Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 06:27 pm GMT

PDB ID	:	4BZI
EMDB ID	:	EMD-2428
Title	:	The structure of the COPII coat assembled on membranes
Authors	:	Zanetti, G.; Prinz, S.; Daum, S.; Meister, A.; Schekman, R.; Bacia, K.; Briggs, J.A.G.
Deposited on	:	2013-07-26
Resolution	:	23.00 Å(reported)
Based on initial model	:	1M2O

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:

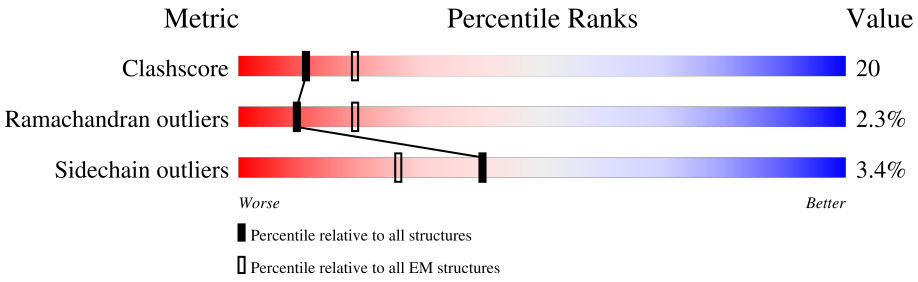
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 23.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
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	768	8% 68% 25% • 5%
1	D	768	10% 68% 25% • 5%
1	G	768	11% 69% 25% • 5%
2	B	190	8% 52% 31% • 14%
2	J	190	8% 53% 31% • 14%
2	K	190	14% 52% 32% • 14%
3	E	926	6% 45% 31% • 21%
3	L	926	11% 45% 31% • 21%

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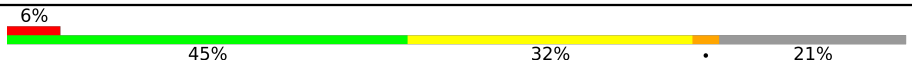
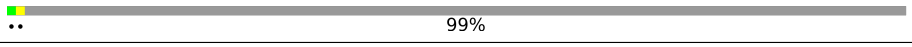
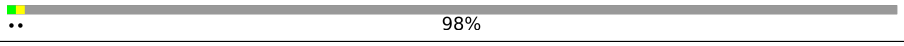
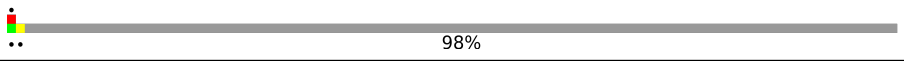
Mol	Chain	Length	Quality of chain
3	M	926	
4	F	926	
4	N	926	
4	O	926	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 39154 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 SEC23P.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	733	Total	C	N	O	S	0	0
			5780	3679	969	1109	23		
1	D	733	Total	C	N	O	S	0	0
			5780	3679	969	1109	23		
1	G	733	Total	C	N	O	S	0	0
			5780	3679	969	1109	23		

- Molecule 2 is a protein called SAR1P.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	164	Total	C	N	O	S	0	0
			1299	836	220	239	4		
2	J	164	Total	C	N	O	S	0	0
			1299	836	220	239	4		
2	K	164	Total	C	N	O	S	0	0
			1299	836	220	239	4		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	139	ALA	GLY	conflict	UNP C8ZIG2
J	139	ALA	GLY	conflict	UNP C8ZIG2
K	139	ALA	GLY	conflict	UNP C8ZIG2

- Molecule 3 is a protein called SEC24P.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	735	Total	C	N	O	S	0	0
			5823	3702	999	1084	38		
3	L	735	Total	C	N	O	S	0	0
			5823	3702	999	1084	38		
3	M	735	Total	C	N	O	S	0	0
			5823	3702	999	1084	38		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	408	THR	ALA	conflict	UNP C8ZAD6
E	865	VAL	ALA	conflict	UNP C8ZAD6
L	408	THR	ALA	conflict	UNP C8ZAD6
L	865	VAL	ALA	conflict	UNP C8ZAD6
M	408	THR	ALA	conflict	UNP C8ZAD6
M	865	VAL	ALA	conflict	UNP C8ZAD6

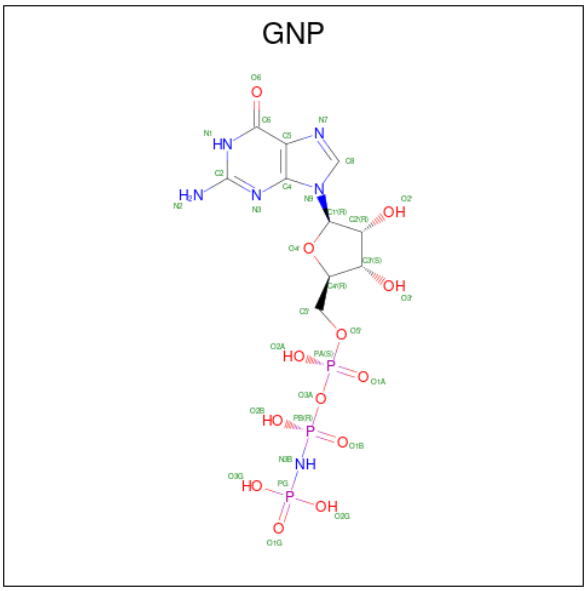
- Molecule 4 is a protein called SEC24P.

Mol	Chain	Residues	Atoms	AltConf	Trace
4	F	13	Total C N O 109 70 19 20	0	0
4	N	14	Total C N O 117 74 21 22	0	0
4	O	14	Total C N O 117 74 21 22	0	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
5	A	1	Total Zn 1 1	0
5	D	1	Total Zn 1 1	0
5	E	1	Total Zn 1 1	0
5	G	1	Total Zn 1 1	0
5	L	1	Total Zn 1 1	0
5	M	1	Total Zn 1 1	0

- Molecule 6 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
6	B	1	Total	C	N	O	P	0
			32	10	6	13	3	
6	J	1	Total	C	N	O	P	0
			32	10	6	13	3	
6	K	1	Total	C	N	O	P	0
			32	10	6	13	3	

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

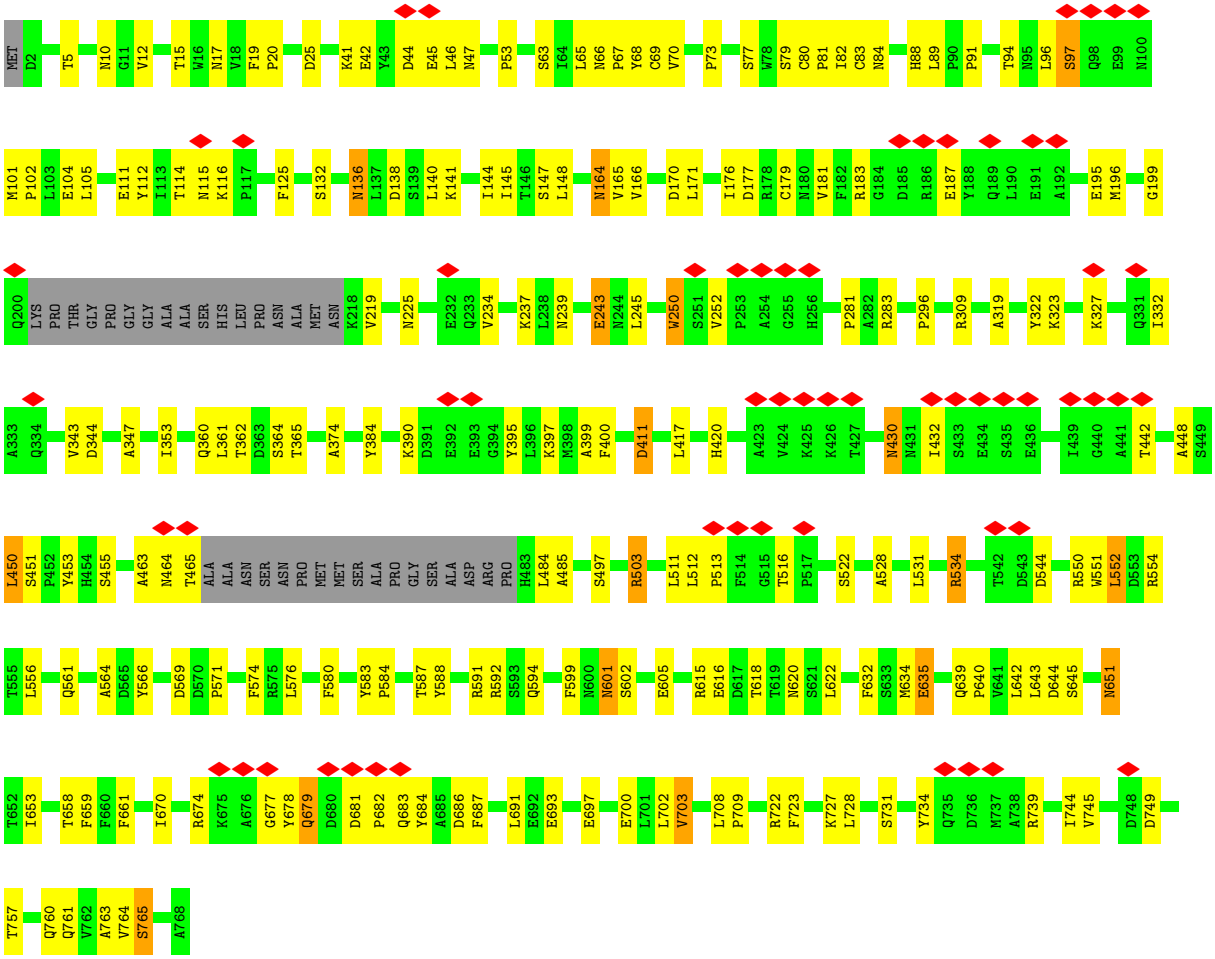
Mol	Chain	Residues	Atoms		AltConf
7	B	1	Total	Mg	0
			1	1	
7	J	1	Total	Mg	0
			1	1	
7	K	1	Total	Mg	0
			1	1	

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.

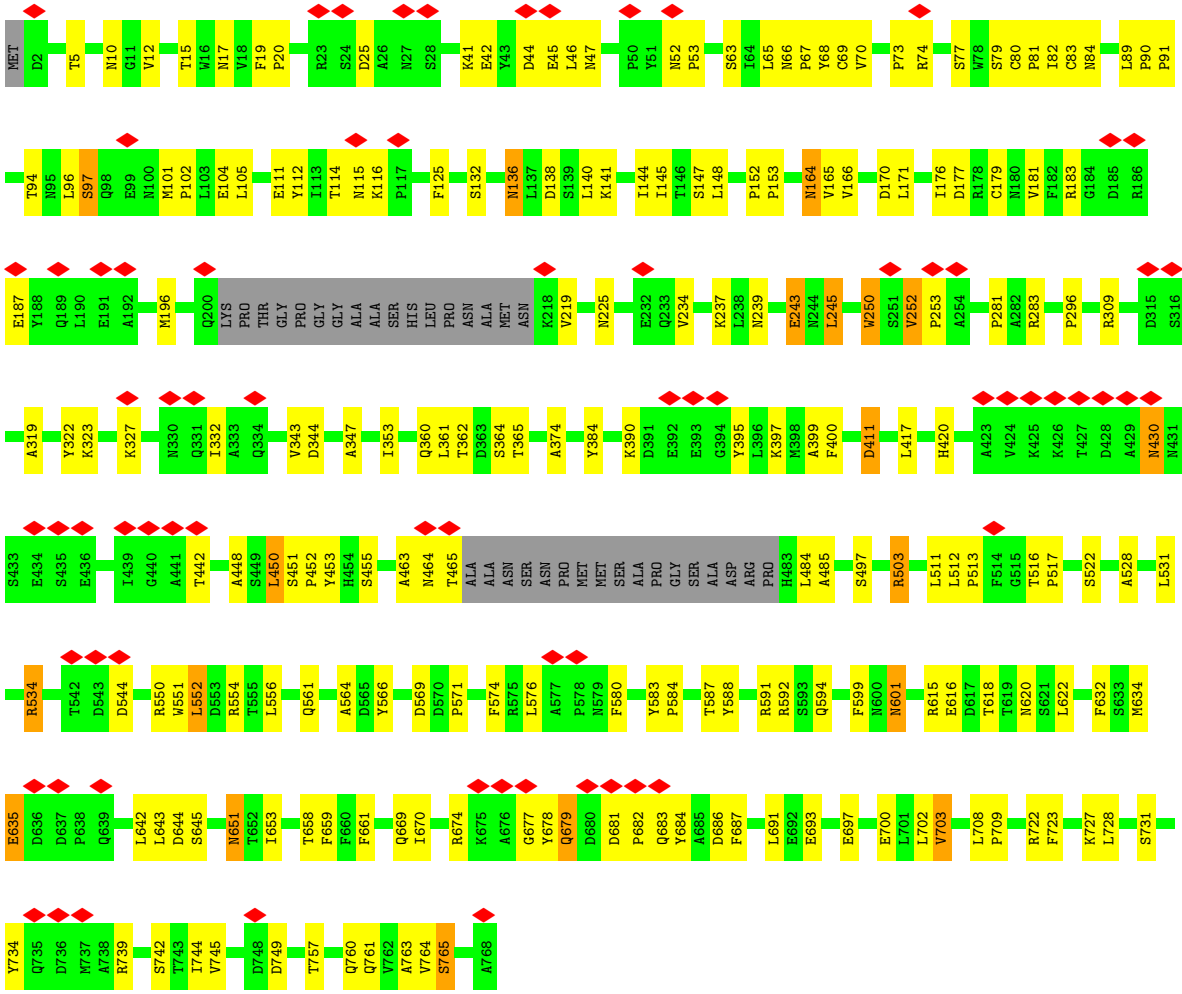
• Molecule 1: SEC23P

Chain A:



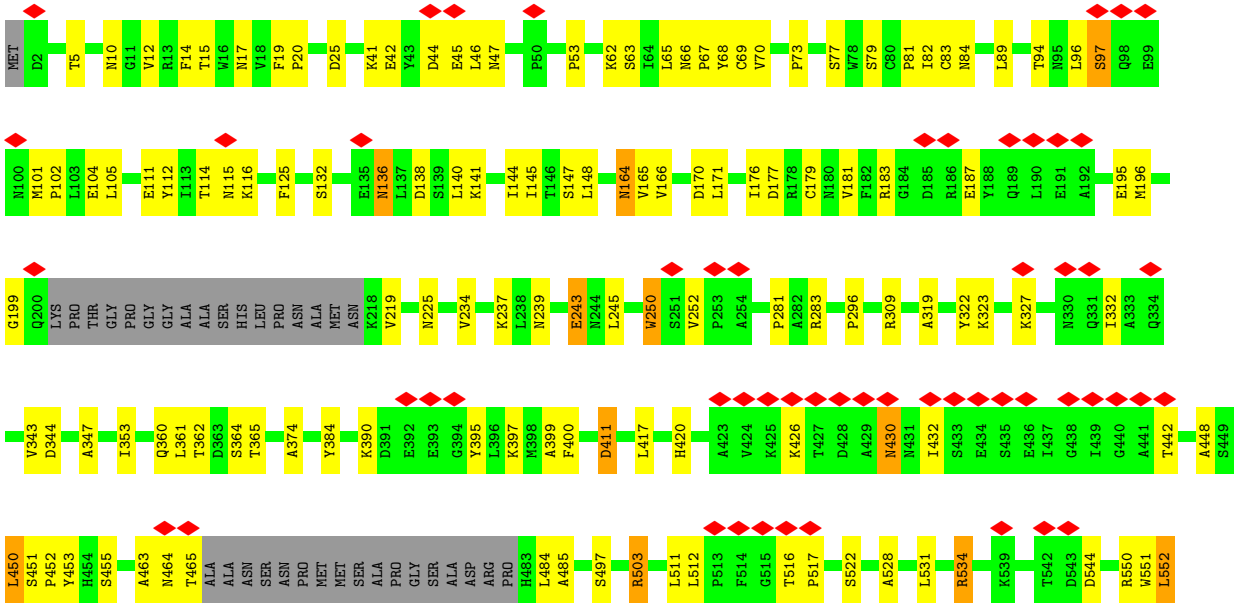
• Molecule 1: SEC23P

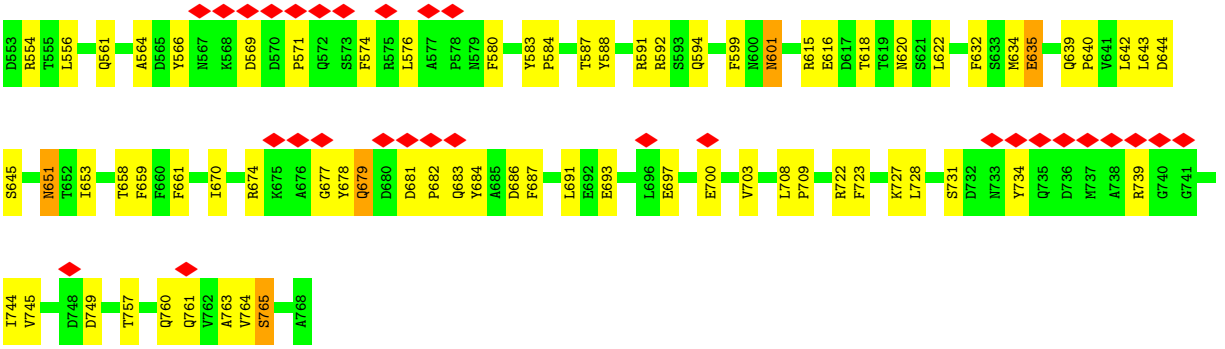
Chain D:



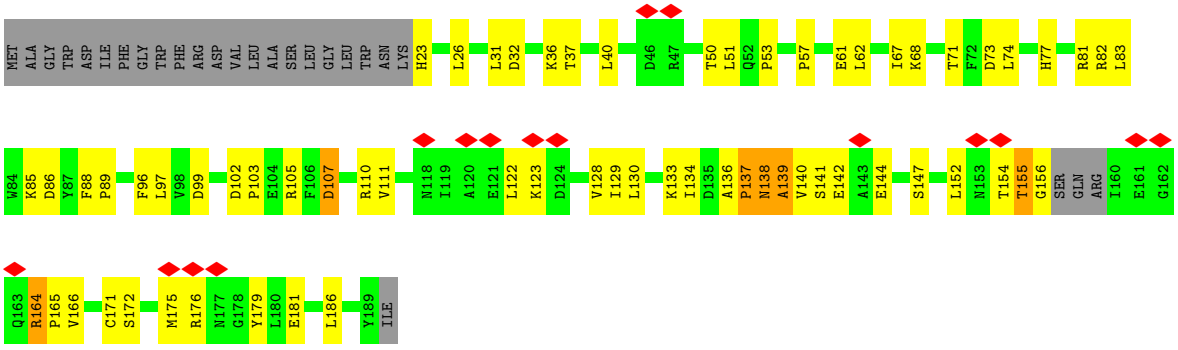
• Molecule 1: SEC23P

Chain G:

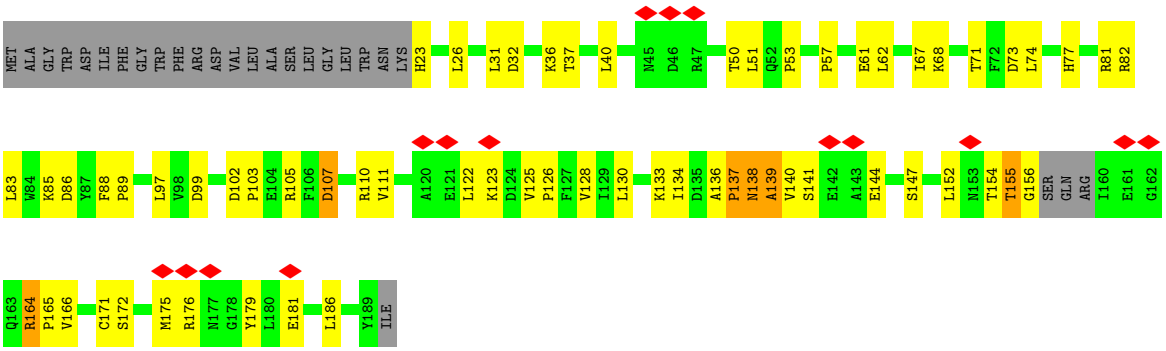




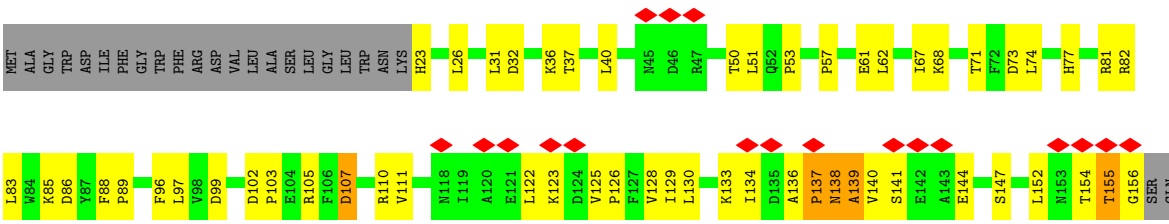
• Molecule 2: SAR1P

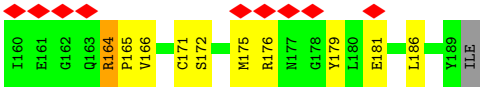


• Molecule 2: SAR1P

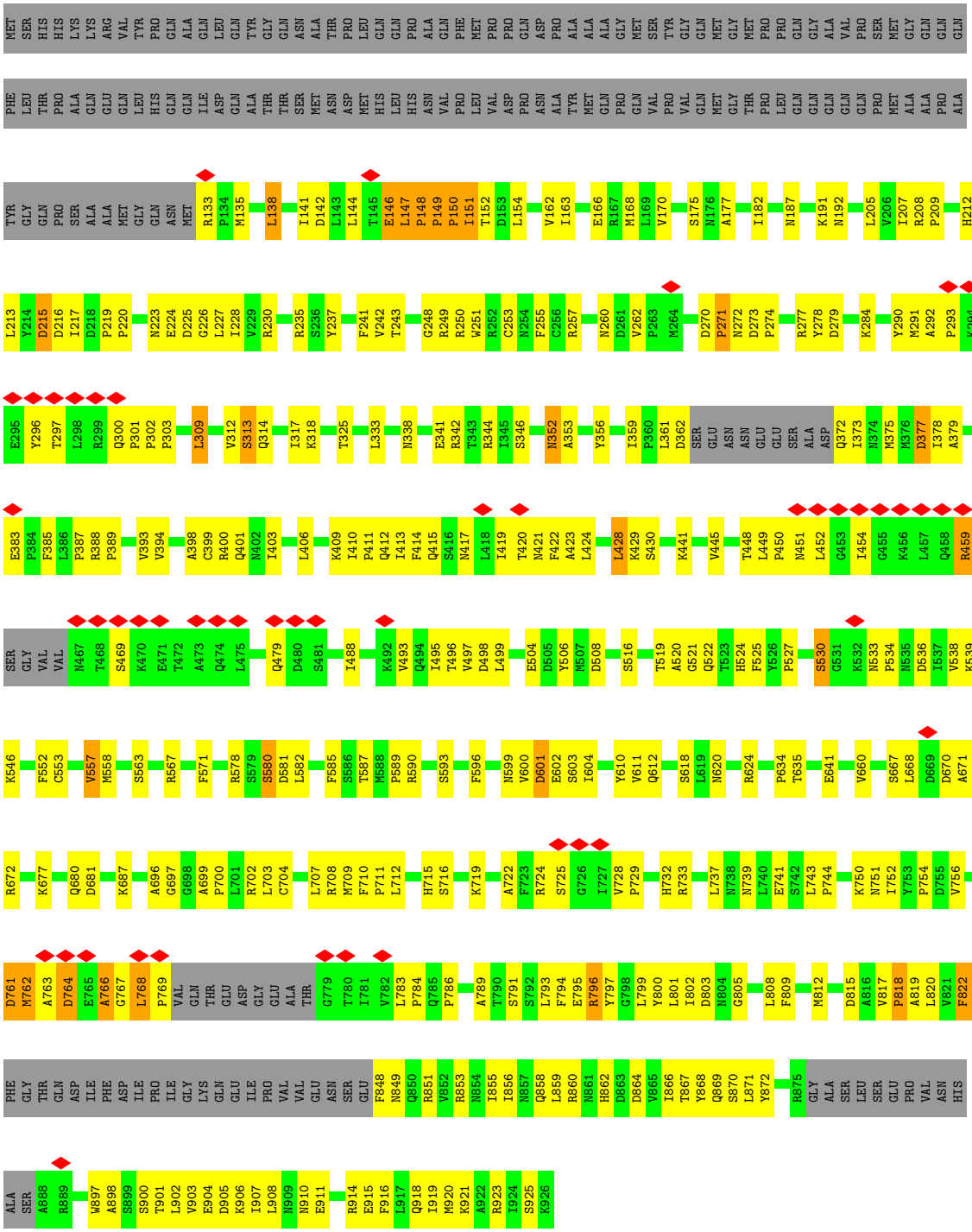


• Molecule 2: SAR1P



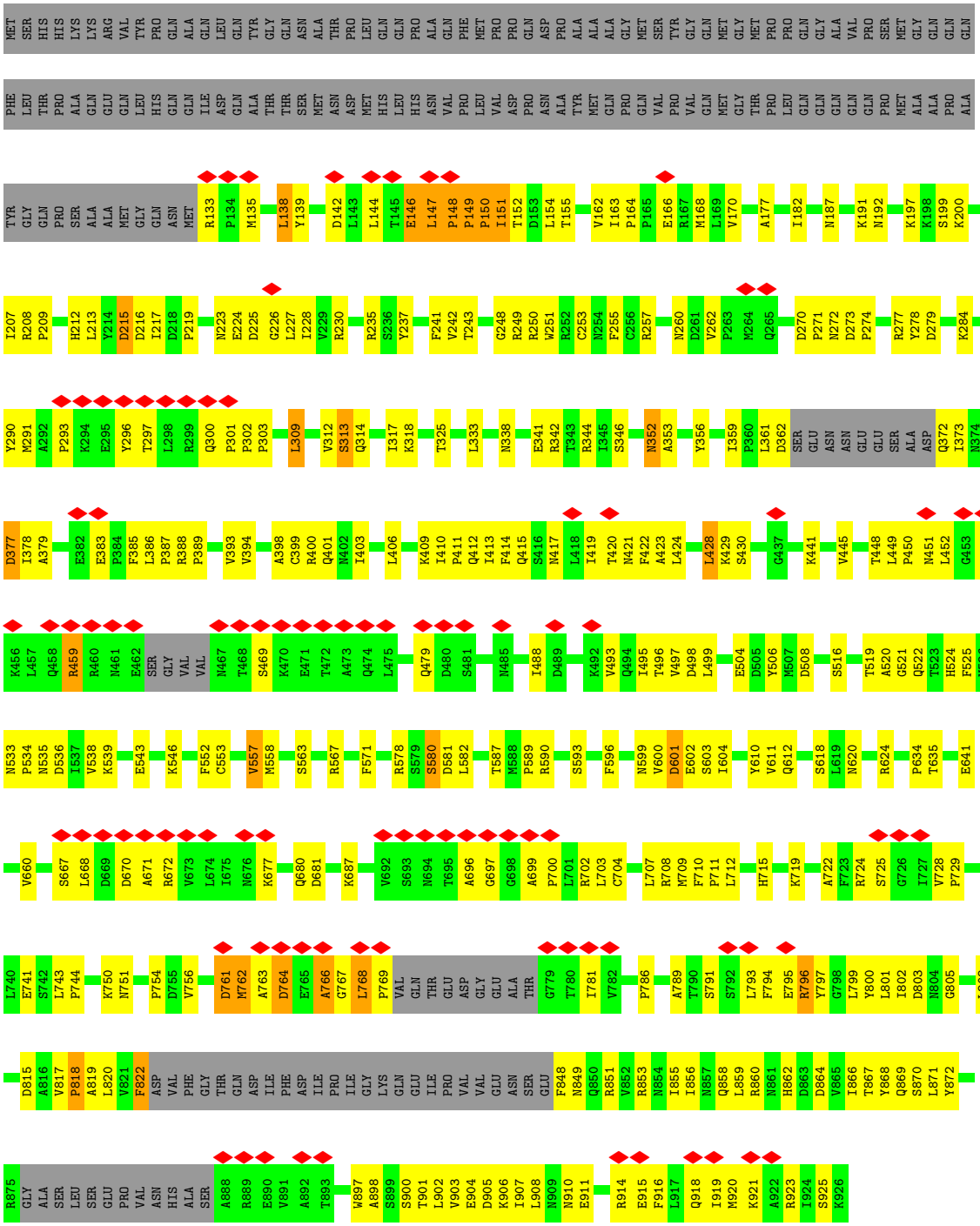


• Molecule 3: SEC24P



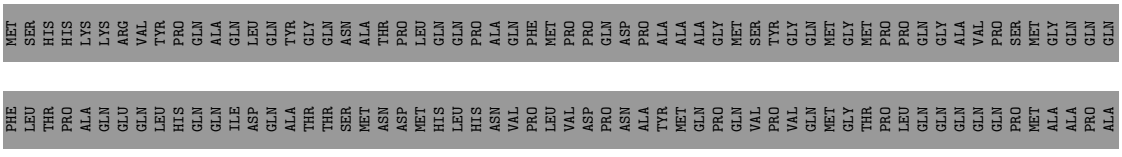
• Molecule 3: SEC24P

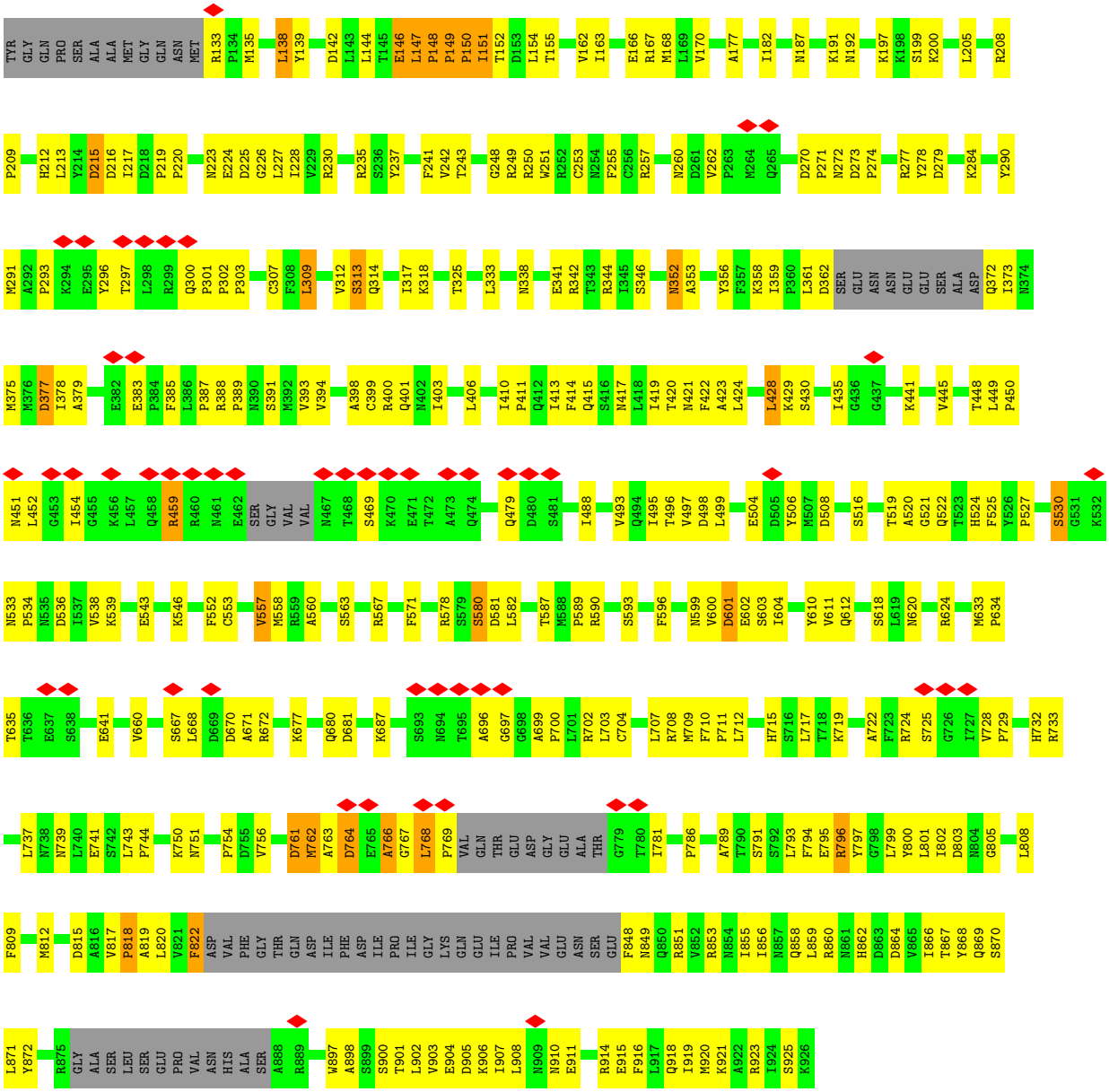
Chain L:



• Molecule 3: SEC24P

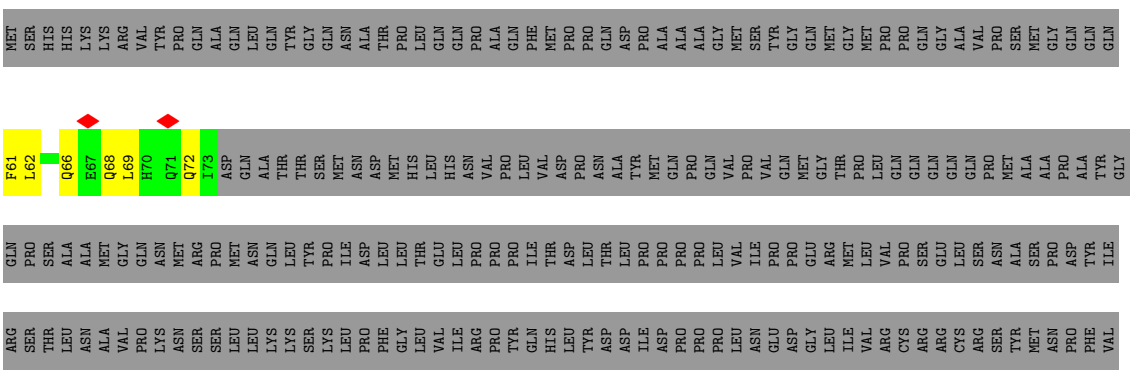
Chain M:

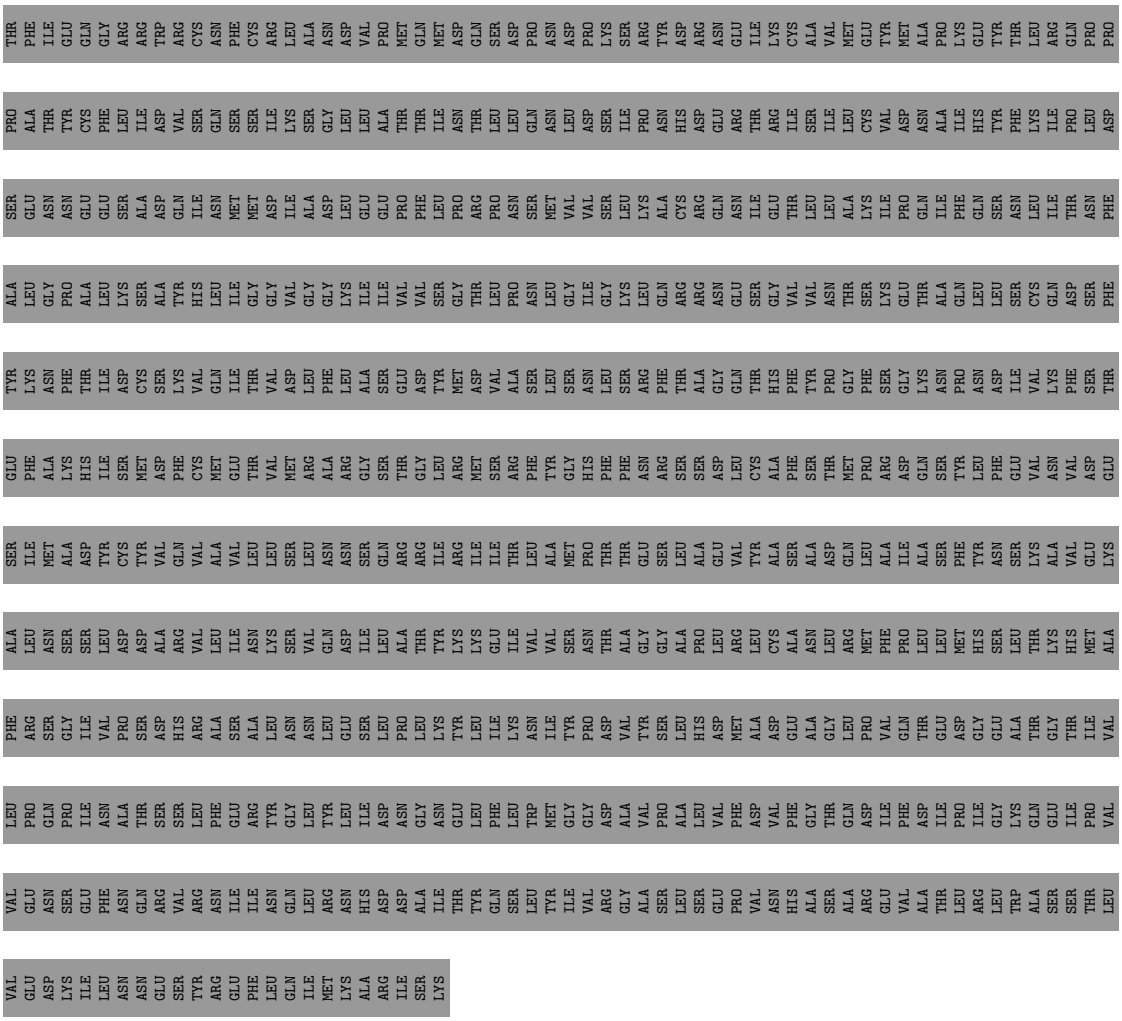




• Molecule 4: SEC24P

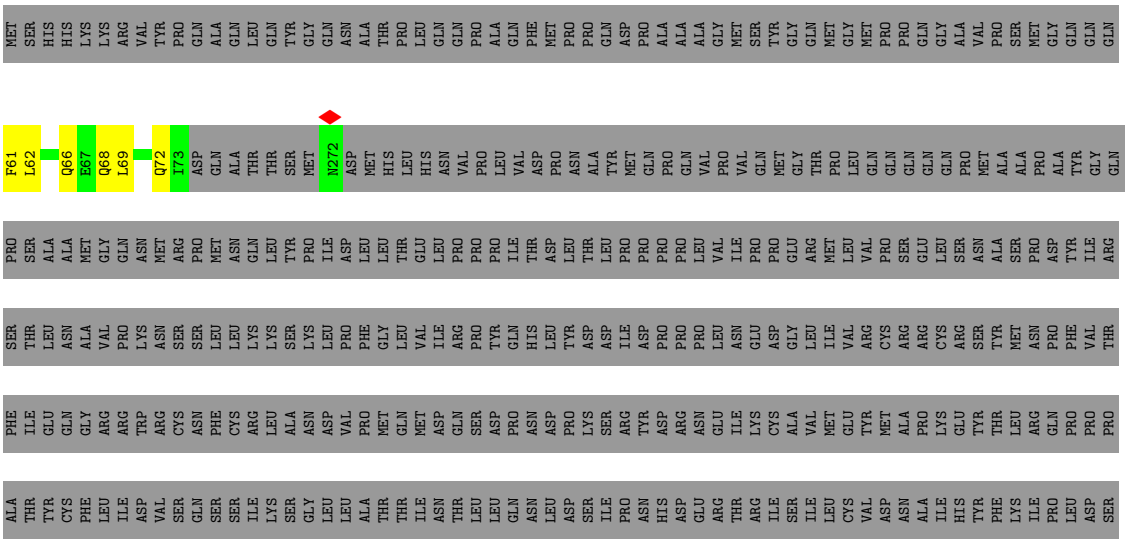
Chain F: 99%

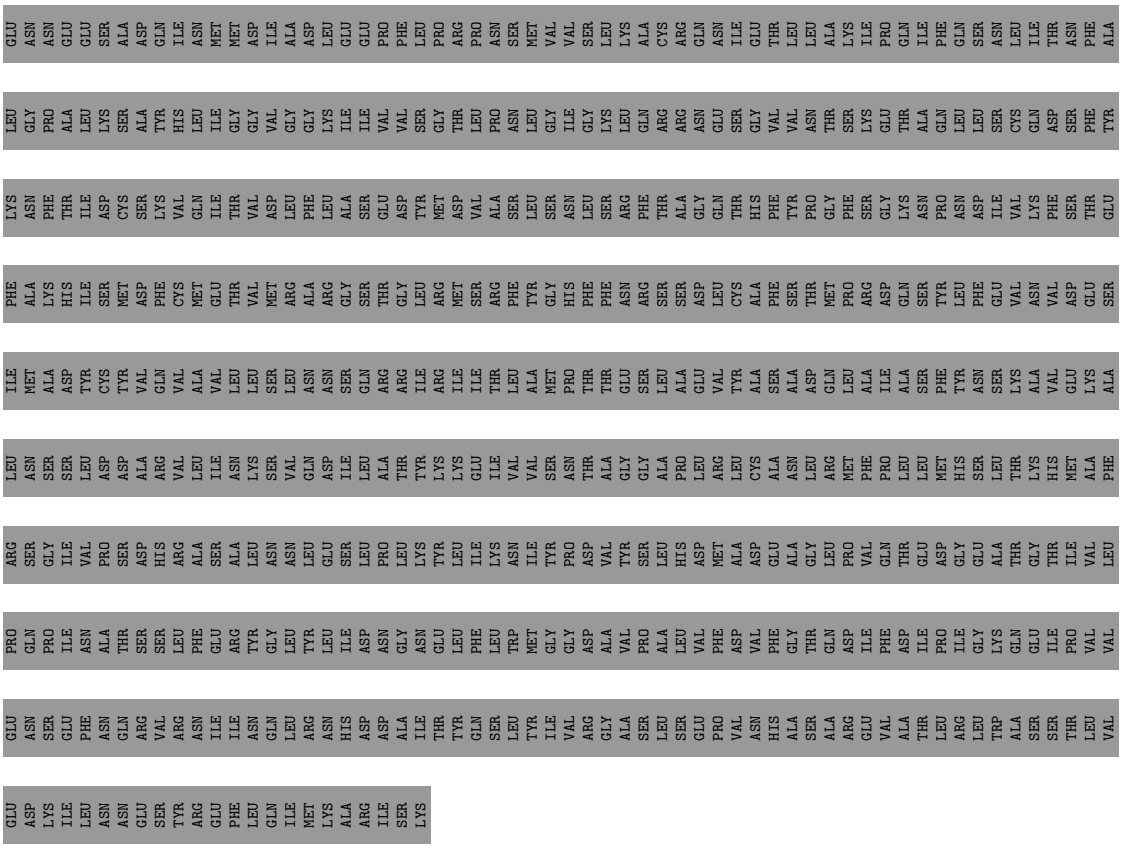




- Molecule 4: SEC24P

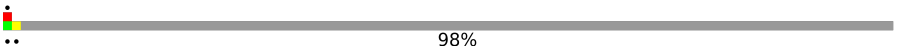
Chain N: 98%

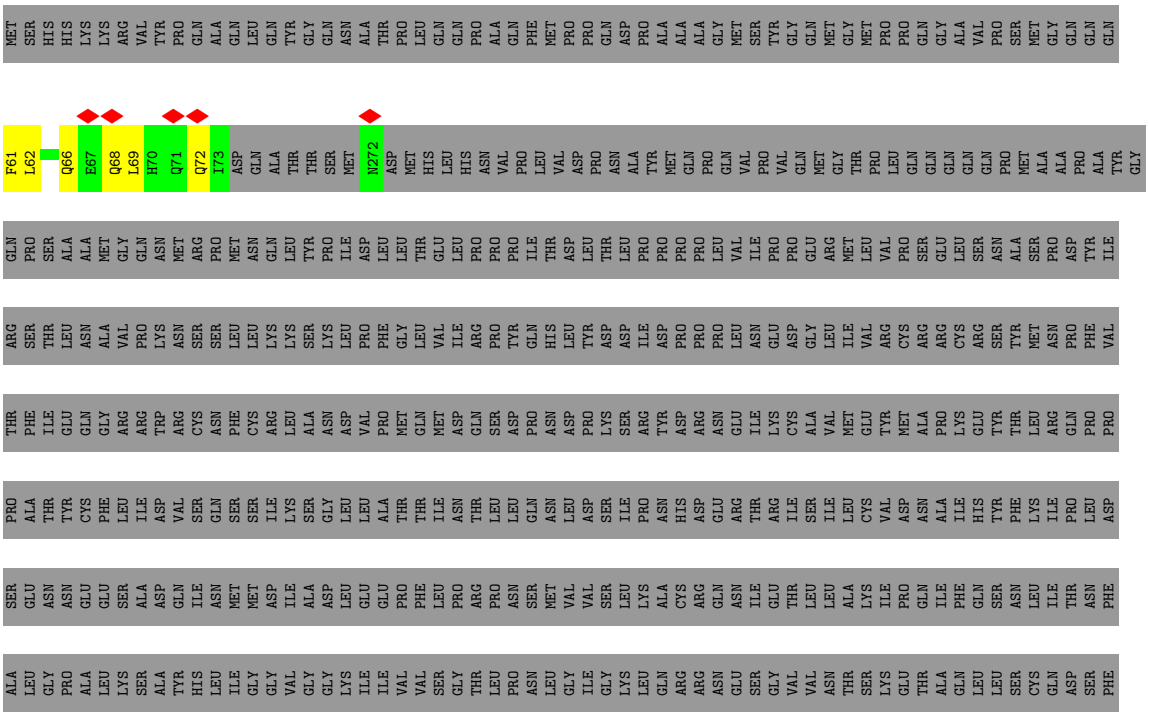


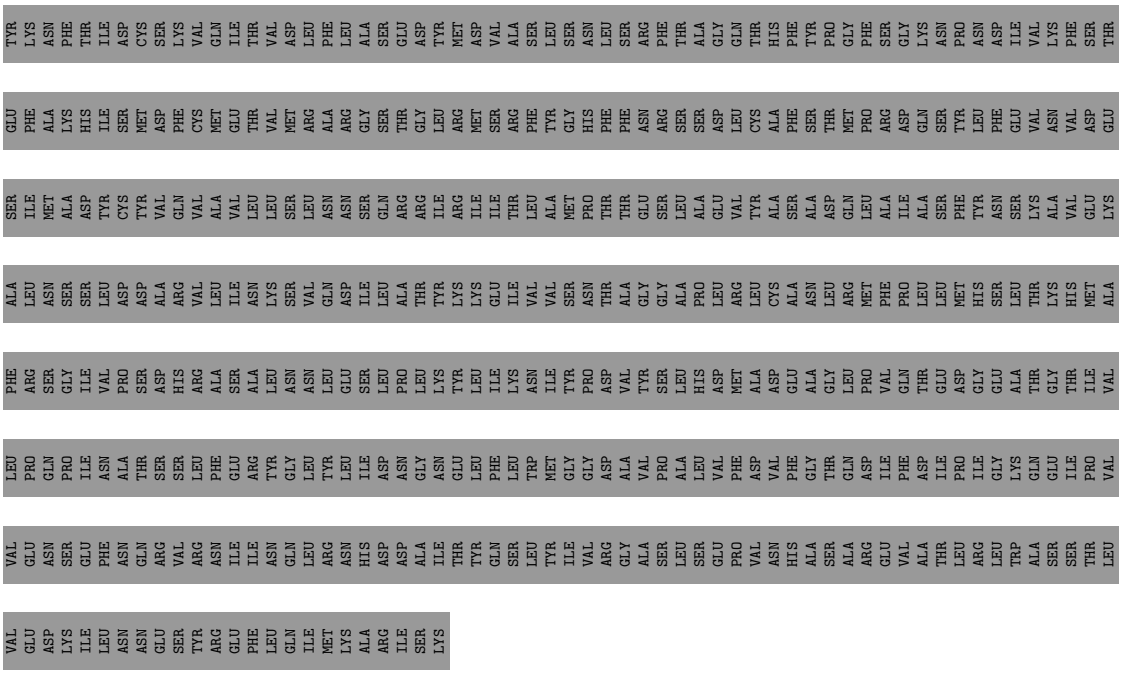


- Molecule 4: SEC24P

Chain O:






TYR LYS ASN PHE THR ILE ASP CYS SER LYS VAL GLN ILE THR VAL ASP LEU PHE LEU ALA SER GLU ASP TYR MET ASP VAL ALA SER LEU SER ASN LEU SER ARG PHE THR ALA GLY GLN THR HIS PHE TYR PRO GLY PHE SER GLY LYS ASN PRO ASN ASP ILE VAL LYS PHE SER THR
GLU PHE ALA LYS HIS ILE SER MET ASP PHE CYS MET GLU THR VAL MET ARG ALA ARG GLY SER THR GLY LEU ARG MET SER ARG PHE TYR GLY HIS PHE PHE ASN ARG SER SER ASP LEU CYS ALA PHE SER THR MET PRO ARG ASP GLN SER TYR LEU PHE GLU VAL ASN SER GLU
SER ILE MET ALA ASP TYR CYS TYR VAL GLN VAL ALA VAL LEU LEU SER LEU ASN ASN SER GLN ARG ARG ILE ARG ILE ILE THR LEU ALA MET PRO THR THR GLU SER LEU ALA GLU VAL TYR ALA SER ALA ASP GLN LEU ALA ILE ALA SER PHE TYR ASN SER LYS ALA VAL GLU LYS
ALA LEU ASN SER SER LEU ASP ASP ALA ARG VAL LEU ILE ASN LYS SER VAL GLN ASP ILE LEU ALA THR TYR LYS LYS GLU ILE VAL VAL SER ASN THR ALA GLY GLY ALA PRO LEU ARG LEU CYS ALA ASN LEU ARG MET PHE PRO LEU LEU MET HIS SER LEU THR LYS HIS MET ALA
PHE ARG SER GLY ILE VAL PRO SER ASP HIS ARG ALA SER ALA LEU ASN LEU GLU LEU SER LEU PRO LEU LYS TYR LEU ILE LYS ASN ILE TYR PRO ASP VAL TYR SER LEU HIS ASP MET ALA ASP GLU ALA GLY LEU PRO VAL GLN THR GLU ASP GLY GLU ALA THR GLY THR ILE VAL
LEU PRO GLN PRO ILE ASN ALA THR SER SER LEU LEU PHE GLU ARG TYR GLY LEU TYR LEU ILE ASP ASN GLY GLU LEU PHE LEU TRP MET GLY GLY ASP ALA VAL PRO ALA LEU VAL PHE ASP VAL PHE GLY THR GLN ASP ILE PHE ASP ILE PRO ILE GLY LYS GLN GLU ILE PRO VAL
VAL GLU ASN SER GLU PHE ASN GLN ARG VAL ARG ASN ILE ILE ASN GLN LEU ARG ASN HIS ASP ASP ALA ILE THR TYR GLN SER LEU TYR ILE VAL ARG GLY ALA SER LEU SER GLU PRO VAL ASN HIS ALA SER ALA ARG GLU VAL ALA THR LEU ARG LEU TRP ALA SER SER THR LEU
VAL GLU ASP LYS ILE LEU ASN ASN GLU SER TYR ARG GLU PHE LEU GLN ILE MET LYS ALA ARG ILE SER LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of tilted images used	15000	Depositor
Resolution determination method	Not provided	
CTF correction method	EACH TILTED IMAGE WITHIN TOMOGRAM	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	80	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	3200	Depositor
Magnification	19500	Depositor
Image detector	GATAN MULTISCAN	Depositor
Maximum voxel value	3.686	Depositor
Minimum voxel value	-2.502	Depositor
Average voxel value	0.000	Depositor
Voxel value standard deviation	1.000	Depositor
Recommended contour level	1.4	Depositor
Tomogram size (Å)	275.2, 275.2, 275.2	wwPDB
Tomogram dimensions	64, 64, 64	wwPDB
Tomogram angles (°)	90.0, 90.0, 90.0	wwPDB
Grid spacing (Å)	4.3, 4.3, 4.3	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, GNP, MG

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	0.38	0/5915	0.62	0/8052
1	D	0.38	0/5915	0.62	0/8052
1	G	0.38	0/5915	0.62	0/8052
2	B	0.34	0/1327	0.61	0/1800
2	J	0.34	0/1327	0.61	0/1800
2	K	0.34	0/1327	0.61	0/1800
3	E	0.39	0/5943	0.68	1/8064 (0.0%)
3	L	0.39	0/5943	0.68	1/8064 (0.0%)
3	M	0.39	0/5943	0.68	1/8064 (0.0%)
4	F	0.35	0/111	0.47	0/150
4	N	0.35	0/118	0.47	0/158
4	O	0.35	0/118	0.48	0/158
All	All	0.38	0/39902	0.64	3/54214 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	768	LEU	CA-CB-CG	5.33	127.56	115.30
3	M	768	LEU	CA-CB-CG	5.33	127.56	115.30
3	L	768	LEU	CA-CB-CG	5.32	127.55	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5780	0	5663	201	0
1	D	5780	0	5663	205	0
1	G	5780	0	5663	193	0
2	B	1299	0	1288	65	0
2	J	1299	0	1288	59	0
2	K	1299	0	1288	61	0
3	E	5823	0	5853	291	0
3	L	5823	0	5853	293	0
3	M	5823	0	5853	301	0
4	F	109	0	105	14	0
4	N	117	0	110	14	0
4	O	117	0	110	12	0
5	A	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
5	L	1	0	0	0	0
5	M	1	0	0	0	0
6	B	32	0	13	5	0
6	J	32	0	13	4	0
6	K	32	0	13	5	0
7	B	1	0	0	0	0
7	J	1	0	0	0	0
7	K	1	0	0	0	0
All	All	39154	0	38776	1589	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 20.

All (1589) 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:A:91:PRO:HB3	1:D:669:GLN:NE2	1.18	1.43
1:A:91:PRO:CB	1:D:669:GLN:HE21	1.35	1.38
1:D:183:ARG:NH1	3:L:383:GLU:HB2	1.53	1.22
1:G:183:ARG:NH1	3:M:383:GLU:HB2	1.53	1.22
1:A:183:ARG:NH1	3:E:383:GLU:HB2	1.53	1.21
3:E:272:ASN:OD1	3:M:906:LYS:HD3	1.41	1.19
1:A:176:ILE:CD1	3:E:413:ILE:HG12	1.73	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:176:ILE:CD1	3:M:413:ILE:HG12	1.73	1.17
1:D:176:ILE:CD1	3:L:413:ILE:HG12	1.73	1.17
3:L:147:LEU:HB3	3:L:148:PRO:HD2	1.16	1.16
1:A:101:MET:CE	4:F:61:PHE:HZ	1.63	1.12
1:D:101:MET:CE	4:N:61:PHE:HZ	1.63	1.11
1:G:101:MET:CE	4:O:61:PHE:HZ	1.63	1.11
3:M:147:LEU:HB3	3:M:148:PRO:HD2	1.16	1.10
3:E:907:ILE:HG22	3:E:908:LEU:HG	1.35	1.08
3:E:147:LEU:HB3	3:E:148:PRO:HD2	1.16	1.08
3:M:907:ILE:HG22	3:M:908:LEU:HG	1.35	1.07
1:A:91:PRO:CB	1:D:669:GLN:NE2	2.05	1.05
3:L:907:ILE:HG22	3:L:908:LEU:HG	1.35	1.05
1:A:101:MET:HE2	4:F:61:PHE:CZ	1.93	1.03
1:G:101:MET:HE2	4:O:61:PHE:CZ	1.93	1.03
1:D:651:ASN:HD22	1:D:651:ASN:H	1.05	1.01
1:G:101:MET:HE2	4:O:61:PHE:HZ	1.22	0.99
1:D:183:ARG:HH12	3:L:383:GLU:HB2	1.23	0.99
1:A:651:ASN:H	1:A:651:ASN:HD22	1.05	0.98
1:D:176:ILE:HD11	3:L:413:ILE:HG12	1.44	0.98
1:D:101:MET:CE	4:N:61:PHE:CZ	2.45	0.98
1:A:101:MET:HE2	4:F:61:PHE:HZ	1.22	0.98
1:G:101:MET:CE	4:O:61:PHE:CZ	2.45	0.98
1:G:176:ILE:HD11	3:M:413:ILE:HG12	1.44	0.98
1:A:101:MET:CE	4:F:61:PHE:CZ	2.46	0.98
1:D:101:MET:HE2	4:N:61:PHE:CZ	1.99	0.97
1:A:176:ILE:HD11	3:E:413:ILE:HG12	1.44	0.96
3:E:147:LEU:CB	3:E:148:PRO:HD2	1.97	0.95
1:D:101:MET:HE2	4:N:61:PHE:HZ	1.27	0.94
3:M:147:LEU:CB	3:M:148:PRO:HD2	1.97	0.94
1:A:183:ARG:HH12	3:E:383:GLU:CB	1.81	0.94
3:L:147:LEU:CB	3:L:148:PRO:HD2	1.97	0.93
1:D:183:ARG:HH12	3:L:383:GLU:CB	1.81	0.93
1:A:183:ARG:HH12	3:E:383:GLU:HB2	1.23	0.93
1:G:183:ARG:HH12	3:M:383:GLU:CB	1.81	0.92
1:G:651:ASN:HD22	1:G:651:ASN:H	1.05	0.92
1:G:183:ARG:HH12	3:M:383:GLU:HB2	1.23	0.91
3:L:375:MET:HE1	3:L:413:ILE:HG21	1.53	0.90
3:L:441:LYS:HE2	3:L:498:ASP:OD2	1.72	0.90
3:M:441:LYS:HE2	3:M:498:ASP:OD2	1.72	0.90
3:M:147:LEU:HB3	3:M:148:PRO:CD	2.02	0.89
2:B:137:PRO:O	1:G:62:LYS:HE3	1.73	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:147:LEU:HB3	3:L:148:PRO:CD	2.02	0.88
1:D:176:ILE:HD11	3:L:413:ILE:CG1	2.03	0.88
3:L:459:ARG:HG2	3:L:459:ARG:HH11	1.38	0.88
1:A:176:ILE:HD11	3:E:413:ILE:CG1	2.03	0.87
3:E:441:LYS:HE2	3:E:498:ASP:OD2	1.72	0.87
1:G:176:ILE:HD11	3:M:413:ILE:CG1	2.03	0.87
3:E:459:ARG:HG2	3:E:459:ARG:HH11	1.39	0.87
3:M:459:ARG:HG2	3:M:459:ARG:HH11	1.39	0.85
1:A:722:ARG:HD3	6:B:1190:GNP:H5'1	1.57	0.85
3:E:352:ASN:HD22	3:E:353:ALA:N	1.75	0.85
3:L:352:ASN:HD22	3:L:353:ALA:N	1.75	0.84
3:E:147:LEU:HB3	3:E:148:PRO:CD	2.02	0.84
1:G:96:LEU:HG	1:G:97:SER:H	1.43	0.84
1:D:722:ARG:HD3	6:J:1190:GNP:H5'1	1.57	0.84
1:G:722:ARG:HD3	6:K:1190:GNP:H5'1	1.57	0.84
3:E:272:ASN:OD1	3:M:906:LYS:CD	2.25	0.83
3:M:333:LEU:HB2	3:M:400:ARG:NH2	1.93	0.83
3:M:352:ASN:HD22	3:M:353:ALA:N	1.75	0.83
1:A:96:LEU:HG	1:A:97:SER:H	1.43	0.82
3:E:333:LEU:HB2	3:E:400:ARG:NH2	1.93	0.82
3:L:333:LEU:HB2	3:L:400:ARG:NH2	1.93	0.82
1:A:176:ILE:HD12	3:E:413:ILE:HG12	1.62	0.81
3:M:375:MET:HE1	3:M:413:ILE:HG21	1.63	0.81
1:D:176:ILE:CD1	3:L:413:ILE:CG1	2.56	0.81
1:G:176:ILE:CD1	3:M:413:ILE:CG1	2.56	0.81
1:G:616:GLU:HG3	1:G:620:ASN:HB2	1.63	0.81
1:D:96:LEU:HG	1:D:97:SER:H	1.43	0.80
1:D:616:GLU:HG3	1:D:620:ASN:HB2	1.63	0.80
1:A:176:ILE:CD1	3:E:413:ILE:CG1	2.56	0.80
1:D:176:ILE:HD12	3:L:413:ILE:HG12	1.62	0.80
3:E:375:MET:HE1	3:E:413:ILE:HG21	1.62	0.79
3:M:147:LEU:HD13	3:M:914:ARG:NH1	1.97	0.79
1:G:176:ILE:HD12	3:M:413:ILE:HG12	1.62	0.79
3:L:147:LEU:HD13	3:L:914:ARG:NH1	1.97	0.79
3:E:147:LEU:HD13	3:E:914:ARG:NH1	1.97	0.79
3:M:709:MET:HE1	3:M:712:LEU:HD23	1.65	0.79
3:L:919:ILE:O	3:L:923:ARG:HG3	1.83	0.79
1:A:616:GLU:HG3	1:A:620:ASN:HB2	1.63	0.79
3:E:680:GLN:HG3	3:E:920:MET:HE1	1.65	0.79
3:E:919:ILE:O	3:E:923:ARG:HG3	1.83	0.79
3:M:919:ILE:O	3:M:923:ARG:HG3	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:ARG:HH11	3:E:383:GLU:HB2	1.46	0.79
2:K:140:VAL:HG12	2:K:141:SER:N	1.99	0.78
3:M:680:GLN:HG3	3:M:920:MET:HE1	1.64	0.77
1:G:164:ASN:N	1:G:164:ASN:HD22	1.81	0.77
2:J:140:VAL:HG12	2:J:141:SER:N	1.99	0.77
1:A:164:ASN:N	1:A:164:ASN:HD22	1.81	0.77
2:B:140:VAL:HG12	2:B:141:SER:N	1.99	0.77
3:L:680:GLN:HG3	3:L:920:MET:HE1	1.65	0.77
3:M:147:LEU:O	3:M:148:PRO:C	2.22	0.77
1:D:114:THR:HG22	1:D:115:ASN:H	1.50	0.76
1:D:164:ASN:H	1:D:164:ASN:HD22	1.33	0.76
3:M:296:TYR:O	3:M:624:ARG:NH1	2.19	0.76
3:L:296:TYR:O	3:L:624:ARG:NH1	2.19	0.76
3:E:147:LEU:O	3:E:148:PRO:C	2.22	0.76
1:G:114:THR:HG22	1:G:115:ASN:H	1.51	0.76
1:A:183:ARG:NH1	3:E:383:GLU:CB	2.39	0.76
3:E:660:VAL:HG11	3:E:741:GLU:HB3	1.68	0.76
3:E:296:TYR:O	3:E:624:ARG:NH1	2.19	0.76
1:G:164:ASN:HD22	1:G:164:ASN:H	1.33	0.75
1:A:164:ASN:HD22	1:A:164:ASN:H	1.33	0.75
2:B:140:VAL:HG12	2:B:141:SER:H	1.52	0.75
3:L:660:VAL:HG11	3:L:741:GLU:HB3	1.68	0.75
1:G:183:ARG:HH11	3:M:383:GLU:HB2	1.46	0.74
2:K:140:VAL:HG12	2:K:141:SER:H	1.52	0.74
3:L:147:LEU:O	3:L:148:PRO:C	2.21	0.74
1:D:512:LEU:HD13	1:D:516:THR:HG21	1.70	0.74
1:G:651:ASN:H	1:G:651:ASN:ND2	1.85	0.74
3:L:567:ARG:HH21	3:L:599:ASN:HD22	1.36	0.74
1:A:512:LEU:HD13	1:A:516:THR:HG21	1.70	0.74
3:L:142:ASP:CG	3:L:700:PRO:HB3	2.08	0.74
1:D:164:ASN:HD22	1:D:164:ASN:N	1.81	0.74
3:L:154:LEU:HG	3:L:709:MET:HE2	1.70	0.74
3:M:660:VAL:HG11	3:M:741:GLU:HB3	1.68	0.74
3:M:567:ARG:HH21	3:M:599:ASN:HD22	1.36	0.73
1:D:183:ARG:HH11	3:L:383:GLU:HB2	1.46	0.73
3:E:142:ASP:CG	3:E:700:PRO:HB3	2.08	0.73
3:E:567:ARG:HH21	3:E:599:ASN:HD22	1.36	0.73
1:A:101:MET:SD	4:F:61:PHE:HZ	2.12	0.73
1:A:114:THR:HG22	1:A:115:ASN:H	1.50	0.73
3:M:557:VAL:HG13	3:M:582:LEU:HD11	1.70	0.73
1:G:512:LEU:HD13	1:G:516:THR:HG21	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:674:ARG:HA	1:G:679:GLN:NE2	2.04	0.72
3:L:557:VAL:HG13	3:L:582:LEU:HD11	1.70	0.72
1:D:101:MET:SD	4:N:61:PHE:HZ	2.12	0.72
1:G:101:MET:SD	4:O:61:PHE:HZ	2.12	0.72
3:M:142:ASP:CG	3:M:700:PRO:HB3	2.08	0.72
1:D:674:ARG:HA	1:D:679:GLN:NE2	2.04	0.72
3:E:709:MET:HE1	3:E:712:LEU:HD23	1.70	0.72
3:E:557:VAL:HG13	3:E:582:LEU:HD11	1.70	0.72
2:J:140:VAL:HG12	2:J:141:SER:H	1.52	0.72
3:E:225:ASP:OD2	3:E:227:LEU:HB3	1.90	0.72
3:L:225:ASP:OD2	3:L:227:LEU:HB3	1.90	0.72
3:L:226:GLY:O	3:L:293:PRO:HG3	1.90	0.71
3:L:142:ASP:O	3:L:146:GLU:HG2	1.91	0.71
1:A:674:ARG:HA	1:A:679:GLN:NE2	2.04	0.71
3:M:142:ASP:O	3:M:146:GLU:HG2	1.91	0.71
1:A:88:HIS:CE1	1:D:742:SER:HB2	2.25	0.71
3:E:154:LEU:HG	3:E:709:MET:HE2	1.73	0.71
3:E:493:VAL:HG23	3:E:495:ILE:HG13	1.73	0.71
3:E:142:ASP:O	3:E:146:GLU:HG2	1.91	0.71
3:E:226:GLY:O	3:E:293:PRO:HG3	1.90	0.71
3:M:225:ASP:OD2	3:M:227:LEU:HB3	1.90	0.71
1:G:616:GLU:CG	1:G:620:ASN:HB2	2.21	0.71
1:A:347:ALA:HB2	1:A:353:ILE:HD13	1.73	0.71
1:G:430:ASN:H	1:G:430:ASN:HD22	1.39	0.70
1:D:616:GLU:CG	1:D:620:ASN:HB2	2.21	0.70
1:G:183:ARG:NH1	3:M:383:GLU:CB	2.39	0.70
1:A:651:ASN:H	1:A:651:ASN:ND2	1.85	0.70
3:L:279:ASP:HA	3:L:284:LYS:HE3	1.74	0.70
1:D:651:ASN:H	1:D:651:ASN:ND2	1.85	0.70
3:M:226:GLY:O	3:M:293:PRO:HG3	1.90	0.70
3:L:696:ALA:HB2	3:L:702:ARG:HH21	1.57	0.70
1:A:616:GLU:CG	1:A:620:ASN:HB2	2.21	0.70
3:L:493:VAL:HG23	3:L:495:ILE:HG13	1.73	0.70
3:M:696:ALA:HB2	3:M:702:ARG:HH21	1.57	0.70
1:D:347:ALA:HB2	1:D:353:ILE:HD13	1.73	0.70
3:M:459:ARG:HG2	3:M:459:ARG:NH1	2.07	0.70
1:G:399:ALA:HB3	1:G:450:LEU:HD13	1.74	0.69
1:A:114:THR:HG22	1:A:115:ASN:N	2.07	0.69
1:D:399:ALA:HB3	1:D:450:LEU:HD13	1.74	0.69
3:E:279:ASP:HA	3:E:284:LYS:HE3	1.74	0.69
3:L:801:LEU:HD11	3:L:808:LEU:HD22	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:801:LEU:HD11	3:M:808:LEU:HD22	1.74	0.69
1:D:430:ASN:H	1:D:430:ASN:HD22	1.39	0.69
2:J:36:LYS:HG2	2:J:97:LEU:HD13	1.75	0.69
1:D:181:VAL:HB	3:L:378:ILE:HG12	1.75	0.69
3:E:801:LEU:HD11	3:E:808:LEU:HD22	1.74	0.69
1:G:114:THR:HG22	1:G:115:ASN:N	2.07	0.69
1:G:181:VAL:HB	3:M:378:ILE:HG12	1.75	0.69
3:L:709:MET:HE1	3:L:712:LEU:HD23	1.73	0.69
3:M:493:VAL:HG23	3:M:495:ILE:HG13	1.73	0.69
1:A:179:CYS:O	3:E:377:ASP:HB2	1.93	0.68
1:D:114:THR:HG22	1:D:115:ASN:N	2.07	0.68
3:E:696:ALA:HB2	3:E:702:ARG:HH21	1.57	0.68
3:E:699:ALA:HB1	3:E:921:LYS:NZ	2.08	0.68
3:E:768:LEU:HG	3:E:769:PRO:HD2	1.74	0.68
3:M:768:LEU:HG	3:M:769:PRO:HD2	1.74	0.68
3:E:766:ALA:O	3:E:768:LEU:N	2.26	0.68
3:L:768:LEU:HG	3:L:769:PRO:HD2	1.74	0.68
2:B:137:PRO:O	1:G:62:LYS:CE	2.42	0.68
1:G:179:CYS:O	3:M:377:ASP:HB2	1.94	0.68
2:K:36:LYS:HG2	2:K:97:LEU:HD13	1.75	0.68
1:G:347:ALA:HB2	1:G:353:ILE:HD13	1.73	0.68
1:G:96:LEU:CG	1:G:97:SER:H	2.07	0.68
3:L:766:ALA:O	3:L:768:LEU:N	2.26	0.68
3:M:279:ASP:HA	3:M:284:LYS:HE3	1.74	0.68
1:A:181:VAL:HB	3:E:378:ILE:HG12	1.75	0.67
3:M:766:ALA:O	3:M:768:LEU:N	2.26	0.67
2:B:36:LYS:HG2	2:B:97:LEU:HD13	1.75	0.67
2:B:130:LEU:HD22	2:B:171:CYS:SG	2.35	0.67
1:G:634:MET:HE1	1:G:686:ASP:O	1.94	0.67
2:K:130:LEU:HD22	2:K:171:CYS:SG	2.35	0.67
3:L:699:ALA:HB1	3:L:921:LYS:NZ	2.08	0.67
3:M:699:ALA:HB1	3:M:921:LYS:NZ	2.08	0.67
1:A:430:ASN:HD22	1:A:430:ASN:H	1.39	0.67
2:J:130:LEU:HD22	2:J:171:CYS:SG	2.35	0.67
1:D:179:CYS:O	3:L:377:ASP:HB2	1.94	0.67
3:M:303:PRO:HG3	3:M:342:ARG:CZ	2.25	0.67
1:A:96:LEU:CG	1:A:97:SER:H	2.07	0.67
1:A:399:ALA:HB3	1:A:450:LEU:HD13	1.74	0.67
1:D:634:MET:HE1	1:D:686:ASP:O	1.95	0.67
1:D:745:VAL:CG1	2:J:50:THR:HG21	2.25	0.67
1:A:634:MET:HE1	1:A:686:ASP:O	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:745:VAL:CG1	2:B:50:THR:HG21	2.25	0.67
2:K:61:GLU:OE1	2:K:68:LYS:HE2	1.95	0.67
2:B:61:GLU:OE1	2:B:68:LYS:HE2	1.95	0.66
3:E:750:LYS:HE3	3:E:805:GLY:HA2	1.77	0.66
1:G:745:VAL:CG1	2:K:50:THR:HG21	2.25	0.66
3:L:312:VAL:HG11	3:L:414:PHE:CD1	2.30	0.66
3:L:812:MET:SD	3:L:820:LEU:HD22	2.36	0.66
3:E:312:VAL:HG11	3:E:414:PHE:CD1	2.30	0.66
3:E:764:ASP:HA	3:E:851:ARG:HH22	1.60	0.66
3:L:750:LYS:HE3	3:L:805:GLY:HA2	1.77	0.66
3:M:312:VAL:HG11	3:M:414:PHE:CD1	2.30	0.66
3:M:750:LYS:HE3	3:M:805:GLY:HA2	1.77	0.66
3:E:271:PRO:O	3:M:906:LYS:NZ	2.25	0.66
3:E:303:PRO:HG3	3:E:342:ARG:CZ	2.25	0.66
3:L:764:ASP:HA	3:L:851:ARG:HH22	1.60	0.66
3:M:362:ASP:OD1	3:M:401:GLN:HB2	1.95	0.66
3:L:312:VAL:HG11	3:L:414:PHE:CG	2.31	0.66
3:M:147:LEU:HD13	3:M:914:ARG:HH12	1.61	0.66
3:L:422:PHE:H	3:L:451:ASN:HB3	1.61	0.66
3:E:362:ASP:OD1	3:E:401:GLN:HB2	1.95	0.66
3:L:818:PRO:C	3:L:820:LEU:H	2.00	0.66
1:A:432:ILE:HD13	1:A:442:THR:HA	1.78	0.65
3:L:149:PRO:O	3:L:151:ILE:HG12	1.97	0.65
3:L:303:PRO:HG3	3:L:342:ARG:CZ	2.25	0.65
3:M:312:VAL:HG11	3:M:414:PHE:CG	2.31	0.65
3:M:422:PHE:H	3:M:451:ASN:HB3	1.61	0.65
3:M:764:ASP:HA	3:M:851:ARG:HH22	1.60	0.65
1:D:323:LYS:O	1:D:327:LYS:HG2	1.97	0.65
3:E:399:CYS:O	3:E:403:ILE:HG13	1.97	0.65
3:E:812:MET:SD	3:E:820:LEU:HD22	2.36	0.65
1:G:432:ILE:HD13	1:G:442:THR:HA	1.78	0.65
1:G:757:THR:O	1:G:761:GLN:HG3	1.97	0.65
3:L:672:ARG:HH11	3:L:725:SER:HB3	1.62	0.65
3:M:149:PRO:O	3:M:151:ILE:HG12	1.97	0.65
3:M:812:MET:SD	3:M:820:LEU:HD22	2.36	0.65
1:G:177:ASP:OD1	1:G:237:LYS:HE3	1.96	0.65
3:L:297:THR:HG22	3:L:624:ARG:HD3	1.79	0.65
1:D:432:ILE:HD13	1:D:442:THR:HA	1.78	0.65
3:L:362:ASP:OD1	3:L:401:GLN:HB2	1.95	0.65
3:M:920:MET:HE3	3:M:920:MET:HA	1.79	0.65
1:A:177:ASP:OD1	1:A:237:LYS:HE3	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:399:CYS:O	3:M:403:ILE:HG13	1.97	0.65
1:D:164:ASN:H	1:D:164:ASN:ND2	1.94	0.65
2:J:61:GLU:OE1	2:J:68:LYS:HE2	1.95	0.65
1:A:164:ASN:H	1:A:164:ASN:ND2	1.94	0.65
3:E:422:PHE:H	3:E:451:ASN:HB3	1.61	0.65
1:G:164:ASN:H	1:G:164:ASN:ND2	1.94	0.65
1:A:757:THR:O	1:A:761:GLN:HG3	1.97	0.64
1:D:96:LEU:CG	1:D:97:SER:H	2.07	0.64
1:D:757:THR:O	1:D:761:GLN:HG3	1.97	0.64
3:L:147:LEU:HD13	3:L:914:ARG:HH12	1.61	0.64
1:D:177:ASP:OD1	1:D:237:LYS:HE3	1.96	0.64
3:M:297:THR:HG22	3:M:624:ARG:HD3	1.79	0.64
1:A:651:ASN:HD22	1:A:651:ASN:N	1.81	0.64
3:E:297:THR:HG22	3:E:624:ARG:HD3	1.79	0.64
3:E:149:PRO:O	3:E:151:ILE:HG12	1.97	0.64
3:E:312:VAL:HG11	3:E:414:PHE:CG	2.31	0.64
1:A:323:LYS:O	1:A:327:LYS:HG2	1.97	0.64
3:L:525:PHE:CE2	3:L:527:PRO:HG3	2.33	0.64
3:E:789:ALA:O	3:E:904:GLU:HB2	1.98	0.64
3:M:672:ARG:HH11	3:M:725:SER:HB3	1.62	0.64
3:E:147:LEU:HD13	3:E:914:ARG:HH12	1.61	0.64
3:E:672:ARG:HH11	3:E:725:SER:HB3	1.62	0.64
3:E:680:GLN:CG	3:E:920:MET:HE1	2.28	0.64
2:K:164:ARG:HG2	2:K:166:VAL:HG23	1.80	0.64
3:L:255:PHE:CZ	3:L:612:GLN:HB2	2.33	0.64
3:M:255:PHE:CZ	3:M:612:GLN:HB2	2.33	0.64
1:D:19:PHE:HB2	1:D:511:LEU:HD23	1.80	0.63
1:G:323:LYS:O	1:G:327:LYS:HG2	1.97	0.63
3:M:817:VAL:C	3:M:819:ALA:H	2.01	0.63
3:M:856:ILE:HD13	3:M:871:LEU:HD22	1.79	0.63
1:G:19:PHE:HB2	1:G:511:LEU:HD23	1.80	0.63
3:L:399:CYS:O	3:L:403:ILE:HG13	1.97	0.63
1:A:19:PHE:HB2	1:A:511:LEU:HD23	1.80	0.63
3:E:818:PRO:C	3:E:820:LEU:H	2.00	0.63
3:L:539:LYS:HA	3:L:868:TYR:CD2	2.34	0.63
3:L:789:ALA:O	3:L:904:GLU:HB2	1.98	0.63
3:L:808:LEU:O	3:L:871:LEU:HD12	1.98	0.63
3:M:525:PHE:CE2	3:M:527:PRO:HG3	2.33	0.63
3:M:808:LEU:O	3:M:871:LEU:HD12	1.99	0.63
3:M:818:PRO:C	3:M:820:LEU:H	2.00	0.63
2:J:164:ARG:HG2	2:J:166:VAL:HG23	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:789:ALA:O	3:M:904:GLU:HB2	1.98	0.63
1:D:484:LEU:CD1	4:N:69:LEU:HD21	2.29	0.63
3:L:856:ILE:HD13	3:L:871:LEU:HD22	1.79	0.63
3:M:154:LEU:HG	3:M:709:MET:HE2	1.80	0.63
3:E:750:LYS:HD2	3:E:803:ASP:OD2	1.98	0.63
3:L:750:LYS:HD2	3:L:803:ASP:OD2	1.98	0.63
3:L:817:VAL:C	3:L:819:ALA:H	2.01	0.63
2:B:164:ARG:HG2	2:B:166:VAL:HG23	1.80	0.63
1:D:183:ARG:NH1	3:L:383:GLU:CB	2.39	0.63
1:D:722:ARG:HH12	6:J:1190:GNP:HNB3	1.46	0.63
3:E:312:VAL:HG12	3:E:312:VAL:O	1.99	0.63
3:E:525:PHE:CE2	3:E:527:PRO:HG3	2.33	0.63
2:J:140:VAL:CG1	2:J:141:SER:H	2.12	0.63
2:K:140:VAL:CG1	2:K:141:SER:H	2.12	0.63
3:E:914:ARG:O	3:E:918:GLN:HG2	1.98	0.63
3:L:449:LEU:HD12	3:L:450:PRO:HD2	1.81	0.63
3:L:914:ARG:O	3:L:918:GLN:HG2	1.98	0.63
3:M:539:LYS:HA	3:M:868:TYR:CD2	2.34	0.63
1:A:96:LEU:HD21	1:A:101:MET:SD	2.39	0.62
3:E:255:PHE:CZ	3:E:612:GLN:HB2	2.33	0.62
1:G:170:ASP:C	1:G:171:LEU:HD12	2.20	0.62
3:M:680:GLN:CG	3:M:920:MET:HE1	2.28	0.62
3:M:914:ARG:O	3:M:918:GLN:HG2	1.98	0.62
1:D:96:LEU:HD21	1:D:101:MET:SD	2.39	0.62
1:D:170:ASP:C	1:D:171:LEU:HD12	2.20	0.62
3:E:539:LYS:HA	3:E:868:TYR:CD2	2.34	0.62
3:L:312:VAL:HG12	3:L:312:VAL:O	1.99	0.62
3:E:808:LEU:O	3:E:871:LEU:HD12	1.99	0.62
3:E:856:ILE:HD13	3:E:871:LEU:HD22	1.79	0.62
1:G:484:LEU:CD1	4:O:69:LEU:HD21	2.29	0.62
3:L:424:LEU:HG	3:L:428:LEU:HD22	1.81	0.62
1:D:136:ASN:HD21	1:D:374:ALA:HB1	1.65	0.62
1:G:96:LEU:HD21	1:G:101:MET:SD	2.39	0.62
1:G:136:ASN:HD21	1:G:374:ALA:HB1	1.65	0.62
1:A:484:LEU:CD1	4:F:69:LEU:HD21	2.29	0.62
3:E:817:VAL:C	3:E:819:ALA:H	2.01	0.62
1:A:219:VAL:HG22	1:A:225:ASN:ND2	2.14	0.62
2:B:140:VAL:CG1	2:B:141:SER:H	2.12	0.62
3:L:680:GLN:CG	3:L:920:MET:HE1	2.28	0.62
1:A:170:ASP:C	1:A:171:LEU:HD12	2.20	0.62
3:E:449:LEU:HD12	3:E:450:PRO:HD2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:722:ARG:HH12	6:K:1190:GNP:HNB3	1.46	0.62
2:B:154:THR:HB	2:B:166:VAL:O	2.00	0.62
3:E:920:MET:HE3	3:E:920:MET:HA	1.81	0.62
3:M:750:LYS:HD2	3:M:803:ASP:OD2	1.98	0.62
1:A:136:ASN:HD21	1:A:374:ALA:HB1	1.65	0.62
3:E:424:LEU:HG	3:E:428:LEU:HD22	1.81	0.62
3:M:449:LEU:HD12	3:M:450:PRO:HD2	1.81	0.62
1:G:219:VAL:HG22	1:G:225:ASN:ND2	2.14	0.61
3:M:312:VAL:HG12	3:M:312:VAL:O	1.99	0.61
3:M:687:LYS:NZ	3:M:925:SER:HA	2.15	0.61
3:E:687:LYS:NZ	3:E:925:SER:HA	2.15	0.61
2:K:154:THR:HB	2:K:166:VAL:O	2.00	0.61
3:E:135:MET:HE2	3:E:641:GLU:OE1	2.01	0.61
3:L:920:MET:HE3	3:L:920:MET:HA	1.82	0.61
1:A:722:ARG:HH12	6:B:1190:GNP:HNB3	1.46	0.61
2:J:154:THR:HB	2:J:166:VAL:O	2.00	0.61
1:D:219:VAL:HG22	1:D:225:ASN:ND2	2.14	0.61
3:M:352:ASN:ND2	3:M:353:ALA:N	2.49	0.61
3:E:272:ASN:HA	3:M:906:LYS:NZ	2.15	0.61
3:M:424:LEU:HG	3:M:428:LEU:HD22	1.81	0.61
3:M:270:ASP:HB2	3:M:273:ASP:HB3	1.83	0.61
1:G:176:ILE:CG1	3:M:413:ILE:HG12	2.31	0.60
3:L:205:LEU:HD13	3:L:611:VAL:HG11	1.83	0.60
1:A:411:ASP:OD1	1:A:411:ASP:N	2.33	0.60
1:D:176:ILE:CG1	3:L:413:ILE:HG12	2.31	0.60
3:E:205:LEU:HD13	3:E:611:VAL:HG11	1.83	0.60
3:E:524:HIS:CE1	3:E:866:ILE:HD11	2.36	0.60
3:L:270:ASP:HB2	3:L:273:ASP:HB3	1.83	0.60
3:L:352:ASN:HD22	3:L:353:ALA:H	1.47	0.60
3:L:352:ASN:ND2	3:L:353:ALA:N	2.49	0.60
1:A:101:MET:SD	4:F:61:PHE:CZ	2.95	0.60
2:K:23:HIS:CD2	2:K:67:ILE:HA	2.36	0.60
1:D:618:THR:O	1:D:622:LEU:HG	2.01	0.60
3:L:687:LYS:NZ	3:L:925:SER:HA	2.15	0.60
3:M:539:LYS:HE3	3:M:543:GLU:OE2	2.02	0.60
3:E:459:ARG:HG2	3:E:459:ARG:NH1	2.07	0.60
3:L:459:ARG:HG2	3:L:459:ARG:NH1	2.07	0.60
1:A:618:THR:O	1:A:622:LEU:HG	2.01	0.60
3:E:375:MET:CE	3:E:413:ILE:HG21	2.31	0.60
2:J:23:HIS:CD2	2:J:67:ILE:HA	2.36	0.60
3:L:539:LYS:HE3	3:L:543:GLU:OE2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:634:MET:HE3	1:D:634:MET:HA	1.83	0.60
1:G:651:ASN:HD22	1:G:651:ASN:N	1.81	0.60
3:L:333:LEU:HB2	3:L:400:ARG:CZ	2.32	0.60
3:L:764:ASP:HA	3:L:851:ARG:NH2	2.16	0.60
1:A:176:ILE:CG1	3:E:413:ILE:HG12	2.31	0.60
1:A:634:MET:HA	1:A:634:MET:HE3	1.84	0.60
1:D:681:ASP:HB2	1:D:682:PRO:HD2	1.84	0.60
1:G:618:THR:O	1:G:622:LEU:HG	2.01	0.60
3:M:205:LEU:HD13	3:M:611:VAL:HG11	1.83	0.60
2:B:23:HIS:CD2	2:B:67:ILE:HA	2.36	0.59
2:B:142:GLU:HB3	1:G:426:LYS:HZ3	1.67	0.59
3:E:668:LEU:HG	3:E:672:ARG:HH21	1.67	0.59
3:E:915:GLU:O	3:E:919:ILE:HG13	2.02	0.59
3:L:524:HIS:CE1	3:L:866:ILE:HD11	2.37	0.59
3:M:375:MET:CE	3:M:413:ILE:HG21	2.31	0.59
3:L:209:PRO:HG3	3:L:558:MET:CE	2.32	0.59
3:M:209:PRO:HG3	3:M:558:MET:CE	2.32	0.59
3:M:668:LEU:HG	3:M:672:ARG:HH21	1.66	0.59
3:E:539:LYS:HE3	3:E:543:GLU:OE2	2.02	0.59
3:L:729:PRO:HB2	3:L:732:HIS:HD2	1.68	0.59
3:M:524:HIS:CE1	3:M:866:ILE:HD11	2.37	0.59
3:E:270:ASP:HB2	3:E:273:ASP:HB3	1.83	0.59
2:K:140:VAL:CG1	2:K:141:SER:N	2.65	0.59
2:K:141:SER:OG	2:K:144:GLU:HG3	2.03	0.59
3:M:915:GLU:O	3:M:919:ILE:HG13	2.02	0.59
1:G:101:MET:SD	4:O:61:PHE:CZ	2.95	0.59
1:D:484:LEU:HD11	4:N:69:LEU:HD21	1.85	0.59
3:E:209:PRO:HG3	3:E:558:MET:CE	2.32	0.59
3:L:668:LEU:HG	3:L:672:ARG:HH21	1.66	0.59
1:D:511:LEU:O	1:D:512:LEU:HD23	2.03	0.59
2:J:140:VAL:CG1	2:J:141:SER:N	2.65	0.59
3:L:133:ARG:NH2	3:L:635:THR:O	2.36	0.59
3:M:333:LEU:HB2	3:M:400:ARG:CZ	2.32	0.59
1:A:68:TYR:HE1	4:F:69:LEU:HD22	1.68	0.59
3:E:764:ASP:HA	3:E:851:ARG:NH2	2.17	0.59
2:B:140:VAL:CG1	2:B:141:SER:N	2.65	0.59
3:E:333:LEU:HB2	3:E:400:ARG:CZ	2.32	0.59
3:E:667:SER:HB3	3:E:670:ASP:HB2	1.85	0.59
1:A:681:ASP:HB2	1:A:682:PRO:HD2	1.84	0.59
3:E:133:ARG:NH2	3:E:635:THR:O	2.36	0.59
3:E:352:ASN:ND2	3:E:353:ALA:N	2.49	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:141:SER:OG	2:J:144:GLU:HG3	2.03	0.59
3:M:352:ASN:HD22	3:M:353:ALA:H	1.47	0.58
3:M:728:VAL:HG21	3:M:733:ARG:NH2	2.18	0.58
3:E:209:PRO:HG3	3:E:558:MET:HE1	1.85	0.58
3:E:849:ASN:OD1	3:E:853:ARG:HD3	2.04	0.58
3:L:667:SER:HB3	3:L:670:ASP:HB2	1.85	0.58
3:M:563:SER:HB3	3:M:610:TYR:H	1.68	0.58
3:M:764:ASP:HA	3:M:851:ARG:NH2	2.17	0.58
1:G:511:LEU:O	1:G:512:LEU:HD23	2.03	0.58
3:M:667:SER:HB3	3:M:670:ASP:HB2	1.85	0.58
1:A:722:ARG:NH1	6:B:1190:GNP:HNB3	2.01	0.58
1:G:10:ASN:O	1:G:12:VAL:HG23	2.03	0.58
1:A:250:TRP:CD1	3:E:389:PRO:HB3	2.38	0.58
2:B:83:LEU:O	2:B:86:ASP:HB2	2.04	0.58
1:G:234:VAL:HG12	1:G:234:VAL:O	2.04	0.58
3:L:147:LEU:CB	3:L:148:PRO:CD	2.74	0.58
3:L:228:ILE:HD13	3:L:290:TYR:CD2	2.39	0.58
3:L:915:GLU:O	3:L:919:ILE:HG13	2.02	0.58
1:A:44:ASP:O	1:A:45:GLU:HG3	2.04	0.58
1:A:511:LEU:O	1:A:512:LEU:HD23	2.03	0.58
1:D:96:LEU:HG	1:D:97:SER:N	2.18	0.58
1:D:722:ARG:NH1	6:J:1190:GNP:HNB3	2.01	0.58
2:J:83:LEU:O	2:J:86:ASP:HB2	2.04	0.58
3:L:672:ARG:NH1	3:L:725:SER:HB3	2.19	0.58
3:M:699:ALA:HB1	3:M:921:LYS:HZ1	1.68	0.58
1:A:10:ASN:O	1:A:12:VAL:HG23	2.03	0.58
3:E:272:ASN:HA	3:M:906:LYS:HZ2	1.67	0.58
3:E:352:ASN:HD22	3:E:353:ALA:H	1.47	0.58
1:G:250:TRP:CD1	3:M:389:PRO:HB3	2.38	0.58
2:J:140:VAL:CG1	2:J:144:GLU:HB2	2.34	0.58
3:L:138:LEU:HD22	3:L:704:CYS:HB3	1.85	0.58
3:M:272:ASN:O	3:M:274:PRO:HD3	2.03	0.58
3:E:672:ARG:NH1	3:E:725:SER:HB3	2.19	0.58
1:G:681:ASP:HB2	1:G:682:PRO:HD2	1.84	0.58
1:A:88:HIS:HE1	1:D:742:SER:HB2	1.66	0.58
1:D:10:ASN:O	1:D:12:VAL:HG23	2.03	0.58
1:D:44:ASP:O	1:D:45:GLU:HG3	2.04	0.58
1:D:250:TRP:CD1	3:L:389:PRO:HB3	2.38	0.58
3:E:729:PRO:HB2	3:E:732:HIS:HD2	1.68	0.58
1:G:68:TYR:HE1	4:O:69:LEU:HD22	1.68	0.58
3:L:728:VAL:HG21	3:L:733:ARG:NH2	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:133:ARG:NH2	3:M:635:THR:O	2.36	0.58
3:M:729:PRO:HB2	3:M:732:HIS:HD2	1.68	0.58
3:E:138:LEU:HD22	3:E:704:CYS:HB3	1.85	0.58
1:G:44:ASP:O	1:G:45:GLU:HG3	2.04	0.58
3:M:138:LEU:HD22	3:M:704:CYS:HB3	1.85	0.58
3:M:228:ILE:HD13	3:M:290:TYR:CD2	2.39	0.58
3:M:849:ASN:OD1	3:M:853:ARG:HD3	2.04	0.58
1:A:484:LEU:HD11	4:F:69:LEU:HD21	1.85	0.57
1:G:484:LEU:HD11	4:O:69:LEU:HD21	1.85	0.57
2:K:83:LEU:O	2:K:86:ASP:HB2	2.04	0.57
3:E:303:PRO:HG3	3:E:342:ARG:NH1	2.19	0.57
3:E:563:SER:HB3	3:E:610:TYR:H	1.68	0.57
1:G:722:ARG:NH1	6:K:1190:GNP:HNB3	2.01	0.57
2:K:140:VAL:CG1	2:K:144:GLU:HB2	2.34	0.57
3:L:209:PRO:HG3	3:L:558:MET:HE1	1.84	0.57
3:M:672:ARG:NH1	3:M:725:SER:HB3	2.19	0.57
3:L:563:SER:HB3	3:L:610:TYR:H	1.68	0.57
3:L:593:SER:HB2	3:L:744:PRO:HA	1.86	0.57
3:L:872:TYR:CE2	3:L:897:TRP:HZ3	2.23	0.57
2:B:141:SER:OG	2:B:144:GLU:HG3	2.03	0.57
1:D:234:VAL:HG12	1:D:234:VAL:O	2.04	0.57
3:L:272:ASN:O	3:L:274:PRO:HD3	2.03	0.57
3:M:378:ILE:HD11	3:M:387:PRO:HG3	1.86	0.57
1:A:450:LEU:N	1:A:450:LEU:HD12	2.19	0.57
2:B:140:VAL:CG1	2:B:144:GLU:HB2	2.34	0.57
1:D:102:PRO:HD2	1:D:105:LEU:HD12	1.87	0.57
1:D:179:CYS:O	3:L:377:ASP:N	2.29	0.57
3:E:272:ASN:O	3:E:274:PRO:HD3	2.03	0.57
3:E:728:VAL:HG21	3:E:733:ARG:NH2	2.18	0.57
1:G:450:LEU:HD12	1:G:450:LEU:N	2.19	0.57
1:D:651:ASN:HD22	1:D:651:ASN:N	1.81	0.57
3:E:228:ILE:HD13	3:E:290:TYR:CD2	2.39	0.57
1:D:68:TYR:HE1	4:N:69:LEU:HD22	1.68	0.57
1:D:450:LEU:N	1:D:450:LEU:HD12	2.19	0.57
1:G:635:GLU:CD	1:G:635:GLU:H	2.08	0.57
3:L:802:ILE:O	3:L:808:LEU:HD23	2.05	0.57
1:G:96:LEU:HG	1:G:97:SER:N	2.18	0.57
1:G:196:MET:HE3	3:M:379:ALA:HB3	1.87	0.57
3:L:147:LEU:HD13	3:L:914:ARG:CZ	2.34	0.57
3:L:849:ASN:OD1	3:L:853:ARG:HD3	2.04	0.57
2:B:142:GLU:HB3	1:G:426:LYS:NZ	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:101:MET:SD	4:N:61:PHE:CZ	2.95	0.57
3:M:872:TYR:CE2	3:M:897:TRP:HZ3	2.22	0.57
1:D:196:MET:HE3	3:L:379:ALA:HB3	1.87	0.56
3:E:593:SER:HB2	3:E:744:PRO:HA	1.86	0.56
3:L:696:ALA:CB	3:L:702:ARG:HH21	2.18	0.56
3:E:378:ILE:HD11	3:E:387:PRO:HG3	1.86	0.56
3:E:872:TYR:CE2	3:E:897:TRP:HZ3	2.23	0.56
3:L:303:PRO:HG3	3:L:342:ARG:NH1	2.19	0.56
3:M:147:LEU:HD13	3:M:914:ARG:CZ	2.34	0.56
3:M:303:PRO:HG3	3:M:342:ARG:NH1	2.19	0.56
1:A:102:PRO:HD2	1:A:105:LEU:HD12	1.87	0.56
1:A:234:VAL:HG12	1:A:234:VAL:O	2.04	0.56
2:K:122:LEU:O	2:K:164:ARG:NH2	2.38	0.56
3:L:135:MET:HE2	3:L:641:GLU:OE1	2.04	0.56
3:L:378:ILE:HD11	3:L:387:PRO:HG3	1.86	0.56
1:G:179:CYS:O	3:M:377:ASP:N	2.29	0.56
3:M:696:ALA:CB	3:M:702:ARG:HH21	2.18	0.56
1:G:65:LEU:HD11	1:G:105:LEU:HD21	1.88	0.56
1:G:145:ILE:HA	1:G:148:LEU:HD12	1.88	0.56
3:M:802:ILE:O	3:M:808:LEU:HD23	2.05	0.56
1:A:145:ILE:HA	1:A:148:LEU:HD12	1.88	0.56
1:A:635:GLU:H	1:A:635:GLU:CD	2.08	0.56
2:B:122:LEU:O	2:B:164:ARG:NH2	2.38	0.56
1:D:145:ILE:HA	1:D:148:LEU:HD12	1.88	0.56
2:J:23:HIS:HD2	2:J:67:ILE:HA	1.70	0.56
3:E:699:ALA:HB1	3:E:921:LYS:HZ1	1.68	0.56
1:G:77:SER:HA	1:G:89:LEU:HB2	1.88	0.56
1:G:102:PRO:HD2	1:G:105:LEU:HD12	1.87	0.56
3:M:593:SER:HB2	3:M:744:PRO:HA	1.86	0.56
1:A:96:LEU:HG	1:A:97:SER:N	2.18	0.56
1:A:219:VAL:HG22	1:A:225:ASN:HD22	1.71	0.56
1:D:77:SER:HA	1:D:89:LEU:HB2	1.88	0.56
1:D:634:MET:HA	1:D:634:MET:CE	2.36	0.56
1:D:679:GLN:HG3	1:D:687:PHE:CE2	2.41	0.56
1:D:635:GLU:CD	1:D:635:GLU:H	2.08	0.56
3:L:375:MET:CE	3:L:413:ILE:HG21	2.31	0.56
1:A:68:TYR:O	1:A:81:PRO:HG3	2.07	0.56
1:A:196:MET:HE3	3:E:379:ALA:HB3	1.87	0.56
1:G:679:GLN:HG3	1:G:687:PHE:CE2	2.41	0.56
3:L:680:GLN:CB	3:L:920:MET:HE1	2.36	0.56
2:B:23:HIS:HD2	2:B:67:ILE:HA	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:57:PRO:HB3	2:B:74:LEU:HD13	1.89	0.55
3:E:147:LEU:HD13	3:E:914:ARG:CZ	2.34	0.55
3:E:802:ILE:O	3:E:808:LEU:HD23	2.05	0.55
1:G:68:TYR:O	1:G:81:PRO:HG3	2.06	0.55
2:J:122:LEU:O	2:J:164:ARG:NH2	2.38	0.55
2:K:23:HIS:HD2	2:K:67:ILE:HA	1.70	0.55
3:L:677:LYS:HG2	3:L:681:ASP:OD2	2.06	0.55
3:E:677:LYS:HG2	3:E:681:ASP:OD2	2.07	0.55
1:G:219:VAL:HG22	1:G:225:ASN:HD22	1.71	0.55
1:G:583:TYR:HB3	1:G:584:PRO:HD3	1.88	0.55
1:G:634:MET:CE	1:G:634:MET:HA	2.36	0.55
1:A:46:LEU:HD12	1:A:47:ASN:H	1.71	0.55
1:A:114:THR:HG22	1:A:116:LYS:H	1.72	0.55
1:D:46:LEU:HD12	1:D:47:ASN:H	1.71	0.55
2:K:57:PRO:HB3	2:K:74:LEU:HD13	1.89	0.55
1:A:679:GLN:HG3	1:A:687:PHE:CE2	2.41	0.55
1:G:455:SER:O	1:G:534:ARG:NH2	2.40	0.55
3:L:699:ALA:HB1	3:L:921:LYS:HZ1	1.70	0.55
1:A:65:LEU:HD11	1:A:105:LEU:HD21	1.88	0.55
3:E:696:ALA:CB	3:E:702:ARG:HH21	2.18	0.55
3:M:209:PRO:HG3	3:M:558:MET:HE1	1.88	0.55
1:A:583:TYR:HB3	1:A:584:PRO:HD3	1.88	0.55
3:E:410:ILE:HB	3:E:411:PRO:HD3	1.89	0.55
3:L:216:ASP:O	3:L:219:PRO:HD3	2.07	0.55
3:L:488:ILE:HD11	3:L:578:ARG:HH22	1.71	0.55
3:L:822:PHE:CD1	3:L:822:PHE:N	2.74	0.55
2:J:57:PRO:HB3	2:J:74:LEU:HD13	1.89	0.55
2:K:50:THR:HG23	2:K:50:THR:O	2.07	0.55
3:M:822:PHE:N	3:M:822:PHE:CD1	2.74	0.55
1:A:564:ALA:HB2	1:A:576:LEU:HD13	1.89	0.55
1:D:68:TYR:O	1:D:81:PRO:HG3	2.07	0.55
1:D:219:VAL:HG22	1:D:225:ASN:HD22	1.71	0.55
1:A:566:TYR:CG	1:A:764:VAL:HG12	2.42	0.54
1:A:761:GLN:O	1:A:765:SER:HB2	2.07	0.54
1:D:564:ALA:HB2	1:D:576:LEU:HD13	1.89	0.54
2:K:137:PRO:HG2	2:K:138:ASN:H	1.71	0.54
3:M:216:ASP:O	3:M:219:PRO:HD3	2.07	0.54
3:M:677:LYS:HG2	3:M:681:ASP:OD2	2.07	0.54
1:D:583:TYR:HB3	1:D:584:PRO:HD3	1.88	0.54
3:E:809:PHE:CD2	3:E:898:ALA:HB2	2.42	0.54
3:E:822:PHE:N	3:E:822:PHE:CD1	2.74	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:102:ASP:N	2:K:103:PRO:HD3	2.23	0.54
3:M:488:ILE:HD11	3:M:578:ARG:HH22	1.71	0.54
2:B:102:ASP:N	2:B:103:PRO:HD3	2.22	0.54
1:D:411:ASP:OD1	1:D:411:ASP:N	2.33	0.54
1:D:566:TYR:CG	1:D:764:VAL:HG12	2.42	0.54
3:M:277:ARG:O	3:M:279:ASP:N	2.41	0.54
1:A:455:SER:O	1:A:534:ARG:NH2	2.40	0.54
1:A:634:MET:HA	1:A:634:MET:CE	2.36	0.54
1:D:114:THR:HG22	1:D:116:LYS:H	1.72	0.54
3:E:162:VAL:O	3:E:634:PRO:HG3	2.08	0.54
3:E:216:ASP:O	3:E:219:PRO:HD3	2.07	0.54
3:E:680:GLN:CB	3:E:920:MET:HE1	2.38	0.54
1:G:46:LEU:HD12	1:G:47:ASN:H	1.71	0.54
1:G:96:LEU:HD11	1:G:102:PRO:HD3	1.90	0.54
3:L:146:GLU:O	3:L:147:LEU:O	2.26	0.54
3:L:496:THR:HA	3:L:519:THR:HB	1.89	0.54
2:B:50:THR:O	2:B:50:THR:HG23	2.07	0.54
1:D:430:ASN:H	1:D:430:ASN:ND2	2.06	0.54
1:D:644:ASP:OD1	1:D:645:SER:N	2.41	0.54
1:G:566:TYR:CG	1:G:764:VAL:HG12	2.42	0.54
1:G:644:ASP:OD1	1:G:645:SER:N	2.41	0.54
3:M:801:LEU:HD12	3:M:809:PHE:O	2.07	0.54
2:B:137:PRO:HG2	2:B:138:ASN:H	1.71	0.54
1:D:679:GLN:HG2	1:D:691:LEU:CD1	2.37	0.54
1:A:96:LEU:HD11	1:A:102:PRO:HD3	1.90	0.54
1:A:179:CYS:O	3:E:377:ASP:N	2.28	0.54
1:D:455:SER:O	1:D:534:ARG:NH2	2.40	0.54
3:E:488:ILE:HD11	3:E:578:ARG:HH22	1.71	0.54
3:L:801:LEU:HD12	3:L:809:PHE:O	2.07	0.54
3:M:135:MET:HE2	3:M:641:GLU:OE1	2.07	0.54
1:A:77:SER:HA	1:A:89:LEU:HB2	1.88	0.54
1:A:679:GLN:HG2	1:A:691:LEU:CD1	2.38	0.54
3:E:277:ARG:O	3:E:279:ASP:N	2.41	0.54
1:G:679:GLN:HG2	1:G:691:LEU:CD1	2.37	0.54
1:G:761:GLN:O	1:G:765:SER:HB2	2.07	0.54
2:J:137:PRO:HG2	2:J:138:ASN:H	1.71	0.54
3:L:162:VAL:O	3:L:634:PRO:HG3	2.08	0.54
3:L:809:PHE:CD2	3:L:898:ALA:HB2	2.42	0.54
3:M:809:PHE:CD2	3:M:898:ALA:HB2	2.42	0.54
3:E:191:LYS:HE3	3:E:604:ILE:O	2.08	0.54
3:E:801:LEU:HD12	3:E:809:PHE:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:277:ARG:O	3:L:279:ASP:N	2.41	0.54
3:M:142:ASP:OD2	3:M:700:PRO:HB3	2.08	0.54
3:M:162:VAL:O	3:M:634:PRO:HG3	2.08	0.54
3:M:601:ASP:OD1	3:M:602:GLU:N	2.41	0.54
3:E:146:GLU:O	3:E:147:LEU:O	2.26	0.54
3:E:429:LYS:HD2	3:E:454:ILE:CD1	2.38	0.54
3:L:601:ASP:OD1	3:L:602:GLU:N	2.41	0.54
3:M:146:GLU:O	3:M:147:LEU:O	2.26	0.54
3:M:352:ASN:HA	3:M:452:LEU:HD23	1.90	0.54
1:D:65:LEU:HD11	1:D:105:LEU:HD21	1.88	0.53
3:E:361:LEU:HD22	3:E:398:ALA:HB1	1.90	0.53
3:E:496:THR:HA	3:E:519:THR:HB	1.89	0.53
3:E:601:ASP:OD1	3:E:602:GLU:N	2.41	0.53
3:L:361:LEU:HD22	3:L:398:ALA:HB1	1.90	0.53
3:L:410:ILE:HB	3:L:411:PRO:HD3	1.89	0.53
3:M:191:LYS:HE3	3:M:604:ILE:O	2.08	0.53
1:G:114:THR:HG22	1:G:116:LYS:H	1.72	0.53
2:J:102:ASP:N	2:J:103:PRO:HD3	2.22	0.53
1:D:96:LEU:HD11	1:D:102:PRO:HD3	1.90	0.53
1:G:564:ALA:HB2	1:G:576:LEU:HD13	1.89	0.53
2:J:50:THR:HG23	2:J:50:THR:O	2.07	0.53
3:M:361:LEU:HD22	3:M:398:ALA:HB1	1.90	0.53
1:A:644:ASP:OD1	1:A:645:SER:N	2.41	0.53
1:D:171:LEU:HD22	1:D:234:VAL:HG11	1.91	0.53
1:D:761:GLN:O	1:D:765:SER:HB2	2.07	0.53
3:E:819:ALA:HA	3:E:822:PHE:CE1	2.44	0.53
2:K:155:THR:CG2	2:K:166:VAL:H	2.21	0.53
3:E:142:ASP:OD2	3:E:700:PRO:HB3	2.08	0.53
3:L:819:ALA:HA	3:L:822:PHE:CE1	2.44	0.53
3:E:699:ALA:N	3:E:700:PRO:HD3	2.24	0.53
1:D:723:PHE:O	1:D:727:LYS:HG2	2.09	0.53
3:E:147:LEU:CB	3:E:148:PRO:CD	2.74	0.53
3:E:346:SER:OG	3:E:393:VAL:HG22	2.09	0.53
3:L:191:LYS:HE3	3:L:604:ILE:O	2.08	0.53
3:M:410:ILE:HB	3:M:411:PRO:HD3	1.89	0.53
3:M:817:VAL:O	3:M:819:ALA:N	2.42	0.53
3:M:819:ALA:HA	3:M:822:PHE:CE1	2.44	0.53
3:E:754:PRO:HG3	3:E:901:THR:O	2.09	0.53
3:L:429:LYS:HD2	3:L:454:ILE:CD1	2.38	0.53
3:M:496:THR:HA	3:M:519:THR:HB	1.89	0.53
1:A:430:ASN:H	1:A:430:ASN:ND2	2.06	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:352:ASN:HA	3:E:452:LEU:HD23	1.90	0.52
1:G:723:PHE:O	1:G:727:LYS:HG2	2.09	0.52
3:L:498:ASP:C	3:L:499:LEU:HD12	2.30	0.52
3:M:498:ASP:C	3:M:499:LEU:HD12	2.30	0.52
3:L:352:ASN:HA	3:L:452:LEU:HD23	1.90	0.52
3:L:817:VAL:O	3:L:819:ALA:N	2.42	0.52
3:E:250:ARG:HB3	3:E:260:ASN:O	2.09	0.52
3:L:142:ASP:OD2	3:L:700:PRO:HB3	2.08	0.52
3:M:346:SER:OG	3:M:393:VAL:HG22	2.09	0.52
3:M:429:LYS:HD2	3:M:454:ILE:CD1	2.38	0.52
3:M:754:PRO:HG3	3:M:901:THR:O	2.09	0.52
3:M:822:PHE:N	3:M:822:PHE:HD1	2.08	0.52
1:D:682:PRO:O	1:D:683:GLN:HB3	2.10	0.52
3:E:817:VAL:O	3:E:819:ALA:N	2.42	0.52
3:M:699:ALA:N	3:M:700:PRO:HD3	2.24	0.52
1:A:682:PRO:C	1:A:684:TYR:H	2.13	0.52
1:A:723:PHE:O	1:A:727:LYS:HG2	2.09	0.52
2:B:32:ASP:OD1	2:B:77:HIS:HA	2.10	0.52
2:J:82:ARG:O	2:J:85:LYS:HE2	2.09	0.52
2:J:155:THR:CG2	2:J:166:VAL:H	2.21	0.52
3:L:303:PRO:HG3	3:L:342:ARG:NH2	2.24	0.52
3:L:822:PHE:N	3:L:822:PHE:HD1	2.08	0.52
3:M:250:ARG:HB3	3:M:260:ASN:O	2.09	0.52
3:E:303:PRO:HG3	3:E:342:ARG:NH2	2.24	0.52
1:G:682:PRO:C	1:G:684:TYR:H	2.13	0.52
2:K:32:ASP:OD1	2:K:77:HIS:HA	2.10	0.52
2:K:128:VAL:HG23	2:K:186:LEU:HD13	1.91	0.52
3:M:303:PRO:HG3	3:M:342:ARG:NH2	2.24	0.52
3:M:519:THR:O	3:M:520:ALA:HB3	2.10	0.52
1:A:171:LEU:HD22	1:A:234:VAL:HG11	1.91	0.52
2:K:82:ARG:O	2:K:85:LYS:HE2	2.09	0.52
3:L:352:ASN:HD22	3:L:352:ASN:C	2.12	0.52
3:L:699:ALA:N	3:L:700:PRO:HD3	2.24	0.52
3:E:498:ASP:C	3:E:499:LEU:HD12	2.30	0.52
3:E:533:ASN:HB3	3:E:536:ASP:OD2	2.10	0.52
3:L:722:ALA:HB1	3:L:737:LEU:HD23	1.92	0.52
3:L:754:PRO:HG3	3:L:901:THR:O	2.09	0.52
3:E:704:CYS:SG	3:E:707:LEU:HD12	2.50	0.52
1:G:430:ASN:H	1:G:430:ASN:ND2	2.06	0.52
2:J:128:VAL:HG23	2:J:186:LEU:HD13	1.91	0.52
3:L:250:ARG:HB3	3:L:260:ASN:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:82:ARG:O	2:B:85:LYS:HE2	2.09	0.52
3:E:822:PHE:N	3:E:822:PHE:HD1	2.08	0.52
1:G:682:PRO:O	1:G:683:GLN:HB3	2.10	0.52
3:L:346:SER:OG	3:L:393:VAL:HG22	2.09	0.52
3:L:519:THR:O	3:L:520:ALA:HB3	2.10	0.52
3:M:162:VAL:O	3:M:163:ILE:HD13	2.10	0.52
3:M:533:ASN:HB3	3:M:536:ASP:OD2	2.10	0.52
1:D:114:THR:CG2	1:D:115:ASN:H	2.22	0.51
3:E:715:HIS:HB2	3:E:916:PHE:CE2	2.45	0.51
1:G:114:THR:CG2	1:G:115:ASN:H	2.23	0.51
1:A:682:PRO:O	1:A:683:GLN:HB3	2.10	0.51
2:K:136:ALA:HB1	2:K:137:PRO:HD2	1.92	0.51
3:L:764:ASP:CA	3:L:851:ARG:HH22	2.24	0.51
3:M:420:THR:O	3:M:420:THR:HG22	2.10	0.51
2:B:155:THR:CG2	2:B:166:VAL:H	2.21	0.51
3:E:420:THR:HG22	3:E:420:THR:O	2.10	0.51
3:L:420:THR:HG22	3:L:420:THR:O	2.10	0.51
3:L:533:ASN:HB3	3:L:536:ASP:OD2	2.10	0.51
3:M:406:LEU:O	3:M:410:ILE:HG13	2.10	0.51
3:M:516:SER:HB2	3:M:522:GLN:N	2.26	0.51
3:M:704:CYS:SG	3:M:707:LEU:HD12	2.50	0.51
1:A:365:THR:HB	1:A:448:ALA:HB3	1.92	0.51
1:D:682:PRO:C	1:D:684:TYR:H	2.13	0.51
1:G:171:LEU:HD22	1:G:234:VAL:HG11	1.91	0.51
3:L:406:LEU:O	3:L:410:ILE:HG13	2.10	0.51
3:E:406:LEU:O	3:E:410:ILE:HG13	2.10	0.51
1:G:171:LEU:HD12	1:G:171:LEU:N	2.26	0.51
1:G:739:ARG:HG3	1:G:739:ARG:HH11	1.76	0.51
1:G:745:VAL:HG13	2:K:50:THR:HG21	1.92	0.51
2:J:155:THR:HG22	2:J:166:VAL:H	1.75	0.51
3:M:715:HIS:HB2	3:M:916:PHE:CE2	2.45	0.51
2:B:107:ASP:O	2:B:111:VAL:HG23	2.11	0.51
1:D:171:LEU:HD12	1:D:171:LEU:N	2.25	0.51
3:L:704:CYS:SG	3:L:707:LEU:HD12	2.50	0.51
2:B:155:THR:HG23	2:B:156:GLY:N	2.26	0.51
3:L:162:VAL:O	3:L:163:ILE:HD13	2.10	0.51
3:L:906:LYS:O	3:L:907:ILE:HD13	2.11	0.51
3:M:722:ALA:HB1	3:M:737:LEU:HD23	1.92	0.51
3:E:516:SER:HB2	3:E:522:GLN:N	2.26	0.51
2:J:107:ASP:O	2:J:111:VAL:HG23	2.11	0.51
2:K:172:SER:OG	2:K:175:MET:HG2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:817:VAL:C	3:L:819:ALA:N	2.64	0.51
2:B:136:ALA:HB1	2:B:137:PRO:HD2	1.92	0.51
2:B:155:THR:HG22	2:B:166:VAL:H	1.75	0.51
3:E:279:ASP:CA	3:E:284:LYS:HE3	2.40	0.51
3:E:722:ALA:HB1	3:E:737:LEU:HD23	1.92	0.51
3:L:715:HIS:CE1	3:L:719:LYS:HE3	2.46	0.51
1:A:171:LEU:HD12	1:A:171:LEU:N	2.26	0.51
3:E:764:ASP:CA	3:E:851:ARG:HH22	2.23	0.51
1:A:144:ILE:O	1:A:148:LEU:HG	2.11	0.50
1:A:739:ARG:HG3	1:A:739:ARG:HH11	1.76	0.50
2:B:128:VAL:HG23	2:B:186:LEU:HD13	1.91	0.50
1:D:745:VAL:HG13	2:J:50:THR:HG21	1.92	0.50
3:E:448:THR:HG22	3:E:449:LEU:O	2.11	0.50
3:E:516:SER:HB2	3:E:521:GLY:C	2.31	0.50
3:L:372:GLN:HG2	3:L:373:ILE:N	2.26	0.50
3:L:516:SER:HB2	3:L:522:GLN:N	2.26	0.50
3:M:372:GLN:HG2	3:M:373:ILE:N	2.27	0.50
2:B:172:SER:OG	2:B:175:MET:HG2	2.11	0.50
1:D:144:ILE:O	1:D:148:LEU:HG	2.12	0.50
1:D:430:ASN:HD22	1:D:430:ASN:N	2.03	0.50
3:E:906:LYS:O	3:E:907:ILE:HD13	2.11	0.50
3:M:710:PHE:HB3	3:M:711:PRO:HD3	1.93	0.50
1:D:365:THR:HB	1:D:448:ALA:HB3	1.92	0.50
3:E:162:VAL:O	3:E:163:ILE:HD13	2.10	0.50
1:G:722:ARG:NH1	6:K:1190:GNP:N3B	2.57	0.50
2:K:107:ASP:O	2:K:111:VAL:HG23	2.11	0.50
3:L:715:HIS:HB2	3:L:916:PHE:CE2	2.45	0.50
3:M:516:SER:HB2	3:M:521:GLY:C	2.31	0.50
1:A:66:ASN:HD22	1:A:68:TYR:H	1.60	0.50
3:E:519:THR:O	3:E:520:ALA:HB3	2.10	0.50
3:E:715:HIS:CE1	3:E:719:LYS:HE3	2.46	0.50
3:E:860:ARG:HG2	3:E:869:GLN:HB2	1.93	0.50
2:J:32:ASP:OD1	2:J:77:HIS:HA	2.10	0.50
2:J:155:THR:HG23	2:J:156:GLY:N	2.26	0.50
3:M:680:GLN:CB	3:M:920:MET:HE1	2.41	0.50
3:M:855:ILE:O	3:M:858:GLN:HB3	2.12	0.50
3:M:906:LYS:O	3:M:907:ILE:HD13	2.11	0.50
1:D:66:ASN:HD22	1:D:68:TYR:H	1.60	0.50
3:E:855:ILE:O	3:E:858:GLN:HB3	2.12	0.50
2:J:136:ALA:HB1	2:J:137:PRO:HD2	1.92	0.50
3:L:250:ARG:HA	3:L:262:VAL:HG23	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:101:MET:HE1	4:N:61:PHE:CZ	2.42	0.50
3:E:722:ALA:HB1	3:E:737:LEU:CD2	2.41	0.50
2:K:155:THR:HG22	2:K:166:VAL:H	1.75	0.50
3:L:499:LEU:HD12	3:L:499:LEU:N	2.27	0.50
3:L:504:GLU:OE2	3:L:530:SER:HB3	2.12	0.50
3:M:715:HIS:CE1	3:M:719:LYS:HE3	2.46	0.50
1:A:745:VAL:HG13	2:B:50:THR:HG21	1.92	0.50
3:L:710:PHE:HB3	3:L:711:PRO:HD3	1.93	0.50
3:M:250:ARG:HA	3:M:262:VAL:HG23	1.94	0.50
1:G:144:ILE:O	1:G:148:LEU:HG	2.11	0.50
1:G:365:THR:HB	1:G:448:ALA:HB3	1.92	0.50
2:J:140:VAL:HG13	2:J:144:GLU:CD	2.32	0.50
3:L:516:SER:HB2	3:L:521:GLY:C	2.31	0.50
3:M:499:LEU:HD12	3:M:499:LEU:N	2.27	0.50
2:K:176:ARG:HA	2:K:179:TYR:HE2	1.77	0.50
3:M:504:GLU:OE2	3:M:530:SER:HB3	2.12	0.50
1:D:739:ARG:HH11	1:D:739:ARG:HG3	1.76	0.49
1:G:645:SER:HA	1:G:728:LEU:HD13	1.94	0.49
2:K:140:VAL:HG13	2:K:144:GLU:CD	2.33	0.49
2:K:155:THR:HG23	2:K:156:GLY:N	2.26	0.49
3:L:448:THR:HG22	3:L:449:LEU:O	2.11	0.49
3:L:907:ILE:HG22	3:L:908:LEU:N	2.27	0.49
3:M:279:ASP:CA	3:M:284:LYS:HE3	2.39	0.49
3:M:448:THR:HG22	3:M:449:LEU:O	2.11	0.49
3:M:818:PRO:C	3:M:820:LEU:N	2.66	0.49
3:M:860:ARG:HG2	3:M:869:GLN:HB2	1.93	0.49
1:G:644:ASP:OD2	1:G:731:SER:HB3	2.13	0.49
3:L:150:PRO:HG2	3:L:708:ARG:HH11	1.78	0.49
3:M:817:VAL:C	3:M:819:ALA:N	2.64	0.49
3:E:768:LEU:CG	3:E:769:PRO:HD2	2.40	0.49
3:E:907:ILE:HG22	3:E:908:LEU:N	2.27	0.49
3:L:722:ALA:HB1	3:L:737:LEU:CD2	2.41	0.49
3:E:423:ALA:HA	3:E:452:LEU:O	2.13	0.49
1:G:390:LYS:HD2	1:G:390:LYS:N	2.28	0.49
3:L:911:GLU:HG3	3:L:919:ILE:HD11	1.94	0.49
3:M:907:ILE:HG22	3:M:908:LEU:N	2.27	0.49
1:D:645:SER:HA	1:D:728:LEU:HD13	1.94	0.49
3:E:504:GLU:OE2	3:E:530:SER:HB3	2.12	0.49
3:M:722:ALA:HB1	3:M:737:LEU:CD2	2.41	0.49
1:A:171:LEU:CD2	1:A:234:VAL:HG11	2.43	0.49
1:D:395:TYR:CD1	1:D:497:SER:HA	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:372:GLN:HG2	3:E:373:ILE:N	2.26	0.49
3:E:589:PRO:O	3:E:590:ARG:HD3	2.13	0.49
3:E:687:LYS:HZ2	3:E:925:SER:HA	1.77	0.49
3:M:794:PHE:HA	3:M:800:TYR:CZ	2.48	0.49
3:M:911:GLU:HG3	3:M:919:ILE:HD11	1.94	0.49
1:G:171:LEU:CD2	1:G:234:VAL:HG11	2.43	0.49
2:K:176:ARG:HA	2:K:179:TYR:CE2	2.48	0.49
3:L:423:ALA:HA	3:L:452:LEU:O	2.13	0.49
3:L:818:PRO:C	3:L:820:LEU:N	2.66	0.49
3:M:150:PRO:HG2	3:M:708:ARG:HH11	1.78	0.49
2:B:140:VAL:HG13	2:B:144:GLU:CD	2.33	0.49
1:D:644:ASP:OD2	1:D:731:SER:HB3	2.13	0.49
3:E:499:LEU:HD12	3:E:499:LEU:N	2.27	0.49
1:G:430:ASN:HD22	1:G:430:ASN:N	2.03	0.49
3:M:764:ASP:CA	3:M:851:ARG:HH22	2.24	0.49
1:A:390:LYS:HD2	1:A:390:LYS:N	2.28	0.49
1:A:395:TYR:CD1	1:A:497:SER:HA	2.48	0.49
1:A:645:SER:HA	1:A:728:LEU:HD13	1.94	0.49
2:B:176:ARG:HA	2:B:179:TYR:CE2	2.48	0.49
1:D:147:SER:HB3	1:D:384:TYR:CE2	2.48	0.49
1:D:390:LYS:N	1:D:390:LYS:HD2	2.28	0.49
3:E:911:GLU:HG3	3:E:919:ILE:HD11	1.94	0.49
2:J:172:SER:OG	2:J:175:MET:HG2	2.11	0.49
3:L:794:PHE:HA	3:L:800:TYR:CZ	2.48	0.49
3:M:703:LEU:HG	3:M:704:CYS:H	1.77	0.49
1:A:91:PRO:CA	1:D:669:GLN:NE2	2.73	0.49
2:B:85:LYS:HA	2:B:88:PHE:CD2	2.48	0.49
3:E:710:PHE:HB3	3:E:711:PRO:HD3	1.93	0.49
1:G:176:ILE:HD12	3:M:413:ILE:CG1	2.38	0.49
2:J:176:ARG:HA	2:J:179:TYR:CE2	2.48	0.49
3:L:279:ASP:CA	3:L:284:LYS:HE3	2.39	0.49
3:L:860:ARG:HG2	3:L:869:GLN:HB2	1.93	0.49
3:M:795:GLU:C	3:M:797:TYR:H	2.17	0.49
3:E:352:ASN:ND2	3:E:352:ASN:C	2.67	0.48
3:E:356:TYR:OH	3:E:430:SER:HB3	2.13	0.48
1:G:147:SER:HB3	1:G:384:TYR:CE2	2.48	0.48
1:G:616:GLU:CG	1:G:620:ASN:CB	2.91	0.48
2:J:88:PHE:N	2:J:89:PRO:CD	2.76	0.48
3:L:312:VAL:O	3:L:312:VAL:CG1	2.61	0.48
3:L:703:LEU:HG	3:L:704:CYS:H	1.77	0.48
3:M:135:MET:HE1	3:M:634:PRO:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:215:ASP:O	3:M:219:PRO:HG3	2.13	0.48
3:E:818:PRO:C	3:E:820:LEU:N	2.66	0.48
1:G:451:SER:C	1:G:453:TYR:H	2.17	0.48
3:M:589:PRO:O	3:M:590:ARG:HD3	2.13	0.48
3:E:338:ASN:OD1	3:E:341:GLU:HA	2.13	0.48
2:J:176:ARG:HA	2:J:179:TYR:HE2	1.77	0.48
2:K:88:PHE:N	2:K:89:PRO:CD	2.76	0.48
1:A:644:ASP:OD2	1:A:731:SER:HB3	2.12	0.48
2:B:88:PHE:N	2:B:89:PRO:CD	2.76	0.48
2:B:134:ILE:HG12	2:B:172:SER:HB2	1.96	0.48
1:D:171:LEU:CD2	1:D:234:VAL:HG11	2.43	0.48
3:E:215:ASP:O	3:E:219:PRO:HG3	2.13	0.48
3:E:794:PHE:HA	3:E:800:TYR:CZ	2.48	0.48
3:E:817:VAL:C	3:E:819:ALA:N	2.64	0.48
1:G:66:ASN:HD22	1:G:68:TYR:H	1.60	0.48
2:J:103:PRO:HG3	2:J:140:VAL:HG21	1.96	0.48
3:L:192:ASN:HA	3:L:603:SER:HA	1.96	0.48
3:L:248:GLY:O	3:L:277:ARG:NH2	2.33	0.48
3:L:534:PRO:O	3:L:538:VAL:HG23	2.13	0.48
3:L:855:ILE:O	3:L:858:GLN:HB3	2.12	0.48
3:M:534:PRO:O	3:M:538:VAL:HG23	2.13	0.48
1:D:616:GLU:CG	1:D:620:ASN:CB	2.91	0.48
3:E:192:ASN:HA	3:E:603:SER:HA	1.96	0.48
3:E:230:ARG:HD3	3:E:237:TYR:CD2	2.49	0.48
2:J:32:ASP:HB3	2:J:77:HIS:N	2.29	0.48
2:K:32:ASP:HB3	2:K:77:HIS:N	2.29	0.48
2:K:99:ASP:OD1	2:K:133:LYS:HD2	2.14	0.48
3:L:230:ARG:HD3	3:L:237:TYR:CD2	2.49	0.48
3:M:423:ALA:HA	3:M:452:LEU:O	2.13	0.48
1:A:147:SER:HB3	1:A:384:TYR:CE2	2.48	0.48
1:D:68:TYR:CE1	4:N:69:LEU:HD22	2.49	0.48
1:D:739:ARG:HG2	1:D:744:ILE:HD11	1.96	0.48
3:E:703:LEU:HG	3:E:704:CYS:H	1.77	0.48
2:J:99:ASP:OD1	2:J:133:LYS:HD2	2.14	0.48
2:J:134:ILE:HG12	2:J:172:SER:HB2	1.96	0.48
3:L:224:GLU:HA	3:L:291:MET:HG3	1.96	0.48
3:L:488:ILE:HD11	3:L:578:ARG:NH2	2.28	0.48
3:M:230:ARG:HD3	3:M:237:TYR:CD2	2.49	0.48
3:M:312:VAL:O	3:M:312:VAL:CG1	2.61	0.48
1:A:17:ASN:HB2	1:A:522:SER:HB2	1.96	0.48
1:A:114:THR:CG2	1:A:115:ASN:H	2.23	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:32:ASP:HB3	2:B:77:HIS:N	2.29	0.48
2:B:176:ARG:HA	2:B:179:TYR:HE2	1.77	0.48
1:D:96:LEU:CG	1:D:97:SER:N	2.76	0.48
3:E:250:ARG:HA	3:E:262:VAL:HG23	1.94	0.48
3:E:312:VAL:O	3:E:312:VAL:CG1	2.61	0.48
2:J:85:LYS:HA	2:J:88:PHE:CD2	2.48	0.48
2:K:134:ILE:HG12	2:K:172:SER:HB2	1.96	0.48
3:L:352:ASN:ND2	3:L:352:ASN:C	2.67	0.48
3:M:192:ASN:HA	3:M:603:SER:HA	1.96	0.48
1:A:739:ARG:HG2	1:A:744:ILE:HD11	1.96	0.48
2:B:103:PRO:HG3	2:B:140:VAL:HG21	1.96	0.48
3:E:534:PRO:O	3:E:538:VAL:HG23	2.13	0.48
3:E:795:GLU:C	3:E:797:TYR:H	2.16	0.48
1:G:395:TYR:CD1	1:G:497:SER:HA	2.48	0.48
3:L:215:ASP:O	3:L:219:PRO:HG3	2.13	0.48
3:L:338:ASN:OD1	3:L:341:GLU:HA	2.13	0.48
3:M:352:ASN:HD22	3:M:352:ASN:N	2.11	0.48
3:M:488:ILE:HD11	3:M:578:ARG:NH2	2.28	0.48
3:M:768:LEU:CG	3:M:769:PRO:HD2	2.40	0.48
1:A:96:LEU:CG	1:A:97:SER:N	2.76	0.48
3:E:150:PRO:HG2	3:E:708:ARG:HH11	1.78	0.48
2:K:85:LYS:HA	2:K:88:PHE:CD2	2.48	0.48
3:L:795:GLU:HB3	3:L:797:TYR:CE2	2.49	0.48
3:M:356:TYR:OH	3:M:430:SER:HB3	2.13	0.48
1:D:42:GLU:OE2	1:D:397:LYS:HE2	2.14	0.48
2:K:137:PRO:C	2:K:139:ALA:H	2.18	0.48
3:L:589:PRO:O	3:L:590:ARG:HD3	2.13	0.48
3:L:796:ARG:NH1	3:L:815:ASP:OD2	2.47	0.48
3:M:338:ASN:OD1	3:M:341:GLU:HA	2.13	0.48
3:E:133:ARG:NE	3:E:135:MET:SD	2.87	0.47
1:G:96:LEU:CG	1:G:97:SER:N	2.76	0.47
1:G:679:GLN:HG3	1:G:687:PHE:HE2	1.79	0.47
2:J:137:PRO:C	2:J:139:ALA:H	2.18	0.47
3:L:230:ARG:HD2	3:L:235:ARG:O	2.14	0.47
3:L:667:SER:HB3	3:L:670:ASP:CB	2.44	0.47
3:L:795:GLU:C	3:L:797:TYR:H	2.17	0.47
3:M:224:GLU:HA	3:M:291:MET:HG3	1.96	0.47
3:M:352:ASN:ND2	3:M:352:ASN:C	2.67	0.47
3:M:580:SER:O	3:M:581:ASP:HB2	2.14	0.47
1:A:68:TYR:CE1	4:F:69:LEU:HD22	2.49	0.47
1:A:616:GLU:CG	1:A:620:ASN:CB	2.91	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:17:ASN:HB2	1:D:522:SER:HB2	1.96	0.47
1:D:19:PHE:HB2	1:D:511:LEU:CD2	2.44	0.47
3:E:580:SER:O	3:E:581:ASP:HB2	2.14	0.47
3:E:796:ARG:NH1	3:E:815:ASP:OD2	2.47	0.47
1:G:195:GLU:O	1:G:199:GLY:N	2.41	0.47
3:L:277:ARG:C	3:L:279:ASP:H	2.17	0.47
3:L:356:TYR:OH	3:L:430:SER:HB3	2.13	0.47
3:L:715:HIS:NE2	3:L:719:LYS:HE3	2.30	0.47
3:M:177:ALA:HB1	3:M:182:ILE:HG22	1.96	0.47
3:M:277:ARG:C	3:M:279:ASP:H	2.18	0.47
3:M:796:ARG:NH1	3:M:815:ASP:OD2	2.47	0.47
3:E:488:ILE:HD11	3:E:578:ARG:NH2	2.28	0.47
3:E:795:GLU:HB3	3:E:797:TYR:CE2	2.49	0.47
1:G:634:MET:HA	1:G:634:MET:HE3	1.94	0.47
2:K:103:PRO:HG3	2:K:140:VAL:HG21	1.96	0.47
2:B:137:PRO:C	2:B:139:ALA:H	2.18	0.47
3:E:352:ASN:HD22	3:E:352:ASN:N	2.11	0.47
3:L:580:SER:O	3:L:581:ASP:HB2	2.14	0.47
3:M:761:ASP:O	3:M:762:MET:O	2.33	0.47
1:A:42:GLU:OE2	1:A:397:LYS:HE2	2.14	0.47
1:A:451:SER:C	1:A:453:TYR:H	2.17	0.47
1:A:679:GLN:HG3	1:A:687:PHE:HE2	1.79	0.47
2:B:99:ASP:OD1	2:B:133:LYS:HD2	2.14	0.47
3:E:149:PRO:O	3:E:150:PRO:C	2.53	0.47
1:G:561:GLN:HG2	1:G:763:ALA:HA	1.96	0.47
3:L:135:MET:HE1	3:L:634:PRO:HB2	1.96	0.47
3:M:795:GLU:HB3	3:M:797:TYR:CE2	2.49	0.47
3:E:248:GLY:O	3:E:277:ARG:NH2	2.33	0.47
2:K:23:HIS:HD2	2:K:68:LYS:H	1.62	0.47
3:M:325:THR:OG1	3:M:445:VAL:HG11	2.15	0.47
3:M:667:SER:HB3	3:M:670:ASP:CB	2.44	0.47
1:A:561:GLN:HG2	1:A:763:ALA:HA	1.96	0.47
1:D:96:LEU:HD11	1:D:101:MET:HA	1.97	0.47
3:E:230:ARG:HD2	3:E:235:ARG:O	2.15	0.47
3:E:378:ILE:CD1	3:E:387:PRO:HG3	2.45	0.47
3:E:388:ARG:HB2	3:E:389:PRO:HD2	1.97	0.47
3:E:761:ASP:O	3:E:762:MET:O	2.33	0.47
3:L:133:ARG:HG3	3:L:135:MET:HG2	1.97	0.47
3:L:151:ILE:HD13	3:L:709:MET:HE1	1.96	0.47
3:L:205:LEU:CD1	3:L:611:VAL:HG11	2.44	0.47
3:L:352:ASN:HD22	3:L:352:ASN:N	2.11	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:149:PRO:O	3:M:150:PRO:C	2.53	0.47
3:M:352:ASN:HD22	3:M:352:ASN:C	2.12	0.47
1:A:66:ASN:HD21	1:A:68:TYR:HB2	1.80	0.47
1:D:164:ASN:HD22	1:D:165:VAL:H	1.63	0.47
3:E:848:PHE:O	3:E:851:ARG:HB2	2.15	0.47
1:G:594:GLN:HE21	1:G:601:ASN:HD21	1.63	0.47
3:M:249:ARG:O	3:M:250:ARG:HG2	2.15	0.47
3:E:177:ALA:HB1	3:E:182:ILE:HG22	1.96	0.47
3:E:224:GLU:HA	3:E:291:MET:HG3	1.96	0.47
3:E:325:THR:OG1	3:E:445:VAL:HG11	2.15	0.47
1:G:651:ASN:ND2	1:G:651:ASN:N	2.53	0.47
1:G:739:ARG:HG2	1:G:744:ILE:HD11	1.96	0.47
3:M:133:ARG:HG3	3:M:135:MET:HG2	1.97	0.47
3:M:248:GLY:O	3:M:277:ARG:NH2	2.33	0.47
1:A:430:ASN:HD22	1:A:430:ASN:N	2.03	0.47
2:B:62:LEU:HD12	2:B:71:THR:HG21	1.97	0.47
1:D:551:TRP:CE3	1:D:552:LEU:HD13	2.50	0.47
1:G:551:TRP:CE3	1:G:552:LEU:HD13	2.50	0.47
2:J:62:LEU:HD12	2:J:71:THR:HG21	1.97	0.47
3:M:133:ARG:HH21	3:M:135:MET:HE2	1.79	0.47
1:D:661:PHE:HA	1:D:709:PRO:HB2	1.97	0.46
3:E:133:ARG:HG3	3:E:135:MET:HG2	1.97	0.46
1:G:17:ASN:HB2	1:G:522:SER:HB2	1.96	0.46
1:G:485:ALA:HB2	1:G:511:LEU:HD11	1.97	0.46
3:L:177:ALA:HB1	3:L:182:ILE:HG22	1.96	0.46
3:L:325:THR:OG1	3:L:445:VAL:HG11	2.15	0.46
3:L:388:ARG:HB2	3:L:389:PRO:HD2	1.97	0.46
3:M:301:PRO:HA	3:M:302:PRO:HD3	1.68	0.46
3:M:600:VAL:HG13	3:M:604:ILE:HD11	1.96	0.46
2:K:62:LEU:HD12	2:K:71:THR:HG21	1.96	0.46
3:L:133:ARG:NE	3:L:135:MET:SD	2.87	0.46
3:M:150:PRO:HG2	3:M:708:ARG:HD3	1.97	0.46
3:M:230:ARG:HD2	3:M:235:ARG:O	2.15	0.46
1:A:485:ALA:HB2	1:A:511:LEU:HD11	1.97	0.46
1:A:556:LEU:HD22	1:A:587:THR:HG21	1.98	0.46
1:D:66:ASN:HD21	1:D:68:TYR:HB2	1.80	0.46
1:D:343:VAL:O	1:D:362:THR:HG22	2.16	0.46
1:D:451:SER:C	1:D:453:TYR:H	2.17	0.46
1:D:594:GLN:HE21	1:D:601:ASN:HD21	1.63	0.46
3:E:168:MET:SD	3:E:175:SER:OG	2.69	0.46
3:E:314:GLN:CG	3:E:318:LYS:HE3	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:600:VAL:HG13	3:E:604:ILE:HD11	1.96	0.46
1:G:42:GLU:OE2	1:G:397:LYS:HE2	2.14	0.46
1:G:661:PHE:HA	1:G:709:PRO:HB2	1.97	0.46
3:L:378:ILE:CD1	3:L:387:PRO:HG3	2.45	0.46
3:M:212:HIS:O	3:M:590:ARG:HB3	2.16	0.46
3:M:715:HIS:NE2	3:M:719:LYS:HE3	2.30	0.46
1:D:679:GLN:HG3	1:D:687:PHE:HE2	1.79	0.46
3:E:277:ARG:C	3:E:279:ASP:H	2.18	0.46
1:G:687:PHE:CE2	1:G:691:LEU:HD11	2.51	0.46
3:L:768:LEU:CG	3:L:769:PRO:HD2	2.40	0.46
3:M:822:PHE:HD1	3:M:822:PHE:H	1.63	0.46
3:M:900:SER:HA	3:M:907:ILE:HG21	1.97	0.46
3:E:715:HIS:NE2	3:E:719:LYS:HE3	2.29	0.46
3:E:822:PHE:HD1	3:E:822:PHE:H	1.63	0.46
1:G:96:LEU:HD11	1:G:101:MET:HA	1.97	0.46
2:J:23:HIS:HD2	2:J:68:LYS:H	1.62	0.46
3:L:144:LEU:HD22	3:L:918:GLN:NE2	2.31	0.46
3:L:314:GLN:CG	3:L:318:LYS:HE3	2.46	0.46
3:L:687:LYS:HZ1	3:L:925:SER:HA	1.80	0.46
3:M:133:ARG:NE	3:M:135:MET:SD	2.88	0.46
3:E:170:VAL:HG12	3:E:170:VAL:O	2.16	0.46
1:G:19:PHE:HB2	1:G:511:LEU:CD2	2.44	0.46
1:G:432:ILE:CD1	1:G:442:THR:HA	2.44	0.46
3:L:149:PRO:O	3:L:150:PRO:C	2.53	0.46
3:L:212:HIS:O	3:L:590:ARG:HB3	2.16	0.46
3:L:600:VAL:HG13	3:L:604:ILE:HD11	1.96	0.46
3:L:761:ASP:O	3:L:762:MET:O	2.33	0.46
3:E:667:SER:HB3	3:E:670:ASP:CB	2.44	0.46
3:L:249:ARG:O	3:L:250:ARG:HG2	2.15	0.46
3:L:279:ASP:C	3:L:284:LYS:HE3	2.36	0.46
3:M:378:ILE:HD13	3:M:385:PHE:CZ	2.51	0.46
3:M:378:ILE:CD1	3:M:387:PRO:HG3	2.45	0.46
3:M:388:ARG:HB2	3:M:389:PRO:HD2	1.97	0.46
1:A:432:ILE:CD1	1:A:442:THR:HA	2.44	0.46
1:D:485:ALA:HB2	1:D:511:LEU:HD11	1.97	0.46
3:E:205:LEU:CD1	3:E:611:VAL:HG11	2.44	0.46
1:G:343:VAL:O	1:G:362:THR:HG22	2.16	0.46
2:K:31:LEU:HD22	2:K:81:ARG:NH2	2.31	0.46
3:L:848:PHE:O	3:L:851:ARG:HB2	2.15	0.46
3:M:314:GLN:CG	3:M:318:LYS:HE3	2.46	0.46
1:D:561:GLN:HG2	1:D:763:ALA:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:31:LEU:HD22	2:J:81:ARG:NH2	2.31	0.46
3:M:795:GLU:O	3:M:797:TYR:N	2.49	0.46
3:M:848:PHE:O	3:M:851:ARG:HB2	2.15	0.46
1:A:164:ASN:HD22	1:A:165:VAL:H	1.63	0.46
2:B:31:LEU:HD22	2:B:81:ARG:NH2	2.31	0.46
1:D:556:LEU:HD22	1:D:587:THR:HG21	1.98	0.46
3:E:249:ARG:O	3:E:250:ARG:HG2	2.15	0.46
3:E:900:SER:HA	3:E:907:ILE:HG21	1.97	0.46
3:M:147:LEU:CB	3:M:148:PRO:CD	2.74	0.46
3:M:197:LYS:HD2	3:M:197:LYS:HA	1.72	0.46
3:M:417:ASN:OD1	3:M:419:ILE:N	2.41	0.46
1:D:734:TYR:HA	1:D:744:ILE:HG21	1.98	0.45
3:E:144:LEU:HD22	3:E:918:GLN:NE2	2.31	0.45
3:E:150:PRO:HG2	3:E:708:ARG:HD3	1.97	0.45
3:L:313:SER:O	3:L:317:ILE:HG12	2.16	0.45
3:L:378:ILE:HD13	3:L:385:PHE:CZ	2.51	0.45
3:L:454:ILE:H	3:L:454:ILE:HG13	1.49	0.45
3:L:795:GLU:O	3:L:797:TYR:N	2.49	0.45
3:M:205:LEU:CD1	3:M:611:VAL:HG11	2.44	0.45
3:M:417:ASN:HD21	3:M:419:ILE:HD12	1.81	0.45
3:M:920:MET:HE3	3:M:920:MET:CA	2.45	0.45
1:A:96:LEU:HD11	1:A:101:MET:HA	1.97	0.45
1:A:687:PHE:CE2	1:A:691:LEU:HD11	2.51	0.45
1:D:687:PHE:CE2	1:D:691:LEU:HD11	2.51	0.45
3:E:417:ASN:HD21	3:E:419:ILE:HD12	1.81	0.45
2:K:32:ASP:O	2:K:105:ARG:NH2	2.49	0.45
2:K:110:ARG:HG3	2:K:110:ARG:HH11	1.82	0.45
3:L:822:PHE:HD1	3:L:822:PHE:H	1.63	0.45
1:A:464:ASN:ND2	1:A:465:THR:H	2.15	0.45
1:A:551:TRP:CE3	1:A:552:LEU:HD13	2.50	0.45
1:A:594:GLN:HE21	1:A:601:ASN:HD21	1.63	0.45
2:B:32:ASP:O	2:B:105:ARG:NH2	2.49	0.45
2:B:97:LEU:HD12	2:B:97:LEU:N	2.31	0.45
1:D:432:ILE:CD1	1:D:442:THR:HA	2.43	0.45
3:E:795:GLU:O	3:E:797:TYR:N	2.49	0.45
3:L:417:ASN:HD21	3:L:419:ILE:HD12	1.81	0.45
3:L:668:LEU:HD21	3:L:733:ARG:NH1	2.31	0.45
1:A:176:ILE:HD12	3:E:413:ILE:CG1	2.38	0.45
1:A:661:PHE:HA	1:A:709:PRO:HB2	1.97	0.45
3:E:135:MET:HE1	3:E:634:PRO:HB2	1.99	0.45
1:G:44:ASP:C	1:G:45:GLU:HG3	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:32:ASP:O	2:J:105:ARG:NH2	2.49	0.45
3:M:144:LEU:HD22	3:M:918:GLN:NE2	2.31	0.45
3:M:170:VAL:HG12	3:M:170:VAL:O	2.16	0.45
1:A:734:TYR:HA	1:A:744:ILE:HG21	1.98	0.45
2:B:23:HIS:HD2	2:B:68:LYS:H	1.62	0.45
1:D:101:MET:HE1	4:N:61:PHE:CE2	2.51	0.45
1:G:164:ASN:HD22	1:G:165:VAL:H	1.63	0.45
3:L:147:LEU:O	3:L:149:PRO:N	2.50	0.45
2:K:97:LEU:N	2:K:97:LEU:HD12	2.31	0.45
3:L:900:SER:HA	3:L:907:ILE:HG21	1.98	0.45
3:M:672:ARG:NH1	3:M:725:SER:HA	2.32	0.45
1:A:19:PHE:HB2	1:A:511:LEU:CD2	2.44	0.45
1:A:44:ASP:C	1:A:45:GLU:HG3	2.37	0.45
2:B:40:LEU:HD22	2:B:73:ASP:HB2	1.99	0.45
2:B:142:GLU:CB	1:G:426:LYS:HZ3	2.30	0.45
3:E:212:HIS:O	3:E:590:ARG:HB3	2.16	0.45
3:E:424:LEU:O	3:E:428:LEU:HB2	2.17	0.45
3:E:506:TYR:CE2	3:E:508:ASP:HB2	2.52	0.45
3:E:756:VAL:O	3:E:786:PRO:HA	2.17	0.45
3:L:791:SER:H	3:L:905:ASP:CG	2.20	0.45
3:M:279:ASP:C	3:M:284:LYS:HE3	2.36	0.45
3:E:313:SER:O	3:E:317:ILE:HG12	2.16	0.45
4:F:62:LEU:HA	4:F:66:GLN:OE1	2.17	0.45
1:G:66:ASN:HD21	1:G:68:TYR:HB2	1.80	0.45
2:J:85:LYS:HA	2:J:88:PHE:CE2	2.52	0.45
2:K:155:THR:OG1	2:K:156:GLY:N	2.50	0.45
3:M:908:LEU:C	3:M:910:ASN:H	2.21	0.45
1:A:343:VAL:O	1:A:362:THR:HG22	2.16	0.45
1:D:464:ASN:ND2	1:D:465:THR:H	2.15	0.45
3:E:279:ASP:C	3:E:284:LYS:HE3	2.36	0.45
3:E:672:ARG:NH1	3:E:725:SER:HA	2.32	0.45
1:G:46:LEU:HG	1:G:47:ASN:N	2.32	0.45
1:G:68:TYR:CE1	4:O:69:LEU:HD22	2.49	0.45
1:G:734:TYR:HA	1:G:744:ILE:HG21	1.98	0.45
2:K:37:THR:HG22	2:K:51:LEU:HD13	1.99	0.45
2:K:125:VAL:HA	2:K:126:PRO:HD3	1.87	0.45
3:M:791:SER:H	3:M:905:ASP:CG	2.21	0.45
4:O:62:LEU:HA	4:O:66:GLN:OE1	2.17	0.45
1:A:187:GLU:HB2	1:A:296:PRO:HG3	1.99	0.45
2:B:110:ARG:HH11	2:B:110:ARG:HG3	1.82	0.45
1:D:44:ASP:C	1:D:45:GLU:HG3	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:187:GLU:HB2	1:D:296:PRO:HG3	1.99	0.45
1:G:411:ASP:OD1	1:G:411:ASP:N	2.33	0.45
1:G:556:LEU:HD22	1:G:587:THR:HG21	1.98	0.45
3:L:150:PRO:HG2	3:L:708:ARG:HD3	1.97	0.45
3:M:756:VAL:O	3:M:786:PRO:HA	2.17	0.45
1:D:588:TYR:O	1:D:591:ARG:HG2	2.18	0.44
3:E:417:ASN:OD1	3:E:419:ILE:N	2.42	0.44
3:E:571:PHE:HD2	3:E:596:PHE:CE1	2.36	0.44
3:L:154:LEU:CG	3:L:709:MET:HE2	2.45	0.44
3:L:309:LEU:HD12	3:L:309:LEU:C	2.38	0.44
3:L:506:TYR:CE2	3:L:508:ASP:HB2	2.52	0.44
3:M:424:LEU:O	3:M:428:LEU:HB2	2.17	0.44
1:A:138:ASP:HA	1:A:141:LYS:HD2	1.99	0.44
1:D:430:ASN:ND2	1:D:430:ASN:N	2.65	0.44
3:L:417:ASN:OD1	3:L:419:ILE:N	2.41	0.44
3:L:672:ARG:NH1	3:L:725:SER:HA	2.32	0.44
3:M:300:GLN:O	3:M:301:PRO:C	2.56	0.44
3:M:313:SER:O	3:M:317:ILE:HG12	2.16	0.44
3:M:668:LEU:HD21	3:M:733:ARG:NH1	2.31	0.44
3:M:919:ILE:HG22	3:M:923:ARG:HD2	1.99	0.44
1:D:561:GLN:CG	1:D:763:ALA:HA	2.48	0.44
3:E:223:ASN:O	3:E:291:MET:HG2	2.17	0.44
3:E:378:ILE:HD13	3:E:385:PHE:CZ	2.51	0.44
3:E:557:VAL:CG1	3:E:582:LEU:HD11	2.44	0.44
3:E:908:LEU:C	3:E:910:ASN:H	2.21	0.44
1:G:599:PHE:HD2	2:K:51:LEU:HD22	1.82	0.44
2:J:40:LEU:HD22	2:J:73:ASP:HB2	1.99	0.44
2:K:85:LYS:HA	2:K:88:PHE:CE2	2.52	0.44
3:L:147:LEU:CD1	3:L:914:ARG:NH1	2.77	0.44
3:L:223:ASN:O	3:L:291:MET:HG2	2.17	0.44
3:L:756:VAL:O	3:L:786:PRO:HA	2.17	0.44
3:M:163:ILE:HD13	3:M:634:PRO:HG3	1.99	0.44
1:A:722:ARG:NH1	6:B:1190:GNP:N3B	2.57	0.44
2:B:134:ILE:CG1	2:B:172:SER:HB2	2.47	0.44
1:D:46:LEU:HG	1:D:47:ASN:N	2.33	0.44
1:D:599:PHE:HD2	2:J:51:LEU:HD22	1.82	0.44
3:E:668:LEU:HD21	3:E:733:ARG:NH1	2.31	0.44
1:G:138:ASP:HA	1:G:141:LYS:HD2	1.99	0.44
1:G:653:ILE:HG13	1:G:670:ILE:HD13	2.00	0.44
2:J:97:LEU:HD12	2:J:97:LEU:N	2.31	0.44
3:L:163:ILE:HD13	3:L:634:PRO:HG3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:170:VAL:HG12	3:L:170:VAL:O	2.16	0.44
3:M:750:LYS:HE3	3:M:805:GLY:CA	2.46	0.44
1:A:15:THR:HG22	1:A:528:ALA:HA	1.99	0.44
1:A:653:ILE:HG13	1:A:670:ILE:HD13	1.99	0.44
2:B:155:THR:OG1	2:B:156:GLY:N	2.50	0.44
1:D:15:THR:HG22	1:D:528:ALA:HA	1.99	0.44
1:D:69:CYS:SG	1:D:81:PRO:HD3	2.58	0.44
3:E:147:LEU:O	3:E:149:PRO:N	2.50	0.44
3:E:309:LEU:C	3:E:309:LEU:HD12	2.38	0.44
3:E:419:ILE:HG22	3:E:421:ASN:H	1.82	0.44
2:K:40:LEU:HD22	2:K:73:ASP:HB2	1.99	0.44
3:L:133:ARG:HH21	3:L:135:MET:HE2	1.81	0.44
3:L:242:VAL:CG1	3:L:251:TRP:HB2	2.48	0.44
3:M:223:ASN:O	3:M:291:MET:HG2	2.17	0.44
3:M:419:ILE:HG22	3:M:421:ASN:H	1.82	0.44
4:O:68:GLN:O	4:O:72:GLN:HG3	2.18	0.44
1:A:111:GLU:HB2	1:A:503:ARG:HD3	1.99	0.44
1:A:550:ARG:O	1:A:554:ARG:HG3	2.18	0.44
1:A:588:TYR:O	1:A:591:ARG:HG2	2.18	0.44
3:E:242:VAL:CG1	3:E:251:TRP:HB2	2.48	0.44
1:G:69:CYS:SG	1:G:81:PRO:HD3	2.57	0.44
1:G:550:ARG:O	1:G:554:ARG:HG3	2.18	0.44
3:L:424:LEU:O	3:L:428:LEU:HB2	2.17	0.44
3:M:167:ARG:HA	3:M:167:ARG:HD3	1.81	0.44
1:A:66:ASN:ND2	1:A:68:TYR:H	2.16	0.44
2:B:85:LYS:HA	2:B:88:PHE:CE2	2.52	0.44
1:D:550:ARG:O	1:D:554:ARG:HG3	2.18	0.44
4:F:68:GLN:O	4:F:72:GLN:HG3	2.17	0.44
1:G:66:ASN:ND2	1:G:68:TYR:H	2.16	0.44
2:J:125:VAL:HA	2:J:126:PRO:HD3	1.87	0.44
2:J:155:THR:HG21	2:J:165:PRO:HA	2.00	0.44
3:M:242:VAL:CG1	3:M:251:TRP:HB2	2.48	0.44
3:M:309:LEU:C	3:M:309:LEU:HD12	2.38	0.44
1:A:69:CYS:SG	1:A:81:PRO:HD3	2.57	0.44
1:D:138:ASP:HA	1:D:141:LYS:HD2	1.99	0.44
3:E:292:ALA:HA	3:E:293:PRO:HD3	1.83	0.44
1:G:464:ASN:ND2	1:G:465:THR:H	2.15	0.44
1:G:561:GLN:CG	1:G:763:ALA:HA	2.48	0.44
2:J:110:ARG:HG3	2:J:110:ARG:HH11	1.82	0.44
2:J:134:ILE:CG1	2:J:172:SER:HB2	2.47	0.44
2:K:134:ILE:CG1	2:K:172:SER:HB2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:506:TYR:CE2	3:M:508:ASP:HB2	2.52	0.44
3:M:668:LEU:O	3:M:671:ALA:HB3	2.18	0.44
1:A:561:GLN:CG	1:A:763:ALA:HA	2.48	0.44
1:D:66:ASN:ND2	1:D:68:TYR:H	2.16	0.44
3:E:764:ASP:O	3:E:851:ARG:NH2	2.51	0.44
3:E:783:LEU:HA	3:E:784:PRO:HD3	1.81	0.44
1:G:588:TYR:O	1:G:591:ARG:HG2	2.18	0.44
3:L:168:MET:HG2	3:L:241:PHE:CE1	2.53	0.44
1:G:187:GLU:HB2	1:G:296:PRO:HG3	1.99	0.43
2:J:37:THR:HG22	2:J:51:LEU:HD13	1.99	0.43
2:J:155:THR:OG1	2:J:156:GLY:N	2.50	0.43
3:L:253:CYS:SG	3:L:255:PHE:HB2	2.58	0.43
3:L:300:GLN:O	3:L:301:PRO:C	2.56	0.43
3:L:361:LEU:HD23	3:L:399:CYS:SG	2.58	0.43
3:L:668:LEU:O	3:L:671:ALA:HB3	2.18	0.43
3:M:344:ARG:HA	3:M:394:VAL:O	2.18	0.43
3:M:571:PHE:HD2	3:M:596:PHE:CE1	2.36	0.43
3:M:717:LEU:HA	3:M:717:LEU:HD12	1.83	0.43
4:N:62:LEU:HA	4:N:66:GLN:OE1	2.17	0.43
1:A:46:LEU:HG	1:A:47:ASN:N	2.32	0.43
1:D:653:ILE:HG13	1:D:670:ILE:HD13	2.00	0.43
3:E:250:ARG:HD2	3:E:260:ASN:O	2.18	0.43
3:L:764:ASP:O	3:L:851:ARG:NH2	2.51	0.43
3:L:808:LEU:O	3:L:872:TYR:N	2.48	0.43
3:M:147:LEU:O	3:M:149:PRO:N	2.50	0.43
3:M:808:LEU:O	3:M:872:TYR:N	2.48	0.43
3:M:872:TYR:CE2	3:M:897:TRP:CZ3	3.06	0.43
2:B:32:ASP:HA	6:B:1190:GNP:O3G	2.18	0.43
1:D:281:PRO:HB3	1:D:400:PHE:HB3	2.00	0.43
3:E:150:PRO:O	3:E:151:ILE:HB	2.18	0.43
3:E:163:ILE:HD13	3:E:634:PRO:HG3	2.00	0.43
3:E:919:ILE:HG22	3:E:923:ARG:HD2	1.99	0.43
3:L:302:PRO:HA	3:L:303:PRO:HD3	1.73	0.43
3:L:872:TYR:CE2	3:L:897:TRP:CZ3	3.06	0.43
1:A:114:THR:CG2	1:A:115:ASN:N	2.76	0.43
1:A:599:PHE:HD2	2:B:51:LEU:HD22	1.82	0.43
3:E:253:CYS:SG	3:E:255:PHE:HB2	2.58	0.43
3:L:147:LEU:HD23	3:L:147:LEU:HA	1.74	0.43
3:L:419:ILE:HG22	3:L:421:ASN:H	1.82	0.43
3:M:253:CYS:SG	3:M:255:PHE:HB2	2.58	0.43
1:A:281:PRO:HB3	1:A:400:PHE:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:512:LEU:HA	1:A:513:PRO:HD3	1.79	0.43
2:B:37:THR:HG22	2:B:51:LEU:HD13	1.99	0.43
1:D:90:PRO:HA	1:D:91:PRO:HD3	1.86	0.43
3:E:668:LEU:O	3:E:671:ALA:HB3	2.18	0.43
1:G:15:THR:HG23	1:G:531:LEU:HD12	2.00	0.43
2:K:155:THR:HG21	2:K:165:PRO:HA	2.00	0.43
3:L:571:PHE:HD2	3:L:596:PHE:CE1	2.36	0.43
1:A:101:MET:HE1	4:F:61:PHE:CZ	2.49	0.43
1:D:283:ARG:NE	1:D:344:ASP:OD2	2.51	0.43
3:E:301:PRO:HA	3:E:302:PRO:HD3	1.68	0.43
3:E:791:SER:H	3:E:905:ASP:CG	2.20	0.43
3:L:359:ILE:HD11	3:L:406:LEU:HD23	2.01	0.43
3:L:919:ILE:HG22	3:L:923:ARG:HD2	1.99	0.43
3:M:147:LEU:HD23	3:M:147:LEU:HA	1.74	0.43
1:A:15:THR:HG23	1:A:531:LEU:HD12	2.01	0.43
1:A:417:LEU:HD23	1:A:417:LEU:C	2.39	0.43
1:D:417:LEU:C	1:D:417:LEU:HD23	2.39	0.43
1:D:642:LEU:O	1:D:644:ASP:N	2.48	0.43
3:E:409:LYS:O	3:E:412:GLN:N	2.48	0.43
3:E:750:LYS:HE3	3:E:805:GLY:CA	2.46	0.43
1:G:111:GLU:HB2	1:G:503:ARG:HD3	1.99	0.43
3:M:217:ILE:H	3:M:217:ILE:HG13	1.64	0.43
3:M:557:VAL:CG1	3:M:582:LEU:HD11	2.44	0.43
1:A:677:GLY:O	1:A:679:GLN:N	2.52	0.43
2:B:181:GLU:H	2:B:181:GLU:CD	2.22	0.43
1:D:111:GLU:HB2	1:D:503:ARG:HD3	1.99	0.43
3:E:168:MET:HG2	3:E:241:PHE:CE1	2.53	0.43
3:E:253:CYS:O	3:E:257:ARG:HA	2.19	0.43
3:E:361:LEU:HD23	3:E:399:CYS:SG	2.58	0.43
1:G:283:ARG:NE	1:G:344:ASP:OD2	2.51	0.43
3:L:344:ARG:HA	3:L:394:VAL:O	2.18	0.43
3:M:154:LEU:HD21	3:M:709:MET:HE3	2.01	0.43
3:M:546:LYS:NZ	3:M:862:HIS:O	2.52	0.43
1:D:152:PRO:HA	1:D:153:PRO:HD3	1.93	0.43
1:D:677:GLY:O	1:D:679:GLN:N	2.52	0.43
1:G:15:THR:HG22	1:G:528:ALA:HA	1.99	0.43
1:G:360:GLN:HG2	1:G:364:SER:OG	2.19	0.43
1:G:642:LEU:O	1:G:644:ASP:N	2.48	0.43
1:G:677:GLY:O	1:G:679:GLN:N	2.52	0.43
3:L:250:ARG:HD2	3:L:260:ASN:O	2.18	0.43
3:L:908:LEU:C	3:L:910:ASN:H	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:168:MET:HG2	3:M:241:PHE:CE1	2.53	0.43
3:M:687:LYS:HZ1	3:M:925:SER:HA	1.84	0.43
3:E:144:LEU:HD22	3:E:918:GLN:HE22	1.84	0.43
3:E:344:ARG:HA	3:E:394:VAL:O	2.18	0.43
1:G:516:THR:HA	1:G:517:PRO:HD3	1.88	0.43
2:J:32:ASP:HA	6:J:1190:GNP:O3G	2.18	0.43
2:K:181:GLU:H	2:K:181:GLU:CD	2.22	0.43
3:M:361:LEU:HD23	3:M:399:CYS:SG	2.58	0.43
4:N:68:GLN:O	4:N:72:GLN:HG3	2.18	0.43
2:B:155:THR:HG21	2:B:165:PRO:HA	2.00	0.42
3:E:428:LEU:HD12	3:E:428:LEU:HA	1.89	0.42
3:E:546:LYS:NZ	3:E:862:HIS:O	2.52	0.42
1:G:281:PRO:HB3	1:G:400:PHE:HB3	2.00	0.42
2:K:32:ASP:HA	6:K:1190:GNP:O3G	2.18	0.42
3:L:144:LEU:HD22	3:L:918:GLN:HE22	1.84	0.42
3:M:209:PRO:CG	3:M:558:MET:CE	2.97	0.42
3:M:250:ARG:HD2	3:M:260:ASN:O	2.18	0.42
3:M:764:ASP:O	3:M:851:ARG:NH2	2.51	0.42
3:M:802:ILE:HB	3:M:809:PHE:HB2	2.01	0.42
1:A:20:PRO:HB3	1:A:25:ASP:HB2	2.02	0.42
2:B:142:GLU:CD	1:G:426:LYS:HZ3	2.22	0.42
1:D:15:THR:HG23	1:D:531:LEU:HD12	2.00	0.42
1:D:74:ARG:H	1:D:74:ARG:HG3	1.66	0.42
1:D:632:PHE:CE2	1:D:693:GLU:HG3	2.55	0.42
3:E:151:ILE:HD13	3:E:709:MET:HE1	2.01	0.42
2:K:147:SER:OG	2:K:152:LEU:HD21	2.19	0.42
3:L:224:GLU:HA	3:L:291:MET:CG	2.49	0.42
3:M:150:PRO:O	3:M:151:ILE:HB	2.18	0.42
3:M:553:CYS:O	3:M:587:THR:HA	2.19	0.42
1:A:63:SER:OG	1:A:82:ILE:HG13	2.20	0.42
1:D:66:ASN:HB2	1:D:67:PRO:CD	2.49	0.42
1:D:360:GLN:HG2	1:D:364:SER:OG	2.19	0.42
3:E:300:GLN:O	3:E:301:PRO:C	2.56	0.42
2:J:181:GLU:H	2:J:181:GLU:CD	2.22	0.42
3:M:224:GLU:HA	3:M:291:MET:CG	2.49	0.42
1:G:66:ASN:HB2	1:G:67:PRO:CD	2.49	0.42
1:G:417:LEU:C	1:G:417:LEU:HD23	2.39	0.42
3:L:209:PRO:CG	3:L:558:MET:CE	2.97	0.42
3:L:546:LYS:NZ	3:L:862:HIS:O	2.52	0.42
3:L:553:CYS:O	3:L:587:THR:HA	2.19	0.42
3:L:750:LYS:HE3	3:L:805:GLY:CA	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:ARG:NE	1:A:344:ASP:OD2	2.51	0.42
2:B:26:LEU:HB2	2:B:71:THR:HG22	2.02	0.42
1:D:66:ASN:ND2	1:D:68:TYR:HB2	2.35	0.42
1:D:512:LEU:HA	1:D:513:PRO:HD3	1.79	0.42
3:E:224:GLU:HA	3:E:291:MET:CG	2.49	0.42
1:G:632:PHE:CE2	1:G:693:GLU:HG3	2.55	0.42
1:G:661:PHE:CD1	1:G:661:PHE:C	2.93	0.42
3:L:150:PRO:O	3:L:151:ILE:HB	2.18	0.42
3:L:864:ASP:OD1	3:L:864:ASP:N	2.53	0.42
3:M:789:ALA:HB1	3:M:902:LEU:HA	2.01	0.42
1:A:360:GLN:HG2	1:A:364:SER:OG	2.19	0.42
1:D:53:PRO:HG3	1:D:112:TYR:CG	2.55	0.42
1:D:574:PHE:CD2	1:D:760:GLN:HG2	2.55	0.42
3:E:151:ILE:HD13	3:E:709:MET:CE	2.50	0.42
3:E:359:ILE:HD11	3:E:406:LEU:HD23	2.01	0.42
3:M:799:LEU:HD13	3:M:812:MET:CE	2.50	0.42
1:A:561:GLN:HG2	1:A:763:ALA:O	2.20	0.42
1:D:63:SER:OG	1:D:82:ILE:HG13	2.20	0.42
1:D:516:THR:HA	1:D:517:PRO:HD3	1.88	0.42
1:D:552:LEU:HD12	1:D:552:LEU:HA	1.91	0.42
3:E:219:PRO:HA	3:E:220:PRO:HD3	1.95	0.42
1:G:243:GLU:OE1	1:G:243:GLU:HA	2.20	0.42
3:L:151:ILE:HD13	3:L:709:MET:CE	2.50	0.42
3:L:386:LEU:HA	3:L:387:PRO:HD3	1.81	0.42
3:L:799:LEU:HD13	3:L:812:MET:CE	2.50	0.42
3:M:212:HIS:CD2	3:M:217:ILE:HB	2.55	0.42
2:B:147:SER:OG	2:B:152:LEU:HD21	2.19	0.42
1:D:181:VAL:N	3:L:377:ASP:O	2.40	0.42
1:D:411:ASP:HA	1:D:463:ALA:HB3	2.02	0.42
3:E:212:HIS:CD2	3:E:217:ILE:HB	2.55	0.42
3:E:789:ALA:HB1	3:E:902:LEU:HA	2.01	0.42
3:E:799:LEU:HD13	3:E:812:MET:CE	2.50	0.42
1:G:658:THR:O	1:G:659:PHE:HB3	2.20	0.42
3:L:212:HIS:CD2	3:L:217:ILE:HB	2.55	0.42
3:L:253:CYS:O	3:L:257:ARG:HA	2.19	0.42
3:M:302:PRO:HA	3:M:303:PRO:HD3	1.73	0.42
3:M:497:VAL:HG12	3:M:499:LEU:HD11	2.01	0.42
1:A:430:ASN:ND2	1:A:430:ASN:N	2.65	0.42
1:D:80:CYS:HA	1:D:81:PRO:HD3	1.86	0.42
1:D:243:GLU:OE1	1:D:243:GLU:HA	2.20	0.42
1:D:561:GLN:HG2	1:D:763:ALA:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:497:VAL:HG12	3:E:499:LEU:HD11	2.01	0.42
3:E:553:CYS:O	3:E:587:THR:HA	2.19	0.42
1:G:53:PRO:HG3	1:G:112:TYR:CG	2.55	0.42
1:G:411:ASP:HA	1:G:463:ALA:HB3	2.02	0.42
1:G:574:PHE:CD2	1:G:760:GLN:HG2	2.55	0.42
1:G:576:LEU:HG	1:G:580:PHE:HB3	2.02	0.42
3:L:242:VAL:CG1	3:L:243:THR:N	2.83	0.42
1:A:66:ASN:HB2	1:A:67:PRO:CD	2.49	0.42
3:E:333:LEU:HD12	3:E:400:ARG:NE	2.35	0.42
1:G:420:HIS:CE1	1:G:615:ARG:HB2	2.55	0.42
3:L:333:LEU:HD12	3:L:400:ARG:NE	2.35	0.42
3:L:789:ALA:HB1	3:L:902:LEU:HA	2.01	0.42
1:A:91:PRO:HB3	1:D:669:GLN:HE21	0.43	0.41
1:A:574:PHE:CD2	1:A:760:GLN:HG2	2.55	0.41
1:D:52:ASN:HA	1:D:53:PRO:HD3	1.87	0.41
1:D:114:THR:CG2	1:D:115:ASN:N	2.76	0.41
1:D:176:ILE:HD12	3:L:413:ILE:CG1	2.38	0.41
1:D:332:ILE:HG22	1:D:361:LEU:HD21	2.02	0.41
3:L:409:LYS:O	3:L:412:GLN:N	2.48	0.41
3:M:144:LEU:HD22	3:M:918:GLN:HE22	1.84	0.41
3:M:496:THR:OG1	3:M:587:THR:HG23	2.20	0.41
1:A:41:LYS:O	1:A:503:ARG:NH2	2.54	0.41
1:A:195:GLU:O	1:A:199:GLY:N	2.41	0.41
1:D:658:THR:O	1:D:659:PHE:HB3	2.20	0.41
1:G:63:SER:OG	1:G:82:ILE:HG13	2.20	0.41
1:G:83:CYS:O	1:G:84:ASN:HB2	2.20	0.41
2:K:26:LEU:HB2	2:K:71:THR:HG22	2.02	0.41
3:L:808:LEU:HD23	3:L:808:LEU:HA	1.88	0.41
3:M:242:VAL:CG1	3:M:243:THR:N	2.83	0.41
3:M:253:CYS:O	3:M:257:ARG:HA	2.19	0.41
3:M:362:ASP:CG	3:M:401:GLN:HB2	2.41	0.41
1:D:96:LEU:O	1:D:97:SER:HB3	2.21	0.41
1:D:420:HIS:CE1	1:D:615:ARG:HB2	2.55	0.41
1:D:569:ASP:O	1:D:571:PRO:HD3	2.20	0.41
1:D:632:PHE:CD1	1:D:632:PHE:N	2.88	0.41
3:E:362:ASP:CG	3:E:401:GLN:HB2	2.40	0.41
3:E:802:ILE:HB	3:E:809:PHE:HB2	2.01	0.41
1:G:42:GLU:HG3	1:G:452:PRO:HB3	2.02	0.41
1:G:96:LEU:O	1:G:97:SER:HB3	2.20	0.41
2:J:26:LEU:HB2	2:J:71:THR:HG22	2.02	0.41
2:J:147:SER:OG	2:J:152:LEU:HD21	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:163:ILE:HA	3:L:164:PRO:HD3	1.90	0.41
3:L:187:ASN:O	3:L:634:PRO:HD2	2.20	0.41
3:L:802:ILE:HB	3:L:809:PHE:HB2	2.01	0.41
1:A:70:VAL:HB	1:A:79:SER:OG	2.21	0.41
1:A:88:HIS:HE1	1:D:742:SER:CB	2.32	0.41
1:A:101:MET:CE	4:F:61:PHE:CE2	3.00	0.41
1:A:411:ASP:HA	1:A:463:ALA:HB3	2.02	0.41
1:A:420:HIS:CE1	1:A:615:ARG:HB2	2.55	0.41
1:A:632:PHE:CD1	1:A:632:PHE:N	2.88	0.41
1:A:632:PHE:CE2	1:A:693:GLU:HG3	2.55	0.41
1:D:83:CYS:O	1:D:84:ASN:HB2	2.20	0.41
3:E:209:PRO:CG	3:E:558:MET:CE	2.97	0.41
1:G:569:ASP:O	1:G:571:PRO:HD3	2.20	0.41
1:G:722:ARG:CZ	2:K:53:PRO:HG3	2.51	0.41
2:K:164:ARG:HG2	2:K:164:ARG:O	2.21	0.41
3:L:209:PRO:CG	3:L:558:MET:HE1	2.51	0.41
3:L:242:VAL:HG12	3:L:243:THR:N	2.34	0.41
3:L:535:ASN:O	3:L:536:ASP:C	2.59	0.41
3:M:729:PRO:HB2	3:M:732:HIS:CD2	2.52	0.41
1:A:67:PRO:HD3	1:A:104:GLU:O	2.21	0.41
1:A:164:ASN:HD22	1:A:165:VAL:N	2.19	0.41
1:A:658:THR:O	1:A:659:PHE:HB3	2.20	0.41
3:E:242:VAL:HG12	3:E:243:THR:N	2.34	0.41
3:E:496:THR:OG1	3:E:587:THR:HG23	2.20	0.41
3:L:277:ARG:C	3:L:279:ASP:N	2.74	0.41
3:M:187:ASN:O	3:M:634:PRO:HD2	2.20	0.41
3:M:781:ILE:HB	3:M:858:GLN:OE1	2.21	0.41
1:A:332:ILE:HG22	1:A:361:LEU:HD21	2.02	0.41
1:A:569:ASP:O	1:A:571:PRO:HD3	2.20	0.41
3:E:242:VAL:CG1	3:E:243:THR:N	2.83	0.41
3:E:920:MET:HE3	3:E:920:MET:CA	2.48	0.41
1:G:140:LEU:O	1:G:144:ILE:HG13	2.21	0.41
1:G:332:ILE:HG22	1:G:361:LEU:HD21	2.02	0.41
3:L:155:THR:O	3:L:155:THR:HG22	2.21	0.41
3:L:496:THR:OG1	3:L:587:THR:HG23	2.20	0.41
3:L:497:VAL:HG12	3:L:499:LEU:HD11	2.01	0.41
3:M:359:ILE:HD11	3:M:406:LEU:HD23	2.01	0.41
3:M:633:MET:HA	3:M:634:PRO:HD3	1.89	0.41
1:A:239:ASN:O	1:A:243:GLU:HB2	2.20	0.41
1:A:243:GLU:HA	1:A:243:GLU:OE1	2.20	0.41
1:A:569:ASP:C	1:A:571:PRO:HD3	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:20:PRO:HB3	1:D:25:ASP:HB2	2.02	0.41
1:D:42:GLU:HG3	1:D:452:PRO:HB3	2.02	0.41
1:D:164:ASN:HD22	1:D:165:VAL:N	2.19	0.41
1:D:643:LEU:HD12	1:D:728:LEU:HD23	2.03	0.41
1:D:661:PHE:CD1	1:D:661:PHE:C	2.93	0.41
3:E:151:ILE:HD13	3:E:151:ILE:HA	1.82	0.41
1:G:239:ASN:O	1:G:243:GLU:HB2	2.20	0.41
1:G:569:ASP:C	1:G:571:PRO:HD3	2.41	0.41
3:L:352:ASN:ND2	3:L:352:ASN:N	2.69	0.41
3:M:151:ILE:HD13	3:M:709:MET:CE	2.50	0.41
3:M:270:ASP:CB	3:M:273:ASP:HB3	2.50	0.41
1:D:41:LYS:O	1:D:503:ARG:NH2	2.54	0.41
1:D:176:ILE:HG13	3:L:413:ILE:HG12	2.02	0.41
1:D:702:LEU:O	1:D:703:VAL:C	2.59	0.41
3:E:133:ARG:HH21	3:E:135:MET:HE2	1.86	0.41
1:G:561:GLN:HG2	1:G:763:ALA:O	2.20	0.41
3:M:242:VAL:HG12	3:M:243:THR:N	2.34	0.41
3:M:820:LEU:C	3:M:822:PHE:N	2.74	0.41
1:A:53:PRO:HG3	1:A:112:TYR:CG	2.55	0.41
1:A:66:ASN:ND2	1:A:68:TYR:HB2	2.35	0.41
1:A:181:VAL:N	3:E:377:ASP:O	2.40	0.41
1:A:576:LEU:HG	1:A:580:PHE:HB3	2.02	0.41
1:D:70:VAL:HB	1:D:79:SER:OG	2.21	0.41
1:D:140:LEU:O	1:D:144:ILE:HG13	2.21	0.41
1:D:239:ASN:O	1:D:243:GLU:HB2	2.20	0.41
1:D:319:ALA:HB1	1:D:322:TYR:HB2	2.03	0.41
1:D:451:SER:C	1:D:453:TYR:N	2.75	0.41
1:D:569:ASP:C	1:D:571:PRO:HD3	2.41	0.41
3:E:187:ASN:O	3:E:634:PRO:HD2	2.20	0.41
3:E:207:ILE:HG22	3:E:209:PRO:HD3	2.03	0.41
3:E:277:ARG:C	3:E:279:ASP:N	2.74	0.41
3:E:820:LEU:C	3:E:822:PHE:N	2.74	0.41
1:G:66:ASN:ND2	1:G:68:TYR:HB2	2.35	0.41
1:G:70:VAL:HB	1:G:79:SER:OG	2.21	0.41
1:G:632:PHE:N	1:G:632:PHE:CD1	2.88	0.41
2:K:96:PHE:HB3	2:K:129:ILE:HD13	2.03	0.41
3:L:557:VAL:CG1	3:L:582:LEU:HD11	2.44	0.41
3:L:808:LEU:O	3:L:871:LEU:HA	2.21	0.41
3:M:217:ILE:C	3:M:219:PRO:HD3	2.41	0.41
3:M:219:PRO:HA	3:M:220:PRO:HD3	1.95	0.41
3:M:560:ALA:HA	3:M:612:GLN:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:809:PHE:HD2	3:M:898:ALA:HB2	1.86	0.41
3:M:864:ASP:OD1	3:M:864:ASP:N	2.53	0.41
1:A:80:CYS:HA	1:A:81:PRO:HD3	1.86	0.41
1:A:176:ILE:HG13	3:E:413:ILE:HG12	2.02	0.41
1:A:661:PHE:CD1	1:A:661:PHE:C	2.93	0.41
1:D:67:PRO:HD3	1:D:104:GLU:O	2.21	0.41
3:E:864:ASP:OD1	3:E:864:ASP:N	2.53	0.41
1:G:41:LYS:O	1:G:503:ARG:NH2	2.54	0.41
1:G:67:PRO:HD3	1:G:104:GLU:O	2.21	0.41
1:G:639:GLN:HA	1:G:640:PRO:HD3	1.90	0.41
3:L:197:LYS:HD2	3:L:197:LYS:HA	1.72	0.41
3:L:207:ILE:HG22	3:L:209:PRO:HD3	2.03	0.41
3:M:199:SER:O	3:M:200:LYS:HB2	2.21	0.41
3:M:307:CYS:HB2	3:M:435:ILE:HG21	2.03	0.41
3:M:333:LEU:HD12	3:M:400:ARG:NE	2.35	0.41
3:M:358:LYS:HA	3:M:391:SER:O	2.21	0.41
1:A:83:CYS:O	1:A:84:ASN:HB2	2.21	0.40
1:A:140:LEU:O	1:A:144:ILE:HG13	2.21	0.40
1:A:319:ALA:HB1	1:A:322:TYR:HB2	2.03	0.40
1:A:464:ASN:ND2	1:A:465:THR:N	2.69	0.40
3:E:312:VAL:CG1	3:E:414:PHE:CD1	3.03	0.40
1:G:20:PRO:HB3	1:G:25:ASP:HB2	2.02	0.40
1:G:164:ASN:HD22	1:G:165:VAL:N	2.19	0.40
1:G:171:LEU:HB3	1:G:237:LYS:HD3	2.03	0.40
3:L:270:ASP:CB	3:L:273:ASP:HB3	2.50	0.40
3:M:699:ALA:HB1	3:M:921:LYS:HZ2	1.86	0.40
1:A:639:GLN:HA	1:A:640:PRO:HD3	1.90	0.40
2:B:96:PHE:HB3	2:B:129:ILE:HD13	2.03	0.40
1:D:141:LYS:NZ	1:D:245:LEU:O	2.50	0.40
1:D:252:VAL:HA	1:D:253:PRO:HD2	1.92	0.40
3:E:154:LEU:CG	3:E:709:MET:HE2	2.48	0.40
3:E:585:PHE:HB3	3:E:587:THR:O	2.22	0.40
3:E:716:SER:HB2	3:E:752:ILE:HG22	2.04	0.40
3:L:699:ALA:HB1	3:L:921:LYS:HZ2	1.84	0.40
3:M:552:PHE:CD1	3:M:552:PHE:C	2.95	0.40
1:A:96:LEU:O	1:A:97:SER:HB3	2.21	0.40
1:A:602:SER:OG	1:A:605:GLU:HB2	2.22	0.40
1:A:643:LEU:HD12	1:A:728:LEU:HD23	2.03	0.40
1:A:722:ARG:CZ	2:B:53:PRO:HG3	2.51	0.40
1:D:722:ARG:CZ	2:J:53:PRO:HG3	2.51	0.40
3:E:141:ILE:HD12	3:E:146:GLU:HG3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:352:ASN:ND2	3:E:352:ASN:N	2.69	0.40
1:G:319:ALA:HB1	1:G:322:TYR:HB2	2.03	0.40
3:L:781:ILE:HB	3:L:858:GLN:OE1	2.21	0.40
1:A:19:PHE:HA	1:A:20:PRO:HD3	1.94	0.40
1:A:451:SER:C	1:A:453:TYR:N	2.75	0.40
1:A:642:LEU:O	1:A:644:ASP:N	2.48	0.40
1:D:171:LEU:HB3	1:D:237:LYS:HD3	2.03	0.40
1:G:464:ASN:ND2	1:G:465:THR:N	2.69	0.40
3:L:199:SER:O	3:L:200:LYS:HB2	2.21	0.40
3:L:362:ASP:CG	3:L:401:GLN:HB2	2.41	0.40
3:M:703:LEU:HD12	3:M:703:LEU:HA	1.96	0.40
3:M:808:LEU:O	3:M:871:LEU:HA	2.21	0.40
1:A:702:LEU:O	1:A:703:VAL:C	2.59	0.40
1:D:576:LEU:HG	1:D:580:PHE:HB3	2.02	0.40
3:E:552:PHE:C	3:E:552:PHE:CD1	2.95	0.40
1:G:12:VAL:HG11	1:G:14:PHE:CE1	2.57	0.40
1:G:451:SER:C	1:G:453:TYR:N	2.74	0.40
1:G:643:LEU:HD12	1:G:728:LEU:HD23	2.03	0.40
3:L:139:TYR:N	3:L:139:TYR:CD1	2.90	0.40
3:L:552:PHE:CD1	3:L:552:PHE:C	2.95	0.40
3:M:139:TYR:CD1	3:M:139:TYR:N	2.90	0.40
3:M:155:THR:O	3:M:155:THR:HG22	2.21	0.40
3:M:417:ASN:OD1	3:M:419:ILE:HB	2.22	0.40
3:M:808:LEU:HD23	3:M:808:LEU:HA	1.89	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	727/768 (95%)	687 (94%)	35 (5%)	5 (1%)	22 63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	727/768 (95%)	688 (95%)	34 (5%)	5 (1%)	22 63
1	G	727/768 (95%)	688 (95%)	34 (5%)	5 (1%)	22 63
2	B	160/190 (84%)	142 (89%)	13 (8%)	5 (3%)	4 27
2	J	160/190 (84%)	142 (89%)	13 (8%)	5 (3%)	4 27
2	K	160/190 (84%)	142 (89%)	13 (8%)	5 (3%)	4 27
3	E	723/926 (78%)	640 (88%)	55 (8%)	28 (4%)	3 23
3	L	723/926 (78%)	641 (89%)	54 (8%)	28 (4%)	3 23
3	M	723/926 (78%)	641 (89%)	54 (8%)	28 (4%)	3 23
4	F	11/926 (1%)	10 (91%)	1 (9%)	0	100 100
4	N	11/926 (1%)	10 (91%)	1 (9%)	0	100 100
4	O	11/926 (1%)	10 (91%)	1 (9%)	0	100 100
All	All	4863/8430 (58%)	4441 (91%)	308 (6%)	114 (2%)	9 34

All (114) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	703	VAL
2	B	139	ALA
2	B	155	THR
1	D	703	VAL
3	E	147	LEU
3	E	148	PRO
3	E	151	ILE
3	E	601	ASP
3	E	762	MET
3	E	766	ALA
3	E	767	GLY
3	E	796	ARG
1	G	703	VAL
2	J	139	ALA
2	J	155	THR
2	K	139	ALA
2	K	155	THR
3	L	147	LEU
3	L	148	PRO
3	L	151	ILE
3	L	601	ASP
3	L	762	MET

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Mol	Chain	Res	Type
3	L	766	ALA
3	L	767	GLY
3	L	796	ARG
3	M	147	LEU
3	M	148	PRO
3	M	151	ILE
3	M	601	ASP
3	M	762	MET
3	M	766	ALA
3	M	767	GLY
3	M	796	ARG
1	A	678	TYR
1	D	678	TYR
3	E	278	TYR
3	E	313	SER
3	E	415	GLN
3	E	469	SER
3	E	580	SER
3	E	697	GLY
3	E	867	THR
3	E	903	VAL
1	G	678	TYR
3	L	278	TYR
3	L	313	SER
3	L	415	GLN
3	L	469	SER
3	L	580	SER
3	L	697	GLY
3	L	867	THR
3	L	903	VAL
3	M	278	TYR
3	M	313	SER
3	M	415	GLN
3	M	469	SER
3	M	580	SER
3	M	697	GLY
3	M	867	THR
3	M	903	VAL
1	A	73	PRO
1	A	97	SER
2	B	123	LYS
1	D	73	PRO

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Mol	Chain	Res	Type
1	D	97	SER
3	E	479	GLN
3	E	530	SER
3	E	620	ASN
3	E	724	ARG
3	E	793	LEU
1	G	73	PRO
1	G	97	SER
2	J	123	LYS
2	K	123	LYS
3	L	479	GLN
3	L	530	SER
3	L	620	ASN
3	L	724	ARG
3	L	793	LEU
3	M	479	GLN
3	M	530	SER
3	M	620	ASN
3	M	724	ARG
3	M	793	LEU
2	B	137	PRO
3	E	149	PRO
2	J	137	PRO
2	K	137	PRO
3	L	149	PRO
3	M	149	PRO
1	A	94	THR
1	D	94	THR
3	E	818	PRO
3	E	859	LEU
1	G	94	THR
3	L	818	PRO
3	L	859	LEU
3	M	818	PRO
3	M	859	LEU
2	B	138	ASN
3	E	146	GLU
3	E	215	ASP
3	E	271	PRO
3	E	763	ALA
2	J	138	ASN
2	K	138	ASN

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Mol	Chain	Res	Type
3	L	146	GLU
3	L	215	ASP
3	L	271	PRO
3	L	763	ALA
3	M	146	GLU
3	M	215	ASP
3	M	271	PRO
3	M	763	ALA

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	644/668 (96%)	616 (96%)	28 (4%)	29	53
1	D	644/668 (96%)	616 (96%)	28 (4%)	29	53
1	G	644/668 (96%)	616 (96%)	28 (4%)	29	53
2	B	138/159 (87%)	136 (99%)	2 (1%)	67	80
2	J	138/159 (87%)	136 (99%)	2 (1%)	67	80
2	K	138/159 (87%)	136 (99%)	2 (1%)	67	80
3	E	660/819 (81%)	640 (97%)	20 (3%)	41	63
3	L	660/819 (81%)	640 (97%)	20 (3%)	41	63
3	M	660/819 (81%)	640 (97%)	20 (3%)	41	63
4	F	12/817 (2%)	12 (100%)	0	100	100
4	N	13/817 (2%)	13 (100%)	0	100	100
4	O	13/817 (2%)	13 (100%)	0	100	100
All	All	4364/7389 (59%)	4214 (97%)	150 (3%)	40	60

All (150) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	125	PHE

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Mol	Chain	Res	Type
1	A	132	SER
1	A	136	ASN
1	A	164	ASN
1	A	166	VAL
1	A	243	GLU
1	A	245	LEU
1	A	250	TRP
1	A	252	VAL
1	A	309	ARG
1	A	411	ASP
1	A	430	ASN
1	A	450	LEU
1	A	503	ARG
1	A	534	ARG
1	A	544	ASP
1	A	552	LEU
1	A	592	ARG
1	A	601	ASN
1	A	635	GLU
1	A	651	ASN
1	A	679	GLN
1	A	697	GLU
1	A	700	GLU
1	A	708	LEU
1	A	749	ASP
1	A	765	SER
2	B	107	ASP
2	B	164	ARG
1	D	5	THR
1	D	125	PHE
1	D	132	SER
1	D	136	ASN
1	D	164	ASN
1	D	166	VAL
1	D	243	GLU
1	D	245	LEU
1	D	250	TRP
1	D	252	VAL
1	D	309	ARG
1	D	411	ASP
1	D	430	ASN
1	D	450	LEU

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Mol	Chain	Res	Type
1	D	503	ARG
1	D	534	ARG
1	D	544	ASP
1	D	552	LEU
1	D	592	ARG
1	D	601	ASN
1	D	635	GLU
1	D	651	ASN
1	D	679	GLN
1	D	697	GLU
1	D	700	GLU
1	D	708	LEU
1	D	749	ASP
1	D	765	SER
3	E	138	LEU
3	E	150	PRO
3	E	152	THR
3	E	166	GLU
3	E	208	ARG
3	E	213	LEU
3	E	309	LEU
3	E	352	ASN
3	E	377	ASP
3	E	428	LEU
3	E	459	ARG
3	E	557	VAL
3	E	618	SER
3	E	739	ASN
3	E	743	LEU
3	E	751	ASN
3	E	761	ASP
3	E	764	ASP
3	E	822	PHE
3	E	870	SER
1	G	5	THR
1	G	125	PHE
1	G	132	SER
1	G	136	ASN
1	G	164	ASN
1	G	166	VAL
1	G	243	GLU
1	G	245	LEU

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Mol	Chain	Res	Type
1	G	250	TRP
1	G	252	VAL
1	G	309	ARG
1	G	411	ASP
1	G	430	ASN
1	G	450	LEU
1	G	503	ARG
1	G	534	ARG
1	G	544	ASP
1	G	552	LEU
1	G	592	ARG
1	G	601	ASN
1	G	635	GLU
1	G	651	ASN
1	G	679	GLN
1	G	697	GLU
1	G	700	GLU
1	G	708	LEU
1	G	749	ASP
1	G	765	SER
2	J	107	ASP
2	J	164	ARG
2	K	107	ASP
2	K	164	ARG
3	L	138	LEU
3	L	150	PRO
3	L	152	THR
3	L	166	GLU
3	L	208	ARG
3	L	213	LEU
3	L	309	LEU
3	L	352	ASN
3	L	377	ASP
3	L	428	LEU
3	L	459	ARG
3	L	557	VAL
3	L	618	SER
3	L	739	ASN
3	L	743	LEU
3	L	751	ASN
3	L	761	ASP
3	L	764	ASP

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Mol	Chain	Res	Type
3	L	822	PHE
3	L	870	SER
3	M	138	LEU
3	M	150	PRO
3	M	152	THR
3	M	166	GLU
3	M	208	ARG
3	M	213	LEU
3	M	309	LEU
3	M	352	ASN
3	M	377	ASP
3	M	428	LEU
3	M	459	ARG
3	M	557	VAL
3	M	618	SER
3	M	739	ASN
3	M	743	LEU
3	M	751	ASN
3	M	761	ASP
3	M	764	ASP
3	M	822	PHE
3	M	870	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (97) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	66	ASN
1	A	88	HIS
1	A	136	ASN
1	A	164	ASN
1	A	189	GLN
1	A	233	GLN
1	A	279	ASN
1	A	430	ASN
1	A	464	ASN
1	A	509	ASN
1	A	601	ASN
1	A	651	ASN
1	A	669	GLN
1	A	679	GLN
1	A	735	GLN

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Mol	Chain	Res	Type
1	A	760	GLN
2	B	23	HIS
2	B	66	ASN
1	D	47	ASN
1	D	66	ASN
1	D	136	ASN
1	D	164	ASN
1	D	189	GLN
1	D	233	GLN
1	D	279	ASN
1	D	430	ASN
1	D	464	ASN
1	D	509	ASN
1	D	601	ASN
1	D	651	ASN
1	D	669	GLN
1	D	679	GLN
1	D	735	GLN
1	D	760	GLN
3	E	352	ASN
3	E	372	GLN
3	E	374	ASN
3	E	421	ASN
3	E	479	GLN
3	E	485	ASN
3	E	524	HIS
3	E	533	ASN
3	E	535	ASN
3	E	599	ASN
3	E	732	HIS
3	E	857	ASN
3	E	918	GLN
4	F	72	GLN
1	G	47	ASN
1	G	66	ASN
1	G	136	ASN
1	G	164	ASN
1	G	189	GLN
1	G	233	GLN
1	G	279	ASN
1	G	430	ASN
1	G	464	ASN

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Mol	Chain	Res	Type
1	G	509	ASN
1	G	601	ASN
1	G	651	ASN
1	G	679	GLN
1	G	735	GLN
1	G	760	GLN
2	J	23	HIS
2	J	66	ASN
2	K	23	HIS
2	K	66	ASN
3	L	272	ASN
3	L	352	ASN
3	L	372	GLN
3	L	374	ASN
3	L	421	ASN
3	L	479	GLN
3	L	485	ASN
3	L	524	HIS
3	L	533	ASN
3	L	535	ASN
3	L	599	ASN
3	L	732	HIS
3	L	857	ASN
3	L	918	GLN
3	M	352	ASN
3	M	372	GLN
3	M	374	ASN
3	M	421	ASN
3	M	479	GLN
3	M	485	ASN
3	M	524	HIS
3	M	533	ASN
3	M	535	ASN
3	M	599	ASN
3	M	732	HIS
3	M	857	ASN
3	M	918	GLN
4	N	72	GLN
4	O	72	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 9 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
6	GNP	K	1190	7	29,34,34	1.85	7 (24%)	33,54,54	2.31	6 (18%)
6	GNP	J	1190	7	29,34,34	1.85	7 (24%)	33,54,54	2.31	6 (18%)
6	GNP	B	1190	7	29,34,34	1.85	7 (24%)	33,54,54	2.31	6 (18%)

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
6	GNP	K	1190	7	-	4/14/38/38	0/3/3/3
6	GNP	J	1190	7	-	4/14/38/38	0/3/3/3
6	GNP	B	1190	7	-	4/14/38/38	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1190	GNP	C6-N1	4.60	1.41	1.33
6	K	1190	GNP	C6-N1	4.59	1.41	1.33
6	J	1190	GNP	C6-N1	4.56	1.41	1.33
6	B	1190	GNP	PB-O2B	-4.16	1.45	1.56
6	J	1190	GNP	PB-O2B	-4.14	1.45	1.56
6	K	1190	GNP	PB-O2B	-4.13	1.45	1.56
6	K	1190	GNP	C5-C6	3.34	1.47	1.41
6	J	1190	GNP	C5-C6	3.33	1.47	1.41
6	B	1190	GNP	C5-C6	3.33	1.47	1.41
6	K	1190	GNP	PG-O2G	-3.27	1.48	1.56
6	B	1190	GNP	PG-O2G	-3.26	1.48	1.56
6	J	1190	GNP	PG-O2G	-3.26	1.48	1.56
6	J	1190	GNP	C2-N1	2.85	1.40	1.35
6	B	1190	GNP	C2-N1	2.80	1.40	1.35
6	K	1190	GNP	C2-N1	2.80	1.40	1.35
6	K	1190	GNP	C8-N7	-2.69	1.29	1.34
6	J	1190	GNP	C8-N7	-2.68	1.29	1.34
6	B	1190	GNP	C8-N7	-2.65	1.30	1.34
6	B	1190	GNP	PB-O3A	2.33	1.62	1.59
6	J	1190	GNP	PB-O3A	2.31	1.62	1.59
6	K	1190	GNP	PB-O3A	2.26	1.61	1.59

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	1190	GNP	C5-C6-N1	-8.39	111.95	123.43
6	K	1190	GNP	C5-C6-N1	-8.38	111.98	123.43
6	J	1190	GNP	C5-C6-N1	-8.36	111.99	123.43
6	B	1190	GNP	C2-N1-C6	6.19	125.77	115.93
6	K	1190	GNP	C2-N1-C6	6.18	125.75	115.93
6	J	1190	GNP	C2-N1-C6	6.18	125.74	115.93
6	K	1190	GNP	O3G-PG-O1G	-4.30	102.63	113.45
6	B	1190	GNP	O3G-PG-O1G	-4.30	102.65	113.45
6	J	1190	GNP	O3G-PG-O1G	-4.29	102.66	113.45
6	J	1190	GNP	N3-C2-N1	-3.84	122.10	127.22
6	B	1190	GNP	N3-C2-N1	-3.81	122.15	127.22
6	K	1190	GNP	N3-C2-N1	-3.80	122.15	127.22
6	J	1190	GNP	O1G-PG-N3B	2.63	115.64	111.77
6	B	1190	GNP	O1G-PG-N3B	2.60	115.59	111.77
6	K	1190	GNP	O1G-PG-N3B	2.59	115.58	111.77
6	B	1190	GNP	C4-C5-C6	-2.32	118.59	120.80
6	K	1190	GNP	C4-C5-C6	-2.32	118.59	120.80
6	J	1190	GNP	C4-C5-C6	-2.31	118.59	120.80

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	1190	GNP	PB-N3B-PG-O1G
6	B	1190	GNP	PG-N3B-PB-O1B
6	B	1190	GNP	PA-O3A-PB-O1B
6	J	1190	GNP	PB-N3B-PG-O1G
6	J	1190	GNP	PG-N3B-PB-O1B
6	J	1190	GNP	PA-O3A-PB-O1B
6	K	1190	GNP	PB-N3B-PG-O1G
6	K	1190	GNP	PG-N3B-PB-O1B
6	K	1190	GNP	PA-O3A-PB-O1B
6	B	1190	GNP	PG-N3B-PB-O3A
6	J	1190	GNP	PG-N3B-PB-O3A
6	K	1190	GNP	PG-N3B-PB-O3A

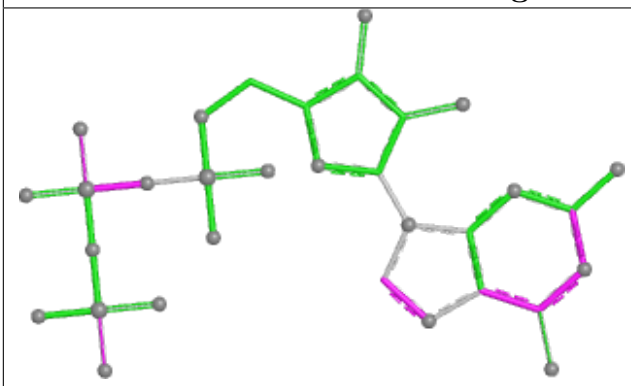
There are no ring outliers.

3 monomers are involved in 14 short contacts:

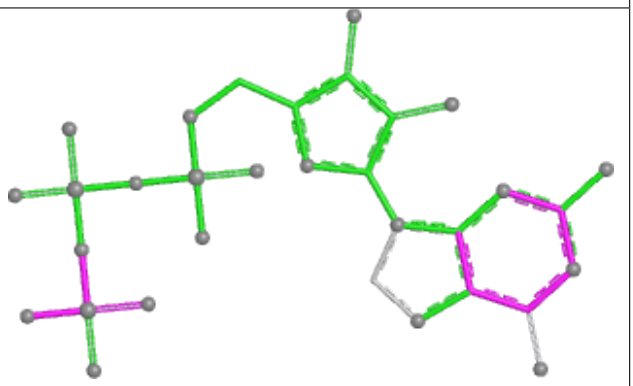
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	K	1190	GNP	5	0
6	J	1190	GNP	4	0
6	B	1190	GNP	5	0

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.

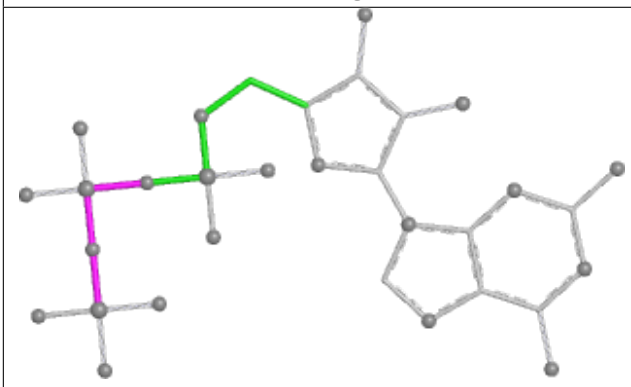
Ligand GNP K 1190



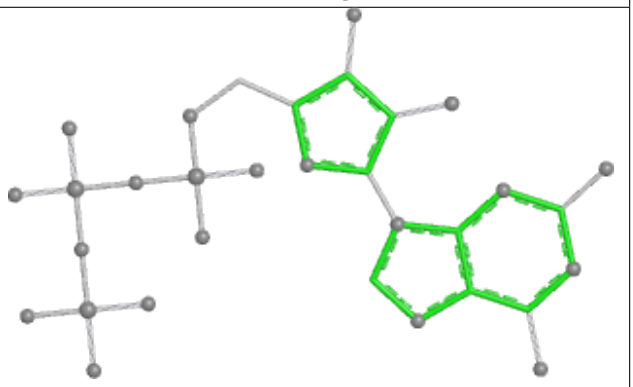
Bond lengths



Bond angles

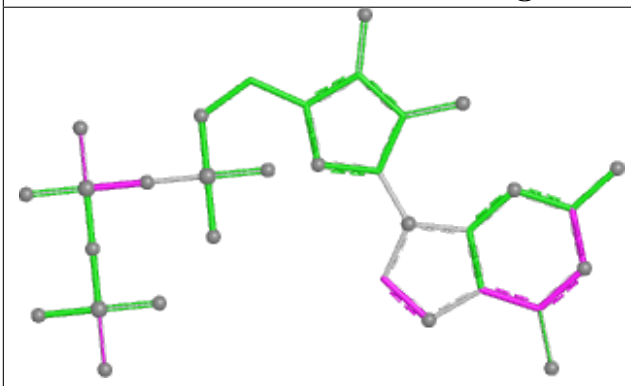


Torsions

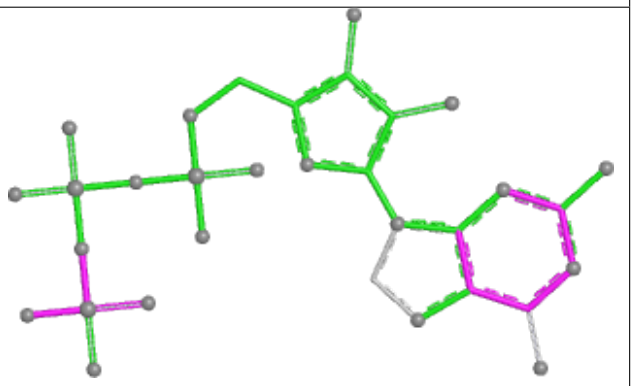


Rings

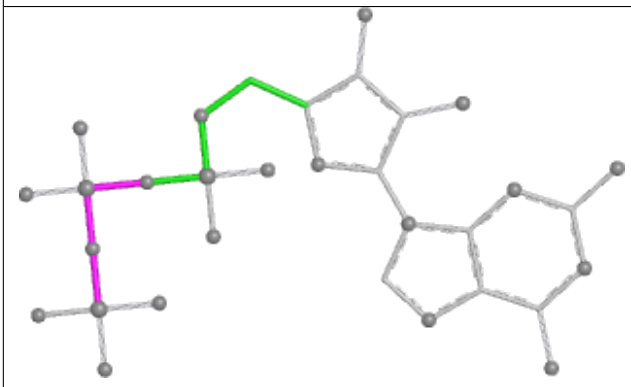
Ligand GNP J 1190



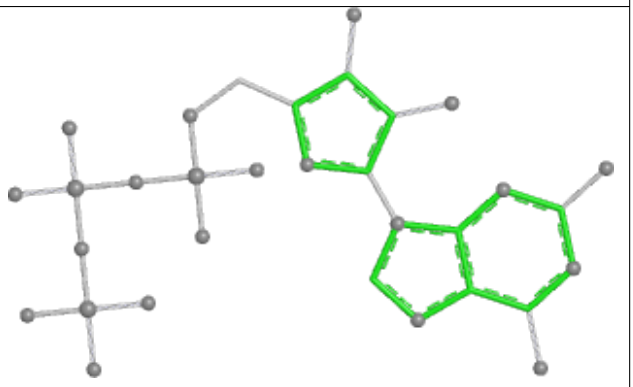
Bond lengths



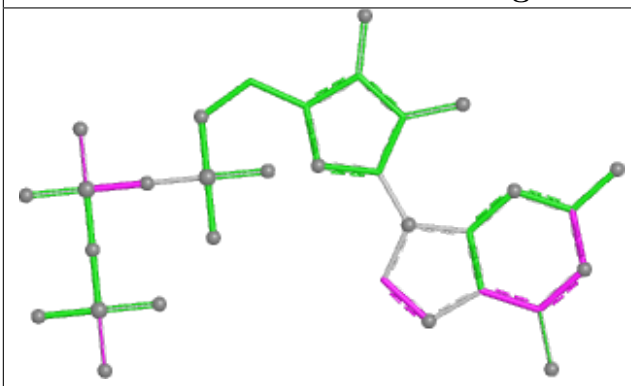
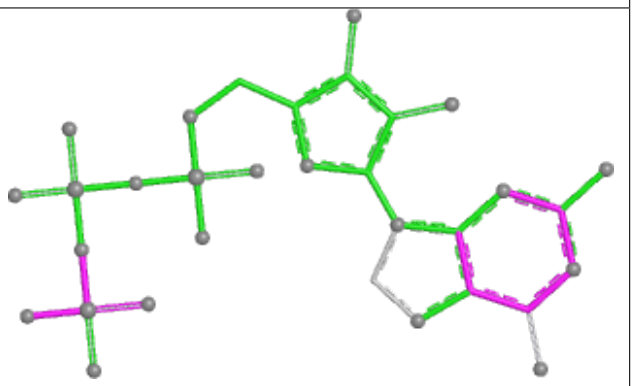
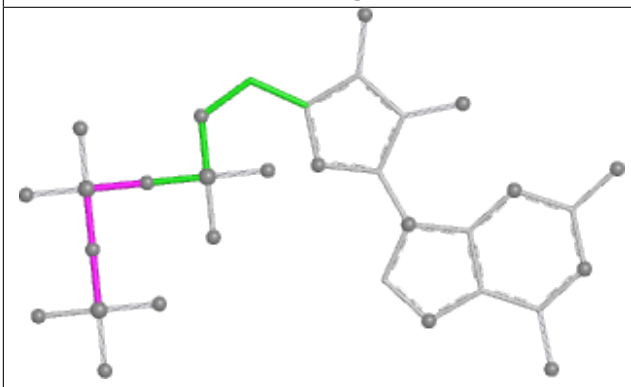
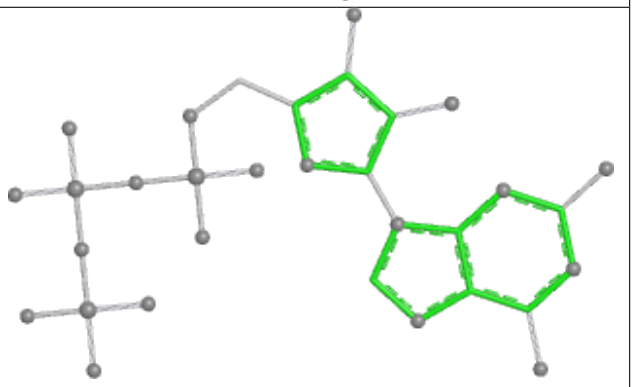
Bond angles



Torsions



Rings

Ligand GNP B 1190	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

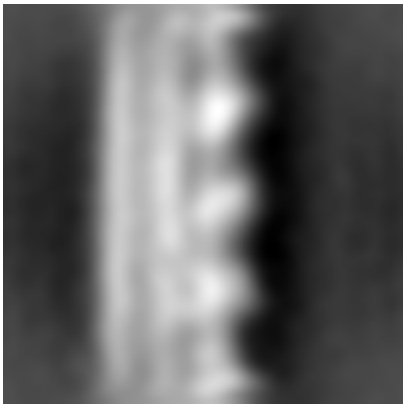
There are no chain breaks in this entry.

6 Tomogram visualisation

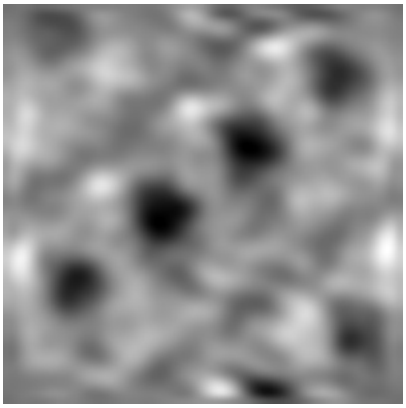
This section contains visualisations of the EMDB entry EMD-2428. These allow visual inspection of the internal detail of the tomogram and identification of artifacts.

6.1 Orthogonal projections

X



Y

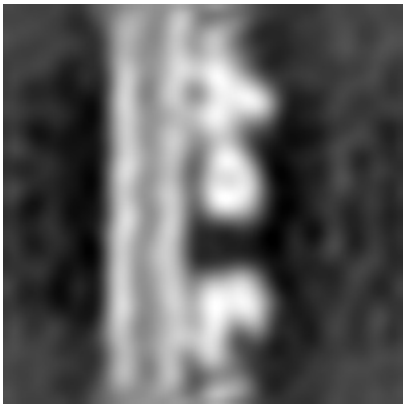


Z

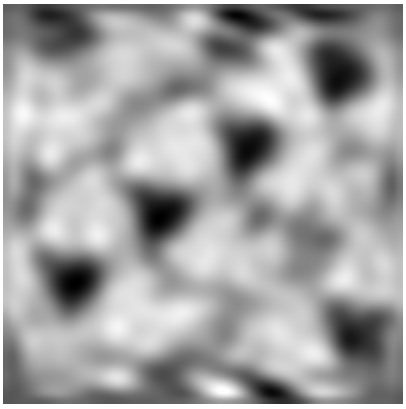
The images above show the tomogram projected in three orthogonal directions.

6.2 Central slices

X Index: 32



Y Index: 32



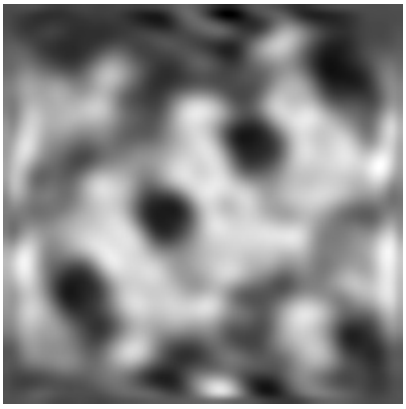
Z Index: 32

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

6.3 Largest variance slices (i)

X Index: 32

Y Index: 26



Z Index: 36

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

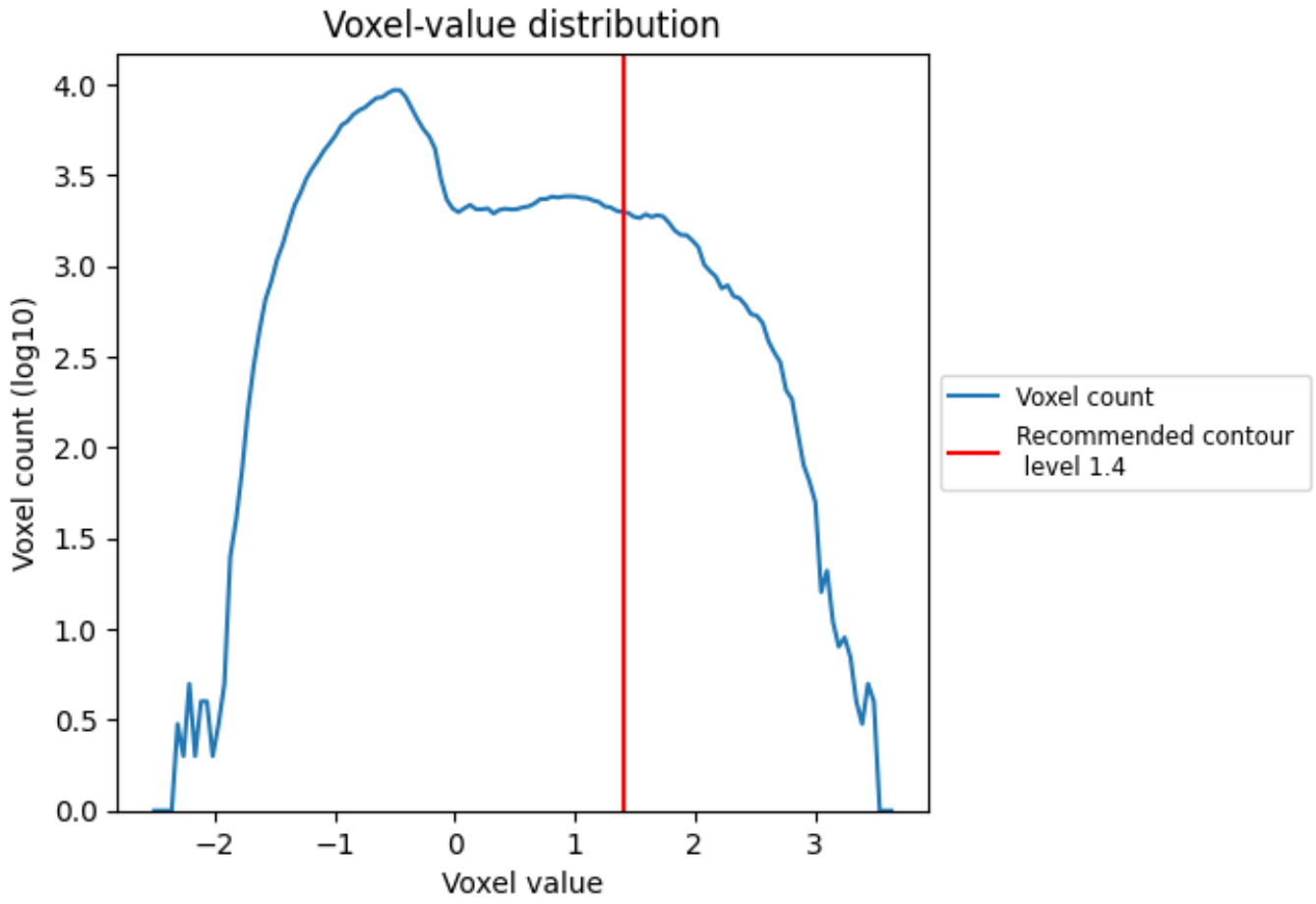
6.4 Mask visualisation (i)

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

7 Tomogram analysis (i)

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

7.1 Voxel-value distribution (i)



The voxel-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic.

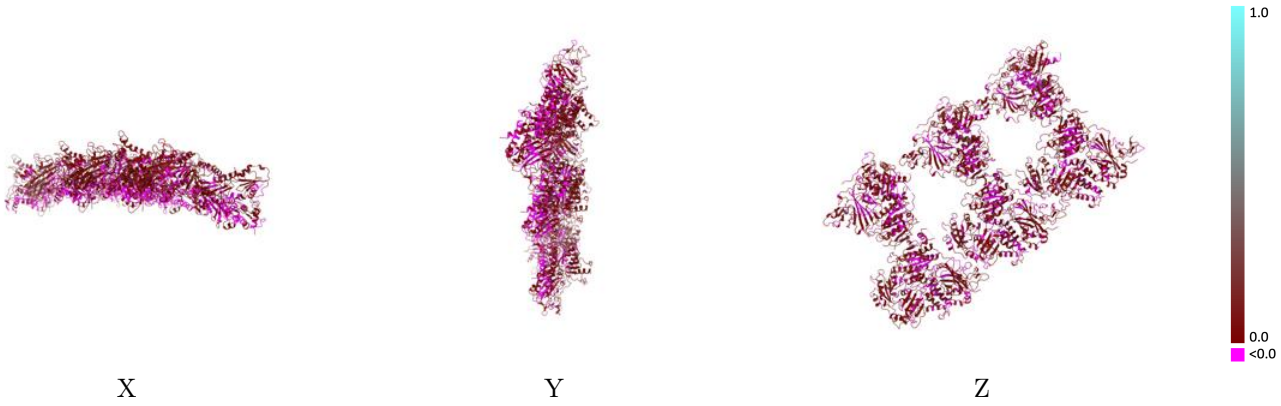
8 Map-model fit

This section contains information regarding the fit between EMDB map EMD-2428 and PDB model 4BZI. Per-residue inclusion information can be found in section 3 on page 7.

8.1 Map-model overlay

This section was not generated.

8.2 Q-score mapped to coordinate model

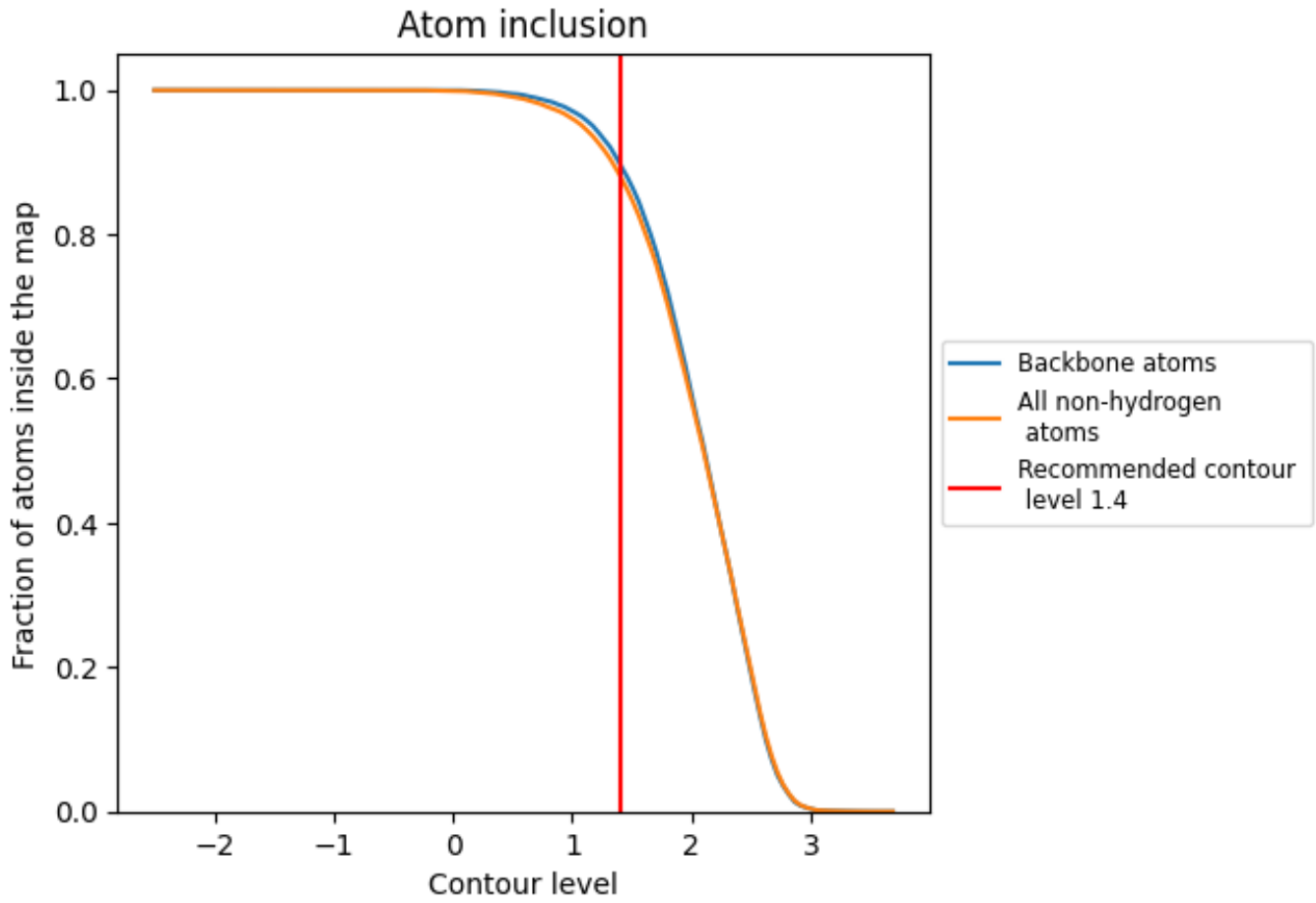


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

8.3 Atom inclusion mapped to coordinate model

This section was not generated.

8.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (1.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8813	0.0470
A	0.8973	0.0440
B	0.8908	0.0620
D	0.8796	0.0450
E	0.9118	0.0470
F	0.7156	0.0410
G	0.8641	0.0520
J	0.9000	0.0480
K	0.8267	0.0500
L	0.8419	0.0410
M	0.9069	0.0450
N	0.9231	0.0770
O	0.6154	0.0390