG1	2.45	0.42
1:M:214:GLU:HG2	1:M:324:VAL:CG1	2.49	0.42
1:N:31:LEU:HG	1:N:454:ILE:HD11	2.01	0.42
1:N:149:THR:CG2	1:N:156:GLU:HA	2.49	0.42
2:Q:17:VAL:HG11	2:Q:33:ALA:O	2.20	0.42
2:R:69:ASP:HA	2:R:73:VAL:HG21	2.01	0.42
2:S:47:ARG:HG2	2:S:49:LEU:H	1.84	0.42
1:A:219:PHE:O	1:A:247:LEU:HD22	2.19	0.42
1:A:348:GLN:HA	1:B:209:GLU:HG3	2.00	0.42
1:B:128:VAL:HG21	1:B:505:GLN:HE21	1.83	0.42
1:B:432:GLN:HB2	1:B:436:GLN:OE1	2.19	0.42
1:B:478:TYR:OH	1:B:483:GLU:HA	2.19	0.42
1:D:73:MET:HG3	1:E:47:PRO:HG2	2.01	0.42
1:D:414:GLY:HA2	1:D:495:ASP:OD2	2.19	0.42
1:H:218:PRO:HG2	1:H:323:VAL:CG1	2.50	0.42
1:H:517:THR:HA	1:N:37:ASN:O	2.19	0.42
1:I:285:ARG:CG	1:I:286:LYS:N	2.81	0.42
1:J:149:THR:HG22	1:J:156:GLU:HA	1.99	0.42
1:J:494:LEU:HD23	1:J:494:LEU:N	2.33	0.42
1:J:496:PRO:O	1:J:499:VAL:HG22	2.19	0.42
1:K:277:LYS:HB2	1:K:277:LYS:NZ	2.34	0.42
1:K:342:ILE:O	1:K:346:VAL:HG23	2.19	0.42
1:L:165:ALA:HB1	1:L:175:ILE:CD1	2.48	0.42
1:L:218:PRO:HG2	1:L:323:VAL:HG12	2.01	0.42
1:L:249:ILE:HB	1:L:275:ALA:CB	2.49	0.42
1:M:19:GLY:HA3	1:M:67:GLU:O	2.20	0.42
1:M:213:VAL:O	1:M:324:VAL:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:248:LEU:HD21	1:M:325:ILE:HD11	2.01	0.42
1:M:360:TYR:O	1:M:364:LYS:HB2	2.19	0.42
2:O:22:ALA:HB3	2:O:28:THR:HG21	2.02	0.42
1:A:124:VAL:HG13	1:A:504:LEU:CD1	2.50	0.42
1:A:392:LYS:O	1:A:396:VAL:HG23	2.20	0.42
1:E:26:ALA:O	1:E:29:VAL:HG22	2.19	0.42
1:F:16:MET:O	1:F:20:VAL:HG23	2.19	0.42
1:F:204:PHE:CD1	1:F:204:PHE:O	2.72	0.42
1:G:496:PRO:HG2	1:G:499:VAL:CG2	2.49	0.42
1:H:247:LEU:HB3	1:H:273:VAL:HG11	2.01	0.42
1:I:47:PRO:HG3	1:J:69:MET:CB	2.49	0.42
1:M:130:GLU:OE1	1:M:130:GLU:HA	2.19	0.42
1:M:324:VAL:CG2	1:M:331:THR:HG23	2.50	0.42
1:N:112:ASN:HA	1:N:113:PRO:HD3	1.92	0.42
1:N:140:ASP:O	1:N:144:ILE:HG12	2.19	0.42
1:N:178:GLU:OE2	1:N:333:ILE:HG21	2.18	0.42
1:N:313:THR:CG2	1:N:314:LEU:H	2.30	0.42
2:P:11:ILE:HG12	2:P:85:ILE:HG12	2.01	0.42
2:Q:76:GLU:O	2:Q:83:VAL:HG22	2.19	0.42
1:A:309:LEU:H	1:A:309:LEU:HD12	1.84	0.42
1:B:266:THR:HG22	1:B:271:VAL:O	2.20	0.42
1:B:496:PRO:HG2	1:B:499:VAL:CG2	2.50	0.42
1:C:199:TYR:HA	1:C:276:VAL:HG12	2.00	0.42
1:D:517:THR:HG23	1:E:39:VAL:HG23	2.00	0.42
1:E:304:GLU:O	1:F:260:ALA:HA	2.19	0.42
1:I:47:PRO:HG2	1:J:73:MET:CG	2.49	0.42
1:I:194:GLN:O	1:I:371:LYS:HD2	2.20	0.42
1:I:443:ALA:O	1:I:447:MET:HG3	2.19	0.42
1:J:496:PRO:HD2	1:J:499:VAL:HG21	2.02	0.42
1:K:223:ALA:HB3	1:K:251:ALA:HB2	2.01	0.42
1:K:455:VAL:HG11	1:K:461:GLU:O	2.20	0.42
1:L:66:PHE:O	1:L:69:MET:HB2	2.19	0.42
1:N:32:GLY:H	1:N:457:ASN:HD22	1.66	0.42
1:N:39:VAL:HG22	1:N:49:ILE:CG1	2.50	0.42
1:N:325:ILE:HG12	1:N:330:THR:HG23	2.01	0.42
1:N:496:PRO:HD2	1:N:499:VAL:CG2	2.49	0.42
1:A:39:VAL:HA	1:A:48:THR:O	2.20	0.42
1:B:217:SER:N	1:B:218:PRO:CD	2.82	0.42
1:B:322:ARG:HG2	1:B:323:VAL:N	2.35	0.42
1:B:475:ASN:OD1	1:B:489:ILE:HD12	2.20	0.42
1:G:279:PRO:HB2	1:G:285:ARG:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:174:VAL:HG13	1:H:194:GLN:OE1	2.20	0.42
1:H:178:GLU:OE2	1:H:322:ARG:HD3	2.20	0.42
1:K:286:LYS:HE2	1:K:286:LYS:HA	2.00	0.42
1:L:24:ALA:HA	1:L:27:VAL:HG12	2.01	0.42
1:L:496:PRO:HD2	1:L:499:VAL:HG21	2.01	0.42
1:N:27:VAL:HG11	1:N:93:THR:HG21	2.00	0.42
1:N:241:ALA:HB2	1:N:271:VAL:HG22	2.02	0.42
2:R:7:HIS:ND1	2:R:48:ILE:HD13	2.35	0.42
2:S:96:GLU:O	2:S:97:ALA:HB3	2.20	0.42
1:A:20:VAL:HG13	1:A:74:VAL:HG11	2.00	0.42
1:A:247:LEU:HB3	1:A:273:VAL:HG13	2.02	0.42
1:A:323:VAL:HG12	1:A:332:ILE:HG12	2.00	0.42
1:A:399:ALA:O	1:A:403:THR:HG23	2.19	0.42
1:B:71:ALA:HA	1:B:74:VAL:HG22	2.00	0.42
1:B:130:GLU:O	1:B:134:LEU:HD13	2.20	0.42
1:C:278:ALA:HB1	1:C:279:PRO:HD2	2.02	0.42
1:E:228:SER:HA	1:E:255:GLU:HB2	2.01	0.42
1:F:149:THR:OG1	1:F:156:GLU:HA	2.19	0.42
1:F:268:ARG:HA	1:F:268:ARG:NE	2.34	0.42
1:G:215:LEU:HB3	1:G:246:PRO:HB2	2.02	0.42
1:G:456:LEU:HB2	1:G:462:PRO:HG3	2.02	0.42
1:J:224:ASP:HB3	1:J:302:SER:HA	2.00	0.42
1:K:174:VAL:HG12	1:K:376:VAL:HG13	2.01	0.42
1:K:496:PRO:O	1:K:499:VAL:HG22	2.19	0.42
1:M:285:ARG:HG3	1:M:286:LYS:N	2.34	0.42
1:N:283:ASP:O	1:N:286:LYS:HB2	2.19	0.42
1:N:420:ILE:HG13	1:N:451:LEU:CD2	2.47	0.42
1:N:421:ARG:O	1:N:425:LYS:HG2	2.19	0.42
1:N:444:LEU:O	1:N:447:MET:HB2	2.19	0.42
1:N:494:LEU:N	1:N:494:LEU:HD23	2.34	0.42
2:O:50:GLU:O	2:O:52:GLY:N	2.53	0.42
2:Q:74:LYS:O	2:Q:84:LEU:HA	2.20	0.42
1:A:31:LEU:HD12	3:A:1:ADP:C5'	2.49	0.42
1:A:414:GLY:O	1:A:417:VAL:HG12	2.20	0.42
1:A:513:LEU:HD11	1:B:388:GLU:HB2	2.00	0.42
1:B:209:GLU:O	1:B:210:THR:CB	2.68	0.42
1:F:28:LYS:HG2	1:F:94:VAL:HG22	2.01	0.42
1:F:225:LYS:HZ2	1:F:309:LEU:HD13	1.84	0.42
1:F:392:LYS:O	1:F:396:VAL:HG23	2.19	0.42
1:G:200:LEU:N	1:G:200:LEU:HD12	2.35	0.42
1:G:214:GLU:HA	1:G:323:VAL:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:278:ALA:HB1	1:G:279:PRO:HD2	2.01	0.42
1:G:349:ILE:HG21	1:G:369:VAL:CG2	2.50	0.42
1:G:409:GLU:O	1:G:409:GLU:HG2	2.19	0.42
1:H:225:LYS:HD3	1:H:303:GLU:CG	2.50	0.42
1:H:308:GLU:HB3	1:H:311:LYS:HD3	2.02	0.42
1:I:165:ALA:HA	1:I:187:LEU:HD11	2.02	0.42
1:J:177:VAL:CG1	1:J:393:LYS:HG3	2.50	0.42
1:K:104:LEU:O	1:K:107:VAL:HG22	2.19	0.42
1:K:339:GLU:O	1:K:343:GLN:HB2	2.20	0.42
2:U:20:LYS:HG2	2:U:27:LEU:CG	2.49	0.42
1:A:352:GLN:HB3	1:A:365:LEU:CD1	2.24	0.42
1:C:291:ASP:HB2	1:C:372:LEU:HD21	2.02	0.42
1:C:405:ALA:HB1	1:C:498:LYS:HB3	2.01	0.42
1:C:432:GLN:HB2	1:C:436:GLN:OE1	2.20	0.42
1:D:24:ALA:O	1:D:28:LYS:HG3	2.19	0.42
1:D:62:LEU:HD12	1:D:62:LEU:HA	1.88	0.42
1:D:252:GLU:HA	1:D:285:ARG:HH12	1.82	0.42
1:D:266:THR:HG22	1:D:271:VAL:O	2.19	0.42
1:E:130:GLU:O	1:E:134:LEU:HD13	2.20	0.42
1:E:215:LEU:HB2	1:E:323:VAL:HG22	2.02	0.42
1:F:305:ILE:O	1:G:264:VAL:HG23	2.19	0.42
1:F:313:THR:HG22	1:F:314:LEU:H	1.85	0.42
1:G:241:ALA:HB3	2:U:25:ILE:HB	2.02	0.42
1:G:358:SER:HA	1:G:362:ARG:HD2	2.02	0.42
1:H:313:THR:HG22	1:H:314:LEU:N	2.33	0.42
1:I:178:GLU:OE2	1:I:322:ARG:HD3	2.20	0.42
1:I:213:VAL:O	1:I:324:VAL:HA	2.20	0.42
1:L:169:VAL:HG22	1:L:173:GLY:HA3	2.02	0.42
1:L:182:GLY:HA2	1:M:284:ARG:HH12	1.83	0.42
1:M:4:LYS:HD2	1:M:521:VAL:HG12	2.01	0.42
1:M:279:PRO:HG3	1:M:292:ILE:HD11	2.01	0.42
2:R:5:PRO:HB2	2:R:9:ARG:O	2.20	0.42
2:T:91:ILE:HB	2:U:6:LEU:HD12	2.02	0.42
1:A:31:LEU:HB2	1:A:90:THR:CG2	2.50	0.42
1:A:130:GLU:O	1:A:134:LEU:HD13	2.19	0.42
1:A:509:SER:HB3	1:B:385:THR:HG23	2.02	0.42
1:D:23:LEU:HD23	1:D:60:ILE:HB	2.02	0.42
1:D:33:PRO:HD3	3:D:1:ADP:C5	2.55	0.42
1:D:399:ALA:O	1:D:403:THR:HG23	2.19	0.42
1:F:419:LEU:HD11	1:F:500:THR:HG23	2.02	0.42
1:H:342:ILE:O	1:H:346:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:518:GLU:HG2	1:N:36:ARG:HB2	2.02	0.42
1:I:353:ILE:HD11	1:I:369:VAL:HG21	2.02	0.42
1:J:321:LYS:HD2	1:J:334:ASP:OD2	2.20	0.42
1:K:66:PHE:CZ	1:K:522:THR:HG22	2.55	0.42
1:K:166:MET:CE	1:K:407:VAL:HG21	2.50	0.42
1:K:434:GLU:HA	1:K:437:ASN:HD22	1.84	0.42
1:L:203:TYR:CB	1:L:263:VAL:HG13	2.50	0.42
1:M:215:LEU:HB3	1:M:218:PRO:CG	2.48	0.42
1:M:323:VAL:HG23	1:M:332:ILE:HG22	2.01	0.42
1:M:346:VAL:O	1:M:350:ARG:HG2	2.20	0.42
2:O:5:PRO:HA	2:U:93:ALA:CB	2.50	0.42
2:O:74:LYS:HG3	2:U:92:LEU:HD11	2.02	0.42
2:S:20:LYS:HD2	2:S:27:LEU:HG	2.01	0.42
2:T:5:PRO:HG2	2:T:43:VAL:C	2.40	0.42
1:A:36:ARG:CB	1:G:518:GLU:HB2	2.50	0.41
1:A:221:LEU:HD11	1:A:301:ILE:CD1	2.50	0.41
1:A:405:ALA:HB1	1:A:498:LYS:HB3	2.01	0.41
1:C:311:LYS:O	1:C:312:ALA:HB2	2.20	0.41
1:D:419:LEU:HA	1:D:422:VAL:HG22	2.01	0.41
1:E:65:LYS:HG3	1:E:523:ASP:O	2.20	0.41
1:E:66:PHE:HA	1:E:69:MET:CE	2.50	0.41
1:E:482:THR:OG1	1:E:484:GLU:HG2	2.19	0.41
1:G:39:VAL:O	1:G:48:THR:O	2.38	0.41
1:G:322:ARG:HG2	1:G:323:VAL:N	2.35	0.41
1:G:512:GLY:O	1:G:516:THR:HG23	2.20	0.41
1:H:15:LYS:O	1:H:67:GLU:HA	2.20	0.41
1:H:47:PRO:HG3	1:I:69:MET:HA	2.02	0.41
1:H:494:LEU:N	1:H:494:LEU:HD23	2.34	0.41
1:J:160:LYS:O	1:J:164:GLU:HG3	2.20	0.41
1:J:524:LEU:HD22	1:J:524:LEU:HA	1.91	0.41
1:K:247:LEU:HB3	1:K:273:VAL:CG1	2.49	0.41
1:K:465:VAL:O	1:K:469:VAL:HG23	2.20	0.41
1:M:40:LEU:HD12	1:M:59:GLU:HG2	2.02	0.41
1:M:353:ILE:HG23	1:M:362:ARG:HG3	2.01	0.41
1:M:478:TYR:HB2	1:M:485:TYR:CE2	2.55	0.41
1:N:254:VAL:HG12	1:N:259:LEU:HB2	2.02	0.41
2:O:43:VAL:CG1	2:O:57:LEU:HD12	2.49	0.41
2:O:47:ARG:HB3	2:O:55:LYS:HG2	2.02	0.41
2:T:31:ALA:O	2:T:32:ALA:HB3	2.19	0.41
1:A:28:LYS:HG2	1:A:94:VAL:HG22	2.02	0.41
1:B:219:PHE:HB2	1:B:247:LEU:CD2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:LEU:HB2	1:C:90:THR:CG2	2.50	0.41
1:D:496:PRO:HG2	1:D:499:VAL:HG22	2.02	0.41
1:E:71:ALA:HA	1:E:74:VAL:HG22	2.02	0.41
1:E:118:ARG:HD2	1:E:436:GLN:NE2	2.35	0.41
1:E:195:PHE:HE1	1:E:330:THR:HB	1.76	0.41
1:E:200:LEU:HD12	1:E:200:LEU:N	2.35	0.41
1:F:262:LEU:HD11	1:F:273:VAL:HB	2.01	0.41
1:G:199:TYR:CE2	1:G:202:PRO:HA	2.55	0.41
1:H:39:VAL:HG23	1:I:517:THR:HG21	2.01	0.41
1:H:281:PHE:CZ	1:N:383:ALA:O	2.74	0.41
1:I:124:VAL:HG21	1:I:508:ALA:CB	2.50	0.41
1:J:263:VAL:O	1:J:267:MET:HG2	2.19	0.41
1:J:447:MET:O	1:J:450:PRO:HD2	2.20	0.41
1:K:13:ARG:HA	1:K:16:MET:CE	2.50	0.41
1:N:69:MET:CE	1:N:522:THR:HB	2.49	0.41
1:N:176:THR:OG1	1:N:378:VAL:HG12	2.20	0.41
2:P:92:LEU:HD11	2:Q:74:LYS:HG3	2.02	0.41
2:R:3:ILE:HD13	2:R:11:ILE:CD1	2.51	0.41
2:R:96:GLU:OE1	2:S:4:ARG:HB2	2.20	0.41
2:S:59:VAL:CG1	2:T:6:LEU:HD21	2.50	0.41
2:T:88:GLU:HG2	2:U:7:HIS:NE2	2.35	0.41
2:U:47:ARG:HD3	2:U:49:LEU:HD12	2.01	0.41
1:A:496:PRO:O	1:A:499:VAL:HG22	2.19	0.41
1:B:278:ALA:HB1	1:B:279:PRO:HD2	2.01	0.41
1:B:359:ASP:O	1:B:360:TYR:CB	2.67	0.41
1:B:518:GLU:CG	1:C:29:VAL:HB	2.50	0.41
1:C:254:VAL:HG21	1:C:275:ALA:HB3	2.01	0.41
1:D:26:ALA:O	1:D:29:VAL:HG22	2.19	0.41
1:D:111:MET:HE1	1:D:438:VAL:HG21	2.01	0.41
1:D:124:VAL:O	1:D:128:VAL:HG23	2.20	0.41
1:D:313:THR:HG22	1:D:314:LEU:HG	2.03	0.41
1:E:31:LEU:HD12	3:E:1:ADP:C5'	2.46	0.41
1:E:85:ALA:HB3	1:E:499:VAL:HG12	2.01	0.41
1:G:5:ASP:HB2	1:G:524:LEU:HD23	2.02	0.41
1:I:107:VAL:HG12	1:I:116:LEU:HD12	2.01	0.41
1:J:112:ASN:HA	1:J:113:PRO:HD3	1.96	0.41
1:K:74:VAL:O	1:K:77:VAL:HG12	2.21	0.41
1:K:193:MET:HG3	1:K:371:LYS:HB3	2.02	0.41
1:L:193:MET:H	1:L:332:ILE:HG13	1.85	0.41
2:T:76:GLU:O	2:T:83:VAL:HG22	2.21	0.41
2:T:92:LEU:HD13	2:U:85:ILE:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:LYS:HE2	1:A:303:GLU:OE2	2.20	0.41
1:A:280:GLY:H	1:A:285:ARG:HB3	1.85	0.41
1:A:325:ILE:HG12	1:A:330:THR:HG23	2.03	0.41
1:A:353:ILE:HG12	1:A:366:GLN:HE22	1.85	0.41
1:B:4:LYS:HD2	1:B:521:VAL:CG1	2.50	0.41
1:B:30:THR:CG2	1:B:38:VAL:HG23	2.50	0.41
1:B:31:LEU:HD23	1:B:453:GLN:CB	2.49	0.41
1:B:199:TYR:HA	1:B:276:VAL:HG12	2.03	0.41
1:B:247:LEU:HB3	1:B:273:VAL:HG22	2.02	0.41
1:C:33:PRO:HG3	1:C:480:ALA:HB3	2.02	0.41
1:D:225:LYS:HB3	1:D:303:GLU:OE1	2.21	0.41
1:D:239:ALA:HB1	1:D:314:LEU:CD2	2.50	0.41
1:D:326:ASN:HB2	1:D:329:THR:H	1.86	0.41
1:D:495:ASP:CG	3:D:1:ADP:HO2'	2.24	0.41
1:G:85:ALA:CB	1:G:499:VAL:HG12	2.50	0.41
1:G:270:ILE:CD1	2:U:27:LEU:HB2	2.50	0.41
1:L:10:ASN:HD21	1:L:108:ALA:HA	1.85	0.41
1:L:214:GLU:HG2	1:L:324:VAL:CG1	2.44	0.41
1:M:107:VAL:HG11	1:M:515:ILE:HG23	2.02	0.41
1:M:169:VAL:HG22	1:M:173:GLY:HA3	2.03	0.41
1:N:130:GLU:OE1	1:N:130:GLU:HA	2.20	0.41
1:N:213:VAL:O	1:N:324:VAL:HA	2.20	0.41
1:A:225:LYS:O	1:A:251:ALA:HB1	2.20	0.41
1:B:313:THR:HG22	1:B:314:LEU:N	2.35	0.41
1:C:226:LYS:HB3	1:C:253:ASP:N	2.35	0.41
1:E:23:LEU:CD1	1:E:23:LEU:C	2.89	0.41
1:E:37:ASN:HB3	1:E:49:ILE:HG23	2.01	0.41
1:E:234:LEU:N	1:E:235:PRO:HD2	2.35	0.41
1:F:62:LEU:O	1:F:68:ASN:HB2	2.20	0.41
1:F:195:PHE:CD1	1:F:197:ARG:HB2	2.55	0.41
1:F:399:ALA:O	1:F:403:THR:HG23	2.21	0.41
1:I:120:ILE:O	1:I:124:VAL:HG23	2.21	0.41
1:K:15:LYS:O	1:K:67:GLU:HG2	2.21	0.41
1:K:202:PRO:HA	1:K:205:ILE:HD13	2.02	0.41
1:K:289:LEU:HG	1:K:300:VAL:HG12	2.03	0.41
1:L:37:ASN:OD1	1:M:513:LEU:HD12	2.21	0.41
1:M:227:ILE:CD1	1:M:309:LEU:HD11	2.51	0.41
1:M:284:ARG:HD3	1:M:284:ARG:H	1.84	0.41
1:M:496:PRO:HD2	1:M:499:VAL:CG2	2.50	0.41
2:O:47:ARG:HB3	2:O:55:LYS:HE2	2.03	0.41
1:A:144:ILE:O	1:A:147:VAL:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:GLU:O	1:A:210:THR:CB	2.68	0.41
1:C:199:TYR:O	1:C:199:TYR:CD1	2.73	0.41
1:E:147:VAL:HG12	1:E:494:LEU:HB2	2.02	0.41
1:H:73:MET:HG2	1:N:49:ILE:HD11	2.01	0.41
1:H:150:ILE:HG21	1:H:494:LEU:HD21	2.01	0.41
1:I:140:ASP:O	1:I:144:ILE:HG12	2.21	0.41
1:K:39:VAL:HB	1:L:520:MET:SD	2.59	0.41
1:K:266:THR:HG21	1:K:273:VAL:O	2.21	0.41
2:O:15:LYS:HD3	2:O:37:ARG:HB3	2.03	0.41
2:R:8:ASP:O	2:R:87:SER:HA	2.20	0.41
1:A:28:LYS:HD2	1:A:453:GLN:NE2	2.36	0.41
1:B:52:ASP:OD1	1:B:54:VAL:HG12	2.21	0.41
1:B:68:ASN:O	1:B:72:GLN:HG2	2.20	0.41
1:C:219:PHE:HB2	1:C:247:LEU:HD22	2.01	0.41
1:D:33:PRO:HA	1:D:153:ASN:ND2	2.35	0.41
1:D:257:GLU:O	1:D:261:THR:HG22	2.21	0.41
1:E:231:ARG:O	1:E:233:MET:HG2	2.20	0.41
1:F:455:VAL:O	1:F:458:CYS:HB2	2.20	0.41
1:G:230:ILE:O	1:G:230:ILE:CG2	2.69	0.41
1:I:277:LYS:HB2	1:I:277:LYS:NZ	2.35	0.41
1:J:459:GLY:HA3	1:K:112:ASN:ND2	2.36	0.41
1:L:496:PRO:O	1:L:499:VAL:HG22	2.20	0.41
1:M:324:VAL:HG22	1:M:331:THR:HG23	2.02	0.41
1:M:409:GLU:OE1	1:M:498:LYS:HA	2.20	0.41
1:N:65:LYS:HB3	1:N:522:THR:OG1	2.20	0.41
1:N:194:GLN:HG3	1:N:331:THR:HB	2.02	0.41
2:Q:7:HIS:O	2:Q:8:ASP:HB3	2.21	0.41
2:Q:48:ILE:HG12	2:Q:54:VAL:HG13	2.02	0.41
2:S:12:VAL:HB	2:S:39:GLU:O	2.20	0.41
1:B:31:LEU:HD12	3:B:1:ADP:C5'	2.49	0.41
1:B:31:LEU:HD23	1:B:453:GLN:HB3	2.02	0.41
1:B:142:LYS:O	1:B:146:GLN:HG3	2.20	0.41
1:B:496:PRO:HG2	1:B:499:VAL:HG22	2.02	0.41
1:B:513:LEU:HD22	1:C:391:GLU:HG2	2.01	0.41
1:C:144:ILE:O	1:C:147:VAL:HG22	2.21	0.41
1:C:212:ALA:HA	1:C:325:ILE:O	2.21	0.41
1:C:234:LEU:N	1:C:235:PRO:HD2	2.35	0.41
1:E:199:TYR:CE2	1:E:202:PRO:HA	2.55	0.41
1:E:479:ASN:CG	1:E:493:ILE:HD11	2.41	0.41
1:F:169:VAL:HG11	1:F:377:ALA:HB2	2.03	0.41
1:F:272:LYS:NZ	1:F:272:LYS:HB2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:120:ILE:O	1:G:124:VAL:HG23	2.21	0.41
1:G:217:SER:N	1:G:218:PRO:CD	2.83	0.41
1:I:24:ALA:HA	1:I:27:VAL:HG12	2.01	0.41
1:J:271:VAL:HG12	1:J:273:VAL:HG13	2.02	0.41
1:J:277:LYS:HB2	1:J:277:LYS:NZ	2.36	0.41
1:K:215:LEU:CB	1:K:218:PRO:HG3	2.51	0.41
1:L:47:PRO:HD3	1:M:72:GLN:CG	2.48	0.41
2:P:31:ALA:O	2:P:32:ALA:CB	2.68	0.41
1:A:254:VAL:HG12	1:A:259:LEU:HG	2.03	0.41
1:A:278:ALA:HB1	1:A:279:PRO:CD	2.50	0.41
1:A:354:GLU:HG3	1:A:354:GLU:O	2.21	0.41
1:B:177:VAL:HG11	1:B:397:GLU:CG	2.51	0.41
1:B:237:LEU:HD21	1:B:271:VAL:HG21	2.03	0.41
1:B:311:LYS:O	1:B:312:ALA:HB2	2.21	0.41
1:C:30:THR:HB	1:C:51:LYS:O	2.21	0.41
1:C:130:GLU:O	1:C:134:LEU:HD13	2.21	0.41
1:C:414:GLY:HA3	1:C:493:ILE:HG22	2.03	0.41
1:C:421:ARG:HG3	1:C:425:LYS:NZ	2.35	0.41
1:D:28:LYS:HD2	1:D:453:GLN:NE2	2.36	0.41
1:D:31:LEU:HB2	1:D:90:THR:CG2	2.51	0.41
1:D:496:PRO:HG2	1:D:499:VAL:CG2	2.51	0.41
1:E:4:LYS:HE2	1:F:59:GLU:HB3	2.02	0.41
1:F:175:ILE:HG12	1:F:377:ALA:HB3	2.03	0.41
1:F:455:VAL:HG13	1:F:460:GLU:HB2	2.02	0.41
1:G:247:LEU:HB3	1:G:273:VAL:HG22	2.03	0.41
1:H:496:PRO:O	1:H:499:VAL:HG22	2.21	0.41
1:I:421:ARG:O	1:I:425:LYS:HG2	2.21	0.41
1:J:26:ALA:O	1:J:29:VAL:HG22	2.20	0.41
1:J:34:LYS:HE2	1:K:118:ARG:NH2	2.36	0.41
1:J:221:LEU:C	1:J:221:LEU:HD13	2.41	0.41
1:K:409:GLU:OE1	1:K:498:LYS:HA	2.21	0.41
1:K:496:PRO:HD2	1:K:499:VAL:CG2	2.51	0.41
1:L:426:LEU:CD1	1:L:444:LEU:HD21	2.50	0.41
1:M:22:VAL:HG11	1:M:62:LEU:HD21	2.02	0.41
1:M:164:GLU:HG3	1:M:187:LEU:HD13	2.01	0.41
1:M:293:ALA:HB2	1:M:300:VAL:HG13	2.01	0.41
1:N:149:THR:HG23	1:N:159:GLY:HA3	2.03	0.41
2:T:42:ALA:HA	2:T:61:VAL:CG1	2.51	0.41
1:A:147:VAL:HG23	1:A:403:THR:HG22	2.03	0.41
1:A:464:VAL:HG21	1:N:467:ASN:ND2	2.36	0.41
1:B:147:VAL:HA	1:B:150:ILE:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:GLY:HA2	1:B:399:ALA:HB1	2.02	0.41
1:B:429:LEU:HG	1:B:440:ILE:HD13	2.03	0.41
1:C:33:PRO:CG	1:C:480:ALA:HB3	2.51	0.41
1:C:200:LEU:HD12	1:C:200:LEU:N	2.35	0.41
1:C:204:PHE:CG	1:C:274:ALA:HB2	2.56	0.41
1:C:281:PHE:O	1:C:285:ARG:HG2	2.21	0.41
1:C:381:VAL:CG1	1:C:392:LYS:HG3	2.51	0.41
1:D:82:ASN:HB2	1:D:89:THR:HG21	2.03	0.41
1:D:178:GLU:O	1:D:380:LYS:HA	2.21	0.41
1:E:229:ASN:C	1:E:231:ARG:H	2.24	0.41
1:F:247:LEU:CB	1:F:273:VAL:HG22	2.51	0.41
1:F:266:THR:CG2	1:F:273:VAL:H	2.31	0.41
1:F:365:LEU:HD22	1:F:365:LEU:O	2.21	0.41
1:H:101:THR:O	1:H:105:LYS:HG3	2.21	0.41
1:I:130:GLU:OE1	1:I:130:GLU:HA	2.20	0.41
1:L:201:SER:HA	1:L:202:PRO:HD3	1.93	0.41
1:M:5:ASP:HB2	1:M:524:LEU:HD23	2.03	0.41
1:N:219:PHE:CE1	1:N:314:LEU:HD23	2.56	0.41
2:O:47:ARG:HD3	2:O:49:LEU:HD12	2.02	0.41
1:B:13:ARG:HD2	1:B:104:LEU:HD22	2.03	0.40
1:B:69:MET:HG2	1:C:41:ASP:HB2	2.03	0.40
1:B:391:GLU:OE1	1:B:391:GLU:HA	2.21	0.40
1:B:510:VAL:HG23	1:B:511:ALA:N	2.36	0.40
1:D:215:LEU:O	1:D:322:ARG:HG3	2.21	0.40
1:D:278:ALA:HB1	1:D:279:PRO:CD	2.51	0.40
1:D:309:LEU:CD1	1:D:309:LEU:H	2.34	0.40
1:D:357:THR:O	1:D:359:ASP:N	2.54	0.40
1:E:280:GLY:CA	1:E:285:ARG:HH21	2.34	0.40
1:G:99:ILE:HD13	1:G:446:ALA:HB3	2.03	0.40
1:I:13:ARG:HA	1:I:16:MET:HE2	2.03	0.40
1:K:166:MET:HE2	1:K:171:LYS:HG2	2.03	0.40
1:L:219:PHE:HB3	1:L:317:LEU:HD23	2.03	0.40
1:M:217:SER:HA	1:M:320:ALA:O	2.21	0.40
1:N:76:GLU:O	1:N:80:LYS:HG3	2.21	0.40
1:N:193:MET:H	1:N:332:ILE:HG13	1.85	0.40
1:N:350:ARG:HE	1:N:369:VAL:HG11	1.85	0.40
2:P:16:GLU:O	2:P:35:SER:HB2	2.21	0.40
1:B:199:TYR:CE2	1:B:202:PRO:HA	2.56	0.40
1:B:517:THR:HA	1:C:37:ASN:O	2.22	0.40
1:C:177:VAL:HG11	1:C:397:GLU:CG	2.51	0.40
1:D:130:GLU:O	1:D:134:LEU:HD13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:228:SER:H	1:D:230:ILE:HG23	1.86	0.40
1:E:199:TYR:H	1:E:199:TYR:HD1	1.69	0.40
1:F:223:ALA:HB3	1:F:251:ALA:HB2	2.02	0.40
1:F:305:ILE:HD11	1:G:203:TYR:CD1	2.56	0.40
1:G:270:ILE:HG23	2:U:25:ILE:HG22	2.03	0.40
1:G:302:SER:CB	1:G:305:ILE:HB	2.51	0.40
1:G:420:ILE:HG13	1:G:448:GLU:HG2	2.03	0.40
1:H:247:LEU:HB3	1:H:273:VAL:CG1	2.51	0.40
1:I:124:VAL:O	1:I:128:VAL:HG23	2.21	0.40
1:J:177:VAL:HG11	1:J:393:LYS:HG3	2.03	0.40
1:J:241:ALA:CB	1:J:271:VAL:HG22	2.50	0.40
1:K:49:ILE:HD11	1:L:73:MET:CE	2.51	0.40
1:K:191:GLU:HB3	1:K:295:LEU:HD11	2.03	0.40
1:L:259:LEU:O	1:L:263:VAL:HG23	2.21	0.40
1:L:271:VAL:HG12	1:L:273:VAL:HG13	2.03	0.40
1:L:349:ILE:O	1:L:352:GLN:HB2	2.20	0.40
1:M:131:LEU:CD1	1:M:422:VAL:HG11	2.50	0.40
1:M:277:LYS:HB2	1:M:277:LYS:NZ	2.35	0.40
1:N:293:ALA:HB2	1:N:300:VAL:HG13	2.03	0.40
2:T:50:GLU:C	2:T:52:GLY:H	2.25	0.40
2:T:73:VAL:HG22	2:T:86:MET:HB3	2.03	0.40
1:A:266:THR:CG2	1:A:273:VAL:H	2.35	0.40
1:B:76:GLU:CD	1:C:386:GLU:HB3	2.41	0.40
1:B:412:VAL:HG13	1:B:497:THR:OG1	2.21	0.40
1:C:33:PRO:HG3	3:C:1:ADP:C6	2.56	0.40
1:C:199:TYR:HB3	1:C:325:ILE:CG2	2.52	0.40
1:D:8:PHE:CE2	1:E:26:ALA:HA	2.56	0.40
1:E:62:LEU:HD22	1:E:67:GLU:HB3	2.03	0.40
1:E:112:ASN:HA	1:E:113:PRO:HD3	1.95	0.40
1:E:209:GLU:O	1:E:210:THR:CB	2.69	0.40
1:F:322:ARG:HG2	1:F:323:VAL:N	2.36	0.40
1:F:353:ILE:HG13	1:F:365:LEU:HD11	2.03	0.40
1:G:37:ASN:OD1	1:G:51:LYS:HB2	2.21	0.40
1:G:453:GLN:NE2	1:G:456:LEU:HD23	2.35	0.40
1:G:455:VAL:O	1:G:458:CYS:HB2	2.21	0.40
1:H:210:THR:HG22	1:H:212:ALA:HB3	2.02	0.40
1:H:270:ILE:HG22	1:H:271:VAL:HG23	2.03	0.40
1:H:288:MET:HA	1:H:288:MET:HE3	2.02	0.40
1:I:475:ASN:ND2	1:I:489:ILE:HD12	2.37	0.40
1:J:65:LYS:O	1:J:66:PHE:HB2	2.20	0.40
1:J:272:LYS:HE3	1:J:272:LYS:HB2	1.95	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:198:GLY:CA	1:K:328:ASP:HA	2.51	0.40
1:K:233:MET:CE	1:K:309:LEU:HD13	2.51	0.40
1:L:160:LYS:O	1:L:164:GLU:HG3	2.22	0.40
1:M:247:LEU:HD22	1:M:248:LEU:N	2.37	0.40
1:M:496:PRO:O	1:M:499:VAL:HG22	2.21	0.40
2:S:93:ALA:HA	2:T:6:LEU:H	1.87	0.40
2:T:47:ARG:HG2	2:T:49:LEU:H	1.87	0.40
2:U:49:LEU:O	2:U:50:GLU:HB3	2.20	0.40
1:A:71:ALA:HA	1:A:74:VAL:HG22	2.03	0.40
1:A:351:GLN:HG2	1:B:210:THR:OG1	2.22	0.40
1:B:28:LYS:HG2	1:B:94:VAL:HG22	2.04	0.40
1:C:461:GLU:HG2	1:C:464:VAL:CG1	2.52	0.40
1:E:5:ASP:OD1	1:E:524:LEU:HD21	2.20	0.40
1:E:82:ASN:ND2	1:E:86:GLY:HA2	2.36	0.40
1:F:42:LYS:HD3	1:F:44:PHE:CE2	2.56	0.40
1:F:115:ASP:O	1:F:436:GLN:HG2	2.21	0.40
1:G:18:ARG:HH11	1:G:18:ARG:HB3	1.86	0.40
1:G:352:GLN:C	1:G:365:LEU:HD11	2.42	0.40
1:G:466:ALA:O	1:G:470:LYS:HG3	2.22	0.40
1:H:19:GLY:HA2	1:H:62:LEU:CD1	2.50	0.40
1:H:200:LEU:CD1	1:H:200:LEU:N	2.85	0.40
1:H:288:MET:HA	1:H:288:MET:CE	2.52	0.40
1:I:47:PRO:HG3	1:J:69:MET:CA	2.51	0.40
1:I:115:ASP:HB3	1:I:436:GLN:HG3	2.03	0.40
1:J:438:VAL:O	1:J:442:VAL:HG23	2.22	0.40
1:K:39:VAL:HA	1:K:48:THR:O	2.21	0.40
1:K:47:PRO:HG2	1:L:73:MET:HG3	2.04	0.40
1:K:438:VAL:O	1:K:442:VAL:HG23	2.21	0.40
1:M:417:VAL:HG21	1:M:488:MET:HG3	2.04	0.40
1:M:455:VAL:HG13	1:M:460:GLU:HB2	2.02	0.40
1:N:247:LEU:HB3	1:N:273:VAL:HG11	2.02	0.40
1:N:276:VAL:CG1	1:N:325:ILE:HD13	2.52	0.40
2:P:8:ASP:O	2:P:87:SER:HA	2.21	0.40
2:U:7:HIS:O	2:U:8:ASP:HB3	2.21	0.40
1:B:247:LEU:CB	1:B:273:VAL:HG22	2.52	0.40
1:B:325:ILE:HD12	1:B:330:THR:HG23	2.02	0.40
1:C:82:ASN:O	1:C:86:GLY:HA2	2.22	0.40
1:C:359:ASP:O	1:C:360:TYR:CB	2.67	0.40
1:C:461:GLU:CD	1:C:461:GLU:H	2.25	0.40
1:C:481:ALA:HB2	3:C:1:ADP:HN62	1.87	0.40
1:D:225:LYS:HZ3	1:D:230:ILE:HD11	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:144:ILE:CD1	1:H:407:VAL:HG22	2.51	0.40
1:I:227:ILE:CD1	1:I:309:LEU:HD11	2.52	0.40
1:L:20:VAL:CG2	1:L:74:VAL:HG21	2.51	0.40
1:L:74:VAL:O	1:L:77:VAL:HG12	2.21	0.40
1:M:124:VAL:O	1:M:128:VAL:HG23	2.22	0.40
1:M:144:ILE:HG21	1:M:163:ALA:HA	2.03	0.40
1:N:35:GLY:HA2	1:N:457:ASN:HB3	2.03	0.40
1:N:66:PHE:HD1	1:N:520:MET:HE2	1.86	0.40
1:N:115:ASP:O	1:N:436:GLN:HG2	2.22	0.40
2:O:7:HIS:C	2:O:9:ARG:H	2.25	0.40
2:P:18:GLU:OE1	2:P:33:ALA:HB3	2.21	0.40
2:Q:66:ILE:HG22	2:Q:92:LEU:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	522/524 (100%)	502 (96%)	12 (2%)	8 (2%)	10	46
1	B	522/524 (100%)	503 (96%)	9 (2%)	10 (2%)	8	38
1	C	522/524 (100%)	505 (97%)	7 (1%)	10 (2%)	8	38
1	D	522/524 (100%)	499 (96%)	17 (3%)	6 (1%)	14	52
1	E	522/524 (100%)	501 (96%)	13 (2%)	8 (2%)	10	46
1	F	522/524 (100%)	500 (96%)	13 (2%)	9 (2%)	9	42
1	G	522/524 (100%)	503 (96%)	9 (2%)	10 (2%)	8	38
1	H	522/524 (100%)	507 (97%)	11 (2%)	4 (1%)	19	60
1	I	522/524 (100%)	513 (98%)	7 (1%)	2 (0%)	34	72
1	J	522/524 (100%)	515 (99%)	5 (1%)	2 (0%)	34	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	522/524 (100%)	511 (98%)	8 (2%)	3 (1%)	25	66
1	L	522/524 (100%)	513 (98%)	6 (1%)	3 (1%)	25	66
1	M	522/524 (100%)	511 (98%)	8 (2%)	3 (1%)	25	66
1	N	522/524 (100%)	508 (97%)	10 (2%)	4 (1%)	19	60
2	O	95/97 (98%)	85 (90%)	3 (3%)	7 (7%)	1	14
2	P	95/97 (98%)	85 (90%)	4 (4%)	6 (6%)	1	17
2	Q	95/97 (98%)	89 (94%)	3 (3%)	3 (3%)	4	26
2	R	95/97 (98%)	89 (94%)	2 (2%)	4 (4%)	3	22
2	S	95/97 (98%)	84 (88%)	7 (7%)	4 (4%)	3	22
2	T	95/97 (98%)	85 (90%)	8 (8%)	2 (2%)	7	36
2	U	95/97 (98%)	86 (90%)	3 (3%)	6 (6%)	1	17
All	All	7973/8015 (100%)	7694 (96%)	165 (2%)	114 (1%)	15	46

All (114) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	306	GLY
1	A	358	SER
1	B	312	ALA
1	B	360	TYR
1	C	233	MET
1	C	312	ALA
1	C	358	SER
1	D	207	LYS
1	D	210	THR
1	D	233	MET
1	D	312	ALA
1	D	358	SER
1	E	210	THR
1	E	233	MET
1	E	312	ALA
1	F	232	GLU
1	G	230	ILE
1	G	233	MET
1	G	279	PRO
1	G	312	ALA
1	G	360	TYR
1	H	66	PHE

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Mol	Chain	Res	Type
1	H	153	ASN
1	H	229	ASN
1	H	356	ALA
1	I	270	ILE
1	J	66	PHE
1	K	66	PHE
1	L	66	PHE
1	M	66	PHE
1	M	154	SER
1	N	66	PHE
2	O	3	ILE
2	O	7	HIS
2	O	20	LYS
2	O	51	ASN
2	P	32	ALA
2	Q	7	HIS
2	Q	20	LYS
2	Q	50	GLU
2	R	21	SER
2	R	32	ALA
2	R	51	ASN
2	S	7	HIS
2	S	51	ASN
2	S	53	GLU
2	S	54	VAL
2	T	7	HIS
2	U	7	HIS
2	U	21	SER
2	U	53	GLU
1	A	282	GLY
1	B	358	SER
1	C	207	LYS
1	C	305	ILE
1	C	309	LEU
1	E	207	LYS
1	F	204	PHE
1	F	207	LYS
1	F	282	GLY
1	G	282	GLY
1	G	306	GLY
1	I	66	PHE
1	L	153	ASN

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Mol	Chain	Res	Type
1	M	153	ASN
1	N	173	GLY
2	O	32	ALA
2	O	52	GLY
2	P	7	HIS
2	P	51	ASN
2	P	52	GLY
2	P	53	GLU
2	U	20	LYS
1	A	207	LYS
1	A	233	MET
1	A	312	ALA
1	B	233	MET
1	B	383	ALA
1	C	210	THR
1	E	383	ALA
1	F	358	SER
1	F	383	ALA
1	G	207	LYS
1	K	173	GLY
1	N	197	ARG
2	T	32	ALA
2	U	80	ASN
1	A	210	THR
1	B	207	LYS
1	B	209	GLU
1	B	306	GLY
1	C	360	TYR
1	D	230	ILE
1	E	358	SER
2	R	7	HIS
1	B	45	GLY
1	B	230	ILE
1	C	311	LYS
1	E	282	GLY
1	F	196	ASP
1	G	109	ALA
1	J	153	ASN
1	L	197	ARG
2	U	79	ASP
1	A	232	GLU
1	F	209	GLU

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Mol	Chain	Res	Type
1	G	356	ALA
2	O	53	GLU
1	N	337	GLY
2	P	54	VAL
1	F	280	GLY
1	K	462	PRO
1	C	230	ILE
1	E	230	ILE

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	A	404/404 (100%)	386 (96%)	18 (4%)	27	52
1	B	404/404 (100%)	387 (96%)	17 (4%)	30	54
1	C	404/404 (100%)	388 (96%)	16 (4%)	31	55
1	D	404/404 (100%)	384 (95%)	20 (5%)	24	49
1	E	404/404 (100%)	372 (92%)	32 (8%)	12	35
1	F	404/404 (100%)	386 (96%)	18 (4%)	27	52
1	G	404/404 (100%)	382 (95%)	22 (5%)	22	47
1	H	404/404 (100%)	384 (95%)	20 (5%)	24	49
1	I	404/404 (100%)	389 (96%)	15 (4%)	34	58
1	J	404/404 (100%)	385 (95%)	19 (5%)	26	51
1	K	404/404 (100%)	387 (96%)	17 (4%)	30	54
1	L	404/404 (100%)	392 (97%)	12 (3%)	41	63
1	M	404/404 (100%)	388 (96%)	16 (4%)	31	55
1	N	404/404 (100%)	385 (95%)	19 (5%)	26	51
2	O	80/80 (100%)	71 (89%)	9 (11%)	6	21
2	P	80/80 (100%)	69 (86%)	11 (14%)	3	17
2	Q	80/80 (100%)	72 (90%)	8 (10%)	7	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	R	80/80 (100%)	74 (92%)	6 (8%)	13 38
2	S	80/80 (100%)	73 (91%)	7 (9%)	10 31
2	T	80/80 (100%)	70 (88%)	10 (12%)	4 19
2	U	80/80 (100%)	72 (90%)	8 (10%)	7 26
All	All	6216/6216 (100%)	5896 (95%)	320 (5%)	27 48

All (320) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	LEU
1	A	77	VAL
1	A	166	MET
1	A	199	TYR
1	A	229	ASN
1	A	234	LEU
1	A	238	GLU
1	A	255	GLU
1	A	257	GLU
1	A	261	THR
1	A	264	VAL
1	A	268	ARG
1	A	314	LEU
1	A	315	GLU
1	A	348	GLN
1	A	360	TYR
1	A	461	GLU
1	A	523	ASP
1	B	77	VAL
1	B	114	MET
1	B	139	SER
1	B	153	ASN
1	B	199	TYR
1	B	207	LYS
1	B	231	ARG
1	B	238	GLU
1	B	271	VAL
1	B	290	GLN
1	B	315	GLU
1	B	325	ILE
1	B	327	LYS
1	B	348	GLN

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Mol	Chain	Res	Type
1	B	360	TYR
1	B	461	GLU
1	B	516	THR
1	C	44	PHE
1	C	77	VAL
1	C	199	TYR
1	C	204	PHE
1	C	225	LYS
1	C	230	ILE
1	C	234	LEU
1	C	247	LEU
1	C	255	GLU
1	C	257	GLU
1	C	261	THR
1	C	288	MET
1	C	313	THR
1	C	315	GLU
1	C	360	TYR
1	C	490	ASP
1	D	62	LEU
1	D	77	VAL
1	D	139	SER
1	D	153	ASN
1	D	199	TYR
1	D	207	LYS
1	D	225	LYS
1	D	230	ILE
1	D	247	LEU
1	D	255	GLU
1	D	257	GLU
1	D	261	THR
1	D	267	MET
1	D	314	LEU
1	D	327	LYS
1	D	348	GLN
1	D	358	SER
1	D	360	TYR
1	D	365	LEU
1	D	461	GLU
1	E	23	LEU
1	E	36	ARG
1	E	42	LYS

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Mol	Chain	Res	Type
1	E	44	PHE
1	E	77	VAL
1	E	141	SER
1	E	153	ASN
1	E	154	SER
1	E	196	ASP
1	E	197	ARG
1	E	199	TYR
1	E	204	PHE
1	E	225	LYS
1	E	228	SER
1	E	238	GLU
1	E	257	GLU
1	E	261	THR
1	E	267	MET
1	E	285	ARG
1	E	313	THR
1	E	315	GLU
1	E	348	GLN
1	E	357	THR
1	E	365	LEU
1	E	379	ILE
1	E	420	ILE
1	E	421	ARG
1	E	452	ARG
1	E	461	GLU
1	E	475	ASN
1	E	513	LEU
1	E	518	GLU
1	F	77	VAL
1	F	139	SER
1	F	197	ARG
1	F	199	TYR
1	F	204	PHE
1	F	210	THR
1	F	234	LEU
1	F	247	LEU
1	F	255	GLU
1	F	261	THR
1	F	268	ARG
1	F	311	LYS
1	F	348	GLN

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Mol	Chain	Res	Type
1	F	360	TYR
1	F	365	LEU
1	F	385	THR
1	F	461	GLU
1	F	521	VAL
1	G	18	ARG
1	G	44	PHE
1	G	77	VAL
1	G	80	LYS
1	G	199	TYR
1	G	210	THR
1	G	216	GLU
1	G	230	ILE
1	G	233	MET
1	G	238	GLU
1	G	257	GLU
1	G	261	THR
1	G	267	MET
1	G	310	GLU
1	G	315	GLU
1	G	348	GLN
1	G	357	THR
1	G	360	TYR
1	G	412	VAL
1	G	445	ARG
1	G	461	GLU
1	G	517	THR
1	H	4	LYS
1	H	7	LYS
1	H	37	ASN
1	H	59	GLU
1	H	129	GLU
1	H	153	ASN
1	H	172	GLU
1	H	200	LEU
1	H	228	SER
1	H	284	ARG
1	H	285	ARG
1	H	286	LYS
1	H	288	MET
1	H	292	ILE
1	H	358	SER

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Mol	Chain	Res	Type
1	H	389	MET
1	H	426	LEU
1	H	433	ASN
1	H	441	LYS
1	H	513	LEU
1	I	41	ASP
1	I	43	SER
1	I	129	GLU
1	I	172	GLU
1	I	255	GLU
1	I	284	ARG
1	I	288	MET
1	I	345	ARG
1	I	364	LYS
1	I	367	GLU
1	I	389	MET
1	I	421	ARG
1	I	426	LEU
1	I	432	GLN
1	I	441	LYS
1	J	28	LYS
1	J	37	ASN
1	J	104	LEU
1	J	139	SER
1	J	154	SER
1	J	157	THR
1	J	233	MET
1	J	268	ARG
1	J	283	ASP
1	J	284	ARG
1	J	285	ARG
1	J	311	LYS
1	J	343	GLN
1	J	367	GLU
1	J	389	MET
1	J	421	ARG
1	J	426	LEU
1	J	513	LEU
1	J	524	LEU
1	K	37	ASN
1	K	41	ASP
1	K	59	GLU

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Mol	Chain	Res	Type
1	K	129	GLU
1	K	151	SER
1	K	172	GLU
1	K	200	LEU
1	K	207	LYS
1	K	226	LYS
1	K	233	MET
1	K	270	ILE
1	K	284	ARG
1	K	288	MET
1	K	343	GLN
1	K	389	MET
1	K	421	ARG
1	K	426	LEU
1	L	37	ASN
1	L	141	SER
1	L	201	SER
1	L	217	SER
1	L	234	LEU
1	L	284	ARG
1	L	288	MET
1	L	300	VAL
1	L	389	MET
1	L	421	ARG
1	L	426	LEU
1	L	513	LEU
1	M	37	ASN
1	M	41	ASP
1	M	139	SER
1	M	154	SER
1	M	175	ILE
1	M	233	MET
1	M	242	LYS
1	M	255	GLU
1	M	267	MET
1	M	367	GLU
1	M	389	MET
1	M	421	ARG
1	M	426	LEU
1	M	432	GLN
1	M	441	LYS
1	M	494	LEU

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Mol	Chain	Res	Type
1	N	36	ARG
1	N	37	ASN
1	N	65	LYS
1	N	114	MET
1	N	139	SER
1	N	154	SER
1	N	172	GLU
1	N	197	ARG
1	N	230	ILE
1	N	233	MET
1	N	284	ARG
1	N	288	MET
1	N	343	GLN
1	N	345	ARG
1	N	389	MET
1	N	421	ARG
1	N	426	LEU
1	N	432	GLN
1	N	441	LYS
2	O	1	MET
2	O	3	ILE
2	O	4	ARG
2	O	6	LEU
2	O	27	LEU
2	O	55	LYS
2	O	64	ILE
2	O	79	ASP
2	O	86	MET
2	P	1	MET
2	P	3	ILE
2	P	6	LEU
2	P	8	ASP
2	P	13	LYS
2	P	20	LYS
2	P	28	THR
2	P	37	ARG
2	P	48	ILE
2	P	55	LYS
2	P	71	TYR
2	Q	1	MET
2	Q	3	ILE
2	Q	7	HIS

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Mol	Chain	Res	Type
2	Q	26	VAL
2	Q	34	LYS
2	Q	37	ARG
2	Q	54	VAL
2	Q	55	LYS
2	R	1	MET
2	R	6	LEU
2	R	8	ASP
2	R	26	VAL
2	R	27	LEU
2	R	55	LYS
2	S	1	MET
2	S	3	ILE
2	S	6	LEU
2	S	8	ASP
2	S	49	LEU
2	S	55	LYS
2	S	77	LYS
2	T	4	ARG
2	T	6	LEU
2	T	27	LEU
2	T	53	GLU
2	T	55	LYS
2	T	61	VAL
2	T	66	ILE
2	T	68	ASN
2	T	78	ILE
2	T	80	ASN
2	U	1	MET
2	U	6	LEU
2	U	48	ILE
2	U	53	GLU
2	U	55	LYS
2	U	71	TYR
2	U	75	SER
2	U	80	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (132) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	82	ASN

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Mol	Chain	Res	Type
1	A	97	GLN
1	A	146	GLN
1	A	153	ASN
1	A	184	GLN
1	A	348	GLN
1	A	366	GLN
1	A	432	GLN
1	A	453	GLN
1	A	457	ASN
1	A	505	GLN
1	B	21	ASN
1	B	82	ASN
1	B	97	GLN
1	B	112	ASN
1	B	146	GLN
1	B	153	ASN
1	B	348	GLN
1	B	366	GLN
1	B	432	GLN
1	B	457	ASN
1	C	21	ASN
1	C	97	GLN
1	C	146	GLN
1	C	343	GLN
1	C	366	GLN
1	C	432	GLN
1	C	453	GLN
1	C	457	ASN
1	C	475	ASN
1	D	21	ASN
1	D	72	GLN
1	D	82	ASN
1	D	146	GLN
1	D	153	ASN
1	D	348	GLN
1	D	432	GLN
1	D	457	ASN
1	D	475	ASN
1	E	21	ASN
1	E	82	ASN
1	E	97	GLN
1	E	146	GLN

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Mol	Chain	Res	Type
1	E	153	ASN
1	E	206	ASN
1	E	348	GLN
1	E	366	GLN
1	E	432	GLN
1	E	457	ASN
1	E	467	ASN
1	E	475	ASN
1	E	505	GLN
1	F	21	ASN
1	F	82	ASN
1	F	97	GLN
1	F	146	GLN
1	F	153	ASN
1	F	348	GLN
1	F	352	GLN
1	F	432	GLN
1	F	457	ASN
1	F	475	ASN
1	G	21	ASN
1	G	153	ASN
1	G	206	ASN
1	G	348	GLN
1	G	366	GLN
1	G	436	GLN
1	G	453	GLN
1	G	457	ASN
1	G	467	ASN
1	G	475	ASN
1	H	21	ASN
1	H	37	ASN
1	H	153	ASN
1	H	319	GLN
1	H	433	ASN
1	H	436	GLN
1	I	10	ASN
1	I	21	ASN
1	I	72	GLN
1	I	97	GLN
1	I	146	GLN
1	I	319	GLN
1	I	433	ASN

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Mol	Chain	Res	Type
1	I	436	GLN
1	J	21	ASN
1	J	37	ASN
1	J	97	GLN
1	J	319	GLN
1	J	343	GLN
1	J	348	GLN
1	J	436	GLN
1	K	21	ASN
1	K	97	GLN
1	K	112	ASN
1	K	153	ASN
1	K	319	GLN
1	K	343	GLN
1	K	436	GLN
1	K	467	ASN
1	L	10	ASN
1	L	21	ASN
1	L	37	ASN
1	L	97	GLN
1	L	153	ASN
1	L	319	GLN
1	M	21	ASN
1	M	37	ASN
1	M	97	GLN
1	M	146	GLN
1	M	153	ASN
1	M	319	GLN
1	M	433	ASN
1	M	436	GLN
1	M	487	ASN
1	N	21	ASN
1	N	37	ASN
1	N	229	ASN
1	N	319	GLN
1	N	343	GLN
1	N	348	GLN
2	O	2	ASN
2	O	68	ASN
2	P	68	ASN
2	R	51	ASN
2	R	68	ASN

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Mol	Chain	Res	Type
2	S	51	ASN
2	S	68	ASN
2	T	68	ASN
2	U	68	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 7 are monoatomic - leaving 7 for Mogul analysis.

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	$\#\|Z\| > 2$
3	ADP	G	1	4	24,29,29	1.31	3 (12%)	29,45,45	2.50	8 (27%)
3	ADP	A	1	4	24,29,29	1.31	3 (12%)	29,45,45	2.50	8 (27%)
3	ADP	F	1	4	24,29,29	1.30	3 (12%)	29,45,45	2.49	7 (24%)
3	ADP	D	1	4	24,29,29	1.30	3 (12%)	29,45,45	2.48	7 (24%)
3	ADP	E	1	4	24,29,29	1.29	3 (12%)	29,45,45	2.52	8 (27%)
3	ADP	B	1	4	24,29,29	1.29	3 (12%)	29,45,45	2.51	8 (27%)
3	ADP	C	1	4	24,29,29	1.28	3 (12%)	29,45,45	2.48	7 (24%)

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
3	ADP	G	1	4	-	4/12/32/32	0/3/3/3
3	ADP	A	1	4	-	4/12/32/32	0/3/3/3
3	ADP	F	1	4	-	4/12/32/32	0/3/3/3
3	ADP	D	1	4	-	4/12/32/32	0/3/3/3
3	ADP	E	1	4	-	4/12/32/32	0/3/3/3
3	ADP	B	1	4	-	5/12/32/32	0/3/3/3
3	ADP	C	1	4	-	5/12/32/32	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1	ADP	O4'-C1'	3.68	1.46	1.41
3	D	1	ADP	O4'-C1'	3.68	1.46	1.41
3	A	1	ADP	O4'-C1'	3.61	1.46	1.41
3	E	1	ADP	O4'-C1'	3.57	1.46	1.41
3	G	1	ADP	O4'-C1'	3.57	1.46	1.41
3	C	1	ADP	O4'-C1'	3.56	1.46	1.41
3	B	1	ADP	O4'-C1'	3.54	1.46	1.41
3	D	1	ADP	C5-N7	-2.24	1.31	1.39
3	E	1	ADP	C5-N7	-2.22	1.31	1.39
3	G	1	ADP	C5-N7	-2.22	1.31	1.39
3	A	1	ADP	C5-N7	-2.21	1.31	1.39
3	C	1	ADP	C5-N7	-2.21	1.31	1.39
3	F	1	ADP	C5-N7	-2.21	1.31	1.39
3	B	1	ADP	C5-N7	-2.17	1.31	1.39
3	A	1	ADP	C2-N3	2.08	1.35	1.32
3	F	1	ADP	C2-N3	2.06	1.35	1.32
3	B	1	ADP	C2-N3	2.04	1.35	1.32
3	G	1	ADP	C2-N3	2.03	1.35	1.32
3	D	1	ADP	C2-N3	2.01	1.35	1.32
3	E	1	ADP	C2-N3	2.01	1.35	1.32
3	C	1	ADP	C2-N3	2.00	1.35	1.32

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	1	ADP	N3-C2-N1	-6.51	118.50	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	1	ADP	N3-C2-N1	-6.47	118.57	128.68
3	F	1	ADP	N3-C2-N1	-6.46	118.59	128.68
3	B	1	ADP	N3-C2-N1	-6.45	118.60	128.68
3	A	1	ADP	N3-C2-N1	-6.45	118.60	128.68
3	C	1	ADP	N3-C2-N1	-6.44	118.62	128.68
3	D	1	ADP	N3-C2-N1	-6.43	118.63	128.68
3	D	1	ADP	O3B-PB-O3A	-6.17	83.93	104.64
3	C	1	ADP	O2B-PB-O3A	-6.12	84.12	104.64
3	E	1	ADP	O2B-PB-O3A	-6.12	84.12	104.64
3	F	1	ADP	O3B-PB-O3A	-6.11	84.14	104.64
3	B	1	ADP	O2B-PB-O3A	-6.10	84.16	104.64
3	D	1	ADP	O2B-PB-O3A	-6.09	84.22	104.64
3	G	1	ADP	O2B-PB-O3A	-6.07	84.29	104.64
3	A	1	ADP	O3B-PB-O3A	-6.06	84.30	104.64
3	A	1	ADP	O2B-PB-O3A	-6.06	84.31	104.64
3	C	1	ADP	O3B-PB-O3A	-6.06	84.31	104.64
3	G	1	ADP	O3B-PB-O3A	-6.05	84.34	104.64
3	B	1	ADP	O3B-PB-O3A	-6.03	84.42	104.64
3	F	1	ADP	O2B-PB-O3A	-6.02	84.44	104.64
3	E	1	ADP	O3B-PB-O3A	-6.00	84.51	104.64
3	E	1	ADP	O3A-PB-O1B	-4.81	84.50	111.19
3	G	1	ADP	O3A-PB-O1B	-4.79	84.63	111.19
3	B	1	ADP	O3A-PB-O1B	-4.78	84.66	111.19
3	A	1	ADP	O3A-PB-O1B	-4.77	84.73	111.19
3	C	1	ADP	O3A-PB-O1B	-4.76	84.78	111.19
3	F	1	ADP	O3A-PB-O1B	-4.75	84.82	111.19
3	D	1	ADP	O3A-PB-O1B	-4.67	85.29	111.19
3	E	1	ADP	O2B-PB-O1B	2.96	122.28	110.68
3	G	1	ADP	O2B-PB-O1B	2.94	122.20	110.68
3	B	1	ADP	O2B-PB-O1B	2.94	122.18	110.68
3	C	1	ADP	O2B-PB-O1B	2.91	122.07	110.68
3	A	1	ADP	O2B-PB-O1B	2.91	122.06	110.68
3	F	1	ADP	O2B-PB-O1B	2.89	121.98	110.68
3	D	1	ADP	O2B-PB-O1B	2.84	121.79	110.68
3	D	1	ADP	O3B-PB-O2B	2.68	117.87	107.64
3	F	1	ADP	O3B-PB-O2B	2.61	117.61	107.64
3	A	1	ADP	O3B-PB-O2B	2.60	117.57	107.64
3	G	1	ADP	O3B-PB-O2B	2.59	117.53	107.64
3	C	1	ADP	O3B-PB-O2B	2.58	117.50	107.64
3	B	1	ADP	O3B-PB-O2B	2.58	117.50	107.64
3	E	1	ADP	O3B-PB-O2B	2.55	117.39	107.64
3	F	1	ADP	C4-C5-N7	-2.22	107.08	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1	ADP	C4-C5-N7	-2.22	107.08	109.40
3	E	1	ADP	C4-C5-N7	-2.21	107.09	109.40
3	B	1	ADP	O5'-C5'-C4'	2.18	116.50	108.99
3	D	1	ADP	C4-C5-N7	-2.17	107.14	109.40
3	A	1	ADP	C4-C5-N7	-2.16	107.14	109.40
3	C	1	ADP	C4-C5-N7	-2.15	107.16	109.40
3	A	1	ADP	O5'-C5'-C4'	2.15	116.38	108.99
3	G	1	ADP	C4-C5-N7	-2.14	107.17	109.40
3	G	1	ADP	O5'-C5'-C4'	2.14	116.34	108.99
3	E	1	ADP	O5'-C5'-C4'	2.09	116.17	108.99

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1	ADP	C5'-O5'-PA-O1A
3	A	1	ADP	C5'-O5'-PA-O2A
3	A	1	ADP	C5'-O5'-PA-O3A
3	B	1	ADP	C5'-O5'-PA-O1A
3	B	1	ADP	C5'-O5'-PA-O2A
3	B	1	ADP	C5'-O5'-PA-O3A
3	C	1	ADP	C5'-O5'-PA-O1A
3	C	1	ADP	C5'-O5'-PA-O2A
3	C	1	ADP	C5'-O5'-PA-O3A
3	D	1	ADP	C5'-O5'-PA-O1A
3	D	1	ADP	C5'-O5'-PA-O2A
3	D	1	ADP	C5'-O5'-PA-O3A
3	E	1	ADP	C5'-O5'-PA-O1A
3	E	1	ADP	C5'-O5'-PA-O2A
3	E	1	ADP	C5'-O5'-PA-O3A
3	F	1	ADP	C5'-O5'-PA-O1A
3	F	1	ADP	C5'-O5'-PA-O2A
3	F	1	ADP	C5'-O5'-PA-O3A
3	G	1	ADP	C5'-O5'-PA-O1A
3	G	1	ADP	C5'-O5'-PA-O2A
3	G	1	ADP	C5'-O5'-PA-O3A
3	D	1	ADP	PB-O3A-PA-O2A
3	F	1	ADP	PB-O3A-PA-O2A
3	G	1	ADP	PB-O3A-PA-O2A
3	A	1	ADP	PB-O3A-PA-O2A
3	B	1	ADP	PB-O3A-PA-O2A
3	C	1	ADP	PB-O3A-PA-O2A

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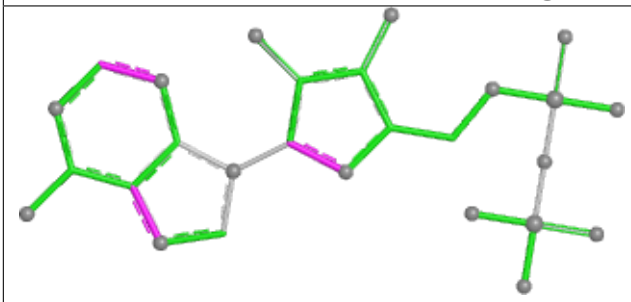
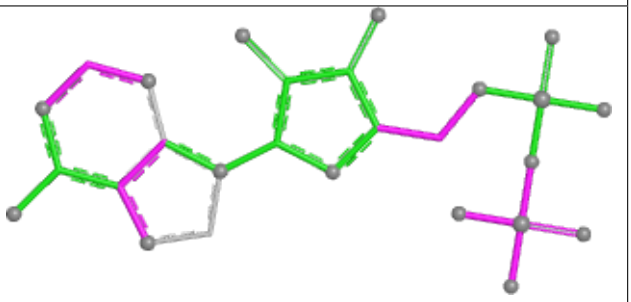
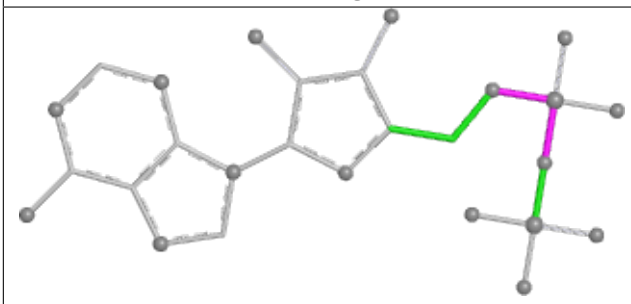
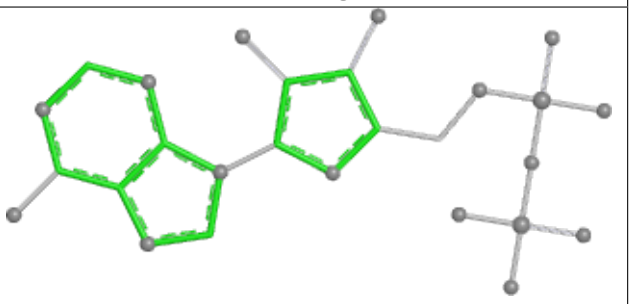
Mol	Chain	Res	Type	Atoms
3	B	1	ADP	PB-O3A-PA-O1A
3	C	1	ADP	PB-O3A-PA-O1A
3	E	1	ADP	PB-O3A-PA-O2A

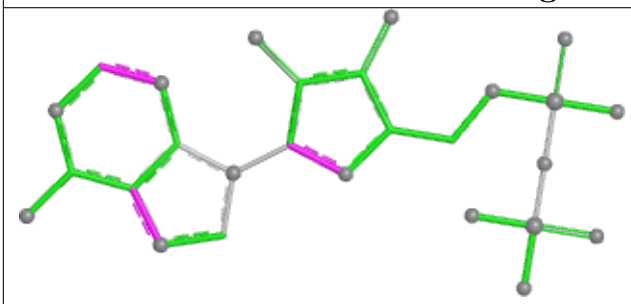
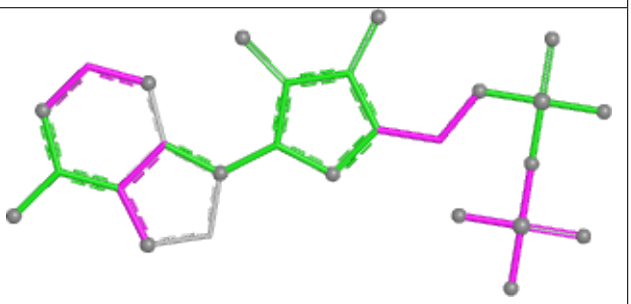
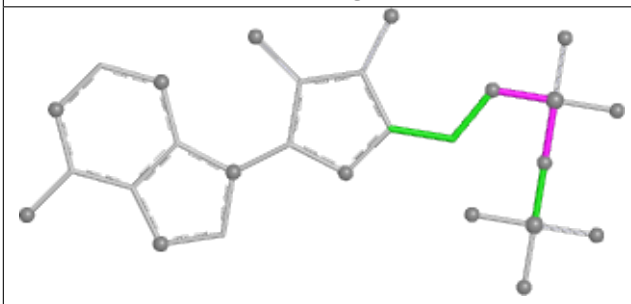
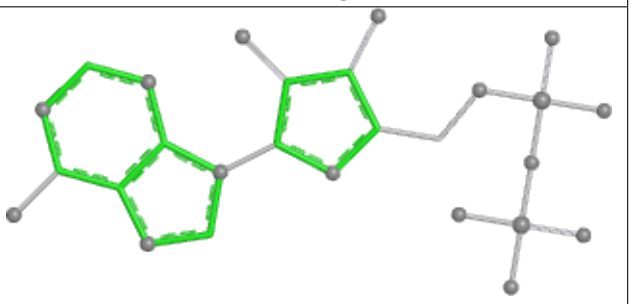
There are no ring outliers.

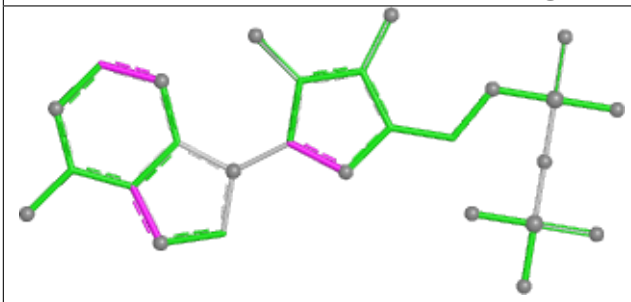
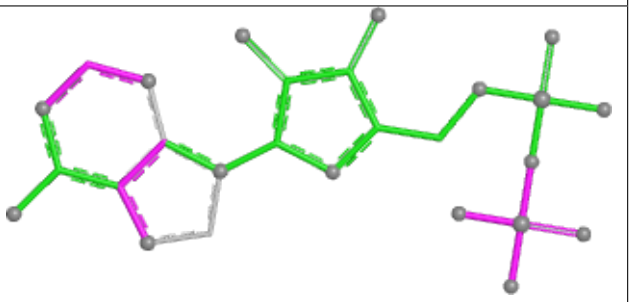
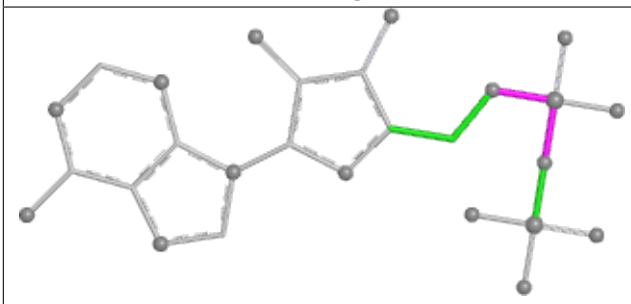
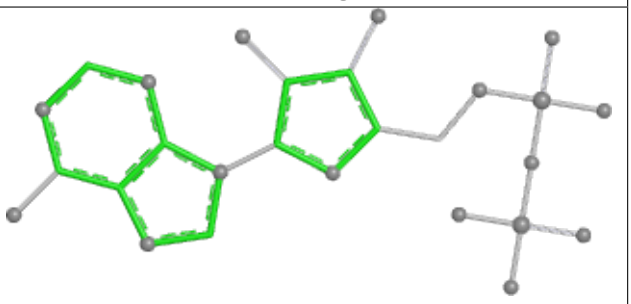
7 monomers are involved in 33 short contacts:

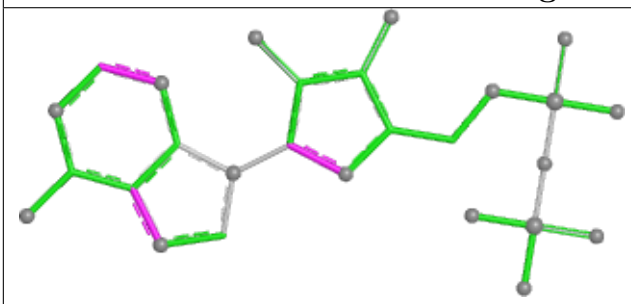
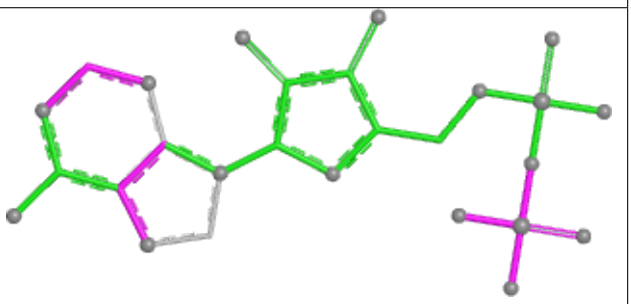
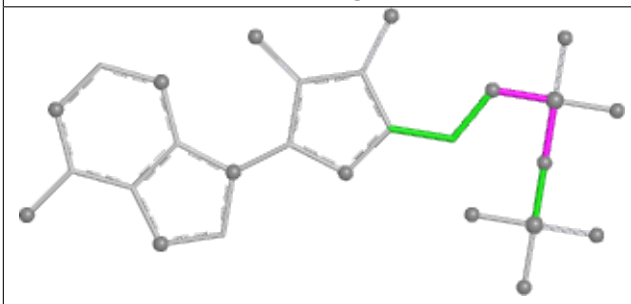
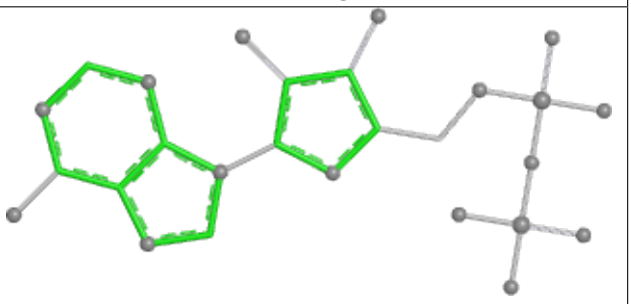
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	1	ADP	3	0
3	A	1	ADP	4	0
3	F	1	ADP	4	0
3	D	1	ADP	3	0
3	E	1	ADP	7	0
3	B	1	ADP	5	0
3	C	1	ADP	7	0

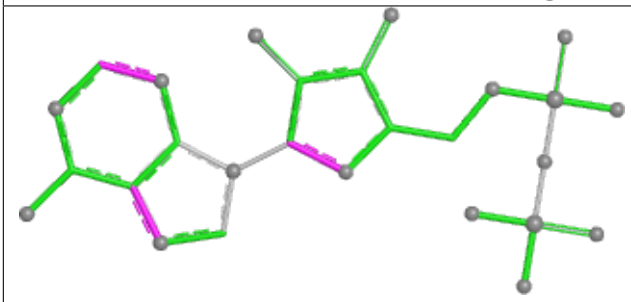
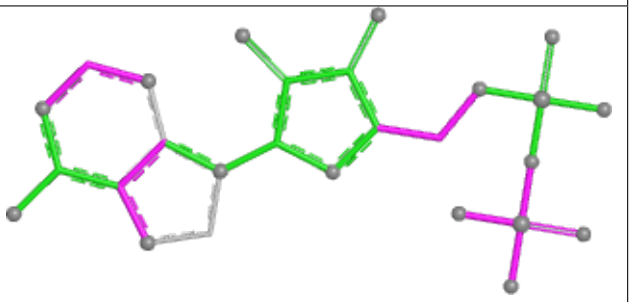
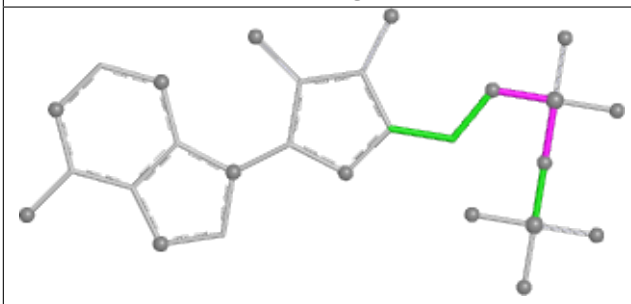
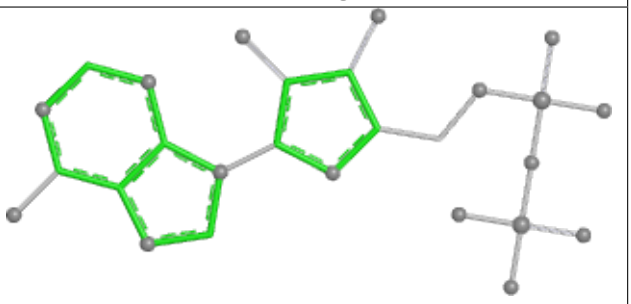
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

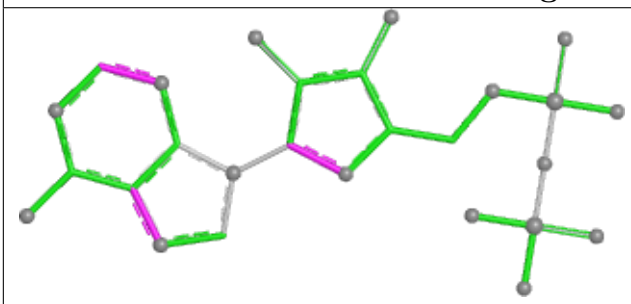
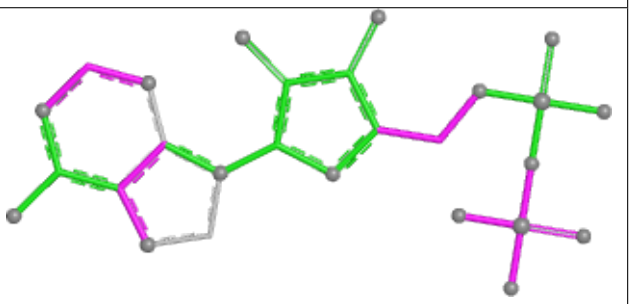
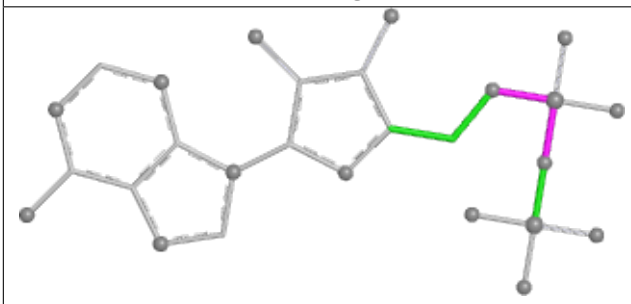
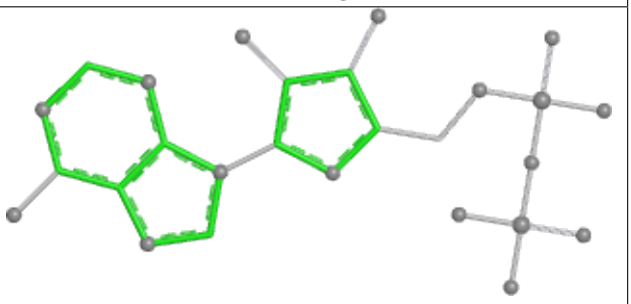
Ligand ADP G 1	
 Bond lengths	 Bond angles
 Torsions	 Rings

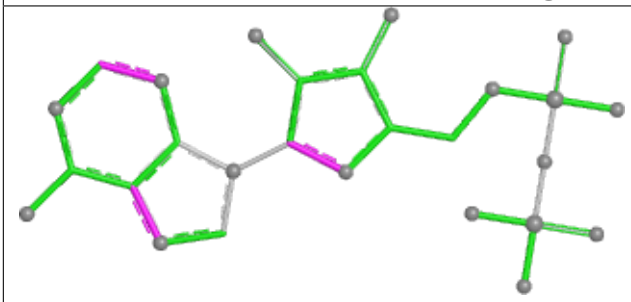
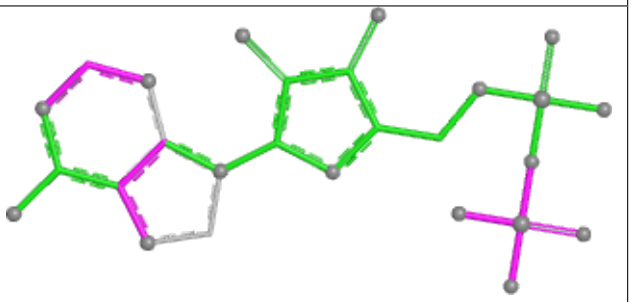
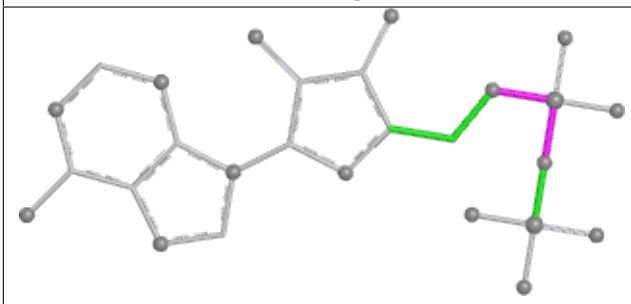
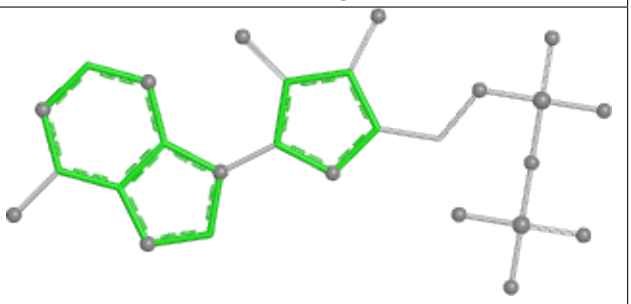
Ligand ADP A 1	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP F 1	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP D 1	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP E 1	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP B 1	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP C 1	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Map visualisation

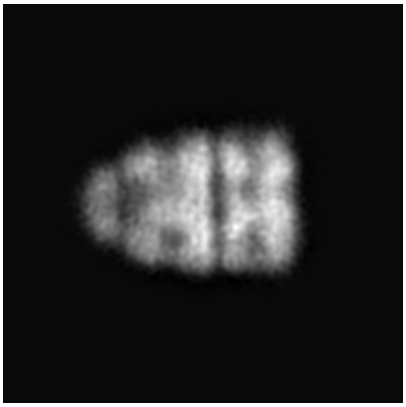
This section contains visualisations of the EMDB entry EMD-2326. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

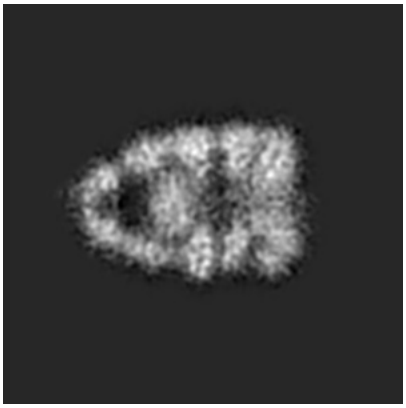
Z

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

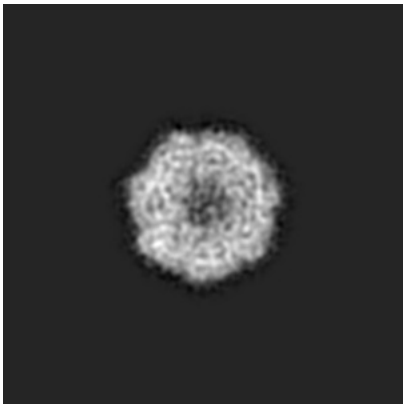
6.2 Central slices

6.2.1 Primary map

X Index: 90



Y Index: 90



Z Index: 90

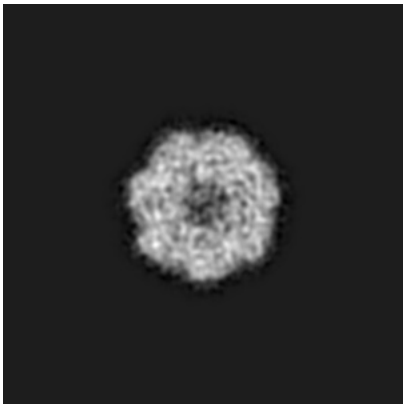
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 104

Y Index: 98

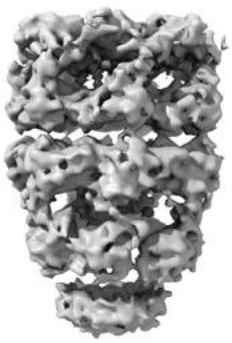


Z Index: 89

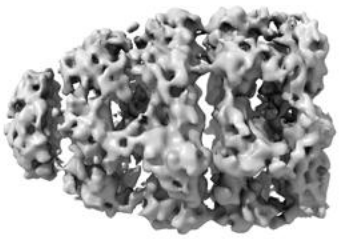
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

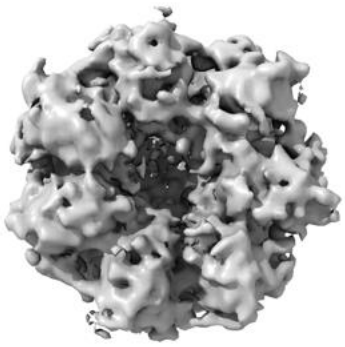
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

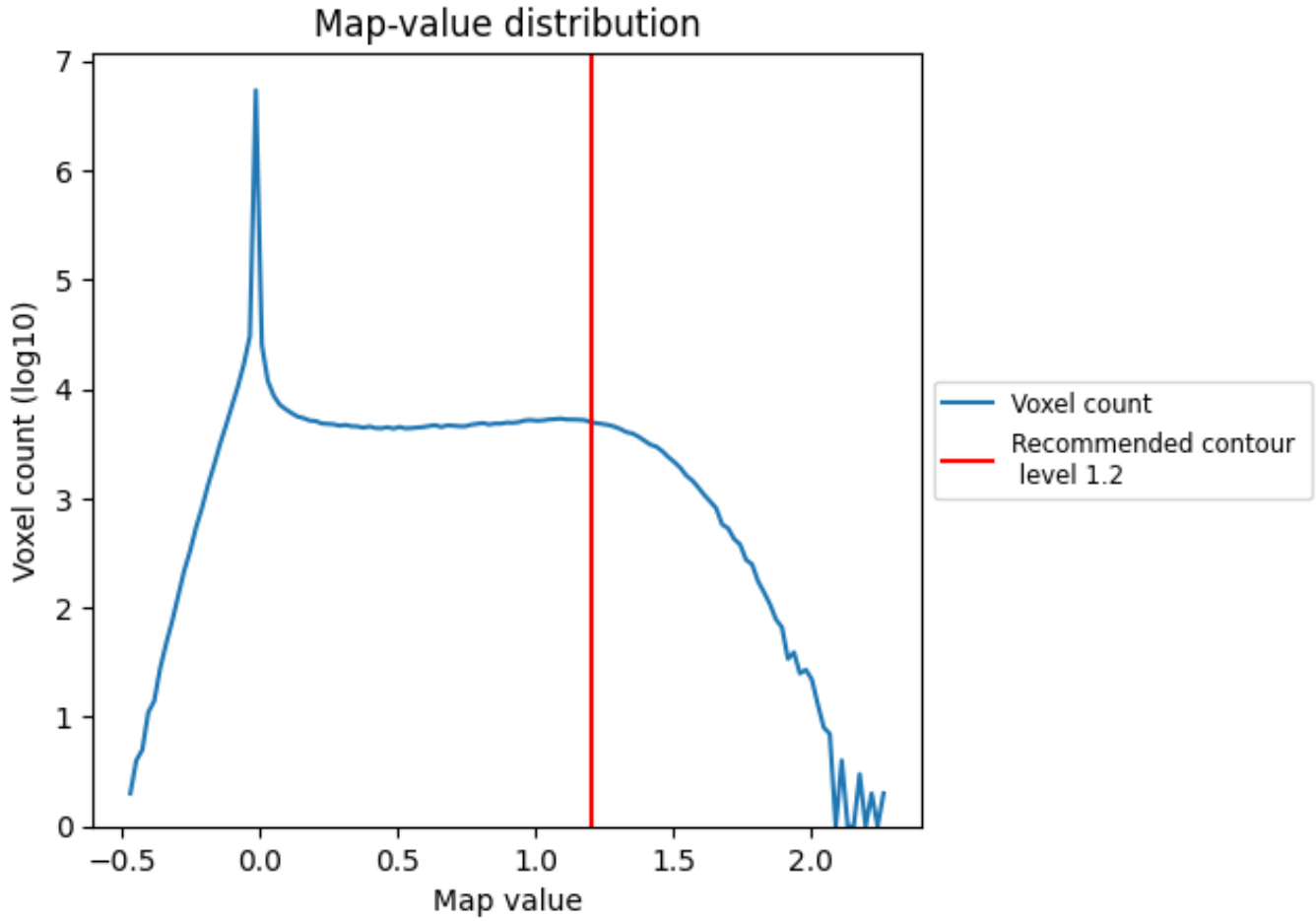
6.5 Mask visualisation (i)

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

7 Map analysis

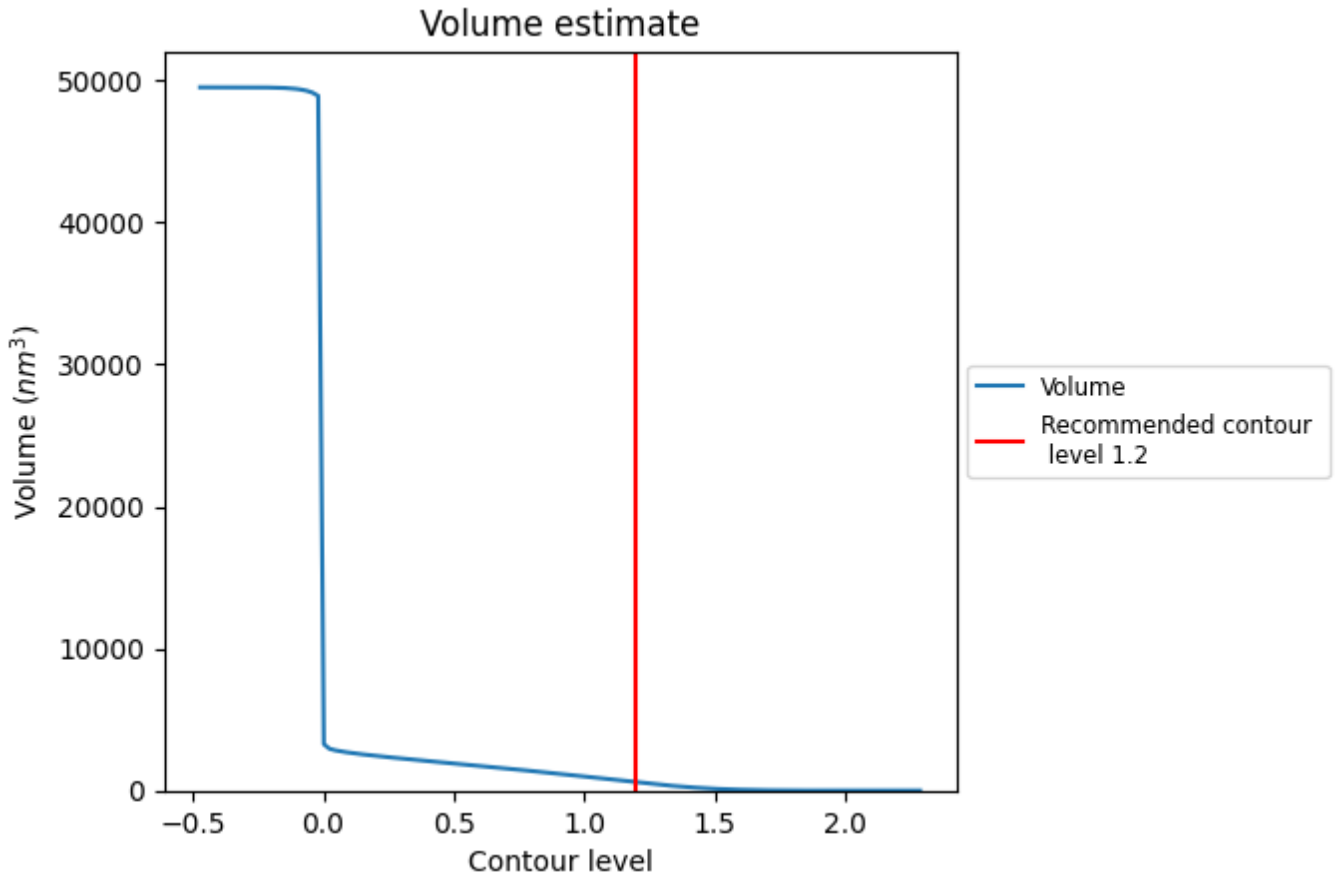
This section contains the results of statistical analysis of the map.

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.

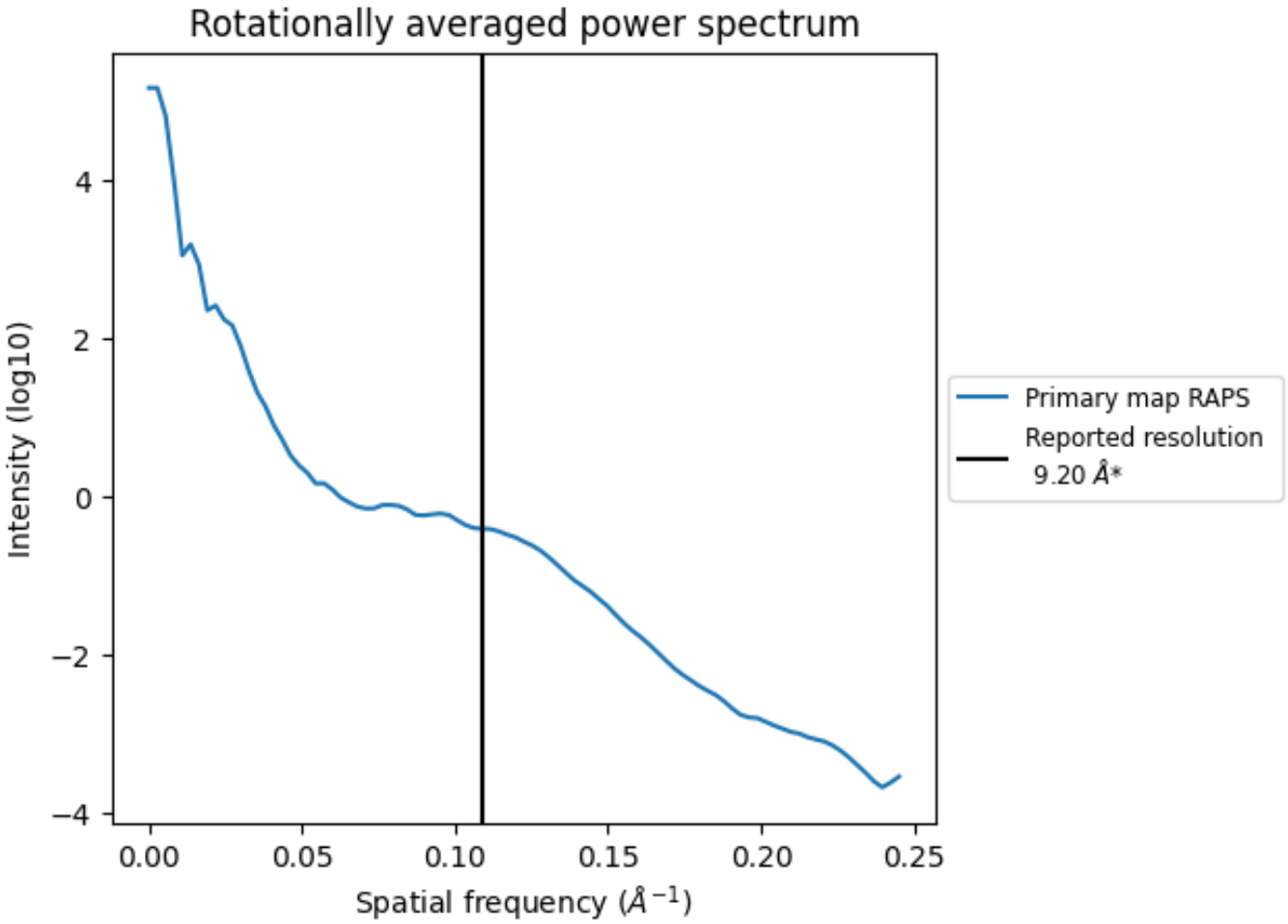
7.2 Volume estimate



The volume at the recommended contour level is 582 nm^3; this corresponds to an approximate mass of 526 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 0.109 $Å^{-1}$

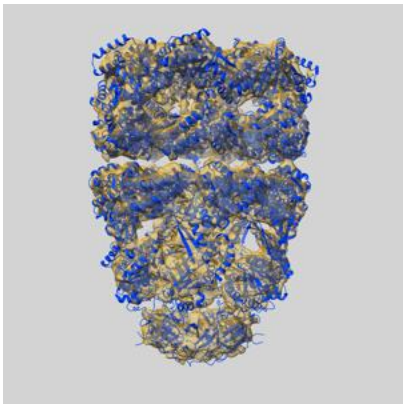
8 Fourier-Shell correlation

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

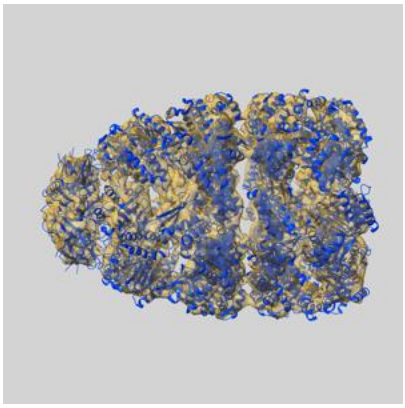
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-2326 and PDB model 3ZQ0. Per-residue inclusion information can be found in section 3 on page 7.

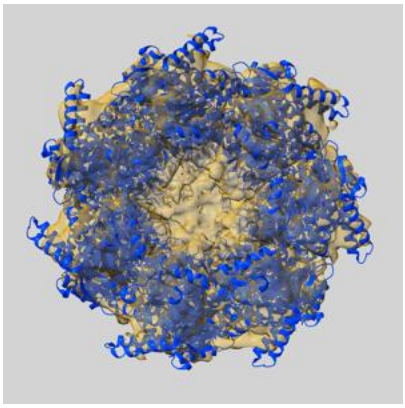
9.1 Map-model overlay



X



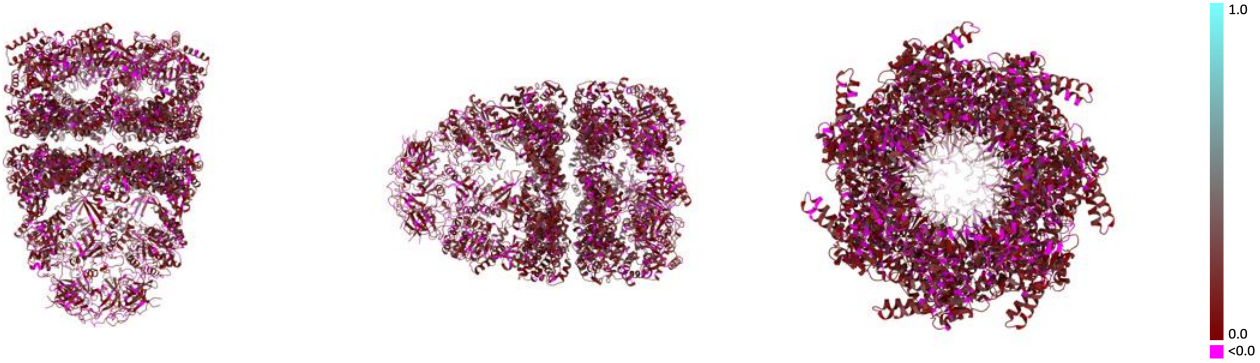
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.2 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.

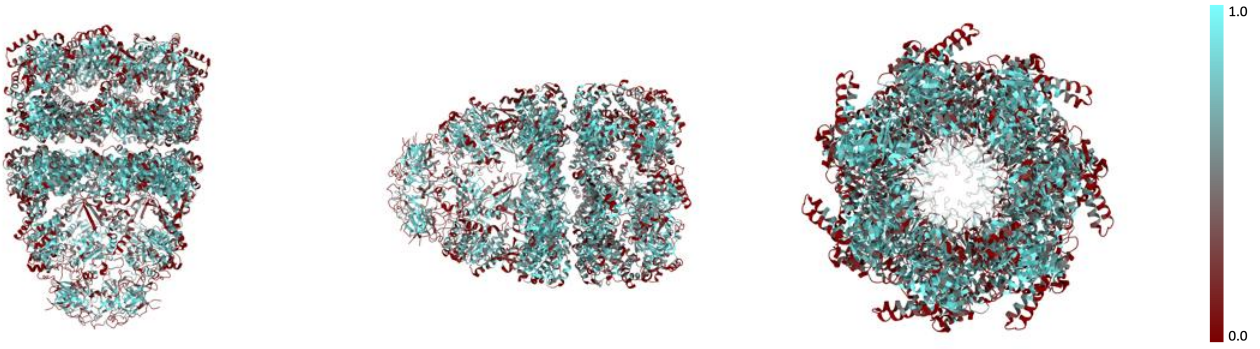
9.2 Q-score mapped to coordinate model



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.

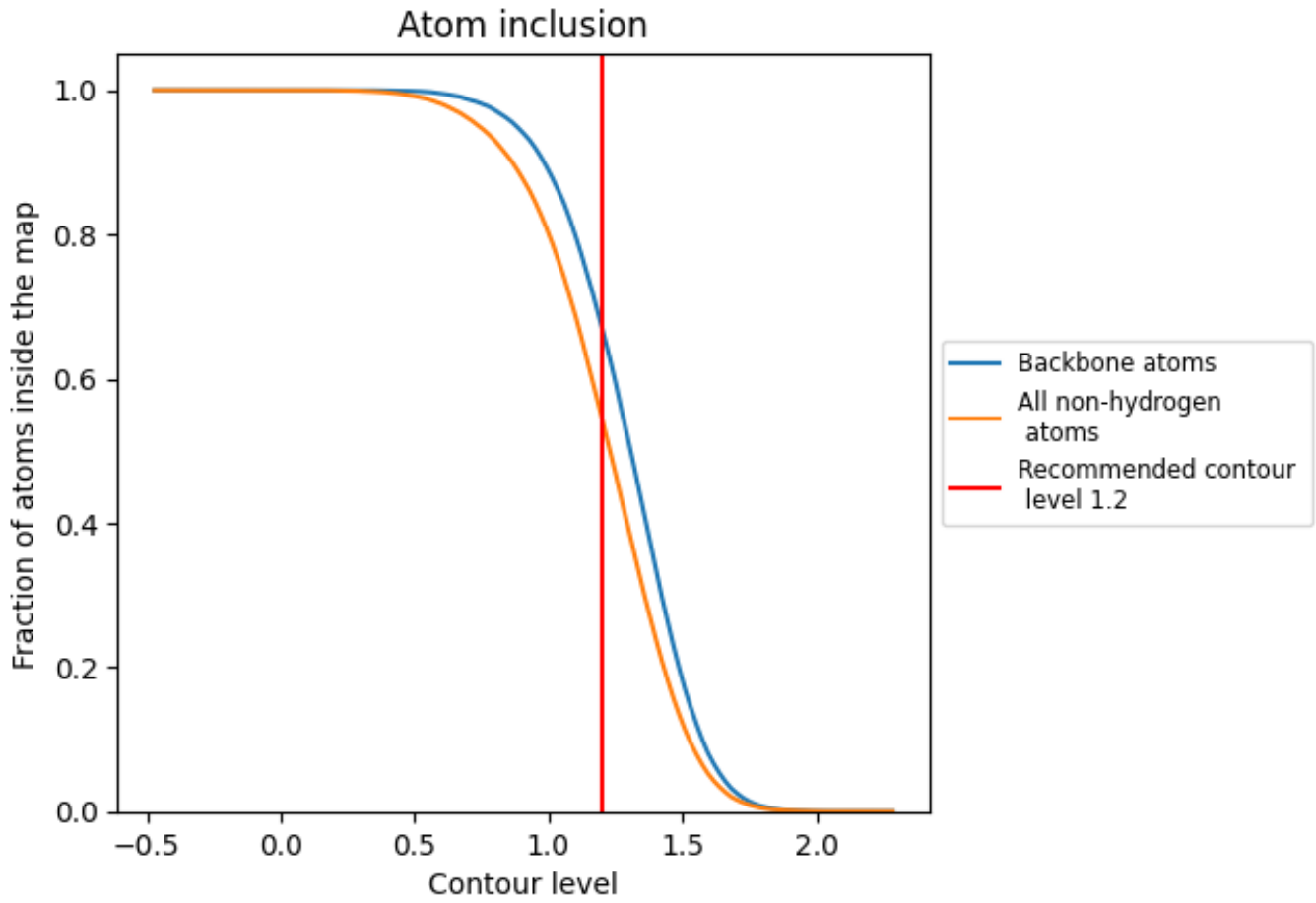
9.3 Atom inclusion mapped to coordinate model



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 (1.2).

9.4 Atom inclusion (i)



At the recommended contour level, 67% of all backbone atoms, 54% 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 (1.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5448	0.1140
A	0.6126	0.1230
B	0.5421	0.1200
C	0.5784	0.1100
D	0.5547	0.1200
E	0.5993	0.1230
F	0.5977	0.1220
G	0.5729	0.1280
H	0.5264	0.1140
I	0.5183	0.1100
J	0.5148	0.1110
K	0.5708	0.1120
L	0.5227	0.1060
M	0.5595	0.1120
N	0.5285	0.1110
O	0.4463	0.0970
P	0.3584	0.0950
Q	0.4324	0.0960
R	0.3989	0.0940
S	0.4212	0.0730
T	0.4338	0.1070
U	0.3989	0.0860