



## Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 06:41 AM UTC

PDB ID : 5UP2 / pdb\_00005up2  
EMDB ID : EMD-8581  
Title : Triheteromeric NMDA receptor GluN1/GluN2A/GluN2B in complex with glycine, glutamate, Ro 25-6981, MK-801 and a GluN2B-specific Fab, at pH 6.5  
Authors : Lu, W.; Du, J.; Goehring, A.; Gouaux, E.  
Deposited on : 2017-02-01  
Resolution : 6.00 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](mailto: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>.

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

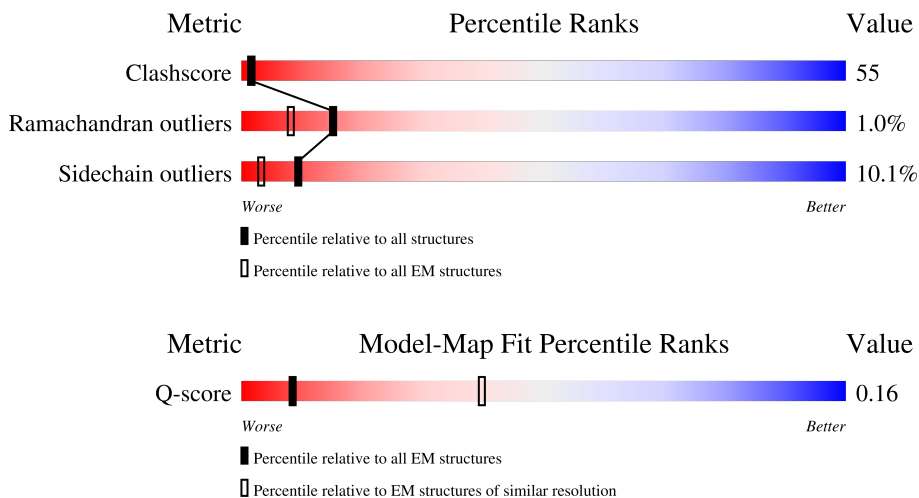
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 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 6.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	525 ( 5.50 - 6.50 )

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  $\geq 3$ , 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	836	
1	C	836	
2	B	831	
3	D	837	

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Mol	Chain	Length	Quality of chain
4	F	216	
4	G	216	
5	E	2	
5	H	2	
5	I	2	
5	J	2	

## 2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 24161 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 N-methyl-D-aspartate receptor subunit NR1-8a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	796	Total	C	N	O	S	0	0
			5745	3691	978	1047	29		
1	C	798	Total	C	N	O	S	0	0
			5442	3460	938	1018	26		

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	ALA	CYS	conflict	UNP C0KD18
A	300	GLN	ASN	conflict	UNP C0KD18
A	350	GLN	ASN	conflict	UNP C0KD18
A	368	ASP	ASN	conflict	UNP C0KD18
A	440	ASP	ASN	conflict	UNP C0KD18
A	469	ASP	ASN	conflict	UNP C0KD18
A	493	ALA	LYS	conflict	UNP C0KD18
A	494	ALA	LYS	conflict	UNP C0KD18
A	495	ALA	GLU	conflict	UNP C0KD18
A	592	ALA	GLU	conflict	UNP C0KD18
A	593	ALA	GLU	conflict	UNP C0KD18
A	594	ALA	GLU	conflict	UNP C0KD18
A	610	ARG	GLY	conflict	UNP C0KD18
A	617	LEU	ILE	conflict	UNP C0KD18
A	636	LEU	GLY	conflict	UNP C0KD18
A	656	ARG	ASP	conflict	UNP C0KD18
A	741	ASP	LYS	conflict	UNP C0KD18
A	769	GLU	ASN	conflict	UNP C0KD18
A	816	TYR	MET	conflict	UNP C0KD18
C	22	ALA	CYS	conflict	UNP C0KD18
C	300	GLN	ASN	conflict	UNP C0KD18
C	350	GLN	ASN	conflict	UNP C0KD18
C	368	ASP	ASN	conflict	UNP C0KD18
C	440	ASP	ASN	conflict	UNP C0KD18
C	469	ASP	ASN	conflict	UNP C0KD18
C	493	ALA	LYS	conflict	UNP C0KD18

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Chain	Residue	Modelled	Actual	Comment	Reference
C	494	ALA	LYS	conflict	UNP C0KD18
C	495	ALA	GLU	conflict	UNP C0KD18
C	592	ALA	GLU	conflict	UNP C0KD18
C	593	ALA	GLU	conflict	UNP C0KD18
C	594	ALA	GLU	conflict	UNP C0KD18
C	610	ARG	GLY	conflict	UNP C0KD18
C	617	LEU	ILE	conflict	UNP C0KD18
C	636	LEU	GLY	conflict	UNP C0KD18
C	656	ARG	ASP	conflict	UNP C0KD18
C	741	ASP	LYS	conflict	UNP C0KD18
C	769	GLU	ASN	conflict	UNP C0KD18
C	816	TYR	MET	conflict	UNP C0KD18

- Molecule 2 is a protein called N-methyl-D-aspartate receptor subunit NR2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	795	5573	3592	931	1019	31	0	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	67	GLN	ASN	conflict	UNP B7ZSK1
B	372	ALA	ASN	conflict	UNP B7ZSK1
B	?	-	THR	deletion	UNP B7ZSK1
B	?	-	ALA	deletion	UNP B7ZSK1
B	?	-	SER	deletion	UNP B7ZSK1
B	?	-	LEU	deletion	UNP B7ZSK1
B	431	ALA	ASN	conflict	UNP B7ZSK1
B	529	ALA	ASN	conflict	UNP B7ZSK1
B	605	LEU	VAL	conflict	UNP B7ZSK1
B	644	ARG	GLU	conflict	UNP B7ZSK1
B	645	ARG	GLU	conflict	UNP B7ZSK1
B	675	GLN	ASN	conflict	UNP B7ZSK1
B	831	LYS	-	expression tag	UNP B7ZSK1

- Molecule 3 is a protein called Ionotropic glutamate receptor subunit NR2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	794	5130	3283	865	957	25	0	0

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	20	SER	MET	conflict	UNP A7XY94
D	21	ARG	GLY	conflict	UNP A7XY94
D	22	ALA	CYS	conflict	UNP A7XY94
D	64	GLU	ALA	conflict	UNP A7XY94
D	69	GLN	ASN	conflict	UNP A7XY94
D	343	ASP	ASN	conflict	UNP A7XY94
D	?	-	LYS	deletion	UNP A7XY94
D	?	-	TYR	deletion	UNP A7XY94
D	?	-	TYR	deletion	UNP A7XY94
D	?	-	VAL	deletion	UNP A7XY94
D	486	VAL	THR	conflict	UNP A7XY94
D	581	ALA	CYS	conflict	UNP A7XY94
D	611	LEU	VAL	conflict	UNP A7XY94
D	650	ARG	GLU	conflict	UNP A7XY94
D	651	ARG	GLU	conflict	UNP A7XY94
D	836	TYR	PHE	conflict	UNP A7XY94
D	837	LYS	-	expression tag	UNP A7XY94

- Molecule 4 is a protein called GluN2B-specific Fab, termed 11D1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	F	214	1070	642	214	214	0	0
4	G	215	1075	645	215	215	0	0

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



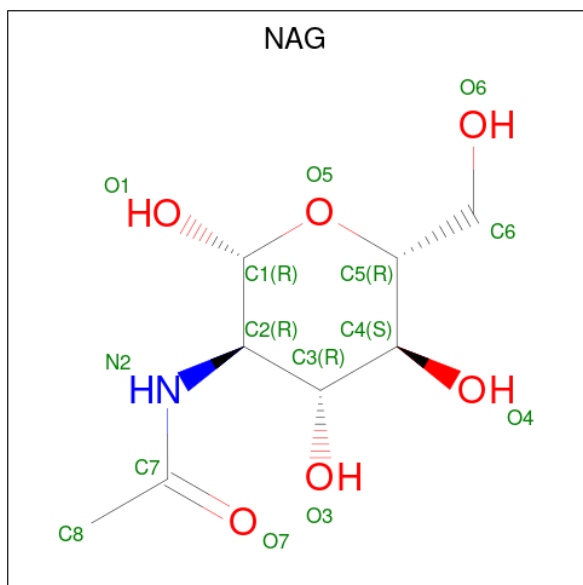
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	E	2	28	16	2	10	0	0
5	H	2	28	16	2	10	0	0
5	I	2	28	16	2	10	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	J	2	28	16	2	10	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).

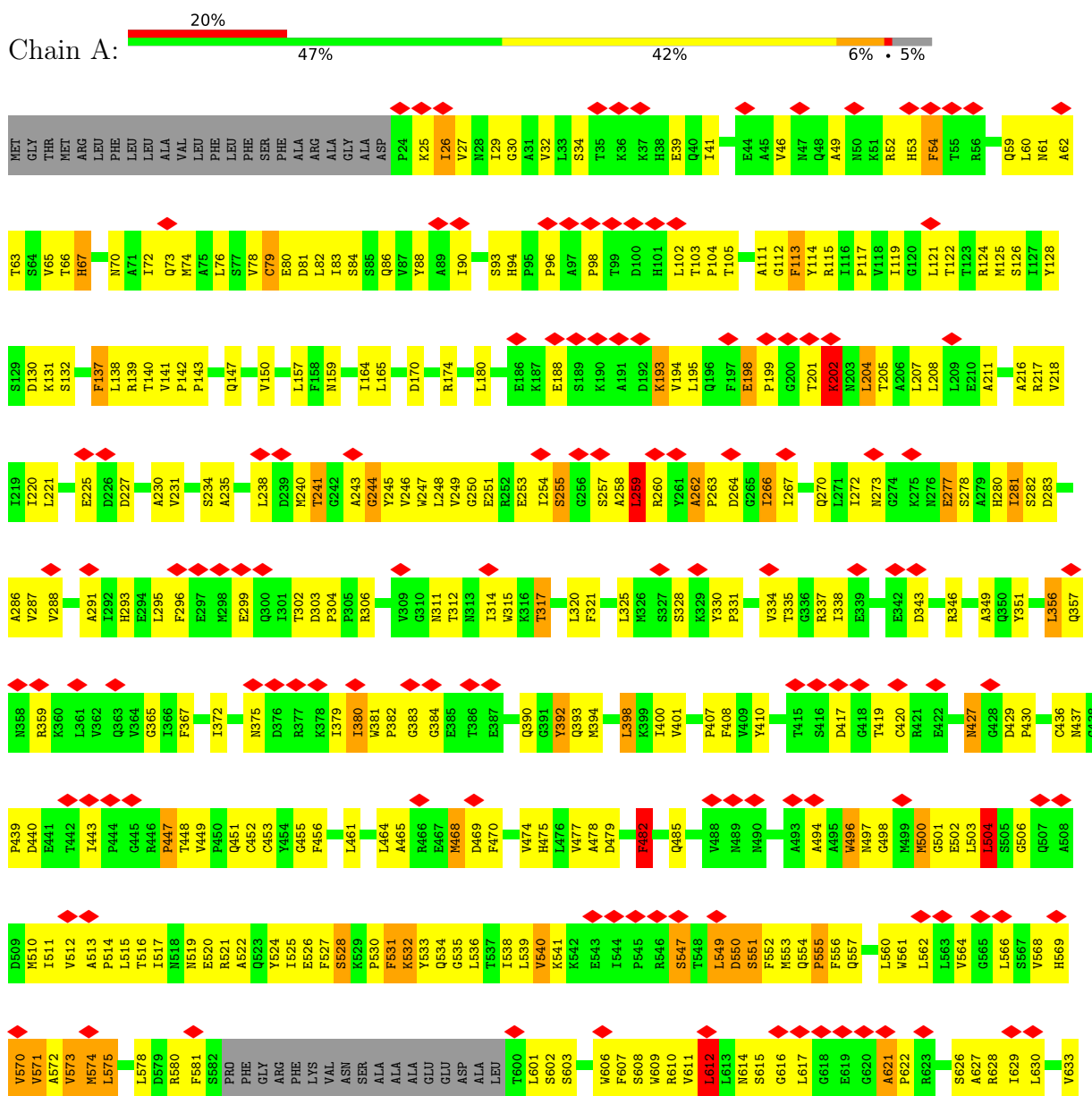


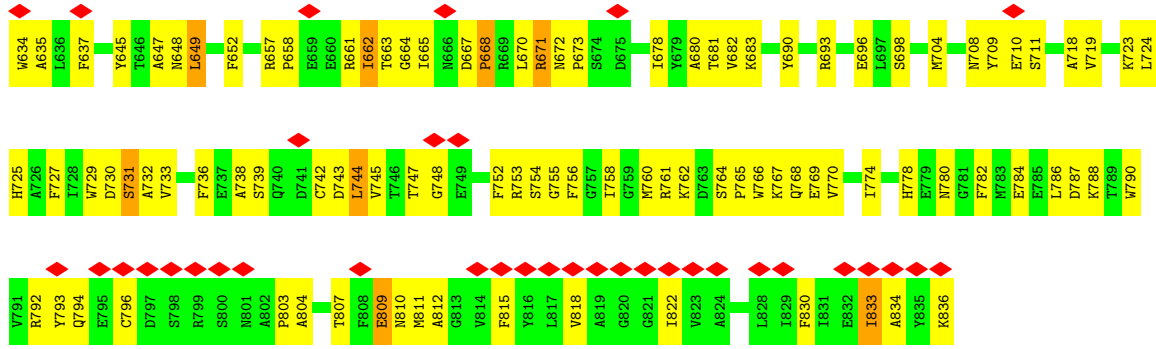
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
6	D	1	14	8	1	5	0

### 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.

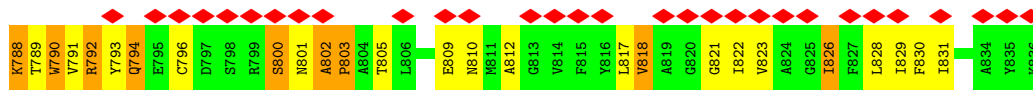
- Molecule 1: N-methyl-D-aspartate receptor subunit NR1-8a



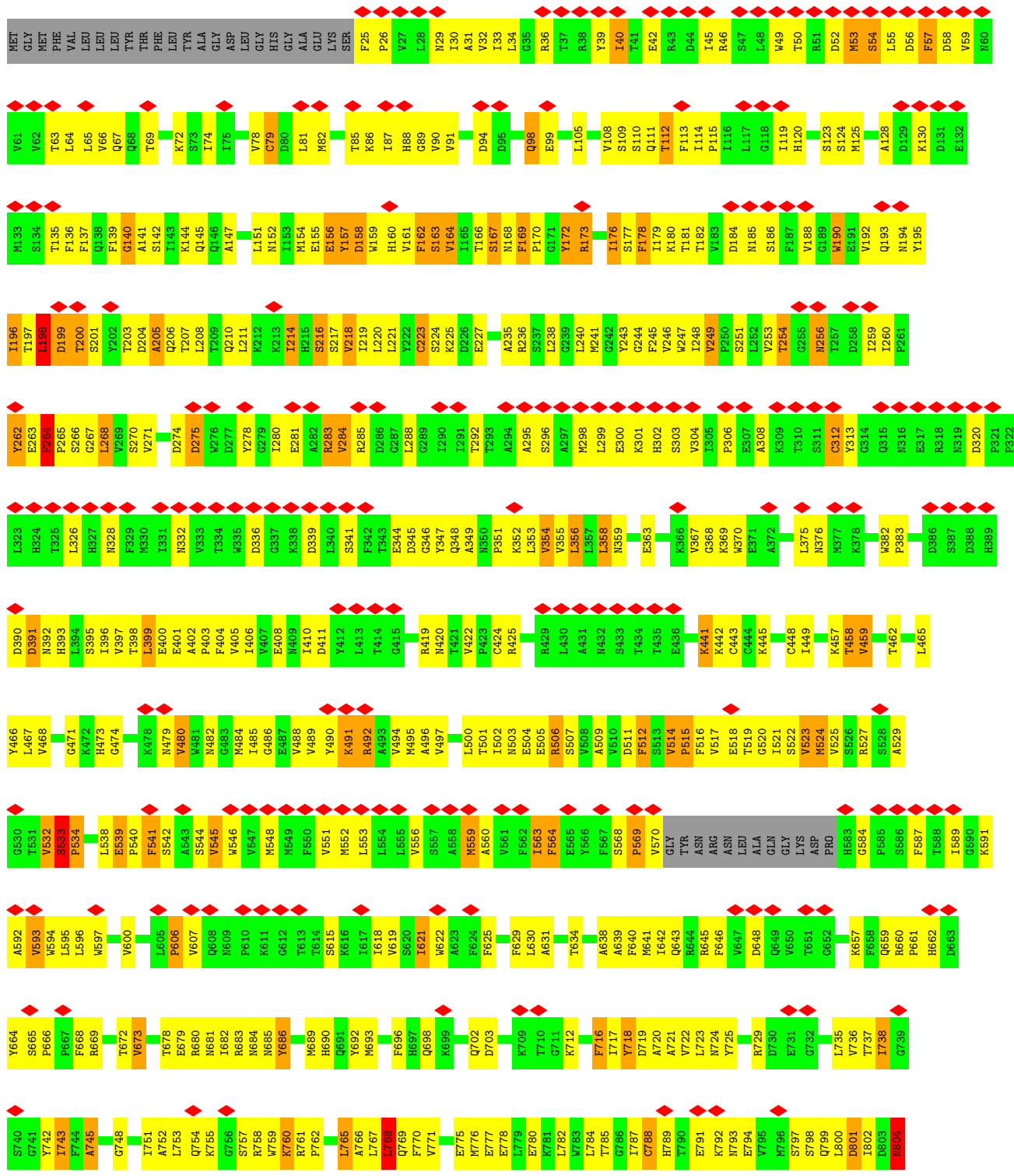


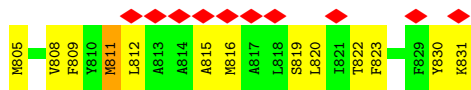
• Molecule 1: N-methyl-D-aspartate receptor subunit NR1-8a



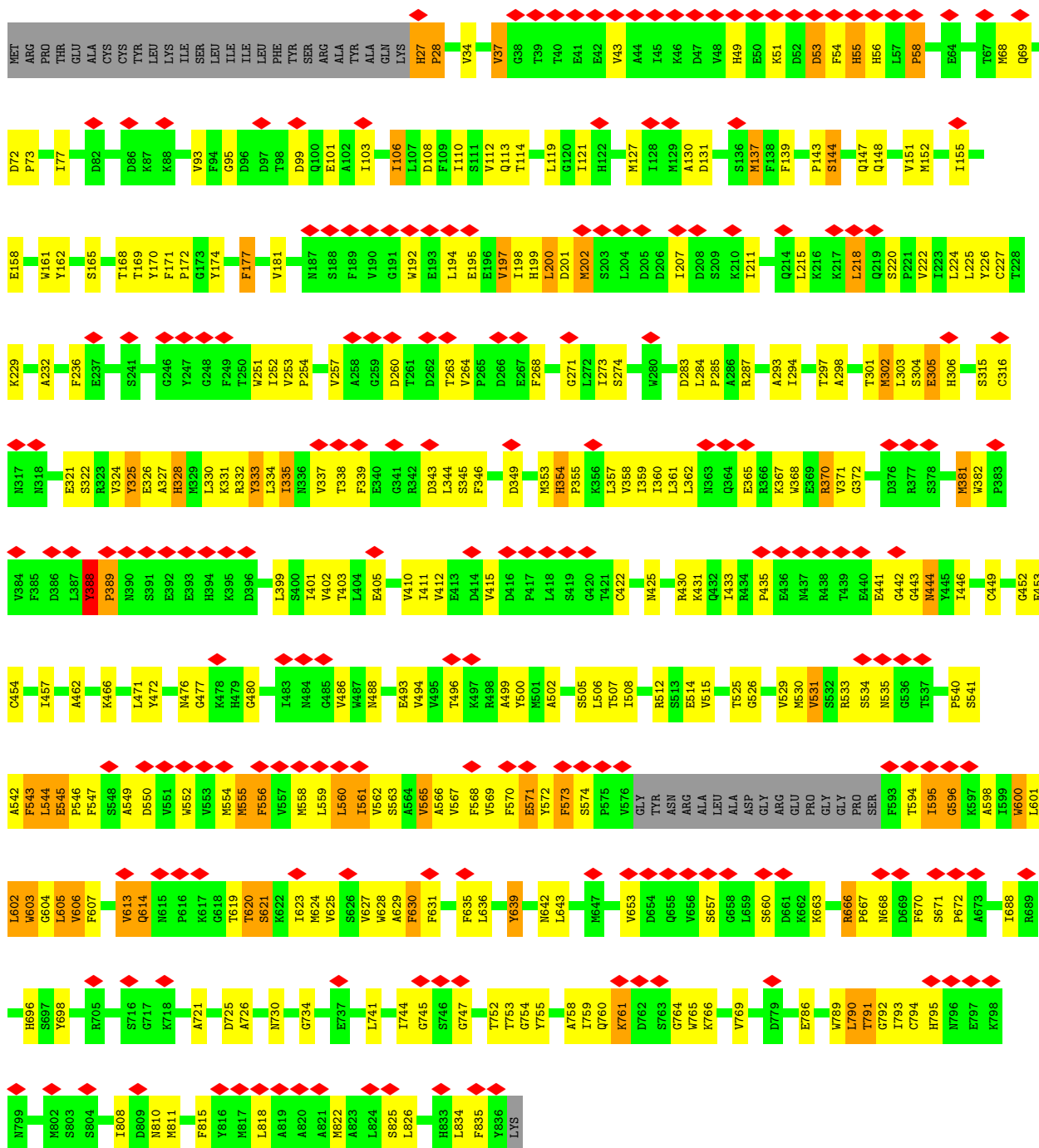


• Molecule 2: N-methyl-D-aspartate receptor subunit NR2A

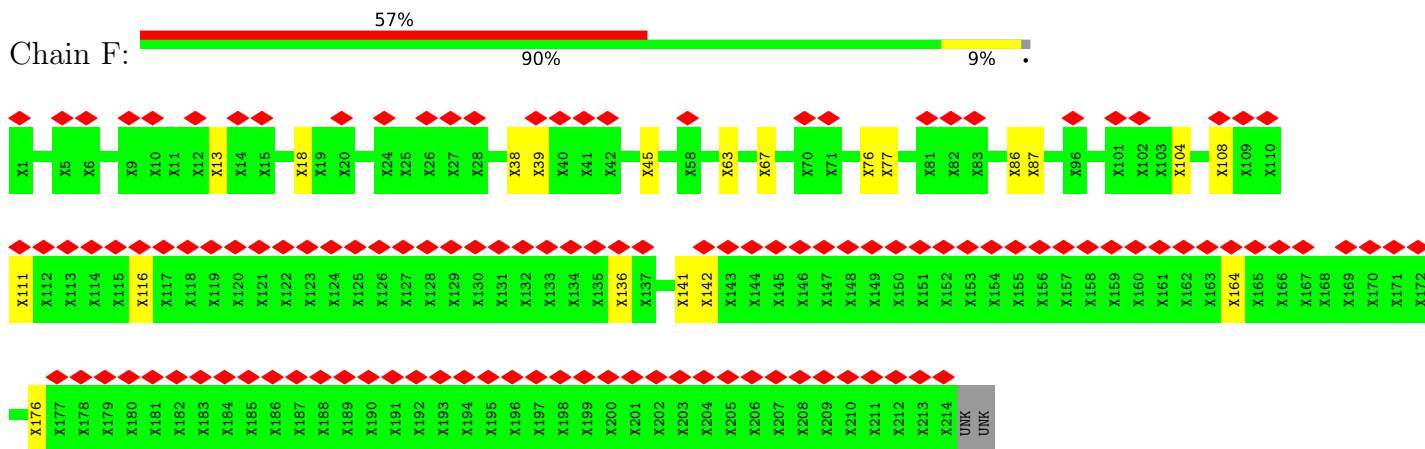




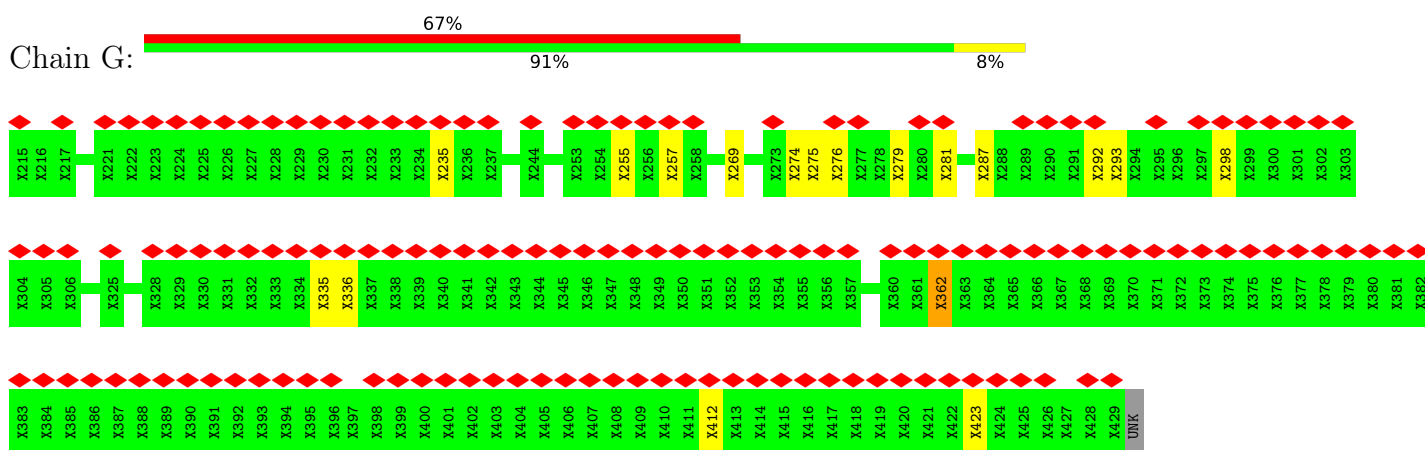
• Molecule 3: Ionotropic glutamate receptor subunit NR2B



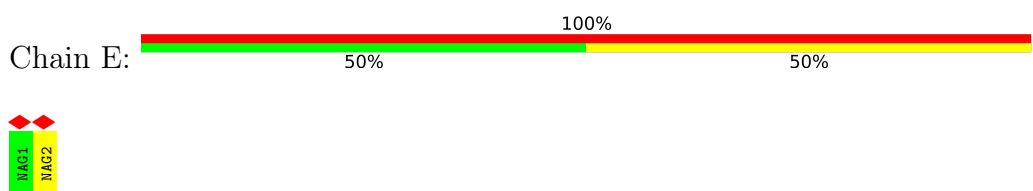
• Molecule 4: GluN2B-specific Fab, termed 11D1



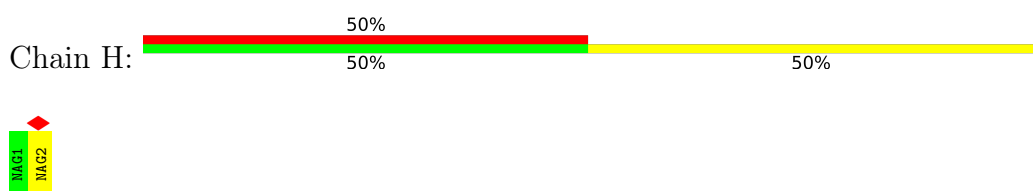
• Molecule 4: GluN2B-specific Fab, termed 11D1



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucofuranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	302052	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	0.84	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.121	Depositor
Minimum map value	-0.025	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.055	Depositor
Map size (Å)	435.2, 435.2, 435.2	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.7, 1.7, 1.7	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:  
NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.64	0/5877	1.20	57/8041 (0.7%)
1	C	0.48	0/5549	1.15	48/7614 (0.6%)
2	B	0.70	1/5697 (0.0%)	1.30	77/7814 (1.0%)
3	D	0.55	1/5233 (0.0%)	1.22	46/7227 (0.6%)
All	All	0.60	2/22356 (0.0%)	1.22	228/30696 (0.7%)

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	1
1	C	0	1
4	F	0	1
4	G	0	1
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	791	THR	C-N	6.61	1.39	1.33
2	B	178	PHE	N-CA	-5.51	1.39	1.46

All (228) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	200	THR	N-CA-C	14.17	126.73	111.28
3	D	613	VAL	N-CA-C	12.52	122.44	110.42
3	D	791	THR	CA-C-N	12.15	134.03	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	791	THR	C-N-CA	12.15	134.03	122.73
1	A	731	SER	N-CA-C	11.95	124.31	111.28
2	B	67	GLN	N-CA-C	10.59	122.90	111.36
1	C	487	ARG	N-CA-C	10.50	122.42	110.97
3	D	534	SER	N-CA-C	10.28	122.57	111.36
3	D	304	SER	N-CA-C	10.19	122.14	111.14
3	D	606	VAL	N-CA-C	10.15	120.97	110.62
1	A	427	ASN	N-CA-C	-10.08	93.05	108.67
2	B	471	GLY	N-CA-C	10.06	128.74	115.36
2	B	39	TYR	N-CA-C	10.02	124.58	109.25
2	B	217	SER	N-CA-C	9.96	121.73	111.07
2	B	54	SER	N-CA-C	9.75	122.81	111.11
1	C	629	ILE	N-CA-C	-9.68	100.74	110.62
1	A	260	ARG	N-CA-C	9.43	121.56	111.28
1	C	77	SER	N-CA-C	-9.38	101.75	113.01
1	A	550	ASP	N-CA-C	9.25	121.36	111.28
2	B	167	SER	N-CA-C	9.21	121.09	111.14
3	D	443	GLY	N-CA-C	8.96	124.98	111.18
2	B	36	ARG	N-CA-C	8.96	122.49	108.79
2	B	533	SER	C-N-CD	-8.95	88.31	125.00
3	D	69	GLN	N-CA-C	-8.88	101.68	111.36
1	C	673	PRO	N-CA-C	-8.85	96.04	110.74
2	B	516	PHE	N-CA-C	8.54	120.58	111.28
3	D	620	THR	N-CA-C	8.52	120.34	111.14
2	B	511	ASP	N-CA-C	8.49	121.98	109.07
3	D	549	ALA	N-CA-C	8.46	122.34	109.23
1	C	557	GLN	N-CA-C	8.28	120.31	111.28
1	A	259	LEU	N-CA-C	8.08	120.08	111.28
1	C	612	LEU	N-CA-C	7.96	119.65	110.97
1	C	790	TRP	N-CA-C	7.96	119.73	111.14
2	B	275	ASP	N-CA-C	7.94	119.94	111.28
2	B	259	ILE	N-CA-C	7.93	119.33	107.75
1	C	205	THR	N-CA-C	7.87	119.86	111.28
3	D	486	VAL	N-CA-C	7.86	119.43	108.12
3	D	101	GLU	N-CA-C	7.85	119.92	111.36
1	C	362	VAL	CA-C-N	-7.79	112.05	123.11
1	C	362	VAL	C-N-CA	-7.79	112.05	123.11
1	A	420	CYS	N-CA-C	7.79	121.16	109.95
2	B	284	VAL	N-CA-C	7.78	118.55	110.62
1	A	282	SER	CA-C-N	7.75	130.67	120.28
1	A	282	SER	C-N-CA	7.75	130.67	120.28
1	C	77	SER	CA-C-N	-7.75	113.41	122.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	77	SER	C-N-CA	-7.75	113.41	122.63
3	D	614	GLN	N-CA-C	7.74	119.91	108.14
3	D	602	LEU	N-CA-C	-7.64	102.95	111.28
2	B	99	GLU	N-CA-C	7.61	119.66	111.36
2	B	112	THR	N-CA-C	7.61	119.65	111.36
1	A	262	ALA	N-CA-C	7.58	121.12	110.20
1	A	551	SER	N-CA-C	7.55	119.15	111.07
3	D	790	LEU	N-CA-C	7.46	119.49	111.36
2	B	249	VAL	CA-C-N	7.42	129.12	119.84
2	B	249	VAL	C-N-CA	7.42	129.12	119.84
2	B	458	THR	N-CA-C	7.40	119.13	111.14
3	D	666	ARG	CA-C-N	7.39	126.90	118.85
3	D	666	ARG	C-N-CA	7.39	126.90	118.85
2	B	216	SER	N-CA-C	7.35	120.09	109.14
2	B	441	LYS	N-CA-C	7.28	121.56	111.74
3	D	671	SER	CA-C-N	-7.26	112.52	119.85
3	D	671	SER	C-N-CA	-7.26	112.52	119.85
2	B	312	CYS	N-CA-C	7.25	122.23	112.88
2	B	514	VAL	C-N-CD	-7.24	95.31	125.00
2	B	545	VAL	N-CA-C	7.21	117.97	110.62
1	C	758	ILE	CA-C-N	-7.19	116.76	121.65
1	C	758	ILE	C-N-CA	-7.19	116.76	121.65
2	B	140	GLY	N-CA-C	7.16	119.74	111.36
1	C	299	GLU	N-CA-C	7.13	120.25	109.41
3	D	305	GLU	N-CA-C	7.02	119.01	111.36
2	B	201	SER	N-CA-C	7.02	118.93	111.28
1	A	743	ASP	N-CA-C	-7.00	103.73	111.36
1	A	494	ALA	N-CA-C	6.99	119.97	108.99
1	C	360	LYS	N-CA-C	6.92	120.24	109.52
1	C	794	GLN	N-CA-C	6.91	120.78	109.24
1	A	804	ALA	N-CA-C	6.89	121.06	112.24
2	B	480	VAL	N-CA-C	6.89	117.75	108.11
1	C	558	SER	N-CA-C	6.88	118.43	111.07
1	A	617	LEU	N-CA-C	6.85	118.75	111.28
1	A	621	ALA	N-CA-C	6.78	118.25	109.64
1	C	438	GLY	C-N-CD	-6.78	97.22	125.00
2	B	218	VAL	N-CA-C	6.77	117.79	107.77
1	C	86	GLN	N-CA-C	6.76	120.90	112.24
1	A	482	PHE	N-CA-C	-6.75	103.92	111.28
2	B	162	PHE	CA-CB-CG	6.72	120.52	113.80
1	A	662	ILE	N-CA-C	6.72	117.47	110.62
3	D	367	LYS	N-CA-C	6.71	120.43	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	489	ASN	N-CA-C	-6.71	96.12	107.99
2	B	514	VAL	N-CA-C	6.70	123.34	108.88
3	D	425	ASN	N-CA-C	6.69	118.58	111.28
2	B	260	ILE	N-CA-C	6.66	114.73	107.60
1	A	193	LYS	N-CA-C	6.65	120.72	111.74
2	B	205	ALA	N-CA-C	6.61	118.48	111.28
1	A	547	SER	N-CA-C	6.59	119.68	109.07
3	D	535	ASN	N-CA-C	6.59	118.22	108.60
1	A	159	ASN	CA-C-N	-6.53	114.09	122.77
1	A	159	ASN	C-N-CA	-6.53	114.09	122.77
3	D	113	GLN	N-CA-C	6.48	118.42	111.36
1	A	672	ASN	CA-C-N	6.46	126.84	119.92
1	A	672	ASN	C-N-CA	6.46	126.84	119.92
1	A	764	SER	CA-C-N	6.43	127.25	120.12
1	A	764	SER	C-N-CA	6.43	127.25	120.12
1	A	137	PHE	N-CA-C	6.41	119.77	110.28
1	A	244	GLY	N-CA-C	-6.35	106.31	115.27
1	A	52	ARG	N-CA-C	6.35	118.20	111.28
1	A	621	ALA	C-N-CD	-6.32	99.07	125.00
3	D	476	ASN	N-CA-C	6.29	119.49	109.24
1	A	202	LYS	CA-C-N	-6.29	114.06	122.42
1	A	202	LYS	C-N-CA	-6.29	114.06	122.42
2	B	177	SER	N-CA-C	6.21	118.13	111.36
1	C	822	ILE	N-CA-C	6.21	116.95	110.62
3	D	619	THR	N-CA-C	6.20	120.96	112.04
2	B	509	ALA	N-CA-C	6.19	118.11	111.36
2	B	313	TYR	N-CA-C	6.17	118.79	109.23
1	C	748	GLY	N-CA-C	6.17	120.13	112.73
1	C	379	ILE	CA-C-N	-6.17	114.55	123.06
1	C	379	ILE	C-N-CA	-6.17	114.55	123.06
2	B	249	VAL	N-CA-C	6.12	114.71	107.73
1	A	504	LEU	CA-C-N	6.12	129.09	120.28
1	A	504	LEU	C-N-CA	6.12	129.09	120.28
1	C	223	ALA	N-CA-C	6.07	117.45	108.60
2	B	479	ASN	N-CA-C	6.03	117.85	111.28
2	B	629	PHE	CA-CB-CG	-6.03	107.77	113.80
2	B	459	VAL	N-CA-C	-6.02	106.87	112.83
3	D	315	SER	N-CA-C	6.01	118.42	109.59
1	A	708	ASN	N-CA-C	6.00	118.29	110.43
2	B	625	PHE	CA-CB-CG	-5.95	107.85	113.80
1	A	419	THR	CA-C-N	-5.93	112.31	123.27
1	A	419	THR	C-N-CA	-5.93	112.31	123.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	531	PHE	N-CA-C	5.91	117.80	111.36
1	C	609	TRP	N-CA-C	-5.89	104.81	112.23
1	C	301	ILE	N-CA-C	5.86	116.55	107.99
3	D	442	GLY	N-CA-C	-5.84	104.52	111.36
3	D	381	MET	N-CA-C	-5.79	99.09	108.41
2	B	804	ASN	N-CA-C	-5.77	105.07	111.36
2	B	111	GLN	N-CA-C	5.77	117.37	111.14
1	C	623	ARG	N-CA-C	5.74	117.61	111.36
1	A	649	LEU	N-CA-C	-5.73	105.11	111.36
1	C	695	VAL	N-CA-C	5.73	116.46	110.62
1	C	542	LYS	N-CA-C	5.71	118.93	110.48
1	A	70	ASN	N-CA-C	-5.70	99.23	108.52
1	A	281	ILE	N-CA-C	5.69	116.42	110.62
1	A	662	ILE	CA-C-N	-5.68	110.70	121.54
1	A	662	ILE	C-N-CA	-5.68	110.70	121.54
3	D	607	PHE	N-CA-C	5.67	119.53	107.67
3	D	660	SER	N-CA-C	-5.67	106.02	113.17
1	A	311	ASN	N-CA-C	5.66	118.13	108.90
1	A	67	HIS	N-CA-C	5.65	119.03	111.24
2	B	506	ARG	N-CA-C	-5.65	105.13	111.28
2	B	673	VAL	N-CA-C	5.63	114.26	109.02
2	B	266	SER	N-CA-C	5.62	117.79	110.43
1	C	72	ILE	N-CA-C	5.62	116.35	110.62
2	B	422	VAL	CA-C-N	5.61	125.37	119.76
2	B	422	VAL	C-N-CA	5.61	125.37	119.76
1	C	803	PRO	N-CA-C	5.60	120.28	111.38
3	D	51	LYS	N-CA-C	-5.60	105.18	111.28
2	B	492	ARG	N-CA-C	-5.58	104.83	111.69
2	B	593	VAL	N-CA-C	-5.57	104.94	110.62
3	D	571	GLU	N-CA-C	-5.56	105.22	111.28
2	B	768	LEU	N-CA-C	5.54	117.01	110.97
3	D	27	HIS	C-N-CD	-5.54	102.28	125.00
1	C	818	VAL	N-CA-C	5.52	116.25	110.62
1	C	449	VAL	C-N-CD	-5.52	102.38	125.00
1	A	317	THR	N-CA-C	5.51	117.29	111.28
2	B	404	PHE	N-CA-C	5.51	120.26	112.93
1	C	151	TRP	N-CA-C	-5.50	105.28	111.28
1	C	800	SER	N-CA-C	5.50	122.50	110.80
1	A	188	GLU	N-CA-C	-5.48	102.28	110.23
3	D	792	GLY	N-CA-C	5.47	119.08	110.71
1	C	547	SER	N-CA-C	5.47	117.75	110.53
1	C	156	ARG	N-CA-C	-5.47	105.32	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	680	ALA	N-CA-C	5.47	115.50	108.34
3	D	127	MET	N-CA-C	5.46	117.78	110.35
2	B	358	LEU	N-CA-C	-5.46	100.90	109.25
2	B	759	TRP	N-CA-C	-5.45	106.33	112.87
2	B	606	PRO	N-CA-C	-5.43	105.98	113.53
1	C	488	VAL	N-CA-C	5.42	120.62	109.34
3	D	177	PHE	N-CA-C	-5.41	104.62	111.11
3	D	477	GLY	N-CA-C	5.39	122.22	115.21
1	C	541	LYS	N-CA-C	5.38	117.47	110.53
1	A	262	ALA	CA-C-N	5.37	125.83	120.52
1	A	262	ALA	C-N-CA	5.37	125.83	120.52
2	B	55	LEU	N-CA-C	5.36	117.20	111.36
2	B	745	ALA	N-CA-C	-5.35	100.18	108.90
2	B	563	ILE	N-CA-C	5.33	116.06	110.62
2	B	703	ASP	N-CA-C	-5.33	105.39	111.14
3	D	596	GLY	N-CA-C	-5.32	106.34	112.73
1	C	563	LEU	N-CA-C	5.32	117.16	111.36
1	A	198	GLU	N-CA-C	-5.31	102.81	110.40
2	B	742	TYR	N-CA-C	-5.30	102.06	109.96
1	C	821	GLY	N-CA-C	5.29	119.08	112.73
1	A	612	LEU	N-CA-C	-5.29	105.51	111.28
2	B	260	ILE	CA-C-N	5.29	126.45	119.84
2	B	260	ILE	C-N-CA	5.29	126.45	119.84
2	B	336	ASP	CA-CB-CG	5.27	117.87	112.60
2	B	719	ASP	N-CA-C	-5.26	102.26	110.10
3	D	106	ILE	N-CA-C	-5.26	105.37	110.42
3	D	53	ASP	N-CA-C	5.25	117.75	111.71
3	D	302	MET	N-CA-C	-5.23	105.58	111.28
1	A	711	SER	N-CA-C	5.20	116.20	108.60
2	B	745	ALA	CA-C-N	-5.20	115.77	123.05
2	B	745	ALA	C-N-CA	-5.20	115.77	123.05
2	B	264	PHE	CA-C-N	5.18	126.31	119.84
2	B	264	PHE	C-N-CA	5.18	126.31	119.84
3	D	444	ASN	N-CA-C	-5.17	100.88	109.46
1	C	817	LEU	O-C-N	-5.17	116.26	122.15
1	A	443	ILE	N-CA-C	-5.15	104.23	109.02
3	D	388	TYR	C-N-CD	-5.14	103.91	125.00
2	B	172	TYR	N-CA-C	-5.11	105.60	111.07
2	B	302	HIS	N-CA-C	5.11	118.49	111.54
2	B	262	TYR	CA-CB-CG	-5.08	104.77	113.90
1	C	611	VAL	N-CA-C	5.07	115.29	110.42
1	A	255	SER	N-CA-C	5.07	117.39	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	163	SER	N-CA-C	5.05	116.74	108.76
2	B	56	ASP	N-CA-C	5.05	116.47	111.07
3	D	621	SER	N-CA-C	5.05	116.86	111.36
1	C	624	SER	N-CA-C	5.04	117.34	109.52
3	D	766	LYS	N-CA-C	5.04	115.98	108.31
2	B	716	PHE	N-CA-C	5.04	117.61	108.69
1	A	384	GLY	N-CA-C	5.03	122.30	115.30
2	B	196	ILE	N-CA-C	5.03	114.95	108.82
1	C	661	ARG	CA-C-N	-5.03	116.42	123.10
1	C	661	ARG	C-N-CA	-5.03	116.42	123.10
1	A	390	GLN	N-CA-C	5.02	116.97	109.59
2	B	328	ASN	N-CA-C	5.02	118.44	112.72
1	A	241	THR	N-CA-C	5.01	118.89	112.87
2	B	158	ASP	N-CA-C	5.01	117.07	108.90
2	B	198	LEU	N-CA-C	5.00	121.46	110.80

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	570	VAL	Mainchain
1	C	792	ARG	Mainchain
4	F	67	UNK	Mainchain
4	G	362	UNK	Peptide

## 5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5745	0	5276	801	0
1	C	5442	0	4757	516	0
2	B	5573	0	4942	894	0
3	D	5130	0	4104	447	0
4	F	1070	0	235	10	0
4	G	1075	0	235	11	0
5	E	28	0	25	4	0
5	H	28	0	25	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	I	28	0	25	3	0
5	J	28	0	25	2	0
6	D	14	0	13	0	0
All	All	24161	0	19662	2406	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 55.

All (2406) 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:630:LEU:HD22	2:B:816:MET:SD	1.39	1.62
1:A:682:VAL:HG21	1:A:729:TRP:CH2	1.17	1.60
2:B:403:PRO:CG	2:B:722:VAL:HG22	1.11	1.57
1:A:506:GLY:CA	1:A:761:ARG:NH2	1.68	1.57
1:A:121:LEU:HD13	1:A:281:ILE:CG1	1.34	1.55
1:A:86:GLN:HE21	1:A:306:ARG:CB	1.16	1.54
2:B:768:LEU:CB	1:C:519:ASN:HB2	1.38	1.54
1:C:673:PRO:HB3	1:C:703:HIS:CG	1.44	1.51
1:C:53:HIS:CD2	1:C:293:HIS:CG	1.99	1.49
2:B:164:VAL:CG2	2:B:220:LEU:HD12	1.44	1.48
2:B:523:VAL:HG22	2:B:717:ILE:CG1	1.45	1.47
2:B:182:THR:HG22	2:B:190:TRP:CZ3	1.52	1.44
1:A:205:THR:CG2	1:A:238:LEU:HD11	1.44	1.44
2:B:768:LEU:HD23	1:C:519:ASN:CA	1.43	1.44
1:A:578:LEU:CD1	1:A:627:ALA:CB	1.95	1.42
1:C:295:LEU:HD22	1:C:321:PHE:CD1	1.53	1.42
1:A:86:GLN:NE2	1:A:306:ARG:CB	1.84	1.41
2:B:169:PHE:CE2	2:B:224:SER:HB3	1.56	1.40
2:B:403:PRO:HG2	2:B:722:VAL:CG2	1.47	1.39
2:B:64:LEU:HD12	2:B:81:LEU:CD1	1.52	1.39
1:A:578:LEU:CD1	1:A:627:ALA:HA	1.51	1.39
2:B:164:VAL:HG23	2:B:220:LEU:CD1	1.53	1.38
1:C:673:PRO:CB	1:C:703:HIS:CD2	2.05	1.37
2:B:768:LEU:CD2	1:C:519:ASN:HA	1.55	1.37
1:C:477:VAL:HG21	1:C:499:MET:CA	1.53	1.37
1:A:578:LEU:CD1	1:A:627:ALA:CA	2.03	1.37
2:B:403:PRO:CG	2:B:722:VAL:CG2	2.02	1.36
1:A:121:LEU:CD1	1:A:281:ILE:CG1	2.00	1.36
1:C:301:ILE:CG2	1:C:317:THR:CG2	2.02	1.36
1:A:26:ILE:CG2	1:A:61:ASN:HB2	1.55	1.35

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:THR:HG23	1:A:238:LEU:CD1	1.56	1.35
2:B:64:LEU:CD1	2:B:81:LEU:HD21	1.54	1.35
1:C:53:HIS:CD2	1:C:293:HIS:CD2	2.12	1.35
1:A:578:LEU:HD13	1:A:627:ALA:CA	1.58	1.34
1:A:682:VAL:CG2	1:A:729:TRP:CH2	2.09	1.34
3:D:158:GLU:HG2	3:D:381:MET:CB	1.58	1.34
2:B:34:LEU:O	2:B:65:LEU:HG	1.21	1.32
2:B:168:ASN:CB	2:B:227:GLU:OE2	1.76	1.32
1:A:682:VAL:CG2	1:A:729:TRP:CZ3	2.13	1.32
1:C:575:LEU:HB2	1:C:634:TRP:CH2	1.65	1.31
1:C:673:PRO:HB3	1:C:703:HIS:CD2	1.61	1.31
2:B:192:VAL:HG21	2:B:195:TYR:CE2	1.66	1.29
1:C:477:VAL:CG2	1:C:499:MET:HA	1.62	1.29
1:A:709:TYR:OH	1:A:724:LEU:HD11	1.20	1.29
1:A:580:ARG:O	2:B:823:PHE:HE1	1.16	1.29
3:D:605:LEU:HD12	3:D:629:ALA:CB	1.62	1.29
1:A:125:MET:O	1:A:139:ARG:NH1	1.64	1.28
1:A:578:LEU:HD12	1:A:627:ALA:CB	1.56	1.28
2:B:673:VAL:CG2	2:B:718:TYR:HE1	1.47	1.27
2:B:192:VAL:HG21	2:B:195:TYR:CD2	1.68	1.27
2:B:182:THR:CG2	2:B:190:TRP:CZ3	2.17	1.27
1:C:301:ILE:CG2	1:C:317:THR:HG21	1.59	1.27
1:A:630:LEU:CD2	2:B:816:MET:SD	2.20	1.26
2:B:179:ILE:CG2	2:B:195:TYR:OH	1.83	1.26
2:B:397:VAL:HG23	2:B:466:TYR:O	1.13	1.26
1:A:815:PHE:CD2	3:D:554:MET:HG2	1.69	1.25
2:B:179:ILE:HG21	2:B:195:TYR:OH	1.20	1.25
1:C:438:GLY:HA3	1:C:451:GLN:NE2	1.50	1.25
2:B:765:LEU:HD11	1:C:523:GLN:NE2	1.50	1.24
3:D:562:VAL:HG22	3:D:621:SER:CB	1.68	1.24
1:A:568:VAL:O	1:A:571:VAL:HG12	1.35	1.23
2:B:57:PHE:CD2	2:B:292:THR:HG23	1.73	1.23
1:C:245:TYR:O	1:C:382:PRO:HG3	1.35	1.23
1:A:119:ILE:CD1	1:A:288:VAL:HG21	1.68	1.22
3:D:562:VAL:CG2	3:D:621:SER:HB2	1.67	1.22
2:B:64:LEU:HD11	2:B:81:LEU:CD2	1.69	1.22
2:B:519:THR:HG22	2:B:721:ALA:CB	1.70	1.22
2:B:42:GLU:CB	2:B:63:THR:HG21	1.69	1.22
1:A:626:SER:CB	2:B:822:THR:OG1	1.88	1.21
3:D:27:HIS:CB	3:D:28:PRO:CD	2.16	1.21
1:A:682:VAL:HG21	1:A:729:TRP:CZ3	1.71	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:575:LEU:HB2	1:C:634:TRP:CZ3	1.75	1.21
1:A:140:THR:O	1:A:346:ARG:HB2	1.37	1.21
1:A:121:LEU:CD1	1:A:281:ILE:HG12	1.64	1.21
1:A:610:ARG:HB3	1:A:615:SER:CB	1.71	1.20
1:A:822:ILE:HD11	3:D:565:VAL:CG1	1.72	1.20
2:B:194:ASN:CG	2:B:214:ILE:HG13	1.65	1.20
1:A:637:PHE:CD1	2:B:808:VAL:HG13	1.78	1.20
2:B:120:HIS:CE1	2:B:280:ILE:HD11	1.77	1.19
1:A:119:ILE:CD1	1:A:288:VAL:CG2	2.18	1.19
2:B:720:ALA:HB2	2:B:743:ILE:CG2	1.69	1.19
2:B:765:LEU:HD11	1:C:523:GLN:CD	1.67	1.19
1:A:93:SER:HB2	1:A:277:GLU:OE2	1.43	1.19
1:A:247:TRP:CB	1:A:266:ILE:HG13	1.71	1.19
1:C:673:PRO:CB	1:C:703:HIS:CG	2.21	1.19
1:C:633:VAL:HG12	3:D:818:LEU:HD12	1.21	1.18
2:B:752:ALA:O	2:B:753:LEU:HD12	1.42	1.18
1:C:673:PRO:HB2	1:C:703:HIS:CD2	1.77	1.18
1:A:506:GLY:HA2	1:A:761:ARG:NH2	0.87	1.18
1:A:815:PHE:CE2	3:D:554:MET:CG	2.26	1.18
1:A:335:THR:CG2	1:A:346:ARG:HH22	1.55	1.18
2:B:552:MET:CE	2:B:622:TRP:CE3	2.27	1.18
1:A:568:VAL:O	1:A:571:VAL:CG1	1.91	1.17
2:B:57:PHE:HB2	2:B:292:THR:HG21	1.22	1.17
2:B:523:VAL:CG2	2:B:717:ILE:HG12	1.74	1.17
2:B:768:LEU:HB2	1:C:519:ASN:CB	1.75	1.16
2:B:151:LEU:HD23	2:B:190:TRP:CH2	1.79	1.16
1:A:815:PHE:CD2	3:D:554:MET:CG	2.28	1.16
2:B:32:VAL:HG22	2:B:91:VAL:HG22	1.22	1.16
2:B:552:MET:CE	2:B:622:TRP:HE3	1.59	1.16
1:A:709:TYR:OH	1:A:724:LEU:CD1	1.92	1.16
2:B:169:PHE:HB3	2:B:170:PRO:CD	1.74	1.16
1:A:560:LEU:CD1	2:B:802:ILE:HB	1.75	1.15
1:A:578:LEU:CD1	1:A:627:ALA:HB2	1.69	1.15
1:A:580:ARG:O	2:B:823:PHE:CE1	1.96	1.15
2:B:522:SER:O	2:B:717:ILE:HA	1.43	1.15
3:D:332:ARG:O	3:D:335:ILE:HG13	1.45	1.15
2:B:179:ILE:CG2	2:B:195:TYR:HH	1.54	1.15
2:B:64:LEU:CD1	2:B:81:LEU:CD2	2.25	1.15
1:C:633:VAL:HG12	3:D:818:LEU:CD1	1.74	1.15
2:B:169:PHE:CE2	2:B:224:SER:CB	2.30	1.15
1:A:126:SER:OG	1:A:143:PRO:HB2	1.46	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:468:VAL:HG21	2:B:484:MET:HG2	1.22	1.14
2:B:523:VAL:HB	2:B:738:ILE:HD11	1.20	1.14
2:B:630:LEU:O	2:B:634:THR:HG23	1.47	1.14
3:D:561:ILE:O	3:D:565:VAL:HG22	1.44	1.14
1:A:637:PHE:CE1	2:B:808:VAL:HG13	1.81	1.14
2:B:524:MET:HE1	2:B:723:LEU:O	1.47	1.14
2:B:659:GLN:NE2	2:B:686:TYR:OH	1.79	1.14
2:B:468:VAL:HG21	2:B:484:MET:CG	1.77	1.14
2:B:57:PHE:HB2	2:B:292:THR:CG2	1.78	1.14
2:B:114:ILE:HD11	2:B:308:ALA:CB	1.78	1.14
1:A:606:TRP:CE2	3:D:623:ILE:HD11	1.82	1.13
3:D:639:TYR:HE1	3:D:643:LEU:HD11	1.12	1.13
2:B:247:TRP:CE3	2:B:268:LEU:HB3	1.83	1.13
2:B:168:ASN:CB	2:B:227:GLU:CD	2.20	1.13
2:B:247:TRP:HB2	2:B:268:LEU:CB	1.78	1.12
1:C:301:ILE:HG21	1:C:317:THR:HG21	1.29	1.12
3:D:294:ILE:HD11	3:D:344:LEU:CB	1.78	1.12
3:D:542:ALA:HB1	3:D:642:ASN:CB	1.79	1.12
1:A:247:TRP:HB2	1:A:266:ILE:HG13	1.13	1.12
1:A:578:LEU:HD13	1:A:627:ALA:CB	1.63	1.12
1:A:398:LEU:HD11	1:A:470:PHE:CD2	1.84	1.12
1:A:560:LEU:HD11	2:B:802:ILE:HB	1.29	1.12
1:C:53:HIS:CG	1:C:293:HIS:CD2	2.37	1.12
1:A:578:LEU:HD12	1:A:627:ALA:HB1	1.23	1.11
1:A:578:LEU:HD11	1:A:627:ALA:HA	1.32	1.11
1:A:606:TRP:NE1	3:D:623:ILE:CD1	2.11	1.11
2:B:673:VAL:HG22	2:B:718:TYR:HE1	1.13	1.11
1:A:815:PHE:CE2	3:D:554:MET:HG2	1.84	1.11
2:B:541:PHE:O	2:B:545:VAL:N	1.83	1.11
3:D:200:LEU:HD22	3:D:201:ASP:H	1.06	1.11
1:C:354:MET:CE	1:C:361:LEU:CB	2.29	1.10
3:D:158:GLU:CG	3:D:381:MET:CB	2.29	1.10
2:B:495:MET:HE3	2:B:753:LEU:HD11	1.30	1.10
1:A:121:LEU:HD13	1:A:281:ILE:CD1	1.79	1.10
2:B:468:VAL:CG2	2:B:484:MET:HG2	1.80	1.10
1:A:530:PRO:HA	1:A:756:PHE:O	1.48	1.10
1:A:551:SER:OG	1:A:649:LEU:CD1	2.01	1.09
2:B:194:ASN:HB2	2:B:214:ILE:HG21	1.30	1.09
3:D:131:ASP:HA	3:D:349:ASP:OD1	1.52	1.09
1:A:606:TRP:HE1	3:D:623:ILE:HD13	1.06	1.09
1:A:496:TRP:HD1	1:A:500:MET:HB3	1.01	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:551:SER:OG	1:A:649:LEU:HD13	1.48	1.09
1:A:610:ARG:CB	1:A:615:SER:CB	2.31	1.09
2:B:673:VAL:CG2	2:B:718:TYR:CE1	2.36	1.08
2:B:247:TRP:HB2	2:B:268:LEU:HB2	1.16	1.08
1:A:822:ILE:HD11	3:D:565:VAL:HG13	1.35	1.08
2:B:502:ILE:HG23	2:B:512:PHE:CZ	1.89	1.08
3:D:388:TYR:N	3:D:389:PRO:CD	2.16	1.08
2:B:42:GLU:CB	2:B:63:THR:CG2	2.32	1.08
1:A:637:PHE:CD1	2:B:808:VAL:CG1	2.36	1.08
1:A:690:TYR:CD2	1:A:752:PHE:CE2	2.41	1.08
1:C:53:HIS:CD2	1:C:293:HIS:ND1	2.19	1.08
1:C:673:PRO:CG	1:C:703:HIS:HB2	1.82	1.08
1:A:26:ILE:HG21	1:A:61:ASN:HB2	1.24	1.07
1:A:398:LEU:CD1	1:A:470:PHE:CD2	2.36	1.07
2:B:114:ILE:HD11	2:B:308:ALA:HB2	1.32	1.07
2:B:669:ARG:HD2	2:B:696:PHE:CD2	1.89	1.07
1:C:633:VAL:CG1	3:D:818:LEU:HD12	1.83	1.07
3:D:605:LEU:CD1	3:D:629:ALA:HB2	1.84	1.07
2:B:34:LEU:O	2:B:65:LEU:CG	2.02	1.07
2:B:768:LEU:CB	1:C:519:ASN:CB	2.33	1.07
1:A:525:ILE:CA	1:A:762:LYS:HE2	1.85	1.07
1:C:53:HIS:CD2	1:C:293:HIS:CE1	2.42	1.07
1:C:53:HIS:NE2	1:C:293:HIS:CG	2.22	1.07
1:C:575:LEU:CD1	1:C:627:ALA:HB1	1.84	1.07
1:C:673:PRO:HG2	1:C:703:HIS:HB2	1.33	1.07
2:B:151:LEU:HD21	2:B:182:THR:HG21	1.30	1.06
1:A:121:LEU:HD13	1:A:281:ILE:HG13	1.07	1.06
2:B:64:LEU:CD1	2:B:81:LEU:HD11	1.84	1.06
2:B:659:GLN:NE2	2:B:686:TYR:CZ	2.23	1.06
1:A:500:MET:HE1	1:A:521:ARG:HB3	1.12	1.06
1:A:511:ILE:O	1:A:758:ILE:CD1	2.03	1.06
1:A:534:GLN:HG3	1:A:732:ALA:HB2	1.30	1.06
1:A:630:LEU:HD21	2:B:816:MET:HA	1.10	1.06
1:A:132:SER:HB3	2:B:172:TYR:CE2	1.90	1.06
2:B:164:VAL:CG2	2:B:220:LEU:CD1	2.20	1.06
2:B:541:PHE:C	2:B:545:VAL:HB	1.80	1.06
1:C:301:ILE:CG2	1:C:317:THR:HG23	1.86	1.06
5:H:2:NAG:H3	5:H:2:NAG:H83	1.35	1.06
1:C:354:MET:HE1	1:C:361:LEU:CB	1.84	1.05
1:A:575:LEU:HD13	1:A:622:PRO:HB3	1.39	1.05
1:A:496:TRP:CD1	1:A:500:MET:HB3	1.90	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:82:MET:HE2	2:B:114:ILE:HD13	1.39	1.05
2:B:765:LEU:HD21	1:C:523:GLN:HG2	1.07	1.05
1:A:140:THR:O	1:A:346:ARG:CD	2.05	1.05
1:A:633:VAL:CG1	2:B:812:LEU:HD12	1.87	1.05
2:B:801:ASP:O	2:B:805:MET:HG3	1.55	1.04
3:D:58:PRO:HG2	3:D:303:LEU:CD1	1.87	1.04
2:B:519:THR:HG22	2:B:721:ALA:HB2	1.07	1.04
1:C:301:ILE:HG21	1:C:317:THR:CG2	1.79	1.04
1:A:121:LEU:CD1	1:A:281:ILE:CD1	2.34	1.04
1:A:606:TRP:NE1	3:D:623:ILE:HD13	1.71	1.04
1:A:621:ALA:HB1	1:A:622:PRO:HD2	1.37	1.04
1:A:633:VAL:HG12	2:B:812:LEU:CD1	1.86	1.04
2:B:397:VAL:CG2	2:B:466:TYR:O	2.05	1.04
1:A:568:VAL:HG12	1:A:608:SER:HB3	1.37	1.04
1:A:335:THR:CG2	1:A:346:ARG:NH2	2.20	1.04
1:A:132:SER:HB3	2:B:172:TYR:HE2	1.15	1.03
2:B:486:GLY:O	2:B:490:TYR:HD2	1.39	1.03
1:C:697:LEU:O	1:C:699:THR:N	1.89	1.03
1:A:335:THR:HG21	1:A:346:ARG:NH2	1.73	1.03
2:B:720:ALA:HB2	2:B:743:ILE:HG23	1.35	1.03
2:B:768:LEU:HD23	1:C:519:ASN:CB	1.86	1.03
3:D:639:TYR:CE1	3:D:643:LEU:CD1	2.42	1.03
2:B:753:LEU:HD22	2:B:760:LYS:HG2	1.38	1.03
1:C:78:VAL:HA	1:C:82:LEU:HB2	1.40	1.03
1:A:121:LEU:HD11	1:A:281:ILE:HG12	1.32	1.03
1:A:500:MET:HE1	1:A:521:ARG:CB	1.89	1.03
3:D:305:GLU:CB	3:D:333:TYR:HE2	1.71	1.03
3:D:600:TRP:CE3	3:D:613:VAL:CB	2.41	1.03
5:E:2:NAG:H3	5:E:2:NAG:H83	1.37	1.03
3:D:332:ARG:HA	3:D:335:ILE:CD1	1.88	1.02
2:B:40:ILE:HD13	2:B:281:GLU:OE2	1.60	1.02
1:A:26:ILE:HG22	1:A:61:ASN:HB2	1.40	1.02
1:A:815:PHE:CZ	3:D:554:MET:HG3	1.94	1.02
1:C:425:THR:HG22	1:C:431:ILE:HG12	1.38	1.02
1:C:575:LEU:HD11	1:C:627:ALA:HB1	1.02	1.02
3:D:542:ALA:HB1	3:D:642:ASN:HB3	1.06	1.02
1:A:512:VAL:HA	1:A:758:ILE:HD11	1.37	1.02
1:A:574:MET:SD	2:B:816:MET:HE3	2.00	1.01
2:B:618:ILE:O	2:B:621:ILE:HG22	1.60	1.01
1:C:53:HIS:HD2	1:C:293:HIS:ND1	1.53	1.01
1:C:301:ILE:HG22	1:C:317:THR:HG21	1.39	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:27:HIS:CB	3:D:28:PRO:HD2	1.85	1.01
1:A:140:THR:O	1:A:346:ARG:CB	2.08	1.01
1:A:578:LEU:HD13	1:A:627:ALA:HB2	1.29	1.01
2:B:765:LEU:HD21	1:C:523:GLN:CG	1.91	1.01
1:C:575:LEU:CB	1:C:634:TRP:CH2	2.43	1.01
2:B:552:MET:HE2	2:B:622:TRP:CE3	1.94	1.01
2:B:600:VAL:CB	2:B:622:TRP:HZ2	1.72	1.01
3:D:305:GLU:CB	3:D:333:TYR:CE2	2.43	1.01
3:D:332:ARG:HA	3:D:335:ILE:HD11	1.39	1.01
2:B:151:LEU:CD2	2:B:182:THR:HG21	1.89	1.01
1:A:512:VAL:HA	1:A:758:ILE:CD1	1.91	1.00
2:B:169:PHE:HB3	2:B:170:PRO:HD2	1.42	1.00
1:C:295:LEU:CD2	1:C:321:PHE:CD1	2.45	1.00
1:C:438:GLY:HA3	1:C:451:GLN:HE21	1.17	1.00
3:D:27:HIS:CB	3:D:28:PRO:HD3	1.87	1.00
3:D:332:ARG:HA	3:D:335:ILE:CG1	1.91	1.00
3:D:765:TRP:HB3	3:D:769:VAL:HG23	1.43	1.00
1:A:815:PHE:CE2	3:D:554:MET:HG3	1.95	1.00
3:D:58:PRO:HG2	3:D:303:LEU:HD11	1.39	1.00
2:B:120:HIS:CE1	2:B:280:ILE:CD1	2.44	1.00
2:B:169:PHE:HE2	2:B:224:SER:HG	1.02	1.00
2:B:720:ALA:CB	2:B:743:ILE:HG23	1.90	1.00
1:A:574:MET:SD	2:B:816:MET:CE	2.50	1.00
3:D:200:LEU:HD22	3:D:201:ASP:N	1.76	1.00
1:A:119:ILE:HD11	1:A:288:VAL:CG2	1.90	1.00
1:A:810:ASN:CB	3:D:631:PHE:HZ	1.76	0.99
1:C:630:LEU:HD22	3:D:822:MET:HG3	1.42	0.99
1:C:477:VAL:HG21	1:C:499:MET:CB	1.92	0.99
1:C:637:PHE:CG	3:D:818:LEU:HD22	1.98	0.99
2:B:523:VAL:CB	2:B:738:ILE:HD11	1.92	0.99
2:B:49:TRP:O	2:B:53:MET:HB2	1.61	0.99
1:C:673:PRO:HB2	1:C:703:HIS:HD2	1.22	0.99
2:B:64:LEU:HD11	2:B:81:LEU:HD21	1.03	0.99
2:B:167:SER:CB	2:B:223:CYS:SG	2.51	0.99
2:B:753:LEU:HD22	2:B:760:LYS:CG	1.92	0.99
2:B:247:TRP:HE3	2:B:268:LEU:HB3	1.23	0.99
2:B:765:LEU:CD1	1:C:523:GLN:NE2	2.25	0.99
1:C:315:TRP:CE3	1:C:317:THR:O	2.16	0.99
2:B:541:PHE:O	2:B:545:VAL:HB	1.61	0.99
1:A:208:LEU:HD23	1:A:240:MET:SD	2.02	0.98
1:A:121:LEU:CD1	1:A:281:ILE:HD11	1.91	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:720:ALA:CB	2:B:743:ILE:CG2	2.41	0.98
2:B:522:SER:OG	2:B:723:LEU:HD12	1.63	0.98
3:D:639:TYR:CE1	3:D:643:LEU:HD11	1.96	0.98
2:B:474:GLY:HA2	2:B:482:ASN:O	1.64	0.98
2:B:673:VAL:HG22	2:B:718:TYR:CE1	1.95	0.98
1:A:498:GLY:O	1:A:502:GLU:HG2	1.61	0.98
1:A:532:LYS:O	1:A:755:GLY:HA2	1.64	0.98
1:A:621:ALA:HB1	1:A:622:PRO:CD	1.92	0.98
2:B:57:PHE:CG	2:B:292:THR:HG23	1.97	0.98
1:C:628:ARG:O	1:C:632:MET:N	1.96	0.98
2:B:74:ILE:HG21	2:B:105:LEU:HD21	1.44	0.98
2:B:154:MET:CE	2:B:248:ILE:HD11	1.92	0.98
1:A:408:PHE:HD2	1:A:514:PRO:HB3	1.29	0.97
1:A:500:MET:CE	1:A:521:ARG:HB3	1.94	0.97
1:A:122:THR:CG2	1:A:277:GLU:HG3	1.95	0.97
1:A:607:PHE:HA	1:A:610:ARG:CD	1.94	0.97
1:A:140:THR:O	1:A:346:ARG:HD3	1.62	0.97
1:A:291:ALA:HB2	1:A:325:LEU:HD13	1.44	0.97
1:C:575:LEU:HD11	1:C:627:ALA:CB	1.96	0.96
1:A:647:ALA:O	2:B:641:MET:SD	2.23	0.96
1:A:738:ALA:O	1:A:742:CYS:SG	2.23	0.96
2:B:520:GLY:O	2:B:743:ILE:HG21	1.65	0.96
1:C:627:ALA:O	1:C:631:GLY:N	1.96	0.96
2:B:520:GLY:HA3	2:B:743:ILE:HG13	1.45	0.96
2:B:53:MET:HE2	2:B:53:MET:HA	1.46	0.96
1:A:119:ILE:HD13	1:A:288:VAL:CG2	1.91	0.96
2:B:673:VAL:HG21	2:B:718:TYR:CE1	1.99	0.96
2:B:57:PHE:CB	2:B:292:THR:CG2	2.44	0.96
1:C:245:TYR:O	1:C:382:PRO:CG	2.14	0.95
2:B:82:MET:CE	2:B:114:ILE:HD13	1.95	0.95
3:D:555:MET:SD	3:D:628:TRP:CZ2	2.59	0.95
1:C:391:GLY:O	1:C:392:TYR:HB2	1.63	0.95
1:A:607:PHE:O	1:A:610:ARG:CG	2.14	0.95
1:A:26:ILE:CG2	1:A:61:ASN:CB	2.43	0.95
1:C:194:VAL:O	1:C:195:LEU:HD23	1.65	0.95
1:C:568:VAL:CG1	1:C:608:SER:OG	2.15	0.95
1:A:560:LEU:HD12	2:B:802:ILE:CB	1.96	0.95
1:A:606:TRP:HE1	3:D:623:ILE:CD1	1.76	0.95
2:B:194:ASN:OD1	2:B:214:ILE:HG13	1.66	0.95
1:C:640:ILE:HG21	3:D:811:MET:HE1	1.45	0.95
2:B:523:VAL:CG2	2:B:717:ILE:CG1	2.40	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:ILE:HG22	1:A:61:ASN:CB	1.97	0.95
2:B:123:SER:O	2:B:139:PHE:CB	2.14	0.95
2:B:194:ASN:CB	2:B:214:ILE:HG13	1.97	0.95
1:C:630:LEU:CD2	3:D:822:MET:HG3	1.96	0.94
1:A:668:PRO:HG3	2:B:785:THR:CG2	1.98	0.94
1:A:811:MET:HE2	3:D:631:PHE:HD2	1.33	0.94
3:D:345:SER:O	3:D:353:MET:N	1.99	0.94
3:D:605:LEU:HG	3:D:625:VAL:CG1	1.98	0.94
1:A:464:LEU:O	1:A:468:MET:N	1.98	0.94
1:A:811:MET:HB2	3:D:635:PHE:CZ	2.00	0.94
1:A:811:MET:HE1	3:D:631:PHE:HB3	1.46	0.94
2:B:673:VAL:HG21	2:B:718:TYR:HE1	1.28	0.94
1:C:53:HIS:CG	1:C:293:HIS:NE2	2.36	0.94
1:A:574:MET:HE3	2:B:820:LEU:CD2	1.97	0.94
1:A:606:TRP:CZ2	3:D:623:ILE:HD11	2.02	0.94
1:C:673:PRO:CB	1:C:703:HIS:CB	2.45	0.94
2:B:151:LEU:HD23	2:B:190:TRP:HH2	1.22	0.94
2:B:514:VAL:N	2:B:515:PRO:HD2	1.82	0.94
2:B:552:MET:HE3	2:B:622:TRP:CE3	2.03	0.94
1:C:575:LEU:CB	1:C:634:TRP:CZ3	2.51	0.94
1:A:283:ASP:OD2	1:A:335:THR:N	2.00	0.94
1:A:503:LEU:HD11	1:A:761:ARG:N	1.82	0.94
1:A:525:ILE:HA	1:A:762:LYS:HE2	1.47	0.94
3:D:605:LEU:HG	3:D:625:VAL:HG12	1.48	0.94
1:A:811:MET:N	3:D:631:PHE:CE2	2.36	0.93
2:B:64:LEU:HD12	2:B:81:LEU:HD11	0.96	0.93
1:A:678:ILE:HG22	1:A:724:LEU:HD22	1.51	0.93
2:B:57:PHE:CB	2:B:292:THR:HG23	1.97	0.93
1:A:610:ARG:O	1:A:614:ASN:N	2.00	0.93
2:B:669:ARG:HD2	2:B:696:PHE:CG	2.04	0.93
2:B:486:GLY:O	2:B:490:TYR:CD2	2.21	0.93
2:B:765:LEU:CD2	1:C:523:GLN:HG2	1.96	0.93
2:B:140:GLY:C	2:B:345:ASP:HB3	1.93	0.93
1:C:574:MET:HG3	3:D:822:MET:HE1	1.48	0.93
2:B:669:ARG:CD	2:B:696:PHE:CD2	2.52	0.93
2:B:768:LEU:CD2	1:C:519:ASN:CA	2.29	0.93
1:C:673:PRO:CG	1:C:703:HIS:CB	2.47	0.93
2:B:198:LEU:HB2	2:B:207:THR:CG2	2.00	0.92
3:D:605:LEU:HD12	3:D:629:ALA:HB2	0.95	0.92
1:C:53:HIS:CD2	1:C:293:HIS:NE2	2.38	0.92
3:D:158:GLU:CD	3:D:381:MET:CB	2.42	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:VAL:HG13	1:A:88:TYR:CD1	2.05	0.92
1:A:606:TRP:CE2	3:D:623:ILE:CD1	2.50	0.92
3:D:284:LEU:N	3:D:285:PRO:CD	2.31	0.92
2:B:592:ALA:O	2:B:596:LEU:CB	2.18	0.92
1:A:119:ILE:HD11	1:A:288:VAL:HG22	1.48	0.91
1:A:552:PHE:O	1:A:555:PRO:HD2	1.71	0.91
2:B:523:VAL:HB	2:B:738:ILE:CD1	2.00	0.91
2:B:801:ASP:O	2:B:805:MET:CG	2.18	0.91
1:C:574:MET:HG3	3:D:822:MET:CE	2.00	0.91
1:A:245:TYR:O	1:A:382:PRO:HG3	1.70	0.91
1:A:822:ILE:CD1	3:D:565:VAL:HG11	2.01	0.91
1:A:682:VAL:HG21	1:A:729:TRP:CZ2	2.04	0.91
2:B:765:LEU:HD11	1:C:523:GLN:CG	2.01	0.91
1:A:607:PHE:O	1:A:610:ARG:HG2	1.71	0.91
1:C:277:GLU:O	1:C:281:ILE:HG13	1.70	0.91
1:C:477:VAL:HG21	1:C:499:MET:HA	0.91	0.91
1:A:630:LEU:CD2	2:B:816:MET:HA	2.01	0.90
2:B:631:ALA:CB	1:C:649:LEU:HG	2.01	0.90
1:A:511:ILE:O	1:A:758:ILE:HD11	1.69	0.90
2:B:241:MET:HA	2:B:247:TRP:CZ2	2.05	0.90
2:B:403:PRO:HG2	2:B:722:VAL:HG22	0.98	0.90
1:C:301:ILE:HG22	1:C:317:THR:CG2	1.97	0.90
1:C:565:GLY:O	1:C:569:HIS:CE1	2.25	0.90
1:C:630:LEU:HD13	1:C:634:TRP:CH2	2.06	0.90
2:B:198:LEU:HB2	2:B:207:THR:HG21	1.52	0.90
2:B:403:PRO:HG3	2:B:722:VAL:CG2	1.82	0.90
2:B:768:LEU:HB3	1:C:519:ASN:HB2	1.53	0.90
1:A:205:THR:HG23	1:A:238:LEU:HD11	0.91	0.90
1:A:506:GLY:HA3	1:A:761:ARG:NH2	1.85	0.90
2:B:403:PRO:HG3	2:B:722:VAL:HG22	0.91	0.90
1:A:208:LEU:HB3	1:A:240:MET:HE3	1.51	0.90
2:B:192:VAL:CG2	2:B:195:TYR:CD2	2.55	0.90
2:B:584:GLY:O	2:B:587:PHE:HD1	1.55	0.89
1:C:568:VAL:HG11	1:C:608:SER:OG	1.73	0.89
1:A:662:ILE:CB	1:A:747:THR:CB	2.51	0.89
2:B:600:VAL:CB	2:B:622:TRP:CZ2	2.55	0.89
1:C:534:GLN:OE1	1:C:730:ASP:HB3	1.73	0.89
5:J:2:NAG:H3	5:J:2:NAG:H83	1.55	0.89
2:B:57:PHE:HD2	2:B:292:THR:HG23	1.35	0.89
1:C:425:THR:CG2	1:C:431:ILE:HG12	2.03	0.89
1:A:633:VAL:HG12	2:B:812:LEU:HD12	1.49	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:ASN:CB	1:A:793:TYR:OH	2.21	0.89
1:A:682:VAL:HG23	1:A:729:TRP:CZ3	2.07	0.89
2:B:194:ASN:HD21	2:B:211:LEU:HD23	1.38	0.89
3:D:388:TYR:N	3:D:389:PRO:HD3	1.87	0.89
1:C:301:ILE:HG23	1:C:317:THR:HG23	1.55	0.89
2:B:382:TRP:CE3	2:B:383:PRO:HD2	2.08	0.89
1:A:408:PHE:CD2	1:A:514:PRO:HB3	2.08	0.88
2:B:403:PRO:HG2	2:B:722:VAL:HG21	1.53	0.88
2:B:502:ILE:HG23	2:B:512:PHE:CE1	2.08	0.88
1:A:822:ILE:CD1	3:D:565:VAL:CG1	2.51	0.88
2:B:631:ALA:HA	1:C:649:LEU:HD11	1.56	0.88
2:B:169:PHE:HE2	2:B:224:SER:CB	1.76	0.88
1:A:560:LEU:CD1	2:B:802:ILE:CB	2.50	0.88
2:B:408:GLU:HG2	2:B:445:LYS:NZ	1.88	0.88
1:C:315:TRP:CE2	1:C:317:THR:HB	2.08	0.88
1:C:634:TRP:O	1:C:637:PHE:CD2	2.27	0.88
2:B:168:ASN:CB	2:B:227:GLU:OE1	2.20	0.88
1:A:668:PRO:HB3	2:B:785:THR:HG23	1.55	0.88
3:D:430:ARG:O	3:D:472:TYR:HB2	1.74	0.87
2:B:194:ASN:HD21	2:B:211:LEU:CD2	1.87	0.87
1:A:574:MET:SD	1:A:630:LEU:HD11	2.14	0.87
1:C:673:PRO:CB	1:C:703:HIS:HB2	2.05	0.87
3:D:505:SER:O	3:D:755:TYR:CE1	2.28	0.87
1:A:822:ILE:HD11	3:D:565:VAL:HG11	1.53	0.87
1:C:53:HIS:HB3	1:C:293:HIS:NE2	1.88	0.87
3:D:639:TYR:CE1	3:D:643:LEU:HD12	2.09	0.87
2:B:192:VAL:CG2	2:B:195:TYR:CE2	2.56	0.87
1:C:53:HIS:NE2	1:C:293:HIS:CB	2.38	0.87
1:C:640:ILE:CG2	3:D:811:MET:HE1	2.04	0.87
1:A:335:THR:HG21	1:A:346:ARG:HH22	1.30	0.87
1:A:525:ILE:N	1:A:762:LYS:HE2	1.89	0.87
1:A:630:LEU:HD21	2:B:816:MET:CA	2.01	0.87
3:D:321:GLU:O	3:D:324:VAL:HG12	1.75	0.87
1:A:811:MET:HE2	3:D:631:PHE:CD2	2.08	0.87
1:A:815:PHE:CE1	3:D:554:MET:HG3	2.09	0.87
2:B:541:PHE:O	2:B:545:VAL:CB	2.22	0.86
1:C:673:PRO:HB3	1:C:703:HIS:CB	2.03	0.86
1:A:131:LYS:NZ	1:A:343:ASP:HA	1.91	0.86
1:A:557:GLN:OE1	2:B:798:SER:OG	1.93	0.86
2:B:182:THR:CG2	2:B:190:TRP:CH2	2.58	0.86
2:B:240:LEU:HA	2:B:245:PHE:HD2	1.40	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:388:TYR:H	3:D:389:PRO:HD3	1.40	0.86
2:B:120:HIS:HB2	2:B:280:ILE:HG23	1.57	0.86
2:B:631:ALA:HB1	1:C:649:LEU:HG	1.55	0.86
1:A:609:TRP:CE3	1:A:612:LEU:CD1	2.58	0.86
1:A:811:MET:CE	3:D:631:PHE:HD2	1.88	0.86
1:A:335:THR:HG23	1:A:346:ARG:HH22	1.38	0.86
1:C:778:HIS:CE1	1:C:783:MET:HG2	2.11	0.86
3:D:297:THR:HG21	3:D:338:THR:O	1.76	0.86
3:D:388:TYR:H	3:D:389:PRO:CD	1.89	0.86
4:G:335:UNK:O	4:G:362:UNK:CB	2.23	0.86
1:A:811:MET:N	3:D:631:PHE:HE2	1.74	0.86
1:C:53:HIS:HD2	1:C:293:HIS:CE1	1.85	0.86
2:B:665:SER:N	2:B:666:PRO:HD2	1.90	0.86
1:A:93:SER:HB2	1:A:277:GLU:CD	2.01	0.86
2:B:169:PHE:HE2	2:B:224:SER:OG	1.56	0.86
5:I:2:NAG:H83	5:I:2:NAG:H3	1.57	0.86
2:B:247:TRP:CB	2:B:268:LEU:HB2	2.02	0.85
1:A:607:PHE:HA	1:A:610:ARG:HD3	1.58	0.85
2:B:398:THR:HG22	2:B:497:VAL:HB	1.59	0.85
3:D:559:LEU:HD21	3:D:598:ALA:HB1	1.58	0.85
2:B:398:THR:HA	2:B:497:VAL:O	1.77	0.85
1:C:283:ASP:OD2	1:C:335:THR:HG22	1.77	0.85
2:B:154:MET:HE1	2:B:248:ILE:HD11	1.56	0.85
1:C:634:TRP:HD1	3:D:818:LEU:HD11	1.40	0.85
1:A:157:LEU:HD22	1:A:372:ILE:HD11	1.59	0.85
2:B:64:LEU:CD1	2:B:81:LEU:CD1	2.47	0.85
1:C:283:ASP:OD2	1:C:335:THR:N	2.08	0.85
1:C:301:ILE:HG23	1:C:317:THR:CG2	2.03	0.85
3:D:283:ASP:C	3:D:285:PRO:HD2	2.02	0.85
1:C:575:LEU:CA	1:C:634:TRP:HH2	1.90	0.84
3:D:294:ILE:HG23	3:D:337:VAL:CB	2.07	0.84
3:D:765:TRP:HB3	3:D:769:VAL:CG2	2.05	0.84
2:B:140:GLY:O	2:B:345:ASP:CB	2.24	0.84
2:B:541:PHE:O	2:B:545:VAL:CA	2.25	0.84
1:C:315:TRP:CD2	1:C:317:THR:O	2.30	0.84
1:A:34:SER:HB2	1:A:96:PRO:CG	2.07	0.84
1:A:122:THR:HG21	1:A:277:GLU:HG3	1.60	0.84
1:A:818:VAL:HG13	3:D:558:MET:HE1	1.59	0.84
2:B:552:MET:CE	2:B:622:TRP:CZ3	2.61	0.84
1:C:295:LEU:HD22	1:C:321:PHE:HD1	1.01	0.84
2:B:522:SER:O	2:B:717:ILE:CA	2.24	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:634:THR:OG1	1:C:649:LEU:HD21	1.77	0.84
3:D:58:PRO:CG	3:D:303:LEU:CD1	2.56	0.84
1:A:647:ALA:HB1	2:B:641:MET:HE3	1.56	0.84
2:B:765:LEU:HD13	1:C:519:ASN:OD1	1.76	0.84
1:A:532:LYS:HE2	1:A:787:ASP:OD2	1.78	0.84
3:D:600:TRP:HE3	3:D:613:VAL:CB	1.86	0.84
1:A:633:VAL:HG21	2:B:815:ALA:CB	2.08	0.84
1:A:690:TYR:CD2	1:A:752:PHE:CZ	2.66	0.84
2:B:32:VAL:HG22	2:B:91:VAL:CG2	2.08	0.84
2:B:114:ILE:CD1	2:B:308:ALA:HB2	2.07	0.83
2:B:154:MET:HA	2:B:158:ASP:CB	2.07	0.83
2:B:791:GLU:O	2:B:792:LYS:C	2.16	0.83
1:A:575:LEU:CD1	1:A:622:PRO:HB3	2.07	0.83
1:A:633:VAL:HG11	2:B:812:LEU:HD12	1.59	0.83
2:B:552:MET:HE2	2:B:622:TRP:CZ3	2.14	0.83
2:B:758:ARG:O	2:B:762:PRO:HD2	1.78	0.83
3:D:639:TYR:HE1	3:D:643:LEU:CD1	1.80	0.83
2:B:268:LEU:HD13	2:B:268:LEU:O	1.78	0.83
1:C:634:TRP:CD1	3:D:818:LEU:HD11	2.13	0.83
2:B:182:THR:HG22	2:B:190:TRP:CE3	2.11	0.83
1:A:105:THR:HA	1:A:128:TYR:HE2	1.44	0.83
2:B:768:LEU:HB2	1:C:519:ASN:HB2	0.84	0.83
1:C:627:ALA:O	1:C:630:LEU:HB2	1.79	0.83
1:C:678:ILE:H	1:C:725:HIS:HD2	1.23	0.83
1:A:263:PRO:O	1:A:356:LEU:HD12	1.78	0.83
1:A:512:VAL:CA	1:A:758:ILE:HD11	2.09	0.83
1:A:810:ASN:HB2	3:D:631:PHE:HZ	1.41	0.83
2:B:520:GLY:O	2:B:743:ILE:CG2	2.27	0.83
1:C:606:TRP:CZ3	1:C:609:TRP:HE3	1.95	0.83
2:B:397:VAL:HG23	2:B:466:TYR:C	2.02	0.82
2:B:458:THR:HG21	2:B:766:ALA:HB1	1.59	0.82
2:B:520:GLY:C	2:B:743:ILE:HG21	2.04	0.82
2:B:768:LEU:CD2	1:C:519:ASN:CB	2.55	0.82
1:C:315:TRP:CZ2	1:C:317:THR:HB	2.14	0.82
2:B:151:LEU:CD2	2:B:190:TRP:CH2	2.61	0.82
2:B:154:MET:CE	2:B:218:VAL:HG11	2.08	0.82
2:B:522:SER:HB3	2:B:743:ILE:HG22	1.59	0.82
1:C:694:GLN:HB2	1:C:697:LEU:HD12	1.60	0.82
1:A:560:LEU:HD12	2:B:802:ILE:CG2	2.09	0.82
1:C:425:THR:HG22	1:C:431:ILE:CG1	2.09	0.82
1:A:560:LEU:HD12	2:B:802:ILE:HB	1.57	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:810:ASN:HB3	3:D:631:PHE:HZ	1.44	0.82
2:B:130:LYS:CB	2:B:137:PHE:CZ	2.62	0.82
1:A:626:SER:CB	2:B:822:THR:CB	2.57	0.82
1:A:530:PRO:CA	1:A:756:PHE:O	2.27	0.82
1:A:690:TYR:CE2	1:A:752:PHE:CD1	2.68	0.82
1:A:381:TRP:HB3	1:A:382:PRO:HD2	1.62	0.82
2:B:495:MET:HE3	2:B:753:LEU:CD1	2.08	0.82
3:D:294:ILE:CD1	3:D:344:LEU:CB	2.57	0.82
1:A:247:TRP:HB3	1:A:266:ILE:HG13	1.62	0.82
1:A:119:ILE:HD12	1:A:288:VAL:HG21	1.60	0.81
1:C:481:LYS:HB2	1:C:498:GLY:HA3	1.61	0.81
1:A:602:SER:HB3	1:A:606:TRP:CZ3	2.15	0.81
1:A:682:VAL:HG21	1:A:729:TRP:HH2	1.35	0.81
3:D:343:ASP:OD2	3:D:354:HIS:CB	2.28	0.81
1:A:678:ILE:CG2	1:A:724:LEU:HD22	2.09	0.81
2:B:424:CYS:HB2	2:B:442:LYS:O	1.80	0.81
1:C:674:SER:HB3	1:C:677:PHE:HB3	1.62	0.81
2:B:568:SER:O	2:B:570:VAL:N	2.13	0.81
1:A:811:MET:CA	3:D:631:PHE:CE2	2.63	0.81
3:D:594:THR:HG23	3:D:598:ALA:HB2	1.63	0.81
1:A:102:LEU:O	1:A:128:TYR:OH	1.98	0.81
1:A:633:VAL:HG21	2:B:815:ALA:HB1	1.61	0.81
1:C:576:TYR:HE2	1:C:604:ALA:HB2	1.45	0.81
1:A:815:PHE:CD2	3:D:554:MET:HG3	2.11	0.80
2:B:559:MET:HG3	2:B:563:ILE:HD11	1.62	0.80
1:A:547:SER:CB	1:A:550:ASP:HB2	2.12	0.80
1:C:782:PHE:CE2	1:C:786:LEU:HD11	2.16	0.80
3:D:338:THR:HG22	3:D:343:ASP:HA	1.62	0.80
2:B:768:LEU:HD23	1:C:519:ASN:HA	0.82	0.80
1:C:298:MET:SD	1:C:320:LEU:HD21	2.21	0.80
2:B:752:ALA:C	2:B:753:LEU:HD12	2.05	0.80
2:B:192:VAL:HG21	2:B:195:TYR:HE2	1.46	0.80
1:C:217:ARG:CB	1:C:392:TYR:N	2.44	0.80
1:A:530:PRO:HB3	1:A:755:GLY:O	1.80	0.80
1:A:729:TRP:HD1	1:A:730:ASP:H	1.29	0.80
2:B:523:VAL:HG22	2:B:717:ILE:HG12	0.81	0.80
3:D:325:TYR:CD1	3:D:326:GLU:N	2.50	0.80
3:D:332:ARG:HA	3:D:335:ILE:HG12	1.61	0.80
2:B:631:ALA:HA	1:C:649:LEU:CD1	2.11	0.80
1:C:639:MET:HE3	1:C:639:MET:HA	1.62	0.80
3:D:562:VAL:HA	3:D:565:VAL:CG2	2.12	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:169:PHE:HB3	2:B:170:PRO:HD3	1.59	0.80
2:B:540:PRO:HB2	1:C:803:PRO:HG2	1.62	0.80
3:D:284:LEU:N	3:D:285:PRO:HD2	1.95	0.80
1:A:124:ARG:O	1:A:143:PRO:HA	1.82	0.79
2:B:194:ASN:OD1	2:B:214:ILE:CG1	2.30	0.79
2:B:514:VAL:HG22	2:B:767:LEU:HD13	1.62	0.79
2:B:541:PHE:HB3	2:B:545:VAL:CB	2.12	0.79
1:A:698:SER:HA	2:B:419:ARG:HH21	1.46	0.79
1:A:818:VAL:HG21	3:D:558:MET:SD	2.22	0.79
2:B:140:GLY:C	2:B:345:ASP:CB	2.55	0.79
2:B:162:PHE:CD2	2:B:219:ILE:HG12	2.16	0.79
2:B:240:LEU:HA	2:B:245:PHE:CD2	2.16	0.79
1:C:391:GLY:O	1:C:392:TYR:CB	2.30	0.79
3:D:500:TYR:HE2	3:D:765:TRP:CD1	1.99	0.79
1:C:503:LEU:HD12	1:C:508:ALA:O	1.81	0.79
1:A:607:PHE:C	1:A:610:ARG:HG2	2.07	0.79
1:A:398:LEU:CD1	1:A:470:PHE:HD2	1.87	0.79
1:A:574:MET:SD	2:B:816:MET:HE1	2.22	0.79
1:A:574:MET:HE3	2:B:820:LEU:HD21	1.64	0.79
1:A:607:PHE:O	1:A:610:ARG:HG3	1.81	0.79
1:C:485:GLN:HA	1:C:495:ALA:HA	1.62	0.79
1:A:552:PHE:CD1	1:A:553:MET:N	2.51	0.79
1:A:811:MET:HB2	3:D:635:PHE:HZ	1.45	0.79
1:A:690:TYR:HD2	1:A:752:PHE:CE2	2.00	0.79
1:A:810:ASN:CB	3:D:631:PHE:CZ	2.64	0.79
2:B:559:MET:O	2:B:563:ILE:HD12	1.82	0.79
2:B:114:ILE:HD11	2:B:308:ALA:HB1	1.61	0.78
1:C:630:LEU:HD13	1:C:634:TRP:CZ2	2.18	0.78
3:D:202:MET:HA	3:D:207:ILE:CB	2.13	0.78
2:B:768:LEU:CG	1:C:519:ASN:HB2	2.13	0.78
1:A:698:SER:CB	2:B:419:ARG:HE	1.95	0.78
1:A:810:ASN:HB3	3:D:631:PHE:CZ	2.18	0.78
2:B:157:TYR:OH	2:B:246:VAL:HG21	1.83	0.78
1:A:560:LEU:HD12	2:B:802:ILE:HG22	1.65	0.78
1:A:609:TRP:HE3	1:A:612:LEU:HD12	1.49	0.78
1:A:568:VAL:CG1	1:A:608:SER:HB3	2.13	0.78
1:C:291:ALA:CB	1:C:325:LEU:HD13	2.13	0.78
1:A:811:MET:CE	3:D:631:PHE:HB3	2.14	0.78
2:B:136:PHE:O	2:B:137:PHE:CG	2.36	0.78
2:B:140:GLY:O	2:B:345:ASP:HB3	1.84	0.78
2:B:157:TYR:OH	2:B:246:VAL:HG11	1.82	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:298:MET:SD	2:B:326:LEU:O	2.42	0.78
2:B:169:PHE:CD2	2:B:224:SER:HB3	2.19	0.78
1:C:287:VAL:HG21	1:C:338:ILE:HD13	1.65	0.78
1:C:397:ARG:HA	1:C:471:THR:OG1	1.84	0.78
1:A:496:TRP:CD1	1:A:500:MET:SD	2.77	0.78
2:B:801:ASP:O	2:B:805:MET:SD	2.41	0.78
2:B:194:ASN:HB2	2:B:214:ILE:CG2	2.10	0.77
1:C:575:LEU:HB2	1:C:634:TRP:HH2	1.46	0.77
1:C:637:PHE:CB	3:D:818:LEU:HD22	2.13	0.77
3:D:600:TRP:CZ3	3:D:613:VAL:CB	2.67	0.77
1:A:525:ILE:C	1:A:762:LYS:NZ	2.43	0.77
1:A:818:VAL:CG1	3:D:558:MET:HE1	2.14	0.77
1:A:690:TYR:CD2	1:A:752:PHE:CD2	2.72	0.77
2:B:399:LEU:HD13	2:B:473:HIS:CE1	2.18	0.77
2:B:468:VAL:HG21	2:B:484:MET:HG3	1.64	0.77
2:B:765:LEU:HD11	1:C:523:GLN:HE21	1.47	0.77
2:B:502:ILE:CG2	2:B:512:PHE:CE1	2.68	0.77
1:C:128:TYR:HB3	1:C:137:PHE:CD2	2.20	0.77
3:D:49:HIS:O	3:D:53:ASP:N	2.17	0.77
1:A:117:PRO:HG2	1:A:321:PHE:CD2	2.19	0.77
1:A:53:HIS:O	1:A:54:PHE:C	2.27	0.77
2:B:241:MET:HA	2:B:247:TRP:HZ2	1.49	0.77
1:C:634:TRP:HE1	3:D:822:MET:HB2	1.49	0.77
3:D:542:ALA:CB	3:D:642:ASN:HB3	2.02	0.77
1:A:637:PHE:HZ	2:B:811:MET:HB3	1.50	0.77
2:B:519:THR:CG2	2:B:721:ALA:HB2	2.03	0.77
3:D:545:GLU:N	3:D:546:PRO:HD2	1.98	0.77
1:A:34:SER:HB2	1:A:96:PRO:HG3	1.67	0.76
1:C:627:ALA:HA	1:C:630:LEU:HB2	1.66	0.76
3:D:152:MET:HE2	3:D:224:LEU:HD22	1.66	0.76
2:B:197:THR:O	2:B:198:LEU:HD12	1.85	0.76
2:B:520:GLY:HA3	2:B:743:ILE:CG1	2.14	0.76
2:B:541:PHE:CA	2:B:545:VAL:HB	2.14	0.76
1:C:634:TRP:O	1:C:637:PHE:HD2	1.65	0.76
3:D:566:ALA:O	3:D:570:PHE:CB	2.33	0.76
1:A:525:ILE:C	1:A:762:LYS:HZ3	1.92	0.76
2:B:169:PHE:CB	2:B:170:PRO:CD	2.57	0.76
2:B:240:LEU:O	2:B:245:PHE:HB2	1.85	0.76
1:A:335:THR:HG23	1:A:346:ARG:NH2	1.93	0.76
2:B:64:LEU:HD12	2:B:81:LEU:CG	2.15	0.76
1:C:53:HIS:CB	1:C:293:HIS:NE2	2.48	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:560:LEU:O	3:D:560:LEU:HD22	1.85	0.76
1:A:554:GLN:HA	2:B:798:SER:C	2.10	0.76
1:C:93:SER:HB3	1:C:121:LEU:HD12	1.67	0.76
1:A:46:VAL:O	1:A:49:ALA:HB3	1.86	0.76
1:A:698:SER:HB3	2:B:419:ARG:HE	1.49	0.76
1:C:394:MET:SD	1:C:766:TRP:NE1	2.59	0.76
1:A:668:PRO:CB	2:B:785:THR:HG23	2.15	0.76
3:D:555:MET:SD	3:D:628:TRP:CE2	2.79	0.76
5:I:2:NAG:H3	5:I:2:NAG:C8	2.16	0.76
2:B:182:THR:CG2	2:B:190:TRP:HZ3	1.95	0.76
3:D:343:ASP:OD2	3:D:354:HIS:HB3	1.86	0.76
2:B:502:ILE:HG12	2:B:512:PHE:CZ	2.21	0.75
2:B:520:GLY:C	2:B:743:ILE:CG2	2.58	0.75
2:B:74:ILE:CG2	2:B:105:LEU:HD21	2.16	0.75
2:B:120:HIS:ND1	2:B:280:ILE:HG12	2.01	0.75
2:B:669:ARG:NH2	2:B:712:LYS:O	2.20	0.75
1:A:115:ARG:HB2	1:A:315:TRP:HB3	1.69	0.75
1:A:247:TRP:HB2	1:A:266:ILE:CG1	2.07	0.75
2:B:402:ALA:HB3	2:B:403:PRO:HD3	1.69	0.75
1:C:425:THR:CG2	1:C:431:ILE:CG1	2.63	0.75
3:D:305:GLU:C	3:D:306:HIS:HD2	1.94	0.75
1:A:621:ALA:CB	1:A:622:PRO:CD	2.59	0.75
1:A:671:ARG:HH11	2:B:782:LEU:HD12	1.51	0.75
1:C:637:PHE:CE1	1:C:641:ILE:HD12	2.21	0.75
3:D:172:PRO:O	3:D:226:TYR:OH	2.02	0.75
1:A:671:ARG:NH1	2:B:782:LEU:HD12	2.02	0.75
3:D:605:LEU:CD1	3:D:629:ALA:CB	2.54	0.75
2:B:82:MET:O	2:B:85:THR:O	2.04	0.75
1:A:510:MET:HG3	1:A:760:MET:CG	2.17	0.75
2:B:408:GLU:HG2	2:B:445:LYS:CE	2.16	0.75
1:C:354:MET:HE3	1:C:361:LEU:CB	2.14	0.75
1:A:690:TYR:CE2	1:A:752:PHE:CG	2.75	0.74
1:A:698:SER:CA	2:B:419:ARG:HH21	2.00	0.74
1:A:552:PHE:O	1:A:555:PRO:CD	2.35	0.74
2:B:25:PHE:CB	2:B:26:PRO:CD	2.66	0.74
2:B:53:MET:HA	2:B:53:MET:CE	2.09	0.74
2:B:524:MET:HG2	2:B:735:LEU:HB3	1.67	0.74
1:A:616:GLY:HA2	2:B:606:PRO:HG3	1.70	0.74
2:B:140:GLY:O	2:B:345:ASP:HB2	1.86	0.74
2:B:519:THR:CG2	2:B:721:ALA:CB	2.59	0.74
3:D:332:ARG:CA	3:D:335:ILE:CG1	2.66	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:435:PRO:HD2	3:D:441:GLU:HA	1.69	0.74
1:A:94:HIS:H	1:A:122:THR:HG1	1.31	0.74
1:A:815:PHE:CG	3:D:554:MET:CG	2.71	0.74
3:D:531:VAL:HG12	3:D:721:ALA:HA	1.69	0.74
1:A:524:TYR:C	1:A:762:LYS:HE2	2.12	0.74
2:B:120:HIS:CD2	2:B:280:ILE:HD13	2.22	0.74
2:B:154:MET:CE	2:B:248:ILE:CD1	2.65	0.74
3:D:161:TRP:HB3	3:D:222:VAL:HG21	1.69	0.74
3:D:200:LEU:CD2	3:D:201:ASP:H	1.96	0.74
3:D:600:TRP:O	3:D:604:GLY:N	2.20	0.74
3:D:559:LEU:HD23	3:D:559:LEU:O	1.88	0.74
1:A:610:ARG:HB2	1:A:615:SER:CB	2.17	0.74
1:A:690:TYR:HD2	1:A:752:PHE:CZ	2.04	0.74
1:C:298:MET:SD	1:C:320:LEU:HD11	2.28	0.74
1:A:211:ALA:HB3	1:A:240:MET:HE1	1.70	0.74
2:B:162:PHE:HD1	2:B:216:SER:H	1.34	0.74
2:B:164:VAL:HG21	2:B:179:ILE:CD1	2.17	0.74
2:B:485:ILE:HD11	2:B:506:ARG:HE	1.52	0.74
1:A:538:ILE:HG23	1:A:727:PHE:O	1.88	0.73
1:A:811:MET:HB2	3:D:631:PHE:CE2	2.22	0.73
2:B:40:ILE:CD1	2:B:281:GLU:OE2	2.36	0.73
1:C:575:LEU:CB	1:C:634:TRP:HH2	1.93	0.73
3:D:331:LYS:O	3:D:335:ILE:HG12	1.87	0.73
1:A:633:VAL:HG12	2:B:812:LEU:HD13	1.68	0.73
1:A:525:ILE:CA	1:A:762:LYS:CE	2.66	0.73
1:A:554:GLN:HA	2:B:798:SER:O	1.87	0.73
2:B:49:TRP:O	2:B:53:MET:N	2.20	0.73
2:B:405:VAL:HG22	2:B:449:ILE:HG12	1.70	0.73
3:D:627:VAL:O	3:D:630:PHE:CD2	2.42	0.73
1:A:510:MET:SD	1:A:760:MET:SD	2.86	0.73
2:B:141:ALA:C	2:B:345:ASP:OD2	2.31	0.73
1:A:121:LEU:CD1	1:A:281:ILE:HG13	1.93	0.73
2:B:124:SER:C	2:B:139:PHE:CB	2.61	0.73
1:C:565:GLY:O	1:C:569:HIS:ND1	2.21	0.73
3:D:332:ARG:CA	3:D:335:ILE:HD11	2.16	0.73
1:C:526:GLU:OE2	1:C:767:LYS:HG3	1.89	0.73
1:C:34:SER:HB2	1:C:96:PRO:HG3	1.69	0.73
1:C:291:ALA:CB	1:C:325:LEU:CD1	2.65	0.73
2:B:631:ALA:HB2	1:C:649:LEU:HD12	1.71	0.73
2:B:753:LEU:HD22	2:B:760:LYS:CB	2.18	0.73
1:C:634:TRP:CZ2	3:D:822:MET:SD	2.82	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:510:MET:HG3	1:A:760:MET:HG2	1.70	0.73
2:B:32:VAL:HG13	2:B:91:VAL:HG23	1.70	0.73
2:B:559:MET:C	2:B:563:ILE:HD12	2.14	0.73
1:A:568:VAL:C	1:A:571:VAL:HG12	2.14	0.72
1:A:815:PHE:CD1	3:D:554:MET:HG3	2.24	0.72
2:B:521:ILE:HG12	2:B:745:ALA:HB2	1.71	0.72
1:C:636:LEU:O	1:C:636:LEU:HD22	1.89	0.72
2:B:791:GLU:O	2:B:793:ASN:N	2.21	0.72
1:C:574:MET:HB3	3:D:822:MET:SD	2.29	0.72
1:C:606:TRP:CZ3	1:C:609:TRP:CE3	2.76	0.72
1:C:766:TRP:O	1:C:770:VAL:HG23	1.89	0.72
1:A:516:THR:HG23	1:A:754:SER:OG	1.89	0.72
1:A:105:THR:HA	1:A:128:TYR:CE2	2.23	0.72
2:B:194:ASN:CG	2:B:214:ILE:CG1	2.56	0.72
3:D:565:VAL:O	3:D:569:VAL:HG23	1.87	0.72
2:B:665:SER:N	2:B:666:PRO:CD	2.53	0.72
1:A:609:TRP:HA	1:A:612:LEU:HD12	1.72	0.72
1:A:621:ALA:CB	1:A:622:PRO:HD2	2.11	0.72
2:B:154:MET:O	2:B:158:ASP:N	2.22	0.72
1:C:637:PHE:CG	3:D:818:LEU:CD2	2.72	0.72
1:C:637:PHE:CE1	1:C:641:ILE:CD1	2.72	0.72
1:A:496:TRP:CH2	1:A:524:TYR:CD2	2.77	0.72
1:A:511:ILE:O	1:A:758:ILE:HD12	1.89	0.72
3:D:388:TYR:N	3:D:389:PRO:HD2	2.02	0.72
2:B:631:ALA:HA	1:C:649:LEU:CG	2.20	0.72
3:D:283:ASP:CB	3:D:285:PRO:HD2	2.20	0.71
3:D:332:ARG:O	3:D:335:ILE:CG1	2.34	0.71
1:A:626:SER:HA	1:A:629:ILE:CD1	2.20	0.71
1:C:634:TRP:HZ2	3:D:822:MET:SD	2.14	0.71
3:D:121:ILE:CB	3:D:287:ARG:CB	2.68	0.71
1:A:530:PRO:CB	1:A:755:GLY:C	2.64	0.71
1:A:609:TRP:CE3	1:A:612:LEU:HD12	2.24	0.71
2:B:753:LEU:CD2	2:B:760:LYS:CG	2.68	0.71
1:A:131:LYS:HZ1	1:A:343:ASP:HA	1.54	0.71
1:A:833:ILE:O	1:A:836:LYS:CB	2.37	0.71
2:B:502:ILE:HG23	2:B:512:PHE:HZ	1.51	0.71
2:B:31:ALA:HB3	2:B:90:VAL:HG12	1.72	0.71
1:A:690:TYR:CE2	1:A:752:PHE:CE1	2.78	0.71
1:C:112:GLY:O	1:C:115:ARG:NH1	2.24	0.71
1:C:138:LEU:HD21	1:C:325:LEU:HG	1.73	0.71
3:D:103:ILE:O	3:D:106:ILE:HG22	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:788:LYS:O	1:A:792:ARG:HB3	1.90	0.70
2:B:544:SER:O	2:B:548:MET:HG2	1.91	0.70
1:C:784:GLU:O	1:C:788:LYS:HB3	1.91	0.70
3:D:305:GLU:C	3:D:306:HIS:CD2	2.69	0.70
1:A:295:LEU:HD22	1:A:321:PHE:CD1	2.26	0.70
1:A:531:PHE:N	1:A:756:PHE:O	2.25	0.70
2:B:241:MET:HA	2:B:247:TRP:CH2	2.25	0.70
2:B:523:VAL:HG22	2:B:717:ILE:CD1	2.19	0.70
1:A:729:TRP:CD1	1:A:730:ASP:H	2.09	0.70
2:B:540:PRO:CB	1:C:803:PRO:HG2	2.20	0.70
2:B:768:LEU:O	2:B:771:VAL:N	2.23	0.70
1:A:126:SER:OG	1:A:143:PRO:CB	2.33	0.70
2:B:182:THR:HG23	2:B:190:TRP:CZ3	2.26	0.70
2:B:539:GLU:O	2:B:542:SER:HB3	1.91	0.70
3:D:119:LEU:CB	3:D:139:PHE:CB	2.69	0.70
1:A:291:ALA:CB	1:A:325:LEU:HD13	2.22	0.70
2:B:192:VAL:HG21	2:B:195:TYR:HD2	1.48	0.70
1:A:115:ARG:HB2	1:A:315:TRP:CB	2.22	0.70
1:A:528:SER:HB2	1:A:758:ILE:HG22	1.73	0.70
1:A:606:TRP:CZ2	3:D:623:ILE:CD1	2.71	0.70
2:B:32:VAL:CG2	2:B:91:VAL:HG22	2.11	0.70
1:C:287:VAL:HG21	1:C:338:ILE:CD1	2.21	0.70
1:A:27:VAL:HG13	1:A:88:TYR:CE1	2.26	0.70
1:A:247:TRP:CB	1:A:266:ILE:CG1	2.62	0.70
1:A:609:TRP:HE3	1:A:612:LEU:CD1	2.03	0.70
1:A:768:GLN:H	1:A:768:GLN:CD	1.98	0.70
2:B:57:PHE:CD2	2:B:292:THR:CG2	2.66	0.70
1:A:530:PRO:HB2	1:A:755:GLY:C	2.17	0.69
1:A:626:SER:HA	1:A:629:ILE:HD12	1.74	0.69
1:A:121:LEU:HD22	1:A:281:ILE:HA	1.73	0.69
3:D:358:VAL:CG1	3:D:370:ARG:HB3	2.22	0.69
1:A:26:ILE:HA	1:A:59:GLN:HG2	1.75	0.69
2:B:396:ILE:O	2:B:465:LEU:HA	1.93	0.69
3:D:358:VAL:HG11	3:D:370:ARG:HB3	1.74	0.69
3:D:594:THR:HG23	3:D:598:ALA:CB	2.21	0.69
1:A:633:VAL:CG1	2:B:812:LEU:CD1	2.56	0.69
1:A:769:GLU:OE1	1:A:769:GLU:N	2.24	0.69
1:A:815:PHE:CG	3:D:554:MET:HG3	2.27	0.69
2:B:541:PHE:CB	2:B:545:VAL:HB	2.22	0.69
3:D:343:ASP:OD2	3:D:354:HIS:HB2	1.90	0.69
3:D:358:VAL:HG13	3:D:372:GLY:O	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:523:VAL:HG22	2:B:717:ILE:HG13	1.68	0.69
2:B:787:ILE:C	2:B:788:CYS:SG	2.75	0.69
1:C:532:LYS:HG3	1:C:533:TYR:N	2.07	0.69
2:B:197:THR:O	2:B:198:LEU:HB2	1.92	0.69
1:A:525:ILE:HA	1:A:762:LYS:CE	2.21	0.69
1:A:668:PRO:CG	2:B:785:THR:HG23	2.23	0.69
1:A:788:LYS:O	1:A:792:ARG:CB	2.41	0.69
1:C:576:TYR:CE2	1:C:604:ALA:HB2	2.28	0.69
3:D:411:ILE:HD12	3:D:789:TRP:CZ3	2.28	0.69
1:A:690:TYR:HE2	1:A:752:PHE:CE1	2.10	0.69
2:B:194:ASN:HB2	2:B:214:ILE:HG13	1.73	0.69
3:D:765:TRP:CB	3:D:769:VAL:CG2	2.71	0.69
2:B:568:SER:O	2:B:569:PRO:C	2.34	0.69
1:C:221:LEU:HD22	1:C:231:VAL:HG11	1.75	0.68
1:A:531:PHE:CZ	1:A:774:ILE:HG21	2.27	0.68
2:B:736:VAL:HG12	2:B:737:THR:N	2.08	0.68
1:A:503:LEU:HD11	1:A:761:ARG:H	1.58	0.68
1:A:517:ILE:HG12	1:A:755:GLY:O	1.92	0.68
1:A:578:LEU:HD13	1:A:627:ALA:N	2.09	0.68
2:B:410:ILE:HG23	2:B:441:LYS:O	1.92	0.68
2:B:534:PRO:HG3	2:B:804:ASN:OD1	1.92	0.68
1:C:34:SER:CB	1:C:96:PRO:HD3	2.23	0.68
2:B:268:LEU:H	2:B:268:LEU:HD12	1.57	0.68
1:A:94:HIS:N	1:A:122:THR:OG1	2.16	0.68
1:A:115:ARG:O	1:A:315:TRP:HE3	1.75	0.68
1:A:122:THR:HG23	1:A:277:GLU:CG	2.24	0.68
1:A:204:LEU:HD11	1:A:230:ALA:C	2.19	0.68
1:A:496:TRP:HD1	1:A:500:MET:CB	1.93	0.68
1:A:465:ALA:O	1:A:468:MET:O	2.11	0.68
1:A:668:PRO:HG3	2:B:785:THR:HG23	1.74	0.68
1:C:138:LEU:HD21	1:C:325:LEU:CD2	2.24	0.68
1:C:568:VAL:HG13	1:C:608:SER:HB2	1.74	0.68
3:D:808:ILE:HG13	3:D:808:ILE:O	1.93	0.68
1:A:439:PRO:HG3	1:A:478:ALA:HA	1.75	0.68
2:B:109:SER:OG	2:B:135:THR:HA	1.94	0.68
2:B:154:MET:HE1	2:B:218:VAL:HG11	1.76	0.68
1:A:394:MET:SD	1:A:766:TRP:CZ2	2.86	0.68
1:A:400:ILE:HD12	1:A:512:VAL:HG23	1.75	0.68
2:B:31:ALA:HB3	2:B:90:VAL:CG1	2.24	0.68
1:C:629:ILE:O	1:C:633:VAL:HG23	1.94	0.68
2:B:408:GLU:HG2	2:B:445:LYS:HE3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:639:MET:HA	1:C:639:MET:CE	2.23	0.68
3:D:332:ARG:C	3:D:335:ILE:HG13	2.18	0.68
4:G:336:UNK:HA	4:G:362:UNK:O	1.95	0.68
1:A:218:VAL:HG13	1:A:246:VAL:HB	1.76	0.67
3:D:500:TYR:CE2	3:D:765:TRP:NE1	2.62	0.67
1:A:811:MET:CE	3:D:631:PHE:CD2	2.71	0.67
2:B:369:LYS:O	2:B:376:ASN:HB2	1.94	0.67
2:B:534:PRO:HD3	2:B:804:ASN:OD1	1.94	0.67
1:A:26:ILE:HG21	1:A:61:ASN:CB	2.15	0.67
1:A:201:THR:O	1:A:204:LEU:HD22	1.95	0.67
1:A:574:MET:CG	2:B:816:MET:CE	2.73	0.67
2:B:753:LEU:HD22	2:B:760:LYS:HB3	1.76	0.67
3:D:37:VAL:HG13	3:D:68:MET:O	1.94	0.67
3:D:327:ALA:O	3:D:330:LEU:HB3	1.95	0.67
1:A:205:THR:CG2	1:A:238:LEU:CD1	2.34	0.67
2:B:180:LYS:NZ	2:B:195:TYR:CE1	2.62	0.67
2:B:524:MET:HG3	2:B:736:VAL:O	1.95	0.67
3:D:606:VAL:CB	3:D:628:TRP:HH2	2.07	0.67
5:I:2:NAG:C1	5:I:2:NAG:H82	2.24	0.67
2:B:765:LEU:CD1	1:C:523:GLN:HE21	2.03	0.67
1:C:481:LYS:HG3	1:C:684:GLN:OE1	1.94	0.67
3:D:505:SER:O	3:D:755:TYR:CD1	2.47	0.67
1:A:73:GLN:O	1:A:73:GLN:CD	2.37	0.67
1:A:398:LEU:CD2	1:A:766:TRP:CZ3	2.77	0.67
1:A:782:PHE:CE2	1:A:786:LEU:HD11	2.30	0.67
3:D:28:PRO:HB3	4:G:269:UNK:CB	2.25	0.67
2:B:125:MET:O	2:B:139:PHE:CB	2.43	0.67
1:C:534:GLN:O	1:C:754:SER:O	2.13	0.67
1:C:673:PRO:HA	1:C:679:TYR:CE2	2.30	0.67
2:B:559:MET:CG	2:B:563:ILE:HD11	2.25	0.67
3:D:594:THR:CG2	3:D:598:ALA:CB	2.73	0.67
1:C:627:ALA:C	1:C:630:LEU:HB2	2.19	0.67
1:A:511:ILE:C	1:A:758:ILE:HD11	2.19	0.66
1:C:140:THR:O	1:C:346:ARG:CB	2.43	0.66
1:C:398:LEU:HB2	1:C:471:THR:O	1.95	0.66
3:D:453:PHE:O	3:D:457:ILE:HG12	1.95	0.66
3:D:562:VAL:HA	3:D:565:VAL:HG23	1.74	0.66
1:A:439:PRO:CG	1:A:478:ALA:HA	2.24	0.66
1:A:621:ALA:CB	2:B:594:TRP:CH2	2.78	0.66
1:A:811:MET:SD	3:D:631:PHE:HD2	2.16	0.66
2:B:552:MET:HE3	2:B:622:TRP:CZ3	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:329:LYS:C	1:C:331:PRO:HD3	2.20	0.66
1:A:115:ARG:CB	1:A:315:TRP:HB3	2.25	0.66
1:A:690:TYR:HE2	1:A:752:PHE:CD1	2.12	0.66
1:C:276:ASN:HB3	1:C:279:ALA:HB3	1.78	0.66
1:C:484:THR:O	1:C:497:ASN:CB	2.43	0.66
3:D:554:MET:HA	3:D:554:MET:HE2	1.76	0.66
1:A:204:LEU:N	1:A:204:LEU:HD23	2.11	0.66
2:B:631:ALA:CA	1:C:649:LEU:HG	2.26	0.66
1:C:575:LEU:N	1:C:634:TRP:HH2	1.92	0.66
1:C:138:LEU:CD2	1:C:325:LEU:CD2	2.73	0.66
1:C:535:GLY:O	1:C:731:SER:HB3	1.96	0.66
2:B:161:VAL:HG21	2:B:220:LEU:HD11	1.78	0.66
2:B:247:TRP:HB2	2:B:268:LEU:CG	2.25	0.66
2:B:405:VAL:O	2:B:406:ILE:HD13	1.96	0.66
2:B:592:ALA:O	2:B:596:LEU:N	2.28	0.66
1:C:53:HIS:NE2	1:C:293:HIS:HB2	2.09	0.66
1:C:291:ALA:HB2	1:C:325:LEU:HD12	1.77	0.66
1:A:609:TRP:CZ3	1:A:612:LEU:HD13	2.30	0.66
2:B:402:ALA:HA	2:B:406:ILE:HD11	1.77	0.66
1:C:673:PRO:HA	1:C:679:TYR:HE2	1.60	0.66
1:A:253:GLU:OE1	1:A:253:GLU:N	2.28	0.66
1:C:217:ARG:CB	1:C:392:TYR:H	2.05	0.66
1:C:301:ILE:CG2	1:C:317:THR:CB	2.74	0.66
1:C:301:ILE:HG21	1:C:317:THR:HG23	1.64	0.66
1:C:513:ALA:HB1	1:C:514:PRO:HD2	1.78	0.66
3:D:171:PHE:O	3:D:174:TYR:HD2	1.79	0.66
1:A:525:ILE:HD11	1:A:527:PHE:CE1	2.30	0.66
1:A:574:MET:SD	1:A:630:LEU:CD1	2.84	0.66
1:C:438:GLY:CA	1:C:451:GLN:NE2	2.44	0.66
1:A:150:VAL:HG21	1:A:351:TYR:HD2	1.61	0.66
1:A:400:ILE:HB	1:A:474:VAL:HG22	1.77	0.66
1:A:578:LEU:CB	1:A:627:ALA:HB2	2.27	0.65
1:A:637:PHE:CE1	2:B:808:VAL:CG1	2.67	0.65
1:C:640:ILE:CG2	3:D:811:MET:CE	2.72	0.65
3:D:543:PHE:CE1	3:D:643:LEU:HD11	2.30	0.65
3:D:620:THR:O	3:D:624:MET:HG2	1.96	0.65
2:B:304:VAL:O	2:B:306:PRO:HD3	1.96	0.65
1:C:575:LEU:CB	1:C:634:TRP:HZ3	2.09	0.65
1:A:122:THR:CG2	1:A:277:GLU:CG	2.71	0.65
2:B:720:ALA:HB2	2:B:743:ILE:HG22	1.73	0.65
1:A:621:ALA:HB1	1:A:622:PRO:HD3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:668:PRO:HG3	2:B:785:THR:HG21	1.78	0.65
2:B:164:VAL:CG2	2:B:220:LEU:HD13	2.23	0.65
2:B:767:LEU:O	2:B:770:PHE:HB2	1.96	0.65
1:A:102:LEU:CB	1:A:128:TYR:HE1	2.10	0.65
1:A:568:VAL:O	1:A:571:VAL:HG13	1.92	0.65
1:C:575:LEU:CD1	1:C:627:ALA:CB	2.66	0.65
1:C:802:ALA:H	1:C:803:PRO:CD	2.09	0.65
1:A:204:LEU:HD21	1:A:230:ALA:HB1	1.76	0.65
1:A:530:PRO:HB2	1:A:755:GLY:HA3	1.76	0.65
2:B:678:THR:O	2:B:679:GLU:C	2.38	0.65
2:B:541:PHE:HB3	2:B:545:VAL:HB	1.77	0.65
1:C:301:ILE:CG2	1:C:317:THR:OG1	2.45	0.65
1:C:301:ILE:HG22	1:C:317:THR:OG1	1.97	0.65
1:C:627:ALA:CA	1:C:630:LEU:HB2	2.26	0.65
3:D:293:ALA:HB1	3:D:339:PHE:CB	2.27	0.65
1:C:74:MET:O	1:C:78:VAL:HG23	1.96	0.65
1:C:650:ALA:O	1:C:653:LEU:HG	1.97	0.65
3:D:253:VAL:HB	3:D:274:SER:HB2	1.79	0.65
1:A:607:PHE:HA	1:A:610:ARG:CG	2.27	0.65
1:A:621:ALA:HB2	2:B:594:TRP:CH2	2.32	0.65
1:A:541:LYS:CB	1:A:745:VAL:N	2.60	0.64
2:B:178:PHE:O	2:B:179:ILE:C	2.37	0.64
1:C:634:TRP:HA	1:C:637:PHE:HD2	1.60	0.64
2:B:197:THR:O	2:B:207:THR:CG2	2.45	0.64
1:C:50:ASN:OD1	1:C:60:LEU:HB2	1.97	0.64
1:A:202:LYS:O	1:A:204:LEU:HD23	1.97	0.64
1:A:810:ASN:HB2	3:D:631:PHE:CZ	2.30	0.64
3:D:346:PHE:O	3:D:353:MET:HB2	1.96	0.64
3:D:603:TRP:CE3	3:D:603:TRP:HA	2.32	0.64
1:A:119:ILE:HD13	1:A:288:VAL:HG23	1.78	0.64
2:B:53:MET:HE2	2:B:53:MET:CA	2.25	0.64
2:B:64:LEU:HD11	2:B:81:LEU:HD22	1.75	0.64
2:B:253:VAL:O	2:B:256:ASN:OD1	2.13	0.64
1:C:574:MET:CG	3:D:822:MET:HE1	2.23	0.64
1:A:29:ILE:HD11	1:A:60:LEU:HD23	1.79	0.64
1:A:818:VAL:CG1	3:D:558:MET:CE	2.75	0.64
2:B:64:LEU:HD13	2:B:81:LEU:HD21	1.74	0.64
2:B:459:VAL:O	2:B:459:VAL:HG12	1.97	0.64
3:D:332:ARG:CA	3:D:335:ILE:HG12	2.26	0.64
2:B:521:ILE:O	2:B:743:ILE:O	2.15	0.64
2:B:631:ALA:CA	1:C:649:LEU:HD11	2.26	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:500:TYR:CE2	3:D:765:TRP:CD1	2.85	0.64
2:B:82:MET:HE2	2:B:114:ILE:CD1	2.22	0.64
2:B:408:GLU:CG	2:B:445:LYS:NZ	2.58	0.64
3:D:480:GLY:HA2	3:D:488:ASN:O	1.98	0.64
3:D:569:VAL:O	3:D:573:PHE:N	2.31	0.64
3:D:765:TRP:CB	3:D:769:VAL:HG21	2.28	0.64
1:A:117:PRO:HG2	1:A:321:PHE:HD2	1.61	0.64
1:A:379:ILE:HG21	1:A:381:TRP:CZ2	2.33	0.64
1:A:540:VAL:HG21	1:A:725:HIS:O	1.97	0.64
2:B:631:ALA:CB	1:C:649:LEU:CG	2.73	0.64
1:C:477:VAL:CG2	1:C:499:MET:HG3	2.28	0.64
1:A:126:SER:HG	1:A:143:PRO:HB2	1.62	0.64
1:A:198:GLU:HG3	1:A:199:PRO:HD2	1.80	0.64
1:A:609:TRP:CE3	1:A:612:LEU:HD13	2.33	0.64
2:B:520:GLY:HA3	2:B:743:ILE:CB	2.28	0.64
2:B:523:VAL:HA	2:B:716:PHE:O	1.97	0.64
2:B:539:GLU:N	2:B:540:PRO:CD	2.61	0.63
2:B:631:ALA:CA	1:C:649:LEU:CD1	2.75	0.63
1:C:415:THR:HG22	1:C:416:SER:H	1.63	0.63
1:C:449:VAL:HG12	1:C:450:PRO:N	2.12	0.63
1:A:736:PHE:HE1	1:A:794:GLN:CD	2.06	0.63
1:C:23:ASP:N	1:C:24:PRO:HD3	2.12	0.63
1:C:265:GLY:HA3	1:C:381:TRP:C	2.23	0.63
1:C:439:PRO:HD2	1:C:476:LEU:HB2	1.79	0.63
3:D:253:VAL:HG11	3:D:257:VAL:HB	1.80	0.63
3:D:301:THR:HB	3:D:333:TYR:CD2	2.32	0.63
1:A:811:MET:HB2	3:D:635:PHE:CE2	2.33	0.63
2:B:408:GLU:HG2	2:B:445:LYS:HZ1	1.63	0.63
2:B:768:LEU:CG	1:C:519:ASN:CA	2.76	0.63
2:B:669:ARG:CD	2:B:696:PHE:CE2	2.81	0.63
2:B:743:ILE:HD13	2:B:743:ILE:H	1.62	0.63
1:C:295:LEU:HD22	1:C:321:PHE:CE1	2.29	0.63
3:D:433:ILE:N	3:D:444:ASN:O	2.31	0.63
1:A:531:PHE:CE1	1:A:774:ILE:HG21	2.32	0.63
2:B:524:MET:HA	2:B:736:VAL:O	1.97	0.63
2:B:768:LEU:HD13	2:B:768:LEU:N	2.11	0.63
1:C:568:VAL:HG13	1:C:608:SER:CB	2.28	0.63
1:A:525:ILE:C	1:A:762:LYS:CE	2.71	0.63
1:A:530:PRO:HB3	1:A:755:GLY:C	2.24	0.63
2:B:527:ARG:CB	2:B:648:ASP:HA	2.29	0.63
1:C:226:ASP:O	1:C:229:THR:OG1	2.17	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:305:GLU:CB	3:D:333:TYR:CZ	2.82	0.63
1:A:147:GLN:HE22	1:A:250:GLY:HA2	1.63	0.63
1:A:205:THR:HG22	1:A:238:LEU:HD11	1.72	0.63
3:D:508:ILE:HG13	3:D:754:GLY:O	1.99	0.63
1:A:115:ARG:HG3	1:A:314:ILE:HB	1.79	0.63
3:D:605:LEU:HD12	3:D:629:ALA:HB1	1.73	0.63
2:B:486:GLY:C	2:B:490:TYR:HD2	2.06	0.62
1:C:802:ALA:N	1:C:803:PRO:HD2	2.14	0.62
1:A:302:THR:O	1:A:315:TRP:CZ2	2.52	0.62
1:C:802:ALA:N	1:C:803:PRO:CD	2.61	0.62
2:B:399:LEU:CD1	2:B:473:HIS:CE1	2.82	0.62
2:B:519:THR:HG22	2:B:721:ALA:HB3	1.74	0.62
2:B:775:GLU:HG3	2:B:776:MET:HE2	1.81	0.62
1:C:535:GLY:O	1:C:731:SER:CB	2.47	0.62
1:C:634:TRP:HD1	3:D:818:LEU:CD1	2.10	0.62
3:D:305:GLU:CB	3:D:333:TYR:OH	2.47	0.62
1:C:34:SER:CA	1:C:96:PRO:HD3	2.29	0.62
1:C:78:VAL:HG11	1:C:110:THR:CG2	2.28	0.62
5:E:2:NAG:H3	5:E:2:NAG:C8	2.18	0.62
1:A:530:PRO:HB2	1:A:755:GLY:CA	2.29	0.62
1:C:142:PRO:HG3	1:C:349:ALA:HB3	1.80	0.62
1:C:485:GLN:CA	1:C:495:ALA:HA	2.29	0.62
3:D:301:THR:HB	3:D:333:TYR:CG	2.35	0.62
1:A:782:PHE:CZ	1:A:786:LEU:HD11	2.32	0.62
2:B:678:THR:O	2:B:681:ASN:N	2.33	0.62
1:C:301:ILE:HG22	1:C:317:THR:CB	2.30	0.62
1:C:425:THR:HG23	1:C:431:ILE:HG13	1.82	0.62
1:C:446:ARG:N	1:C:447:PRO:HD3	2.15	0.62
2:B:94:ASP:O	2:B:120:HIS:HD2	1.82	0.62
2:B:474:GLY:CA	2:B:482:ASN:O	2.45	0.62
2:B:787:ILE:O	2:B:788:CYS:SG	2.58	0.62
1:C:283:ASP:OD1	1:C:334:VAL:HG23	1.99	0.62
3:D:554:MET:HE2	3:D:554:MET:CA	2.29	0.62
3:D:667:PRO:HG2	3:D:668:ASN:HD22	1.65	0.62
1:A:578:LEU:HB3	1:A:627:ALA:HB2	1.82	0.62
1:A:630:LEU:HD13	2:B:816:MET:SD	2.40	0.62
2:B:192:VAL:CG2	2:B:195:TYR:HD2	2.08	0.62
2:B:502:ILE:CG2	2:B:512:PHE:CZ	2.74	0.62
1:C:630:LEU:HD21	3:D:822:MET:HG3	1.80	0.62
3:D:493:GLU:O	3:D:499:ALA:N	2.31	0.62
1:A:140:THR:C	1:A:346:ARG:CD	2.73	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:736:PHE:CE1	1:A:794:GLN:CD	2.78	0.62
2:B:34:LEU:O	2:B:65:LEU:CD1	2.48	0.62
2:B:214:ILE:HD13	2:B:214:ILE:N	2.13	0.62
2:B:396:ILE:HG23	2:B:495:MET:O	1.98	0.62
2:B:559:MET:HB2	2:B:618:ILE:HG21	1.81	0.62
1:C:114:TYR:OH	1:C:308:CYS:SG	2.54	0.62
1:A:102:LEU:CB	1:A:128:TYR:CE1	2.83	0.62
2:B:225:LYS:HD2	2:B:256:ASN:ND2	2.14	0.62
2:B:753:LEU:CD2	2:B:760:LYS:HB3	2.29	0.62
1:C:673:PRO:HD3	1:C:699:THR:HG22	1.82	0.62
2:B:120:HIS:NE2	2:B:280:ILE:CD1	2.62	0.61
2:B:141:ALA:CA	2:B:345:ASP:OD2	2.48	0.61
2:B:179:ILE:CB	2:B:195:TYR:OH	2.48	0.61
2:B:504:GLU:OE1	1:C:772:LEU:O	2.16	0.61
2:B:768:LEU:CD2	1:C:519:ASN:HB2	2.26	0.61
2:B:769:GLN:NE2	1:C:520:GLU:OE2	2.33	0.61
1:C:609:TRP:O	1:C:610:ARG:C	2.43	0.61
1:A:131:LYS:HZ3	1:A:343:ASP:HA	1.64	0.61
1:A:286:ALA:CB	1:A:330:TYR:CE2	2.83	0.61
2:B:559:MET:CG	2:B:563:ILE:CD1	2.78	0.61
1:C:287:VAL:CG2	1:C:338:ILE:HD12	2.30	0.61
1:A:150:VAL:HG21	1:A:351:TYR:CD2	2.35	0.61
1:A:551:SER:OG	1:A:649:LEU:HD11	1.99	0.61
2:B:541:PHE:HD1	2:B:541:PHE:H	1.47	0.61
1:C:477:VAL:HB	1:C:499:MET:HG3	1.81	0.61
1:C:679:TYR:H	1:C:703:HIS:HE1	1.48	0.61
1:A:25:LYS:O	1:A:59:GLN:HB3	2.00	0.61
2:B:154:MET:O	2:B:158:ASP:O	2.17	0.61
1:C:287:VAL:CG2	1:C:338:ILE:CD1	2.78	0.61
1:A:525:ILE:CD1	1:A:527:PHE:CE1	2.83	0.61
1:C:568:VAL:CG1	1:C:608:SER:CB	2.78	0.61
1:A:204:LEU:HG	1:A:234:SER:OG	2.00	0.61
3:D:543:PHE:O	3:D:546:PRO:HG2	2.00	0.61
1:A:668:PRO:HG3	2:B:785:THR:OG1	1.99	0.61
1:A:709:TYR:OH	1:A:724:LEU:HD12	1.97	0.61
2:B:541:PHE:CZ	1:C:803:PRO:HB3	2.35	0.61
1:C:477:VAL:HG21	1:C:499:MET:CG	2.29	0.61
3:D:77:ILE:HD11	3:D:106:ILE:HD11	1.83	0.61
1:A:204:LEU:CD1	1:A:231:VAL:HA	2.31	0.61
1:A:630:LEU:HD21	2:B:816:MET:SD	2.37	0.61
1:C:138:LEU:HD21	1:C:325:LEU:CG	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:SER:CB	2:B:172:TYR:CE2	2.77	0.61
1:A:682:VAL:HG22	1:A:729:TRP:CZ3	2.31	0.61
1:A:811:MET:CB	3:D:631:PHE:CE2	2.83	0.61
2:B:179:ILE:HG21	2:B:195:TYR:HH	0.62	0.61
2:B:638:ALA:CB	1:C:653:LEU:HD22	2.29	0.61
1:C:78:VAL:CA	1:C:82:LEU:HB2	2.25	0.61
3:D:543:PHE:CD1	3:D:639:TYR:CE1	2.89	0.61
1:A:496:TRP:CH2	1:A:524:TYR:CG	2.88	0.61
1:A:568:VAL:HG12	1:A:608:SER:CB	2.23	0.61
1:A:671:ARG:NH1	2:B:782:LEU:HA	2.15	0.61
1:A:811:MET:HB2	3:D:631:PHE:CD2	2.35	0.61
2:B:166:THR:O	2:B:197:THR:OG1	2.16	0.61
2:B:559:MET:HG2	2:B:563:ILE:CD1	2.30	0.61
2:B:669:ARG:HD2	2:B:696:PHE:CE2	2.36	0.61
2:B:631:ALA:HA	1:C:649:LEU:HG	1.82	0.60
2:B:753:LEU:CD2	2:B:760:LYS:CB	2.79	0.60
1:C:415:THR:HG22	1:C:416:SER:N	2.16	0.60
1:C:631:GLY:O	1:C:635:ALA:CB	2.48	0.60
3:D:37:VAL:CG1	3:D:68:MET:O	2.48	0.60
1:A:496:TRP:CZ2	1:A:524:TYR:HB3	2.36	0.60
1:A:553:MET:O	2:B:798:SER:O	2.19	0.60
1:A:709:TYR:CZ	1:A:724:LEU:CD1	2.84	0.60
2:B:541:PHE:HB3	2:B:545:VAL:HG11	1.82	0.60
2:B:640:PHE:O	2:B:643:GLN:N	2.34	0.60
2:B:775:GLU:O	2:B:778:GLU:N	2.33	0.60
1:C:692:ARG:HD3	1:C:701:TYR:OH	2.02	0.60
1:A:690:TYR:CE2	1:A:752:PHE:CD2	2.89	0.60
1:A:811:MET:HB2	3:D:631:PHE:HE2	1.66	0.60
2:B:270:SER:O	2:B:356:LEU:O	2.19	0.60
2:B:659:GLN:CD	2:B:686:TYR:OH	2.43	0.60
3:D:225:LEU:HD12	3:D:251:TRP:HZ3	1.66	0.60
2:B:154:MET:HE3	2:B:248:ILE:HG13	1.81	0.60
2:B:178:PHE:O	2:B:181:THR:N	2.34	0.60
2:B:193:GLN:HG3	2:B:214:ILE:HG23	1.83	0.60
1:C:118:VAL:O	1:C:138:LEU:HB2	2.00	0.60
1:C:128:TYR:CD2	1:C:137:PHE:CZ	2.90	0.60
1:A:394:MET:CE	1:A:765:PRO:HG3	2.31	0.60
1:A:496:TRP:HE1	1:A:504:LEU:HD23	1.66	0.60
2:B:164:VAL:HG21	2:B:179:ILE:HD11	1.83	0.60
1:C:398:LEU:N	1:C:471:THR:O	2.34	0.60
1:C:627:ALA:O	1:C:630:LEU:CB	2.50	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:ARG:HA	1:A:141:VAL:HG23	1.84	0.60
1:A:671:ARG:HH12	2:B:782:LEU:HA	1.67	0.60
2:B:182:THR:HG21	2:B:190:TRP:CH2	2.35	0.60
2:B:355:VAL:N	2:B:368:GLY:O	2.30	0.60
2:B:765:LEU:HA	1:C:519:ASN:OD1	2.02	0.60
1:C:785:GLU:O	1:C:789:THR:OG1	2.10	0.60
3:D:422:CYS:SG	3:D:449:CYS:CB	2.90	0.60
3:D:734:GLY:O	3:D:793:ILE:CB	2.50	0.60
2:B:49:TRP:O	2:B:53:MET:CB	2.42	0.60
1:A:140:THR:CA	1:A:346:ARG:HD2	2.31	0.59
2:B:163:SER:CB	2:B:194:ASN:HD22	2.15	0.59
2:B:502:ILE:HG12	2:B:512:PHE:CE2	2.36	0.59
2:B:621:ILE:HG13	1:C:818:VAL:HG22	1.83	0.59
3:D:663:LYS:O	3:D:666:ARG:O	2.20	0.59
1:A:39:GLU:OE1	1:A:66:THR:OG1	2.15	0.59
2:B:164:VAL:HG22	2:B:220:LEU:CD1	2.25	0.59
2:B:593:VAL:O	2:B:597:TRP:HB2	2.01	0.59
2:B:664:TYR:C	2:B:666:PRO:HD2	2.27	0.59
1:C:58:ILE:HG21	1:C:296:PHE:CE2	2.37	0.59
1:C:272:ILE:CB	1:C:350:GLN:O	2.51	0.59
3:D:734:GLY:O	3:D:793:ILE:N	2.35	0.59
2:B:42:GLU:CB	2:B:63:THR:HG22	2.31	0.59
3:D:411:ILE:HD12	3:D:789:TRP:HZ3	1.64	0.59
1:A:140:THR:O	1:A:346:ARG:CG	2.50	0.59
1:A:208:LEU:HD22	1:A:235:ALA:HA	1.84	0.59
1:A:247:TRP:HB3	1:A:266:ILE:CG1	2.31	0.59
1:A:648:ASN:ND2	2:B:800:LEU:HD11	2.18	0.59
1:A:668:PRO:CG	2:B:785:THR:CG2	2.74	0.59
2:B:151:LEU:CD2	2:B:182:THR:CG2	2.75	0.59
2:B:529:ALA:HB3	2:B:646:PHE:HA	1.84	0.59
2:B:541:PHE:HB3	2:B:545:VAL:CG1	2.31	0.59
1:C:264:ASP:OD1	1:C:265:GLY:N	2.35	0.59
2:B:164:VAL:HG21	2:B:179:ILE:HD12	1.83	0.59
2:B:197:THR:O	2:B:207:THR:HG22	2.02	0.59
2:B:631:ALA:HB2	1:C:649:LEU:CD1	2.32	0.59
3:D:430:ARG:O	3:D:472:TYR:CB	2.49	0.59
3:D:541:SER:HA	3:D:544:LEU:HG	1.83	0.59
1:A:86:GLN:HE22	1:A:306:ARG:CB	2.05	0.59
1:A:449:VAL:HG12	1:A:451:GLN:HG2	1.85	0.59
1:A:557:GLN:CD	2:B:798:SER:OG	2.46	0.59
2:B:548:MET:HA	2:B:551:VAL:HB	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:606:TRP:HZ3	1:C:609:TRP:HE3	1.47	0.59
3:D:170:TYR:HE1	3:D:199:HIS:HB3	1.68	0.59
1:A:86:GLN:HE21	1:A:306:ARG:CA	2.08	0.59
1:A:570:VAL:O	1:A:573:VAL:HG23	2.02	0.59
1:C:354:MET:HA	1:C:362:VAL:O	2.03	0.59
3:D:741:LEU:HD12	3:D:741:LEU:N	2.18	0.59
3:D:202:MET:O	3:D:202:MET:HE3	2.03	0.59
1:A:698:SER:HB3	2:B:419:ARG:NE	2.17	0.59
2:B:247:TRP:CB	2:B:268:LEU:HD23	2.33	0.59
2:B:410:ILE:HG23	2:B:441:LYS:C	2.27	0.59
2:B:541:PHE:HB3	2:B:545:VAL:HG21	1.85	0.59
2:B:621:ILE:HG13	1:C:818:VAL:HG13	1.84	0.59
1:C:691:PHE:CD2	1:C:704:MET:HE1	2.38	0.59
1:A:283:ASP:OD2	1:A:334:VAL:N	2.35	0.59
1:A:607:PHE:CA	1:A:610:ARG:HG2	2.33	0.59
2:B:504:GLU:O	2:B:507:SER:HB2	2.02	0.59
2:B:669:ARG:NE	2:B:696:PHE:CD2	2.71	0.59
2:B:777:GLU:OE1	2:B:777:GLU:N	2.34	0.59
3:D:603:TRP:HA	3:D:603:TRP:HE3	1.68	0.59
1:C:73:GLN:O	1:C:77:SER:HB2	2.02	0.58
1:A:302:THR:O	1:A:315:TRP:NE1	2.36	0.58
1:A:549:LEU:O	1:A:553:MET:HB2	2.04	0.58
1:A:575:LEU:HD13	1:A:622:PRO:CB	2.22	0.58
1:A:663:THR:O	1:A:667:ASP:HB2	2.03	0.58
2:B:33:ILE:HG23	2:B:64:LEU:O	2.03	0.58
2:B:631:ALA:CB	1:C:649:LEU:CD1	2.81	0.58
2:B:702:GLN:OE1	2:B:702:GLN:N	2.27	0.58
3:D:332:ARG:C	3:D:335:ILE:CG1	2.76	0.58
3:D:526:GLY:O	3:D:726:ALA:N	2.36	0.58
1:A:140:THR:C	1:A:346:ARG:HD3	2.27	0.58
1:A:205:THR:HA	1:A:208:LEU:HD13	1.85	0.58
1:A:398:LEU:HD12	1:A:470:PHE:HD2	1.67	0.58
1:A:526:GLU:O	1:A:527:PHE:HD1	1.87	0.58
1:A:803:PRO:HG3	3:D:642:ASN:CG	2.28	0.58
2:B:541:PHE:HB3	2:B:545:VAL:CG2	2.34	0.58
3:D:77:ILE:HG12	3:D:110:ILE:HD11	1.84	0.58
1:A:142:PRO:HG3	1:A:349:ALA:CB	2.33	0.58
1:A:217:ARG:HB3	1:A:244:GLY:O	2.02	0.58
2:B:686:TYR:HB2	2:B:689:MET:HB3	1.86	0.58
2:B:520:GLY:CA	2:B:743:ILE:HG13	2.27	0.58
3:D:345:SER:O	3:D:353:MET:HB3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:ILE:HA	1:A:59:GLN:CG	2.34	0.58
1:A:500:MET:O	1:A:503:LEU:HB3	2.03	0.58
1:A:525:ILE:CD1	1:A:527:PHE:HE1	2.17	0.58
2:B:196:ILE:HD11	2:B:211:LEU:HG	1.84	0.58
2:B:521:ILE:H	2:B:745:ALA:HB3	1.68	0.58
2:B:584:GLY:O	2:B:587:PHE:CD1	2.46	0.58
1:C:195:LEU:HB3	1:C:207:LEU:HD21	1.85	0.58
1:C:787:ASP:O	1:C:791:VAL:HB	2.03	0.58
3:D:301:THR:HB	3:D:333:TYR:CE2	2.38	0.58
3:D:502:ALA:H	3:D:758:ALA:HB3	1.69	0.58
1:A:698:SER:HB2	2:B:419:ARG:HE	1.68	0.58
2:B:521:ILE:HG12	2:B:745:ALA:CB	2.33	0.58
2:B:559:MET:O	2:B:563:ILE:CD1	2.51	0.58
2:B:775:GLU:HA	2:B:778:GLU:HG2	1.85	0.58
1:C:141:VAL:HA	1:C:346:ARG:CB	2.33	0.58
1:C:697:LEU:O	1:C:698:SER:C	2.46	0.58
1:C:809:GLU:O	1:C:812:ALA:HB3	2.04	0.58
2:B:120:HIS:ND1	2:B:280:ILE:CD1	2.67	0.58
2:B:162:PHE:HD2	2:B:219:ILE:HG12	1.67	0.58
2:B:568:SER:C	2:B:570:VAL:N	2.60	0.58
3:D:322:SER:O	3:D:325:TYR:HB3	2.03	0.58
3:D:565:VAL:O	3:D:569:VAL:CG2	2.51	0.58
1:A:671:ARG:O	1:A:673:PRO:HD3	2.03	0.58
1:A:768:GLN:CD	1:A:768:GLN:N	2.62	0.58
2:B:25:PHE:CB	2:B:26:PRO:HD3	2.33	0.58
2:B:64:LEU:HD12	2:B:81:LEU:CD2	2.15	0.58
2:B:799:GLN:HG2	2:B:799:GLN:O	2.03	0.58
3:D:512:ARG:HA	3:D:515:VAL:HG22	1.85	0.58
1:A:709:TYR:CZ	1:A:724:LEU:HD11	2.30	0.58
2:B:264:PHE:CE1	2:B:268:LEU:HD11	2.38	0.58
1:C:34:SER:HA	1:C:96:PRO:HD3	1.85	0.58
1:C:606:TRP:HA	1:C:606:TRP:CE3	2.39	0.58
1:C:634:TRP:CA	1:C:637:PHE:HD2	2.16	0.58
1:A:121:LEU:CD2	1:A:281:ILE:HG12	2.34	0.57
1:A:516:THR:HG23	1:A:754:SER:CB	2.33	0.57
1:A:811:MET:SD	3:D:631:PHE:CD2	2.96	0.57
2:B:197:THR:O	2:B:198:LEU:CB	2.51	0.57
2:B:765:LEU:HD13	1:C:519:ASN:CG	2.29	0.57
1:C:412:ARG:NH1	1:C:454:TYR:OH	2.37	0.57
1:A:121:LEU:HD12	1:A:281:ILE:HD11	1.85	0.57
2:B:49:TRP:HA	2:B:49:TRP:HE3	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:64:LEU:CD1	2:B:81:LEU:CG	2.77	0.57
2:B:552:MET:HE1	2:B:622:TRP:HE3	1.63	0.57
1:C:637:PHE:HE1	1:C:641:ILE:CD1	2.16	0.57
3:D:170:TYR:CE1	3:D:199:HIS:HB3	2.38	0.57
3:D:305:GLU:O	3:D:306:HIS:CD2	2.57	0.57
1:A:500:MET:HE1	1:A:521:ARG:CG	2.34	0.57
2:B:49:TRP:HA	2:B:49:TRP:CE3	2.39	0.57
1:C:34:SER:HB2	1:C:96:PRO:CG	2.34	0.57
1:A:157:LEU:HD22	1:A:372:ILE:CD1	2.32	0.57
2:B:151:LEU:O	2:B:155:GLU:N	2.31	0.57
2:B:770:PHE:N	2:B:770:PHE:CD1	2.72	0.57
1:C:34:SER:HB2	1:C:96:PRO:HD3	1.86	0.57
3:D:530:MET:O	3:D:531:VAL:HG12	2.04	0.57
1:A:76:LEU:C	1:A:76:LEU:HD23	2.29	0.57
1:A:150:VAL:CG2	1:A:351:TYR:HD2	2.17	0.57
2:B:163:SER:HB2	2:B:194:ASN:HB3	1.85	0.57
2:B:458:THR:CG2	2:B:766:ALA:HB1	2.32	0.57
1:C:194:VAL:O	1:C:195:LEU:CD2	2.47	0.57
1:A:811:MET:HA	3:D:631:PHE:CE2	2.39	0.57
2:B:180:LYS:NZ	2:B:195:TYR:CZ	2.72	0.57
2:B:271:VAL:HG21	2:B:355:VAL:HA	1.86	0.57
2:B:390:ASP:O	2:B:391:ASP:C	2.48	0.57
1:A:398:LEU:HD11	1:A:470:PHE:CG	2.38	0.57
1:A:511:ILE:O	1:A:758:ILE:CG1	2.53	0.57
1:A:607:PHE:HA	1:A:610:ARG:NE	2.20	0.57
2:B:112:THR:O	2:B:113:PHE:HB2	2.04	0.57
2:B:244:GLY:O	2:B:245:PHE:HD1	1.88	0.57
1:C:283:ASP:CG	1:C:335:THR:HG22	2.29	0.57
1:C:716:ILE:HD13	1:C:737:GLU:HG3	1.85	0.57
1:A:195:LEU:HD13	1:A:207:LEU:HD21	1.85	0.57
2:B:163:SER:CB	2:B:194:ASN:HB3	2.35	0.57
2:B:354:VAL:HA	2:B:369:LYS:HA	1.86	0.57
1:C:449:VAL:CG1	1:C:450:PRO:N	2.68	0.57
3:D:541:SER:HA	3:D:544:LEU:HD23	1.86	0.57
1:A:205:THR:HG23	1:A:238:LEU:HD13	1.72	0.57
1:A:497:ASN:HA	1:A:501:GLY:HA3	1.85	0.57
2:B:130:LYS:CB	2:B:137:PHE:CE2	2.88	0.57
2:B:424:CYS:CB	2:B:442:LYS:O	2.52	0.57
2:B:523:VAL:CA	2:B:738:ILE:HD11	2.34	0.57
1:C:128:TYR:HB3	1:C:137:PHE:CE2	2.40	0.57
3:D:301:THR:HB	3:D:333:TYR:CD1	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:569:VAL:O	3:D:572:TYR:CB	2.53	0.57
1:A:540:VAL:N	1:A:745:VAL:O	2.38	0.57
1:A:630:LEU:CD1	2:B:816:MET:SD	2.93	0.57
1:A:818:VAL:HG13	3:D:558:MET:CE	2.33	0.57
2:B:399:LEU:HB2	2:B:484:MET:HE1	1.87	0.57
3:D:253:VAL:HG12	3:D:254:PRO:O	2.05	0.57
3:D:500:TYR:HE2	3:D:765:TRP:NE1	2.02	0.57
2:B:197:THR:C	2:B:198:LEU:HD12	2.30	0.56
3:D:399:LEU:O	3:D:401:ILE:HG13	2.04	0.56
3:D:594:THR:CG2	3:D:598:ALA:HB2	2.35	0.56
2:B:152:ASN:HB3	2:B:375:LEU:CB	2.35	0.56
2:B:485:ILE:HD11	2:B:506:ARG:NE	2.20	0.56
1:A:121:LEU:HD11	1:A:281:ILE:CG1	1.99	0.56
1:A:243:ALA:HB2	1:A:383:GLY:HA3	1.85	0.56
1:A:286:ALA:HB1	1:A:330:TYR:CE2	2.40	0.56
1:A:554:GLN:CA	2:B:798:SER:O	2.54	0.56
1:A:710:GLU:OE1	1:A:710:GLU:N	2.38	0.56
1:A:739:SER:HA	1:A:796:CYS:SG	2.45	0.56
2:B:29:ASN:O	2:B:88:HIS:N	2.31	0.56
2:B:140:GLY:CA	2:B:345:ASP:HB3	2.35	0.56
2:B:640:PHE:CD1	2:B:643:GLN:CB	2.88	0.56
2:B:659:GLN:OE1	2:B:686:TYR:CE2	2.58	0.56
2:B:775:GLU:CG	2:B:776:MET:HE2	2.35	0.56
1:C:575:LEU:HA	1:C:630:LEU:CD1	2.35	0.56
1:C:631:GLY:O	1:C:635:ALA:HB3	2.05	0.56
1:C:634:TRP:HA	1:C:637:PHE:CD2	2.40	0.56
3:D:541:SER:HA	3:D:544:LEU:CG	2.36	0.56
3:D:606:VAL:HA	3:D:628:TRP:CZ3	2.40	0.56
2:B:247:TRP:HB2	2:B:268:LEU:HD23	1.86	0.56
3:D:606:VAL:HA	3:D:628:TRP:CH2	2.40	0.56
2:B:268:LEU:H	2:B:268:LEU:CD1	2.18	0.56
2:B:275:ASP:O	2:B:278:TYR:O	2.23	0.56
2:B:548:MET:O	2:B:552:MET:N	2.38	0.56
1:C:142:PRO:HD3	1:C:349:ALA:HB2	1.86	0.56
3:D:600:TRP:O	3:D:603:TRP:HB2	2.06	0.56
1:A:140:THR:O	1:A:346:ARG:HD2	1.99	0.56
1:A:574:MET:CE	2:B:820:LEU:CD2	2.80	0.56
1:A:664:GLY:HA2	1:A:667:ASP:HB2	1.86	0.56
2:B:736:VAL:CG1	2:B:737:THR:N	2.68	0.56
3:D:541:SER:HA	3:D:544:LEU:CD2	2.36	0.56
1:A:122:THR:HG23	1:A:277:GLU:HG3	1.79	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:ILE:CA	1:A:59:GLN:HG2	2.35	0.56
1:A:117:PRO:CG	1:A:321:PHE:HD2	2.18	0.56
1:A:283:ASP:CG	1:A:334:VAL:H	2.13	0.56
1:A:532:LYS:CE	1:A:787:ASP:OD2	2.50	0.56
2:B:249:VAL:CG2	2:B:268:LEU:CD2	2.84	0.56
2:B:640:PHE:HD1	2:B:643:GLN:CB	2.18	0.56
1:C:53:HIS:NE2	1:C:293:HIS:CD2	2.57	0.56
1:C:291:ALA:HB3	1:C:325:LEU:HD13	1.86	0.56
3:D:525:THR:OG1	3:D:725:ASP:OD1	2.23	0.56
4:G:274:UNK:CB	4:G:279:UNK:HA	2.35	0.56
1:A:130:ASP:C	1:A:130:ASP:OD1	2.48	0.56
1:A:365:GLY:HA2	1:A:375:ASN:HB2	1.87	0.56
5:H:2:NAG:H3	5:H:2:NAG:C8	2.13	0.56
1:A:286:ALA:HB3	1:A:330:TYR:CE2	2.41	0.56
1:A:690:TYR:CE2	1:A:752:PHE:CZ	2.94	0.56
2:B:197:THR:HG23	2:B:198:LEU:HG	1.88	0.56
1:A:657:ARG:N	1:A:658:PRO:CD	2.69	0.55
2:B:154:MET:HE3	2:B:218:VAL:HG11	1.87	0.55
2:B:347:TYR:O	2:B:348:GLN:C	2.49	0.55
1:C:477:VAL:HG11	1:C:499:MET:HB2	1.88	0.55
1:C:634:TRP:C	1:C:637:PHE:HD2	2.14	0.55
1:A:331:PRO:O	1:A:337:ARG:HA	2.06	0.55
1:A:440:ASP:CB	1:A:449:VAL:HG21	2.36	0.55
1:A:574:MET:CG	2:B:816:MET:HE1	2.36	0.55
1:A:580:ARG:O	2:B:823:PHE:CZ	2.57	0.55
2:B:496:ALA:H	2:B:752:ALA:HB3	1.71	0.55
2:B:659:GLN:OE1	2:B:686:TYR:HE2	1.89	0.55
1:A:500:MET:HE3	1:A:521:ARG:HD3	1.88	0.55
2:B:621:ILE:HG13	1:C:818:VAL:CG1	2.36	0.55
1:C:560:LEU:N	1:C:560:LEU:HD23	2.21	0.55
3:D:540:PRO:HD2	3:D:810:ASN:CB	2.36	0.55
3:D:627:VAL:O	3:D:630:PHE:HD2	1.88	0.55
1:A:338:ILE:HG12	1:A:346:ARG:HH21	1.72	0.55
2:B:520:GLY:CA	2:B:743:ILE:HG21	2.36	0.55
2:B:768:LEU:CG	1:C:519:ASN:CB	2.81	0.55
1:C:517:ILE:HD12	1:C:530:PRO:HB3	1.87	0.55
1:A:611:VAL:CG1	1:A:635:ALA:HA	2.36	0.55
2:B:205:ALA:HA	2:B:208:LEU:HB2	1.89	0.55
2:B:538:LEU:CB	2:B:541:PHE:CD1	2.90	0.55
2:B:761:ARG:CB	2:B:762:PRO:HD3	2.37	0.55
1:C:291:ALA:HB2	1:C:325:LEU:CD1	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:782:PHE:CZ	1:C:786:LEU:HD11	2.42	0.55
1:A:662:ILE:O	1:A:664:GLY:N	2.40	0.55
2:B:621:ILE:HG13	1:C:818:VAL:CG2	2.36	0.55
1:C:575:LEU:N	1:C:634:TRP:CH2	2.74	0.55
1:A:26:ILE:HG22	1:A:61:ASN:HB3	1.85	0.55
1:A:249:VAL:HG22	1:A:267:ILE:O	2.06	0.55
1:A:815:PHE:CZ	3:D:554:MET:CG	2.68	0.55
1:C:630:LEU:HD22	1:C:634:TRP:CZ2	2.42	0.55
3:D:545:GLU:N	3:D:546:PRO:CD	2.67	0.55
2:B:559:MET:HG2	2:B:563:ILE:HD12	1.89	0.55
1:C:168:SER:HA	1:C:197:PHE:CE1	2.42	0.55
1:A:32:VAL:HG22	1:A:65:VAL:HG12	1.87	0.55
1:A:287:VAL:HG22	1:A:330:TYR:HB3	1.88	0.55
2:B:399:LEU:HD13	2:B:473:HIS:NE2	2.21	0.55
2:B:512:PHE:HB3	2:B:751:ILE:H	1.72	0.55
2:B:541:PHE:CD1	2:B:541:PHE:N	2.75	0.55
1:C:34:SER:HB2	1:C:96:PRO:CD	2.37	0.55
3:D:530:MET:O	3:D:531:VAL:CG1	2.55	0.55
1:A:93:SER:CB	1:A:277:GLU:CD	2.78	0.54
2:B:162:PHE:HD1	2:B:216:SER:N	2.04	0.54
2:B:207:THR:O	2:B:211:LEU:HG	2.06	0.54
1:C:150:VAL:O	1:C:154:MET:N	2.35	0.54
1:C:425:THR:HG23	1:C:431:ILE:CG1	2.35	0.54
1:C:691:PHE:CG	1:C:704:MET:HE1	2.42	0.54
3:D:543:PHE:CD1	3:D:543:PHE:N	2.74	0.54
2:B:120:HIS:ND1	2:B:280:ILE:CG1	2.70	0.54
2:B:179:ILE:HG22	2:B:195:TYR:OH	1.98	0.54
2:B:192:VAL:HG11	2:B:195:TYR:CE2	2.42	0.54
1:C:792:ARG:O	1:C:793:TYR:C	2.48	0.54
3:D:531:VAL:HG11	3:D:721:ALA:CB	2.38	0.54
3:D:543:PHE:CE1	3:D:639:TYR:HE1	2.24	0.54
3:D:565:VAL:O	3:D:569:VAL:N	2.32	0.54
1:A:621:ALA:HB3	2:B:594:TRP:CH2	2.41	0.54
1:C:637:PHE:CE1	1:C:641:ILE:HD11	2.42	0.54
1:A:73:GLN:CD	1:A:73:GLN:C	2.75	0.54
2:B:673:VAL:HG21	2:B:718:TYR:CZ	2.41	0.54
1:A:626:SER:CB	2:B:822:THR:HB	2.38	0.54
1:A:647:ALA:C	2:B:641:MET:SD	2.91	0.54
2:B:247:TRP:HB2	2:B:268:LEU:CD2	2.37	0.54
2:B:278:TYR:HB2	2:B:283:ARG:NH1	2.22	0.54
1:A:407:PRO:HG3	1:A:733:VAL:HA	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:682:VAL:HG23	1:A:729:TRP:CE3	2.42	0.54
1:A:811:MET:CB	3:D:631:PHE:HE2	2.20	0.54
2:B:164:VAL:HA	2:B:220:LEU:HB2	1.89	0.54
1:C:128:TYR:CB	1:C:137:PHE:CE2	2.90	0.54
1:C:329:LYS:HD2	1:C:329:LYS:O	2.07	0.54
1:A:698:SER:CB	2:B:419:ARG:HH21	2.20	0.54
2:B:194:ASN:ND2	2:B:211:LEU:HD23	2.18	0.54
2:B:522:SER:HB3	2:B:743:ILE:CG2	2.35	0.54
1:A:221:LEU:HG	1:A:249:VAL:HG12	1.88	0.54
1:A:365:GLY:HA2	1:A:375:ASN:H	1.72	0.54
1:A:637:PHE:CZ	2:B:811:MET:HB3	2.36	0.54
2:B:78:VAL:O	2:B:82:MET:HG2	2.07	0.54
1:C:132:SER:HB3	3:D:174:TYR:OH	2.07	0.54
1:C:516:THR:HA	1:C:756:PHE:HA	1.90	0.54
1:C:696:GLU:H	1:C:696:GLU:CD	2.16	0.54
3:D:559:LEU:O	3:D:563:SER:N	2.40	0.54
1:A:25:LYS:C	1:A:59:GLN:HB3	2.33	0.54
1:A:496:TRP:NE1	1:A:504:LEU:HD23	2.23	0.54
1:A:818:VAL:CG2	3:D:558:MET:SD	2.95	0.54
2:B:46:ARG:HH21	2:B:63:THR:HB	1.73	0.54
1:C:32:VAL:HG22	1:C:65:VAL:HG12	1.89	0.54
3:D:325:TYR:CD1	3:D:325:TYR:C	2.85	0.54
1:C:149:LEU:O	1:C:153:GLU:N	2.35	0.54
1:C:292:ILE:HG12	1:C:321:PHE:CZ	2.43	0.54
1:A:782:PHE:CE2	1:A:786:LEU:CD1	2.92	0.53
2:B:249:VAL:HG21	2:B:268:LEU:CD2	2.37	0.53
2:B:517:VAL:O	2:B:748:GLY:HA2	2.08	0.53
1:A:552:PHE:CD1	1:A:552:PHE:C	2.86	0.53
2:B:29:ASN:CB	2:B:87:ILE:HA	2.38	0.53
2:B:393:HIS:N	2:B:462:THR:O	2.40	0.53
1:C:164:ILE:HG12	1:C:193:LYS:CB	2.37	0.53
3:D:58:PRO:HG2	3:D:303:LEU:HD12	1.86	0.53
3:D:331:LYS:O	3:D:334:LEU:HB3	2.08	0.53
1:A:132:SER:CB	2:B:172:TYR:HE2	2.04	0.53
1:A:784:GLU:O	1:A:788:LYS:HG2	2.07	0.53
1:C:565:GLY:O	1:C:569:HIS:HE1	1.87	0.53
3:D:543:PHE:CE1	3:D:639:TYR:CE1	2.96	0.53
3:D:565:VAL:O	3:D:569:VAL:CB	2.56	0.53
3:D:631:PHE:CE2	3:D:635:PHE:CZ	2.96	0.53
2:B:120:HIS:NE2	2:B:280:ILE:HD13	2.24	0.53
2:B:136:PHE:O	2:B:137:PHE:CD1	2.61	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:520:GLY:HA3	2:B:743:ILE:HB	1.89	0.53
1:C:770:VAL:O	1:C:774:ILE:HG12	2.08	0.53
1:A:150:VAL:CG2	1:A:351:TYR:CD2	2.92	0.53
2:B:219:ILE:N	2:B:246:VAL:O	2.39	0.53
2:B:244:GLY:O	2:B:245:PHE:CD1	2.61	0.53
2:B:514:VAL:N	2:B:515:PRO:CD	2.65	0.53
2:B:592:ALA:C	2:B:596:LEU:H	2.17	0.53
2:B:765:LEU:O	1:C:519:ASN:OD1	2.27	0.53
1:C:398:LEU:O	1:C:472:TYR:HA	2.09	0.53
1:C:481:LYS:HD2	1:C:684:GLN:HB2	1.90	0.53
3:D:325:TYR:HD1	3:D:326:GLU:N	2.03	0.53
2:B:120:HIS:CG	2:B:280:ILE:HD13	2.43	0.53
1:C:637:PHE:HE1	1:C:641:ILE:HD11	1.74	0.53
3:D:77:ILE:CD1	3:D:106:ILE:HD11	2.38	0.53
1:A:29:ILE:CD1	1:A:60:LEU:HD23	2.38	0.53
1:A:74:MET:O	1:A:74:MET:HE3	2.08	0.53
1:A:121:LEU:HD11	1:A:281:ILE:CD1	2.29	0.53
1:A:205:THR:HG21	1:A:238:LEU:HD11	1.70	0.53
1:A:678:ILE:CG2	1:A:724:LEU:CD2	2.84	0.53
1:A:822:ILE:CD1	3:D:565:VAL:HG13	2.22	0.53
2:B:163:SER:O	2:B:220:LEU:N	2.36	0.53
2:B:197:THR:O	2:B:198:LEU:CD1	2.54	0.53
2:B:223:CYS:SG	2:B:227:GLU:OE2	2.55	0.53
2:B:351:PRO:HD2	2:B:370:TRP:HZ3	1.74	0.53
3:D:563:SER:OG	3:D:594:THR:OG1	2.23	0.53
1:A:479:ASP:CB	1:A:498:GLY:HA2	2.39	0.53
2:B:120:HIS:NE2	2:B:280:ILE:HD11	2.18	0.53
2:B:395:SER:O	2:B:396:ILE:HG13	2.09	0.53
2:B:758:ARG:C	2:B:760:LYS:H	2.15	0.53
1:C:398:LEU:HD12	1:C:470:PHE:CD1	2.44	0.53
1:C:628:ARG:HB2	1:C:628:ARG:CZ	2.36	0.53
3:D:834:LEU:O	3:D:835:PHE:C	2.52	0.53
1:A:536:LEU:HA	1:A:730:ASP:HA	1.90	0.53
2:B:57:PHE:CG	2:B:292:THR:CG2	2.78	0.53
2:B:621:ILE:CG1	1:C:818:VAL:HG22	2.39	0.53
2:B:758:ARG:O	2:B:762:PRO:CD	2.55	0.53
1:C:673:PRO:HG2	1:C:703:HIS:CB	2.19	0.53
3:D:301:THR:HB	3:D:333:TYR:CZ	2.44	0.53
2:B:495:MET:HE2	2:B:751:ILE:HG21	1.91	0.53
1:C:330:TYR:N	1:C:331:PRO:HD3	2.24	0.53
3:D:567:VAL:O	3:D:571:GLU:CB	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:LEU:HD11	1:A:470:PHE:HD2	1.50	0.52
1:A:482:PHE:CG	1:A:515:LEU:HD21	2.45	0.52
1:C:295:LEU:O	1:C:298:MET:HB2	2.09	0.52
1:C:534:GLN:NE2	1:C:730:ASP:OD1	2.31	0.52
1:C:576:TYR:CE1	1:C:600:THR:HB	2.43	0.52
1:C:621:ALA:HB1	1:C:622:PRO:HD2	1.91	0.52
1:A:220:ILE:HG12	1:A:248:LEU:HD12	1.91	0.52
1:A:302:THR:OG1	1:A:315:TRP:NE1	2.41	0.52
1:A:811:MET:CA	3:D:631:PHE:HE2	2.11	0.52
2:B:720:ALA:HB3	2:B:743:ILE:CG2	2.37	0.52
2:B:768:LEU:HD23	1:C:519:ASN:CG	2.34	0.52
1:C:745:VAL:HG12	1:C:746:THR:N	2.24	0.52
3:D:500:TYR:OH	3:D:764:GLY:HA2	2.09	0.52
3:D:506:LEU:O	3:D:755:TYR:HA	2.09	0.52
3:D:559:LEU:HD21	3:D:598:ALA:CB	2.35	0.52
3:D:559:LEU:HD23	3:D:559:LEU:C	2.33	0.52
1:A:401:VAL:CG2	1:A:477:VAL:HB	2.38	0.52
1:A:510:MET:HG3	1:A:760:MET:SD	2.49	0.52
2:B:147:ALA:O	2:B:151:LEU:HD13	2.10	0.52
2:B:396:ILE:O	2:B:465:LEU:HD23	2.10	0.52
1:A:287:VAL:HG23	1:A:330:TYR:HD2	1.74	0.52
2:B:194:ASN:CB	2:B:214:ILE:HG21	2.22	0.52
2:B:410:ILE:HG22	2:B:443:CYS:SG	2.49	0.52
2:B:638:ALA:HB2	1:C:653:LEU:HD22	1.91	0.52
1:C:519:ASN:ND2	1:C:523:GLN:HE21	2.08	0.52
1:C:778:HIS:ND1	1:C:783:MET:HG2	2.24	0.52
1:A:111:ALA:O	1:A:114:TYR:N	2.41	0.52
1:A:815:PHE:HZ	3:D:628:TRP:HE1	1.57	0.52
3:D:37:VAL:HG23	3:D:95:GLY:O	2.10	0.52
3:D:200:LEU:HD12	3:D:211:ILE:CB	2.39	0.52
3:D:606:VAL:CB	3:D:628:TRP:CH2	2.92	0.52
3:D:741:LEU:N	3:D:741:LEU:CD1	2.73	0.52
1:A:248:LEU:HD23	1:A:267:ILE:HB	1.92	0.52
2:B:296:SER:O	2:B:300:GLU:HB2	2.10	0.52
1:C:667:ASP:CG	1:C:668:PRO:HD2	2.34	0.52
1:A:606:TRP:NE1	3:D:623:ILE:CG1	2.72	0.52
2:B:775:GLU:O	2:B:776:MET:C	2.50	0.52
1:C:94:HIS:N	1:C:122:THR:OG1	2.33	0.52
1:C:478:ALA:CB	1:C:502:GLU:OE2	2.57	0.52
1:C:532:LYS:HG3	1:C:533:TYR:H	1.75	0.52
3:D:301:THR:HB	3:D:333:TYR:CE1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:563:SER:OG	3:D:594:THR:CB	2.57	0.52
1:A:429:ASP:CB	1:A:430:PRO:HD2	2.40	0.52
2:B:491:LYS:HD2	2:B:491:LYS:O	2.10	0.52
2:B:672:THR:H	2:B:693:MET:HG2	1.75	0.52
2:B:758:ARG:C	2:B:760:LYS:N	2.66	0.52
1:C:138:LEU:CD2	1:C:325:LEU:HD21	2.39	0.52
1:C:477:VAL:CG2	1:C:499:MET:CG	2.88	0.52
1:A:32:VAL:HA	1:A:65:VAL:HG12	1.91	0.52
1:A:788:LYS:O	1:A:792:ARG:HB2	2.09	0.52
2:B:31:ALA:CB	2:B:90:VAL:HG12	2.40	0.52
2:B:154:MET:CA	2:B:158:ASP:CB	2.85	0.52
2:B:284:VAL:O	2:B:288:LEU:HG	2.09	0.52
2:B:527:ARG:CB	2:B:648:ASP:CB	2.88	0.52
3:D:224:LEU:HD23	3:D:252:ILE:HB	1.91	0.52
1:A:551:SER:CB	1:A:649:LEU:CD1	2.88	0.51
1:A:678:ILE:HG21	1:A:724:LEU:CD2	2.40	0.51
1:A:811:MET:HE2	3:D:635:PHE:CE2	2.45	0.51
1:A:818:VAL:HG11	3:D:558:MET:CE	2.40	0.51
2:B:720:ALA:CB	2:B:743:ILE:HG21	2.33	0.51
1:C:30:GLY:HA2	1:C:63:THR:O	2.11	0.51
1:C:365:GLY:HA2	1:C:375:ASN:H	1.75	0.51
3:D:415:VAL:HB	3:D:449:CYS:SG	2.51	0.51
3:D:531:VAL:CG1	3:D:721:ALA:HA	2.39	0.51
3:D:741:LEU:CD1	3:D:741:LEU:H	2.23	0.51
1:A:607:PHE:HA	1:A:610:ARG:HG2	1.88	0.51
2:B:485:ILE:CD1	2:B:506:ARG:HE	2.21	0.51
2:B:522:SER:HG	2:B:723:LEU:HD12	1.70	0.51
2:B:591:LYS:C	2:B:595:LEU:CB	2.79	0.51
5:E:2:NAG:H83	5:E:2:NAG:C3	2.21	0.51
2:B:164:VAL:HG23	2:B:220:LEU:HD12	0.60	0.51
3:D:168:THR:HG21	3:D:174:TYR:HB2	1.92	0.51
3:D:765:TRP:HB2	3:D:769:VAL:HG21	1.92	0.51
1:A:30:GLY:HA2	1:A:63:THR:O	2.10	0.51
1:A:496:TRP:NE1	1:A:500:MET:SD	2.84	0.51
1:A:574:MET:CG	2:B:816:MET:HE3	2.39	0.51
1:C:78:VAL:HG11	1:C:110:THR:HG22	1.90	0.51
1:C:477:VAL:CB	1:C:499:MET:HG3	2.40	0.51
1:A:105:THR:CA	1:A:128:TYR:HE2	2.20	0.51
1:A:468:MET:HG2	1:A:470:PHE:HD1	1.76	0.51
1:C:27:VAL:HG13	1:C:88:TYR:CD1	2.45	0.51
1:C:291:ALA:CB	1:C:325:LEU:HD12	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:295:LEU:HB2	1:C:324:VAL:HG11	1.92	0.51
1:A:429:ASP:CB	1:A:430:PRO:CD	2.88	0.51
1:A:784:GLU:OE1	1:A:784:GLU:N	2.37	0.51
2:B:154:MET:HE3	2:B:248:ILE:CG1	2.40	0.51
2:B:393:HIS:HA	2:B:462:THR:O	2.11	0.51
2:B:693:MET:SD	2:B:693:MET:C	2.94	0.51
3:D:301:THR:CB	3:D:333:TYR:CG	2.93	0.51
2:B:753:LEU:CD2	2:B:760:LYS:HG2	2.26	0.51
1:A:140:THR:C	1:A:346:ARG:HD2	2.35	0.51
1:A:286:ALA:HB3	1:A:330:TYR:HE2	1.73	0.51
1:C:75:ALA:O	1:C:78:VAL:N	2.35	0.51
3:D:562:VAL:O	3:D:565:VAL:HG23	2.11	0.51
1:A:392:TYR:CD2	1:A:394:MET:HE2	2.46	0.51
1:A:447:PRO:O	1:A:448:THR:C	2.53	0.51
1:A:575:LEU:CD1	1:A:622:PRO:CB	2.84	0.51
1:C:25:LYS:O	1:C:59:GLN:HB2	2.10	0.51
1:C:694:GLN:HB2	1:C:697:LEU:CD1	2.37	0.51
1:A:367:PHE:HD1	1:A:372:ILE:HA	1.76	0.51
1:A:477:VAL:HG23	1:A:502:GLU:HG3	1.93	0.51
1:A:661:ARG:O	1:A:667:ASP:OD2	2.28	0.51
2:B:262:TYR:CD2	2:B:262:TYR:C	2.87	0.51
2:B:673:VAL:HG12	2:B:698:GLN:NE2	2.26	0.51
1:C:73:GLN:O	1:C:77:SER:N	2.37	0.51
3:D:405:GLU:HB3	3:D:412:VAL:HG23	1.91	0.51
1:A:32:VAL:HG22	1:A:65:VAL:CG1	2.41	0.50
1:A:291:ALA:O	1:A:321:PHE:HE1	1.94	0.50
1:A:302:THR:O	1:A:315:TRP:HZ2	1.92	0.50
1:A:581:PHE:HB2	2:B:823:PHE:CZ	2.46	0.50
1:A:606:TRP:NE1	3:D:623:ILE:HD11	1.94	0.50
1:A:739:SER:OG	1:A:794:GLN:HB3	2.11	0.50
2:B:69:THR:CB	2:B:98:GLN:OE1	2.59	0.50
3:D:371:VAL:O	3:D:382:TRP:CB	2.58	0.50
1:A:103:THR:O	1:A:105:THR:N	2.44	0.50
1:A:536:LEU:N	1:A:536:LEU:HD12	2.26	0.50
2:B:31:ALA:O	2:B:90:VAL:CB	2.59	0.50
2:B:268:LEU:CD1	2:B:268:LEU:N	2.73	0.50
2:B:390:ASP:O	2:B:392:ASN:N	2.43	0.50
2:B:615:SER:O	2:B:619:VAL:HG23	2.10	0.50
2:B:659:GLN:C	2:B:661:PRO:HD3	2.37	0.50
1:C:67:HIS:CE1	1:C:95:PRO:HG3	2.46	0.50
1:C:119:ILE:HG12	1:C:138:LEU:CD2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:288:VAL:O	1:C:292:ILE:HG13	2.11	0.50
1:C:326:MET:HA	1:C:340:PHE:HD2	1.75	0.50
1:A:204:LEU:HD12	1:A:231:VAL:HA	1.92	0.50
3:D:360:ILE:HG22	3:D:368:TRP:HE3	1.75	0.50
3:D:541:SER:O	3:D:544:LEU:HB2	2.10	0.50
1:A:468:MET:HE1	1:A:770:VAL:HG22	1.92	0.50
2:B:485:ILE:O	2:B:489:VAL:HG23	2.12	0.50
2:B:522:SER:O	2:B:717:ILE:HG23	2.12	0.50
1:A:357:GLN:HG3	1:A:380:ILE:HG21	1.94	0.50
1:A:811:MET:CB	3:D:635:PHE:CE2	2.95	0.50
2:B:192:VAL:CB	2:B:195:TYR:HE2	2.24	0.50
2:B:395:SER:C	2:B:396:ILE:HG13	2.36	0.50
2:B:399:LEU:HD23	2:B:400:GLU:H	1.76	0.50
2:B:411:ASP:C	2:B:411:ASP:OD1	2.50	0.50
2:B:534:PRO:CD	2:B:804:ASN:OD1	2.60	0.50
1:C:128:TYR:CD2	1:C:137:PHE:CE1	2.99	0.50
1:A:436:CYS:HA	1:A:474:VAL:O	2.11	0.50
1:A:578:LEU:CG	1:A:627:ALA:HB2	2.38	0.50
1:A:581:PHE:HB2	2:B:823:PHE:HZ	1.75	0.50
2:B:172:TYR:CD1	2:B:173:ARG:N	2.79	0.50
2:B:621:ILE:CG2	2:B:622:TRP:N	2.75	0.50
2:B:659:GLN:CD	2:B:686:TYR:CZ	2.90	0.50
1:C:78:VAL:HG11	1:C:110:THR:HG21	1.93	0.50
1:C:80:GLU:O	1:C:84:SER:HB3	2.12	0.50
1:C:575:LEU:HD23	1:C:575:LEU:C	2.37	0.50
1:C:803:PRO:O	1:C:805:THR:HG23	2.12	0.50
1:A:554:GLN:HG2	2:B:797:SER:O	2.12	0.50
2:B:768:LEU:N	2:B:768:LEU:CD1	2.75	0.50
1:C:481:LYS:O	1:C:499:MET:HB2	2.12	0.50
1:C:636:LEU:HD22	1:C:636:LEU:C	2.36	0.50
3:D:554:MET:HA	3:D:554:MET:CE	2.39	0.50
1:A:668:PRO:CB	2:B:785:THR:CG2	2.89	0.50
1:A:690:TYR:CE2	1:A:752:PHE:CE2	2.99	0.50
2:B:197:THR:HG23	2:B:198:LEU:CD1	2.42	0.50
2:B:660:ARG:N	2:B:661:PRO:HD3	2.25	0.50
1:C:53:HIS:CE1	1:C:293:HIS:CD2	3.00	0.50
3:D:494:VAL:HA	3:D:499:ALA:O	2.12	0.50
1:A:427:ASN:CB	1:A:793:TYR:CZ	2.95	0.50
1:A:698:SER:HA	2:B:419:ARG:NH2	2.22	0.50
2:B:765:LEU:CD1	1:C:523:GLN:CG	2.82	0.50
1:C:634:TRP:CD1	1:C:634:TRP:N	2.79	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:345:SER:OG	3:D:353:MET:HB3	2.12	0.50
3:D:630:PHE:CD1	3:D:630:PHE:C	2.90	0.50
2:B:267:GLY:HA2	2:B:358:LEU:O	2.12	0.49
1:A:496:TRP:CZ2	1:A:524:TYR:CB	2.96	0.49
1:A:510:MET:CG	1:A:760:MET:SD	3.00	0.49
1:A:526:GLU:N	1:A:762:LYS:HD3	2.27	0.49
2:B:359:ASN:CB	2:B:363:GLU:O	2.60	0.49
2:B:397:VAL:HG23	2:B:467:LEU:HA	1.95	0.49
2:B:399:LEU:HB2	2:B:484:MET:CE	2.42	0.49
2:B:505:GLU:CD	2:B:680:ARG:NH1	2.70	0.49
1:C:57:LYS:C	1:C:58:ILE:HG13	2.36	0.49
1:C:75:ALA:O	1:C:78:VAL:HB	2.12	0.49
3:D:283:ASP:CA	3:D:285:PRO:HD2	2.42	0.49
4:F:18:UNK:HA	4:F:77:UNK:C	2.42	0.49
2:B:31:ALA:O	2:B:90:VAL:HA	2.13	0.49
2:B:725:TYR:CZ	2:B:729:ARG:HG3	2.48	0.49
1:C:78:VAL:CG1	1:C:110:THR:HG21	2.42	0.49
1:C:478:ALA:N	1:C:502:GLU:OE2	2.34	0.49
1:C:481:LYS:HB2	1:C:498:GLY:CA	2.37	0.49
1:C:802:ALA:H	1:C:803:PRO:HD2	1.74	0.49
3:D:570:PHE:O	3:D:574:SER:N	2.32	0.49
1:A:574:MET:CB	2:B:816:MET:HE1	2.42	0.49
1:A:637:PHE:CE2	2:B:812:LEU:HB2	2.47	0.49
2:B:249:VAL:HG23	2:B:268:LEU:HD23	1.94	0.49
2:B:517:VAL:HG12	2:B:518:GLU:N	2.25	0.49
1:C:576:TYR:O	1:C:577:LEU:C	2.53	0.49
1:C:653:LEU:O	1:C:653:LEU:HD12	2.13	0.49
3:D:73:PRO:O	3:D:77:ILE:HD12	2.12	0.49
3:D:143:PRO:O	3:D:144:SER:C	2.55	0.49
3:D:202:MET:O	3:D:202:MET:HG2	2.11	0.49
3:D:321:GLU:O	3:D:324:VAL:CG1	2.55	0.49
3:D:562:VAL:CA	3:D:565:VAL:CG2	2.87	0.49
1:A:811:MET:CB	3:D:635:PHE:CZ	2.86	0.49
3:D:53:ASP:O	3:D:54:PHE:C	2.52	0.49
3:D:143:PRO:O	3:D:144:SER:O	2.30	0.49
1:A:283:ASP:OD2	1:A:335:THR:HG22	2.12	0.49
1:A:398:LEU:HD23	1:A:766:TRP:CZ3	2.46	0.49
1:A:811:MET:H	3:D:631:PHE:HE2	1.56	0.49
2:B:151:LEU:O	2:B:155:GLU:HG2	2.11	0.49
2:B:523:VAL:CG2	2:B:717:ILE:CD1	2.87	0.49
1:C:73:GLN:O	1:C:77:SER:CB	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:SER:O	1:C:81:ASP:HB3	2.12	0.49
3:D:361:LEU:HD23	3:D:362:LEU:N	2.28	0.49
3:D:540:PRO:CD	3:D:810:ASN:HB2	2.42	0.49
3:D:636:LEU:HD12	3:D:639:TYR:HD2	1.78	0.49
1:A:60:LEU:HD11	1:A:293:HIS:HE1	1.76	0.49
1:A:117:PRO:HG2	1:A:321:PHE:CE2	2.47	0.49
1:A:496:TRP:O	1:A:497:ASN:CB	2.59	0.49
2:B:249:VAL:HG21	2:B:268:LEU:HD21	1.94	0.49
1:C:168:SER:CA	1:C:197:PHE:CE1	2.96	0.49
1:C:551:SER:O	1:C:555:PRO:HD2	2.12	0.49
1:C:653:LEU:HD12	1:C:653:LEU:C	2.38	0.49
3:D:165:SER:OG	3:D:195:GLU:HB3	2.13	0.49
1:A:533:TYR:HA	1:A:754:SER:O	2.13	0.49
2:B:142:SER:HB2	2:B:344:GLU:OE2	2.13	0.49
2:B:163:SER:O	2:B:220:LEU:HB2	2.13	0.49
2:B:405:VAL:CG1	2:B:406:ILE:N	2.76	0.49
3:D:422:CYS:SG	3:D:449:CYS:HB3	2.53	0.49
3:D:530:MET:C	3:D:531:VAL:CG1	2.85	0.49
1:A:67:HIS:ND1	1:A:67:HIS:O	2.45	0.49
2:B:397:VAL:CG2	2:B:467:LEU:HA	2.43	0.49
2:B:402:ALA:N	2:B:403:PRO:CD	2.75	0.49
1:C:290:GLN:OE1	1:C:330:TYR:HB2	2.13	0.49
1:C:292:ILE:HG12	1:C:321:PHE:HZ	1.78	0.49
3:D:540:PRO:HD2	3:D:810:ASN:HB2	1.95	0.49
1:A:147:GLN:NE2	1:A:250:GLY:HA2	2.28	0.49
1:A:574:MET:HE1	2:B:819:SER:OG	2.12	0.49
2:B:192:VAL:CG2	2:B:195:TYR:HE2	2.11	0.49
2:B:204:ASP:N	2:B:204:ASP:OD1	2.44	0.49
1:C:78:VAL:HB	1:C:110:THR:HG21	1.93	0.49
1:C:315:TRP:CZ3	1:C:317:THR:O	2.66	0.49
3:D:34:VAL:HG13	3:D:93:VAL:HB	1.95	0.49
1:A:834:ALA:C	1:A:836:LYS:H	2.21	0.48
2:B:724:ASN:OD1	2:B:737:THR:HG21	2.13	0.48
1:C:697:LEU:C	1:C:699:THR:N	2.65	0.48
3:D:284:LEU:N	3:D:285:PRO:HD3	2.22	0.48
1:A:221:LEU:HD11	1:A:253:GLU:HG2	1.95	0.48
1:A:668:PRO:HG3	2:B:785:THR:CB	2.43	0.48
1:C:673:PRO:HG3	1:C:679:TYR:OH	2.12	0.48
3:D:530:MET:C	3:D:531:VAL:HG13	2.37	0.48
1:A:267:ILE:HD13	1:A:267:ILE:N	2.27	0.48
1:A:830:PHE:O	1:A:834:ALA:N	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:247:TRP:CB	2:B:268:LEU:CB	2.70	0.48
2:B:425:ARG:O	2:B:466:TYR:HA	2.13	0.48
1:C:229:THR:HG22	1:C:258:ALA:HA	1.95	0.48
1:A:103:THR:N	1:A:104:PRO:CD	2.76	0.48
1:A:221:LEU:CD1	1:A:253:GLU:HG2	2.44	0.48
1:A:225:GLU:OE2	1:A:255:SER:OG	2.21	0.48
1:A:778:HIS:HD2	3:D:752:THR:OG1	1.95	0.48
1:A:811:MET:HG2	3:D:635:PHE:HE2	1.78	0.48
2:B:109:SER:O	2:B:110:SER:C	2.56	0.48
2:B:119:ILE:CB	2:B:283:ARG:HB3	2.44	0.48
1:C:455:GLY:HA2	1:C:790:TRP:CH2	2.48	0.48
1:C:823:VAL:O	1:C:826:ILE:HG13	2.13	0.48
3:D:734:GLY:C	3:D:793:ILE:H	2.21	0.48
1:A:140:THR:HB	1:A:346:ARG:HD2	1.96	0.48
1:A:461:LEU:HD13	1:A:512:VAL:HG21	1.95	0.48
1:A:468:MET:HE1	1:A:770:VAL:CG2	2.44	0.48
1:A:540:VAL:O	1:A:745:VAL:O	2.31	0.48
1:A:609:TRP:CZ3	1:A:612:LEU:CD1	2.93	0.48
2:B:30:ILE:HA	2:B:89:GLY:O	2.13	0.48
2:B:79:CYS:CB	2:B:312:CYS:HG	2.24	0.48
2:B:534:PRO:CG	2:B:804:ASN:OD1	2.61	0.48
2:B:768:LEU:HG	1:C:519:ASN:N	2.28	0.48
1:A:80:GLU:HG2	1:A:81:ASP:OD1	2.14	0.48
1:A:291:ALA:C	1:A:321:PHE:HE1	2.20	0.48
1:A:325:LEU:HD12	1:A:328:SER:OG	2.14	0.48
1:A:496:TRP:HE1	1:A:504:LEU:CD2	2.27	0.48
1:A:539:LEU:O	1:A:539:LEU:HG	2.13	0.48
1:A:574:MET:HE3	2:B:820:LEU:CG	2.42	0.48
1:A:602:SER:O	1:A:606:TRP:CE3	2.67	0.48
1:A:609:TRP:CE3	1:A:609:TRP:HA	2.48	0.48
2:B:235:ALA:HA	2:B:238:LEU:HB2	1.95	0.48
2:B:539:GLU:N	2:B:540:PRO:HD2	2.29	0.48
2:B:659:GLN:CD	2:B:686:TYR:HH	2.19	0.48
1:C:535:GLY:O	1:C:731:SER:OG	2.31	0.48
3:D:410:VAL:HG22	3:D:454:CYS:HB2	1.95	0.48
1:A:208:LEU:HB3	1:A:240:MET:CE	2.33	0.48
2:B:124:SER:O	2:B:139:PHE:CB	2.62	0.48
2:B:639:ALA:O	2:B:642:ILE:HB	2.13	0.48
2:B:664:TYR:HB3	2:B:666:PRO:HD2	1.95	0.48
2:B:683:ARG:HD3	2:B:690:HIS:CE1	2.49	0.48
3:D:561:ILE:O	3:D:565:VAL:CG2	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:606:VAL:N	3:D:628:TRP:HZ3	2.12	0.48
5:J:2:NAG:H3	5:J:2:NAG:C8	2.29	0.48
1:A:34:SER:CB	1:A:96:PRO:HG3	2.41	0.48
1:A:202:LYS:O	1:A:204:LEU:CD2	2.62	0.48
2:B:659:GLN:CD	2:B:686:TYR:CE2	2.91	0.48
1:C:50:ASN:O	1:C:55:THR:OG1	2.31	0.48
1:C:468:MET:HE2	1:C:773:ASN:OD1	2.14	0.48
3:D:543:PHE:CD1	3:D:639:TYR:CD1	3.02	0.48
3:D:606:VAL:CA	3:D:628:TRP:CH2	2.96	0.48
5:E:2:NAG:C8	5:E:2:NAG:C1	2.92	0.48
1:A:202:LYS:C	1:A:204:LEU:HD23	2.38	0.48
1:A:500:MET:CE	1:A:521:ARG:CG	2.92	0.48
1:A:541:LYS:CB	1:A:744:LEU:HA	2.44	0.48
1:A:657:ARG:N	1:A:658:PRO:HD2	2.29	0.48
2:B:775:GLU:HA	2:B:778:GLU:CG	2.44	0.48
1:C:103:THR:CB	1:C:104:PRO:HD3	2.44	0.48
3:D:562:VAL:CA	3:D:565:VAL:HG23	2.42	0.48
1:A:302:THR:O	1:A:315:TRP:CE2	2.67	0.48
1:A:440:ASP:CB	1:A:447:PRO:HD2	2.43	0.48
1:A:511:ILE:O	1:A:758:ILE:HG13	2.14	0.48
2:B:31:ALA:H	2:B:90:VAL:HG12	1.79	0.48
2:B:680:ARG:HG3	2:B:683:ARG:HH21	1.79	0.48
1:C:301:ILE:HG23	1:C:317:THR:OG1	2.12	0.48
1:C:640:ILE:HG22	3:D:811:MET:CE	2.42	0.48
3:D:543:PHE:HE1	3:D:643:LEU:HD11	1.79	0.48
1:A:150:VAL:HG22	1:A:367:PHE:CD2	2.49	0.47
1:A:287:VAL:HG22	1:A:330:TYR:CB	2.44	0.47
1:A:519:ASN:HA	1:A:522:ALA:HB3	1.96	0.47
1:A:607:PHE:C	1:A:610:ARG:CG	2.79	0.47
2:B:31:ALA:O	2:B:90:VAL:HB	2.14	0.47
2:B:347:TYR:CG	2:B:348:GLN:N	2.82	0.47
2:B:401:GLU:O	2:B:406:ILE:HD11	2.13	0.47
3:D:559:LEU:C	3:D:559:LEU:CD2	2.88	0.47
2:B:172:TYR:CG	2:B:173:ARG:N	2.82	0.47
2:B:458:THR:HG21	2:B:770:PHE:CZ	2.49	0.47
2:B:484:MET:O	2:B:488:VAL:HG23	2.14	0.47
1:C:138:LEU:HD22	1:C:325:LEU:CD2	2.44	0.47
1:C:142:PRO:CG	1:C:349:ALA:HB3	2.43	0.47
1:C:354:MET:SD	1:C:361:LEU:CB	3.01	0.47
1:C:629:ILE:CG2	3:D:825:SER:HB3	2.45	0.47
1:C:731:SER:O	1:C:735:GLU:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:GLY:O	1:A:502:GLU:C	2.54	0.47
1:A:516:THR:CG2	1:A:754:SER:OG	2.60	0.47
1:A:630:LEU:CG	2:B:816:MET:SD	2.98	0.47
1:C:142:PRO:CD	1:C:349:ALA:CB	2.92	0.47
3:D:600:TRP:HA	3:D:603:TRP:HB2	1.96	0.47
4:F:164:UNK:HA	4:F:176:UNK:HA	1.97	0.47
1:A:574:MET:CE	2:B:820:LEU:HD23	2.44	0.47
2:B:124:SER:O	2:B:139:PHE:HA	2.14	0.47
2:B:128:ALA:HB2	2:B:170:PRO:HG3	1.95	0.47
2:B:243:TYR:HD1	2:B:243:TYR:H	1.60	0.47
2:B:801:ASP:HB3	2:B:804:ASN:HB3	1.95	0.47
1:C:83:ILE:HD13	1:C:114:TYR:CE2	2.49	0.47
3:D:328:HIS:ND1	3:D:328:HIS:C	2.73	0.47
1:A:535:GLY:O	1:A:731:SER:HB2	2.14	0.47
1:A:621:ALA:HB2	2:B:594:TRP:CZ2	2.50	0.47
2:B:341:SER:O	2:B:349:ALA:N	2.36	0.47
1:C:649:LEU:C	1:C:649:LEU:HD23	2.39	0.47
3:D:507:THR:HG22	3:D:508:ILE:H	1.79	0.47
1:A:121:LEU:CD2	1:A:281:ILE:CG1	2.91	0.47
2:B:517:VAL:CG1	2:B:518:GLU:N	2.77	0.47
3:D:195:GLU:CD	3:D:220:SER:HB3	2.39	0.47
1:A:113:PHE:CE2	1:A:312:THR:HA	2.50	0.47
1:A:220:ILE:HG12	1:A:248:LEU:HB2	1.97	0.47
1:A:574:MET:HG3	2:B:816:MET:CE	2.43	0.47
1:A:767:LYS:HD2	1:A:767:LYS:C	2.40	0.47
2:B:512:PHE:HB3	2:B:751:ILE:N	2.29	0.47
2:B:524:MET:HE1	2:B:723:LEU:C	2.34	0.47
2:B:540:PRO:HB2	1:C:803:PRO:CG	2.38	0.47
2:B:682:ILE:HG22	2:B:690:HIS:HB2	1.97	0.47
2:B:765:LEU:CD2	1:C:523:GLN:CG	2.74	0.47
1:C:142:PRO:CD	1:C:349:ALA:HB2	2.44	0.47
1:C:398:LEU:HD23	1:C:398:LEU:HA	1.81	0.47
1:C:483:GLY:HA2	1:C:497:ASN:O	2.15	0.47
1:C:503:LEU:CD1	1:C:508:ALA:O	2.59	0.47
1:C:700:MET:C	1:C:704:MET:HE2	2.40	0.47
3:D:177:PHE:O	3:D:181:VAL:HG23	2.14	0.47
3:D:761:LYS:HA	3:D:761:LYS:HD2	1.48	0.47
1:A:150:VAL:HG22	1:A:367:PHE:CE2	2.50	0.47
1:A:379:ILE:HG21	1:A:381:TRP:CE2	2.50	0.47
1:A:538:ILE:HG22	1:A:540:VAL:HG12	1.95	0.47
1:A:681:THR:HG22	1:A:704:MET:SD	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:50:THR:O	2:B:54:SER:HB2	2.14	0.47
2:B:74:ILE:HG21	2:B:105:LEU:CD2	2.31	0.47
2:B:256:ASN:OD1	2:B:256:ASN:N	2.40	0.47
2:B:370:TRP:CD1	2:B:375:LEU:HA	2.50	0.47
2:B:532:VAL:O	2:B:533:SER:HB2	2.15	0.47
3:D:670:PHE:CG	3:D:672:PRO:HD2	2.50	0.47
1:A:621:ALA:CB	1:A:622:PRO:HD3	2.38	0.47
2:B:542:SER:HA	2:B:546:TRP:HB2	1.96	0.47
3:D:560:LEU:HD22	3:D:560:LEU:C	2.36	0.47
3:D:744:ILE:O	3:D:747:GLY:N	2.37	0.47
2:B:32:VAL:HG13	2:B:91:VAL:CG2	2.43	0.47
2:B:151:LEU:HA	2:B:154:MET:HB2	1.95	0.47
2:B:657:LYS:O	2:B:668:PHE:HE1	1.98	0.47
1:C:30:GLY:O	1:C:90:ILE:HA	2.15	0.47
1:A:34:SER:CB	1:A:96:PRO:HD3	2.45	0.46
1:A:258:ALA:O	1:A:262:ALA:HB2	2.15	0.46
2:B:145:GLN:NE2	2:B:351:PRO:HG2	2.29	0.46
2:B:249:VAL:HG23	2:B:268:LEU:CD2	2.45	0.46
2:B:249:VAL:HB	2:B:270:SER:HA	1.97	0.46
2:B:448:CYS:SG	2:B:497:VAL:CG1	3.03	0.46
1:C:630:LEU:HD11	3:D:826:LEU:HD21	1.96	0.46
3:D:565:VAL:O	3:D:569:VAL:HB	2.14	0.46
3:D:639:TYR:CD1	3:D:639:TYR:C	2.92	0.46
1:A:204:LEU:HD11	1:A:231:VAL:HA	1.98	0.46
1:A:398:LEU:HD21	1:A:766:TRP:CZ3	2.51	0.46
1:A:485:GLN:HA	1:A:496:TRP:HA	1.97	0.46
1:A:551:SER:O	1:A:645:TYR:HE1	1.98	0.46
1:A:564:VAL:HG21	2:B:809:PHE:CZ	2.51	0.46
1:A:663:THR:O	1:A:667:ASP:N	2.48	0.46
2:B:157:TYR:OH	2:B:246:VAL:CG1	2.59	0.46
1:C:117:PRO:HG2	1:C:321:PHE:HD2	1.79	0.46
1:C:283:ASP:CB	1:C:335:THR:HG22	2.46	0.46
1:C:575:LEU:HB3	1:C:634:TRP:HZ3	1.77	0.46
3:D:148:GLN:O	3:D:152:MET:HG3	2.15	0.46
2:B:268:LEU:HD13	2:B:268:LEU:C	2.38	0.46
1:C:201:THR:CB	1:C:204:LEU:HD21	2.45	0.46
1:C:669:ARG:O	1:C:672:ASN:O	2.34	0.46
4:G:235:UNK:HA	4:G:293:UNK:O	2.16	0.46
1:A:140:THR:HB	1:A:346:ARG:CD	2.46	0.46
1:A:496:TRP:HZ2	1:A:524:TYR:HB3	1.79	0.46
1:A:574:MET:HE3	2:B:820:LEU:HD23	1.89	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:197:THR:O	2:B:207:THR:HG21	2.15	0.46
2:B:405:VAL:HA	2:B:445:LYS:O	2.16	0.46
2:B:520:GLY:CA	2:B:743:ILE:CB	2.93	0.46
1:C:117:PRO:HG2	1:C:321:PHE:CD2	2.51	0.46
2:B:680:ARG:O	2:B:684:ASN:ND2	2.44	0.46
1:C:58:ILE:HG21	1:C:296:PHE:HE2	1.81	0.46
1:C:77:SER:O	1:C:81:ASP:CB	2.63	0.46
1:C:771:SER:O	1:C:772:LEU:C	2.58	0.46
3:D:58:PRO:HG3	3:D:303:LEU:CD1	2.45	0.46
1:A:811:MET:CB	3:D:631:PHE:CD2	2.98	0.46
1:C:76:LEU:C	1:C:78:VAL:N	2.70	0.46
1:C:184:LEU:CB	1:C:189:SER:HA	2.46	0.46
1:C:643:ALA:O	1:C:646:THR:OG1	2.25	0.46
2:B:31:ALA:CA	2:B:90:VAL:HG12	2.45	0.46
2:B:192:VAL:HG22	2:B:193:GLN:N	2.30	0.46
2:B:194:ASN:HB2	2:B:214:ILE:CG1	2.45	0.46
1:C:92:VAL:HG11	1:C:104:PRO:HB3	1.97	0.46
3:D:302:MET:HE2	3:D:330:LEU:HD21	1.98	0.46
1:A:46:VAL:HG21	1:A:62:ALA:HB2	1.98	0.46
1:A:259:LEU:O	1:A:359:ARG:NH2	2.49	0.46
1:A:637:PHE:HD1	2:B:808:VAL:CG1	2.21	0.46
2:B:163:SER:HB2	2:B:194:ASN:HD22	1.79	0.46
1:C:32:VAL:HG12	1:C:67:HIS:NE2	2.31	0.46
1:A:30:GLY:O	1:A:90:ILE:HA	2.15	0.46
1:A:53:HIS:O	1:A:54:PHE:O	2.33	0.46
1:A:249:VAL:HG13	1:A:266:ILE:HD11	1.98	0.46
1:A:696:GLU:H	1:A:696:GLU:CD	2.17	0.46
2:B:64:LEU:HD12	2:B:81:LEU:HD13	1.75	0.46
1:C:46:VAL:HG21	1:C:62:ALA:HB2	1.98	0.46
3:D:514:GLU:O	3:D:761:LYS:NZ	2.49	0.46
1:A:241:THR:HG21	1:A:263:PRO:HB3	1.98	0.45
1:A:603:SER:O	1:A:607:PHE:CG	2.69	0.45
1:A:626:SER:HA	1:A:629:ILE:HD11	1.98	0.45
2:B:91:VAL:HG21	2:B:284:VAL:HG13	1.98	0.45
2:B:420:ASN:OD1	2:B:420:ASN:C	2.59	0.45
2:B:457:LYS:HE2	2:B:457:LYS:HB2	1.71	0.45
3:D:218:LEU:C	3:D:218:LEU:HD12	2.41	0.45
1:A:27:VAL:HG13	1:A:88:TYR:CG	2.50	0.45
1:A:93:SER:CB	1:A:277:GLU:OE2	2.37	0.45
1:A:291:ALA:HB2	1:A:325:LEU:CD1	2.32	0.45
2:B:160:HIS:CG	2:B:160:HIS:O	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:264:PHE:HE1	2:B:268:LEU:HD21	1.81	0.45
2:B:448:CYS:SG	2:B:497:VAL:HG11	2.56	0.45
2:B:522:SER:HB3	2:B:720:ALA:HB2	1.97	0.45
1:A:170:ASP:O	1:A:174:ARG:HG3	2.16	0.45
1:A:295:LEU:HD22	1:A:321:PHE:CE1	2.51	0.45
1:A:379:ILE:CG2	1:A:381:TRP:NE1	2.80	0.45
1:A:778:HIS:CD2	3:D:752:THR:OG1	2.69	0.45
2:B:634:THR:OG1	1:C:649:LEU:CD2	2.58	0.45
2:B:669:ARG:HD3	2:B:696:PHE:CE2	2.52	0.45
1:C:26:ILE:HD11	1:C:61:ASN:HB2	1.97	0.45
1:C:295:LEU:CD2	1:C:321:PHE:CE1	2.96	0.45
1:C:630:LEU:O	1:C:634:TRP:CG	2.69	0.45
3:D:559:LEU:CD2	3:D:598:ALA:HB1	2.39	0.45
1:A:93:SER:HB3	1:A:121:LEU:HD12	1.98	0.45
1:A:811:MET:HA	3:D:631:PHE:CD2	2.52	0.45
1:C:80:GLU:O	1:C:84:SER:CB	2.64	0.45
1:C:439:PRO:CD	1:C:476:LEU:HB2	2.45	0.45
3:D:726:ALA:O	3:D:730:ASN:ND2	2.34	0.45
4:G:255:UNK:C	4:G:257:UNK:N	2.79	0.45
1:A:357:GLN:HE21	1:A:380:ILE:HB	1.82	0.45
1:A:503:LEU:HD11	1:A:761:ARG:CA	2.46	0.45
2:B:58:ASP:C	2:B:59:VAL:HG23	2.41	0.45
2:B:166:THR:CB	2:B:172:TYR:HB2	2.46	0.45
2:B:523:VAL:O	2:B:738:ILE:CD1	2.64	0.45
2:B:621:ILE:HD11	1:C:818:VAL:HG22	1.98	0.45
1:C:519:ASN:HD21	1:C:523:GLN:HE21	1.65	0.45
1:C:674:SER:HB3	1:C:677:PHE:CB	2.42	0.45
1:C:679:TYR:H	1:C:703:HIS:CE1	2.33	0.45
1:A:251:GLU:O	1:A:254:ILE:HG12	2.17	0.45
1:A:550:ASP:OD1	1:A:652:PHE:CD1	2.69	0.45
1:A:560:LEU:HD12	2:B:802:ILE:CA	2.45	0.45
2:B:57:PHE:CB	2:B:292:THR:HG21	2.11	0.45
2:B:490:TYR:O	2:B:491:LYS:HB3	2.16	0.45
2:B:502:ILE:C	2:B:503:ASN:HD22	2.24	0.45
2:B:621:ILE:CD1	1:C:818:VAL:HG22	2.46	0.45
1:C:204:LEU:O	1:C:208:LEU:HD12	2.17	0.45
3:D:147:GLN:O	3:D:151:VAL:HG23	2.16	0.45
3:D:332:ARG:HG3	3:D:335:ILE:HD11	1.99	0.45
3:D:666:ARG:HA	3:D:667:PRO:HD2	1.80	0.45
1:A:607:PHE:CA	1:A:610:ARG:CG	2.93	0.45
2:B:31:ALA:N	2:B:90:VAL:HG12	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:163:SER:O	2:B:220:LEU:CB	2.64	0.45
2:B:393:HIS:HA	2:B:462:THR:C	2.41	0.45
2:B:393:HIS:CA	2:B:462:THR:O	2.65	0.45
1:C:438:GLY:HA2	1:C:476:LEU:HD12	1.98	0.45
3:D:533:ARG:CB	3:D:653:VAL:HA	2.46	0.45
3:D:566:ALA:O	3:D:570:PHE:N	2.41	0.45
2:B:247:TRP:HB3	2:B:268:LEU:HD23	1.98	0.45
2:B:399:LEU:HD12	2:B:473:HIS:ND1	2.32	0.45
2:B:800:LEU:HD12	2:B:800:LEU:HA	1.85	0.45
1:C:53:HIS:CG	1:C:293:HIS:CE1	2.90	0.45
2:B:520:GLY:C	2:B:743:ILE:HB	2.41	0.45
1:C:23:ASP:N	1:C:24:PRO:CD	2.79	0.45
1:A:122:THR:HG23	1:A:277:GLU:HG2	1.98	0.45
1:A:254:ILE:HD11	1:A:270:GLN:HG3	1.99	0.45
2:B:408:GLU:CG	2:B:445:LYS:HZ2	2.29	0.45
2:B:830:TYR:O	2:B:831:LYS:C	2.59	0.45
1:C:678:ILE:N	1:C:725:HIS:HD2	2.02	0.45
3:D:507:THR:CG2	3:D:753:THR:HG21	2.47	0.45
1:A:398:LEU:HD12	1:A:470:PHE:CD2	2.40	0.44
1:A:440:ASP:CB	1:A:449:VAL:CG2	2.96	0.44
1:A:510:MET:HA	1:A:760:MET:HG2	1.99	0.44
1:A:524:TYR:O	1:A:762:LYS:HE2	2.15	0.44
2:B:204:ASP:O	2:B:207:THR:OG1	2.28	0.44
2:B:527:ARG:CB	2:B:648:ASP:CA	2.94	0.44
1:C:138:LEU:CD2	1:C:325:LEU:HD23	2.47	0.44
3:D:284:LEU:O	3:D:285:PRO:C	2.60	0.44
3:D:526:GLY:HA2	3:D:753:THR:HG22	1.99	0.44
3:D:657:SER:O	3:D:744:ILE:HD11	2.16	0.44
1:A:663:THR:O	1:A:667:ASP:CB	2.64	0.44
2:B:157:TYR:OH	2:B:246:VAL:CG2	2.60	0.44
2:B:169:PHE:CB	2:B:170:PRO:HD3	2.39	0.44
3:D:556:PHE:HD1	3:D:556:PHE:HA	1.69	0.44
1:A:34:SER:CB	1:A:96:PRO:CG	2.89	0.44
1:A:115:ARG:HG3	1:A:315:TRP:H	1.83	0.44
1:A:456:PHE:N	1:A:790:TRP:CH2	2.85	0.44
1:A:555:PRO:O	1:A:556:PHE:C	2.60	0.44
2:B:42:GLU:O	2:B:46:ARG:N	2.49	0.44
2:B:169:PHE:CE2	2:B:227:GLU:OE1	2.70	0.44
2:B:243:TYR:N	2:B:243:TYR:CD1	2.86	0.44
2:B:405:VAL:O	2:B:406:ILE:CD1	2.63	0.44
1:C:134:HIS:N	1:C:134:HIS:CD2	2.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:162:TYR:O	3:D:192:TRP:HB2	2.17	0.44
3:D:326:GLU:C	3:D:328:HIS:N	2.75	0.44
1:A:78:VAL:O	1:A:82:LEU:HB2	2.17	0.44
2:B:50:THR:HA	2:B:53:MET:HB2	1.99	0.44
2:B:490:TYR:O	2:B:491:LYS:CB	2.64	0.44
2:B:522:SER:OG	2:B:720:ALA:HA	2.17	0.44
1:A:46:VAL:O	1:A:49:ALA:CB	2.60	0.44
2:B:65:LEU:HD23	2:B:66:VAL:N	2.32	0.44
2:B:775:GLU:C	2:B:778:GLU:H	2.24	0.44
1:C:425:THR:CG2	1:C:431:ILE:HG13	2.38	0.44
1:A:41:ILE:HG21	1:A:278:SER:OG	2.18	0.44
1:A:283:ASP:CG	1:A:334:VAL:N	2.75	0.44
2:B:120:HIS:CG	2:B:280:ILE:CD1	3.00	0.44
1:C:397:ARG:CA	1:C:471:THR:OG1	2.60	0.44
3:D:360:ILE:HG22	3:D:368:TRP:CE3	2.51	0.44
1:A:257:SER:O	1:A:258:ALA:C	2.60	0.44
1:A:264:ASP:OD1	1:A:356:LEU:O	2.36	0.44
1:A:554:GLN:HB2	1:A:555:PRO:CD	2.48	0.44
2:B:221:LEU:HD12	2:B:221:LEU:N	2.33	0.44
2:B:459:VAL:O	2:B:459:VAL:CG1	2.64	0.44
2:B:520:GLY:O	2:B:743:ILE:HG22	2.15	0.44
1:C:276:ASN:HB3	1:C:279:ALA:CB	2.46	0.44
1:C:367:PHE:HD1	1:C:372:ILE:HA	1.82	0.44
1:C:569:HIS:H	1:C:569:HIS:HD1	1.64	0.44
1:A:65:VAL:HG13	1:A:67:HIS:H	1.83	0.44
2:B:173:ARG:HD3	2:B:173:ARG:HA	1.32	0.44
2:B:176:ILE:O	2:B:180:LYS:HG2	2.17	0.44
1:C:138:LEU:HD22	1:C:325:LEU:HD21	1.99	0.44
1:C:629:ILE:HG21	3:D:825:SER:HB3	1.99	0.44
1:A:736:PHE:HD1	1:A:794:GLN:OE1	2.01	0.44
1:A:807:THR:HG22	1:A:807:THR:O	2.17	0.44
1:A:818:VAL:CG2	3:D:558:MET:HE1	2.47	0.44
2:B:58:ASP:O	2:B:59:VAL:HG23	2.18	0.44
2:B:124:SER:O	2:B:139:PHE:CA	2.66	0.44
2:B:140:GLY:HA3	2:B:345:ASP:HB3	1.99	0.44
2:B:355:VAL:HG12	2:B:367:VAL:CB	2.47	0.44
2:B:504:GLU:CG	1:C:775:LEU:HB3	2.48	0.44
1:C:78:VAL:CG1	1:C:110:THR:CG2	2.95	0.44
1:C:298:MET:SD	1:C:320:LEU:CD2	3.01	0.44
3:D:198:ILE:HD12	3:D:215:LEU:HD23	2.00	0.44
1:A:204:LEU:HD11	1:A:230:ALA:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:704:MET:SD	1:A:704:MET:C	3.01	0.43
2:B:58:ASP:O	2:B:59:VAL:CG2	2.66	0.43
2:B:520:GLY:C	2:B:743:ILE:CB	2.91	0.43
3:D:759:ILE:HG22	3:D:760:GLN:N	2.33	0.43
2:B:108:VAL:O	2:B:112:THR:HG23	2.18	0.43
2:B:182:THR:HG23	2:B:190:TRP:HZ3	1.75	0.43
2:B:339:ASP:C	2:B:339:ASP:OD1	2.61	0.43
2:B:491:LYS:HD3	2:B:491:LYS:HA	1.58	0.43
2:B:621:ILE:HD12	2:B:621:ILE:O	2.17	0.43
1:C:438:GLY:HA2	1:C:439:PRO:HD2	1.80	0.43
1:A:102:LEU:CB	1:A:128:TYR:HH	2.31	0.43
1:A:780:ASN:C	1:A:780:ASN:OD1	2.59	0.43
2:B:198:LEU:HB2	2:B:207:THR:HG23	1.92	0.43
2:B:425:ARG:NH1	2:B:466:TYR:HB3	2.34	0.43
2:B:559:MET:SD	2:B:618:ILE:HG21	2.58	0.43
2:B:685:ASN:HB3	2:B:686:TYR:CD1	2.53	0.43
1:C:517:ILE:CD1	1:C:530:PRO:HB3	2.48	0.43
1:C:575:LEU:HB3	1:C:634:TRP:CZ3	2.46	0.43
1:C:606:TRP:HA	1:C:606:TRP:HE3	1.80	0.43
1:C:731:SER:O	1:C:735:GLU:CG	2.66	0.43
1:C:802:ALA:H	1:C:803:PRO:HD3	1.82	0.43
1:A:554:GLN:HG2	2:B:798:SER:HA	2.00	0.43
2:B:240:LEU:O	2:B:245:PHE:CB	2.63	0.43
2:B:630:LEU:O	2:B:634:THR:CG2	2.41	0.43
1:C:78:VAL:CB	1:C:110:THR:HG21	2.48	0.43
1:C:141:VAL:HB	1:C:142:PRO:HD2	2.00	0.43
4:F:13:UNK:O	4:F:108:UNK:N	2.52	0.43
1:A:105:THR:CA	1:A:128:TYR:CE2	2.98	0.43
1:A:317:THR:O	1:A:320:LEU:N	2.50	0.43
1:A:606:TRP:CD1	3:D:623:ILE:HG12	2.54	0.43
1:A:756:PHE:N	1:A:756:PHE:CD1	2.86	0.43
1:A:818:VAL:HG22	3:D:558:MET:HE1	2.00	0.43
2:B:128:ALA:HB2	2:B:170:PRO:CG	2.48	0.43
2:B:768:LEU:O	2:B:771:VAL:HB	2.18	0.43
1:C:53:HIS:HD1	1:C:53:HIS:HA	1.73	0.43
1:C:408:PHE:HA	1:C:456:PHE:HB3	2.00	0.43
1:C:729:TRP:CG	1:C:730:ASP:H	2.36	0.43
3:D:168:THR:HG22	3:D:169:THR:N	2.33	0.43
3:D:345:SER:O	3:D:353:MET:CB	2.66	0.43
1:A:80:GLU:O	1:A:84:SER:OG	2.31	0.43
1:A:520:GLU:CB	1:A:693:ARG:NH2	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:668:PRO:HB3	2:B:785:THR:CG2	2.40	0.43
1:A:709:TYR:CE1	1:A:724:LEU:CD1	3.01	0.43
1:A:784:GLU:H	1:A:784:GLU:CD	2.26	0.43
2:B:401:GLU:O	2:B:405:VAL:O	2.36	0.43
2:B:401:GLU:O	2:B:406:ILE:CD1	2.67	0.43
2:B:405:VAL:HG12	2:B:406:ILE:N	2.33	0.43
2:B:468:VAL:CG2	2:B:484:MET:CG	2.59	0.43
2:B:761:ARG:N	2:B:762:PRO:CD	2.81	0.43
3:D:229:LYS:O	3:D:232:ALA:HB3	2.19	0.43
1:A:121:LEU:CG	1:A:281:ILE:HG12	2.41	0.43
1:A:249:VAL:CG1	1:A:266:ILE:HD11	2.48	0.43
1:A:379:ILE:CG2	1:A:381:TRP:CE2	3.02	0.43
1:A:557:GLN:HB2	2:B:798:SER:O	2.19	0.43
1:A:809:GLU:O	1:A:812:ALA:HB3	2.18	0.43
2:B:560:ALA:HB1	2:B:589:ILE:HG12	2.00	0.43
2:B:682:ILE:CG2	2:B:690:HIS:HB2	2.47	0.43
1:C:227:ASP:O	1:C:231:VAL:HG23	2.18	0.43
3:D:130:ALA:O	3:D:131:ASP:C	2.62	0.43
3:D:595:ILE:HB	3:D:596:GLY:H	1.64	0.43
3:D:667:PRO:HG2	3:D:668:ASN:ND2	2.31	0.43
3:D:744:ILE:O	3:D:745:GLY:C	2.62	0.43
1:A:496:TRP:CZ3	1:A:524:TYR:CD2	3.06	0.43
1:C:401:VAL:HG21	1:C:477:VAL:HG23	2.01	0.43
2:B:163:SER:OG	2:B:194:ASN:ND2	2.51	0.43
2:B:194:ASN:OD1	2:B:214:ILE:CD1	2.67	0.43
2:B:196:ILE:HD11	2:B:211:LEU:CD2	2.49	0.43
2:B:249:VAL:CG2	2:B:268:LEU:HD23	2.49	0.43
2:B:640:PHE:O	2:B:641:MET:C	2.57	0.43
1:C:354:MET:HE3	1:C:361:LEU:CA	2.48	0.43
1:C:667:ASP:OD2	1:C:668:PRO:HD2	2.19	0.43
1:A:113:PHE:HD1	1:A:113:PHE:HA	1.76	0.43
1:A:128:TYR:HB3	1:A:137:PHE:CD2	2.54	0.43
2:B:194:ASN:ND2	2:B:211:LEU:CD2	2.69	0.43
2:B:264:PHE:CE1	2:B:268:LEU:HD21	2.54	0.43
2:B:659:GLN:NE2	2:B:686:TYR:CE2	2.80	0.43
2:B:736:VAL:CG1	2:B:737:THR:H	2.32	0.43
1:C:398:LEU:H	1:C:472:TYR:HA	1.83	0.43
1:C:629:ILE:O	1:C:633:VAL:N	2.46	0.43
3:D:200:LEU:CD2	3:D:201:ASP:N	2.65	0.43
4:F:86:UNK:HA	4:F:104:UNK:HA	2.01	0.43
4:G:281:UNK:O	4:G:298:UNK:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:GLN:O	1:A:73:GLN:NE2	2.52	0.42
1:A:164:ILE:HG23	1:A:193:LYS:O	2.18	0.42
1:A:302:THR:HG1	1:A:315:TRP:CD1	2.37	0.42
1:A:303:ASP:HB3	1:A:304:PRO:HD2	2.01	0.42
1:A:525:ILE:HA	1:A:762:LYS:CD	2.48	0.42
2:B:236:ARG:NH1	2:B:263:GLU:OE1	2.51	0.42
2:B:533:SER:HA	2:B:534:PRO:HD2	1.47	0.42
2:B:645:ARG:HA	2:B:794:GLU:HA	2.00	0.42
3:D:236:PHE:HD2	3:D:268:PHE:CD1	2.37	0.42
3:D:402:VAL:HB	3:D:472:TYR:CZ	2.54	0.42
4:F:39:UNK:HA	4:F:45:UNK:HA	2.01	0.42
4:F:141:UNK:CA	4:F:142:UNK:C	2.96	0.42
4:G:336:UNK:HA	4:G:362:UNK:CB	2.49	0.42
1:A:79:CYS:O	1:A:83:ILE:HB	2.19	0.42
1:A:94:HIS:N	1:A:122:THR:HG1	2.05	0.42
2:B:156:GLU:OE2	2:B:157:TYR:HB3	2.20	0.42
2:B:458:THR:HG21	2:B:770:PHE:HZ	1.84	0.42
3:D:452:GLY:HA2	3:D:789:TRP:CE2	2.54	0.42
3:D:786:GLU:O	3:D:791:THR:N	2.50	0.42
4:F:63:UNK:HA	4:F:76:UNK:HA	2.01	0.42
1:A:132:SER:HB3	2:B:172:TYR:CD2	2.50	0.42
1:A:221:LEU:HD23	1:A:247:TRP:CZ3	2.54	0.42
1:A:286:ALA:CB	1:A:330:TYR:HE2	2.28	0.42
2:B:199:ASP:HB3	2:B:200:THR:H	1.67	0.42
3:D:525:THR:HG22	3:D:754:GLY:HA2	2.01	0.42
1:A:121:LEU:CD2	1:A:281:ILE:HA	2.47	0.42
1:A:272:ILE:O	1:A:273:ASN:CB	2.66	0.42
1:A:398:LEU:CD1	1:A:470:PHE:CE2	2.99	0.42
1:A:410:TYR:O	1:A:453:CYS:HA	2.20	0.42
1:A:517:ILE:CD1	1:A:755:GLY:O	2.68	0.42
1:A:662:ILE:CB	1:A:748:GLY:N	2.83	0.42
2:B:32:VAL:CG2	2:B:91:VAL:CG2	2.86	0.42
2:B:405:VAL:C	2:B:406:ILE:HG12	2.44	0.42
1:C:538:ILE:O	1:C:746:THR:HA	2.19	0.42
3:D:225:LEU:HD21	3:D:227:CYS:SG	2.59	0.42
3:D:283:ASP:C	3:D:285:PRO:CD	2.77	0.42
3:D:332:ARG:CG	3:D:335:ILE:HD11	2.49	0.42
3:D:403:THR:HG22	3:D:471:LEU:HD11	2.01	0.42
1:A:140:THR:CB	1:A:346:ARG:HD2	2.50	0.42
2:B:114:ILE:HG23	2:B:115:PRO:HD2	2.00	0.42
2:B:523:VAL:CG2	2:B:717:ILE:HD11	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:673:PRO:CG	1:C:703:HIS:HB3	2.44	0.42
3:D:155:ILE:HD11	3:D:359:ILE:HG12	2.01	0.42
3:D:667:PRO:HG3	3:D:698:TYR:CZ	2.55	0.42
1:A:437:ASN:HB2	1:A:475:HIS:HB2	2.00	0.42
1:A:517:ILE:CG1	1:A:755:GLY:O	2.62	0.42
1:A:554:GLN:HB3	2:B:800:LEU:HD13	2.01	0.42
1:A:575:LEU:HD12	1:A:575:LEU:O	2.20	0.42
2:B:271:VAL:CG2	2:B:354:VAL:O	2.68	0.42
3:D:99:ASP:OD1	3:D:260:ASP:N	2.53	0.42
3:D:298:ALA:O	3:D:301:THR:OG1	2.31	0.42
3:D:433:ILE:H	3:D:444:ASN:C	2.24	0.42
1:A:455:GLY:HA2	1:A:790:TRP:HH2	1.84	0.42
1:A:525:ILE:C	1:A:762:LYS:HE2	2.35	0.42
1:A:540:VAL:HG23	1:A:719:VAL:CG1	2.50	0.42
1:A:566:LEU:O	1:A:569:HIS:HB2	2.20	0.42
2:B:50:THR:O	2:B:54:SER:N	2.52	0.42
2:B:673:VAL:HG21	2:B:718:TYR:OH	2.19	0.42
3:D:332:ARG:CB	3:D:335:ILE:HD11	2.49	0.42
3:D:688:ILE:HG22	3:D:696:HIS:HB2	2.00	0.42
4:F:111:UNK:HA	4:F:141:UNK:O	2.19	0.42
1:A:115:ARG:O	1:A:315:TRP:CE3	2.65	0.42
1:A:621:ALA:HB1	1:A:628:ARG:CB	2.50	0.42
2:B:768:LEU:O	2:B:769:GLN:C	2.61	0.42
3:D:606:VAL:CA	3:D:628:TRP:HH2	2.33	0.42
1:A:102:LEU:C	1:A:128:TYR:HH	2.20	0.42
1:A:739:SER:HA	1:A:742:CYS:SG	2.60	0.42
2:B:251:SER:HA	2:B:254:THR:HB	2.02	0.42
1:C:483:GLY:HA3	1:C:500:MET:HB2	2.00	0.42
3:D:151:VAL:O	3:D:155:ILE:HG13	2.20	0.42
4:F:38:UNK:HA	4:F:87:UNK:HA	2.01	0.42
1:A:140:THR:HA	1:A:346:ARG:HD2	2.02	0.42
1:A:554:GLN:HB2	1:A:555:PRO:HD3	2.01	0.42
2:B:271:VAL:HG23	2:B:354:VAL:O	2.20	0.42
1:C:94:HIS:HA	1:C:95:PRO:HD3	1.88	0.42
3:D:200:LEU:CD1	3:D:211:ILE:CB	2.98	0.42
1:A:561:TRP:CG	1:A:562:LEU:N	2.87	0.41
1:A:626:SER:CA	1:A:629:ILE:HD12	2.47	0.41
1:A:670:LEU:HD23	1:A:670:LEU:C	2.45	0.41
1:A:803:PRO:HG3	3:D:642:ASN:OD1	2.20	0.41
1:A:811:MET:CE	3:D:635:PHE:CE2	3.03	0.41
2:B:135:THR:CB	2:B:137:PHE:CE2	3.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:137:PHE:O	2:B:346:GLY:HA3	2.20	0.41
2:B:154:MET:HE3	2:B:248:ILE:CD1	2.48	0.41
1:C:124:ARG:NH1	1:C:271:LEU:CB	2.83	0.41
1:C:394:MET:SD	1:C:766:TRP:CE2	3.12	0.41
1:C:800:SER:O	1:C:801:ASN:C	2.62	0.41
3:D:562:VAL:O	3:D:566:ALA:N	2.37	0.41
3:D:594:THR:HG22	3:D:598:ALA:CB	2.50	0.41
3:D:606:VAL:CA	3:D:628:TRP:CZ3	3.02	0.41
1:A:517:ILE:HD13	1:A:530:PRO:HB3	2.01	0.41
1:A:630:LEU:HD22	2:B:816:MET:CG	2.37	0.41
2:B:501:THR:HG22	2:B:502:ILE:N	2.35	0.41
2:B:645:ARG:CB	2:B:793:ASN:O	2.68	0.41
1:C:477:VAL:CG2	1:C:499:MET:CB	2.82	0.41
1:C:634:TRP:HZ2	3:D:822:MET:HG3	1.85	0.41
3:D:137:MET:HE3	3:D:137:MET:HB3	1.96	0.41
3:D:325:TYR:CD1	3:D:326:GLU:CA	3.03	0.41
1:A:736:PHE:CD1	1:A:794:GLN:OE1	2.72	0.41
2:B:502:ILE:HG12	2:B:512:PHE:CE1	2.53	0.41
2:B:754:GLN:O	2:B:755:LYS:C	2.62	0.41
2:B:754:GLN:HB3	2:B:757:SER:CB	2.50	0.41
1:C:496:TRP:HA	1:C:501:GLY:HA3	2.01	0.41
1:C:611:VAL:O	1:C:642:VAL:HG21	2.19	0.41
3:D:168:THR:CG2	3:D:174:TYR:HB2	2.51	0.41
3:D:362:LEU:HD23	3:D:362:LEU:HA	1.92	0.41
1:A:637:PHE:CD2	2:B:812:LEU:HB2	2.55	0.41
2:B:34:LEU:HD11	2:B:45:ILE:CD1	2.50	0.41
2:B:390:ASP:C	2:B:392:ASN:N	2.77	0.41
2:B:523:VAL:HG13	2:B:717:ILE:HG13	2.01	0.41
1:C:627:ALA:O	1:C:630:LEU:CA	2.69	0.41
3:D:325:TYR:O	3:D:328:HIS:HB3	2.20	0.41
3:D:431:LYS:O	3:D:446:ILE:N	2.52	0.41
3:D:462:ALA:O	3:D:466:LYS:N	2.48	0.41
4:F:116:UNK:HA	4:F:136:UNK:O	2.21	0.41
1:A:34:SER:HB3	1:A:96:PRO:HD3	2.01	0.41
1:A:72:ILE:O	1:A:72:ILE:HG12	2.20	0.41
1:A:291:ALA:O	1:A:295:LEU:HB3	2.20	0.41
1:A:400:ILE:HD12	1:A:512:VAL:CG2	2.47	0.41
1:A:464:LEU:O	1:A:468:MET:CB	2.69	0.41
1:A:496:TRP:CE3	1:A:496:TRP:N	2.86	0.41
1:A:788:LYS:HB3	1:A:792:ARG:HH11	1.85	0.41
2:B:495:MET:HE2	2:B:751:ILE:CG2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:519:THR:CG2	2:B:721:ALA:HB3	2.41	0.41
1:C:132:SER:HB2	3:D:174:TYR:HE2	1.85	0.41
1:C:482:PHE:HA	1:C:499:MET:HE3	2.02	0.41
1:C:526:GLU:CD	1:C:767:LYS:HG3	2.45	0.41
3:D:58:PRO:CG	3:D:303:LEU:HD12	2.44	0.41
3:D:198:ILE:C	3:D:199:HIS:HD2	2.28	0.41
1:A:194:VAL:O	1:A:195:LEU:HD23	2.21	0.41
1:A:266:ILE:HG23	1:A:266:ILE:O	2.20	0.41
1:A:637:PHE:HD2	2:B:812:LEU:HD13	1.85	0.41
1:A:657:ARG:CB	1:A:658:PRO:HD3	2.50	0.41
1:A:704:MET:HE3	1:A:704:MET:HB3	1.92	0.41
2:B:157:TYR:CD1	2:B:157:TYR:C	2.95	0.41
2:B:238:LEU:HD23	2:B:238:LEU:HA	1.90	0.41
2:B:295:ALA:O	2:B:299:LEU:N	2.53	0.41
2:B:502:ILE:HG21	2:B:512:PHE:CE1	2.52	0.41
2:B:541:PHE:CZ	1:C:803:PRO:CB	3.03	0.41
2:B:621:ILE:HD13	2:B:621:ILE:HA	1.77	0.41
2:B:768:LEU:C	2:B:770:PHE:N	2.77	0.41
1:C:572:ALA:HB1	1:C:604:ALA:HB1	2.02	0.41
1:A:513:ALA:HB1	1:A:514:PRO:HD2	2.02	0.41
1:A:550:ASP:O	1:A:553:MET:HB3	2.21	0.41
1:A:718:ALA:HB1	1:A:724:LEU:HG	2.02	0.41
2:B:353:LEU:HB2	2:B:370:TRP:HB3	2.02	0.41
2:B:399:LEU:HD12	2:B:484:MET:HE2	2.03	0.41
2:B:514:VAL:CG2	2:B:767:LEU:HD13	2.44	0.41
2:B:538:LEU:CB	2:B:541:PHE:CE1	3.04	0.41
2:B:672:THR:H	2:B:693:MET:CG	2.32	0.41
3:D:252:ILE:HA	3:D:273:ILE:O	2.20	0.41
3:D:345:SER:C	3:D:353:MET:HB3	2.46	0.41
3:D:725:ASP:OD1	3:D:726:ALA:N	2.54	0.41
4:G:287:UNK:N	4:G:292:UNK:O	2.54	0.41
1:A:111:ALA:O	1:A:112:GLY:C	2.62	0.41
1:A:115:ARG:HB3	1:A:315:TRP:HB3	2.02	0.41
2:B:592:ALA:O	2:B:596:LEU:CA	2.66	0.41
2:B:680:ARG:CG	2:B:683:ARG:HH21	2.33	0.41
2:B:780:GLU:O	2:B:784:LEU:N	2.54	0.41
1:C:29:ILE:HD11	1:C:60:LEU:HD23	2.03	0.41
1:C:283:ASP:O	1:C:287:VAL:HG23	2.21	0.41
3:D:786:GLU:HA	3:D:790:LEU:HB2	2.03	0.41
1:A:34:SER:HB2	1:A:96:PRO:HG2	1.97	0.41
1:A:165:LEU:HD22	1:A:180:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:ALA:CB	1:A:240:MET:HE1	2.47	0.41
1:A:216:ALA:O	1:A:217:ARG:HD3	2.20	0.41
1:A:357:GLN:HG2	1:A:380:ILE:HD13	2.03	0.41
1:A:531:PHE:CE1	1:A:774:ILE:CG2	3.04	0.41
1:A:570:VAL:O	1:A:572:ALA:N	2.54	0.41
2:B:52:ASP:HB3	2:B:285:ARG:HD2	2.02	0.41
2:B:184:ASP:O	2:B:185:ASN:C	2.63	0.41
2:B:203:THR:O	2:B:203:THR:HG23	2.19	0.41
2:B:271:VAL:HA	2:B:356:LEU:HD12	2.03	0.41
2:B:424:CYS:N	2:B:442:LYS:O	2.54	0.41
2:B:553:LEU:O	2:B:556:VAL:HB	2.19	0.41
2:B:678:THR:C	2:B:680:ARG:N	2.79	0.41
1:C:76:LEU:C	1:C:78:VAL:H	2.28	0.41
1:C:532:LYS:CG	1:C:533:TYR:N	2.82	0.41
1:C:576:TYR:HA	1:C:579:ASP:HB3	2.02	0.41
1:C:663:THR:N	1:C:667:ASP:HB2	2.35	0.41
1:C:769:GLU:H	1:C:769:GLU:HG2	1.66	0.41
3:D:346:PHE:C	3:D:353:MET:HB2	2.45	0.41
3:D:545:GLU:H	3:D:545:GLU:HG2	1.70	0.41
3:D:815:PHE:N	3:D:815:PHE:CD1	2.88	0.41
1:A:204:LEU:HD11	1:A:231:VAL:N	2.36	0.41
1:A:512:VAL:N	1:A:758:ILE:HD11	2.35	0.41
1:A:541:LYS:CB	1:A:745:VAL:H	2.33	0.41
1:A:718:ALA:O	1:A:723:LYS:N	2.54	0.41
2:B:468:VAL:HG23	2:B:484:MET:HG2	1.89	0.41
1:C:575:LEU:HD23	1:C:576:TYR:N	2.36	0.41
1:C:637:PHE:CD2	3:D:818:LEU:CD2	3.03	0.41
3:D:667:PRO:HG3	3:D:698:TYR:CE2	2.56	0.41
1:A:105:THR:HB	1:A:128:TYR:OH	2.21	0.40
1:A:198:GLU:CG	1:A:199:PRO:HD2	2.49	0.40
1:A:540:VAL:CG2	1:A:541:LYS:N	2.82	0.40
2:B:31:ALA:O	2:B:90:VAL:CA	2.69	0.40
2:B:144:LYS:HA	2:B:178:PHE:CD2	2.56	0.40
2:B:274:ASP:O	2:B:278:TYR:CE1	2.74	0.40
1:C:265:GLY:HA3	1:C:381:TRP:O	2.21	0.40
1:C:446:ARG:N	1:C:447:PRO:CD	2.83	0.40
1:C:550:ASP:CB	1:C:810:ASN:CB	2.99	0.40
3:D:55:HIS:HB3	3:D:56:HIS:H	1.51	0.40
4:G:412:UNK:HA	4:G:423:UNK:HA	2.03	0.40
1:A:204:LEU:O	1:A:208:LEU:HD12	2.21	0.40
1:A:221:LEU:HD12	1:A:221:LEU:C	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:494:VAL:HG12	2:B:495:MET:HG3	2.01	0.40
2:B:559:MET:SD	2:B:618:ILE:CG2	3.09	0.40
1:C:415:THR:CG2	1:C:416:SER:N	2.83	0.40
3:D:49:HIS:O	3:D:53:ASP:CB	2.70	0.40
3:D:143:PRO:HG3	3:D:357:LEU:HD12	2.02	0.40
3:D:263:THR:C	3:D:264:VAL:HG23	2.46	0.40
4:G:275:UNK:O	4:G:276:UNK:C	2.69	0.40
1:A:121:LEU:HD22	1:A:281:ILE:CA	2.46	0.40
1:A:531:PHE:HE1	1:A:774:ILE:CG1	2.35	0.40
1:A:532:LYS:O	1:A:755:GLY:CA	2.52	0.40
1:A:602:SER:C	1:A:606:TRP:CE3	3.00	0.40
1:A:682:VAL:O	1:A:683:LYS:C	2.65	0.40
2:B:564:PHE:CD1	2:B:564:PHE:C	2.98	0.40
1:C:408:PHE:HB3	1:C:457:CYS:SG	2.62	0.40
1:C:575:LEU:HA	1:C:630:LEU:HD13	2.02	0.40
1:C:771:SER:O	1:C:774:ILE:N	2.55	0.40
3:D:630:PHE:CG	3:D:631:PHE:N	2.87	0.40
1:A:119:ILE:HD13	1:A:288:VAL:HG21	1.63	0.40
1:A:199:PRO:HA	1:A:227:ASP:OD2	2.21	0.40
1:A:530:PRO:C	1:A:756:PHE:O	2.64	0.40
1:A:553:MET:HG3	2:B:798:SER:HB2	2.04	0.40
2:B:206:GLN:O	2:B:210:GLN:HG3	2.22	0.40
2:B:474:GLY:HA3	2:B:485:ILE:HD12	2.02	0.40
2:B:673:VAL:CG1	2:B:698:GLN:NE2	2.85	0.40
1:C:27:VAL:HB	1:C:59:GLN:O	2.21	0.40
3:D:108:ASP:O	3:D:112:VAL:HG23	2.20	0.40
3:D:194:LEU:HD11	3:D:197:VAL:CG2	2.52	0.40
3:D:734:GLY:O	3:D:793:ILE:CA	2.70	0.40
1:A:266:ILE:HG22	1:A:356:LEU:HG	2.04	0.40
1:A:540:VAL:HG23	1:A:719:VAL:HG13	2.02	0.40
1:A:551:SER:O	1:A:645:TYR:CE1	2.75	0.40
1:A:554:GLN:HA	2:B:798:SER:CA	2.52	0.40
1:A:560:LEU:CD1	2:B:802:ILE:CG2	2.90	0.40
1:A:634:TRP:CD1	2:B:812:LEU:HD11	2.56	0.40
1:A:753:ARG:H	1:A:753:ARG:HG3	1.72	0.40
2:B:49:TRP:CE3	2:B:49:TRP:CA	3.04	0.40
1:C:26:ILE:CG1	1:C:61:ASN:HB2	2.52	0.40
1:C:119:ILE:HG12	1:C:138:LEU:HD23	2.04	0.40
3:D:271:GLY:HA2	3:D:361:LEU:HD21	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [\(i\)](#)

### 5.3.1 Protein backbone [\(i\)](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	792/836 (95%)	756 (96%)	31 (4%)	5 (1%)	21	59
1	C	794/836 (95%)	758 (96%)	30 (4%)	6 (1%)	16	54
2	B	791/831 (95%)	733 (93%)	44 (6%)	14 (2%)	6	34
3	D	790/837 (94%)	752 (95%)	31 (4%)	7 (1%)	14	50
All	All	3167/3340 (95%)	2999 (95%)	136 (4%)	32 (1%)	15	48

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	447	PRO
2	B	169	PHE
2	B	515	PRO
2	B	534	PRO
1	C	392	TYR
1	C	698	SER
3	D	28	PRO
3	D	144	SER
2	B	569	PRO
1	A	98	PRO
2	B	199	ASP
2	B	254	THR
2	B	265	PRO
2	B	391	ASP
3	D	58	PRO
1	A	54	PHE
2	B	198	LEU
2	B	533	SER
2	B	607	VAL
1	C	98	PRO
1	A	555	PRO
1	A	668	PRO

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Mol	Chain	Res	Type
2	B	188	VAL
2	B	264	PHE
1	C	439	PRO
1	C	450	PRO
1	C	802	ALA
3	D	43	VAL
3	D	389	PRO
2	B	320	ASP
3	D	355	PRO
3	D	388	TYR

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	534/714 (75%)	494 (92%)	40 (8%)	12	33
1	C	461/714 (65%)	414 (90%)	47 (10%)	7	23
2	B	490/724 (68%)	435 (89%)	55 (11%)	6	19
3	D	375/735 (51%)	330 (88%)	45 (12%)	5	17
All	All	1860/2887 (64%)	1673 (90%)	187 (10%)	9	23

All (187) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ILE
1	A	79	CYS
1	A	113	PHE
1	A	138	LEU
1	A	202	LYS
1	A	204	LEU
1	A	259	LEU
1	A	266	ILE
1	A	277	GLU
1	A	280	HIS
1	A	296	PHE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	299	GLU
1	A	356	LEU
1	A	380	ILE
1	A	392	TYR
1	A	393	GLN
1	A	398	LEU
1	A	417	ASP
1	A	452	CYS
1	A	468	MET
1	A	469	ASP
1	A	482	PHE
1	A	496	TRP
1	A	500	MET
1	A	504	LEU
1	A	528	SER
1	A	532	LYS
1	A	540	VAL
1	A	549	LEU
1	A	571	VAL
1	A	573	VAL
1	A	574	MET
1	A	575	LEU
1	A	601	LEU
1	A	612	LEU
1	A	665	ILE
1	A	671	ARG
1	A	744	LEU
1	A	809	GLU
1	A	833	ILE
2	B	40	ILE
2	B	53	MET
2	B	57	PHE
2	B	72	LYS
2	B	79	CYS
2	B	86	LYS
2	B	98	GLN
2	B	156	GLU
2	B	157	TYR
2	B	159	TRP
2	B	164	VAL
2	B	173	ARG
2	B	176	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	186	SER
2	B	190	TRP
2	B	214	ILE
2	B	223	CYS
2	B	256	ASN
2	B	268	LEU
2	B	283	ARG
2	B	301	LYS
2	B	303	SER
2	B	332	ASN
2	B	352	LYS
2	B	354	VAL
2	B	356	LEU
2	B	399	LEU
2	B	480	VAL
2	B	491	LYS
2	B	492	ARG
2	B	500	LEU
2	B	512	PHE
2	B	523	VAL
2	B	524	MET
2	B	525	VAL
2	B	532	VAL
2	B	539	GLU
2	B	541	PHE
2	B	559	MET
2	B	564	PHE
2	B	621	ILE
2	B	662	HIS
2	B	686	TYR
2	B	692	TYR
2	B	718	TYR
2	B	738	ILE
2	B	743	ILE
2	B	760	LYS
2	B	765	LEU
2	B	768	LEU
2	B	788	CYS
2	B	789	HIS
2	B	801	ASP
2	B	804	ASN
2	B	811	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	26	ILE
1	C	53	HIS
1	C	58	ILE
1	C	59	GLN
1	C	79	CYS
1	C	81	ASP
1	C	82	LEU
1	C	138	LEU
1	C	260	ARG
1	C	277	GLU
1	C	301	ILE
1	C	308	CYS
1	C	309	VAL
1	C	329	LYS
1	C	334	VAL
1	C	335	THR
1	C	426	ILE
1	C	477	VAL
1	C	500	MET
1	C	534	GLN
1	C	560	LEU
1	C	574	MET
1	C	577	LEU
1	C	601	LEU
1	C	628	ARG
1	C	636	LEU
1	C	637	PHE
1	C	639	MET
1	C	640	ILE
1	C	667	ASP
1	C	695	VAL
1	C	696	GLU
1	C	724	LEU
1	C	742	CYS
1	C	753	ARG
1	C	767	LYS
1	C	771	SER
1	C	775	LEU
1	C	783	MET
1	C	788	LYS
1	C	794	GLN
1	C	796	CYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	826	ILE
1	C	828	LEU
1	C	829	ILE
1	C	830	PHE
1	C	831	ILE
3	D	37	VAL
3	D	55	HIS
3	D	72	ASP
3	D	114	THR
3	D	137	MET
3	D	197	VAL
3	D	200	LEU
3	D	202	MET
3	D	218	LEU
3	D	316	CYS
3	D	325	TYR
3	D	328	HIS
3	D	333	TYR
3	D	335	ILE
3	D	354	HIS
3	D	365	GLU
3	D	370	ARG
3	D	496	THR
3	D	529	VAL
3	D	531	VAL
3	D	543	PHE
3	D	544	LEU
3	D	545	GLU
3	D	547	PHE
3	D	550	ASP
3	D	552	TRP
3	D	555	MET
3	D	556	PHE
3	D	560	LEU
3	D	561	ILE
3	D	565	VAL
3	D	568	PHE
3	D	573	PHE
3	D	595	ILE
3	D	600	TRP
3	D	601	LEU
3	D	602	LEU

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Mol	Chain	Res	Type
3	D	603	TRP
3	D	605	LEU
3	D	614	GLN
3	D	630	PHE
3	D	639	TYR
3	D	761	LYS
3	D	794	CYS
3	D	795	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	HIS
1	A	70	ASN
1	A	86	GLN
1	A	146	HIS
1	A	147	GLN
1	A	162	HIS
1	A	196	GLN
1	A	293	HIS
1	A	311	ASN
1	A	475	HIS
1	A	648	ASN
1	A	778	HIS
2	B	120	HIS
2	B	152	ASN
2	B	160	HIS
2	B	194	ASN
2	B	302	HIS
2	B	332	ASN
2	B	389	HIS
2	B	473	HIS
2	B	503	ASN
2	B	659	GLN
2	B	675	GLN
2	B	754	GLN
2	B	827	HIS
1	C	38	HIS
1	C	53	HIS
1	C	59	GLN
1	C	451	GLN
1	C	523	GLN

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Mol	Chain	Res	Type
1	C	694	GLN
1	C	703	HIS
1	C	725	HIS
1	C	778	HIS
3	D	29	ASN
3	D	55	HIS
3	D	154	ASN
3	D	199	HIS
3	D	306	HIS
3	D	354	HIS
3	D	668	ASN
3	D	691	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

8 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	$\# Z  > 2$
5	NAG	E	1	5,1	14,14,15	0.29	0	17,19,21	0.56	0
5	NAG	E	2	5	14,14,15	0.29	0	17,19,21	0.56	0
5	NAG	H	1	5,1	14,14,15	0.30	0	17,19,21	0.56	0
5	NAG	H	2	5	14,14,15	0.29	0	17,19,21	0.55	0
5	NAG	I	1	5,1	14,14,15	0.29	0	17,19,21	0.56	0
5	NAG	I	2	5	14,14,15	0.29	0	17,19,21	0.56	0
5	NAG	J	1	3,5	14,14,15	0.29	0	17,19,21	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	J	2	5	14,14,15	0.30	0	17,19,21	0.56	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	E	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	E	2	5	-	5/6/23/26	0/1/1/1
5	NAG	H	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	H	2	5	-	5/6/23/26	0/1/1/1
5	NAG	I	1	5,1	-	5/6/23/26	0/1/1/1
5	NAG	I	2	5	-	5/6/23/26	0/1/1/1
5	NAG	J	1	3,5	-	2/6/23/26	0/1/1/1
5	NAG	J	2	5	-	5/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	2	NAG	C3-C2-N2-C7
5	E	2	NAG	C8-C7-N2-C2
5	E	2	NAG	O7-C7-N2-C2
5	H	2	NAG	C3-C2-N2-C7
5	H	2	NAG	C8-C7-N2-C2
5	H	2	NAG	O7-C7-N2-C2
5	I	1	NAG	C8-C7-N2-C2
5	I	1	NAG	O7-C7-N2-C2
5	I	2	NAG	C1-C2-N2-C7
5	I	2	NAG	C8-C7-N2-C2
5	I	2	NAG	O7-C7-N2-C2
5	J	1	NAG	C8-C7-N2-C2
5	J	1	NAG	O7-C7-N2-C2
5	J	2	NAG	C3-C2-N2-C7
5	J	2	NAG	C8-C7-N2-C2
5	J	2	NAG	O7-C7-N2-C2

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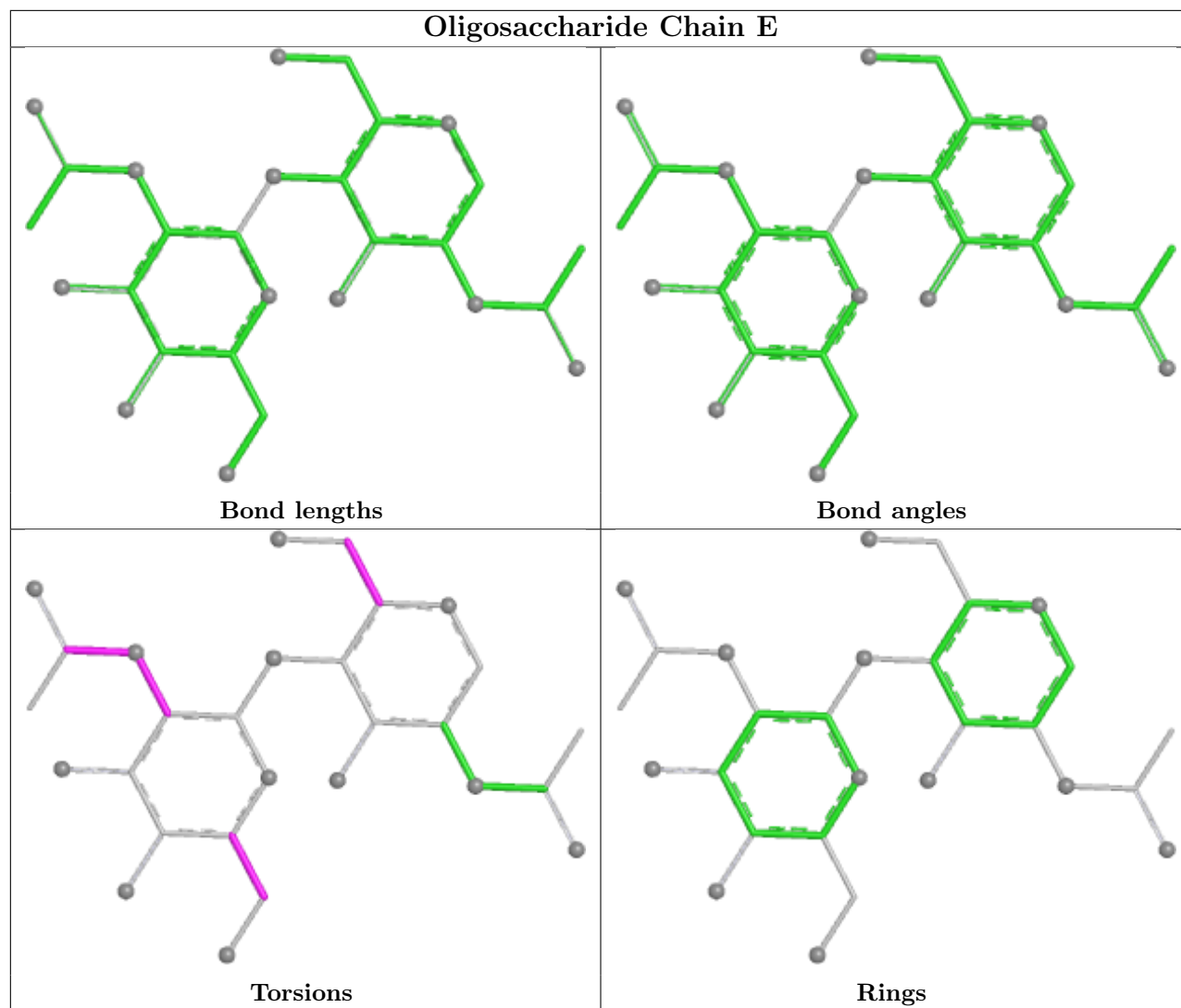
Mol	Chain	Res	Type	Atoms
5	E	2	NAG	O5-C5-C6-O6
5	H	2	NAG	O5-C5-C6-O6
5	J	2	NAG	O5-C5-C6-O6
5	I	2	NAG	O5-C5-C6-O6
5	H	2	NAG	C4-C5-C6-O6
5	E	2	NAG	C4-C5-C6-O6
5	J	2	NAG	C4-C5-C6-O6
5	I	2	NAG	C4-C5-C6-O6
5	I	1	NAG	C4-C5-C6-O6
5	I	1	NAG	O5-C5-C6-O6
5	E	1	NAG	C4-C5-C6-O6
5	E	1	NAG	O5-C5-C6-O6
5	I	1	NAG	C3-C2-N2-C7

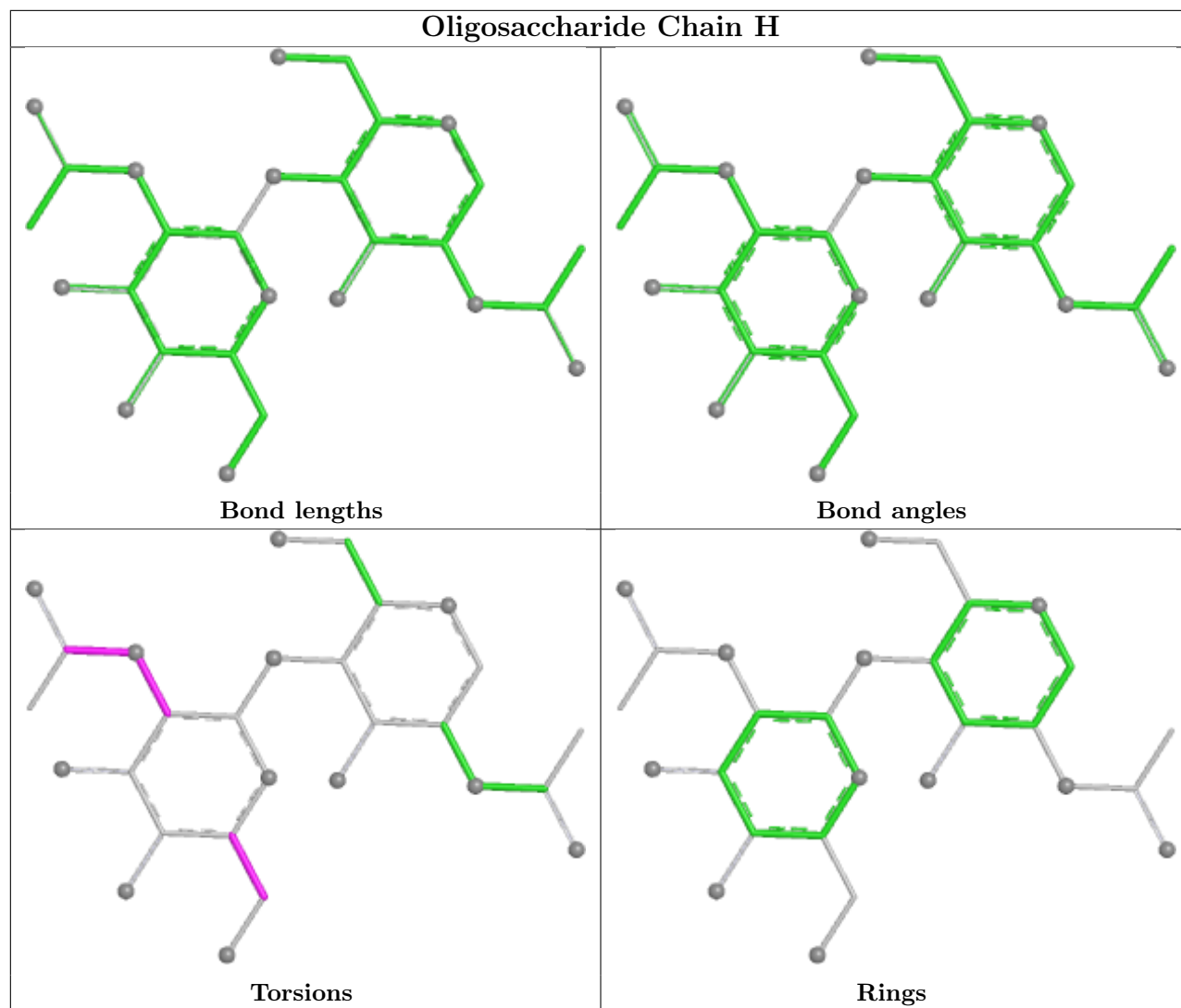
There are no ring outliers.

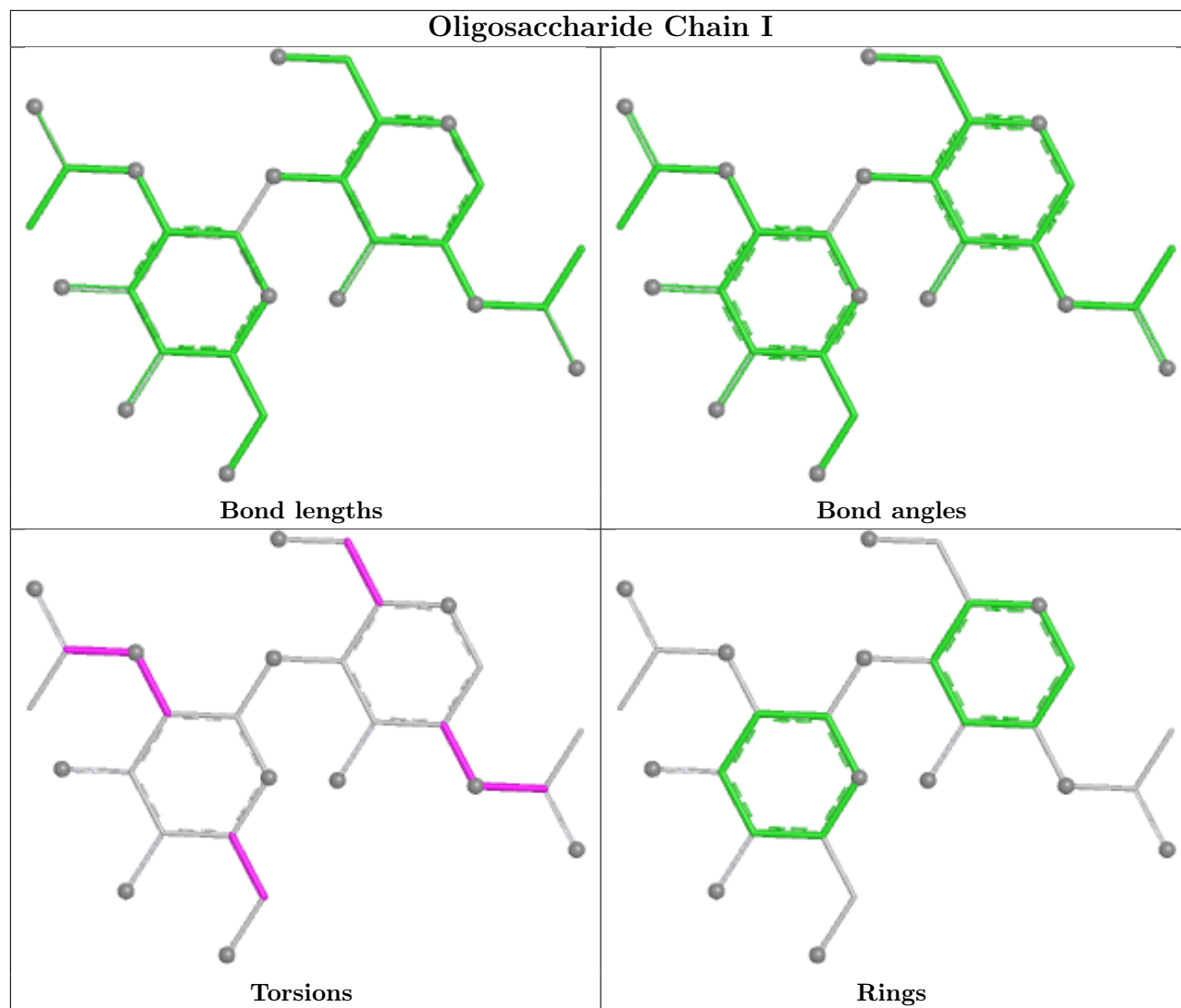
4 monomers are involved in 11 short contacts:

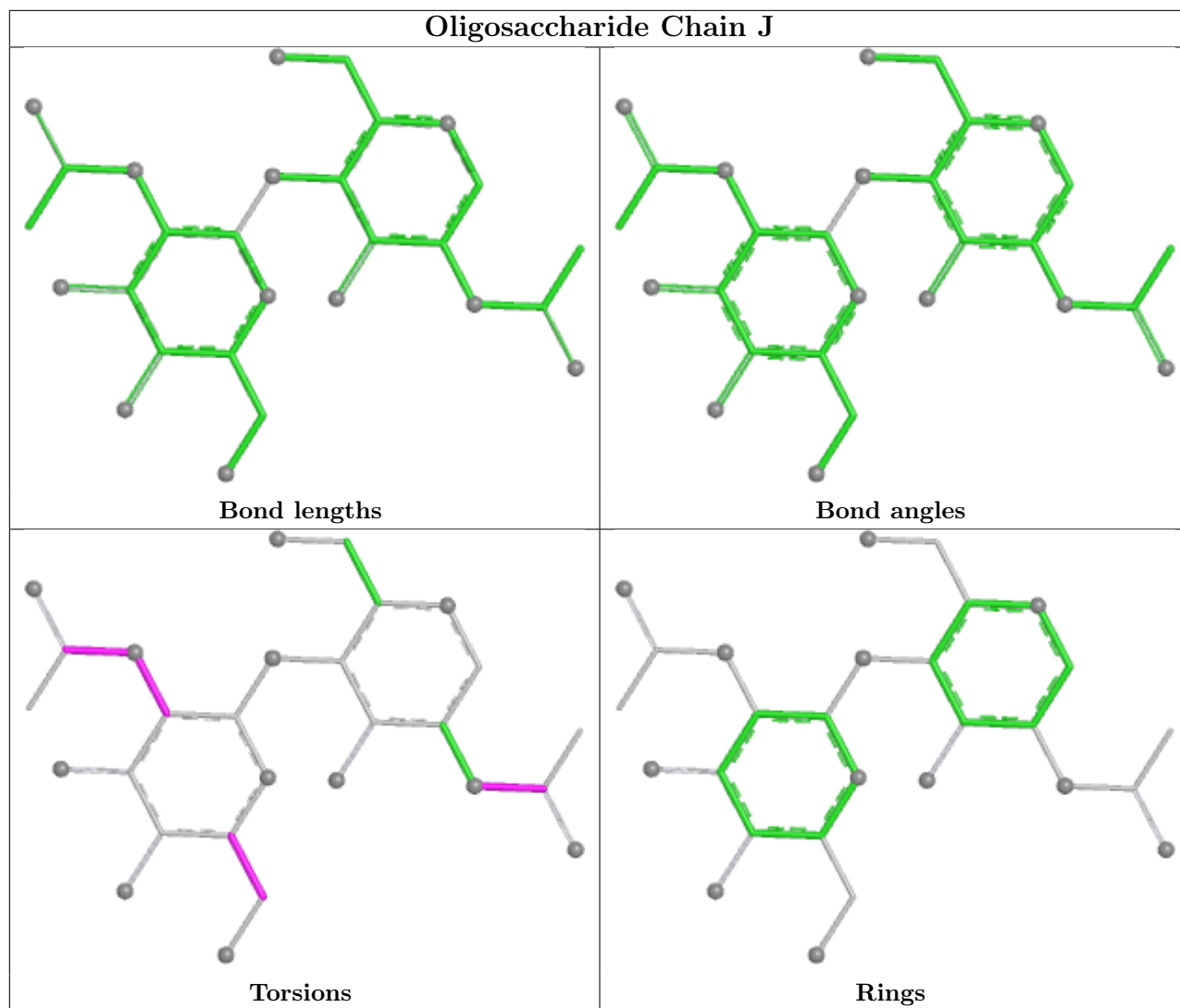
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	I	2	NAG	3	0
5	J	2	NAG	2	0
5	H	2	NAG	2	0
5	E	2	NAG	4	0

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](#)

1 ligand is 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	$\# Z  > 2$
6	NAG	D	1003	3	14,14,15	0.29	0	17,19,21	0.56	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	D	1003	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	1003	NAG	C8-C7-N2-C2
6	D	1003	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	G	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	348:UNK	C	349:UNK	N	14.40

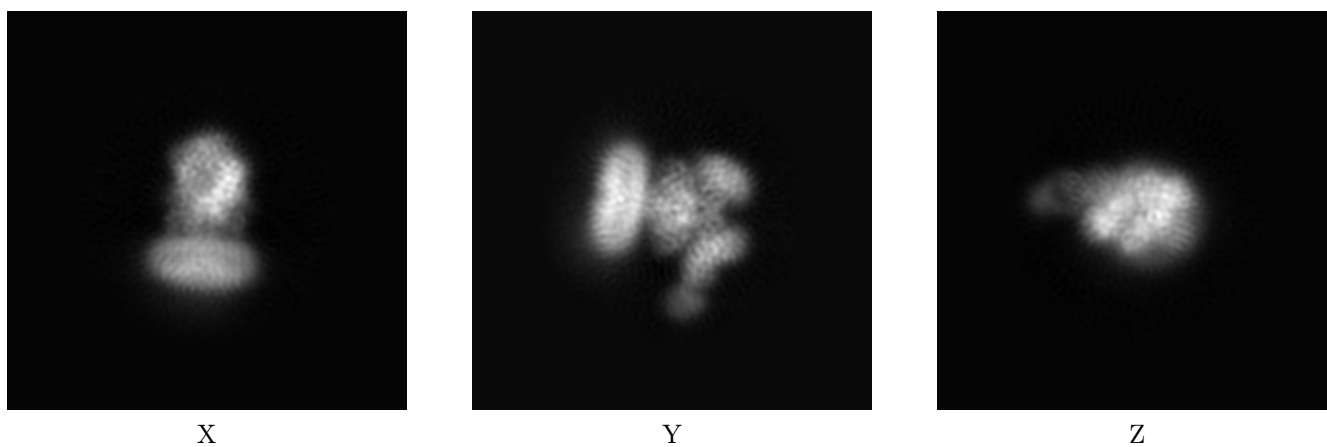
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8581. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

### 6.1 Orthogonal projections [i](#)

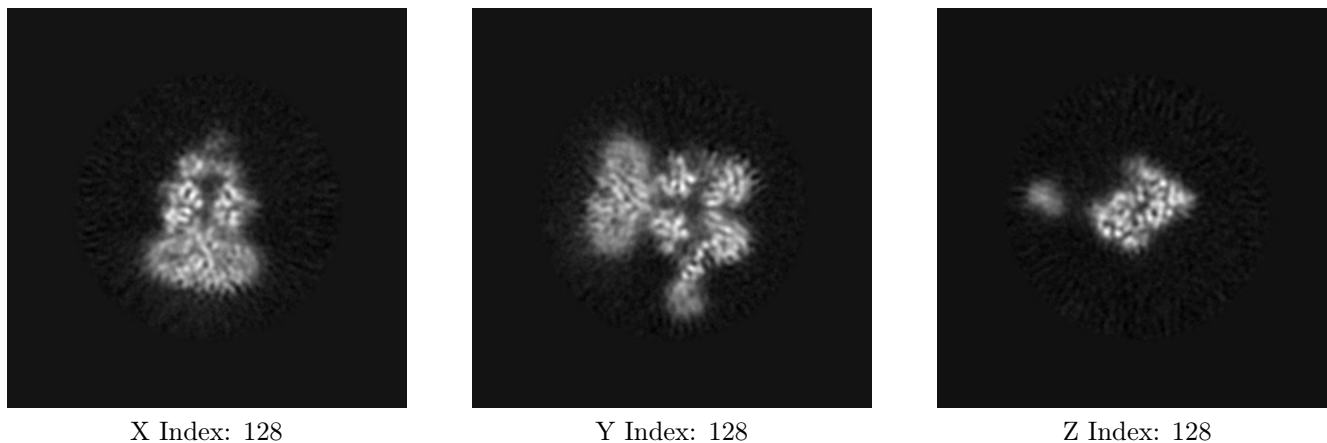
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

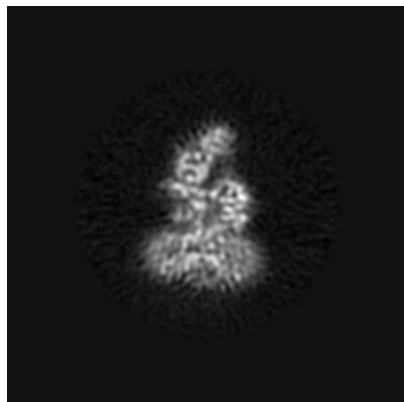
#### 6.2.1 Primary map



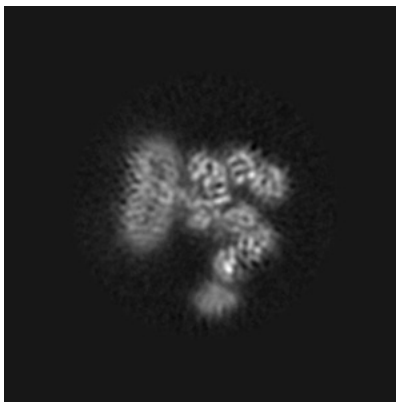
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

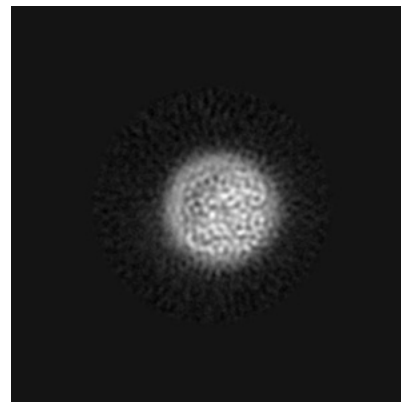
### 6.3.1 Primary map



X Index: 135



Y Index: 136



Z Index: 90

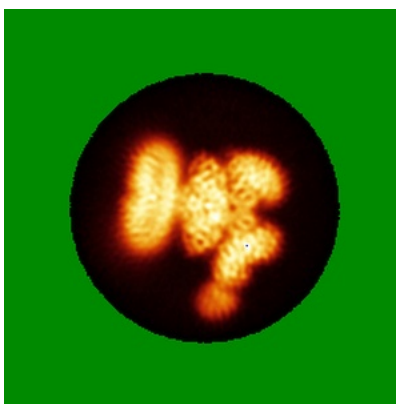
The images above show the largest variance slices of the map in three orthogonal directions.

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

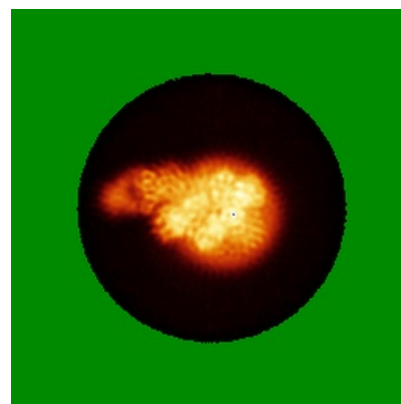
### 6.4.1 Primary map



X



Y



Z

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

## 6.5 Orthogonal surface views [i](#)

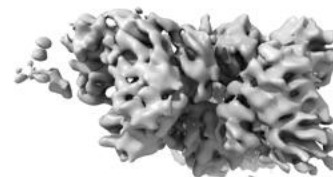
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.055. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

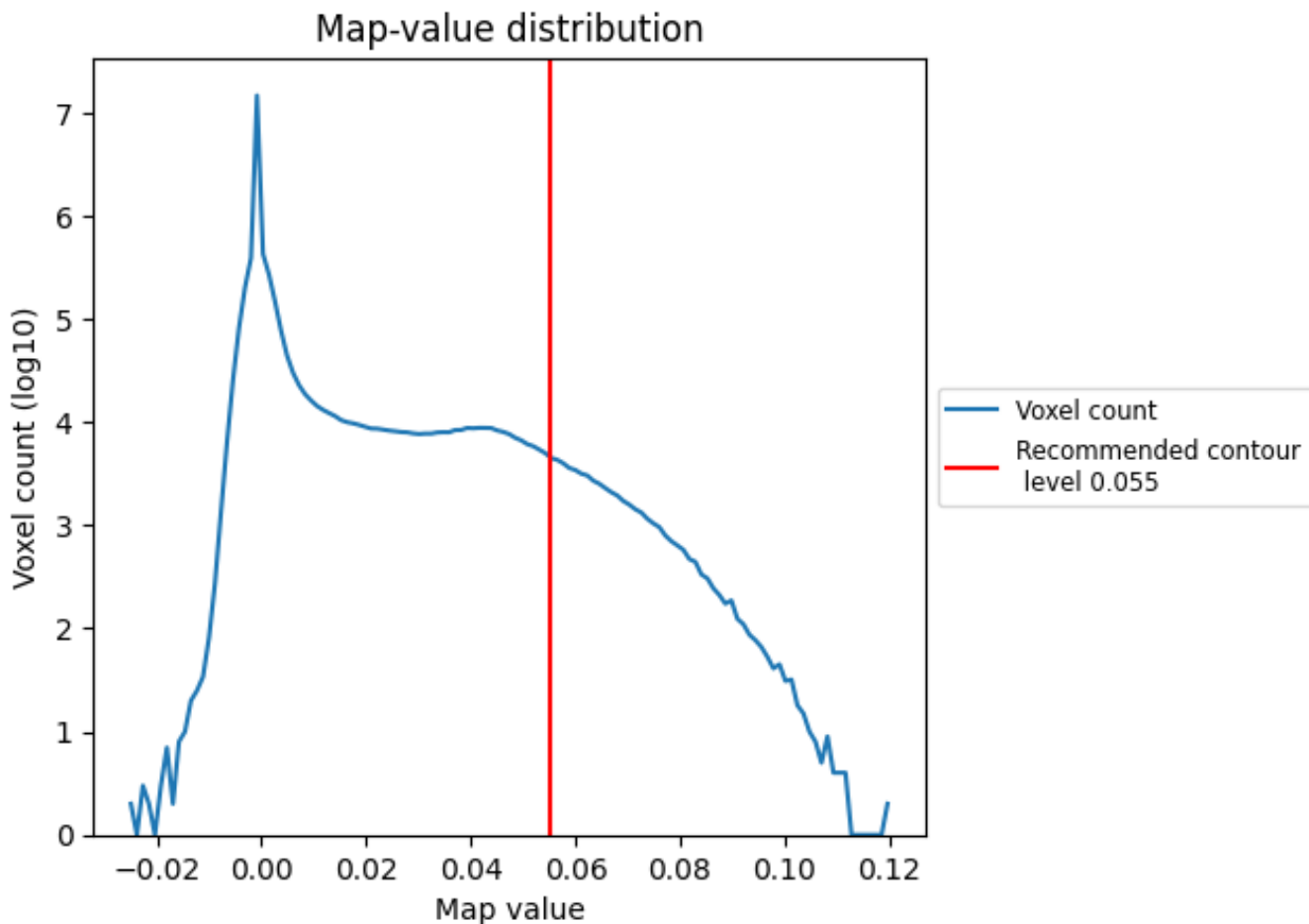
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

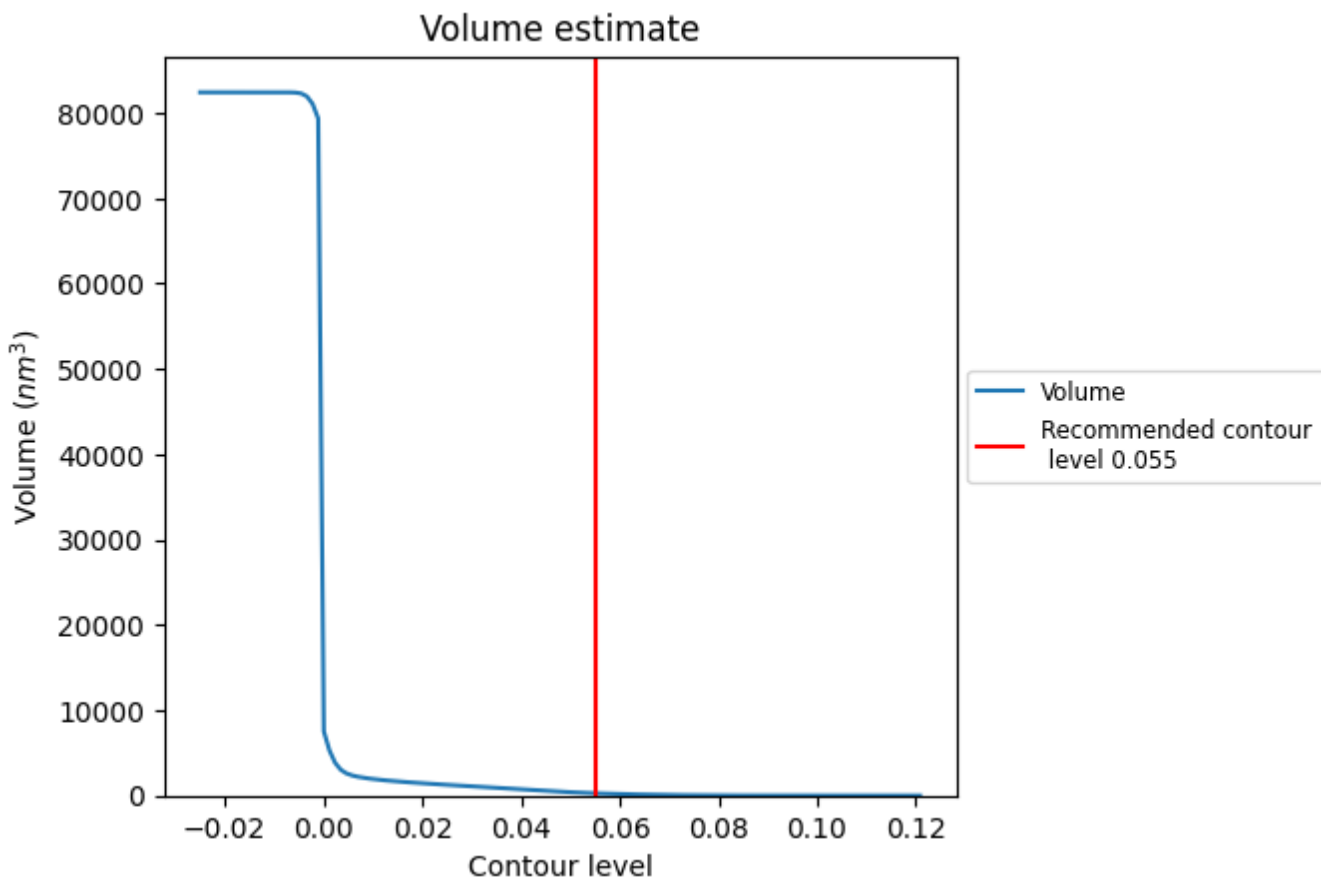
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

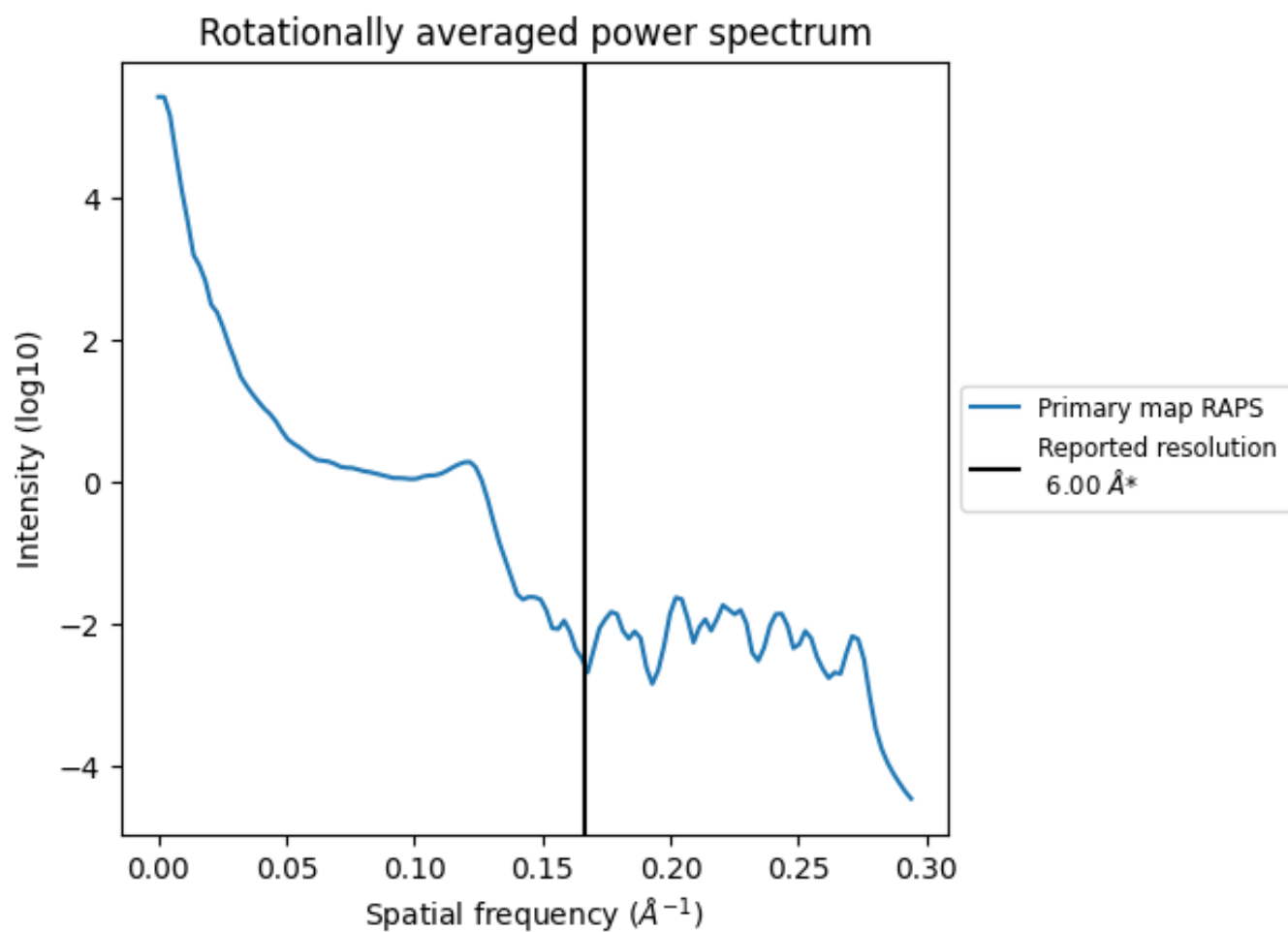
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 267 nm<sup>3</sup>; this corresponds to an approximate mass of 241 kDa.

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

### 7.3 Rotationally averaged power spectrum [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.167 \text{\AA}^{-1}$

## 8 Fourier-Shell correlation

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

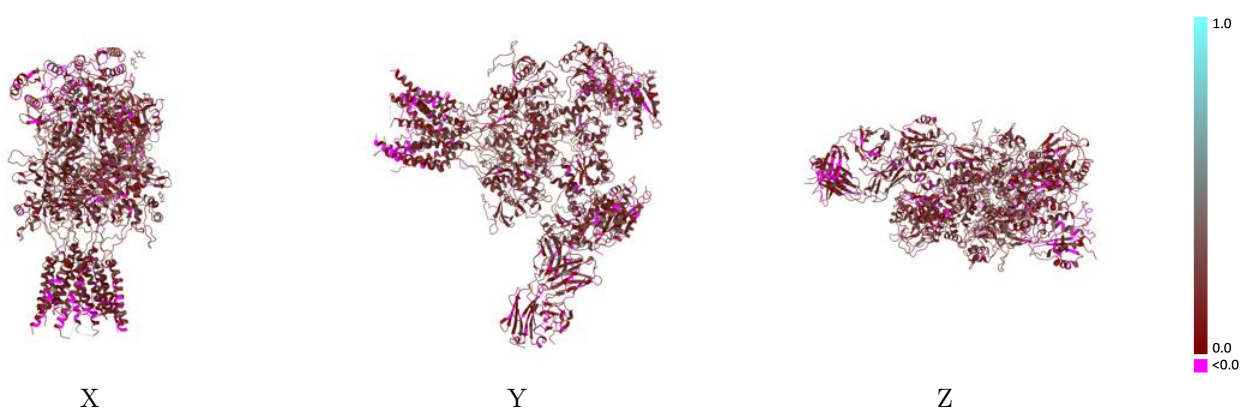
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8581 and PDB model 5UP2. Per-residue inclusion information can be found in section 3 on page 8.

### 9.1 Map-model overlay [i](#)

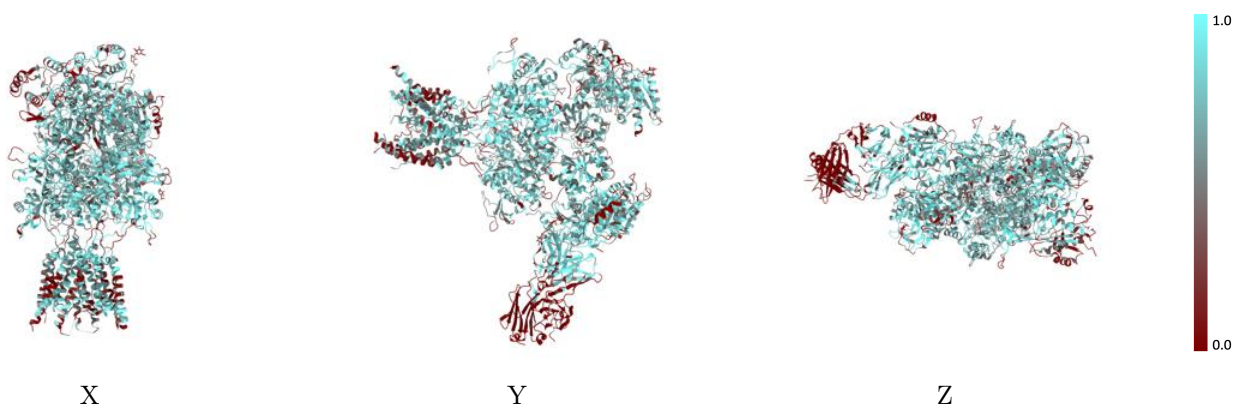
This section was not generated.

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



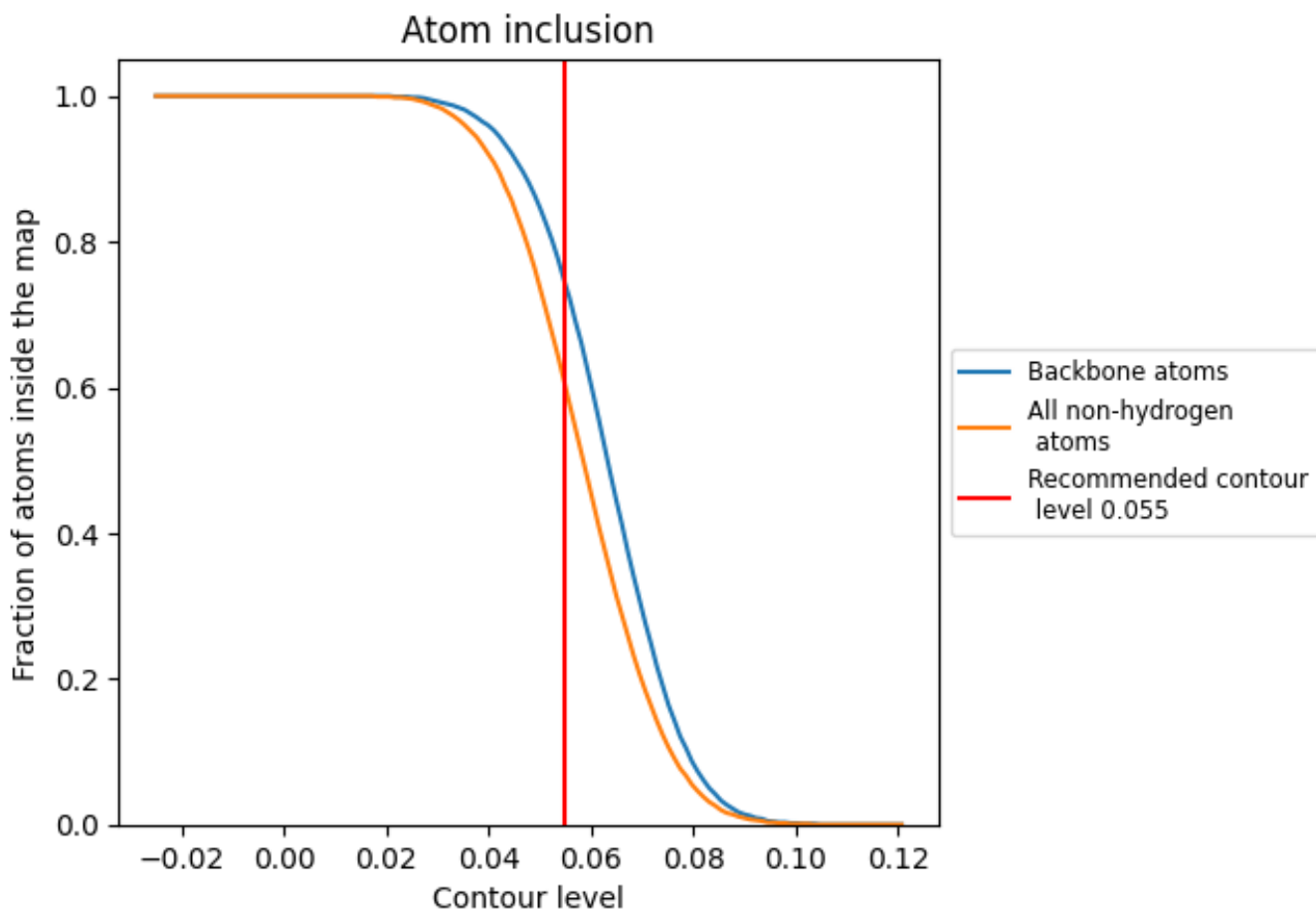
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.055).























## 9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 60% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.055) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6040	 0.1600
A	 0.6510	 0.1570
B	 0.5820	 0.1570
C	 0.6490	 0.1630
D	 0.6440	 0.1680
E	 0.1430	 0.3020
F	 0.4080	 0.1570
G	 0.3070	 0.1310
H	 0.2500	 0.1770
I	 0.0710	 0.1920
J	 0.0000	 0.1690

