



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 02:59 AM UTC

PDB ID : 8GNH / pdb_00008gnh
EMDB ID : EMD-34164
Title : Complex structure of BD-218 and Spike protein
Authors : Wang, B.; Xu, H.; Su, X.D.
Deposited on : 2022-08-23
Resolution : 3.74 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

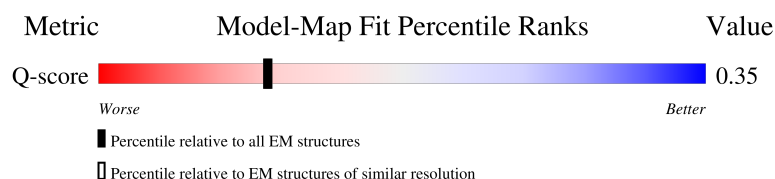
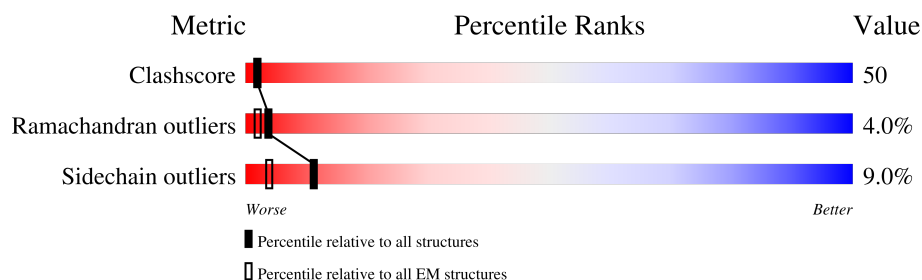
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.74 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	10346 (3.24 - 4.24)

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

Mol	Chain	Length	Quality of chain
1	A	1208	
1	B	1208	
1	C	1208	
2	H	321	

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Mol	Chain	Length	Quality of chain
3	L	232	
4	D	2	
4	N	2	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	B	1302	-	-	X	-
5	NAG	B	1304	-	-	X	-
5	NAG	C	1301	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 26171 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1032	Total	C	N	O	S	0	0
			7816	4963	1312	1505	36		
1	B	1058	Total	C	N	O	S	0	0
			8083	5141	1354	1551	37		
1	C	1048	Total	C	N	O	S	0	0
			8096	5160	1346	1553	37		

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	682	GLY	ARG	engineered mutation	UNP P0DTC2
A	683	SER	ARG	engineered mutation	UNP P0DTC2
A	685	SER	ARG	engineered mutation	UNP P0DTC2
A	817	PRO	PHE	engineered mutation	UNP P0DTC2
A	892	PRO	ALA	engineered mutation	UNP P0DTC2
A	899	PRO	ALA	engineered mutation	UNP P0DTC2
A	942	PRO	ALA	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	682	GLY	ARG	engineered mutation	UNP P0DTC2
B	683	SER	ARG	engineered mutation	UNP P0DTC2
B	685	SER	ARG	engineered mutation	UNP P0DTC2
B	817	PRO	PHE	engineered mutation	UNP P0DTC2
B	892	PRO	ALA	engineered mutation	UNP P0DTC2
B	899	PRO	ALA	engineered mutation	UNP P0DTC2
B	942	PRO	ALA	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	682	GLY	ARG	engineered mutation	UNP P0DTC2
C	683	SER	ARG	engineered mutation	UNP P0DTC2
C	685	SER	ARG	engineered mutation	UNP P0DTC2
C	817	PRO	PHE	engineered mutation	UNP P0DTC2
C	892	PRO	ALA	engineered mutation	UNP P0DTC2
C	899	PRO	ALA	engineered mutation	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	942	PRO	ALA	engineered mutation	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2

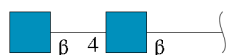
- Molecule 2 is a protein called Heavy chain of BD-218.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	121	Total	C	N	O	S	0	0
			903	569	155	177	2		

- Molecule 3 is a protein called Light chain of BD-218.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	106	Total	C	N	O	S	0	0
			769	482	130	155	2		

- Molecule 4 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
4	N	2	Total	C	N	O	0	0
			28	16	2	10		
4	D	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	

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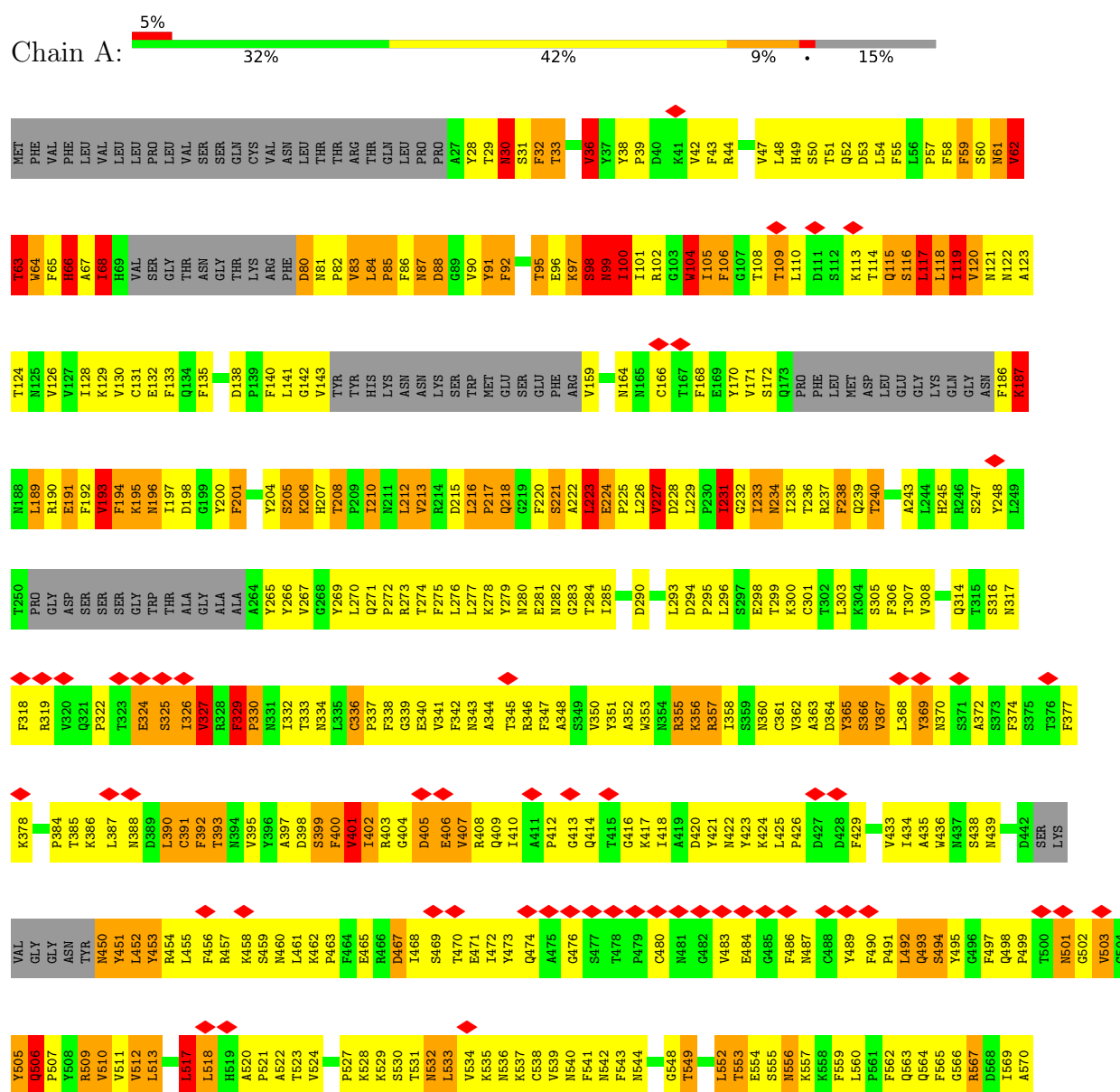
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Mol	Chain	Residues	Atoms				AltConf
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C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

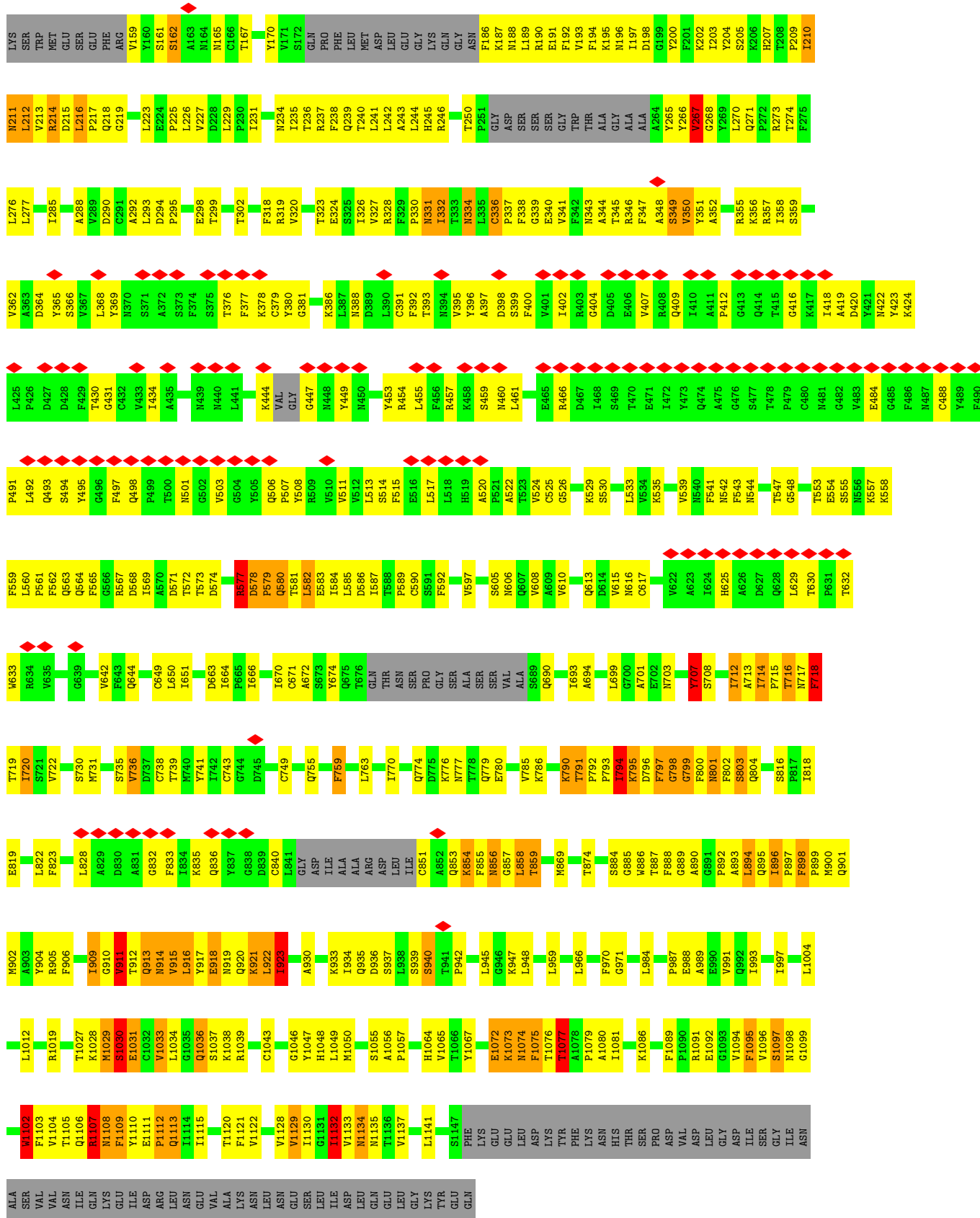
3 Residue-property plots

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

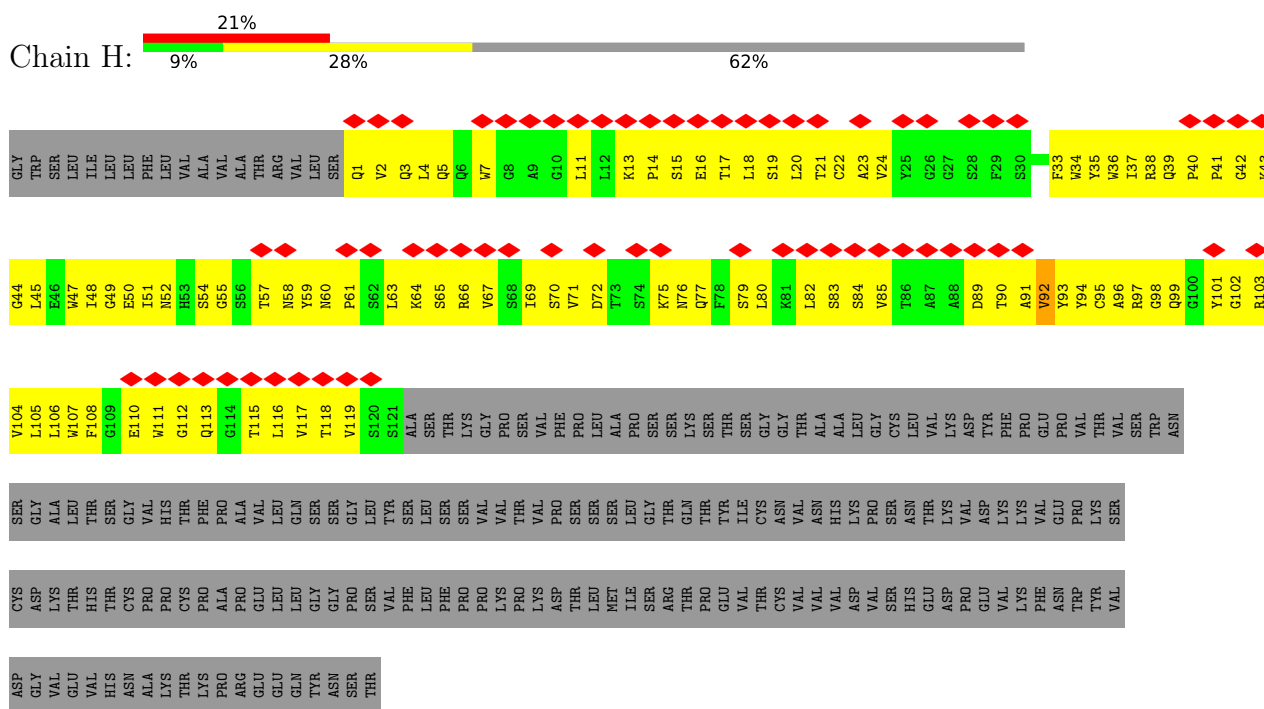
• Molecule 1: Spike glycoprotein



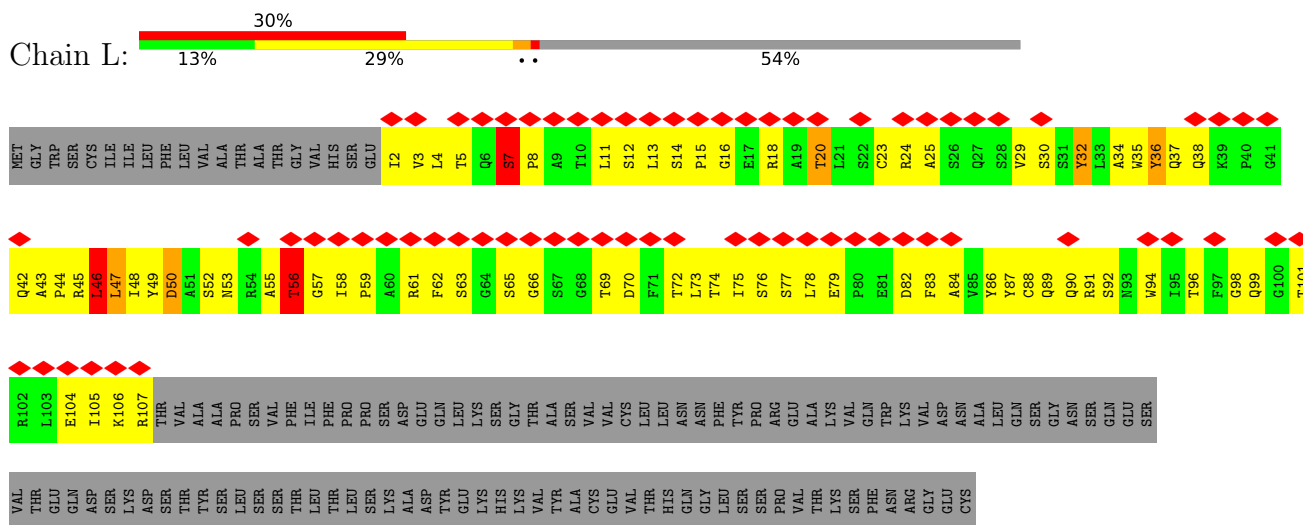




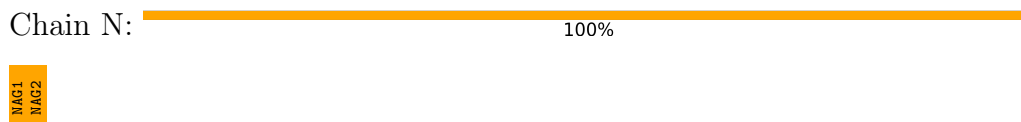
- Molecule 2: Heavy chain of BD-218



- Molecule 3: Light chain of BD-218



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



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



MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	297084	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 ($e^-/\text{\AA}^2$)	1.78125	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.623	Depositor
Minimum map value	-0.541	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.040	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	421.99997, 421.99997, 421.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.055, 1.055, 1.055	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	0.74	7/7981 (0.1%)	1.08	50/10890 (0.5%)
1	B	0.67	3/8263 (0.0%)	0.94	46/11270 (0.4%)
1	C	0.71	6/8278 (0.1%)	0.88	27/11279 (0.2%)
2	H	0.29	0/923	0.60	0/1257
3	L	0.34	0/784	0.82	4/1069 (0.4%)
All	All	0.69	16/26229 (0.1%)	0.95	127/35765 (0.4%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	32	PHE	CA-C	-8.45	1.43	1.52
1	B	1104	VAL	C-O	-7.38	1.16	1.24
1	C	707	TYR	CA-C	-7.26	1.43	1.52
1	B	279	TYR	CA-C	-6.73	1.46	1.53
1	B	1104	VAL	CA-C	-6.69	1.44	1.52
1	A	804	GLN	N-CA	-6.37	1.40	1.46
1	A	802	PHE	CA-C	-6.37	1.44	1.52
1	A	804	GLN	CA-C	-6.34	1.47	1.52
1	C	1104	VAL	C-O	-6.34	1.17	1.24
1	A	1094	VAL	CA-CB	-6.22	1.46	1.54
1	A	900	MET	CA-C	-5.76	1.45	1.52
1	C	1075	PHE	CA-CB	-5.70	1.45	1.53
1	C	1077	THR	CA-C	-5.51	1.45	1.53
1	C	267	VAL	CA-C	-5.38	1.46	1.52
1	C	1133	VAL	CA-CB	-5.35	1.47	1.53
1	A	357	ARG	CA-C	-5.07	1.46	1.52

All (127) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	712	ILE	N-CA-C	18.45	126.20	111.62
1	C	580	GLN	N-CA-C	-13.48	96.07	111.03
1	A	98	SER	N-CA-C	-11.15	95.76	111.81
1	C	31	SER	N-CA-C	9.82	124.83	113.15
1	C	214	ARG	N-CA-C	9.64	122.78	111.02
1	B	367	VAL	N-CA-C	-9.54	101.26	110.42
1	C	923	ILE	N-CA-C	-9.39	103.73	111.81
1	A	392	PHE	N-CA-C	8.97	124.06	113.20
1	A	195	LYS	N-CA-C	8.77	125.70	109.56
1	A	804	GLN	N-CA-C	-8.73	98.33	111.34
1	A	66	HIS	N-CA-C	8.67	123.29	110.46
1	A	192	PHE	N-CA-C	8.55	119.53	108.24
1	A	104	TRP	N-CA-C	-8.14	97.75	109.96
1	C	352	ALA	N-CA-C	-8.01	99.55	110.68
1	B	361	CYS	N-CA-C	7.70	127.19	110.80
1	A	194	PHE	N-CA-C	7.65	120.01	107.23
1	A	201	PHE	N-CA-C	-7.35	103.90	114.12
1	A	553	THR	CB-CA-C	7.28	124.90	110.42
1	B	108	THR	N-CA-C	7.22	120.06	111.33
1	A	227	VAL	N-CA-C	7.17	124.26	109.34
1	C	349	SER	N-CA-C	7.11	117.63	108.24
1	B	345	THR	CB-CA-C	-6.97	107.50	115.79
1	B	216	LEU	CA-C-N	-6.91	113.19	120.03
1	B	216	LEU	C-N-CA	-6.91	113.19	120.03
1	A	218	GLN	N-CA-C	6.89	119.75	108.52
1	A	191	GLU	N-CA-C	6.87	125.43	110.80
1	C	720	ILE	CB-CA-C	-6.76	104.63	111.80
1	C	1132	ILE	CB-CA-C	-6.65	100.48	111.32
1	B	1135	ASN	N-CA-C	6.64	118.90	107.28
1	C	211	ASN	N-CA-C	-6.63	103.98	111.07
1	A	68	ILE	N-CA-C	6.61	118.31	108.46
3	L	55	ALA	N-CA-C	-6.57	100.11	109.96
1	B	520	ALA	CA-C-N	-6.56	110.82	120.46
1	B	520	ALA	C-N-CA	-6.56	110.82	120.46
1	B	711	SER	CA-C-N	-6.54	116.23	123.16
1	B	711	SER	C-N-CA	-6.54	116.23	123.16
1	B	923	ILE	N-CA-C	-6.51	95.80	109.34
1	B	529	LYS	N-CA-C	6.50	118.40	110.41
1	A	327	VAL	N-CA-C	6.48	117.69	108.42
1	A	357	ARG	CA-C-N	-6.39	112.03	120.91
1	A	357	ARG	C-N-CA	-6.39	112.03	120.91
1	B	712	ILE	CA-C-O	-6.34	115.16	120.80
1	B	316	SER	N-CA-C	6.33	116.81	108.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1098	ASN	N-CA-C	-6.30	102.99	111.87
1	C	892	PRO	N-CA-C	-6.25	100.69	110.50
1	A	100	ILE	CB-CA-C	-6.20	102.91	111.65
1	A	803	SER	N-CA-C	-6.20	102.94	110.88
1	A	36	VAL	CB-CA-C	6.18	121.43	111.29
1	C	716	THR	N-CA-C	6.18	120.13	112.59
1	B	603	ASN	CA-C-N	-6.17	110.51	121.81
1	B	603	ASN	C-N-CA	-6.17	110.51	121.81
1	C	267	VAL	CB-CA-C	-6.14	103.01	111.49
1	B	201	PHE	N-CA-C	-6.10	101.25	110.28
3	L	36	TYR	N-CA-C	6.10	119.65	109.95
1	A	220	PHE	N-CA-C	6.10	119.34	109.40
1	A	585	LEU	N-CA-C	6.03	117.82	107.28
1	A	223	LEU	N-CA-C	6.02	123.62	110.80
1	B	92	PHE	N-CA-C	6.00	118.05	107.61
1	A	510	VAL	N-CA-C	5.94	117.14	108.58
1	B	137	ASN	N-CA-C	5.94	119.63	112.38
1	A	492	LEU	O-C-N	5.93	129.91	123.10
1	A	329	PHE	CA-C-N	-5.90	112.47	119.84
1	A	329	PHE	C-N-CA	-5.90	112.47	119.84
1	B	131	CYS	N-CA-C	5.87	123.30	110.80
1	A	187	LYS	N-CA-C	5.82	120.22	112.30
1	C	714	ILE	CA-C-N	5.82	127.12	119.84
1	C	714	ILE	C-N-CA	5.82	127.12	119.84
1	B	279	TYR	N-CA-C	-5.82	100.89	109.62
1	B	134	GLN	N-CA-C	5.79	123.13	110.80
1	B	345	THR	N-CA-C	5.78	119.94	109.32
1	A	556	ASN	N-CA-C	5.74	117.73	108.32
1	C	1137	VAL	N-CA-C	-5.73	99.50	107.80
1	B	444	LYS	N-CA-C	-5.71	103.37	111.24
1	C	577	ARG	N-CA-C	-5.70	99.23	108.52
1	A	395	VAL	O-C-N	-5.69	116.73	123.04
1	A	84	LEU	CA-C-N	5.60	126.84	119.84
1	A	84	LEU	C-N-CA	5.60	126.84	119.84
3	L	46	LEU	N-CA-C	5.60	117.80	107.73
1	C	898	PHE	N-CA-C	5.58	122.14	109.81
1	C	267	VAL	N-CA-C	5.58	117.20	109.45
1	B	86	PHE	N-CA-C	5.57	121.49	114.31
1	C	1133	VAL	CB-CA-C	-5.56	103.76	110.99
1	A	1105	THR	CA-C-N	-5.56	110.92	121.54
1	A	1105	THR	C-N-CA	-5.56	110.92	121.54
1	B	1099	GLY	N-CA-C	-5.56	100.00	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	133	PHE	N-CA-C	5.56	118.16	107.44
1	B	98	SER	N-CA-C	-5.55	97.03	108.18
1	B	215	ASP	N-CA-C	5.53	117.97	109.07
1	C	1102	TRP	N-CA-C	5.51	122.53	110.80
1	B	84	LEU	CA-C-N	5.48	125.94	120.52
1	B	84	LEU	C-N-CA	5.48	125.94	120.52
1	B	1130	ILE	CB-CA-C	-5.46	103.55	111.68
1	A	899	PRO	N-CA-C	-5.44	101.26	112.47
1	B	736	VAL	N-CA-C	5.43	116.55	108.46
1	B	216	LEU	N-CA-C	5.43	121.81	109.81
1	B	712	ILE	O-C-N	5.40	126.14	121.98
1	C	718	PHE	N-CA-C	5.39	117.86	108.76
1	A	759	PHE	CA-C-N	-5.37	112.37	121.18
1	A	759	PHE	C-N-CA	-5.37	112.37	121.18
1	A	898	PHE	N-CA-C	5.35	121.64	109.81
1	A	554	GLU	N-CA-C	-5.33	105.00	112.25
1	A	30	ASN	N-CA-C	5.31	118.09	109.06
1	C	1073	LYS	N-CA-C	-5.31	99.17	107.93
1	A	493	GLN	N-CA-C	-5.31	99.49	110.80
1	A	116	SER	N-CA-C	5.27	122.02	110.80
1	A	467	ASP	N-CA-C	5.22	117.14	110.61
1	A	117	LEU	CA-C-N	5.22	131.51	121.54
1	A	117	LEU	C-N-CA	5.22	131.51	121.54
1	A	587	ILE	N-CA-C	5.21	114.73	108.06
1	A	324	GLU	O-C-N	-5.18	115.59	122.74
1	C	213	VAL	CB-CA-C	-5.18	105.25	111.88
1	C	33	THR	CB-CA-C	-5.16	101.77	110.44
1	B	717	ASN	N-CA-C	-5.15	102.24	109.96
1	B	361	CYS	N-CA-CB	-5.15	101.79	110.49
1	B	1100	THR	CB-CA-C	-5.15	107.97	114.40
1	B	1132	ILE	N-CA-C	-5.14	102.87	109.30
1	C	63	THR	N-CA-C	5.13	117.91	108.58
1	B	710	ASN	N-CA-C	-5.12	99.89	110.80
1	C	909	ILE	N-CA-C	-5.12	107.84	112.96
1	C	334	ASN	N-CA-C	5.08	117.36	111.02
3	L	56	THR	N-CA-C	5.07	121.60	110.80
1	B	100	ILE	N-CA-C	5.05	119.85	109.34
1	A	505	TYR	N-CA-C	-5.04	104.61	111.56
1	B	946	GLY	N-CA-C	-5.03	106.67	112.50
1	A	1042	PHE	N-CA-C	-5.02	107.11	113.18
1	B	201	PHE	CB-CA-C	5.01	118.22	109.65
1	A	1094	VAL	CB-CA-C	-5.00	103.09	111.29

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7816	0	7501	933	0
1	B	8083	0	7787	821	0
1	C	8096	0	7837	687	0
2	H	903	0	862	129	0
3	L	769	0	726	102	0
4	D	28	0	25	7	0
4	N	28	0	25	5	0
5	A	168	0	156	14	0
5	B	154	0	143	33	0
5	C	126	0	117	19	0
All	All	26171	0	25179	2560	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 50.

All (2560) 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:559:PHE:CE1	1:A:584:ILE:HD11	1.52	1.45
1:B:201:PHE:CE2	1:B:203:ILE:HD11	1.51	1.43
1:A:86:PHE:CE1	1:A:90:VAL:HG22	1.54	1.40
1:C:712:ILE:CG2	1:C:1077:THR:HG22	1.52	1.40
1:A:917:TYR:HB3	1:C:1129:VAL:CG1	1.54	1.38
1:B:282:ASN:OD1	5:B:1306:NAG:C1	1.76	1.31
1:B:318:PHE:CE2	1:B:623:ALA:HB1	1.65	1.31
1:A:347:PHE:HD2	1:A:509:ARG:CB	1.43	1.29
1:B:336:CYS:HB3	1:B:337:PRO:CD	1.55	1.29
1:C:1134:ASN:OD1	5:C:1302:NAG:C1	1.81	1.26
1:B:718:PHE:HD1	1:B:1067:TYR:CE2	1.53	1.26
1:B:38:TYR:CD1	1:B:285:ILE:HD11	1.69	1.25
1:A:559:PHE:CZ	1:A:584:ILE:HD11	1.69	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:VAL:HG13	1:C:267:VAL:O	1.25	1.24
1:B:497:PHE:CD2	1:B:507:PRO:HB3	1.70	1.24
1:A:506:GLN:HB2	1:A:507:PRO:CD	1.62	1.24
2:H:82:LEU:HD21	2:H:93:TYR:CE2	1.72	1.23
1:A:904:TYR:HE2	1:C:1094:VAL:CG1	1.54	1.21
1:B:38:TYR:CE1	1:B:285:ILE:HD11	1.77	1.20
1:B:718:PHE:CD1	1:B:1067:TYR:CE2	2.30	1.19
1:C:712:ILE:HB	1:C:1077:THR:CG2	1.72	1.19
3:L:7:SER:HB3	3:L:8:PRO:CD	1.72	1.19
1:A:904:TYR:CE2	1:C:1094:VAL:CG1	2.27	1.18
1:B:336:CYS:CB	1:B:337:PRO:CD	2.18	1.18
1:A:347:PHE:CD2	1:A:509:ARG:CB	2.26	1.17
1:C:133:PHE:HA	1:C:162:SER:O	1.44	1.17
1:B:417:LYS:O	1:B:421:TYR:HB2	1.44	1.17
1:B:116:SER:OG	1:B:235:ILE:HG12	1.46	1.16
1:B:712:ILE:CD1	1:C:896:ILE:HG22	1.74	1.16
1:B:97:LYS:CE	1:B:100:ILE:HD11	1.75	1.16
1:C:919:ASN:O	1:C:923:ILE:HG22	1.47	1.15
1:A:200:TYR:CB	1:A:228:ASP:CG	2.20	1.14
1:A:206:LYS:CD	1:A:223:LEU:CB	2.26	1.14
1:C:712:ILE:CG2	1:C:1077:THR:CG2	2.26	1.14
1:B:360:ASN:HA	1:B:523:THR:HB	1.22	1.14
1:B:117:LEU:CD2	1:B:233:ILE:HD11	1.78	1.13
1:A:1090:PRO:HD3	1:A:1095:PHE:CE1	1.83	1.12
1:C:718:PHE:CD1	1:C:1067:TYR:HE1	1.68	1.12
1:A:533:LEU:CD1	1:A:541:PHE:HA	1.78	1.12
1:B:712:ILE:HD12	1:C:896:ILE:CG2	1.77	1.12
1:C:1075:PHE:CE1	1:C:1110:TYR:HE1	1.68	1.11
1:B:336:CYS:CB	1:B:337:PRO:HD2	1.78	1.10
1:C:64:TRP:HA	1:C:266:TYR:HB3	1.18	1.10
1:C:351:TYR:HE1	1:C:453:TYR:HA	1.08	1.10
1:A:917:TYR:HB3	1:C:1129:VAL:HG11	1.11	1.09
1:B:336:CYS:HB3	1:B:337:PRO:HD3	1.15	1.09
1:C:712:ILE:HG22	1:C:1077:THR:HG22	1.21	1.09
1:C:888:PHE:CZ	1:C:1034:LEU:CD2	2.36	1.09
1:B:497:PHE:CE2	1:B:507:PRO:HB3	1.87	1.09
1:B:389:ASP:HA	1:B:526:GLY:HA3	1.34	1.09
1:B:362:VAL:HG12	1:B:526:GLY:O	1.51	1.08
1:C:564:GLN:HA	1:C:577:ARG:HD3	1.32	1.08
1:C:712:ILE:HB	1:C:1077:THR:HG21	1.14	1.08
1:C:712:ILE:CB	1:C:1077:THR:CG2	2.29	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:82:LEU:CD2	2:H:93:TYR:CE2	2.35	1.08
2:H:104:VAL:HG23	3:L:49:TYR:CD2	1.89	1.08
1:A:533:LEU:HD11	1:A:541:PHE:HA	1.29	1.07
1:A:1090:PRO:CD	1:A:1095:PHE:HE1	1.66	1.07
1:B:456:PHE:HB3	1:B:491:PRO:HA	1.32	1.07
1:A:580:GLN:CG	5:A:1306:NAG:HN2	1.66	1.07
1:B:318:PHE:HE2	1:B:623:ALA:HB1	0.94	1.06
1:A:506:GLN:HB2	1:A:507:PRO:HD2	1.38	1.06
1:C:922:LEU:HD11	5:C:1301:NAG:C6	1.84	1.06
1:B:711:SER:O	1:C:897:PRO:HD3	1.54	1.05
1:C:717:ASN:OD1	5:C:1301:NAG:H82	1.56	1.05
2:H:82:LEU:CD2	2:H:93:TYR:HE2	1.68	1.05
1:A:451:TYR:HB2	1:A:495:TYR:CB	1.84	1.05
1:B:360:ASN:O	1:B:524:VAL:HA	1.55	1.05
1:C:1075:PHE:CZ	1:C:1110:TYR:HE1	1.74	1.05
1:A:114:THR:O	1:A:132:GLU:HG3	1.57	1.04
1:A:393:THR:OG1	1:A:522:ALA:HA	1.56	1.04
1:A:33:THR:HB	1:A:58:PHE:HA	1.36	1.04
1:B:336:CYS:HB2	1:B:337:PRO:HD2	1.36	1.04
1:C:1075:PHE:CZ	1:C:1110:TYR:CE1	2.46	1.04
1:A:1090:PRO:HD3	1:A:1095:PHE:HE1	1.14	1.04
1:A:106:PHE:O	1:A:110:LEU:HD21	1.55	1.04
1:A:904:TYR:HE2	1:C:1094:VAL:HG11	1.16	1.04
1:A:326:ILE:HD11	1:A:539:VAL:CG1	1.88	1.04
1:A:801:ASN:OD1	5:A:1301:NAG:C1	2.03	1.03
1:C:912:THR:H	1:C:1107:ARG:NH1	1.54	1.03
1:A:544:ASN:HB3	1:A:579:PRO:HG3	1.39	1.03
1:B:282:ASN:CG	5:B:1306:NAG:C1	2.30	1.03
3:L:8:PRO:HB2	3:L:11:LEU:HB2	1.40	1.03
1:A:32:PHE:CB	1:A:218:GLN:HG2	1.86	1.03
1:B:104:TRP:HZ3	1:B:194:PHE:CB	1.71	1.03
1:B:97:LYS:HE2	1:B:100:ILE:HD11	1.09	1.02
1:C:888:PHE:CZ	1:C:1034:LEU:HD22	1.94	1.02
1:B:736:VAL:HG23	1:B:858:LEU:HD13	1.39	1.02
1:A:580:GLN:HG2	5:A:1306:NAG:HN2	0.91	1.02
2:H:82:LEU:HD21	2:H:93:TYR:CD2	1.93	1.02
1:A:32:PHE:CB	1:A:218:GLN:CG	2.37	1.01
1:B:717:ASN:CG	5:B:1302:NAG:C8	2.32	1.01
1:A:97:LYS:HD3	1:A:187:LYS:HD2	1.35	1.01
1:A:559:PHE:CE1	1:A:584:ILE:CD1	2.42	1.01
1:A:104:TRP:CZ3	1:A:194:PHE:CB	2.44	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:LYS:HD2	1:A:223:LEU:CB	1.90	1.01
1:B:337:PRO:HG3	1:B:358:ILE:CD1	1.91	1.01
1:B:718:PHE:CD1	1:B:1067:TYR:HE2	1.75	1.01
1:B:117:LEU:CD2	1:B:233:ILE:CD1	2.39	1.01
1:A:439:ASN:CB	1:A:503:VAL:HG21	1.91	1.00
1:B:318:PHE:HE2	1:B:623:ALA:CB	1.73	1.00
1:A:104:TRP:HZ3	1:A:194:PHE:CB	1.74	1.00
1:A:1081:ILE:HD12	1:A:1095:PHE:CE2	1.97	0.99
1:B:529:LYS:NZ	1:B:529:LYS:HA	1.76	0.99
1:C:712:ILE:CB	1:C:1077:THR:HG21	1.88	0.99
3:L:7:SER:HB3	3:L:8:PRO:HD3	1.42	0.99
3:L:88:CYS:H	3:L:99:GLN:HG2	1.22	0.99
1:C:64:TRP:HA	1:C:266:TYR:CB	1.91	0.98
2:H:104:VAL:CG2	3:L:49:TYR:CD2	2.46	0.98
1:B:201:PHE:CE2	1:B:203:ILE:CD1	2.45	0.98
1:A:580:GLN:HG2	5:A:1306:NAG:N2	1.76	0.98
1:A:33:THR:CB	1:A:58:PHE:HA	1.94	0.98
1:A:355:ARG:HB3	1:A:398:ASP:OD2	1.63	0.98
1:C:718:PHE:HD1	1:C:1067:TYR:CE1	1.80	0.97
1:A:196:ASN:ND2	1:A:235:ILE:CD1	2.27	0.97
1:C:894:LEU:HD22	1:C:894:LEU:H	1.25	0.97
1:A:196:ASN:HD22	1:A:235:ILE:HD12	1.29	0.97
1:B:712:ILE:HD12	1:C:896:ILE:HG22	0.99	0.97
1:A:439:ASN:CB	1:A:503:VAL:CG2	2.42	0.97
1:A:805:ILE:HD13	1:A:805:ILE:H	1.30	0.97
1:B:83:VAL:HG22	1:B:237:ARG:CG	1.95	0.97
1:A:904:TYR:OH	1:C:1094:VAL:HG13	1.64	0.96
1:C:62:VAL:HG13	1:C:267:VAL:C	1.90	0.96
1:A:326:ILE:HD11	1:A:539:VAL:HG13	1.47	0.96
1:A:86:PHE:CE1	1:A:90:VAL:CG2	2.48	0.96
1:A:196:ASN:ND2	1:A:235:ILE:HD11	1.80	0.96
1:A:404:GLY:O	1:A:407:VAL:HG23	1.65	0.96
1:B:83:VAL:CG2	1:B:237:ARG:HG2	1.95	0.96
1:C:351:TYR:CE1	1:C:453:TYR:HA	1.99	0.96
1:C:718:PHE:HD1	1:C:1067:TYR:HE1	0.97	0.95
1:B:93:ALA:HB2	1:B:191:GLU:HA	1.46	0.95
1:B:139:PRO:O	1:B:243:ALA:HB2	1.66	0.95
1:A:82:PRO:CB	1:A:240:THR:H	1.80	0.95
1:A:805:ILE:HG22	1:A:1054:GLN:NE2	1.81	0.95
1:B:497:PHE:CD2	1:B:507:PRO:CB	2.49	0.95
2:H:106:LEU:HA	3:L:46:LEU:HD23	1.48	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:759:PHE:O	1:C:763:LEU:HD23	1.66	0.95
1:B:97:LYS:HE2	1:B:100:ILE:CD1	1.97	0.95
1:B:282:ASN:ND2	5:B:1306:NAG:C1	2.31	0.94
1:B:337:PRO:HG3	1:B:358:ILE:HG12	1.49	0.94
1:B:337:PRO:HG3	1:B:358:ILE:CG1	1.97	0.94
1:B:38:TYR:CE1	1:B:285:ILE:CD1	2.50	0.94
1:B:104:TRP:CZ3	1:B:194:PHE:CB	2.49	0.94
1:B:122:ASN:HB2	1:B:127:VAL:HG13	1.48	0.94
1:C:921:LYS:H	1:C:921:LYS:HZ3	1.10	0.94
3:L:37:GLN:H	3:L:47:LEU:CD1	1.81	0.94
1:C:92:PHE:CE1	1:C:265:TYR:CE1	2.55	0.93
1:C:351:TYR:CD1	1:C:422:ASN:OD1	2.21	0.93
1:C:712:ILE:HG21	1:C:1077:THR:HG22	1.50	0.93
1:B:201:PHE:HE2	1:B:203:ILE:HD11	1.24	0.93
3:L:37:GLN:H	3:L:47:LEU:HD13	1.32	0.93
1:A:506:GLN:HB2	1:A:507:PRO:HD3	1.50	0.93
1:B:117:LEU:HD21	1:B:233:ILE:HD11	1.49	0.92
1:B:132:GLU:O	1:B:164:ASN:HB2	1.69	0.92
1:C:922:LEU:HD11	5:C:1301:NAG:O6	1.68	0.92
1:A:66:HIS:HB2	1:A:68:ILE:HD12	1.51	0.92
1:A:536:ASN:OD1	1:A:552:LEU:HD13	1.70	0.92
1:A:557:LYS:NZ	1:B:43:PHE:HE2	1.68	0.92
1:A:196:ASN:HD22	1:A:235:ILE:CD1	1.81	0.92
1:A:338:PHE:HB3	1:A:342:PHE:CE2	2.05	0.91
1:A:453:TYR:O	1:A:492:LEU:HD22	1.71	0.91
1:C:1075:PHE:HZ	1:C:1110:TYR:CE1	1.87	0.91
1:A:206:LYS:HG2	1:A:223:LEU:CB	1.99	0.91
1:B:1082:CYS:HB2	1:B:1132:ILE:HD11	1.49	0.91
2:H:13:LYS:HG2	2:H:118:THR:HG22	1.49	0.91
1:A:435:ALA:HB2	1:A:510:VAL:HG23	1.51	0.91
1:A:418:ILE:HA	1:A:422:ASN:HB2	1.53	0.91
1:A:552:LEU:HD23	1:B:848:ASP:OD2	1.70	0.90
1:A:809:PRO:HA	1:A:814:LYS:HE3	1.50	0.90
1:B:718:PHE:HE2	1:B:919:ASN:OD1	1.54	0.90
1:A:338:PHE:HA	1:A:341:VAL:HG12	1.53	0.90
1:B:497:PHE:HD2	1:B:507:PRO:HB3	1.31	0.90
1:C:92:PHE:CE1	1:C:265:TYR:HE1	1.90	0.90
1:A:506:GLN:CB	1:A:507:PRO:CD	2.46	0.90
1:C:922:LEU:CD1	5:C:1301:NAG:H62	2.02	0.90
1:B:718:PHE:CE2	1:B:919:ASN:OD1	2.24	0.90
1:B:712:ILE:HG22	1:B:1075:PHE:O	1.70	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:THR:O	1:A:186:PHE:HB3	1.71	0.90
1:A:436:TRP:CD1	1:A:438:SER:HG	1.89	0.90
1:B:310:LYS:HG3	1:B:600:PRO:HA	1.52	0.90
1:A:68:ILE:H	1:A:68:ILE:HD13	1.35	0.90
1:A:350:VAL:CG2	1:A:453:TYR:HA	2.03	0.89
1:A:1081:ILE:HD12	1:A:1095:PHE:HE2	1.33	0.89
2:H:39:GLN:HB2	2:H:45:LEU:HG	1.50	0.89
3:L:34:ALA:HB3	3:L:89:GLN:HB3	1.55	0.89
1:B:282:ASN:HD21	5:B:1306:NAG:C1	1.83	0.89
1:C:141:LEU:HB3	1:C:243:ALA:HB2	1.52	0.89
1:C:912:THR:H	1:C:1107:ARG:HH11	1.07	0.89
1:A:361:CYS:H	1:A:524:VAL:HG22	1.35	0.89
1:C:920:GLN:O	1:C:923:ILE:HG23	1.73	0.89
1:A:206:LYS:CG	1:A:223:LEU:CB	2.51	0.89
1:A:452:LEU:HD11	1:A:492:LEU:HD13	1.55	0.89
1:C:564:GLN:HA	1:C:577:ARG:CD	2.03	0.89
1:B:57:PRO:HB3	1:B:273:ARG:HH22	1.37	0.89
2:H:1:GLN:HG2	2:H:2:VAL:H	1.37	0.89
1:B:282:ASN:OD1	5:B:1306:NAG:O5	1.89	0.89
1:A:540:ASN:HA	1:A:549:THR:HG23	1.53	0.88
1:C:544:ASN:HD21	1:C:579:PRO:HG3	1.36	0.88
1:A:336:CYS:SG	1:A:337:PRO:HD2	2.11	0.88
1:A:97:LYS:HD3	1:A:187:LYS:CD	2.03	0.88
1:A:904:TYR:CE2	1:C:1094:VAL:HG13	2.04	0.88
1:C:533:LEU:HD22	1:C:578:ASP:OD2	1.73	0.88
1:C:1075:PHE:CE1	1:C:1110:TYR:CE1	2.59	0.88
1:C:1075:PHE:HZ	1:C:1110:TYR:CZ	1.91	0.88
1:B:83:VAL:CG2	1:B:237:ARG:CG	2.52	0.88
1:A:896:ILE:HG12	1:C:712:ILE:CD1	2.04	0.88
1:A:280:ASN:HD21	1:A:284:THR:HB	1.38	0.88
1:A:559:PHE:CZ	1:A:584:ILE:CD1	2.56	0.88
1:A:187:LYS:O	1:A:187:LYS:NZ	2.07	0.87
1:B:712:ILE:HG22	1:B:1075:PHE:C	1.99	0.87
1:C:922:LEU:CD1	5:C:1301:NAG:C6	2.51	0.87
3:L:7:SER:CB	3:L:8:PRO:CD	2.52	0.87
1:C:1075:PHE:HZ	1:C:1110:TYR:OH	1.57	0.87
1:A:298:GLU:HG2	1:A:633:TRP:HZ2	1.40	0.87
1:B:717:ASN:ND2	5:B:1302:NAG:O5	2.07	0.87
1:A:455:LEU:HD11	1:A:493:GLN:HB2	1.55	0.87
1:B:206:LYS:CA	1:B:206:LYS:HE3	2.03	0.87
1:C:62:VAL:CG1	1:C:267:VAL:O	2.20	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:LEU:HD12	1:C:266:TYR:OH	1.73	0.87
1:C:856:ASN:OD1	1:C:858:LEU:CD2	2.23	0.87
1:A:330:PRO:HA	1:A:580:GLN:NE2	1.90	0.87
1:A:917:TYR:CB	1:C:1129:VAL:CG1	2.49	0.86
1:A:279:TYR:HB3	1:A:283:GLY:HA2	1.55	0.86
1:A:200:TYR:CB	1:A:228:ASP:OD2	2.23	0.86
1:B:915:VAL:O	1:B:919:ASN:HB2	1.75	0.86
1:A:904:TYR:CZ	1:C:1094:VAL:HG13	2.08	0.86
1:A:308:VAL:HG12	1:A:602:THR:HB	1.55	0.86
1:C:856:ASN:O	1:C:858:LEU:HD23	1.76	0.85
1:A:100:ILE:CG2	1:A:243:ALA:H	1.89	0.85
1:A:712:ILE:HG13	1:B:896:ILE:HG22	1.57	0.85
1:B:93:ALA:HB2	1:B:191:GLU:CA	2.05	0.85
1:B:1103:PHE:HB3	1:B:1113:GLN:O	1.76	0.85
1:A:196:ASN:HA	1:A:201:PHE:HA	1.59	0.85
1:C:568:ASP:H	1:C:571:ASP:HA	1.41	0.85
1:C:349:SER:O	1:C:400:PHE:HB3	1.77	0.85
1:B:83:VAL:HG22	1:B:237:ARG:HD2	1.59	0.85
1:C:100:ILE:HG22	1:C:242:LEU:HD23	1.59	0.85
1:C:888:PHE:CE1	1:C:1034:LEU:CD2	2.59	0.85
1:A:503:VAL:HG22	1:A:506:GLN:NE2	1.92	0.85
1:A:552:LEU:CD2	1:B:848:ASP:OD2	2.25	0.85
1:C:717:ASN:OD1	5:C:1301:NAG:C8	2.25	0.85
1:A:413:GLY:HA3	1:C:987:PRO:HG3	1.59	0.85
1:A:560:LEU:H	1:A:563:GLN:HB2	1.41	0.85
1:B:712:ILE:CD1	1:C:896:ILE:CG2	2.46	0.85
1:A:534:VAL:HB	1:A:539:VAL:HG21	1.59	0.85
1:C:244:LEU:HD12	1:C:245:HIS:H	1.42	0.84
1:B:337:PRO:CG	1:B:358:ILE:HG12	2.07	0.84
1:A:917:TYR:CB	1:C:1129:VAL:HG11	2.03	0.84
1:C:888:PHE:HA	1:C:893:ALA:CB	2.06	0.84
1:B:84:LEU:O	1:B:237:ARG:HG3	1.76	0.84
1:A:326:ILE:HG13	1:A:533:LEU:HD22	1.59	0.84
1:A:33:THR:HB	1:A:58:PHE:CA	2.07	0.84
1:B:83:VAL:HG22	1:B:237:ARG:CD	2.07	0.84
1:C:888:PHE:CE1	1:C:1034:LEU:HD22	2.13	0.84
1:C:1075:PHE:HZ	1:C:1110:TYR:HH	0.96	0.84
1:A:567:ARG:HD3	1:A:571:ASP:HA	1.60	0.83
1:B:921:LYS:HA	1:B:921:LYS:NZ	1.92	0.83
1:A:1039:ARG:HD2	1:C:1039:ARG:HD3	1.60	0.83
1:B:717:ASN:CG	5:B:1302:NAG:H82	2.02	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:717:ASN:OD1	5:B:1302:NAG:C8	2.26	0.83
1:C:332:ILE:HG22	1:C:362:VAL:HG13	1.58	0.83
1:C:921:LYS:H	1:C:921:LYS:NZ	1.75	0.83
1:A:348:ALA:O	1:A:451:TYR:CD1	2.32	0.83
1:C:888:PHE:HZ	1:C:1034:LEU:HD21	1.43	0.83
1:B:360:ASN:O	1:B:524:VAL:CA	2.27	0.83
1:B:402:ILE:HD12	1:B:406:GLU:HB2	1.60	0.83
2:H:39:GLN:O	2:H:92:VAL:HG23	1.78	0.83
1:A:106:PHE:HE2	1:A:118:LEU:HA	1.44	0.82
1:A:452:LEU:CD1	1:A:492:LEU:HD13	2.07	0.82
1:A:457:ARG:HD2	1:A:458:LYS:HG2	1.60	0.82
1:A:1090:PRO:CG	1:A:1095:PHE:HE1	1.91	0.82
1:B:941:THR:H	1:B:942:PRO:HD3	1.44	0.82
1:B:412:PRO:HB3	1:B:427:ASP:HA	1.60	0.82
1:B:1082:CYS:HB3	1:B:1134:ASN:HB2	1.60	0.82
1:B:442:ASP:OD2	1:B:507:PRO:HG3	1.79	0.82
1:A:330:PRO:CA	1:A:580:GLN:HE22	1.91	0.82
1:B:337:PRO:CD	1:B:358:ILE:HG12	2.09	0.82
2:H:98:GLY:HA3	2:H:105:LEU:HD23	1.59	0.82
1:B:736:VAL:CG2	1:B:858:LEU:HD13	2.08	0.82
1:C:128:ILE:HD13	1:C:229:LEU:HD11	1.62	0.82
2:H:82:LEU:HD23	2:H:93:TYR:HE2	1.44	0.82
1:B:279:TYR:HA	1:B:285:ILE:HA	1.61	0.82
1:B:360:ASN:CA	1:B:523:THR:HB	2.07	0.82
1:A:429:PHE:HZ	1:A:512:VAL:HG22	1.44	0.81
1:C:741:TYR:CE1	1:C:966:LEU:HD21	2.15	0.81
1:C:922:LEU:CD1	5:C:1301:NAG:O6	2.28	0.81
1:A:86:PHE:HE1	1:A:90:VAL:HG22	1.08	0.81
1:B:108:THR:H	1:B:235:ILE:HG13	1.45	0.81
1:B:529:LYS:HA	1:B:529:LYS:CE	2.07	0.81
1:A:553:THR:CB	1:A:587:ILE:HA	2.10	0.81
1:B:337:PRO:HG3	1:B:358:ILE:HD11	1.59	0.81
1:B:714:ILE:HG12	1:B:715:PRO:HD2	1.62	0.81
1:C:544:ASN:ND2	1:C:579:PRO:HG3	1.95	0.81
1:A:436:TRP:CD1	1:A:438:SER:OG	2.32	0.81
1:B:351:TYR:HB2	1:B:454:ARG:HG2	1.62	0.81
1:A:210:ILE:HG23	1:A:212:LEU:HD23	1.62	0.81
1:A:348:ALA:O	1:A:451:TYR:HD1	1.63	0.81
1:B:362:VAL:CG1	1:B:526:GLY:O	2.28	0.81
1:B:106:PHE:CZ	1:B:201:PHE:HE1	1.98	0.81
1:C:714:ILE:CG2	1:C:1109:PHE:O	2.28	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1081:ILE:CD1	1:A:1095:PHE:CD2	2.64	0.81
1:C:712:ILE:HG22	1:C:1077:THR:CG2	2.04	0.81
1:A:85:PRO:HD2	1:A:269:TYR:OH	1.80	0.81
1:B:201:PHE:CZ	1:B:203:ILE:HD11	2.16	0.81
1:A:32:PHE:CB	1:A:218:GLN:HG3	2.10	0.80
1:A:322:PRO:HB2	1:A:538:CYS:H	1.45	0.80
1:B:96:GLU:HG2	1:B:99:ASN:HA	1.63	0.80
1:A:731:MET:HG3	1:A:955:ASN:HD21	1.45	0.80
1:A:1098:ASN:OD1	1:A:1098:ASN:N	2.14	0.80
1:C:718:PHE:CD1	1:C:1067:TYR:CE1	2.60	0.80
2:H:104:VAL:CG2	3:L:49:TYR:HD2	1.93	0.80
1:B:117:LEU:HD22	1:B:233:ILE:CD1	2.12	0.80
1:B:318:PHE:CD2	1:B:623:ALA:HB1	2.17	0.80
1:B:389:ASP:HA	1:B:526:GLY:CA	2.11	0.80
1:A:592:PHE:H	1:B:853:GLN:HG3	1.46	0.80
1:C:355:ARG:HH22	1:C:514:SER:HB2	1.46	0.79
1:B:83:VAL:CG2	1:B:237:ARG:CD	2.60	0.79
1:B:715:PRO:HA	1:B:1072:GLU:CB	2.11	0.79
1:B:673:SER:HB3	1:B:675:GLN:HE22	1.47	0.79
1:C:62:VAL:HG22	1:C:268:GLY:HA2	1.62	0.79
1:A:393:THR:O	1:A:523:THR:HG22	1.82	0.79
1:C:109:THR:HG23	1:C:111:ASP:H	1.45	0.79
1:C:718:PHE:HB2	1:C:1067:TYR:CE1	2.18	0.79
1:B:206:LYS:HE3	1:B:206:LYS:HA	1.62	0.79
1:C:193:VAL:HG23	1:C:223:LEU:HD22	1.65	0.79
1:C:210:ILE:H	1:C:210:ILE:HD12	1.47	0.79
1:A:330:PRO:CB	1:A:580:GLN:HE22	1.96	0.79
1:B:110:LEU:HD22	1:B:135:PHE:CB	2.13	0.79
1:B:122:ASN:HD22	1:B:127:VAL:CG1	1.96	0.79
1:A:347:PHE:HB3	1:A:400:PHE:O	1.83	0.78
1:B:717:ASN:ND2	5:B:1302:NAG:H82	1.98	0.78
2:H:20:LEU:HD11	2:H:93:TYR:HB2	1.64	0.78
2:H:39:GLN:NE2	2:H:43:LYS:H	1.81	0.78
1:B:454:ARG:HE	1:B:457:ARG:HD2	1.49	0.78
1:C:888:PHE:HA	1:C:893:ALA:HB2	1.63	0.78
1:B:1106:GLN:HE21	1:B:1109:PHE:HB3	1.47	0.78
1:B:93:ALA:HB2	1:B:190:ARG:C	2.08	0.78
1:A:200:TYR:CB	1:A:228:ASP:OD1	2.32	0.78
1:C:351:TYR:HD1	1:C:422:ASN:OD1	1.66	0.78
1:A:84:LEU:HD12	1:A:84:LEU:H	1.48	0.78
3:L:56:THR:C	3:L:58:ILE:H	1.92	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:553:THR:CB	1:A:587:ILE:HG22	2.14	0.77
1:A:1090:PRO:CD	1:A:1095:PHE:CE1	2.55	0.77
1:C:936:ASP:OD1	1:C:937:SER:N	2.17	0.77
1:A:826:VAL:HG23	1:A:945:LEU:HD13	1.65	0.77
1:C:856:ASN:OD1	1:C:858:LEU:HD23	1.84	0.77
1:C:919:ASN:C	1:C:923:ILE:HG22	2.10	0.77
1:A:82:PRO:CG	1:A:240:THR:H	1.97	0.77
1:A:575:ALA:HA	1:A:586:ASP:HA	1.66	0.77
1:A:587:ILE:HD12	1:A:587:ILE:N	2.00	0.77
1:C:718:PHE:H	1:C:718:PHE:HD2	1.30	0.77
1:A:518:LEU:N	1:A:518:LEU:HD23	1.99	0.77
1:B:121:ASN:O	1:B:121:ASN:ND2	2.17	0.77
1:A:322:PRO:HB2	1:A:537:LYS:HB2	1.67	0.77
1:A:784:GLN:HE22	1:A:1030:SER:HB3	1.50	0.77
1:B:83:VAL:CG2	1:B:237:ARG:HD2	2.14	0.77
1:B:130:VAL:HG21	1:B:168:PHE:HB3	1.67	0.77
1:B:714:ILE:CG1	1:B:715:PRO:HD2	2.15	0.77
1:B:106:PHE:HB3	1:B:235:ILE:HG21	1.66	0.76
1:B:93:ALA:CB	1:B:190:ARG:C	2.58	0.76
1:B:825:LYS:HB2	1:B:945:LEU:HD21	1.67	0.76
1:A:66:HIS:O	1:A:80:ASP:HB3	1.84	0.76
1:B:462:LYS:HG3	1:B:465:GLU:HB2	1.66	0.76
1:A:212:LEU:HD11	1:A:217:PRO:HB3	1.66	0.76
1:A:506:GLN:CB	1:A:507:PRO:HD3	2.09	0.76
1:B:337:PRO:HB2	1:B:341:VAL:HG22	1.68	0.76
1:B:497:PHE:HD2	1:B:507:PRO:CB	1.91	0.76
1:C:64:TRP:CA	1:C:266:TYR:HB3	2.10	0.76
1:C:887:THR:CG2	1:C:894:LEU:CD2	2.64	0.76
1:C:888:PHE:CZ	1:C:1034:LEU:HD21	2.17	0.76
1:A:82:PRO:CB	1:A:240:THR:N	2.48	0.76
1:A:83:VAL:H	1:A:84:LEU:HD12	1.51	0.76
1:A:1081:ILE:CD1	1:A:1095:PHE:CE2	2.69	0.76
1:C:736:VAL:HG23	1:C:858:LEU:HB3	1.68	0.76
1:B:122:ASN:HB2	1:B:127:VAL:CG1	2.15	0.76
2:H:17:THR:HG22	2:H:84:SER:H	1.51	0.76
3:L:88:CYS:N	3:L:99:GLN:HG2	2.00	0.75
1:C:898:PHE:HB3	1:C:899:PRO:HD3	1.67	0.75
1:A:322:PRO:CB	1:A:537:LYS:HB2	2.17	0.75
1:A:408:ARG:HD2	1:A:408:ARG:C	2.12	0.75
1:B:388:ASN:O	1:B:526:GLY:HA2	1.87	0.75
1:C:349:SER:O	1:C:400:PHE:CB	2.34	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:409:GLN:NE2	1:C:419:ALA:H	1.85	0.75
1:A:84:LEU:O	1:A:237:ARG:HA	1.86	0.75
1:B:90:VAL:HG21	1:B:238:PHE:CZ	2.21	0.75
1:B:970:PHE:N	1:C:755:GLN:HE22	1.84	0.75
1:A:206:LYS:HD3	1:A:223:LEU:CB	2.17	0.75
1:A:97:LYS:HA	1:A:97:LYS:CE	2.10	0.74
1:B:909:ILE:HD12	1:B:1047:TYR:HB3	1.69	0.74
1:A:330:PRO:HA	1:A:580:GLN:HE22	1.49	0.74
1:A:759:PHE:HA	1:A:762:GLN:HE22	1.50	0.74
1:C:33:THR:HG22	1:C:58:PHE:CZ	2.22	0.74
1:A:43:PHE:CD2	1:C:557:LYS:HE3	2.23	0.74
1:A:67:ALA:HB2	1:A:80:ASP:HB2	1.68	0.74
1:A:204:TYR:CE1	1:A:225:PRO:HB3	2.23	0.74
1:B:992:GLN:OE1	1:B:995:ARG:NH2	2.20	0.74
5:B:1304:NAG:H83	5:B:1304:NAG:H3	1.67	0.74
1:B:503:VAL:HA	1:B:506:GLN:HB2	1.70	0.74
1:A:355:ARG:HB3	1:A:398:ASP:CG	2.13	0.74
1:A:855:PHE:HB3	1:C:589:PRO:HG2	1.68	0.74
1:B:34:ARG:NH2	1:B:219:GLY:O	2.20	0.74
1:C:351:TYR:OH	1:C:492:LEU:HD23	1.87	0.74
1:B:101:ILE:CD1	1:B:240:THR:HG21	2.18	0.74
1:C:214:ARG:HG2	1:C:214:ARG:NH1	2.01	0.74
1:B:438:SER:H	1:B:508:TYR:HA	1.51	0.74
1:A:385:THR:HG23	1:A:386:LYS:HG3	1.68	0.74
3:L:8:PRO:HG3	3:L:11:LEU:HD22	1.69	0.74
1:C:776:LYS:HG3	1:C:779:GLN:HE21	1.53	0.73
2:H:117:VAL:HG12	2:H:119:VAL:H	1.53	0.73
1:A:205:SER:O	1:A:223:LEU:CB	2.36	0.73
1:A:212:LEU:HD21	1:A:217:PRO:HG3	1.69	0.73
1:B:140:PHE:CE2	1:B:249:LEU:HD12	2.22	0.73
1:C:355:ARG:NH1	1:C:398:ASP:OD2	2.22	0.73
1:C:1043:CYS:SG	1:C:1048:HIS:ND1	2.60	0.73
1:C:1113:GLN:OE1	1:C:1113:GLN:N	2.21	0.73
1:A:131:CYS:HA	1:A:166:CYS:HB3	1.69	0.73
1:C:571:ASP:O	1:C:573:THR:N	2.21	0.73
1:B:189:LEU:HG	1:B:210:ILE:HD11	1.69	0.73
1:C:803:SER:HB3	4:D:1:NAG:H81	1.70	0.73
1:A:529:LYS:HG3	1:A:530:SER:H	1.53	0.73
3:L:83:PHE:HD1	3:L:106:LYS:H	1.36	0.73
1:C:887:THR:CG2	1:C:894:LEU:HD21	2.18	0.73
2:H:20:LEU:HG	2:H:82:LEU:HD11	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:LYS:HG3	1:B:186:PHE:HE2	1.54	0.73
1:C:887:THR:HG21	1:C:894:LEU:HD21	1.71	0.73
1:B:943:SER:C	1:B:945:LEU:N	2.43	0.73
1:C:912:THR:N	1:C:1107:ARG:NH1	2.36	0.73
1:B:110:LEU:HD13	1:B:135:PHE:CB	2.19	0.73
1:B:943:SER:O	1:B:946:GLY:N	2.21	0.72
1:B:970:PHE:H	1:C:755:GLN:HE22	1.35	0.72
1:C:554:GLU:HG3	1:C:555:SER:H	1.54	0.72
1:C:770:ILE:HD11	1:C:1012:LEU:HD23	1.71	0.72
1:A:422:ASN:OD1	1:A:453:TYR:HB2	1.88	0.72
1:C:92:PHE:HE1	1:C:265:TYR:HE1	1.36	0.72
1:C:894:LEU:HD13	1:C:894:LEU:N	2.04	0.72
2:H:104:VAL:HG21	3:L:49:TYR:CD2	2.24	0.72
1:A:82:PRO:HB2	1:A:239:GLN:HA	1.71	0.72
1:B:899:PRO:HB3	1:B:920:GLN:HE22	1.52	0.72
1:A:372:ALA:HB1	1:A:374:PHE:CD2	2.24	0.72
1:A:533:LEU:HD12	1:A:541:PHE:HA	1.69	0.72
1:B:93:ALA:HB2	1:B:191:GLU:N	2.04	0.72
1:B:189:LEU:HB2	1:B:208:THR:HB	1.70	0.72
3:L:7:SER:HB3	3:L:8:PRO:HD2	1.67	0.72
1:B:712:ILE:HD12	1:B:712:ILE:O	1.90	0.72
3:L:7:SER:CB	3:L:8:PRO:HD2	2.20	0.72
1:A:454:ARG:NH2	1:A:467:ASP:O	2.23	0.72
1:A:86:PHE:HD1	1:A:90:VAL:HG13	1.54	0.71
1:A:402:ILE:HD13	1:A:402:ILE:C	2.14	0.71
1:A:429:PHE:CZ	1:A:512:VAL:HG22	2.25	0.71
1:C:564:GLN:O	1:C:577:ARG:HG2	1.90	0.71
1:A:455:LEU:CD1	1:A:493:GLN:HB2	2.19	0.71
1:C:642:VAL:HG22	1:C:651:ILE:HG22	1.71	0.71
1:A:393:THR:H	1:A:522:ALA:HB1	1.54	0.71
1:A:106:PHE:CE2	1:A:118:LEU:HA	2.26	0.71
1:C:357:ARG:HB2	1:C:396:TYR:CE2	2.24	0.71
1:B:484:GLU:HG3	1:B:489:TYR:HA	1.70	0.71
1:C:92:PHE:CZ	1:C:265:TYR:CE1	2.77	0.71
2:H:36:TRP:CE3	2:H:80:LEU:HD23	2.25	0.71
1:A:1091:ARG:HG2	1:A:1119:ASN:O	1.90	0.71
1:B:346:ARG:HB2	1:B:346:ARG:NH2	2.05	0.71
1:B:712:ILE:CG2	1:B:1075:PHE:C	2.64	0.71
1:A:904:TYR:CZ	1:C:1094:VAL:CG1	2.70	0.71
1:A:1081:ILE:HD11	1:A:1095:PHE:HD2	1.54	0.71
1:B:458:LYS:HG2	1:B:473:TYR:HD2	1.56	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:ILE:HD12	1:C:210:ILE:N	2.05	0.71
1:A:110:LEU:HB3	1:A:135:PHE:HD2	1.56	0.70
1:A:330:PRO:HB3	1:A:580:GLN:HE22	1.54	0.70
1:A:755:GLN:HE22	1:C:970:PHE:H	1.38	0.70
1:A:805:ILE:HB	1:A:878:LEU:HD11	1.72	0.70
1:A:36:VAL:CB	1:A:55:PHE:CB	2.68	0.70
1:A:130:VAL:HG11	1:A:168:PHE:HB3	1.73	0.70
1:A:712:ILE:HB	1:A:1077:THR:CG2	2.20	0.70
1:A:326:ILE:HD12	1:A:533:LEU:HA	1.73	0.70
1:B:115:GLN:NE2	1:B:115:GLN:H	1.88	0.70
1:B:337:PRO:HD3	1:B:358:ILE:HG12	1.72	0.70
1:B:712:ILE:HG23	1:B:1075:PHE:HB2	1.73	0.70
3:L:56:THR:O	3:L:58:ILE:N	2.23	0.70
1:A:54:LEU:CB	1:A:272:PRO:HA	2.22	0.70
1:A:503:VAL:CG2	1:A:506:GLN:NE2	2.54	0.70
1:A:904:TYR:CE2	1:C:1094:VAL:HG11	2.09	0.70
1:B:921:LYS:HA	1:B:921:LYS:HZ3	1.54	0.70
1:C:357:ARG:NH1	1:C:359:SER:HB3	2.05	0.70
1:C:567:ARG:HE	1:C:571:ASP:HB3	1.57	0.70
1:C:854:LYS:HG2	1:C:858:LEU:HD11	1.73	0.70
3:L:2:ILE:HG21	3:L:90:GLN:HE22	1.57	0.70
1:B:480:CYS:O	1:B:483:VAL:N	2.23	0.70
1:B:497:PHE:HD2	1:B:507:PRO:CG	2.04	0.70
3:L:37:GLN:N	3:L:47:LEU:HD13	2.06	0.70
1:B:497:PHE:HB3	1:B:507:PRO:HD3	1.73	0.70
1:C:1086:LYS:HE2	1:C:1122:VAL:HG21	1.73	0.70
1:A:319:ARG:HB2	1:A:592:PHE:CZ	2.26	0.70
1:B:1117:THR:HG22	1:B:1140:PRO:HD2	1.72	0.70
1:C:357:ARG:CZ	1:C:359:SER:HB3	2.22	0.70
2:H:39:GLN:HE21	2:H:43:LYS:H	1.37	0.70
1:A:1102:TRP:CD1	1:A:1102:TRP:H	2.09	0.70
1:B:318:PHE:HZ	1:B:615:VAL:HG21	1.56	0.70
1:B:529:LYS:HA	1:B:529:LYS:HZ2	1.53	0.70
1:C:133:PHE:HD1	1:C:162:SER:O	1.75	0.70
1:C:922:LEU:HD11	5:C:1301:NAG:H62	1.63	0.70
1:A:54:LEU:HB2	1:A:272:PRO:HA	1.74	0.69
1:A:84:LEU:HD12	1:A:84:LEU:N	2.05	0.69
1:B:100:ILE:HD12	1:B:242:LEU:CD1	2.22	0.69
1:B:101:ILE:HD11	1:B:240:THR:HG21	1.73	0.69
1:B:208:THR:HG22	1:B:209:PRO:HD2	1.74	0.69
1:B:337:PRO:CB	1:B:341:VAL:HG22	2.21	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1304:NAG:H83	5:B:1304:NAG:C5	2.22	0.69
1:C:409:GLN:HE22	1:C:416:GLY:C	2.00	0.69
3:L:83:PHE:HE1	3:L:105:ILE:HG23	1.57	0.69
1:A:390:LEU:HD23	1:A:390:LEU:N	2.07	0.69
1:C:188:ASN:HA	1:C:209:PRO:HA	1.71	0.69
1:B:924:ALA:O	1:B:928:ASN:ND2	2.26	0.69
2:H:90:THR:HA	2:H:116:LEU:HD22	1.74	0.69
1:A:540:ASN:CA	1:A:549:THR:HG23	2.20	0.69
1:C:133:PHE:CD1	1:C:162:SER:C	2.71	0.69
1:C:1074:ASN:O	1:C:1074:ASN:ND2	2.26	0.69
3:L:35:TRP:O	3:L:47:LEU:HB3	1.92	0.69
1:B:713:ALA:HA	1:B:1074:ASN:HA	1.73	0.69
1:C:117:LEU:HD12	1:C:231:ILE:HG21	1.74	0.69
1:C:921:LYS:H	1:C:921:LYS:CE	2.05	0.69
1:A:417:LYS:HA	1:A:420:ASP:HB3	1.75	0.69
1:B:63:THR:O	1:B:267:VAL:HG22	1.91	0.69
1:C:567:ARG:NE	1:C:571:ASP:HB3	2.07	0.69
3:L:56:THR:C	3:L:58:ILE:N	2.50	0.69
1:A:63:THR:O	1:A:63:THR:OG1	2.09	0.69
1:A:326:ILE:CG1	1:A:533:LEU:HD22	2.23	0.69
1:C:33:THR:HG22	1:C:58:PHE:CE1	2.27	0.69
1:C:63:THR:OG1	1:C:63:THR:O	2.10	0.69
1:C:214:ARG:O	1:C:214:ARG:HD3	1.93	0.69
1:B:334:ASN:ND2	1:B:361:CYS:HA	2.07	0.69
1:B:984:LEU:HD23	1:B:988:GLU:HG3	1.73	0.69
1:A:86:PHE:CD1	1:A:90:VAL:HG22	2.26	0.69
1:A:206:LYS:HD3	1:A:221:SER:OG	1.93	0.69
1:B:200:TYR:CA	1:B:230:PRO:HA	2.22	0.69
1:C:214:ARG:HG2	1:C:214:ARG:HH11	1.55	0.69
1:C:617:CYS:SG	1:C:644:GLN:NE2	2.65	0.69
2:H:97:ARG:HH21	2:H:106:LEU:HD22	1.57	0.69
1:A:457:ARG:NH2	1:A:467:ASP:OD2	2.26	0.68
1:B:365:TYR:O	1:B:368:LEU:N	2.26	0.68
2:H:82:LEU:HD23	2:H:93:TYR:CE2	2.22	0.68
2:H:48:ILE:HG13	2:H:49:GLY:H	1.58	0.68
1:B:360:ASN:HA	1:B:523:THR:CB	2.12	0.68
2:H:43:LYS:HG3	2:H:44:GLY:H	1.58	0.68
1:A:656:VAL:CG2	1:A:695:TYR:HB3	2.23	0.68
3:L:35:TRP:O	3:L:47:LEU:CB	2.42	0.68
1:A:566:GLY:HA2	1:B:43:PHE:HB3	1.76	0.68
1:A:712:ILE:CG2	1:A:1077:THR:HG22	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:PRO:HB3	1:A:240:THR:N	2.09	0.68
1:A:805:ILE:HD13	1:A:805:ILE:N	2.05	0.68
1:A:917:TYR:HB3	1:C:1129:VAL:HG13	1.72	0.68
1:A:1090:PRO:HB3	1:A:1095:PHE:CE1	2.29	0.68
1:C:216:LEU:HD13	1:C:216:LEU:O	1.94	0.68
1:B:351:TYR:O	1:B:454:ARG:NH1	2.27	0.68
1:B:48:LEU:HD22	1:B:304:LYS:HG2	1.75	0.68
1:C:803:SER:HB3	4:D:1:NAG:C8	2.24	0.68
1:C:854:LYS:O	1:C:855:PHE:CD1	2.46	0.68
1:B:972:ALA:HA	1:B:995:ARG:NH2	2.09	0.68
1:C:856:ASN:OD1	1:C:858:LEU:HD21	1.93	0.68
2:H:66:ARG:HH21	2:H:85:VAL:HA	1.59	0.68
1:A:402:ILE:H	1:A:402:ILE:HD12	1.57	0.68
1:A:580:GLN:CG	5:A:1306:NAG:N2	2.46	0.68
1:A:894:LEU:HD12	1:C:713:ALA:O	1.94	0.68
1:B:715:PRO:HA	1:B:1072:GLU:HB2	1.75	0.68
1:A:98:SER:O	1:A:98:SER:OG	2.08	0.67
5:A:1301:NAG:C1	5:A:1301:NAG:H82	2.22	0.67
1:B:38:TYR:CZ	1:B:285:ILE:CD1	2.76	0.67
1:B:357:ARG:NH2	1:B:396:TYR:OH	2.26	0.67
1:B:1075:PHE:HB3	1:B:1096:VAL:HG22	1.75	0.67
1:A:457:ARG:HD2	1:A:458:LYS:H	1.59	0.67
1:A:1090:PRO:CG	1:A:1095:PHE:CE1	2.77	0.67
1:A:64:TRP:CB	1:A:266:TYR:CE2	2.76	0.67
1:B:318:PHE:CE2	1:B:623:ALA:CB	2.57	0.67
1:B:629:LEU:HD23	1:B:633:TRP:HB3	1.76	0.67
1:B:718:PHE:H	1:B:718:PHE:HD2	1.42	0.67
1:A:567:ARG:HH12	1:B:47:VAL:HG21	1.59	0.67
1:B:68:ILE:O	1:B:69:HIS:ND1	2.28	0.67
1:B:445:VAL:HA	1:B:499:PRO:HD3	1.76	0.67
1:C:922:LEU:O	1:C:922:LEU:HD13	1.94	0.67
2:H:104:VAL:HG12	2:H:105:LEU:H	1.60	0.67
1:C:901:GLN:HE21	1:C:905:ARG:HE	1.43	0.67
1:A:517:LEU:C	1:A:517:LEU:HD22	2.18	0.67
1:A:553:THR:CB	1:A:587:ILE:CG2	2.73	0.67
1:A:755:GLN:HE22	1:C:970:PHE:N	1.93	0.67
1:C:1074:ASN:HD22	1:C:1074:ASN:C	2.02	0.67
1:B:93:ALA:CB	1:B:191:GLU:N	2.58	0.67
1:B:100:ILE:O	1:B:242:LEU:HB2	1.94	0.67
1:B:714:ILE:HD11	1:B:1107:ARG:C	2.20	0.67
1:C:856:ASN:HD22	1:C:966:LEU:HD11	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:GLU:CD	1:A:224:GLU:H	2.02	0.67
1:A:350:VAL:HG22	1:A:453:TYR:HA	1.75	0.67
1:A:592:PHE:N	1:B:853:GLN:HG3	2.10	0.67
1:B:337:PRO:HD3	1:B:358:ILE:CG1	2.24	0.67
1:C:736:VAL:HG23	1:C:858:LEU:HA	1.76	0.67
1:B:334:ASN:ND2	1:B:334:ASN:O	2.27	0.66
1:C:216:LEU:O	1:C:216:LEU:HD22	1.94	0.66
2:H:110:GLU:HG2	2:H:111:TRP:H	1.60	0.66
1:C:457:ARG:NH2	1:C:459:SER:O	2.27	0.66
1:A:67:ALA:HB2	1:A:80:ASP:CB	2.26	0.66
1:A:298:GLU:HG2	1:A:633:TRP:CZ2	2.26	0.66
1:A:424:LYS:NZ	1:A:425:LEU:O	2.28	0.66
1:B:93:ALA:CB	1:B:191:GLU:HA	2.23	0.66
1:C:212:LEU:C	1:C:212:LEU:HD22	2.20	0.66
1:C:736:VAL:HG23	1:C:858:LEU:CB	2.26	0.66
1:B:922:LEU:HD12	1:B:922:LEU:O	1.95	0.66
1:A:42:VAL:HG11	1:C:567:ARG:HD3	1.77	0.66
1:A:540:ASN:OD1	1:A:549:THR:CG2	2.43	0.66
1:A:729:VAL:HG12	1:A:1059:GLY:HA2	1.76	0.66
1:C:736:VAL:HG23	1:C:858:LEU:CA	2.26	0.66
1:C:887:THR:HG23	1:C:894:LEU:CD2	2.24	0.66
1:A:806:LEU:HD11	1:A:878:LEU:CD2	2.25	0.66
1:A:1081:ILE:CD1	1:A:1095:PHE:HD2	2.07	0.66
1:B:206:LYS:HB3	1:B:223:LEU:HG	1.78	0.66
1:A:388:ASN:HB2	1:A:527:PRO:HD2	1.78	0.66
1:A:216:LEU:HD23	1:A:216:LEU:H	1.60	0.66
1:B:96:GLU:HB3	1:B:188:ASN:ND2	2.11	0.66
1:C:93:ALA:O	1:C:265:TYR:HB2	1.95	0.66
1:C:355:ARG:HB3	1:C:396:TYR:HB3	1.77	0.66
2:H:11:LEU:HA	2:H:115:THR:HB	1.77	0.66
1:A:1077:THR:CB	1:A:1095:PHE:O	2.44	0.66
1:C:36:VAL:HG11	1:C:277:LEU:HD21	1.77	0.66
1:A:82:PRO:HG3	1:A:240:THR:H	1.60	0.66
1:A:456:PHE:CD1	1:A:473:TYR:HB3	2.31	0.66
1:B:971:GLY:O	1:B:995:ARG:NH1	2.29	0.66
1:B:287:ASP:OD1	1:B:288:ALA:N	2.29	0.65
1:B:334:ASN:HD21	1:B:361:CYS:HA	1.60	0.65
1:B:346:ARG:HG2	1:B:509:ARG:HH22	1.60	0.65
1:B:438:SER:O	1:B:442:ASP:N	2.29	0.65
1:B:581:THR:HA	4:N:1:NAG:O6	1.96	0.65
1:C:887:THR:HG21	1:C:894:LEU:CD2	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:67:VAL:HG13	2:H:82:LEU:HA	1.78	0.65
5:B:1304:NAG:H83	5:B:1304:NAG:C3	2.25	0.65
2:H:20:LEU:HD11	2:H:93:TYR:CB	2.26	0.65
1:A:95:THR:O	1:A:186:PHE:CB	2.42	0.65
1:A:324:GLU:HB3	1:A:539:VAL:HA	1.78	0.65
1:A:388:ASN:O	1:A:528:LYS:NZ	2.28	0.65
1:A:567:ARG:HA	1:A:571:ASP:O	1.95	0.65
1:A:1077:THR:HB	1:A:1095:PHE:O	1.95	0.65
1:C:216:LEU:CD1	1:C:266:TYR:OH	2.43	0.65
1:A:917:TYR:C	1:C:1129:VAL:HG13	2.21	0.65
1:B:273:ARG:HH21	1:B:273:ARG:CG	2.09	0.65
1:C:579:PRO:HA	1:C:582:LEU:HD22	1.79	0.65
3:L:36:TYR:HA	3:L:47:LEU:HD22	1.79	0.65
1:A:532:ASN:O	1:A:535:LYS:NZ	2.24	0.65
1:B:38:TYR:CD1	1:B:285:ILE:CD1	2.64	0.65
1:C:777:ASN:OD1	1:C:1019:ARG:NH1	2.26	0.65
1:C:922:LEU:O	1:C:922:LEU:HD22	1.96	0.65
1:A:326:ILE:CD1	1:A:539:VAL:CG1	2.73	0.65
1:B:57:PRO:CB	1:B:273:ARG:HH22	2.08	0.65
1:B:293:LEU:HD12	1:B:630:THR:HG21	1.79	0.65
1:B:337:PRO:CG	1:B:358:ILE:CG1	2.70	0.65
1:B:438:SER:HB3	1:B:442:ASP:CB	2.26	0.65
1:B:497:PHE:CD2	1:B:507:PRO:CG	2.80	0.65
1:C:902:MET:HE1	1:C:1050:MET:SD	2.36	0.65
1:A:377:PHE:CD1	1:A:434:ILE:HD13	2.30	0.65
1:A:406:GLU:C	1:A:408:ARG:H	2.04	0.65
1:B:543:PHE:HD1	1:B:579:PRO:HD2	1.61	0.65
1:A:82:PRO:HB2	1:A:239:GLN:CA	2.25	0.65
1:A:120:VAL:HG22	1:A:121:ASN:H	1.62	0.65
1:A:86:PHE:CZ	1:A:194:PHE:O	2.50	0.65
1:B:200:TYR:CB	1:B:230:PRO:HA	2.26	0.65
1:C:355:ARG:NH2	1:C:396:TYR:HB2	2.12	0.65
4:N:1:NAG:H61	4:N:2:NAG:H2	1.78	0.65
1:A:406:GLU:H	1:A:406:GLU:CD	2.05	0.64
1:A:759:PHE:CE2	1:C:970:PHE:HE1	2.15	0.64
1:C:529:LYS:HG3	1:C:530:SER:H	1.62	0.64
4:D:1:NAG:H61	4:D:2:NAG:H2	1.78	0.64
5:B:1304:NAG:H3	5:B:1304:NAG:C8	2.17	0.64
1:C:780:GLU:OE2	1:C:1019:ARG:NH2	2.23	0.64
1:A:295:PRO:O	1:A:298:GLU:HG3	1.97	0.64
1:A:806:LEU:CD1	1:A:878:LEU:CD2	2.75	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:736:VAL:HG23	1:B:858:LEU:HA	1.79	0.64
1:C:92:PHE:CZ	1:C:265:TYR:CD1	2.86	0.64
1:A:336:CYS:SG	1:A:337:PRO:CD	2.86	0.64
1:A:577:ARG:HA	1:A:583:GLU:O	1.96	0.64
1:B:714:ILE:HD11	1:B:1107:ARG:O	1.97	0.64
1:C:133:PHE:CD1	1:C:162:SER:O	2.49	0.64
1:A:307:THR:HA	1:A:602:THR:HG21	1.77	0.64
1:A:1091:ARG:CG	1:A:1119:ASN:O	2.46	0.64
2:H:41:PRO:HD3	2:H:91:ALA:HA	1.78	0.64
3:L:11:LEU:HB3	3:L:104:GLU:HG2	1.80	0.64
1:A:533:LEU:CD1	1:A:541:PHE:CA	2.68	0.64
1:A:805:ILE:CG2	1:A:1054:GLN:NE2	2.60	0.64
1:B:902:MET:HE1	1:B:1050:MET:HE3	1.80	0.64
1:C:398:ASP:O	1:C:511:VAL:HA	1.96	0.64
1:A:63:THR:O	1:A:65:PHE:N	2.30	0.64
1:A:322:PRO:HD3	1:A:625:HIS:CE1	2.33	0.64
1:B:421:TYR:O	1:B:454:ARG:HG3	1.97	0.64
1:B:712:ILE:CG2	1:B:1075:PHE:HB2	2.27	0.64
1:C:64:TRP:HH2	1:C:214:ARG:CD	2.10	0.64
1:C:84:LEU:HB2	1:C:238:PHE:CE1	2.33	0.64
1:C:718:PHE:CB	1:C:1067:TYR:CE1	2.80	0.64
1:B:117:LEU:HD23	1:B:233:ILE:CD1	2.28	0.64
1:B:404:GLY:HA2	1:B:508:TYR:HB2	1.80	0.64
2:H:18:LEU:HB3	2:H:82:LEU:HB2	1.80	0.64
1:A:104:TRP:CH2	1:A:194:PHE:CB	2.81	0.64
1:A:557:LYS:HD2	1:B:43:PHE:CZ	2.32	0.64
1:A:1075:PHE:HZ	1:A:1110:TYR:CE2	2.16	0.64
1:A:1116:THR:HG22	1:A:1138:TYR:HD2	1.62	0.64
1:B:380:TYR:CZ	1:B:412:PRO:HD2	2.33	0.64
1:C:541:PHE:HB2	1:C:543:PHE:CE2	2.33	0.64
1:A:461:LEU:HD13	1:A:465:GLU:HB3	1.80	0.63
1:A:377:PHE:HD1	1:A:434:ILE:HD13	1.63	0.63
1:A:567:ARG:HH22	1:B:49:HIS:HB2	1.63	0.63
1:B:133:PHE:O	1:B:135:PHE:N	2.23	0.63
1:B:360:ASN:O	1:B:362:VAL:N	2.30	0.63
1:B:921:LYS:HA	1:B:921:LYS:CE	2.29	0.63
1:C:856:ASN:ND2	1:C:966:LEU:HD11	2.13	0.63
1:C:940:SER:C	1:C:942:PRO:HD3	2.23	0.63
1:A:66:HIS:H	1:A:66:HIS:CD2	2.16	0.63
1:A:909:ILE:HD12	1:A:1047:TYR:HB3	1.80	0.63
1:B:116:SER:HG	1:B:235:ILE:HG12	1.60	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:943:SER:O	1:B:944:ALA:C	2.41	0.63
1:A:457:ARG:HD2	1:A:458:LYS:N	2.13	0.63
1:A:571:ASP:O	1:A:572:THR:C	2.41	0.63
1:A:97:LYS:C	1:A:97:LYS:HZ3	2.06	0.63
1:A:100:ILE:HG21	1:A:243:ALA:H	1.62	0.63
1:C:355:ARG:NH2	1:C:514:SER:HB2	2.13	0.63
1:A:904:TYR:OH	1:C:1094:VAL:CG1	2.44	0.63
1:B:115:GLN:HB2	1:B:130:VAL:HG12	1.81	0.63
1:B:341:VAL:HG23	1:B:341:VAL:O	1.99	0.63
1:B:736:VAL:CG2	1:B:858:LEU:HD22	2.28	0.63
1:C:64:TRP:HH2	1:C:214:ARG:HD2	1.63	0.63
1:C:351:TYR:O	1:C:466:ARG:HB2	1.98	0.63
1:C:920:GLN:HA	1:C:923:ILE:CG2	2.29	0.63
2:H:92:VAL:CG1	2:H:113:GLN:HA	2.28	0.63
1:A:33:THR:HB	1:A:58:PHE:CB	2.29	0.63
1:A:480:CYS:HB3	1:A:483:VAL:O	1.99	0.63
1:A:626:ALA:O	1:A:634:ARG:NE	2.27	0.63
1:B:244:LEU:H	1:B:247:SER:HB3	1.62	0.63
1:B:941:THR:H	1:B:942:PRO:CD	2.11	0.63
1:B:1081:ILE:O	1:B:1088:HIS:N	2.21	0.63
1:A:674:TYR:CZ	1:A:690:GLN:HB3	2.34	0.63
1:A:784:GLN:NE2	1:A:1030:SER:HB3	2.13	0.63
1:C:568:ASP:OD1	1:C:571:ASP:N	2.32	0.63
1:A:316:SER:OG	1:A:595:VAL:N	2.30	0.63
1:B:122:ASN:HD22	1:B:127:VAL:HG11	1.64	0.63
1:A:347:PHE:CE2	1:A:509:ARG:CB	2.82	0.62
1:A:356:LYS:H	1:A:397:ALA:HB3	1.63	0.62
1:A:984:LEU:O	1:C:386:LYS:NZ	2.31	0.62
1:B:240:THR:CG2	1:B:265:TYR:CE2	2.82	0.62
1:B:722:VAL:O	1:B:934:ILE:HD11	1.99	0.62
3:L:24:ARG:HA	3:L:70:ASP:HA	1.79	0.62
1:A:187:LYS:HB2	1:A:210:ILE:O	2.00	0.62
1:B:717:ASN:OD1	5:B:1302:NAG:H81	1.98	0.62
3:L:29:VAL:HG21	3:L:90:GLN:HG3	1.81	0.62
1:A:905:ARG:NH1	1:A:1049:LEU:O	2.32	0.62
1:B:52:GLN:HG2	1:B:274:THR:OG1	1.98	0.62
1:B:106:PHE:CZ	1:B:201:PHE:CE1	2.86	0.62
1:B:279:TYR:CA	1:B:285:ILE:HA	2.29	0.62
1:B:1106:GLN:NE2	1:B:1109:PHE:HB3	2.14	0.62
1:C:568:ASP:N	1:C:571:ASP:HA	2.12	0.62
1:C:1075:PHE:HE1	1:C:1110:TYR:HE1	1.38	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:72:ASP:O	2:H:76:ASN:N	2.23	0.62
1:A:369:TYR:HE1	1:A:387:LEU:HD23	1.63	0.62
1:B:342:PHE:CZ	1:B:434:ILE:HG21	2.34	0.62
1:C:380:TYR:HE2	1:C:412:PRO:HD3	1.64	0.62
1:A:50:SER:HA	1:A:276:LEU:HA	1.81	0.62
1:A:142:GLY:H	1:A:159:VAL:HG21	1.64	0.62
1:A:407:VAL:O	1:A:407:VAL:HG12	2.00	0.62
1:B:777:ASN:OD1	1:B:1019:ARG:NH1	2.31	0.62
3:L:61:ARG:O	3:L:76:SER:N	2.29	0.62
1:A:218:GLN:N	1:A:218:GLN:OE1	2.33	0.62
1:A:567:ARG:CD	1:A:571:ASP:HA	2.29	0.62
1:A:587:ILE:HD12	1:A:587:ILE:H	1.62	0.62
1:C:888:PHE:HA	1:C:893:ALA:HB1	1.80	0.62
1:B:231:ILE:HD13	1:B:231:ILE:N	2.13	0.62
1:B:717:ASN:CG	5:B:1302:NAG:H81	2.23	0.62
1:B:204:TYR:CE1	1:B:225:PRO:HB3	2.35	0.62
3:L:36:TYR:CD2	3:L:44:PRO:HB2	2.34	0.62
1:A:334:ASN:HD21	1:A:360:ASN:HB3	1.65	0.62
1:A:353:TRP:CZ3	1:A:355:ARG:HG2	2.35	0.62
1:B:352:ALA:HB2	1:B:468:ILE:HG21	1.81	0.62
1:A:338:PHE:HA	1:A:341:VAL:CG1	2.30	0.61
1:A:401:VAL:HG21	1:A:451:TYR:CG	2.34	0.61
1:A:656:VAL:HG23	1:A:695:TYR:HB3	1.82	0.61
1:C:989:ALA:O	1:C:993:ILE:HG12	2.00	0.61
2:H:48:ILE:HA	2:H:60:ASN:HB2	1.81	0.61
3:L:8:PRO:CG	3:L:11:LEU:HD22	2.30	0.61
1:A:187:LYS:HD3	1:A:187:LYS:H	1.64	0.61
1:A:204:TYR:HA	1:A:225:PRO:HA	1.82	0.61
1:A:401:VAL:HG21	1:A:451:TYR:CD1	2.35	0.61
1:C:241:LEU:C	1:C:242:LEU:HD12	2.25	0.61
1:C:741:TYR:HE1	1:C:966:LEU:HD21	1.63	0.61
3:L:86:TYR:HE1	3:L:104:GLU:HB2	1.64	0.61
1:A:357:ARG:HG3	1:A:357:ARG:HH11	1.65	0.61
1:A:38:TYR:CE1	1:A:222:ALA:O	2.53	0.61
1:A:330:PRO:HA	1:A:580:GLN:CD	2.25	0.61
1:A:787:GLN:HE21	1:C:703:ASN:HB2	1.66	0.61
1:B:949:GLN:O	1:B:950:ASP:C	2.44	0.61
1:B:1075:PHE:HB3	1:B:1096:VAL:CG2	2.30	0.61
1:B:717:ASN:ND2	5:B:1302:NAG:C8	2.59	0.61
1:C:899:PRO:HB3	1:C:920:GLN:HE21	1.66	0.61
3:L:61:ARG:NH2	3:L:82:ASP:OD1	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:THR:CA	1:A:58:PHE:HA	2.30	0.61
1:A:742:ILE:O	1:A:1000:ARG:NH1	2.31	0.61
1:A:800:PHE:H	1:A:800:PHE:HD2	1.47	0.61
1:B:311:GLY:HA2	1:B:664:ILE:HD12	1.83	0.61
2:H:38:ARG:NE	2:H:93:TYR:HE1	1.97	0.61
1:A:416:GLY:O	1:A:420:ASP:N	2.29	0.61
1:A:429:PHE:HZ	1:A:512:VAL:CG2	2.13	0.61
1:A:896:ILE:HG12	1:C:712:ILE:HD11	1.81	0.61
1:C:64:TRP:CH2	1:C:214:ARG:HD2	2.35	0.61
1:C:358:ILE:HG23	1:C:524:VAL:HG21	1.83	0.61
1:C:922:LEU:HG	5:C:1301:NAG:H62	1.81	0.61
1:A:540:ASN:OD1	1:A:549:THR:HG21	1.99	0.61
1:B:1125:ASN:ND2	1:B:1127:ASP:OD1	2.34	0.61
1:C:244:LEU:HD12	1:C:245:HIS:N	2.15	0.61
2:H:34:TRP:O	2:H:51:ILE:HG22	2.00	0.61
1:A:350:VAL:HG23	1:A:351:TYR:H	1.64	0.61
1:A:661:GLU:OE1	1:A:661:GLU:HA	2.01	0.61
1:A:797:PHE:CD1	1:C:707:TYR:OH	2.51	0.61
1:B:58:PHE:CD2	1:B:290:ASP:HB2	2.36	0.61
1:B:418:ILE:HG23	1:B:422:ASN:HB2	1.83	0.61
1:C:214:ARG:HD3	1:C:214:ARG:C	2.26	0.61
1:C:858:LEU:HD12	1:C:858:LEU:O	2.01	0.61
3:L:66:GLY:HA3	3:L:72:THR:H	1.65	0.61
1:A:187:LYS:HD3	1:A:187:LYS:N	2.16	0.60
1:B:273:ARG:HH21	1:B:273:ARG:HG2	1.65	0.60
1:B:384:PRO:HA	1:B:387:LEU:HG	1.83	0.60
1:B:437:ASN:C	1:B:509:ARG:H	2.08	0.60
1:C:580:GLN:OE1	1:C:580:GLN:HA	2.00	0.60
1:C:895:GLN:N	1:C:895:GLN:OE1	2.30	0.60
1:A:86:PHE:HZ	1:A:194:PHE:O	1.84	0.60
1:A:97:LYS:C	1:A:99:ASN:H	2.09	0.60
1:A:295:PRO:O	1:A:299:THR:HG23	2.01	0.60
1:A:365:TYR:O	1:A:366:SER:C	2.45	0.60
1:A:577:ARG:NH1	1:A:583:GLU:O	2.34	0.60
1:B:38:TYR:CG	1:B:285:ILE:HD11	2.30	0.60
1:B:106:PHE:N	1:B:106:PHE:HD1	1.99	0.60
1:B:402:ILE:HD11	1:B:510:VAL:HG21	1.84	0.60
2:H:66:ARG:NH2	2:H:89:ASP:OD2	2.34	0.60
1:A:567:ARG:HG2	1:A:571:ASP:CG	2.26	0.60
1:B:56:LEU:HD12	1:B:57:PRO:HD2	1.83	0.60
1:C:921:LYS:HZ3	1:C:921:LYS:N	1.91	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:ARG:HH11	1:A:460:ASN:HA	1.66	0.60
1:A:760:CYS:HA	1:A:763:LEU:HD13	1.84	0.60
1:A:1091:ARG:HG2	1:A:1119:ASN:C	2.25	0.60
1:A:1091:ARG:NE	1:A:1121:PHE:HB3	2.16	0.60
1:C:822:LEU:HD12	1:C:945:LEU:HD21	1.82	0.60
1:C:1029:MET:O	1:C:1030:SER:C	2.44	0.60
2:H:38:ARG:NE	2:H:93:TYR:CE1	2.69	0.60
1:A:104:TRP:H	1:A:104:TRP:CD1	2.18	0.60
1:A:756:TYR:O	1:A:759:PHE:HD2	1.84	0.60
1:B:58:PHE:CZ	1:B:275:PHE:CE2	2.90	0.60
1:B:346:ARG:HH21	1:B:346:ARG:HG3	1.65	0.60
1:B:1132:ILE:HG23	1:B:1132:ILE:O	2.01	0.60
1:A:39:PRO:HG3	1:A:51:THR:HG21	1.82	0.60
1:A:68:ILE:H	1:A:68:ILE:CD1	2.10	0.60
1:B:83:VAL:HG21	1:B:237:ARG:CD	2.31	0.60
1:B:722:VAL:HG11	1:B:931:ILE:HD13	1.83	0.60
1:B:1094:VAL:O	1:B:1094:VAL:HG13	2.02	0.60
1:C:190:ARG:HA	1:C:207:HIS:HB3	1.82	0.60
1:C:921:LYS:HE2	1:C:922:LEU:H	1.66	0.60
1:B:718:PHE:HB2	1:B:1067:TYR:CZ	2.36	0.60
1:C:90:VAL:HG21	1:C:238:PHE:CE2	2.36	0.60
1:C:984:LEU:HB3	1:C:988:GLU:OE2	2.02	0.60
2:H:51:ILE:HG12	2:H:71:VAL:HG23	1.83	0.60
1:B:360:ASN:O	1:B:524:VAL:CG1	2.50	0.60
1:B:1094:VAL:O	1:B:1094:VAL:HG22	2.02	0.60
1:C:320:VAL:HB	1:C:590:CYS:HB3	1.83	0.60
1:C:356:LYS:O	1:C:396:TYR:HA	2.01	0.60
1:C:785:VAL:CG1	1:C:888:PHE:HE2	2.15	0.60
1:C:898:PHE:HB3	1:C:899:PRO:CD	2.32	0.60
1:A:805:ILE:H	1:A:805:ILE:CD1	1.98	0.60
1:B:168:PHE:HE2	1:B:229:LEU:HD22	1.67	0.60
1:B:298:GLU:OE1	1:B:633:TRP:HH2	1.84	0.60
1:B:1121:PHE:HZ	1:C:913:GLN:HE22	1.48	0.60
1:C:424:LYS:HE3	1:C:461:LEU:HB2	1.83	0.60
1:C:816:SER:N	1:C:819:GLU:OE1	2.34	0.60
1:C:916:LEU:HA	1:C:919:ASN:HD21	1.67	0.60
3:L:42:GLN:NE2	3:L:43:ALA:O	2.35	0.60
1:A:44:ARG:HD2	1:A:279:TYR:CE1	2.37	0.60
1:A:454:ARG:NH1	1:A:469:SER:OG	2.31	0.60
1:B:93:ALA:HB1	1:B:190:ARG:C	2.26	0.60
1:B:108:THR:HB	1:B:235:ILE:CD1	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:THR:O	1:B:274:THR:HG22	2.01	0.60
1:C:134:GLN:H	1:C:162:SER:HB3	1.66	0.60
1:C:212:LEU:HD21	1:C:214:ARG:HB3	1.84	0.60
2:H:70:SER:O	2:H:79:SER:N	2.35	0.60
1:B:93:ALA:HB2	1:B:190:ARG:O	2.02	0.59
1:B:416:GLY:N	1:B:420:ASP:OD2	2.35	0.59
1:C:887:THR:HG23	1:C:887:THR:O	2.02	0.59
1:A:457:ARG:CD	1:A:458:LYS:HG2	2.32	0.59
1:B:117:LEU:CD2	1:B:233:ILE:HD12	2.33	0.59
1:B:916:LEU:O	1:B:919:ASN:N	2.35	0.59
1:C:447:GLY:N	1:C:449:TYR:HH	2.00	0.59
1:A:429:PHE:CZ	1:A:512:VAL:CG2	2.84	0.59
1:A:452:LEU:HD13	1:A:492:LEU:HB3	1.83	0.59
1:A:567:ARG:NH2	1:B:44:ARG:HD3	2.18	0.59
1:B:337:PRO:CG	1:B:358:ILE:HD11	2.30	0.59
1:C:330:PRO:HG3	1:C:579:PRO:HB2	1.82	0.59
1:C:922:LEU:CG	5:C:1301:NAG:H62	2.32	0.59
1:C:1075:PHE:HE1	1:C:1110:TYR:CE1	2.15	0.59
1:A:68:ILE:HD13	1:A:68:ILE:N	2.13	0.59
1:A:83:VAL:O	1:A:83:VAL:HG22	2.03	0.59
1:A:278:LYS:HB2	1:A:306:PHE:CE2	2.37	0.59
1:A:800:PHE:N	1:A:800:PHE:CD2	2.70	0.59
1:B:477:SER:N	3:L:92:SER:HB2	2.17	0.59
1:C:1096:VAL:HG22	1:C:1096:VAL:O	2.01	0.59
3:L:4:LEU:O	3:L:5:THR:OG1	2.16	0.59
1:A:340:GLU:HA	1:A:343:ASN:HB2	1.84	0.59
1:A:401:VAL:HG11	1:A:451:TYR:CZ	2.37	0.59
1:A:660:TYR:HB2	1:A:695:TYR:CE2	2.36	0.59
1:B:171:VAL:HG12	1:B:172:SER:H	1.68	0.59
1:B:1089:PHE:HE2	1:C:914:ASN:HA	1.68	0.59
1:C:58:PHE:HB2	1:C:293:LEU:HD21	1.82	0.59
1:B:105:ILE:HG13	1:B:118:LEU:HD12	1.83	0.59
2:H:48:ILE:HG13	2:H:49:GLY:N	2.17	0.59
1:A:54:LEU:HB2	1:A:271:GLN:O	2.02	0.59
1:A:350:VAL:HG21	1:A:453:TYR:CB	2.32	0.59
1:A:787:GLN:NE2	1:C:701:ALA:O	2.35	0.59
1:B:279:TYR:CB	1:B:285:ILE:HA	2.33	0.59
2:H:60:ASN:HB3	2:H:63:LEU:HB2	1.83	0.59
1:A:713:ALA:HB3	1:B:894:LEU:HB3	1.85	0.59
1:A:806:LEU:CD1	1:A:878:LEU:HD21	2.31	0.59
1:B:165:ASN:HB2	5:B:1311:NAG:N2	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:716:THR:HG23	1:C:716:THR:O	2.02	0.59
1:A:33:THR:H	1:A:59:PHE:H	1.49	0.59
1:A:206:LYS:HZ3	1:A:206:LYS:HB3	1.67	0.59
1:A:541:PHE:N	1:A:548:GLY:O	2.35	0.59
1:A:712:ILE:HB	1:A:1077:THR:HG21	1.85	0.59
1:B:410:ILE:HG22	1:B:425:LEU:HD11	1.85	0.59
1:B:454:ARG:NE	1:B:457:ARG:HD2	2.17	0.59
1:A:366:SER:HA	1:A:369:TYR:CE2	2.37	0.59
1:A:420:ASP:O	1:A:422:ASN:N	2.35	0.59
1:A:715:PRO:HG3	1:A:1069:PRO:HB3	1.85	0.59
1:C:96:GLU:OE2	1:C:101:ILE:HG12	2.02	0.59
2:H:16:GLU:O	2:H:85:VAL:N	2.26	0.59
1:A:85:PRO:HD2	1:A:269:TYR:HH	1.67	0.58
1:A:110:LEU:HB3	1:A:135:PHE:CD2	2.37	0.58
1:A:204:TYR:CD1	1:A:225:PRO:HB3	2.37	0.58
1:A:708:SER:O	1:A:710:ASN:N	2.36	0.58
1:A:741:TYR:CE1	1:A:966:LEU:HD12	2.38	0.58
1:B:346:ARG:HH21	1:B:346:ARG:CG	2.13	0.58
1:B:501:ASN:HD22	1:B:501:ASN:C	2.11	0.58
1:B:749:CYS:SG	1:B:997:ILE:HD11	2.42	0.58
1:C:190:ARG:HD2	1:C:192:PHE:HZ	1.68	0.58
3:L:5:THR:HB	3:L:24:ARG:CZ	2.32	0.58
1:A:100:ILE:HG22	1:A:243:ALA:H	1.66	0.58
1:A:128:ILE:HD13	1:A:170:TYR:HD2	1.68	0.58
1:A:620:VAL:HG21	1:A:649:CYS:SG	2.43	0.58
1:B:438:SER:HB3	1:B:442:ASP:HB3	1.85	0.58
1:C:884:SER:OG	1:C:893:ALA:HB1	2.03	0.58
1:A:57:PRO:HB3	1:A:273:ARG:CZ	2.32	0.58
1:A:280:ASN:ND2	5:A:1305:NAG:H82	2.18	0.58
1:A:873:TYR:HE1	1:C:699:LEU:HB3	1.69	0.58
1:A:1076:THR:HG22	1:A:1076:THR:O	2.02	0.58
1:B:48:LEU:CD2	1:B:304:LYS:HG2	2.34	0.58
1:B:110:LEU:C	1:B:112:SER:H	2.10	0.58
1:B:950:ASP:O	1:B:951:VAL:C	2.45	0.58
2:H:18:LEU:HD23	2:H:82:LEU:HD22	1.84	0.58
1:A:393:THR:HA	1:A:523:THR:H	1.68	0.58
1:A:898:PHE:CZ	1:A:1050:MET:HE1	2.38	0.58
1:B:107:GLY:H	1:B:235:ILE:HG21	1.69	0.58
1:B:234:ASN:OD1	1:B:234:ASN:N	2.35	0.58
1:B:239:GLN:HG2	1:B:239:GLN:O	2.03	0.58
1:B:332:ILE:HD12	1:B:332:ILE:H	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:564:GLN:O	1:C:577:ARG:CG	2.50	0.58
1:C:1096:VAL:O	1:C:1096:VAL:HG13	2.02	0.58
1:A:421:TYR:CD1	1:A:457:ARG:HB3	2.39	0.58
1:A:567:ARG:HD2	1:A:567:ARG:C	2.29	0.58
1:A:819:GLU:HA	1:A:822:LEU:HD12	1.85	0.58
1:A:1090:PRO:CB	1:A:1095:PHE:CE1	2.86	0.58
1:A:1102:TRP:CD1	1:A:1102:TRP:N	2.72	0.58
1:B:92:PHE:C	1:B:92:PHE:CD2	2.80	0.58
1:B:273:ARG:HG2	1:B:273:ARG:NH2	2.19	0.58
1:B:1103:PHE:C	1:B:1115:ILE:HD11	2.28	0.58
1:A:30:ASN:HA	1:A:60:SER:O	2.03	0.58
1:A:208:THR:HG23	1:A:210:ILE:HD13	1.85	0.58
1:A:557:LYS:HZ2	1:B:43:PHE:HE2	0.80	0.58
1:C:885:GLY:HA2	1:C:901:GLN:CD	2.29	0.58
1:A:941:THR:HG22	1:A:941:THR:O	2.02	0.58
1:C:718:PHE:HD2	1:C:718:PHE:N	2.00	0.58
1:A:984:LEU:HD22	1:A:988:GLU:HG3	1.84	0.58
1:B:346:ARG:HB3	1:B:451:TYR:OH	2.04	0.58
2:H:66:ARG:H	2:H:66:ARG:HD3	1.69	0.58
3:L:37:GLN:H	3:L:47:LEU:HD11	1.68	0.58
1:B:1104:VAL:HG12	1:B:1115:ILE:HD13	1.86	0.58
1:C:326:ILE:O	1:C:326:ILE:HG13	2.02	0.58
1:A:86:PHE:CD1	1:A:90:VAL:HG13	2.37	0.58
1:A:140:PHE:HZ	1:A:248:TYR:H	1.50	0.58
1:A:350:VAL:HG21	1:A:422:ASN:OD1	2.04	0.58
1:B:393:THR:H	1:B:517:LEU:HA	1.68	0.58
1:B:520:ALA:HB1	1:B:521:PRO:HD2	1.85	0.58
1:A:108:THR:O	1:A:110:LEU:HG	2.04	0.57
1:A:566:GLY:HA2	1:B:43:PHE:HD2	1.68	0.57
1:B:93:ALA:HB1	1:B:190:ARG:H	1.69	0.57
1:B:717:ASN:OD1	5:B:1302:NAG:H83	2.01	0.57
1:B:1104:VAL:O	1:B:1104:VAL:HG13	2.02	0.57
1:B:1139:ASP:OD1	1:B:1141:LEU:HG	2.04	0.57
1:C:797:PHE:O	1:C:798:GLY:C	2.47	0.57
3:L:38:GLN:HA	3:L:44:PRO:HB3	1.85	0.57
1:B:187:LYS:HA	1:B:210:ILE:O	2.03	0.57
1:B:334:ASN:HD22	1:B:334:ASN:C	2.11	0.57
1:C:391:CYS:SG	1:C:526:GLY:N	2.70	0.57
1:C:735:SER:O	1:C:859:THR:N	2.36	0.57
2:H:33:PHE:HD1	2:H:52:ASN:HA	1.68	0.57
2:H:61:PRO:HA	2:H:64:LYS:HG2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:36:TYR:HA	3:L:47:LEU:HB2	1.84	0.57
1:B:956:ALA:O	1:B:957:GLN:C	2.45	0.57
2:H:58:ASN:HD21	2:H:64:LYS:HE3	1.69	0.57
3:L:61:ARG:NH1	3:L:79:GLU:OE1	2.37	0.57
1:A:187:LYS:HZ2	1:A:187:LYS:C	2.05	0.57
1:A:317:ASN:HA	1:A:592:PHE:HE2	1.69	0.57
1:A:1102:TRP:H	1:A:1102:TRP:HD1	1.50	0.57
1:B:214:ARG:HG2	1:B:214:ARG:O	2.05	0.57
1:C:1094:VAL:HG23	1:C:1094:VAL:O	2.05	0.57
1:A:337:PRO:CD	1:A:358:ILE:HD11	2.35	0.57
1:A:1081:ILE:HD12	1:A:1095:PHE:CD2	2.30	0.57
1:B:943:SER:O	1:B:945:LEU:N	2.37	0.57
1:C:105:ILE:HG12	1:C:110:LEU:HD11	1.87	0.57
1:C:823:PHE:CD1	1:C:1057:PRO:HG3	2.39	0.57
1:A:105:ILE:HA	1:A:118:LEU:CB	2.35	0.57
1:B:346:ARG:HG2	1:B:509:ARG:NH2	2.20	0.57
1:C:720:ILE:O	1:C:720:ILE:HG22	2.03	0.57
1:C:785:VAL:HG11	1:C:888:PHE:HE2	1.68	0.57
1:A:106:PHE:N	1:A:106:PHE:CD2	2.72	0.57
1:A:374:PHE:HB2	1:A:434:ILE:HD11	1.87	0.57
1:A:534:VAL:O	1:A:535:LYS:HB2	2.04	0.57
1:B:1091:ARG:HH11	1:B:1091:ARG:HG3	1.69	0.57
1:C:118:LEU:HD23	1:C:119:ILE:N	2.18	0.57
1:C:444:LYS:H	1:C:447:GLY:HA2	1.69	0.57
1:A:337:PRO:O	1:A:340:GLU:HG2	2.04	0.57
1:B:309:GLU:HG2	1:B:313:TYR:OH	2.04	0.57
1:C:1074:ASN:ND2	1:C:1074:ASN:H	2.02	0.57
1:C:1107:ARG:O	1:C:1107:ARG:NE	2.37	0.57
2:H:7:TRP:O	2:H:21:THR:N	2.38	0.57
2:H:99:GLN:HB2	2:H:103:ARG:H	1.69	0.57
1:A:84:LEU:HB3	1:A:85:PRO:CD	2.35	0.57
1:A:474:GLN:OE1	1:A:474:GLN:N	2.31	0.57
1:A:904:TYR:CE2	1:C:1094:VAL:HG12	2.34	0.57
1:B:90:VAL:HG21	1:B:238:PHE:HZ	1.69	0.57
1:B:328:ARG:NH2	1:B:580:GLN:OE1	2.37	0.57
1:B:718:PHE:CB	1:B:1067:TYR:CZ	2.87	0.57
1:C:393:THR:HG22	1:C:522:ALA:HA	1.87	0.57
1:C:419:ALA:HA	1:C:423:TYR:O	2.05	0.57
2:H:104:VAL:HG23	3:L:49:TYR:CE2	2.36	0.57
1:A:104:TRP:CD1	1:A:104:TRP:N	2.72	0.57
1:C:822:LEU:HD21	1:C:1056:ALA:HB2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:804:GLN:O	1:A:817:PRO:HD2	2.04	0.56
1:A:1030:SER:HA	1:A:1034:LEU:HG	1.86	0.56
1:B:406:GLU:O	1:B:410:ILE:HG13	2.05	0.56
1:B:458:LYS:HG2	1:B:473:TYR:CD2	2.40	0.56
1:B:497:PHE:HD2	1:B:507:PRO:HG3	1.70	0.56
1:B:712:ILE:CG2	1:B:1075:PHE:CB	2.83	0.56
1:B:718:PHE:HD1	1:B:1067:TYR:CD2	2.16	0.56
2:H:106:LEU:CA	3:L:46:LEU:HD23	2.29	0.56
1:A:366:SER:O	1:A:370:ASN:N	2.38	0.56
1:B:285:ILE:O	1:B:285:ILE:HG22	2.05	0.56
1:C:94:SER:O	1:C:189:LEU:HD12	2.04	0.56
1:C:541:PHE:HB2	1:C:543:PHE:HE2	1.68	0.56
1:C:912:THR:OG1	1:C:1107:ARG:NH1	2.38	0.56
1:A:318:PHE:HB3	1:A:633:TRP:HZ3	1.70	0.56
1:A:402:ILE:H	1:A:402:ILE:CD1	2.19	0.56
1:A:418:ILE:O	1:A:423:TYR:N	2.38	0.56
1:A:1128:VAL:HG21	1:B:918:GLU:HG2	1.86	0.56
1:B:116:SER:OG	1:B:235:ILE:CG1	2.36	0.56
1:B:407:VAL:HA	1:B:410:ILE:HD12	1.85	0.56
1:B:474:GLN:HA	1:B:480:CYS:SG	2.45	0.56
1:B:532:ASN:OD1	1:B:533:LEU:N	2.37	0.56
1:B:708:SER:HB3	1:B:711:SER:HB2	1.88	0.56
1:B:715:PRO:HA	1:B:1072:GLU:CA	2.35	0.56
1:C:577:ARG:HA	1:C:584:ILE:HA	1.87	0.56
1:C:707:TYR:CD2	1:C:707:TYR:C	2.83	0.56
3:L:3:VAL:HG12	3:L:4:LEU:O	2.05	0.56
3:L:34:ALA:HB1	3:L:48:ILE:O	2.06	0.56
1:A:92:PHE:CE1	1:A:265:TYR:HB2	2.41	0.56
1:A:471:GLU:O	1:A:491:PRO:HD3	2.04	0.56
1:B:106:PHE:N	1:B:106:PHE:CD1	2.71	0.56
1:B:140:PHE:N	1:B:140:PHE:CD1	2.73	0.56
1:B:979:ASP:O	1:B:982:SER:N	2.39	0.56
1:C:334:ASN:O	1:C:334:ASN:ND2	2.38	0.56
1:C:355:ARG:HA	1:C:397:ALA:O	2.06	0.56
1:C:554:GLU:O	1:C:586:ASP:N	2.39	0.56
3:L:36:TYR:HD2	3:L:44:PRO:HB2	1.68	0.56
1:A:319:ARG:HG2	1:A:624:ILE:HB	1.87	0.56
1:B:90:VAL:O	1:B:90:VAL:HG12	2.03	0.56
1:B:202:LYS:HE2	1:B:202:LYS:HA	1.87	0.56
1:B:825:LYS:HB2	1:B:945:LEU:CD2	2.35	0.56
1:C:350:VAL:HA	1:C:400:PHE:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:559:PHE:HB3	1:C:563:GLN:HB2	1.87	0.56
2:H:92:VAL:HG13	2:H:113:GLN:HA	1.86	0.56
1:A:208:THR:HG23	1:A:210:ILE:CD1	2.36	0.56
1:A:277:LEU:HD12	1:A:285:ILE:HD12	1.88	0.56
1:A:788:ILE:H	1:A:788:ILE:HD12	1.71	0.56
1:B:38:TYR:CZ	1:B:285:ILE:HD12	2.41	0.56
1:B:718:PHE:CZ	1:B:919:ASN:OD1	2.58	0.56
1:B:939:SER:O	1:B:940:SER:C	2.49	0.56
3:L:46:LEU:HD11	3:L:49:TYR:CD1	2.41	0.56
1:A:319:ARG:HB2	1:A:592:PHE:CE1	2.41	0.56
1:A:557:LYS:CD	1:B:43:PHE:CZ	2.89	0.56
1:A:726:ILE:HG12	1:A:1061:VAL:HG22	1.88	0.56
1:B:707:TYR:CE2	1:C:897:PRO:HA	2.41	0.56
1:C:86:PHE:C	1:C:86:PHE:CD2	2.84	0.56
2:H:59:TYR:HE1	2:H:80:LEU:HD13	1.70	0.56
1:A:299:THR:HG22	1:A:597:VAL:HG11	1.88	0.56
1:A:1039:ARG:HH12	1:B:1039:ARG:CZ	2.19	0.56
1:B:970:PHE:N	1:C:755:GLN:NE2	2.52	0.56
1:A:364:ASP:O	1:A:367:VAL:HG22	2.06	0.56
1:A:559:PHE:CD1	1:A:584:ILE:CD1	2.89	0.56
1:A:600:PRO:HD3	1:A:692:ILE:HD11	1.88	0.56
1:B:115:GLN:H	1:B:115:GLN:CD	2.11	0.56
1:A:189:LEU:HD23	1:A:189:LEU:C	2.31	0.56
1:A:712:ILE:CG2	1:A:1077:THR:CG2	2.83	0.56
1:B:295:PRO:HG2	1:B:636:TYR:HD2	1.71	0.56
1:B:616:ASN:HD22	5:B:1308:NAG:H83	1.70	0.56
1:B:846:ALA:HB3	1:B:849:LEU:HG	1.88	0.56
1:B:1071:GLN:CA	1:B:1071:GLN:HE21	2.17	0.56
1:C:64:TRP:CD1	1:C:64:TRP:C	2.83	0.56
1:A:28:TYR:CZ	1:A:61:ASN:HB3	2.41	0.55
1:A:557:LYS:HD2	1:B:43:PHE:CE2	2.41	0.55
1:B:86:PHE:C	1:B:86:PHE:CD2	2.84	0.55
1:B:201:PHE:C	1:B:201:PHE:CD2	2.84	0.55
1:C:920:GLN:O	1:C:923:ILE:CG2	2.51	0.55
2:H:34:TRP:CZ3	2:H:97:ARG:HB2	2.40	0.55
1:A:43:PHE:HD2	1:C:557:LYS:HE3	1.70	0.55
1:A:350:VAL:CG2	1:A:453:TYR:CA	2.81	0.55
1:A:420:ASP:CG	1:A:421:TYR:H	2.14	0.55
1:A:559:PHE:CD1	1:A:584:ILE:HD11	2.30	0.55
1:A:712:ILE:HG22	1:A:1077:THR:HG22	1.88	0.55
1:B:104:TRP:N	1:B:104:TRP:CD1	2.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:409:GLN:OE1	1:B:419:ALA:N	2.39	0.55
1:C:89:GLY:C	1:C:270:LEU:HG	2.31	0.55
1:C:731:MET:HG2	1:C:774:GLN:NE2	2.21	0.55
3:L:8:PRO:HB3	3:L:11:LEU:HD13	1.88	0.55
1:A:393:THR:CB	1:A:522:ALA:HA	2.35	0.55
1:B:108:THR:HG22	1:B:109:THR:HG22	1.87	0.55
1:B:438:SER:N	1:B:508:TYR:HA	2.20	0.55
1:C:894:LEU:HD22	1:C:894:LEU:N	2.03	0.55
1:A:117:LEU:HB3	1:A:130:VAL:HG23	1.87	0.55
1:C:54:LEU:HD13	1:C:88:ASP:OD2	2.06	0.55
1:C:564:GLN:CA	1:C:577:ARG:HD3	2.22	0.55
1:C:1076:THR:O	1:C:1076:THR:OG1	2.15	0.55
2:H:39:GLN:NE2	2:H:40:PRO:O	2.39	0.55
1:A:707:TYR:C	1:A:707:TYR:CD2	2.85	0.55
1:A:748:GLU:OE1	1:A:748:GLU:N	2.29	0.55
1:B:33:THR:O	1:B:34:ARG:NE	2.24	0.55
1:B:69:HIS:HE1	1:B:80:ASP:HB2	1.71	0.55
1:B:97:LYS:CE	1:B:100:ILE:CD1	2.68	0.55
1:B:1071:GLN:HE21	1:B:1071:GLN:HA	1.70	0.55
2:H:18:LEU:HG	2:H:19:SER:H	1.72	0.55
2:H:33:PHE:HE1	2:H:54:SER:H	1.54	0.55
2:H:104:VAL:HG23	3:L:49:TYR:HD2	1.55	0.55
1:A:563:GLN:HE22	1:B:44:ARG:H	1.54	0.55
1:A:612:TYR:CE2	1:A:620:VAL:HG13	2.41	0.55
1:B:404:GLY:O	1:B:407:VAL:HG23	2.07	0.55
1:B:449:TYR:C	1:B:451:TYR:H	2.14	0.55
1:B:519:HIS:ND1	1:B:519:HIS:O	2.39	0.55
5:B:1305:NAG:H83	5:B:1305:NAG:H3	1.88	0.55
1:C:344:ALA:O	1:C:346:ARG:N	2.39	0.55
1:A:338:PHE:O	1:A:342:PHE:CD2	2.60	0.55
1:A:412:PRO:C	1:A:414:GLN:H	2.14	0.55
1:B:91:TYR:C	1:B:91:TYR:CD2	2.84	0.55
1:B:140:PHE:N	1:B:140:PHE:HD1	2.04	0.55
1:B:275:PHE:N	1:B:275:PHE:HD1	2.04	0.55
1:B:409:GLN:CD	1:B:419:ALA:HB2	2.31	0.55
1:B:736:VAL:CG2	1:B:858:LEU:CD1	2.83	0.55
1:C:115:GLN:NE2	1:C:165:ASN:HD21	2.04	0.55
1:C:351:TYR:OH	1:C:492:LEU:CD2	2.55	0.55
1:C:738:CYS:SG	1:C:739:THR:N	2.79	0.55
2:H:17:THR:HB	2:H:83:SER:HA	1.88	0.55
2:H:104:VAL:HG12	2:H:105:LEU:N	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:518:LEU:HD23	1:A:518:LEU:H	1.72	0.55
1:A:734:THR:O	1:A:734:THR:HG23	2.07	0.55
1:A:977:LEU:O	1:A:981:LEU:HD12	2.07	0.55
1:A:1139:ASP:OD2	1:A:1141:LEU:N	2.40	0.55
1:B:346:ARG:HB2	1:B:346:ARG:CZ	2.36	0.55
1:C:212:LEU:HD13	1:C:215:ASP:O	2.07	0.55
1:C:718:PHE:N	1:C:718:PHE:CD2	2.70	0.55
1:C:888:PHE:CE1	1:C:1034:LEU:HD23	2.41	0.55
1:A:85:PRO:O	1:A:269:TYR:HE1	1.89	0.55
1:A:92:PHE:CD2	1:A:92:PHE:C	2.85	0.55
1:A:995:ARG:O	1:A:998:THR:OG1	2.25	0.55
1:B:1002:GLN:OE1	1:B:1002:GLN:HA	2.07	0.55
1:A:33:THR:HG23	1:A:33:THR:O	2.07	0.55
1:A:238:PHE:CD1	1:A:238:PHE:C	2.84	0.55
1:A:364:ASP:O	1:A:366:SER:N	2.40	0.55
1:B:302:THR:HG23	1:B:303:LEU:HD12	1.88	0.55
1:B:332:ILE:HG23	1:B:362:VAL:HG21	1.89	0.55
1:B:426:PRO:HG3	1:B:464:PHE:CZ	2.42	0.55
1:C:355:ARG:CZ	1:C:396:TYR:HB2	2.36	0.55
1:A:338:PHE:CA	1:A:341:VAL:HG12	2.33	0.54
1:B:93:ALA:CB	1:B:191:GLU:CA	2.83	0.54
1:C:606:ASN:O	1:C:608:VAL:HG13	2.07	0.54
2:H:3:GLN:OE1	2:H:3:GLN:HA	2.07	0.54
1:B:277:LEU:HA	1:B:288:ALA:HA	1.88	0.54
1:B:360:ASN:HA	1:B:524:VAL:N	2.23	0.54
1:B:921:LYS:O	1:B:921:LYS:HD3	2.07	0.54
1:C:107:GLY:H	1:C:235:ILE:HG23	1.72	0.54
1:C:715:PRO:HD2	1:C:1108:ASN:O	2.07	0.54
1:C:1095:PHE:CE1	1:C:1105:THR:CB	2.90	0.54
3:L:30:SER:C	3:L:32:TYR:H	2.16	0.54
1:A:712:ILE:HB	1:A:1077:THR:HG22	1.87	0.54
1:B:456:PHE:CE1	2:H:101:TYR:HE1	2.25	0.54
1:B:483:VAL:O	1:B:488:CYS:HB3	2.08	0.54
1:C:1103:PHE:O	1:C:1115:ILE:HG13	2.07	0.54
1:A:870:ILE:O	1:A:874:THR:HG23	2.07	0.54
1:A:917:TYR:HB3	1:C:1129:VAL:HG12	1.73	0.54
1:B:331:ASN:O	1:B:333:THR:HG23	2.07	0.54
1:B:337:PRO:CD	1:B:358:ILE:CG1	2.82	0.54
1:C:214:ARG:HH11	1:C:214:ARG:CG	2.20	0.54
1:C:535:LYS:HE2	1:C:585:LEU:HD21	1.89	0.54
1:C:1089:PHE:CE1	1:C:1129:VAL:HG21	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:592:PHE:HE1	1:A:624:ILE:HG22	1.72	0.54
1:B:712:ILE:O	1:C:895:GLN:O	2.26	0.54
1:C:101:ILE:HG22	1:C:242:LEU:HD11	1.89	0.54
1:A:91:TYR:CD1	1:A:91:TYR:C	2.85	0.54
1:A:299:THR:CG2	1:A:597:VAL:HG11	2.37	0.54
1:A:453:TYR:O	1:A:492:LEU:CD2	2.52	0.54
1:B:64:TRP:HB3	1:B:265:TYR:O	2.08	0.54
1:C:722:VAL:HA	1:C:1064:HIS:O	2.08	0.54
1:C:988:GLU:O	1:C:991:VAL:HG12	2.07	0.54
1:C:993:ILE:O	1:C:997:ILE:HG12	2.08	0.54
3:L:38:GLN:O	3:L:84:ALA:HB1	2.07	0.54
1:A:317:ASN:HA	1:A:592:PHE:CE2	2.42	0.54
1:A:322:PRO:HB3	1:A:537:LYS:HB2	1.88	0.54
1:A:759:PHE:HE2	1:C:970:PHE:HE1	1.54	0.54
1:B:409:GLN:HB3	1:B:419:ALA:HB2	1.89	0.54
1:B:471:GLU:H	1:B:491:PRO:HG3	1.73	0.54
2:H:37:ILE:HD13	2:H:108:PHE:HE2	1.73	0.54
1:A:85:PRO:O	1:A:269:TYR:CE1	2.60	0.54
1:A:628:GLN:O	1:A:629:LEU:HD23	2.08	0.54
1:B:141:LEU:HB2	1:B:159:VAL:HG22	1.89	0.54
1:B:343:ASN:OD1	1:B:343:ASN:N	2.40	0.54
1:B:1046:GLY:HA2	1:C:890:ALA:HB1	1.88	0.54
1:A:97:LYS:C	1:A:99:ASN:N	2.66	0.54
1:A:399:SER:HB3	1:A:511:VAL:HA	1.90	0.54
1:A:802:PHE:O	1:A:802:PHE:HD2	1.91	0.54
1:A:1050:MET:O	1:A:1065:VAL:HG22	2.08	0.54
5:C:1301:NAG:H82	5:C:1301:NAG:C1	2.38	0.54
1:A:1091:ARG:CG	1:A:1119:ASN:C	2.81	0.54
1:B:34:ARG:HB3	1:B:91:TYR:CE1	2.43	0.54
1:B:165:ASN:HB2	5:B:1311:NAG:C7	2.37	0.54
1:B:398:ASP:HB2	1:B:512:VAL:HB	1.89	0.54
1:B:944:ALA:C	1:B:946:GLY:H	2.16	0.54
5:B:1302:NAG:H82	5:B:1302:NAG:C1	2.38	0.54
5:B:1303:NAG:C1	5:B:1303:NAG:H82	2.38	0.54
1:C:140:PHE:HE2	1:C:250:THR:H	1.55	0.54
1:A:99:ASN:O	1:A:99:ASN:ND2	2.41	0.53
1:A:293:LEU:HG	1:A:294:ASP:H	1.73	0.53
1:A:303:LEU:HD13	1:A:308:VAL:HG23	1.88	0.53
1:B:438:SER:C	1:B:442:ASP:HB3	2.33	0.53
1:B:669:GLY:HA3	1:C:869:MET:HE1	1.89	0.53
1:B:993:ILE:O	1:B:997:ILE:HG12	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:LEU:CD1	1:C:216:LEU:H	2.21	0.53
1:B:210:ILE:HG22	1:B:212:LEU:H	1.73	0.53
1:B:1076:THR:O	1:B:1076:THR:HG22	2.06	0.53
1:C:913:GLN:C	1:C:915:VAL:H	2.15	0.53
2:H:39:GLN:HE22	2:H:42:GLY:H	1.55	0.53
1:A:559:PHE:CD1	1:A:584:ILE:HG12	2.42	0.53
1:C:915:VAL:O	1:C:918:GLU:HG2	2.07	0.53
2:H:59:TYR:OH	2:H:69:ILE:N	2.41	0.53
2:H:66:ARG:HG3	2:H:84:SER:HB3	1.89	0.53
1:A:90:VAL:HG21	1:A:238:PHE:CD2	2.44	0.53
1:A:1130:ILE:HG13	1:A:1130:ILE:O	2.08	0.53
1:C:887:THR:HG23	1:C:894:LEU:HD21	1.90	0.53
1:A:117:LEU:N	1:A:117:LEU:CD2	2.72	0.53
1:A:664:ILE:HB	1:A:672:ALA:O	2.08	0.53
1:B:94:SER:HB2	1:B:265:TYR:HB2	1.91	0.53
1:B:346:ARG:CZ	1:B:346:ARG:CB	2.85	0.53
1:B:916:LEU:O	1:B:920:GLN:N	2.42	0.53
4:D:1:NAG:C1	4:D:1:NAG:H82	2.38	0.53
1:A:319:ARG:HB3	1:A:624:ILE:O	2.09	0.53
1:A:365:TYR:HB3	1:A:387:LEU:HD23	1.90	0.53
1:B:456:PHE:CB	1:B:491:PRO:HA	2.22	0.53
1:C:57:PRO:HB3	1:C:273:ARG:NH1	2.23	0.53
1:C:64:TRP:HZ3	1:C:215:ASP:CG	2.16	0.53
1:C:722:VAL:HG12	1:C:930:ALA:HB1	1.90	0.53
1:C:801:ASN:OD1	4:D:1:NAG:H81	2.08	0.53
1:A:97:LYS:NZ	1:A:97:LYS:CB	2.72	0.53
1:A:216:LEU:HD23	1:A:216:LEU:N	2.23	0.53
1:A:1090:PRO:CB	1:A:1095:PHE:HE1	2.21	0.53
1:B:200:TYR:HA	1:B:230:PRO:HA	1.91	0.53
1:B:275:PHE:N	1:B:275:PHE:CD1	2.73	0.53
1:C:64:TRP:CH2	1:C:214:ARG:CD	2.92	0.53
1:C:533:LEU:HD22	1:C:578:ASP:CG	2.34	0.53
1:C:560:LEU:HB2	1:C:563:GLN:CD	2.33	0.53
1:C:714:ILE:HG23	1:C:715:PRO:HD2	1.89	0.53
4:N:1:NAG:C1	4:N:1:NAG:H82	2.38	0.53
1:A:187:LYS:NZ	1:A:187:LYS:HB2	2.23	0.53
1:A:338:PHE:HB3	1:A:342:PHE:HE2	1.68	0.53
1:A:436:TRP:NE1	1:A:438:SER:OG	2.40	0.53
1:A:619:GLU:O	1:A:619:GLU:HG2	2.09	0.53
1:B:226:LEU:HD12	1:B:227:VAL:HG22	1.89	0.53
1:B:1144:GLU:OE1	1:B:1147:SER:OG	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1075:PHE:CZ	1:C:1110:TYR:OH	2.41	0.53
1:A:468:ILE:H	1:A:468:ILE:HD12	1.72	0.53
1:B:106:PHE:HZ	1:B:201:PHE:HE1	1.51	0.53
1:B:201:PHE:CZ	1:B:203:ILE:CD1	2.86	0.53
1:C:351:TYR:HH	1:C:492:LEU:HD23	1.74	0.53
5:C:1304:NAG:H3	5:C:1304:NAG:H83	1.89	0.53
1:A:44:ARG:HG3	1:A:44:ARG:O	2.09	0.53
1:A:818:ILE:O	1:A:822:LEU:HG	2.09	0.53
1:B:238:PHE:C	1:B:238:PHE:CD1	2.86	0.53
1:B:409:GLN:NE2	1:B:415:THR:O	2.42	0.53
1:C:229:LEU:HB3	1:C:231:ILE:HG12	1.91	0.53
1:C:1091:ARG:HE	1:C:1121:PHE:HB3	1.73	0.53
5:C:1302:NAG:C1	5:C:1302:NAG:H82	2.38	0.53
3:L:59:PRO:HD2	3:L:62:PHE:HE1	1.74	0.53
1:A:36:VAL:HA	1:A:55:PHE:CB	2.39	0.52
1:A:216:LEU:N	1:A:216:LEU:CD2	2.72	0.52
1:A:776:LYS:O	1:A:780:GLU:HG2	2.10	0.52
1:A:1037:SER:HB3	1:A:1043:CYS:SG	2.50	0.52
1:B:456:PHE:CE2	1:B:473:TYR:HB3	2.45	0.52
1:B:714:ILE:CD1	1:B:1107:ARG:O	2.56	0.52
1:B:974:SER:HB3	1:B:980:ILE:HD11	1.90	0.52
1:A:49:HIS:CG	1:A:50:SER:H	2.27	0.52
5:A:1301:NAG:C1	5:A:1301:NAG:C8	2.85	0.52
5:A:1302:NAG:H82	5:A:1302:NAG:C1	2.38	0.52
1:B:136:CYS:O	1:B:139:PRO:HD3	2.10	0.52
1:A:66:HIS:C	1:A:80:ASP:HB3	2.34	0.52
1:A:626:ALA:HB1	1:A:634:ARG:HG3	1.91	0.52
1:A:712:ILE:CB	1:A:1077:THR:CG2	2.88	0.52
1:B:202:LYS:C	1:B:203:ILE:HD13	2.35	0.52
1:B:949:GLN:HG3	1:B:953:ASN:HD21	1.73	0.52
1:B:956:ALA:O	1:B:959:LEU:N	2.43	0.52
1:B:1101:HIS:HB3	1:B:1103:PHE:CZ	2.45	0.52
1:C:350:VAL:HA	1:C:400:PHE:CB	2.40	0.52
1:C:1134:ASN:ND2	1:C:1134:ASN:H	2.07	0.52
1:A:318:PHE:HB3	1:A:633:TRP:CZ3	2.45	0.52
1:C:380:TYR:HE2	1:C:412:PRO:CD	2.23	0.52
1:C:906:PHE:CE2	1:C:916:LEU:HB2	2.44	0.52
1:A:97:LYS:CB	1:A:97:LYS:HZ2	2.22	0.52
1:A:187:LYS:NZ	1:A:187:LYS:CB	2.73	0.52
1:A:278:LYS:HB2	1:A:306:PHE:HE2	1.74	0.52
1:A:353:TRP:HZ3	1:A:355:ARG:HG2	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:VAL:HG13	1:B:422:ASN:HB3	1.90	0.52
1:C:83:VAL:HG22	1:C:237:ARG:HG2	1.91	0.52
1:C:736:VAL:CG2	1:C:857:GLY:O	2.57	0.52
3:L:11:LEU:O	3:L:105:ILE:N	2.36	0.52
1:B:193:VAL:HG12	1:B:204:TYR:HB2	1.90	0.52
1:C:449:TYR:OH	1:C:498:GLN:OE1	2.27	0.52
1:C:785:VAL:O	1:C:786:LYS:HE2	2.10	0.52
1:C:1080:ALA:HB3	1:C:1132:ILE:HG22	1.92	0.52
2:H:24:VAL:H	2:H:77:GLN:HB3	1.74	0.52
1:A:97:LYS:NZ	1:A:97:LYS:CA	2.73	0.52
1:B:131:CYS:HB3	1:B:166:CYS:HA	1.91	0.52
1:B:324:GLU:HB3	1:B:539:VAL:HG12	1.92	0.52
1:B:480:CYS:HA	1:B:483:VAL:HB	1.91	0.52
1:C:130:VAL:CG1	1:C:167:THR:HB	2.40	0.52
2:H:20:LEU:CD1	2:H:93:TYR:HB2	2.35	0.52
3:L:37:GLN:HB2	3:L:47:LEU:HD21	1.92	0.52
3:L:86:TYR:CE1	3:L:104:GLU:HB2	2.44	0.52
1:A:238:PHE:C	1:A:238:PHE:HD1	2.17	0.52
1:A:391:CYS:HB3	1:A:524:VAL:O	2.10	0.52
1:A:455:LEU:N	1:A:491:PRO:O	2.43	0.52
1:A:617:CYS:HA	1:A:620:VAL:HG23	1.92	0.52
1:B:189:LEU:HG	1:B:210:ILE:CD1	2.39	0.52
1:B:921:LYS:HD3	1:B:921:LYS:C	2.35	0.52
5:B:1301:NAG:C1	5:B:1301:NAG:H82	2.38	0.52
1:C:712:ILE:HG21	1:C:1077:THR:CG2	2.21	0.52
1:C:899:PRO:HB3	1:C:920:GLN:NE2	2.24	0.52
1:C:909:ILE:HD12	1:C:1047:TYR:HB3	1.90	0.52
1:A:122:ASN:CG	1:A:124:THR:HB	2.35	0.52
1:A:345:THR:C	1:A:346:ARG:HD2	2.35	0.52
1:A:476:GLY:H	1:A:487:ASN:HB3	1.75	0.52
1:A:711:SER:O	1:B:897:PRO:HD3	2.10	0.52
1:B:139:PRO:O	1:B:243:ALA:CB	2.49	0.52
1:B:887:THR:HG21	1:B:894:LEU:H	1.74	0.52
1:C:515:PHE:HE2	1:C:517:LEU:HG	1.74	0.52
1:C:790:LYS:O	1:C:791:THR:C	2.52	0.52
1:A:327:VAL:HG12	1:A:542:ASN:HB3	1.90	0.52
1:A:402:ILE:HD12	1:A:402:ILE:N	2.24	0.52
1:A:878:LEU:HD23	1:A:878:LEU:C	2.35	0.52
1:B:346:ARG:NH2	1:B:346:ARG:CB	2.73	0.52
1:B:833:PHE:HE1	1:B:855:PHE:HB3	1.75	0.52
1:B:1073:LYS:CB	1:B:1073:LYS:NZ	2.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:722:VAL:O	1:C:934:ILE:HD11	2.10	0.52
3:L:36:TYR:HA	3:L:47:LEU:HD13	1.92	0.52
1:A:540:ASN:OD1	1:A:549:THR:HG23	2.10	0.51
1:B:298:GLU:OE1	1:B:633:TRP:CH2	2.63	0.51
1:B:901:GLN:HE21	1:B:905:ARG:HE	1.58	0.51
1:C:216:LEU:CD1	1:C:216:LEU:N	2.73	0.51
1:C:327:VAL:CB	1:C:542:ASN:O	2.58	0.51
1:C:796:ASP:O	1:C:798:GLY:N	2.43	0.51
1:C:937:SER:O	1:C:942:PRO:HG2	2.10	0.51
1:A:95:THR:O	1:A:186:PHE:CG	2.63	0.51
1:A:712:ILE:CB	1:A:1077:THR:HG22	2.40	0.51
1:B:992:GLN:CD	1:B:995:ARG:HH21	2.18	0.51
1:C:884:SER:HB3	1:C:888:PHE:HB3	1.91	0.51
1:A:408:ARG:HH11	1:A:409:GLN:HA	1.73	0.51
1:A:566:GLY:HA2	1:B:43:PHE:CD2	2.45	0.51
1:A:1091:ARG:HE	1:A:1121:PHE:HB3	1.74	0.51
1:A:1094:VAL:O	1:A:1094:VAL:HG23	2.10	0.51
1:B:929:SER:HB2	1:B:933:LYS:NZ	2.26	0.51
1:C:216:LEU:HD12	1:C:216:LEU:H	1.74	0.51
1:C:1130:ILE:HG23	1:C:1130:ILE:O	2.10	0.51
3:L:91:ARG:HA	3:L:96:THR:HA	1.92	0.51
1:A:273:ARG:HH21	1:A:290:ASP:HB3	1.76	0.51
1:A:374:PHE:CB	1:A:434:ILE:HD11	2.40	0.51
1:A:628:GLN:O	1:A:628:GLN:HG2	2.11	0.51
1:A:917:TYR:O	1:C:1129:VAL:HG13	2.10	0.51
1:B:69:HIS:CE1	1:B:80:ASP:HB2	2.45	0.51
1:B:559:PHE:HB2	1:B:563:GLN:OE1	2.11	0.51
1:A:405:ASP:OD1	1:A:505:TYR:HA	2.11	0.51
1:A:759:PHE:HE2	1:C:970:PHE:CE1	2.28	0.51
1:B:337:PRO:CB	1:B:341:VAL:CG2	2.87	0.51
1:B:439:ASN:HB2	1:B:506:GLN:HB3	1.92	0.51
1:B:518:LEU:N	1:B:518:LEU:CD1	2.73	0.51
1:B:921:LYS:NZ	1:B:921:LYS:CA	2.71	0.51
1:C:358:ILE:HG22	1:C:395:VAL:HB	1.92	0.51
2:H:20:LEU:HG	2:H:82:LEU:CD1	2.39	0.51
1:A:143:VAL:HG22	1:A:245:HIS:HA	1.92	0.51
1:A:966:LEU:O	1:A:966:LEU:HD23	2.11	0.51
1:B:104:TRP:CH2	1:B:194:PHE:CB	2.92	0.51
1:B:290:ASP:OD2	1:B:292:ALA:N	2.42	0.51
1:A:350:VAL:O	1:A:353:TRP:HD1	1.93	0.51
1:B:50:SER:HA	1:B:276:LEU:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:48:ILE:HG22	2:H:63:LEU:HD12	1.92	0.51
3:L:46:LEU:CD1	3:L:49:TYR:CD1	2.94	0.51
1:A:30:ASN:O	1:A:30:ASN:ND2	2.43	0.51
1:A:68:ILE:CD1	1:A:68:ILE:N	2.72	0.51
1:B:100:ILE:HD12	1:B:242:LEU:HD12	1.91	0.51
1:B:392:PHE:O	1:B:523:THR:OG1	2.29	0.51
1:B:714:ILE:HG13	1:B:715:PRO:HD2	1.93	0.51
1:B:1143:PRO:O	1:B:1146:ASP:N	2.37	0.51
1:C:86:PHE:C	1:C:86:PHE:HD2	2.18	0.51
1:C:337:PRO:C	1:C:339:GLY:H	2.19	0.51
1:C:888:PHE:CA	1:C:893:ALA:HB2	2.35	0.51
1:A:393:THR:H	1:A:522:ALA:CB	2.23	0.51
1:A:393:THR:HA	1:A:522:ALA:HA	1.93	0.51
1:A:604:THR:HA	5:A:1308:NAG:C8	2.41	0.51
1:A:758:SER:O	1:A:760:CYS:N	2.43	0.51
1:A:864:LEU:HG	1:A:865:LEU:HD22	1.91	0.51
1:B:89:GLY:C	1:B:270:LEU:HD23	2.36	0.51
1:B:352:ALA:HB2	1:B:468:ILE:CG2	2.41	0.51
1:B:377:PHE:O	1:B:379:CYS:HB2	2.11	0.51
5:B:1304:NAG:H83	5:B:1304:NAG:C4	2.41	0.51
1:C:86:PHE:HB3	1:C:236:THR:C	2.36	0.51
1:C:886:TRP:CD1	1:C:886:TRP:C	2.88	0.51
2:H:1:GLN:HG2	2:H:2:VAL:N	2.16	0.51
3:L:83:PHE:HB2	3:L:106:LYS:HE3	1.93	0.51
1:A:47:VAL:HG22	1:A:48:LEU:H	1.76	0.51
1:A:88:ASP:OD1	1:A:88:ASP:N	2.34	0.51
1:A:189:LEU:HB3	1:A:208:THR:HG22	1.91	0.51
1:A:204:TYR:CZ	1:A:225:PRO:HB3	2.45	0.51
1:A:457:ARG:NH1	1:A:460:ASN:HA	2.25	0.51
1:B:27:ALA:O	1:B:63:THR:HA	2.10	0.51
1:B:574:ASP:OD1	1:B:574:ASP:N	2.44	0.51
2:H:59:TYR:CE1	2:H:80:LEU:HD13	2.45	0.51
1:A:364:ASP:O	1:A:365:TYR:C	2.54	0.50
1:A:452:LEU:CD1	1:A:492:LEU:HB3	2.41	0.50
1:A:809:PRO:CA	1:A:814:LYS:HE3	2.34	0.50
1:A:890:ALA:HB1	1:C:1046:GLY:HA2	1.93	0.50
1:B:940:SER:O	1:B:941:THR:HB	2.10	0.50
1:C:347:PHE:CE2	1:C:399:SER:HB3	2.46	0.50
1:C:358:ILE:CG2	1:C:395:VAL:HB	2.41	0.50
1:C:736:VAL:CG2	1:C:858:LEU:HB3	2.39	0.50
2:H:104:VAL:HG21	3:L:49:TYR:HD2	1.68	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:108:PHE:CE1	3:L:45:ARG:HA	2.46	0.50
1:A:322:PRO:HG2	1:A:538:CYS:SG	2.51	0.50
1:A:410:ILE:HD11	1:A:512:VAL:CG2	2.41	0.50
1:A:566:GLY:O	1:A:573:THR:HA	2.11	0.50
1:B:122:ASN:HD22	1:B:127:VAL:HG12	1.76	0.50
1:C:106:PHE:HB3	1:C:235:ILE:HG21	1.92	0.50
1:C:327:VAL:HA	1:C:542:ASN:O	2.11	0.50
1:C:714:ILE:HG22	1:C:1109:PHE:O	2.10	0.50
1:A:377:PHE:HE2	1:A:384:PRO:HB3	1.76	0.50
1:A:599:THR:OG1	1:A:600:PRO:O	2.25	0.50
1:B:68:ILE:O	1:B:80:ASP:HB3	2.12	0.50
1:B:168:PHE:CE2	1:B:170:TYR:HB2	2.46	0.50
1:B:442:ASP:OD2	1:B:507:PRO:CG	2.54	0.50
1:C:318:PHE:CZ	1:C:615:VAL:HG21	2.46	0.50
1:C:457:ARG:HH22	1:C:460:ASN:C	2.19	0.50
3:L:65:SER:OG	3:L:72:THR:O	2.24	0.50
1:A:212:LEU:CD2	1:A:212:LEU:N	2.74	0.50
1:A:350:VAL:HG21	1:A:453:TYR:CA	2.42	0.50
1:A:604:THR:HA	5:A:1308:NAG:H82	1.94	0.50
1:A:755:GLN:NE2	1:C:970:PHE:N	2.59	0.50
1:B:279:TYR:HA	1:B:285:ILE:CA	2.39	0.50
1:B:492:LEU:O	1:B:493:GLN:NE2	2.45	0.50
1:B:953:ASN:O	1:B:954:GLN:C	2.55	0.50
1:C:921:LYS:CE	1:C:921:LYS:N	2.73	0.50
2:H:35:TYR:HA	2:H:50:GLU:HA	1.93	0.50
3:L:11:LEU:HG	3:L:13:LEU:HG	1.92	0.50
1:A:746:SER:OG	1:A:748:GLU:OE2	2.26	0.50
1:B:187:LYS:HA	1:B:210:ILE:HB	1.93	0.50
1:B:543:PHE:CD1	1:B:579:PRO:HD2	2.43	0.50
1:B:1078:ALA:HB1	1:B:1133:VAL:CG2	2.41	0.50
3:L:12:SER:HA	3:L:105:ILE:HB	1.92	0.50
1:A:738:CYS:SG	1:A:739:THR:N	2.84	0.50
1:B:206:LYS:CD	1:B:206:LYS:C	2.85	0.50
1:C:52:GLN:NE2	1:C:273:ARG:O	2.44	0.50
1:C:828:LEU:HG	1:C:835:LYS:HB2	1.93	0.50
1:A:403:ARG:O	1:A:405:ASP:OD1	2.30	0.50
1:A:410:ILE:HG12	1:A:433:VAL:HG12	1.93	0.50
1:A:880:GLY:O	1:A:884:SER:N	2.45	0.50
1:A:914:ASN:HA	1:C:1089:PHE:CE2	2.47	0.50
1:A:1030:SER:HA	1:A:1034:LEU:CG	2.41	0.50
1:C:347:PHE:CZ	1:C:399:SER:HB3	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:381:GLY:HA3	1:C:430:THR:HG23	1.92	0.50
1:C:749:CYS:SG	1:C:997:ILE:HD11	2.52	0.50
3:L:20:THR:HB	3:L:74:THR:HG23	1.94	0.50
1:A:187:LYS:C	1:A:187:LYS:CE	2.85	0.50
1:A:314:GLN:OE1	1:A:596:SER:HB2	2.11	0.50
1:A:406:GLU:C	1:A:408:ARG:N	2.69	0.50
1:A:543:PHE:CD2	1:A:576:VAL:HG11	2.47	0.50
1:B:436:TRP:CD1	1:B:437:ASN:H	2.29	0.50
2:H:65:SER:OG	2:H:66:ARG:HD3	2.11	0.50
2:H:65:SER:OG	2:H:66:ARG:NH1	2.44	0.50
3:L:36:TYR:CE2	3:L:44:PRO:CG	2.95	0.50
1:A:99:ASN:HD22	1:A:99:ASN:C	2.19	0.50
1:A:350:VAL:C	1:A:352:ALA:H	2.20	0.50
1:A:720:ILE:HG13	1:A:923:ILE:HG13	1.93	0.50
1:A:964:LYS:HZ1	1:B:758:SER:CB	2.25	0.50
1:C:128:ILE:HD12	1:C:170:TYR:HD2	1.77	0.50
1:C:794:ILE:HG13	1:C:795:LYS:H	1.77	0.50
2:H:48:ILE:O	2:H:60:ASN:N	2.45	0.50
1:A:367:VAL:HG23	1:A:368:LEU:H	1.77	0.49
1:A:450:ASN:N	1:A:450:ASN:ND2	2.60	0.49
1:A:565:PHE:HA	1:A:576:VAL:HA	1.94	0.49
1:A:806:LEU:CD1	1:A:878:LEU:HD22	2.42	0.49
1:B:115:GLN:H	1:B:115:GLN:HE21	1.59	0.49
1:B:445:VAL:HG22	1:B:499:PRO:HG3	1.93	0.49
1:B:578:ASP:OD2	1:B:581:THR:HG22	2.12	0.49
1:C:298:GLU:O	1:C:302:THR:HG23	2.12	0.49
2:H:104:VAL:HG21	3:L:49:TYR:HB2	1.94	0.49
1:A:563:GLN:NE2	1:B:43:PHE:HA	2.26	0.49
1:A:712:ILE:HA	1:B:895:GLN:O	2.11	0.49
1:B:337:PRO:HB3	1:B:341:VAL:CG2	2.42	0.49
1:B:969:ASN:CG	1:C:755:GLN:HE21	2.20	0.49
1:C:755:GLN:NE2	1:C:755:GLN:O	2.45	0.49
1:C:920:GLN:CA	1:C:923:ILE:CG2	2.91	0.49
2:H:52:ASN:HB2	2:H:55:GLY:O	2.12	0.49
1:A:43:PHE:HB3	1:C:557:LYS:NZ	2.27	0.49
1:A:189:LEU:C	1:A:189:LEU:CD2	2.85	0.49
1:A:208:THR:CG2	1:A:210:ILE:HD13	2.43	0.49
1:A:234:ASN:N	1:A:234:ASN:ND2	2.60	0.49
1:A:417:LYS:HG3	1:A:422:ASN:ND2	2.27	0.49
1:A:572:THR:O	1:A:573:THR:C	2.56	0.49
1:A:755:GLN:C	1:A:757:GLY:H	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:13:LYS:O	2:H:15:SER:N	2.37	0.49
1:A:66:HIS:CD2	1:A:66:HIS:N	2.78	0.49
1:A:97:LYS:CE	1:A:97:LYS:CA	2.86	0.49
1:A:115:GLN:O	1:A:131:CYS:O	2.30	0.49
1:A:452:LEU:HD13	1:A:492:LEU:HD13	1.93	0.49
1:A:979:ASP:HB3	1:A:983:ARG:NH1	2.27	0.49
1:B:472:ILE:HG21	1:B:483:VAL:O	2.11	0.49
1:B:703:ASN:N	1:C:790:LYS:HZ2	2.11	0.49
1:A:33:THR:CB	1:A:58:PHE:CA	2.75	0.49
1:A:390:LEU:HD23	1:A:390:LEU:H	1.76	0.49
1:A:1005:GLN:O	1:A:1008:VAL:HG12	2.13	0.49
1:B:943:SER:C	1:B:945:LEU:H	2.16	0.49
1:B:1141:LEU:HD22	1:C:1141:LEU:CD1	2.42	0.49
1:C:190:ARG:HD2	1:C:192:PHE:CZ	2.47	0.49
1:C:212:LEU:C	1:C:212:LEU:CD2	2.85	0.49
1:C:290:ASP:O	1:C:292:ALA:N	2.42	0.49
3:L:32:TYR:HA	3:L:50:ASP:HA	1.95	0.49
1:A:52:GLN:HB2	1:A:274:THR:HG22	1.94	0.49
1:A:129:LYS:HE2	5:A:1304:NAG:H82	1.95	0.49
1:A:296:LEU:O	1:A:299:THR:OG1	2.27	0.49
1:A:350:VAL:HG21	1:A:453:TYR:HA	1.93	0.49
1:A:708:SER:C	1:A:710:ASN:H	2.20	0.49
1:A:850:ILE:HA	1:A:853:GLN:NE2	2.28	0.49
1:B:96:GLU:HB3	1:B:188:ASN:CG	2.38	0.49
1:B:189:LEU:CG	1:B:210:ILE:HD11	2.41	0.49
1:B:417:LYS:O	1:B:421:TYR:CB	2.37	0.49
1:B:948:LEU:O	1:B:949:GLN:C	2.56	0.49
1:C:244:LEU:CD1	1:C:245:HIS:H	2.19	0.49
1:C:674:TYR:CZ	1:C:690:GLN:HB3	2.48	0.49
1:C:833:PHE:CZ	1:C:854:LYS:HD2	2.47	0.49
1:A:366:SER:O	1:A:367:VAL:C	2.55	0.49
1:A:367:VAL:HG23	1:A:368:LEU:N	2.26	0.49
1:A:517:LEU:C	1:A:517:LEU:CD2	2.85	0.49
1:A:563:GLN:CD	1:B:43:PHE:HA	2.38	0.49
1:A:1075:PHE:HZ	1:A:1110:TYR:CD2	2.31	0.49
1:B:49:HIS:ND1	1:B:50:SER:N	2.61	0.49
1:B:140:PHE:HD1	1:B:140:PHE:H	1.59	0.49
1:B:615:VAL:HG12	1:B:616:ASN:O	2.12	0.49
1:B:752:LEU:HD12	1:B:993:ILE:HG21	1.94	0.49
2:H:37:ILE:HG22	2:H:47:TRP:HA	1.93	0.49
2:H:99:GLN:HE22	2:H:103:ARG:NH2	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:110:GLU:HG2	2:H:111:TRP:N	2.26	0.49
1:A:804:GLN:HB3	1:A:805:ILE:HD13	1.95	0.49
1:A:989:ALA:O	1:A:993:ILE:HG12	2.12	0.49
5:A:1302:NAG:C1	5:A:1302:NAG:C8	2.91	0.49
1:B:202:LYS:O	1:B:203:ILE:HD13	2.12	0.49
1:B:418:ILE:HG13	1:B:422:ASN:HD22	1.78	0.49
1:C:133:PHE:CE2	1:C:161:SER:HA	2.48	0.49
1:A:402:ILE:CD1	1:A:402:ILE:N	2.72	0.49
1:A:503:VAL:HA	1:A:506:GLN:CG	2.43	0.49
1:B:27:ALA:HB3	1:B:64:TRP:CZ2	2.47	0.49
1:B:476:GLY:HA3	3:L:92:SER:HA	1.95	0.49
1:C:117:LEU:HD23	1:C:118:LEU:N	2.28	0.49
1:C:337:PRO:O	1:C:339:GLY:N	2.41	0.49
1:C:802:PHE:C	1:C:804:GLN:N	2.66	0.49
1:C:888:PHE:C	1:C:888:PHE:CD2	2.90	0.49
1:C:913:GLN:HE21	1:C:914:ASN:N	2.11	0.49
2:H:96:ALA:HA	2:H:107:TRP:O	2.13	0.49
1:A:353:TRP:O	1:A:353:TRP:CE3	2.66	0.49
1:A:571:ASP:O	1:A:573:THR:N	2.45	0.49
1:B:115:GLN:CD	1:B:115:GLN:N	2.71	0.49
1:B:405:ASP:HB3	1:B:408:ARG:HH12	1.78	0.49
1:B:426:PRO:HB3	1:B:463:PRO:HB3	1.95	0.49
1:B:822:LEU:HD21	1:B:1056:ALA:HB2	1.95	0.49
5:B:1307:NAG:O7	5:B:1307:NAG:O3	2.21	0.49
1:C:108:THR:OG1	1:C:234:ASN:O	2.21	0.49
1:C:424:LYS:HE3	1:C:461:LEU:H	1.77	0.49
1:C:791:THR:O	1:C:792:PRO:C	2.55	0.49
4:D:1:NAG:C8	4:D:1:NAG:C1	2.91	0.49
1:A:1075:PHE:CD2	1:A:1096:VAL:HG11	2.47	0.48
1:A:1135:ASN:ND2	1:A:1136:THR:H	2.11	0.48
1:B:117:LEU:HD23	1:B:233:ILE:HD12	1.93	0.48
1:B:235:ILE:HD12	1:B:235:ILE:HA	1.66	0.48
1:C:730:SER:HA	1:C:774:GLN:OE1	2.13	0.48
1:C:936:ASP:HA	1:C:939:SER:OG	2.13	0.48
1:A:97:LYS:HZ2	1:A:97:LYS:HB3	1.78	0.48
1:A:187:LYS:CD	1:A:187:LYS:C	2.85	0.48
1:A:386:LYS:HZ2	1:B:983:ARG:N	2.11	0.48
1:B:578:ASP:OD2	1:B:581:THR:N	2.35	0.48
1:B:736:VAL:HG23	1:B:858:LEU:CD1	2.28	0.48
1:B:989:ALA:O	1:B:993:ILE:HG12	2.13	0.48
1:B:1078:ALA:HB1	1:B:1133:VAL:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:393:THR:HG21	1:C:520:ALA:HB3	1.95	0.48
1:C:497:PHE:CG	1:C:507:PRO:HG3	2.48	0.48
1:A:187:LYS:HB2	1:A:187:LYS:HZ3	1.78	0.48
1:A:308:VAL:H	1:A:602:THR:CG2	2.26	0.48
1:A:350:VAL:HG23	1:A:351:TYR:N	2.28	0.48
1:A:410:ILE:HD11	1:A:512:VAL:HG21	1.95	0.48
1:A:785:VAL:HG22	1:A:787:GLN:H	1.78	0.48
1:A:851:CYS:O	1:A:854:LYS:HB3	2.13	0.48
1:B:529:LYS:HD2	1:B:529:LYS:N	2.27	0.48
5:B:1302:NAG:C8	5:B:1302:NAG:C1	2.91	0.48
1:C:189:LEU:O	1:C:207:HIS:HB2	2.13	0.48
1:C:544:ASN:CG	1:C:579:PRO:HG3	2.37	0.48
1:C:912:THR:HB	1:C:914:ASN:OD1	2.13	0.48
1:C:1027:THR:O	1:C:1028:LYS:C	2.56	0.48
2:H:47:TRP:CZ3	2:H:60:ASN:HA	2.48	0.48
3:L:35:TRP:O	3:L:47:LEU:HB2	2.12	0.48
1:A:703:ASN:O	1:B:789:TYR:HA	2.13	0.48
1:B:168:PHE:CE2	1:B:229:LEU:HD22	2.47	0.48
1:B:423:TYR:HE1	1:B:425:LEU:HD23	1.77	0.48
1:B:475:ALA:HA	2:H:101:TYR:CD1	2.48	0.48
1:B:577:ARG:HA	1:B:583:GLU:O	2.14	0.48
1:C:357:ARG:NH2	1:C:359:SER:HB3	2.28	0.48
1:C:447:GLY:N	1:C:498:GLN:OE1	2.46	0.48
1:A:567:ARG:NH2	1:B:49:HIS:HB2	2.29	0.48
1:A:624:ILE:HD11	1:A:637:SER:CB	2.43	0.48
1:B:108:THR:HB	1:B:235:ILE:HD12	1.96	0.48
1:B:321:GLN:HA	1:B:321:GLN:OE1	2.12	0.48
1:B:743:CYS:HB3	1:B:749:CYS:HB3	1.72	0.48
1:B:940:SER:OG	1:B:941:THR:N	2.46	0.48
1:B:985:ASP:CG	1:B:987:PRO:HD2	2.38	0.48
5:B:1301:NAG:C1	5:B:1301:NAG:C8	2.91	0.48
5:B:1303:NAG:C1	5:B:1303:NAG:C8	2.91	0.48
1:C:84:LEU:HB2	1:C:238:PHE:CZ	2.48	0.48
1:C:101:ILE:HA	1:C:242:LEU:HG	1.95	0.48
1:C:378:LYS:HB3	1:C:380:TYR:HE1	1.77	0.48
1:C:717:ASN:OD1	5:C:1301:NAG:O5	2.32	0.48
1:C:1113:GLN:N	1:C:1113:GLN:CD	2.70	0.48
2:H:61:PRO:HG2	3:L:94:TRP:CE3	2.49	0.48
1:A:402:ILE:HD13	1:A:402:ILE:O	2.14	0.48
1:B:240:THR:HG23	1:B:265:TYR:CE2	2.48	0.48
1:B:712:ILE:HB	1:B:1077:THR:HB	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:921:LYS:C	1:B:921:LYS:CD	2.84	0.48
1:C:197:ILE:HG13	1:C:198:ASP:H	1.77	0.48
1:C:376:THR:O	1:C:434:ILE:HA	2.13	0.48
1:C:377:PHE:CD1	1:C:434:ILE:HG12	2.48	0.48
1:C:1110:TYR:O	1:C:1112:PRO:HD3	2.14	0.48
2:H:4:LEU:HD21	2:H:34:TRP:CZ3	2.49	0.48
4:N:1:NAG:C1	4:N:1:NAG:C8	2.91	0.48
1:A:353:TRP:HZ2	1:A:465:GLU:C	2.21	0.48
1:A:797:PHE:C	1:A:799:GLY:H	2.20	0.48
1:A:1072:GLU:CD	1:A:1072:GLU:N	2.71	0.48
1:B:273:ARG:CG	1:B:273:ARG:NH2	2.72	0.48
1:B:457:ARG:NH1	1:B:459:SER:O	2.47	0.48
1:B:555:SER:HB3	1:B:586:ASP:CG	2.38	0.48
1:B:1076:THR:HB	1:B:1097:SER:HB3	1.94	0.48
1:C:554:GLU:CG	1:C:555:SER:H	2.25	0.48
1:C:629:LEU:HD23	1:C:633:TRP:CG	2.49	0.48
1:C:663:ASP:O	1:C:664:ILE:C	2.56	0.48
1:C:671:CYS:O	1:C:694:ALA:HA	2.13	0.48
5:C:1301:NAG:C8	5:C:1301:NAG:C1	2.91	0.48
1:A:332:ILE:HG22	1:A:332:ILE:O	2.14	0.48
1:A:559:PHE:CE1	1:A:584:ILE:CG1	2.97	0.48
1:A:643:PHE:N	1:A:650:LEU:O	2.47	0.48
1:B:97:LYS:HE3	1:B:100:ILE:HD11	1.81	0.48
1:B:115:GLN:NE2	1:B:115:GLN:N	2.60	0.48
1:B:438:SER:HB2	1:B:507:PRO:C	2.39	0.48
1:C:836:GLN:HB2	1:C:854:LYS:NZ	2.29	0.48
5:C:1302:NAG:C1	5:C:1302:NAG:C8	2.91	0.48
1:A:122:ASN:O	1:A:123:ALA:C	2.57	0.48
1:B:206:LYS:CA	1:B:206:LYS:CE	2.85	0.48
1:C:391:CYS:CB	1:C:525:CYS:HA	2.44	0.48
1:C:666:ILE:HB	1:C:670:ILE:O	2.14	0.48
1:C:736:VAL:HG13	1:C:736:VAL:O	2.13	0.48
1:A:567:ARG:HB2	1:B:42:VAL:HG22	1.96	0.48
1:A:592:PHE:HB2	1:A:625:HIS:NE2	2.28	0.48
1:A:666:ILE:HG12	1:A:671:CYS:HA	1.96	0.48
1:A:797:PHE:HD1	1:C:707:TYR:OH	1.94	0.48
1:B:955:ASN:O	1:B:956:ALA:C	2.55	0.48
1:C:143:VAL:HA	1:C:159:VAL:HG21	1.96	0.48
1:C:718:PHE:CG	1:C:1067:TYR:HE1	2.23	0.48
1:C:1134:ASN:ND2	1:C:1134:ASN:N	2.60	0.48
2:H:97:ARG:O	2:H:106:LEU:N	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:5:THR:HB	3:L:24:ARG:NH1	2.29	0.48
1:A:133:PHE:HB2	1:A:135:PHE:CZ	2.49	0.47
1:A:187:LYS:HD3	1:A:187:LYS:C	2.36	0.47
1:A:308:VAL:CG1	1:A:602:THR:HB	2.36	0.47
1:A:357:ARG:HG3	1:A:357:ARG:NH1	2.29	0.47
1:A:577:ARG:HG3	1:A:582:LEU:HA	1.96	0.47
1:A:619:GLU:O	1:A:623:ALA:HB3	2.14	0.47
1:A:914:ASN:HD21	1:A:918:GLU:CD	2.22	0.47
1:A:932:GLY:O	1:A:935:GLN:HG3	2.13	0.47
1:B:62:VAL:HG23	1:B:64:TRP:HZ3	1.79	0.47
1:B:128:ILE:HD13	1:B:170:TYR:CE2	2.49	0.47
1:B:318:PHE:CD1	1:B:318:PHE:C	2.91	0.47
1:B:601:GLY:O	1:B:604:THR:N	2.48	0.47
1:B:902:MET:HB3	1:B:916:LEU:HD11	1.95	0.47
1:B:920:GLN:O	1:B:920:GLN:HG3	2.12	0.47
1:C:326:ILE:HG12	1:C:539:VAL:HG21	1.96	0.47
1:C:424:LYS:HE3	1:C:461:LEU:CB	2.44	0.47
1:A:39:PRO:HB3	1:A:53:ASP:CB	2.43	0.47
1:A:569:ILE:HD13	1:B:47:VAL:HG12	1.95	0.47
1:B:337:PRO:HB2	1:B:341:VAL:CG2	2.43	0.47
1:B:726:ILE:C	1:B:727:LEU:HD22	2.39	0.47
1:C:212:LEU:HD13	1:C:215:ASP:H	1.79	0.47
1:C:364:ASP:OD2	1:C:366:SER:OG	2.23	0.47
2:H:72:ASP:OD1	2:H:77:GLN:HG3	2.14	0.47
1:A:469:SER:HB2	1:A:471:GLU:OE2	2.13	0.47
1:A:490:PHE:CD1	1:A:491:PRO:HD2	2.50	0.47
1:A:510:VAL:O	1:A:510:VAL:HG13	2.12	0.47
1:A:555:SER:CB	1:A:586:ASP:H	2.27	0.47
1:A:852:ALA:HA	1:A:855:PHE:CD2	2.49	0.47
1:A:917:TYR:C	1:C:1129:VAL:CG1	2.88	0.47
1:A:1010:GLN:O	1:A:1013:ILE:HG22	2.14	0.47
1:B:659:SER:HB3	1:B:698:SER:HB2	1.96	0.47
1:B:1130:ILE:HG13	1:C:920:GLN:OE1	2.15	0.47
1:C:203:ILE:HB	1:C:227:VAL:HG22	1.95	0.47
2:H:92:VAL:HG12	2:H:113:GLN:HA	1.95	0.47
3:L:37:GLN:N	3:L:47:LEU:CD1	2.64	0.47
3:L:76:SER:OG	3:L:77:SER:N	2.47	0.47
1:A:873:TYR:CE1	1:C:699:LEU:HB3	2.48	0.47
1:B:715:PRO:HA	1:B:1072:GLU:HA	1.96	0.47
1:B:1028:LYS:NZ	1:B:1042:PHE:O	2.48	0.47
1:C:299:THR:OG1	1:C:597:VAL:HG21	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:581:THR:O	1:C:581:THR:OG1	2.24	0.47
1:C:795:LYS:HZ2	1:C:802:PHE:H	1.62	0.47
1:C:886:TRP:CH2	1:C:904:TYR:HD2	2.32	0.47
1:A:318:PHE:C	1:A:319:ARG:HD2	2.39	0.47
1:A:322:PRO:CB	1:A:538:CYS:H	2.21	0.47
1:A:421:TYR:HB3	1:A:454:ARG:HD2	1.95	0.47
1:A:1135:ASN:CG	1:A:1136:THR:H	2.22	0.47
1:B:121:ASN:ND2	1:B:121:ASN:C	2.73	0.47
1:B:519:HIS:ND1	1:B:519:HIS:C	2.72	0.47
1:C:323:THR:OG1	1:C:324:GLU:OE1	2.24	0.47
1:C:494:SER:OG	1:C:495:TYR:N	2.43	0.47
1:C:933:LYS:O	1:C:934:ILE:C	2.56	0.47
1:A:49:HIS:CG	1:A:50:SER:N	2.82	0.47
1:A:91:TYR:HA	1:A:193:VAL:HA	1.97	0.47
1:A:357:ARG:NH2	1:B:230:PRO:HB2	2.29	0.47
1:A:393:THR:CA	1:A:522:ALA:HA	2.44	0.47
1:A:405:ASP:OD1	1:A:405:ASP:N	2.47	0.47
1:A:784:GLN:OE1	1:A:1029:MET:HG2	2.14	0.47
1:B:201:PHE:CD2	1:B:201:PHE:O	2.68	0.47
1:B:337:PRO:HD3	1:B:358:ILE:HG13	1.97	0.47
1:B:337:PRO:CB	1:B:358:ILE:HD11	2.45	0.47
1:B:362:VAL:HA	1:B:525:CYS:H	1.78	0.47
1:B:746:SER:OG	1:B:981:LEU:HD11	2.15	0.47
5:B:1304:NAG:H83	5:B:1304:NAG:H5	1.94	0.47
1:C:195:LYS:HG2	1:C:196:ASN:N	2.30	0.47
1:C:541:PHE:N	1:C:548:GLY:O	2.48	0.47
1:C:922:LEU:HD12	5:C:1301:NAG:O6	2.14	0.47
3:L:13:LEU:O	3:L:107:ARG:N	2.48	0.47
3:L:37:GLN:HG2	3:L:84:ALA:HB3	1.95	0.47
1:A:187:LYS:CB	1:A:210:ILE:O	2.63	0.47
1:A:731:MET:HG3	1:A:955:ASN:ND2	2.22	0.47
1:A:816:SER:N	1:A:819:GLU:OE1	2.37	0.47
1:A:964:LYS:NZ	1:A:965:GLN:OE1	2.29	0.47
1:B:110:LEU:C	1:B:112:SER:N	2.73	0.47
1:B:193:VAL:CG1	1:B:204:TYR:HB2	2.45	0.47
1:B:358:ILE:CG2	1:B:395:VAL:HB	2.45	0.47
1:C:351:TYR:HE1	1:C:453:TYR:CA	2.00	0.47
1:C:905:ARG:NH1	1:C:1049:LEU:O	2.41	0.47
1:C:915:VAL:O	1:C:916:LEU:C	2.57	0.47
1:A:195:LYS:O	1:A:197:ILE:HG12	2.15	0.47
1:A:462:LYS:O	1:A:463:PRO:C	2.58	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:986:PRO:HA	1:A:989:ALA:HB3	1.97	0.47
1:B:327:VAL:N	1:B:531:THR:OG1	2.27	0.47
1:C:93:ALA:HA	1:C:190:ARG:O	2.14	0.47
1:C:197:ILE:HG13	1:C:198:ASP:N	2.29	0.47
1:C:900:MET:HG3	1:C:917:TYR:OH	2.15	0.47
2:H:72:ASP:O	2:H:75:LYS:N	2.48	0.47
3:L:34:ALA:O	3:L:88:CYS:HA	2.14	0.47
1:A:90:VAL:HG21	1:A:238:PHE:CE2	2.49	0.47
1:A:119:ILE:HD11	1:A:126:VAL:HG13	1.97	0.47
1:A:218:GLN:N	1:A:218:GLN:CD	2.72	0.47
1:A:1089:PHE:CE1	1:A:1123:SER:HB3	2.50	0.47
1:B:100:ILE:O	1:B:242:LEU:CB	2.62	0.47
1:B:409:GLN:NE2	1:B:416:GLY:HA3	2.30	0.47
1:B:1142:GLN:N	1:B:1143:PRO:HD2	2.30	0.47
1:C:1134:ASN:OD1	5:C:1302:NAG:C2	2.60	0.47
2:H:18:LEU:N	2:H:82:LEU:O	2.45	0.47
3:L:75:ILE:HD11	3:L:86:TYR:CE2	2.50	0.47
1:A:30:ASN:ND2	1:A:30:ASN:C	2.72	0.46
1:A:399:SER:HB3	1:A:511:VAL:CB	2.45	0.46
1:A:423:TYR:CG	1:A:424:LYS:N	2.83	0.46
1:A:779:GLN:O	1:A:783:ALA:HB3	2.16	0.46
1:A:813:SER:HB3	1:A:815:ARG:NH1	2.30	0.46
1:B:805:ILE:HB	1:B:1054:GLN:NE2	2.30	0.46
1:B:981:LEU:HD23	1:B:981:LEU:HA	1.55	0.46
1:C:940:SER:OG	1:C:942:PRO:HD3	2.15	0.46
3:L:16:GLY:N	3:L:78:LEU:O	2.28	0.46
1:A:196:ASN:ND2	1:A:235:ILE:HD12	2.02	0.46
1:A:806:LEU:HA	1:A:806:LEU:HD12	1.62	0.46
1:B:101:ILE:HG23	1:B:101:ILE:O	2.15	0.46
1:B:360:ASN:C	1:B:524:VAL:HG13	2.40	0.46
1:B:952:VAL:O	1:B:953:ASN:C	2.58	0.46
1:C:128:ILE:HD12	1:C:170:TYR:CD2	2.50	0.46
1:C:455:LEU:HD13	1:C:493:GLN:HE22	1.80	0.46
1:C:484:GLU:HA	1:C:488:CYS:HB3	1.96	0.46
1:C:853:GLN:CD	1:C:854:LYS:N	2.73	0.46
1:C:1036:GLN:O	1:C:1037:SER:C	2.58	0.46
2:H:4:LEU:HD13	2:H:95:CYS:SG	2.56	0.46
1:A:275:PHE:HE2	1:A:290:ASP:OD1	1.99	0.46
1:A:316:SER:CB	1:A:595:VAL:H	2.27	0.46
1:A:364:ASP:C	1:A:366:SER:N	2.74	0.46
1:A:406:GLU:O	1:A:406:GLU:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1043:CYS:O	1:A:1064:HIS:CG	2.68	0.46
1:B:201:PHE:O	1:B:201:PHE:HD2	1.99	0.46
1:B:318:PHE:CD1	1:B:318:PHE:O	2.68	0.46
1:B:714:ILE:O	1:B:1072:GLU:HB2	2.15	0.46
1:B:938:LEU:O	1:B:942:PRO:HD2	2.15	0.46
1:B:946:GLY:C	1:B:948:LEU:N	2.71	0.46
1:C:241:LEU:O	1:C:242:LEU:HD12	2.16	0.46
1:C:707:TYR:CD2	1:C:707:TYR:O	2.69	0.46
1:C:1081:ILE:HG12	1:C:1095:PHE:HD2	1.80	0.46
1:A:99:ASN:N	1:A:99:ASN:ND2	2.63	0.46
1:A:523:THR:HG23	1:A:524:VAL:HG23	1.97	0.46
1:A:564:GLN:CD	1:A:577:ARG:HB3	2.40	0.46
1:A:969:ASN:HA	1:A:975:SER:HB3	1.97	0.46
1:A:1082:CYS:HB2	1:A:1132:ILE:HD11	1.98	0.46
1:B:382:VAL:HG12	1:B:386:LYS:HB3	1.97	0.46
1:B:382:VAL:HG12	1:B:383:SER:N	2.30	0.46
1:B:452:LEU:HD22	1:B:494:SER:HA	1.96	0.46
1:B:903:ALA:HB1	1:B:913:GLN:HG2	1.98	0.46
1:C:62:VAL:HG22	1:C:268:GLY:CA	2.38	0.46
1:C:194:PHE:CD1	1:C:203:ILE:HG12	2.51	0.46
1:C:398:ASP:O	1:C:511:VAL:HG13	2.14	0.46
1:C:455:LEU:HB2	1:C:493:GLN:HE22	1.81	0.46
2:H:39:GLN:HE22	2:H:42:GLY:N	2.13	0.46
1:A:408:ARG:C	1:A:408:ARG:CD	2.85	0.46
1:A:421:TYR:HE1	1:A:459:SER:HA	1.80	0.46
1:A:436:TRP:HD1	1:A:438:SER:HG	1.56	0.46
1:A:708:SER:C	1:A:710:ASN:N	2.73	0.46
1:B:140:PHE:CG	1:B:140:PHE:O	2.68	0.46
1:B:204:TYR:HE1	1:B:225:PRO:HB3	1.80	0.46
1:B:379:CYS:HA	1:B:432:CYS:HA	1.97	0.46
1:B:921:LYS:CE	1:B:921:LYS:CA	2.84	0.46
1:C:186:PHE:HE2	1:C:187:LYS:HE2	1.81	0.46
1:C:409:GLN:OE1	1:C:418:ILE:HB	2.16	0.46
1:C:560:LEU:O	1:C:562:PHE:N	2.48	0.46
1:C:922:LEU:HD22	1:C:922:LEU:C	2.38	0.46
1:C:1072:GLU:CD	1:C:1072:GLU:N	2.73	0.46
3:L:48:ILE:CD1	3:L:73:LEU:HD13	2.45	0.46
1:A:421:TYR:HE1	1:A:459:SER:CA	2.27	0.46
1:A:776:LYS:HE2	1:A:776:LYS:HB3	1.64	0.46
1:A:900:MET:HA	1:A:917:TYR:OH	2.15	0.46
1:B:405:ASP:HB3	1:B:408:ARG:NH1	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:951:VAL:O	1:B:952:VAL:C	2.59	0.46
1:B:1103:PHE:HA	1:B:1115:ILE:HD11	1.97	0.46
1:C:615:VAL:HG12	1:C:616:ASN:O	2.15	0.46
2:H:65:SER:HG	2:H:66:ARG:HH11	1.62	0.46
3:L:4:LEU:HD12	3:L:23:CYS:SG	2.56	0.46
3:L:16:GLY:HA2	3:L:77:SER:OG	2.16	0.46
1:A:556:ASN:ND2	1:A:556:ASN:C	2.73	0.46
1:A:707:TYR:CD2	1:A:707:TYR:O	2.69	0.46
1:A:1091:ARG:HE	1:A:1121:PHE:N	2.14	0.46
1:B:65:PHE:CZ	1:B:265:TYR:CE2	3.04	0.46
1:B:69:HIS:CE1	1:B:80:ASP:CB	2.99	0.46
1:B:187:LYS:CA	1:B:210:ILE:HB	2.46	0.46
1:B:650:LEU:O	1:B:651:ILE:HD13	2.15	0.46
1:B:886:TRP:HH2	1:B:904:TYR:HB3	1.80	0.46
1:B:983:ARG:C	1:B:984:LEU:HD12	2.40	0.46
1:C:65:PHE:HE2	1:C:84:LEU:HD11	1.79	0.46
1:C:188:ASN:N	1:C:210:ILE:HD11	2.30	0.46
1:C:1089:PHE:HE1	1:C:1129:VAL:HG21	1.81	0.46
1:A:278:LYS:HE3	1:A:278:LYS:HB3	1.80	0.46
1:A:350:VAL:HG21	1:A:453:TYR:HB3	1.97	0.46
1:A:1029:MET:HE2	1:A:1062:PHE:CZ	2.51	0.46
1:B:318:PHE:CZ	1:B:615:VAL:HG21	2.44	0.46
1:B:342:PHE:HZ	1:B:434:ILE:HG21	1.79	0.46
1:B:1048:HIS:HA	1:B:1066:THR:HG22	1.98	0.46
1:B:1071:GLN:HB3	1:B:1072:GLU:H	1.61	0.46
1:C:214:ARG:CD	1:C:214:ARG:C	2.85	0.46
1:C:455:LEU:HD22	1:C:493:GLN:NE2	2.31	0.46
1:C:836:GLN:CD	1:C:836:GLN:H	2.24	0.46
1:A:86:PHE:CD1	1:A:86:PHE:O	2.69	0.46
1:A:329:PHE:CE1	1:A:544:ASN:HA	2.51	0.46
1:A:1029:MET:HE2	1:A:1062:PHE:HZ	1.80	0.46
1:A:1141:LEU:HD13	1:C:1141:LEU:HD21	1.98	0.46
1:B:100:ILE:HD12	1:B:242:LEU:HD11	1.98	0.46
1:B:437:ASN:OD1	1:B:438:SER:N	2.48	0.46
1:B:828:LEU:CD2	1:B:952:VAL:HG11	2.46	0.46
1:B:1110:TYR:CZ	1:B:1112:PRO:HD3	2.51	0.46
2:H:14:PRO:HG3	2:H:116:LEU:O	2.16	0.46
2:H:18:LEU:O	2:H:82:LEU:N	2.49	0.46
1:A:91:TYR:CD1	1:A:91:TYR:O	2.68	0.46
1:A:324:GLU:OE1	1:A:537:LYS:NZ	2.41	0.46
1:B:65:PHE:CE2	1:B:82:PRO:HD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:ILE:HD13	1:B:170:TYR:CD2	2.51	0.46
1:B:471:GLU:O	1:B:491:PRO:HD3	2.16	0.46
1:C:96:GLU:HB2	1:C:188:ASN:OD1	2.16	0.46
1:C:197:ILE:HG22	1:C:202:LYS:HZ3	1.81	0.46
1:C:454:ARG:NH1	1:C:491:PRO:HB2	2.31	0.46
1:C:741:TYR:HD2	1:C:1004:LEU:HD11	1.80	0.46
1:C:832:GLY:O	1:C:836:GLN:NE2	2.49	0.46
1:A:138:ASP:OD1	1:A:138:ASP:N	2.49	0.45
1:A:140:PHE:C	1:A:141:LEU:HD12	2.41	0.45
1:A:393:THR:O	1:A:523:THR:CG2	2.57	0.45
1:A:825:LYS:HE2	1:A:825:LYS:HB3	1.79	0.45
1:A:1039:ARG:HD2	1:C:1039:ARG:CD	2.40	0.45
1:B:193:VAL:HG13	1:B:193:VAL:O	2.17	0.45
1:B:265:TYR:O	1:B:267:VAL:HG13	2.15	0.45
1:B:714:ILE:HG12	1:B:715:PRO:CD	2.41	0.45
1:B:722:VAL:HA	1:B:1064:HIS:O	2.15	0.45
1:C:64:TRP:CD1	1:C:64:TRP:O	2.70	0.45
1:C:886:TRP:CD1	1:C:886:TRP:O	2.69	0.45
1:C:916:LEU:HA	1:C:919:ASN:ND2	2.31	0.45
3:L:63:SER:OG	3:L:74:THR:O	2.25	0.45
3:L:89:GLN:HA	3:L:98:GLY:HA2	1.98	0.45
1:A:43:PHE:CZ	1:A:282:ASN:C	2.94	0.45
1:A:68:ILE:O	1:A:68:ILE:HG12	2.16	0.45
1:A:131:CYS:HB3	1:A:164:ASN:O	2.16	0.45
1:A:564:GLN:OE1	1:A:577:ARG:HB3	2.16	0.45
1:A:898:PHE:CE1	1:A:1050:MET:HE1	2.51	0.45
1:B:86:PHE:O	1:B:86:PHE:CG	2.70	0.45
1:B:126:VAL:HG23	1:B:128:ILE:HG13	1.97	0.45
1:B:712:ILE:O	1:C:896:ILE:CG2	2.64	0.45
1:B:718:PHE:CD2	1:B:718:PHE:N	2.82	0.45
1:B:1089:PHE:CE2	1:C:914:ASN:HA	2.50	0.45
1:C:64:TRP:HH2	1:C:214:ARG:HD3	1.80	0.45
1:C:100:ILE:O	1:C:242:LEU:HG	2.17	0.45
1:C:217:PRO:O	1:C:219:GLY:N	2.50	0.45
1:C:564:GLN:OE1	1:C:565:PHE:HB2	2.16	0.45
1:A:38:TYR:CD1	1:A:222:ALA:O	2.70	0.45
1:A:498:GLN:CB	1:A:499:PRO:HD2	2.46	0.45
1:A:542:ASN:O	1:A:543:PHE:C	2.59	0.45
1:A:595:VAL:HG22	1:A:612:TYR:CD1	2.50	0.45
1:A:802:PHE:O	1:A:802:PHE:CD2	2.70	0.45
1:A:1024:LEU:O	1:A:1027:THR:OG1	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:TYR:CE2	1:B:285:ILE:HD12	2.51	0.45
1:B:106:PHE:CE2	1:B:201:PHE:HE1	2.32	0.45
1:B:363:ALA:O	1:B:526:GLY:O	2.33	0.45
1:B:814:LYS:HA	1:B:814:LYS:HD3	1.70	0.45
1:B:887:THR:CG2	1:B:894:LEU:H	2.28	0.45
1:B:971:GLY:H	1:C:755:GLN:CD	2.24	0.45
1:C:714:ILE:CG2	1:C:715:PRO:HD2	2.46	0.45
1:C:714:ILE:HG23	1:C:714:ILE:HD12	1.59	0.45
1:C:720:ILE:HD11	1:C:923:ILE:CD1	2.46	0.45
1:C:736:VAL:HG23	1:C:857:GLY:O	2.17	0.45
1:C:874:THR:HG21	1:C:1055:SER:HB3	1.98	0.45
1:C:894:LEU:H	1:C:894:LEU:CD2	2.02	0.45
2:H:4:LEU:HB3	2:H:95:CYS:SG	2.55	0.45
1:A:140:PHE:CZ	1:A:247:SER:HA	2.51	0.45
1:A:378:LYS:HB2	1:A:433:VAL:HG22	1.98	0.45
1:A:898:PHE:O	1:A:898:PHE:CG	2.69	0.45
1:A:1012:LEU:HD23	1:A:1012:LEU:HA	1.76	0.45
1:B:40:ASP:OD2	1:B:42:VAL:HG12	2.16	0.45
1:B:90:VAL:HG12	1:B:92:PHE:HB3	1.98	0.45
1:C:142:GLY:C	1:C:159:VAL:HG11	2.41	0.45
1:C:290:ASP:HB3	1:C:293:LEU:HG	1.99	0.45
1:C:672:ALA:HA	1:C:693:ILE:O	2.17	0.45
1:A:803:SER:O	1:A:803:SER:OG	2.24	0.45
1:B:57:PRO:HB2	1:B:60:SER:OG	2.16	0.45
1:B:94:SER:HB2	1:B:265:TYR:CB	2.47	0.45
1:B:438:SER:N	1:B:509:ARG:H	2.14	0.45
1:B:710:ASN:OD1	1:B:710:ASN:N	2.48	0.45
1:B:825:LYS:CB	1:B:945:LEU:HD11	2.47	0.45
1:B:996:LEU:HD23	1:B:996:LEU:HA	1.83	0.45
1:C:52:GLN:HG2	1:C:274:THR:OG1	2.17	0.45
1:C:369:TYR:OH	1:C:388:ASN:ND2	2.49	0.45
1:C:569:ILE:H	1:C:569:ILE:HD12	1.80	0.45
1:C:712:ILE:H	1:C:1077:THR:HG23	1.82	0.45
3:L:36:TYR:CA	3:L:47:LEU:HD13	2.47	0.45
3:L:59:PRO:HG2	3:L:61:ARG:NH1	2.32	0.45
1:A:92:PHE:CD2	1:A:92:PHE:O	2.70	0.45
1:A:361:CYS:C	1:A:524:VAL:HG13	2.42	0.45
1:A:624:ILE:HD11	1:A:637:SER:HB2	1.98	0.45
1:A:640:SER:C	1:A:642:VAL:H	2.23	0.45
1:A:667:GLY:O	1:B:864:LEU:HD12	2.16	0.45
1:B:68:ILE:O	1:B:69:HIS:CG	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:ASN:HD22	1:B:361:CYS:HB3	1.82	0.45
1:B:712:ILE:HG23	1:B:1075:PHE:CB	2.43	0.45
1:B:1030:SER:O	1:B:1034:LEU:HB2	2.16	0.45
1:C:83:VAL:HG13	1:C:83:VAL:O	2.17	0.45
1:C:554:GLU:HG3	1:C:555:SER:N	2.29	0.45
1:C:574:ASP:HA	1:C:587:ILE:CG2	2.47	0.45
1:C:718:PHE:CG	1:C:718:PHE:O	2.70	0.45
1:C:935:GLN:O	1:C:939:SER:HB3	2.16	0.45
1:A:82:PRO:HB2	1:A:239:GLN:CB	2.47	0.45
1:B:45:SER:O	1:B:47:VAL:N	2.49	0.45
1:B:122:ASN:ND2	1:B:127:VAL:CG1	2.73	0.45
1:B:140:PHE:CD1	1:B:140:PHE:O	2.70	0.45
1:B:238:PHE:CD1	1:B:238:PHE:O	2.70	0.45
1:B:933:LYS:HA	1:B:936:ASP:OD1	2.16	0.45
1:C:109:THR:O	1:C:237:ARG:NH2	2.48	0.45
1:C:802:PHE:O	1:C:804:GLN:N	2.50	0.45
3:L:56:THR:O	3:L:58:ILE:HD12	2.16	0.45
1:A:63:THR:HG22	1:A:267:VAL:O	2.17	0.45
1:A:621:PRO:HA	1:A:624:ILE:HG12	1.99	0.45
1:B:91:TYR:CD2	1:B:91:TYR:O	2.69	0.45
1:B:334:ASN:ND2	1:B:361:CYS:CA	2.76	0.45
1:B:366:SER:OG	1:B:385:THR:HA	2.16	0.45
1:B:426:PRO:HB2	1:B:428:ASP:OD1	2.17	0.45
1:B:884:SER:O	1:B:887:THR:HG22	2.17	0.45
1:B:988:GLU:HA	1:B:988:GLU:OE1	2.17	0.45
1:C:424:LYS:NZ	1:C:460:ASN:HB2	2.32	0.45
1:C:582:LEU:HA	1:C:582:LEU:HD13	1.58	0.45
1:C:613:GLN:O	1:C:615:VAL:HG23	2.16	0.45
1:C:718:PHE:CD2	1:C:718:PHE:O	2.70	0.45
1:C:818:ILE:HG12	1:C:935:GLN:HG2	1.98	0.45
1:C:886:TRP:HH2	1:C:904:TYR:HD2	1.63	0.45
1:A:84:LEU:O	1:A:237:ARG:CA	2.62	0.45
1:A:391:CYS:HB2	1:A:522:ALA:HB3	1.99	0.45
1:B:714:ILE:CG1	1:B:715:PRO:CD	2.90	0.45
1:B:1130:ILE:H	1:B:1130:ILE:HG12	1.57	0.45
2:H:5:GLN:O	2:H:22:CYS:HA	2.17	0.45
1:A:206:LYS:HZ3	1:A:207:HIS:H	1.65	0.45
1:A:529:LYS:HG3	1:A:530:SER:N	2.27	0.45
1:A:813:SER:OG	1:A:868:GLU:HG3	2.17	0.45
1:A:1018:ILE:HD13	1:A:1018:ILE:HA	1.85	0.45
1:B:346:ARG:HA	1:B:509:ARG:HH22	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:GLN:HB3	1:A:494:SER:H	1.60	0.44
1:B:92:PHE:O	1:B:92:PHE:CG	2.70	0.44
1:B:206:LYS:HG3	1:B:206:LYS:O	2.17	0.44
1:B:346:ARG:NH2	1:B:346:ARG:CG	2.73	0.44
1:B:390:LEU:HG	1:B:392:PHE:CE2	2.52	0.44
1:B:605:SER:OG	1:B:606:ASN:N	2.50	0.44
1:B:825:LYS:HB3	1:B:945:LEU:HD11	1.99	0.44
1:B:969:ASN:CG	1:C:755:GLN:NE2	2.75	0.44
1:C:104:TRP:HE3	1:C:104:TRP:H	1.64	0.44
1:C:365:TYR:O	1:C:368:LEU:HB2	2.17	0.44
1:C:799:GLY:O	1:C:800:PHE:C	2.60	0.44
1:A:84:LEU:CB	1:A:85:PRO:CD	2.95	0.44
1:A:215:ASP:HB3	1:A:216:LEU:HD23	1.99	0.44
1:A:403:ARG:O	1:A:405:ASP:CG	2.60	0.44
1:A:421:TYR:CG	1:A:457:ARG:HB3	2.52	0.44
1:A:577:ARG:HB2	1:A:577:ARG:HH11	1.81	0.44
1:A:612:TYR:OH	1:A:624:ILE:HD13	2.17	0.44
1:A:773:GLU:OE2	1:A:1019:ARG:HD3	2.17	0.44
1:B:83:VAL:HG23	1:B:237:ARG:HG2	1.90	0.44
1:B:454:ARG:HA	1:B:492:LEU:HD23	1.99	0.44
1:B:1004:LEU:HD23	1:B:1004:LEU:HA	1.85	0.44
1:C:794:ILE:HG23	1:C:795:LYS:N	2.31	0.44
1:A:221:SER:O	1:A:223:LEU:N	2.51	0.44
1:A:403:ARG:O	1:A:405:ASP:N	2.45	0.44
1:A:452:LEU:CB	1:A:494:SER:HA	2.48	0.44
1:B:356:LYS:O	1:B:396:TYR:HA	2.17	0.44
1:B:895:GLN:O	1:B:895:GLN:HG2	2.17	0.44
1:B:929:SER:HB2	1:B:933:LYS:HZ2	1.82	0.44
1:B:1012:LEU:HA	1:B:1012:LEU:HD23	1.68	0.44
1:B:1104:VAL:HG12	1:B:1115:ILE:CD1	2.46	0.44
1:C:420:ASP:HA	1:C:424:LYS:NZ	2.32	0.44
3:L:87:TYR:HA	3:L:99:GLN:HB2	1.99	0.44
1:A:54:LEU:HD12	1:A:270:LEU:HD21	2.00	0.44
1:A:282:ASN:C	1:A:284:THR:H	2.26	0.44
1:A:805:ILE:HG22	1:A:1054:GLN:HE21	1.72	0.44
1:A:909:ILE:HD11	1:A:1048:HIS:O	2.18	0.44
1:B:204:TYR:HB3	1:B:223:LEU:HB3	1.99	0.44
1:B:940:SER:OG	1:B:942:PRO:HD3	2.17	0.44
1:C:714:ILE:HA	1:C:714:ILE:HD13	1.57	0.44
1:C:856:ASN:OD1	1:C:856:ASN:O	2.34	0.44
1:C:887:THR:HG23	1:C:894:LEU:HD22	1.96	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1095:PHE:CZ	1:C:1120:THR:HG22	2.52	0.44
3:L:87:TYR:CE2	3:L:101:THR:HG22	2.52	0.44
1:A:131:CYS:HB3	1:A:164:ASN:H	1.81	0.44
1:A:324:GLU:HB2	1:A:537:LYS:HE2	1.98	0.44
1:A:340:GLU:O	1:A:344:ALA:N	2.50	0.44
1:A:823:PHE:HD1	1:A:1057:PRO:HD3	1.83	0.44
1:A:906:PHE:CD2	1:A:911:VAL:HG21	2.52	0.44
1:B:457:ARG:HG2	1:B:458:LYS:N	2.32	0.44
1:C:358:ILE:HG23	1:C:524:VAL:CG2	2.48	0.44
1:C:802:PHE:C	1:C:804:GLN:H	2.26	0.44
1:C:885:GLY:HA2	1:C:901:GLN:NE2	2.31	0.44
1:A:417:LYS:HZ1	1:A:421:TYR:HB2	1.82	0.44
1:A:435:ALA:CB	1:A:510:VAL:HG23	2.36	0.44
1:A:559:PHE:CD1	1:A:584:ILE:CG1	3.01	0.44
1:A:597:VAL:O	1:A:597:VAL:HG13	2.16	0.44
1:A:1027:THR:O	1:A:1028:LYS:C	2.59	0.44
1:B:349:SER:HB3	1:B:452:LEU:O	2.18	0.44
1:C:216:LEU:CG	1:C:266:TYR:OH	2.66	0.44
1:C:365:TYR:HE2	1:C:392:PHE:CE1	2.35	0.44
1:C:802:PHE:HZ	1:C:898:PHE:CE2	2.36	0.44
2:H:99:GLN:HE22	2:H:103:ARG:HH21	1.66	0.44
1:A:86:PHE:HE1	1:A:90:VAL:H	1.66	0.44
1:A:231:ILE:HD12	1:A:232:GLY:H	1.81	0.44
1:A:324:GLU:HG2	1:A:325:SER:H	1.82	0.44
1:A:570:ALA:C	1:A:572:THR:H	2.24	0.44
1:B:189:LEU:HG	1:B:210:ILE:CG1	2.47	0.44
1:B:436:TRP:CD1	1:B:437:ASN:N	2.86	0.44
1:B:466:ARG:O	1:B:466:ARG:HD3	2.18	0.44
1:C:62:VAL:CG1	1:C:267:VAL:C	2.78	0.44
1:C:795:LYS:NZ	1:C:802:PHE:H	2.16	0.44
2:H:92:VAL:HG12	2:H:112:GLY:O	2.17	0.44
4:D:2:NAG:H5	4:D:2:NAG:HN2	1.83	0.44
1:B:941:THR:N	1:B:942:PRO:CD	2.80	0.44
1:C:112:SER:OG	1:C:134:GLN:HA	2.18	0.44
1:C:404:GLY:HA2	1:C:508:TYR:CD2	2.53	0.44
1:C:557:LYS:HE2	1:C:559:PHE:CZ	2.52	0.44
1:A:391:CYS:HB2	1:A:522:ALA:CB	2.48	0.44
1:A:563:GLN:NE2	1:B:43:PHE:HD1	2.16	0.44
1:A:801:ASN:H	1:A:928:ASN:ND2	2.15	0.44
1:B:62:VAL:CG2	1:B:64:TRP:HZ3	2.31	0.44
1:B:91:TYR:O	1:B:91:TYR:HD2	2.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:452:LEU:CD2	1:B:494:SER:HA	2.48	0.44
1:B:529:LYS:HA	1:B:529:LYS:HZ3	1.72	0.44
1:C:379:CYS:C	1:C:380:TYR:HD1	2.26	0.44
1:C:755:GLN:CD	1:C:755:GLN:C	2.86	0.44
1:C:948:LEU:HD23	1:C:948:LEU:HA	1.80	0.44
1:A:38:TYR:CE2	1:A:285:ILE:HD11	2.52	0.43
1:A:233:ILE:HD12	1:A:234:ASN:H	1.81	0.43
1:A:426:PRO:HD3	1:A:463:PRO:HB3	2.00	0.43
1:A:705:VAL:HG21	1:B:883:THR:OG1	2.18	0.43
1:A:1025:ALA:O	1:A:1026:ALA:C	2.61	0.43
1:A:1031:GLU:OE2	1:C:1039:ARG:HD2	2.18	0.43
1:B:31:SER:O	1:B:32:PHE:C	2.60	0.43
1:B:121:ASN:HA	1:B:126:VAL:HA	1.99	0.43
1:B:360:ASN:O	1:B:524:VAL:HG12	2.18	0.43
1:B:360:ASN:HB3	1:B:523:THR:HG22	2.00	0.43
1:B:708:SER:OG	1:B:710:ASN:OD1	2.36	0.43
1:B:729:VAL:HG12	1:B:1058:HIS:C	2.43	0.43
1:A:215:ASP:HB3	1:A:216:LEU:H	1.55	0.43
1:A:393:THR:C	1:A:523:THR:HG22	2.43	0.43
1:A:451:TYR:CB	1:A:495:TYR:CB	2.76	0.43
1:B:100:ILE:HB	1:B:242:LEU:HD12	2.00	0.43
1:B:562:PHE:CE2	1:C:225:PRO:HD2	2.53	0.43
1:B:715:PRO:CA	1:B:1072:GLU:HB2	2.45	0.43
1:B:724:THR:OG1	1:B:934:ILE:HD12	2.18	0.43
1:B:1077:THR:OG1	1:B:1078:ALA:N	2.52	0.43
1:C:64:TRP:CH2	1:C:214:ARG:O	2.71	0.43
1:C:191:GLU:OE1	1:C:191:GLU:N	2.50	0.43
1:C:244:LEU:HD12	1:C:246:ARG:H	1.82	0.43
1:C:743:CYS:HB3	1:C:749:CYS:HB3	1.83	0.43
2:H:22:CYS:HB2	2:H:36:TRP:CH2	2.53	0.43
4:N:2:NAG:H5	4:N:2:NAG:HN2	1.83	0.43
1:A:408:ARG:HD2	1:A:409:GLN:N	2.33	0.43
1:A:425:LEU:HD11	1:A:429:PHE:CD1	2.53	0.43
1:A:462:LYS:N	1:A:462:LYS:HD3	2.32	0.43
1:A:612:TYR:CD1	1:A:612:TYR:N	2.86	0.43
1:A:892:PRO:HG2	1:A:894:LEU:HD21	2.00	0.43
1:A:1097:SER:HB2	1:A:1102:TRP:CD2	2.54	0.43
1:B:295:PRO:O	1:B:298:GLU:N	2.51	0.43
1:B:1141:LEU:HD22	1:C:1141:LEU:HD11	1.99	0.43
1:C:98:SER:H	1:C:100:ILE:HG12	1.84	0.43
1:C:204:TYR:CD2	1:C:225:PRO:HA	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:ASP:CG	1:A:421:TYR:N	2.77	0.43
1:A:470:THR:OG1	1:A:490:PHE:HE1	2.02	0.43
1:A:874:THR:HG21	1:A:1055:SER:HB2	2.00	0.43
1:B:712:ILE:HG23	1:B:1075:PHE:H	1.83	0.43
1:B:878:LEU:O	1:B:882:ILE:HG12	2.19	0.43
1:C:553:THR:HG23	1:C:554:GLU:N	2.33	0.43
1:C:910:GLY:O	1:C:911:VAL:HG23	2.18	0.43
1:C:1048:HIS:NE2	1:C:1050:MET:C	2.77	0.43
1:A:96:GLU:CB	1:A:99:ASN:HA	2.49	0.43
1:A:1075:PHE:CZ	1:A:1110:TYR:CE2	3.01	0.43
1:A:1139:ASP:O	1:A:1143:PRO:HG2	2.19	0.43
1:B:34:ARG:HH22	1:B:220:PHE:HA	1.84	0.43
1:B:282:ASN:CG	5:B:1306:NAG:O5	2.55	0.43
1:B:324:GLU:CD	1:B:325:SER:H	2.27	0.43
1:B:346:ARG:HA	1:B:509:ARG:NH2	2.33	0.43
1:B:434:ILE:HD11	1:B:513:LEU:HD12	2.01	0.43
1:B:497:PHE:CE2	1:B:507:PRO:CB	2.79	0.43
1:B:865:LEU:HD22	1:B:869:MET:HE2	1.99	0.43
1:B:1078:ALA:CB	1:B:1133:VAL:CG2	2.97	0.43
1:C:64:TRP:C	1:C:64:TRP:HD1	2.27	0.43
1:C:106:PHE:HB3	1:C:235:ILE:HD13	1.99	0.43
1:C:741:TYR:CE2	1:C:1004:LEU:HG	2.53	0.43
1:C:795:LYS:HE2	1:C:795:LYS:HB3	1.64	0.43
1:C:801:ASN:OD1	1:C:801:ASN:C	2.62	0.43
2:H:4:LEU:HD23	2:H:24:VAL:HA	1.99	0.43
1:A:717:ASN:HD22	1:A:1071:GLN:HE22	1.66	0.43
1:A:922:LEU:HD11	1:A:926:GLN:HE21	1.84	0.43
1:A:1142:GLN:O	1:A:1145:LEU:HB2	2.18	0.43
1:B:971:GLY:N	1:C:755:GLN:OE1	2.51	0.43
1:B:973:ILE:HD11	1:B:984:LEU:HD11	2.00	0.43
1:C:714:ILE:HG23	1:C:1109:PHE:O	2.12	0.43
1:A:339:GLY:O	1:A:343:ASN:OD1	2.36	0.43
1:A:626:ALA:HA	1:A:629:LEU:HG	2.00	0.43
1:B:46:SER:HA	1:B:280:ASN:C	2.44	0.43
1:B:129:LYS:HG2	1:B:169:GLU:OE2	2.17	0.43
1:B:273:ARG:HD3	1:B:273:ARG:HA	1.22	0.43
1:B:714:ILE:HG13	1:B:1107:ARG:O	2.18	0.43
1:B:756:TYR:OH	1:B:994:ASP:OD1	2.34	0.43
1:B:767:LEU:HD23	1:B:767:LEU:HA	1.68	0.43
1:B:1019:ARG:HA	1:B:1019:ARG:HD2	1.86	0.43
1:B:1078:ALA:HB2	1:B:1102:TRP:CZ3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1141:LEU:O	1:B:1145:LEU:HB2	2.19	0.43
1:C:718:PHE:HB3	1:C:1067:TYR:OH	2.19	0.43
2:H:66:ARG:HD3	2:H:66:ARG:N	2.33	0.43
1:A:454:ARG:HH12	1:A:469:SER:HG	1.60	0.43
1:A:564:GLN:NE2	1:A:577:ARG:HB3	2.33	0.43
1:A:589:PRO:O	1:A:590:CYS:C	2.61	0.43
1:A:755:GLN:OE1	1:C:971:GLY:N	2.52	0.43
1:B:117:LEU:HA	1:B:117:LEU:HD13	1.58	0.43
1:B:290:ASP:CG	1:B:291:CYS:H	2.26	0.43
1:B:642:VAL:HG22	1:B:651:ILE:HD12	1.99	0.43
1:B:1006:THR:O	1:B:1010:GLN:HG2	2.18	0.43
1:C:190:ARG:HB3	1:C:192:PHE:CE1	2.54	0.43
1:C:407:VAL:HG11	1:C:508:TYR:HD2	1.82	0.43
1:C:501:ASN:O	1:C:506:GLN:NE2	2.51	0.43
1:C:529:LYS:HG3	1:C:530:SER:N	2.30	0.43
1:C:988:GLU:O	1:C:989:ALA:C	2.61	0.43
1:C:1049:LEU:HD23	1:C:1049:LEU:HA	1.68	0.43
1:A:171:VAL:HG22	1:A:172:SER:H	1.83	0.43
1:A:392:PHE:HA	1:A:517:LEU:HD23	2.01	0.43
1:A:629:LEU:H	1:A:634:ARG:NH1	2.16	0.43
1:A:825:LYS:CB	1:A:945:LEU:HD11	2.49	0.43
1:B:65:PHE:CE2	1:B:265:TYR:CZ	3.06	0.43
1:B:106:PHE:CE2	1:B:201:PHE:CE1	3.07	0.43
1:B:116:SER:HB3	1:B:117:LEU:H	1.65	0.43
1:B:458:LYS:HE2	1:B:471:GLU:OE1	2.18	0.43
1:B:1049:LEU:HD23	1:B:1049:LEU:HA	1.79	0.43
1:B:1082:CYS:HB3	1:B:1134:ASN:CB	2.39	0.43
1:B:1082:CYS:HA	1:B:1086:LYS:O	2.19	0.43
1:C:141:LEU:HG	1:C:142:GLY:H	1.84	0.43
1:C:165:ASN:O	1:C:165:ASN:ND2	2.52	0.43
1:A:43:PHE:CD1	1:C:563:GLN:OE1	2.71	0.43
1:A:296:LEU:HB2	1:A:608:VAL:HG11	2.01	0.43
1:A:322:PRO:HG2	1:A:538:CYS:CB	2.49	0.43
1:A:356:LYS:HE3	1:A:358:ILE:HD13	2.01	0.43
1:A:360:ASN:HA	1:A:523:THR:O	2.18	0.43
1:A:533:LEU:HD12	1:A:541:PHE:CA	2.43	0.43
1:A:626:ALA:HA	1:A:629:LEU:CD1	2.49	0.43
1:A:705:VAL:HG21	1:B:883:THR:CB	2.49	0.43
1:B:210:ILE:CG2	1:B:212:LEU:HB2	2.48	0.43
1:B:249:LEU:HD23	1:B:249:LEU:O	2.18	0.43
1:B:271:GLN:HG3	1:B:272:PRO:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1017:GLU:OE1	1:B:1017:GLU:HA	2.19	0.43
1:C:294:ASP:N	1:C:294:ASP:OD1	2.51	0.43
1:C:409:GLN:NE2	1:C:416:GLY:O	2.52	0.43
1:C:798:GLY:O	1:C:800:PHE:N	2.47	0.43
1:C:802:PHE:O	1:C:803:SER:C	2.61	0.43
1:A:513:LEU:HD12	1:A:513:LEU:HA	1.61	0.42
1:A:633:TRP:O	1:A:637:SER:N	2.52	0.42
1:A:764:ASN:O	1:A:768:THR:HG23	2.19	0.42
1:A:917:TYR:O	1:C:1129:VAL:CG1	2.66	0.42
1:A:929:SER:HB2	1:A:933:LYS:NZ	2.34	0.42
1:A:965:GLN:C	1:A:967:SER:H	2.27	0.42
1:B:46:SER:HA	1:B:280:ASN:CA	2.49	0.42
1:C:318:PHE:HZ	1:C:615:VAL:HG21	1.83	0.42
1:C:542:ASN:CG	1:C:547:THR:HG22	2.44	0.42
1:C:597:VAL:HG12	1:C:610:VAL:HG12	2.02	0.42
1:C:947:LYS:HE2	1:C:947:LYS:HB3	1.86	0.42
2:H:94:TYR:CD2	2:H:111:TRP:HA	2.54	0.42
2:H:113:GLN:OE1	2:H:115:THR:OG1	2.21	0.42
1:A:273:ARG:HG3	1:A:275:PHE:CZ	2.54	0.42
1:A:850:ILE:HA	1:A:853:GLN:HE22	1.83	0.42
1:A:872:GLN:HG2	1:C:699:LEU:HD12	2.02	0.42
1:A:1049:LEU:HB2	1:A:1065:VAL:HG23	2.01	0.42
1:A:1130:ILE:HG12	1:B:920:GLN:OE1	2.19	0.42
1:B:226:LEU:HD12	1:B:227:VAL:HG13	2.01	0.42
1:B:878:LEU:HD23	1:B:878:LEU:HA	1.80	0.42
1:B:933:LYS:O	1:B:934:ILE:C	2.62	0.42
1:C:625:HIS:HB2	1:C:629:LEU:HD13	2.01	0.42
1:A:393:THR:HA	1:A:523:THR:N	2.34	0.42
1:A:727:LEU:HA	1:A:728:PRO:HD3	1.93	0.42
1:A:855:PHE:HB3	1:C:589:PRO:CG	2.46	0.42
1:A:1144:GLU:O	1:A:1146:ASP:N	2.52	0.42
1:B:35:GLY:HA3	1:B:56:LEU:HB3	2.00	0.42
1:B:129:LYS:NZ	1:B:161:SER:OG	2.47	0.42
1:B:712:ILE:CG2	1:B:1075:PHE:O	2.55	0.42
1:B:972:ALA:HA	1:B:995:ARG:CZ	2.49	0.42
1:C:66:HIS:O	1:C:66:HIS:CG	2.69	0.42
1:C:1031:GLU:HB3	1:C:1037:SER:HB2	2.00	0.42
1:C:1097:SER:CB	1:C:1102:TRP:CA	2.97	0.42
2:H:24:VAL:H	2:H:77:GLN:CB	2.33	0.42
3:L:18:ARG:HA	3:L:76:SER:O	2.19	0.42
1:A:62:VAL:HB	1:A:63:THR:H	1.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:740:MET:HB2	1:C:319:ARG:HH21	1.84	0.42
1:A:825:LYS:HB3	1:A:945:LEU:CD1	2.49	0.42
1:A:912:THR:O	1:A:913:GLN:C	2.61	0.42
1:B:122:ASN:ND2	1:B:127:VAL:HG11	2.33	0.42
1:B:335:LEU:HD23	1:B:335:LEU:HA	1.88	0.42
1:B:718:PHE:O	1:B:718:PHE:CG	2.71	0.42
1:B:913:GLN:O	1:B:914:ASN:C	2.61	0.42
1:B:942:PRO:O	1:B:943:SER:C	2.63	0.42
1:C:104:TRP:N	1:C:104:TRP:CE3	2.87	0.42
1:C:122:ASN:C	1:C:124:THR:H	2.27	0.42
1:C:431:GLY:HA3	1:C:513:LEU:O	2.20	0.42
1:C:911:VAL:O	1:C:911:VAL:HG12	2.19	0.42
2:H:33:PHE:HD1	2:H:52:ASN:CA	2.32	0.42
3:L:34:ALA:HA	3:L:49:TYR:HA	2.01	0.42
1:A:277:LEU:HD12	1:A:285:ILE:HG23	2.01	0.42
1:A:564:GLN:NE2	1:A:577:ARG:H	2.17	0.42
1:A:748:GLU:O	1:A:752:LEU:HD23	2.20	0.42
1:A:797:PHE:C	1:A:799:GLY:N	2.77	0.42
1:B:754:LEU:HD23	1:B:754:LEU:HA	1.82	0.42
1:B:857:GLY:O	1:B:859:THR:HG23	2.19	0.42
1:B:1011:GLN:OE1	1:B:1014:ARG:NH1	2.52	0.42
1:C:58:PHE:CD2	1:C:290:ASP:HB2	2.55	0.42
1:C:205:SER:HA	1:C:223:LEU:HD23	2.01	0.42
1:C:917:TYR:HB2	1:C:918:GLU:OE1	2.20	0.42
3:L:36:TYR:HE2	3:L:44:PRO:HG3	1.84	0.42
1:A:298:GLU:O	1:A:301:CYS:HB2	2.19	0.42
1:A:402:ILE:HG12	1:A:404:GLY:H	1.85	0.42
1:A:894:LEU:HD12	1:C:713:ALA:HB3	2.01	0.42
1:A:1013:ILE:HA	1:A:1013:ILE:HD12	1.82	0.42
1:B:168:PHE:CD2	1:B:231:ILE:HD11	2.54	0.42
1:C:529:LYS:CG	1:C:530:SER:H	2.29	0.42
2:H:99:GLN:CD	2:H:103:ARG:HB2	2.44	0.42
1:A:280:ASN:ND2	1:A:284:THR:HB	2.18	0.42
1:A:406:GLU:CD	1:A:406:GLU:N	2.72	0.42
1:A:602:THR:HG23	1:A:603:ASN:N	2.34	0.42
1:A:898:PHE:HZ	1:A:1050:MET:HE1	1.84	0.42
1:B:130:VAL:HG23	1:B:168:PHE:O	2.20	0.42
1:B:295:PRO:HG2	1:B:636:TYR:CD2	2.53	0.42
1:B:1073:LYS:NZ	1:B:1073:LYS:HB3	2.32	0.42
1:C:328:ARG:HA	1:C:580:GLN:HG2	2.01	0.42
1:C:355:ARG:NE	1:C:396:TYR:HB2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:503:VAL:HA	1:C:506:GLN:OE1	2.20	0.42
1:C:718:PHE:CB	1:C:1067:TYR:HE1	2.28	0.42
1:C:1072:GLU:N	1:C:1072:GLU:OE1	2.52	0.42
2:H:98:GLY:CA	2:H:105:LEU:HD23	2.40	0.42
1:A:572:THR:O	1:A:574:ASP:N	2.53	0.42
1:A:990:GLU:CD	1:A:990:GLU:C	2.87	0.42
1:A:1039:ARG:HD3	1:A:1042:PHE:CD2	2.54	0.42
1:A:1080:ALA:O	1:A:1132:ILE:HG13	2.19	0.42
1:B:38:TYR:CG	1:B:285:ILE:CD1	3.00	0.42
1:C:240:THR:HG22	1:C:241:LEU:H	1.83	0.42
1:C:277:LEU:HD23	1:C:288:ALA:HB2	2.02	0.42
1:C:357:ARG:HH12	1:C:359:SER:HB3	1.84	0.42
1:C:391:CYS:HA	1:C:525:CYS:HA	2.01	0.42
1:C:605:SER:OG	1:C:606:ASN:N	2.53	0.42
1:C:1049:LEU:HB2	1:C:1065:VAL:O	2.19	0.42
3:L:15:PRO:HA	3:L:78:LEU:HB3	2.00	0.42
1:A:86:PHE:HD1	1:A:90:VAL:CG1	2.27	0.42
1:A:92:PHE:HE1	1:A:265:TYR:HB2	1.82	0.42
1:A:299:THR:OG1	1:A:300:LYS:N	2.52	0.42
1:A:303:LEU:CD2	1:A:305:SER:HB3	2.49	0.42
1:A:326:ILE:CD1	1:A:533:LEU:HD22	2.49	0.42
1:A:486:PHE:HD1	1:A:487:ASN:ND2	2.18	0.42
1:A:755:GLN:NE2	1:A:755:GLN:O	2.52	0.42
1:B:37:TYR:CD2	1:B:204:TYR:HD2	2.37	0.42
1:B:38:TYR:CE1	1:B:285:ILE:CG1	3.03	0.42
1:B:186:PHE:HE1	1:B:214:ARG:HG3	1.84	0.42
1:B:379:CYS:HA	1:B:432:CYS:CB	2.50	0.42
1:B:885:GLY:HA2	1:B:901:GLN:NE2	2.35	0.42
1:B:988:GLU:O	1:B:989:ALA:C	2.63	0.42
1:C:130:VAL:O	1:C:130:VAL:HG22	2.19	0.42
1:C:402:ILE:HD11	1:C:407:VAL:HG12	2.01	0.42
1:C:720:ILE:HD11	1:C:923:ILE:HD12	2.02	0.42
2:H:43:LYS:HG3	2:H:44:GLY:N	2.30	0.42
2:H:66:ARG:NE	2:H:84:SER:O	2.53	0.42
1:A:109:THR:HG21	1:A:113:LYS:NZ	2.35	0.42
1:A:594:GLY:O	1:A:613:GLN:HG2	2.20	0.42
1:A:755:GLN:C	1:A:755:GLN:CD	2.88	0.42
1:A:806:LEU:HD12	1:A:878:LEU:HD22	2.02	0.42
1:B:211:ASN:C	1:B:212:LEU:HD22	2.45	0.42
1:B:218:GLN:OE1	1:B:218:GLN:N	2.53	0.42
1:B:343:ASN:ND2	5:B:1304:NAG:O6	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1103:PHE:CA	1:B:1115:ILE:HD11	2.49	0.42
1:C:64:TRP:HH2	1:C:214:ARG:O	2.03	0.42
1:C:89:GLY:HA3	1:C:270:LEU:HD12	2.01	0.42
1:C:336:CYS:SG	1:C:358:ILE:HD11	2.60	0.42
1:C:1036:GLN:HG2	1:C:1048:HIS:O	2.20	0.42
3:L:36:TYR:CA	3:L:47:LEU:HD22	2.47	0.42
1:A:100:ILE:HG22	1:A:243:ALA:N	2.35	0.41
1:A:303:LEU:CD1	1:A:308:VAL:HG23	2.50	0.41
1:A:357:ARG:NH1	1:A:357:ARG:CG	2.81	0.41
1:A:362:VAL:O	1:A:363:ALA:C	2.63	0.41
1:A:365:TYR:O	1:A:368:LEU:N	2.52	0.41
1:A:378:LYS:HB2	1:A:433:VAL:CG2	2.50	0.41
1:A:390:LEU:H	1:A:390:LEU:CD2	2.30	0.41
1:A:1039:ARG:HB2	1:A:1042:PHE:HB3	2.00	0.41
1:A:1105:THR:OG1	1:A:1106:GLN:N	2.53	0.41
1:B:128:ILE:HB	1:B:170:TYR:O	2.20	0.41
1:B:206:LYS:O	1:B:206:LYS:CG	2.68	0.41
1:B:300:LYS:HG3	1:B:308:VAL:CG2	2.50	0.41
1:B:353:TRP:HZ3	1:B:355:ARG:HD2	1.85	0.41
1:B:455:LEU:N	1:B:491:PRO:O	2.53	0.41
1:B:770:ILE:HD11	1:B:1012:LEU:HD23	2.02	0.41
1:C:203:ILE:O	1:C:226:LEU:HB3	2.20	0.41
1:A:97:LYS:HB2	1:A:186:PHE:HD1	1.85	0.41
1:A:295:PRO:O	1:A:296:LEU:C	2.63	0.41
1:A:350:VAL:CG2	1:A:453:TYR:HB3	2.50	0.41
1:A:565:PHE:HB3	1:A:576:VAL:HG23	2.01	0.41
1:A:887:THR:C	1:A:889:GLY:H	2.27	0.41
1:A:1075:PHE:CD2	1:A:1096:VAL:CG1	3.03	0.41
1:A:1078:ALA:HB2	1:A:1102:TRP:CH2	2.55	0.41
1:A:1104:VAL:HG13	1:A:1104:VAL:O	2.20	0.41
1:B:366:SER:HA	1:B:369:TYR:HB3	2.01	0.41
1:B:800:PHE:CE1	1:B:898:PHE:HE2	2.37	0.41
1:C:276:LEU:O	1:C:288:ALA:HA	2.20	0.41
1:C:337:PRO:C	1:C:339:GLY:N	2.78	0.41
1:C:1089:PHE:CZ	1:C:1129:VAL:HG21	2.56	0.41
2:H:57:THR:OG1	2:H:69:ILE:HG23	2.20	0.41
2:H:117:VAL:HG12	2:H:119:VAL:N	2.29	0.41
1:A:748:GLU:HG2	1:A:749:CYS:N	2.35	0.41
1:A:1082:CYS:HB2	1:A:1132:ILE:CD1	2.50	0.41
1:B:57:PRO:HB3	1:B:273:ARG:NH2	2.19	0.41
1:B:909:ILE:HD13	1:B:909:ILE:HA	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:914:ASN:OD1	1:B:914:ASN:N	2.52	0.41
1:B:944:ALA:C	1:B:946:GLY:N	2.79	0.41
1:B:1139:ASP:HB3	1:B:1142:GLN:HB2	2.01	0.41
1:C:840:CYS:HB2	1:C:851:CYS:O	2.20	0.41
2:H:7:TRP:CE3	2:H:21:THR:OG1	2.70	0.41
3:L:14:SER:C	3:L:78:LEU:HD23	2.45	0.41
3:L:20:THR:HB	3:L:74:THR:HA	2.02	0.41
1:A:87:ASN:OD1	1:A:87:ASN:N	2.51	0.41
1:B:445:VAL:HG13	1:B:499:PRO:HG3	2.02	0.41
1:B:800:PHE:CZ	1:B:898:PHE:HE2	2.39	0.41
1:B:903:ALA:O	1:B:904:TYR:C	2.63	0.41
1:B:909:ILE:HD11	1:B:1048:HIS:O	2.19	0.41
1:B:1045:LYS:HE3	1:C:889:GLY:O	2.20	0.41
1:C:270:LEU:O	1:C:271:GLN:HG3	2.20	0.41
1:A:54:LEU:HA	1:A:273:ARG:O	2.21	0.41
1:B:293:LEU:O	1:B:632:THR:OG1	2.27	0.41
1:B:712:ILE:O	1:C:896:ILE:HG23	2.21	0.41
1:B:938:LEU:HD23	1:B:938:LEU:HA	1.80	0.41
1:C:457:ARG:CZ	1:C:461:LEU:HD23	2.51	0.41
1:C:491:PRO:HG2	1:C:492:LEU:HD12	2.03	0.41
1:C:559:PHE:HD2	1:C:563:GLN:HB3	1.86	0.41
1:C:715:PRO:CD	1:C:1108:ASN:O	2.67	0.41
1:C:720:ILE:HD13	1:C:720:ILE:HG21	1.75	0.41
1:C:785:VAL:HG11	1:C:888:PHE:CE2	2.53	0.41
1:C:909:ILE:HD13	1:C:909:ILE:HA	1.79	0.41
2:H:20:LEU:HD11	2:H:93:TYR:CD2	2.56	0.41
1:A:48:LEU:CD2	1:A:278:LYS:HG3	2.51	0.41
1:A:386:LYS:HZ2	1:B:984:LEU:N	2.19	0.41
1:A:760:CYS:CB	1:A:763:LEU:HD22	2.51	0.41
1:A:1109:PHE:O	1:A:1110:TYR:C	2.64	0.41
1:B:168:PHE:O	1:B:170:TYR:N	2.51	0.41
1:B:235:ILE:O	1:B:235:ILE:HG22	2.20	0.41
1:B:409:GLN:HE22	1:B:416:GLY:HA3	1.86	0.41
1:B:421:TYR:CD1	1:B:457:ARG:HB3	2.55	0.41
1:B:457:ARG:NH1	1:B:459:SER:C	2.78	0.41
1:C:277:LEU:HB3	1:C:285:ILE:HD12	2.03	0.41
1:A:31:SER:CB	1:A:216:LEU:HD21	2.51	0.41
1:A:308:VAL:H	1:A:602:THR:HB	1.85	0.41
1:A:458:LYS:HG3	1:A:459:SER:N	2.35	0.41
1:A:461:LEU:C	1:A:462:LYS:HD3	2.46	0.41
1:A:560:LEU:N	1:A:563:GLN:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:912:THR:O	1:A:914:ASN:N	2.53	0.41
1:A:1072:GLU:HB3	1:A:1073:LYS:H	1.72	0.41
1:C:392:PHE:HD2	1:C:515:PHE:CD2	2.38	0.41
1:C:560:LEU:O	1:C:561:PRO:C	2.63	0.41
1:C:792:PRO:O	1:C:793:PRO:C	2.64	0.41
1:A:363:ALA:O	1:A:365:TYR:N	2.52	0.41
1:A:1038:LYS:HE2	1:A:1038:LYS:HB2	1.44	0.41
1:B:80:ASP:OD1	1:B:80:ASP:N	2.54	0.41
1:C:200:TYR:HB2	1:C:202:LYS:HZ2	1.86	0.41
1:C:900:MET:HE3	1:C:900:MET:HB2	1.80	0.41
1:C:1091:ARG:HG3	1:C:1092:GLU:OE1	2.21	0.41
1:A:472:ILE:HA	1:A:489:TYR:O	2.21	0.41
1:A:476:GLY:N	1:A:487:ASN:HB3	2.36	0.41
1:A:562:PHE:O	1:B:41:LYS:HE2	2.21	0.41
1:A:592:PHE:CE1	1:A:624:ILE:HA	2.56	0.41
1:A:854:LYS:O	1:A:856:ASN:N	2.46	0.41
1:A:883:THR:HG1	1:C:707:TYR:CB	2.34	0.41
1:A:896:ILE:HG12	1:C:712:ILE:HD13	1.98	0.41
1:A:1034:LEU:HD12	1:A:1034:LEU:C	2.46	0.41
1:B:58:PHE:CE1	1:B:275:PHE:CE2	3.09	0.41
1:B:97:LYS:HB2	1:B:100:ILE:HG12	2.03	0.41
1:B:171:VAL:HG12	1:B:172:SER:N	2.33	0.41
1:B:292:ALA:C	1:B:633:TRP:HE1	2.29	0.41
1:B:386:LYS:HE2	1:B:386:LYS:HB2	1.88	0.41
1:B:423:TYR:CE1	1:B:425:LEU:HD23	2.55	0.41
1:B:736:VAL:CG2	1:B:858:LEU:CD2	2.99	0.41
1:B:950:ASP:N	1:B:950:ASP:OD1	2.53	0.41
1:B:966:LEU:HA	1:B:966:LEU:HD23	1.70	0.41
1:B:1073:LYS:HB3	1:B:1073:LYS:HE2	1.78	0.41
1:C:266:TYR:CD1	1:C:266:TYR:O	2.74	0.41
1:C:294:ASP:O	1:C:295:PRO:C	2.64	0.41
1:C:573:THR:O	1:C:587:ILE:HG21	2.21	0.41
1:C:715:PRO:O	1:C:715:PRO:CG	2.69	0.41
1:C:884:SER:HB3	1:C:888:PHE:CB	2.51	0.41
1:C:1095:PHE:HZ	1:C:1120:THR:HG22	1.83	0.41
2:H:66:ARG:HH21	2:H:85:VAL:CA	2.31	0.41
3:L:25:ALA:N	3:L:69:THR:O	2.46	0.41
1:A:280:ASN:CG	1:A:281:GLU:H	2.29	0.41
1:A:329:PHE:CE1	1:A:391:CYS:SG	3.14	0.41
1:A:345:THR:O	1:A:346:ARG:HD2	2.21	0.41
1:A:425:LEU:HD12	1:A:425:LEU:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:GLU:OE2	1:A:484:GLU:N	2.53	0.41
1:A:660:TYR:HB2	1:A:695:TYR:CZ	2.56	0.41
1:A:767:LEU:HD23	1:A:770:ILE:HD12	2.02	0.41
1:A:894:LEU:HD12	1:C:713:ALA:CB	2.51	0.41
1:B:37:TYR:HD2	1:B:204:TYR:CD2	2.38	0.41
1:B:337:PRO:HB3	1:B:358:ILE:HD11	2.03	0.41
1:B:554:GLU:N	1:B:554:GLU:OE1	2.54	0.41
1:B:726:ILE:HD13	1:B:944:ALA:HB1	2.03	0.41
1:C:712:ILE:O	1:C:712:ILE:HG23	2.19	0.41
1:C:822:LEU:CD1	1:C:945:LEU:HD21	2.50	0.41
1:C:922:LEU:O	1:C:922:LEU:CD2	2.68	0.41
1:C:1038:LYS:O	1:C:1039:ARG:C	2.63	0.41
3:L:36:TYR:HA	3:L:47:LEU:CD2	2.50	0.41
3:L:62:PHE:HB3	3:L:73:LEU:HD11	2.03	0.41
1:A:39:PRO:HB3	1:A:53:ASP:HB2	2.02	0.40
1:A:54:LEU:HB3	1:A:272:PRO:HA	2.01	0.40
1:A:142:GLY:N	1:A:159:VAL:HG21	2.31	0.40
1:A:224:GLU:HA	1:A:225:PRO:HD3	1.95	0.40
1:A:401:VAL:HG11	1:A:451:TYR:CE2	2.55	0.40
1:A:580:GLN:HG3	5:A:1306:NAG:O7	2.21	0.40
1:A:594:GLY:O	1:A:613:GLN:N	2.55	0.40
1:B:53:ASP:CG	1:B:54:LEU:N	2.79	0.40
1:B:349:SER:OG	1:B:451:TYR:HA	2.21	0.40
1:B:351:TYR:HB3	1:B:453:TYR:HA	2.01	0.40
1:B:454:ARG:CA	1:B:492:LEU:HD23	2.50	0.40
1:B:474:GLN:HG2	1:B:480:CYS:SG	2.61	0.40
1:B:475:ALA:HA	2:H:101:TYR:HD1	1.85	0.40
1:B:598:ILE:HG23	1:B:664:ILE:HG21	2.03	0.40
1:B:946:GLY:O	1:B:948:LEU:N	2.55	0.40
1:C:92:PHE:CE1	1:C:265:TYR:CD1	3.04	0.40
1:C:139:PRO:HD2	1:C:239:GLN:HE22	1.86	0.40
1:C:246:ARG:O	1:C:246:ARG:HG2	2.20	0.40
1:C:741:TYR:HE2	1:C:1004:LEU:HG	1.85	0.40
1:C:1072:GLU:OE1	1:C:1072:GLU:CA	2.69	0.40
1:A:86:PHE:CD1	1:A:90:VAL:CG2	2.96	0.40
1:A:501:ASN:HB2	1:A:502:GLY:H	1.72	0.40
1:A:542:ASN:O	1:A:542:ASN:ND2	2.55	0.40
1:A:596:SER:OG	1:A:597:VAL:N	2.53	0.40
1:A:634:ARG:O	1:A:637:SER:OG	2.31	0.40
1:A:854:LYS:O	1:C:592:PHE:HZ	2.04	0.40
1:A:1130:ILE:CD1	1:B:920:GLN:OE1	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:TYR:CD2	1:B:204:TYR:CD2	3.09	0.40
1:B:106:PHE:HB3	1:B:235:ILE:CG2	2.43	0.40
1:B:332:ILE:HD11	1:B:528:LYS:CB	2.50	0.40
1:B:457:ARG:NH2	1:B:467:ASP:OD2	2.46	0.40
1:B:714:ILE:CG1	1:B:1107:ARG:O	2.69	0.40
1:C:610:VAL:O	1:C:650:LEU:HA	2.21	0.40
1:C:644:GLN:HE22	1:C:649:CYS:HB2	1.86	0.40
1:C:736:VAL:O	1:C:736:VAL:CG1	2.69	0.40
1:C:736:VAL:HA	1:C:857:GLY:O	2.20	0.40
1:C:933:LYS:O	1:C:936:ASP:N	2.54	0.40
1:C:1107:ARG:O	1:C:1107:ARG:CD	2.69	0.40
1:A:90:VAL:HG12	1:A:269:TYR:CD1	2.56	0.40
1:A:560:LEU:HB2	1:A:563:GLN:HG3	2.04	0.40
1:A:1039:ARG:HH12	1:B:1039:ARG:NH1	2.20	0.40
1:A:1049:LEU:HD23	1:A:1049:LEU:HA	1.86	0.40
1:A:1144:GLU:C	1:A:1146:ASP:N	2.79	0.40
1:B:403:ARG:HA	1:B:507:PRO:HA	2.02	0.40
1:B:989:ALA:O	1:B:990:GLU:C	2.64	0.40
1:B:1091:ARG:HG3	1:B:1091:ARG:NH1	2.34	0.40
1:C:630:THR:HG22	1:C:632:THR:H	1.87	0.40
1:C:959:LEU:HD13	1:C:959:LEU:HA	1.91	0.40
1:A:97:LYS:HZ3	1:A:97:LYS:CA	2.32	0.40
1:A:187:LYS:NZ	1:A:187:LYS:C	2.73	0.40
1:A:557:LYS:HZ1	1:A:574:ASP:HB2	1.86	0.40
1:A:619:GLU:CD	1:A:619:GLU:H	2.30	0.40
1:A:854:LYS:O	1:C:592:PHE:CZ	2.75	0.40
1:B:190:ARG:HB3	1:B:192:PHE:CZ	2.55	0.40
1:B:418:ILE:HG13	1:B:422:ASN:ND2	2.35	0.40
1:B:569:ILE:H	1:B:569:ILE:HD12	1.87	0.40
1:C:36:VAL:HG11	1:C:277:LEU:CD2	2.50	0.40
1:C:110:LEU:HA	1:C:110:LEU:HD12	1.81	0.40
1:C:558:LYS:O	1:C:559:PHE:C	2.64	0.40
2:H:21:THR:O	2:H:23:ALA:N	2.54	0.40
2:H:69:ILE:HA	2:H:80:LEU:H	1.87	0.40
2:H:102:GLY:O	2:H:103:ARG:HD3	2.21	0.40
1:A:324:GLU:O	1:A:540:ASN:ND2	2.55	0.40
1:A:421:TYR:HA	1:A:457:ARG:NH1	2.36	0.40
1:A:453:TYR:HB2	1:A:454:ARG:H	1.65	0.40
1:A:1081:ILE:CG1	1:A:1095:PHE:CE2	3.04	0.40
1:A:1125:ASN:OD1	1:A:1125:ASN:N	2.55	0.40
1:B:108:THR:HB	1:B:235:ILE:HD11	2.01	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:462:LYS:HE3	1:B:465:GLU:HA	2.03	0.40
1:B:518:LEU:N	1:B:518:LEU:HD13	2.36	0.40
1:C:913:GLN:C	1:C:915:VAL:N	2.79	0.40
1:C:916:LEU:HD12	1:C:923:ILE:HD13	2.02	0.40
2:H:15:SER:HA	2:H:85:VAL:O	2.22	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	1016/1208 (84%)	705 (69%)	255 (25%)	56 (6%)	1	16
1	B	1046/1208 (87%)	828 (79%)	182 (17%)	36 (3%)	3	24
1	C	1032/1208 (85%)	818 (79%)	181 (18%)	33 (3%)	3	25
2	H	119/321 (37%)	86 (72%)	33 (28%)	0	100	100
3	L	104/232 (45%)	73 (70%)	23 (22%)	8 (8%)	1	10
All	All	3317/4177 (79%)	2510 (76%)	674 (20%)	133 (4%)	4	21

All (133) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	33	THR
1	A	83	VAL
1	A	99	ASN
1	A	120	VAL
1	A	198	ASP
1	A	223	LEU
1	A	231	ILE
1	A	1145	LEU
1	B	336	CYS

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Mol	Chain	Res	Type
1	B	361	CYS
1	B	369	TYR
1	B	941	THR
1	B	951	VAL
1	C	218	GLN
1	C	345	THR
1	C	572	THR
1	C	1079	PRO
1	C	1099	GLY
1	C	1102	TRP
1	A	62	VAL
1	A	63	THR
1	A	64	TRP
1	A	101	ILE
1	A	118	LEU
1	A	189	LEU
1	A	191	GLU
1	A	217	PRO
1	A	333	THR
1	A	365	TYR
1	A	401	VAL
1	A	407	VAL
1	A	451	TYR
1	A	497	PHE
1	A	572	THR
1	A	574	ASP
1	A	709	ASN
1	A	759	PHE
1	A	1101	HIS
1	B	134	GLN
1	B	199	GLY
1	B	214	ARG
1	B	445	VAL
1	B	944	ALA
1	B	1094	VAL
1	C	64	TRP
1	C	797	PHE
1	C	798	GLY
1	C	854	LYS
1	C	1033	VAL
1	C	1097	SER
1	C	1107	ARG

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Mol	Chain	Res	Type
3	L	7	SER
3	L	32	TYR
3	L	50	ASP
3	L	53	ASN
1	A	85	PRO
1	A	193	VAL
1	A	196	ASN
1	A	330	PRO
1	A	506	GLN
1	A	509	ARG
1	A	517	LEU
1	A	573	THR
1	A	1099	GLY
1	A	1144	GLU
1	B	116	SER
1	B	121	ASN
1	B	123	ALA
1	B	136	CYS
1	B	281	GLU
1	B	450	ASN
1	B	518	LEU
1	B	713	ALA
1	B	919	ASN
1	B	940	SER
1	B	950	ASP
1	C	88	ASP
1	C	331	ASN
1	C	338	PHE
1	C	856	ASN
1	C	1029	MET
1	C	1095	PHE
1	C	1109	PHE
1	C	1112	PRO
1	C	1135	ASN
3	L	56	THR
1	A	59	PHE
1	A	213	VAL
1	A	400	PHE
1	A	706	ALA
1	A	707	TYR
1	A	1097	SER
1	B	99	ASN

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Mol	Chain	Res	Type
1	B	131	CYS
1	B	283	GLY
1	B	429	PHE
1	B	430	THR
1	B	945	LEU
1	C	940	SER
1	C	1108	ASN
3	L	57	GLY
1	A	36	VAL
1	A	102	ARG
1	A	109	THR
1	A	329	PHE
1	A	520	ALA
1	A	944	ALA
1	A	1033	VAL
1	B	87	ASN
1	B	345	THR
1	B	496	GLY
1	C	348	ALA
1	C	794	ILE
1	C	911	VAL
1	C	914	ASN
1	C	1030	SER
1	C	1106	GLN
3	L	47	LEU
1	B	362	VAL
3	L	52	SER
1	A	227	VAL
1	A	521	PRO
1	B	952	VAL
1	C	799	GLY
1	A	367	VAL
1	A	119	ILE
1	A	705	VAL
1	B	139	PRO
1	A	942	PRO
1	B	100	ILE
1	C	579	PRO
1	C	915	VAL
1	B	120	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	852/1056 (81%)	749 (88%)	103 (12%)	5	22
1	B	888/1056 (84%)	807 (91%)	81 (9%)	9	32
1	C	897/1056 (85%)	834 (93%)	63 (7%)	14	41
2	H	95/279 (34%)	94 (99%)	1 (1%)	65	73
3	L	80/200 (40%)	76 (95%)	4 (5%)	22	47
All	All	2812/3647 (77%)	2560 (91%)	252 (9%)	11	33

All (252) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	THR
1	A	30	ASN
1	A	61	ASN
1	A	62	VAL
1	A	63	THR
1	A	66	HIS
1	A	68	ILE
1	A	80	ASP
1	A	81	ASN
1	A	87	ASN
1	A	88	ASP
1	A	91	TYR
1	A	92	PHE
1	A	95	THR
1	A	97	LYS
1	A	98	SER
1	A	99	ASN
1	A	100	ILE
1	A	104	TRP
1	A	105	ILE
1	A	106	PHE
1	A	115	GLN
1	A	116	SER

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Mol	Chain	Res	Type
1	A	117	LEU
1	A	119	ILE
1	A	187	LYS
1	A	190	ARG
1	A	193	VAL
1	A	205	SER
1	A	206	LYS
1	A	208	THR
1	A	210	ILE
1	A	212	LEU
1	A	213	VAL
1	A	216	LEU
1	A	221	SER
1	A	224	GLU
1	A	226	LEU
1	A	227	VAL
1	A	229	LEU
1	A	231	ILE
1	A	233	ILE
1	A	234	ASN
1	A	236	THR
1	A	238	PHE
1	A	240	THR
1	A	325	SER
1	A	326	ILE
1	A	327	VAL
1	A	329	PHE
1	A	336	CYS
1	A	355	ARG
1	A	356	LYS
1	A	366	SER
1	A	369	TYR
1	A	390	LEU
1	A	391	CYS
1	A	393	THR
1	A	399	SER
1	A	401	VAL
1	A	402	ILE
1	A	405	ASP
1	A	406	GLU
1	A	450	ASN
1	A	452	LEU

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Mol	Chain	Res	Type
1	A	453	TYR
1	A	494	SER
1	A	501	ASN
1	A	503	VAL
1	A	506	GLN
1	A	512	VAL
1	A	513	LEU
1	A	517	LEU
1	A	518	LEU
1	A	531	THR
1	A	532	ASN
1	A	533	LEU
1	A	549	THR
1	A	552	LEU
1	A	567	ARG
1	A	574	ASP
1	A	577	ARG
1	A	580	GLN
1	A	584	ILE
1	A	587	ILE
1	A	661	GLU
1	A	705	VAL
1	A	736	VAL
1	A	802	PHE
1	A	805	ILE
1	A	806	LEU
1	A	859	THR
1	A	900	MET
1	A	901	GLN
1	A	945	LEU
1	A	1029	MET
1	A	1033	VAL
1	A	1037	SER
1	A	1038	LYS
1	A	1073	LYS
1	A	1096	VAL
1	A	1097	SER
1	A	1098	ASN
1	B	92	PHE
1	B	101	ILE
1	B	104	TRP
1	B	105	ILE

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Mol	Chain	Res	Type
1	B	106	PHE
1	B	108	THR
1	B	109	THR
1	B	115	GLN
1	B	116	SER
1	B	117	LEU
1	B	121	ASN
1	B	131	CYS
1	B	136	CYS
1	B	137	ASN
1	B	139	PRO
1	B	140	PHE
1	B	201	PHE
1	B	206	LYS
1	B	208	THR
1	B	215	ASP
1	B	216	LEU
1	B	228	ASP
1	B	231	ILE
1	B	233	ILE
1	B	235	ILE
1	B	240	THR
1	B	273	ARG
1	B	275	PHE
1	B	284	THR
1	B	301	CYS
1	B	302	THR
1	B	304	LYS
1	B	306	PHE
1	B	307	THR
1	B	318	PHE
1	B	320	VAL
1	B	334	ASN
1	B	341	VAL
1	B	343	ASN
1	B	345	THR
1	B	346	ARG
1	B	358	ILE
1	B	359	SER
1	B	361	CYS
1	B	367	VAL
1	B	428	ASP

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Mol	Chain	Res	Type
1	B	468	ILE
1	B	500	THR
1	B	501	ASN
1	B	513	LEU
1	B	518	LEU
1	B	524	VAL
1	B	525	CYS
1	B	529	LYS
1	B	718	PHE
1	B	719	THR
1	B	736	VAL
1	B	919	ASN
1	B	921	LYS
1	B	922	LEU
1	B	923	ILE
1	B	945	LEU
1	B	947	LYS
1	B	953	ASN
1	B	954	GLN
1	B	1071	GLN
1	B	1072	GLU
1	B	1073	LYS
1	B	1076	THR
1	B	1091	ARG
1	B	1092	GLU
1	B	1094	VAL
1	B	1096	VAL
1	B	1097	SER
1	B	1104	VAL
1	B	1130	ILE
1	B	1132	ILE
1	B	1133	VAL
1	B	1134	ASN
1	B	1136	THR
1	B	1137	VAL
1	C	29	THR
1	C	33	THR
1	C	63	THR
1	C	64	TRP
1	C	86	PHE
1	C	87	ASN
1	C	162	SER

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Mol	Chain	Res	Type
1	C	210	ILE
1	C	211	ASN
1	C	212	LEU
1	C	216	LEU
1	C	267	VAL
1	C	331	ASN
1	C	332	ILE
1	C	336	CYS
1	C	340	GLU
1	C	341	VAL
1	C	343	ASN
1	C	350	VAL
1	C	577	ARG
1	C	578	ASP
1	C	582	LEU
1	C	583	GLU
1	C	707	TYR
1	C	708	SER
1	C	712	ILE
1	C	718	PHE
1	C	719	THR
1	C	736	VAL
1	C	759	PHE
1	C	790	LYS
1	C	791	THR
1	C	794	ILE
1	C	795	LYS
1	C	801	ASN
1	C	803	SER
1	C	858	LEU
1	C	859	THR
1	C	894	LEU
1	C	896	ILE
1	C	911	VAL
1	C	913	GLN
1	C	916	LEU
1	C	918	GLU
1	C	921	LYS
1	C	922	LEU
1	C	923	ILE
1	C	1030	SER
1	C	1031	GLU

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Mol	Chain	Res	Type
1	C	1033	VAL
1	C	1036	GLN
1	C	1072	GLU
1	C	1073	LYS
1	C	1074	ASN
1	C	1077	THR
1	C	1098	ASN
1	C	1107	ARG
1	C	1111	GLU
1	C	1113	GLN
1	C	1128	VAL
1	C	1129	VAL
1	C	1132	ILE
1	C	1134	ASN
2	H	92	VAL
3	L	7	SER
3	L	20	THR
3	L	46	LEU
3	L	56	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	49	HIS
1	A	66	HIS
1	A	99	ASN
1	A	125	ASN
1	A	134	GLN
1	A	196	ASN
1	A	207	HIS
1	A	234	ASN
1	A	450	ASN
1	A	506	GLN
1	A	556	ASN
1	A	563	GLN
1	A	564	GLN
1	A	755	GLN
1	A	787	GLN
1	A	955	ASN
1	A	1071	GLN
1	B	115	GLN

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Mol	Chain	Res	Type
1	B	121	ASN
1	B	122	ASN
1	B	125	ASN
1	B	134	GLN
1	B	334	ASN
1	B	422	ASN
1	B	439	ASN
1	B	501	ASN
1	B	853	GLN
1	B	872	GLN
1	B	901	GLN
1	B	953	ASN
1	B	1071	GLN
1	B	1074	ASN
1	B	1106	GLN
1	C	69	HIS
1	C	165	ASN
1	C	334	ASN
1	C	343	ASN
1	C	409	GLN
1	C	755	GLN
1	C	779	GLN
1	C	901	GLN
1	C	913	GLN
1	C	919	ASN
1	C	1011	GLN
1	C	1071	GLN
1	C	1074	ASN
2	H	39	GLN
3	L	53	ASN
3	L	90	GLN
3	L	99	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

4 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
4	NAG	D	1	4	14,14,15	1.85	4 (28%)	17,19,21	3.23	9 (52%)
4	NAG	D	2	4	14,14,15	0.93	1 (7%)	17,19,21	1.10	1 (5%)
4	NAG	N	1	4	14,14,15	1.85	4 (28%)	17,19,21	3.23	9 (52%)
4	NAG	N	2	4	14,14,15	0.92	1 (7%)	17,19,21	1.09	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	1	4	-	3/6/23/26	0/1/1/1
4	NAG	D	2	4	-	1/6/23/26	0/1/1/1
4	NAG	N	1	4	-	3/6/23/26	0/1/1/1
4	NAG	N	2	4	-	1/6/23/26	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1	NAG	O5-C1	4.51	1.51	1.43
4	N	1	NAG	O5-C1	4.50	1.51	1.43
4	N	2	NAG	C1-C2	2.68	1.56	1.52
4	N	1	NAG	C8-C7	-2.67	1.45	1.50
4	D	2	NAG	C1-C2	2.67	1.56	1.52
4	D	1	NAG	C4-C5	-2.65	1.47	1.53
4	D	1	NAG	C8-C7	-2.64	1.45	1.50
4	N	1	NAG	C4-C5	-2.63	1.47	1.53
4	D	1	NAG	O7-C7	-2.37	1.17	1.23
4	N	1	NAG	O7-C7	-2.34	1.18	1.23

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	N	1	NAG	C2-N2-C7	6.39	131.46	122.90
4	D	1	NAG	C2-N2-C7	6.37	131.44	122.90
4	N	1	NAG	O4-C4-C5	5.02	121.68	109.32
4	N	1	NAG	O4-C4-C3	4.99	122.13	110.38
4	D	1	NAG	O4-C4-C3	4.98	122.12	110.38
4	D	1	NAG	O4-C4-C5	4.98	121.59	109.32
4	D	1	NAG	C4-C3-C2	-4.46	104.49	111.02
4	N	1	NAG	C4-C3-C2	-4.43	104.52	111.02
4	D	1	NAG	C1-O5-C5	4.18	117.79	112.19
4	N	1	NAG	C1-O5-C5	4.16	117.76	112.19
4	D	1	NAG	O5-C5-C4	-3.94	101.24	110.83
4	N	1	NAG	O5-C5-C4	-3.92	101.29	110.83
4	N	1	NAG	C8-C7-N2	3.16	121.36	116.12
4	D	1	NAG	C8-C7-N2	3.15	121.34	116.12
4	D	1	NAG	C1-C2-N2	3.12	115.34	110.43
4	N	1	NAG	C1-C2-N2	3.10	115.32	110.43
4	N	2	NAG	C1-C2-N2	2.71	114.71	110.43
4	D	2	NAG	C1-C2-N2	2.68	114.66	110.43
4	N	1	NAG	C3-C4-C5	-2.26	106.14	110.23
4	D	1	NAG	C3-C4-C5	-2.24	106.17	110.23

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	N	1	NAG	C1-C2-N2-C7
4	D	1	NAG	C1-C2-N2-C7
4	N	1	NAG	C8-C7-N2-C2
4	D	1	NAG	C8-C7-N2-C2
4	N	1	NAG	O7-C7-N2-C2
4	D	1	NAG	O7-C7-N2-C2
4	N	2	NAG	O5-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 12 short contacts:

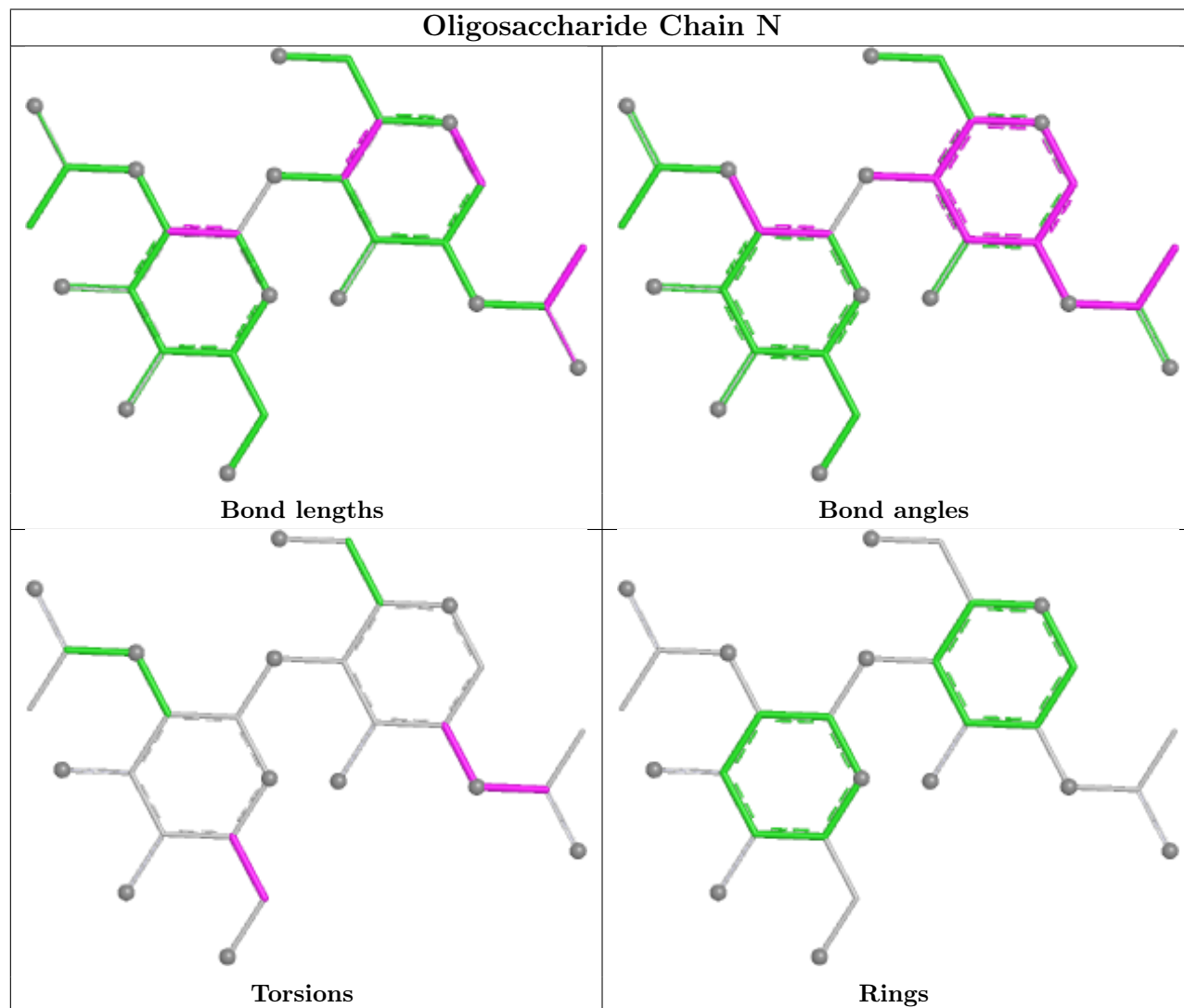
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1	NAG	6	0
4	N	1	NAG	4	0

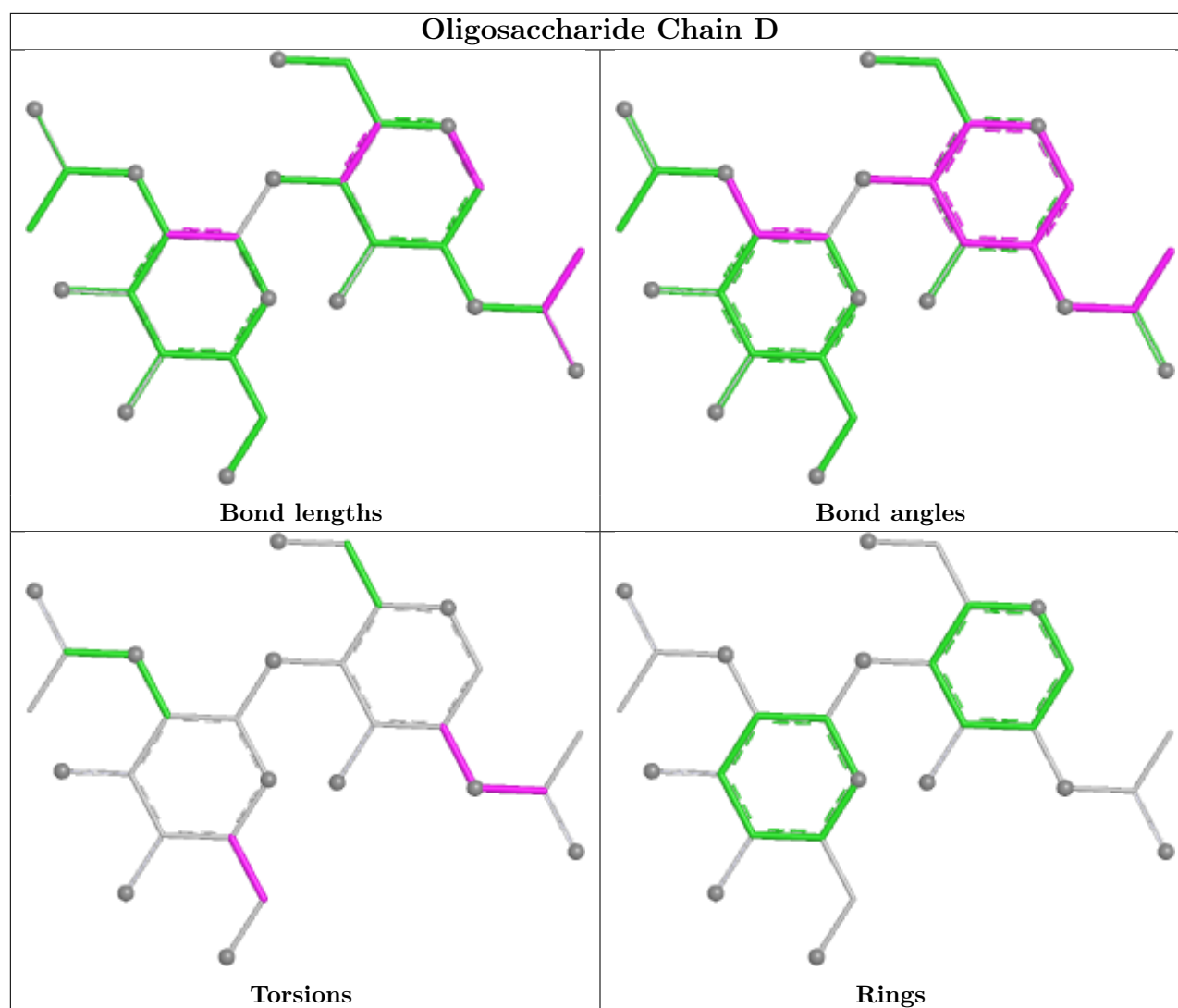
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	N	2	NAG	2	0
4	D	2	NAG	2	0

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





5.6 Ligand geometry [i](#)

32 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	A	1303	-	14,14,15	0.32	0	17,19,21	0.47	0
5	NAG	C	1303	1	14,14,15	0.19	0	17,19,21	0.68	0
5	NAG	A	1312	-	14,14,15	0.34	0	17,19,21	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	1306	1	14,14,15	0.16	0	17,19,21	0.42	0
5	NAG	A	1308	1	14,14,15	0.21	0	17,19,21	0.59	0
5	NAG	A	1302	-	14,14,15	1.86	4 (28%)	17,19,21	3.22	9 (52%)
5	NAG	A	1309	1	14,14,15	0.21	0	17,19,21	0.49	0
5	NAG	A	1311	1	14,14,15	0.23	0	17,19,21	0.52	0
5	NAG	A	1307	1	14,14,15	0.24	0	17,19,21	0.46	0
5	NAG	C	1309	-	14,14,15	0.21	0	17,19,21	0.48	0
5	NAG	A	1310	1	14,14,15	0.31	0	17,19,21	0.49	0
5	NAG	B	1304	-	14,14,15	0.44	0	17,19,21	1.67	3 (17%)
5	NAG	B	1302	-	14,14,15	1.85	4 (28%)	17,19,21	3.23	9 (52%)
5	NAG	B	1309	1	14,14,15	0.30	0	17,19,21	0.39	0
5	NAG	C	1305	-	14,14,15	0.37	0	17,19,21	0.58	0
5	NAG	B	1308	1	14,14,15	0.29	0	17,19,21	0.54	0
5	NAG	B	1310	1	14,14,15	0.40	0	17,19,21	0.47	0
5	NAG	B	1311	1	14,14,15	0.67	1 (7%)	17,19,21	0.61	0
5	NAG	B	1307	1	14,14,15	0.63	0	17,19,21	1.12	1 (5%)
5	NAG	A	1301	-	14,14,15	0.97	0	17,19,21	2.38	9 (52%)
5	NAG	C	1302	-	14,14,15	1.86	4 (28%)	17,19,21	3.22	9 (52%)
5	NAG	B	1303	-	14,14,15	1.84	4 (28%)	17,19,21	3.23	9 (52%)
5	NAG	B	1301	-	14,14,15	1.87	4 (28%)	17,19,21	3.22	9 (52%)
5	NAG	C	1306	1	14,14,15	0.21	0	17,19,21	0.40	0
5	NAG	A	1304	-	14,14,15	0.23	0	17,19,21	0.40	0
5	NAG	A	1305	1	14,14,15	0.45	0	17,19,21	0.80	0
5	NAG	C	1301	-	14,14,15	1.85	4 (28%)	17,19,21	3.23	9 (52%)
5	NAG	C	1307	1	14,14,15	0.27	0	17,19,21	0.46	0
5	NAG	B	1306	-	14,14,15	1.19	2 (14%)	17,19,21	0.78	1 (5%)
5	NAG	C	1304	1	14,14,15	0.36	0	17,19,21	1.30	1 (5%)
5	NAG	B	1305	1	14,14,15	0.50	0	17,19,21	1.32	1 (5%)
5	NAG	C	1308	-	14,14,15	0.33	0	17,19,21	0.76	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	1303	-	-	4/6/23/26	0/1/1/1
5	NAG	C	1303	1	-	4/6/23/26	0/1/1/1
5	NAG	A	1312	-	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	1306	1	-	4/6/23/26	0/1/1/1
5	NAG	A	1308	1	-	1/6/23/26	0/1/1/1
5	NAG	A	1302	-	-	3/6/23/26	0/1/1/1
5	NAG	A	1309	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1311	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1307	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1309	-	-	4/6/23/26	0/1/1/1
5	NAG	A	1310	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1304	-	-	5/6/23/26	0/1/1/1
5	NAG	B	1302	-	-	3/6/23/26	0/1/1/1
5	NAG	B	1309	1	-	4/6/23/26	0/1/1/1
5	NAG	C	1305	-	-	3/6/23/26	0/1/1/1
5	NAG	B	1308	1	-	4/6/23/26	0/1/1/1
5	NAG	B	1310	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1311	1	-	4/6/23/26	0/1/1/1
5	NAG	B	1307	1	-	4/6/23/26	0/1/1/1
5	NAG	A	1301	-	-	6/6/23/26	0/1/1/1
5	NAG	C	1302	-	-	3/6/23/26	0/1/1/1
5	NAG	B	1303	-	-	3/6/23/26	0/1/1/1
5	NAG	B	1301	-	-	3/6/23/26	0/1/1/1
5	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1304	-	-	2/6/23/26	0/1/1/1
5	NAG	A	1305	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1301	-	-	3/6/23/26	0/1/1/1
5	NAG	C	1307	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1306	-	-	0/6/23/26	0/1/1/1
5	NAG	C	1304	1	-	6/6/23/26	0/1/1/1
5	NAG	B	1305	1	-	4/6/23/26	0/1/1/1
5	NAG	C	1308	-	-	2/6/23/26	0/1/1/1

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1302	NAG	O5-C1	4.60	1.51	1.43
5	B	1301	NAG	O5-C1	4.57	1.51	1.43
5	A	1302	NAG	O5-C1	4.54	1.51	1.43
5	B	1302	NAG	O5-C1	4.48	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1301	NAG	O5-C1	4.47	1.51	1.43
5	B	1303	NAG	O5-C1	4.47	1.51	1.43
5	B	1306	NAG	O5-C1	3.44	1.49	1.43
5	B	1301	NAG	C4-C5	-2.72	1.47	1.53
5	C	1301	NAG	C4-C5	-2.71	1.47	1.53
5	A	1302	NAG	C4-C5	-2.69	1.47	1.53
5	B	1303	NAG	C8-C7	-2.67	1.45	1.50
5	B	1302	NAG	C8-C7	-2.67	1.45	1.50
5	C	1301	NAG	C8-C7	-2.67	1.45	1.50
5	A	1302	NAG	C8-C7	-2.66	1.45	1.50
5	B	1302	NAG	C4-C5	-2.66	1.47	1.53
5	C	1302	NAG	C8-C7	-2.65	1.45	1.50
5	C	1302	NAG	C4-C5	-2.64	1.47	1.53
5	B	1301	NAG	C8-C7	-2.63	1.45	1.50
5	B	1303	NAG	C4-C5	-2.61	1.47	1.53
5	B	1306	NAG	C1-C2	2.60	1.55	1.52
5	B	1303	NAG	O7-C7	-2.36	1.18	1.23
5	C	1302	NAG	O7-C7	-2.35	1.18	1.23
5	B	1301	NAG	O7-C7	-2.34	1.18	1.23
5	B	1302	NAG	O7-C7	-2.34	1.18	1.23
5	C	1301	NAG	O7-C7	-2.33	1.18	1.23
5	A	1302	NAG	O7-C7	-2.33	1.18	1.23
5	B	1311	NAG	C1-C2	2.27	1.55	1.52

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1302	NAG	C2-N2-C7	6.38	131.46	122.90
5	B	1301	NAG	C2-N2-C7	6.38	131.44	122.90
5	B	1302	NAG	C2-N2-C7	6.38	131.44	122.90
5	C	1301	NAG	C2-N2-C7	6.37	131.43	122.90
5	A	1302	NAG	C2-N2-C7	6.35	131.41	122.90
5	B	1303	NAG	C2-N2-C7	6.34	131.40	122.90
5	B	1302	NAG	O4-C4-C5	5.04	121.73	109.32
5	B	1301	NAG	O4-C4-C5	5.03	121.72	109.32
5	C	1301	NAG	O4-C4-C5	5.03	121.70	109.32
5	C	1302	NAG	O4-C4-C5	5.02	121.69	109.32
5	B	1303	NAG	O4-C4-C5	5.02	121.68	109.32
5	A	1302	NAG	O4-C4-C5	5.01	121.67	109.32
5	A	1302	NAG	O4-C4-C3	4.97	122.10	110.38
5	C	1301	NAG	O4-C4-C3	4.97	122.09	110.38
5	C	1302	NAG	O4-C4-C3	4.96	122.08	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1302	NAG	O4-C4-C3	4.96	122.07	110.38
5	B	1301	NAG	O4-C4-C3	4.95	122.04	110.38
5	B	1303	NAG	O4-C4-C3	4.95	122.04	110.38
5	A	1301	NAG	O4-C4-C5	-4.74	97.65	109.32
5	B	1305	NAG	C2-N2-C7	4.67	129.15	122.90
5	B	1303	NAG	C4-C3-C2	-4.50	104.43	111.02
5	B	1301	NAG	C4-C3-C2	-4.49	104.43	111.02
5	A	1302	NAG	C4-C3-C2	-4.49	104.44	111.02
5	C	1304	NAG	C2-N2-C7	4.48	128.90	122.90
5	C	1301	NAG	C4-C3-C2	-4.46	104.48	111.02
5	C	1302	NAG	C4-C3-C2	-4.45	104.50	111.02
5	B	1302	NAG	C4-C3-C2	-4.43	104.53	111.02
5	B	1304	NAG	O5-C1-C2	-4.22	104.77	111.29
5	B	1303	NAG	C1-O5-C5	4.21	117.83	112.19
5	C	1301	NAG	C1-O5-C5	4.19	117.80	112.19
5	B	1302	NAG	C1-O5-C5	4.14	117.73	112.19
5	A	1302	NAG	C1-O5-C5	4.14	117.73	112.19
5	B	1301	NAG	C1-O5-C5	4.14	117.73	112.19
5	C	1302	NAG	C1-O5-C5	4.12	117.70	112.19
5	A	1301	NAG	O5-C5-C4	-4.11	100.83	110.83
5	B	1303	NAG	O5-C5-C4	-3.95	101.22	110.83
5	C	1302	NAG	O5-C5-C4	-3.92	101.28	110.83
5	B	1302	NAG	O5-C5-C4	-3.92	101.30	110.83
5	C	1301	NAG	O5-C5-C4	-3.91	101.32	110.83
5	B	1301	NAG	O5-C5-C4	-3.90	101.34	110.83
5	A	1302	NAG	O5-C5-C4	-3.90	101.35	110.83
5	B	1304	NAG	C6-C5-C4	-3.41	104.64	113.02
5	B	1307	NAG	C1-O5-C5	-3.25	107.83	112.19
5	C	1302	NAG	C8-C7-N2	3.17	121.38	116.12
5	B	1302	NAG	C8-C7-N2	3.16	121.36	116.12
5	B	1303	NAG	C8-C7-N2	3.15	121.34	116.12
5	A	1302	NAG	C8-C7-N2	3.14	121.33	116.12
5	B	1301	NAG	C8-C7-N2	3.14	121.33	116.12
5	A	1302	NAG	C1-C2-N2	3.14	115.38	110.43
5	C	1301	NAG	C8-C7-N2	3.13	121.32	116.12
5	B	1302	NAG	C1-C2-N2	3.13	115.37	110.43
5	B	1303	NAG	C1-C2-N2	3.13	115.36	110.43
5	C	1302	NAG	C1-C2-N2	3.12	115.36	110.43
5	B	1301	NAG	C1-C2-N2	3.10	115.32	110.43
5	C	1301	NAG	C1-C2-N2	3.10	115.31	110.43
5	A	1301	NAG	O4-C4-C3	3.02	117.50	110.38
5	A	1301	NAG	C1-C2-N2	-2.92	105.84	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1306	NAG	C1-O5-C5	2.90	116.07	112.19
5	A	1301	NAG	O5-C1-C2	2.89	115.76	111.29
5	A	1301	NAG	C4-C3-C2	2.70	114.97	111.02
5	C	1308	NAG	C1-O5-C5	2.68	115.78	112.19
5	A	1301	NAG	O3-C3-C2	-2.66	103.88	109.40
5	B	1304	NAG	C3-C4-C5	2.35	114.48	110.23
5	B	1302	NAG	C3-C4-C5	-2.28	106.10	110.23
5	C	1302	NAG	C3-C4-C5	-2.26	106.14	110.23
5	C	1301	NAG	C3-C4-C5	-2.26	106.14	110.23
5	B	1303	NAG	C3-C4-C5	-2.23	106.19	110.23
5	A	1302	NAG	C3-C4-C5	-2.22	106.21	110.23
5	B	1301	NAG	C3-C4-C5	-2.22	106.21	110.23
5	A	1301	NAG	C3-C4-C5	2.08	114.00	110.23
5	A	1301	NAG	O3-C3-C4	2.05	115.21	110.38

There are no chirality outliers.

All (91) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1301	NAG	C1-C2-N2-C7
5	A	1301	NAG	C8-C7-N2-C2
5	A	1301	NAG	O7-C7-N2-C2
5	A	1302	NAG	C1-C2-N2-C7
5	B	1301	NAG	C1-C2-N2-C7
5	B	1302	NAG	C1-C2-N2-C7
5	B	1303	NAG	C1-C2-N2-C7
5	B	1304	NAG	C3-C2-N2-C7
5	B	1304	NAG	C8-C7-N2-C2
5	B	1304	NAG	O7-C7-N2-C2
5	C	1301	NAG	C1-C2-N2-C7
5	C	1302	NAG	C1-C2-N2-C7
5	C	1305	NAG	C1-C2-N2-C7
5	C	1307	NAG	O5-C5-C6-O6
5	C	1309	NAG	O5-C5-C6-O6
5	C	1305	NAG	C4-C5-C6-O6
5	C	1306	NAG	C4-C5-C6-O6
5	B	1309	NAG	O5-C5-C6-O6
5	A	1310	NAG	O5-C5-C6-O6
5	A	1311	NAG	O5-C5-C6-O6
5	A	1303	NAG	O5-C5-C6-O6
5	B	1311	NAG	C4-C5-C6-O6
5	A	1306	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	A	1311	NAG	C4-C5-C6-O6
5	C	1304	NAG	O5-C5-C6-O6
5	B	1309	NAG	C4-C5-C6-O6
5	C	1305	NAG	O5-C5-C6-O6
5	C	1308	NAG	O5-C5-C6-O6
5	C	1307	NAG	C4-C5-C6-O6
5	A	1306	NAG	O5-C5-C6-O6
5	B	1307	NAG	O5-C5-C6-O6
5	C	1303	NAG	O5-C5-C6-O6
5	A	1303	NAG	C4-C5-C6-O6
5	C	1309	NAG	C4-C5-C6-O6
5	C	1306	NAG	O5-C5-C6-O6
5	C	1304	NAG	C4-C5-C6-O6
5	C	1308	NAG	C4-C5-C6-O6
5	A	1302	NAG	C8-C7-N2-C2
5	B	1301	NAG	C8-C7-N2-C2
5	B	1302	NAG	C8-C7-N2-C2
5	B	1303	NAG	C8-C7-N2-C2
5	C	1301	NAG	C8-C7-N2-C2
5	C	1302	NAG	C8-C7-N2-C2
5	A	1310	NAG	C4-C5-C6-O6
5	B	1307	NAG	C4-C5-C6-O6
5	A	1302	NAG	O7-C7-N2-C2
5	A	1306	NAG	C8-C7-N2-C2
5	A	1306	NAG	O7-C7-N2-C2
5	B	1301	NAG	O7-C7-N2-C2
5	B	1302	NAG	O7-C7-N2-C2
5	B	1303	NAG	O7-C7-N2-C2
5	B	1305	NAG	C8-C7-N2-C2
5	B	1305	NAG	O7-C7-N2-C2
5	B	1308	NAG	C8-C7-N2-C2
5	B	1308	NAG	O7-C7-N2-C2
5	B	1309	NAG	C8-C7-N2-C2
5	B	1309	NAG	O7-C7-N2-C2
5	B	1310	NAG	C8-C7-N2-C2
5	B	1310	NAG	O7-C7-N2-C2
5	B	1311	NAG	C8-C7-N2-C2
5	B	1311	NAG	O7-C7-N2-C2
5	C	1301	NAG	O7-C7-N2-C2
5	C	1302	NAG	O7-C7-N2-C2
5	C	1304	NAG	C8-C7-N2-C2
5	C	1304	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
5	C	1309	NAG	C8-C7-N2-C2
5	C	1309	NAG	O7-C7-N2-C2
5	A	1304	NAG	O5-C5-C6-O6
5	B	1311	NAG	O5-C5-C6-O6
5	B	1308	NAG	C4-C5-C6-O6
5	A	1312	NAG	C4-C5-C6-O6
5	B	1308	NAG	O5-C5-C6-O6
5	C	1303	NAG	C4-C5-C6-O6
5	A	1312	NAG	O5-C5-C6-O6
5	A	1301	NAG	O5-C5-C6-O6
5	B	1304	NAG	O5-C5-C6-O6
5	A	1303	NAG	C1-C2-N2-C7
5	B	1307	NAG	C1-C2-N2-C7
5	C	1303	NAG	C1-C2-N2-C7
5	C	1304	NAG	C1-C2-N2-C7
5	B	1304	NAG	C4-C5-C6-O6
5	A	1303	NAG	C3-C2-N2-C7
5	B	1307	NAG	C3-C2-N2-C7
5	C	1304	NAG	C3-C2-N2-C7
5	A	1301	NAG	C4-C5-C6-O6
5	A	1304	NAG	C4-C5-C6-O6
5	A	1308	NAG	C4-C5-C6-O6
5	B	1305	NAG	C1-C2-N2-C7
5	A	1301	NAG	C3-C2-N2-C7
5	B	1305	NAG	C3-C2-N2-C7
5	C	1303	NAG	C3-C2-N2-C7

There are no ring outliers.

18 monomers are involved in 66 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1306	NAG	5	0
5	A	1308	NAG	2	0
5	A	1302	NAG	2	0
5	B	1304	NAG	7	0
5	B	1302	NAG	11	0
5	B	1308	NAG	1	0
5	B	1311	NAG	2	0
5	B	1307	NAG	1	0
5	A	1301	NAG	3	0
5	C	1302	NAG	4	0
5	B	1303	NAG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1301	NAG	2	0
5	A	1304	NAG	1	0
5	A	1305	NAG	1	0
5	C	1301	NAG	14	0
5	B	1306	NAG	6	0
5	C	1304	NAG	1	0
5	B	1305	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

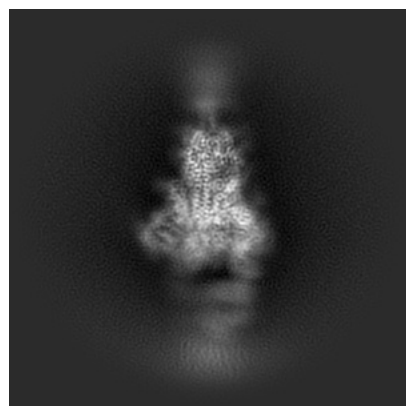
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34164. These allow visual inspection of the internal detail of the map and identification of artifacts.

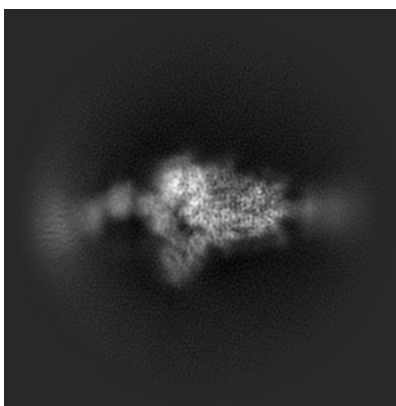
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

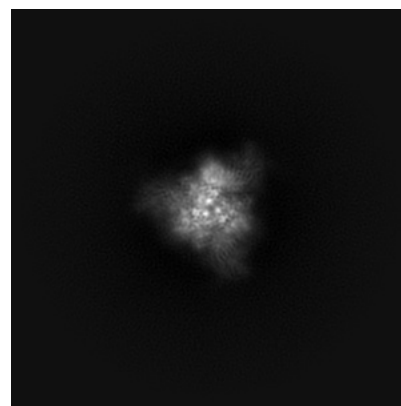
6.1.1 Primary map



X

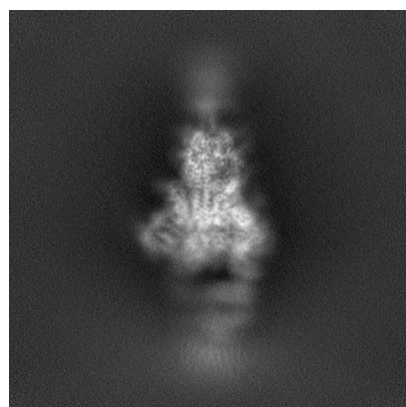


Y

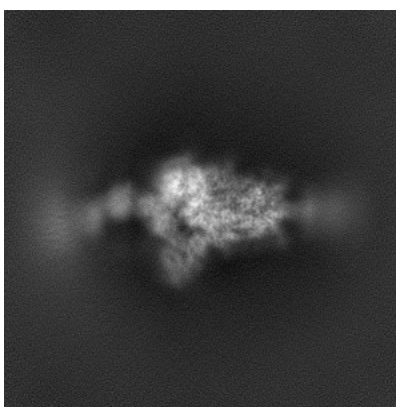


Z

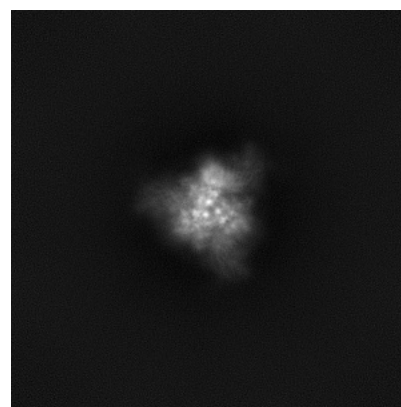
6.1.2 Raw map



X



Y



Z

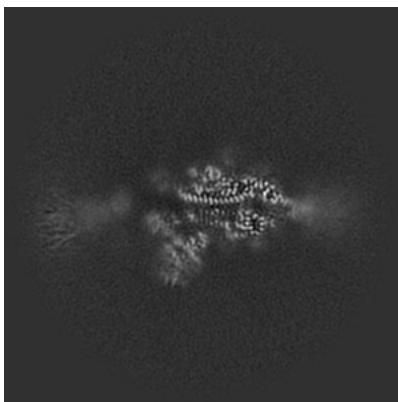
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

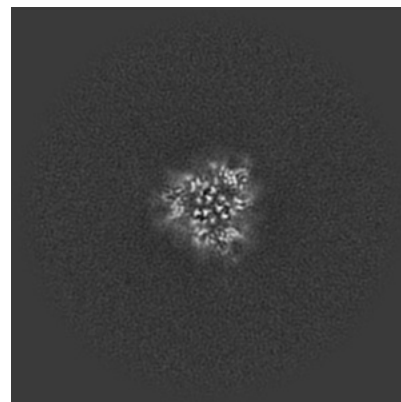
6.2.1 Primary map



X Index: 200

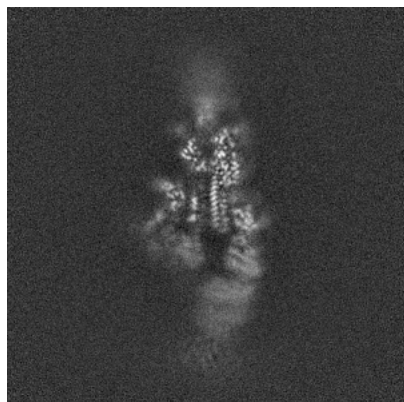


Y Index: 200

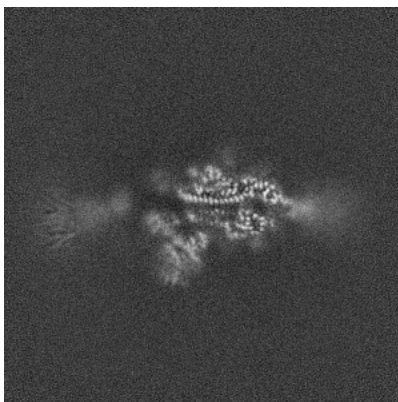


Z Index: 200

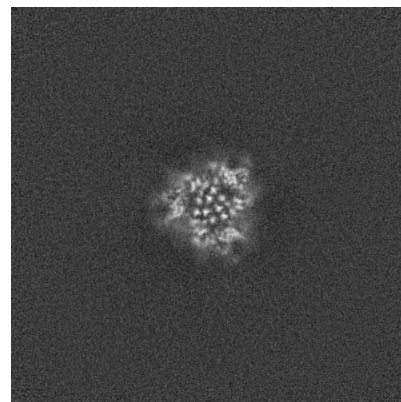
6.2.2 Raw map



X Index: 200



Y Index: 200

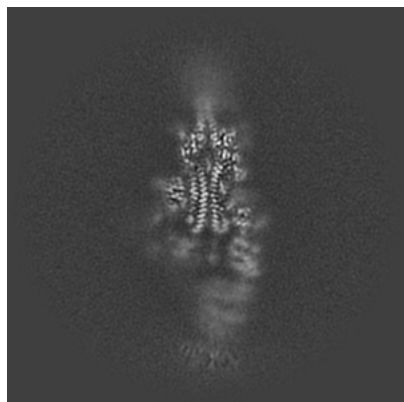


Z Index: 200

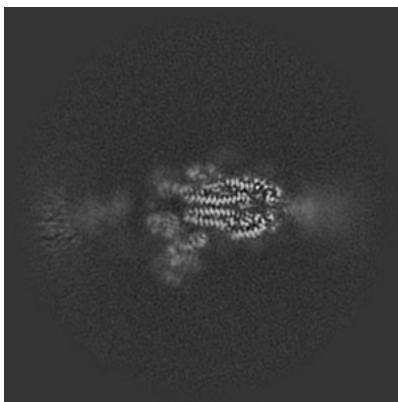
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

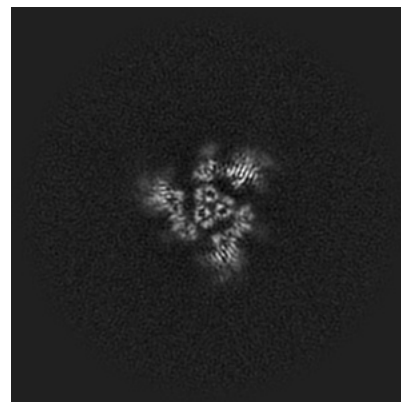
6.3.1 Primary map



X Index: 196

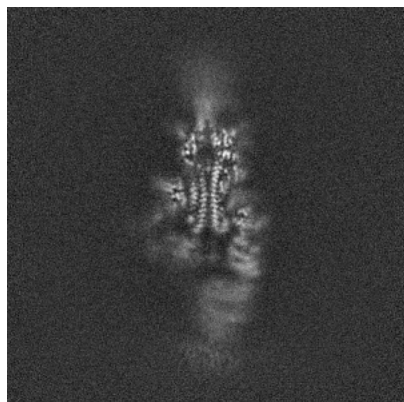


Y Index: 197

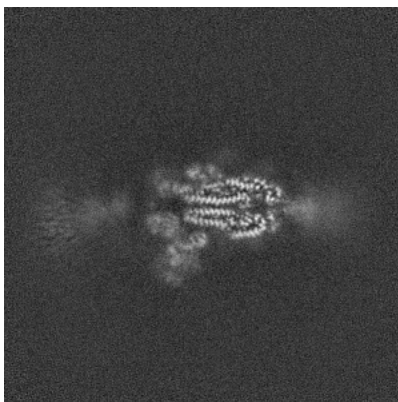


Z Index: 186

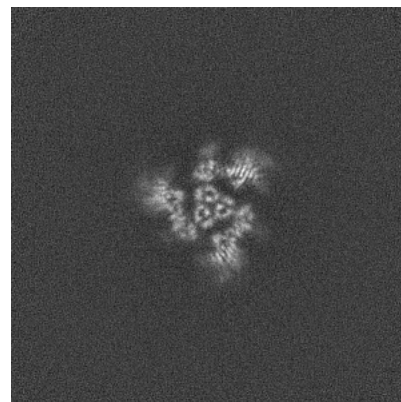
6.3.2 Raw map



X Index: 197



Y Index: 197

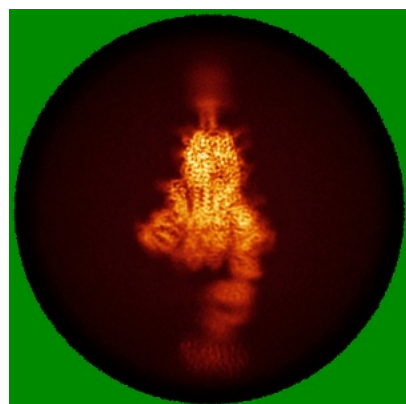


Z Index: 186

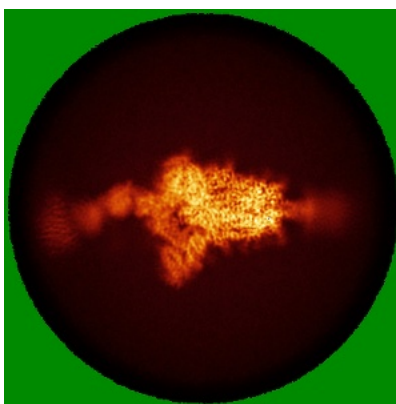
The images above show the largest variance slices of the map in three orthogonal directions.

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

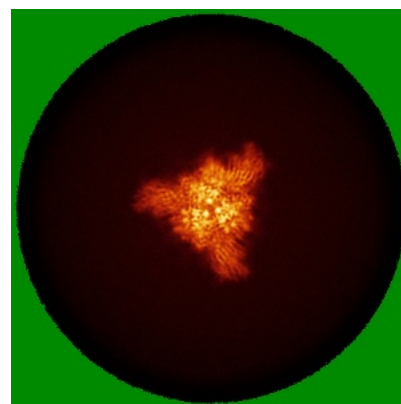
6.4.1 Primary map



X

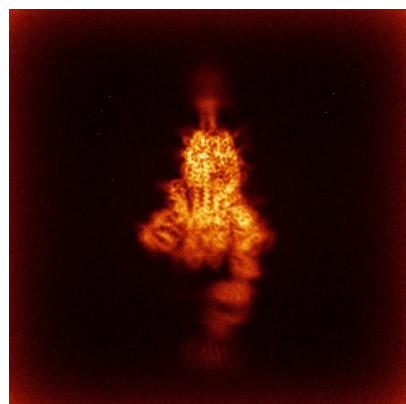


Y

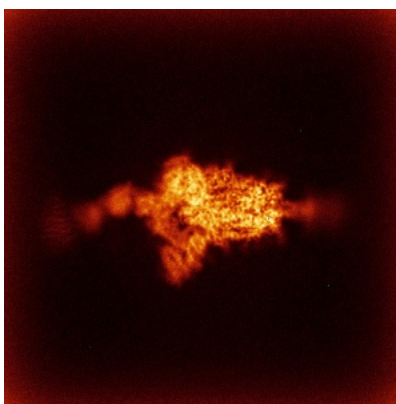


Z

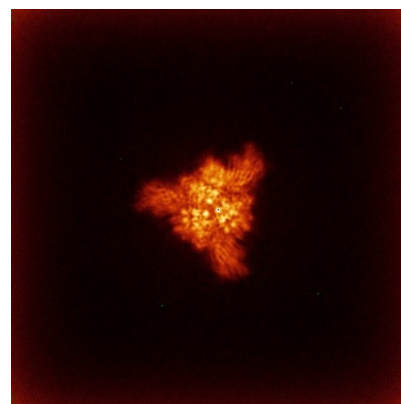
6.4.2 Raw map



X



Y

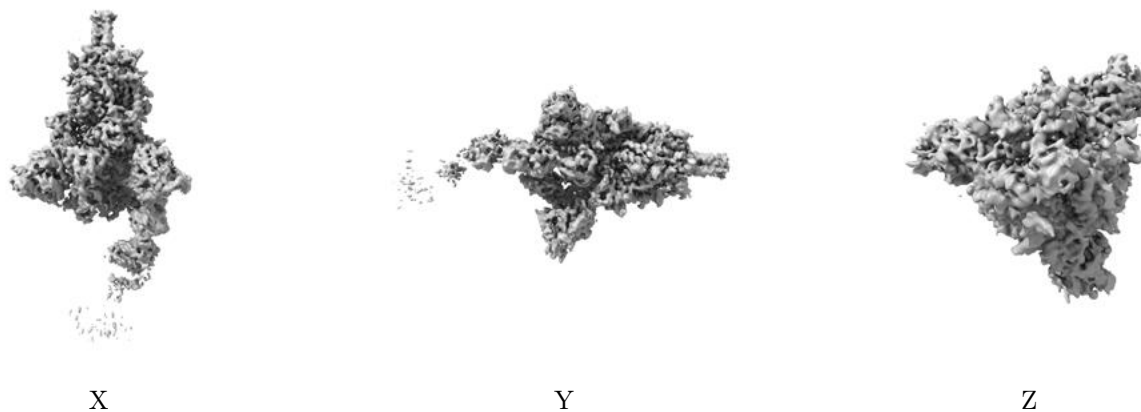


Z

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

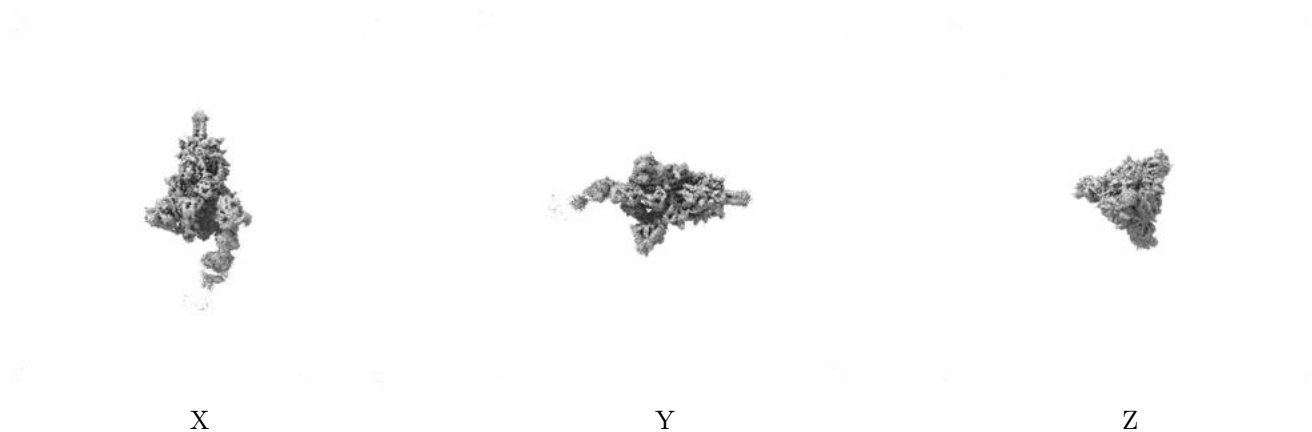
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

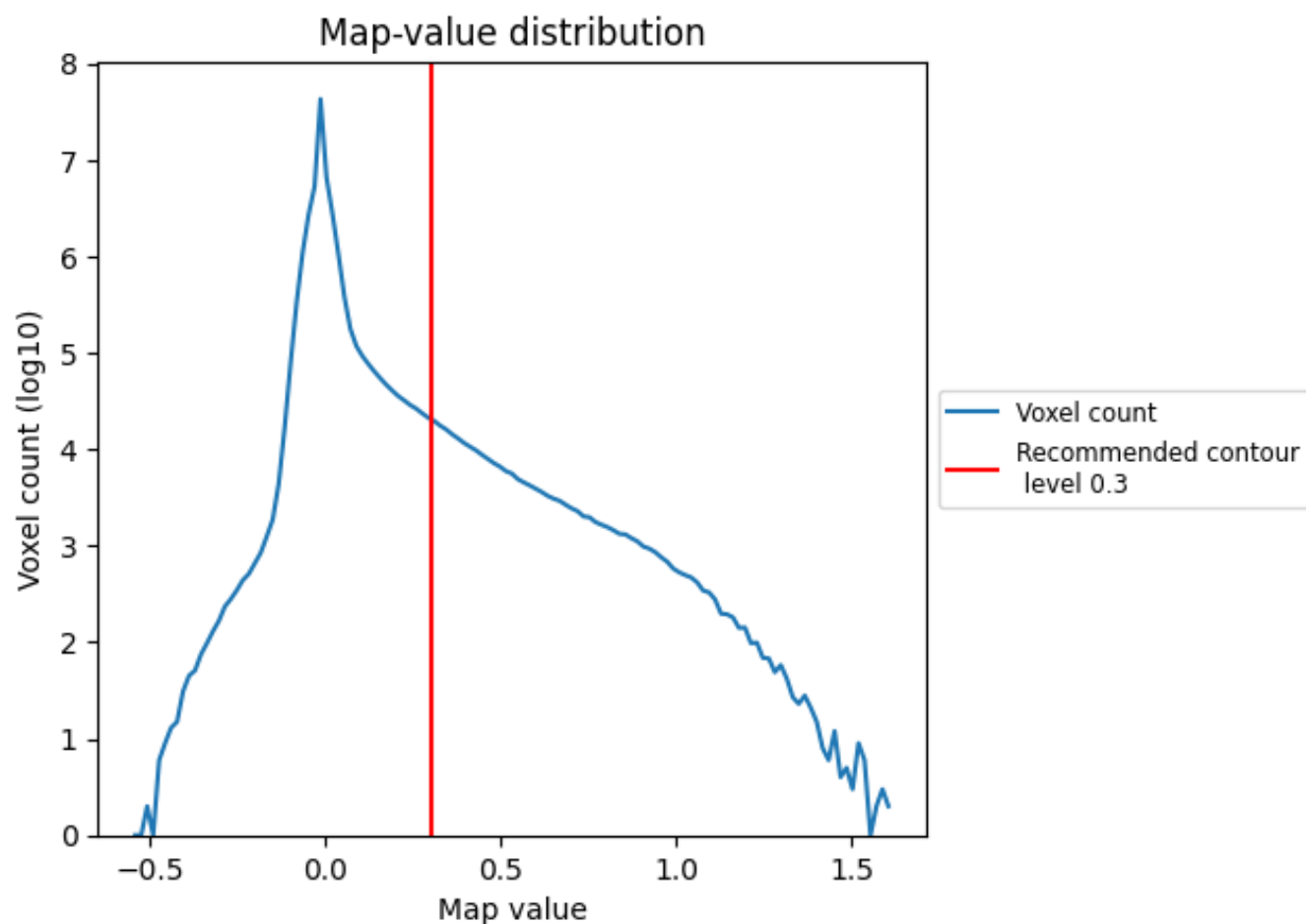
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

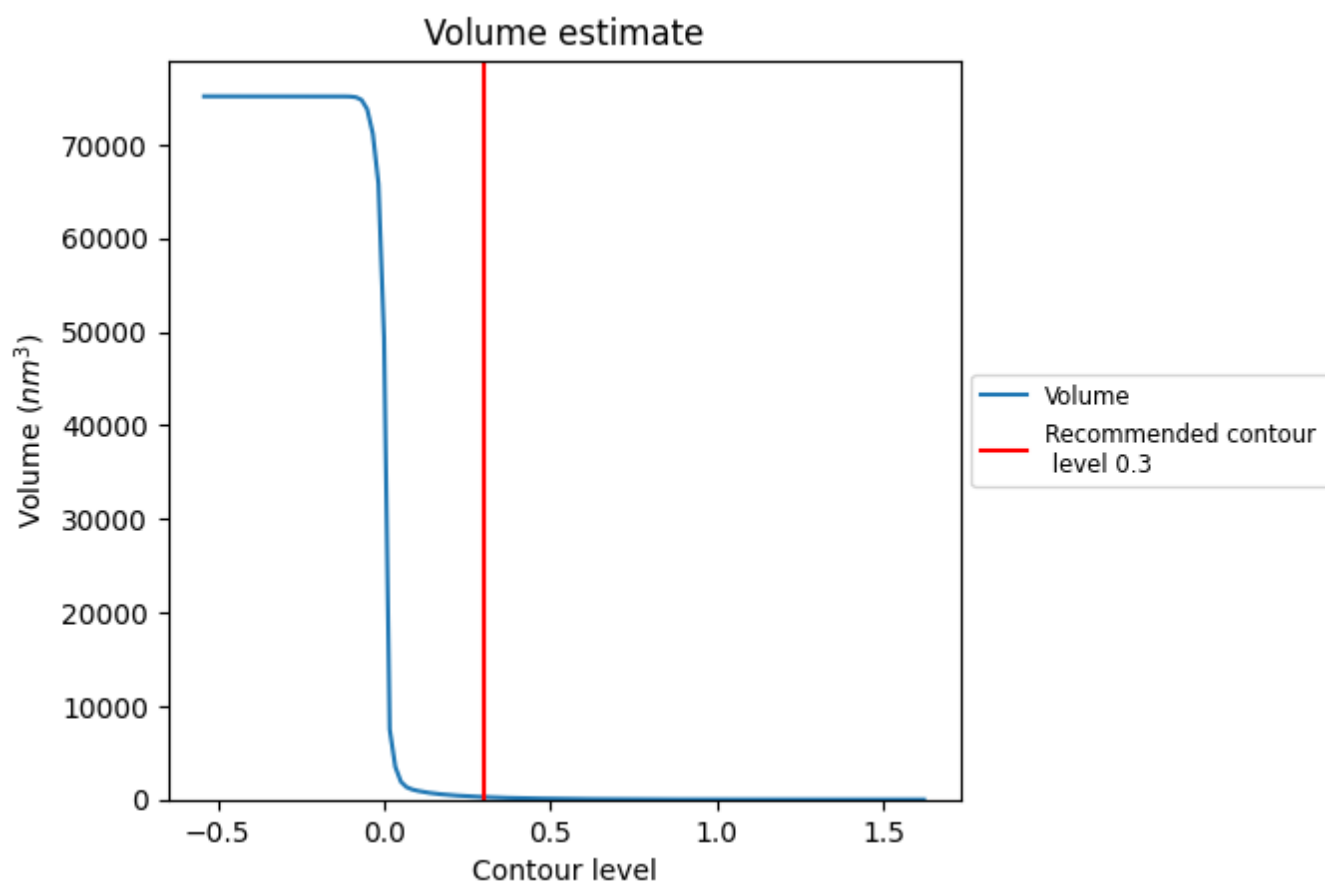
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

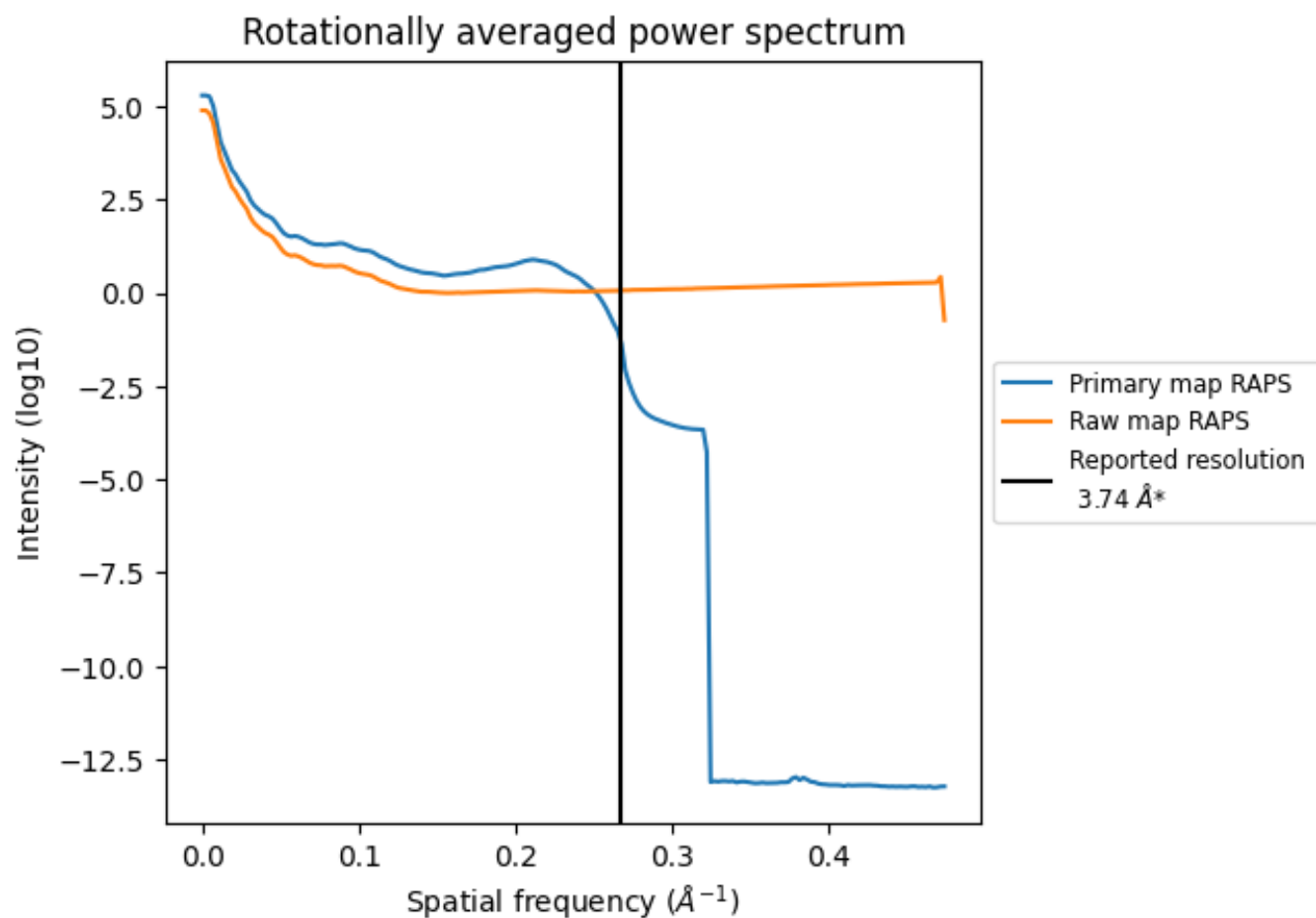
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 271 nm^3 ; this corresponds to an approximate mass of 245 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

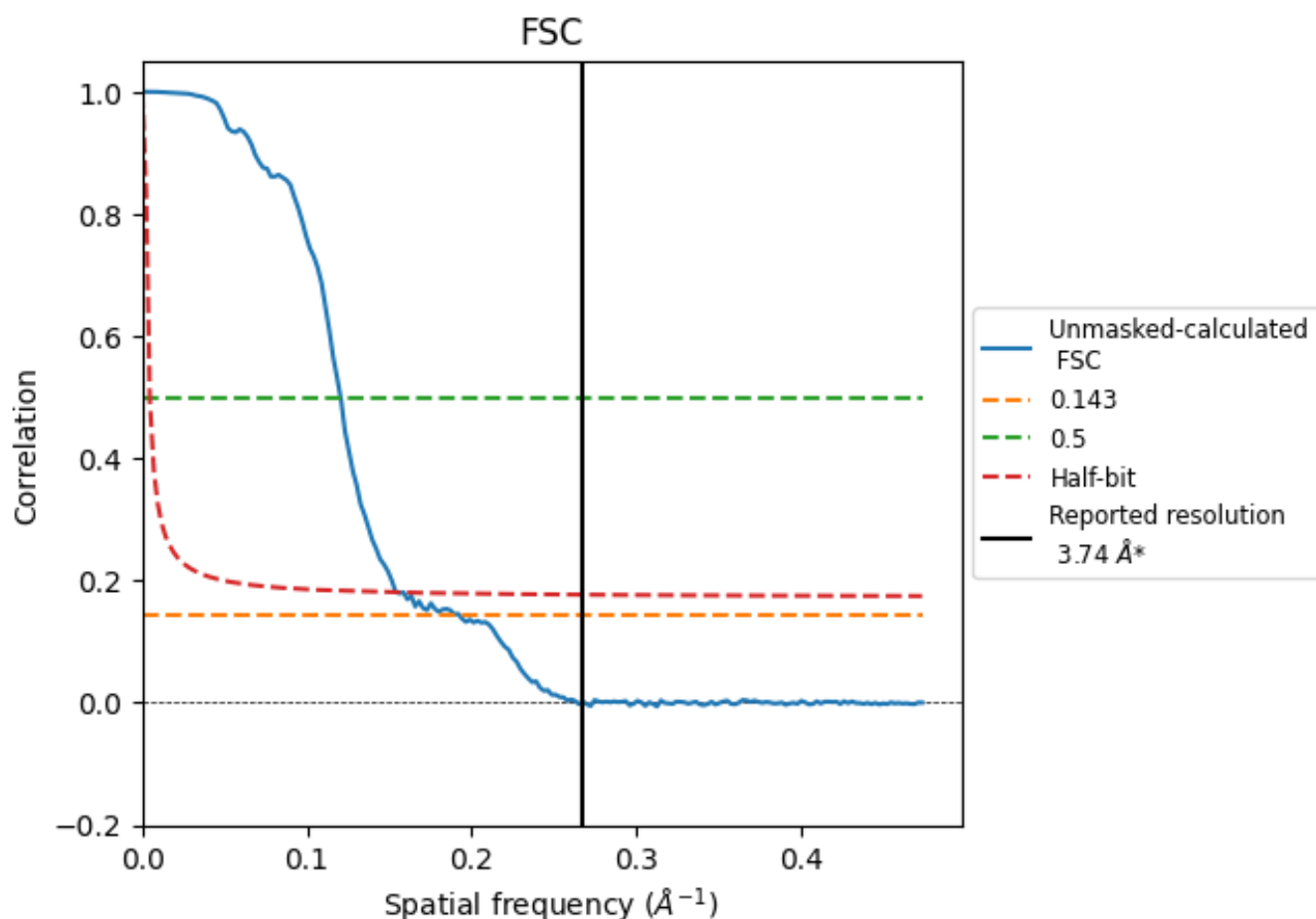


*Reported resolution corresponds to spatial frequency of 0.267 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.267 Å⁻¹

8.2 Resolution estimates [i](#)

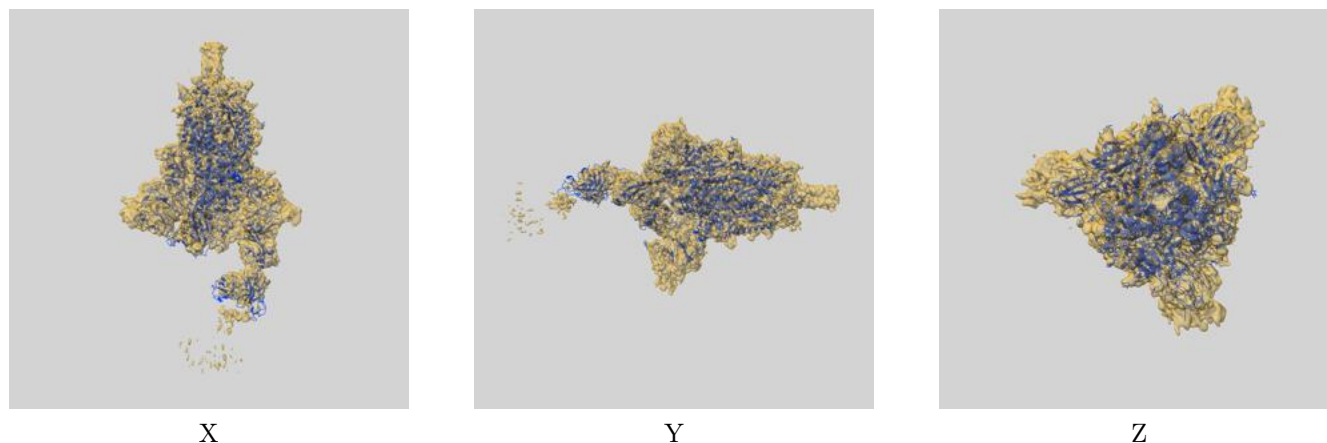
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.74	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	5.19	8.30	6.46

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.19 differs from the reported value 3.74 by more than 10 %

9 Map-model fit [i](#)

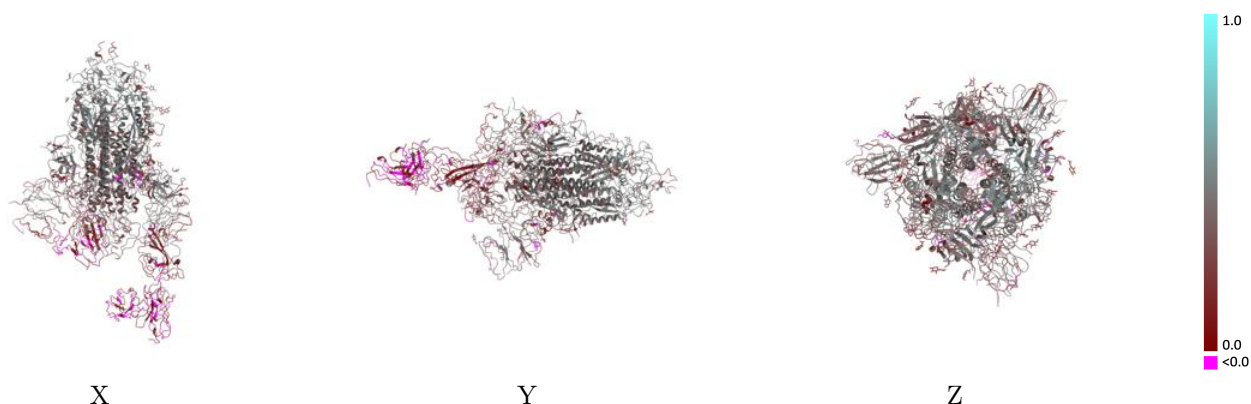
This section contains information regarding the fit between EMDB map EMD-34164 and PDB model 8GNH. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



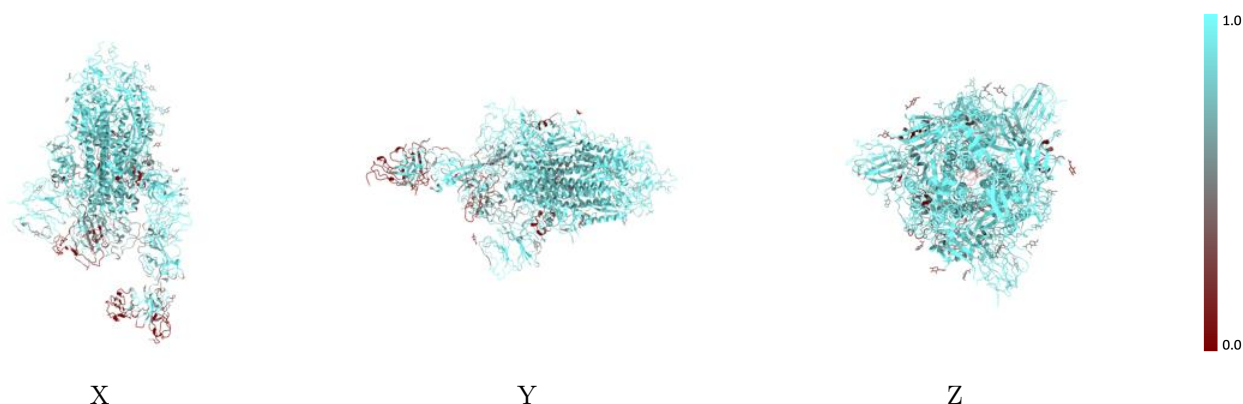
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



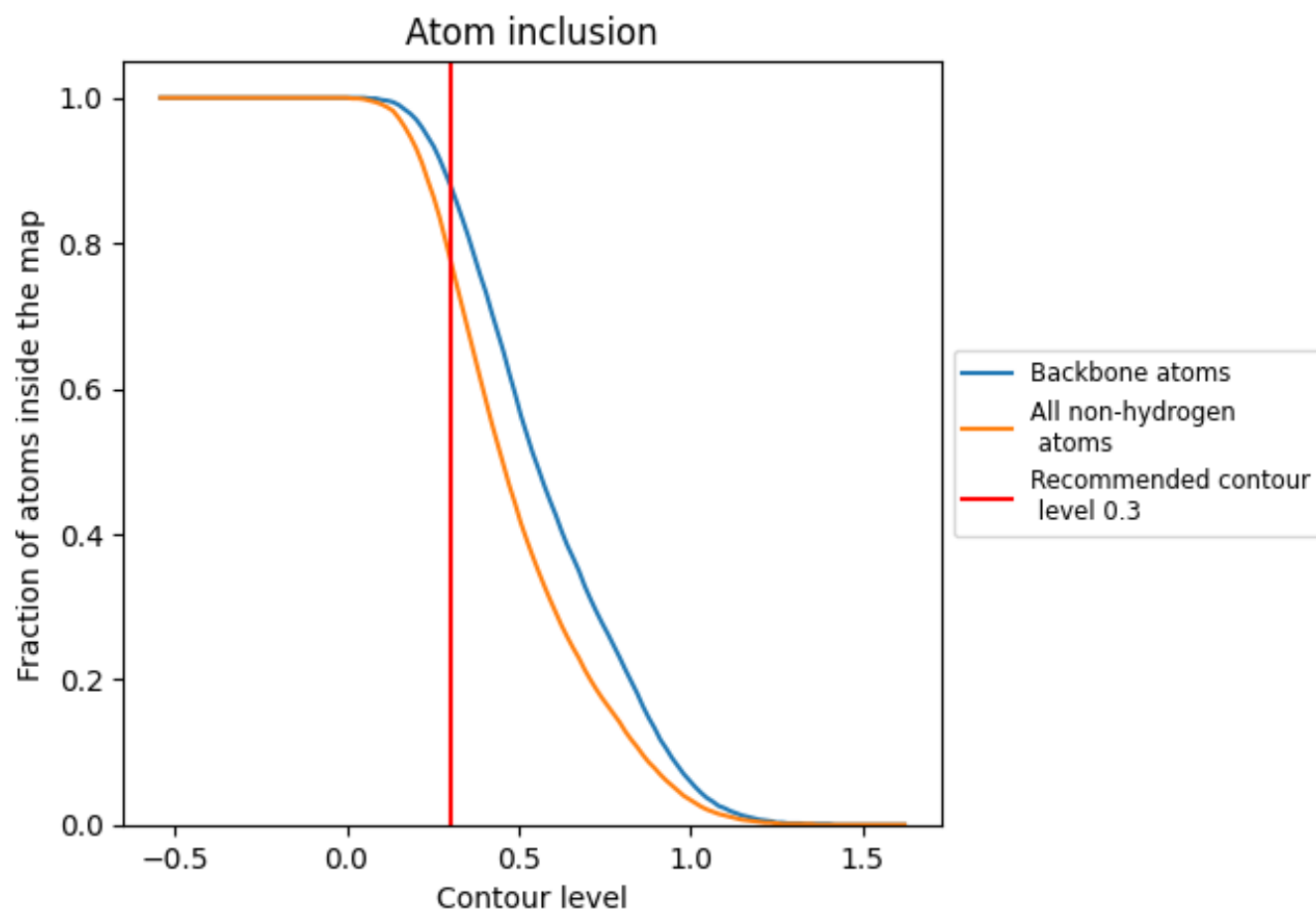
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7820	0.3500
A	0.8150	0.3810
B	0.8300	0.3660
C	0.7830	0.3600
D	0.6070	0.1810
H	0.4320	0.0870
L	0.3180	0.0720
N	0.7860	0.1780

1.0

0.0

<0.0