



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 12:15 AM UTC

PDB ID : 8WYJ / pdb_00008wyj
EMDB ID : EMD-37930
Title : The global map of Omicron Subvariants Spike with two antibodies
Authors : Yan, R.H.; Wang, A.J.; Yang, H.N.
Deposited on : 2023-10-31
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

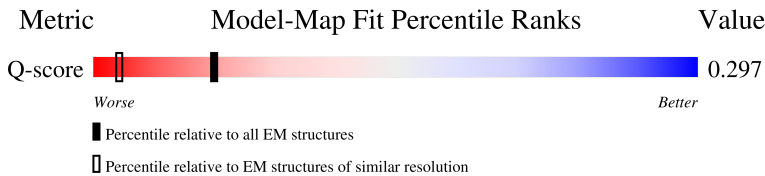
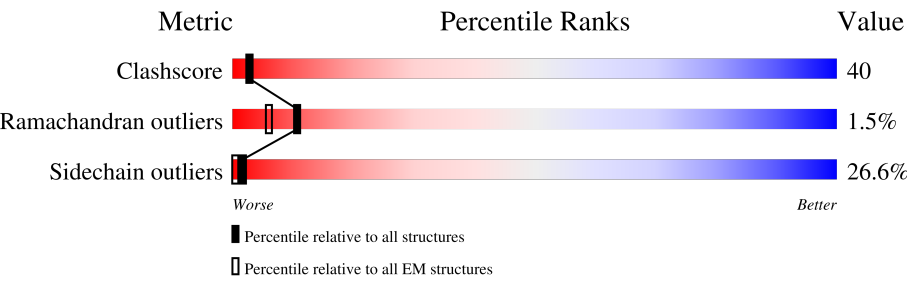
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

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

Mol	Chain	Length	Quality of chain
1	A	1123	6% 40% 39% 11% 8%
1	B	1123	41% 39% 11% 8%
1	C	1123	13% 41% 39% 11% 8%
2	E	127	24% 58% 17%

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Mol	Chain	Length	Quality of chain
2	I	127	
2	S	127	
3	G	106	
3	K	106	
3	T	106	
4	D	125	
4	H	125	
4	Q	125	
5	F	108	
5	J	108	
5	R	108	
6	M	6	
6	O	6	
6	V	6	
7	L	2	
7	N	2	
7	P	2	
7	U	2	
7	W	2	
7	X	2	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 35013 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1030	Total	C	N	O	S	0	0
			8083	5183	1342	1522	36		
1	B	1030	Total	C	N	O	S	0	0
			8083	5183	1342	1522	36		
1	C	1030	Total	C	N	O	S	0	0
			8083	5183	1342	1522	36		

There are 207 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	ILE	THR	conflict	UNP P0DTC2
A	24	THR	ARG	conflict	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	27	SER	ALA	conflict	UNP P0DTC2
A	50	LEU	SER	conflict	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	127	PHE	VAL	conflict	UNP P0DTC2
A	142	ASP	GLY	conflict	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	157	SER	PHE	conflict	UNP P0DTC2
A	158	GLY	ARG	conflict	UNP P0DTC2
A	?	-	ASN	deletion	UNP P0DTC2
A	211	ILE	LEU	conflict	UNP P0DTC2
A	212	GLY	VAL	conflict	UNP P0DTC2
A	215	PHE	LEU	conflict	UNP P0DTC2
A	245	ASN	HIS	conflict	UNP P0DTC2
A	264	ASP	ALA	conflict	UNP P0DTC2
A	332	VAL	ILE	conflict	UNP P0DTC2
A	339	HIS	GLY	conflict	UNP P0DTC2
A	356	THR	LYS	conflict	UNP P0DTC2
A	371	PHE	SER	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	373	PRO	SER	conflict	UNP P0DTC2
A	375	PHE	SER	conflict	UNP P0DTC2
A	376	ALA	THR	conflict	UNP P0DTC2
A	403	LYS	ARG	conflict	UNP P0DTC2
A	405	ASN	ASP	conflict	UNP P0DTC2
A	408	SER	ARG	conflict	UNP P0DTC2
A	417	ASN	LYS	conflict	UNP P0DTC2
A	440	LYS	ASN	conflict	UNP P0DTC2
A	445	HIS	VAL	conflict	UNP P0DTC2
A	446	SER	GLY	conflict	UNP P0DTC2
A	450	ASP	ASN	conflict	UNP P0DTC2
A	452	TRP	LEU	conflict	UNP P0DTC2
A	460	LYS	ASN	conflict	UNP P0DTC2
A	477	ASN	SER	conflict	UNP P0DTC2
A	478	LYS	THR	conflict	UNP P0DTC2
A	481	LYS	ASN	conflict	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	483	LYS	GLU	conflict	UNP P0DTC2
A	485	PRO	PHE	conflict	UNP P0DTC2
A	497	ARG	GLN	conflict	UNP P0DTC2
A	500	TYR	ASN	conflict	UNP P0DTC2
A	504	HIS	TYR	conflict	UNP P0DTC2
A	553	LYS	GLU	conflict	UNP P0DTC2
A	569	VAL	ALA	conflict	UNP P0DTC2
A	613	GLY	ASP	conflict	UNP P0DTC2
A	620	SER	PRO	conflict	UNP P0DTC2
A	654	TYR	HIS	conflict	UNP P0DTC2
A	669	VAL	ILE	conflict	UNP P0DTC2
A	679	LYS	ASN	conflict	UNP P0DTC2
A	681	ARG	PRO	conflict	UNP P0DTC2
A	682	GLY	ARG	conflict	UNP P0DTC2
A	683	SER	ARG	conflict	UNP P0DTC2
A	685	SER	ARG	conflict	UNP P0DTC2
A	764	LYS	ASN	conflict	UNP P0DTC2
A	796	TYR	ASP	conflict	UNP P0DTC2
A	817	PRO	PHE	conflict	UNP P0DTC2
A	892	PRO	ALA	conflict	UNP P0DTC2
A	899	PRO	ALA	conflict	UNP P0DTC2
A	939	PHE	SER	conflict	UNP P0DTC2
A	942	PRO	ALA	conflict	UNP P0DTC2
A	954	HIS	GLN	conflict	UNP P0DTC2
A	969	LYS	ASN	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	UNP P0DTC2
A	1143	LEU	PRO	conflict	UNP P0DTC2
B	22	ILE	THR	conflict	UNP P0DTC2
B	24	THR	ARG	conflict	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	27	SER	ALA	conflict	UNP P0DTC2
B	50	LEU	SER	conflict	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	127	PHE	VAL	conflict	UNP P0DTC2
B	142	ASP	GLY	conflict	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	157	SER	PHE	conflict	UNP P0DTC2
B	158	GLY	ARG	conflict	UNP P0DTC2
B	?	-	ASN	deletion	UNP P0DTC2
B	211	ILE	LEU	conflict	UNP P0DTC2
B	212	GLY	VAL	conflict	UNP P0DTC2
B	215	PHE	LEU	conflict	UNP P0DTC2
B	245	ASN	HIS	conflict	UNP P0DTC2
B	264	ASP	ALA	conflict	UNP P0DTC2
B	332	VAL	ILE	conflict	UNP P0DTC2
B	339	HIS	GLY	conflict	UNP P0DTC2
B	356	THR	LYS	conflict	UNP P0DTC2
B	371	PHE	SER	conflict	UNP P0DTC2
B	373	PRO	SER	conflict	UNP P0DTC2
B	375	PHE	SER	conflict	UNP P0DTC2
B	376	ALA	THR	conflict	UNP P0DTC2
B	403	LYS	ARG	conflict	UNP P0DTC2
B	405	ASN	ASP	conflict	UNP P0DTC2
B	408	SER	ARG	conflict	UNP P0DTC2
B	417	ASN	LYS	conflict	UNP P0DTC2
B	440	LYS	ASN	conflict	UNP P0DTC2
B	445	HIS	VAL	conflict	UNP P0DTC2
B	446	SER	GLY	conflict	UNP P0DTC2
B	450	ASP	ASN	conflict	UNP P0DTC2
B	452	TRP	LEU	conflict	UNP P0DTC2
B	460	LYS	ASN	conflict	UNP P0DTC2
B	477	ASN	SER	conflict	UNP P0DTC2
B	478	LYS	THR	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	481	LYS	ASN	conflict	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	483	LYS	GLU	conflict	UNP P0DTC2
B	485	PRO	PHE	conflict	UNP P0DTC2
B	497	ARG	GLN	conflict	UNP P0DTC2
B	500	TYR	ASN	conflict	UNP P0DTC2
B	504	HIS	TYR	conflict	UNP P0DTC2
B	553	LYS	GLU	conflict	UNP P0DTC2
B	569	VAL	ALA	conflict	UNP P0DTC2
B	613	GLY	ASP	conflict	UNP P0DTC2
B	620	SER	PRO	conflict	UNP P0DTC2
B	654	TYR	HIS	conflict	UNP P0DTC2
B	669	VAL	ILE	conflict	UNP P0DTC2
B	679	LYS	ASN	conflict	UNP P0DTC2
B	681	ARG	PRO	conflict	UNP P0DTC2
B	682	GLY	ARG	conflict	UNP P0DTC2
B	683	SER	ARG	conflict	UNP P0DTC2
B	685	SER	ARG	conflict	UNP P0DTC2
B	764	LYS	ASN	conflict	UNP P0DTC2
B	796	TYR	ASP	conflict	UNP P0DTC2
B	817	PRO	PHE	conflict	UNP P0DTC2
B	892	PRO	ALA	conflict	UNP P0DTC2
B	899	PRO	ALA	conflict	UNP P0DTC2
B	939	PHE	SER	conflict	UNP P0DTC2
B	942	PRO	ALA	conflict	UNP P0DTC2
B	954	HIS	GLN	conflict	UNP P0DTC2
B	969	LYS	ASN	conflict	UNP P0DTC2
B	986	PRO	LYS	conflict	UNP P0DTC2
B	987	PRO	VAL	conflict	UNP P0DTC2
B	1143	LEU	PRO	conflict	UNP P0DTC2
C	22	ILE	THR	conflict	UNP P0DTC2
C	24	THR	ARG	conflict	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	27	SER	ALA	conflict	UNP P0DTC2
C	50	LEU	SER	conflict	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	127	PHE	VAL	conflict	UNP P0DTC2
C	142	ASP	GLY	conflict	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	157	SER	PHE	conflict	UNP P0DTC2
C	158	GLY	ARG	conflict	UNP P0DTC2
C	?	-	ASN	deletion	UNP P0DTC2
C	211	ILE	LEU	conflict	UNP P0DTC2
C	212	GLY	VAL	conflict	UNP P0DTC2
C	215	PHE	LEU	conflict	UNP P0DTC2
C	245	ASN	HIS	conflict	UNP P0DTC2
C	264	ASP	ALA	conflict	UNP P0DTC2
C	332	VAL	ILE	conflict	UNP P0DTC2
C	339	HIS	GLY	conflict	UNP P0DTC2
C	356	THR	LYS	conflict	UNP P0DTC2
C	371	PHE	SER	conflict	UNP P0DTC2
C	373	PRO	SER	conflict	UNP P0DTC2
C	375	PHE	SER	conflict	UNP P0DTC2
C	376	ALA	THR	conflict	UNP P0DTC2
C	403	LYS	ARG	conflict	UNP P0DTC2
C	405	ASN	ASP	conflict	UNP P0DTC2
C	408	SER	ARG	conflict	UNP P0DTC2
C	417	ASN	LYS	conflict	UNP P0DTC2
C	440	LYS	ASN	conflict	UNP P0DTC2
C	445	HIS	VAL	conflict	UNP P0DTC2
C	446	SER	GLY	conflict	UNP P0DTC2
C	450	ASP	ASN	conflict	UNP P0DTC2
C	452	TRP	LEU	conflict	UNP P0DTC2
C	460	LYS	ASN	conflict	UNP P0DTC2
C	477	ASN	SER	conflict	UNP P0DTC2
C	478	LYS	THR	conflict	UNP P0DTC2
C	481	LYS	ASN	conflict	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	483	LYS	GLU	conflict	UNP P0DTC2
C	485	PRO	PHE	conflict	UNP P0DTC2
C	497	ARG	GLN	conflict	UNP P0DTC2
C	500	TYR	ASN	conflict	UNP P0DTC2
C	504	HIS	TYR	conflict	UNP P0DTC2
C	553	LYS	GLU	conflict	UNP P0DTC2
C	569	VAL	ALA	conflict	UNP P0DTC2
C	613	GLY	ASP	conflict	UNP P0DTC2
C	620	SER	PRO	conflict	UNP P0DTC2
C	654	TYR	HIS	conflict	UNP P0DTC2
C	669	VAL	ILE	conflict	UNP P0DTC2
C	679	LYS	ASN	conflict	UNP P0DTC2
C	681	ARG	PRO	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	682	GLY	ARG	conflict	UNP P0DTC2
C	683	SER	ARG	conflict	UNP P0DTC2
C	685	SER	ARG	conflict	UNP P0DTC2
C	764	LYS	ASN	conflict	UNP P0DTC2
C	796	TYR	ASP	conflict	UNP P0DTC2
C	817	PRO	PHE	conflict	UNP P0DTC2
C	892	PRO	ALA	conflict	UNP P0DTC2
C	899	PRO	ALA	conflict	UNP P0DTC2
C	939	PHE	SER	conflict	UNP P0DTC2
C	942	PRO	ALA	conflict	UNP P0DTC2
C	954	HIS	GLN	conflict	UNP P0DTC2
C	969	LYS	ASN	conflict	UNP P0DTC2
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	UNP P0DTC2
C	1143	LEU	PRO	conflict	UNP P0DTC2

- Molecule 2 is a protein called S309-HC.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	126	Total	C	N	O	S	0	0
			956	605	164	182	5		
2	I	126	Total	C	N	O	S	0	0
			956	605	164	182	5		
2	S	126	Total	C	N	O	S	0	0
			956	605	164	182	5		

- Molecule 3 is a protein called S309-KC.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	106	Total	C	N	O	S	0	0
			740	466	124	148	2		
3	K	106	Total	C	N	O	S	0	0
			740	466	124	148	2		
3	T	106	Total	C	N	O	S	0	0
			740	466	124	148	2		

- Molecule 4 is a protein called SA55-HC.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	123	Total	C	N	O	S	0	0
			930	588	157	180	5		

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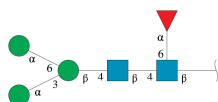
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Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	123	Total	C	N	O	S	0	0
			930	588	157	180	5		
4	Q	123	Total	C	N	O	S	0	0
			930	588	157	180	5		

- Molecule 5 is a protein called SA55_KC.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	108	Total	C	N	O	S	0	0
			835	524	136	172	3		
5	J	108	Total	C	N	O	S	0	0
			835	524	136	172	3		
5	R	108	Total	C	N	O	S	0	0
			835	524	136	172	3		

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
6	M	6	Total	C	N	O	0	0
			71	40	2	29		
6	O	6	Total	C	N	O	0	0
			71	40	2	29		
6	V	6	Total	C	N	O	0	0
			71	40	2	29		

- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
7	L	2	Total	C	N	O	0	0
			28	16	2	10		

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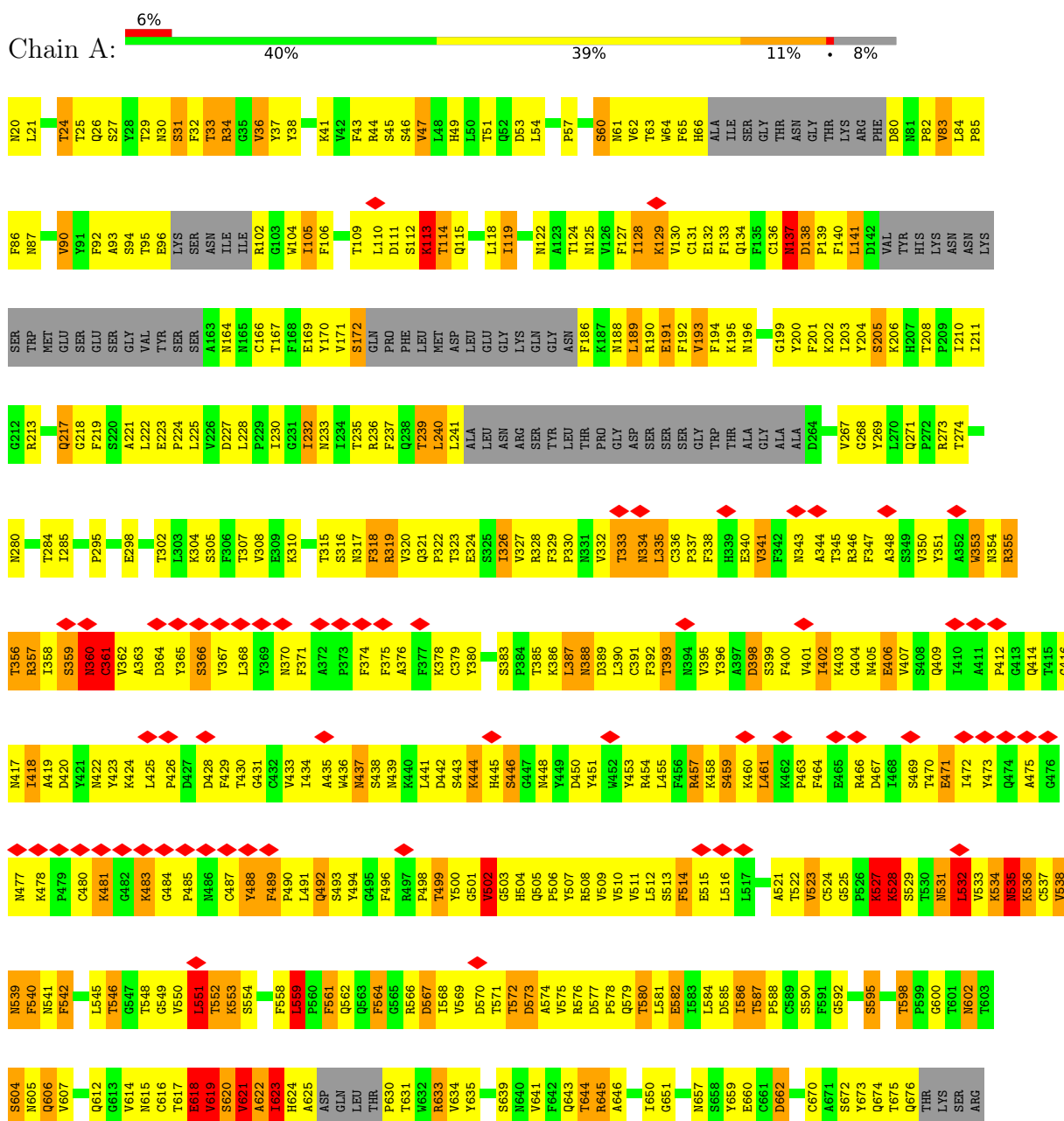
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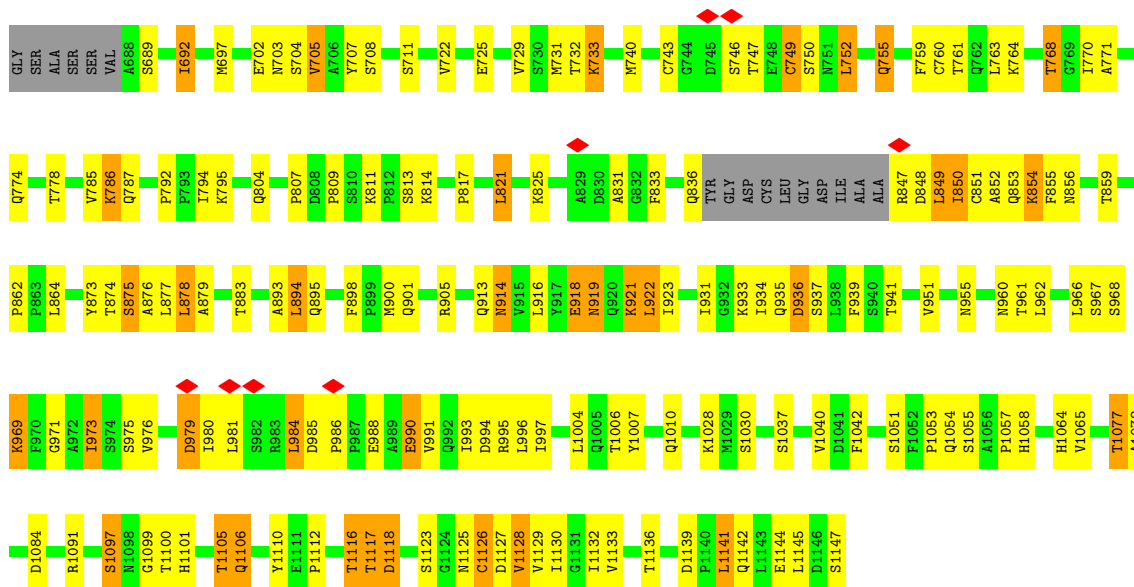
Mol	Chain	Residues	Atoms				AltConf	Trace
7	N	2	Total	C	N	O	0	0
			28	16	2	10		
7	P	2	Total	C	N	O	0	0
			28	16	2	10		
7	U	2	Total	C	N	O	0	0
			28	16	2	10		
7	W	2	Total	C	N	O	0	0
			28	16	2	10		
7	X	2	Total	C	N	O	0	0
			28	16	2	10		

3 Residue-property plots

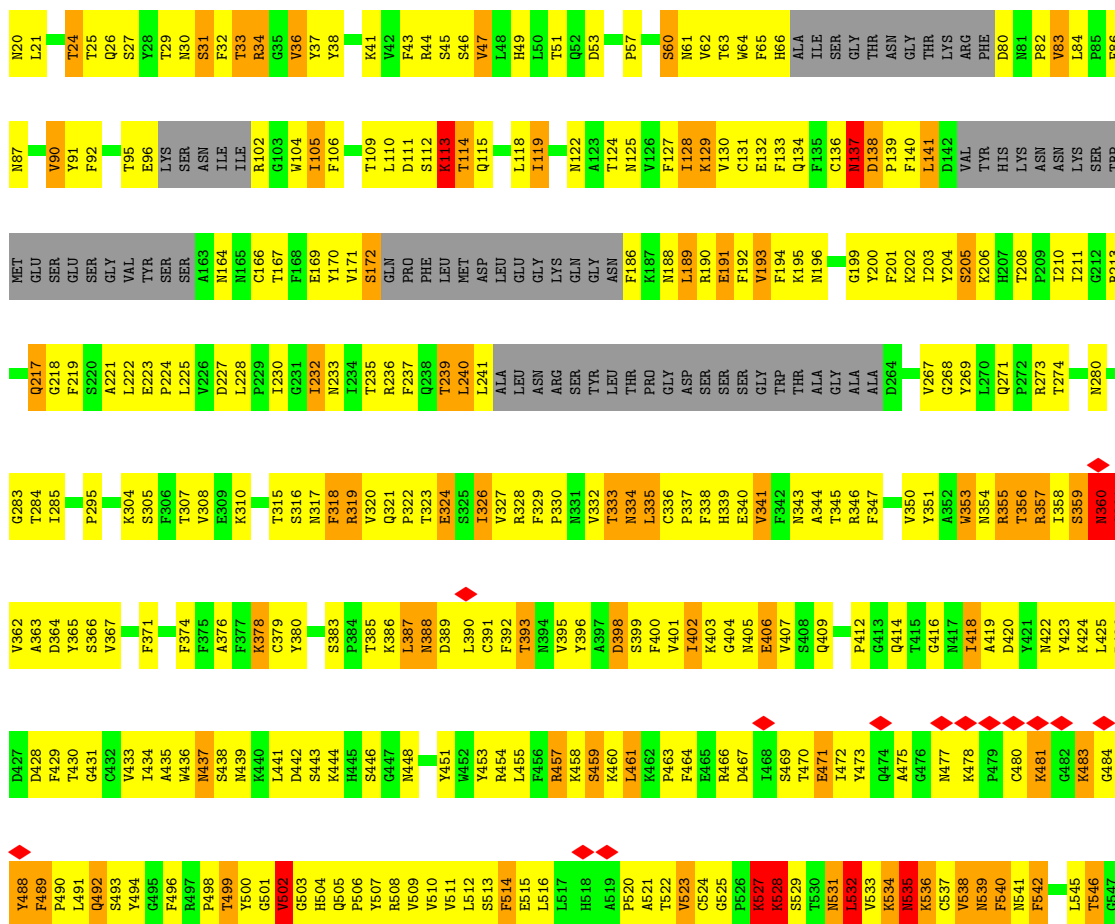
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

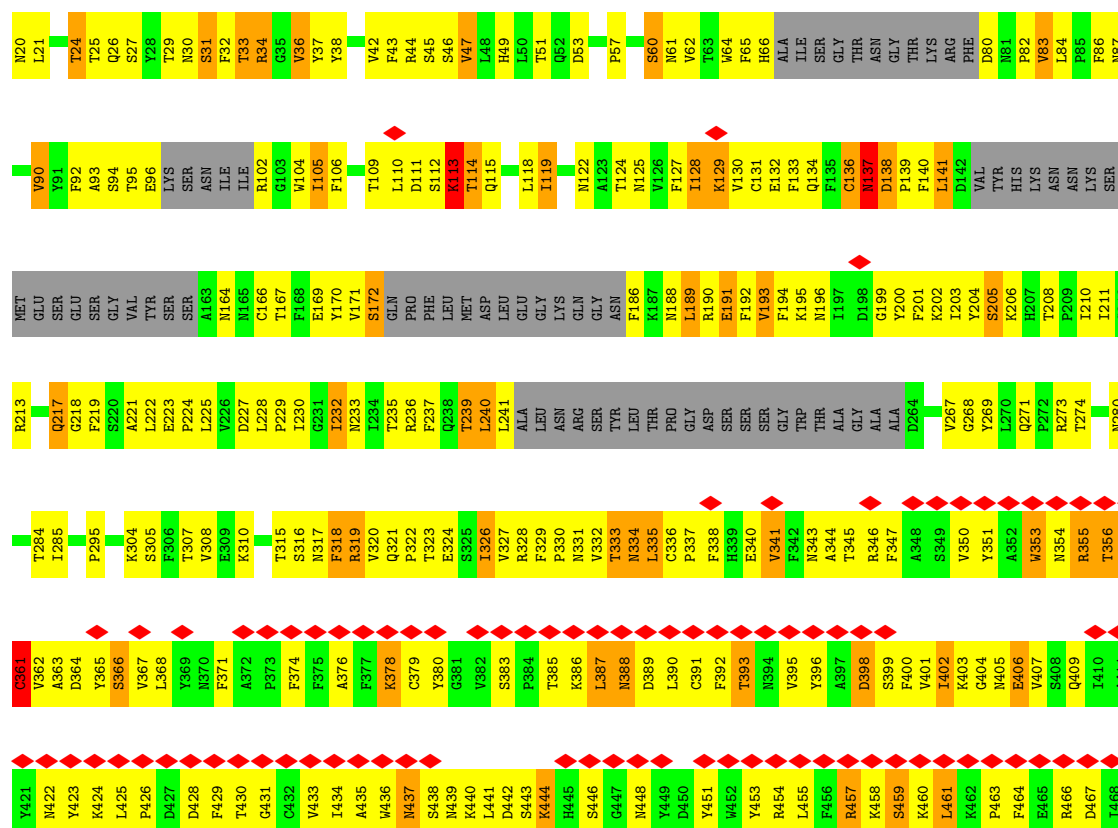
• Molecule 1: Spike glycoprotein

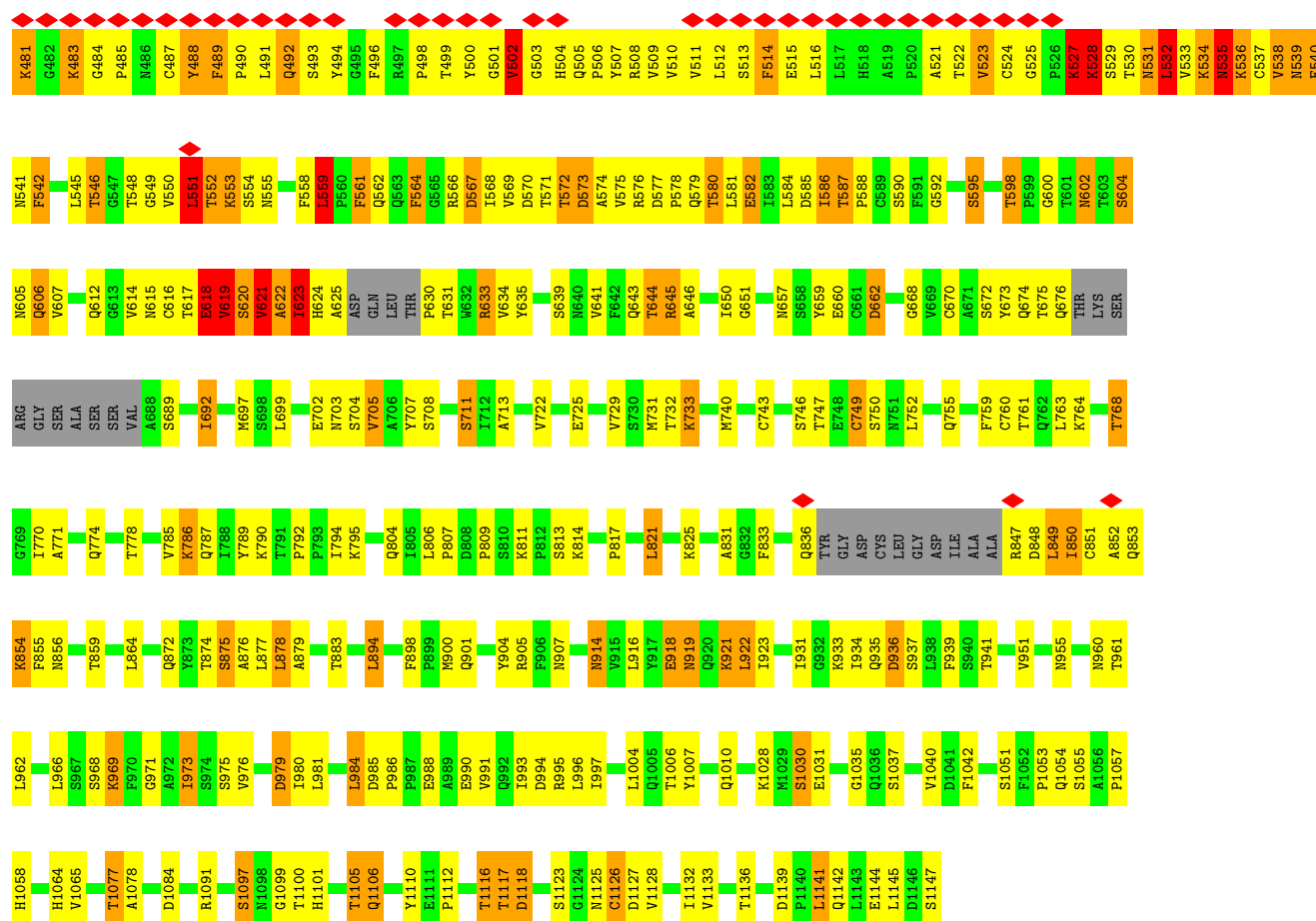




- Molecule 1: Spike glycoprotein









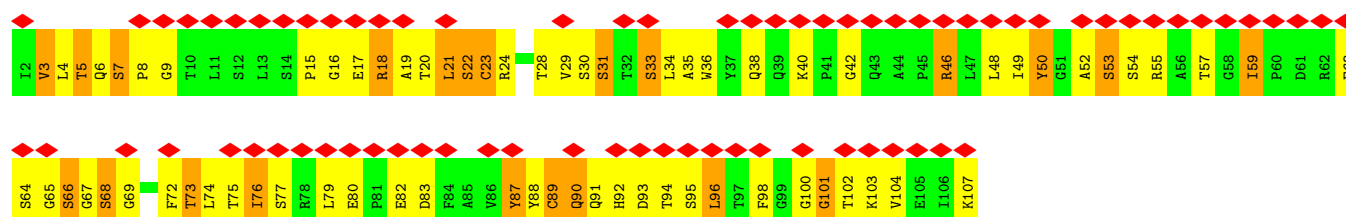
• Molecule 2: S309-HC



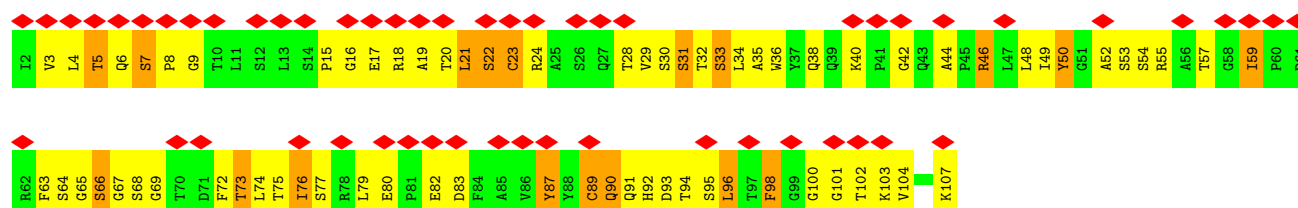
• Molecule 3: S309-KC



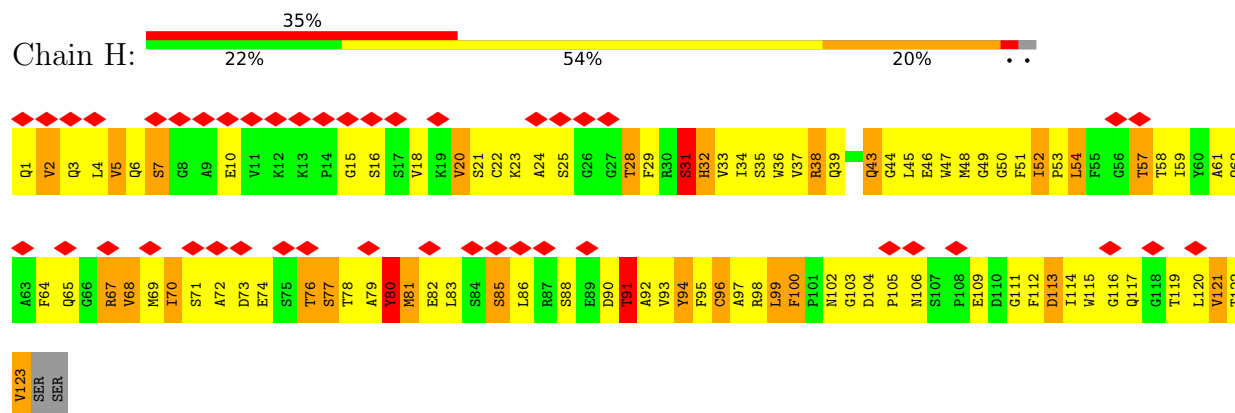
• Molecule 3: S309-KC



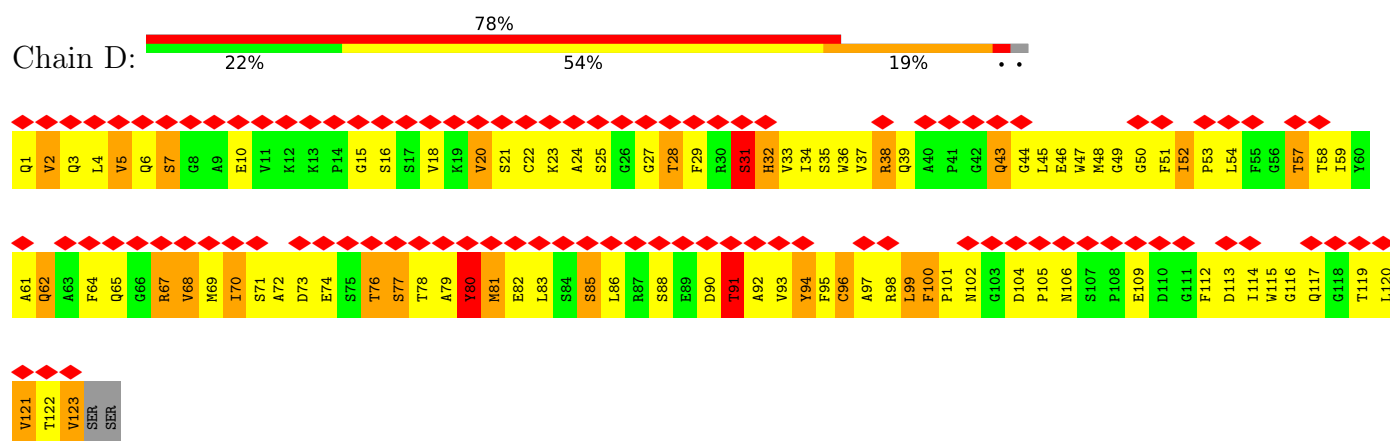
• Molecule 3: S309-KC



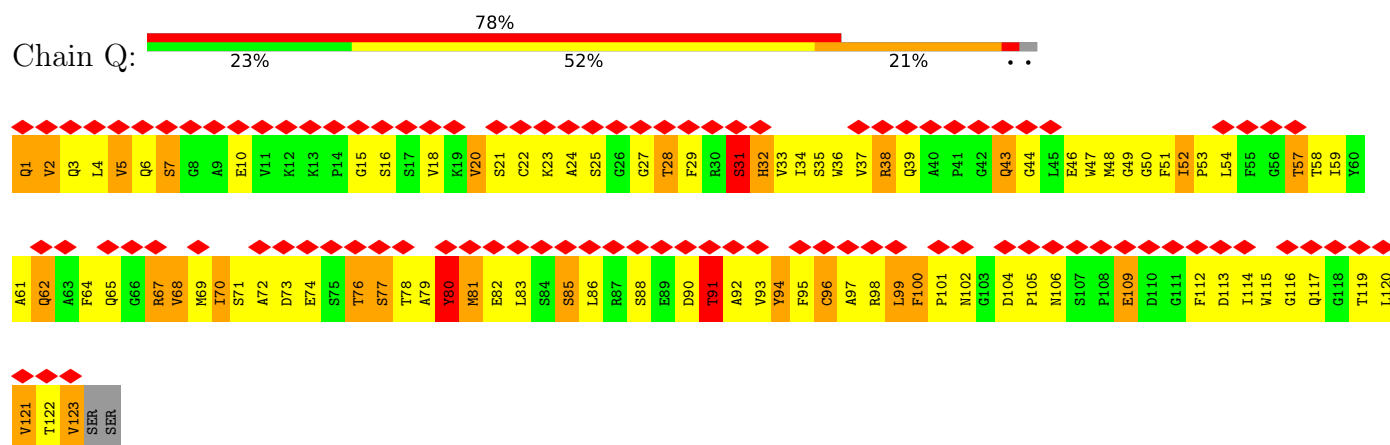
- Molecule 4: SA55-HC



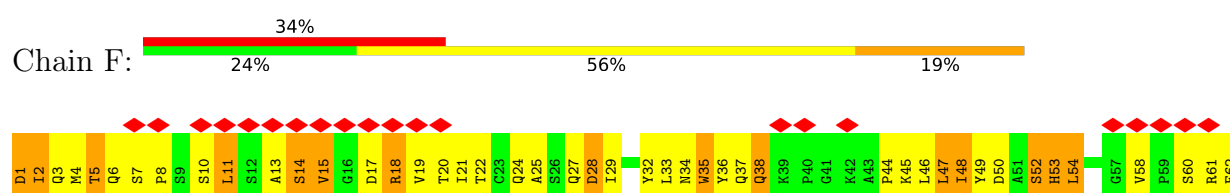
- Molecule 4: SA55-HC



- Molecule 4: SA55-HC



- Molecule 5: SA55_KC

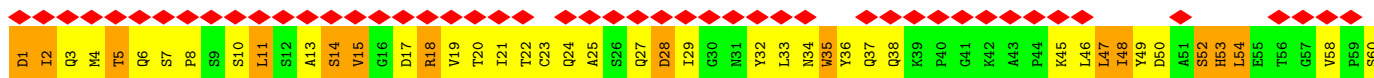
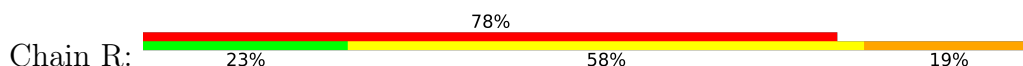




• Molecule 5: SA55_KC



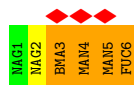
• Molecule 5: SA55_KC



• Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamid o-2-deoxy-beta-D-glucopyranose



• Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamid o-2-deoxy-beta-D-glucopyranose



• Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamid o-2-deoxy-beta-D-glucopyranose





- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L: 100%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N: 50% 50%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P: 50% 100%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U: 50% 50%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W: 50% 50%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X: 50% 50%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	125226	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.5625	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.303	Depositor
Minimum map value	-1.180	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.038	Depositor
Recommended contour level	0.15	Depositor
Map size ($\text{\AA}$)	448.19998, 448.19998, 448.19998	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.83, 0.83, 0.83	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	1.11	7/8277 (0.1%)	0.86	16/11261 (0.1%)
1	B	1.11	7/8277 (0.1%)	0.86	16/11261 (0.1%)
1	C	1.11	7/8277 (0.1%)	0.86	16/11261 (0.1%)
2	E	0.29	0/980	0.72	0/1332
2	I	0.29	0/980	0.72	0/1332
2	S	0.29	0/980	0.72	0/1332
3	G	0.32	0/756	0.86	0/1034
3	K	0.32	0/756	0.86	0/1034
3	T	0.31	0/756	0.86	0/1034
4	D	0.32	0/952	0.87	1/1291 (0.1%)
4	H	0.32	0/952	0.87	1/1291 (0.1%)
4	Q	0.32	0/952	0.87	1/1291 (0.1%)
5	F	0.31	0/854	0.86	1/1160 (0.1%)
5	J	0.31	0/854	0.85	1/1160 (0.1%)
5	R	0.31	0/854	0.86	1/1160 (0.1%)
All	All	0.94	21/35457 (0.1%)	0.85	54/48234 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	18
1	B	0	18
1	C	0	19
3	G	0	2
3	K	0	2
3	T	0	2
4	D	0	1
4	H	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
4	Q	0	1
5	F	0	1
5	J	0	1
5	R	0	1
All	All	0	67

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	540	PHE	CE2-CZ	32.32	2.35	1.38
1	C	540	PHE	CE2-CZ	32.30	2.35	1.38
1	A	540	PHE	CE2-CZ	32.29	2.35	1.38
1	B	551	LEU	CA-C	31.10	1.94	1.53
1	A	551	LEU	CA-C	31.08	1.94	1.53
1	B	540	PHE	CD1-CE1	31.08	2.31	1.38
1	A	540	PHE	CD1-CE1	31.07	2.31	1.38
1	C	551	LEU	CA-C	31.07	1.94	1.53
1	C	540	PHE	CD1-CE1	31.06	2.31	1.38
1	B	540	PHE	CE1-CZ	30.87	2.31	1.38
1	C	540	PHE	CE1-CZ	30.86	2.31	1.38
1	A	540	PHE	CE1-CZ	30.84	2.31	1.38
1	A	540	PHE	CD2-CE2	30.35	2.29	1.38
1	B	540	PHE	CD2-CE2	30.35	2.29	1.38
1	C	540	PHE	CD2-CE2	30.35	2.29	1.38
1	A	540	PHE	CG-CD1	21.50	1.84	1.38
1	C	540	PHE	CG-CD1	21.50	1.83	1.38
1	B	540	PHE	CG-CD1	21.49	1.83	1.38
1	C	540	PHE	CG-CD2	20.19	1.81	1.38
1	B	540	PHE	CG-CD2	20.16	1.81	1.38
1	A	540	PHE	CG-CD2	20.15	1.81	1.38

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	551	LEU	O-C-N	-15.74	103.96	122.84
1	C	551	LEU	O-C-N	-15.73	103.96	122.84
1	B	551	LEU	O-C-N	-15.66	104.04	122.84
1	A	551	LEU	CB-CA-C	9.76	127.99	111.41
1	B	551	LEU	CB-CA-C	9.75	127.99	111.41
1	C	551	LEU	CB-CA-C	9.73	127.95	111.41
1	A	551	LEU	N-CA-CB	-7.87	95.92	110.56
1	B	551	LEU	N-CA-CB	-7.86	95.94	110.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	551	LEU	N-CA-CB	-7.85	95.96	110.56
1	C	551	LEU	CA-C-O	7.81	130.72	121.11
1	A	551	LEU	CA-C-O	7.78	130.67	121.11
1	B	551	LEU	CA-C-O	7.75	130.65	121.11
1	A	551	LEU	N-CA-C	7.27	122.10	107.41
1	B	551	LEU	N-CA-C	7.27	122.09	107.41
1	C	551	LEU	N-CA-C	7.26	122.08	107.41
1	C	619	VAL	CA-C-N	6.51	132.76	122.93
1	C	619	VAL	C-N-CA	6.51	132.76	122.93
1	B	619	VAL	CA-C-N	6.49	132.73	122.93
1	B	619	VAL	C-N-CA	6.49	132.73	122.93
1	A	619	VAL	CA-C-N	6.47	132.70	122.93
1	A	619	VAL	C-N-CA	6.47	132.70	122.93
1	A	551	LEU	CA-C-N	6.20	135.92	123.20
1	A	551	LEU	C-N-CA	6.20	135.92	123.20
1	C	551	LEU	CA-C-N	6.19	135.89	123.20
1	C	551	LEU	C-N-CA	6.19	135.89	123.20
1	B	551	LEU	CA-C-N	6.17	135.84	123.20
1	B	551	LEU	C-N-CA	6.17	135.84	123.20
1	B	602	ASN	N-CA-C	-6.14	105.44	113.12
1	C	602	ASN	N-CA-C	-6.13	105.46	113.12
1	A	602	ASN	N-CA-C	-6.09	105.51	113.12
5	J	2	ILE	N-CA-C	-5.88	105.07	113.07
5	F	2	ILE	N-CA-C	-5.88	105.08	113.07
5	R	2	ILE	N-CA-C	-5.85	105.11	113.07
1	B	341	VAL	N-CA-C	-5.66	106.94	111.81
1	C	341	VAL	N-CA-C	-5.63	106.96	111.81
1	A	341	VAL	N-CA-C	-5.62	106.98	111.81
1	B	539	ASN	N-CA-C	-5.39	108.47	114.62
1	C	539	ASN	N-CA-C	-5.39	108.47	114.62
1	A	539	ASN	N-CA-C	-5.38	108.49	114.62
1	A	527	LYS	CA-C-N	5.34	131.73	121.54
1	A	527	LYS	C-N-CA	5.34	131.73	121.54
1	C	527	LYS	CA-C-N	5.33	131.73	121.54
1	C	527	LYS	C-N-CA	5.33	131.73	121.54
1	B	527	LYS	CA-C-N	5.32	131.70	121.54
1	B	527	LYS	C-N-CA	5.32	131.70	121.54
1	C	561	PHE	N-CA-C	-5.21	108.19	114.75
1	A	561	PHE	N-CA-C	-5.20	108.19	114.75
4	H	80	TYR	CA-CB-CG	5.19	123.25	113.90
4	Q	80	TYR	CA-CB-CG	5.19	123.24	113.90
1	B	561	PHE	N-CA-C	-5.18	108.22	114.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	80	TYR	CA-CB-CG	5.18	123.23	113.90
1	B	502	VAL	N-CA-C	-5.14	106.32	113.00
1	A	502	VAL	N-CA-C	-5.12	106.34	113.00
1	C	502	VAL	N-CA-C	-5.09	106.39	113.00

There are no chirality outliers.

All (67) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	LYS	Peptide
1	A	137	ASN	Peptide
1	A	318	PHE	Peptide
1	A	359	SER	Peptide
1	A	360	ASN	Peptide
1	A	361	CYS	Peptide
1	A	457	ARG	Peptide
1	A	489	PHE	Peptide
1	A	527	LYS	Peptide
1	A	528	LYS	Peptide
1	A	531	ASN	Peptide
1	A	532	LEU	Peptide
1	A	535	ASN	Peptide
1	A	559	LEU	Peptide
1	A	618	GLU	Peptide
1	A	620	SER	Peptide
1	A	622	ALA	Peptide
1	A	623	ILE	Peptide
1	B	113	LYS	Peptide
1	B	137	ASN	Peptide
1	B	318	PHE	Peptide
1	B	359	SER	Peptide
1	B	360	ASN	Peptide
1	B	361	CYS	Peptide
1	B	457	ARG	Peptide
1	B	489	PHE	Peptide
1	B	527	LYS	Peptide
1	B	528	LYS	Peptide
1	B	531	ASN	Peptide
1	B	532	LEU	Peptide
1	B	535	ASN	Peptide
1	B	559	LEU	Peptide
1	B	618	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	B	620	SER	Peptide
1	B	622	ALA	Peptide
1	B	623	ILE	Peptide
1	C	113	LYS	Peptide
1	C	136	CYS	Peptide
1	C	137	ASN	Peptide
1	C	318	PHE	Peptide
1	C	359	SER	Peptide
1	C	360	ASN	Peptide
1	C	361	CYS	Peptide
1	C	457	ARG	Peptide
1	C	489	PHE	Peptide
1	C	527	LYS	Peptide
1	C	528	LYS	Peptide
1	C	531	ASN	Peptide
1	C	532	LEU	Peptide
1	C	535	ASN	Peptide
1	C	559	LEU	Peptide
1	C	618	GLU	Peptide
1	C	620	SER	Peptide
1	C	622	ALA	Peptide
1	C	623	ILE	Peptide
4	D	31	SER	Peptide
5	F	7	SER	Peptide
3	G	101	GLY	Peptide
3	G	23	CYS	Peptide
4	H	31	SER	Peptide
5	J	7	SER	Peptide
3	K	101	GLY	Peptide
3	K	23	CYS	Peptide
4	Q	31	SER	Peptide
5	R	7	SER	Peptide
3	T	101	GLY	Peptide
3	T	23	CYS	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8083	0	7912	613	0
1	B	8083	0	7912	604	0
1	C	8083	0	7912	599	0
2	E	956	0	897	109	0
2	I	956	0	897	116	0
2	S	956	0	897	103	0
3	G	740	0	666	78	0
3	K	740	0	666	90	0
3	T	740	0	666	71	0
4	D	930	0	899	103	0
4	H	930	0	899	113	0
4	Q	930	0	899	96	0
5	F	835	0	797	99	0
5	J	835	0	797	83	0
5	R	835	0	797	86	0
6	M	71	0	61	4	0
6	O	71	0	61	8	0
6	V	71	0	61	5	0
7	L	28	0	25	0	0
7	N	28	0	25	1	0
7	P	28	0	25	0	0
7	U	28	0	25	1	0
7	W	28	0	25	1	0
7	X	28	0	25	1	0
All	All	35013	0	33846	2778	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 40.

All (2778) 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:540:PHE:CD2	1:A:540:PHE:CG	1.81	1.66
1:C:540:PHE:CD2	1:C:540:PHE:CG	1.81	1.65
1:B:540:PHE:CD2	1:B:540:PHE:CG	1.81	1.65
1:C:540:PHE:CG	1:C:540:PHE:CD1	1.84	1.65
1:A:540:PHE:CG	1:A:540:PHE:CD1	1.84	1.63
1:B:540:PHE:CG	1:B:540:PHE:CD1	1.84	1.59
1:C:540:PHE:CZ	1:C:551:LEU:HA	1.41	1.56
1:A:540:PHE:CZ	1:A:551:LEU:HA	1.41	1.52
1:B:540:PHE:CZ	1:B:551:LEU:HA	1.41	1.51
1:A:551:LEU:CA	1:A:551:LEU:C	1.94	1.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:551:LEU:C	1:C:551:LEU:CA	1.94	1.39
1:B:551:LEU:CA	1:B:551:LEU:C	1.94	1.39
1:C:540:PHE:CZ	1:C:552:THR:N	1.99	1.30
1:B:540:PHE:CZ	1:B:552:THR:N	1.99	1.30
1:A:540:PHE:CZ	1:A:552:THR:N	1.99	1.29
1:B:540:PHE:CE1	1:B:551:LEU:C	2.19	1.20
1:C:540:PHE:CD2	1:C:540:PHE:CE2	2.29	1.20
1:A:540:PHE:CE2	1:A:551:LEU:C	2.20	1.20
1:C:540:PHE:CE1	1:C:551:LEU:C	2.19	1.20
1:A:540:PHE:CE1	1:A:551:LEU:C	2.19	1.19
1:B:540:PHE:CE2	1:B:551:LEU:C	2.20	1.19
1:A:540:PHE:CD2	1:A:540:PHE:CE2	2.29	1.18
1:A:540:PHE:CD1	1:A:540:PHE:CE1	2.31	1.18
1:B:540:PHE:CD2	1:B:540:PHE:CE2	2.29	1.18
1:B:540:PHE:CD1	1:B:540:PHE:CE1	2.31	1.18
1:B:540:PHE:CZ	1:B:540:PHE:CE1	2.31	1.18
1:C:540:PHE:CZ	1:C:540:PHE:CE1	2.31	1.18
1:C:540:PHE:CE2	1:C:551:LEU:C	2.20	1.18
1:A:540:PHE:CZ	1:A:540:PHE:CE1	2.31	1.18
1:C:540:PHE:CD1	1:C:540:PHE:CE1	2.31	1.17
1:C:540:PHE:CZ	1:C:551:LEU:CA	2.28	1.17
1:A:540:PHE:CZ	1:A:551:LEU:CA	2.28	1.17
1:A:540:PHE:CZ	1:A:540:PHE:CE2	2.35	1.15
1:B:540:PHE:CZ	1:B:551:LEU:CA	2.28	1.15
1:B:540:PHE:CZ	1:B:540:PHE:CE2	2.35	1.14
1:C:540:PHE:CZ	1:C:551:LEU:C	2.26	1.14
1:C:540:PHE:CZ	1:C:540:PHE:CE2	2.35	1.14
1:A:540:PHE:CZ	1:A:551:LEU:C	2.26	1.14
1:A:588:PRO:HG2	1:B:855:PHE:HB3	1.26	1.14
1:B:540:PHE:CZ	1:B:551:LEU:C	2.26	1.12
1:A:540:PHE:CD2	1:A:551:LEU:C	2.31	1.09
1:C:540:PHE:CD2	1:C:551:LEU:C	2.31	1.09
1:B:540:PHE:CD2	1:B:551:LEU:C	2.31	1.08
1:A:502:VAL:HG22	4:D:46:GLU:HA	1.34	1.07
1:C:540:PHE:CD1	1:C:551:LEU:C	2.33	1.07
1:B:540:PHE:CD1	1:B:551:LEU:C	2.33	1.07
1:C:540:PHE:CE1	1:C:551:LEU:CA	2.39	1.06
1:A:540:PHE:CD1	1:A:551:LEU:C	2.33	1.06
1:B:540:PHE:CE1	1:B:551:LEU:CA	2.39	1.06
1:A:540:PHE:CG	1:A:551:LEU:O	2.09	1.06
1:A:540:PHE:CE1	1:A:551:LEU:CA	2.39	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:540:PHE:CG	1:C:551:LEU:O	2.09	1.06
1:A:540:PHE:CE2	1:A:551:LEU:CA	2.39	1.05
1:B:540:PHE:CG	1:B:551:LEU:O	2.09	1.05
1:B:540:PHE:CE2	1:B:551:LEU:CA	2.39	1.05
1:C:540:PHE:CE2	1:C:551:LEU:CA	2.39	1.04
1:A:540:PHE:CE1	1:A:551:LEU:HA	1.94	1.02
1:B:540:PHE:CE1	1:B:551:LEU:HA	1.94	1.02
1:C:540:PHE:CE1	1:C:551:LEU:HA	1.94	1.02
3:T:36:TRP:HB2	3:T:49:ILE:HB	1.42	1.01
3:G:36:TRP:HB2	3:G:49:ILE:HB	1.42	1.00
3:K:36:TRP:HB2	3:K:49:ILE:HB	1.42	1.00
1:C:540:PHE:CD1	1:C:551:LEU:O	2.15	0.99
1:B:540:PHE:CD1	1:B:551:LEU:O	2.15	0.99
1:A:540:PHE:CD1	1:A:551:LEU:O	2.15	0.98
1:A:330:PRO:O	1:A:528:LYS:NZ	1.96	0.98
1:B:330:PRO:O	1:B:528:LYS:NZ	1.97	0.97
1:C:551:LEU:HD23	1:C:586:ILE:HB	1.46	0.97
1:B:339:HIS:O	2:E:100:TYR:OH	1.82	0.96
4:Q:38:ARG:HB3	4:Q:46:GLU:HB3	1.47	0.96
1:B:27:SER:HB2	1:B:64:TRP:HB3	1.48	0.96
1:C:343:ASN:ND2	6:V:1:NAG:O3	1.98	0.96
1:C:330:PRO:O	1:C:528:LYS:NZ	1.96	0.96
4:D:38:ARG:HB3	4:D:46:GLU:HB3	1.47	0.96
1:A:540:PHE:CE2	1:A:552:THR:N	2.34	0.95
1:B:551:LEU:HD23	1:B:586:ILE:HB	1.46	0.95
1:A:551:LEU:HD23	1:A:586:ILE:HB	1.46	0.95
1:B:540:PHE:CE2	1:B:552:THR:N	2.34	0.95
1:C:540:PHE:CD1	1:C:551:LEU:CB	2.50	0.95
1:B:540:PHE:CE2	1:B:551:LEU:N	2.35	0.95
4:H:38:ARG:HB3	4:H:46:GLU:HB3	1.47	0.95
1:A:540:PHE:CD1	1:A:551:LEU:CB	2.50	0.95
1:B:528:LYS:HZ1	1:B:579:GLN:HB3	1.31	0.95
1:A:540:PHE:CE2	1:A:551:LEU:N	2.35	0.95
1:B:540:PHE:CD1	1:B:551:LEU:CB	2.50	0.94
1:C:540:PHE:CE2	1:C:551:LEU:N	2.35	0.94
1:C:27:SER:HB2	1:C:64:TRP:HB3	1.48	0.94
1:B:504:HIS:CE1	4:H:105:PRO:HD3	2.03	0.93
1:C:540:PHE:CE2	1:C:552:THR:N	2.34	0.93
1:A:27:SER:HB2	1:A:64:TRP:HB3	1.48	0.93
3:K:55:ARG:HH12	3:K:64:SER:HA	1.33	0.93
1:A:540:PHE:CG	1:A:551:LEU:C	2.47	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:540:PHE:CG	1:C:551:LEU:C	2.47	0.92
1:B:540:PHE:CG	1:B:551:LEU:C	2.47	0.92
1:A:1116:THR:OG1	1:A:1118:ASP:OD2	1.89	0.91
1:A:444:LYS:NZ	3:K:100:GLY:H	1.69	0.91
1:B:1116:THR:OG1	1:B:1118:ASP:OD2	1.89	0.90
3:G:55:ARG:HH12	3:G:64:SER:HA	1.33	0.90
1:C:1116:THR:OG1	1:C:1118:ASP:OD2	1.89	0.90
1:A:540:PHE:CD2	1:A:551:LEU:CA	2.55	0.90
1:B:418:ILE:HG12	1:B:422:ASN:HB3	1.54	0.90
1:C:540:PHE:CD2	1:C:551:LEU:CA	2.56	0.89
3:T:55:ARG:HH12	3:T:64:SER:HA	1.33	0.89
1:A:616:CYS:O	1:A:619:VAL:N	2.06	0.89
1:C:616:CYS:O	1:C:619:VAL:N	2.06	0.89
1:C:137:ASN:OD1	1:C:138:ASP:N	2.06	0.89
1:B:540:PHE:CD2	1:B:551:LEU:CA	2.56	0.89
1:C:418:ILE:HG12	1:C:422:ASN:HB3	1.54	0.89
1:B:616:CYS:O	1:B:619:VAL:N	2.06	0.89
1:A:448:ASN:ND2	3:K:5:THR:HG22	1.88	0.88
1:B:345:THR:OG1	2:E:111:ILE:HA	1.73	0.88
1:A:346:ARG:HB2	2:I:112:GLY:HA2	1.55	0.88
1:A:418:ILE:HG12	1:A:422:ASN:HB3	1.54	0.88
1:A:540:PHE:CD1	1:A:551:LEU:HB2	2.09	0.88
1:A:500:TYR:O	4:D:45:LEU:HD13	1.74	0.88
1:C:540:PHE:CD1	1:C:551:LEU:HB2	2.09	0.87
1:A:551:LEU:HA	1:A:551:LEU:C	1.98	0.87
1:B:622:ALA:O	1:B:624:HIS:N	2.07	0.87
1:B:137:ASN:OD1	1:B:138:ASP:N	2.05	0.87
1:B:551:LEU:HA	1:B:551:LEU:C	1.98	0.87
1:A:622:ALA:O	1:A:624:HIS:N	2.07	0.87
1:C:528:LYS:HZ1	1:C:579:GLN:HB3	1.40	0.86
1:A:137:ASN:OD1	1:A:138:ASP:N	2.06	0.86
1:B:540:PHE:CD1	1:B:551:LEU:HB2	2.09	0.86
1:C:540:PHE:CD2	1:C:551:LEU:N	2.44	0.86
4:H:34:ILE:HA	4:H:98:ARG:HH12	1.40	0.86
1:C:622:ALA:O	1:C:624:HIS:N	2.07	0.86
4:Q:34:ILE:HA	4:Q:98:ARG:HH12	1.40	0.86
1:B:540:PHE:CD2	1:B:551:LEU:N	2.44	0.86
1:B:617:THR:O	1:B:621:VAL:HA	1.76	0.86
1:A:540:PHE:CD2	1:A:551:LEU:N	2.44	0.85
1:A:540:PHE:CD1	1:A:551:LEU:CA	2.59	0.85
1:B:540:PHE:CD1	1:B:551:LEU:CA	2.59	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:ASN:HD21	3:K:5:THR:HG22	1.41	0.85
1:A:617:THR:O	1:A:621:VAL:HA	1.76	0.85
1:B:702:GLU:OE2	1:C:790:LYS:NZ	2.08	0.85
1:C:617:THR:O	1:C:621:VAL:HA	1.76	0.85
3:G:48:LEU:HG	3:G:49:ILE:HG12	1.59	0.85
1:C:540:PHE:CD1	1:C:551:LEU:CA	2.59	0.85
4:D:34:ILE:HA	4:D:98:ARG:HH12	1.40	0.84
1:B:345:THR:HG22	1:B:346:ARG:HG2	1.59	0.84
1:C:345:THR:HG22	1:C:346:ARG:HG2	1.59	0.84
3:T:48:LEU:HG	3:T:49:ILE:HG12	1.59	0.84
1:C:551:LEU:HA	1:C:551:LEU:C	1.98	0.83
1:A:345:THR:HG22	1:A:346:ARG:HG2	1.59	0.83
1:C:552:THR:OG1	1:C:553:LYS:N	2.12	0.83
1:C:532:LEU:O	1:C:534:LYS:N	2.12	0.83
3:K:48:LEU:HG	3:K:49:ILE:HG12	1.59	0.82
4:D:36:TRP:HB3	4:D:48:MET:HB3	1.59	0.82
1:A:532:LEU:O	1:A:534:LYS:N	2.12	0.82
4:Q:98:ARG:HB2	4:Q:114:ILE:H	1.44	0.82
1:B:395:VAL:HA	1:B:514:PHE:HA	1.61	0.82
4:H:36:TRP:HB3	4:H:48:MET:HB3	1.59	0.82
1:B:532:LEU:O	1:B:534:LYS:N	2.12	0.82
4:H:39:GLN:CD	5:F:38:GLN:HE22	1.88	0.82
4:Q:36:TRP:HB3	4:Q:48:MET:HB3	1.59	0.82
1:A:395:VAL:HA	1:A:514:PHE:HA	1.61	0.82
1:C:395:VAL:HA	1:C:514:PHE:HA	1.61	0.82
1:A:350:VAL:HG23	1:A:400:PHE:HD1	1.45	0.81
1:C:321:GLN:HG2	1:C:630:PRO:HG2	1.63	0.81
1:A:321:GLN:HG2	1:A:630:PRO:HG2	1.63	0.81
1:C:350:VAL:HG23	1:C:400:PHE:HD1	1.45	0.81
3:T:5:THR:OG1	3:T:24:ARG:O	1.98	0.81
4:H:98:ARG:HB2	4:H:114:ILE:H	1.44	0.81
2:I:35:SER:N	2:I:97:ALA:O	2.14	0.81
4:Q:35:SER:HA	4:Q:50:GLY:HA3	1.63	0.81
1:A:528:LYS:HZ1	1:A:579:GLN:HB3	1.44	0.81
2:I:116:ASN:CG	6:O:6:FUC:HO3	1.87	0.80
2:S:35:SER:N	2:S:97:ALA:O	2.14	0.80
5:R:4:MET:HE2	5:R:90:ARG:HB2	1.62	0.80
1:B:568:ILE:HG13	1:C:47:VAL:HG12	1.63	0.80
4:D:98:ARG:HB2	4:D:114:ILE:H	1.44	0.80
1:A:112:SER:HA	1:A:132:GLU:HB3	1.63	0.80
1:A:345:THR:O	1:A:508:ARG:NH1	2.15	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:ILE:HG21	1:A:483:LYS:HE2	1.64	0.80
1:A:855:PHE:HB3	1:C:588:PRO:HG2	1.64	0.80
1:B:345:THR:HA	2:E:111:ILE:HD12	1.63	0.80
3:G:5:THR:OG1	3:G:24:ARG:O	1.98	0.80
1:C:112:SER:HA	1:C:132:GLU:HB3	1.63	0.80
1:C:442:ASP:HB2	1:C:506:PRO:HB3	1.62	0.80
1:C:472:ILE:HG21	1:C:483:LYS:HE2	1.64	0.80
4:H:35:SER:HA	4:H:50:GLY:HA3	1.63	0.80
1:B:321:GLN:HG2	1:B:630:PRO:HG2	1.63	0.80
1:B:345:THR:O	1:B:508:ARG:NH1	2.15	0.80
3:K:5:THR:OG1	3:K:24:ARG:O	1.98	0.80
1:B:504:HIS:NE2	4:H:105:PRO:HD3	1.96	0.80
5:F:4:MET:HE2	5:F:90:ARG:HB2	1.62	0.80
5:J:4:MET:HE2	5:J:90:ARG:HB2	1.62	0.80
1:B:112:SER:HA	1:B:132:GLU:HB3	1.63	0.79
1:B:350:VAL:HG23	1:B:400:PHE:HD1	1.45	0.79
1:B:539:ASN:O	1:B:541:ASN:N	2.15	0.79
1:C:539:ASN:O	1:C:541:ASN:N	2.15	0.79
1:A:552:THR:OG1	1:A:553:LYS:N	2.12	0.79
1:B:552:THR:OG1	1:B:553:LYS:N	2.12	0.79
1:A:442:ASP:HB2	1:A:506:PRO:HB3	1.62	0.79
1:C:620:SER:O	1:C:622:ALA:N	2.16	0.79
1:A:570:ASP:OD1	1:B:967:SER:OG	2.00	0.79
1:B:405:ASN:O	1:B:409:GLN:NE2	2.16	0.79
1:A:620:SER:O	1:A:622:ALA:N	2.16	0.79
1:C:345:THR:O	1:C:508:ARG:NH1	2.15	0.79
2:E:35:SER:N	2:E:97:ALA:O	2.14	0.79
1:A:539:ASN:O	1:A:541:ASN:N	2.15	0.79
1:B:472:ILE:HG21	1:B:483:LYS:HE2	1.64	0.79
3:G:15:PRO:HA	3:G:79:LEU:HB2	1.65	0.79
3:T:77:SER:OG	5:R:18:ARG:NH2	2.16	0.79
1:B:442:ASP:HB2	1:B:506:PRO:HB3	1.62	0.79
1:C:540:PHE:CG	1:C:551:LEU:CA	2.66	0.79
1:C:540:PHE:CD2	1:C:551:LEU:O	2.37	0.78
4:D:35:SER:HA	4:D:50:GLY:HA3	1.63	0.78
1:C:559:LEU:O	1:C:561:PHE:N	2.16	0.78
1:B:620:SER:O	1:B:622:ALA:N	2.16	0.78
1:A:540:PHE:CG	1:A:551:LEU:CA	2.66	0.78
1:A:894:LEU:HB3	1:C:713:ALA:HB3	1.63	0.78
1:A:574:ALA:HA	1:A:585:ASP:HA	1.66	0.78
1:C:921:LYS:HE2	1:C:921:LYS:H	1.49	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:540:PHE:CG	1:B:551:LEU:CA	2.66	0.78
1:B:574:ALA:HA	1:B:585:ASP:HA	1.66	0.78
1:B:559:LEU:O	1:B:561:PHE:N	2.16	0.77
1:A:450:ASP:CG	3:K:3:VAL:HG11	2.08	0.77
1:B:921:LYS:H	1:B:921:LYS:HE2	1.49	0.77
1:A:334:ASN:O	1:A:362:VAL:N	2.18	0.77
2:I:2:VAL:HB	6:O:6:FUC:H4	1.64	0.77
1:B:334:ASN:O	1:B:362:VAL:N	2.18	0.77
2:I:24:ALA:N	2:I:77:THR:O	2.18	0.77
1:A:559:LEU:O	1:A:561:PHE:N	2.16	0.77
3:K:15:PRO:HA	3:K:79:LEU:HB2	1.65	0.77
1:B:540:PHE:CD2	1:B:551:LEU:O	2.36	0.77
1:A:540:PHE:CD2	1:A:551:LEU:O	2.36	0.77
1:A:500:TYR:C	4:D:45:LEU:HD13	2.10	0.76
1:C:574:ALA:HA	1:C:585:ASP:HA	1.66	0.76
1:A:138:ASP:HB2	1:A:139:PRO:HD3	1.66	0.76
1:A:109:THR:OG1	1:A:114:THR:OG1	2.02	0.76
1:C:405:ASN:O	1:C:409:GLN:NE2	2.16	0.76
3:G:64:SER:OG	5:F:28:ASP:OD2	2.01	0.76
1:C:334:ASN:O	1:C:362:VAL:N	2.18	0.76
1:B:138:ASP:HB2	1:B:139:PRO:HD3	1.67	0.76
1:A:921:LYS:H	1:A:921:LYS:HE2	1.49	0.76
1:C:363:ALA:HB3	1:C:523:VAL:HG13	1.68	0.76
1:B:747:THR:HG22	1:B:749:CYS:H	1.50	0.75
1:B:1040:VAL:HG21	1:C:1035:GLY:HA3	1.67	0.75
1:C:138:ASP:HB2	1:C:139:PRO:HD3	1.67	0.75
1:C:344:ALA:HB3	1:C:347:PHE:HE2	1.51	0.75
3:G:50:TYR:CE1	6:M:1:NAG:H61	2.21	0.75
3:G:36:TRP:HB3	3:G:48:LEU:HD23	1.69	0.75
3:T:15:PRO:HA	3:T:79:LEU:HB2	1.65	0.75
1:A:344:ALA:HB3	1:A:347:PHE:HE2	1.51	0.75
1:A:405:ASN:O	1:A:409:GLN:NE2	2.16	0.75
1:B:424:LYS:NZ	1:B:425:LEU:O	2.19	0.75
3:T:6:GLN:HA	3:T:23:CYS:HA	1.69	0.75
1:A:457:ARG:NH2	1:A:471:GLU:OE1	2.20	0.75
1:A:540:PHE:HE2	1:A:550:VAL:HG12	1.52	0.75
1:B:540:PHE:HE2	1:B:550:VAL:HG12	1.52	0.75
1:B:363:ALA:HB3	1:B:523:VAL:HG13	1.68	0.75
1:C:747:THR:HG22	1:C:749:CYS:H	1.50	0.75
1:C:424:LYS:NZ	1:C:425:LEU:O	2.19	0.74
1:A:363:ALA:HB3	1:A:523:VAL:HG13	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:LYS:NZ	1:A:425:LEU:O	2.19	0.74
1:C:500:TYR:HA	4:Q:101:PRO:HB3	1.69	0.74
2:I:51:ILE:HG22	2:I:70:MET:HB3	1.69	0.74
2:S:24:ALA:N	2:S:77:THR:O	2.18	0.74
1:A:502:VAL:HG22	4:D:46:GLU:CA	2.16	0.74
2:S:51:ILE:HG22	2:S:70:MET:HB3	1.69	0.74
1:C:402:ILE:HD12	1:C:407:VAL:HG22	1.69	0.74
2:E:51:ILE:HG22	2:E:70:MET:HB3	1.69	0.74
1:B:402:ILE:HD12	1:B:407:VAL:HG22	1.69	0.74
1:B:1126:CYS:HB3	1:B:1132:ILE:HD13	1.69	0.74
3:G:6:GLN:HA	3:G:23:CYS:HA	1.69	0.74
2:I:42:GLY:HA2	3:K:54:SER:OG	1.87	0.74
3:K:36:TRP:HB3	3:K:48:LEU:HD23	1.69	0.74
1:B:1041:ASP:HB2	1:C:1030:SER:HB3	1.67	0.74
2:E:24:ALA:N	2:E:77:THR:O	2.18	0.74
1:A:502:VAL:CG2	4:D:46:GLU:HA	2.17	0.74
1:A:747:THR:HG22	1:A:749:CYS:H	1.50	0.74
1:B:344:ALA:HB3	1:B:347:PHE:HE2	1.51	0.74
1:A:393:THR:HA	1:A:522:THR:H	1.53	0.73
1:B:540:PHE:CE2	1:B:552:THR:HG22	2.23	0.73
3:T:36:TRP:HB3	3:T:48:LEU:HD23	1.69	0.73
1:A:540:PHE:CE2	1:A:552:THR:HG22	2.23	0.73
3:K:6:GLN:HA	3:K:23:CYS:HA	1.69	0.73
1:A:743:CYS:SG	1:A:750:SER:N	2.62	0.73
1:C:457:ARG:NH2	1:C:471:GLU:OE1	2.20	0.73
1:C:540:PHE:HE2	1:C:550:VAL:HG12	1.52	0.73
1:A:333:THR:OG1	1:A:361:CYS:O	2.07	0.73
1:B:393:THR:HA	1:B:522:THR:H	1.53	0.73
1:C:333:THR:OG1	1:C:361:CYS:O	2.07	0.73
1:C:540:PHE:CE2	1:C:552:THR:HG22	2.23	0.73
1:B:457:ARG:NH2	1:B:471:GLU:OE1	2.20	0.73
1:A:1126:CYS:HB3	1:A:1132:ILE:HD13	1.69	0.73
1:B:478:LYS:HE2	1:B:480:CYS:HB3	1.71	0.73
3:K:55:ARG:NH1	3:K:64:SER:HA	2.04	0.73
1:A:478:LYS:HE2	1:A:480:CYS:HB3	1.71	0.72
1:B:743:CYS:SG	1:B:750:SER:N	2.62	0.72
3:T:55:ARG:NH1	3:T:64:SER:HA	2.04	0.72
1:C:393:THR:HA	1:C:522:THR:H	1.53	0.72
1:C:743:CYS:SG	1:C:750:SER:N	2.62	0.72
2:E:33:GLY:HA3	2:E:50:TRP:HE1	1.54	0.72
1:A:104:TRP:HB2	1:A:106:PHE:CE2	2.24	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:TRP:HB2	1:B:106:PHE:CE2	2.25	0.72
3:G:55:ARG:NH1	3:G:64:SER:HA	2.04	0.72
1:A:402:ILE:HD12	1:A:407:VAL:HG22	1.69	0.72
1:B:333:THR:OG1	1:B:361:CYS:O	2.07	0.72
2:E:101:THR:HG21	3:G:96:LEU:HD11	1.72	0.72
1:C:104:TRP:HB2	1:C:106:PHE:CE2	2.24	0.72
1:C:786:LYS:HB2	1:C:787:GLN:HG3	1.72	0.72
1:C:1126:CYS:HB3	1:C:1132:ILE:HD13	1.69	0.72
2:E:70:MET:HG3	2:E:81:MET:HG3	1.72	0.72
2:S:29:PHE:HE1	2:S:74:THR:HA	1.55	0.72
1:A:102:ARG:N	1:A:241:LEU:O	2.23	0.71
1:B:786:LYS:HB2	1:B:787:GLN:HG3	1.72	0.71
1:C:478:LYS:HE2	1:C:480:CYS:HB3	1.71	0.71
2:I:60:TYR:HE1	2:I:70:MET:HB2	1.56	0.71
1:B:437:ASN:HD21	1:B:439:ASN:HB2	1.55	0.71
2:E:60:TYR:HE1	2:E:70:MET:HB2	1.55	0.71
1:C:118:LEU:HB2	1:C:129:LYS:HB3	1.72	0.71
1:B:115:GLN:NE2	1:B:132:GLU:OE1	2.24	0.71
1:C:437:ASN:HD21	1:C:439:ASN:HB2	1.55	0.71
3:G:21:LEU:HB3	3:G:74:LEU:HB3	1.71	0.71
3:G:38:GLN:O	3:G:46:ARG:N	2.20	0.71
2:S:33:GLY:HA3	2:S:50:TRP:HE1	1.54	0.71
1:A:115:GLN:NE2	1:A:132:GLU:OE1	2.24	0.71
1:A:444:LYS:HD3	3:K:101:GLY:HA3	1.72	0.71
1:A:786:LYS:HB2	1:A:787:GLN:HG3	1.72	0.71
2:E:33:GLY:O	2:E:99:ASP:N	2.24	0.71
2:I:33:GLY:O	2:I:99:ASP:N	2.24	0.71
2:S:60:TYR:HE1	2:S:70:MET:HB2	1.55	0.71
1:C:102:ARG:N	1:C:241:LEU:O	2.23	0.71
1:C:420:ASP:HA	1:C:460:LYS:HB2	1.73	0.71
2:I:70:MET:HG3	2:I:81:MET:HG3	1.72	0.71
2:S:38:ARG:HB3	2:S:46:GLU:HB2	1.73	0.71
2:E:29:PHE:HE1	2:E:74:THR:HA	1.55	0.71
3:K:21:LEU:HB3	3:K:74:LEU:HB3	1.72	0.71
1:A:405:ASN:HD21	4:D:99:LEU:HD23	1.56	0.70
1:B:566:ARG:HG2	1:C:42:VAL:HG11	1.73	0.70
2:S:33:GLY:O	2:S:99:ASP:N	2.24	0.70
2:S:70:MET:HG3	2:S:81:MET:HG3	1.72	0.70
2:I:33:GLY:HA3	2:I:50:TRP:HE1	1.54	0.70
1:A:420:ASP:HA	1:A:460:LYS:HB2	1.73	0.70
1:A:1118:ASP:OD2	1:A:1118:ASP:N	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:443:SER:HB2	1:C:496:PHE:CE2	2.26	0.70
2:I:29:PHE:HE1	2:I:74:THR:HA	1.55	0.70
1:A:443:SER:HB2	1:A:496:PHE:CE2	2.26	0.70
1:B:102:ARG:N	1:B:241:LEU:O	2.23	0.70
1:A:437:ASN:HD21	1:A:439:ASN:HB2	1.55	0.70
1:B:118:LEU:HB2	1:B:129:LYS:HB3	1.72	0.70
1:C:115:GLN:NE2	1:C:132:GLU:OE1	2.24	0.70
2:I:5:VAL:HB	2:I:23:LYS:HB2	1.73	0.70
3:T:33:SER:O	3:T:92:HIS:ND1	2.25	0.70
1:A:853:GLN:NE2	1:A:960:ASN:OD1	2.23	0.70
1:B:344:ALA:HA	2:E:110:LEU:HG	1.73	0.70
1:B:1118:ASP:OD2	1:B:1118:ASP:N	2.24	0.70
1:A:118:LEU:HB2	1:A:129:LYS:HB3	1.72	0.70
1:A:1105:THR:OG1	1:A:1106:GLN:O	2.10	0.70
1:B:1105:THR:OG1	1:B:1106:GLN:O	2.10	0.70
1:C:1105:THR:OG1	1:C:1106:GLN:O	2.10	0.70
1:C:109:THR:OG1	1:C:114:THR:OG1	2.02	0.70
3:T:21:LEU:HB3	3:T:74:LEU:HB3	1.72	0.70
3:T:38:GLN:O	3:T:46:ARG:N	2.20	0.70
3:K:33:SER:O	3:K:92:HIS:ND1	2.25	0.69
1:A:505:GLN:HG2	4:D:45:LEU:HD12	1.72	0.69
1:A:453:TYR:O	1:A:492:GLN:N	2.24	0.69
1:B:109:THR:OG1	1:B:114:THR:OG1	2.02	0.69
3:K:4:LEU:HD11	3:K:91:GLN:HB2	1.74	0.69
1:A:625:ALA:HA	1:A:630:PRO:HA	1.75	0.69
3:G:61:ASP:O	5:F:27:GLN:NE2	2.26	0.69
1:B:540:PHE:CG	1:B:551:LEU:HB2	2.28	0.69
1:B:625:ALA:HA	1:B:630:PRO:HA	1.75	0.69
1:C:625:ALA:HA	1:C:630:PRO:HA	1.75	0.69
2:S:5:VAL:HB	2:S:23:LYS:HB2	1.74	0.69
1:A:505:GLN:HE21	4:D:45:LEU:CD1	2.06	0.69
1:A:895:GLN:NE2	1:C:711:SER:OG	2.25	0.69
1:B:443:SER:HB2	1:B:496:PHE:CE2	2.26	0.69
2:E:38:ARG:HB3	2:E:46:GLU:HB2	1.73	0.69
2:I:23:LYS:NZ	2:I:76:THR:O	2.26	0.69
1:A:350:VAL:HG11	1:A:453:TYR:HB2	1.74	0.69
1:B:350:VAL:HG11	1:B:453:TYR:HB2	1.74	0.69
1:B:420:ASP:HA	1:B:460:LYS:HB2	1.73	0.69
1:C:540:PHE:CG	1:C:551:LEU:HB2	2.28	0.69
2:E:23:LYS:NZ	2:E:76:THR:O	2.26	0.69
1:B:426:PRO:HD2	1:B:430:THR:HG22	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:33:SER:O	3:G:92:HIS:ND1	2.25	0.69
3:T:4:LEU:HD11	3:T:91:GLN:HB2	1.74	0.69
1:A:528:LYS:NZ	1:A:579:GLN:HB3	2.08	0.69
3:G:4:LEU:HD11	3:G:91:GLN:HB2	1.74	0.69
2:I:38:ARG:HB3	2:I:46:GLU:HB2	1.73	0.69
1:B:566:ARG:HG2	1:C:42:VAL:CG1	2.23	0.68
1:C:426:PRO:HD2	1:C:430:THR:HG22	1.75	0.68
1:C:528:LYS:NZ	1:C:579:GLN:HB3	2.08	0.68
2:E:5:VAL:HB	2:E:23:LYS:HB2	1.74	0.68
5:J:19:VAL:HG21	5:J:75:ILE:HB	1.75	0.68
1:A:426:PRO:HD2	1:A:430:THR:HG22	1.75	0.68
1:A:540:PHE:CG	1:A:551:LEU:HB2	2.28	0.68
4:H:15:GLY:N	4:H:86:LEU:O	2.26	0.68
2:S:23:LYS:NZ	2:S:76:THR:O	2.26	0.68
1:A:540:PHE:CE2	1:A:550:VAL:HG12	2.29	0.68
1:A:1117:THR:O	1:A:1117:THR:OG1	2.10	0.68
1:A:595:SER:OG	1:A:612:GLN:NE2	2.26	0.68
1:B:914:ASN:OD1	1:B:914:ASN:N	2.25	0.68
1:C:540:PHE:CE2	1:C:550:VAL:HG12	2.29	0.68
1:A:540:PHE:CE1	1:A:551:LEU:HB3	2.29	0.68
1:C:618:GLU:O	1:C:620:SER:N	2.27	0.68
1:C:1117:THR:O	1:C:1117:THR:OG1	2.10	0.68
3:G:20:THR:HA	3:G:75:THR:HA	1.76	0.68
5:R:19:VAL:HG21	5:R:75:ILE:HB	1.75	0.68
1:B:122:ASN:ND2	1:B:124:THR:OG1	2.27	0.68
1:B:853:GLN:NE2	1:B:960:ASN:OD1	2.23	0.68
1:C:595:SER:OG	1:C:612:GLN:NE2	2.26	0.68
1:A:457:ARG:NH1	1:A:459:SER:O	2.27	0.68
1:B:595:SER:OG	1:B:612:GLN:NE2	2.26	0.68
4:H:33:VAL:HG11	4:H:52:ILE:HD13	1.76	0.68
1:A:537:CYS:O	1:A:539:ASN:N	2.28	0.67
1:B:457:ARG:NH1	1:B:459:SER:O	2.27	0.67
1:C:620:SER:HB2	1:C:631:THR:OG1	1.94	0.67
3:K:20:THR:HA	3:K:75:THR:HA	1.76	0.67
3:T:6:GLN:HE21	3:T:89:CYS:H	1.42	0.67
1:C:457:ARG:NH1	1:C:459:SER:O	2.27	0.67
5:F:19:VAL:HG21	5:F:75:ILE:HB	1.75	0.67
1:A:618:GLU:O	1:A:620:SER:N	2.27	0.67
1:A:620:SER:HB2	1:A:631:THR:OG1	1.94	0.67
1:C:540:PHE:CE1	1:C:551:LEU:HB3	2.29	0.67
1:C:350:VAL:HG11	1:C:453:TYR:HB2	1.74	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:7:SER:HB3	4:H:21:SER:H	1.59	0.67
4:D:33:VAL:HG11	4:D:52:ILE:HD13	1.76	0.67
5:J:1:ASP:OD2	5:J:96:SER:OG	2.12	0.67
1:B:540:PHE:CE1	1:B:551:LEU:HB3	2.29	0.67
1:C:122:ASN:ND2	1:C:124:THR:OG1	2.27	0.67
3:G:6:GLN:HE21	3:G:89:CYS:H	1.42	0.67
2:I:101:THR:O	2:I:110:LEU:N	2.22	0.67
1:A:847:ARG:NH1	1:C:555:ASN:OD1	2.28	0.67
1:A:951:VAL:O	1:A:955:ASN:ND2	2.28	0.67
2:I:31:SER:HA	2:I:105:TRP:HZ2	1.59	0.67
1:A:122:ASN:ND2	1:A:124:THR:OG1	2.27	0.67
1:B:540:PHE:CE2	1:B:550:VAL:HG12	2.29	0.67
1:B:825:LYS:HD2	1:B:939:PHE:HA	1.77	0.67
1:C:540:PHE:CE2	1:C:550:VAL:C	2.73	0.67
1:A:328:ARG:HB3	1:A:528:LYS:HD2	1.77	0.67
1:C:371:PHE:HD1	6:V:2:NAG:H62	1.59	0.67
1:B:537:CYS:O	1:B:539:ASN:N	2.28	0.67
1:B:620:SER:HB2	1:B:631:THR:OG1	1.94	0.67
1:C:537:CYS:O	1:C:539:ASN:N	2.28	0.67
4:Q:7:SER:HB3	4:Q:21:SER:H	1.59	0.67
1:B:395:VAL:HG12	1:B:512:LEU:HB3	1.77	0.66
4:H:24:ALA:HA	4:H:29:PHE:CE2	2.30	0.66
1:B:1117:THR:O	1:B:1117:THR:OG1	2.10	0.66
1:C:951:VAL:O	1:C:955:ASN:ND2	2.28	0.66
2:E:31:SER:HA	2:E:105:TRP:HZ2	1.59	0.66
4:H:47:TRP:CE2	5:F:97:TYR:HD1	2.12	0.66
5:F:6:GLN:HE22	5:F:102:GLY:H	1.43	0.66
3:K:38:GLN:O	3:K:46:ARG:N	2.20	0.66
4:Q:33:VAL:HG11	4:Q:52:ILE:HD13	1.76	0.66
1:B:618:GLU:O	1:B:620:SER:N	2.27	0.66
4:Q:24:ALA:HA	4:Q:29:PHE:CE2	2.30	0.66
4:H:70:ILE:HG23	4:H:81:MET:HA	1.77	0.66
3:K:6:GLN:HE21	3:K:89:CYS:H	1.42	0.66
4:D:7:SER:HB3	4:D:21:SER:H	1.59	0.66
2:S:31:SER:HA	2:S:105:TRP:HZ2	1.59	0.66
4:Q:70:ILE:HG23	4:Q:81:MET:HA	1.77	0.66
1:C:329:PHE:HA	1:C:578:PRO:HB3	1.78	0.66
4:D:70:ILE:HG23	4:D:81:MET:HA	1.77	0.66
5:J:6:GLN:HE22	5:J:102:GLY:H	1.43	0.66
1:A:443:SER:HB3	1:A:506:PRO:HG3	1.78	0.66
1:A:540:PHE:CE2	1:A:550:VAL:C	2.73	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:SER:N	1:B:60:SER:O	2.28	0.66
1:B:328:ARG:HB3	1:B:528:LYS:HD2	1.77	0.66
1:B:329:PHE:HA	1:B:578:PRO:HB3	1.78	0.66
1:C:395:VAL:HG12	1:C:512:LEU:HB3	1.77	0.66
1:C:914:ASN:N	1:C:914:ASN:OD1	2.25	0.66
4:D:24:ALA:HA	4:D:29:PHE:CE2	2.30	0.66
1:A:914:ASN:N	1:A:914:ASN:OD1	2.25	0.66
1:B:361:CYS:HB3	1:B:523:VAL:HA	1.78	0.66
1:C:328:ARG:HB3	1:C:528:LYS:HD2	1.77	0.66
2:S:101:THR:O	2:S:110:LEU:N	2.22	0.66
1:A:825:LYS:HD2	1:A:939:PHE:HA	1.77	0.65
1:B:540:PHE:CE2	1:B:550:VAL:C	2.73	0.65
1:B:951:VAL:O	1:B:955:ASN:ND2	2.28	0.65
1:C:443:SER:HB3	1:C:506:PRO:HG3	1.78	0.65
1:C:1142:GLN:OE1	1:C:1142:GLN:N	2.29	0.65
3:T:20:THR:HA	3:T:75:THR:HA	1.76	0.65
1:A:361:CYS:HB3	1:A:523:VAL:HA	1.78	0.65
1:A:443:SER:CB	1:A:506:PRO:HG3	2.26	0.65
1:B:443:SER:HB3	1:B:506:PRO:HG3	1.78	0.65
1:C:853:GLN:C	1:C:855:PHE:H	2.04	0.65
1:A:65:PHE:HE2	1:A:84:LEU:HD11	1.62	0.65
1:A:395:VAL:HG12	1:A:512:LEU:HB3	1.77	0.65
4:D:33:VAL:N	4:D:102:ASN:OD1	2.29	0.65
4:Q:15:GLY:N	4:Q:86:LEU:O	2.26	0.65
1:C:825:LYS:HD2	1:C:939:PHE:HA	1.77	0.65
1:C:853:GLN:NE2	1:C:960:ASN:OD1	2.23	0.65
4:Q:33:VAL:N	4:Q:102:ASN:OD1	2.30	0.65
4:Q:52:ILE:HD11	4:Q:59:ILE:HD13	1.77	0.65
1:A:505:GLN:HE21	4:D:45:LEU:HD12	1.61	0.65
1:C:44:ARG:HB3	1:C:47:VAL:HG21	1.79	0.65
1:A:540:PHE:CE1	1:A:551:LEU:CB	2.80	0.65
1:B:453:TYR:O	1:B:492:GLN:N	2.24	0.65
1:C:422:ASN:HD22	1:C:454:ARG:HG2	1.61	0.65
4:H:52:ILE:HD11	4:H:59:ILE:HD13	1.77	0.65
1:A:540:PHE:CE1	1:A:552:THR:N	2.65	0.65
1:A:1142:GLN:N	1:A:1142:GLN:OE1	2.29	0.65
1:B:422:ASN:HD22	1:B:454:ARG:HG2	1.61	0.65
1:B:443:SER:CB	1:B:506:PRO:HG3	2.26	0.65
5:J:1:ASP:HB3	5:J:3:GLN:H	1.62	0.65
1:A:31:SER:N	1:A:60:SER:O	2.28	0.65
1:A:853:GLN:C	1:A:855:PHE:H	2.04	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:453:TYR:O	1:C:492:GLN:N	2.24	0.65
1:B:540:PHE:CE1	1:B:552:THR:N	2.65	0.65
4:H:33:VAL:N	4:H:102:ASN:OD1	2.29	0.65
4:D:15:GLY:N	4:D:86:LEU:O	2.26	0.65
1:A:326:ILE:HA	1:A:542:PHE:CD1	2.32	0.64
1:A:569:VAL:O	1:A:571:THR:HG23	1.97	0.64
1:B:44:ARG:HB3	1:B:47:VAL:HG21	1.79	0.64
4:Q:5:VAL:O	4:Q:23:LYS:N	2.25	0.64
1:A:562:GLN:HA	1:B:41:LYS:O	1.96	0.64
1:B:65:PHE:HE2	1:B:84:LEU:HD11	1.62	0.64
1:B:326:ILE:HA	1:B:542:PHE:CD1	2.33	0.64
1:C:361:CYS:HB3	1:C:523:VAL:HA	1.78	0.64
1:C:639:SER:HB3	1:C:651:GLY:HA2	1.78	0.64
1:A:344:ALA:HB3	1:A:347:PHE:CE2	2.32	0.64
1:B:1142:GLN:OE1	1:B:1142:GLN:N	2.29	0.64
5:F:1:ASP:OD2	5:F:96:SER:OG	2.12	0.64
5:R:6:GLN:HE22	5:R:102:GLY:H	1.43	0.64
1:A:44:ARG:HB3	1:A:47:VAL:HG21	1.79	0.64
1:A:329:PHE:HA	1:A:578:PRO:HB3	1.78	0.64
1:B:354:ASN:HA	1:B:466:ARG:NH2	2.13	0.64
1:C:569:VAL:O	1:C:571:THR:HG23	1.97	0.64
1:B:604:SER:OG	1:B:605:ASN:N	2.30	0.64
1:B:620:SER:HB3	1:B:623:ILE:HA	1.80	0.64
1:C:65:PHE:HE2	1:C:84:LEU:HD11	1.62	0.64
1:C:360:ASN:O	1:C:361:CYS:HB3	1.97	0.64
1:C:540:PHE:CE1	1:C:551:LEU:CB	2.80	0.64
4:D:52:ILE:HD11	4:D:59:ILE:HD13	1.77	0.64
5:R:1:ASP:HB3	5:R:3:GLN:H	1.62	0.64
1:B:639:SER:HB3	1:B:651:GLY:HA2	1.78	0.64
1:C:540:PHE:CE1	1:C:552:THR:N	2.65	0.64
5:F:83:ILE:HD11	5:F:107:ILE:HG22	1.78	0.64
1:A:230:ILE:HG22	1:A:232:ILE:HB	1.80	0.64
1:A:422:ASN:HD22	1:A:454:ARG:HG2	1.61	0.64
1:A:604:SER:OG	1:A:605:ASN:N	2.30	0.64
1:B:569:VAL:O	1:B:571:THR:HG23	1.97	0.64
1:C:31:SER:N	1:C:60:SER:O	2.28	0.64
2:S:35:SER:HA	2:S:50:TRP:HA	1.80	0.64
1:B:540:PHE:CE1	1:B:551:LEU:CB	2.80	0.64
1:C:393:THR:HG23	1:C:521:ALA:HA	1.79	0.64
1:C:443:SER:CB	1:C:506:PRO:HG3	2.26	0.64
1:A:393:THR:HG23	1:A:521:ALA:HA	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:ASN:ND2	3:K:5:THR:CG2	2.61	0.64
1:B:230:ILE:HG22	1:B:232:ILE:HB	1.80	0.64
1:B:792:PRO:O	1:B:795:LYS:NZ	2.31	0.64
2:E:35:SER:HA	2:E:50:TRP:HA	1.80	0.64
1:A:105:ILE:O	1:A:237:PHE:HA	1.99	0.63
1:B:393:THR:HG23	1:B:521:ALA:HA	1.79	0.63
1:A:337:PRO:HD3	1:A:359:SER:H	1.64	0.63
1:A:360:ASN:O	1:A:361:CYS:HB3	1.98	0.63
1:A:792:PRO:O	1:A:795:LYS:NZ	2.31	0.63
1:B:559:LEU:HD21	1:C:284:THR:HG22	1.80	0.63
1:C:620:SER:HB3	1:C:623:ILE:HA	1.80	0.63
2:I:35:SER:HA	2:I:50:TRP:HA	1.80	0.63
1:B:722:VAL:HG22	1:B:1065:VAL:HG22	1.80	0.63
1:B:853:GLN:C	1:B:855:PHE:H	2.04	0.63
1:C:354:ASN:HA	1:C:466:ARG:NH2	2.13	0.63
2:S:40:ALA:HB3	2:S:43:GLN:HB2	1.80	0.63
1:A:140:PHE:HB3	1:A:241:LEU:HD11	1.79	0.63
1:A:398:ASP:N	1:A:398:ASP:OD1	2.32	0.63
1:C:334:ASN:N	1:C:334:ASN:OD1	2.30	0.63
1:C:337:PRO:HD3	1:C:359:SER:H	1.64	0.63
1:C:550:VAL:HB	1:C:587:THR:HG22	1.81	0.63
1:C:792:PRO:O	1:C:795:LYS:NZ	2.31	0.63
1:C:1118:ASP:OD2	1:C:1118:ASP:N	2.24	0.63
2:E:20:VAL:O	2:E:80:TYR:HA	1.99	0.63
1:A:334:ASN:N	1:A:334:ASN:OD1	2.30	0.63
1:A:639:SER:HB3	1:A:651:GLY:HA2	1.78	0.63
1:B:140:PHE:HB3	1:B:241:LEU:HD11	1.79	0.63
1:C:140:PHE:HB3	1:C:241:LEU:HD11	1.79	0.63
1:C:326:ILE:HA	1:C:542:PHE:CD1	2.33	0.63
5:F:1:ASP:HB3	5:F:3:GLN:H	1.62	0.63
2:I:33:GLY:HA2	2:I:53:THR:HG23	1.81	0.63
3:K:28:THR:HA	3:K:69:GLY:HA2	1.81	0.63
1:A:722:VAL:HG22	1:A:1065:VAL:HG22	1.80	0.63
1:B:528:LYS:NZ	1:B:579:GLN:HB3	2.08	0.63
1:C:344:ALA:HB3	1:C:347:PHE:CE2	2.32	0.63
1:C:1110:TYR:CZ	1:C:1112:PRO:HG3	2.34	0.63
2:E:101:THR:O	2:E:110:LEU:N	2.22	0.63
2:S:20:VAL:O	2:S:80:TYR:HA	1.99	0.63
3:T:55:ARG:NH1	3:T:63:PHE:O	2.31	0.63
1:B:699:LEU:HD12	1:C:872:GLN:CD	2.23	0.63
1:B:1110:TYR:CZ	1:B:1112:PRO:HG3	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:ILE:O	1:C:237:PHE:HA	1.98	0.63
5:J:83:ILE:HD11	5:J:107:ILE:HG22	1.79	0.63
1:A:354:ASN:HA	1:A:466:ARG:NH2	2.13	0.63
1:B:337:PRO:HD3	1:B:359:SER:H	1.64	0.63
1:B:550:VAL:HB	1:B:587:THR:HG22	1.81	0.63
1:A:620:SER:HB3	1:A:623:ILE:HA	1.80	0.63
1:B:25:THR:H	1:B:66:HIS:HB3	1.64	0.63
1:B:360:ASN:O	1:B:361:CYS:HB3	1.97	0.63
1:C:230:ILE:HG22	1:C:232:ILE:HB	1.80	0.63
2:E:33:GLY:HA2	2:E:53:THR:HG23	1.81	0.63
5:R:83:ILE:HD11	5:R:107:ILE:HG22	1.79	0.63
1:B:344:ALA:HB3	1:B:347:PHE:CE2	2.32	0.62
1:C:722:VAL:HG22	1:C:1065:VAL:HG22	1.80	0.62
3:G:55:ARG:NH1	3:G:63:PHE:O	2.31	0.62
3:K:55:ARG:NH1	3:K:63:PHE:O	2.31	0.62
1:B:334:ASN:OD1	1:B:334:ASN:N	2.30	0.62
2:E:40:ALA:HB3	2:E:43:GLN:HB2	1.80	0.62
1:A:1110:TYR:CZ	1:A:1112:PRO:HG3	2.34	0.62
1:B:564:PHE:CZ	1:C:42:VAL:HG22	2.33	0.62
1:C:84:LEU:HD13	1:C:267:VAL:HG21	1.82	0.62
1:C:604:SER:OG	1:C:605:ASN:N	2.30	0.62
2:I:20:VAL:O	2:I:80:TYR:HA	1.99	0.62
4:D:68:VAL:HB	4:D:70:ILE:HD11	1.80	0.62
4:Q:68:VAL:HB	4:Q:70:ILE:HD11	1.80	0.62
1:C:502:VAL:HG11	5:R:93:ASP:O	1.98	0.62
3:G:28:THR:HA	3:G:69:GLY:HA2	1.81	0.62
2:I:35:SER:HB3	2:I:99:ASP:HB2	1.81	0.62
1:B:60:SER:OG	1:B:61:ASN:N	2.32	0.62
1:A:527:LYS:HD2	1:A:528:LYS:H	1.65	0.62
1:B:105:ILE:O	1:B:237:PHE:HA	1.98	0.62
3:G:8:PRO:HG2	3:G:21:LEU:HA	1.82	0.62
2:I:40:ALA:HB3	2:I:43:GLN:HB2	1.80	0.62
3:T:49:ILE:HG23	3:T:54:SER:O	2.00	0.62
1:A:84:LEU:HD13	1:A:267:VAL:HG21	1.82	0.62
1:A:550:VAL:HB	1:A:587:THR:HG22	1.81	0.62
1:B:472:ILE:HG23	1:B:490:PRO:HD3	1.82	0.62
1:B:527:LYS:HD2	1:B:528:LYS:H	1.65	0.62
1:B:971:GLY:O	1:B:995:ARG:NH1	2.33	0.62
1:C:527:LYS:HD2	1:C:528:LYS:H	1.65	0.62
4:H:68:VAL:HB	4:H:70:ILE:HD11	1.79	0.62
3:T:8:PRO:HG2	3:T:21:LEU:HA	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:398:ASP:N	1:C:398:ASP:OD1	2.32	0.62
1:B:398:ASP:OD1	1:B:398:ASP:N	2.32	0.61
1:C:60:SER:OG	1:C:61:ASN:N	2.32	0.61
2:E:35:SER:HB3	2:E:99:ASP:HB2	1.81	0.61
3:G:35:ALA:O	3:G:90:GLN:N	2.32	0.61
3:G:49:ILE:HG23	3:G:54:SER:O	2.00	0.61
2:S:33:GLY:HA2	2:S:53:THR:HG23	1.81	0.61
2:S:35:SER:HB3	2:S:99:ASP:HB2	1.81	0.61
1:A:25:THR:H	1:A:66:HIS:HB3	1.64	0.61
1:B:457:ARG:HA	1:B:490:PRO:HB3	1.81	0.61
1:A:457:ARG:HA	1:A:490:PRO:HB3	1.81	0.61
4:H:100:PHE:HD1	4:H:112:PHE:HB2	1.65	0.61
4:D:5:VAL:O	4:D:23:LYS:N	2.25	0.61
3:T:28:THR:HA	3:T:69:GLY:HA2	1.81	0.61
3:T:35:ALA:O	3:T:90:GLN:N	2.32	0.61
1:B:568:ILE:HG13	1:C:47:VAL:CG1	2.30	0.61
1:C:25:THR:H	1:C:66:HIS:HB3	1.64	0.61
1:C:337:PRO:HG2	1:C:358:ILE:HA	1.83	0.61
1:C:361:CYS:CB	1:C:523:VAL:HA	2.31	0.61
5:J:21:ILE:O	5:J:73:PHE:N	2.33	0.61
1:A:343:ASN:ND2	6:O:6:FUC:H63	2.15	0.61
1:A:444:LYS:CD	3:K:101:GLY:HA3	2.30	0.61
1:A:549:GLY:H	1:A:551:LEU:HD11	1.66	0.61
1:B:567:ASP:HB3	1:B:573:ASP:OD2	2.01	0.61
1:C:457:ARG:HA	1:C:490:PRO:HB3	1.81	0.61
1:C:971:GLY:O	1:C:995:ARG:NH1	2.33	0.61
1:A:502:VAL:HG21	4:D:46:GLU:OE2	2.00	0.61
1:A:567:ASP:HB3	1:A:573:ASP:OD2	2.01	0.61
1:A:971:GLY:O	1:A:995:ARG:NH1	2.33	0.61
1:A:472:ILE:HG23	1:A:490:PRO:HD3	1.82	0.61
1:B:549:GLY:H	1:B:551:LEU:HD11	1.66	0.61
1:C:433:VAL:HG22	1:C:511:VAL:HG13	1.83	0.61
1:C:472:ILE:HG23	1:C:490:PRO:HD3	1.82	0.61
2:S:31:SER:HA	2:S:105:TRP:CZ2	2.36	0.61
4:Q:100:PHE:HD1	4:Q:112:PHE:HB2	1.65	0.61
1:A:328:ARG:O	1:A:528:LYS:NZ	2.31	0.61
1:A:337:PRO:HA	2:I:31:SER:OG	2.00	0.61
1:A:405:ASN:ND2	4:D:99:LEU:HD23	2.15	0.61
1:A:433:VAL:HG22	1:A:511:VAL:HG13	1.83	0.61
1:A:787:GLN:OE1	1:C:703:ASN:ND2	2.34	0.61
3:K:8:PRO:HG2	3:K:21:LEU:HA	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:100:PHE:HD1	4:D:112:PHE:HB2	1.65	0.61
1:A:502:VAL:HA	1:A:505:GLN:HB2	1.82	0.61
3:T:9:GLY:HA2	3:T:102:THR:HA	1.83	0.61
1:A:831:ALA:HA	1:A:851:CYS:HB3	1.83	0.61
1:B:475:ALA:HB3	1:B:484:GLY:N	2.16	0.61
1:B:502:VAL:HA	1:B:505:GLN:HB2	1.82	0.61
3:G:7:SER:HB2	3:G:22:SER:HB3	1.83	0.61
3:G:9:GLY:HA2	3:G:102:THR:HA	1.83	0.61
4:H:36:TRP:HD1	4:H:50:GLY:HA2	1.66	0.61
3:K:9:GLY:HA2	3:K:102:THR:HA	1.83	0.61
5:J:11:LEU:H	5:J:103:THR:HG23	1.66	0.61
1:A:475:ALA:HB3	1:A:484:GLY:N	2.16	0.60
1:B:582:GLU:OE1	1:B:582:GLU:HA	2.00	0.60
1:C:1116:THR:OG1	1:C:1117:THR:N	2.34	0.60
3:K:7:SER:HB2	3:K:22:SER:HB3	1.83	0.60
4:D:36:TRP:HD1	4:D:50:GLY:HA2	1.66	0.60
1:A:1116:THR:OG1	1:A:1117:THR:N	2.34	0.60
1:B:84:LEU:HD13	1:B:267:VAL:HG21	1.81	0.60
5:R:11:LEU:H	5:R:103:THR:HG23	1.66	0.60
1:A:328:ARG:HD2	1:A:329:PHE:H	1.67	0.60
1:A:361:CYS:CB	1:A:523:VAL:HA	2.31	0.60
1:B:328:ARG:HD2	1:B:329:PHE:H	1.67	0.60
1:B:328:ARG:HG3	1:B:330:PRO:HD2	1.83	0.60
1:C:454:ARG:HD2	1:C:457:ARG:HG3	1.84	0.60
1:C:582:GLU:OE1	1:C:582:GLU:HA	2.00	0.60
1:C:804:GLN:OE1	1:C:935:GLN:NE2	2.35	0.60
4:H:5:VAL:O	4:H:23:LYS:N	2.26	0.60
5:R:13:ALA:HB1	5:R:17:ASP:HB3	1.84	0.60
1:A:618:GLU:N	1:A:618:GLU:OE2	2.35	0.60
1:B:361:CYS:CB	1:B:523:VAL:HA	2.31	0.60
1:B:429:PHE:HB2	1:B:514:PHE:HE1	1.67	0.60
1:B:618:GLU:OE2	1:B:618:GLU:N	2.35	0.60
1:C:321:GLN:NE2	1:C:539:ASN:OD1	2.35	0.60
1:C:549:GLY:H	1:C:551:LEU:HD11	1.66	0.60
1:C:567:ASP:HB3	1:C:573:ASP:OD2	2.01	0.60
3:K:35:ALA:O	3:K:90:GLN:N	2.32	0.60
3:K:49:ILE:HG23	3:K:54:SER:O	2.00	0.60
5:J:14:SER:OG	5:J:15:VAL:N	2.33	0.60
1:A:454:ARG:HD2	1:A:457:ARG:HG3	1.84	0.60
1:B:321:GLN:NE2	1:B:539:ASN:OD1	2.35	0.60
1:B:804:GLN:OE1	1:B:935:GLN:NE2	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:831:ALA:HA	1:B:851:CYS:HB3	1.83	0.60
2:I:31:SER:HA	2:I:105:TRP:CZ2	2.36	0.60
1:A:321:GLN:NE2	1:A:539:ASN:OD1	2.35	0.60
1:A:328:ARG:HG3	1:A:330:PRO:HD2	1.83	0.60
1:C:328:ARG:O	1:C:528:LYS:NZ	2.31	0.60
1:C:502:VAL:HA	1:C:505:GLN:HB2	1.82	0.60
3:G:19:ALA:N	3:G:76:ILE:O	2.32	0.60
1:C:475:ALA:HB3	1:C:484:GLY:N	2.16	0.60
2:E:31:SER:HA	2:E:105:TRP:CZ2	2.36	0.60
5:F:79:GLN:HB2	5:F:80:PRO:HD2	1.83	0.60
5:J:79:GLN:HB2	5:J:80:PRO:HD2	1.83	0.60
1:A:337:PRO:HG2	1:A:358:ILE:HA	1.83	0.60
1:A:804:GLN:OE1	1:A:935:GLN:NE2	2.35	0.60
1:C:618:GLU:N	1:C:618:GLU:OE2	2.35	0.60
5:J:13:ALA:HB1	5:J:17:ASP:HB3	1.84	0.60
2:S:24:ALA:HB3	2:S:77:THR:HB	1.84	0.60
4:Q:36:TRP:HD1	4:Q:50:GLY:HA2	1.66	0.60
1:A:419:ALA:HB1	1:A:424:LYS:HD2	1.84	0.59
2:E:103:GLY:HA3	2:E:110:LEU:HD22	1.84	0.59
5:F:11:LEU:H	5:F:103:THR:HG23	1.66	0.59
5:R:5:THR:HA	5:R:101:GLN:HE22	1.67	0.59
1:A:429:PHE:HB2	1:A:514:PHE:HE1	1.67	0.59
1:A:862:PRO:HB2	1:C:645:ARG:HH11	1.66	0.59
1:C:328:ARG:HD2	1:C:329:PHE:H	1.67	0.59
1:C:662:ASP:HB2	1:C:672:SER:HB2	1.84	0.59
3:T:7:SER:HB2	3:T:22:SER:HB3	1.83	0.59
1:B:87:ASN:HB2	1:B:269:TYR:CD1	2.37	0.59
1:B:419:ALA:HB1	1:B:424:LYS:HD2	1.84	0.59
1:C:328:ARG:HG3	1:C:330:PRO:HD2	1.83	0.59
4:D:85:SER:O	4:D:85:SER:OG	2.18	0.59
2:S:94:TYR:CE2	2:S:123:VAL:HG21	2.38	0.59
5:R:21:ILE:O	5:R:73:PHE:N	2.33	0.59
5:R:79:GLN:HB2	5:R:80:PRO:HD2	1.83	0.59
1:B:90:VAL:HG11	1:B:237:PHE:CZ	2.37	0.59
1:B:321:GLN:NE2	1:B:322:PRO:O	2.36	0.59
1:B:433:VAL:HG22	1:B:511:VAL:HG13	1.83	0.59
1:B:1130:ILE:HD11	1:C:921:LYS:HD3	1.85	0.59
1:C:321:GLN:NE2	1:C:322:PRO:O	2.36	0.59
1:C:458:LYS:HG2	1:C:459:SER:OG	2.03	0.59
1:A:446:SER:HA	5:J:57:GLY:HA2	1.83	0.59
1:A:458:LYS:HG2	1:A:459:SER:OG	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:554:SER:HB3	1:A:585:ASP:H	1.68	0.59
1:A:662:ASP:HB2	1:A:672:SER:HB2	1.84	0.59
1:B:337:PRO:HG2	1:B:358:ILE:HA	1.83	0.59
2:E:36:TRP:C	2:E:48:MET:HB2	2.27	0.59
2:S:36:TRP:C	2:S:48:MET:HB2	2.27	0.59
1:A:321:GLN:NE2	1:A:322:PRO:O	2.36	0.59
1:A:550:VAL:C	1:A:551:LEU:HG	2.28	0.59
1:A:582:GLU:HA	1:A:582:GLU:OE1	2.00	0.59
1:B:139:PRO:HG2	1:B:140:PHE:CE1	2.38	0.59
1:B:458:LYS:HG2	1:B:459:SER:OG	2.03	0.59
1:C:32:PHE:HB2	1:C:217:GLN:HB2	1.85	0.59
1:C:429:PHE:HB2	1:C:514:PHE:HE1	1.67	0.59
1:C:550:VAL:C	1:C:551:LEU:HG	2.28	0.59
2:E:94:TYR:CE2	2:E:123:VAL:HG21	2.38	0.59
2:I:94:TYR:CE2	2:I:123:VAL:HG21	2.38	0.59
1:A:536:LYS:O	1:A:537:CYS:HB2	2.03	0.59
1:A:538:VAL:HG13	1:A:538:VAL:O	2.03	0.59
1:B:32:PHE:HB2	1:B:217:GLN:HB2	1.85	0.59
1:B:591:PHE:CZ	1:C:854:LYS:O	2.56	0.59
1:C:90:VAL:HG11	1:C:237:PHE:CZ	2.37	0.59
2:S:37:VAL:HB	2:S:45:LEU:HB3	1.85	0.59
1:A:32:PHE:HB2	1:A:217:GLN:HB2	1.85	0.59
1:B:622:ALA:C	1:B:624:HIS:H	2.08	0.59
1:C:130:VAL:O	1:C:167:THR:OG1	2.18	0.59
4:D:98:ARG:HG3	4:D:114:ILE:HD12	1.85	0.59
4:Q:98:ARG:HG3	4:Q:114:ILE:HD12	1.85	0.59
4:Q:122:THR:HG22	4:Q:123:VAL:H	1.68	0.59
1:A:90:VAL:HG11	1:A:237:PHE:CZ	2.37	0.59
1:B:662:ASP:HB2	1:B:672:SER:HB2	1.84	0.59
1:C:536:LYS:O	1:C:537:CYS:HB2	2.03	0.59
2:E:24:ALA:HB3	2:E:77:THR:HB	1.84	0.59
2:I:36:TRP:C	2:I:48:MET:HB2	2.27	0.59
5:J:5:THR:HA	5:J:101:GLN:HE22	1.67	0.59
3:T:48:LEU:HD11	3:T:63:PHE:CE2	2.38	0.59
1:A:87:ASN:HB2	1:A:269:TYR:CD1	2.37	0.59
1:A:616:CYS:HA	1:A:619:VAL:HG12	1.85	0.59
1:C:426:PRO:HD3	1:C:464:PHE:HD2	1.68	0.59
1:C:538:VAL:O	1:C:538:VAL:HG13	2.03	0.59
5:F:5:THR:HA	5:F:101:GLN:HE22	1.67	0.59
1:A:60:SER:OG	1:A:61:ASN:N	2.32	0.58
1:C:440:LYS:HD3	5:R:49:TYR:HE2	1.66	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:36:TRP:O	4:H:48:MET:N	2.36	0.58
5:F:13:ALA:HB1	5:F:17:ASP:HB3	1.84	0.58
4:D:36:TRP:O	4:D:48:MET:N	2.36	0.58
1:C:87:ASN:HB2	1:C:269:TYR:CD1	2.37	0.58
1:C:616:CYS:HA	1:C:619:VAL:HG12	1.85	0.58
4:D:92:ALA:HB3	4:D:94:TYR:CE1	2.38	0.58
4:Q:36:TRP:O	4:Q:48:MET:N	2.36	0.58
1:B:130:VAL:O	1:B:167:THR:OG1	2.18	0.58
1:B:585:ASP:OD2	1:C:847:ARG:NH2	2.35	0.58
1:C:831:ALA:HA	1:C:851:CYS:HB3	1.83	0.58
3:K:48:LEU:HD11	3:K:63:PHE:CE2	2.38	0.58
1:A:139:PRO:HG2	1:A:140:PHE:CE1	2.38	0.58
1:C:554:SER:HB3	1:C:585:ASP:H	1.67	0.58
2:S:103:GLY:HA3	2:S:110:LEU:HD22	1.84	0.58
1:B:454:ARG:HD2	1:B:457:ARG:HG3	1.84	0.58
1:B:616:CYS:HA	1:B:619:VAL:HG12	1.85	0.58
4:H:122:THR:HG22	4:H:123:VAL:H	1.68	0.58
2:S:117:TRP:HB2	3:T:44:ALA:HB1	1.86	0.58
1:A:876:ALA:O	1:A:877:LEU:HB2	2.02	0.58
3:G:48:LEU:HD11	3:G:63:PHE:CE2	2.38	0.58
4:H:98:ARG:HG3	4:H:114:ILE:HD12	1.85	0.58
5:R:1:ASP:OD2	5:R:96:SER:OG	2.12	0.58
1:B:422:ASN:HA	1:B:454:ARG:HE	1.69	0.58
5:F:47:LEU:H	5:F:47:LEU:HD12	1.69	0.58
3:K:40:LYS:O	3:K:42:GLY:N	2.37	0.58
1:B:538:VAL:O	1:B:538:VAL:HG13	2.03	0.58
1:B:554:SER:HB3	1:B:585:ASP:H	1.67	0.58
4:H:85:SER:O	4:H:85:SER:OG	2.18	0.58
2:I:24:ALA:HB3	2:I:77:THR:HB	1.84	0.58
2:I:103:GLY:HA3	2:I:110:LEU:HD22	1.84	0.58
1:A:130:VAL:O	1:A:167:THR:OG1	2.18	0.58
1:B:536:LYS:O	1:B:537:CYS:HB2	2.03	0.58
1:B:876:ALA:O	1:B:877:LEU:HB2	2.02	0.58
4:H:92:ALA:HB3	4:H:94:TYR:CE1	2.38	0.58
5:F:14:SER:OG	5:F:15:VAL:N	2.33	0.58
1:B:115:GLN:HE22	1:B:166:CYS:HA	1.69	0.58
1:B:564:PHE:O	1:C:43:PHE:N	2.18	0.58
1:C:139:PRO:HG2	1:C:140:PHE:CE1	2.38	0.58
4:D:5:VAL:HA	4:D:117:GLN:HE22	1.69	0.58
4:D:6:GLN:HG3	4:D:7:SER:H	1.68	0.58
3:T:40:LYS:O	3:T:42:GLY:N	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:5:VAL:HA	4:Q:117:GLN:HE22	1.69	0.58
1:C:112:SER:CA	1:C:132:GLU:HB3	2.34	0.57
1:C:419:ALA:HB1	1:C:424:LYS:HD2	1.84	0.57
4:H:115:TRP:CH2	5:F:44:PRO:HB2	2.38	0.57
1:C:876:ALA:O	1:C:877:LEU:HB2	2.02	0.57
1:A:406:GLU:HG2	1:A:494:TYR:HE1	1.69	0.57
1:A:564:PHE:H	1:A:564:PHE:HD2	1.52	0.57
1:C:564:PHE:H	1:C:564:PHE:HD2	1.52	0.57
2:E:37:VAL:HB	2:E:45:LEU:HB3	1.85	0.57
3:G:21:LEU:O	3:G:74:LEU:N	2.31	0.57
4:Q:92:ALA:HB3	4:Q:94:TYR:CE1	2.38	0.57
1:B:438:SER:HB2	1:B:441:LEU:HB2	1.86	0.57
1:B:528:LYS:HG3	1:B:529:SER:N	2.19	0.57
1:C:20:ASN:OD1	1:C:21:LEU:N	2.38	0.57
1:C:542:PHE:HD2	1:C:546:THR:HG23	1.69	0.57
2:E:25:SER:O	2:E:27:TYR:N	2.34	0.57
4:H:5:VAL:HA	4:H:117:GLN:HE22	1.69	0.57
2:S:38:ARG:HE	2:S:92:ALA:HB3	1.69	0.57
1:A:115:GLN:HE22	1:A:166:CYS:HA	1.69	0.57
1:A:346:ARG:NH2	3:K:24:ARG:CB	2.68	0.57
1:A:505:GLN:OE1	1:A:506:PRO:HD2	2.05	0.57
1:B:20:ASN:OD1	1:B:21:LEU:N	2.38	0.57
1:B:358:ILE:HD11	1:B:395:VAL:H	1.69	0.57
1:B:600:GLY:C	1:B:602:ASN:H	2.13	0.57
2:I:38:ARG:HE	2:I:92:ALA:HB3	1.70	0.57
3:K:79:LEU:HD22	3:K:104:VAL:HG11	1.86	0.57
4:D:122:THR:HG22	4:D:123:VAL:H	1.68	0.57
5:J:47:LEU:H	5:J:47:LEU:HD12	1.69	0.57
1:A:20:ASN:OD1	1:A:21:LEU:N	2.38	0.57
1:A:438:SER:HB2	1:A:441:LEU:HB2	1.86	0.57
1:B:318:PHE:O	1:B:319:ARG:HB2	2.05	0.57
1:B:542:PHE:HD2	1:B:546:THR:HG23	1.69	0.57
1:B:550:VAL:C	1:B:551:LEU:HG	2.28	0.57
1:C:406:GLU:HG2	1:C:494:TYR:HE1	1.69	0.57
1:C:505:GLN:OE1	1:C:506:PRO:HD2	2.05	0.57
5:R:47:LEU:H	5:R:47:LEU:HD12	1.69	0.57
1:A:422:ASN:HA	1:A:454:ARG:HE	1.69	0.57
1:A:572:THR:O	1:A:572:THR:OG1	2.23	0.57
1:A:936:ASP:N	1:A:936:ASP:OD1	2.36	0.57
1:C:193:VAL:HG13	1:C:204:TYR:HB2	1.86	0.57
1:C:358:ILE:HD11	1:C:395:VAL:H	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:438:SER:HB2	1:C:441:LEU:HB2	1.86	0.57
1:A:318:PHE:O	1:A:319:ARG:HB2	2.05	0.57
1:A:475:ALA:HB3	1:A:484:GLY:H	1.70	0.57
1:A:528:LYS:HG3	1:A:529:SER:N	2.19	0.57
2:E:67:ARG:NH2	2:E:90:ASP:OD2	2.38	0.57
5:F:79:GLN:HG3	5:F:82:ASP:OD2	2.04	0.57
1:A:112:SER:CA	1:A:132:GLU:HB3	2.34	0.57
1:A:358:ILE:HD11	1:A:395:VAL:H	1.69	0.57
1:B:406:GLU:HG2	1:B:494:TYR:HE1	1.69	0.57
1:B:426:PRO:HD3	1:B:464:PHE:HD2	1.68	0.57
1:B:1141:LEU:HD12	1:B:1145:LEU:HD23	1.87	0.57
1:C:475:ALA:HB3	1:C:484:GLY:H	1.70	0.57
2:E:50:TRP:CH2	2:E:107:GLY:HA2	2.40	0.57
3:T:79:LEU:HD22	3:T:104:VAL:HG11	1.86	0.57
4:Q:24:ALA:HB3	4:Q:77:SER:OG	2.05	0.57
5:R:78:LEU:HD23	5:R:78:LEU:H	1.70	0.57
1:B:112:SER:CA	1:B:132:GLU:HB3	2.34	0.57
1:B:475:ALA:HB2	1:B:488:TYR:CD2	2.40	0.57
1:C:318:PHE:O	1:C:319:ARG:HB2	2.05	0.57
1:C:350:VAL:HG23	1:C:400:PHE:CD1	2.35	0.57
1:C:528:LYS:HG3	1:C:529:SER:N	2.19	0.57
1:C:878:LEU:HD12	1:C:1053:PRO:HD2	1.87	0.57
2:E:38:ARG:HE	2:E:92:ALA:HB3	1.70	0.57
3:G:18:ARG:NH1	5:F:70:ASP:OD1	2.38	0.57
3:G:40:LYS:O	3:G:42:GLY:N	2.37	0.57
4:H:6:GLN:HG3	4:H:7:SER:H	1.68	0.57
5:F:21:ILE:O	5:F:73:PHE:N	2.32	0.57
5:F:78:LEU:HD23	5:F:78:LEU:H	1.70	0.57
2:S:50:TRP:CH2	2:S:107:GLY:HA2	2.40	0.57
1:A:542:PHE:HD2	1:A:546:THR:HG23	1.69	0.56
1:C:936:ASP:OD1	1:C:936:ASP:N	2.36	0.56
2:I:50:TRP:CH2	2:I:107:GLY:HA2	2.40	0.56
5:J:78:LEU:HD23	5:J:78:LEU:H	1.70	0.56
1:A:426:PRO:HD3	1:A:464:PHE:HD2	1.68	0.56
1:A:600:GLY:C	1:A:602:ASN:H	2.13	0.56
1:C:622:ALA:C	1:C:624:HIS:H	2.08	0.56
2:I:6:GLN:HG3	2:I:21:SER:O	2.06	0.56
3:T:38:GLN:H	3:T:48:LEU:HB2	1.70	0.56
1:A:317:ASN:ND2	1:A:592:GLY:O	2.39	0.56
1:B:328:ARG:O	1:B:528:LYS:NZ	2.31	0.56
1:B:568:ILE:HA	1:C:47:VAL:CG1	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:GLN:HE22	1:C:166:CYS:HA	1.69	0.56
1:C:403:LYS:HG3	1:C:504:HIS:HA	1.87	0.56
1:C:422:ASN:HA	1:C:454:ARG:HE	1.69	0.56
2:I:37:VAL:HB	2:I:45:LEU:HB3	1.85	0.56
2:I:98:ARG:HB2	2:I:115:ASP:HB3	1.87	0.56
5:J:79:GLN:HG3	5:J:82:ASP:OD2	2.04	0.56
2:S:6:GLN:HG3	2:S:21:SER:O	2.06	0.56
3:T:83:ASP:O	3:T:87:TYR:OH	2.09	0.56
5:R:14:SER:OG	5:R:15:VAL:N	2.33	0.56
5:R:79:GLN:HG3	5:R:82:ASP:OD2	2.04	0.56
1:A:193:VAL:HG13	1:A:204:TYR:HB2	1.86	0.56
1:A:1141:LEU:HD12	1:A:1145:LEU:HD23	1.87	0.56
1:B:371:PHE:HB2	1:B:374:PHE:CE2	2.41	0.56
1:B:405:ASN:N	1:B:503:GLY:O	2.31	0.56
1:C:443:SER:HA	1:C:448:ASN:ND2	2.21	0.56
4:H:24:ALA:HB3	4:H:77:SER:OG	2.05	0.56
4:D:24:ALA:HB3	4:D:77:SER:OG	2.05	0.56
4:Q:6:GLN:HG3	4:Q:7:SER:H	1.68	0.56
4:Q:38:ARG:HD2	4:Q:46:GLU:HB3	1.88	0.56
1:B:403:LYS:HG3	1:B:504:HIS:HA	1.87	0.56
1:B:443:SER:HA	1:B:448:ASN:ND2	2.21	0.56
2:E:98:ARG:HB2	2:E:115:ASP:HB3	1.87	0.56
2:I:42:GLY:HA2	3:K:54:SER:HG	1.69	0.56
4:D:38:ARG:HD2	4:D:46:GLU:HB3	1.88	0.56
5:J:22:THR:HG21	5:J:70:ASP:HB2	1.88	0.56
4:Q:62:GLN:HE21	5:R:94:LEU:HB3	1.70	0.56
5:R:22:THR:HG21	5:R:70:ASP:HB2	1.88	0.56
1:A:346:ARG:HH21	3:K:24:ARG:CB	2.18	0.56
1:A:443:SER:HA	1:A:448:ASN:ND2	2.21	0.56
1:A:622:ALA:C	1:A:624:HIS:H	2.08	0.56
1:A:878:LEU:HD12	1:A:1053:PRO:HD2	1.87	0.56
1:B:591:PHE:HZ	1:C:855:PHE:HA	1.70	0.56
3:G:79:LEU:HD22	3:G:104:VAL:HG11	1.86	0.56
4:H:33:VAL:O	4:H:102:ASN:ND2	2.38	0.56
1:A:426:PRO:HD2	1:A:430:THR:CG2	2.36	0.56
1:A:475:ALA:HB2	1:A:488:TYR:CD2	2.40	0.56
1:B:337:PRO:CD	1:B:359:SER:H	2.18	0.56
1:B:600:GLY:O	1:B:602:ASN:N	2.39	0.56
1:C:475:ALA:HB2	1:C:488:TYR:CD2	2.40	0.56
2:I:25:SER:O	2:I:27:TYR:N	2.34	0.56
7:X:2:NAG:H3	7:X:2:NAG:H83	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:PRO:CD	1:A:359:SER:H	2.18	0.56
1:A:371:PHE:HB2	1:A:374:PHE:CE2	2.41	0.56
1:A:588:PRO:HG2	1:B:855:PHE:CB	2.19	0.56
1:C:426:PRO:HD2	1:C:430:THR:CG2	2.36	0.56
2:S:67:ARG:NH2	2:S:90:ASP:OD2	2.38	0.56
1:A:125:ASN:HB3	1:A:127:PHE:HD2	1.71	0.56
1:A:451:TYR:O	1:A:494:TYR:N	2.38	0.56
1:B:193:VAL:HG13	1:B:204:TYR:HB2	1.86	0.56
1:B:936:ASP:N	1:B:936:ASP:OD1	2.36	0.56
1:C:618:GLU:O	1:C:619:VAL:C	2.49	0.56
3:K:19:ALA:N	3:K:76:ILE:O	2.31	0.56
2:S:98:ARG:HB2	2:S:115:ASP:HB3	1.87	0.56
4:Q:33:VAL:O	4:Q:102:ASN:ND2	2.38	0.56
1:B:24:THR:HB	1:B:66:HIS:HB3	1.88	0.56
1:C:371:PHE:HB2	1:C:374:PHE:CE2	2.41	0.56
1:C:600:GLY:C	1:C:602:ASN:H	2.13	0.56
4:Q:85:SER:O	4:Q:85:SER:OG	2.18	0.56
3:G:38:GLN:H	3:G:48:LEU:HB2	1.70	0.55
3:G:74:LEU:HD23	3:G:76:ILE:HD11	1.89	0.55
5:F:19:VAL:HB	5:F:75:ILE:H	1.71	0.55
4:Q:21:SER:HA	4:Q:79:ALA:O	2.07	0.55
5:R:19:VAL:HB	5:R:75:ILE:H	1.71	0.55
1:A:600:GLY:O	1:A:602:ASN:N	2.39	0.55
1:B:426:PRO:HD2	1:B:430:THR:CG2	2.36	0.55
1:C:317:ASN:ND2	1:C:592:GLY:O	2.39	0.55
1:C:426:PRO:HA	1:C:463:PRO:HB3	1.89	0.55
1:C:443:SER:HB2	1:C:496:PHE:HE2	1.70	0.55
1:C:540:PHE:CD1	1:C:551:LEU:HB3	2.41	0.55
3:T:74:LEU:HD23	3:T:76:ILE:HD11	1.89	0.55
1:B:317:ASN:ND2	1:B:592:GLY:O	2.39	0.55
1:B:353:TRP:CD1	1:B:353:TRP:H	2.24	0.55
1:B:426:PRO:HA	1:B:463:PRO:HB3	1.89	0.55
1:B:475:ALA:HB3	1:B:484:GLY:H	1.70	0.55
1:C:206:LYS:HZ2	1:C:208:THR:HA	1.70	0.55
1:C:337:PRO:CD	1:C:359:SER:H	2.18	0.55
1:C:643:GLN:NE2	1:C:644:THR:O	2.35	0.55
2:E:6:GLN:HG3	2:E:21:SER:O	2.06	0.55
2:I:67:ARG:NH2	2:I:90:ASP:OD2	2.38	0.55
3:K:21:LEU:O	3:K:74:LEU:N	2.31	0.55
3:K:38:GLN:H	3:K:48:LEU:HB2	1.71	0.55
5:J:19:VAL:HB	5:J:75:ILE:H	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:2:NAG:H83	7:N:2:NAG:H3	1.87	0.55
1:A:403:LYS:HG3	1:A:504:HIS:HA	1.87	0.55
1:B:505:GLN:OE1	1:B:506:PRO:HD2	2.05	0.55
1:B:618:GLU:O	1:B:619:VAL:C	2.49	0.55
1:C:1141:LEU:HD12	1:C:1145:LEU:HD23	1.87	0.55
4:H:38:ARG:HD2	4:H:46:GLU:HB3	1.87	0.55
2:I:39:GLN:HE22	3:K:53:SER:HB2	1.72	0.55
5:R:89:GLN:HA	5:R:99:PHE:HA	1.89	0.55
7:U:2:NAG:H3	7:U:2:NAG:H83	1.87	0.55
1:B:125:ASN:HB3	1:B:127:PHE:HD2	1.71	0.55
1:B:189:LEU:HD22	1:B:210:ILE:HD13	1.88	0.55
1:B:441:LEU:HA	3:G:32:THR:HG22	1.89	0.55
1:B:901:GLN:HE21	1:B:905:ARG:HE	1.55	0.55
1:C:189:LEU:HD22	1:C:210:ILE:HD13	1.88	0.55
4:H:21:SER:HA	4:H:79:ALA:O	2.07	0.55
4:H:39:GLN:O	4:H:92:ALA:HB1	2.06	0.55
1:B:118:LEU:N	1:B:129:LYS:O	2.37	0.55
1:B:334:ASN:HB2	2:E:105:TRP:HH2	1.71	0.55
1:B:984:LEU:HB3	1:B:988:GLU:OE1	2.07	0.55
1:B:1107:ARG:HD3	1:C:904:TYR:CZ	2.40	0.55
2:I:12:LYS:HG3	2:I:86:LEU:HD13	1.89	0.55
1:B:356:THR:OG1	1:B:357:ARG:N	2.40	0.55
1:B:561:PHE:CE2	1:C:224:PRO:HD2	2.41	0.55
1:C:984:LEU:HB3	1:C:988:GLU:OE1	2.07	0.55
5:F:89:GLN:HB2	5:F:99:PHE:CD2	2.42	0.55
2:I:14:PRO:HA	2:I:86:LEU:O	2.07	0.55
1:A:118:LEU:N	1:A:129:LYS:O	2.37	0.55
1:A:535:ASN:HA	1:A:552:THR:HA	1.88	0.55
1:A:568:ILE:HD13	1:B:850:ILE:HD12	1.89	0.55
1:B:355:ARG:HG2	1:B:466:ARG:HD2	1.89	0.55
1:B:848:ASP:OD1	1:B:849:LEU:N	2.40	0.55
1:B:878:LEU:HD12	1:B:1053:PRO:HD2	1.87	0.55
1:C:600:GLY:O	1:C:602:ASN:N	2.39	0.55
4:H:39:GLN:NE2	5:F:38:GLN:HE22	2.05	0.55
3:K:74:LEU:HD23	3:K:76:ILE:HD11	1.89	0.55
2:S:98:ARG:O	2:S:115:ASP:N	2.31	0.55
1:A:353:TRP:CD1	1:A:353:TRP:H	2.24	0.55
1:B:31:SER:O	1:B:31:SER:OG	2.22	0.55
1:B:395:VAL:CG1	1:B:512:LEU:HB3	2.37	0.55
1:C:395:VAL:CG1	1:C:512:LEU:HB3	2.37	0.55
4:H:48:MET:HE1	4:H:83:LEU:HD13	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:39:GLN:O	4:D:92:ALA:HB1	2.06	0.55
2:S:14:PRO:HA	2:S:86:LEU:O	2.07	0.55
3:T:21:LEU:O	3:T:74:LEU:N	2.31	0.55
1:B:350:VAL:HG23	1:B:400:PHE:CD1	2.35	0.55
1:C:355:ARG:HG2	1:C:466:ARG:HD2	1.89	0.55
3:T:19:ALA:N	3:T:76:ILE:O	2.32	0.55
1:A:618:GLU:O	1:A:619:VAL:C	2.49	0.54
1:A:921:LYS:HE2	1:A:921:LYS:N	2.21	0.54
1:B:343:ASN:HD21	6:M:1:NAG:HO3	1.55	0.54
1:B:540:PHE:CD1	1:B:551:LEU:HB3	2.41	0.54
1:C:24:THR:HB	1:C:66:HIS:HB3	1.88	0.54
1:C:31:SER:O	1:C:31:SER:OG	2.22	0.54
1:C:322:PRO:O	1:C:323:THR:OG1	2.25	0.54
1:C:572:THR:O	1:C:572:THR:OG1	2.23	0.54
1:C:848:ASP:OD1	1:C:849:LEU:N	2.40	0.54
5:J:47:LEU:HD23	5:J:58:VAL:HB	1.89	0.54
5:R:89:GLN:HB2	5:R:99:PHE:CD2	2.42	0.54
1:A:34:ARG:NH1	1:A:218:GLY:O	2.40	0.54
1:B:334:ASN:CB	2:E:105:TRP:HH2	2.20	0.54
1:B:494:TYR:HB3	1:B:496:PHE:CE1	2.42	0.54
2:E:14:PRO:HA	2:E:86:LEU:O	2.07	0.54
5:F:47:LEU:HD13	5:F:73:PHE:HE1	1.72	0.54
5:F:72:THR:HG22	5:F:74:THR:HG22	1.89	0.54
5:J:72:THR:HG22	5:J:74:THR:HG22	1.89	0.54
1:A:540:PHE:CD1	1:A:551:LEU:HB3	2.41	0.54
1:A:848:ASP:OD1	1:A:849:LEU:N	2.40	0.54
1:A:901:GLN:HE21	1:A:905:ARG:HE	1.55	0.54
5:J:89:GLN:HB2	5:J:99:PHE:CD2	2.42	0.54
4:Q:28:THR:HG23	4:Q:104:ASP:OD1	2.07	0.54
1:A:355:ARG:HG2	1:A:466:ARG:HD2	1.89	0.54
1:A:356:THR:OG1	1:A:357:ARG:N	2.40	0.54
1:A:1053:PRO:O	1:A:1054:GLN:NE2	2.40	0.54
1:B:472:ILE:HA	1:B:490:PRO:HG3	1.90	0.54
1:B:554:SER:HB3	1:B:585:ASP:N	2.23	0.54
1:B:572:THR:O	1:B:572:THR:OG1	2.23	0.54
1:C:239:THR:HG22	1:C:240:LEU:H	1.72	0.54
4:H:28:THR:HG23	4:H:104:ASP:OD1	2.07	0.54
5:F:22:THR:HG21	5:F:70:ASP:HB2	1.88	0.54
1:A:189:LEU:HD22	1:A:210:ILE:HD13	1.88	0.54
1:A:470:THR:O	1:A:470:THR:HG22	2.08	0.54
1:A:472:ILE:HA	1:A:490:PRO:HG3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:TYR:HB3	1:A:496:PHE:CE1	2.42	0.54
1:A:984:LEU:HB3	1:A:988:GLU:OE1	2.07	0.54
1:B:206:LYS:HZ2	1:B:208:THR:HA	1.71	0.54
1:B:470:THR:O	1:B:470:THR:HG22	2.08	0.54
1:C:356:THR:OG1	1:C:357:ARG:N	2.40	0.54
3:G:18:ARG:NE	5:F:69:THR:OG1	2.41	0.54
1:A:166:CYS:SG	1:A:167:THR:N	2.81	0.54
1:C:125:ASN:HB3	1:C:127:PHE:HD2	1.71	0.54
1:C:353:TRP:CD1	1:C:353:TRP:H	2.24	0.54
1:C:535:ASN:HA	1:C:552:THR:HA	1.89	0.54
1:C:554:SER:HB3	1:C:585:ASP:N	2.23	0.54
2:S:32:TYR:HD2	2:S:33:GLY:H	1.56	0.54
4:Q:39:GLN:O	4:Q:92:ALA:HB1	2.06	0.54
5:R:47:LEU:HD23	5:R:58:VAL:HB	1.89	0.54
1:A:443:SER:HB2	1:A:496:PHE:HE2	1.70	0.54
1:A:620:SER:C	1:A:622:ALA:N	2.65	0.54
1:B:112:SER:HB2	1:B:134:GLN:HB2	1.90	0.54
1:B:540:PHE:CZ	1:B:586:ILE:HA	2.43	0.54
1:B:643:GLN:NE2	1:B:644:THR:O	2.35	0.54
1:B:1116:THR:OG1	1:B:1117:THR:N	2.34	0.54
2:E:32:TYR:HD2	2:E:33:GLY:H	1.56	0.54
2:I:18:VAL:CG1	2:I:83:LEU:H	2.21	0.54
1:A:125:ASN:ND2	1:A:171:VAL:HB	2.23	0.54
1:A:502:VAL:HG12	1:A:505:GLN:HG3	1.89	0.54
1:B:535:ASN:HA	1:B:552:THR:HA	1.89	0.54
1:B:1053:PRO:O	1:B:1054:GLN:NE2	2.40	0.54
1:C:451:TYR:O	1:C:494:TYR:N	2.38	0.54
1:C:494:TYR:HB3	1:C:496:PHE:CE1	2.42	0.54
1:C:502:VAL:HG12	1:C:505:GLN:HG3	1.89	0.54
1:C:971:GLY:HA3	1:C:995:ARG:HH11	1.73	0.54
4:H:38:ARG:HD2	4:H:46:GLU:CB	2.38	0.54
4:D:28:THR:HG23	4:D:104:ASP:OD1	2.07	0.54
1:A:426:PRO:HA	1:A:463:PRO:HB3	1.89	0.54
1:B:564:PHE:H	1:B:564:PHE:HD2	1.52	0.54
1:C:118:LEU:N	1:C:129:LYS:O	2.37	0.54
1:C:403:LYS:HG2	1:C:406:GLU:OE2	2.08	0.54
1:C:540:PHE:CZ	1:C:586:ILE:HA	2.43	0.54
1:C:759:PHE:O	1:C:763:LEU:HG	2.08	0.54
1:C:1053:PRO:O	1:C:1054:GLN:NE2	2.40	0.54
4:H:47:TRP:CE2	5:F:97:TYR:CD1	2.96	0.54
5:J:36:TYR:CE2	5:J:46:LEU:HD13	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:LEU:O	1:A:129:LYS:N	2.41	0.54
1:A:239:THR:HG22	1:A:240:LEU:H	1.73	0.54
1:B:1107:ARG:HD3	1:C:904:TYR:CE2	2.42	0.54
5:J:89:GLN:HA	5:J:99:PHE:HA	1.89	0.54
5:R:47:LEU:HD13	5:R:73:PHE:HE1	1.72	0.54
1:A:322:PRO:O	1:A:323:THR:OG1	2.25	0.53
1:A:395:VAL:CG1	1:A:512:LEU:HB3	2.37	0.53
1:A:554:SER:HB3	1:A:585:ASP:N	2.23	0.53
1:B:759:PHE:O	1:B:763:LEU:HG	2.08	0.53
3:G:18:ARG:NH1	5:F:69:THR:H	2.06	0.53
2:I:32:TYR:HD2	2:I:33:GLY:H	1.56	0.53
4:D:38:ARG:HD2	4:D:46:GLU:CB	2.38	0.53
2:S:18:VAL:HG12	2:S:83:LEU:O	2.08	0.53
1:A:24:THR:HB	1:A:66:HIS:HB3	1.88	0.53
1:B:971:GLY:HA3	1:B:995:ARG:HH11	1.73	0.53
2:E:18:VAL:CG1	2:E:83:LEU:H	2.21	0.53
5:F:89:GLN:HA	5:F:99:PHE:HA	1.89	0.53
2:I:18:VAL:HG12	2:I:83:LEU:O	2.08	0.53
4:D:21:SER:HA	4:D:79:ALA:O	2.07	0.53
5:J:47:LEU:HD13	5:J:73:PHE:HE1	1.72	0.53
2:S:25:SER:O	2:S:27:TYR:N	2.34	0.53
1:A:540:PHE:CG	1:A:551:LEU:CB	2.91	0.53
1:A:703:ASN:O	1:B:789:TYR:HA	2.07	0.53
1:B:502:VAL:HG12	1:B:505:GLN:HG3	1.89	0.53
1:C:118:LEU:O	1:C:129:LYS:N	2.41	0.53
1:C:125:ASN:ND2	1:C:171:VAL:HB	2.23	0.53
1:C:166:CYS:SG	1:C:167:THR:N	2.81	0.53
4:H:100:PHE:HD2	5:F:91:TYR:HB2	1.72	0.53
4:D:48:MET:HE1	4:D:83:LEU:HD13	1.89	0.53
5:J:2:ILE:HB	5:J:90:ARG:NH1	2.24	0.53
1:A:112:SER:HB2	1:A:134:GLN:HB2	1.90	0.53
1:A:540:PHE:CZ	1:A:586:ILE:HA	2.43	0.53
1:B:118:LEU:O	1:B:129:LYS:N	2.41	0.53
1:B:166:CYS:SG	1:B:167:THR:N	2.81	0.53
1:B:641:VAL:HG22	1:B:650:ILE:HG12	1.91	0.53
5:F:36:TYR:CE2	5:F:46:LEU:HD13	2.43	0.53
3:K:92:HIS:HA	3:K:96:LEU:HD13	1.91	0.53
2:S:50:TRP:HH2	2:S:107:GLY:HA2	1.73	0.53
1:A:403:LYS:HD2	1:A:496:PHE:HB3	1.90	0.53
1:A:538:VAL:HG23	1:A:550:VAL:N	2.24	0.53
1:A:971:GLY:HA3	1:A:995:ARG:HH11	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:THR:HG22	1:B:240:LEU:H	1.72	0.53
1:B:371:PHE:HA	6:M:2:NAG:H62	1.91	0.53
1:B:764:LYS:O	1:B:768:THR:OG1	2.27	0.53
1:C:641:VAL:HG22	1:C:650:ILE:HG12	1.91	0.53
2:E:18:VAL:HG12	2:E:83:LEU:O	2.08	0.53
5:F:2:ILE:HB	5:F:90:ARG:NH1	2.24	0.53
5:F:47:LEU:HD13	5:F:73:PHE:CE1	2.44	0.53
2:S:12:LYS:HG3	2:S:86:LEU:HD13	1.89	0.53
1:B:403:LYS:HG2	1:B:406:GLU:OE2	2.08	0.53
1:C:34:ARG:NH1	1:C:218:GLY:O	2.40	0.53
1:C:403:LYS:HD2	1:C:496:PHE:HB3	1.91	0.53
1:C:405:ASN:N	1:C:503:GLY:O	2.31	0.53
2:S:18:VAL:CG1	2:S:83:LEU:H	2.21	0.53
3:T:92:HIS:HA	3:T:96:LEU:HD13	1.91	0.53
4:Q:48:MET:HE1	4:Q:83:LEU:HD13	1.89	0.53
1:B:322:PRO:O	1:B:323:THR:OG1	2.25	0.53
1:C:901:GLN:HE21	1:C:905:ARG:HE	1.55	0.53
4:H:2:VAL:HG11	4:H:28:THR:HB	1.91	0.53
4:Q:38:ARG:HD2	4:Q:46:GLU:CB	2.38	0.53
5:R:36:TYR:CE2	5:R:46:LEU:HD13	2.43	0.53
1:A:588:PRO:HD2	1:B:855:PHE:CD1	2.44	0.53
1:B:24:THR:H	1:B:80:ASP:HB2	1.74	0.53
1:B:125:ASN:ND2	1:B:171:VAL:HB	2.23	0.53
1:C:24:THR:H	1:C:80:ASP:HB2	1.74	0.53
1:C:538:VAL:HG23	1:C:550:VAL:N	2.24	0.53
2:E:12:LYS:HG3	2:E:86:LEU:HD13	1.89	0.53
1:A:24:THR:H	1:A:80:ASP:HB2	1.74	0.53
1:A:403:LYS:HG2	1:A:406:GLU:OE2	2.08	0.53
1:B:403:LYS:HD2	1:B:496:PHE:HB3	1.91	0.53
1:B:472:ILE:HG22	1:B:473:TYR:H	1.74	0.53
1:B:540:PHE:CG	1:B:551:LEU:CB	2.91	0.53
1:C:470:THR:HG22	1:C:470:THR:O	2.08	0.53
1:C:764:LYS:O	1:C:768:THR:OG1	2.27	0.53
4:Q:2:VAL:HG11	4:Q:28:THR:HB	1.91	0.53
1:A:500:TYR:HB3	1:A:504:HIS:HB2	1.91	0.53
1:A:641:VAL:HG22	1:A:650:ILE:HG12	1.91	0.53
1:A:759:PHE:O	1:A:763:LEU:HG	2.08	0.53
1:B:95:THR:HA	1:B:188:ASN:O	2.09	0.53
1:B:538:VAL:HG23	1:B:550:VAL:N	2.24	0.53
1:C:528:LYS:HG3	1:C:529:SER:OG	2.09	0.53
2:E:50:TRP:HH2	2:E:107:GLY:HA2	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:27:GLN:CG	5:F:28:ASP:H	2.22	0.53
1:A:405:ASN:N	1:A:503:GLY:O	2.31	0.52
1:C:112:SER:HB2	1:C:134:GLN:HB2	1.90	0.52
1:C:357:ARG:HA	1:C:396:TYR:HD2	1.74	0.52
5:F:1:ASP:HB3	5:F:3:GLN:N	2.24	0.52
5:F:10:SER:O	5:F:10:SER:OG	2.25	0.52
5:F:47:LEU:HD23	5:F:58:VAL:HB	1.89	0.52
4:D:2:VAL:HG11	4:D:28:THR:HB	1.91	0.52
5:R:27:GLN:CG	5:R:28:ASP:H	2.23	0.52
5:R:72:THR:HG22	5:R:74:THR:HG22	1.89	0.52
1:A:95:THR:HA	1:A:188:ASN:O	2.09	0.52
1:A:499:THR:OG1	5:J:81:GLU:OE1	2.27	0.52
1:B:831:ALA:O	1:B:854:LYS:HB2	2.09	0.52
1:C:95:THR:HA	1:C:188:ASN:O	2.09	0.52
1:C:540:PHE:CG	1:C:551:LEU:CB	2.91	0.52
3:G:92:HIS:HA	3:G:96:LEU:HD13	1.91	0.52
4:D:31:SER:O	4:D:33:VAL:N	2.43	0.52
1:A:328:ARG:H	1:A:528:LYS:HE3	1.74	0.52
1:B:514:PHE:N	1:B:514:PHE:CD1	2.72	0.52
1:C:921:LYS:HE2	1:C:921:LYS:N	2.21	0.52
3:K:16:GLY:H	3:K:79:LEU:H	1.57	0.52
1:C:472:ILE:HA	1:C:490:PRO:HG3	1.90	0.52
1:A:498:PRO:HA	1:A:505:GLN:NE2	2.25	0.52
1:B:985:ASP:OD1	1:B:988:GLU:HG2	2.10	0.52
1:C:328:ARG:H	1:C:528:LYS:HE3	1.74	0.52
1:C:472:ILE:HG22	1:C:473:TYR:H	1.74	0.52
4:H:31:SER:O	4:H:33:VAL:N	2.43	0.52
2:I:40:ALA:HA	2:I:92:ALA:HB1	1.92	0.52
1:A:200:TYR:O	1:A:202:LYS:HG3	2.10	0.52
1:A:514:PHE:N	1:A:514:PHE:CD1	2.72	0.52
1:A:733:LYS:HE3	1:A:771:ALA:O	2.10	0.52
1:A:1051:SER:OG	1:A:1064:HIS:ND1	2.31	0.52
1:B:328:ARG:H	1:B:528:LYS:HE3	1.74	0.52
1:B:733:LYS:HE3	1:B:771:ALA:O	2.10	0.52
2:E:40:ALA:HA	2:E:92:ALA:HB1	1.92	0.52
5:F:48:ILE:HG23	5:F:49:TYR:O	2.10	0.52
3:K:6:GLN:HB3	3:K:102:THR:H	1.74	0.52
3:T:64:SER:HB2	3:T:77:SER:HB2	1.91	0.52
5:R:2:ILE:HB	5:R:90:ARG:NH1	2.24	0.52
5:R:34:ASN:OD1	5:R:91:TYR:HB3	2.10	0.52
1:A:350:VAL:HG23	1:A:400:PHE:CD1	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:LYS:NZ	3:K:100:GLY:N	2.49	0.52
1:B:189:LEU:HB2	1:B:210:ILE:HD13	1.92	0.52
1:B:200:TYR:O	1:B:202:LYS:HG3	2.10	0.52
1:B:443:SER:HB2	1:B:496:PHE:HE2	1.70	0.52
1:B:1039:ARG:NH1	1:C:1031:GLU:OE2	2.42	0.52
1:C:200:TYR:O	1:C:202:LYS:HG3	2.09	0.52
5:F:34:ASN:OD1	5:F:91:TYR:HB3	2.10	0.52
5:J:1:ASP:HB3	5:J:3:GLN:N	2.24	0.52
5:J:47:LEU:HD13	5:J:73:PHE:CE1	2.44	0.52
5:R:1:ASP:HB3	5:R:3:GLN:N	2.24	0.52
5:R:48:ILE:HG23	5:R:49:TYR:O	2.10	0.52
1:A:505:GLN:NE2	4:D:45:LEU:HD12	2.23	0.52
1:A:528:LYS:HG3	1:A:529:SER:OG	2.09	0.52
1:A:643:GLN:NE2	1:A:644:THR:O	2.35	0.52
1:B:425:LEU:HD23	1:B:430:THR:HG21	1.92	0.52
1:C:514:PHE:CD1	1:C:514:PHE:N	2.72	0.52
3:G:16:GLY:H	3:G:79:LEU:H	1.57	0.52
5:J:27:GLN:CG	5:J:28:ASP:H	2.23	0.52
5:J:48:ILE:HG23	5:J:49:TYR:O	2.10	0.52
1:A:425:LEU:HD23	1:A:430:THR:HG21	1.92	0.52
1:C:371:PHE:HA	6:V:2:NAG:C6	2.40	0.52
1:C:620:SER:C	1:C:622:ALA:N	2.65	0.52
1:C:733:LYS:HE3	1:C:771:ALA:O	2.10	0.52
1:C:831:ALA:O	1:C:854:LYS:HB2	2.09	0.52
4:H:79:ALA:C	4:H:80:TYR:HD1	2.17	0.52
2:I:50:TRP:HH2	2:I:107:GLY:HA2	1.73	0.52
5:J:34:ASN:OD1	5:J:91:TYR:HB3	2.10	0.52
2:S:18:VAL:HB	2:S:86:LEU:HD11	1.92	0.52
1:A:401:VAL:HG12	1:A:508:ARG:HE	1.75	0.52
1:A:764:LYS:O	1:A:768:THR:OG1	2.27	0.52
1:A:876:ALA:C	1:A:878:LEU:H	2.18	0.52
1:B:194:PHE:CD1	1:B:203:ILE:HG23	2.45	0.52
1:B:498:PRO:HA	1:B:505:GLN:NE2	2.25	0.52
1:B:528:LYS:HG3	1:B:529:SER:OG	2.09	0.52
1:B:591:PHE:CZ	1:C:855:PHE:HA	2.44	0.52
1:B:921:LYS:HE2	1:B:921:LYS:N	2.21	0.52
1:C:194:PHE:CD1	1:C:203:ILE:HG23	2.45	0.52
1:C:395:VAL:O	1:C:513:SER:N	2.21	0.52
1:C:604:SER:OG	1:C:606:GLN:HG3	2.10	0.52
5:F:86:TYR:HB2	5:F:103:THR:O	2.10	0.52
4:D:91:THR:HA	4:D:121:VAL:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:117:TRP:CB	3:T:44:ALA:HB1	2.40	0.52
5:R:47:LEU:HD13	5:R:73:PHE:CE1	2.44	0.52
1:A:357:ARG:HA	1:A:396:TYR:HD2	1.74	0.51
1:B:315:THR:OG1	1:B:316:SER:N	2.43	0.51
1:B:451:TYR:O	1:B:494:TYR:N	2.38	0.51
1:B:1051:SER:OG	1:B:1064:HIS:ND1	2.32	0.51
1:C:876:ALA:C	1:C:878:LEU:H	2.18	0.51
3:G:6:GLN:NE2	3:G:89:CYS:H	2.08	0.51
3:G:6:GLN:HB3	3:G:102:THR:H	1.74	0.51
4:D:33:VAL:O	4:D:102:ASN:ND2	2.38	0.51
5:J:86:TYR:HB2	5:J:103:THR:O	2.10	0.51
3:T:16:GLY:H	3:T:79:LEU:H	1.57	0.51
4:Q:31:SER:O	4:Q:33:VAL:N	2.43	0.51
4:Q:91:THR:HA	4:Q:121:VAL:O	2.10	0.51
1:A:189:LEU:HB2	1:A:210:ILE:HD13	1.92	0.51
1:C:189:LEU:HB2	1:C:210:ILE:HD13	1.92	0.51
1:C:498:PRO:HA	1:C:505:GLN:NE2	2.25	0.51
1:C:985:ASP:OD1	1:C:988:GLU:HG2	2.10	0.51
4:Q:79:ALA:C	4:Q:80:TYR:HD1	2.17	0.51
1:B:340:GLU:HB3	2:E:110:LEU:HD21	1.93	0.51
1:B:577:ASP:OD1	1:B:580:THR:HG23	2.10	0.51
1:C:315:THR:OG1	1:C:316:SER:N	2.43	0.51
1:C:577:ASP:OD1	1:C:580:THR:HG23	2.11	0.51
5:F:5:THR:HA	5:F:101:GLN:NE2	2.26	0.51
5:R:5:THR:HA	5:R:101:GLN:NE2	2.25	0.51
1:A:615:ASN:O	1:A:618:GLU:HB2	2.11	0.51
1:A:831:ALA:O	1:A:854:LYS:HB2	2.09	0.51
1:B:416:GLY:O	1:B:419:ALA:N	2.44	0.51
1:C:1006:THR:O	1:C:1010:GLN:HG2	2.10	0.51
1:C:1091:ARG:HH11	1:C:1118:ASP:HA	1.76	0.51
4:D:51:PHE:HB3	4:D:72:ALA:HB3	1.93	0.51
5:J:95:PRO:HB3	5:J:97:TYR:CE1	2.46	0.51
1:B:34:ARG:NH1	1:B:218:GLY:O	2.40	0.51
1:B:357:ARG:HA	1:B:396:TYR:HD2	1.74	0.51
1:B:1091:ARG:HH11	1:B:1118:ASP:HA	1.76	0.51
1:C:500:TYR:HB3	1:C:504:HIS:HB2	1.91	0.51
1:C:919:ASN:OD1	1:C:919:ASN:N	2.44	0.51
2:I:39:GLN:NE2	3:K:53:SER:HB2	2.25	0.51
3:K:64:SER:HB2	3:K:77:SER:HB2	1.91	0.51
4:D:100:PHE:CD1	4:D:112:PHE:HB2	2.46	0.51
4:Q:64:PHE:HB2	4:Q:68:VAL:HG13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:6:GLN:HB3	5:R:88:CYS:SG	2.51	0.51
1:A:125:ASN:CG	1:A:172:SER:H	2.19	0.51
1:A:472:ILE:HG22	1:A:473:TYR:H	1.74	0.51
1:B:61:ASN:N	1:B:61:ASN:OD1	2.41	0.51
1:B:318:PHE:O	1:B:318:PHE:CG	2.64	0.51
1:B:620:SER:C	1:B:622:ALA:N	2.65	0.51
1:C:33:THR:O	1:C:33:THR:OG1	2.24	0.51
1:C:425:LEU:HD23	1:C:430:THR:HG21	1.92	0.51
2:I:18:VAL:HB	2:I:86:LEU:HD11	1.92	0.51
4:D:64:PHE:HB2	4:D:68:VAL:HG13	1.92	0.51
4:Q:100:PHE:CD1	4:Q:112:PHE:HB2	2.46	0.51
1:A:985:ASP:OD1	1:A:988:GLU:HG2	2.10	0.51
1:B:919:ASN:N	1:B:919:ASN:OD1	2.44	0.51
4:H:98:ARG:CD	4:H:102:ASN:HB3	2.41	0.51
5:F:6:GLN:HB3	5:F:88:CYS:SG	2.51	0.51
5:F:90:ARG:NH2	5:F:98:THR:OG1	2.44	0.51
5:J:6:GLN:HB3	5:J:88:CYS:SG	2.51	0.51
1:A:346:ARG:CB	2:I:112:GLY:HA2	2.36	0.51
1:B:615:ASN:O	1:B:618:GLU:HB2	2.11	0.51
4:D:79:ALA:C	4:D:80:TYR:HD1	2.17	0.51
5:J:5:THR:HA	5:J:101:GLN:NE2	2.25	0.51
3:T:6:GLN:HB3	3:T:102:THR:H	1.74	0.51
5:R:86:TYR:HB2	5:R:103:THR:O	2.10	0.51
5:R:95:PRO:HB3	5:R:97:TYR:CE1	2.46	0.51
1:A:551:LEU:CD2	1:A:586:ILE:HB	2.31	0.51
1:A:1006:THR:O	1:A:1010:GLN:HG2	2.10	0.51
1:B:401:VAL:HG12	1:B:508:ARG:HE	1.75	0.51
1:C:401:VAL:HG12	1:C:508:ARG:HE	1.75	0.51
3:G:64:SER:HB2	3:G:77:SER:HB2	1.92	0.51
5:R:46:LEU:HD11	5:R:48:ILE:O	2.11	0.51
1:A:416:GLY:O	1:A:419:ALA:N	2.44	0.51
1:A:604:SER:OG	1:A:606:GLN:HG3	2.10	0.51
1:C:340:GLU:HB3	2:S:110:LEU:HD21	1.93	0.51
1:A:206:LYS:HZ2	1:A:208:THR:HA	1.75	0.50
1:A:577:ASP:OD1	1:A:580:THR:HG23	2.10	0.50
1:A:1091:ARG:HH11	1:A:1118:ASP:HA	1.76	0.50
1:B:338:PHE:CE2	1:B:363:ALA:HB1	2.46	0.50
1:B:499:THR:HB	4:H:112:PHE:CD1	2.46	0.50
1:B:604:SER:OG	1:B:606:GLN:HG3	2.10	0.50
1:B:981:LEU:HD21	1:B:993:ILE:HD11	1.92	0.50
1:C:37:TYR:HA	1:C:222:LEU:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:36:TYR:CE2	5:F:89:GLN:HB3	2.46	0.50
1:B:37:TYR:HB3	1:B:222:LEU:HB2	1.93	0.50
1:C:37:TYR:HB3	1:C:222:LEU:HB2	1.93	0.50
1:C:334:ASN:HB3	2:S:105:TRP:HH2	1.74	0.50
4:H:64:PHE:HB2	4:H:68:VAL:HG13	1.92	0.50
4:Q:92:ALA:HB3	4:Q:94:TYR:HE1	1.76	0.50
4:Q:98:ARG:CD	4:Q:102:ASN:HB3	2.41	0.50
1:A:37:TYR:HB3	1:A:222:LEU:HB2	1.93	0.50
1:A:37:TYR:HA	1:A:222:LEU:H	1.76	0.50
1:A:43:PHE:HA	1:C:562:GLN:NE2	2.26	0.50
1:C:615:ASN:O	1:C:618:GLU:HB2	2.11	0.50
1:C:981:LEU:HD21	1:C:993:ILE:HD11	1.92	0.50
5:J:48:ILE:HD13	5:J:73:PHE:CE2	2.47	0.50
2:S:65:GLN:OE1	2:S:65:GLN:HA	2.12	0.50
1:A:338:PHE:CE2	1:A:363:ALA:HB1	2.46	0.50
1:A:618:GLU:O	1:A:621:VAL:N	2.45	0.50
1:B:334:ASN:HB3	2:E:30:THR:OG1	2.10	0.50
1:B:500:TYR:HB3	1:B:504:HIS:HB2	1.91	0.50
1:B:618:GLU:O	1:B:621:VAL:N	2.45	0.50
1:C:125:ASN:CG	1:C:172:SER:H	2.19	0.50
1:C:318:PHE:O	1:C:318:PHE:CG	2.64	0.50
1:C:393:THR:OG1	1:C:515:GLU:O	2.23	0.50
2:E:18:VAL:HB	2:E:86:LEU:HD11	1.93	0.50
4:H:91:THR:HA	4:H:121:VAL:O	2.11	0.50
5:F:95:PRO:HB3	5:F:97:TYR:CE1	2.46	0.50
4:D:98:ARG:CD	4:D:102:ASN:HB3	2.41	0.50
1:C:416:GLY:O	1:C:419:ALA:N	2.44	0.50
2:E:67:ARG:HE	2:E:85:ARG:HB3	1.76	0.50
4:H:47:TRP:CZ3	4:H:61:ALA:HA	2.47	0.50
5:J:90:ARG:NH2	5:J:98:THR:OG1	2.44	0.50
4:Q:47:TRP:CZ3	4:Q:61:ALA:HA	2.47	0.50
5:R:36:TYR:CE2	5:R:89:GLN:HB3	2.46	0.50
5:R:90:ARG:NH2	5:R:98:THR:OG1	2.44	0.50
1:A:194:PHE:CD1	1:A:203:ILE:HG23	2.45	0.50
1:C:919:ASN:HB3	1:C:922:LEU:HD23	1.94	0.50
2:E:69:THR:O	2:E:69:THR:OG1	2.30	0.50
2:I:67:ARG:HE	2:I:85:ARG:HB3	1.76	0.50
4:D:47:TRP:CZ3	4:D:61:ALA:HA	2.47	0.50
5:J:36:TYR:CE2	5:J:89:GLN:HB3	2.47	0.50
3:T:7:SER:N	3:T:22:SER:O	2.36	0.50
3:T:65:GLY:HA2	3:T:75:THR:N	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:ASN:CG	4:D:101:PRO:HG3	2.36	0.50
1:B:374:PHE:C	1:B:376:ALA:H	2.20	0.50
1:B:564:PHE:CD2	1:B:564:PHE:N	2.80	0.50
1:C:338:PHE:CE2	1:C:363:ALA:HB1	2.46	0.50
4:H:51:PHE:HB3	4:H:72:ALA:HB3	1.93	0.50
5:F:48:ILE:HD13	5:F:73:PHE:CE2	2.47	0.50
2:I:65:GLN:HA	2:I:65:GLN:OE1	2.12	0.50
4:D:35:SER:HB2	4:D:99:LEU:HD13	1.94	0.50
1:A:318:PHE:O	1:A:318:PHE:CG	2.64	0.50
1:B:33:THR:O	1:B:33:THR:OG1	2.24	0.50
1:B:36:VAL:O	1:B:221:ALA:HA	2.12	0.50
1:B:1006:THR:O	1:B:1010:GLN:HG2	2.10	0.50
1:C:1051:SER:OG	1:C:1064:HIS:ND1	2.32	0.50
1:A:538:VAL:HG23	1:A:550:VAL:CA	2.42	0.50
1:B:91:TYR:OH	1:B:191:GLU:OE1	2.14	0.50
1:B:551:LEU:CD2	1:B:586:ILE:HB	2.31	0.50
1:B:919:ASN:HB3	1:B:922:LEU:HD23	1.94	0.50
1:C:425:LEU:HB3	1:C:430:THR:HG21	1.94	0.50
3:G:65:GLY:HA3	3:G:74:LEU:HD12	1.93	0.50
5:F:46:LEU:HD11	5:F:48:ILE:O	2.11	0.50
4:D:37:VAL:HG21	4:D:115:TRP:CZ3	2.47	0.50
4:D:79:ALA:C	4:D:80:TYR:CD1	2.90	0.50
5:J:46:LEU:HD11	5:J:48:ILE:O	2.11	0.50
4:Q:33:VAL:HG13	4:Q:52:ILE:HA	1.94	0.50
4:Q:51:PHE:HB3	4:Q:72:ALA:HB3	1.93	0.50
5:R:48:ILE:HD13	5:R:73:PHE:CE2	2.47	0.50
1:A:351:TYR:HB3	1:A:422:ASN:ND2	2.27	0.49
1:A:370:ASN:OD1	6:O:5:MAN:H3	2.12	0.49
1:A:981:LEU:HD21	1:A:993:ILE:HD11	1.92	0.49
1:B:1141:LEU:O	1:B:1145:LEU:N	2.29	0.49
1:C:374:PHE:C	1:C:376:ALA:H	2.20	0.49
1:C:538:VAL:HG23	1:C:550:VAL:CA	2.42	0.49
1:C:618:GLU:O	1:C:621:VAL:N	2.45	0.49
3:G:63:PHE:CZ	3:G:74:LEU:HD21	2.47	0.49
4:H:37:VAL:HG21	4:H:115:TRP:CZ3	2.47	0.49
4:H:80:TYR:HD1	4:H:80:TYR:N	2.10	0.49
4:H:92:ALA:HB3	4:H:94:TYR:HE1	1.77	0.49
3:K:48:LEU:HD12	3:K:59:ILE:CD1	2.42	0.49
2:S:40:ALA:HA	2:S:92:ALA:HB1	1.92	0.49
3:T:63:PHE:CZ	3:T:74:LEU:HD21	2.47	0.49
3:T:65:GLY:HA3	3:T:74:LEU:HD12	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:38:ARG:HH22	4:Q:90:ASP:HA	1.77	0.49
1:C:36:VAL:O	1:C:221:ALA:HA	2.12	0.49
3:K:65:GLY:HA2	3:K:75:THR:N	2.27	0.49
4:Q:80:TYR:HD1	4:Q:80:TYR:N	2.10	0.49
1:B:534:LYS:HB3	1:B:540:PHE:HB3	1.94	0.49
1:C:657:ASN:ND2	1:C:659:TYR:OH	2.46	0.49
1:C:853:GLN:C	1:C:855:PHE:N	2.68	0.49
3:K:50:TYR:C	3:K:50:TYR:CD2	2.90	0.49
4:D:24:ALA:HA	4:D:29:PHE:CZ	2.47	0.49
4:D:80:TYR:HD1	4:D:80:TYR:N	2.10	0.49
4:Q:79:ALA:C	4:Q:80:TYR:CD1	2.90	0.49
5:R:10:SER:O	5:R:10:SER:OG	2.25	0.49
1:A:534:LYS:HB3	1:A:540:PHE:HB3	1.94	0.49
1:B:579:GLN:HG3	1:B:580:THR:HG23	1.94	0.49
1:C:351:TYR:HB3	1:C:422:ASN:ND2	2.27	0.49
1:C:747:THR:O	1:C:750:SER:N	2.44	0.49
4:H:33:VAL:HG13	4:H:52:ILE:HA	1.94	0.49
4:H:34:ILE:HB	4:H:98:ARG:HH22	1.77	0.49
4:D:33:VAL:HG13	4:D:52:ILE:HA	1.94	0.49
5:J:10:SER:O	5:J:10:SER:OG	2.24	0.49
3:T:48:LEU:HD12	3:T:59:ILE:CD1	2.42	0.49
5:R:24:GLN:HG3	5:R:70:ASP:HB3	1.94	0.49
1:B:937:SER:O	1:B:941:THR:HB	2.13	0.49
1:C:1100:THR:HG1	1:C:1101:HIS:CE1	2.30	0.49
3:K:63:PHE:CZ	3:K:74:LEU:HD21	2.47	0.49
3:K:65:GLY:HA3	3:K:74:LEU:HD12	1.93	0.49
4:D:34:ILE:HB	4:D:98:ARG:HH22	1.77	0.49
5:J:8:PRO:HD2	5:J:22:THR:O	2.13	0.49
1:A:33:THR:O	1:A:33:THR:OG1	2.24	0.49
1:A:916:LEU:HD12	1:A:923:ILE:HD12	1.95	0.49
1:A:937:SER:O	1:A:941:THR:HB	2.13	0.49
1:C:579:GLN:HG3	1:C:580:THR:HG23	1.94	0.49
2:E:65:GLN:OE1	2:E:65:GLN:HA	2.12	0.49
3:G:6:GLN:OE1	3:G:102:THR:N	2.46	0.49
4:H:98:ARG:HD2	4:H:102:ASN:HB3	1.94	0.49
2:S:67:ARG:HE	2:S:85:ARG:HB3	1.76	0.49
4:Q:35:SER:HB2	4:Q:99:LEU:HD13	1.94	0.49
1:A:36:VAL:O	1:A:221:ALA:HA	2.12	0.49
1:A:86:PHE:N	1:A:235:THR:O	2.46	0.49
1:A:315:THR:OG1	1:A:316:SER:N	2.43	0.49
1:A:919:ASN:OD1	1:A:919:ASN:N	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:LEU:HB3	1:B:430:THR:HG21	1.94	0.49
1:B:565:GLY:CA	1:C:43:PHE:HB3	2.43	0.49
1:B:568:ILE:HA	1:C:47:VAL:HG11	1.93	0.49
1:B:876:ALA:C	1:B:878:LEU:H	2.18	0.49
4:H:79:ALA:C	4:H:80:TYR:CD1	2.90	0.49
5:J:28:ASP:OD2	5:J:69:THR:HG23	2.13	0.49
4:Q:37:VAL:HG21	4:Q:115:TRP:CZ3	2.47	0.49
1:A:337:PRO:HD2	1:A:358:ILE:HB	1.95	0.49
1:A:579:GLN:HG3	1:A:580:THR:HG23	1.94	0.49
1:B:44:ARG:HB3	1:B:47:VAL:CG2	2.43	0.49
1:C:1141:LEU:O	1:C:1145:LEU:N	2.29	0.49
4:H:80:TYR:N	4:H:80:TYR:CD1	2.81	0.49
5:F:8:PRO:HD2	5:F:22:THR:O	2.13	0.49
5:J:24:GLN:HG3	5:J:70:ASP:HB3	1.94	0.49
1:A:25:THR:N	1:A:66:HIS:HB3	2.28	0.49
1:A:337:PRO:HD3	1:A:359:SER:OG	2.13	0.49
1:B:86:PHE:N	1:B:235:THR:O	2.46	0.49
1:B:125:ASN:CG	1:B:172:SER:H	2.19	0.49
1:C:337:PRO:HD2	1:C:358:ILE:HB	1.95	0.49
1:C:350:VAL:HG13	1:C:422:ASN:HD21	1.78	0.49
3:G:36:TRP:HA	3:G:89:CYS:HA	1.95	0.49
3:G:65:GLY:HA2	3:G:75:THR:N	2.27	0.49
5:F:68:GLY:H	5:F:71:PHE:HE1	1.60	0.49
4:Q:80:TYR:N	4:Q:80:TYR:CD1	2.81	0.49
5:R:2:ILE:CG2	5:R:27:GLN:H	2.26	0.49
1:A:568:ILE:HB	1:B:850:ILE:CD1	2.43	0.49
1:B:337:PRO:HD3	1:B:359:SER:OG	2.13	0.49
1:B:350:VAL:HG13	1:B:422:ASN:HD21	1.78	0.49
1:B:535:ASN:O	1:B:536:LYS:O	2.31	0.49
1:B:916:LEU:HD12	1:B:923:ILE:HD12	1.95	0.49
1:C:337:PRO:HD3	1:C:359:SER:OG	2.12	0.49
4:H:38:ARG:HH22	4:H:90:ASP:HA	1.78	0.49
4:H:45:LEU:HG	5:F:87:TYR:CG	2.47	0.49
4:H:100:PHE:CD1	4:H:112:PHE:HB2	2.46	0.49
4:D:98:ARG:HD2	4:D:102:ASN:HB3	1.94	0.49
4:Q:34:ILE:HB	4:Q:98:ARG:HH22	1.77	0.49
1:A:374:PHE:C	1:A:376:ALA:H	2.20	0.48
1:A:406:GLU:HG3	1:A:418:ILE:HD12	1.95	0.48
1:A:561:PHE:HB2	1:B:41:LYS:HE2	1.94	0.48
1:A:919:ASN:HB3	1:A:922:LEU:HD23	1.94	0.48
1:B:37:TYR:OH	1:B:53:ASP:OD2	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:TYR:HB3	1:B:422:ASN:ND2	2.27	0.48
1:B:357:ARG:HB3	1:B:396:TYR:HE2	1.78	0.48
1:B:393:THR:HG22	1:B:522:THR:HG23	1.95	0.48
1:C:25:THR:N	1:C:66:HIS:HB3	2.28	0.48
1:C:37:TYR:OH	1:C:53:ASP:OD2	2.31	0.48
1:C:200:TYR:HB3	1:C:227:ASP:OD1	2.13	0.48
1:C:406:GLU:HG3	1:C:418:ILE:HD12	1.95	0.48
1:C:564:PHE:N	1:C:564:PHE:CD2	2.80	0.48
1:C:833:PHE:HE2	1:C:851:CYS:HB2	1.78	0.48
1:C:937:SER:O	1:C:941:THR:HB	2.13	0.48
3:T:36:TRP:HA	3:T:89:CYS:HA	1.95	0.48
1:A:393:THR:HG22	1:A:522:THR:HG23	1.95	0.48
1:A:425:LEU:HB3	1:A:430:THR:HG21	1.95	0.48
1:A:900:MET:HE2	1:A:900:MET:HB3	1.60	0.48
1:B:657:ASN:ND2	1:B:659:TYR:OH	2.46	0.48
1:C:393:THR:HG22	1:C:522:THR:HG23	1.95	0.48
1:C:402:ILE:HD11	1:C:509:VAL:HG21	1.95	0.48
1:C:426:PRO:HD3	1:C:464:PHE:CD2	2.48	0.48
1:C:527:LYS:HD2	1:C:528:LYS:N	2.28	0.48
4:H:39:GLN:O	4:H:39:GLN:HG3	2.13	0.48
5:F:22:THR:CG2	5:F:70:ASP:HB2	2.43	0.48
2:I:38:ARG:HH12	2:I:90:ASP:HA	1.78	0.48
2:S:93:VAL:HB	2:S:122:LEU:HA	1.95	0.48
4:Q:24:ALA:HA	4:Q:29:PHE:CZ	2.47	0.48
4:Q:39:GLN:O	4:Q:39:GLN:HG3	2.13	0.48
5:R:28:ASP:OD2	5:R:69:THR:HG23	2.13	0.48
1:A:657:ASN:ND2	1:A:659:TYR:OH	2.46	0.48
1:A:833:PHE:HE2	1:A:851:CYS:HB2	1.78	0.48
1:B:37:TYR:HA	1:B:222:LEU:H	1.76	0.48
1:B:140:PHE:HD1	1:B:241:LEU:HD11	1.79	0.48
1:B:200:TYR:HB3	1:B:227:ASP:OD1	2.13	0.48
1:B:538:VAL:HG23	1:B:550:VAL:CA	2.42	0.48
1:B:833:PHE:HE2	1:B:851:CYS:HB2	1.78	0.48
1:C:500:TYR:CA	4:Q:101:PRO:HB3	2.40	0.48
1:C:916:LEU:HD12	1:C:923:ILE:HD12	1.95	0.48
2:E:33:GLY:HA2	2:E:53:THR:H	1.79	0.48
2:E:38:ARG:HH12	2:E:90:ASP:HA	1.78	0.48
3:G:6:GLN:HG2	3:G:23:CYS:HB2	1.95	0.48
3:G:50:TYR:C	3:G:50:TYR:CD2	2.90	0.48
2:I:33:GLY:HA2	2:I:53:THR:H	1.79	0.48
2:I:70:MET:HE2	2:I:81:MET:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:15:VAL:HA	5:J:78:LEU:HG	1.96	0.48
2:S:102:ARG:HA	2:S:109:SER:HA	1.95	0.48
3:T:6:GLN:OE1	3:T:102:THR:N	2.46	0.48
3:T:50:TYR:C	3:T:50:TYR:CD2	2.90	0.48
1:A:204:TYR:HA	1:A:224:PRO:HA	1.95	0.48
1:A:358:ILE:HD11	1:A:395:VAL:HG23	1.95	0.48
1:B:340:GLU:O	1:B:344:ALA:HB2	2.13	0.48
1:C:204:TYR:HA	1:C:224:PRO:HA	1.95	0.48
1:C:422:ASN:OD1	1:C:423:TYR:HB2	2.14	0.48
3:G:7:SER:N	3:G:22:SER:O	2.36	0.48
5:F:6:GLN:NE2	5:F:86:TYR:O	2.46	0.48
4:D:38:ARG:NH2	4:D:90:ASP:HA	2.28	0.48
2:S:4:LEU:N	2:S:25:SER:OG	2.46	0.48
5:R:22:THR:CG2	5:R:70:ASP:HB2	2.43	0.48
1:A:350:VAL:HG13	1:A:422:ASN:HD21	1.78	0.48
1:B:49:HIS:CD2	1:B:51:THR:HG22	2.49	0.48
1:B:496:PHE:HB2	1:B:504:HIS:O	2.13	0.48
1:B:703:ASN:O	1:C:789:TYR:HA	2.14	0.48
5:F:24:GLN:HG3	5:F:70:ASP:HB3	1.94	0.48
4:D:38:ARG:HH22	4:D:90:ASP:HA	1.78	0.48
4:D:80:TYR:CD1	4:D:80:TYR:N	2.81	0.48
5:J:6:GLN:NE2	5:J:86:TYR:O	2.46	0.48
1:A:49:HIS:CD2	1:A:51:THR:HG22	2.48	0.48
1:A:200:TYR:HB3	1:A:227:ASP:OD1	2.13	0.48
1:A:527:LYS:HD2	1:A:528:LYS:N	2.28	0.48
1:B:83:VAL:HG12	1:B:236:ARG:HH21	1.79	0.48
1:C:96:GLU:HA	1:C:186:PHE:N	2.29	0.48
1:C:535:ASN:O	1:C:536:LYS:O	2.31	0.48
4:H:24:ALA:HA	4:H:29:PHE:CZ	2.47	0.48
4:H:37:VAL:HG21	4:H:115:TRP:HZ3	1.78	0.48
5:F:2:ILE:CG2	5:F:27:GLN:H	2.26	0.48
5:F:28:ASP:OD2	5:F:69:THR:HG23	2.13	0.48
3:K:6:GLN:NE2	3:K:89:CYS:H	2.08	0.48
2:S:72:THR:OG1	2:S:79:GLY:HA2	2.14	0.48
4:Q:37:VAL:HG21	4:Q:115:TRP:HZ3	1.77	0.48
5:R:8:PRO:HD2	5:R:22:THR:O	2.13	0.48
1:A:44:ARG:HB3	1:A:47:VAL:CG2	2.43	0.48
1:A:422:ASN:OD1	1:A:423:TYR:HB2	2.14	0.48
1:B:96:GLU:HA	1:B:186:PHE:N	2.29	0.48
1:B:406:GLU:HG3	1:B:418:ILE:HD12	1.94	0.48
1:C:44:ARG:HB3	1:C:47:VAL:CG2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:GLU:CD	1:C:170:TYR:H	2.22	0.48
2:E:70:MET:HE2	2:E:81:MET:HG3	1.95	0.48
3:G:38:GLN:N	3:G:48:LEU:HB2	2.29	0.48
3:K:6:GLN:OE1	3:K:102:THR:N	2.46	0.48
2:S:20:VAL:O	2:S:80:TYR:HD1	1.97	0.48
1:A:37:TYR:OH	1:A:53:ASP:OD2	2.31	0.48
1:A:140:PHE:HD1	1:A:241:LEU:HD11	1.79	0.48
1:A:319:ARG:HD2	1:A:320:VAL:H	1.79	0.48
1:A:535:ASN:O	1:A:536:LYS:O	2.31	0.48
1:B:25:THR:N	1:B:66:HIS:HB3	2.28	0.48
1:B:204:TYR:HA	1:B:224:PRO:HA	1.95	0.48
3:G:48:LEU:HD12	3:G:59:ILE:CD1	2.42	0.48
5:F:15:VAL:HA	5:F:78:LEU:HG	1.96	0.48
5:F:35:TRP:HB2	5:F:48:ILE:HG22	1.96	0.48
2:S:38:ARG:HH12	2:S:90:ASP:HA	1.78	0.48
5:R:15:VAL:HA	5:R:78:LEU:HG	1.96	0.48
1:A:96:GLU:HA	1:A:186:PHE:N	2.29	0.48
1:A:853:GLN:O	1:A:855:PHE:N	2.47	0.48
1:C:340:GLU:O	1:C:344:ALA:HB2	2.13	0.48
1:C:853:GLN:O	1:C:855:PHE:N	2.47	0.48
2:E:102:ARG:HA	2:E:109:SER:HA	1.95	0.48
4:H:38:ARG:NH2	4:H:90:ASP:HA	2.28	0.48
2:I:4:LEU:N	2:I:25:SER:OG	2.46	0.48
2:I:93:VAL:HB	2:I:122:LEU:HA	1.95	0.48
4:D:37:VAL:HG21	4:D:115:TRP:HZ3	1.78	0.48
5:J:2:ILE:CG2	5:J:27:GLN:H	2.26	0.48
4:Q:98:ARG:HD2	4:Q:102:ASN:HB3	1.94	0.48
1:A:340:GLU:O	1:A:344:ALA:HB2	2.13	0.48
1:B:337:PRO:HD2	1:B:358:ILE:HB	1.95	0.48
1:B:853:GLN:O	1:B:855:PHE:N	2.47	0.48
4:H:35:SER:HB2	4:H:99:LEU:HD13	1.94	0.48
4:H:45:LEU:HD11	5:F:87:TYR:CD2	2.49	0.48
4:D:39:GLN:O	4:D:39:GLN:HG3	2.13	0.48
5:J:22:THR:CG2	5:J:70:ASP:HB2	2.43	0.48
5:J:33:LEU:HD21	5:J:35:TRP:CD1	2.49	0.48
2:S:33:GLY:HA2	2:S:53:THR:H	1.79	0.48
2:S:70:MET:HE2	2:S:81:MET:HG3	1.95	0.48
3:T:6:GLN:NE2	3:T:89:CYS:H	2.08	0.48
1:B:53:ASP:OD2	1:B:195:LYS:NZ	2.42	0.47
1:B:125:ASN:HB3	1:B:127:PHE:CD2	2.49	0.47
1:B:502:VAL:HG21	4:H:54:LEU:HD22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:ASN:HB3	1:C:127:PHE:CD2	2.49	0.47
2:E:4:LEU:N	2:E:25:SER:OG	2.46	0.47
3:K:7:SER:N	3:K:22:SER:O	2.36	0.47
3:K:36:TRP:HA	3:K:89:CYS:HA	1.95	0.47
5:R:6:GLN:NE2	5:R:86:TYR:O	2.46	0.47
1:A:731:MET:H	1:A:774:GLN:HE21	1.62	0.47
1:C:49:HIS:CD2	1:C:51:THR:HG22	2.49	0.47
1:C:1097:SER:C	1:C:1099:GLY:H	2.22	0.47
2:I:102:ARG:HA	2:I:109:SER:HA	1.95	0.47
3:K:6:GLN:HG2	3:K:23:CYS:HB2	1.95	0.47
5:J:35:TRP:HB2	5:J:48:ILE:HG22	1.96	0.47
5:J:78:LEU:HB2	5:J:82:ASP:HB2	1.96	0.47
3:T:48:LEU:HD12	3:T:59:ILE:HD11	1.96	0.47
1:B:346:ARG:NH2	3:G:32:THR:OG1	2.21	0.47
1:B:422:ASN:OD1	1:B:423:TYR:HB2	2.14	0.47
1:B:1028:LYS:NZ	1:B:1042:PHE:O	2.47	0.47
1:C:371:PHE:CD1	6:V:2:NAG:H62	2.45	0.47
4:D:6:GLN:HG3	4:D:7:SER:N	2.29	0.47
2:S:2:VAL:HG13	2:S:25:SER:HB3	1.97	0.47
5:R:33:LEU:HD21	5:R:35:TRP:CD1	2.49	0.47
1:A:358:ILE:CD1	1:A:395:VAL:H	2.27	0.47
1:A:549:GLY:N	1:A:551:LEU:HD11	2.28	0.47
1:A:575:VAL:N	1:A:584:LEU:O	2.42	0.47
1:B:731:MET:H	1:B:774:GLN:HE21	1.62	0.47
1:C:140:PHE:HD1	1:C:241:LEU:HD11	1.79	0.47
1:C:328:ARG:O	1:C:578:PRO:HB2	2.14	0.47
1:C:362:VAL:O	1:C:362:VAL:HG13	2.15	0.47
1:C:496:PHE:HB2	1:C:504:HIS:O	2.13	0.47
1:C:534:LYS:HB3	1:C:540:PHE:HB3	1.94	0.47
2:E:72:THR:OG1	2:E:79:GLY:HA2	2.14	0.47
2:E:93:VAL:HB	2:E:122:LEU:HA	1.95	0.47
5:F:87:TYR:HB3	5:F:100:GLY:C	2.40	0.47
2:I:32:TYR:O	2:I:53:THR:OG1	2.32	0.47
3:K:48:LEU:HD12	3:K:59:ILE:HD11	1.96	0.47
4:Q:38:ARG:NH2	4:Q:90:ASP:HA	2.28	0.47
5:R:35:TRP:CD1	5:R:73:PHE:HB2	2.49	0.47
5:R:87:TYR:HB3	5:R:100:GLY:C	2.40	0.47
1:A:357:ARG:HB3	1:A:396:TYR:HE2	1.78	0.47
1:A:444:LYS:HE3	1:A:444:LYS:HB3	1.56	0.47
1:A:496:PHE:HB2	1:A:504:HIS:O	2.13	0.47
1:A:564:PHE:N	1:A:564:PHE:CD2	2.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1028:LYS:NZ	1:A:1042:PHE:O	2.47	0.47
1:B:119:ILE:HD13	1:B:128:ILE:HG23	1.96	0.47
1:B:588:PRO:HG2	1:C:855:PHE:HB3	1.96	0.47
1:C:357:ARG:HB3	1:C:396:TYR:HE2	1.78	0.47
1:C:1141:LEU:HD13	1:C:1141:LEU:HA	1.67	0.47
3:G:48:LEU:HD12	3:G:59:ILE:HD11	1.96	0.47
4:H:6:GLN:HG3	4:H:7:SER:N	2.29	0.47
3:T:36:TRP:N	3:T:49:ILE:O	2.46	0.47
4:Q:34:ILE:HA	4:Q:98:ARG:NH1	2.20	0.47
1:A:37:TYR:OH	1:A:54:LEU:O	2.29	0.47
1:B:140:PHE:HD2	1:B:140:PHE:O	1.98	0.47
1:B:169:GLU:OE1	1:B:169:GLU:HA	2.14	0.47
1:B:1097:SER:C	1:B:1099:GLY:H	2.22	0.47
1:B:1141:LEU:HD13	1:B:1141:LEU:HA	1.67	0.47
1:C:358:ILE:HD11	1:C:395:VAL:HG23	1.95	0.47
2:E:98:ARG:O	2:E:115:ASP:N	2.31	0.47
5:F:33:LEU:HD21	5:F:35:TRP:CD1	2.49	0.47
2:I:72:THR:OG1	2:I:79:GLY:HA2	2.14	0.47
5:J:35:TRP:CD1	5:J:73:PHE:HB2	2.49	0.47
2:S:50:TRP:O	2:S:58:THR:HA	2.15	0.47
3:T:6:GLN:HG2	3:T:23:CYS:HB2	1.95	0.47
4:Q:6:GLN:HG3	4:Q:7:SER:N	2.29	0.47
1:A:169:GLU:CD	1:A:170:TYR:H	2.22	0.47
1:A:402:ILE:HD11	1:A:509:VAL:HG21	1.95	0.47
1:A:527:LYS:HB3	1:A:528:LYS:H	1.46	0.47
1:A:914:ASN:HB2	1:A:918:GLU:OE2	2.15	0.47
1:A:1097:SER:C	1:A:1099:GLY:H	2.22	0.47
1:B:319:ARG:HD2	1:B:320:VAL:H	1.79	0.47
1:B:355:ARG:NH1	1:B:464:PHE:HE1	2.13	0.47
1:B:358:ILE:HD11	1:B:395:VAL:HG23	1.95	0.47
1:B:398:ASP:HB2	1:B:511:VAL:HB	1.97	0.47
1:B:565:GLY:HA2	1:C:43:PHE:O	2.14	0.47
1:B:625:ALA:HA	1:B:630:PRO:CA	2.43	0.47
1:B:879:ALA:O	1:B:883:THR:OG1	2.27	0.47
1:C:319:ARG:HD2	1:C:320:VAL:H	1.79	0.47
1:C:355:ARG:NH1	1:C:464:PHE:HE1	2.13	0.47
1:C:404:GLY:HA3	1:C:503:GLY:HA2	1.97	0.47
1:C:502:VAL:HG21	5:R:93:ASP:O	2.14	0.47
1:C:633:ARG:NE	1:C:633:ARG:HA	2.30	0.47
2:E:20:VAL:O	2:E:80:TYR:HD1	1.97	0.47
2:E:29:PHE:CE2	2:E:53:THR:HB	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:83:LEU:HD23	2:I:84:ARG:O	2.15	0.47
2:I:103:GLY:H	2:I:110:LEU:HB2	1.80	0.47
4:D:51:PHE:CD1	4:D:71:SER:HA	2.49	0.47
4:D:92:ALA:HB3	4:D:94:TYR:HE1	1.76	0.47
5:J:86:TYR:HB2	5:J:103:THR:HB	1.97	0.47
2:S:29:PHE:CE2	2:S:53:THR:HB	2.50	0.47
2:S:63:LYS:H	2:S:63:LYS:HG3	1.37	0.47
2:S:83:LEU:HD23	2:S:84:ARG:O	2.15	0.47
3:T:38:GLN:N	3:T:48:LEU:HB2	2.29	0.47
5:R:35:TRP:HB2	5:R:48:ILE:HG22	1.96	0.47
1:A:83:VAL:HG12	1:A:236:ARG:HH21	1.79	0.47
1:A:140:PHE:HD2	1:A:140:PHE:O	1.98	0.47
1:A:328:ARG:O	1:A:578:PRO:HB2	2.14	0.47
1:A:355:ARG:NH1	1:A:464:PHE:HE1	2.13	0.47
1:A:426:PRO:HD3	1:A:464:PHE:CD2	2.49	0.47
1:B:328:ARG:O	1:B:578:PRO:HB2	2.14	0.47
1:B:402:ILE:HD11	1:B:509:VAL:HG21	1.95	0.47
1:C:93:ALA:O	1:C:94:SER:OG	2.30	0.47
1:C:189:LEU:O	1:C:191:GLU:N	2.48	0.47
4:H:112:PHE:CE2	5:F:46:LEU:HD23	2.49	0.47
4:H:115:TRP:CZ2	5:F:44:PRO:HB2	2.49	0.47
5:F:35:TRP:CD1	5:F:73:PHE:HB2	2.49	0.47
5:F:75:ILE:HG21	5:F:78:LEU:HB3	1.97	0.47
5:J:87:TYR:HB3	5:J:100:GLY:C	2.40	0.47
5:R:17:ASP:O	5:R:18:ARG:C	2.58	0.47
5:R:68:GLY:H	5:R:71:PHE:HE1	1.60	0.47
5:R:68:GLY:O	5:R:71:PHE:HE1	1.98	0.47
1:B:549:GLY:N	1:B:551:LEU:HD11	2.28	0.47
1:B:633:ARG:HA	1:B:633:ARG:NE	2.30	0.47
1:C:140:PHE:O	1:C:140:PHE:HD2	1.98	0.47
5:F:15:VAL:HG22	5:F:107:ILE:HD12	1.97	0.47
2:I:20:VAL:O	2:I:80:TYR:HD1	1.97	0.47
2:I:69:THR:O	2:I:69:THR:OG1	2.30	0.47
3:K:66:SER:OG	3:K:67:GLY:N	2.47	0.47
5:J:75:ILE:HG21	5:J:78:LEU:HB3	1.97	0.47
4:Q:98:ARG:HD3	4:Q:98:ARG:HA	1.51	0.47
5:R:75:ILE:HG21	5:R:78:LEU:HB3	1.97	0.47
1:B:362:VAL:HG13	1:B:362:VAL:O	2.15	0.47
1:C:444:LYS:HB3	1:C:444:LYS:HE3	1.56	0.47
1:C:645:ARG:HE	1:C:645:ARG:HB3	1.52	0.47
3:G:96:LEU:HD23	3:G:96:LEU:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:32:TYR:O	2:S:53:THR:OG1	2.33	0.47
3:T:66:SER:OG	3:T:67:GLY:N	2.47	0.47
3:T:96:LEU:HD23	3:T:96:LEU:H	1.80	0.47
1:A:57:PRO:HG3	1:A:271:GLN:OE1	2.16	0.46
1:A:1125:ASN:O	1:A:1127:ASP:N	2.48	0.46
1:C:1028:LYS:NZ	1:C:1042:PHE:O	2.47	0.46
4:H:34:ILE:HA	4:H:98:ARG:NH1	2.20	0.46
5:F:17:ASP:O	5:F:18:ARG:C	2.58	0.46
2:I:29:PHE:CE2	2:I:53:THR:HB	2.50	0.46
2:I:42:GLY:CA	3:K:54:SER:OG	2.61	0.46
3:K:38:GLN:N	3:K:48:LEU:HB2	2.29	0.46
2:S:29:PHE:O	2:S:53:THR:OG1	2.19	0.46
4:Q:51:PHE:CD1	4:Q:71:SER:HA	2.49	0.46
1:A:93:ALA:O	1:A:94:SER:OG	2.30	0.46
1:A:393:THR:OG1	1:A:515:GLU:O	2.23	0.46
1:A:879:ALA:O	1:A:883:THR:OG1	2.27	0.46
1:A:1145:LEU:HD11	1:B:1145:LEU:HD11	1.97	0.46
1:B:169:GLU:CD	1:B:170:TYR:H	2.22	0.46
1:C:398:ASP:HB2	1:C:511:VAL:HB	1.97	0.46
2:E:64:PHE:HA	2:E:67:ARG:HD3	1.97	0.46
5:J:68:GLY:O	5:J:71:PHE:HE1	1.98	0.46
5:R:6:GLN:NE2	5:R:102:GLY:H	2.12	0.46
1:A:398:ASP:HB2	1:A:511:VAL:HB	1.97	0.46
1:A:406:GLU:CG	1:A:418:ILE:HD12	2.45	0.46
1:A:862:PRO:HB2	1:C:645:ARG:NH1	2.29	0.46
1:B:189:LEU:O	1:B:191:GLU:N	2.48	0.46
1:B:1125:ASN:O	1:B:1127:ASP:N	2.48	0.46
1:C:57:PRO:HG3	1:C:271:GLN:OE1	2.15	0.46
1:C:331:ASN:HD21	7:W:1:NAG:C1	2.28	0.46
1:C:406:GLU:CG	1:C:418:ILE:HD12	2.45	0.46
1:C:879:ALA:O	1:C:883:THR:OG1	2.27	0.46
1:C:914:ASN:HB2	1:C:918:GLU:OE2	2.15	0.46
3:G:66:SER:OG	3:G:67:GLY:N	2.47	0.46
3:K:42:GLY:HA3	5:J:34:ASN:HD21	1.80	0.46
5:J:15:VAL:HG22	5:J:107:ILE:HD12	1.97	0.46
1:A:169:GLU:OE1	1:A:169:GLU:HA	2.14	0.46
1:A:280:ASN:CG	1:A:284:THR:HG1	2.23	0.46
1:C:111:ASP:HB2	1:C:134:GLN:OE1	2.16	0.46
1:C:898:PHE:O	1:C:900:MET:N	2.49	0.46
4:H:51:PHE:CD1	4:H:71:SER:HA	2.49	0.46
2:I:50:TRP:O	2:I:58:THR:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:37:GLN:HB3	5:J:47:LEU:HD11	1.98	0.46
2:S:103:GLY:H	2:S:110:LEU:HB2	1.80	0.46
1:A:63:THR:O	1:A:63:THR:OG1	2.34	0.46
1:A:119:ILE:HD13	1:A:128:ILE:HG23	1.96	0.46
1:A:189:LEU:O	1:A:191:GLU:N	2.48	0.46
1:A:235:THR:C	1:A:236:ARG:HG2	2.41	0.46
1:A:362:VAL:O	1:A:362:VAL:HG13	2.14	0.46
1:A:569:VAL:HG12	1:B:964:LYS:HB3	1.97	0.46
1:B:114:THR:O	1:B:115:GLN:HB2	2.16	0.46
1:B:336:CYS:SG	1:B:337:PRO:HD2	2.56	0.46
1:C:119:ILE:HD13	1:C:128:ILE:HG23	1.96	0.46
1:C:365:TYR:OH	1:C:395:VAL:HG21	2.16	0.46
1:C:1125:ASN:O	1:C:1127:ASP:N	2.48	0.46
2:E:32:TYR:O	2:E:53:THR:OG1	2.33	0.46
2:I:98:ARG:O	2:I:115:ASP:N	2.31	0.46
1:A:31:SER:O	1:A:31:SER:OG	2.22	0.46
1:A:53:ASP:OD2	1:A:195:LYS:NZ	2.42	0.46
1:A:404:GLY:HA3	1:A:503:GLY:HA2	1.97	0.46
1:A:633:ARG:NE	1:A:633:ARG:HA	2.30	0.46
1:B:318:PHE:HZ	1:B:614:VAL:HG11	1.80	0.46
1:B:319:ARG:HD2	1:B:320:VAL:N	2.31	0.46
1:B:378:LYS:HD3	1:B:378:LYS:HA	1.55	0.46
1:C:358:ILE:CD1	1:C:395:VAL:H	2.27	0.46
1:C:481:LYS:HE2	1:C:481:LYS:HB3	1.69	0.46
2:E:50:TRP:O	2:E:58:THR:HA	2.15	0.46
2:I:2:VAL:HG13	2:I:25:SER:HB3	1.97	0.46
2:I:117:TRP:CH2	3:K:68:SER:N	2.84	0.46
5:J:18:ARG:HA	5:J:18:ARG:HD2	1.64	0.46
1:A:453:TYR:CD1	1:A:492:GLN:HB2	2.51	0.46
1:A:559:LEU:HD12	1:A:559:LEU:HA	1.70	0.46
1:B:132:GLU:HB2	1:B:164:ASN:HB2	1.98	0.46
1:B:280:ASN:CG	1:B:284:THR:HG1	2.23	0.46
1:B:527:LYS:HD2	1:B:528:LYS:N	2.28	0.46
1:C:194:PHE:HD1	1:C:203:ILE:HG23	1.80	0.46
1:C:319:ARG:HD2	1:C:320:VAL:N	2.31	0.46
1:A:80:ASP:O	1:A:82:PRO:HD3	2.16	0.46
1:A:132:GLU:HB2	1:A:164:ASN:HB2	1.98	0.46
1:B:194:PHE:HD1	1:B:203:ILE:HG23	1.80	0.46
1:B:404:GLY:HA3	1:B:503:GLY:HA2	1.97	0.46
1:C:353:TRP:CD1	1:C:353:TRP:N	2.84	0.46
1:C:549:GLY:N	1:C:551:LEU:HD11	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:64:PHE:HA	2:I:67:ARG:HD3	1.97	0.46
2:S:64:PHE:HA	2:S:67:ARG:HD3	1.97	0.46
1:A:36:VAL:HG11	1:A:219:PHE:CE2	2.51	0.46
1:A:41:LYS:HG2	1:C:561:PHE:HD2	1.81	0.46
1:A:318:PHE:HZ	1:A:614:VAL:HG11	1.80	0.46
1:A:898:PHE:O	1:A:900:MET:N	2.49	0.46
1:B:38:TYR:CE2	1:B:285:ILE:HG13	2.51	0.46
1:B:199:GLY:HA2	1:B:230:ILE:O	2.16	0.46
1:B:353:TRP:CD1	1:B:353:TRP:N	2.83	0.46
1:B:566:ARG:CG	1:C:42:VAL:HG11	2.45	0.46
1:C:36:VAL:HG11	1:C:219:PHE:CE2	2.51	0.46
1:C:83:VAL:HG12	1:C:236:ARG:HH21	1.79	0.46
1:C:169:GLU:OE1	1:C:169:GLU:HA	2.14	0.46
1:C:336:CYS:SG	1:C:337:PRO:HD2	2.55	0.46
1:C:559:LEU:HD12	1:C:559:LEU:HA	1.70	0.46
2:E:83:LEU:HD23	2:E:84:ARG:O	2.14	0.46
5:J:17:ASP:O	5:J:18:ARG:C	2.58	0.46
3:T:92:HIS:HA	3:T:96:LEU:CD1	2.46	0.46
4:Q:97:ALA:HB3	4:Q:99:LEU:HD12	1.98	0.46
1:A:199:GLY:HA2	1:A:230:ILE:O	2.16	0.46
1:A:351:TYR:HB2	1:A:467:ASP:O	2.16	0.46
1:A:1145:LEU:HA	1:A:1145:LEU:HD13	1.77	0.46
1:B:193:VAL:HG12	1:B:222:LEU:HD12	1.98	0.46
1:B:196:ASN:ND2	1:B:201:PHE:HB2	2.31	0.46
1:B:353:TRP:O	1:B:466:ARG:NE	2.49	0.46
1:B:358:ILE:CD1	1:B:395:VAL:H	2.27	0.46
1:B:501:GLY:N	4:H:103:GLY:O	2.49	0.46
1:B:579:GLN:HG3	1:B:580:THR:CG2	2.46	0.46
1:C:114:THR:O	1:C:115:GLN:HB2	2.16	0.46
1:C:196:ASN:ND2	1:C:201:PHE:HB2	2.31	0.46
1:C:558:PHE:O	1:C:559:LEU:C	2.59	0.46
1:C:579:GLN:HG3	1:C:580:THR:CG2	2.46	0.46
1:C:625:ALA:HA	1:C:630:PRO:CA	2.43	0.46
5:F:78:LEU:HB2	5:F:82:ASP:HB2	1.96	0.46
3:K:96:LEU:HD23	3:K:96:LEU:H	1.80	0.46
4:D:47:TRP:CE2	4:D:49:GLY:HA2	2.51	0.46
5:J:49:TYR:CE2	5:J:53:HIS:HB2	2.51	0.46
2:S:38:ARG:HD2	2:S:94:TYR:HE1	1.81	0.46
4:Q:94:TYR:O	4:Q:119:THR:HG22	2.16	0.46
1:A:193:VAL:HG12	1:A:222:LEU:HD12	1.98	0.45
1:A:747:THR:O	1:A:750:SER:N	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:PRO:HG3	1:B:271:GLN:OE1	2.15	0.45
1:B:111:ASP:HB2	1:B:134:GLN:OE1	2.16	0.45
1:B:111:ASP:OD2	1:B:113:LYS:HB2	2.16	0.45
1:B:453:TYR:CD1	1:B:492:GLN:HB2	2.51	0.45
1:B:1077:THR:HG23	1:B:1078:ALA:N	2.30	0.45
1:C:38:TYR:CE2	1:C:285:ILE:HG13	2.51	0.45
1:C:128:ILE:HG22	1:C:129:LYS:H	1.81	0.45
1:C:1077:THR:HG23	1:C:1078:ALA:N	2.30	0.45
2:E:103:GLY:H	2:E:110:LEU:HB2	1.80	0.45
3:K:83:ASP:O	3:K:87:TYR:OH	2.09	0.45
2:S:67:ARG:O	2:S:83:LEU:HA	2.16	0.45
3:T:64:SER:HB3	3:T:75:THR:O	2.17	0.45
5:R:37:GLN:HB3	5:R:47:LEU:HD11	1.98	0.45
1:A:336:CYS:SG	1:A:337:PRO:HD2	2.55	0.45
1:A:445:HIS:NE2	5:J:42:LYS:HE3	2.31	0.45
1:B:80:ASP:O	1:B:82:PRO:HD3	2.16	0.45
1:B:235:THR:C	1:B:236:ARG:HG2	2.41	0.45
1:B:406:GLU:CG	1:B:418:ILE:HD12	2.45	0.45
1:B:705:VAL:O	1:B:707:TYR:N	2.48	0.45
1:C:235:THR:C	1:C:236:ARG:HG2	2.41	0.45
1:C:318:PHE:HZ	1:C:614:VAL:HG11	1.80	0.45
1:C:351:TYR:HB2	1:C:467:ASP:O	2.16	0.45
2:E:2:VAL:HG13	2:E:25:SER:HB3	1.97	0.45
5:F:37:GLN:HB3	5:F:47:LEU:HD11	1.98	0.45
5:F:49:TYR:CE2	5:F:53:HIS:HB2	2.51	0.45
5:F:68:GLY:O	5:F:71:PHE:HE1	1.98	0.45
2:I:39:GLN:HE22	3:K:53:SER:C	2.24	0.45
4:D:94:TYR:O	4:D:119:THR:HG22	2.16	0.45
1:A:38:TYR:CE2	1:A:285:ILE:HG13	2.51	0.45
1:A:353:TRP:CD1	1:A:353:TRP:N	2.83	0.45
1:A:505:GLN:CG	4:D:45:LEU:HD12	2.44	0.45
1:A:1100:THR:HG1	1:A:1101:HIS:CE1	2.33	0.45
1:B:395:VAL:O	1:B:513:SER:N	2.21	0.45
1:B:898:PHE:O	1:B:900:MET:N	2.49	0.45
1:B:921:LYS:HE2	1:B:921:LYS:HB2	1.59	0.45
4:H:67:ARG:HG3	4:H:67:ARG:HH11	1.82	0.45
5:F:86:TYR:HB2	5:F:103:THR:HB	1.97	0.45
2:I:38:ARG:HB2	2:I:48:MET:SD	2.56	0.45
5:J:68:GLY:H	5:J:71:PHE:HE1	1.60	0.45
2:S:10:GLU:O	2:S:124:THR:N	2.50	0.45
2:S:38:ARG:HB2	2:S:48:MET:SD	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:38:ARG:NH1	4:Q:90:ASP:HA	2.32	0.45
4:Q:67:ARG:HH11	4:Q:67:ARG:HG3	1.82	0.45
1:A:125:ASN:HB3	1:A:127:PHE:CD2	2.49	0.45
1:A:295:PRO:HB2	1:A:607:VAL:HG21	1.98	0.45
1:B:407:VAL:HG21	1:B:507:TYR:CG	2.51	0.45
1:B:914:ASN:HB2	1:B:918:GLU:OE2	2.15	0.45
1:C:86:PHE:N	1:C:235:THR:O	2.46	0.45
1:C:334:ASN:HB3	2:S:105:TRP:CH2	2.50	0.45
1:C:350:VAL:HG13	1:C:422:ASN:ND2	2.32	0.45
1:C:453:TYR:CD1	1:C:492:GLN:HB2	2.51	0.45
1:C:623:ILE:H	1:C:623:ILE:HG12	1.23	0.45
4:D:67:ARG:HH11	4:D:67:ARG:HG3	1.82	0.45
4:Q:47:TRP:CE2	4:Q:49:GLY:HA2	2.50	0.45
5:R:78:LEU:HB2	5:R:82:ASP:HB2	1.97	0.45
1:A:111:ASP:HB2	1:A:134:GLN:OE1	2.16	0.45
1:A:348:ALA:HA	2:I:111:ILE:CG1	2.46	0.45
1:B:295:PRO:HB2	1:B:607:VAL:HG21	1.98	0.45
1:B:380:TYR:CD2	1:B:433:VAL:HB	2.52	0.45
1:B:558:PHE:O	1:B:559:LEU:C	2.59	0.45
1:B:623:ILE:H	1:B:623:ILE:HG12	1.23	0.45
1:C:132:GLU:HB2	1:C:164:ASN:HB2	1.98	0.45
1:C:380:TYR:CD2	1:C:433:VAL:HB	2.52	0.45
1:C:406:GLU:OE1	1:C:406:GLU:N	2.49	0.45
1:C:407:VAL:HG21	1:C:507:TYR:CG	2.51	0.45
1:C:440:LYS:NZ	3:T:32:THR:HG22	2.30	0.45
1:C:502:VAL:HA	1:C:505:GLN:CB	2.47	0.45
1:C:731:MET:H	1:C:774:GLN:HE21	1.62	0.45
3:G:83:ASP:O	3:G:87:TYR:OH	2.09	0.45
2:I:10:GLU:O	2:I:124:THR:N	2.50	0.45
2:I:55:ASN:HD21	2:I:57:ASN:HB2	1.82	0.45
2:I:119:GLN:HG2	3:K:18:ARG:HH11	1.81	0.45
3:K:64:SER:HB3	3:K:75:THR:O	2.17	0.45
4:D:38:ARG:NH2	4:D:90:ASP:O	2.43	0.45
4:D:97:ALA:HB3	4:D:99:LEU:HD12	1.98	0.45
4:Q:109:GLU:H	4:Q:109:GLU:HG2	1.43	0.45
5:R:94:LEU:HG	5:R:95:PRO:HD2	1.99	0.45
1:A:61:ASN:N	1:A:61:ASN:OD1	2.41	0.45
1:A:92:PHE:HZ	1:A:239:THR:OG1	2.00	0.45
1:A:114:THR:O	1:A:115:GLN:HB2	2.16	0.45
1:A:196:ASN:ND2	1:A:201:PHE:HB2	2.31	0.45
1:A:319:ARG:HD2	1:A:320:VAL:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:GLY:HA3	1:A:502:VAL:O	2.16	0.45
1:A:407:VAL:HG21	1:A:507:TYR:CG	2.51	0.45
1:A:558:PHE:O	1:A:559:LEU:C	2.59	0.45
1:A:579:GLN:HG3	1:A:580:THR:CG2	2.46	0.45
1:A:625:ALA:HA	1:A:630:PRO:CA	2.43	0.45
1:A:1077:THR:HG23	1:A:1078:ALA:N	2.30	0.45
1:B:25:THR:OG1	1:B:26:GLN:N	2.50	0.45
1:B:128:ILE:HB	1:B:169:GLU:OE1	2.17	0.45
1:B:406:GLU:OE1	1:B:406:GLU:N	2.49	0.45
1:B:409:GLN:OE1	1:B:416:GLY:HA3	2.17	0.45
1:B:422:ASN:HD22	1:B:454:ARG:CG	2.28	0.45
1:C:213:ARG:HA	1:C:213:ARG:HD2	1.78	0.45
1:C:353:TRP:O	1:C:466:ARG:NE	2.49	0.45
1:C:575:VAL:O	1:C:584:LEU:N	2.49	0.45
1:C:575:VAL:N	1:C:584:LEU:O	2.42	0.45
1:C:619:VAL:O	1:C:619:VAL:HG13	2.16	0.45
2:E:38:ARG:HB2	2:E:48:MET:SD	2.56	0.45
3:G:64:SER:HB3	3:G:75:THR:O	2.17	0.45
4:H:47:TRP:CE2	4:H:49:GLY:HA2	2.51	0.45
4:H:73:ASP:O	4:H:76:THR:OG1	2.32	0.45
5:F:94:LEU:HG	5:F:95:PRO:HD2	1.99	0.45
2:S:85:ARG:HA	2:S:85:ARG:HD3	1.87	0.45
4:Q:29:PHE:O	4:Q:32:HIS:HB2	2.17	0.45
1:A:57:PRO:HB3	1:A:273:ARG:NE	2.32	0.45
1:A:128:ILE:HG22	1:A:129:LYS:H	1.81	0.45
1:A:348:ALA:HA	2:I:111:ILE:HG12	1.98	0.45
1:A:350:VAL:HG13	1:A:422:ASN:ND2	2.32	0.45
1:A:406:GLU:OE1	1:A:406:GLU:N	2.49	0.45
1:B:92:PHE:HZ	1:B:239:THR:OG1	2.00	0.45
1:B:350:VAL:HG13	1:B:422:ASN:ND2	2.32	0.45
1:B:393:THR:OG1	1:B:515:GLU:O	2.23	0.45
1:B:502:VAL:HA	1:B:505:GLN:CB	2.47	0.45
1:C:199:GLY:HA2	1:C:230:ILE:O	2.16	0.45
1:C:361:CYS:SG	1:C:524:CYS:N	2.87	0.45
1:C:380:TYR:HB3	1:C:412:PRO:CD	2.46	0.45
1:C:568:ILE:H	1:C:568:ILE:HD12	1.82	0.45
4:H:98:ARG:HD3	4:H:98:ARG:HA	1.51	0.45
4:Q:52:ILE:HB	4:Q:57:THR:O	2.17	0.45
5:R:15:VAL:HG22	5:R:107:ILE:HD12	1.97	0.45
5:R:49:TYR:CE2	5:R:53:HIS:HB2	2.51	0.45
1:A:194:PHE:HD1	1:A:203:ILE:HG23	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:VAL:O	1:A:513:SER:N	2.21	0.45
1:A:568:ILE:HB	1:B:850:ILE:HD12	1.98	0.45
1:A:575:VAL:O	1:A:584:LEU:N	2.49	0.45
1:A:1129:VAL:HG13	1:B:917:TYR:HB3	1.99	0.45
1:B:404:GLY:HA3	1:B:502:VAL:O	2.17	0.45
1:B:418:ILE:C	1:B:420:ASP:H	2.25	0.45
1:B:619:VAL:HG13	1:B:619:VAL:O	2.16	0.45
1:C:228:LEU:O	1:C:230:ILE:HG12	2.17	0.45
2:E:60:TYR:CE1	2:E:70:MET:HB2	2.44	0.45
2:E:67:ARG:O	2:E:83:LEU:HA	2.16	0.45
4:H:38:ARG:NH1	4:H:90:ASP:HA	2.32	0.45
2:I:35:SER:C	2:I:36:TRP:CD1	2.95	0.45
3:K:79:LEU:CD2	3:K:104:VAL:HG11	2.47	0.45
4:D:38:ARG:NH1	4:D:90:ASP:HA	2.32	0.45
5:R:32:TYR:HA	5:R:91:TYR:CE1	2.52	0.45
1:A:380:TYR:HB3	1:A:412:PRO:CD	2.46	0.45
1:A:619:VAL:O	1:A:619:VAL:HG13	2.16	0.45
1:B:129:LYS:NZ	1:B:131:CYS:SG	2.75	0.45
1:B:365:TYR:OH	1:B:395:VAL:HG21	2.16	0.45
1:B:907:ASN:HD22	1:B:907:ASN:HA	1.56	0.45
1:C:92:PHE:HZ	1:C:239:THR:OG1	2.00	0.45
1:C:907:ASN:HD22	1:C:907:ASN:HA	1.56	0.45
2:E:9:ALA:HA	2:E:122:LEU:O	2.17	0.45
2:I:38:ARG:HD2	2:I:94:TYR:HE1	1.81	0.45
1:A:111:ASP:OD2	1:A:113:LYS:HB2	2.17	0.45
1:B:128:ILE:HG22	1:B:129:LYS:H	1.81	0.45
1:B:228:LEU:O	1:B:230:ILE:HG12	2.17	0.45
1:B:351:TYR:HB2	1:B:467:ASP:O	2.16	0.45
1:B:401:VAL:HG11	1:B:508:ARG:HH21	1.82	0.45
1:B:568:ILE:HA	1:C:47:VAL:HG12	1.98	0.45
1:C:83:VAL:CG1	1:C:236:ARG:HH21	2.30	0.45
4:H:94:TYR:O	4:H:119:THR:HG22	2.16	0.45
5:J:94:LEU:HG	5:J:95:PRO:HD2	1.99	0.45
2:S:48:MET:HE2	2:S:94:TYR:CD1	2.52	0.45
5:R:2:ILE:HG23	5:R:27:GLN:H	1.82	0.45
5:R:86:TYR:HB2	5:R:103:THR:HB	1.97	0.45
1:A:192:PHE:CD1	1:A:205:SER:HB2	2.52	0.44
1:A:233:ASN:N	1:A:233:ASN:OD1	2.50	0.44
1:A:345:THR:HB	2:I:115:ASP:OD1	2.17	0.44
1:A:409:GLN:OE1	1:A:416:GLY:HA3	2.17	0.44
1:B:542:PHE:CD2	1:B:546:THR:HG23	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:984:LEU:HB3	1:B:988:GLU:CD	2.42	0.44
1:C:111:ASP:OD2	1:C:113:LYS:HB2	2.17	0.44
1:C:705:VAL:O	1:C:707:TYR:N	2.48	0.44
2:E:10:GLU:HB2	2:E:123:VAL:HA	1.98	0.44
2:E:48:MET:HE2	2:E:94:TYR:CD1	2.52	0.44
4:H:4:LEU:HD22	4:H:114:ILE:O	2.17	0.44
4:H:94:TYR:H	4:H:94:TYR:HD1	1.65	0.44
4:H:100:PHE:HD2	5:F:91:TYR:CB	2.30	0.44
5:F:52:SER:HB3	5:F:53:HIS:CD2	2.53	0.44
2:I:10:GLU:HB2	2:I:123:VAL:HA	1.98	0.44
4:D:34:ILE:HA	4:D:98:ARG:NH1	2.20	0.44
4:D:52:ILE:HB	4:D:57:THR:O	2.17	0.44
5:J:52:SER:HB3	5:J:53:HIS:CD2	2.53	0.44
2:S:10:GLU:HB2	2:S:123:VAL:HA	1.98	0.44
2:S:35:SER:C	2:S:36:TRP:CD1	2.95	0.44
3:T:38:GLN:HA	3:T:87:TYR:HA	1.99	0.44
1:A:353:TRP:O	1:A:466:ARG:NE	2.49	0.44
1:A:365:TYR:OH	1:A:395:VAL:HG21	2.16	0.44
1:A:418:ILE:C	1:A:420:ASP:H	2.25	0.44
1:A:705:VAL:O	1:A:707:TYR:N	2.48	0.44
1:A:853:GLN:C	1:A:855:PHE:N	2.68	0.44
1:B:36:VAL:HG11	1:B:219:PHE:CE2	2.51	0.44
1:B:707:TYR:HB3	1:C:792:PRO:HG3	1.99	0.44
1:C:233:ASN:N	1:C:233:ASN:OD1	2.50	0.44
1:C:295:PRO:HB2	1:C:607:VAL:HG21	1.98	0.44
1:C:329:PHE:HA	1:C:578:PRO:CB	2.47	0.44
1:C:404:GLY:HA3	1:C:502:VAL:O	2.16	0.44
1:C:409:GLN:OE1	1:C:416:GLY:HA3	2.17	0.44
2:E:55:ASN:HD21	2:E:57:ASN:HB2	1.82	0.44
4:H:45:LEU:HD21	5:F:87:TYR:CE2	2.52	0.44
4:H:97:ALA:HB3	4:H:99:LEU:HD12	1.98	0.44
4:D:4:LEU:HD22	4:D:114:ILE:O	2.18	0.44
5:J:32:TYR:HA	5:J:91:TYR:CE1	2.52	0.44
2:S:55:ASN:HD21	2:S:57:ASN:HB2	1.82	0.44
3:T:79:LEU:CD2	3:T:104:VAL:HG11	2.47	0.44
1:A:228:LEU:O	1:A:230:ILE:HG12	2.17	0.44
1:A:401:VAL:HG11	1:A:508:ARG:HH21	1.82	0.44
1:A:984:LEU:HB3	1:A:988:GLU:CD	2.42	0.44
1:A:1125:ASN:OD1	1:A:1125:ASN:N	2.50	0.44
1:A:1130:ILE:HD11	1:B:921:LYS:HD3	1.99	0.44
1:B:57:PRO:HB3	1:B:273:ARG:NE	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:LYS:HA	1:B:113:LYS:HD2	1.69	0.44
1:B:380:TYR:HB3	1:B:412:PRO:CD	2.46	0.44
1:B:426:PRO:HD3	1:B:464:PHE:CD2	2.48	0.44
1:B:568:ILE:H	1:B:568:ILE:HD12	1.82	0.44
1:B:575:VAL:N	1:B:584:LEU:O	2.42	0.44
1:C:422:ASN:HD22	1:C:454:ARG:CG	2.28	0.44
1:C:440:LYS:HD3	5:R:49:TYR:CE2	2.49	0.44
1:C:600:GLY:C	1:C:602:ASN:N	2.75	0.44
1:C:1057:PRO:O	1:C:1058:HIS:HB2	2.18	0.44
4:H:29:PHE:O	4:H:32:HIS:HB2	2.17	0.44
5:F:33:LEU:HD22	5:F:71:PHE:CB	2.48	0.44
3:K:92:HIS:HA	3:K:96:LEU:CD1	2.46	0.44
5:J:54:LEU:HD11	5:J:58:VAL:O	2.18	0.44
4:Q:4:LEU:HD22	4:Q:114:ILE:O	2.17	0.44
5:R:52:SER:HB3	5:R:53:HIS:CD2	2.53	0.44
1:A:365:TYR:O	1:A:367:VAL:N	2.51	0.44
1:A:444:LYS:HZ3	3:K:101:GLY:H	1.65	0.44
1:B:192:PHE:CD1	1:B:205:SER:HB2	2.52	0.44
1:C:57:PRO:HB3	1:C:273:ARG:NE	2.32	0.44
1:C:280:ASN:CG	1:C:284:THR:HG1	2.24	0.44
1:C:436:TRP:CZ3	1:C:510:VAL:HG23	2.53	0.44
2:E:38:ARG:HD2	2:E:94:TYR:HE1	1.81	0.44
5:F:32:TYR:HA	5:F:91:TYR:CE1	2.52	0.44
4:D:29:PHE:O	4:D:32:HIS:HB2	2.17	0.44
4:D:91:THR:OG1	4:D:91:THR:O	2.32	0.44
1:A:90:VAL:HA	1:A:268:GLY:O	2.17	0.44
1:A:444:LYS:HZ2	3:K:100:GLY:H	1.59	0.44
1:A:566:ARG:HH11	1:A:566:ARG:HG3	1.82	0.44
1:B:233:ASN:OD1	1:B:233:ASN:N	2.50	0.44
1:B:365:TYR:O	1:B:367:VAL:N	2.51	0.44
1:B:436:TRP:CZ3	1:B:510:VAL:HG23	2.52	0.44
1:B:527:LYS:HB3	1:B:528:LYS:H	1.46	0.44
1:B:566:ARG:HH11	1:B:566:ARG:HG3	1.82	0.44
1:C:53:ASP:OD2	1:C:195:LYS:NZ	2.42	0.44
1:C:80:ASP:O	1:C:82:PRO:HD3	2.16	0.44
1:C:365:TYR:O	1:C:367:VAL:N	2.51	0.44
1:C:407:VAL:HG21	1:C:507:TYR:CD2	2.53	0.44
1:C:418:ILE:C	1:C:420:ASP:H	2.25	0.44
1:C:553:LYS:HG2	1:C:554:SER:N	2.33	0.44
2:I:9:ALA:HA	2:I:122:LEU:O	2.17	0.44
2:I:67:ARG:O	2:I:83:LEU:HA	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:97:ALA:HB2	4:D:115:TRP:CE3	2.53	0.44
2:S:9:ALA:HA	2:S:122:LEU:O	2.17	0.44
5:R:21:ILE:HG23	5:R:103:THR:HG21	2.00	0.44
1:A:112:SER:C	1:A:132:GLU:HB3	2.43	0.44
1:A:343:ASN:HD22	6:O:6:FUC:H63	1.80	0.44
1:A:380:TYR:CD2	1:A:433:VAL:HB	2.52	0.44
1:A:553:LYS:HG2	1:A:554:SER:N	2.33	0.44
1:B:441:LEU:HA	3:G:32:THR:CG2	2.47	0.44
1:B:553:LYS:HG2	1:B:554:SER:N	2.33	0.44
1:B:699:LEU:HD12	1:C:872:GLN:NE2	2.33	0.44
1:C:25:THR:OG1	1:C:26:GLN:N	2.50	0.44
1:C:90:VAL:HA	1:C:268:GLY:O	2.17	0.44
1:C:401:VAL:HG11	1:C:508:ARG:HH21	1.82	0.44
1:C:426:PRO:HD3	1:C:464:PHE:HB2	2.00	0.44
2:E:10:GLU:O	2:E:124:THR:N	2.50	0.44
2:E:35:SER:C	2:E:36:TRP:CD1	2.95	0.44
4:H:52:ILE:HB	4:H:57:THR:O	2.17	0.44
5:F:21:ILE:HG23	5:F:103:THR:HG21	2.00	0.44
2:I:36:TRP:O	2:I:48:MET:HB2	2.18	0.44
3:K:38:GLN:HA	3:K:87:TYR:HA	1.99	0.44
5:J:33:LEU:HD22	5:J:71:PHE:CB	2.48	0.44
5:R:33:LEU:HD22	5:R:71:PHE:CB	2.48	0.44
1:A:83:VAL:CG1	1:A:236:ARG:HH21	2.30	0.44
1:A:849:LEU:HB3	1:A:851:CYS:SG	2.58	0.44
1:A:855:PHE:CD1	1:C:588:PRO:HD2	2.53	0.44
1:A:1057:PRO:O	1:A:1058:HIS:HB2	2.18	0.44
1:B:426:PRO:HD3	1:B:464:PHE:HB2	2.00	0.44
1:B:1125:ASN:OD1	1:B:1125:ASN:N	2.50	0.44
1:C:112:SER:C	1:C:132:GLU:HB3	2.43	0.44
1:C:437:ASN:HB3	5:R:93:ASP:OD2	2.18	0.44
1:C:1145:LEU:HA	1:C:1145:LEU:HD13	1.77	0.44
2:E:113:GLY:HA3	3:G:37:TYR:OH	2.18	0.44
2:S:29:PHE:CE1	2:S:74:THR:HA	2.44	0.44
2:S:69:THR:O	2:S:69:THR:OG1	2.30	0.44
4:Q:38:ARG:HH12	4:Q:90:ASP:HA	1.82	0.44
1:A:426:PRO:HD3	1:A:464:PHE:HB2	2.00	0.44
1:A:893:ALA:HB3	1:C:705:VAL:HG11	2.00	0.44
1:B:380:TYR:HB3	1:B:412:PRO:HD3	1.99	0.44
1:B:618:GLU:O	1:B:621:VAL:HA	2.18	0.44
1:B:715:PRO:HD3	1:C:894:LEU:HD13	1.98	0.44
1:B:1100:THR:HG1	1:B:1101:HIS:CE1	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:PHE:CD1	1:C:205:SER:HB2	2.52	0.44
1:C:380:TYR:HB3	1:C:412:PRO:HD3	1.99	0.44
1:A:128:ILE:HB	1:A:169:GLU:OE1	2.17	0.44
1:A:380:TYR:HB3	1:A:412:PRO:HD3	1.99	0.44
1:A:433:VAL:HG13	1:A:511:VAL:HG22	2.00	0.44
1:A:618:GLU:O	1:A:621:VAL:HA	2.18	0.44
1:A:1128:VAL:CG2	1:B:918:GLU:HG3	2.48	0.44
1:A:1141:LEU:O	1:A:1145:LEU:N	2.29	0.44
1:B:131:CYS:HA	1:B:166:CYS:CB	2.48	0.44
1:B:329:PHE:HA	1:B:578:PRO:CB	2.46	0.44
1:B:747:THR:O	1:B:750:SER:N	2.44	0.44
1:B:849:LEU:HB3	1:B:851:CYS:SG	2.58	0.44
1:C:128:ILE:HB	1:C:169:GLU:OE1	2.17	0.44
1:C:193:VAL:HG12	1:C:222:LEU:HD12	1.98	0.44
1:C:433:VAL:HG13	1:C:511:VAL:HG22	2.00	0.44
3:G:92:HIS:HA	3:G:96:LEU:CD1	2.46	0.44
4:H:38:ARG:HH12	4:H:90:ASP:HA	1.83	0.44
5:J:2:ILE:HG23	5:J:27:GLN:H	1.82	0.44
4:Q:97:ALA:HB2	4:Q:115:TRP:CE3	2.53	0.44
1:A:133:PHE:CZ	1:A:141:LEU:HD13	2.53	0.43
1:A:295:PRO:HG3	1:A:635:TYR:CE1	2.53	0.43
1:B:44:ARG:HD3	1:B:47:VAL:HG21	2.00	0.43
1:B:133:PHE:CZ	1:B:141:LEU:HD13	2.53	0.43
1:C:44:ARG:HD3	1:C:47:VAL:HG21	2.00	0.43
1:C:61:ASN:N	1:C:61:ASN:OD1	2.41	0.43
1:C:131:CYS:HA	1:C:166:CYS:CB	2.48	0.43
1:C:502:VAL:HG22	5:R:95:PRO:HD3	1.99	0.43
2:E:36:TRP:O	2:E:48:MET:HB2	2.18	0.43
2:E:73:ASP:O	2:E:77:THR:N	2.51	0.43
5:J:6:GLN:NE2	5:J:102:GLY:H	2.12	0.43
1:A:375:PHE:CZ	4:D:62:GLN:HB3	2.53	0.43
1:A:568:ILE:H	1:A:568:ILE:HD12	1.82	0.43
1:B:112:SER:C	1:B:132:GLU:HB3	2.43	0.43
1:B:213:ARG:HA	1:B:213:ARG:HD2	1.78	0.43
1:B:344:ALA:HA	2:E:111:ILE:H	1.82	0.43
1:B:407:VAL:HG21	1:B:507:TYR:CD2	2.53	0.43
1:B:747:THR:CG2	1:B:749:CYS:HB3	2.49	0.43
1:B:933:LYS:HB2	1:B:933:LYS:HE3	1.78	0.43
1:C:442:ASP:HB2	1:C:506:PRO:CB	2.41	0.43
1:C:566:ARG:HG3	1:C:566:ARG:HH11	1.82	0.43
5:F:54:LEU:HD11	5:F:58:VAL:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:48:MET:HE2	2:I:94:TYR:CD1	2.52	0.43
2:I:85:ARG:HA	2:I:85:ARG:HD3	1.86	0.43
4:D:61:ALA:HB3	4:D:68:VAL:HG11	2.00	0.43
2:S:73:ASP:O	2:S:77:THR:N	2.51	0.43
1:A:502:VAL:HA	1:A:505:GLN:CB	2.47	0.43
1:A:864:LEU:O	1:C:668:GLY:N	2.52	0.43
1:B:83:VAL:CG1	1:B:236:ARG:HH21	2.30	0.43
1:B:1072:GLU:HB3	1:C:894:LEU:HD22	1.99	0.43
1:C:326:ILE:CG2	1:C:326:ILE:O	2.67	0.43
2:E:29:PHE:CE1	2:E:74:THR:HA	2.44	0.43
3:G:79:LEU:CD2	3:G:104:VAL:HG11	2.47	0.43
4:H:37:VAL:HB	4:H:95:PHE:HB2	2.01	0.43
4:H:97:ALA:HB2	4:H:115:TRP:CE3	2.53	0.43
4:Q:93:VAL:HG13	4:Q:120:LEU:HD22	2.00	0.43
5:R:3:GLN:N	5:R:90:ARG:HH22	2.17	0.43
6:V:3:BMA:H3	6:V:4:MAN:H2	1.41	0.43
1:A:436:TRP:CZ3	1:A:510:VAL:HG23	2.53	0.43
1:A:585:ASP:OD2	1:B:847:ARG:NH2	2.52	0.43
1:B:295:PRO:HG3	1:B:635:TYR:CE1	2.53	0.43
1:B:1040:VAL:HB	1:C:1030:SER:O	2.19	0.43
1:C:133:PHE:CZ	1:C:141:LEU:HD13	2.53	0.43
5:F:2:ILE:HG23	5:F:27:GLN:H	1.82	0.43
5:F:65:SER:O	5:F:72:THR:N	2.51	0.43
3:K:36:TRP:CZ3	3:K:87:TYR:HB2	2.54	0.43
2:S:18:VAL:HG13	2:S:83:LEU:H	1.84	0.43
1:A:488:TYR:HD1	1:A:488:TYR:HA	1.68	0.43
1:A:542:PHE:CD2	1:A:546:THR:HA	2.54	0.43
1:B:65:PHE:CE2	1:B:84:LEU:HD11	2.48	0.43
1:B:90:VAL:HA	1:B:268:GLY:O	2.17	0.43
1:B:542:PHE:CD2	1:B:546:THR:HA	2.53	0.43
1:B:575:VAL:O	1:B:584:LEU:N	2.50	0.43
1:C:295:PRO:HG3	1:C:635:TYR:CE1	2.53	0.43
1:C:357:ARG:HA	1:C:396:TYR:CD2	2.54	0.43
1:C:542:PHE:CD2	1:C:546:THR:HG23	2.51	0.43
1:C:900:MET:HB3	1:C:900:MET:HE2	1.60	0.43
3:G:38:GLN:HA	3:G:87:TYR:HA	1.99	0.43
3:G:64:SER:OG	5:F:28:ASP:CG	2.62	0.43
2:I:23:LYS:HE3	2:I:23:LYS:HB3	1.81	0.43
4:D:38:ARG:HH12	4:D:90:ASP:HA	1.83	0.43
4:D:53:PRO:HG2	4:D:74:GLU:HG3	2.01	0.43
4:D:93:VAL:HG13	4:D:120:LEU:HD22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:36:TRP:O	2:S:48:MET:HB2	2.18	0.43
1:A:326:ILE:O	1:A:326:ILE:CG2	2.67	0.43
1:A:407:VAL:HG21	1:A:507:TYR:CD2	2.53	0.43
1:A:821:LEU:HD12	1:A:821:LEU:HA	1.87	0.43
1:A:976:VAL:HB	1:A:979:ASP:HB2	2.01	0.43
1:B:319:ARG:HG2	1:B:319:ARG:HH11	1.84	0.43
1:C:540:PHE:CD1	1:C:540:PHE:CB	2.88	0.43
1:C:849:LEU:HB3	1:C:851:CYS:SG	2.58	0.43
1:C:984:LEU:HB3	1:C:988:GLU:CD	2.42	0.43
2:E:38:ARG:N	2:E:46:GLU:O	2.31	0.43
3:G:36:TRP:N	3:G:49:ILE:O	2.46	0.43
3:G:36:TRP:CE2	3:G:89:CYS:HB2	2.54	0.43
4:H:22:CYS:HB3	4:H:79:ALA:HB3	2.01	0.43
2:I:18:VAL:HG13	2:I:83:LEU:H	1.84	0.43
2:S:117:TRP:HH2	3:T:98:PHE:HE2	1.67	0.43
5:R:54:LEU:HD11	5:R:58:VAL:O	2.18	0.43
6:O:3:BMA:H3	6:O:4:MAN:H2	1.41	0.43
1:A:348:ALA:HA	2:I:111:ILE:HD13	1.99	0.43
1:A:673:TYR:HD1	1:A:692:ILE:HG12	1.84	0.43
1:B:326:ILE:O	1:B:326:ILE:CG2	2.67	0.43
1:B:433:VAL:HG13	1:B:511:VAL:HG22	2.00	0.43
1:C:489:PHE:O	1:C:492:GLN:NE2	2.52	0.43
1:C:598:THR:HB	1:C:607:VAL:HG12	2.01	0.43
1:C:821:LEU:HD12	1:C:821:LEU:HA	1.87	0.43
1:C:976:VAL:O	1:C:980:ILE:HG12	2.19	0.43
2:E:19:LYS:HD2	2:E:80:TYR:HB3	2.01	0.43
2:S:54:TYR:HD2	2:S:105:TRP:HA	1.84	0.43
4:Q:94:TYR:HD1	4:Q:94:TYR:H	1.65	0.43
1:A:44:ARG:HD3	1:A:47:VAL:HG21	2.00	0.43
1:A:65:PHE:CE2	1:A:84:LEU:HD11	2.48	0.43
1:A:402:ILE:HA	1:A:494:TYR:CZ	2.54	0.43
1:A:620:SER:O	1:A:622:ALA:C	2.62	0.43
1:A:747:THR:CG2	1:A:749:CYS:HB3	2.49	0.43
1:A:976:VAL:O	1:A:980:ILE:HG12	2.19	0.43
1:B:402:ILE:HA	1:B:494:TYR:CZ	2.54	0.43
1:C:343:ASN:HB3	2:S:111:ILE:CG2	2.48	0.43
1:C:618:GLU:O	1:C:621:VAL:HA	2.18	0.43
1:C:973:ILE:H	1:C:973:ILE:HG12	1.45	0.43
4:H:45:LEU:HG	5:F:87:TYR:CD1	2.53	0.43
4:H:93:VAL:HG13	4:H:120:LEU:HD22	2.01	0.43
5:F:3:GLN:N	5:F:90:ARG:HH22	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:60:TYR:CE1	2:I:70:MET:HB2	2.44	0.43
2:I:63:LYS:H	2:I:63:LYS:HG3	1.37	0.43
3:K:36:TRP:CE2	3:K:89:CYS:HB2	2.54	0.43
4:D:98:ARG:HD3	4:D:98:ARG:HA	1.51	0.43
3:T:36:TRP:CZ3	3:T:87:TYR:HB2	2.54	0.43
4:Q:1:GLN:HB3	4:Q:2:VAL:H	1.66	0.43
4:Q:61:ALA:HB3	4:Q:68:VAL:HG11	2.00	0.43
5:R:35:TRP:HB3	5:R:73:PHE:CD1	2.54	0.43
1:A:133:PHE:CE1	1:A:136:CYS:HB2	2.54	0.43
1:A:357:ARG:HA	1:A:396:TYR:CD2	2.54	0.43
1:A:1145:LEU:HG	1:B:1145:LEU:HD21	2.00	0.43
1:B:357:ARG:HA	1:B:396:TYR:CD2	2.54	0.43
1:B:581:LEU:CG	1:B:582:GLU:H	2.32	0.43
1:B:673:TYR:HD1	1:B:692:ILE:HG12	1.84	0.43
1:B:976:VAL:O	1:B:980:ILE:HG12	2.19	0.43
1:C:500:TYR:C	4:Q:101:PRO:HG3	2.44	0.43
1:C:538:VAL:HA	1:C:550:VAL:HA	2.01	0.43
1:C:620:SER:O	1:C:622:ALA:C	2.62	0.43
1:C:747:THR:CG2	1:C:749:CYS:HB3	2.49	0.43
2:E:52:SER:O	2:E:56:GLY:N	2.47	0.43
5:F:18:ARG:HD2	5:F:18:ARG:HA	1.64	0.43
2:I:29:PHE:CE1	2:I:74:THR:HA	2.44	0.43
2:S:33:GLY:CA	2:S:50:TRP:HE1	2.29	0.43
3:T:36:TRP:CE2	3:T:89:CYS:HB2	2.54	0.43
1:A:131:CYS:HA	1:A:166:CYS:CB	2.48	0.43
1:A:361:CYS:SG	1:A:524:CYS:N	2.87	0.43
1:A:442:ASP:HB2	1:A:506:PRO:CB	2.41	0.43
1:A:538:VAL:HA	1:A:550:VAL:HA	2.01	0.43
1:B:133:PHE:CE1	1:B:136:CYS:HB2	2.54	0.43
1:B:319:ARG:HD2	1:B:319:ARG:HA	1.54	0.43
1:B:564:PHE:HD2	1:B:564:PHE:N	2.17	0.43
1:C:319:ARG:HG2	1:C:319:ARG:HH11	1.84	0.43
1:C:402:ILE:HA	1:C:494:TYR:CZ	2.54	0.43
1:C:581:LEU:CG	1:C:582:GLU:H	2.32	0.43
2:E:33:GLY:CA	2:E:50:TRP:HE1	2.29	0.43
2:I:52:SER:O	2:I:56:GLY:N	2.47	0.43
4:D:94:TYR:HD1	4:D:94:TYR:H	1.65	0.43
3:T:64:SER:O	3:T:76:ILE:HG13	2.19	0.43
5:R:95:PRO:HB3	5:R:97:TYR:CZ	2.54	0.43
1:A:29:THR:HG22	1:A:30:ASN:H	1.84	0.42
1:A:329:PHE:HA	1:A:578:PRO:CB	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:598:THR:HB	1:A:607:VAL:HG12	2.01	0.42
1:B:334:ASN:O	1:B:361:CYS:C	2.62	0.42
1:B:457:ARG:HE	1:B:457:ARG:HB3	1.73	0.42
1:B:481:LYS:HE2	1:B:481:LYS:HB3	1.69	0.42
1:B:531:ASN:O	1:B:532:LEU:C	2.62	0.42
1:B:581:LEU:HD23	1:B:582:GLU:H	1.84	0.42
1:B:664:PRO:CB	1:C:864:LEU:HD13	2.49	0.42
1:C:334:ASN:O	1:C:361:CYS:C	2.62	0.42
1:C:378:LYS:HD3	1:C:378:LYS:HA	1.55	0.42
3:G:36:TRP:CZ3	3:G:87:TYR:HB2	2.54	0.42
5:J:95:PRO:HB3	5:J:97:TYR:CZ	2.54	0.42
4:Q:53:PRO:HG2	4:Q:74:GLU:HG3	2.00	0.42
1:A:319:ARG:HG2	1:A:319:ARG:HH11	1.84	0.42
1:A:559:LEU:HD22	1:B:283:GLY:O	2.19	0.42
1:A:581:LEU:CG	1:A:582:GLU:H	2.32	0.42
1:A:913:GLN:O	1:A:916:LEU:N	2.51	0.42
1:B:598:THR:HB	1:B:607:VAL:HG12	2.01	0.42
1:B:962:LEU:HD13	1:B:1007:TYR:HB2	2.01	0.42
1:C:133:PHE:CE1	1:C:136:CYS:HB2	2.54	0.42
1:C:365:TYR:N	1:C:388:ASN:HB3	2.35	0.42
1:C:673:TYR:HD1	1:C:692:ILE:HG12	1.84	0.42
1:C:976:VAL:HB	1:C:979:ASP:HB2	2.01	0.42
3:G:49:ILE:CD1	3:G:59:ILE:HD12	2.50	0.42
4:H:61:ALA:HB3	4:H:68:VAL:HG11	2.00	0.42
5:J:65:SER:O	5:J:72:THR:N	2.51	0.42
4:Q:51:PHE:HA	4:Q:58:THR:OG1	2.19	0.42
5:R:65:SER:O	5:R:72:THR:N	2.51	0.42
6:M:3:BMA:H3	6:M:4:MAN:H2	1.41	0.42
1:A:489:PHE:O	1:A:492:GLN:NE2	2.52	0.42
1:A:581:LEU:HD23	1:A:582:GLU:H	1.84	0.42
1:A:770:ILE:O	1:A:774:GLN:HG2	2.19	0.42
1:B:324:GLU:OE2	1:B:324:GLU:HA	2.17	0.42
1:B:524:CYS:SG	1:B:525:GLY:N	2.93	0.42
1:B:620:SER:O	1:B:622:ALA:C	2.62	0.42
1:B:1057:PRO:O	1:B:1058:HIS:HB2	2.18	0.42
1:C:29:THR:HG22	1:C:30:ASN:H	1.84	0.42
4:H:51:PHE:HA	4:H:58:THR:OG1	2.19	0.42
3:K:23:CYS:N	3:K:72:PHE:O	2.50	0.42
5:J:21:ILE:HG23	5:J:103:THR:HG21	2.00	0.42
1:A:334:ASN:O	1:A:361:CYS:C	2.62	0.42
1:A:1117:THR:CG2	1:A:1139:ASP:HA	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1141:LEU:HD13	1:A:1141:LEU:HA	1.67	0.42
1:B:63:THR:O	1:B:63:THR:OG1	2.34	0.42
1:B:361:CYS:SG	1:B:524:CYS:N	2.87	0.42
1:B:380:TYR:HB2	1:B:430:THR:OG1	2.19	0.42
1:B:387:LEU:H	1:B:387:LEU:CD2	2.33	0.42
1:C:65:PHE:CE2	1:C:84:LEU:HD11	2.48	0.42
1:C:405:ASN:ND2	1:C:504:HIS:HE1	2.17	0.42
1:C:524:CYS:SG	1:C:525:GLY:N	2.93	0.42
1:C:770:ILE:O	1:C:774:GLN:HG2	2.19	0.42
2:E:18:VAL:HG13	2:E:83:LEU:H	1.84	0.42
4:H:73:ASP:HB3	4:H:76:THR:OG1	2.20	0.42
4:H:91:THR:O	4:H:91:THR:OG1	2.32	0.42
5:F:95:PRO:HB3	5:F:97:TYR:CZ	2.54	0.42
2:I:73:ASP:O	2:I:77:THR:N	2.51	0.42
3:K:48:LEU:O	3:K:59:ILE:HD11	2.20	0.42
4:D:22:CYS:HB3	4:D:79:ALA:HB3	2.01	0.42
2:S:97:ALA:HB1	2:S:114:PHE:HB3	2.02	0.42
4:Q:38:ARG:HH22	4:Q:90:ASP:C	2.27	0.42
1:A:548:THR:HG23	1:A:548:THR:O	2.19	0.42
1:B:36:VAL:HG11	1:B:219:PHE:CZ	2.55	0.42
1:B:102:ARG:HD3	1:B:241:LEU:HB2	2.02	0.42
1:B:502:VAL:CG2	4:H:54:LEU:HD22	2.49	0.42
1:C:581:LEU:HD23	1:C:582:GLU:H	1.84	0.42
2:E:23:LYS:HE3	2:E:23:LYS:HB3	1.81	0.42
3:G:48:LEU:O	3:G:59:ILE:HD11	2.20	0.42
4:H:95:PHE:CE2	5:F:44:PRO:HD3	2.54	0.42
5:F:35:TRP:HB3	5:F:73:PHE:CD1	2.54	0.42
3:K:49:ILE:CD1	3:K:59:ILE:HD12	2.50	0.42
5:J:35:TRP:HB3	5:J:73:PHE:CD1	2.54	0.42
2:S:34:ILE:HA	2:S:98:ARG:HA	2.02	0.42
3:T:49:ILE:CD1	3:T:59:ILE:HD12	2.50	0.42
4:Q:37:VAL:HB	4:Q:95:PHE:HB2	2.01	0.42
1:A:102:ARG:HD3	1:A:241:LEU:HB2	2.02	0.42
1:A:365:TYR:N	1:A:388:ASN:HB3	2.35	0.42
1:A:405:ASN:ND2	1:A:504:HIS:HE1	2.17	0.42
1:A:786:LYS:H	1:A:786:LYS:HG2	1.72	0.42
1:B:122:ASN:HD21	1:B:127:PHE:HE2	1.67	0.42
1:B:365:TYR:N	1:B:388:ASN:HB3	2.35	0.42
1:B:409:GLN:HG3	1:B:418:ILE:H	1.85	0.42
1:B:538:VAL:HA	1:B:550:VAL:HA	2.01	0.42
1:C:393:THR:O	1:C:522:THR:OG1	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:542:PHE:CD2	1:C:546:THR:HA	2.53	0.42
1:C:548:THR:HG23	1:C:548:THR:O	2.20	0.42
2:E:34:ILE:HA	2:E:98:ARG:HA	2.02	0.42
3:K:38:GLN:HB2	3:K:48:LEU:HD13	2.01	0.42
1:A:444:LYS:NZ	3:K:101:GLY:N	2.68	0.42
1:B:344:ALA:C	2:E:111:ILE:HB	2.45	0.42
1:B:393:THR:O	1:B:522:THR:OG1	2.36	0.42
1:C:431:GLY:HA3	1:C:512:LEU:HB2	2.02	0.42
1:C:531:ASN:O	1:C:532:LEU:C	2.62	0.42
1:C:540:PHE:CD2	1:C:540:PHE:CB	2.87	0.42
1:C:551:LEU:CD2	1:C:586:ILE:HB	2.31	0.42
1:C:806:LEU:HD23	1:C:806:LEU:HA	1.92	0.42
2:E:34:ILE:N	2:E:51:ILE:O	2.53	0.42
2:E:38:ARG:HD2	2:E:94:TYR:CE1	2.55	0.42
4:H:53:PRO:HG2	4:H:74:GLU:HG3	2.01	0.42
4:H:59:ILE:HD12	5:F:95:PRO:HB2	2.02	0.42
2:I:19:LYS:HD2	2:I:80:TYR:HB3	2.01	0.42
2:S:38:ARG:HD2	2:S:94:TYR:CE1	2.55	0.42
4:Q:47:TRP:CZ2	4:Q:49:GLY:HA2	2.55	0.42
1:A:450:ASP:CB	3:K:3:VAL:HG11	2.50	0.42
1:A:531:ASN:O	1:A:532:LEU:C	2.62	0.42
1:B:405:ASN:ND2	1:B:504:HIS:HE1	2.17	0.42
1:C:112:SER:HB2	1:C:134:GLN:H	1.85	0.42
1:C:122:ASN:C	1:C:124:THR:H	2.28	0.42
1:C:371:PHE:HB2	1:C:374:PHE:CZ	2.55	0.42
1:C:1117:THR:CG2	1:C:1139:ASP:HA	2.49	0.42
4:H:98:ARG:HD3	4:H:98:ARG:HH11	1.67	0.42
5:F:6:GLN:NE2	5:F:102:GLY:H	2.12	0.42
5:F:86:TYR:C	5:F:103:THR:H	2.28	0.42
2:I:34:ILE:N	2:I:51:ILE:O	2.53	0.42
2:I:54:TYR:HD2	2:I:105:TRP:HA	1.84	0.42
3:K:31:SER:HB3	3:K:52:ALA:HB3	2.01	0.42
4:D:96:CYS:O	4:D:116:GLY:N	2.53	0.42
5:J:3:GLN:N	5:J:90:ARG:HH22	2.16	0.42
5:J:4:MET:SD	5:J:25:ALA:HB2	2.60	0.42
1:A:36:VAL:HG11	1:A:219:PHE:CZ	2.55	0.42
1:A:319:ARG:HD2	1:A:319:ARG:HA	1.54	0.42
1:A:524:CYS:SG	1:A:525:GLY:N	2.93	0.42
1:A:542:PHE:CD2	1:A:546:THR:HG23	2.51	0.42
1:A:962:LEU:HD13	1:A:1007:TYR:HB2	2.01	0.42
1:B:770:ILE:O	1:B:774:GLN:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:935:GLN:O	1:B:939:PHE:HB3	2.20	0.42
1:C:102:ARG:HD3	1:C:241:LEU:HB2	2.02	0.42
1:C:122:ASN:HD21	1:C:127:PHE:HE2	1.67	0.42
2:E:12:LYS:HB2	2:E:125:VAL:HG22	2.02	0.42
2:E:39:GLN:HB3	2:E:93:VAL:HG22	2.02	0.42
5:F:4:MET:SD	5:F:25:ALA:HB2	2.60	0.42
4:D:73:ASP:HB3	4:D:76:THR:OG1	2.20	0.42
5:J:86:TYR:C	5:J:103:THR:H	2.28	0.42
3:T:48:LEU:O	3:T:59:ILE:HD11	2.20	0.42
4:Q:22:CYS:HB3	4:Q:79:ALA:HB3	2.01	0.42
5:R:4:MET:SD	5:R:25:ALA:HB2	2.60	0.42
5:R:62:PHE:HA	5:R:75:ILE:HG12	2.01	0.42
1:A:348:ALA:CA	2:I:111:ILE:HG21	2.49	0.42
1:A:371:PHE:HB2	1:A:374:PHE:CZ	2.55	0.42
1:A:393:THR:O	1:A:522:THR:OG1	2.36	0.42
1:A:873:TYR:OH	1:C:699:LEU:HD22	2.20	0.42
1:A:985:ASP:HB2	1:A:986:PRO:HD2	2.02	0.42
1:B:122:ASN:C	1:B:124:THR:H	2.28	0.42
1:B:431:GLY:HA3	1:B:512:LEU:HB2	2.02	0.42
1:B:559:LEU:HD12	1:B:559:LEU:HA	1.70	0.42
1:C:192:PHE:HB3	1:C:194:PHE:CZ	2.55	0.42
2:E:22:CYS:O	2:E:79:GLY:N	2.36	0.42
2:I:97:ALA:HB1	2:I:114:PHE:HB3	2.02	0.42
4:D:20:VAL:HG21	4:D:119:THR:HG21	2.02	0.42
4:D:37:VAL:HB	4:D:95:PHE:HB2	2.01	0.42
2:S:19:LYS:HD2	2:S:80:TYR:HB3	2.01	0.42
3:T:31:SER:HB3	3:T:52:ALA:HB3	2.01	0.42
4:Q:83:LEU:HD23	4:Q:86:LEU:HD13	2.01	0.42
4:Q:96:CYS:O	4:Q:116:GLY:N	2.53	0.42
1:A:122:ASN:C	1:A:124:THR:H	2.28	0.41
1:A:387:LEU:CD2	1:A:387:LEU:H	2.33	0.41
1:A:935:GLN:O	1:A:939:PHE:HB3	2.20	0.41
1:B:192:PHE:HB3	1:B:194:PHE:CZ	2.55	0.41
1:B:494:TYR:HB3	1:B:496:PHE:CD1	2.55	0.41
1:B:500:TYR:C	4:H:103:GLY:H	2.28	0.41
1:B:548:THR:O	1:B:548:THR:HG23	2.19	0.41
1:B:985:ASP:HB2	1:B:986:PRO:HD2	2.02	0.41
1:C:494:TYR:HB3	1:C:496:PHE:CD1	2.55	0.41
1:C:962:LEU:HD13	1:C:1007:TYR:HB2	2.01	0.41
3:G:61:ASP:C	5:F:27:GLN:HE22	2.28	0.41
2:I:29:PHE:CE1	2:I:77:THR:HA	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:49:GLY:CA	2:I:70:MET:HE1	2.50	0.41
4:D:51:PHE:HA	4:D:58:THR:OG1	2.19	0.41
5:J:62:PHE:HA	5:J:75:ILE:HG12	2.01	0.41
4:Q:20:VAL:HG21	4:Q:119:THR:HG21	2.02	0.41
5:R:37:GLN:CD	5:R:47:LEU:HD21	2.45	0.41
1:A:370:ASN:HB3	6:O:5:MAN:H5	2.02	0.41
1:A:409:GLN:HG3	1:A:418:ILE:H	1.85	0.41
1:A:967:SER:OG	1:C:570:ASP:OD1	2.22	0.41
1:A:973:ILE:H	1:A:973:ILE:HG12	1.44	0.41
1:A:1130:ILE:HD11	1:B:921:LYS:NZ	2.34	0.41
1:B:29:THR:HG22	1:B:30:ASN:H	1.84	0.41
1:B:112:SER:HB2	1:B:134:GLN:H	1.85	0.41
1:B:130:VAL:HB	1:B:167:THR:OG1	2.20	0.41
1:B:355:ARG:NH1	1:B:464:PHE:CE1	2.89	0.41
1:B:365:TYR:H	1:B:388:ASN:HA	1.85	0.41
1:B:371:PHE:HB2	1:B:374:PHE:CZ	2.55	0.41
1:B:437:ASN:HB2	1:B:507:TYR:CE1	2.55	0.41
1:B:489:PHE:O	1:B:492:GLN:NE2	2.52	0.41
1:B:976:VAL:HB	1:B:979:ASP:HB2	2.00	0.41
1:B:1117:THR:CG2	1:B:1139:ASP:HA	2.49	0.41
1:C:552:THR:O	1:C:584:LEU:HB3	2.20	0.41
1:C:850:ILE:C	1:C:852:ALA:N	2.79	0.41
2:E:54:TYR:HD2	2:E:105:TRP:HA	1.84	0.41
3:G:31:SER:HB3	3:G:52:ALA:HB3	2.01	0.41
3:G:38:GLN:HB2	3:G:48:LEU:HD13	2.01	0.41
4:H:96:CYS:O	4:H:116:GLY:N	2.53	0.41
5:F:37:GLN:CD	5:F:47:LEU:HD21	2.45	0.41
2:I:38:ARG:N	2:I:46:GLU:O	2.31	0.41
2:I:39:GLN:HB3	2:I:93:VAL:HG22	2.02	0.41
3:K:6:GLN:NE2	3:K:88:TYR:HA	2.36	0.41
4:D:47:TRP:CZ2	4:D:49:GLY:HA2	2.55	0.41
2:S:34:ILE:N	2:S:51:ILE:O	2.53	0.41
2:S:44:GLY:CA	3:T:100:GLY:HA2	2.50	0.41
1:A:192:PHE:HB3	1:A:194:PHE:CZ	2.55	0.41
1:A:232:ILE:HA	1:A:232:ILE:HD13	1.81	0.41
1:A:587:THR:HA	1:A:588:PRO:HD3	1.93	0.41
1:A:809:PRO:HA	1:A:814:LYS:NZ	2.36	0.41
1:A:969:LYS:H	1:A:969:LYS:HG3	1.73	0.41
1:B:442:ASP:HB2	1:B:506:PRO:CB	2.41	0.41
1:B:552:THR:O	1:B:584:LEU:HB3	2.20	0.41
1:C:36:VAL:HG11	1:C:219:PHE:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1125:ASN:OD1	1:C:1125:ASN:N	2.50	0.41
2:I:55:ASN:ND2	2:I:57:ASN:HB2	2.36	0.41
4:Q:73:ASP:HB3	4:Q:76:THR:OG1	2.20	0.41
4:Q:104:ASP:CG	4:Q:105:PRO:HD2	2.45	0.41
1:A:340:GLU:OE1	2:I:28:PRO:HD2	2.20	0.41
1:A:645:ARG:HE	1:A:645:ARG:HB3	1.52	0.41
1:B:84:LEU:HD23	1:B:84:LEU:HA	1.86	0.41
1:B:874:THR:O	1:B:878:LEU:HB2	2.20	0.41
1:B:1145:LEU:HA	1:B:1145:LEU:HD13	1.77	0.41
1:C:1040:VAL:C	1:C:1042:PHE:H	2.28	0.41
4:H:48:MET:O	4:H:61:ALA:HB2	2.21	0.41
2:I:34:ILE:HA	2:I:98:ARG:HA	2.02	0.41
2:I:116:ASN:CG	6:O:6:FUC:O3	2.58	0.41
4:D:104:ASP:CG	4:D:105:PRO:HD2	2.45	0.41
2:S:49:GLY:CA	2:S:70:MET:HE1	2.50	0.41
2:S:55:ASN:ND2	2:S:57:ASN:HB2	2.36	0.41
2:S:81:MET:HE1	2:S:94:TYR:CD2	2.56	0.41
3:T:38:GLN:HB2	3:T:48:LEU:HD13	2.01	0.41
5:R:18:ARG:HA	5:R:18:ARG:HD2	1.64	0.41
1:A:122:ASN:HD21	1:A:127:PHE:HE2	1.67	0.41
1:A:380:TYR:HB2	1:A:430:THR:OG1	2.19	0.41
1:A:1040:VAL:C	1:A:1042:PHE:H	2.28	0.41
1:B:395:VAL:HA	1:B:514:PHE:CA	2.43	0.41
1:C:343:ASN:HB3	2:S:111:ILE:HG21	2.03	0.41
1:C:483:LYS:H	1:C:483:LYS:HG3	1.52	0.41
1:C:985:ASP:HB2	1:C:986:PRO:HD2	2.02	0.41
4:H:43:GLN:HG2	4:H:44:GLY:N	2.36	0.41
5:J:89:GLN:HA	5:J:98:THR:O	2.21	0.41
3:T:87:TYR:CE2	3:T:103:LYS:HA	2.56	0.41
1:A:494:TYR:HB3	1:A:496:PHE:CD1	2.55	0.41
1:A:616:CYS:O	1:A:619:VAL:HG12	2.21	0.41
1:A:623:ILE:H	1:A:623:ILE:HG12	1.23	0.41
1:B:402:ILE:CD1	1:B:407:VAL:HG22	2.46	0.41
1:B:435:ALA:HA	1:B:509:VAL:HG13	2.03	0.41
1:B:488:TYR:HD1	1:B:488:TYR:HA	1.68	0.41
1:C:435:ALA:HA	1:C:509:VAL:HG13	2.03	0.41
1:C:616:CYS:O	1:C:618:GLU:C	2.63	0.41
1:C:731:MET:HB2	1:C:955:ASN:HD21	1.85	0.41
1:C:874:THR:O	1:C:878:LEU:HB2	2.20	0.41
2:E:6:GLN:HB3	2:E:120:GLY:H	1.86	0.41
2:E:49:GLY:CA	2:E:70:MET:HE1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:6:GLN:HB3	2:I:120:GLY:H	1.86	0.41
3:T:23:CYS:N	3:T:72:PHE:O	2.50	0.41
5:R:86:TYR:C	5:R:103:THR:H	2.28	0.41
1:A:112:SER:HB2	1:A:134:GLN:H	1.85	0.41
1:A:365:TYR:H	1:A:388:ASN:HA	1.85	0.41
1:A:422:ASN:HD22	1:A:454:ARG:CG	2.28	0.41
1:A:437:ASN:HB2	1:A:507:TYR:CE1	2.55	0.41
1:A:600:GLY:C	1:A:602:ASN:N	2.75	0.41
1:A:933:LYS:HB2	1:A:933:LYS:HE3	1.78	0.41
1:B:520:PRO:HD2	1:C:229:PRO:HB2	2.02	0.41
1:B:616:CYS:O	1:B:619:VAL:HG12	2.21	0.41
1:C:355:ARG:NH1	1:C:464:PHE:CE1	2.88	0.41
1:C:380:TYR:HB2	1:C:430:THR:OG1	2.19	0.41
1:C:437:ASN:HB2	1:C:507:TYR:CE1	2.55	0.41
1:C:501:GLY:H	1:C:504:HIS:HD2	1.69	0.41
1:C:933:LYS:HB2	1:C:933:LYS:HE3	1.78	0.41
2:E:71:THR:HG22	2:E:80:TYR:HB2	2.02	0.41
2:E:115:ASP:CG	2:E:116:ASN:H	2.29	0.41
4:H:20:VAL:HG21	4:H:119:THR:HG21	2.02	0.41
4:H:47:TRP:CZ2	4:H:49:GLY:HA2	2.55	0.41
2:I:38:ARG:HD2	2:I:94:TYR:CE1	2.55	0.41
3:K:64:SER:O	3:K:76:ILE:HG13	2.19	0.41
4:D:48:MET:O	4:D:61:ALA:HB2	2.21	0.41
4:D:83:LEU:HD23	4:D:86:LEU:HD13	2.01	0.41
1:A:64:TRP:CD1	1:A:64:TRP:C	2.99	0.41
1:A:194:PHE:HB3	1:A:201:PHE:CE1	2.56	0.41
1:A:431:GLY:HA3	1:A:512:LEU:HB2	2.02	0.41
1:A:731:MET:HB2	1:A:955:ASN:HD21	1.86	0.41
1:A:852:ALA:HB1	1:A:855:PHE:HD2	1.86	0.41
1:B:501:GLY:H	1:B:504:HIS:HD2	1.69	0.41
1:B:809:PRO:HA	1:B:814:LYS:NZ	2.36	0.41
1:C:130:VAL:HB	1:C:167:THR:OG1	2.20	0.41
1:C:387:LEU:H	1:C:387:LEU:CD2	2.33	0.41
1:C:402:ILE:CD1	1:C:407:VAL:HG22	2.46	0.41
1:C:409:GLN:HG3	1:C:418:ILE:H	1.85	0.41
1:C:616:CYS:O	1:C:619:VAL:HG12	2.21	0.41
1:C:935:GLN:O	1:C:939:PHE:HB3	2.20	0.41
3:G:64:SER:O	3:G:76:ILE:HG13	2.19	0.41
4:D:117:GLN:HA	5:J:107:ILE:CD1	2.51	0.41
4:Q:43:GLN:HG2	4:Q:44:GLY:N	2.36	0.41
1:A:355:ARG:NH1	1:A:464:PHE:CE1	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:THR:O	1:A:433:VAL:HG23	2.21	0.41
1:A:558:PHE:HA	1:B:43:PHE:CD2	2.56	0.41
1:A:566:ARG:HG3	1:A:566:ARG:NH1	2.36	0.41
1:A:807:PRO:CG	1:A:875:SER:HB2	2.51	0.41
1:A:874:THR:O	1:A:878:LEU:HB2	2.20	0.41
1:A:969:LYS:O	1:A:971:GLY:N	2.54	0.41
1:A:1128:VAL:HG21	1:B:918:GLU:HG3	2.02	0.41
1:B:502:VAL:C	1:B:504:HIS:N	2.78	0.41
1:B:536:LYS:O	1:B:537:CYS:CB	2.69	0.41
1:B:752:LEU:HD11	1:B:990:GLU:OE1	2.21	0.41
1:B:850:ILE:HD13	1:B:960:ASN:HD21	1.86	0.41
1:B:913:GLN:O	1:B:916:LEU:N	2.51	0.41
1:C:194:PHE:HB3	1:C:201:PHE:CE1	2.56	0.41
1:C:205:SER:OG	1:C:206:LYS:N	2.54	0.41
1:C:366:SER:C	1:C:368:LEU:N	2.79	0.41
1:C:430:THR:O	1:C:433:VAL:HG23	2.21	0.41
1:C:817:PRO:O	1:C:821:LEU:HD22	2.21	0.41
2:E:39:GLN:HE22	3:G:39:GLN:HE22	1.68	0.41
2:E:97:ALA:HB1	2:E:114:PHE:HB3	2.02	0.41
3:G:22:SER:HA	3:G:73:THR:HA	2.02	0.41
4:H:51:PHE:C	4:H:53:PRO:HD3	2.46	0.41
5:F:62:PHE:HA	5:F:75:ILE:HG12	2.01	0.41
5:F:70:ASP:C	5:F:71:PHE:HD1	2.29	0.41
2:I:29:PHE:O	2:I:53:THR:OG1	2.19	0.41
3:K:87:TYR:CE2	3:K:103:LYS:HA	2.56	0.41
2:S:12:LYS:HB2	2:S:125:VAL:HG22	2.02	0.41
2:S:71:THR:HG22	2:S:80:TYR:HB2	2.02	0.41
3:T:22:SER:HA	3:T:73:THR:HA	2.02	0.41
4:Q:4:LEU:HD21	4:Q:98:ARG:NE	2.36	0.41
4:Q:48:MET:O	4:Q:61:ALA:HB2	2.20	0.41
5:R:70:ASP:C	5:R:71:PHE:HD1	2.29	0.41
1:A:501:GLY:H	1:A:504:HIS:HD2	1.69	0.41
1:A:552:THR:O	1:A:584:LEU:HB3	2.20	0.41
1:B:357:ARG:HB3	1:B:396:TYR:CE2	2.56	0.41
1:B:439:ASN:HA	1:B:506:PRO:HG2	2.03	0.41
2:E:55:ASN:ND2	2:E:57:ASN:HB2	2.36	0.41
3:G:34:LEU:HG	3:G:90:GLN:O	2.21	0.41
2:I:71:THR:HG22	2:I:80:TYR:HB2	2.02	0.41
5:J:70:ASP:C	5:J:71:PHE:HD1	2.29	0.41
2:S:86:LEU:HB3	2:S:125:VAL:HG11	2.03	0.41
2:S:97:ALA:HB2	2:S:117:TRP:CE3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:THR:OG1	1:A:26:GLN:N	2.50	0.40
1:A:435:ALA:HA	1:A:509:VAL:HG13	2.03	0.40
1:A:481:LYS:HE2	1:A:481:LYS:HB3	1.69	0.40
1:A:644:THR:HB	1:A:646:ALA:H	1.86	0.40
1:A:817:PRO:O	1:A:821:LEU:HD22	2.21	0.40
1:A:850:ILE:HD12	1:C:568:ILE:HB	2.03	0.40
1:B:457:ARG:NH1	1:B:461:LEU:HB3	2.37	0.40
1:B:1040:VAL:C	1:B:1042:PHE:H	2.28	0.40
1:C:357:ARG:HB3	1:C:396:TYR:CE2	2.56	0.40
1:C:644:THR:HB	1:C:646:ALA:H	1.86	0.40
1:C:809:PRO:HA	1:C:814:LYS:NZ	2.36	0.40
3:G:46:ARG:HH22	3:G:58:GLY:C	2.29	0.40
3:K:22:SER:HA	3:K:73:THR:HA	2.02	0.40
4:D:27:GLY:O	4:D:29:PHE:HD2	2.04	0.40
4:D:43:GLN:HG2	4:D:44:GLY:N	2.36	0.40
4:D:51:PHE:C	4:D:53:PRO:HD3	2.46	0.40
2:S:115:ASP:CG	2:S:116:ASN:H	2.29	0.40
4:Q:38:ARG:NH2	4:Q:90:ASP:O	2.43	0.40
4:Q:91:THR:HA	4:Q:122:THR:HA	2.04	0.40
1:A:84:LEU:HA	1:A:85:PRO:HD2	1.96	0.40
1:A:298:GLU:O	1:A:302:THR:HG23	2.21	0.40
1:A:457:ARG:NH1	1:A:461:LEU:HB3	2.37	0.40
1:A:670:CYS:SG	1:A:697:MET:HB3	2.61	0.40
1:A:674:GLN:C	1:A:676:GLN:HE21	2.30	0.40
1:B:616:CYS:O	1:B:618:GLU:C	2.63	0.40
1:C:232:ILE:HD13	1:C:232:ILE:HA	1.81	0.40
1:C:566:ARG:HG3	1:C:566:ARG:NH1	2.36	0.40
1:C:807:PRO:CG	1:C:875:SER:HB2	2.51	0.40
1:C:850:ILE:HG23	1:C:853:GLN:CD	2.46	0.40
1:C:969:LYS:C	1:C:971:GLY:N	2.79	0.40
2:E:81:MET:HE1	2:E:94:TYR:CD2	2.56	0.40
2:E:113:GLY:HA2	3:G:92:HIS:NE2	2.36	0.40
4:H:83:LEU:HD23	4:H:86:LEU:HD13	2.01	0.40
2:I:38:ARG:O	2:I:46:GLU:N	2.33	0.40
3:K:36:TRP:N	3:K:49:ILE:O	2.46	0.40
3:K:42:GLY:HA2	5:J:46:LEU:CD2	2.51	0.40
4:Q:27:GLY:O	4:Q:29:PHE:HD2	2.04	0.40
4:Q:51:PHE:C	4:Q:53:PRO:HD3	2.46	0.40
5:R:23:CYS:HB2	5:R:35:TRP:CE2	2.56	0.40
1:A:139:PRO:HG2	1:A:140:PHE:CZ	2.56	0.40
1:A:366:SER:C	1:A:368:LEU:N	2.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:GLY:O	1:A:417:ASN:C	2.64	0.40
1:A:752:LEU:HD11	1:A:990:GLU:OE1	2.21	0.40
1:A:850:ILE:HG23	1:A:853:GLN:CD	2.46	0.40
1:B:194:PHE:HB3	1:B:201:PHE:CE1	2.56	0.40
1:B:326:ILE:HG12	1:B:542:PHE:CD1	2.57	0.40
1:B:566:ARG:HG3	1:B:566:ARG:NH1	2.36	0.40
1:B:587:THR:HA	1:B:588:PRO:HD3	1.93	0.40
1:C:29:THR:HG22	1:C:30:ASN:N	2.36	0.40
1:C:326:ILE:N	1:C:530:THR:OG1	2.51	0.40
1:C:457:ARG:NH1	1:C:461:LEU:HB3	2.37	0.40
1:C:674:GLN:C	1:C:676:GLN:HE21	2.30	0.40
1:C:969:LYS:O	1:C:971:GLY:N	2.54	0.40
3:G:87:TYR:CE2	3:G:103:LYS:HA	2.56	0.40
4:H:4:LEU:HD21	4:H:98:ARG:NE	2.36	0.40
4:H:45:LEU:HD12	5:F:99:PHE:HB3	2.03	0.40
4:H:91:THR:HA	4:H:122:THR:HA	2.04	0.40
4:H:104:ASP:CG	4:H:105:PRO:HD2	2.45	0.40
4:H:111:GLY:C	4:H:113:ASP:H	2.29	0.40
2:I:12:LYS:HB2	2:I:125:VAL:HG22	2.02	0.40
2:I:38:ARG:NE	2:I:92:ALA:HB3	2.35	0.40
5:J:45:LYS:HD2	5:J:45:LYS:HA	1.91	0.40
2:S:29:PHE:CE1	2:S:77:THR:HA	2.55	0.40
3:T:23:CYS:HB3	3:T:36:TRP:CZ2	2.57	0.40
1:A:130:VAL:HB	1:A:167:THR:OG1	2.20	0.40
1:A:205:SER:OG	1:A:206:LYS:N	2.54	0.40
1:A:213:ARG:HA	1:A:213:ARG:HD2	1.78	0.40
1:A:326:ILE:HG12	1:A:542:PHE:CD1	2.57	0.40
1:A:752:LEU:O	1:A:755:GLN:HB2	2.22	0.40
1:B:353:TRP:O	1:B:355:ARG:N	2.52	0.40
1:B:850:ILE:C	1:B:852:ALA:N	2.79	0.40
1:B:969:LYS:O	1:B:971:GLY:N	2.54	0.40
1:C:616:CYS:C	1:C:619:VAL:H	2.29	0.40
1:C:670:CYS:SG	1:C:697:MET:HB3	2.62	0.40
1:C:850:ILE:HD13	1:C:960:ASN:HD21	1.86	0.40
2:E:29:PHE:CE1	2:E:77:THR:HA	2.55	0.40
2:E:50:TRP:HZ2	2:E:104:ALA:HA	1.87	0.40
2:E:86:LEU:HB3	2:E:125:VAL:HG11	2.03	0.40
2:I:35:SER:O	2:I:97:ALA:N	2.54	0.40
2:I:51:ILE:CG2	2:I:70:MET:HB3	2.46	0.40
2:I:115:ASP:CG	2:I:116:ASN:H	2.29	0.40
3:K:23:CYS:HB3	3:K:36:TRP:CZ2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:34:LEU:HG	3:T:90:GLN:O	2.21	0.40
3:T:38:GLN:HB2	3:T:48:LEU:HB2	2.03	0.40
4:Q:98:ARG:HB2	4:Q:114:ILE:N	2.25	0.40
5:R:89:GLN:NE2	5:R:97:TYR:HD2	2.20	0.40
1:A:969:LYS:C	1:A:971:GLY:N	2.79	0.40
1:B:139:PRO:HG2	1:B:140:PHE:CZ	2.56	0.40
1:B:430:THR:O	1:B:433:VAL:HG23	2.21	0.40
1:B:670:CYS:SG	1:B:697:MET:HB3	2.61	0.40
1:B:850:ILE:HG23	1:B:853:GLN:CD	2.46	0.40
1:C:139:PRO:HG2	1:C:140:PHE:CZ	2.56	0.40
1:C:326:ILE:HG12	1:C:542:PHE:CD1	2.57	0.40
2:E:34:ILE:C	2:E:50:TRP:HD1	2.30	0.40
2:E:69:THR:N	2:E:82:GLU:O	2.36	0.40
2:I:33:GLY:CA	2:I:50:TRP:HE1	2.29	0.40
3:K:34:LEU:HG	3:K:90:GLN:O	2.21	0.40
3:K:38:GLN:HB2	3:K:48:LEU:HB2	2.03	0.40
2:S:23:LYS:HB3	2:S:23:LYS:HE3	1.81	0.40
2:S:34:ILE:HB	2:S:51:ILE:HG12	2.04	0.40
2:S:50:TRP:HZ2	2:S:104:ALA:HA	1.87	0.40
2:S:51:ILE:CG2	2:S:70:MET:HB3	2.46	0.40
2:S:52:SER:O	2:S:56:GLY:N	2.47	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	1012/1123 (90%)	772 (76%)	221 (22%)	19 (2%)	6	27
1	B	1012/1123 (90%)	772 (76%)	221 (22%)	19 (2%)	6	27
1	C	1012/1123 (90%)	773 (76%)	220 (22%)	19 (2%)	6	27
2	E	124/127 (98%)	91 (73%)	33 (27%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	I	124/127 (98%)	91 (73%)	33 (27%)	0	100	100
2	S	124/127 (98%)	91 (73%)	33 (27%)	0	100	100
3	G	104/106 (98%)	79 (76%)	25 (24%)	0	100	100
3	K	104/106 (98%)	78 (75%)	26 (25%)	0	100	100
3	T	104/106 (98%)	78 (75%)	26 (25%)	0	100	100
4	D	121/125 (97%)	91 (75%)	27 (22%)	3 (2%)	4	21
4	H	121/125 (97%)	91 (75%)	27 (22%)	3 (2%)	4	21
4	Q	121/125 (97%)	91 (75%)	27 (22%)	3 (2%)	4	21
5	F	106/108 (98%)	76 (72%)	30 (28%)	0	100	100
5	J	106/108 (98%)	76 (72%)	30 (28%)	0	100	100
5	R	106/108 (98%)	76 (72%)	30 (28%)	0	100	100
All	All	4401/4767 (92%)	3326 (76%)	1009 (23%)	66 (2%)	11	32

All (66) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	533	VAL
1	A	536	LYS
1	A	538	VAL
1	A	619	VAL
1	A	621	VAL
1	A	623	ILE
1	B	533	VAL
1	B	536	LYS
1	B	538	VAL
1	B	619	VAL
1	B	621	VAL
1	B	623	ILE
1	C	533	VAL
1	C	536	LYS
1	C	538	VAL
1	C	619	VAL
1	C	621	VAL
1	C	623	ILE
1	A	477	ASN
1	A	527	LYS
1	A	528	LYS
1	B	477	ASN

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Mol	Chain	Res	Type
1	B	527	LYS
1	B	528	LYS
1	C	477	ASN
1	C	527	LYS
1	C	528	LYS
4	H	32	HIS
4	H	91	THR
4	D	32	HIS
4	D	91	THR
4	Q	32	HIS
4	Q	91	THR
1	A	137	ASN
1	A	360	ASN
1	A	361	CYS
1	A	854	LYS
1	B	137	ASN
1	B	360	ASN
1	B	361	CYS
1	B	854	LYS
1	C	137	ASN
1	C	360	ASN
1	C	361	CYS
1	C	854	LYS
1	A	535	ASN
1	B	535	ASN
1	C	535	ASN
1	A	138	ASP
1	A	190	ARG
1	A	335	LEU
1	A	485	PRO
1	A	532	LEU
1	B	138	ASP
1	B	190	ARG
1	B	335	LEU
1	B	485	PRO
1	B	532	LEU
1	C	138	ASP
1	C	190	ARG
1	C	335	LEU
1	C	485	PRO
1	C	532	LEU
4	H	31	SER

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Mol	Chain	Res	Type
4	D	31	SER
4	Q	31	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	903/978 (92%)	700 (78%)	203 (22%)	1	4
1	B	903/978 (92%)	700 (78%)	203 (22%)	1	4
1	C	903/978 (92%)	700 (78%)	203 (22%)	1	4
2	E	96/103 (93%)	67 (70%)	29 (30%)	0	0
2	I	96/103 (93%)	67 (70%)	29 (30%)	0	0
2	S	96/103 (93%)	67 (70%)	29 (30%)	0	0
3	G	71/88 (81%)	40 (56%)	31 (44%)	0	0
3	K	71/88 (81%)	40 (56%)	31 (44%)	0	0
3	T	71/88 (81%)	40 (56%)	31 (44%)	0	0
4	D	100/102 (98%)	59 (59%)	41 (41%)	0	0
4	H	100/102 (98%)	59 (59%)	41 (41%)	0	0
4	Q	100/102 (98%)	59 (59%)	41 (41%)	0	0
5	F	94/94 (100%)	62 (66%)	32 (34%)	0	0
5	J	94/94 (100%)	62 (66%)	32 (34%)	0	0
5	R	94/94 (100%)	62 (66%)	32 (34%)	0	0
All	All	3792/4095 (93%)	2784 (73%)	1008 (27%)	2	2

All (1008) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	THR
1	A	31	SER
1	A	33	THR
1	A	34	ARG

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Mol	Chain	Res	Type
1	A	36	VAL
1	A	45	SER
1	A	46	SER
1	A	47	VAL
1	A	60	SER
1	A	62	VAL
1	A	83	VAL
1	A	90	VAL
1	A	105	ILE
1	A	110	LEU
1	A	113	LYS
1	A	114	THR
1	A	119	ILE
1	A	128	ILE
1	A	129	LYS
1	A	137	ASN
1	A	141	LEU
1	A	172	SER
1	A	189	LEU
1	A	191	GLU
1	A	193	VAL
1	A	205	SER
1	A	211	ILE
1	A	217	GLN
1	A	223	GLU
1	A	225	LEU
1	A	232	ILE
1	A	239	THR
1	A	240	LEU
1	A	274	THR
1	A	304	LYS
1	A	305	SER
1	A	307	THR
1	A	308	VAL
1	A	310	LYS
1	A	319	ARG
1	A	324	GLU
1	A	326	ILE
1	A	327	VAL
1	A	332	VAL
1	A	333	THR
1	A	334	ASN

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Mol	Chain	Res	Type
1	A	335	LEU
1	A	341	VAL
1	A	353	TRP
1	A	355	ARG
1	A	356	THR
1	A	357	ARG
1	A	364	ASP
1	A	366	SER
1	A	378	LYS
1	A	379	CYS
1	A	383	SER
1	A	385	THR
1	A	386	LYS
1	A	387	LEU
1	A	388	ASN
1	A	389	ASP
1	A	390	LEU
1	A	391	CYS
1	A	392	PHE
1	A	393	THR
1	A	398	ASP
1	A	399	SER
1	A	402	ILE
1	A	406	GLU
1	A	414	GLN
1	A	418	ILE
1	A	428	ASP
1	A	434	ILE
1	A	437	ASN
1	A	444	LYS
1	A	446	SER
1	A	455	LEU
1	A	459	SER
1	A	461	LEU
1	A	469	SER
1	A	471	GLU
1	A	481	LYS
1	A	483	LYS
1	A	487	CYS
1	A	488	TYR
1	A	491	LEU
1	A	492	GLN

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Mol	Chain	Res	Type
1	A	493	SER
1	A	499	THR
1	A	502	VAL
1	A	514	PHE
1	A	516	LEU
1	A	523	VAL
1	A	527	LYS
1	A	532	LEU
1	A	534	LYS
1	A	542	PHE
1	A	545	LEU
1	A	546	THR
1	A	551	LEU
1	A	552	THR
1	A	553	LYS
1	A	559	LEU
1	A	564	PHE
1	A	567	ASP
1	A	572	THR
1	A	573	ASP
1	A	576	ARG
1	A	580	THR
1	A	582	GLU
1	A	586	ILE
1	A	587	THR
1	A	590	SER
1	A	595	SER
1	A	598	THR
1	A	604	SER
1	A	606	GLN
1	A	618	GLU
1	A	621	VAL
1	A	623	ILE
1	A	633	ARG
1	A	634	VAL
1	A	644	THR
1	A	645	ARG
1	A	660	GLU
1	A	662	ASP
1	A	675	THR
1	A	689	SER
1	A	692	ILE

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Mol	Chain	Res	Type
1	A	702	GLU
1	A	704	SER
1	A	705	VAL
1	A	708	SER
1	A	711	SER
1	A	725	GLU
1	A	729	VAL
1	A	732	THR
1	A	733	LYS
1	A	740	MET
1	A	746	SER
1	A	749	CYS
1	A	752	LEU
1	A	755	GLN
1	A	760	CYS
1	A	761	THR
1	A	768	THR
1	A	778	THR
1	A	785	VAL
1	A	786	LYS
1	A	794	ILE
1	A	811	LYS
1	A	813	SER
1	A	821	LEU
1	A	836	GLN
1	A	849	LEU
1	A	850	ILE
1	A	856	ASN
1	A	859	THR
1	A	875	SER
1	A	878	LEU
1	A	894	LEU
1	A	914	ASN
1	A	918	GLU
1	A	919	ASN
1	A	921	LYS
1	A	922	LEU
1	A	931	ILE
1	A	934	ILE
1	A	936	ASP
1	A	961	THR
1	A	966	LEU

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Mol	Chain	Res	Type
1	A	968	SER
1	A	969	LYS
1	A	973	ILE
1	A	975	SER
1	A	979	ASP
1	A	984	LEU
1	A	990	GLU
1	A	991	VAL
1	A	994	ASP
1	A	996	LEU
1	A	997	ILE
1	A	1004	LEU
1	A	1030	SER
1	A	1037	SER
1	A	1055	SER
1	A	1077	THR
1	A	1084	ASP
1	A	1097	SER
1	A	1105	THR
1	A	1106	GLN
1	A	1116	THR
1	A	1117	THR
1	A	1118	ASP
1	A	1123	SER
1	A	1126	CYS
1	A	1128	VAL
1	A	1133	VAL
1	A	1136	THR
1	A	1141	LEU
1	A	1144	GLU
1	A	1147	SER
1	B	24	THR
1	B	31	SER
1	B	33	THR
1	B	34	ARG
1	B	36	VAL
1	B	45	SER
1	B	46	SER
1	B	47	VAL
1	B	60	SER
1	B	62	VAL
1	B	83	VAL

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Mol	Chain	Res	Type
1	B	90	VAL
1	B	105	ILE
1	B	110	LEU
1	B	113	LYS
1	B	114	THR
1	B	119	ILE
1	B	128	ILE
1	B	129	LYS
1	B	137	ASN
1	B	141	LEU
1	B	172	SER
1	B	189	LEU
1	B	191	GLU
1	B	193	VAL
1	B	205	SER
1	B	211	ILE
1	B	217	GLN
1	B	223	GLU
1	B	225	LEU
1	B	232	ILE
1	B	239	THR
1	B	240	LEU
1	B	274	THR
1	B	304	LYS
1	B	305	SER
1	B	307	THR
1	B	308	VAL
1	B	310	LYS
1	B	319	ARG
1	B	324	GLU
1	B	326	ILE
1	B	327	VAL
1	B	332	VAL
1	B	333	THR
1	B	334	ASN
1	B	335	LEU
1	B	341	VAL
1	B	353	TRP
1	B	355	ARG
1	B	356	THR
1	B	357	ARG
1	B	364	ASP

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Mol	Chain	Res	Type
1	B	366	SER
1	B	378	LYS
1	B	379	CYS
1	B	383	SER
1	B	385	THR
1	B	386	LYS
1	B	387	LEU
1	B	388	ASN
1	B	389	ASP
1	B	390	LEU
1	B	391	CYS
1	B	392	PHE
1	B	393	THR
1	B	398	ASP
1	B	399	SER
1	B	402	ILE
1	B	406	GLU
1	B	414	GLN
1	B	418	ILE
1	B	428	ASP
1	B	434	ILE
1	B	437	ASN
1	B	444	LYS
1	B	446	SER
1	B	455	LEU
1	B	459	SER
1	B	461	LEU
1	B	469	SER
1	B	471	GLU
1	B	481	LYS
1	B	483	LYS
1	B	487	CYS
1	B	488	TYR
1	B	491	LEU
1	B	492	GLN
1	B	493	SER
1	B	499	THR
1	B	502	VAL
1	B	514	PHE
1	B	516	LEU
1	B	523	VAL
1	B	527	LYS

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Mol	Chain	Res	Type
1	B	532	LEU
1	B	534	LYS
1	B	542	PHE
1	B	545	LEU
1	B	546	THR
1	B	551	LEU
1	B	552	THR
1	B	553	LYS
1	B	559	LEU
1	B	564	PHE
1	B	567	ASP
1	B	572	THR
1	B	573	ASP
1	B	576	ARG
1	B	580	THR
1	B	582	GLU
1	B	586	ILE
1	B	587	THR
1	B	590	SER
1	B	595	SER
1	B	598	THR
1	B	604	SER
1	B	606	GLN
1	B	618	GLU
1	B	621	VAL
1	B	623	ILE
1	B	633	ARG
1	B	634	VAL
1	B	644	THR
1	B	645	ARG
1	B	660	GLU
1	B	662	ASP
1	B	675	THR
1	B	689	SER
1	B	692	ILE
1	B	702	GLU
1	B	704	SER
1	B	705	VAL
1	B	708	SER
1	B	711	SER
1	B	725	GLU
1	B	729	VAL

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Mol	Chain	Res	Type
1	B	732	THR
1	B	733	LYS
1	B	740	MET
1	B	746	SER
1	B	749	CYS
1	B	752	LEU
1	B	755	GLN
1	B	760	CYS
1	B	761	THR
1	B	768	THR
1	B	778	THR
1	B	785	VAL
1	B	786	LYS
1	B	794	ILE
1	B	811	LYS
1	B	813	SER
1	B	821	LEU
1	B	836	GLN
1	B	849	LEU
1	B	850	ILE
1	B	856	ASN
1	B	859	THR
1	B	875	SER
1	B	878	LEU
1	B	894	LEU
1	B	914	ASN
1	B	918	GLU
1	B	919	ASN
1	B	921	LYS
1	B	922	LEU
1	B	931	ILE
1	B	934	ILE
1	B	936	ASP
1	B	961	THR
1	B	966	LEU
1	B	968	SER
1	B	969	LYS
1	B	973	ILE
1	B	975	SER
1	B	979	ASP
1	B	984	LEU
1	B	990	GLU

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Mol	Chain	Res	Type
1	B	991	VAL
1	B	994	ASP
1	B	996	LEU
1	B	997	ILE
1	B	1004	LEU
1	B	1030	SER
1	B	1037	SER
1	B	1055	SER
1	B	1077	THR
1	B	1084	ASP
1	B	1097	SER
1	B	1105	THR
1	B	1106	GLN
1	B	1116	THR
1	B	1117	THR
1	B	1118	ASP
1	B	1123	SER
1	B	1126	CYS
1	B	1128	VAL
1	B	1133	VAL
1	B	1136	THR
1	B	1141	LEU
1	B	1144	GLU
1	B	1147	SER
1	C	24	THR
1	C	31	SER
1	C	33	THR
1	C	34	ARG
1	C	36	VAL
1	C	45	SER
1	C	46	SER
1	C	47	VAL
1	C	60	SER
1	C	62	VAL
1	C	83	VAL
1	C	90	VAL
1	C	105	ILE
1	C	110	LEU
1	C	113	LYS
1	C	114	THR
1	C	119	ILE
1	C	128	ILE

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Mol	Chain	Res	Type
1	C	129	LYS
1	C	137	ASN
1	C	141	LEU
1	C	172	SER
1	C	189	LEU
1	C	191	GLU
1	C	193	VAL
1	C	205	SER
1	C	211	ILE
1	C	217	GLN
1	C	223	GLU
1	C	225	LEU
1	C	232	ILE
1	C	239	THR
1	C	240	LEU
1	C	274	THR
1	C	304	LYS
1	C	305	SER
1	C	307	THR
1	C	308	VAL
1	C	310	LYS
1	C	319	ARG
1	C	324	GLU
1	C	326	ILE
1	C	327	VAL
1	C	332	VAL
1	C	333	THR
1	C	334	ASN
1	C	335	LEU
1	C	341	VAL
1	C	353	TRP
1	C	355	ARG
1	C	356	THR
1	C	357	ARG
1	C	364	ASP
1	C	366	SER
1	C	378	LYS
1	C	379	CYS
1	C	383	SER
1	C	385	THR
1	C	386	LYS
1	C	387	LEU

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Mol	Chain	Res	Type
1	C	388	ASN
1	C	389	ASP
1	C	390	LEU
1	C	391	CYS
1	C	392	PHE
1	C	393	THR
1	C	398	ASP
1	C	399	SER
1	C	402	ILE
1	C	406	GLU
1	C	414	GLN
1	C	418	ILE
1	C	428	ASP
1	C	434	ILE
1	C	437	ASN
1	C	444	LYS
1	C	446	SER
1	C	455	LEU
1	C	459	SER
1	C	461	LEU
1	C	469	SER
1	C	471	GLU
1	C	481	LYS
1	C	483	LYS
1	C	487	CYS
1	C	488	TYR
1	C	491	LEU
1	C	492	GLN
1	C	493	SER
1	C	499	THR
1	C	502	VAL
1	C	514	PHE
1	C	516	LEU
1	C	523	VAL
1	C	527	LYS
1	C	532	LEU
1	C	534	LYS
1	C	542	PHE
1	C	545	LEU
1	C	546	THR
1	C	551	LEU
1	C	552	THR

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Mol	Chain	Res	Type
1	C	553	LYS
1	C	559	LEU
1	C	564	PHE
1	C	567	ASP
1	C	572	THR
1	C	573	ASP
1	C	576	ARG
1	C	580	THR
1	C	582	GLU
1	C	586	ILE
1	C	587	THR
1	C	590	SER
1	C	595	SER
1	C	598	THR
1	C	604	SER
1	C	606	GLN
1	C	618	GLU
1	C	621	VAL
1	C	623	ILE
1	C	633	ARG
1	C	634	VAL
1	C	644	THR
1	C	645	ARG
1	C	660	GLU
1	C	662	ASP
1	C	675	THR
1	C	689	SER
1	C	692	ILE
1	C	702	GLU
1	C	704	SER
1	C	705	VAL
1	C	708	SER
1	C	711	SER
1	C	725	GLU
1	C	729	VAL
1	C	732	THR
1	C	733	LYS
1	C	740	MET
1	C	746	SER
1	C	749	CYS
1	C	752	LEU
1	C	755	GLN

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Mol	Chain	Res	Type
1	C	760	CYS
1	C	761	THR
1	C	768	THR
1	C	778	THR
1	C	785	VAL
1	C	786	LYS
1	C	794	ILE
1	C	811	LYS
1	C	813	SER
1	C	821	LEU
1	C	836	GLN
1	C	849	LEU
1	C	850	ILE
1	C	856	ASN
1	C	859	THR
1	C	875	SER
1	C	878	LEU
1	C	894	LEU
1	C	914	ASN
1	C	918	GLU
1	C	919	ASN
1	C	921	LYS
1	C	922	LEU
1	C	931	ILE
1	C	934	ILE
1	C	936	ASP
1	C	961	THR
1	C	966	LEU
1	C	968	SER
1	C	969	LYS
1	C	973	ILE
1	C	975	SER
1	C	979	ASP
1	C	984	LEU
1	C	990	GLU
1	C	991	VAL
1	C	994	ASP
1	C	996	LEU
1	C	997	ILE
1	C	1004	LEU
1	C	1030	SER
1	C	1037	SER

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Mol	Chain	Res	Type
1	C	1055	SER
1	C	1077	THR
1	C	1084	ASP
1	C	1097	SER
1	C	1105	THR
1	C	1106	GLN
1	C	1116	THR
1	C	1117	THR
1	C	1118	ASP
1	C	1123	SER
1	C	1126	CYS
1	C	1128	VAL
1	C	1133	VAL
1	C	1136	THR
1	C	1141	LEU
1	C	1144	GLU
1	C	1147	SER
2	E	2	VAL
2	E	7	SER
2	E	13	LYS
2	E	19	LYS
2	E	23	LYS
2	E	30	THR
2	E	32	TYR
2	E	35	SER
2	E	37	VAL
2	E	43	GLN
2	E	48	MET
2	E	52	SER
2	E	63	LYS
2	E	65	GLN
2	E	68	VAL
2	E	71	THR
2	E	72	THR
2	E	74	THR
2	E	75	SER
2	E	83	LEU
2	E	85	ARG
2	E	93	VAL
2	E	94	TYR
2	E	109	SER
2	E	110	LEU

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Mol	Chain	Res	Type
2	E	111	ILE
2	E	122	LEU
2	E	126	SER
2	E	127	SER
3	G	3	VAL
3	G	5	THR
3	G	7	SER
3	G	17	GLU
3	G	18	ARG
3	G	21	LEU
3	G	22	SER
3	G	29	VAL
3	G	30	SER
3	G	31	SER
3	G	33	SER
3	G	46	ARG
3	G	50	TYR
3	G	53	SER
3	G	57	THR
3	G	59	ILE
3	G	66	SER
3	G	68	SER
3	G	73	THR
3	G	76	ILE
3	G	80	GLU
3	G	82	GLU
3	G	87	TYR
3	G	89	CYS
3	G	90	GLN
3	G	93	ASP
3	G	94	THR
3	G	95	SER
3	G	96	LEU
3	G	98	PHE
3	G	107	LYS
4	H	1	GLN
4	H	2	VAL
4	H	3	GLN
4	H	5	VAL
4	H	7	SER
4	H	10	GLU
4	H	16	SER

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Mol	Chain	Res	Type
4	H	18	VAL
4	H	20	VAL
4	H	25	SER
4	H	28	THR
4	H	31	SER
4	H	38	ARG
4	H	43	GLN
4	H	52	ILE
4	H	54	LEU
4	H	57	THR
4	H	62	GLN
4	H	65	GLN
4	H	67	ARG
4	H	68	VAL
4	H	69	MET
4	H	70	ILE
4	H	76	THR
4	H	77	SER
4	H	78	THR
4	H	80	TYR
4	H	81	MET
4	H	82	GLU
4	H	85	SER
4	H	88	SER
4	H	91	THR
4	H	94	TYR
4	H	96	CYS
4	H	99	LEU
4	H	100	PHE
4	H	106	ASN
4	H	109	GLU
4	H	113	ASP
4	H	121	VAL
4	H	123	VAL
5	F	1	ASP
5	F	5	THR
5	F	11	LEU
5	F	14	SER
5	F	15	VAL
5	F	18	ARG
5	F	20	THR
5	F	28	ASP

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Mol	Chain	Res	Type
5	F	29	ILE
5	F	35	TRP
5	F	38	GLN
5	F	45	LYS
5	F	47	LEU
5	F	48	ILE
5	F	50	ASP
5	F	52	SER
5	F	53	HIS
5	F	54	LEU
5	F	60	SER
5	F	61	ARG
5	F	69	THR
5	F	72	THR
5	F	74	THR
5	F	76	SER
5	F	77	SER
5	F	79	GLN
5	F	85	THR
5	F	87	TYR
5	F	98	THR
5	F	104	LYS
5	F	105	VAL
5	F	106	GLU
2	I	2	VAL
2	I	7	SER
2	I	13	LYS
2	I	19	LYS
2	I	23	LYS
2	I	30	THR
2	I	32	TYR
2	I	35	SER
2	I	37	VAL
2	I	43	GLN
2	I	48	MET
2	I	52	SER
2	I	63	LYS
2	I	65	GLN
2	I	68	VAL
2	I	71	THR
2	I	72	THR
2	I	74	THR

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Mol	Chain	Res	Type
2	I	75	SER
2	I	83	LEU
2	I	85	ARG
2	I	93	VAL
2	I	94	TYR
2	I	109	SER
2	I	110	LEU
2	I	111	ILE
2	I	122	LEU
2	I	126	SER
2	I	127	SER
3	K	3	VAL
3	K	5	THR
3	K	7	SER
3	K	17	GLU
3	K	18	ARG
3	K	21	LEU
3	K	22	SER
3	K	29	VAL
3	K	30	SER
3	K	31	SER
3	K	33	SER
3	K	46	ARG
3	K	50	TYR
3	K	53	SER
3	K	57	THR
3	K	59	ILE
3	K	66	SER
3	K	68	SER
3	K	73	THR
3	K	76	ILE
3	K	80	GLU
3	K	82	GLU
3	K	87	TYR
3	K	89	CYS
3	K	90	GLN
3	K	93	ASP
3	K	94	THR
3	K	95	SER
3	K	96	LEU
3	K	98	PHE
3	K	107	LYS

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Mol	Chain	Res	Type
4	D	1	GLN
4	D	2	VAL
4	D	3	GLN
4	D	5	VAL
4	D	7	SER
4	D	10	GLU
4	D	16	SER
4	D	18	VAL
4	D	20	VAL
4	D	25	SER
4	D	28	THR
4	D	31	SER
4	D	38	ARG
4	D	43	GLN
4	D	52	ILE
4	D	54	LEU
4	D	57	THR
4	D	62	GLN
4	D	65	GLN
4	D	67	ARG
4	D	68	VAL
4	D	69	MET
4	D	70	ILE
4	D	76	THR
4	D	77	SER
4	D	78	THR
4	D	80	TYR
4	D	81	MET
4	D	82	GLU
4	D	85	SER
4	D	88	SER
4	D	91	THR
4	D	94	TYR
4	D	96	CYS
4	D	99	LEU
4	D	100	PHE
4	D	106	ASN
4	D	109	GLU
4	D	113	ASP
4	D	121	VAL
4	D	123	VAL
5	J	1	ASP

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Mol	Chain	Res	Type
5	J	5	THR
5	J	11	LEU
5	J	14	SER
5	J	15	VAL
5	J	18	ARG
5	J	20	THR
5	J	28	ASP
5	J	29	ILE
5	J	35	TRP
5	J	38	GLN
5	J	45	LYS
5	J	47	LEU
5	J	48	ILE
5	J	50	ASP
5	J	52	SER
5	J	53	HIS
5	J	54	LEU
5	J	60	SER
5	J	61	ARG
5	J	69	THR
5	J	72	THR
5	J	74	THR
5	J	76	SER
5	J	77	SER
5	J	79	GLN
5	J	85	THR
5	J	87	TYR
5	J	98	THR
5	J	104	LYS
5	J	105	VAL
5	J	106	GLU
2	S	2	VAL
2	S	7	SER
2	S	13	LYS
2	S	19	LYS
2	S	23	LYS
2	S	30	THR
2	S	32	TYR
2	S	35	SER
2	S	37	VAL
2	S	43	GLN
2	S	48	MET

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Mol	Chain	Res	Type
2	S	52	SER
2	S	63	LYS
2	S	65	GLN
2	S	68	VAL
2	S	71	THR
2	S	72	THR
2	S	74	THR
2	S	75	SER
2	S	83	LEU
2	S	85	ARG
2	S	93	VAL
2	S	94	TYR
2	S	109	SER
2	S	110	LEU
2	S	111	ILE
2	S	122	LEU
2	S	126	SER
2	S	127	SER
3	T	3	VAL
3	T	5	THR
3	T	7	SER
3	T	17	GLU
3	T	18	ARG
3	T	21	LEU
3	T	22	SER
3	T	29	VAL
3	T	30	SER
3	T	31	SER
3	T	33	SER
3	T	46	ARG
3	T	50	TYR
3	T	53	SER
3	T	57	THR
3	T	59	ILE
3	T	66	SER
3	T	68	SER
3	T	73	THR
3	T	76	ILE
3	T	80	GLU
3	T	82	GLU
3	T	87	TYR
3	T	89	CYS

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Mol	Chain	Res	Type
3	T	90	GLN
3	T	93	ASP
3	T	94	THR
3	T	95	SER
3	T	96	LEU
3	T	98	PHE
3	T	107	LYS
4	Q	1	GLN
4	Q	2	VAL
4	Q	3	GLN
4	Q	5	VAL
4	Q	7	SER
4	Q	10	GLU
4	Q	16	SER
4	Q	18	VAL
4	Q	20	VAL
4	Q	25	SER
4	Q	28	THR
4	Q	31	SER
4	Q	38	ARG
4	Q	43	GLN
4	Q	52	ILE
4	Q	54	LEU
4	Q	57	THR
4	Q	62	GLN
4	Q	65	GLN
4	Q	67	ARG
4	Q	68	VAL
4	Q	69	MET
4	Q	70	ILE
4	Q	76	THR
4	Q	77	SER
4	Q	78	THR
4	Q	80	TYR
4	Q	81	MET
4	Q	82	GLU
4	Q	85	SER
4	Q	88	SER
4	Q	91	THR
4	Q	94	TYR
4	Q	96	CYS
4	Q	99	LEU

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Mol	Chain	Res	Type
4	Q	100	PHE
4	Q	106	ASN
4	Q	109	GLU
4	Q	113	ASP
4	Q	121	VAL
4	Q	123	VAL
5	R	1	ASP
5	R	5	THR
5	R	11	LEU
5	R	14	SER
5	R	15	VAL
5	R	18	ARG
5	R	20	THR
5	R	28	ASP
5	R	29	ILE
5	R	35	TRP
5	R	38	GLN
5	R	45	LYS
5	R	47	LEU
5	R	48	ILE
5	R	50	ASP
5	R	52	SER
5	R	53	HIS
5	R	54	LEU
5	R	60	SER
5	R	61	ARG
5	R	69	THR
5	R	72	THR
5	R	74	THR
5	R	76	SER
5	R	77	SER
5	R	79	GLN
5	R	85	THR
5	R	87	TYR
5	R	98	THR
5	R	104	LYS
5	R	105	VAL
5	R	106	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	ASN
1	A	238	GLN
1	A	331	ASN
1	A	339	HIS
1	A	422	ASN
1	A	437	ASN
1	A	612	GLN
1	A	657	ASN
1	A	676	GLN
1	A	710	ASN
1	A	774	GLN
1	A	901	GLN
1	A	913	GLN
1	A	935	GLN
1	A	955	ASN
1	A	965	GLN
1	A	1088	HIS
1	A	1106	GLN
1	A	1135	ASN
1	B	122	ASN
1	B	238	GLN
1	B	339	HIS
1	B	370	ASN
1	B	405	ASN
1	B	417	ASN
1	B	422	ASN
1	B	437	ASN
1	B	612	GLN
1	B	657	ASN
1	B	676	GLN
1	B	774	GLN
1	B	804	GLN
1	B	901	GLN
1	B	935	GLN
1	B	955	ASN
1	B	957	GLN
1	B	965	GLN
1	B	1088	HIS
1	B	1106	GLN
1	B	1135	ASN
1	C	122	ASN
1	C	238	GLN
1	C	331	ASN

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Mol	Chain	Res	Type
1	C	339	HIS
1	C	343	ASN
1	C	370	ASN
1	C	405	ASN
1	C	417	ASN
1	C	422	ASN
1	C	437	ASN
1	C	612	GLN
1	C	657	ASN
1	C	676	GLN
1	C	709	ASN
1	C	710	ASN
1	C	774	GLN
1	C	804	GLN
1	C	901	GLN
1	C	913	GLN
1	C	935	GLN
1	C	955	ASN
1	C	965	GLN
1	C	1088	HIS
1	C	1106	GLN
1	C	1135	ASN
2	E	39	GLN
2	E	116	ASN
3	G	91	GLN
5	F	3	GLN
5	F	6	GLN
5	F	38	GLN
5	F	89	GLN
2	I	39	GLN
3	K	91	GLN
5	J	3	GLN
5	J	6	GLN
5	J	89	GLN
2	S	39	GLN
2	S	116	ASN
3	T	91	GLN
5	R	3	GLN
5	R	6	GLN
5	R	89	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

30 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
7	NAG	L	1	7	14,14,15	0.36	0	17,19,21	0.41	0
7	NAG	L	2	7	14,14,15	0.38	0	17,19,21	0.46	0
6	NAG	M	1	6	14,14,15	0.18	0	17,19,21	0.51	0
6	NAG	M	2	6	14,14,15	0.62	1 (7%)	17,19,21	1.15	2 (11%)
6	BMA	M	3	6	11,11,12	1.08	1 (9%)	15,15,17	1.24	1 (6%)
6	MAN	M	4	6	11,11,12	1.05	1 (9%)	15,15,17	0.81	1 (6%)
6	MAN	M	5	6	11,11,12	1.21	2 (18%)	15,15,17	1.24	2 (13%)
6	FUC	M	6	6	10,10,11	0.65	0	14,14,16	1.19	1 (7%)
7	NAG	N	1	7	14,14,15	0.21	0	17,19,21	0.96	1 (5%)
7	NAG	N	2	7	14,14,15	0.55	0	17,19,21	1.30	2 (11%)
6	NAG	O	1	6	14,14,15	0.18	0	17,19,21	0.50	0
6	NAG	O	2	6	14,14,15	0.62	1 (7%)	17,19,21	1.15	2 (11%)
6	BMA	O	3	6	11,11,12	1.10	1 (9%)	15,15,17	1.24	1 (6%)
6	MAN	O	4	6	11,11,12	1.04	1 (9%)	15,15,17	0.81	1 (6%)
6	MAN	O	5	6	11,11,12	1.20	2 (18%)	15,15,17	1.25	2 (13%)
6	FUC	O	6	6	10,10,11	0.64	0	14,14,16	1.19	1 (7%)
7	NAG	P	1	7	14,14,15	0.36	0	17,19,21	0.41	0
7	NAG	P	2	7	14,14,15	0.39	0	17,19,21	0.46	0
7	NAG	U	1	7	14,14,15	0.21	0	17,19,21	0.95	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	U	2	7	14,14,15	0.56	0	17,19,21	1.30	2 (11%)
6	NAG	V	1	6	14,14,15	0.18	0	17,19,21	0.50	0
6	NAG	V	2	6	14,14,15	0.63	1 (7%)	17,19,21	1.15	2 (11%)
6	BMA	V	3	6	11,11,12	1.09	1 (9%)	15,15,17	1.24	1 (6%)
6	MAN	V	4	6	11,11,12	1.04	1 (9%)	15,15,17	0.81	1 (6%)
6	MAN	V	5	6	11,11,12	1.20	2 (18%)	15,15,17	1.25	2 (13%)
6	FUC	V	6	6	10,10,11	0.66	0	14,14,16	1.20	2 (14%)
7	NAG	W	1	7	14,14,15	0.36	0	17,19,21	0.40	0
7	NAG	W	2	7	14,14,15	0.41	0	17,19,21	0.46	0
7	NAG	X	1	7	14,14,15	0.20	0	17,19,21	0.97	1 (5%)
7	NAG	X	2	7	14,14,15	0.54	0	17,19,21	1.31	2 (11%)

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
7	NAG	L	1	7	-	2/6/23/26	0/1/1/1
7	NAG	L	2	7	-	2/6/23/26	0/1/1/1
6	NAG	M	1	6	-	4/6/23/26	0/1/1/1
6	NAG	M	2	6	-	4/6/23/26	0/1/1/1
6	BMA	M	3	6	-	0/2/19/22	0/1/1/1
6	MAN	M	4	6	-	2/2/19/22	0/1/1/1
6	MAN	M	5	6	-	0/2/19/22	0/1/1/1
6	FUC	M	6	6	-	-	0/1/1/1
7	NAG	N	1	7	-	2/6/23/26	0/1/1/1
7	NAG	N	2	7	-	4/6/23/26	0/1/1/1
6	NAG	O	1	6	-	4/6/23/26	0/1/1/1
6	NAG	O	2	6	-	4/6/23/26	0/1/1/1
6	BMA	O	3	6	-	0/2/19/22	0/1/1/1
6	MAN	O	4	6	-	2/2/19/22	0/1/1/1
6	MAN	O	5	6	-	0/2/19/22	0/1/1/1
6	FUC	O	6	6	-	-	0/1/1/1
7	NAG	P	1	7	-	2/6/23/26	0/1/1/1
7	NAG	P	2	7	-	2/6/23/26	0/1/1/1
7	NAG	U	1	7	-	2/6/23/26	0/1/1/1
7	NAG	U	2	7	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	V	1	6	-	4/6/23/26	0/1/1/1
6	NAG	V	2	6	-	4/6/23/26	0/1/1/1
6	BMA	V	3	6	-	0/2/19/22	0/1/1/1
6	MAN	V	4	6	-	2/2/19/22	0/1/1/1
6	MAN	V	5	6	-	0/2/19/22	0/1/1/1
6	FUC	V	6	6	-	-	0/1/1/1
7	NAG	W	1	7	-	2/6/23/26	0/1/1/1
7	NAG	W	2	7	-	2/6/23/26	0/1/1/1
7	NAG	X	1	7	-	2/6/23/26	0/1/1/1
7	NAG	X	2	7	-	4/6/23/26	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	5	MAN	C2-C3	2.37	1.56	1.52
6	V	5	MAN	C2-C3	2.36	1.56	1.52
6	O	3	BMA	C4-C5	2.29	1.57	1.53
6	M	3	BMA	C4-C5	2.27	1.57	1.53
6	V	3	BMA	C4-C5	2.26	1.57	1.53
6	O	5	MAN	C2-C3	2.26	1.55	1.52
6	O	5	MAN	C1-C2	2.20	1.57	1.52
6	V	5	MAN	C1-C2	2.20	1.57	1.52
6	V	2	NAG	O5-C1	-2.20	1.40	1.43
6	M	2	NAG	O5-C1	-2.18	1.40	1.43
6	M	5	MAN	C1-C2	2.18	1.57	1.52
6	O	2	NAG	O5-C1	-2.17	1.40	1.43
6	M	4	MAN	C1-C2	2.13	1.57	1.52
6	O	4	MAN	C1-C2	2.11	1.57	1.52
6	V	4	MAN	C1-C2	2.10	1.57	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	X	2	NAG	C2-N2-C7	4.48	128.91	122.90
7	N	2	NAG	C2-N2-C7	4.44	128.85	122.90
7	U	2	NAG	C2-N2-C7	4.42	128.83	122.90
6	V	3	BMA	C1-C2-C3	-3.67	104.30	109.64
6	O	3	BMA	C1-C2-C3	-3.67	104.30	109.64
6	M	3	BMA	C1-C2-C3	-3.65	104.33	109.64
7	N	1	NAG	C1-O5-C5	3.34	116.66	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	X	1	NAG	C1-O5-C5	3.33	116.65	112.19
7	U	1	NAG	C1-O5-C5	3.30	116.61	112.19
6	V	5	MAN	O5-C5-C4	-2.63	104.44	110.83
6	M	5	MAN	O5-C5-C4	-2.61	104.48	110.83
6	O	5	MAN	O5-C5-C4	-2.61	104.48	110.83
6	O	6	FUC	O3-C3-C4	-2.43	104.64	110.38
6	O	2	NAG	C3-C4-C5	2.43	114.64	110.23
6	V	6	FUC	O3-C3-C4	-2.42	104.67	110.38
6	M	6	FUC	O3-C3-C4	-2.42	104.68	110.38
6	V	2	NAG	C3-C4-C5	2.41	114.61	110.23
6	M	2	NAG	C3-C4-C5	2.41	114.60	110.23
6	M	2	NAG	O4-C4-C5	-2.38	103.47	109.32
6	O	2	NAG	O4-C4-C5	-2.37	103.49	109.32
6	V	2	NAG	O4-C4-C5	-2.37	103.50	109.32
7	N	2	NAG	C1-C2-N2	2.06	113.68	110.43
6	M	4	MAN	O2-C2-C3	-2.06	105.89	110.15
6	M	5	MAN	O2-C2-C3	-2.05	105.90	110.15
6	O	4	MAN	O2-C2-C3	-2.05	105.91	110.15
7	X	2	NAG	C1-C2-N2	2.04	113.66	110.43
6	O	5	MAN	O2-C2-C3	-2.04	105.92	110.15
7	U	2	NAG	C1-C2-N2	2.04	113.65	110.43
6	V	5	MAN	O2-C2-C3	-2.04	105.92	110.15
6	V	4	MAN	O2-C2-C3	-2.04	105.92	110.15
6	V	6	FUC	C1-O5-C5	2.00	117.69	112.97

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	M	1	NAG	C4-C5-C6-O6
6	O	1	NAG	C4-C5-C6-O6
6	V	1	NAG	C4-C5-C6-O6
6	M	4	MAN	O5-C5-C6-O6
6	O	4	MAN	O5-C5-C6-O6
6	V	4	MAN	O5-C5-C6-O6
6	M	4	MAN	C4-C5-C6-O6
6	O	4	MAN	C4-C5-C6-O6
6	V	4	MAN	C4-C5-C6-O6
6	M	1	NAG	O5-C5-C6-O6
6	O	1	NAG	O5-C5-C6-O6
6	V	1	NAG	O5-C5-C6-O6
7	L	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	P	1	NAG	O5-C5-C6-O6
7	W	1	NAG	O5-C5-C6-O6
7	L	2	NAG	O5-C5-C6-O6
7	P	2	NAG	O5-C5-C6-O6
7	W	2	NAG	O5-C5-C6-O6
7	L	2	NAG	C4-C5-C6-O6
7	P	2	NAG	C4-C5-C6-O6
7	W	2	NAG	C4-C5-C6-O6
6	M	1	NAG	C8-C7-N2-C2
6	M	1	NAG	O7-C7-N2-C2
6	O	1	NAG	C8-C7-N2-C2
6	O	1	NAG	O7-C7-N2-C2
6	V	1	NAG	C8-C7-N2-C2
6	V	1	NAG	O7-C7-N2-C2
7	N	1	NAG	C8-C7-N2-C2
7	N	1	NAG	O7-C7-N2-C2
7	N	2	NAG	C8-C7-N2-C2
7	N	2	NAG	O7-C7-N2-C2
7	U	1	NAG	C8-C7-N2-C2
7	U	1	NAG	O7-C7-N2-C2
7	U	2	NAG	C8-C7-N2-C2
7	U	2	NAG	O7-C7-N2-C2
7	X	1	NAG	C8-C7-N2-C2
7	X	1	NAG	O7-C7-N2-C2
7	X	2	NAG	C8-C7-N2-C2
7	X	2	NAG	O7-C7-N2-C2
7	L	1	NAG	C4-C5-C6-O6
7	P	1	NAG	C4-C5-C6-O6
7	W	1	NAG	C4-C5-C6-O6
6	M	2	NAG	C4-C5-C6-O6
6	O	2	NAG	C4-C5-C6-O6
6	V	2	NAG	C4-C5-C6-O6
6	M	2	NAG	O5-C5-C6-O6
6	O	2	NAG	O5-C5-C6-O6
6	V	2	NAG	O5-C5-C6-O6
6	M	2	NAG	C3-C2-N2-C7
6	O	2	NAG	C3-C2-N2-C7
6	V	2	NAG	C3-C2-N2-C7
6	M	2	NAG	C1-C2-N2-C7
6	O	2	NAG	C1-C2-N2-C7
6	V	2	NAG	C1-C2-N2-C7
7	N	2	NAG	C1-C2-N2-C7

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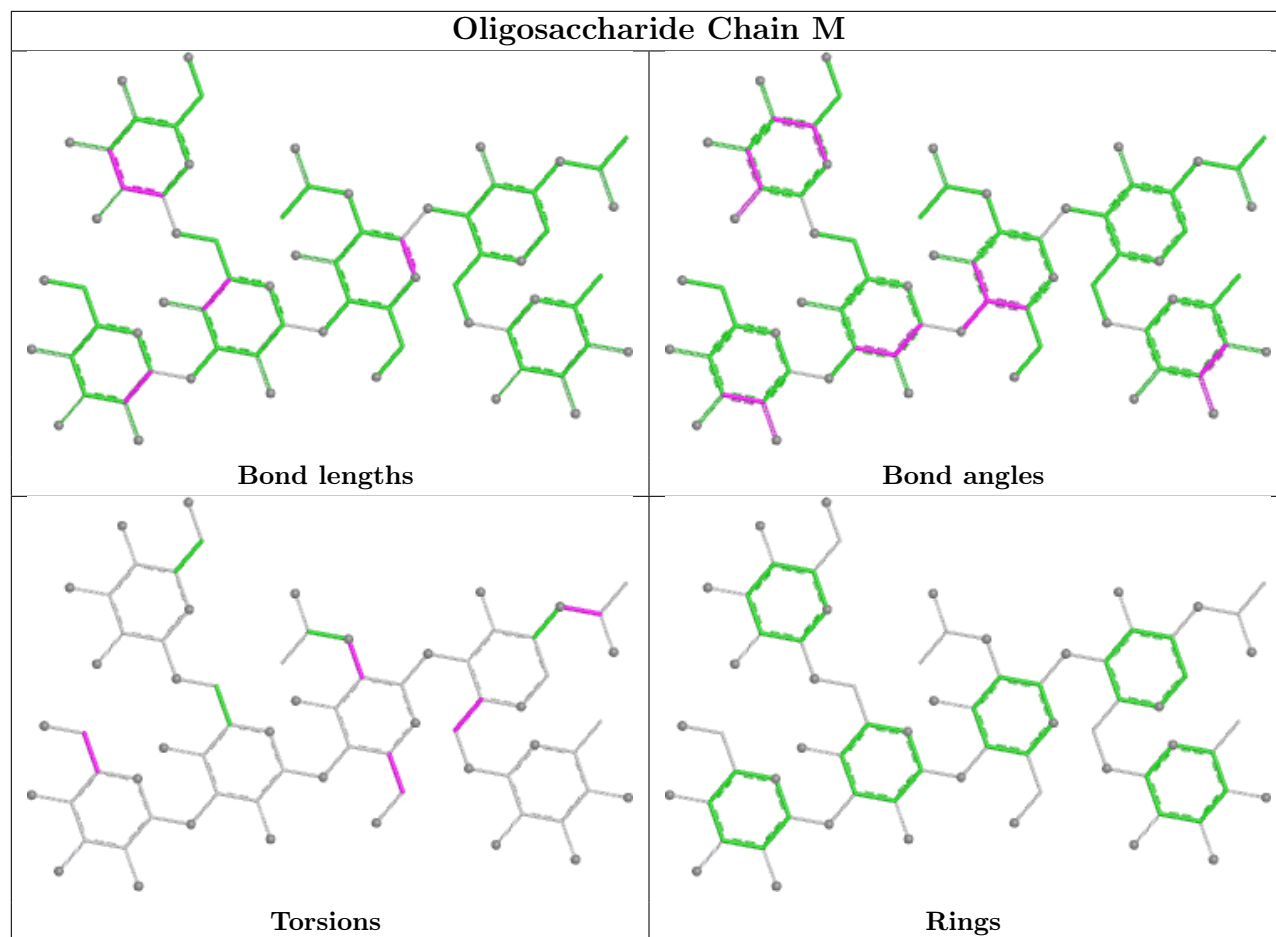
Mol	Chain	Res	Type	Atoms
7	U	2	NAG	C1-C2-N2-C7
7	X	2	NAG	C1-C2-N2-C7
7	N	2	NAG	C3-C2-N2-C7
7	U	2	NAG	C3-C2-N2-C7
7	X	2	NAG	C3-C2-N2-C7

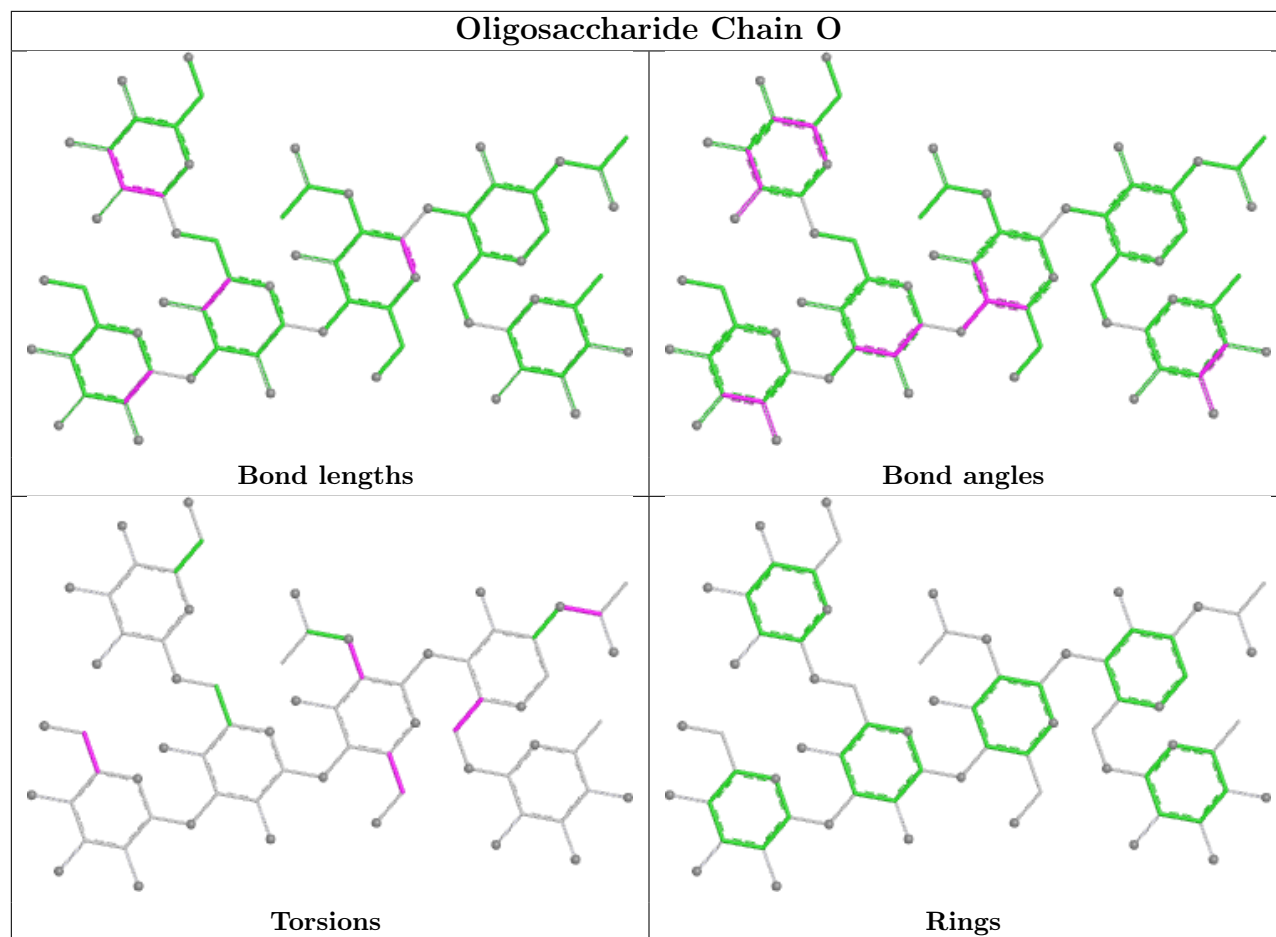
There are no ring outliers.

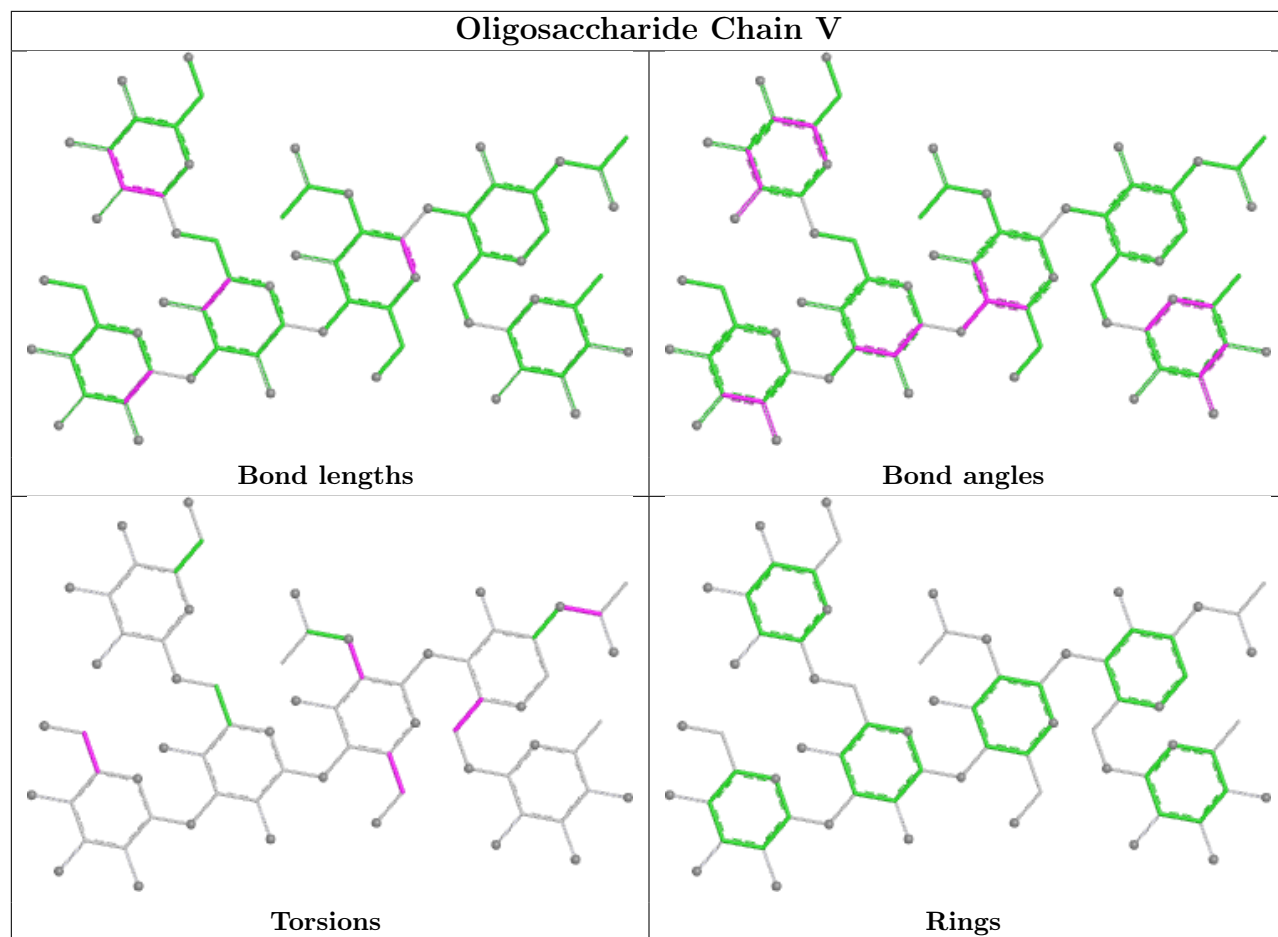
16 monomers are involved in 21 short contacts:

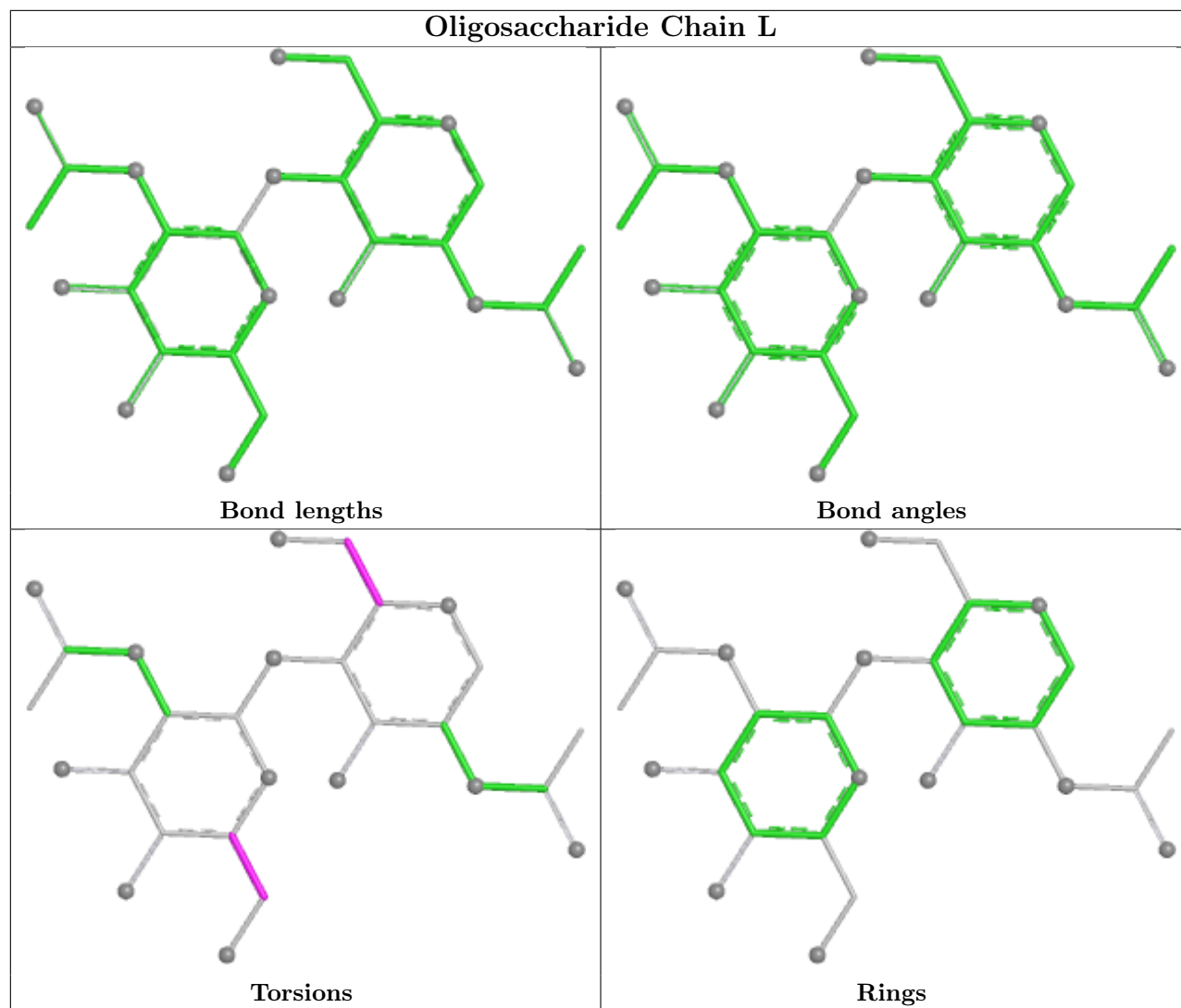
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	O	6	FUC	5	0
6	V	1	NAG	1	0
7	X	2	NAG	1	0
6	O	4	MAN	1	0
6	M	1	NAG	2	0
6	V	3	BMA	1	0
6	V	2	NAG	3	0
6	O	3	BMA	1	0
6	O	5	MAN	2	0
6	M	3	BMA	1	0
7	W	1	NAG	1	0
6	M	4	MAN	1	0
7	N	2	NAG	1	0
7	U	2	NAG	1	0
6	V	4	MAN	1	0
6	M	2	NAG	1	0

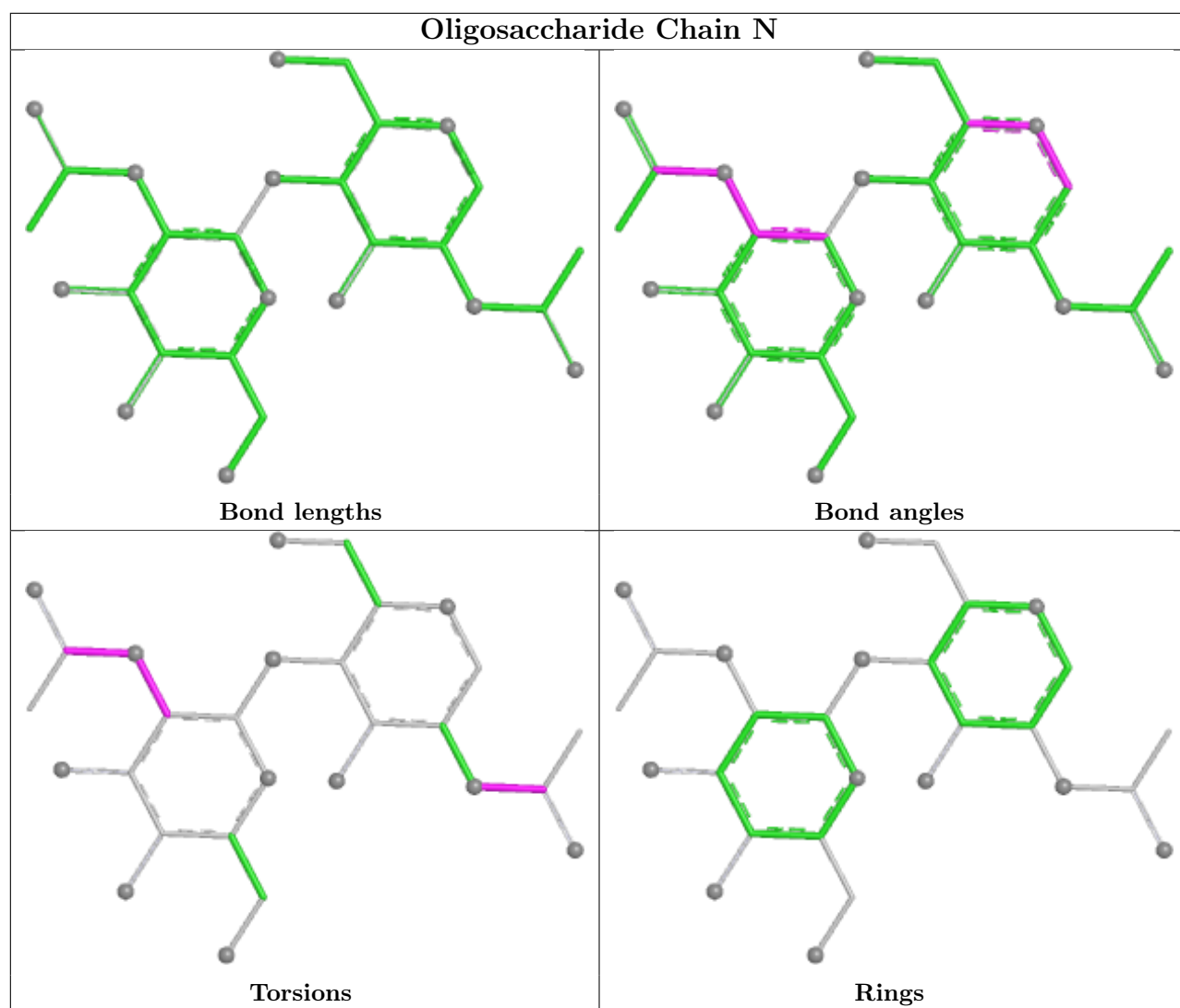
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

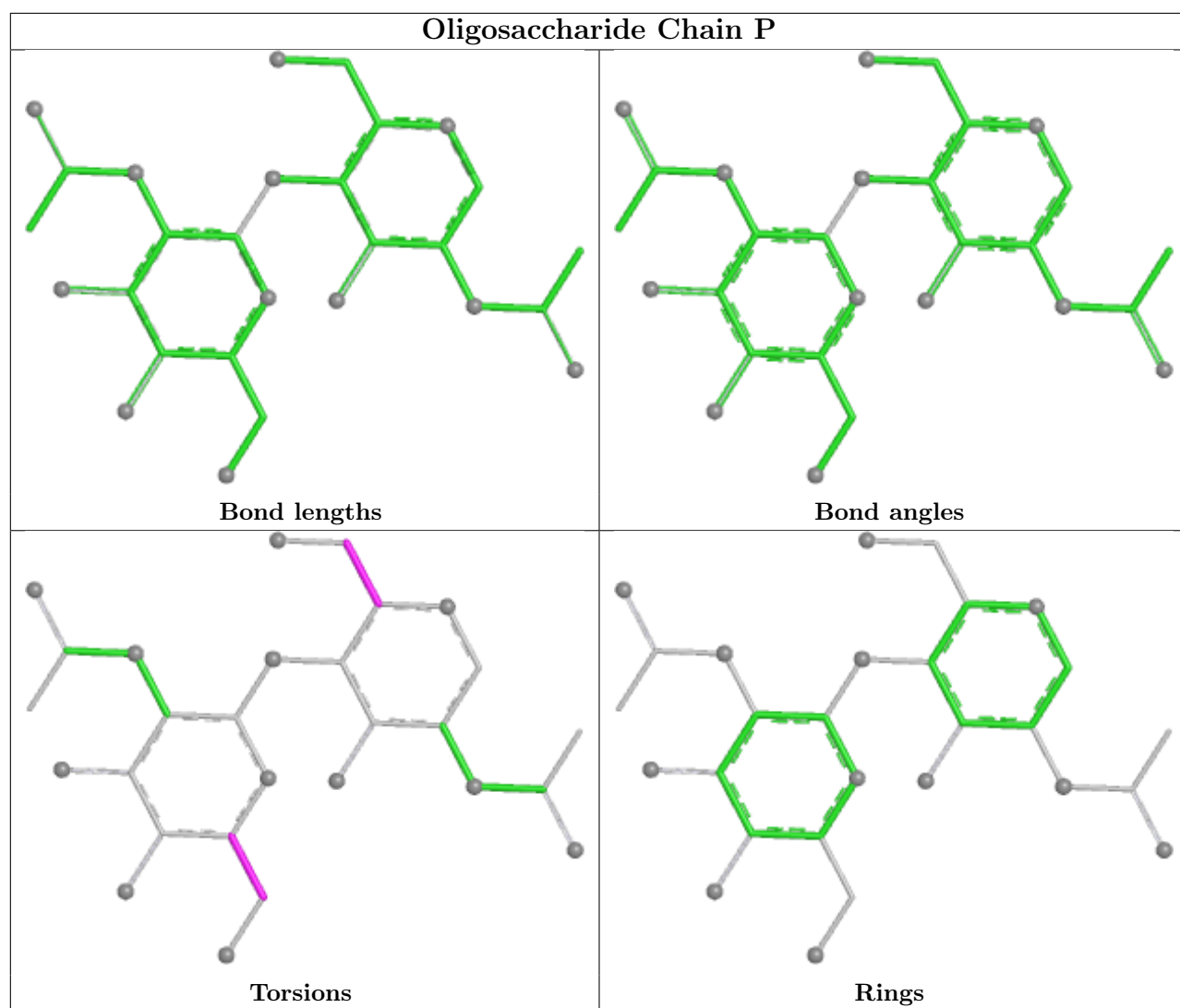


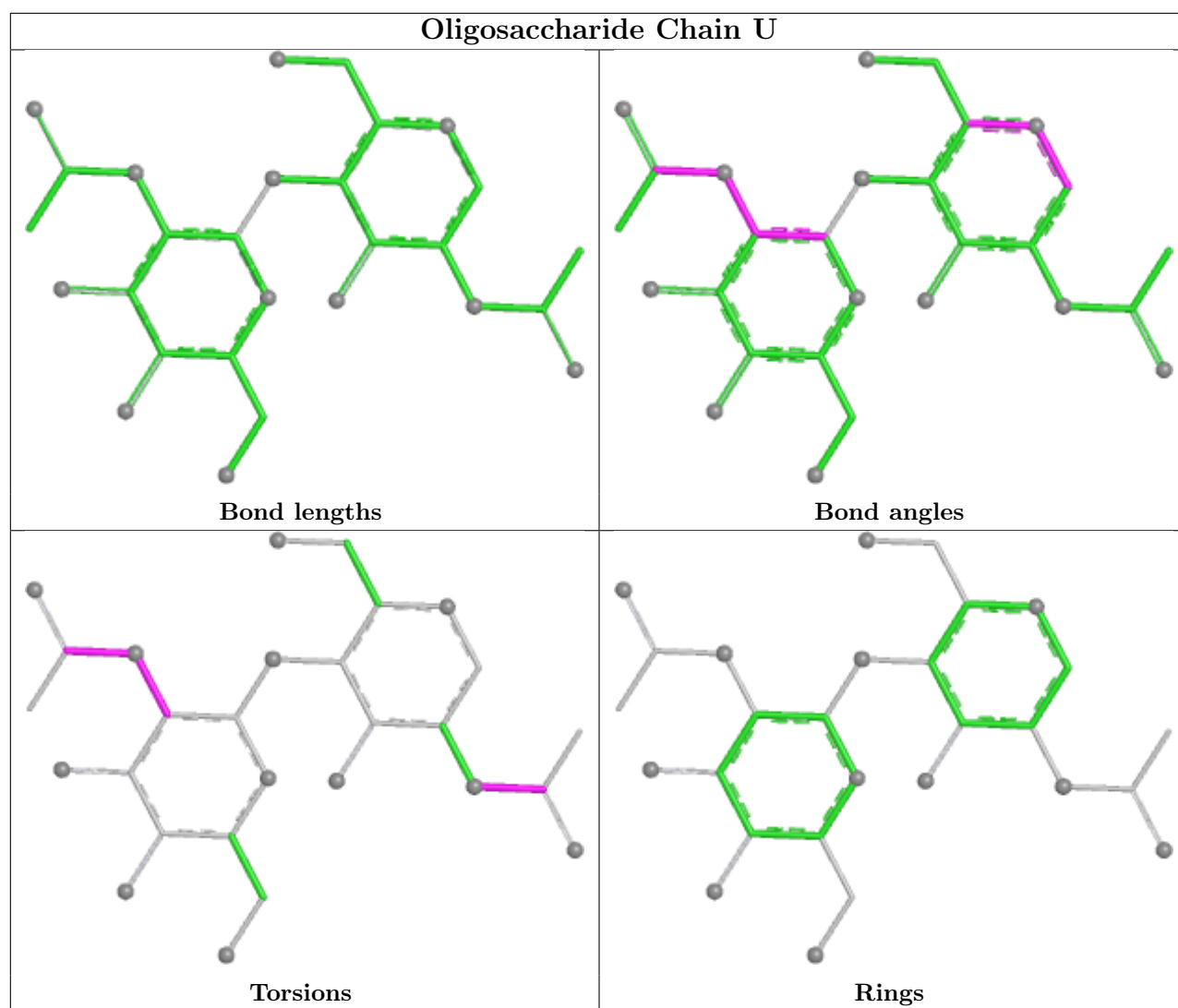


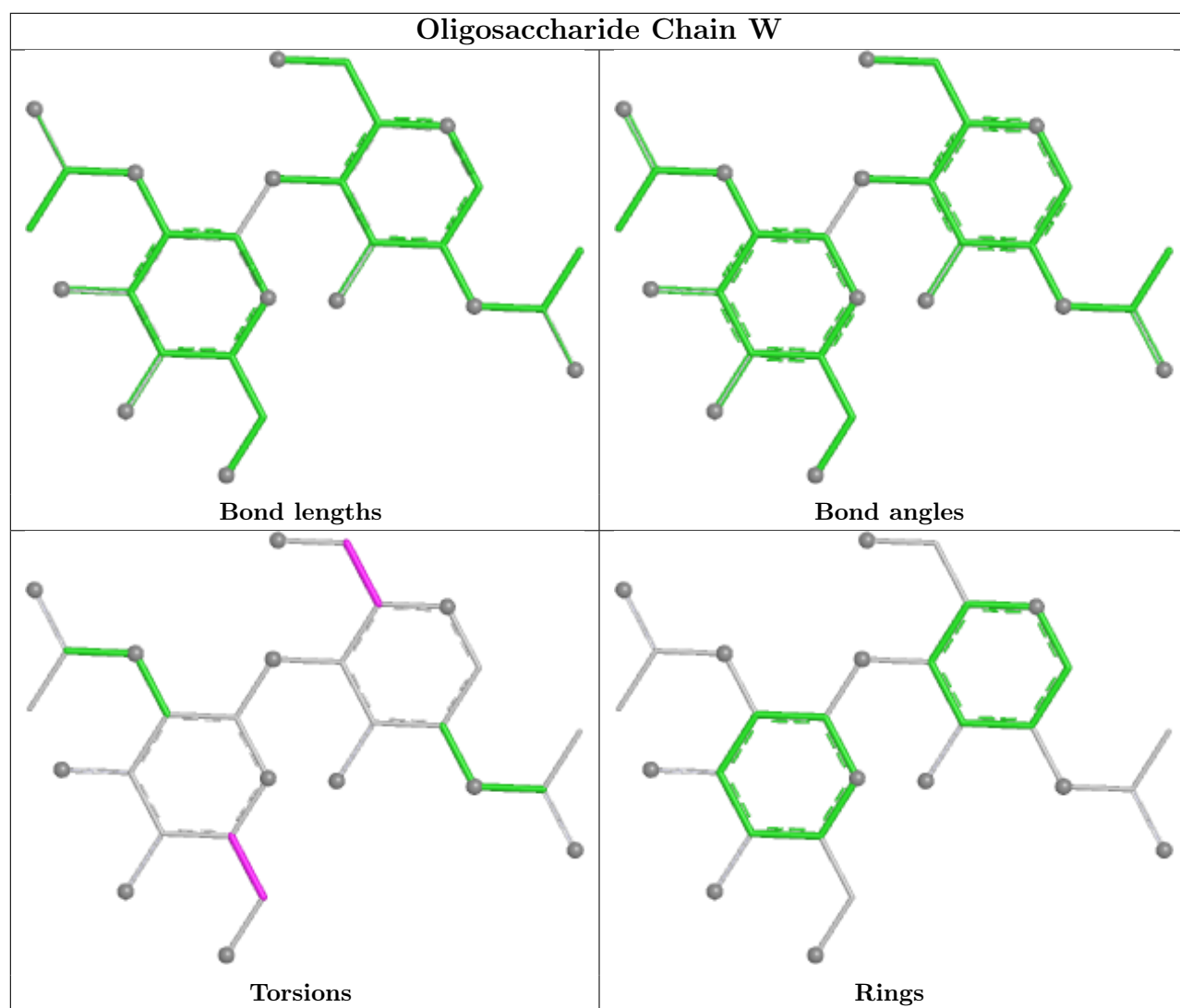


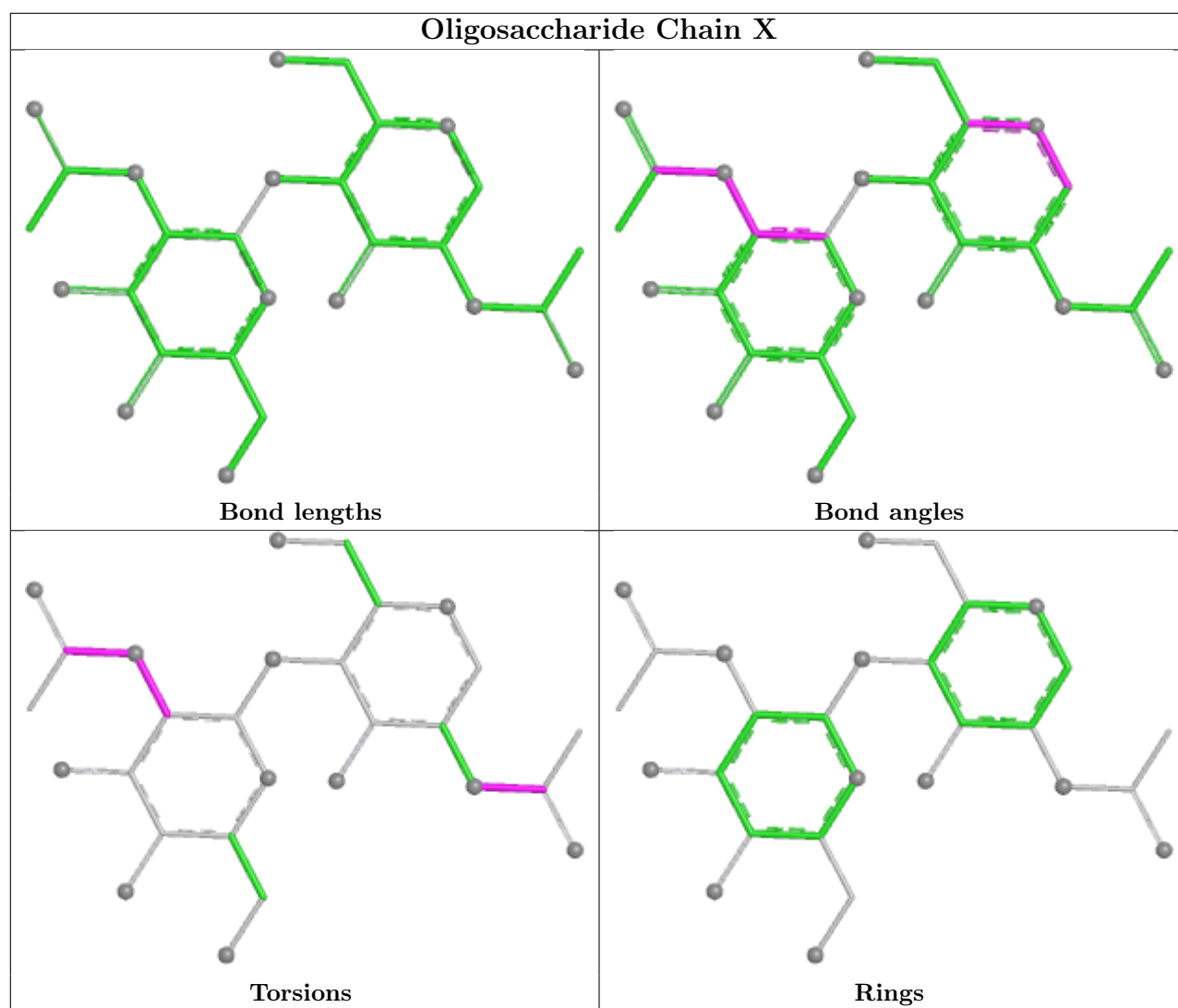












5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

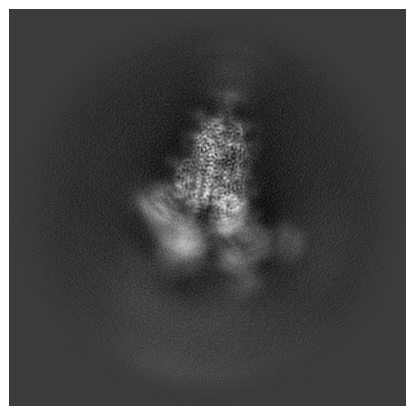
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37930. These allow visual inspection of the internal detail of the map and identification of artifacts.

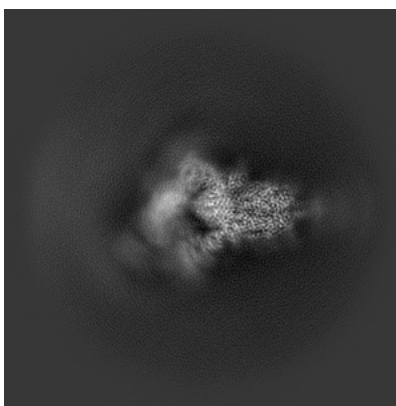
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

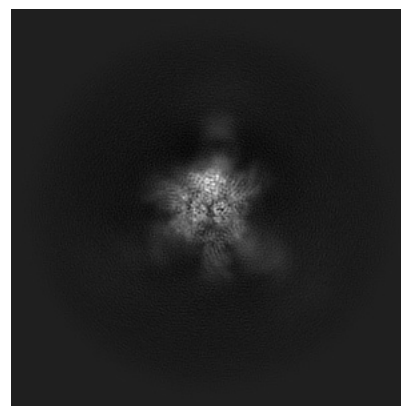
6.1.1 Primary map



X

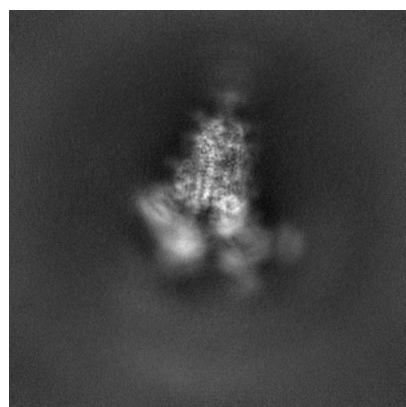


Y

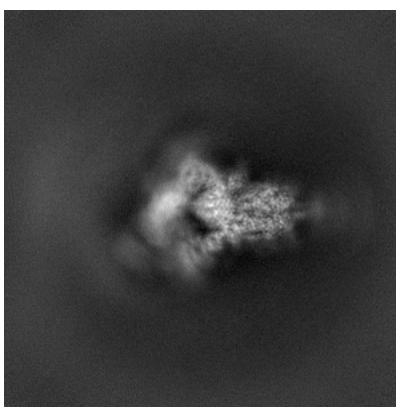


Z

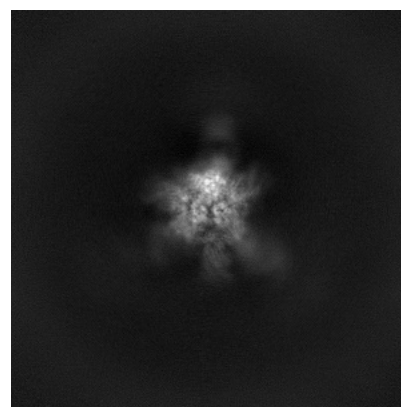
6.1.2 Raw map



X



Y

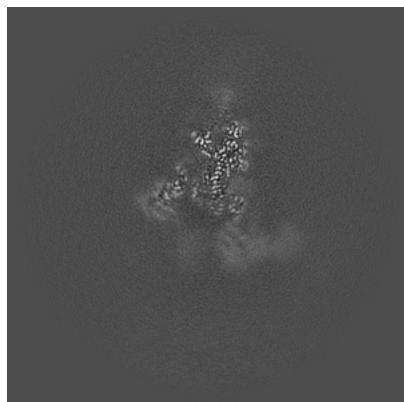


Z

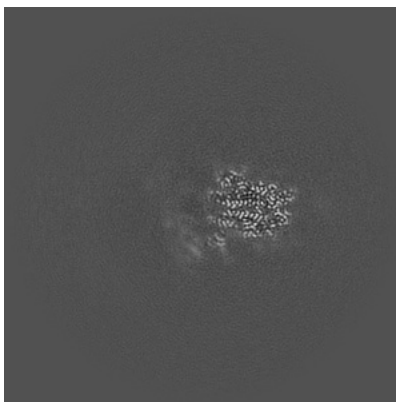
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

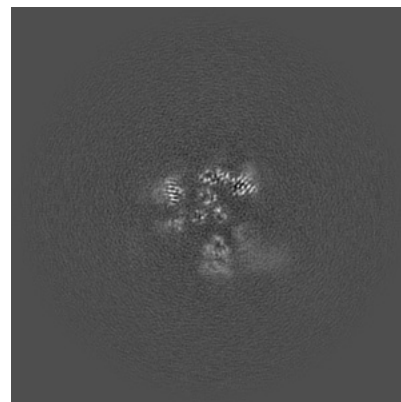
6.2.1 Primary map



X Index: 270

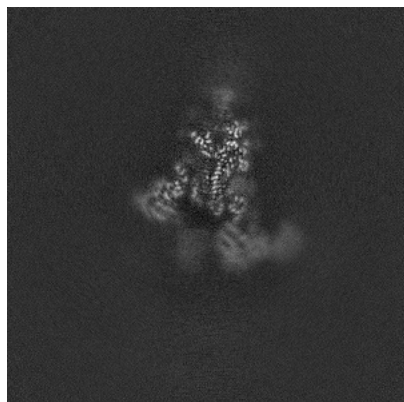


Y Index: 270

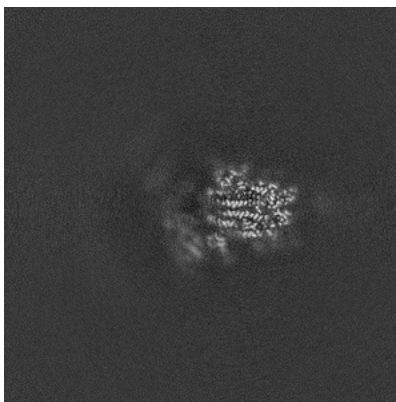


Z Index: 270

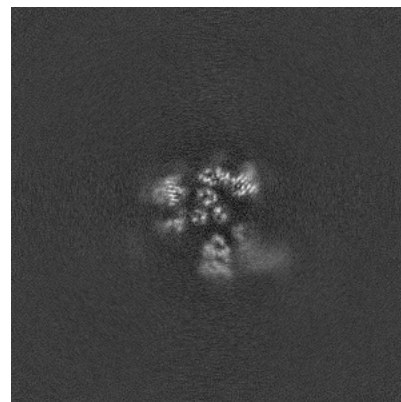
6.2.2 Raw map



X Index: 270



Y Index: 270



Z Index: 270

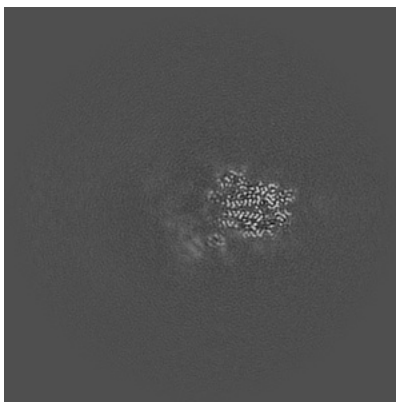
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

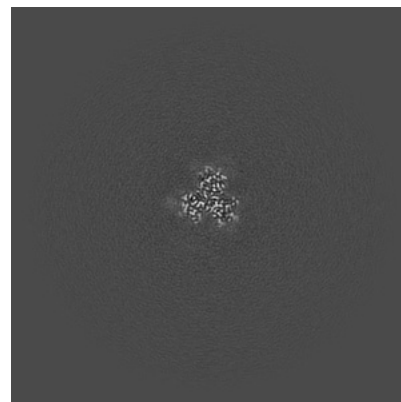
6.3.1 Primary map



X Index: 278



Y Index: 271

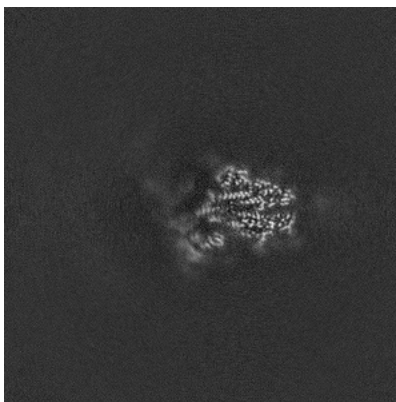


Z Index: 343

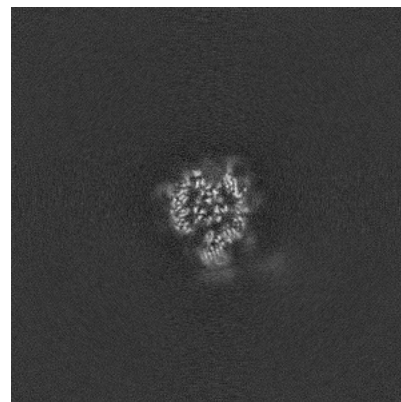
6.3.2 Raw map



X Index: 277



Y Index: 275

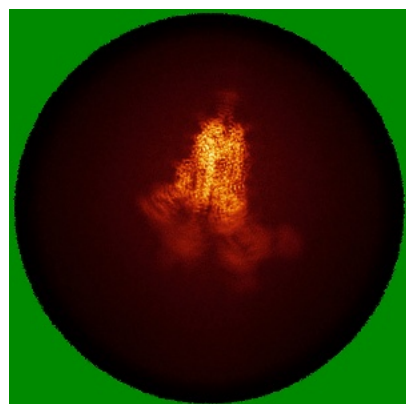


Z Index: 288

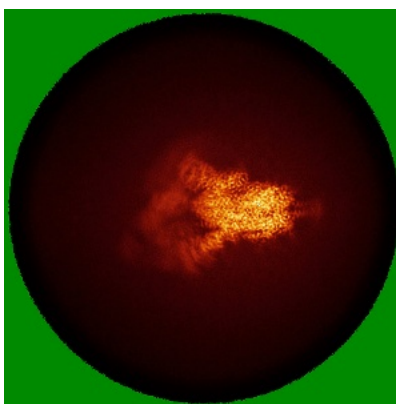
The images above show the largest variance slices of the map in three orthogonal directions.

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

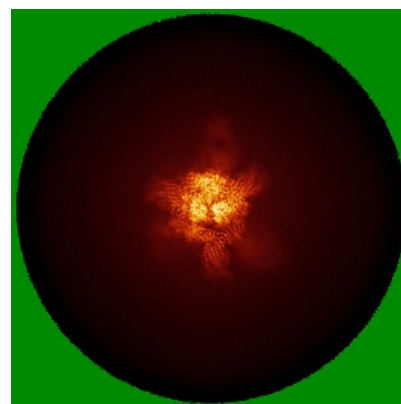
6.4.1 Primary map



X

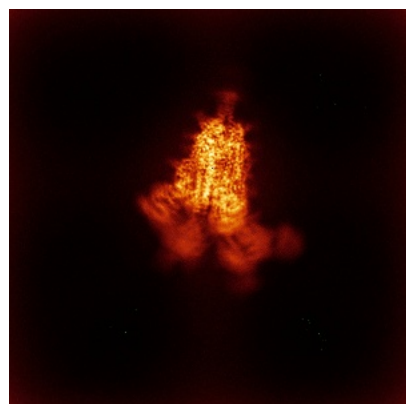


Y

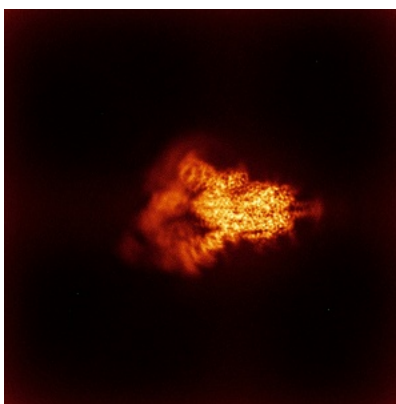


Z

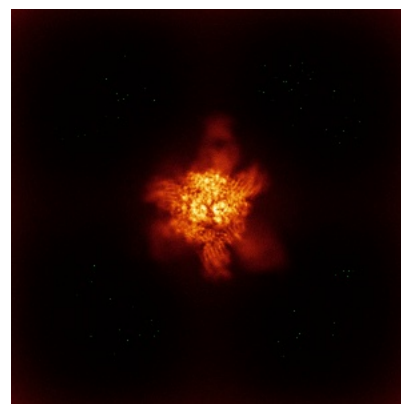
6.4.2 Raw map



X



Y



Z

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

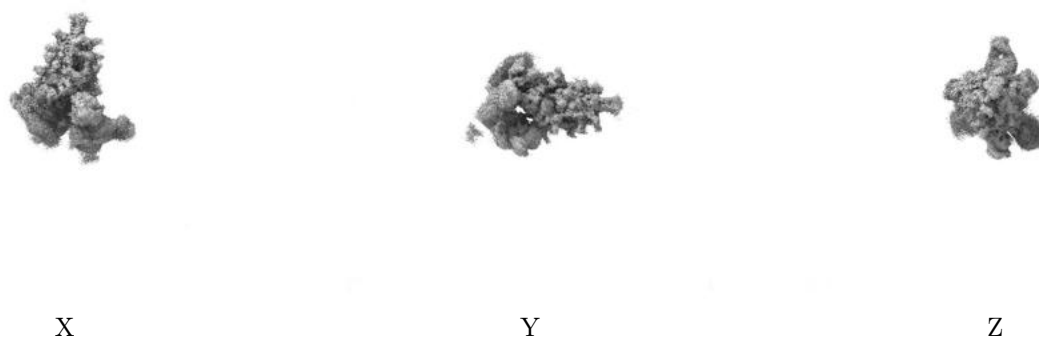
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

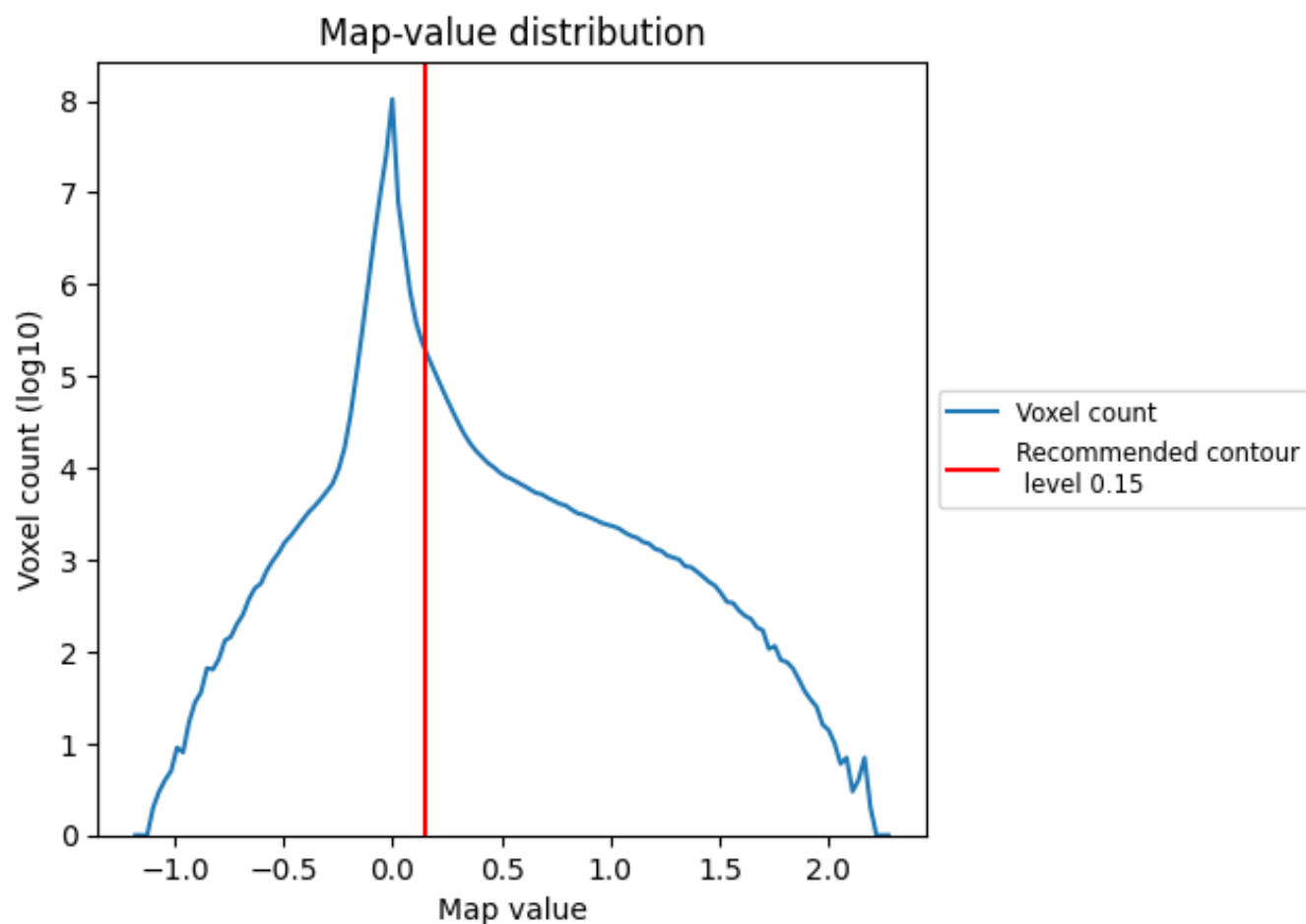
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

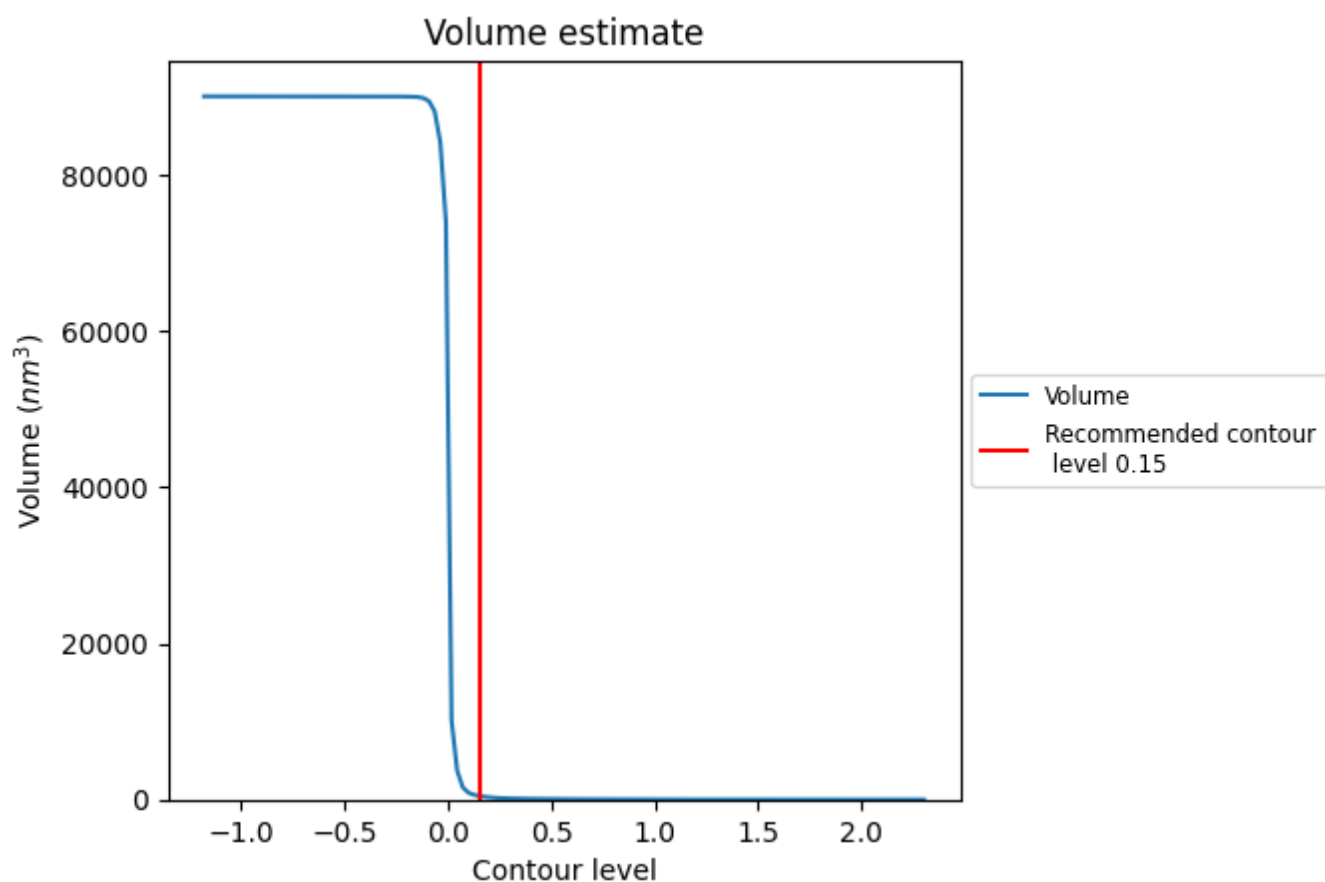
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

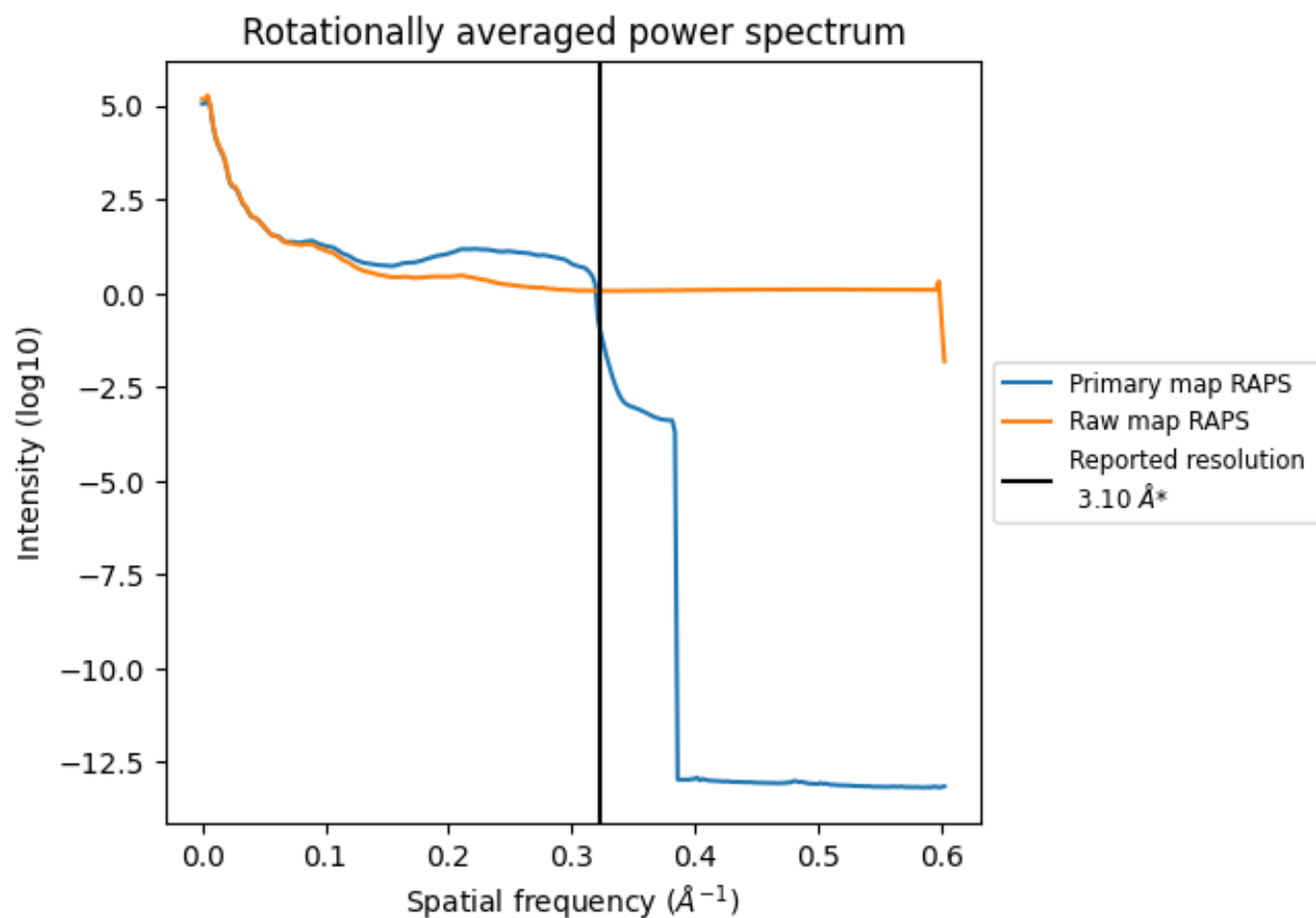
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 464 nm³; this corresponds to an approximate mass of 419 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

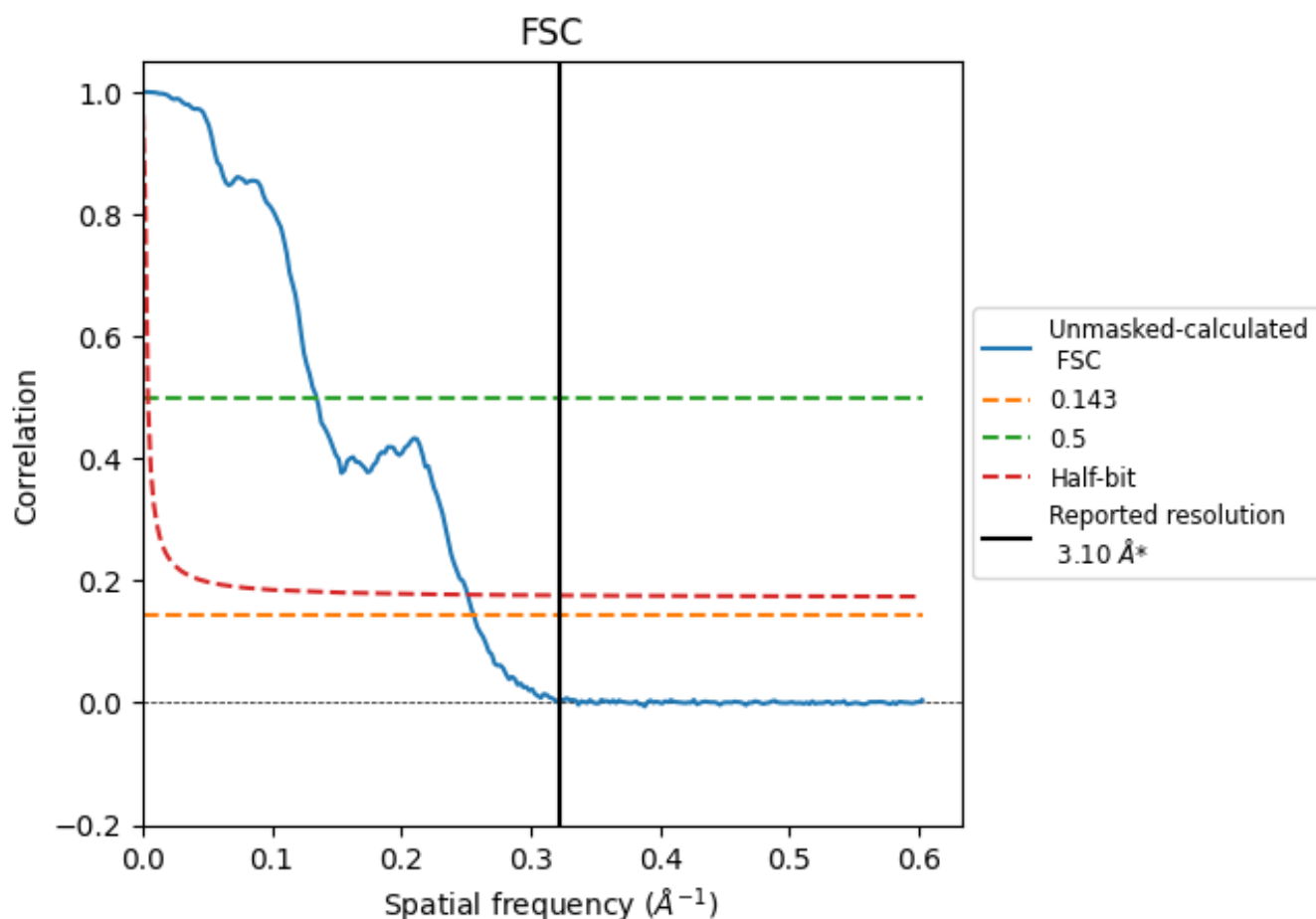


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.323 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

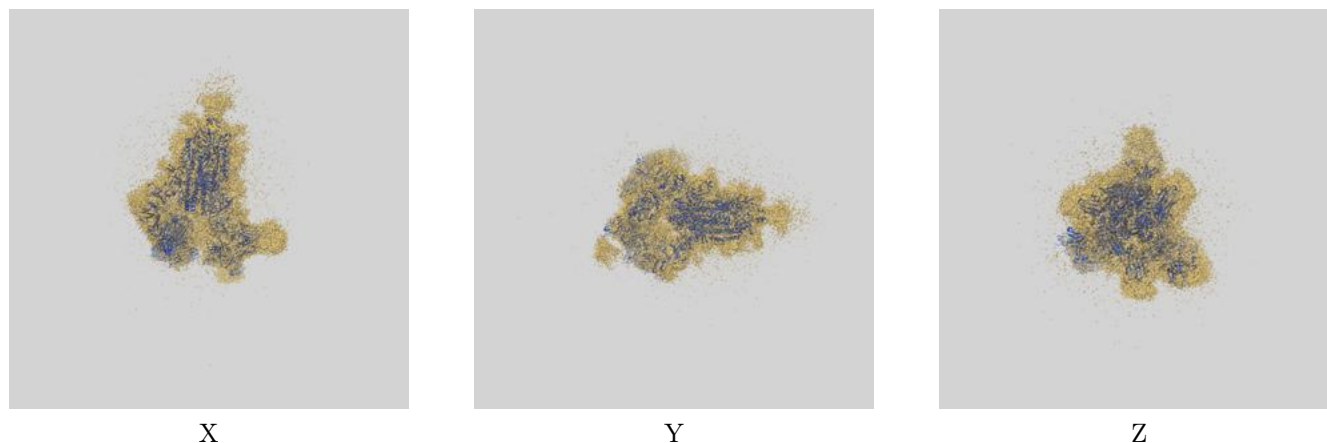
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.91	7.43	3.98

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.91 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

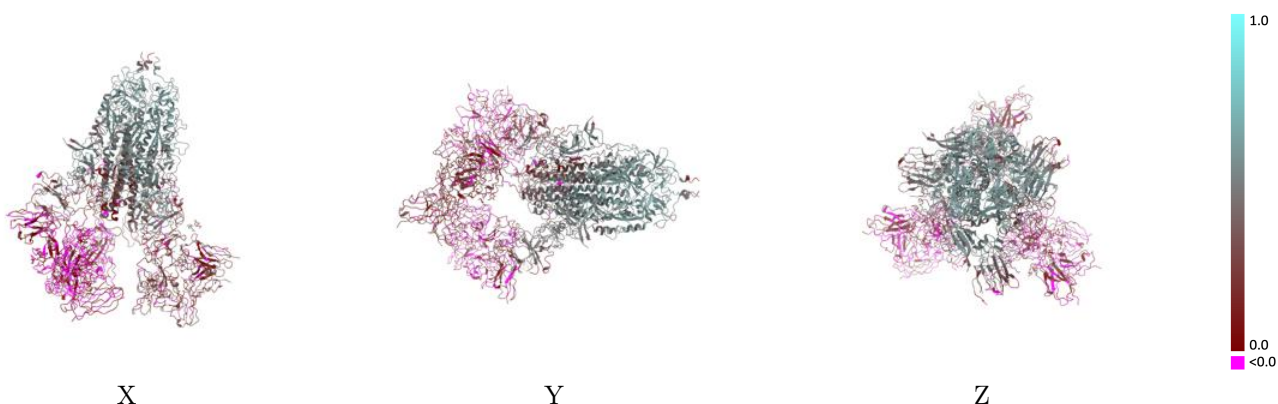
This section contains information regarding the fit between EMDB map EMD-37930 and PDB model 8WYJ. Per-residue inclusion information can be found in [section 3](#) on [page 12](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

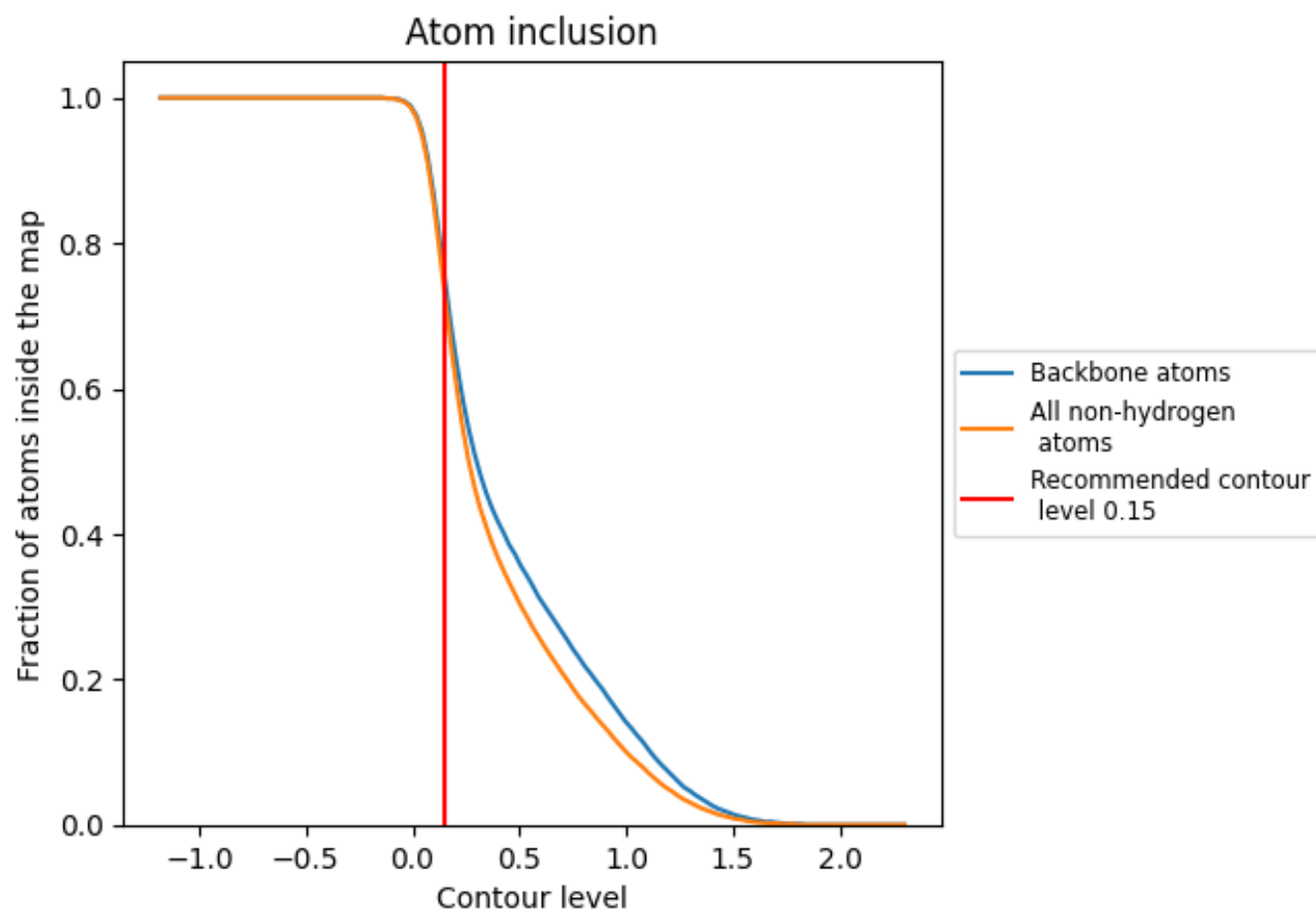


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 73% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7310	 0.2970
A	 0.8500	 0.3420
B	 0.9270	 0.4370
C	 0.8130	 0.3690
D	 0.2150	 0.0630
E	 0.8840	 0.2110
F	 0.6080	 0.2060
G	 0.8750	 0.2110
H	 0.5790	 0.2070
I	 0.2680	 0.0610
J	 0.1010	 0.0370
K	 0.2550	 0.0090
L	 0.8570	 0.3460
M	 0.7320	 0.2240
N	 0.5360	 0.1940
O	 0.4510	 0.0430
P	 0.4640	 0.1150
Q	 0.2240	 0.0640
R	 0.2160	 0.0420
S	 0.4910	 0.0710
T	 0.4460	 0.0430
U	 0.3930	 0.0290
V	 0.3380	 0.0540
W	 0.7860	 0.1350
X	 0.1430	 0.0590

