



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 12:18 AM UTC

PDB ID : 7EEB / pdb_00007eeb
EMDB ID : EMD-31076
Title : Structure of the CatSpermasome
Authors : Wu, J.P.; Ke, M.
Deposited on : 2021-03-18
Resolution : 2.90 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:

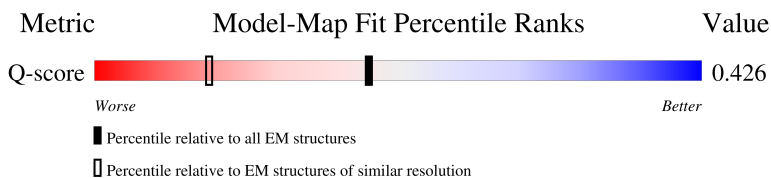
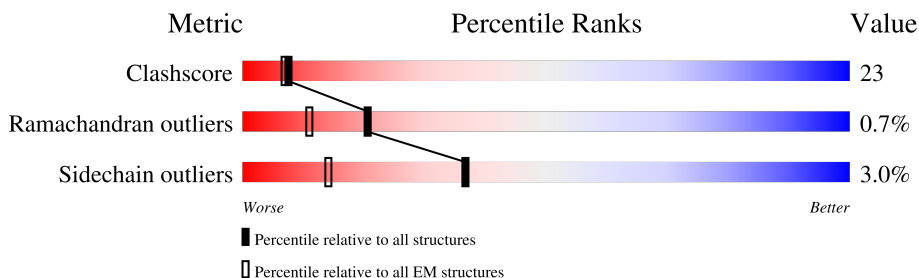
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.90 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	13054 (2.40 - 3.40)

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	955	5% (red), 15% (orange), 11% (yellow), 73% (grey)
2	B	588	20% (red), 28% (orange), 19% (yellow), 52% (grey)
3	C	395	18% (red), 50% (orange), 20% (yellow), 30% (grey)
4	D	442	8% (red), 38% (orange), 17% (yellow), 45% (grey)

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Mol	Chain	Length	Quality of chain
5	E	1109	58% 30% 5% 5%
6	F	1145	65% 22% 9%
7	G	805	60% 25% 11%
8	H	985	64% 28% 7%
9	L	706	48% 35% 15%
10	J	171	82% 12% 6%
11	M	116	60% 37%
12	N	28	93% 7%
13	I	216	78% 19%
14	K	194	69% 26%
15	O	7	29% 43% 29%
16	P	2	50% 50%
16	S	2	50% 50%
16	T	2	50% 50%
16	V	2	100%
16	X	2	50% 50%
16	a	2	100%
16	d	2	50% 50%
17	Q	3	33% 33% 33%
17	R	3	33% 67%
17	U	3	100%
17	W	3	67% 33%
17	b	3	67% 33%
18	Y	5	40% 20% 40% 40%
18	c	5	80% 20%

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Mol	Chain	Length	Quality of chain
19	Z	7	

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
16	NAG	X	1	-	-	X	-
17	NAG	U	1	-	-	X	-
18	NAG	c	1	-	-	X	-
18	NAG	c	2	-	-	X	-
19	NAG	Z	1	-	-	X	-

2 Entry composition i

There are 22 unique types of molecules in this entry. The entry contains 47874 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 Enhanced green fluorescent protein, Cation channel sperm-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	258	2112	1422	322	357	11	0	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-268	ASP	-	expression tag	UNP C5MKY7
A	-267	TYR	-	expression tag	UNP C5MKY7
A	-266	LYS	-	expression tag	UNP C5MKY7
A	-265	ASP	-	expression tag	UNP C5MKY7
A	-264	HIS	-	expression tag	UNP C5MKY7
A	-263	ASP	-	expression tag	UNP C5MKY7
A	-262	GLY	-	expression tag	UNP C5MKY7
A	-261	ASP	-	expression tag	UNP C5MKY7
A	-260	TYR	-	expression tag	UNP C5MKY7
A	-259	LYS	-	expression tag	UNP C5MKY7
A	-258	ASP	-	expression tag	UNP C5MKY7
A	-257	HIS	-	expression tag	UNP C5MKY7
A	-256	ASP	-	expression tag	UNP C5MKY7
A	-255	ILE	-	expression tag	UNP C5MKY7
A	-254	ASP	-	expression tag	UNP C5MKY7
A	-253	TYR	-	expression tag	UNP C5MKY7
A	-252	LYS	-	expression tag	UNP C5MKY7
A	-251	ASP	-	expression tag	UNP C5MKY7
A	-250	ASP	-	expression tag	UNP C5MKY7
A	-249	ASP	-	expression tag	UNP C5MKY7
A	-248	ASP	-	expression tag	UNP C5MKY7
A	-247	LYS	-	expression tag	UNP C5MKY7
A	-7	GLU	-	linker	UNP C5MKY7
A	-6	ASN	-	linker	UNP C5MKY7
A	-5	LEU	-	linker	UNP C5MKY7
A	-4	TYR	-	linker	UNP C5MKY7
A	-3	PHE	-	linker	UNP C5MKY7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLN	-	linker	UNP C5MKY7
A	-1	GLY	-	linker	UNP C5MKY7
A	0	SER	-	linker	UNP C5MKY7

- Molecule 2 is a protein called Cation channel sperm-associated protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	281	2343	1585	363	384	11	0	0

- Molecule 3 is a protein called Cation channel sperm-associated protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	278	2277	1506	359	400	12	0	0

- Molecule 4 is a protein called Cation channel sperm-associated protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	242	1965	1325	300	325	15	0	0

- Molecule 5 is a protein called Cation channel sperm-associated protein subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	1053	8470	5502	1387	1537	44	0	0

- Molecule 6 is a protein called Cation channel sperm-associated protein subunit gamma 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	1042	8454	5515	1354	1538	47	0	0

- Molecule 7 is a protein called Cation channel sperm-associated protein subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	714	5680	3669	923	1056	32	0	0

- Molecule 8 is a protein called Cation channel sperm-associated protein subunit epsilon.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	916	7502	4865	1208	1389	40	0	0

- Molecule 9 is a protein called Kazal-like domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	L	597	4694	3079	747	829	39	0	0

- Molecule 10 is a protein called Transmembrane protein 249.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	J	161	794	472	161	161	0	0

- Molecule 11 is a protein called Transmembrane protein 262.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	M	116	946	625	159	151	11	0	0

- Molecule 12 is a protein called Unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	N	28	140	84	28	28	0	0

- Molecule 13 is a protein called EF-hand calcium-binding domain-containing protein 9.

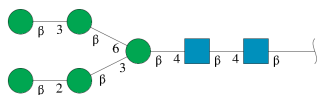
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	I	174	863	515	174	174	0	0

- Molecule 14 is a protein called Cation channel sperm-associated protein subunit zeta.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
14	K	143	710	424	143	143	0	0

- Molecule 15 is an oligosaccharide called beta-D-mannopyranose-(1-2)-beta-D-mannopyranos e-(1-3)-[beta-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopy

ranose.



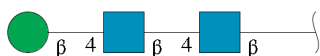
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
15	O	7	83	46	2	35	0	0

- Molecule 16 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
16	P	2	28	16	2	10	0	0
16	S	2	28	16	2	10	0	0
16	T	2	28	16	2	10	0	0
16	V	2	28	16	2	10	0	0
16	X	2	28	16	2	10	0	0
16	a	2	28	16	2	10	0	0
16	d	2	28	16	2	10	0	0

- Molecule 17 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



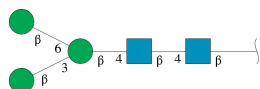
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
17	Q	3	39	22	2	15	0	0

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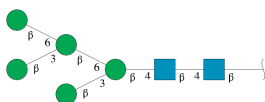
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
17	R	3	Total	C	N	O	0	0
			39	22	2	15		
17	U	3	Total	C	N	O	0	0
			39	22	2	15		
17	W	3	Total	C	N	O	0	0
			39	22	2	15		
17	b	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 18 is an oligosaccharide called beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
18	Y	5	Total	C	N	O	0	0
			61	34	2	25		
18	c	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 19 is an oligosaccharide called beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-6)-[beta-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
19	Z	7	Total	C	N	O	0	0
			83	46	2	35		

- Molecule 20 is SODIUM ION (CCD ID: NA) (formula: Na).

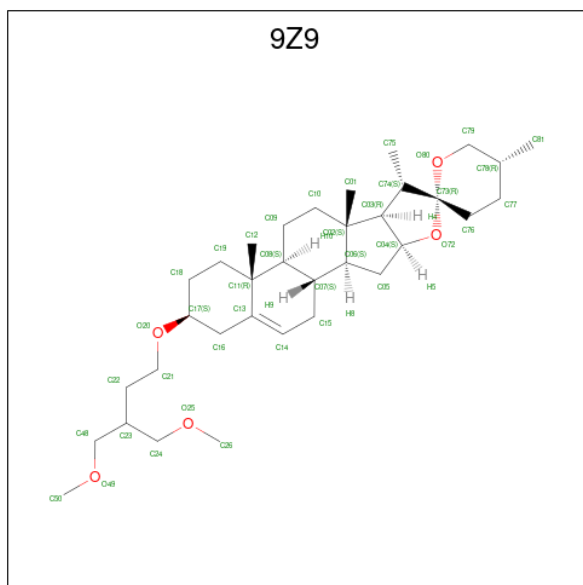
Mol	Chain	Residues	Atoms	AltConf
20	A	1	Total Na 1 1	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	Na	
20	D	1	1	1	0

- Molecule 21 is (3beta,14beta,17beta,25R)-3-[4-methoxy-3-(methoxymethyl)butoxy]spirost-5-en (CCD ID: 9Z9) (formula: $C_{34}H_{56}O_5$).

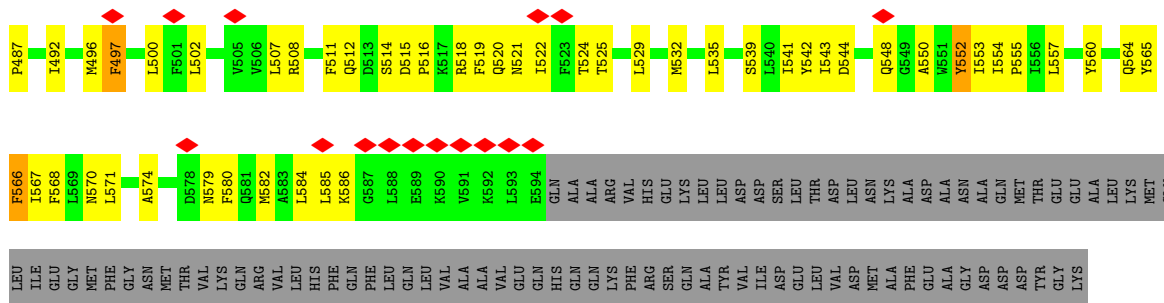


Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
21	A	1	39	34	5	0
21	A	1	39	34	5	0
21	A	1	39	34	5	0

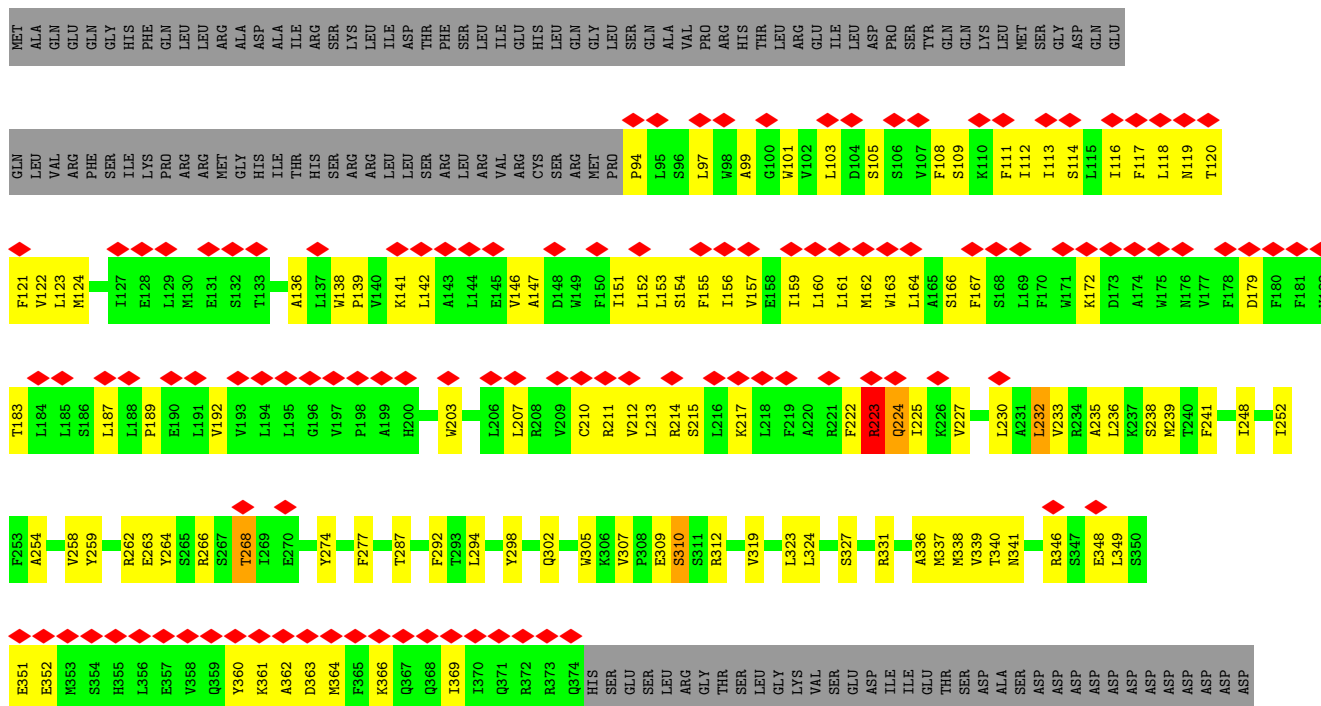
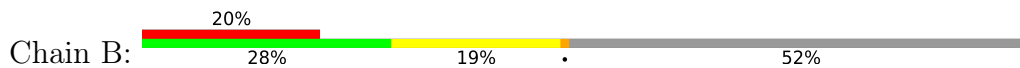
- Molecule 22 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



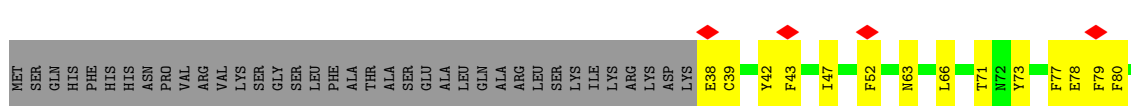
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
22	E	1	Total 14	C 8	N 1	O 5	0
22	E	1	Total 14	C 8	N 1	O 5	0
22	E	1	Total 14	C 8	N 1	O 5	0
22	E	1	Total 14	C 8	N 1	O 5	0
22	F	1	Total 14	C 8	N 1	O 5	0
22	G	1	Total 14	C 8	N 1	O 5	0
22	G	1	Total 14	C 8	N 1	O 5	0
22	G	1	Total 14	C 8	N 1	O 5	0
22	H	1	Total 14	C 8	N 1	O 5	0

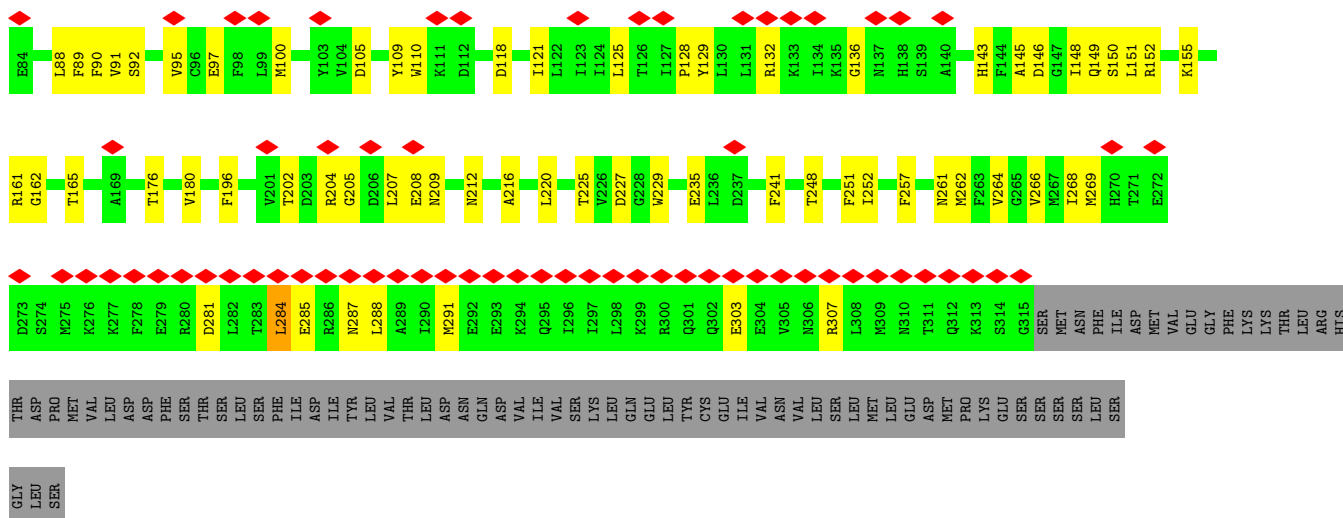


• Molecule 2: Cation channel sperm-associated protein 2

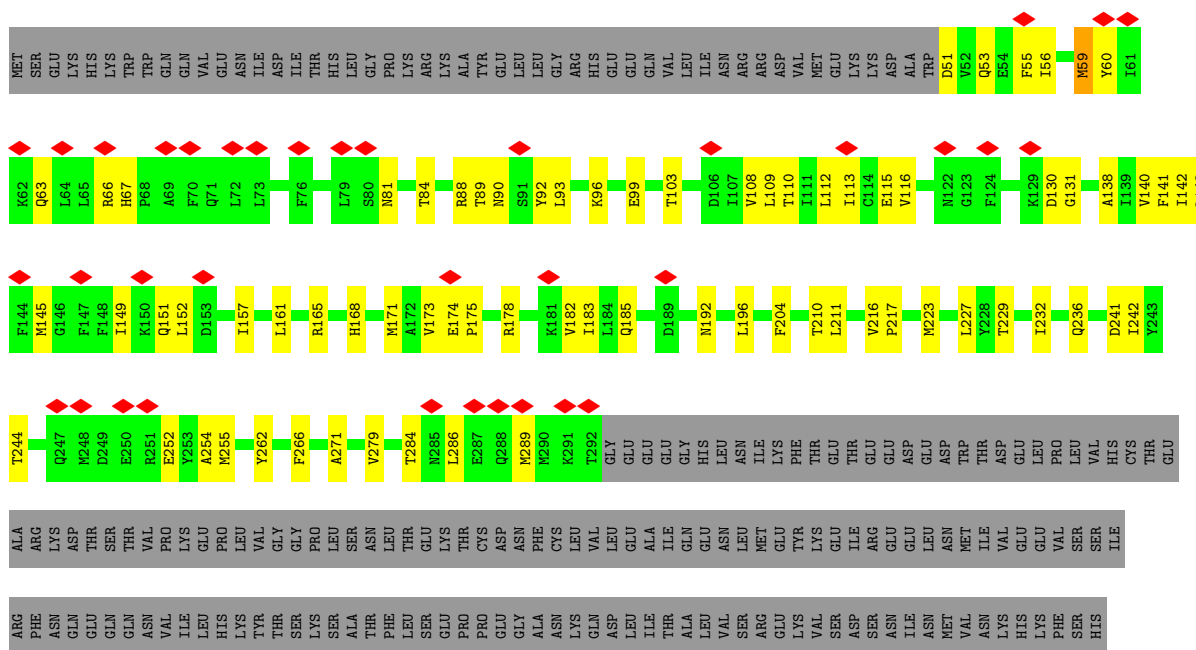


• Molecule 3: Cation channel sperm-associated protein 3

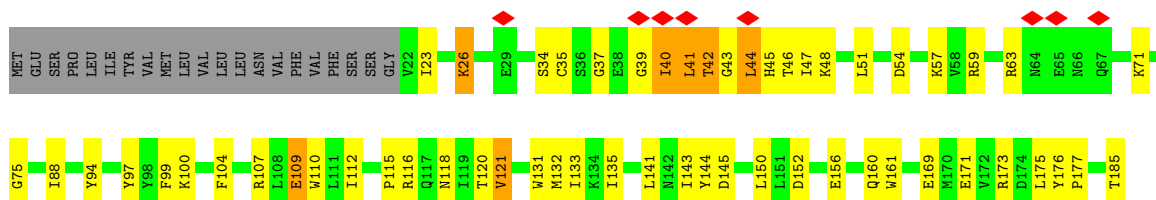


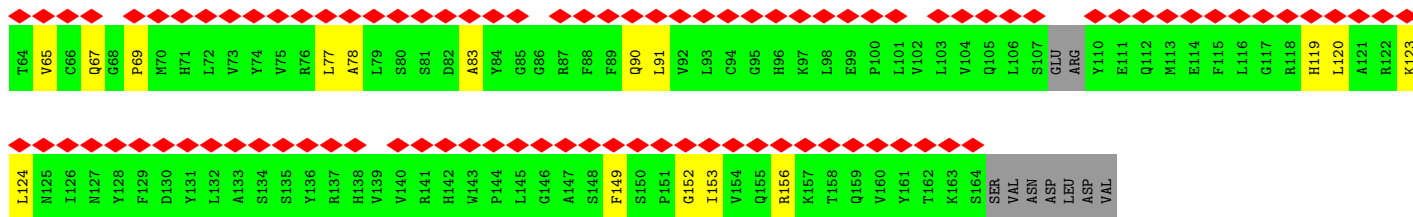


• Molecule 4: Cation channel sperm-associated protein 4

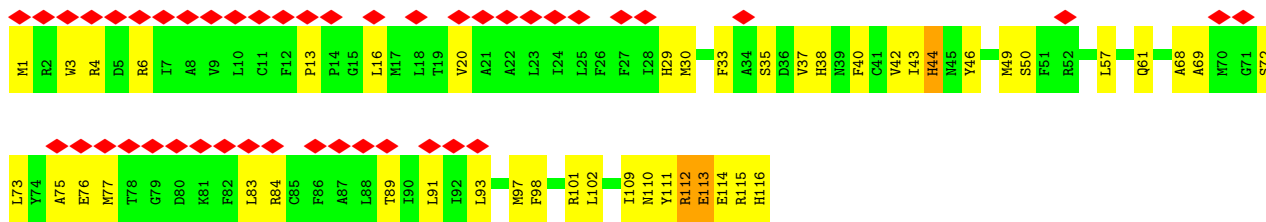
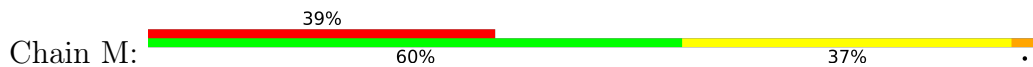


• Molecule 5: Cation channel sperm-associated protein subunit beta

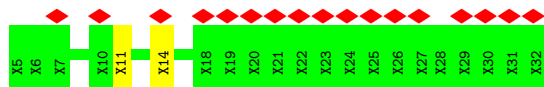
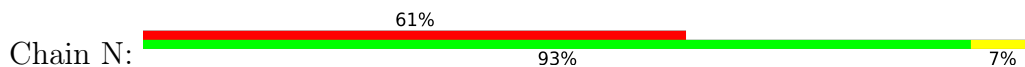




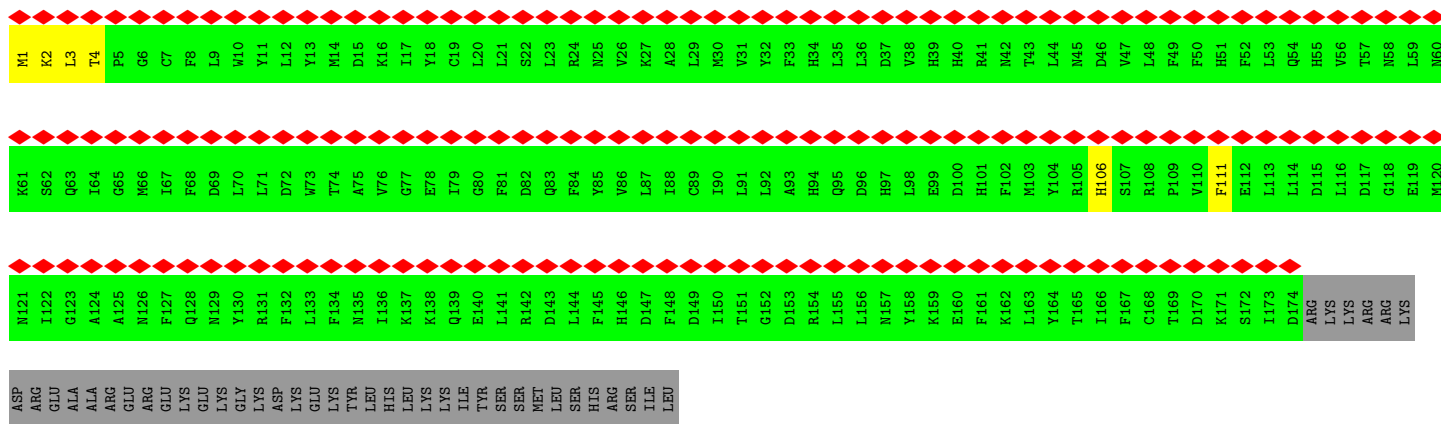
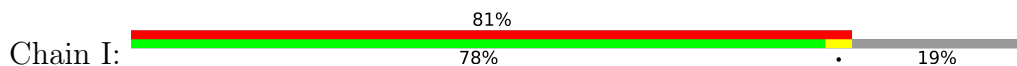
• Molecule 11: Transmembrane protein 262



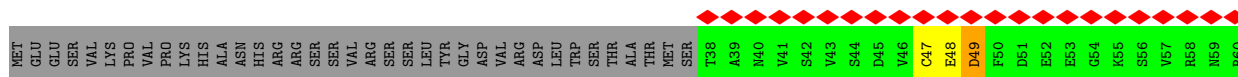
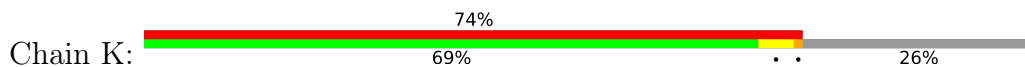
• Molecule 12: Unknown

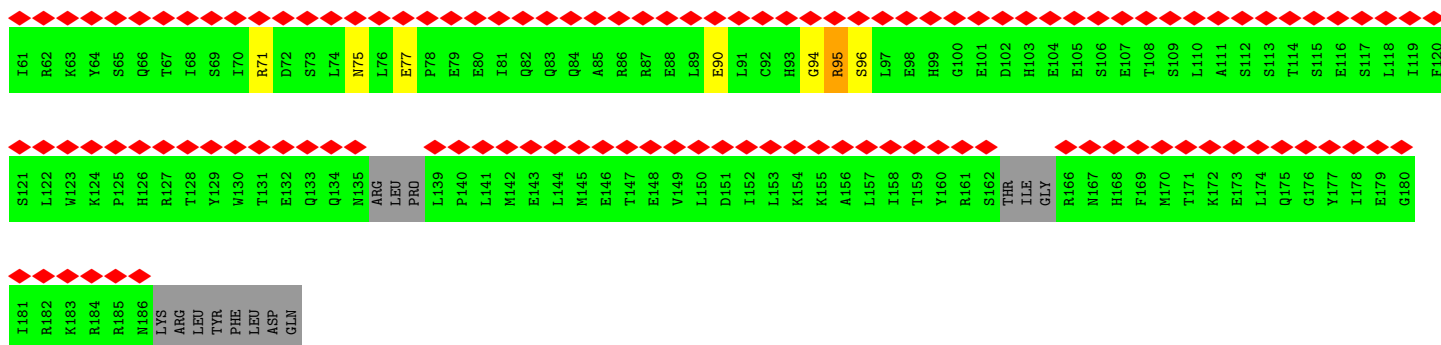


• Molecule 13: EF-hand calcium-binding domain-containing protein 9



• Molecule 14: Cation channel sperm-associated protein subunit zeta





- Molecule 15: beta-D-mannopyranose-(1-2)-beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 16: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 16: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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- Molecule 16: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



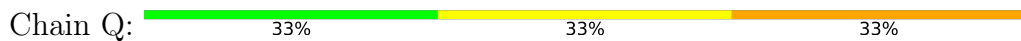
- Molecule 16: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



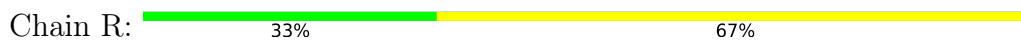
- Molecule 16: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



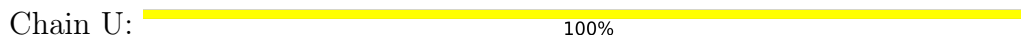
- Molecule 17: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 17: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 17: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





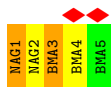
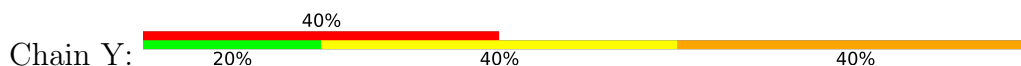
- Molecule 17: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



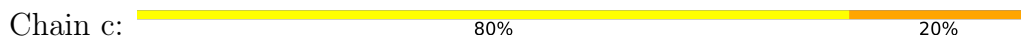
- Molecule 17: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 18: beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 18: beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 19: beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-6)-[beta-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	560730	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.093	Depositor
Minimum map value	-2.371	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.083	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	430.91998, 430.91998, 430.91998	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0773, 1.0773, 1.0773	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NA, NAG, 9Z9

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	0.40	0/2159	0.70	3/2933 (0.1%)
2	B	0.39	0/2406	0.66	3/3270 (0.1%)
3	C	0.34	0/2324	0.51	0/3141
4	D	0.37	0/2015	0.53	0/2739
5	E	0.61	13/8706 (0.1%)	0.94	49/11819 (0.4%)
6	F	0.59	23/8695 (0.3%)	0.78	26/11809 (0.2%)
7	G	0.42	1/5823 (0.0%)	0.74	13/7921 (0.2%)
8	H	0.32	0/7706	0.57	7/10491 (0.1%)
9	L	0.29	0/4817	0.51	2/6543 (0.0%)
10	J	0.33	0/791	0.51	0/1096
11	M	0.37	0/972	0.62	0/1314
13	I	1.18	0/862	1.50	1/1201 (0.1%)
14	K	0.72	0/707	1.25	5/982 (0.5%)
All	All	0.49	37/47983 (0.1%)	0.75	109/65259 (0.2%)

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	807	ILE	C-O	-9.34	1.13	1.24
6	F	442	ILE	C-O	-8.38	1.14	1.23
5	E	999	LYS	C-O	-7.89	1.14	1.24
6	F	138	TYR	C-O	-7.81	1.14	1.24
6	F	498	ASN	C-O	-7.66	1.15	1.24
6	F	351	VAL	C-O	-7.44	1.16	1.24
6	F	691	LYS	C-O	-7.15	1.14	1.24
6	F	229	LYS	C-O	-6.94	1.15	1.23
6	F	731	ILE	C-O	-6.64	1.15	1.24
6	F	468	THR	C-O	-6.50	1.17	1.23
5	E	719	GLN	C-O	-6.49	1.15	1.23
6	F	501	GLU	C-O	-6.45	1.16	1.24
6	F	603	LEU	C-O	-6.21	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	82	LEU	C-O	-6.15	1.16	1.24
6	F	252	ILE	C-O	-6.10	1.17	1.24
6	F	467	TYR	C-O	-6.05	1.16	1.23
5	E	109	GLU	C-O	-6.05	1.16	1.23
6	F	260	LYS	C-O	-5.92	1.16	1.23
5	E	427	GLY	C-O	-5.79	1.16	1.23
5	E	556	PRO	C-O	-5.75	1.16	1.23
7	G	264	SER	C-O	-5.52	1.17	1.24
6	F	641	LEU	C-O	-5.49	1.17	1.24
6	F	914	CYS	C-O	-5.47	1.17	1.23
5	E	1041	LEU	C-O	-5.47	1.17	1.23
5	E	886	ASN	C-O	-5.46	1.17	1.24
6	F	916	LEU	C-O	-5.44	1.17	1.23
6	F	1039	SER	C-O	-5.41	1.17	1.24
5	E	832	SER	CA-CB	-5.36	1.46	1.53
5	E	695	PHE	C-O	-5.36	1.17	1.23
6	F	627	ALA	C-O	-5.31	1.17	1.23
5	E	696	LEU	C-O	-5.28	1.18	1.24
6	F	259	GLU	C-O	-5.25	1.17	1.23
6	F	335	ARG	C-O	-5.25	1.17	1.23
5	E	721	ASN	C-O	-5.19	1.16	1.24
6	F	497	TYR	C-O	-5.18	1.17	1.24
5	E	329	SER	C-O	-5.12	1.17	1.24
6	F	465	VAL	C-O	-5.01	1.18	1.23

All (109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	471	ILE	N-CA-C	-9.98	102.95	112.83
5	E	655	ASP	CA-C-N	8.46	133.30	121.96
5	E	655	ASP	C-N-CA	8.46	133.30	121.96
5	E	895	PRO	N-CA-C	8.05	124.71	113.53
9	L	486	ASN	N-CA-C	-8.03	102.53	111.28
2	B	222	PHE	CA-C-N	7.82	130.61	120.44
2	B	222	PHE	C-N-CA	7.82	130.61	120.44
14	K	95	ARG	N-CA-C	-7.64	100.42	110.43
8	H	875	GLY	N-CA-C	7.38	121.06	112.50
6	F	270	GLN	N-CA-C	-7.35	103.57	112.54
5	E	770	GLY	N-CA-C	7.24	121.25	112.49
6	F	951	ARG	N-CA-C	-6.98	103.67	111.28
5	E	692	ASN	N-CA-C	-6.82	101.53	110.53
6	F	466	THR	CA-C-O	-6.79	113.80	121.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	223	ARG	N-CA-C	6.74	118.28	111.07
5	E	46	THR	CA-C-N	-6.71	114.13	123.13
5	E	46	THR	C-N-CA	-6.71	114.13	123.13
5	E	1041	LEU	N-CA-C	-6.65	98.86	109.76
6	F	613	LEU	CA-C-O	-6.60	111.12	120.16
5	E	757	MET	N-CA-C	-6.58	102.32	110.41
6	F	953	LEU	N-CA-C	-6.46	102.00	110.53
6	F	1022	PRO	O-C-N	6.39	124.15	121.15
5	E	891	ASP	N-CA-C	-6.35	97.77	108.94
7	G	719	LYS	N-CA-C	-6.33	104.38	111.28
8	H	756	ARG	CA-C-N	6.28	130.40	121.42
8	H	756	ARG	C-N-CA	6.28	130.40	121.42
5	E	648	LEU	N-CA-C	-6.24	105.65	113.20
7	G	185	THR	CB-CA-C	-6.21	100.49	110.79
5	E	897	PRO	N-CA-C	6.18	122.12	113.53
5	E	1053	PRO	N-CA-C	6.16	122.27	113.47
7	G	184	ASN	CA-C-N	6.15	128.52	120.28
7	G	184	ASN	C-N-CA	6.15	128.52	120.28
5	E	805	THR	CA-C-O	-6.13	114.47	121.40
5	E	757	MET	CA-C-O	-6.10	115.04	121.99
8	H	875	GLY	CA-C-O	-6.06	114.45	121.00
7	G	571	ARG	CA-C-O	-5.97	114.76	121.81
5	E	917	THR	CA-CB-OG1	-5.97	100.65	109.60
5	E	283	PHE	N-CA-C	-5.94	100.32	109.52
5	E	283	PHE	CA-C-N	-5.88	113.35	122.59
5	E	283	PHE	C-N-CA	-5.88	113.35	122.59
5	E	292	ILE	CA-C-N	-5.82	113.33	122.65
5	E	292	ILE	C-N-CA	-5.82	113.33	122.65
5	E	913	CYS	CA-C-N	5.82	130.52	120.58
5	E	913	CYS	C-N-CA	5.82	130.52	120.58
5	E	803	GLY	CA-C-O	-5.79	115.27	121.35
7	G	662	TRP	CA-C-N	5.79	126.25	120.52
7	G	662	TRP	C-N-CA	5.79	126.25	120.52
7	G	183	MET	CA-C-N	5.78	129.08	120.87
7	G	183	MET	C-N-CA	5.78	129.08	120.87
5	E	610	ILE	O-C-N	5.76	129.40	122.03
6	F	955	THR	CA-CB-OG1	-5.76	100.97	109.60
5	E	760	PHE	CA-C-N	-5.72	112.80	119.32
5	E	760	PHE	C-N-CA	-5.72	112.80	119.32
5	E	42	THR	CA-CB-OG1	-5.70	101.05	109.60
14	K	49	ASP	CA-C-N	5.70	128.48	120.28
14	K	49	ASP	C-N-CA	5.70	128.48	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	627	ALA	CA-C-O	-5.68	114.80	121.44
6	F	903	PHE	CA-C-N	-5.65	112.63	122.64
6	F	903	PHE	C-N-CA	-5.65	112.63	122.64
5	E	336	PRO	N-CA-C	-5.62	102.38	111.03
5	E	1039	CYS	CA-C-O	-5.61	114.15	120.32
5	E	288	ARG	N-CA-C	-5.59	105.28	111.71
6	F	642	ILE	CA-C-O	-5.56	115.77	121.67
5	E	318	PHE	CB-CA-C	-5.55	101.25	110.14
1	A	469	LEU	N-CA-C	-5.54	105.24	111.28
7	G	571	ARG	N-CA-C	-5.53	103.09	110.55
6	F	351	VAL	N-CA-C	-5.50	99.63	107.77
5	E	557	LEU	CA-C-O	-5.45	115.78	121.55
6	F	627	ALA	CA-C-N	5.35	129.17	122.43
6	F	627	ALA	C-N-CA	5.35	129.17	122.43
6	F	1036	VAL	CA-C-O	-5.34	114.70	120.47
8	H	939	TYR	CA-C-N	-5.33	113.35	120.54
8	H	939	TYR	C-N-CA	-5.33	113.35	120.54
5	E	656	VAL	N-CA-C	-5.32	100.53	107.88
5	E	1056	PHE	O-C-N	5.32	125.61	120.55
6	F	498	ASN	N-CA-C	-5.30	99.77	108.41
6	F	1038	ASN	CB-CA-C	-5.28	101.27	110.09
6	F	612	ASN	N-CA-C	-5.27	102.24	110.10
5	E	285	GLY	N-CA-C	-5.25	108.37	115.36
6	F	612	ASN	CA-C-O	-5.25	114.94	120.92
6	F	613	LEU	N-CA-C	5.22	121.34	109.81
7	G	235	SER	CA-C-O	-5.22	116.13	121.87
5	E	884	THR	CA-C-O	-5.21	115.03	120.55
7	G	580	LYS	CA-C-N	5.19	125.09	119.85
7	G	580	LYS	C-N-CA	5.19	125.09	119.85
6	F	613	LEU	CA-C-N	-5.19	114.23	119.83
6	F	613	LEU	C-N-CA	-5.19	114.23	119.83
13	I	106	HIS	CB-CA-C	-5.16	110.64	116.63
5	E	807	ILE	CA-C-O	-5.16	114.97	120.59
5	E	994	ASN	N-CA-C	-5.16	107.66	114.31
5	E	692	ASN	CA-C-O	-5.14	115.90	121.87
5	E	656	VAL	CA-C-O	-5.13	116.65	120.96
8	H	949	MET	N-CA-C	-5.11	105.71	111.28
9	L	484	LEU	N-CA-C	-5.10	102.50	110.10
5	E	1052	VAL	CA-C-N	5.08	124.25	118.97
5	E	1052	VAL	C-N-CA	5.08	124.25	118.97
5	E	948	PHE	CA-CB-CG	-5.06	108.74	113.80
5	E	657	GLU	CA-C-N	5.06	130.53	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	657	GLU	C-N-CA	5.06	130.53	122.59
5	E	109	GLU	CA-C-N	5.04	128.36	120.75
5	E	109	GLU	C-N-CA	5.04	128.36	120.75
6	F	468	THR	CA-C-O	-5.03	115.33	121.67
1	A	566	PHE	N-CA-C	5.03	116.84	111.36
6	F	1015	ILE	CA-C-O	-5.03	115.16	120.39
6	F	1016	ILE	CA-C-O	-5.02	116.40	119.51
14	K	77	GLU	CA-C-N	5.02	125.04	119.32
14	K	77	GLU	C-N-CA	5.02	125.04	119.32
6	F	468	THR	CA-CB-OG1	-5.01	102.08	109.60
5	E	632	TYR	CB-CA-C	-5.00	102.75	110.26

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2112	0	2211	161	0
2	B	2343	0	2435	133	0
3	C	2277	0	2339	90	0
4	D	1965	0	2022	64	0
5	E	8470	0	8412	564	0
6	F	8454	0	8306	305	0
7	G	5680	0	5593	371	0
8	H	7502	0	7359	325	0
9	L	4694	0	4699	216	0
10	J	794	0	346	11	0
11	M	946	0	950	72	0
12	N	140	0	30	1	0
13	I	863	0	370	1	0
14	K	710	0	297	5	0
15	O	83	0	70	1	0
16	P	28	0	25	1	0
16	S	28	0	25	2	0
16	T	28	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	V	28	0	25	2	0
16	X	28	0	25	9	0
16	a	28	0	25	3	0
16	d	28	0	25	0	0
17	Q	39	0	34	1	0
17	R	39	0	34	3	0
17	U	39	0	34	11	0
17	W	39	0	34	3	0
17	b	39	0	34	4	0
18	Y	61	0	52	4	0
18	c	61	0	52	21	0
19	Z	83	0	70	18	0
20	A	1	0	0	0	0
20	D	1	0	0	0	0
21	A	117	0	0	20	0
22	E	56	0	52	2	0
22	F	14	0	13	2	0
22	G	42	0	39	3	0
22	H	14	0	13	1	0
All	All	47874	0	46075	2158	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 23.

All (2158) 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:535:LEU:HD11	1:A:565:TYR:CD2	1.32	1.62
8:H:91:ASN:HD21	16:V:1:NAG:C1	1.03	1.58
8:H:888:ASN:HD21	18:c:1:NAG:C1	1.07	1.58
8:H:292:ASN:HD22	16:X:1:NAG:C1	1.04	1.58
8:H:565:ASN:HD22	19:Z:1:NAG:C1	0.93	1.52
5:E:759:THR:HG22	6:F:861:TYR:CZ	1.47	1.46
1:A:378:ILE:HD12	6:F:903:PHE:CE2	1.53	1.44
7:G:165:ILE:CG2	7:G:166:PRO:HD3	1.47	1.41
8:H:565:ASN:ND2	19:Z:1:NAG:C1	1.72	1.40
8:H:888:ASN:ND2	18:c:1:NAG:C1	1.80	1.40
8:H:91:ASN:ND2	16:V:1:NAG:C1	1.86	1.38
1:A:535:LEU:CD1	1:A:565:TYR:CD2	2.07	1.37
5:E:948:PHE:CE1	5:E:1052:VAL:HG13	1.65	1.31
1:A:378:ILE:CD1	6:F:903:PHE:CE2	2.13	1.31

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:153:LEU:HD13	8:H:949:MET:SD	1.71	1.31
8:H:292:ASN:ND2	16:X:1:NAG:C1	1.90	1.30
7:G:579:TRP:O	7:G:678:ILE:CG2	1.80	1.30
5:E:1023:SER:CB	5:E:1052:VAL:HG21	1.62	1.29
7:G:663:PRO:HG3	17:U:2:NAG:C6	1.60	1.28
5:E:643:LEU:CD1	5:E:694:LYS:NZ	1.95	1.28
8:H:933:ILE:CD1	8:H:934:PRO:HD2	1.65	1.27
1:A:535:LEU:CD1	1:A:565:TYR:HD2	1.41	1.27
5:E:761:PRO:HG2	6:F:861:TYR:O	1.32	1.25
9:L:565:LEU:O	9:L:568:PRO:HD2	1.12	1.25
5:E:996:LYS:O	5:E:1000:HIS:HD2	1.15	1.25
9:L:472:ALA:HB1	9:L:512:GLU:CB	1.67	1.25
7:G:571:ARG:NH2	7:G:707:PHE:HB2	1.53	1.24
5:E:646:ASN:ND2	5:E:647:PRO:HD2	1.50	1.24
7:G:721:GLN:CG	7:G:722:PRO:HD3	1.68	1.24
5:E:646:ASN:HD22	5:E:647:PRO:CD	1.49	1.23
7:G:516:GLN:NE2	7:G:518:LYS:CE	2.01	1.23
8:H:933:ILE:HD12	8:H:934:PRO:CD	1.68	1.23
6:F:1020:ILE:O	6:F:1021:TYR:CG	1.93	1.22
7:G:721:GLN:HG2	7:G:722:PRO:CD	1.71	1.21
1:A:467:ARG:HH22	21:A:703:9Z9:C26	1.53	1.21
5:E:895:PRO:O	5:E:896:ILE:HD13	1.34	1.21
5:E:689:ILE:O	5:E:690:LYS:HG2	1.04	1.20
7:G:723:LEU:O	7:G:727:LEU:HG	1.40	1.20
3:C:80:PHE:CD2	7:G:716:PRO:HG2	1.77	1.18
7:G:663:PRO:CG	17:U:2:NAG:H62	1.71	1.18
1:A:378:ILE:HD12	6:F:903:PHE:CZ	1.80	1.17
5:E:643:LEU:HD11	5:E:694:LYS:NZ	1.57	1.16
7:G:516:GLN:NE2	7:G:518:LYS:HE3	1.60	1.16
5:E:759:THR:HG22	6:F:861:TYR:CE2	1.81	1.15
5:E:895:PRO:O	5:E:896:ILE:CD1	1.94	1.14
9:L:634:TYR:CB	9:L:648:ILE:HD12	1.76	1.14
5:E:895:PRO:C	5:E:896:ILE:HD12	1.71	1.14
6:F:257:TYR:O	6:F:297:THR:CG2	1.94	1.14
5:E:428:SER:O	5:E:446:LEU:HB2	1.44	1.14
3:C:42:TYR:HB2	7:G:746:GLN:HG3	1.25	1.13
6:F:1020:ILE:HG23	6:F:1021:TYR:CE1	1.81	1.13
8:H:565:ASN:HD22	19:Z:1:NAG:C2	1.59	1.13
3:C:73:TYR:CE1	7:G:715:LEU:HD21	1.84	1.13
5:E:996:LYS:O	5:E:1000:HIS:CD2	2.01	1.13
6:F:1008:GLU:HA	6:F:1013:TYR:CD2	1.82	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:721:ASN:HD22	5:E:721:ASN:N	1.46	1.12
7:G:575:TYR:CE1	7:G:714:ALA:HB2	1.83	1.12
7:G:682:GLN:HA	7:G:714:ALA:CB	1.79	1.12
8:H:758:PHE:CZ	9:L:553:ILE:HD11	1.84	1.12
5:E:916:VAL:HG21	5:E:921:MET:HB2	1.26	1.11
7:G:516:GLN:HB2	7:G:582:VAL:HG13	1.30	1.11
5:E:689:ILE:O	5:E:690:LYS:CG	1.98	1.11
5:E:895:PRO:C	5:E:896:ILE:CD1	2.22	1.11
8:H:933:ILE:HD12	8:H:934:PRO:HD2	1.16	1.11
5:E:1052:VAL:CG1	11:M:116:HIS:CE1	2.33	1.10
7:G:165:ILE:HG21	7:G:192:THR:CA	1.82	1.10
2:B:153:LEU:CD1	8:H:949:MET:SD	2.39	1.10
5:E:646:ASN:HD22	5:E:647:PRO:HD2	0.93	1.10
9:L:565:LEU:O	9:L:568:PRO:CD	2.00	1.09
7:G:165:ILE:HG23	7:G:166:PRO:CD	1.81	1.09
7:G:165:ILE:HB	7:G:193:GLY:O	1.52	1.09
7:G:575:TYR:HD1	7:G:714:ALA:N	1.51	1.09
3:C:42:TYR:CB	7:G:746:GLN:HG3	1.82	1.08
5:E:1057:PRO:HG3	11:M:112:ARG:NE	1.68	1.07
9:L:547:ASP:OD1	9:L:548:ASP:N	1.88	1.07
21:A:702:9Z9:C26	21:A:704:9Z9:C23	2.33	1.07
5:E:629:GLU:OE2	5:E:631:THR:HG22	1.52	1.07
5:E:762:ILE:HG13	6:F:195:PHE:CZ	1.89	1.07
5:E:762:ILE:CG2	5:E:763:PRO:HD2	1.85	1.07
6:F:641:LEU:CD1	6:F:750:ILE:HD11	1.84	1.07
7:G:579:TRP:O	7:G:678:ILE:HG22	0.90	1.07
7:G:516:GLN:NE2	7:G:518:LYS:HE2	1.66	1.06
11:M:113:GLU:HG3	11:M:114:GLU:H	1.20	1.06
2:B:223:ARG:H	2:B:223:ARG:HD3	1.15	1.05
5:E:759:THR:CG2	6:F:861:TYR:CZ	2.38	1.05
6:F:257:TYR:O	6:F:297:THR:HG22	1.53	1.05
5:E:886:ASN:HD22	5:E:886:ASN:N	1.53	1.05
8:H:750:LYS:HD3	8:H:750:LYS:H	1.17	1.05
9:L:472:ALA:HB1	9:L:512:GLU:HB3	1.35	1.05
2:B:223:ARG:HH22	2:B:224:GLN:CG	1.70	1.05
7:G:165:ILE:CG2	7:G:193:GLY:H	1.69	1.05
8:H:870:PHE:CE1	18:c:2:NAG:H5	1.91	1.05
5:E:962:GLU:HG3	5:E:963:ARG:H	1.20	1.04
6:F:1020:ILE:O	6:F:1021:TYR:CD2	2.10	1.04
7:G:165:ILE:HG21	7:G:192:THR:HA	1.06	1.04
7:G:579:TRP:C	7:G:678:ILE:HG22	1.80	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:559:MET:HE2	5:E:563:ILE:O	1.58	1.04
1:A:377:GLU:O	1:A:381:GLU:HG2	1.58	1.03
7:G:575:TYR:O	7:G:576:ASP:HB2	1.54	1.03
7:G:715:LEU:HB3	7:G:716:PRO:HD2	1.40	1.03
5:E:762:ILE:HG23	5:E:763:PRO:HD2	1.38	1.03
5:E:1023:SER:HB3	5:E:1052:VAL:CG2	1.86	1.03
7:G:165:ILE:CG2	7:G:166:PRO:CD	2.35	1.03
9:L:472:ALA:HB1	9:L:512:GLU:CG	1.88	1.02
2:B:262:ARG:O	2:B:266:ARG:HG3	1.59	1.02
5:E:1023:SER:HB3	5:E:1052:VAL:HG21	1.05	1.01
5:E:1052:VAL:HG12	11:M:116:HIS:CE1	1.94	1.01
8:H:871:SER:HB2	8:H:874:ILE:HB	1.43	1.00
7:G:720:PHE:CD2	7:G:722:PRO:HD2	1.96	1.00
1:A:519:PHE:HB2	1:A:525:THR:HG22	1.43	1.00
6:F:189:THR:CG2	6:F:191:GLY:H	1.73	1.00
7:G:571:ARG:HH21	7:G:708:SER:H	1.04	1.00
5:E:1023:SER:CB	5:E:1052:VAL:CG2	2.40	1.00
8:H:870:PHE:HE1	18:c:2:NAG:H3	1.24	0.99
1:A:439:SER:HB2	6:F:1003:GLU:OE2	1.60	0.99
5:E:759:THR:HG22	6:F:861:TYR:CE1	1.97	0.99
5:E:890:ALA:O	5:E:919:ARG:NH1	1.94	0.99
8:H:292:ASN:ND2	16:X:1:NAG:O7	1.94	0.99
6:F:641:LEU:HD11	6:F:750:ILE:HD11	1.42	0.99
7:G:212:VAL:HG21	7:G:236:TYR:CE2	1.98	0.99
7:G:572:LEU:HD12	7:G:573:VAL:N	1.77	0.99
2:B:223:ARG:HH22	2:B:224:GLN:HG3	1.24	0.99
7:G:717:VAL:HG22	7:G:719:LYS:CE	1.91	0.98
5:E:1057:PRO:HG3	11:M:112:ARG:CD	1.91	0.98
5:E:948:PHE:CE1	5:E:1052:VAL:CG1	2.45	0.98
7:G:682:GLN:HA	7:G:714:ALA:HB3	1.41	0.98
2:B:223:ARG:HH21	2:B:223:ARG:HB2	1.27	0.98
5:E:685:MET:HA	5:E:687:GLN:HE22	1.27	0.98
5:E:960:PHE:HE1	5:E:965:LYS:HD2	1.26	0.98
7:G:571:ARG:HH21	7:G:708:SER:N	1.62	0.98
8:H:840:ASN:CG	8:H:876:LYS:O	2.07	0.97
1:A:467:ARG:NH2	21:A:703:9Z9:C26	2.25	0.97
9:L:476:GLU:O	9:L:477:ASP:O	1.81	0.97
5:E:902:HIS:O	5:E:905:LYS:HG2	1.63	0.97
5:E:916:VAL:CG2	5:E:921:MET:HB2	1.95	0.97
7:G:516:GLN:HE22	7:G:518:LYS:CE	1.70	0.97
7:G:575:TYR:CD1	7:G:714:ALA:HB2	1.98	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:901:HIS:HD2	6:F:903:PHE:CE2	1.83	0.97
7:G:165:ILE:CG2	7:G:192:THR:HA	1.94	0.97
8:H:755:ARG:NH1	9:L:552:PHE:CD1	2.33	0.96
1:A:550:ALA:HB3	1:A:552:TYR:CZ	2.00	0.96
5:E:759:THR:CG2	6:F:861:TYR:CE2	2.48	0.96
7:G:571:ARG:NH2	7:G:708:SER:H	1.62	0.96
5:E:721:ASN:H	5:E:721:ASN:ND2	1.53	0.95
7:G:573:VAL:CG1	7:G:711:VAL:HG22	1.95	0.95
5:E:755:LYS:HE2	5:E:755:LYS:HA	1.45	0.95
8:H:752:ARG:NH1	8:H:753:CYS:HB3	1.81	0.95
5:E:23:ILE:HB	5:E:26:LYS:HG3	1.48	0.95
7:G:575:TYR:CD1	7:G:714:ALA:N	2.34	0.95
1:A:535:LEU:HD12	1:A:565:TYR:CE2	2.01	0.95
6:F:452:GLU:HB3	6:F:468:THR:HG23	1.48	0.95
6:F:901:HIS:CD2	6:F:903:PHE:HE2	1.85	0.95
6:F:266:ASP:O	6:F:267:SER:OG	1.85	0.95
7:G:184:ASN:HB3	7:G:187:LYS:NZ	1.81	0.95
5:E:1023:SER:CA	5:E:1052:VAL:HG21	1.97	0.94
8:H:565:ASN:CB	19:Z:1:NAG:C1	2.45	0.94
7:G:719:LYS:H	7:G:719:LYS:HD3	1.30	0.94
5:E:1057:PRO:CG	11:M:112:ARG:HD3	1.98	0.94
7:G:165:ILE:HG22	7:G:166:PRO:HD3	1.48	0.94
5:E:559:MET:HE2	5:E:563:ILE:C	1.93	0.93
5:E:643:LEU:CD1	5:E:694:LYS:HZ2	1.82	0.93
21:A:703:9Z9:C48	21:A:704:9Z9:C26	2.47	0.93
8:H:933:ILE:HD12	8:H:934:PRO:N	1.83	0.93
8:H:292:ASN:HD22	16:X:1:NAG:C2	1.82	0.93
1:A:535:LEU:CD1	1:A:565:TYR:CE2	2.51	0.92
8:H:565:ASN:CG	19:Z:1:NAG:C1	2.42	0.92
1:A:579:ASN:HA	1:A:582:MET:HE2	1.49	0.92
7:G:165:ILE:HG23	7:G:166:PRO:HD3	0.92	0.92
2:B:142:LEU:HB2	8:H:941:VAL:CG1	1.99	0.92
5:E:609:ILE:CG2	5:E:611:VAL:O	2.18	0.92
1:A:361:VAL:HG21	1:A:461:ARG:HG2	1.51	0.92
5:E:989:HIS:HE1	5:E:999:LYS:HZ3	1.01	0.91
6:F:916:LEU:HD23	6:F:918:ARG:HG2	1.49	0.91
7:G:722:PRO:O	7:G:723:LEU:HD23	1.70	0.91
5:E:643:LEU:HD11	5:E:694:LYS:HZ3	1.32	0.91
8:H:752:ARG:HG3	8:H:752:ARG:HH11	1.36	0.91
5:E:870:ASN:HB2	5:E:897:PRO:HD3	1.53	0.91
1:A:566:PHE:O	1:A:570:ASN:ND2	2.04	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:157:PHE:CE2	7:G:200:HIS:CE1	2.59	0.91
2:B:142:LEU:HB2	8:H:941:VAL:HG12	1.50	0.91
1:A:378:ILE:CD1	6:F:903:PHE:HE2	1.84	0.90
3:C:73:TYR:HE1	7:G:715:LEU:HD21	1.25	0.90
8:H:888:ASN:HD21	18:c:1:NAG:C2	1.83	0.90
5:E:755:LYS:O	5:E:756:ALA:HB2	1.70	0.90
5:E:1057:PRO:HG3	11:M:112:ARG:HD3	1.53	0.90
9:L:472:ALA:HB1	9:L:512:GLU:HG2	1.52	0.90
6:F:907:ILE:HD12	6:F:907:ILE:H	1.35	0.90
9:L:472:ALA:CB	9:L:512:GLU:CB	2.49	0.90
6:F:1061:ARG:HH21	6:F:1061:ARG:HG2	1.36	0.90
5:E:286:PHE:CE2	5:E:320:ARG:NH1	2.40	0.90
5:E:913:CYS:SG	5:E:922:CYS:CB	2.59	0.90
8:H:919:CYS:HB2	16:a:1:NAG:H82	1.53	0.90
5:E:762:ILE:CG1	6:F:195:PHE:CZ	2.54	0.89
6:F:904:ASP:OD1	6:F:905:CYS:N	2.04	0.89
7:G:516:GLN:HB2	7:G:582:VAL:CG1	2.01	0.89
5:E:557:LEU:O	5:E:558:THR:OG1	1.88	0.89
7:G:575:TYR:HD1	7:G:714:ALA:H	1.13	0.89
7:G:717:VAL:HG22	7:G:719:LYS:HE2	1.51	0.89
8:H:888:ASN:CG	18:c:1:NAG:C1	2.46	0.89
5:E:989:HIS:CE1	5:E:999:LYS:NZ	2.40	0.89
8:H:292:ASN:ND2	16:X:1:NAG:C2	2.36	0.89
5:E:989:HIS:HE1	5:E:999:LYS:NZ	1.69	0.89
6:F:892:ILE:HD11	6:F:913:PRO:CB	2.03	0.89
5:E:559:MET:CE	5:E:563:ILE:O	2.20	0.89
6:F:901:HIS:HD2	6:F:903:PHE:HE2	0.94	0.89
1:A:467:ARG:HH12	21:A:703:9Z9:C26	1.85	0.89
7:G:663:PRO:HG3	17:U:2:NAG:H62	0.89	0.89
8:H:870:PHE:CD1	18:c:2:NAG:O4	2.26	0.89
5:E:249:LEU:CD1	5:E:254:LEU:HD13	2.03	0.89
6:F:265:SER:OG	6:F:271:ASP:O	1.91	0.89
9:L:486:ASN:O	9:L:488:THR:N	2.04	0.89
3:C:42:TYR:CG	7:G:746:GLN:HG3	2.08	0.89
6:F:966:ARG:HG3	6:F:972:ASP:OD2	1.73	0.88
8:H:759:SER:OG	8:H:776:LYS:HE2	1.73	0.88
5:E:287:GLU:HB2	5:E:289:VAL:HG12	1.53	0.88
5:E:643:LEU:HD11	5:E:694:LYS:HZ2	1.36	0.88
6:F:1016:ILE:HD12	6:F:1016:ILE:H	1.39	0.88
7:G:575:TYR:CE1	7:G:714:ALA:CB	2.57	0.88
6:F:257:TYR:O	6:F:297:THR:HG21	1.71	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:L:634:TYR:CG	9:L:648:ILE:HD12	2.09	0.88
2:B:309:GLU:O	2:B:310:SER:OG	1.91	0.88
8:H:870:PHE:CZ	18:c:2:NAG:H5	2.08	0.88
3:C:42:TYR:HB2	7:G:746:GLN:CG	2.05	0.87
6:F:355:GLY:HA3	6:F:412:ALA:HB1	1.56	0.87
6:F:498:ASN:HD22	8:H:183:THR:HG21	1.38	0.87
9:L:474:ILE:HD12	9:L:648:ILE:HG12	1.54	0.87
5:E:585:LEU:N	5:E:611:VAL:CG2	2.37	0.87
6:F:189:THR:HG23	6:F:191:GLY:H	1.39	0.87
1:A:378:ILE:HD13	6:F:903:PHE:CE2	2.09	0.86
5:E:643:LEU:CD1	5:E:694:LYS:HZ1	1.86	0.86
5:E:692:ASN:O	5:E:693:LEU:HD23	1.74	0.86
5:E:389:LYS:NZ	6:F:163:GLU:OE2	2.07	0.86
5:E:948:PHE:CD1	5:E:1052:VAL:HG13	2.11	0.86
2:B:223:ARG:HB2	2:B:223:ARG:NH2	1.90	0.86
8:H:933:ILE:HD13	8:H:934:PRO:HD2	1.56	0.86
8:H:752:ARG:HH12	8:H:753:CYS:HB3	1.41	0.86
5:E:989:HIS:CE1	5:E:999:LYS:HZ3	1.89	0.86
8:H:839:ILE:HG21	8:H:872:TYR:CD1	2.11	0.86
5:E:23:ILE:CB	5:E:26:LYS:HG3	2.06	0.85
5:E:945:ARG:NE	5:E:1050:ASP:OD1	2.09	0.85
5:E:1052:VAL:HG12	11:M:116:HIS:ND1	1.90	0.85
5:E:249:LEU:HD12	5:E:254:LEU:HD13	1.57	0.85
5:E:286:PHE:HD2	5:E:290:ASP:CB	1.88	0.85
5:E:643:LEU:HD12	5:E:694:LYS:NZ	1.92	0.85
7:G:163:GLY:HA3	7:G:168:THR:HG21	1.59	0.85
7:G:184:ASN:HB3	7:G:187:LYS:HZ2	1.37	0.85
8:H:292:ASN:HD21	16:X:1:NAG:C7	1.90	0.85
8:H:839:ILE:HG21	8:H:872:TYR:HD1	1.40	0.85
5:E:948:PHE:HE1	5:E:1052:VAL:HG13	1.35	0.84
6:F:620:VAL:HG22	6:F:621:ASN:H	1.42	0.84
9:L:634:TYR:HB3	9:L:648:ILE:HD12	1.57	0.84
1:A:414:PRO:HG2	21:A:703:9Z9:C18	2.06	0.84
7:G:184:ASN:O	7:G:187:LYS:HG3	1.76	0.84
9:L:269:LEU:HB2	9:L:419:LEU:HD13	1.58	0.84
7:G:157:PHE:CE2	7:G:200:HIS:ND1	2.45	0.84
1:A:382:TRP:CZ2	6:F:1016:ILE:HG23	2.12	0.84
7:G:720:PHE:CE2	7:G:722:PRO:HD2	2.12	0.84
1:A:382:TRP:CZ2	6:F:1016:ILE:CG2	2.60	0.84
3:C:80:PHE:CD2	7:G:716:PRO:CG	2.61	0.84
8:H:870:PHE:CE1	18:c:2:NAG:H3	2.11	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:721:GLN:HG2	7:G:722:PRO:HD3	0.87	0.84
9:L:465:GLU:CD	9:L:655:VAL:HG13	2.01	0.84
3:C:42:TYR:OH	7:G:742:ALA:HB1	1.77	0.84
5:E:832:SER:O	5:E:834:LEU:N	2.11	0.83
7:G:719:LYS:HD3	7:G:719:LYS:N	1.92	0.83
6:F:641:LEU:HD12	6:F:750:ILE:HD11	1.58	0.83
11:M:46:TYR:CE2	11:M:111:TYR:HE2	1.96	0.83
3:C:80:PHE:HD2	7:G:716:PRO:HG2	1.41	0.83
5:E:689:ILE:C	5:E:690:LYS:HG2	2.02	0.83
2:B:223:ARG:NH2	2:B:224:GLN:HG3	1.93	0.83
3:C:73:TYR:HE1	7:G:715:LEU:CD2	1.92	0.83
5:E:1052:VAL:HG11	11:M:116:HIS:CE1	2.13	0.83
5:E:1057:PRO:CG	11:M:112:ARG:CD	2.56	0.83
7:G:682:GLN:HG3	7:G:714:ALA:HB1	1.61	0.83
5:E:656:VAL:HG13	5:E:671:MET:O	1.80	0.82
7:G:579:TRP:N	7:G:678:ILE:O	2.10	0.82
7:G:720:PHE:CZ	7:G:722:PRO:HG2	2.15	0.82
1:A:519:PHE:HA	1:A:524:THR:HG23	1.60	0.82
6:F:1020:ILE:O	6:F:1021:TYR:CD1	2.33	0.82
5:E:870:ASN:O	5:E:897:PRO:HD2	1.78	0.82
7:G:573:VAL:HG13	7:G:711:VAL:HG22	1.59	0.82
9:L:546:SER:O	9:L:547:ASP:HB2	1.79	0.82
7:G:157:PHE:HE2	7:G:200:HIS:ND1	1.78	0.81
9:L:488:THR:HA	9:L:492:ASN:HD22	1.44	0.81
8:H:919:CYS:CB	16:a:1:NAG:H82	2.09	0.81
5:E:761:PRO:HD3	6:F:860:THR:HB	1.61	0.81
5:E:960:PHE:CE1	5:E:965:LYS:HD2	2.14	0.81
6:F:498:ASN:O	6:F:500:GLU:N	2.13	0.81
7:G:375:MET:HE3	8:H:650:ASN:HB2	1.62	0.81
11:M:46:TYR:CE2	11:M:111:TYR:CE2	2.69	0.81
5:E:993:GLU:OE1	5:E:996:LYS:HG3	1.80	0.81
7:G:682:GLN:CA	7:G:714:ALA:CB	2.59	0.81
8:H:840:ASN:CB	8:H:876:LYS:O	2.29	0.81
8:H:939:TYR:HE2	9:L:566:LYS:HZ2	1.28	0.81
5:E:880:SER:C	5:E:881:ILE:HD12	2.06	0.81
1:A:483:SER:HA	21:A:702:9Z9:C12	2.11	0.81
5:E:632:TYR:OH	5:E:635:LYS:O	1.99	0.81
5:E:948:PHE:HB3	5:E:949:PRO:HD3	1.61	0.81
6:F:916:LEU:HD12	6:F:1053:HIS:CE1	2.15	0.81
5:E:961:ASN:HB3	5:E:964:ASP:OD1	1.81	0.80
6:F:279:ILE:HG22	6:F:281:SER:H	1.45	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:749:ASN:HB3	8:H:752:ARG:HB3	1.62	0.80
1:A:374:THR:HA	1:A:377:GLU:HG2	1.64	0.80
5:E:948:PHE:HB3	5:E:949:PRO:CD	2.12	0.80
2:B:268:THR:O	2:B:268:THR:CG2	2.28	0.80
5:E:879:ILE:CD1	5:E:1023:SER:OG	2.29	0.80
5:E:1050:ASP:O	5:E:1051:GLU:HB2	1.81	0.80
6:F:453:ALA:HB1	6:F:456:LEU:HB2	1.62	0.80
8:H:792:LEU:HD12	8:H:932:MET:SD	2.22	0.80
5:E:762:ILE:HG13	6:F:195:PHE:HZ	1.47	0.80
5:E:886:ASN:N	5:E:886:ASN:ND2	2.29	0.80
6:F:622:GLN:N	6:F:625:TYR:O	2.12	0.80
7:G:165:ILE:CG2	7:G:193:GLY:N	2.45	0.80
8:H:750:LYS:HD3	8:H:750:LYS:N	1.97	0.80
5:E:39:GLY:O	5:E:40:ILE:HG12	1.82	0.80
8:H:757:ASP:O	8:H:758:PHE:HD1	1.65	0.80
7:G:165:ILE:HG21	7:G:193:GLY:N	1.97	0.79
8:H:341:GLU:OE1	8:H:343:THR:HG23	1.83	0.79
9:L:472:ALA:CB	9:L:512:GLU:HB3	2.11	0.79
5:E:646:ASN:HD22	5:E:647:PRO:N	1.79	0.79
5:E:762:ILE:HG12	6:F:195:PHE:CE2	2.18	0.79
8:H:839:ILE:CG2	8:H:872:TYR:HD1	1.96	0.79
5:E:559:MET:HE3	5:E:563:ILE:HG22	1.62	0.79
7:G:188:LEU:HA	7:G:190:HIS:CE1	2.18	0.79
5:E:829:SER:O	5:E:830:SER:OG	2.00	0.78
6:F:1020:ILE:HG23	6:F:1021:TYR:CD1	2.19	0.78
8:H:565:ASN:ND2	19:Z:1:NAG:N2	2.31	0.78
6:F:966:ARG:HG2	6:F:976:SER:CB	2.14	0.78
8:H:839:ILE:HG21	8:H:872:TYR:HB2	1.63	0.78
5:E:774:LEU:HD12	5:E:775:VAL:HG23	1.65	0.78
2:B:235:ALA:HA	2:B:341:ASN:HD22	1.47	0.78
5:E:913:CYS:SG	5:E:922:CYS:HB2	2.22	0.78
7:G:215:ASN:OD1	7:G:237:LYS:HG3	1.84	0.78
7:G:239:LEU:HD12	7:G:239:LEU:N	1.99	0.78
9:L:462:PHE:HA	9:L:465:GLU:OE2	1.83	0.78
1:A:382:TRP:CH2	6:F:1016:ILE:HG22	2.18	0.78
8:H:598:GLN:HE22	19:Z:2:NAG:H83	1.49	0.78
5:E:559:MET:CE	5:E:563:ILE:HG22	2.14	0.78
7:G:516:GLN:CB	7:G:582:VAL:HG13	2.13	0.78
7:G:571:ARG:CZ	7:G:707:PHE:HB2	2.13	0.78
7:G:165:ILE:CG1	7:G:211:MET:HE1	2.14	0.78
9:L:286:LYS:HB3	9:L:526:VAL:HG11	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:281:LEU:HD22	8:H:319:VAL:HG11	1.66	0.77
5:E:685:MET:HA	5:E:687:GLN:NE2	1.97	0.77
5:E:870:ASN:HB2	5:E:897:PRO:CD	2.14	0.77
7:G:224:TYR:O	7:G:227:ASN:N	2.13	0.77
8:H:758:PHE:CE1	9:L:553:ILE:HD11	2.19	0.77
4:D:182:VAL:HG11	4:D:286:LEU:HD12	1.66	0.77
6:F:52:ASN:O	6:F:98:TYR:HA	1.85	0.77
8:H:749:ASN:ND2	8:H:752:ARG:HG2	1.99	0.77
1:A:483:SER:HB2	21:A:702:9Z9:C16	2.15	0.77
1:A:467:ARG:NH1	21:A:703:9Z9:C26	2.48	0.77
5:E:899:ASN:OD1	5:E:905:LYS:HB3	1.83	0.77
7:G:188:LEU:N	7:G:188:LEU:HD23	1.99	0.77
9:L:504:SER:HA	9:L:514:PHE:HA	1.66	0.77
7:G:184:ASN:ND2	7:G:186:ASP:OD2	2.17	0.77
7:G:516:GLN:CB	7:G:582:VAL:CG1	2.63	0.77
8:H:292:ASN:ND2	16:X:1:NAG:C7	2.47	0.77
6:F:501:GLU:OE1	8:H:179:LYS:HD3	1.86	0.76
5:E:621:SER:OG	5:E:655:ASP:OD2	2.03	0.76
8:H:852:ASN:HB2	8:H:855:ILE:HD13	1.67	0.76
5:E:489:LYS:HA	5:E:489:LYS:CE	2.15	0.76
6:F:186:ASP:OD1	6:F:200:ARG:HD3	1.85	0.76
11:M:57:LEU:HD23	11:M:101:ARG:HE	1.50	0.76
11:M:112:ARG:HB2	11:M:112:ARG:NH2	2.00	0.76
5:E:875:SER:HB2	5:E:883:LEU:HD12	1.67	0.76
9:L:548:ASP:OD1	9:L:549:GLU:N	2.18	0.76
2:B:138:TRP:HE3	2:B:139:PRO:CD	1.99	0.76
5:E:761:PRO:HB2	5:E:762:ILE:HD12	1.65	0.76
7:G:575:TYR:CD1	7:G:714:ALA:CB	2.68	0.76
8:H:840:ASN:HB3	8:H:876:LYS:O	1.86	0.76
11:M:113:GLU:HG3	11:M:114:GLU:N	1.92	0.76
7:G:157:PHE:HE2	7:G:200:HIS:CE1	2.02	0.76
9:L:634:TYR:CG	9:L:648:ILE:CD1	2.69	0.76
5:E:200:MET:HB2	5:E:243:THR:HG21	1.67	0.75
5:E:879:ILE:HD13	5:E:1023:SER:OG	1.84	0.75
7:G:720:PHE:CE2	7:G:722:PRO:CD	2.69	0.75
1:A:419:ASP:HB2	1:A:461:ARG:NH2	2.01	0.75
7:G:165:ILE:O	7:G:165:ILE:HD13	1.86	0.75
3:C:42:TYR:CE2	7:G:742:ALA:HB1	2.21	0.75
5:E:762:ILE:HG22	5:E:763:PRO:HD2	1.68	0.75
6:F:129:ILE:HG12	6:F:185:VAL:HG22	1.68	0.75
7:G:226:LEU:O	7:G:227:ASN:C	2.29	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:106:ILE:HG12	8:H:123:THR:HG22	1.68	0.75
4:D:60:TYR:HB3	5:E:1078:PHE:CE2	2.21	0.75
5:E:897:PRO:O	5:E:898:ARG:HD3	1.86	0.75
6:F:355:GLY:O	6:F:356:ASN:HB3	1.86	0.75
9:L:634:TYR:HB2	9:L:648:ILE:HD12	1.66	0.75
8:H:139:ASP:HB2	8:H:216:MET:HE2	1.69	0.75
2:B:223:ARG:HH21	2:B:223:ARG:CB	1.99	0.75
7:G:665:VAL:CG2	17:U:1:NAG:O7	2.35	0.75
5:E:555:VAL:HG13	5:E:559:MET:SD	2.26	0.75
5:E:755:LYS:HE2	5:E:755:LYS:CA	2.15	0.75
8:H:836:ASN:ND2	18:c:1:NAG:O6	2.20	0.75
1:A:382:TRP:HZ2	6:F:1016:ILE:HG23	1.50	0.75
5:E:897:PRO:C	5:E:898:ARG:HD3	2.11	0.75
9:L:430:GLY:HA2	9:L:586:ILE:HG21	1.68	0.75
6:F:1020:ILE:C	6:F:1021:TYR:CG	2.64	0.74
5:E:495:LEU:HD23	5:E:503:ILE:HD11	1.67	0.74
6:F:613:LEU:O	6:F:613:LEU:HD22	1.87	0.74
7:G:573:VAL:HG11	7:G:711:VAL:HG22	1.69	0.74
2:B:179:ASP:OD2	2:B:217:LYS:NZ	2.18	0.74
7:G:682:GLN:CA	7:G:714:ALA:HB3	2.17	0.74
8:H:874:ILE:HG23	8:H:875:GLY:N	2.02	0.74
8:H:965:LYS:HD2	9:L:436:LEU:HD22	1.67	0.74
9:L:120:ILE:HD11	9:L:303:TRP:HE1	1.51	0.74
5:E:609:ILE:HG23	5:E:611:VAL:O	1.88	0.74
5:E:1023:SER:HA	5:E:1052:VAL:CG2	2.18	0.74
6:F:1016:ILE:HD12	6:F:1016:ILE:N	2.01	0.74
7:G:579:TRP:CE3	7:G:678:ILE:HG21	2.23	0.74
5:E:286:PHE:HD2	5:E:290:ASP:HB3	1.52	0.74
7:G:165:ILE:CB	7:G:193:GLY:O	2.35	0.74
5:E:318:PHE:O	5:E:329:SER:HB3	1.87	0.74
8:H:965:LYS:CD	9:L:436:LEU:HD22	2.17	0.74
8:H:871:SER:C	8:H:873:ALA:H	1.92	0.73
8:H:937:SER:O	8:H:941:VAL:HG22	1.88	0.73
9:L:472:ALA:CB	9:L:512:GLU:HG2	2.17	0.73
1:A:381:GLU:O	1:A:385:MET:CE	2.37	0.73
6:F:189:THR:HG22	6:F:191:GLY:H	1.52	0.73
6:F:355:GLY:O	6:F:356:ASN:CB	2.34	0.73
8:H:871:SER:CB	8:H:874:ILE:HB	2.17	0.73
6:F:620:VAL:HG22	6:F:621:ASN:N	2.01	0.73
7:G:571:ARG:NH2	7:G:707:PHE:CB	2.43	0.73
3:C:128:PRO:HG3	3:C:149:GLN:HE22	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:41:LEU:HD13	5:E:41:LEU:N	2.03	0.73
7:G:579:TRP:HE3	7:G:678:ILE:HG21	1.53	0.73
5:E:585:LEU:H	5:E:611:VAL:CG2	1.98	0.73
8:H:245:THR:HG22	8:H:246:TYR:H	1.54	0.73
8:H:610:ASN:ND2	8:H:723:THR:OG1	2.20	0.73
9:L:129:ARG:NH1	9:L:644:GLU:O	2.22	0.73
8:H:329:LEU:HB2	8:H:359:PHE:HE2	1.53	0.73
2:B:223:ARG:H	2:B:223:ARG:CD	1.89	0.73
5:E:885:ASP:C	5:E:886:ASN:HD22	1.96	0.73
5:E:45:HIS:H	5:E:45:HIS:CD2	2.06	0.72
5:E:1056:PHE:HB3	11:M:115:ARG:HB2	1.70	0.72
6:F:966:ARG:HG2	6:F:976:SER:HB2	1.71	0.72
8:H:759:SER:OG	8:H:776:LYS:CE	2.37	0.72
7:G:516:GLN:HE21	7:G:518:LYS:HE2	1.54	0.72
5:E:947:LYS:O	5:E:948:PHE:O	2.07	0.72
7:G:579:TRP:O	7:G:678:ILE:N	2.20	0.72
5:E:762:ILE:HD12	5:E:762:ILE:N	2.05	0.71
5:E:1023:SER:CA	5:E:1052:VAL:CG2	2.68	0.71
6:F:419:LEU:H	6:F:419:LEU:HD23	1.55	0.71
9:L:174:SER:HB3	9:L:311:ALA:HB2	1.71	0.71
5:E:835:ARG:HH11	5:E:835:ARG:HG3	1.55	0.71
8:H:87:CYS:HG	8:H:101:CYS:HG	0.72	0.71
8:H:870:PHE:CE1	18:c:2:NAG:C5	2.71	0.71
5:E:156:GLU:O	5:E:160:GLN:NE2	2.24	0.71
5:E:870:ASN:O	5:E:897:PRO:HG2	1.89	0.71
7:G:665:VAL:HG21	17:U:1:NAG:H2	1.72	0.71
2:B:235:ALA:HA	2:B:341:ASN:ND2	2.05	0.71
5:E:42:THR:O	5:E:43:GLY:C	2.31	0.71
6:F:951:ARG:HH21	6:F:951:ARG:HG2	1.56	0.71
1:A:550:ALA:CB	1:A:552:TYR:CZ	2.73	0.71
9:L:520:GLY:HA3	9:L:538:CYS:H	1.56	0.71
7:G:519:ILE:C	7:G:519:ILE:HD13	2.15	0.71
7:G:165:ILE:HG22	7:G:193:GLY:H	1.54	0.71
5:E:629:GLU:OE2	5:E:631:THR:CG2	2.36	0.71
7:G:682:GLN:CB	7:G:714:ALA:HB1	2.21	0.71
8:H:933:ILE:HD12	8:H:933:ILE:C	2.15	0.71
5:E:428:SER:O	5:E:446:LEU:CB	2.33	0.71
6:F:284:VAL:HG21	6:F:338:ARG:HH12	1.55	0.71
9:L:287:THR:HG22	9:L:288:VAL:H	1.55	0.71
9:L:465:GLU:OE1	9:L:655:VAL:HG13	1.90	0.71
5:E:649:HIS:C	5:E:650:GLU:HG3	2.15	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:632:TYR:CE1	5:E:635:LYS:O	2.44	0.70
6:F:371:GLY:HA3	6:F:393:SER:HB2	1.73	0.70
7:G:165:ILE:HB	7:G:211:MET:HE1	1.73	0.70
8:H:757:ASP:C	8:H:758:PHE:HD1	1.99	0.70
5:E:34:SER:OG	5:E:44:LEU:CD1	2.39	0.70
5:E:896:ILE:HD12	5:E:896:ILE:N	2.05	0.70
6:F:95:SER:HB2	6:F:679:GLN:HG2	1.71	0.70
7:G:575:TYR:CD1	7:G:714:ALA:CA	2.75	0.70
7:G:579:TRP:HB3	7:G:678:ILE:HG23	1.72	0.70
11:M:89:THR:O	11:M:93:LEU:N	2.21	0.70
6:F:498:ASN:O	6:F:498:ASN:OD1	2.10	0.70
7:G:575:TYR:CE1	7:G:714:ALA:CA	2.75	0.70
8:H:754:GLN:HE21	8:H:754:GLN:H	1.40	0.70
2:B:138:TRP:CE3	2:B:139:PRO:HG3	2.26	0.70
2:B:223:ARG:HH22	2:B:224:GLN:HG2	1.54	0.70
2:B:223:ARG:NH2	2:B:224:GLN:CG	2.50	0.70
8:H:876:LYS:HG2	8:H:877:PRO:N	2.05	0.70
3:C:42:TYR:CZ	7:G:742:ALA:HB1	2.26	0.70
5:E:689:ILE:N	5:E:689:ILE:HD12	2.07	0.70
2:B:262:ARG:HD3	2:B:266:ARG:HH11	1.55	0.69
6:F:420:LEU:HD23	6:F:477:LEU:HD23	1.72	0.69
7:G:226:LEU:O	7:G:229:SER:N	2.24	0.69
5:E:759:THR:HA	6:F:861:TYR:CD1	2.27	0.69
6:F:892:ILE:HD11	6:F:913:PRO:HB3	1.72	0.69
1:A:483:SER:CB	21:A:702:9Z9:C16	2.69	0.69
1:A:486:LEU:CD1	21:A:702:9Z9:C12	2.69	0.69
2:B:268:THR:O	2:B:268:THR:HG23	1.92	0.69
7:G:575:TYR:CD2	7:G:681:GLY:O	2.45	0.69
8:H:353:GLU:HG2	8:H:354:THR:HG23	1.73	0.69
8:H:939:TYR:HE2	9:L:566:LYS:NZ	1.89	0.69
9:L:486:ASN:C	9:L:488:THR:H	1.99	0.69
1:A:474:SER:O	4:D:192:ASN:ND2	2.26	0.69
5:E:1057:PRO:HG3	11:M:112:ARG:CZ	2.23	0.69
8:H:598:GLN:NE2	19:Z:2:NAG:H83	2.06	0.69
5:E:286:PHE:CD2	5:E:290:ASP:HB3	2.28	0.69
6:F:419:LEU:HD23	6:F:419:LEU:N	2.08	0.69
7:G:715:LEU:HB3	7:G:716:PRO:CD	2.20	0.69
21:A:702:9Z9:O25	21:A:704:9Z9:C23	2.40	0.69
5:E:585:LEU:N	5:E:611:VAL:HG21	2.08	0.69
8:H:935:ARG:HB3	8:H:935:ARG:CZ	2.21	0.69
1:A:508:ARG:HB2	1:A:525:THR:HG21	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:534:ILE:HD13	6:F:548:VAL:HG21	1.74	0.69
7:G:722:PRO:C	7:G:723:LEU:HD23	2.18	0.69
8:H:90:GLU:O	8:H:97:THR:OG1	2.10	0.69
8:H:320:ILE:HG22	8:H:327:LEU:HB2	1.75	0.69
8:H:781:VAL:HG13	8:H:785:GLY:O	1.93	0.69
8:H:752:ARG:NH1	8:H:752:ARG:HG3	2.05	0.69
5:E:962:GLU:HG3	5:E:963:ARG:N	2.01	0.68
9:L:546:SER:O	9:L:547:ASP:CB	2.41	0.68
6:F:402:ASN:ND2	22:F:1201:NAG:O5	2.25	0.68
5:E:429:GLN:HG2	5:E:445:ASN:HA	1.76	0.68
5:E:960:PHE:HD1	5:E:965:LYS:HB3	1.59	0.68
7:G:682:GLN:CG	7:G:714:ALA:HB1	2.23	0.68
5:E:287:GLU:N	5:E:287:GLU:OE1	2.26	0.68
8:H:939:TYR:HE2	9:L:566:LYS:CE	2.06	0.68
5:E:1006:LEU:HD11	5:E:1033:VAL:HG23	1.74	0.68
6:F:750:ILE:HB	6:F:870:LYS:HE3	1.73	0.68
7:G:165:ILE:HG21	7:G:192:THR:C	2.18	0.68
13:I:1:MET:O	13:I:3:LEU:N	2.26	0.68
6:F:300:ASP:HB3	6:F:348:LEU:HB3	1.74	0.68
6:F:785:ILE:HD11	6:F:811:VAL:HG21	1.76	0.68
7:G:684:ASN:OD1	7:G:712:HIS:HA	1.93	0.68
8:H:565:ASN:HB3	19:Z:1:NAG:C1	2.24	0.68
6:F:1020:ILE:CG2	6:F:1021:TYR:CE1	2.71	0.68
7:G:165:ILE:HG22	7:G:166:PRO:CD	2.15	0.68
1:A:467:ARG:CZ	21:A:703:9Z9:C26	2.72	0.68
3:C:73:TYR:CZ	7:G:715:LEU:HD21	2.28	0.68
5:E:651:LEU:HD23	5:E:651:LEU:H	1.59	0.67
9:L:552:PHE:O	9:L:553:ILE:O	2.12	0.67
5:E:646:ASN:OD1	5:E:648:LEU:CD1	2.42	0.67
5:E:870:ASN:O	5:E:897:PRO:CD	2.40	0.67
5:E:882:PRO:C	5:E:883:LEU:HG	2.17	0.67
8:H:485:MET:HE1	18:Y:1:NAG:C8	2.24	0.67
9:L:549:GLU:CD	9:L:550:GLY:H	2.01	0.67
5:E:911:LYS:HD2	5:E:935:ALA:HA	1.75	0.67
1:A:550:ALA:CB	1:A:552:TYR:CE1	2.77	0.67
2:B:223:ARG:HD3	2:B:223:ARG:N	2.00	0.67
5:E:319:ASN:O	5:E:320:ARG:HG3	1.94	0.67
8:H:750:LYS:H	8:H:750:LYS:CD	2.00	0.67
5:E:948:PHE:CB	5:E:949:PRO:CD	2.71	0.67
8:H:225:ILE:HG22	8:H:240:LEU:HB3	1.77	0.67
8:H:781:VAL:O	8:H:785:GLY:HA2	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:574:ALA:HA	2:B:339:VAL:HG22	1.76	0.67
1:A:535:LEU:HD12	1:A:565:TYR:HE2	1.59	0.67
3:C:80:PHE:CE2	7:G:716:PRO:HG2	2.27	0.67
5:E:1056:PHE:CB	11:M:115:ARG:HB2	2.25	0.67
9:L:433:VAL:HG13	9:L:438:MET:HB2	1.75	0.67
1:A:374:THR:HA	1:A:377:GLU:CG	2.25	0.67
6:F:51:LEU:HD21	6:F:66:PHE:HD1	1.57	0.67
5:E:637:TYR:HD2	5:E:680:SER:HB3	1.59	0.67
5:E:960:PHE:CD1	5:E:965:LYS:HB3	2.29	0.67
6:F:419:LEU:HD23	6:F:431:VAL:O	1.95	0.67
7:G:572:LEU:HD12	7:G:572:LEU:C	2.18	0.67
8:H:749:ASN:HD22	8:H:752:ARG:HG2	1.60	0.67
1:A:483:SER:OG	21:A:702:9Z9:C16	2.43	0.67
7:G:190:HIS:HE2	7:G:228:HIS:CD2	2.12	0.67
7:G:529:PRO:HA	7:G:532:LEU:HD12	1.77	0.67
1:A:532:MET:O	1:A:535:LEU:HD23	1.95	0.66
6:F:227:VAL:HG23	6:F:229:LYS:HZ3	1.59	0.66
8:H:758:PHE:CE1	9:L:553:ILE:CD1	2.78	0.66
2:B:153:LEU:HD11	8:H:949:MET:SD	2.31	0.66
5:E:875:SER:CB	5:E:883:LEU:HD12	2.25	0.66
7:G:187:LYS:O	7:G:190:HIS:HE1	1.78	0.66
5:E:760:PHE:HD1	5:E:787:GLU:OE1	1.77	0.66
7:G:165:ILE:HD13	7:G:165:ILE:C	2.21	0.66
8:H:478:PHE:HB3	8:H:490:MET:HG2	1.75	0.66
5:E:48:LYS:NZ	5:E:214:SER:O	2.28	0.66
4:D:60:TYR:HB3	5:E:1078:PHE:HE2	1.60	0.66
7:G:717:VAL:HG22	7:G:719:LYS:NZ	2.10	0.66
9:L:253:CYS:O	9:L:257:LEU:N	2.26	0.66
5:E:755:LYS:O	5:E:756:ALA:CB	2.38	0.66
6:F:189:THR:HG23	6:F:190:ASN:N	2.09	0.66
3:C:63:ASN:HD21	3:C:152:ARG:HH11	1.43	0.65
5:E:636:LEU:HD23	5:E:636:LEU:H	1.60	0.65
2:B:138:TRP:HE3	2:B:139:PRO:HG3	1.60	0.65
5:E:695:PHE:HB3	5:E:699:SER:OG	1.97	0.65
6:F:75:VAL:HG21	6:F:95:SER:HB3	1.78	0.65
7:G:165:ILE:CG1	7:G:211:MET:CE	2.74	0.65
11:M:114:GLU:HG3	11:M:116:HIS:HD2	1.61	0.65
2:B:262:ARG:HD3	2:B:266:ARG:NH1	2.12	0.65
5:E:23:ILE:CG2	5:E:26:LYS:HG3	2.26	0.65
5:E:831:CYS:SG	5:E:1038:PHE:C	2.80	0.65
5:E:948:PHE:CD2	5:E:949:PRO:HD3	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:138:TRP:HE3	2:B:139:PRO:CG	2.08	0.65
7:G:106:VAL:HG23	7:G:119:TYR:CE2	2.31	0.65
8:H:476:LEU:HD12	8:H:490:MET:HE2	1.78	0.65
5:E:636:LEU:HD21	5:E:637:TYR:CE1	2.32	0.65
6:F:452:GLU:HB3	6:F:468:THR:CG2	2.26	0.65
16:T:1:NAG:O3	16:T:1:NAG:O7	2.14	0.65
3:C:262:MET:HE2	4:D:183:ILE:HD11	1.78	0.65
5:E:722:TYR:O	5:E:723:TRP:HD1	1.79	0.65
8:H:874:ILE:HG23	8:H:875:GLY:H	1.61	0.65
5:E:643:LEU:CD1	5:E:694:LYS:HZ3	1.89	0.65
8:H:754:GLN:HE21	8:H:754:GLN:N	1.95	0.65
9:L:372:PRO:HG2	9:L:679:ILE:HG21	1.79	0.65
5:E:135:ILE:O	5:E:145:ASP:HA	1.96	0.65
5:E:249:LEU:HD13	5:E:254:LEU:HD13	1.78	0.65
6:F:450:ILE:O	6:F:468:THR:OG1	2.14	0.65
6:F:641:LEU:CD1	6:F:750:ILE:CD1	2.69	0.65
7:G:573:VAL:O	7:G:711:VAL:HA	1.97	0.65
1:A:382:TRP:CH2	6:F:1016:ILE:CG2	2.78	0.64
2:B:262:ARG:CD	2:B:266:ARG:HH11	2.10	0.64
5:E:286:PHE:CZ	5:E:320:ARG:NH1	2.65	0.64
5:E:489:LYS:HA	5:E:489:LYS:HE2	1.79	0.64
8:H:870:PHE:CE1	18:c:2:NAG:C4	2.80	0.64
1:A:521:ASN:O	1:A:525:THR:HG23	1.98	0.64
6:F:1061:ARG:HH21	6:F:1061:ARG:CG	2.10	0.64
7:G:713:GLY:O	7:G:715:LEU:HD23	1.97	0.64
7:G:718:THR:O	7:G:720:PHE:HD1	1.81	0.64
1:A:486:LEU:HD12	21:A:702:9Z9:C12	2.28	0.64
5:E:301:LYS:NZ	5:E:364:GLN:OE1	2.29	0.64
7:G:90:VAL:HG12	7:G:115:TYR:OH	1.97	0.64
7:G:189:SER:C	7:G:191:LEU:H	2.05	0.64
9:L:112:ALA:HB3	9:L:271:GLY:HA3	1.78	0.64
1:A:552:TYR:O	1:A:555:PRO:HD2	1.97	0.64
6:F:151:ALA:HB1	6:F:170:TRP:HB3	1.79	0.64
6:F:279:ILE:HD11	6:F:310:ILE:HD11	1.80	0.64
4:D:157:ILE:O	4:D:161:LEU:HD13	1.98	0.64
5:E:738:LYS:HB3	5:E:746:ILE:HD13	1.79	0.64
5:E:39:GLY:C	5:E:40:ILE:HG12	2.23	0.64
5:E:286:PHE:CD2	5:E:290:ASP:CB	2.77	0.64
7:G:720:PHE:CD2	7:G:722:PRO:CD	2.79	0.64
8:H:755:ARG:NH1	9:L:552:PHE:CG	2.57	0.64
4:D:168:HIS:HA	4:D:171:MET:HG3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:L:646:CYS:SG	9:L:647:TRP:N	2.71	0.64
2:B:262:ARG:CD	2:B:266:ARG:NH1	2.61	0.64
4:D:252:GLU:OE2	4:D:254:ALA:N	2.31	0.64
5:E:1052:VAL:HB	11:M:116:HIS:HE1	1.62	0.64
5:E:808:ALA:HB2	5:E:824:LEU:HD23	1.80	0.63
6:F:917:PHE:CE2	6:F:1056:PRO:HG3	2.33	0.63
9:L:373:LEU:HD21	9:L:680:HIS:HB2	1.80	0.63
11:M:114:GLU:C	11:M:115:ARG:HG2	2.22	0.63
5:E:118:ASN:OD1	22:E:1202:NAG:O5	2.16	0.63
5:E:762:ILE:CG2	5:E:763:PRO:CD	2.72	0.63
7:G:165:ILE:HG12	7:G:211:MET:HE1	1.79	0.63
7:G:286:VAL:HG13	7:G:291:ILE:HG13	1.79	0.63
6:F:501:GLU:OE1	8:H:179:LYS:CD	2.45	0.63
7:G:575:TYR:O	7:G:576:ASP:CB	2.35	0.63
11:M:114:GLU:OE1	11:M:114:GLU:HA	1.98	0.63
1:A:382:TRP:CZ2	6:F:1016:ILE:HG22	2.30	0.63
5:E:879:ILE:HD11	5:E:1023:SER:OG	1.97	0.63
5:E:918:SER:C	5:E:920:ALA:H	2.07	0.63
1:A:550:ALA:HB1	1:A:552:TYR:CE1	2.32	0.63
5:E:993:GLU:C	5:E:994:ASN:HD22	2.07	0.63
6:F:189:THR:HG23	6:F:191:GLY:N	2.11	0.63
3:C:77:PHE:HA	7:G:715:LEU:HD11	1.79	0.63
6:F:73:ASP:HA	6:F:94:LEU:HB2	1.80	0.63
11:M:40:PHE:HD2	11:M:49:MET:HE1	1.61	0.63
5:E:1065:ALA:HB2	11:M:102:LEU:HD11	1.80	0.63
6:F:622:GLN:O	6:F:625:TYR:N	2.32	0.63
8:H:758:PHE:HZ	9:L:553:ILE:HD11	1.52	0.63
3:C:52:PHE:HZ	3:C:97:GLU:HG3	1.64	0.63
5:E:651:LEU:HD23	5:E:651:LEU:N	2.14	0.63
7:G:603:GLU:OE1	7:G:606:GLY:N	2.31	0.63
9:L:503:THR:O	9:L:515:SER:N	2.32	0.63
5:E:834:LEU:HD12	5:E:962:GLU:HB3	1.80	0.62
7:G:212:VAL:HG21	7:G:236:TYR:CD2	2.34	0.62
7:G:516:GLN:HE22	7:G:518:LYS:HE2	1.39	0.62
1:A:378:ILE:CD1	6:F:901:HIS:HD2	2.12	0.62
3:C:77:PHE:HA	7:G:715:LEU:CD1	2.29	0.62
5:E:34:SER:OG	5:E:44:LEU:HD11	1.99	0.62
5:E:585:LEU:N	5:E:611:VAL:HG22	2.13	0.62
6:F:295:SER:O	6:F:313:ASN:ND2	2.32	0.62
6:F:1008:GLU:CA	6:F:1013:TYR:CD2	2.72	0.62
7:G:626:GLN:HB2	7:G:643:TRP:HH2	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:VAL:CG2	1:A:461:ARG:HG2	2.28	0.62
7:G:667:TYR:HE2	7:G:674:THR:HG21	1.65	0.62
7:G:520:SER:O	7:G:522:CYS:O	2.18	0.62
5:E:286:PHE:HD2	5:E:290:ASP:HB2	1.64	0.62
6:F:1008:GLU:HA	6:F:1013:TYR:CG	2.31	0.62
7:G:519:ILE:HG23	7:G:519:ILE:O	1.99	0.62
7:G:165:ILE:HG21	7:G:193:GLY:H	1.47	0.62
7:G:168:THR:C	7:G:169:ASN:HD22	2.07	0.62
2:B:120:THR:HG22	2:B:212:VAL:HG13	1.82	0.62
5:E:612:PRO:O	5:E:613:PHE:HB2	2.00	0.62
5:E:636:LEU:H	5:E:636:LEU:CD2	2.12	0.62
7:G:296:VAL:HG12	7:G:305:PHE:HB3	1.81	0.62
7:G:572:LEU:HD12	7:G:573:VAL:H	1.59	0.62
9:L:551:GLN:HA	9:L:551:GLN:OE1	1.98	0.62
1:A:532:MET:HE2	1:A:541:ILE:HD11	1.81	0.62
2:B:189:PRO:HA	2:B:192:VAL:HG22	1.82	0.62
6:F:641:LEU:HD12	6:F:750:ILE:CD1	2.29	0.62
7:G:165:ILE:HD12	7:G:191:LEU:O	1.99	0.62
2:B:119:ASN:HA	2:B:122:VAL:HG22	1.82	0.62
5:E:540:VAL:HG11	5:E:669:LEU:HB2	1.81	0.62
5:E:880:SER:O	5:E:881:ILE:HD12	1.99	0.62
5:E:1056:PHE:HD1	5:E:1057:PRO:HD3	1.64	0.62
7:G:186:ASP:OD1	7:G:187:LYS:N	2.33	0.62
9:L:539:ILE:HG22	9:L:540:LYS:O	2.00	0.62
5:E:239:HIS:ND1	5:E:288:ARG:HD3	2.14	0.61
7:G:165:ILE:CB	7:G:211:MET:HE1	2.29	0.61
8:H:762:ILE:HG13	8:H:824:ARG:HH22	1.65	0.61
7:G:583:VAL:HG21	7:G:595:MET:HE3	1.81	0.61
4:D:55:PHE:O	4:D:59:MET:N	2.33	0.61
5:E:71:LYS:O	5:E:71:LYS:HG2	2.00	0.61
5:E:685:MET:CA	5:E:687:GLN:HE22	2.08	0.61
8:H:633:MET:HB2	8:H:637:GLU:HB2	1.82	0.61
5:E:612:PRO:HB2	6:F:627:ALA:HB1	1.82	0.61
5:E:643:LEU:HD13	5:E:694:LYS:NZ	2.12	0.61
5:E:738:LYS:CB	5:E:746:ILE:HD13	2.31	0.61
6:F:908:LYS:NZ	6:F:908:LYS:HB3	2.14	0.61
6:F:464:THR:O	6:F:464:THR:HG23	2.01	0.61
8:H:835:GLN:HE22	8:H:892:LYS:HG3	1.65	0.61
1:A:381:GLU:O	1:A:385:MET:SD	2.58	0.61
1:A:535:LEU:HD11	1:A:565:TYR:HD2	0.59	0.61
5:E:34:SER:OG	5:E:44:LEU:HD12	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:760:PHE:CD1	5:E:787:GLU:OE1	2.53	0.61
5:E:831:CYS:SG	5:E:1038:PHE:O	2.59	0.61
5:E:918:SER:C	5:E:920:ALA:N	2.57	0.61
5:E:1056:PHE:CD1	5:E:1057:PRO:N	2.68	0.61
5:E:1057:PRO:CG	11:M:112:ARG:NE	2.56	0.61
8:H:876:LYS:HG3	8:H:877:PRO:HD2	1.83	0.61
5:E:632:TYR:CZ	5:E:635:LYS:O	2.53	0.61
5:E:761:PRO:HB2	5:E:762:ILE:CD1	2.30	0.61
7:G:339:ILE:HG22	7:G:349:VAL:HG22	1.81	0.61
1:A:560:TYR:HE1	1:A:564:GLN:HE21	1.47	0.61
5:E:895:PRO:O	5:E:896:ILE:HB	1.99	0.61
6:F:987:THR:HG22	6:F:992:PHE:H	1.65	0.61
8:H:870:PHE:CE1	18:c:2:NAG:C3	2.83	0.61
1:A:358:PHE:HB3	1:A:465:VAL:HG22	1.83	0.61
4:D:130:ASP:OD1	4:D:131:GLY:N	2.31	0.61
5:E:48:LYS:HZ1	5:E:217:TRP:CD1	2.19	0.61
6:F:1057:LEU:CD2	6:F:1062:THR:OG1	2.49	0.61
8:H:565:ASN:CB	19:Z:1:NAG:O5	2.49	0.61
6:F:184:SER:HB2	6:F:200:ARG:HD2	1.83	0.60
8:H:876:LYS:CG	8:H:877:PRO:N	2.64	0.60
17:U:1:NAG:H62	17:U:2:NAG:C1	2.31	0.60
1:A:361:VAL:HG11	1:A:461:ARG:CG	2.30	0.60
5:E:647:PRO:O	5:E:650:GLU:CD	2.44	0.60
6:F:469:ASN:ND2	6:F:469:ASN:H	1.99	0.60
7:G:732:THR:HA	7:G:735:LEU:HD12	1.83	0.60
8:H:565:ASN:ND2	19:Z:1:NAG:C2	2.34	0.60
2:B:248:ILE:O	2:B:252:ILE:HG12	2.01	0.60
2:B:259:TYR:HE1	3:C:71:THR:HG22	1.65	0.60
7:G:42:LEU:HD22	7:G:95:ILE:HD11	1.82	0.60
8:H:839:ILE:HG21	8:H:872:TYR:CB	2.28	0.60
8:H:892:LYS:O	17:b:1:NAG:H3	2.02	0.60
1:A:414:PRO:HB2	21:A:703:9Z9:C19	2.31	0.60
2:B:120:THR:HG21	2:B:215:SER:HB2	1.83	0.60
3:C:43:PHE:HZ	3:C:100:MET:HB2	1.66	0.60
5:E:902:HIS:O	5:E:905:LYS:CG	2.46	0.60
6:F:647:LYS:HG3	6:F:751:PRO:HB3	1.83	0.60
7:G:535:ASN:ND2	22:G:902:NAG:C7	2.63	0.60
8:H:757:ASP:C	8:H:758:PHE:CD1	2.79	0.60
1:A:584:LEU:HD21	4:D:284:THR:HG23	1.83	0.60
2:B:121:PHE:HA	2:B:124:MET:HG3	1.83	0.60
5:E:675:ASP:OD1	5:E:676:LYS:N	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:687:GLN:NE2	5:E:687:GLN:H	2.00	0.60
5:E:870:ASN:O	5:E:897:PRO:CG	2.49	0.60
8:H:337:ARG:NH1	8:H:338:THR:O	2.34	0.60
9:L:519:ALA:HB1	9:L:539:ILE:HD11	1.84	0.60
9:L:640:CYS:HB3	9:L:644:GLU:HB2	1.83	0.60
1:A:565:TYR:HE1	2:B:331:ARG:HH11	1.49	0.60
5:E:627:ASP:HB2	5:E:643:LEU:HB2	1.84	0.60
5:E:898:ARG:HG2	5:E:898:ARG:HH21	1.66	0.60
5:E:960:PHE:CD1	5:E:965:LYS:CB	2.85	0.60
6:F:641:LEU:HD11	6:F:750:ILE:CD1	2.27	0.60
7:G:184:ASN:OD1	7:G:185:THR:N	2.34	0.60
5:E:40:ILE:C	5:E:41:LEU:HD13	2.26	0.60
5:E:239:HIS:CE1	5:E:288:ARG:HD3	2.37	0.60
5:E:636:LEU:CD2	5:E:637:TYR:CD1	2.84	0.60
5:E:885:ASP:OD1	5:E:907:THR:HB	2.02	0.60
5:E:1052:VAL:HG12	5:E:1053:PRO:HD2	1.84	0.60
5:E:1055:PRO:HG2	11:M:109:ILE:HG13	1.82	0.60
6:F:242:TRP:CD1	6:F:352:TYR:HH	2.19	0.60
9:L:86:PHE:O	9:L:90:PHE:N	2.32	0.60
1:A:455:LYS:O	1:A:458:ARG:HD2	2.02	0.60
5:E:881:ILE:HG22	5:E:881:ILE:O	2.01	0.60
6:F:226:LEU:HD11	6:F:276:GLU:HB2	1.82	0.60
6:F:887:ASP:HB2	6:F:926:LEU:HD22	1.84	0.60
5:E:629:GLU:CD	5:E:631:THR:HG22	2.27	0.60
5:E:697:THR:HG23	5:E:698:GLY:H	1.67	0.60
7:G:106:VAL:HG23	7:G:119:TYR:HE2	1.67	0.60
8:H:839:ILE:CG2	8:H:872:TYR:CD1	2.79	0.60
8:H:935:ARG:HH11	8:H:935:ARG:CG	2.15	0.60
8:H:935:ARG:HH11	8:H:935:ARG:HG3	1.67	0.60
9:L:255:PHE:N	9:L:434:ASP:OD2	2.35	0.60
9:L:376:THR:HG23	9:L:672:LEU:HB3	1.83	0.60
5:E:921:MET:O	22:E:1204:NAG:N2	2.25	0.60
5:E:948:PHE:CB	5:E:949:PRO:HD3	2.30	0.60
5:E:1073:LEU:HA	5:E:1076:ILE:HD12	1.84	0.60
8:H:182:ASN:HD22	8:H:204:LEU:HD22	1.67	0.60
8:H:870:PHE:CE1	18:c:2:NAG:O4	2.54	0.60
9:L:549:GLU:OE1	9:L:550:GLY:N	2.31	0.60
10:J:149:PHE:O	10:J:153:ILE:N	2.22	0.60
14:K:95:ARG:O	14:K:96:SER:C	2.45	0.60
3:C:77:PHE:CD1	7:G:715:LEU:HD13	2.36	0.59
3:C:257:PHE:O	3:C:261:ASN:HB2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:35:CYS:HB2	5:E:47:ILE:HG21	1.83	0.59
5:E:918:SER:O	5:E:920:ALA:N	2.35	0.59
5:E:1057:PRO:CD	11:M:112:ARG:HD3	2.32	0.59
6:F:176:PHE:CE1	17:R:1:NAG:C8	2.85	0.59
7:G:609:THR:HG1	7:G:687:TYR:HH	1.47	0.59
8:H:391:GLY:HA2	8:H:397:PHE:HB3	1.84	0.59
10:J:152:GLY:O	10:J:156:ARG:N	2.34	0.59
3:C:63:ASN:ND2	3:C:152:ARG:HH11	2.00	0.59
5:E:993:GLU:OE1	5:E:996:LYS:CG	2.50	0.59
7:G:717:VAL:HG13	7:G:717:VAL:O	2.02	0.59
8:H:530:VAL:HG22	8:H:540:VAL:HG22	1.84	0.59
2:B:262:ARG:O	2:B:266:ARG:CG	2.44	0.59
5:E:762:ILE:CG1	6:F:195:PHE:CE2	2.81	0.59
6:F:842:LYS:HG3	6:F:875:PHE:CE1	2.38	0.59
5:E:319:ASN:O	5:E:320:ARG:CG	2.50	0.59
8:H:598:GLN:NE2	19:Z:2:NAG:C8	2.65	0.59
9:L:444:LEU:HB3	9:L:677:ILE:HG12	1.84	0.59
6:F:568:HIS:NE2	6:F:601:ARG:HD2	2.17	0.59
8:H:149:THR:HG22	8:H:211:VAL:HG22	1.84	0.59
11:M:46:TYR:HA	11:M:49:MET:HE3	1.85	0.59
2:B:141:LYS:NZ	8:H:937:SER:OG	2.35	0.59
5:E:37:GLY:O	5:E:39:GLY:N	2.27	0.59
5:E:508:PRO:O	5:E:509:GLU:HG2	2.02	0.59
5:E:997:LYS:NZ	6:F:714:ASP:OD2	2.36	0.59
7:G:717:VAL:O	7:G:719:LYS:HE2	2.01	0.59
8:H:565:ASN:HB2	19:Z:1:NAG:O5	2.03	0.59
9:L:142:ALA:HB1	9:L:231:ILE:HG13	1.83	0.59
5:E:989:HIS:CE1	5:E:999:LYS:HZ1	2.20	0.59
6:F:907:ILE:HD12	6:F:907:ILE:N	2.10	0.59
8:H:76:ASN:OD1	8:H:77:SER:N	2.34	0.59
1:A:582:MET:SD	2:B:346:ARG:NH1	2.76	0.59
6:F:901:HIS:CD2	6:F:903:PHE:CE2	2.72	0.59
8:H:87:CYS:CB	8:H:101:CYS:HG	2.14	0.59
5:E:893:SER:HB2	5:E:917:THR:O	2.03	0.59
7:G:544:ALA:HB2	7:G:607:LEU:HD23	1.83	0.59
7:G:592:GLU:HG3	7:G:593:GLU:OE2	2.03	0.59
9:L:216:SER:HA	9:L:219:ILE:HD12	1.85	0.59
4:D:92:TYR:HD2	4:D:93:LEU:HD12	1.68	0.58
5:E:1082:LEU:O	5:E:1086:HIS:ND1	2.35	0.58
8:H:245:THR:HG22	8:H:246:TYR:N	2.17	0.58
11:M:110:ASN:C	11:M:111:TYR:CD1	2.80	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:77:PHE:CD1	7:G:715:LEU:CD1	2.86	0.58
5:E:623:CYS:SG	5:E:651:LEU:HB3	2.43	0.58
5:E:833:TYR:CE2	5:E:834:LEU:CD2	2.85	0.58
8:H:317:ARG:NH1	8:H:331:ASP:OD1	2.35	0.58
5:E:636:LEU:HD23	5:E:637:TYR:CD1	2.38	0.58
6:F:498:ASN:C	6:F:500:GLU:H	2.10	0.58
6:F:656:TYR:OH	6:F:689:HIS:ND1	2.31	0.58
9:L:170:MET:HE1	9:L:229:HIS:HA	1.85	0.58
11:M:115:ARG:O	11:M:116:HIS:HB2	2.03	0.58
1:A:378:ILE:HD11	6:F:901:HIS:CD2	2.37	0.58
2:B:152:LEU:O	2:B:156:ILE:HD12	2.03	0.58
5:E:646:ASN:OD1	5:E:648:LEU:HD11	2.01	0.58
5:E:833:TYR:CE2	5:E:834:LEU:HD23	2.38	0.58
8:H:635:LYS:NZ	8:H:914:PRO:O	2.36	0.58
8:H:749:ASN:CB	8:H:752:ARG:HB3	2.33	0.58
9:L:505:ILE:N	9:L:513:TYR:O	2.22	0.58
5:E:656:VAL:CG1	5:E:671:MET:O	2.52	0.58
8:H:871:SER:C	8:H:873:ALA:N	2.61	0.58
5:E:761:PRO:CG	6:F:861:TYR:O	2.28	0.58
5:E:833:TYR:CD2	5:E:834:LEU:HD23	2.37	0.58
5:E:961:ASN:O	5:E:964:ASP:N	2.30	0.58
3:C:73:TYR:CE1	7:G:715:LEU:CD2	2.69	0.58
3:C:287:ASN:O	3:C:291:MET:HG2	2.04	0.58
5:E:723:TRP:CE2	5:E:755:LYS:HD2	2.37	0.58
7:G:475:LYS:NZ	7:G:475:LYS:HB3	2.18	0.58
9:L:492:ASN:OD1	9:L:497:CYS:HB2	2.03	0.58
1:A:518:ARG:CZ	1:A:541:ILE:HG22	2.34	0.58
5:E:646:ASN:OD1	5:E:648:LEU:HD12	2.04	0.58
5:E:895:PRO:O	5:E:896:ILE:CB	2.51	0.58
7:G:237:LYS:O	7:G:238:ASN:HB2	2.03	0.58
8:H:888:ASN:OD1	18:c:1:NAG:C1	2.52	0.58
9:L:104:VAL:HG22	9:L:237:TYR:HE1	1.69	0.58
5:E:288:ARG:HG2	5:E:288:ARG:HH11	1.67	0.58
9:L:549:GLU:CG	9:L:550:GLY:H	2.16	0.58
5:E:832:SER:C	5:E:834:LEU:H	2.11	0.58
5:E:993:GLU:HG3	5:E:993:GLU:O	2.04	0.58
6:F:815:ARG:NH2	8:H:674:GLU:OE2	2.34	0.58
7:G:573:VAL:HG13	7:G:573:VAL:O	2.02	0.58
9:L:376:THR:HG21	9:L:676:ALA:HB2	1.84	0.58
9:L:406:THR:O	9:L:410:ALA:N	2.29	0.58
2:B:211:ARG:O	2:B:214:ARG:HG2	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:646:ASN:ND2	5:E:647:PRO:CD	2.28	0.57
5:E:991:GLU:HG3	5:E:991:GLU:O	2.04	0.57
6:F:1080:TYR:HA	6:F:1083:PHE:HB2	1.86	0.57
8:H:759:SER:HB3	9:L:541:GLU:HB2	1.84	0.57
1:A:560:TYR:CE1	1:A:564:GLN:HG3	2.39	0.57
5:E:1003:GLU:HG3	5:E:1004:PRO:HD3	1.87	0.57
6:F:402:ASN:ND2	6:F:424:ASP:HB3	2.19	0.57
6:F:409:THR:HG22	6:F:418:LEU:HB2	1.87	0.57
6:F:774:THR:O	6:F:790:LYS:NZ	2.36	0.57
7:G:226:LEU:HB3	7:G:229:SER:HB3	1.86	0.57
8:H:632:HIS:NE2	8:H:736:GLY:O	2.38	0.57
1:A:542:TYR:CD1	1:A:554:ILE:HD13	2.39	0.57
5:E:610:ILE:O	5:E:610:ILE:HG22	2.04	0.57
8:H:888:ASN:ND2	18:c:1:NAG:C2	2.53	0.57
9:L:504:SER:OG	9:L:559:THR:OG1	2.21	0.57
17:W:1:NAG:O3	17:W:2:NAG:O5	2.19	0.57
2:B:119:ASN:OD1	2:B:120:THR:N	2.38	0.57
6:F:955:THR:O	6:F:955:THR:HG22	2.05	0.57
7:G:227:ASN:OD1	22:G:901:NAG:O5	2.16	0.57
9:L:263:ALA:HA	9:L:266:ILE:HG12	1.86	0.57
2:B:117:PHE:O	2:B:120:THR:OG1	2.22	0.57
3:C:264:VAL:HG13	4:D:279:VAL:HG13	1.86	0.57
4:D:173:VAL:HG12	4:D:173:VAL:O	2.05	0.57
5:E:916:VAL:HG21	5:E:921:MET:CB	2.18	0.57
5:E:1082:LEU:HD13	11:M:76:GLU:HG3	1.85	0.57
11:M:114:GLU:O	11:M:115:ARG:HG2	2.04	0.57
2:B:336:ALA:HA	3:C:268:ILE:HG12	1.86	0.57
3:C:145:ALA:O	3:C:148:ILE:HG22	2.05	0.57
5:E:37:GLY:C	5:E:39:GLY:H	2.13	0.57
5:E:365:GLU:O	5:E:771:ASN:ND2	2.38	0.57
5:E:638:TYR:N	5:E:638:TYR:CD1	2.72	0.57
5:E:645:LYS:O	5:E:677:TRP:CZ2	2.58	0.57
5:E:747:ASP:OD1	5:E:794:HIS:ND1	2.33	0.57
5:E:833:TYR:HE2	5:E:834:LEU:CD2	2.18	0.57
7:G:224:TYR:CD1	7:G:224:TYR:C	2.82	0.57
11:M:42:VAL:HG23	11:M:43:ILE:H	1.69	0.57
2:B:258:VAL:HG11	3:C:71:THR:HB	1.87	0.57
3:C:284:LEU:HD22	3:C:288:LEU:HG	1.87	0.57
8:H:362:ARG:NH1	8:H:429:PRO:O	2.37	0.57
1:A:378:ILE:CD1	6:F:901:HIS:CD2	2.87	0.57
1:A:553:ILE:HG12	1:A:557:LEU:HG	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:866:THR:OG1	5:E:942:LYS:NZ	2.26	0.57
2:B:103:LEU:HD11	2:B:161:LEU:HB3	1.86	0.57
3:C:129:TYR:CE1	7:G:724:LEU:HG	2.40	0.57
5:E:636:LEU:HD23	5:E:637:TYR:HD1	1.70	0.57
7:G:573:VAL:HG13	7:G:711:VAL:HA	1.87	0.57
9:L:170:MET:HE2	9:L:170:MET:HA	1.86	0.57
5:E:855:HIS:ND1	5:E:863:MET:HG3	2.20	0.56
5:E:898:ARG:HG2	5:E:898:ARG:NH2	2.20	0.56
7:G:189:SER:O	7:G:191:LEU:N	2.37	0.56
7:G:275:LEU:HD22	7:G:284:LEU:HD12	1.87	0.56
1:A:471:ILE:HG21	1:A:475:LEU:HD21	1.86	0.56
5:E:584:GLY:C	5:E:611:VAL:HG21	2.30	0.56
5:E:1052:VAL:CB	11:M:116:HIS:CE1	2.88	0.56
6:F:644:VAL:HG11	6:F:749:GLY:C	2.30	0.56
7:G:715:LEU:CB	7:G:716:PRO:HD2	2.26	0.56
7:G:719:LYS:H	7:G:719:LYS:CD	2.11	0.56
5:E:575:GLY:O	5:E:718:ARG:HD3	2.04	0.56
5:E:686:PRO:HD2	5:E:687:GLN:HE21	1.69	0.56
6:F:688:LEU:HD21	6:F:707:TRP:HB2	1.87	0.56
6:F:951:ARG:HG2	6:F:951:ARG:NH2	2.17	0.56
7:G:88:LEU:O	7:G:90:VAL:HG13	2.05	0.56
7:G:226:LEU:O	7:G:229:SER:CB	2.52	0.56
7:G:532:LEU:HA	7:G:536:TYR:HB2	1.88	0.56
7:G:572:LEU:HA	7:G:710:TYR:O	2.05	0.56
10:J:12:CYS:O	10:J:16:ARG:N	2.38	0.56
7:G:665:VAL:HG22	17:U:1:NAG:O7	2.06	0.56
1:A:344:ILE:HG22	1:A:405:ALA:HB2	1.87	0.56
1:A:374:THR:O	6:F:903:PHE:CZ	2.59	0.56
1:A:378:ILE:HD13	6:F:903:PHE:CD2	2.41	0.56
5:E:948:PHE:CG	5:E:949:PRO:N	2.68	0.56
6:F:176:PHE:CE1	17:R:1:NAG:H83	2.40	0.56
6:F:1020:ILE:C	6:F:1021:TYR:CD1	2.83	0.56
1:A:456:SER:OG	4:D:210:THR:HG21	2.06	0.56
2:B:179:ASP:OD2	2:B:217:LYS:HD3	2.05	0.56
7:G:334:SER:O	7:G:335:THR:OG1	2.24	0.56
9:L:472:ALA:CB	9:L:512:GLU:HB2	2.34	0.56
4:D:63:GLN:O	4:D:67:HIS:HB2	2.06	0.56
4:D:99:GLU:O	4:D:103:THR:HG23	2.06	0.56
4:D:241:ASP:O	4:D:244:THR:OG1	2.24	0.56
5:E:762:ILE:HG23	6:F:195:PHE:CE1	2.41	0.56
7:G:720:PHE:CG	7:G:722:PRO:HD2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:820:GLU:HA	8:H:907:TYR:HA	1.86	0.56
9:L:526:VAL:HG13	9:L:531:LYS:HG2	1.88	0.56
5:E:290:ASP:OD2	5:E:320:ARG:CZ	2.54	0.56
5:E:835:ARG:HG3	5:E:835:ARG:NH1	2.20	0.56
6:F:1079:PHE:O	6:F:1083:PHE:N	2.39	0.56
3:C:207:LEU:O	3:C:208:GLU:HG3	2.06	0.56
5:E:900:GLN:O	5:E:901:PHE:CB	2.54	0.56
6:F:1061:ARG:HG2	6:F:1061:ARG:NH2	2.15	0.56
8:H:488:ILE:HG12	8:H:499:SER:HB3	1.87	0.56
5:E:1002:LEU:HD13	5:E:1033:VAL:HG21	1.88	0.56
7:G:70:LEU:HD21	7:G:119:TYR:HB3	1.86	0.56
9:L:475:ASN:O	9:L:476:GLU:O	2.24	0.56
18:c:3:BMA:H3	18:c:4:BMA:O2	2.05	0.56
7:G:575:TYR:CE1	7:G:714:ALA:HA	2.41	0.55
8:H:817:ILE:HD13	8:H:861:TRP:CD1	2.41	0.55
2:B:113:ILE:HA	2:B:116:ILE:HD12	1.87	0.55
7:G:274:ARG:NH2	7:G:321:GLY:HA3	2.20	0.55
8:H:888:ASN:O	8:H:891:ASN:HB2	2.05	0.55
9:L:331:ALA:O	9:L:335:ARG:N	2.32	0.55
10:J:65:VAL:O	11:M:6:ARG:NH2	2.39	0.55
1:A:475:LEU:HD12	4:D:196:LEU:HD13	1.88	0.55
1:A:567:ILE:HG22	1:A:567:ILE:O	2.06	0.55
5:E:334:LYS:HG2	5:E:335:GLU:H	1.72	0.55
5:E:808:ALA:HB2	5:E:824:LEU:CD2	2.37	0.55
8:H:381:ILE:HG21	8:H:423:VAL:HG11	1.89	0.55
2:B:119:ASN:HB3	2:B:151:ILE:HG21	1.86	0.55
3:C:225:THR:O	3:C:227:ASP:N	2.39	0.55
8:H:426:LEU:HD21	8:H:431:GLU:HB3	1.87	0.55
9:L:212:VAL:HG23	9:L:213:PRO:HD3	1.88	0.55
4:D:116:VAL:HG21	4:D:140:VAL:HG11	1.88	0.55
5:E:651:LEU:N	5:E:651:LEU:CD2	2.70	0.55
5:E:862:ASN:HB3	5:E:945:ARG:NH1	2.22	0.55
6:F:909:ASP:OD2	6:F:911:GLU:N	2.39	0.55
8:H:830:ASN:OD1	8:H:831:SER:N	2.38	0.55
11:M:13:PRO:HG2	11:M:16:LEU:HD12	1.89	0.55
1:A:449:ARG:HD2	4:D:211:LEU:O	2.06	0.55
2:B:336:ALA:O	2:B:340:THR:HG23	2.06	0.55
5:E:740:ILE:HG22	5:E:746:ILE:HG13	1.88	0.55
6:F:796:THR:HB	6:F:846:MET:HB3	1.89	0.55
6:F:1020:ILE:O	6:F:1021:TYR:CE2	2.57	0.55
7:G:165:ILE:HG13	7:G:211:MET:HE2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:286:LEU:HA	4:D:289:MET:HE2	1.87	0.55
5:E:315:THR:HG22	5:E:332:PHE:HB2	1.88	0.55
7:G:164:GLN:O	7:G:168:THR:OG1	2.18	0.55
7:G:575:TYR:HE1	7:G:714:ALA:HA	1.72	0.55
5:E:248:VAL:O	5:E:254:LEU:HD12	2.07	0.55
5:E:464:VAL:HG11	5:E:495:LEU:HD22	1.89	0.55
5:E:960:PHE:HD1	5:E:965:LYS:CB	2.19	0.55
7:G:575:TYR:CZ	7:G:682:GLN:OE1	2.60	0.55
7:G:721:GLN:CD	7:G:722:PRO:HD3	2.30	0.55
8:H:762:ILE:HG13	8:H:824:ARG:NH2	2.22	0.55
2:B:153:LEU:HD13	8:H:949:MET:CE	2.35	0.55
5:E:761:PRO:HD2	6:F:861:TYR:HB2	1.88	0.55
6:F:271:ASP:OD1	6:F:272:TYR:N	2.40	0.55
2:B:263:GLU:OE1	2:B:263:GLU:N	2.29	0.55
6:F:908:LYS:HB3	6:F:908:LYS:HZ3	1.72	0.55
7:G:443:ASN:HD22	7:G:443:ASN:C	2.14	0.55
1:A:419:ASP:CG	1:A:461:ARG:HH21	2.13	0.54
5:E:629:GLU:CD	5:E:631:THR:CG2	2.80	0.54
6:F:917:PHE:C	6:F:917:PHE:CD2	2.85	0.54
9:L:398:HIS:HA	9:L:401:THR:HG22	1.88	0.54
3:C:42:TYR:HE2	7:G:742:ALA:HB1	1.72	0.54
5:E:671:MET:HE1	5:E:682:LEU:HD12	1.90	0.54
5:E:850:TRP:HA	5:E:864:ILE:HD13	1.89	0.54
6:F:766:VAL:HG23	6:F:820:ASN:HD22	1.72	0.54
7:G:186:ASP:OD1	7:G:187:LYS:HG2	2.07	0.54
7:G:190:HIS:O	7:G:191:LEU:HD23	2.07	0.54
8:H:492:ASP:O	8:H:493:GLN:HG2	2.07	0.54
2:B:109:SER:HA	2:B:112:ILE:HG12	1.88	0.54
8:H:218:SER:HB2	8:H:246:TYR:HE1	1.72	0.54
7:G:571:ARG:NH2	7:G:708:SER:N	2.36	0.54
9:L:150:ILE:O	9:L:154:GLY:N	2.33	0.54
5:E:45:HIS:CD2	5:E:45:HIS:N	2.75	0.54
6:F:966:ARG:HD2	6:F:976:SER:OG	2.06	0.54
1:A:497:PHE:CD1	1:A:497:PHE:C	2.85	0.54
3:C:248:THR:O	3:C:252:ILE:HG12	2.07	0.54
5:E:263:TYR:CE2	5:E:280:ARG:HB2	2.43	0.54
8:H:870:PHE:HD1	18:c:2:NAG:O4	1.89	0.54
1:A:438:LEU:HD11	1:A:443:TYR:HE1	1.73	0.54
2:B:363:ASP:HA	2:B:366:LYS:HG2	1.88	0.54
7:G:121:GLU:HB3	7:G:123:THR:HG23	1.89	0.54
8:H:284:THR:OG1	8:H:287:GLU:O	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:L:589:ILE:HA	9:L:592:ILE:HD12	1.89	0.54
3:C:43:PHE:CZ	3:C:100:MET:HB2	2.43	0.54
8:H:225:ILE:CG2	8:H:240:LEU:HB3	2.38	0.54
4:D:204:PHE:HD2	4:D:266:PHE:HD1	1.56	0.54
5:E:457:SER:HB3	5:E:497:TYR:HB3	1.90	0.54
6:F:952:THR:HG23	6:F:955:THR:OG1	2.08	0.54
8:H:800:VAL:HG23	8:H:812:VAL:HB	1.90	0.54
9:L:458:PHE:O	9:L:659:MET:HE3	2.08	0.54
3:C:229:TRP:CZ2	4:D:232:ILE:HD13	2.43	0.54
5:E:973:LEU:HD21	5:E:995:VAL:HG11	1.90	0.54
7:G:184:ASN:HB3	7:G:187:LYS:HZ1	1.70	0.54
7:G:188:LEU:HD23	7:G:188:LEU:H	1.72	0.54
7:G:516:GLN:CD	7:G:518:LYS:HE3	2.29	0.54
8:H:87:CYS:HB3	8:H:101:CYS:SG	2.48	0.53
8:H:870:PHE:HE1	18:c:2:NAG:C3	2.08	0.53
8:H:872:TYR:C	8:H:872:TYR:CD2	2.87	0.53
2:B:156:ILE:HD11	2:B:187:LEU:HD21	1.90	0.53
3:C:303:GLU:HB3	3:C:307:ARG:CZ	2.38	0.53
7:G:576:ASP:O	7:G:577:LYS:HG3	2.07	0.53
8:H:818:LEU:HD11	8:H:907:TYR:HB3	1.90	0.53
1:A:466:LEU:HB3	1:A:471:ILE:HD11	1.89	0.53
2:B:268:THR:O	2:B:268:THR:HG22	2.07	0.53
3:C:284:LEU:HD22	3:C:284:LEU:C	2.33	0.53
5:E:613:PHE:O	6:F:627:ALA:CB	2.56	0.53
7:G:717:VAL:O	7:G:719:LYS:HD3	2.09	0.53
5:E:319:ASN:C	5:E:320:ARG:HG3	2.33	0.53
7:G:626:GLN:HB2	7:G:643:TRP:CH2	2.44	0.53
8:H:804:ASP:OD1	8:H:805:GLU:N	2.40	0.53
10:J:78:ALA:N	10:J:90:GLN:O	2.41	0.53
1:A:515:ASP:OD2	1:A:544:ASP:HB3	2.08	0.53
4:D:145:MET:O	4:D:149:ILE:HG22	2.09	0.53
4:D:174:GLU:HG2	4:D:175:PRO:HD3	1.90	0.53
5:E:953:TYR:HB3	5:E:1018:LEU:HB3	1.90	0.53
6:F:908:LYS:NZ	6:F:908:LYS:CB	2.72	0.53
8:H:250:ILE:HG12	16:X:1:NAG:H61	1.90	0.53
8:H:565:ASN:HB2	19:Z:1:NAG:C1	2.34	0.53
1:A:345:LEU:O	1:A:348:THR:N	2.41	0.53
1:A:368:LEU:HD21	1:A:456:SER:HA	1.90	0.53
2:B:155:PHE:O	2:B:159:ILE:HG12	2.09	0.53
2:B:138:TRP:HE3	2:B:139:PRO:HD3	1.71	0.53
5:E:689:ILE:N	5:E:689:ILE:CD1	2.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:908:GLY:O	5:E:909:LYS:HG3	2.09	0.53
7:G:225:PRO:O	7:G:226:LEU:HD12	2.08	0.53
9:L:238:ILE:HG12	9:L:609:TYR:CD2	2.44	0.53
9:L:460:LEU:O	9:L:464:VAL:HG23	2.09	0.53
1:A:565:TYR:O	1:A:565:TYR:HD1	1.92	0.53
2:B:138:TRP:CE3	2:B:139:PRO:CD	2.88	0.53
3:C:42:TYR:OH	7:G:742:ALA:CB	2.55	0.53
5:E:839:HIS:N	5:E:1043:GLU:OE1	2.38	0.53
8:H:876:LYS:CB	8:H:876:LYS:NZ	2.72	0.53
9:L:99:LEU:HD22	9:L:321:MET:HE3	1.91	0.53
9:L:549:GLU:CG	9:L:550:GLY:N	2.72	0.53
2:B:309:GLU:C	2:B:310:SER:HG	2.04	0.53
5:E:41:LEU:N	5:E:41:LEU:CD1	2.71	0.53
5:E:1075:PHE:CE1	11:M:69:ALA:HB1	2.44	0.53
3:C:121:ILE:HD12	3:C:152:ARG:HA	1.91	0.53
6:F:121:MET:HE2	6:F:193:GLY:HA2	1.91	0.53
7:G:19:LEU:HD12	7:G:330:GLN:HB2	1.91	0.53
8:H:537:ASN:HB2	8:H:549:TYR:CE1	2.43	0.53
9:L:395:LEU:HD11	9:L:570:PHE:CE2	2.44	0.53
11:M:112:ARG:CZ	11:M:112:ARG:CB	2.87	0.53
5:E:950:VAL:O	5:E:1019:THR:HA	2.09	0.52
6:F:251:PHE:HB3	6:F:269:PHE:HE2	1.74	0.52
7:G:224:TYR:O	7:G:227:ASN:CG	2.52	0.52
8:H:351:ILE:HD12	8:H:389:TYR:CD2	2.44	0.52
8:H:792:LEU:HD12	8:H:932:MET:H	1.73	0.52
8:H:835:GLN:HG3	17:b:1:NAG:H81	1.90	0.52
4:D:149:ILE:HD13	4:D:152:LEU:HD13	1.91	0.52
5:E:175:LEU:HB3	5:E:200:MET:HE1	1.89	0.52
5:E:623:CYS:SG	5:E:651:LEU:HA	2.49	0.52
5:E:862:ASN:HB3	5:E:945:ARG:HH11	1.73	0.52
5:E:884:THR:O	5:E:885:ASP:HB2	2.10	0.52
7:G:307:VAL:HB	7:G:311:HIS:HB2	1.92	0.52
7:G:475:LYS:NZ	7:G:475:LYS:CB	2.73	0.52
8:H:598:GLN:HE22	19:Z:2:NAG:C8	2.18	0.52
2:B:230:LEU:O	2:B:233:VAL:HG22	2.09	0.52
3:C:77:PHE:HD1	7:G:715:LEU:CD1	2.22	0.52
5:E:75:GLY:HA2	5:E:104:PHE:CD1	2.45	0.52
5:E:632:TYR:CD1	5:E:632:TYR:C	2.87	0.52
5:E:724:ILE:HD11	5:E:811:LEU:HD11	1.91	0.52
5:E:761:PRO:CD	6:F:860:THR:HB	2.36	0.52
7:G:71:THR:HG22	7:G:79:LEU:HD22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:965:LYS:HD3	9:L:436:LEU:HD22	1.88	0.52
18:Y:1:NAG:H62	18:Y:2:NAG:H82	1.92	0.52
5:E:417:HIS:ND1	5:E:463:ILE:HD11	2.23	0.52
7:G:333:TRP:HA	7:G:337:THR:HG21	1.92	0.52
7:G:665:VAL:HG21	17:U:1:NAG:O7	2.08	0.52
8:H:161:GLU:HG3	8:H:167:ALA:HB2	1.91	0.52
8:H:391:GLY:HA2	8:H:397:PHE:CB	2.39	0.52
8:H:418:LEU:HD11	8:H:436:LEU:HD23	1.91	0.52
8:H:797:GLN:HB2	8:H:894:HIS:CD2	2.44	0.52
9:L:432:ILE:HG21	9:L:446:PHE:CE1	2.44	0.52
7:G:186:ASP:OD1	7:G:186:ASP:N	2.40	0.52
7:G:573:VAL:CG1	7:G:711:VAL:CG2	2.80	0.52
8:H:791:GLU:HB2	8:H:794:GLN:HG3	1.90	0.52
5:E:629:GLU:OE1	5:E:631:THR:CG2	2.58	0.52
5:E:835:ARG:NH1	5:E:835:ARG:CG	2.72	0.52
7:G:516:GLN:HB3	7:G:582:VAL:CG1	2.40	0.52
7:G:682:GLN:HA	7:G:714:ALA:HB2	1.83	0.52
8:H:181:MET:HG3	8:H:186:GLN:HB3	1.91	0.52
8:H:504:THR:HG23	8:H:505:VAL:HG23	1.90	0.52
9:L:645:ARG:NH1	9:L:646:CYS:O	2.42	0.52
1:A:449:ARG:NE	4:D:255:MET:HE1	2.24	0.52
5:E:51:LEU:HG	5:E:150:LEU:HD11	1.90	0.52
5:E:632:TYR:HE1	5:E:635:LYS:O	1.91	0.52
5:E:876:HIS:CE1	5:E:877:MET:HG3	2.44	0.52
7:G:95:ILE:HD13	7:G:110:ILE:HG12	1.92	0.52
7:G:723:LEU:O	7:G:727:LEU:CG	2.34	0.52
21:A:702:9Z9:C26	21:A:704:9Z9:C48	2.86	0.52
2:B:232:LEU:O	2:B:236:LEU:HG	2.10	0.52
3:C:78:GLU:O	3:C:79:PHE:HB2	2.10	0.52
5:E:356:ARG:NH2	5:E:374:ASN:HD22	2.08	0.52
5:E:829:SER:C	5:E:830:SER:HG	2.13	0.52
5:E:916:VAL:CG2	5:E:921:MET:CB	2.81	0.52
8:H:752:ARG:NH1	8:H:752:ARG:CG	2.73	0.52
8:H:791:GLU:HA	8:H:930:LEU:HD12	1.91	0.52
10:J:57:HIS:HA	10:J:67:GLN:HA	1.92	0.52
2:B:160:LEU:HA	2:B:163:TRP:HD1	1.75	0.52
5:E:609:ILE:HG22	5:E:611:VAL:O	2.07	0.52
5:E:685:MET:CA	5:E:687:GLN:NE2	2.70	0.52
5:E:978:GLU:OE1	5:E:982:ARG:N	2.43	0.52
6:F:517:MET:HE2	6:F:527:VAL:HG22	1.91	0.52
6:F:709:GLN:HG3	6:F:710:HIS:H	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:105:LEU:HD12	7:G:116:SER:HB2	1.92	0.52
8:H:919:CYS:HB3	16:a:1:NAG:H82	1.91	0.52
8:H:935:ARG:CB	8:H:935:ARG:NH1	2.73	0.52
5:E:116:ARG:NH2	5:E:120:THR:OG1	2.34	0.52
5:E:761:PRO:C	5:E:762:ILE:HD12	2.34	0.52
6:F:402:ASN:HD21	6:F:424:ASP:HB3	1.74	0.52
6:F:941:SER:HB2	6:F:1036:VAL:CG1	2.40	0.52
9:L:631:ALA:O	9:L:650:ASN:N	2.35	0.52
1:A:554:ILE:HG22	1:A:555:PRO:HD3	1.92	0.51
5:E:267:ASP:OD2	5:E:269:ARG:NH2	2.37	0.51
6:F:577:LEU:HD13	6:F:584:LEU:HD11	1.91	0.51
7:G:682:GLN:HG3	7:G:714:ALA:CB	2.38	0.51
8:H:792:LEU:CD1	8:H:932:MET:SD	2.98	0.51
5:E:670:ILE:HA	5:E:681:ALA:HB2	1.91	0.51
5:E:721:ASN:HD22	5:E:721:ASN:H	0.69	0.51
6:F:918:ARG:HG3	6:F:919:ASP:N	2.23	0.51
8:H:897:TRP:NE1	8:H:907:TYR:OH	2.37	0.51
8:H:935:ARG:CZ	8:H:935:ARG:CB	2.86	0.51
9:L:508:ARG:HB3	9:L:543:LEU:HA	1.92	0.51
4:D:174:GLU:OE1	4:D:174:GLU:N	2.44	0.51
6:F:266:ASP:C	6:F:267:SER:HG	1.99	0.51
7:G:580:LYS:HD2	7:G:670:LEU:HD12	1.92	0.51
8:H:335:TYR:CE2	8:H:344:LYS:HB3	2.45	0.51
8:H:554:ILE:HD11	8:H:721:SER:HA	1.93	0.51
5:E:798:ARG:NH1	6:F:663:VAL:O	2.43	0.51
5:E:947:LYS:O	5:E:948:PHE:C	2.52	0.51
6:F:189:THR:CG2	6:F:191:GLY:N	2.58	0.51
9:L:94:ASP:HA	9:L:97:MET:HB3	1.92	0.51
9:L:181:PHE:HD1	9:L:300:GLN:HG2	1.74	0.51
9:L:424:ILE:HA	9:L:427:PHE:HB2	1.92	0.51
5:E:747:ASP:CG	5:E:794:HIS:HD1	2.17	0.51
5:E:762:ILE:HD11	6:F:862:LEU:CD1	2.41	0.51
6:F:620:VAL:CG2	6:F:621:ASN:N	2.73	0.51
7:G:165:ILE:HG13	7:G:211:MET:CE	2.40	0.51
7:G:239:LEU:N	7:G:239:LEU:CD1	2.73	0.51
9:L:254:GLY:HA2	9:L:257:LEU:HB2	1.91	0.51
5:E:319:ASN:C	5:E:319:ASN:HD22	2.19	0.51
5:E:791:LEU:HD12	5:E:793:ILE:HD11	1.92	0.51
8:H:512:PRO:HG3	8:H:556:GLU:OE2	2.10	0.51
9:L:624:PHE:O	9:L:628:SER:N	2.42	0.51
3:C:176:THR:O	3:C:180:VAL:HG23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:402:ASN:HD22	6:F:402:ASN:N	2.06	0.51
6:F:569:SER:HB3	6:F:590:LEU:HD23	1.92	0.51
7:G:603:GLU:HG3	7:G:607:LEU:HB2	1.93	0.51
8:H:856:PRO:O	8:H:860:VAL:HG23	2.11	0.51
1:A:377:GLU:HG3	1:A:378:ILE:N	2.26	0.51
3:C:143:HIS:HA	3:C:146:ASP:HB3	1.92	0.51
8:H:876:LYS:HZ2	8:H:876:LYS:HB2	1.75	0.51
11:M:16:LEU:O	11:M:20:VAL:HG22	2.11	0.51
5:E:185:THR:CG2	5:E:247:LEU:HG	2.41	0.51
7:G:624:GLN:OE1	7:G:662:TRP:HB2	2.11	0.51
8:H:854:ASP:OD1	8:H:855:ILE:HD12	2.11	0.51
1:A:469:LEU:HD23	1:A:469:LEU:O	2.11	0.51
1:A:568:PHE:O	1:A:571:LEU:HB2	2.10	0.51
5:E:594:HIS:ND1	5:E:594:HIS:O	2.43	0.51
5:E:646:ASN:ND2	5:E:647:PRO:N	2.55	0.51
9:L:446:PHE:O	9:L:450:THR:OG1	2.25	0.51
9:L:661:ILE:O	9:L:665:SER:N	2.40	0.51
2:B:232:LEU:O	2:B:232:LEU:HD22	2.10	0.50
6:F:53:LYS:HG3	6:F:64:ASP:OD2	2.10	0.50
6:F:110:ASN:OD1	6:F:113:GLU:HG2	2.11	0.50
6:F:419:LEU:N	6:F:419:LEU:CD2	2.73	0.50
8:H:848:MET:HE3	8:H:848:MET:HA	1.92	0.50
11:M:1:MET:SD	11:M:4:ARG:NH2	2.84	0.50
1:A:518:ARG:NH1	1:A:544:ASP:OD2	2.44	0.50
2:B:159:ILE:HA	2:B:162:MET:HE2	1.93	0.50
2:B:337:MET:O	2:B:340:THR:OG1	2.23	0.50
5:E:467:VAL:HG12	5:E:471:ARG:O	2.11	0.50
5:E:818:CYS:HB2	5:E:821:ILE:HD11	1.92	0.50
7:G:317:GLN:HG3	7:G:322:THR:HG21	1.92	0.50
9:L:521:CYS:HA	9:L:536:CYS:HA	1.93	0.50
1:A:361:VAL:HG11	1:A:461:ARG:HG3	1.92	0.50
1:A:419:ASP:HB2	1:A:461:ARG:HH22	1.74	0.50
8:H:834:GLU:OE2	8:H:880:LEU:HG	2.11	0.50
8:H:935:ARG:CG	8:H:935:ARG:NH1	2.73	0.50
1:A:362:CYS:HA	1:A:365:THR:HG22	1.93	0.50
3:C:209:ASN:ND2	3:C:235:GLU:OE2	2.43	0.50
5:E:636:LEU:HD23	5:E:636:LEU:N	2.24	0.50
6:F:189:THR:CG2	6:F:190:ASN:N	2.72	0.50
7:G:372:SER:OG	8:H:651:ARG:NH1	2.44	0.50
7:G:717:VAL:CG2	7:G:719:LYS:NZ	2.73	0.50
9:L:461:ILE:O	9:L:465:GLU:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:94:PRO:HA	2:B:97:LEU:HD12	1.92	0.50
3:C:207:LEU:HD23	3:C:208:GLU:HB3	1.94	0.50
5:E:762:ILE:N	5:E:762:ILE:CD1	2.73	0.50
7:G:580:LYS:HD3	7:G:676:ASN:O	2.12	0.50
9:L:406:THR:HB	9:L:409:ILE:HB	1.94	0.50
12:N:11:UNK:O	12:N:14:UNK:N	2.45	0.50
21:A:703:9Z9:C26	21:A:704:9Z9:C22	2.90	0.50
7:G:526:ILE:HG22	7:G:527:LEU:HG	1.94	0.50
7:G:717:VAL:HG22	7:G:719:LYS:CD	2.41	0.50
1:A:529:LEU:HD12	1:A:560:TYR:CE2	2.47	0.50
4:D:60:TYR:HA	4:D:63:GLN:HG3	1.93	0.50
5:E:176:TYR:CZ	5:E:509:GLU:HB3	2.46	0.50
5:E:560:PRO:HB2	5:E:563:ILE:HG12	1.93	0.50
5:E:638:TYR:N	5:E:638:TYR:HD1	2.10	0.50
5:E:736:LEU:HD13	5:E:738:LYS:HD3	1.94	0.50
6:F:966:ARG:HG2	6:F:976:SER:HB3	1.94	0.50
7:G:516:GLN:HE21	7:G:518:LYS:CE	2.08	0.50
8:H:51:TRP:CZ2	8:H:120:ARG:HG3	2.46	0.50
3:C:80:PHE:HD2	7:G:716:PRO:CG	2.13	0.50
5:E:88:ILE:HD12	5:E:97:TYR:CE2	2.47	0.50
6:F:621:ASN:ND2	6:F:626:GLN:NE2	2.60	0.50
7:G:519:ILE:HD13	7:G:519:ILE:O	2.11	0.50
8:H:894:HIS:CE1	17:b:1:NAG:H5	2.47	0.50
9:L:212:VAL:CG2	9:L:213:PRO:HD3	2.42	0.50
2:B:138:TRP:CE3	2:B:139:PRO:CG	2.90	0.50
5:E:613:PHE:O	6:F:627:ALA:HB1	2.12	0.50
8:H:351:ILE:HB	8:H:397:PHE:CZ	2.47	0.50
8:H:758:PHE:CZ	9:L:553:ILE:CD1	2.75	0.50
3:C:125:LEU:HD13	3:C:152:ARG:NH2	2.27	0.49
5:E:40:ILE:C	5:E:41:LEU:CD1	2.85	0.49
5:E:43:GLY:C	5:E:45:HIS:H	2.19	0.49
6:F:372:TYR:HA	6:F:389:PRO:HG2	1.94	0.49
6:F:709:GLN:HG3	6:F:710:HIS:N	2.27	0.49
7:G:542:LYS:NZ	7:G:556:ASP:OD2	2.44	0.49
9:L:515:SER:HB3	9:L:518:PHE:HB3	1.93	0.49
9:L:584:CYS:C	9:L:587:PRO:HD2	2.36	0.49
7:G:276:ILE:HD11	7:G:323:TYR:HD2	1.77	0.49
9:L:270:LEU:HA	9:L:273:VAL:HB	1.93	0.49
5:E:759:THR:HG21	6:F:861:TYR:CE2	2.42	0.49
7:G:165:ILE:C	7:G:165:ILE:CD1	2.86	0.49
7:G:196:GLY:HA3	7:G:210:LEU:HD22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:L:94:ASP:O	9:L:98:THR:N	2.41	0.49
9:L:99:LEU:O	9:L:103:ALA:N	2.43	0.49
16:S:1:NAG:H62	16:S:2:NAG:HN2	1.76	0.49
1:A:522:ILE:O	1:A:525:THR:OG1	2.26	0.49
2:B:223:ARG:NH2	2:B:224:GLN:HG2	2.24	0.49
7:G:169:ASN:N	7:G:169:ASN:ND2	2.60	0.49
11:M:68:ALA:HB1	11:M:91:LEU:HD22	1.94	0.49
5:E:176:TYR:CE2	5:E:509:GLU:HB3	2.47	0.49
5:E:643:LEU:HD12	5:E:694:LYS:HZ1	1.63	0.49
5:E:898:ARG:HH21	5:E:898:ARG:CG	2.26	0.49
6:F:406:ASP:O	6:F:407:TRP:HB2	2.12	0.49
7:G:579:TRP:C	7:G:678:ILE:CG2	2.62	0.49
8:H:135:PHE:HA	8:H:149:THR:O	2.11	0.49
8:H:268:LEU:HD12	8:H:282:LEU:HD11	1.94	0.49
8:H:334:VAL:HG13	8:H:345:LEU:HB2	1.93	0.49
11:M:110:ASN:C	11:M:111:TYR:HD1	2.18	0.49
5:E:23:ILE:HG21	5:E:26:LYS:HG3	1.94	0.49
5:E:689:ILE:HG22	5:E:690:LYS:N	2.27	0.49
5:E:1052:VAL:CB	11:M:116:HIS:HE1	2.24	0.49
2:B:263:GLU:HG3	2:B:309:GLU:HB3	1.94	0.49
3:C:284:LEU:C	3:C:284:LEU:CD2	2.85	0.49
5:E:354:ILE:HG23	5:E:354:ILE:O	2.12	0.49
6:F:227:VAL:HG23	6:F:229:LYS:NZ	2.25	0.49
6:F:402:ASN:HD22	6:F:402:ASN:H	1.59	0.49
8:H:150:ILE:HG12	8:H:225:ILE:CD1	2.43	0.49
8:H:802:LEU:HD23	8:H:809:ILE:HD11	1.94	0.49
8:H:839:ILE:HD13	8:H:872:TYR:HB2	1.93	0.49
9:L:238:ILE:HG12	9:L:609:TYR:HD2	1.78	0.49
14:K:90:GLU:O	14:K:94:GLY:N	2.46	0.49
4:D:53:GLN:CD	4:D:53:GLN:H	2.19	0.49
5:E:833:TYR:CD2	5:E:833:TYR:C	2.91	0.49
5:E:881:ILE:N	5:E:881:ILE:CD1	2.76	0.49
9:L:396:PRO:HB3	9:L:411:SER:HA	1.94	0.49
14:K:47:CYS:O	14:K:49:ASP:N	2.45	0.49
5:E:554:HIS:NE2	5:E:556:PRO:HA	2.27	0.49
5:E:849:ASP:O	5:E:853:GLY:N	2.36	0.49
6:F:1016:ILE:HG22	6:F:1017:PRO:HD2	1.94	0.49
7:G:22:VAL:HG13	7:G:364:ASP:OD1	2.13	0.49
9:L:327:SER:HB2	9:L:332:HIS:HE2	1.77	0.49
11:M:112:ARG:NH2	11:M:112:ARG:CB	2.73	0.49
1:A:475:LEU:HD23	1:A:475:LEU:H	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:SER:HA	1:A:486:LEU:HD12	1.94	0.49
1:A:516:PRO:O	1:A:520:GLN:HB3	2.12	0.49
21:A:702:9Z9:C15	21:A:704:9Z9:C15	2.91	0.49
5:E:808:ALA:CB	5:E:824:LEU:HD23	2.42	0.49
5:E:857:ASP:C	5:E:859:GLN:H	2.21	0.49
6:F:269:PHE:CD1	6:F:587:LEU:HD13	2.47	0.49
8:H:188:PRO:HA	8:H:226:ARG:O	2.13	0.49
8:H:273:ASP:HB3	8:H:276:ILE:O	2.12	0.49
9:L:335:ARG:O	9:L:339:ARG:N	2.46	0.49
9:L:525:LYS:HB3	9:L:534:TYR:CE1	2.48	0.49
4:D:182:VAL:HA	4:D:289:MET:HE3	1.95	0.48
5:E:762:ILE:HG22	5:E:763:PRO:CD	2.41	0.48
5:E:880:SER:C	5:E:881:ILE:CD1	2.83	0.48
5:E:895:PRO:O	5:E:896:ILE:CG1	2.60	0.48
8:H:939:TYR:CE2	9:L:566:LYS:NZ	2.72	0.48
9:L:502:TYR:HB2	9:L:647:TRP:CH2	2.48	0.48
1:A:361:VAL:HG11	1:A:461:ARG:HG2	1.95	0.48
5:E:43:GLY:O	5:E:45:HIS:N	2.46	0.48
5:E:232:TYR:HA	5:E:235:LEU:HB3	1.94	0.48
7:G:106:VAL:CG2	7:G:119:TYR:CE2	2.96	0.48
8:H:634:ASP:OD2	8:H:741:LYS:NZ	2.37	0.48
8:H:816:PHE:HB3	8:H:911:ILE:HD13	1.94	0.48
9:L:170:MET:HE3	9:L:232:ALA:HB3	1.95	0.48
9:L:210:ASN:C	9:L:213:PRO:HD2	2.38	0.48
9:L:433:VAL:HA	9:L:438:MET:HG3	1.95	0.48
10:J:119:HIS:O	10:J:123:LYS:N	2.40	0.48
14:K:47:CYS:C	14:K:49:ASP:H	2.20	0.48
1:A:450:ILE:O	1:A:453:VAL:HG12	2.14	0.48
2:B:349:LEU:O	2:B:352:GLU:HG3	2.13	0.48
5:E:141:LEU:HD11	7:G:422:PRO:HG2	1.94	0.48
5:E:895:PRO:C	5:E:896:ILE:HD13	2.07	0.48
5:E:1054:LEU:HD23	5:E:1058:GLY:HA3	1.96	0.48
7:G:106:VAL:CG2	7:G:119:TYR:HE2	2.26	0.48
7:G:164:GLN:HG3	7:G:166:PRO:HD2	1.95	0.48
8:H:414:GLN:O	8:H:415:THR:HG22	2.12	0.48
8:H:947:VAL:HG12	8:H:948:LEU:HD22	1.94	0.48
9:L:451:THR:HG1	9:L:584:CYS:HG	1.60	0.48
9:L:499:THR:HA	9:L:502:TYR:CE2	2.49	0.48
1:A:374:THR:CA	1:A:377:GLU:HG2	2.41	0.48
5:E:489:LYS:HE2	5:E:489:LYS:CA	2.40	0.48
7:G:165:ILE:HB	7:G:211:MET:CE	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:273:VAL:HG23	7:G:322:THR:OG1	2.13	0.48
7:G:278:GLN:O	7:G:280:ILE:HD12	2.12	0.48
3:C:38:GLU:O	7:G:746:GLN:OE1	2.31	0.48
4:D:115:GLU:OE1	4:D:115:GLU:HA	2.14	0.48
5:E:358:ILE:HD11	5:E:374:ASN:HB2	1.94	0.48
5:E:918:SER:O	5:E:919:ARG:C	2.56	0.48
5:E:948:PHE:HE1	5:E:1052:VAL:CG1	2.10	0.48
8:H:959:SER:O	8:H:963:TYR:N	2.36	0.48
9:L:486:ASN:C	9:L:488:THR:N	2.59	0.48
9:L:613:LYS:O	9:L:617:SER:OG	2.26	0.48
11:M:38:HIS:O	11:M:42:VAL:HG22	2.14	0.48
1:A:565:TYR:C	1:A:565:TYR:CD1	2.92	0.48
6:F:360:TYR:CD1	6:F:377:THR:HG22	2.49	0.48
6:F:966:ARG:CG	6:F:976:SER:HB2	2.42	0.48
7:G:155:ASN:O	7:G:156:LEU:HD12	2.14	0.48
8:H:839:ILE:HG21	8:H:872:TYR:CG	2.49	0.48
8:H:884:TYR:CE2	8:H:886:ILE:HB	2.48	0.48
9:L:505:ILE:HD12	9:L:516:PRO:HB3	1.95	0.48
5:E:42:THR:OG1	5:E:43:GLY:N	2.46	0.48
5:E:1023:SER:O	5:E:1024:GLU:HG2	2.14	0.48
6:F:637:LYS:N	6:F:769:LEU:O	2.47	0.48
7:G:142:CYS:C	7:G:149:CYS:HB3	2.38	0.48
7:G:190:HIS:ND1	7:G:190:HIS:N	2.59	0.48
9:L:201:ASN:HB3	9:L:204:ARG:HB2	1.95	0.48
5:E:35:CYS:HB2	5:E:47:ILE:HD13	1.94	0.48
5:E:557:LEU:C	5:E:558:THR:HG1	2.08	0.48
5:E:672:ASN:HB3	5:E:680:SER:HB2	1.95	0.48
6:F:515:LYS:HG2	6:F:516:TYR:HD1	1.79	0.48
7:G:190:HIS:NE2	7:G:228:HIS:CD2	2.80	0.48
3:C:266:VAL:HG12	4:D:286:LEU:HD11	1.96	0.48
5:E:39:GLY:C	5:E:40:ILE:CG1	2.85	0.48
5:E:43:GLY:C	5:E:45:HIS:N	2.71	0.48
5:E:636:LEU:CD2	5:E:636:LEU:N	2.73	0.48
8:H:664:VAL:HG23	8:H:665:MET:HG2	1.95	0.48
9:L:431:LEU:HD13	9:L:435:ARG:NH2	2.28	0.48
1:A:580:PHE:O	1:A:584:LEU:HD23	2.14	0.48
5:E:54:ASP:OD2	5:E:57:LYS:NZ	2.47	0.48
5:E:687:GLN:H	5:E:687:GLN:HE21	1.61	0.48
5:E:1056:PHE:CD1	5:E:1057:PRO:CD	2.97	0.48
6:F:785:ILE:HD13	6:F:813:LEU:HD21	1.95	0.48
7:G:515:VAL:HG12	7:G:516:GLN:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:516:GLN:HG3	7:G:584:GLU:OE2	2.14	0.48
7:G:528:ASN:O	7:G:531:GLN:HG2	2.14	0.48
8:H:639:LEU:HD21	8:H:733:ILE:HD13	1.96	0.48
9:L:166:SER:HB2	9:L:232:ALA:O	2.14	0.48
9:L:417:PHE:HD2	9:L:575:PHE:CZ	2.32	0.48
1:A:419:ASP:CB	1:A:461:ARG:HH21	2.27	0.47
5:E:646:ASN:HD22	5:E:646:ASN:C	2.19	0.47
6:F:966:ARG:HG3	6:F:972:ASP:CG	2.39	0.47
6:F:1057:LEU:HD23	6:F:1062:THR:OG1	2.14	0.47
7:G:519:ILE:C	7:G:519:ILE:CD1	2.85	0.47
8:H:901:TYR:HA	8:H:931:GLY:O	2.14	0.47
3:C:132:ARG:O	3:C:136:GLY:HA2	2.14	0.47
4:D:178:ARG:O	4:D:182:VAL:HG23	2.14	0.47
5:E:319:ASN:C	5:E:319:ASN:ND2	2.71	0.47
5:E:319:ASN:ND2	5:E:320:ARG:N	2.61	0.47
5:E:962:GLU:CG	5:E:963:ARG:H	2.03	0.47
6:F:239:ARG:HG3	6:F:253:LEU:HD11	1.96	0.47
7:G:508:ASP:N	7:G:701:CYS:SG	2.87	0.47
7:G:517:ASN:ND2	7:G:517:ASN:C	2.72	0.47
8:H:143:ASN:HD21	17:W:1:NAG:C7	2.24	0.47
9:L:505:ILE:HG13	9:L:556:ILE:O	2.14	0.47
17:U:1:NAG:C6	17:U:2:NAG:C1	2.92	0.47
6:F:832:GLU:O	6:F:839:ASN:ND2	2.32	0.47
7:G:236:TYR:CD2	7:G:236:TYR:O	2.67	0.47
7:G:623:SER:HB3	7:G:659:PRO:HG2	1.96	0.47
8:H:87:CYS:CB	8:H:101:CYS:SG	3.01	0.47
8:H:267:PRO:HB2	8:H:528:HIS:CD2	2.49	0.47
8:H:913:ASP:HB3	8:H:916:TYR:HB2	1.96	0.47
9:L:112:ALA:HB2	9:L:268:TYR:HA	1.97	0.47
9:L:214:ASN:H	9:L:217:LYS:HE2	1.79	0.47
9:L:548:ASP:CG	9:L:549:GLU:N	2.72	0.47
11:M:33:PHE:O	11:M:37:VAL:HG12	2.14	0.47
11:M:40:PHE:CD2	11:M:49:MET:HE1	2.45	0.47
11:M:46:TYR:CE2	11:M:111:TYR:CD2	3.02	0.47
11:M:112:ARG:HB2	11:M:112:ARG:CZ	2.43	0.47
1:A:566:PHE:CZ	2:B:292:PHE:CE2	3.02	0.47
5:E:59:ARG:NH1	5:E:109:GLU:OE2	2.46	0.47
5:E:94:TYR:CZ	5:E:729:LEU:HD11	2.49	0.47
5:E:737:VAL:HG22	5:E:826:THR:HB	1.95	0.47
5:E:759:THR:O	5:E:762:ILE:O	2.33	0.47
5:E:855:HIS:HB3	5:E:863:MET:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:692:TYR:OH	6:F:701:HIS:ND1	2.48	0.47
8:H:754:GLN:N	8:H:754:GLN:NE2	2.60	0.47
9:L:455:VAL:HA	9:L:458:PHE:HD2	1.78	0.47
10:J:77:LEU:HA	10:J:91:LEU:HA	1.95	0.47
2:B:183:THR:OG1	2:B:214:ARG:NH2	2.47	0.47
3:C:212:ASN:OD1	3:C:212:ASN:N	2.46	0.47
5:E:116:ARG:HH21	5:E:120:THR:HG1	1.60	0.47
6:F:966:ARG:CG	6:F:976:SER:CB	2.91	0.47
8:H:665:MET:HE3	8:H:665:MET:HB3	1.73	0.47
1:A:346:SER:O	1:A:350:SER:OG	2.32	0.47
1:A:519:PHE:HB3	1:A:525:THR:HA	1.97	0.47
1:A:550:ALA:HB3	1:A:552:TYR:OH	2.13	0.47
2:B:298:TYR:O	2:B:302:GLN:HG3	2.15	0.47
2:B:366:LYS:HA	2:B:369:ILE:HD12	1.97	0.47
4:D:141:PHE:O	4:D:145:MET:HG2	2.14	0.47
5:E:833:TYR:CE2	5:E:834:LEU:HG	2.50	0.47
5:E:839:HIS:HB2	5:E:1043:GLU:HG2	1.95	0.47
5:E:880:SER:OG	5:E:898:ARG:NH2	2.48	0.47
5:E:1030:VAL:O	5:E:1042:SER:HA	2.15	0.47
6:F:892:ILE:HD11	6:F:913:PRO:CG	2.45	0.47
7:G:37:LEU:HD21	7:G:83:THR:HG21	1.97	0.47
7:G:293:ILE:HG22	7:G:307:VAL:HG22	1.96	0.47
9:L:417:PHE:HD2	9:L:575:PHE:HZ	1.62	0.47
9:L:634:TYR:CG	9:L:648:ILE:HD13	2.48	0.47
1:A:532:MET:CE	1:A:541:ILE:HD11	2.43	0.47
2:B:307:VAL:HG12	2:B:309:GLU:H	1.79	0.47
3:C:89:PHE:O	3:C:92:SER:OG	2.30	0.47
5:E:636:LEU:CD2	5:E:637:TYR:HD1	2.27	0.47
5:E:643:LEU:HD12	5:E:694:LYS:HZ2	1.64	0.47
5:E:881:ILE:HD12	5:E:881:ILE:N	2.29	0.47
5:E:881:ILE:N	5:E:882:PRO:HD3	2.30	0.47
6:F:120:LEU:HD11	6:F:165:MET:HE1	1.96	0.47
6:F:823:LYS:HE2	6:F:825:ILE:HD11	1.96	0.47
7:G:571:ARG:HH21	7:G:707:PHE:HB2	1.65	0.47
7:G:720:PHE:CE2	7:G:722:PRO:HG2	2.50	0.47
7:G:736:THR:O	7:G:740:ALA:N	2.43	0.47
8:H:320:ILE:HB	8:H:359:PHE:HE1	1.79	0.47
9:L:164:ALA:O	9:L:168:ILE:N	2.48	0.47
9:L:368:ILE:HD13	9:L:607:VAL:HG11	1.95	0.47
9:L:502:TYR:CG	9:L:515:SER:HB2	2.50	0.47
17:U:2:NAG:H4	17:U:3:BMA:O2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:88:ILE:HG12	5:E:133:ILE:CD1	2.45	0.47
5:E:399:PHE:HA	6:F:162:ALA:HB1	1.97	0.47
5:E:428:SER:HA	5:E:449:HIS:O	2.15	0.47
7:G:165:ILE:CD1	7:G:191:LEU:O	2.62	0.47
7:G:184:ASN:ND2	7:G:186:ASP:CG	2.72	0.47
7:G:579:TRP:CE3	7:G:678:ILE:CG2	2.97	0.47
7:G:722:PRO:HB3	7:G:727:LEU:HD21	1.96	0.47
8:H:874:ILE:CG2	8:H:875:GLY:N	2.72	0.47
9:L:473:GLY:O	9:L:474:ILE:C	2.58	0.47
1:A:455:LYS:HG3	1:A:458:ARG:HD2	1.96	0.47
5:E:514:GLY:HA2	5:E:526:ILE:HD13	1.96	0.47
5:E:561:THR:HA	5:E:564:GLN:HG2	1.95	0.47
5:E:585:LEU:O	5:E:611:VAL:HG22	2.14	0.47
5:E:616:GLU:OE1	5:E:658:LYS:NZ	2.48	0.47
5:E:686:PRO:CD	5:E:687:GLN:HE21	2.28	0.47
6:F:261:SER:HA	6:F:275:LEU:O	2.15	0.47
7:G:168:THR:C	7:G:169:ASN:ND2	2.73	0.47
7:G:710:TYR:CE2	7:G:712:HIS:HD2	2.33	0.47
8:H:261:THR:HG1	8:H:314:HIS:HD1	1.62	0.47
11:M:114:GLU:CG	11:M:116:HIS:HD2	2.27	0.47
1:A:433:LEU:HD11	1:A:438:LEU:HD13	1.97	0.47
2:B:147:ALA:O	2:B:151:ILE:HG12	2.15	0.47
4:D:204:PHE:CD2	4:D:266:PHE:HD1	2.33	0.47
6:F:322:THR:HG22	6:F:332:GLY:HA3	1.97	0.47
6:F:641:LEU:HD12	6:F:750:ILE:CG1	2.45	0.47
8:H:221:ILE:O	8:H:243:MET:HA	2.15	0.47
1:A:432:LEU:HA	1:A:435:ILE:HG22	1.96	0.46
1:A:582:MET:O	1:A:585:LEU:HG	2.15	0.46
6:F:257:TYR:C	6:F:297:THR:HG22	2.34	0.46
6:F:814:ASN:ND2	6:F:815:ARG:HG2	2.29	0.46
6:F:1076:LEU:HA	6:F:1076:LEU:HD23	1.80	0.46
7:G:223:GLU:O	7:G:227:ASN:CA	2.64	0.46
7:G:544:ALA:CB	7:G:607:LEU:HD23	2.44	0.46
8:H:259:PRO:O	8:H:313:ARG:HD2	2.15	0.46
8:H:261:THR:OG1	8:H:314:HIS:ND1	2.48	0.46
8:H:659:HIS:HD1	8:H:667:TRP:HH2	1.63	0.46
1:A:381:GLU:O	1:A:385:MET:HE1	2.14	0.46
6:F:256:PHE:O	6:F:257:TYR:C	2.59	0.46
6:F:620:VAL:CG2	6:F:621:ASN:H	2.20	0.46
6:F:717:TYR:CZ	6:F:721:LEU:HD11	2.50	0.46
6:F:978:ILE:HG12	6:F:1010:SER:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:615:THR:HG22	7:G:618:THR:HG22	1.97	0.46
9:L:143:SER:O	9:L:147:ALA:N	2.47	0.46
1:A:492:ILE:HD11	1:A:568:PHE:CD1	2.50	0.46
1:A:511:PHE:O	1:A:519:PHE:HE1	1.98	0.46
4:D:81:ASN:O	4:D:84:THR:OG1	2.27	0.46
5:E:408:PHE:CE2	5:E:411:PRO:HB3	2.50	0.46
5:E:721:ASN:N	5:E:721:ASN:ND2	2.21	0.46
6:F:914:CYS:SG	6:F:1051:HIS:ND1	2.88	0.46
6:F:917:PHE:CD2	6:F:1056:PRO:HD3	2.51	0.46
8:H:222:ALA:HA	8:H:243:MET:HG2	1.96	0.46
8:H:231:ALA:HB2	8:H:236:PHE:CE1	2.50	0.46
9:L:503:THR:O	9:L:516:PRO:HD3	2.15	0.46
1:A:453:VAL:O	1:A:456:SER:N	2.48	0.46
5:E:831:CYS:SG	5:E:1039:CYS:N	2.71	0.46
5:E:948:PHE:CG	5:E:949:PRO:HD3	2.51	0.46
6:F:518:VAL:HG12	6:F:579:PHE:HD2	1.80	0.46
6:F:1061:ARG:CG	6:F:1061:ARG:NH2	2.72	0.46
7:G:643:TRP:HE1	7:G:694:VAL:HG13	1.79	0.46
8:H:245:THR:CG2	8:H:246:TYR:H	2.26	0.46
8:H:633:MET:CE	8:H:665:MET:HE1	2.45	0.46
8:H:755:ARG:HG3	9:L:552:PHE:CD2	2.51	0.46
8:H:908:ARG:NH2	8:H:924:ILE:HD11	2.30	0.46
9:L:87:VAL:HA	9:L:90:PHE:HB2	1.97	0.46
1:A:363:LEU:O	1:A:366:VAL:HG12	2.14	0.46
2:B:224:GLN:O	2:B:227:VAL:N	2.49	0.46
3:C:38:GLU:HG2	3:C:39:CYS:H	1.79	0.46
5:E:431:TRP:CE2	5:E:442:MET:HB2	2.51	0.46
5:E:655:ASP:HA	5:E:658:LYS:CD	2.45	0.46
5:E:969:GLU:HB3	5:E:971:PRO:HD2	1.98	0.46
8:H:287:GLU:HG2	8:H:300:ARG:HG2	1.97	0.46
8:H:292:ASN:ND2	16:X:1:NAG:N2	2.63	0.46
6:F:899:ASN:O	6:F:901:HIS:ND1	2.32	0.46
6:F:904:ASP:HB3	6:F:908:LYS:NZ	2.31	0.46
6:F:981:THR:HG23	6:F:983:VAL:HG12	1.96	0.46
8:H:583:LEU:HD21	8:H:595:LEU:CD1	2.45	0.46
5:E:37:GLY:C	5:E:39:GLY:N	2.71	0.46
5:E:591:VAL:HG22	5:E:605:ILE:HG22	1.98	0.46
5:E:1052:VAL:HB	11:M:116:HIS:CE1	2.46	0.46
7:G:715:LEU:CB	7:G:716:PRO:CD	2.89	0.46
8:H:449:ILE:HG13	8:H:470:LEU:HD23	1.98	0.46
8:H:804:ASP:CG	8:H:805:GLU:H	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:L:613:LYS:O	9:L:618:VAL:HG23	2.16	0.46
11:M:30:MET:SD	11:M:97:MET:HE1	2.55	0.46
2:B:114:SER:O	2:B:118:LEU:HD23	2.15	0.46
4:D:145:MET:HA	4:D:145:MET:HE3	1.97	0.46
5:E:44:LEU:HD12	5:E:63:ARG:HH21	1.80	0.46
5:E:45:HIS:H	5:E:45:HIS:HD2	1.61	0.46
5:E:632:TYR:CD1	5:E:633:SER:O	2.69	0.46
5:E:1056:PHE:HD1	5:E:1057:PRO:CD	2.29	0.46
6:F:176:PHE:HE1	17:R:1:NAG:H83	1.81	0.46
6:F:300:ASP:CB	6:F:348:LEU:HB3	2.45	0.46
6:F:898:ILE:O	6:F:900:LYS:HD2	2.16	0.46
6:F:1008:GLU:HA	6:F:1013:TYR:CE2	2.41	0.46
7:G:188:LEU:N	7:G:188:LEU:CD2	2.70	0.46
7:G:682:GLN:CB	7:G:714:ALA:CB	2.88	0.46
9:L:201:ASN:O	9:L:205:ASN:ND2	2.49	0.46
11:M:75:ALA:HB1	11:M:83:LEU:HB3	1.98	0.46
4:D:204:PHE:O	4:D:262:TYR:OH	2.32	0.46
5:E:849:ASP:HA	5:E:852:SER:HB3	1.97	0.46
6:F:621:ASN:ND2	6:F:626:GLN:HE21	2.13	0.46
6:F:758:LYS:HG2	6:F:1039:SER:O	2.16	0.46
6:F:907:ILE:H	6:F:907:ILE:CD1	2.14	0.46
7:G:575:TYR:N	7:G:712:HIS:O	2.40	0.46
2:B:348:GLU:O	2:B:351:GLU:HG3	2.16	0.46
4:D:90:ASN:ND2	4:D:93:LEU:HD13	2.31	0.46
5:E:884:THR:O	5:E:886:ASN:ND2	2.49	0.46
8:H:308:LEU:HD12	8:H:312:GLN:HG2	1.98	0.46
9:L:100:TYR:O	9:L:104:VAL:N	2.48	0.46
9:L:400:GLN:HG3	9:L:407:PRO:HG3	1.97	0.46
1:A:453:VAL:O	1:A:456:SER:HB2	2.16	0.45
5:E:597:GLU:HB2	5:E:598:PRO:HD3	1.98	0.45
5:E:875:SER:CB	5:E:883:LEU:CD1	2.94	0.45
8:H:52:ARG:HD2	8:H:54:TYR:OH	2.16	0.45
9:L:164:ALA:HB2	9:L:321:MET:HB3	1.98	0.45
9:L:476:GLU:O	9:L:477:ASP:C	2.53	0.45
11:M:29:HIS:ND1	11:M:61:GLN:HG2	2.31	0.45
2:B:203:TRP:O	2:B:207:LEU:HG	2.16	0.45
5:E:44:LEU:HD22	5:E:44:LEU:HA	1.77	0.45
5:E:1015:GLY:O	16:P:1:NAG:H82	2.16	0.45
5:E:1053:PRO:HD2	11:M:116:HIS:ND1	2.31	0.45
6:F:165:MET:HG2	6:F:669:PHE:CZ	2.51	0.45
7:G:212:VAL:CG2	7:G:236:TYR:CD2	2.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:239:LEU:O	7:G:256:ASN:ND2	2.49	0.45
8:H:315:SER:O	8:H:317:ARG:NH1	2.49	0.45
8:H:357:LEU:HD11	8:H:385:LYS:HB2	1.96	0.45
8:H:793:GLY:HA2	8:H:899:MET:HE2	1.98	0.45
9:L:431:LEU:HD13	9:L:435:ARG:HH21	1.80	0.45
1:A:566:PHE:CZ	2:B:292:PHE:HE2	2.34	0.45
2:B:323:LEU:O	2:B:327:SER:HB3	2.16	0.45
4:D:216:VAL:N	4:D:217:PRO:HD3	2.32	0.45
7:G:720:PHE:CE2	7:G:722:PRO:CG	3.00	0.45
8:H:485:MET:HE1	18:Y:1:NAG:H82	1.96	0.45
8:H:872:TYR:CD2	8:H:872:TYR:O	2.69	0.45
9:L:178:ALA:HB2	9:L:307:PHE:HB2	1.98	0.45
18:Y:2:NAG:H4	18:Y:3:BMA:O2	2.16	0.45
2:B:305:TRP:CD1	2:B:312:ARG:HG2	2.51	0.45
5:E:94:TYR:CE2	5:E:729:LEU:HD21	2.52	0.45
5:E:99:PHE:HD1	5:E:112:ILE:HD12	1.82	0.45
5:E:848:GLU:HG2	5:E:849:ASP:N	2.32	0.45
8:H:533:ASP:OD1	8:H:533:ASP:N	2.44	0.45
8:H:746:ARG:NH2	8:H:811:ILE:HD11	2.31	0.45
8:H:755:ARG:O	8:H:756:ARG:HB2	2.16	0.45
1:A:471:ILE:O	1:A:472:LEU:HB2	2.17	0.45
1:A:473:THR:HB	1:A:476:HIS:HB2	1.99	0.45
2:B:138:TRP:HB3	2:B:139:PRO:HD3	1.98	0.45
3:C:77:PHE:CD1	7:G:715:LEU:HD11	2.51	0.45
5:E:41:LEU:C	5:E:41:LEU:HD22	2.40	0.45
5:E:843:ARG:HE	5:E:863:MET:CE	2.29	0.45
5:E:912:GLN:NE2	5:E:913:CYS:SG	2.90	0.45
6:F:501:GLU:OE2	8:H:180:GLN:HG2	2.16	0.45
6:F:1012:CYS:O	6:F:1015:ILE:HG13	2.16	0.45
7:G:239:LEU:HD12	7:G:239:LEU:H	1.78	0.45
7:G:743:ILE:HB	7:G:744:PRO:HD3	1.98	0.45
1:A:440:TYR:HB3	6:F:1003:GLU:HG2	1.98	0.45
1:A:518:ARG:NH2	1:A:541:ILE:HG22	2.31	0.45
3:C:261:ASN:HA	3:C:264:VAL:HG12	1.99	0.45
5:E:88:ILE:HD12	5:E:97:TYR:HE2	1.82	0.45
5:E:161:TRP:HE1	5:E:268:LEU:HA	1.82	0.45
5:E:173:ARG:HA	5:E:176:TYR:CE1	2.51	0.45
5:E:585:LEU:H	5:E:611:VAL:HG22	1.76	0.45
7:G:224:TYR:O	7:G:227:ASN:CB	2.65	0.45
7:G:582:VAL:HG13	7:G:582:VAL:O	2.16	0.45
9:L:518:PHE:C	9:L:520:GLY:H	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:L:549:GLU:HG2	9:L:550:GLY:N	2.31	0.45
1:A:419:ASP:CB	1:A:461:ARG:NH2	2.75	0.45
1:A:492:ILE:HD11	1:A:568:PHE:CE1	2.52	0.45
2:B:252:ILE:HD12	3:C:151:LEU:HA	1.99	0.45
3:C:269:MET:SD	4:D:286:LEU:HD22	2.56	0.45
4:D:223:MET:O	4:D:227:LEU:HD23	2.15	0.45
5:E:269:ARG:O	5:E:271:PRO:HD3	2.17	0.45
5:E:1056:PHE:O	5:E:1058:GLY:N	2.46	0.45
6:F:916:LEU:CD2	6:F:918:ARG:HG2	2.35	0.45
7:G:578:PRO:CB	7:G:677:LYS:HB2	2.47	0.45
7:G:719:LYS:O	7:G:720:PHE:CD1	2.70	0.45
9:L:243:PHE:CZ	9:L:328:LEU:HD22	2.52	0.45
9:L:472:ALA:CA	9:L:512:GLU:HB3	2.46	0.45
15:O:4:BMA:H2	15:O:5:BMA:O2	2.15	0.45
1:A:515:ASP:OD1	1:A:548:GLN:NE2	2.49	0.45
2:B:112:ILE:O	2:B:116:ILE:HG13	2.17	0.45
5:E:48:LYS:HE2	5:E:48:LYS:HB3	1.80	0.45
5:E:48:LYS:HD2	5:E:214:SER:HB2	1.99	0.45
5:E:453:LYS:NZ	5:E:493:PHE:O	2.50	0.45
5:E:928:GLN:HG2	5:E:936:PHE:CE2	2.52	0.45
5:E:1023:SER:HA	5:E:1052:VAL:HG22	1.97	0.45
6:F:917:PHE:CD2	6:F:917:PHE:O	2.69	0.45
8:H:759:SER:HB3	9:L:541:GLU:OE1	2.16	0.45
8:H:939:TYR:O	8:H:940:LEU:C	2.56	0.45
9:L:246:ASP:OD1	9:L:601:THR:OG1	2.27	0.45
9:L:392:LEU:HD11	9:L:418:VAL:HG21	1.99	0.45
11:M:42:VAL:HG23	11:M:43:ILE:N	2.30	0.45
5:E:900:GLN:OE1	11:M:44:HIS:CE1	2.70	0.45
6:F:486:LEU:HD22	6:F:499:ARG:HG2	1.98	0.45
6:F:691:LYS:HA	6:F:691:LYS:HD3	1.71	0.45
8:H:134:TYR:HB2	8:H:153:TYR:CD1	2.52	0.45
8:H:268:LEU:HD23	8:H:268:LEU:H	1.82	0.45
8:H:583:LEU:HD21	8:H:595:LEU:HD12	1.97	0.45
5:E:152:ASP:O	5:E:156:GLU:HG2	2.16	0.45
5:E:559:MET:HE2	5:E:563:ILE:HG22	1.95	0.45
6:F:623:GLY:O	6:F:625:TYR:CD2	2.70	0.45
6:F:892:ILE:HD11	6:F:913:PRO:HB2	1.92	0.45
1:A:345:LEU:HD12	1:A:405:ALA:HB1	1.99	0.44
4:D:151:GLN:N	4:D:151:GLN:OE1	2.50	0.44
5:E:335:GLU:O	5:E:337:PHE:CE1	2.70	0.44
5:E:884:THR:HG21	5:E:980:ASN:OD1	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:548:VAL:HB	6:F:549:PRO:HD3	1.99	0.44
7:G:539:THR:O	7:G:540:ILE:HD13	2.17	0.44
8:H:590:ASP:C	8:H:592:LYS:H	2.25	0.44
8:H:841:GLU:HB2	8:H:878:GLY:H	1.81	0.44
11:M:112:ARG:O	11:M:113:GLU:HB2	2.17	0.44
1:A:497:PHE:CD1	1:A:497:PHE:O	2.70	0.44
2:B:138:TRP:CE3	2:B:139:PRO:N	2.85	0.44
2:B:362:ALA:O	2:B:366:LYS:N	2.50	0.44
5:E:288:ARG:HG2	5:E:288:ARG:NH1	2.31	0.44
6:F:914:CYS:SG	6:F:1051:HIS:CG	3.10	0.44
7:G:145:LYS:HD3	7:G:145:LYS:HA	1.74	0.44
7:G:226:LEU:HA	7:G:229:SER:HB2	1.99	0.44
9:L:114:VAL:HA	9:L:117:THR:HB	1.99	0.44
9:L:140:TYR:HA	9:L:613:LYS:HD2	1.98	0.44
9:L:634:TYR:HB2	9:L:648:ILE:HB	1.98	0.44
2:B:146:VAL:HG12	8:H:941:VAL:HB	1.99	0.44
2:B:166:SER:O	2:B:167:PHE:HB3	2.17	0.44
2:B:277:PHE:HB3	2:B:287:THR:OG1	2.17	0.44
3:C:284:LEU:HD22	3:C:284:LEU:O	2.17	0.44
5:E:960:PHE:CD1	5:E:965:LYS:HB2	2.53	0.44
7:G:59:ASP:HB3	7:G:72:ILE:O	2.18	0.44
7:G:468:PHE:O	7:G:468:PHE:CD2	2.70	0.44
7:G:687:TYR:HB3	7:G:689:PHE:CE1	2.52	0.44
5:E:554:HIS:ND1	5:E:600:GLY:O	2.51	0.44
6:F:270:GLN:NE2	6:F:270:GLN:HA	2.33	0.44
6:F:402:ASN:ND2	6:F:402:ASN:N	2.66	0.44
7:G:92:VAL:HA	7:G:93:PRO:HD3	1.77	0.44
8:H:309:SER:O	8:H:313:ARG:HG3	2.17	0.44
9:L:303:TRP:HB3	9:L:307:PHE:CE1	2.53	0.44
1:A:452:LYS:O	1:A:455:LYS:HB3	2.18	0.44
7:G:315:GLY:HA3	7:G:324:VAL:HG22	1.99	0.44
8:H:329:LEU:HB2	8:H:359:PHE:CE2	2.43	0.44
8:H:839:ILE:CD1	8:H:872:TYR:HB2	2.48	0.44
9:L:148:ILE:HD11	9:L:610:ALA:HB2	1.98	0.44
9:L:150:ILE:HG21	9:L:235:PRO:HG3	1.99	0.44
1:A:395:TYR:HB3	1:A:423:MET:SD	2.58	0.44
2:B:111:PHE:O	2:B:114:SER:HB3	2.16	0.44
3:C:66:LEU:HD12	3:C:90:PHE:HE2	1.83	0.44
5:E:143:ILE:HG13	5:E:144:TYR:H	1.83	0.44
5:E:239:HIS:ND1	5:E:288:ARG:CD	2.79	0.44
5:E:561:THR:O	5:E:564:GLN:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:879:ILE:O	5:E:879:ILE:HG22	2.17	0.44
5:E:970:PRO:N	5:E:971:PRO:HD2	2.32	0.44
5:E:1057:PRO:HG2	11:M:109:ILE:HD12	2.00	0.44
6:F:1053:HIS:ND1	6:F:1053:HIS:C	2.75	0.44
7:G:578:PRO:HB2	7:G:677:LYS:HB2	1.99	0.44
1:A:378:ILE:HG12	6:F:918:ARG:HH21	1.83	0.44
1:A:477:GLU:OE1	1:A:477:GLU:N	2.33	0.44
8:H:218:SER:HB2	8:H:246:TYR:CE1	2.53	0.44
8:H:391:GLY:HA2	8:H:397:PHE:CG	2.53	0.44
8:H:830:ASN:OD1	8:H:893:ASN:HA	2.18	0.44
8:H:876:LYS:CB	8:H:876:LYS:HZ2	2.30	0.44
9:L:187:ILE:HG22	9:L:188:ILE:HG22	2.00	0.44
1:A:471:ILE:O	1:A:471:ILE:HG22	2.18	0.44
1:A:532:MET:HE1	1:A:557:LEU:HD22	2.00	0.44
1:A:554:ILE:HD12	1:A:554:ILE:HA	1.91	0.44
1:A:570:ASN:HB2	2:B:338:MET:HE1	1.99	0.44
2:B:179:ASP:OD2	2:B:217:LYS:CD	2.66	0.44
5:E:131:TRP:CZ3	5:E:152:ASP:HB2	2.53	0.44
5:E:570:LYS:HB2	5:E:572:ILE:HG22	1.98	0.44
5:E:869:ILE:HD12	5:E:869:ILE:H	1.83	0.44
6:F:462:LEU:HD23	6:F:462:LEU:HA	1.77	0.44
7:G:165:ILE:CB	7:G:193:GLY:H	2.25	0.44
8:H:426:LEU:HD23	8:H:426:LEU:H	1.83	0.44
1:A:429:ASP:OD1	1:A:430:PHE:N	2.50	0.44
3:C:216:ALA:O	3:C:220:LEU:HB2	2.18	0.44
5:E:689:ILE:HG22	5:E:691:SER:H	1.83	0.44
6:F:952:THR:OG1	6:F:953:LEU:N	2.51	0.44
7:G:643:TRP:HE1	7:G:694:VAL:CG1	2.31	0.44
8:H:565:ASN:HD21	19:Z:1:NAG:C7	2.30	0.44
8:H:577:SER:OG	8:H:579:GLU:OE1	2.27	0.44
1:A:582:MET:O	1:A:586:LYS:HG2	2.18	0.43
7:G:224:TYR:O	7:G:225:PRO:C	2.61	0.43
7:G:412:MET:HE3	7:G:414:PRO:HG3	2.00	0.43
8:H:809:ILE:HG13	8:H:810:LYS:HG2	2.00	0.43
8:H:820:GLU:OE2	8:H:824:ARG:N	2.51	0.43
1:A:486:LEU:N	1:A:487:PRO:HD2	2.34	0.43
5:E:656:VAL:HG13	5:E:671:MET:C	2.43	0.43
5:E:759:THR:HG22	6:F:861:TYR:CD2	2.46	0.43
9:L:419:LEU:O	9:L:423:ILE:HG12	2.17	0.43
9:L:515:SER:O	9:L:518:PHE:N	2.51	0.43
2:B:324:LEU:HD23	2:B:324:LEU:HA	1.89	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:148:ILE:O	3:C:151:LEU:HG	2.18	0.43
5:E:169:GLU:C	5:E:171:GLU:H	2.26	0.43
5:E:335:GLU:HB3	5:E:336:PRO:CD	2.48	0.43
5:E:410:LEU:HD12	5:E:410:LEU:O	2.18	0.43
6:F:235:LEU:HD23	6:F:235:LEU:H	1.83	0.43
7:G:225:PRO:C	7:G:226:LEU:HG	2.43	0.43
7:G:317:GLN:HG3	7:G:322:THR:CG2	2.48	0.43
1:A:502:LEU:HD23	1:A:502:LEU:HA	1.86	0.43
3:C:161:ARG:O	3:C:165:THR:HG23	2.17	0.43
5:E:415:ILE:O	5:E:423:LEU:HD12	2.19	0.43
5:E:835:ARG:HH11	5:E:835:ARG:CG	2.20	0.43
6:F:99:TYR:CZ	6:F:679:GLN:NE2	2.86	0.43
6:F:623:GLY:O	6:F:625:TYR:HD2	2.01	0.43
7:G:572:LEU:CD1	7:G:710:TYR:O	2.66	0.43
7:G:612:TYR:HD1	7:G:676:ASN:HD21	1.66	0.43
7:G:665:VAL:CG2	17:U:1:NAG:H2	2.45	0.43
8:H:827:TYR:HB2	8:H:895:ILE:HD11	2.00	0.43
9:L:163:ILE:O	9:L:167:CYS:N	2.48	0.43
5:E:335:GLU:O	5:E:336:PRO:C	2.60	0.43
5:E:626:SER:OG	5:E:627:ASP:N	2.50	0.43
5:E:1064:VAL:HG12	11:M:98:PHE:HZ	1.83	0.43
6:F:469:ASN:ND2	6:F:469:ASN:N	2.60	0.43
6:F:773:ASP:OD1	6:F:773:ASP:N	2.52	0.43
6:F:995:MET:HE2	6:F:995:MET:HB3	1.81	0.43
7:G:206:GLN:OE1	7:G:223:GLU:HB2	2.18	0.43
7:G:245:LYS:HD2	7:G:299:ASN:O	2.19	0.43
7:G:441:PHE:CG	7:G:441:PHE:O	2.71	0.43
8:H:320:ILE:HD11	8:H:361:LYS:HB3	2.00	0.43
8:H:576:LYS:HB2	8:H:576:LYS:HE3	1.79	0.43
8:H:819:TRP:CZ3	8:H:821:ILE:HD12	2.53	0.43
8:H:871:SER:O	8:H:873:ALA:N	2.50	0.43
9:L:597:PRO:HB2	9:L:600:PHE:HD2	1.84	0.43
1:A:565:TYR:O	1:A:565:TYR:CD1	2.70	0.43
3:C:42:TYR:CD1	7:G:746:GLN:HG3	2.53	0.43
3:C:205:GLY:HA3	3:C:241:PHE:CZ	2.53	0.43
5:E:185:THR:HG23	5:E:247:LEU:HG	1.99	0.43
5:E:337:PHE:CD1	5:E:337:PHE:N	2.87	0.43
5:E:646:ASN:HD21	5:E:648:LEU:HG	1.83	0.43
5:E:999:LYS:HE3	5:E:1010:VAL:O	2.18	0.43
6:F:692:TYR:CD1	6:F:703:PRO:HB3	2.53	0.43
7:G:165:ILE:N	7:G:193:GLY:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:579:TRP:HE3	7:G:678:ILE:CG2	2.24	0.43
7:G:714:ALA:O	7:G:715:LEU:HD22	2.18	0.43
9:L:413:LEU:O	9:L:417:PHE:HB2	2.19	0.43
9:L:549:GLU:CD	9:L:549:GLU:H	2.27	0.43
2:B:146:VAL:CG1	8:H:941:VAL:HB	2.49	0.43
4:D:66:ARG:HH21	10:J:83:ALA:HB1	1.84	0.43
4:D:236:GLN:NE2	4:D:271:ALA:HB1	2.32	0.43
5:E:628:LEU:HD12	5:E:629:GLU:N	2.33	0.43
5:E:880:SER:C	5:E:882:PRO:HD3	2.43	0.43
6:F:424:ASP:HA	22:F:1201:NAG:H62	2.00	0.43
7:G:62:VAL:HG22	7:G:70:LEU:HD13	2.00	0.43
8:H:593:TYR:OH	19:Z:5:BMA:H62	2.19	0.43
8:H:710:LEU:HD13	8:H:734:ASP:HB3	2.00	0.43
2:B:259:TYR:CE1	3:C:71:THR:HG22	2.50	0.43
3:C:43:PHE:O	3:C:47:ILE:HG12	2.19	0.43
7:G:573:VAL:CG1	7:G:711:VAL:HA	2.49	0.43
1:A:507:LEU:HD12	1:A:529:LEU:HD11	2.00	0.43
2:B:319:VAL:O	2:B:323:LEU:HG	2.18	0.43
5:E:656:VAL:O	5:E:657:GLU:HB2	2.19	0.43
5:E:832:SER:O	5:E:835:ARG:N	2.44	0.43
6:F:68:ASP:OD1	6:F:211:ARG:NH2	2.52	0.43
6:F:360:TYR:HA	6:F:376:GLY:O	2.19	0.43
8:H:414:GLN:C	8:H:416:ASP:H	2.27	0.43
1:A:508:ARG:HA	1:A:508:ARG:HD2	1.67	0.43
2:B:154:SER:O	2:B:157:VAL:HG12	2.19	0.43
2:B:230:LEU:HA	2:B:233:VAL:HG22	2.00	0.43
2:B:252:ILE:O	3:C:150:SER:OG	2.35	0.43
5:E:242:LEU:HA	5:E:259:SER:HB3	2.01	0.43
7:G:475:LYS:HB3	7:G:475:LYS:HZ3	1.83	0.43
8:H:330:VAL:O	8:H:333:THR:HG22	2.18	0.43
8:H:478:PHE:CB	8:H:490:MET:HG2	2.47	0.43
8:H:565:ASN:ND2	19:Z:1:NAG:C7	2.81	0.43
9:L:171:GLY:O	9:L:175:MET:HG2	2.19	0.43
9:L:406:THR:HG22	9:L:409:ILE:H	1.84	0.43
2:B:224:GLN:O	2:B:225:ILE:C	2.62	0.42
5:E:761:PRO:CB	5:E:762:ILE:HD12	2.43	0.42
5:E:947:LYS:HG2	5:E:1051:GLU:OE2	2.19	0.42
6:F:485:MET:HE2	6:F:485:MET:HB2	1.94	0.42
6:F:1015:ILE:HG22	6:F:1023:PRO:HB2	2.01	0.42
7:G:443:ASN:C	7:G:443:ASN:ND2	2.77	0.42
7:G:528:ASN:OD1	7:G:529:PRO:HD2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:578:PRO:HA	7:G:678:ILE:O	2.19	0.42
8:H:754:GLN:H	8:H:754:GLN:NE2	2.11	0.42
8:H:790:LEU:HD11	8:H:796:PHE:HB2	2.01	0.42
8:H:939:TYR:CE2	9:L:566:LYS:CD	3.02	0.42
9:L:426:HIS:HE1	9:L:585:SER:HB3	1.82	0.42
9:L:500:SER:HB3	9:L:639:ARG:NH1	2.33	0.42
1:A:525:THR:O	1:A:529:LEU:HD23	2.19	0.42
3:C:77:PHE:CA	7:G:715:LEU:HD11	2.48	0.42
5:E:115:PRO:HD2	5:E:118:ASN:HD22	1.84	0.42
5:E:646:ASN:ND2	5:E:646:ASN:C	2.77	0.42
5:E:649:HIS:C	5:E:650:GLU:CG	2.84	0.42
5:E:723:TRP:CD2	5:E:755:LYS:HD2	2.54	0.42
5:E:742:VAL:HG21	5:E:800:PHE:HD1	1.83	0.42
5:E:1082:LEU:HD23	5:E:1082:LEU:HA	1.86	0.42
6:F:363:ALA:HB3	6:F:374:HIS:HB2	2.00	0.42
7:G:187:LYS:HB2	7:G:188:LEU:HD23	2.01	0.42
7:G:517:ASN:C	7:G:517:ASN:HD22	2.26	0.42
7:G:558:LEU:HG	7:G:560:VAL:HG23	2.01	0.42
7:G:575:TYR:CG	7:G:681:GLY:O	2.72	0.42
7:G:676:ASN:OD1	7:G:677:LYS:N	2.53	0.42
9:L:627:SER:HA	9:L:630:ILE:HD12	2.01	0.42
11:M:112:ARG:HH21	11:M:112:ARG:CG	2.31	0.42
2:B:238:SER:HB3	2:B:341:ASN:HD21	1.84	0.42
3:C:88:LEU:HA	3:C:91:VAL:HG12	2.00	0.42
4:D:229:THR:HG23	4:D:242:ILE:HD13	2.02	0.42
5:E:120:THR:O	5:E:121:VAL:HG12	2.19	0.42
5:E:467:VAL:CG1	5:E:471:ARG:HB2	2.49	0.42
5:E:540:VAL:HG12	5:E:659:SER:HB3	2.01	0.42
5:E:760:PHE:O	5:E:761:PRO:C	2.61	0.42
5:E:843:ARG:HE	5:E:863:MET:HE1	1.84	0.42
7:G:210:LEU:HD12	7:G:219:PHE:CZ	2.54	0.42
7:G:598:GLU:HG3	7:G:672:GLY:HA3	2.00	0.42
9:L:93:ILE:HB	9:L:248:ILE:CD1	2.49	0.42
9:L:218:CYS:HA	9:L:221:PHE:HD2	1.83	0.42
2:B:154:SER:HA	2:B:157:VAL:HG12	2.01	0.42
7:G:17:HIS:CG	7:G:18:THR:H	2.36	0.42
7:G:600:VAL:HG13	7:G:694:VAL:HG21	2.01	0.42
8:H:222:ALA:HB2	8:H:243:MET:HE2	2.01	0.42
8:H:844:THR:C	8:H:861:TRP:HZ3	2.27	0.42
9:L:189:PRO:HG2	9:L:192:GLN:HB2	2.02	0.42
9:L:494:TYR:HB3	9:L:522:LYS:NZ	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:S:1:NAG:H62	16:S:2:NAG:N2	2.34	0.42
2:B:136:ALA:C	2:B:139:PRO:HD2	2.44	0.42
3:C:207:LEU:C	3:C:209:ASN:H	2.27	0.42
4:D:53:GLN:HB2	11:M:77:MET:HG2	2.01	0.42
5:E:623:CYS:SG	5:E:651:LEU:CB	3.08	0.42
5:E:636:LEU:CD2	5:E:637:TYR:CE1	3.00	0.42
6:F:75:VAL:HG12	6:F:79:PHE:HD2	1.85	0.42
6:F:916:LEU:HD12	6:F:1053:HIS:HE1	1.74	0.42
7:G:223:GLU:O	7:G:227:ASN:HA	2.19	0.42
8:H:350:GLY:HA3	8:H:397:PHE:O	2.20	0.42
8:H:476:LEU:HD13	8:H:492:ASP:HB3	2.01	0.42
9:L:299:LEU:HD12	9:L:300:GLN:N	2.34	0.42
9:L:336:LEU:HG	9:L:340:LYS:HE3	2.02	0.42
9:L:549:GLU:HG2	9:L:550:GLY:H	1.83	0.42
1:A:396:VAL:N	1:A:423:MET:HE1	2.34	0.42
5:E:176:TYR:HB2	5:E:177:PRO:CD	2.49	0.42
7:G:511:LYS:HE3	7:G:587:LYS:HD3	2.00	0.42
8:H:349:ARG:HG2	8:H:396:ARG:HD2	2.01	0.42
9:L:482:GLY:HA3	9:L:486:ASN:ND2	2.34	0.42
9:L:649:TYR:CE2	9:L:654:LEU:HD22	2.54	0.42
10:J:120:LEU:O	10:J:124:LEU:N	2.44	0.42
1:A:483:SER:CA	21:A:702:9Z9:C12	2.91	0.42
2:B:105:SER:HB2	2:B:108:PHE:HB3	2.01	0.42
5:E:952:GLN:HA	5:E:1017:ASN:OD1	2.19	0.42
6:F:164:ALA:HB1	6:F:667:LEU:HD21	2.02	0.42
6:F:496:SER:HB2	6:F:502:PHE:CD2	2.55	0.42
7:G:175:ASN:ND2	7:G:179:SER:OG	2.36	0.42
9:L:290:ILE:O	9:L:294:LYS:N	2.53	0.42
9:L:509:ASP:C	9:L:511:LYS:H	2.27	0.42
4:D:110:THR:HA	4:D:113:ILE:HD12	2.01	0.42
5:E:186:LYS:NZ	5:E:456:ASN:O	2.53	0.42
5:E:948:PHE:CG	5:E:949:PRO:CD	3.02	0.42
6:F:755:PHE:O	6:F:756:LEU:HD23	2.20	0.42
7:G:573:VAL:HG13	7:G:711:VAL:CG2	2.41	0.42
8:H:143:ASN:ND2	17:W:1:NAG:C7	2.83	0.42
8:H:961:PHE:O	8:H:965:LYS:HG3	2.20	0.42
9:L:502:TYR:HB2	9:L:647:TRP:CZ2	2.55	0.42
2:B:118:LEU:O	2:B:122:VAL:HG13	2.20	0.42
3:C:281:ASP:O	3:C:285:GLU:HG2	2.19	0.42
5:E:288:ARG:NH1	5:E:288:ARG:CG	2.82	0.42
5:E:655:ASP:HA	5:E:658:LYS:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:696:LEU:O	5:E:697:THR:C	2.62	0.42
7:G:291:ILE:HA	7:G:309:GLU:OE1	2.19	0.42
7:G:467:ASP:OD2	22:G:903:NAG:O7	2.37	0.42
8:H:858:ASP:OD1	8:H:859:ASP:N	2.52	0.42
9:L:505:ILE:HG21	9:L:516:PRO:HA	2.01	0.42
1:A:414:PRO:HA	1:A:417:ASN:HB2	2.01	0.42
1:A:454:PHE:O	1:A:457:MET:HB2	2.20	0.42
3:C:266:VAL:HG12	4:D:286:LEU:CD1	2.50	0.42
5:E:1075:PHE:CD1	11:M:69:ALA:HB1	2.55	0.42
6:F:1018:GLN:CA	6:F:1018:GLN:HE21	2.33	0.42
7:G:225:PRO:HB3	7:G:472:ALA:HB2	2.02	0.42
7:G:726:ILE:O	7:G:730:VAL:HG23	2.20	0.42
8:H:633:MET:HE1	8:H:665:MET:HE1	2.01	0.42
9:L:458:PHE:CZ	9:L:577:ALA:HB1	2.54	0.42
11:M:61:GLN:OE1	11:M:98:PHE:HA	2.20	0.42
1:A:378:ILE:CD1	6:F:903:PHE:CD2	2.90	0.41
2:B:160:LEU:HD23	2:B:163:TRP:CD1	2.55	0.41
2:B:294:LEU:CD2	2:B:323:LEU:HD22	2.50	0.41
3:C:118:ASP:OD1	3:C:155:LYS:HG2	2.20	0.41
4:D:138:ALA:O	4:D:142:ILE:HG12	2.20	0.41
5:E:755:LYS:CA	5:E:755:LYS:CE	2.93	0.41
5:E:865:LYS:HB2	5:E:945:ARG:HD2	2.00	0.41
6:F:498:ASN:HD22	8:H:183:THR:CG2	2.21	0.41
6:F:623:GLY:C	6:F:624:ASN:CG	2.87	0.41
7:G:188:LEU:HA	7:G:190:HIS:HE1	1.75	0.41
7:G:516:GLN:CB	7:G:582:VAL:HG11	2.49	0.41
9:L:287:THR:HG22	9:L:288:VAL:N	2.30	0.41
4:D:51:ASP:N	4:D:53:GLN:HE22	2.18	0.41
5:E:132:MET:HE1	5:E:499:GLN:HG3	2.02	0.41
5:E:357:VAL:HG22	5:E:373:PHE:CE1	2.55	0.41
5:E:762:ILE:HD11	6:F:862:LEU:HD11	2.02	0.41
6:F:165:MET:HG2	6:F:669:PHE:HZ	1.84	0.41
6:F:515:LYS:HE3	6:F:515:LYS:HB2	1.85	0.41
6:F:644:VAL:HA	6:F:645:PRO:HD3	1.62	0.41
8:H:205:THR:HG22	8:H:206:SER:N	2.36	0.41
8:H:715:PHE:O	8:H:729:PRO:HD2	2.20	0.41
8:H:888:ASN:ND2	18:c:1:NAG:N2	2.68	0.41
9:L:422:GLY:HA2	9:L:582:ASN:ND2	2.35	0.41
9:L:455:VAL:HG22	9:L:666:GLN:HB3	2.02	0.41
9:L:483:GLN:O	9:L:484:LEU:C	2.61	0.41
10:J:55:MET:HA	10:J:69:PRO:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:LEU:HD23	1:A:469:LEU:C	2.46	0.41
3:C:110:TRP:CD1	3:C:110:TRP:N	2.88	0.41
4:D:109:LEU:HD13	4:D:143:LEU:HD13	2.02	0.41
5:E:193:VAL:O	5:E:193:VAL:HG12	2.21	0.41
5:E:557:LEU:O	5:E:558:THR:CB	2.69	0.41
5:E:960:PHE:CE1	5:E:965:LYS:CB	3.04	0.41
6:F:722:PHE:CD1	6:F:732:TYR:HB2	2.55	0.41
6:F:1018:GLN:HE21	6:F:1018:GLN:HA	1.85	0.41
7:G:106:VAL:HG23	7:G:119:TYR:CD2	2.55	0.41
8:H:815:ASN:HA	8:H:888:ASN:HB3	2.01	0.41
9:L:387:THR:HG23	9:L:662:TRP:CG	2.56	0.41
9:L:497:CYS:HB3	9:L:502:TYR:CE1	2.55	0.41
2:B:360:TYR:CE2	2:B:364:MET:HE3	2.55	0.41
4:D:96:LYS:HE3	4:D:96:LYS:HB2	1.83	0.41
4:D:236:GLN:HE21	4:D:271:ALA:HB1	1.84	0.41
5:E:1003:GLU:CG	5:E:1004:PRO:HD3	2.48	0.41
5:E:1040:GLU:OE1	5:E:1040:GLU:HA	2.21	0.41
6:F:187:ILE:HD12	6:F:201:PHE:CE1	2.56	0.41
6:F:550:SER:O	6:F:554:GLU:HG2	2.20	0.41
6:F:1082:LEU:HA	6:F:1085:LEU:HG	2.03	0.41
7:G:223:GLU:OE2	7:G:223:GLU:CA	2.69	0.41
8:H:752:ARG:HB2	22:H:1001:NAG:O6	2.20	0.41
8:H:903:GLY:N	8:H:929:SER:OG	2.45	0.41
9:L:116:MET:O	9:L:120:ILE:HG12	2.20	0.41
9:L:197:CYS:HB3	9:L:205:ASN:HA	2.02	0.41
2:B:120:THR:O	2:B:124:MET:HG3	2.20	0.41
5:E:107:ARG:H	5:E:107:ARG:HG2	1.65	0.41
5:E:290:ASP:OD2	5:E:320:ARG:NH2	2.53	0.41
5:E:628:LEU:CD1	5:E:640:ILE:HG23	2.51	0.41
5:E:730:ASP:OD1	5:E:730:ASP:C	2.63	0.41
6:F:49:LEU:HD12	6:F:187:ILE:HD11	2.01	0.41
6:F:941:SER:HB2	6:F:1036:VAL:HG11	2.03	0.41
7:G:383:PRO:CB	7:G:415:ARG:NH2	2.83	0.41
8:H:304:PRO:HD2	8:H:342:PHE:CD2	2.55	0.41
8:H:439:CYS:O	8:H:442:CYS:HB3	2.20	0.41
8:H:515:GLU:O	8:H:516:THR:HG22	2.20	0.41
2:B:123:LEU:HA	2:B:123:LEU:HD12	1.87	0.41
5:E:335:GLU:HB3	5:E:336:PRO:HD3	2.02	0.41
5:E:1083:ARG:NE	11:M:84:ARG:HH21	2.19	0.41
6:F:696:TYR:CD2	6:F:888:VAL:HG11	2.55	0.41
6:F:802:CYS:HB3	6:F:829:ARG:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:914:CYS:SG	6:F:1051:HIS:HB3	2.61	0.41
6:F:916:LEU:HD23	6:F:918:ARG:CG	2.33	0.41
7:G:344:ILE:H	7:G:344:ILE:HD12	1.85	0.41
7:G:573:VAL:N	7:G:710:TYR:O	2.45	0.41
7:G:576:ASP:O	7:G:577:LYS:CB	2.68	0.41
8:H:269:MET:HG3	8:H:283:ALA:HB3	2.03	0.41
8:H:795:MET:HG3	17:b:1:NAG:O6	2.20	0.41
8:H:967:TYR:CZ	8:H:968:ARG:HG2	2.56	0.41
11:M:72:SER:HB3	11:M:91:LEU:HD21	2.01	0.41
2:B:101:TRP:CE2	8:H:963:TYR:CE1	3.09	0.41
4:D:165:ARG:HA	4:D:165:ARG:HD2	1.78	0.41
6:F:112:GLU:HB3	17:Q:1:NAG:C8	2.50	0.41
6:F:490:GLY:C	6:F:492:PHE:H	2.29	0.41
6:F:587:LEU:HA	6:F:600:LYS:HA	2.02	0.41
6:F:758:LYS:CB	6:F:1040:THR:HA	2.50	0.41
7:G:169:ASN:HD22	7:G:169:ASN:N	2.18	0.41
7:G:224:TYR:CG	7:G:225:PRO:N	2.88	0.41
8:H:891:ASN:ND2	18:c:1:NAG:O6	2.54	0.41
8:H:904:MET:HB3	8:H:904:MET:HE3	1.85	0.41
9:L:451:THR:O	9:L:455:VAL:HG23	2.21	0.41
1:A:471:ILE:CG2	1:A:475:LEU:HD21	2.49	0.41
1:A:539:SER:O	1:A:543:ILE:HG13	2.21	0.41
2:B:238:SER:CB	2:B:341:ASN:HD21	2.33	0.41
3:C:73:TYR:CE2	7:G:712:HIS:CE1	3.08	0.41
4:D:81:ASN:C	4:D:81:ASN:HD22	2.28	0.41
4:D:88:ARG:C	4:D:90:ASN:H	2.29	0.41
5:E:581:SER:HB2	5:E:712:LYS:HB3	2.02	0.41
5:E:1079:VAL:HG23	11:M:73:LEU:HD21	2.02	0.41
6:F:624:ASN:OD1	6:F:624:ASN:N	2.53	0.41
8:H:242:PHE:CE2	8:H:244:LEU:HD22	2.56	0.41
11:M:73:LEU:O	11:M:77:MET:N	2.32	0.41
1:A:468:ARG:O	1:A:468:ARG:HD2	2.21	0.41
1:A:512:GLN:C	1:A:514:SER:H	2.29	0.41
2:B:254:ALA:O	2:B:258:VAL:HG23	2.21	0.41
2:B:309:GLU:O	2:B:310:SER:CB	2.68	0.41
3:C:91:VAL:HG23	3:C:125:LEU:HD21	2.02	0.41
5:E:42:THR:HG21	5:E:48:LYS:HE3	2.02	0.41
5:E:361:LEU:HD13	5:E:416:PHE:HD1	1.86	0.41
5:E:489:LYS:CE	5:E:489:LYS:CA	2.86	0.41
5:E:540:VAL:HG23	5:E:552:PHE:HB2	2.02	0.41
5:E:961:ASN:O	5:E:963:ARG:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:1003:GLU:HG3	5:E:1004:PRO:CD	2.51	0.41
6:F:758:LYS:HD3	6:F:1041:TYR:CE1	2.56	0.41
6:F:809:GLN:OE1	6:F:818:VAL:HG13	2.21	0.41
6:F:858:GLN:OE1	6:F:867:GLN:NE2	2.54	0.41
7:G:43:PHE:O	7:G:94:SER:HA	2.21	0.41
7:G:429:PRO:O	7:G:460:GLN:NE2	2.50	0.41
7:G:441:PHE:CE1	7:G:452:LYS:HB2	2.56	0.41
7:G:657:ASP:OD1	7:G:657:ASP:N	2.52	0.41
8:H:254:PRO:HB2	8:H:257:TYR:CE1	2.56	0.41
8:H:694:TYR:O	8:H:697:VAL:HG12	2.21	0.41
8:H:814:ALA:HB1	8:H:913:ASP:HB2	2.02	0.41
9:L:122:GLN:HG3	9:L:132:TRP:HB2	2.03	0.41
9:L:426:HIS:CE1	9:L:585:SER:HB3	2.56	0.41
2:B:99:ALA:HB2	2:B:164:LEU:HD22	2.02	0.41
2:B:241:PHE:CE2	3:C:162:GLY:HA3	2.56	0.41
2:B:294:LEU:HD13	3:C:225:THR:HB	2.03	0.41
6:F:974:THR:O	6:F:976:SER:N	2.53	0.41
7:G:723:LEU:C	7:G:727:LEU:HG	2.33	0.41
1:A:492:ILE:O	1:A:496:MET:HG2	2.21	0.40
1:A:497:PHE:O	1:A:500:LEU:HB3	2.21	0.40
2:B:138:TRP:CZ3	2:B:139:PRO:HG3	2.55	0.40
2:B:210:CYS:O	2:B:213:LEU:HB2	2.22	0.40
3:C:196:PHE:CD2	4:D:89:THR:HG23	2.56	0.40
4:D:109:LEU:HG	4:D:113:ILE:HD11	2.04	0.40
5:E:230:ILE:H	5:E:230:ILE:HG13	1.77	0.40
5:E:1074:ILE:O	5:E:1078:PHE:HD1	2.03	0.40
6:F:237:LYS:H	6:F:237:LYS:HG2	1.68	0.40
7:G:48:ASN:ND2	7:G:255:TRP:HH2	2.19	0.40
7:G:624:GLN:OE1	7:G:624:GLN:HA	2.20	0.40
7:G:720:PHE:CZ	7:G:722:PRO:CG	2.97	0.40
8:H:207:GLU:OE1	8:H:207:GLU:N	2.51	0.40
8:H:675:ILE:HG12	8:H:680:CYS:SG	2.60	0.40
9:L:88:GLN:HA	9:L:91:ASN:ND2	2.36	0.40
11:M:35:SER:O	11:M:38:HIS:HB3	2.21	0.40
1:A:392:LEU:O	1:A:396:VAL:HG23	2.21	0.40
2:B:179:ASP:O	2:B:214:ARG:NH2	2.48	0.40
2:B:239:MET:HE1	2:B:338:MET:HG3	2.02	0.40
4:D:56:ILE:HD12	11:M:77:MET:HE1	2.03	0.40
5:E:882:PRO:O	5:E:883:LEU:HD23	2.21	0.40
5:E:948:PHE:CD2	5:E:949:PRO:CD	3.02	0.40
6:F:531:ASN:O	6:F:531:ASN:ND2	2.41	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:558:ASN:O	6:F:562:MET:HG2	2.20	0.40
6:F:941:SER:CB	6:F:1036:VAL:HG11	2.51	0.40
7:G:224:TYR:HB3	7:G:225:PRO:HD3	2.03	0.40
7:G:601:ILE:HD11	7:G:707:PHE:HZ	1.87	0.40
7:G:602:SER:HB2	7:G:628:TRP:CZ2	2.56	0.40
8:H:755:ARG:O	8:H:756:ARG:CB	2.70	0.40
9:L:91:ASN:HB2	9:L:329:PRO:HD2	2.02	0.40
9:L:122:GLN:HE21	9:L:128:THR:C	2.29	0.40
9:L:139:ASP:HB2	9:L:226:GLN:NE2	2.36	0.40
9:L:158:ASN:ND2	9:L:161:ARG:HG3	2.36	0.40
9:L:450:THR:CG2	9:L:583:MET:HE2	2.51	0.40
9:L:533:TYR:CE1	9:L:557:ALA:HB2	2.56	0.40
1:A:340:LEU:HD12	1:A:341:GLN:N	2.37	0.40
1:A:521:ASN:OD1	1:A:522:ILE:N	2.55	0.40
2:B:172:LYS:HD3	2:B:172:LYS:HA	1.85	0.40
2:B:361:LYS:HA	2:B:361:LYS:HD3	1.93	0.40
3:C:105:ASP:OD2	3:C:109:TYR:N	2.54	0.40
4:D:185:GLN:HG2	4:D:289:MET:SD	2.61	0.40
5:E:651:LEU:C	5:E:652:LYS:O	2.58	0.40
5:E:908:GLY:O	5:E:909:LYS:CG	2.69	0.40
5:E:966:ILE:H	5:E:966:ILE:HG13	1.62	0.40
7:G:163:GLY:CA	7:G:168:THR:HG21	2.42	0.40
7:G:585:LEU:O	7:G:592:GLU:HB3	2.21	0.40
8:H:803:TYR:CE1	8:H:808:PHE:HB3	2.57	0.40
8:H:967:TYR:OH	8:H:968:ARG:NE	2.52	0.40
9:L:634:TYR:CD2	9:L:648:ILE:CD1	3.04	0.40
11:M:3:TRP:H	11:M:3:TRP:CD1	2.39	0.40
2:B:142:LEU:H	2:B:142:LEU:HD23	1.86	0.40
3:C:95:VAL:HG11	7:G:728:LEU:HD22	2.03	0.40
3:C:202:THR:C	3:C:204:ARG:H	2.30	0.40
3:C:220:LEU:HG	3:C:251:PHE:CZ	2.56	0.40
4:D:108:VAL:O	4:D:112:LEU:HD23	2.22	0.40
5:E:99:PHE:CD2	5:E:110:TRP:HB3	2.56	0.40
5:E:575:GLY:O	5:E:718:ARG:CD	2.69	0.40
5:E:870:ASN:HB2	5:E:897:PRO:HD2	2.00	0.40
6:F:48:LEU:HB2	6:F:103:ASN:OD1	2.21	0.40
6:F:687:TRP:HE3	6:F:688:LEU:HD12	1.87	0.40
7:G:719:LYS:C	7:G:720:PHE:CD1	2.99	0.40
9:L:93:ILE:HB	9:L:248:ILE:HD12	2.02	0.40
9:L:571:PHE:HB3	9:L:575:PHE:CE2	2.56	0.40
2:B:136:ALA:O	2:B:139:PRO:HD2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:264:TYR:OH	2:B:274:TYR:O	2.39	0.40
5:E:335:GLU:O	5:E:337:PHE:CD1	2.74	0.40
5:E:485:LEU:HD23	5:E:485:LEU:HA	1.94	0.40
5:E:563:ILE:O	5:E:563:ILE:HG22	2.22	0.40
5:E:870:ASN:C	5:E:897:PRO:HG2	2.47	0.40
5:E:899:ASN:OD1	5:E:905:LYS:CB	2.63	0.40
6:F:724:ASN:O	6:F:725:ARG:HG2	2.20	0.40
6:F:952:THR:CG2	6:F:955:THR:OG1	2.69	0.40
6:F:955:THR:O	6:F:955:THR:CG2	2.70	0.40
7:G:226:LEU:O	7:G:229:SER:HB2	2.20	0.40
8:H:242:PHE:HE2	8:H:244:LEU:HD22	1.87	0.40
14:K:71:ARG:O	14:K:75:ASN:N	2.55	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	256/955 (27%)	240 (94%)	15 (6%)	1 (0%)	30	59
2	B	279/588 (47%)	256 (92%)	22 (8%)	1 (0%)	30	59
3	C	276/395 (70%)	249 (90%)	27 (10%)	0	100	100
4	D	240/442 (54%)	225 (94%)	15 (6%)	0	100	100
5	E	1047/1109 (94%)	968 (92%)	67 (6%)	12 (1%)	11	36
6	F	1040/1145 (91%)	975 (94%)	59 (6%)	6 (1%)	21	51
7	G	708/805 (88%)	663 (94%)	39 (6%)	6 (1%)	16	44
8	H	912/985 (93%)	861 (94%)	46 (5%)	5 (0%)	24	54
9	L	593/706 (84%)	549 (93%)	38 (6%)	6 (1%)	12	39
10	J	155/171 (91%)	142 (92%)	13 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	M	114/116 (98%)	101 (89%)	11 (10%)	2 (2%)	6	25
13	I	172/216 (80%)	163 (95%)	6 (4%)	3 (2%)	7	26
14	K	137/194 (71%)	135 (98%)	1 (1%)	1 (1%)	18	48
All	All	5929/7827 (76%)	5527 (93%)	359 (6%)	43 (1%)	20	48

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	335	GLU
5	E	689	ILE
5	E	756	ALA
5	E	833	TYR
5	E	948	PHE
5	E	962	GLU
6	F	257	TYR
6	F	499	ARG
7	G	190	HIS
7	G	224	TYR
7	G	576	ASP
8	H	877	PRO
9	L	476	GLU
9	L	477	ASP
9	L	487	LEU
9	L	547	ASP
9	L	548	ASP
11	M	113	GLU
13	I	2	LYS
1	A	470	SER
2	B	310	SER
5	E	121	VAL
5	E	896	ILE
6	F	356	ASN
6	F	900	LYS
7	G	93	PRO
8	H	874	ILE
9	L	553	ILE
13	I	111	PHE
5	E	613	PHE
5	E	901	PHE
5	E	1051	GLU
6	F	836	ILE

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Mol	Chain	Res	Type
7	G	577	LYS
8	H	787	PRO
5	E	919	ARG
8	H	755	ARG
8	H	756	ARG
14	K	48	GLU
6	F	1021	TYR
7	G	166	PRO
11	M	50	SER
13	I	4	THR

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	237/846 (28%)	233 (98%)	4 (2%)	53	82
2	B	262/546 (48%)	258 (98%)	4 (2%)	57	84
3	C	253/363 (70%)	252 (100%)	1 (0%)	84	94
4	D	213/399 (53%)	212 (100%)	1 (0%)	81	93
5	E	957/1009 (95%)	912 (95%)	45 (5%)	23	56
6	F	946/1035 (91%)	904 (96%)	42 (4%)	25	59
7	G	642/720 (89%)	618 (96%)	24 (4%)	30	64
8	H	842/897 (94%)	828 (98%)	14 (2%)	53	82
9	L	516/613 (84%)	505 (98%)	11 (2%)	47	77
11	M	100/100 (100%)	98 (98%)	2 (2%)	48	78
All	All	4968/6528 (76%)	4820 (97%)	148 (3%)	37	70

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	461	ARG
1	A	482	LEU
1	A	497	PHE

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Mol	Chain	Res	Type
1	A	552	TYR
2	B	223	ARG
2	B	224	GLN
2	B	232	LEU
2	B	268	THR
3	C	284	LEU
4	D	59	MET
5	E	26	LYS
5	E	40	ILE
5	E	41	LEU
5	E	44	LEU
5	E	100	LYS
5	E	287	GLU
5	E	288	ARG
5	E	318	PHE
5	E	319	ASN
5	E	453	LYS
5	E	468	GLU
5	E	469	ASP
5	E	489	LYS
5	E	522	ASN
5	E	631	THR
5	E	635	LYS
5	E	636	LEU
5	E	639	THR
5	E	648	LEU
5	E	650	GLU
5	E	651	LEU
5	E	687	GLN
5	E	689	ILE
5	E	691	SER
5	E	696	LEU
5	E	721	ASN
5	E	749	GLN
5	E	755	LYS
5	E	762	ILE
5	E	802	LYS
5	E	805	THR
5	E	834	LEU
5	E	881	ILE
5	E	884	THR
5	E	886	ASN

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Mol	Chain	Res	Type
5	E	896	ILE
5	E	898	ARG
5	E	899	ASN
5	E	916	VAL
5	E	966	ILE
5	E	997	LYS
5	E	1049	VAL
5	E	1052	VAL
5	E	1054	LEU
5	E	1056	PHE
6	F	147	ILE
6	F	189	THR
6	F	260	LYS
6	F	335	ARG
6	F	401	LYS
6	F	402	ASN
6	F	406	ASP
6	F	455	GLU
6	F	465	VAL
6	F	468	THR
6	F	469	ASN
6	F	603	LEU
6	F	612	ASN
6	F	613	LEU
6	F	621	ASN
6	F	622	GLN
6	F	624	ASN
6	F	626	GLN
6	F	641	LEU
6	F	644	VAL
6	F	691	LYS
6	F	704	THR
6	F	731	ILE
6	F	900	LYS
6	F	906	VAL
6	F	907	ILE
6	F	908	LYS
6	F	912	MET
6	F	917	PHE
6	F	951	ARG
6	F	953	LEU
6	F	956	ILE

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Mol	Chain	Res	Type
6	F	961	GLU
6	F	1016	ILE
6	F	1018	GLN
6	F	1021	TYR
6	F	1038	ASN
6	F	1053	HIS
6	F	1055	LEU
6	F	1060	LYS
6	F	1061	ARG
6	F	1062	THR
7	G	86	LYS
7	G	88	LEU
7	G	165	ILE
7	G	168	THR
7	G	169	ASN
7	G	186	ASP
7	G	188	LEU
7	G	200	HIS
7	G	223	GLU
7	G	224	TYR
7	G	226	LEU
7	G	237	LYS
7	G	239	LEU
7	G	443	ASN
7	G	475	LYS
7	G	519	ILE
7	G	572	LEU
7	G	575	TYR
7	G	627	ASN
7	G	719	LYS
7	G	721	GLN
7	G	724	LEU
7	G	725	THR
7	G	746	GLN
8	H	91	ASN
8	H	750	LYS
8	H	752	ARG
8	H	754	GLN
8	H	755	ARG
8	H	756	ARG
8	H	776	LYS
8	H	786	CYS

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Mol	Chain	Res	Type
8	H	789	THR
8	H	795	MET
8	H	876	LYS
8	H	932	MET
8	H	933	ILE
8	H	935	ARG
9	L	385	TYR
9	L	466	CYS
9	L	469	THR
9	L	471	PHE
9	L	474	ILE
9	L	475	ASN
9	L	510	GLU
9	L	549	GLU
9	L	551	GLN
9	L	552	PHE
9	L	566	LYS
11	M	44	HIS
11	M	112	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	548	GLN
2	B	205	GLN
2	B	296	HIS
2	B	341	ASN
3	C	270	HIS
4	D	236	GLN
4	D	285	ASN
5	E	45	HIS
5	E	319	ASN
5	E	374	ASN
5	E	376	GLN
5	E	403	HIS
5	E	429	GLN
5	E	520	HIS
5	E	646	ASN
5	E	687	GLN
5	E	719	GLN
5	E	721	ASN
5	E	749	GLN

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Mol	Chain	Res	Type
5	E	780	GLN
5	E	839	HIS
5	E	862	ASN
5	E	876	HIS
5	E	886	ASN
5	E	912	GLN
5	E	986	GLN
5	E	989	HIS
5	E	994	ASN
5	E	1000	HIS
5	E	1046	GLN
6	F	52	ASN
6	F	67	GLN
6	F	101	GLN
6	F	109	GLN
6	F	270	GLN
6	F	402	ASN
6	F	469	ASN
6	F	498	ASN
6	F	621	ASN
6	F	622	GLN
6	F	626	GLN
6	F	679	GLN
6	F	771	HIS
6	F	1018	GLN
7	G	99	HIS
7	G	155	ASN
7	G	169	ASN
7	G	228	HIS
7	G	443	ASN
7	G	517	ASN
7	G	712	HIS
7	G	746	GLN
8	H	91	ASN
8	H	180	GLN
8	H	182	ASN
8	H	292	ASN
8	H	438	HIS
8	H	517	ASN
8	H	561	HIS
8	H	565	ASN
8	H	610	ASN

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Mol	Chain	Res	Type
8	H	754	GLN
8	H	836	ASN
8	H	888	ASN
8	H	894	HIS
9	L	364	ASN
9	L	367	HIS
9	L	475	ASN
9	L	492	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

53 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
15	NAG	O	1	15,5	14,14,15	0.61	1 (7%)	17,19,21	0.78	1 (5%)
15	NAG	O	2	15	14,14,15	0.52	0	17,19,21	0.62	0
15	BMA	O	3	15	11,11,12	1.71	3 (27%)	15,15,17	1.27	2 (13%)
15	BMA	O	4	15	11,11,12	1.30	1 (9%)	15,15,17	1.21	1 (6%)
15	BMA	O	5	15	11,11,12	1.19	2 (18%)	15,15,17	1.42	2 (13%)
15	BMA	O	6	15	11,11,12	1.08	0	15,15,17	1.09	1 (6%)
15	BMA	O	7	15	11,11,12	0.61	0	15,15,17	0.90	0
16	NAG	P	1	5,16	14,14,15	0.65	1 (7%)	17,19,21	0.42	0
16	NAG	P	2	16	14,14,15	0.21	0	17,19,21	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	NAG	Q	1	6,17	14,14,15	0.66	1 (7%)	17,19,21	0.51	0
17	NAG	Q	2	17	14,14,15	0.42	0	17,19,21	0.59	0
17	BMA	Q	3	17	11,11,12	0.55	0	15,15,17	1.05	2 (13%)
17	NAG	R	1	6,17	14,14,15	0.49	0	17,19,21	0.52	0
17	NAG	R	2	17	14,14,15	0.31	0	17,19,21	0.64	0
17	BMA	R	3	17	11,11,12	0.95	1 (9%)	15,15,17	1.35	2 (13%)
16	NAG	S	1	6,16	14,14,15	0.75	1 (7%)	17,19,21	0.44	0
16	NAG	S	2	16	14,14,15	0.21	0	17,19,21	0.49	0
16	NAG	T	1	6,16	14,14,15	0.29	0	17,19,21	0.52	0
16	NAG	T	2	16	14,14,15	0.28	0	17,19,21	0.49	0
17	NAG	U	1	7,17	14,14,15	0.28	0	17,19,21	0.55	0
17	NAG	U	2	17	14,14,15	0.28	0	17,19,21	0.55	0
17	BMA	U	3	17	11,11,12	0.22	0	15,15,17	0.55	0
16	NAG	V	1	16	14,14,15	0.45	0	17,19,21	0.62	0
16	NAG	V	2	16	14,14,15	0.33	0	17,19,21	0.62	1 (5%)
17	NAG	W	1	8,17	14,14,15	0.32	0	17,19,21	0.66	0
17	NAG	W	2	17	14,14,15	0.54	0	17,19,21	1.33	3 (17%)
17	BMA	W	3	17	11,11,12	0.60	0	15,15,17	1.02	2 (13%)
16	NAG	X	1	16	14,14,15	0.77	1 (7%)	17,19,21	0.61	0
16	NAG	X	2	16	14,14,15	0.17	0	17,19,21	0.47	0
18	NAG	Y	1	18,8	14,14,15	0.80	1 (7%)	17,19,21	0.64	0
18	NAG	Y	2	18	14,14,15	0.36	0	17,19,21	0.62	0
18	BMA	Y	3	18	11,11,12	0.92	1 (9%)	15,15,17	1.23	2 (13%)
18	BMA	Y	4	18	11,11,12	0.81	1 (9%)	15,15,17	0.86	1 (6%)
18	BMA	Y	5	18	11,11,12	0.74	0	15,15,17	0.83	0
19	NAG	Z	1	19	14,14,15	0.57	0	17,19,21	0.54	0
19	NAG	Z	2	19	14,14,15	0.66	1 (7%)	17,19,21	0.50	0
19	BMA	Z	3	19	11,11,12	0.84	0	15,15,17	0.91	1 (6%)
19	BMA	Z	4	19	11,11,12	1.07	1 (9%)	15,15,17	1.10	1 (6%)
19	BMA	Z	5	19	11,11,12	0.98	1 (9%)	15,15,17	1.08	1 (6%)
19	BMA	Z	6	19	11,11,12	0.61	0	15,15,17	0.88	0
19	BMA	Z	7	19	11,11,12	0.54	0	15,15,17	0.77	0
16	NAG	a	1	16	14,14,15	0.38	0	17,19,21	0.62	0
16	NAG	a	2	16	14,14,15	0.48	0	17,19,21	0.63	1 (5%)
17	NAG	b	1	8,17	14,14,15	0.46	0	17,19,21	0.75	1 (5%)
17	NAG	b	2	17	14,14,15	0.37	0	17,19,21	0.53	0
17	BMA	b	3	17	11,11,12	0.75	0	15,15,17	0.68	0
18	NAG	c	1	18	14,14,15	0.28	0	17,19,21	0.48	0
18	NAG	c	2	18	14,14,15	0.39	0	17,19,21	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	BMA	c	3	18	11,11,12	0.53	0	15,15,17	1.06	0
18	BMA	c	4	18	11,11,12	1.09	1 (9%)	15,15,17	1.18	2 (13%)
18	BMA	c	5	18	11,11,12	0.75	0	15,15,17	0.94	1 (6%)
16	NAG	d	1	9,16	14,14,15	0.74	1 (7%)	17,19,21	0.76	0
16	NAG	d	2	16	14,14,15	0.36	0	17,19,21	0.41	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	NAG	O	1	15,5	-	1/6/23/26	0/1/1/1
15	NAG	O	2	15	-	2/6/23/26	0/1/1/1
15	BMA	O	3	15	-	2/2/19/22	0/1/1/1
15	BMA	O	4	15	-	2/2/19/22	0/1/1/1
15	BMA	O	5	15	-	2/2/19/22	0/1/1/1
15	BMA	O	6	15	-	2/2/19/22	0/1/1/1
15	BMA	O	7	15	-	2/2/19/22	0/1/1/1
16	NAG	P	1	5,16	-	2/6/23/26	0/1/1/1
16	NAG	P	2	16	-	2/6/23/26	0/1/1/1
17	NAG	Q	1	6,17	-	2/6/23/26	0/1/1/1
17	NAG	Q	2	17	-	2/6/23/26	0/1/1/1
17	BMA	Q	3	17	-	0/2/19/22	0/1/1/1
17	NAG	R	1	6,17	-	2/6/23/26	0/1/1/1
17	NAG	R	2	17	-	0/6/23/26	0/1/1/1
17	BMA	R	3	17	-	2/2/19/22	0/1/1/1
16	NAG	S	1	6,16	-	0/6/23/26	0/1/1/1
16	NAG	S	2	16	-	2/6/23/26	0/1/1/1
16	NAG	T	1	6,16	-	3/6/23/26	0/1/1/1
16	NAG	T	2	16	-	0/6/23/26	0/1/1/1
17	NAG	U	1	7,17	-	1/6/23/26	0/1/1/1
17	NAG	U	2	17	-	0/6/23/26	0/1/1/1
17	BMA	U	3	17	-	1/2/19/22	0/1/1/1
16	NAG	V	1	16	-	2/6/23/26	0/1/1/1
16	NAG	V	2	16	-	2/6/23/26	0/1/1/1
17	NAG	W	1	8,17	-	2/6/23/26	0/1/1/1
17	NAG	W	2	17	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BMA	W	3	17	-	0/2/19/22	0/1/1/1
16	NAG	X	1	16	-	2/6/23/26	0/1/1/1
16	NAG	X	2	16	-	2/6/23/26	0/1/1/1
18	NAG	Y	1	18,8	-	2/6/23/26	0/1/1/1
18	NAG	Y	2	18	-	2/6/23/26	0/1/1/1
18	BMA	Y	3	18	-	1/2/19/22	0/1/1/1
18	BMA	Y	4	18	-	1/2/19/22	0/1/1/1
18	BMA	Y	5	18	-	2/2/19/22	0/1/1/1
19	NAG	Z	1	19	-	2/6/23/26	0/1/1/1
19	NAG	Z	2	19	-	2/6/23/26	0/1/1/1
19	BMA	Z	3	19	-	2/2/19/22	0/1/1/1
19	BMA	Z	4	19	-	1/2/19/22	0/1/1/1
19	BMA	Z	5	19	-	2/2/19/22	0/1/1/1
19	BMA	Z	6	19	-	0/2/19/22	0/1/1/1
19	BMA	Z	7	19	-	2/2/19/22	0/1/1/1
16	NAG	a	1	16	-	1/6/23/26	0/1/1/1
16	NAG	a	2	16	-	2/6/23/26	0/1/1/1
17	NAG	b	1	8,17	-	2/6/23/26	0/1/1/1
17	NAG	b	2	17	-	2/6/23/26	0/1/1/1
17	BMA	b	3	17	-	1/2/19/22	0/1/1/1
18	NAG	c	1	18	-	0/6/23/26	0/1/1/1
18	NAG	c	2	18	-	0/6/23/26	0/1/1/1
18	BMA	c	3	18	-	1/2/19/22	0/1/1/1
18	BMA	c	4	18	-	0/2/19/22	0/1/1/1
18	BMA	c	5	18	-	1/2/19/22	0/1/1/1
16	NAG	d	1	9,16	-	2/6/23/26	0/1/1/1
16	NAG	d	2	16	-	2/6/23/26	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	O	3	BMA	C2-C3	3.04	1.57	1.52
18	c	4	BMA	C1-C2	3.01	1.59	1.52
15	O	3	BMA	C4-C5	-2.88	1.46	1.53
18	Y	1	NAG	O5-C1	-2.76	1.39	1.43
16	S	1	NAG	O5-C1	-2.72	1.39	1.43
15	O	4	BMA	O5-C1	-2.69	1.39	1.43
16	d	1	NAG	O5-C1	-2.66	1.39	1.43
19	Z	5	BMA	C1-C2	2.59	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	O	3	BMA	C1-C2	2.49	1.58	1.52
15	O	5	BMA	C2-C3	-2.45	1.48	1.52
18	Y	3	BMA	C1-C2	2.41	1.58	1.52
16	X	1	NAG	O5-C1	-2.41	1.39	1.43
18	Y	4	BMA	C1-C2	2.38	1.57	1.52
19	Z	2	NAG	O5-C1	-2.34	1.39	1.43
16	P	1	NAG	O5-C1	-2.23	1.40	1.43
17	Q	1	NAG	O5-C1	-2.22	1.40	1.43
19	Z	4	BMA	C1-C2	2.11	1.57	1.52
17	R	3	BMA	C4-C5	2.09	1.57	1.53
15	O	1	NAG	O5-C1	-2.08	1.40	1.43
15	O	5	BMA	C1-C2	2.01	1.57	1.52

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	W	2	NAG	C1-O5-C5	3.76	117.22	112.19
15	O	4	BMA	O2-C2-C3	-3.39	103.13	110.15
15	O	5	BMA	O2-C2-C3	-3.38	103.14	110.15
15	O	5	BMA	C1-C2-C3	-3.34	104.77	109.64
18	c	4	BMA	O2-C2-C3	-3.13	103.66	110.15
18	Y	3	BMA	O2-C2-C3	-3.10	103.72	110.15
17	R	3	BMA	C3-C4-C5	3.09	115.83	110.23
19	Z	5	BMA	O2-C2-C3	-2.91	104.11	110.15
17	W	3	BMA	C1-O5-C5	2.70	115.81	112.19
15	O	1	NAG	C1-O5-C5	2.68	115.78	112.19
15	O	3	BMA	C3-C4-C5	-2.63	105.47	110.23
18	c	5	BMA	O2-C2-C3	-2.44	105.10	110.15
17	Q	3	BMA	O2-C2-C3	-2.43	105.11	110.15
18	Y	3	BMA	C1-C2-C3	-2.39	106.17	109.64
15	O	6	BMA	O2-C2-C3	-2.39	105.21	110.15
15	O	3	BMA	O3-C3-C2	2.38	114.91	110.05
19	Z	3	BMA	O2-C2-C3	-2.37	105.25	110.15
18	Y	4	BMA	O2-C2-C3	-2.32	105.34	110.15
19	Z	4	BMA	O2-C2-C3	-2.28	105.44	110.15
17	W	3	BMA	O2-C2-C3	-2.18	105.64	110.15
17	b	1	NAG	C1-O5-C5	2.18	115.10	112.19
17	Q	3	BMA	C1-O5-C5	2.17	115.09	112.19
17	W	2	NAG	O4-C4-C5	2.12	114.55	109.32
18	c	4	BMA	O2-C2-C1	2.11	114.05	109.22
17	R	3	BMA	C1-C2-C3	-2.10	106.59	109.64
16	a	2	NAG	C1-O5-C5	2.03	114.91	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	V	2	NAG	C1-O5-C5	2.02	114.89	112.19
17	W	2	NAG	O4-C4-C3	2.01	115.12	110.38

There are no chirality outliers.

All (77) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	T	1	NAG	C3-C2-N2-C7
16	V	2	NAG	O5-C5-C6-O6
17	Q	1	NAG	O5-C5-C6-O6
15	O	4	BMA	O5-C5-C6-O6
16	V	1	NAG	O5-C5-C6-O6
17	W	2	NAG	C4-C5-C6-O6
15	O	2	NAG	O5-C5-C6-O6
19	Z	1	NAG	C4-C5-C6-O6
17	W	1	NAG	O5-C5-C6-O6
19	Z	2	NAG	C4-C5-C6-O6
17	R	1	NAG	O5-C5-C6-O6
18	Y	1	NAG	O5-C5-C6-O6
15	O	2	NAG	C4-C5-C6-O6
16	V	1	NAG	C4-C5-C6-O6
16	S	2	NAG	O5-C5-C6-O6
16	X	1	NAG	O5-C5-C6-O6
16	d	1	NAG	O5-C5-C6-O6
18	Y	5	BMA	O5-C5-C6-O6
15	O	3	BMA	C4-C5-C6-O6
16	V	2	NAG	C4-C5-C6-O6
16	X	1	NAG	C4-C5-C6-O6
17	Q	1	NAG	C4-C5-C6-O6
15	O	3	BMA	O5-C5-C6-O6
17	W	2	NAG	O5-C5-C6-O6
19	Z	5	BMA	O5-C5-C6-O6
19	Z	3	BMA	O5-C5-C6-O6
16	d	2	NAG	O5-C5-C6-O6
17	Q	2	NAG	O5-C5-C6-O6
19	Z	3	BMA	C4-C5-C6-O6
18	Y	1	NAG	C4-C5-C6-O6
17	Q	2	NAG	C4-C5-C6-O6
19	Z	1	NAG	O5-C5-C6-O6
17	W	1	NAG	C4-C5-C6-O6
15	O	6	BMA	O5-C5-C6-O6
15	O	4	BMA	C4-C5-C6-O6

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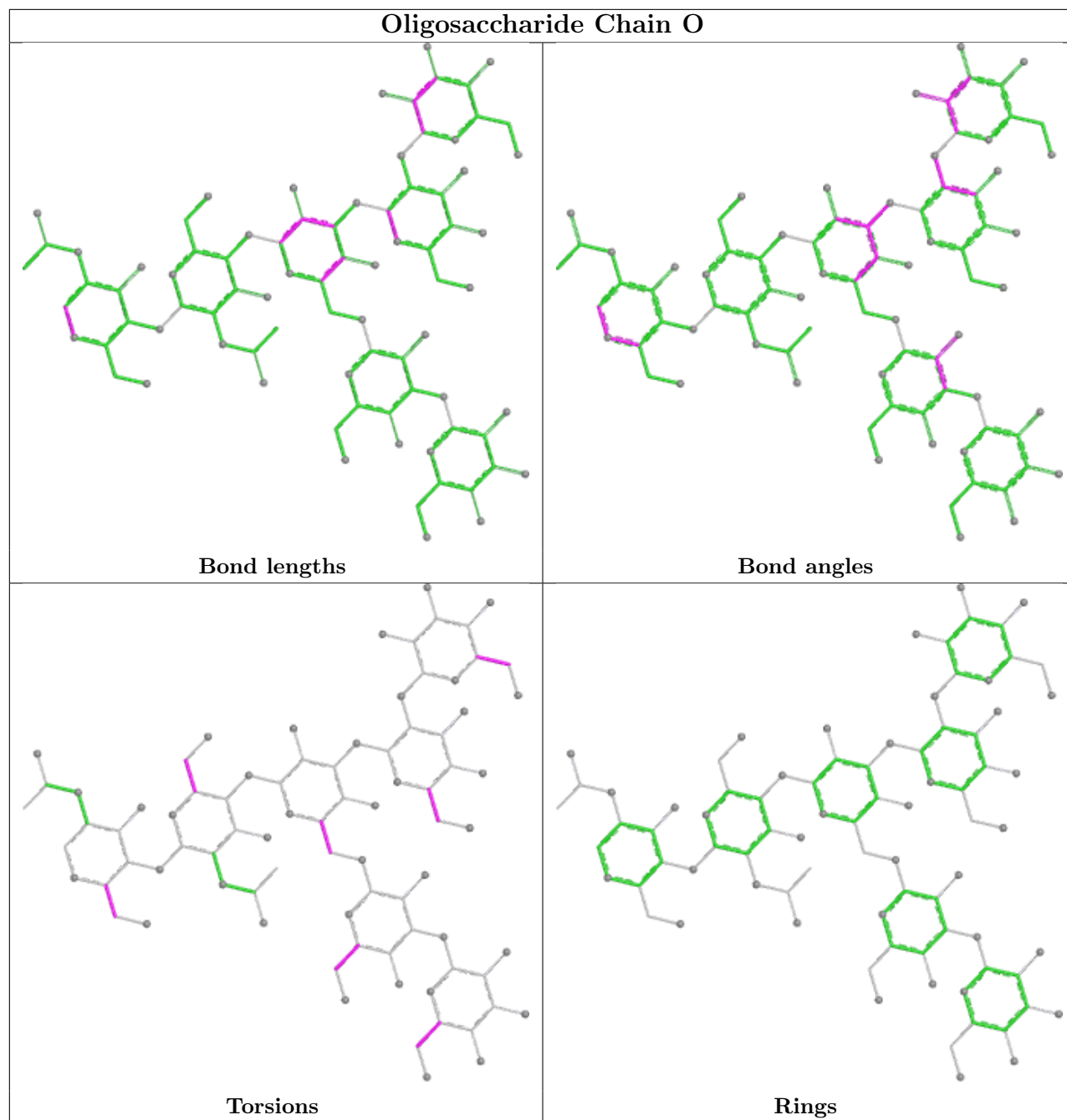
Mol	Chain	Res	Type	Atoms
19	Z	2	NAG	O5-C5-C6-O6
16	d	2	NAG	C4-C5-C6-O6
17	R	1	NAG	C4-C5-C6-O6
15	O	6	BMA	C4-C5-C6-O6
16	P	1	NAG	C4-C5-C6-O6
19	Z	7	BMA	C4-C5-C6-O6
16	X	2	NAG	C4-C5-C6-O6
16	d	1	NAG	C4-C5-C6-O6
18	Y	4	BMA	O5-C5-C6-O6
16	a	2	NAG	O5-C5-C6-O6
19	Z	7	BMA	O5-C5-C6-O6
17	R	3	BMA	C4-C5-C6-O6
15	O	7	BMA	C4-C5-C6-O6
18	Y	2	NAG	O5-C5-C6-O6
17	R	3	BMA	O5-C5-C6-O6
17	b	1	NAG	C4-C5-C6-O6
16	P	1	NAG	O5-C5-C6-O6
16	T	1	NAG	C8-C7-N2-C2
18	Y	5	BMA	C4-C5-C6-O6
16	S	2	NAG	C4-C5-C6-O6
16	X	2	NAG	O5-C5-C6-O6
15	O	7	BMA	O5-C5-C6-O6
17	b	2	NAG	O5-C5-C6-O6
15	O	5	BMA	O5-C5-C6-O6
16	a	1	NAG	O5-C5-C6-O6
17	U	3	BMA	O5-C5-C6-O6
16	T	1	NAG	O7-C7-N2-C2
18	c	3	BMA	O5-C5-C6-O6
19	Z	4	BMA	O5-C5-C6-O6
15	O	1	NAG	O5-C5-C6-O6
17	b	3	BMA	O5-C5-C6-O6
17	b	1	NAG	O5-C5-C6-O6
16	P	2	NAG	C4-C5-C6-O6
19	Z	5	BMA	C4-C5-C6-O6
18	c	5	BMA	O5-C5-C6-O6
16	a	2	NAG	C3-C2-N2-C7
18	Y	2	NAG	C4-C5-C6-O6
16	P	2	NAG	O5-C5-C6-O6
17	b	2	NAG	C4-C5-C6-O6
15	O	5	BMA	C4-C5-C6-O6
17	U	1	NAG	C1-C2-N2-C7
18	Y	3	BMA	C4-C5-C6-O6

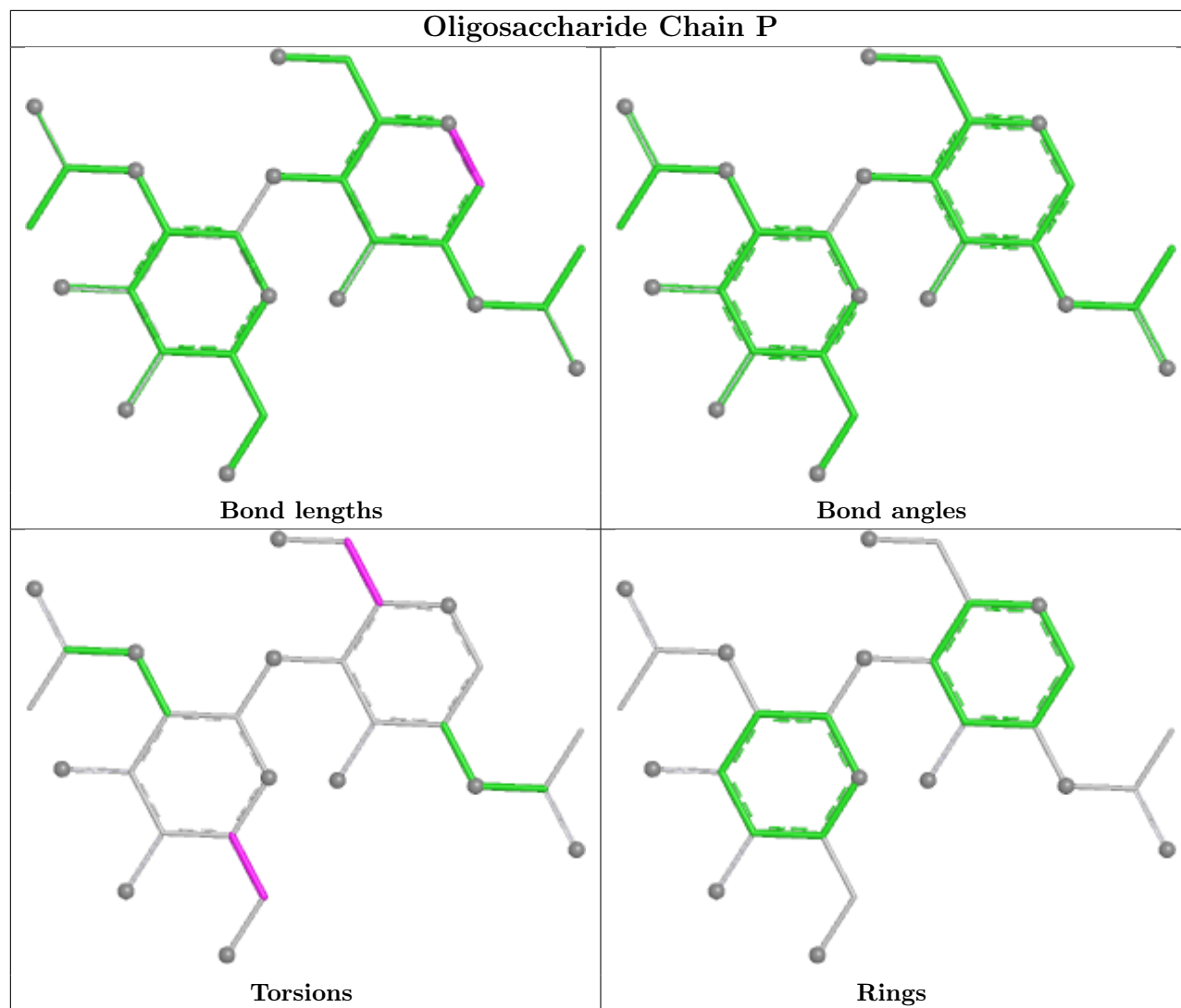
There are no ring outliers.

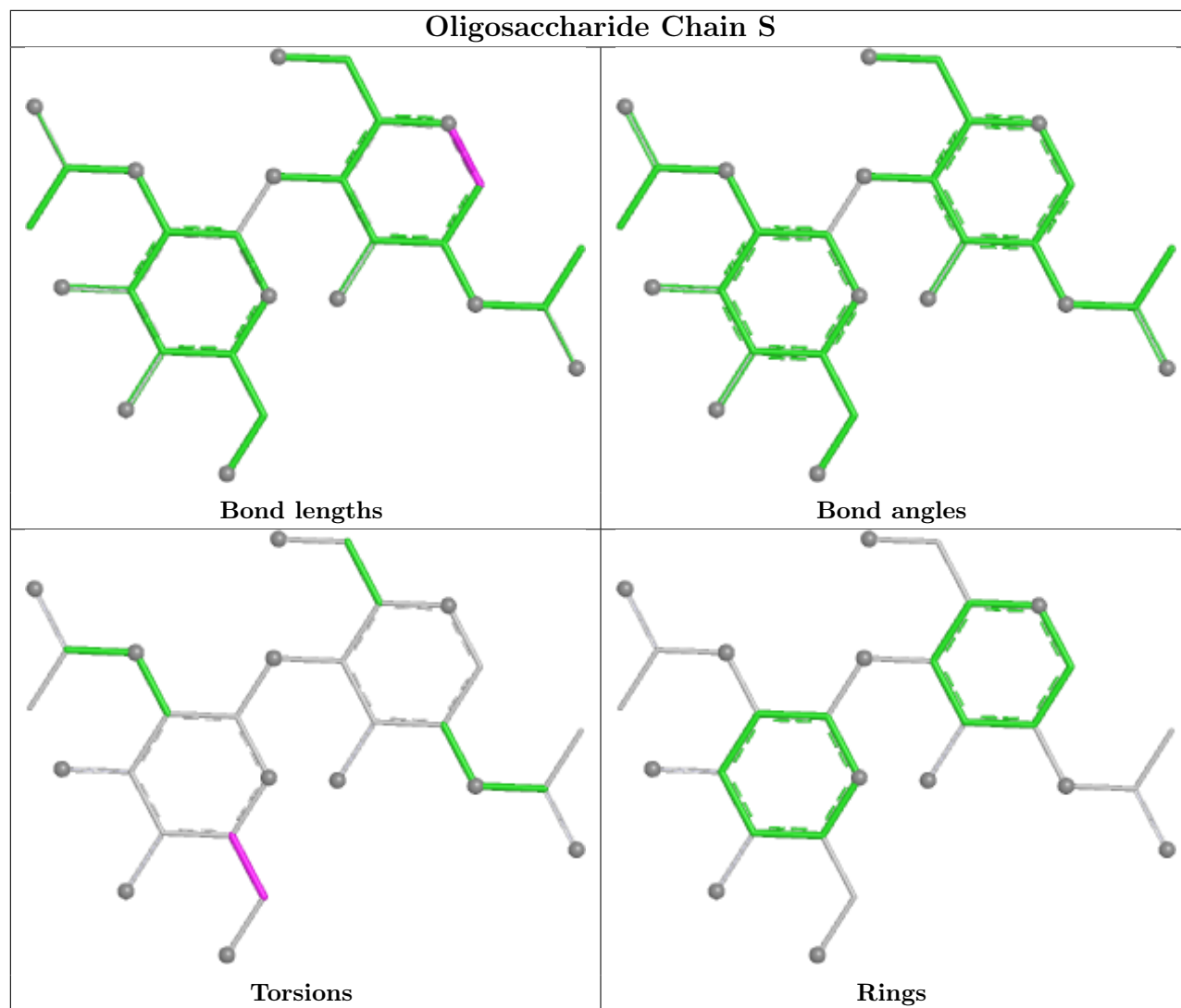
27 monomers are involved in 84 short contacts:

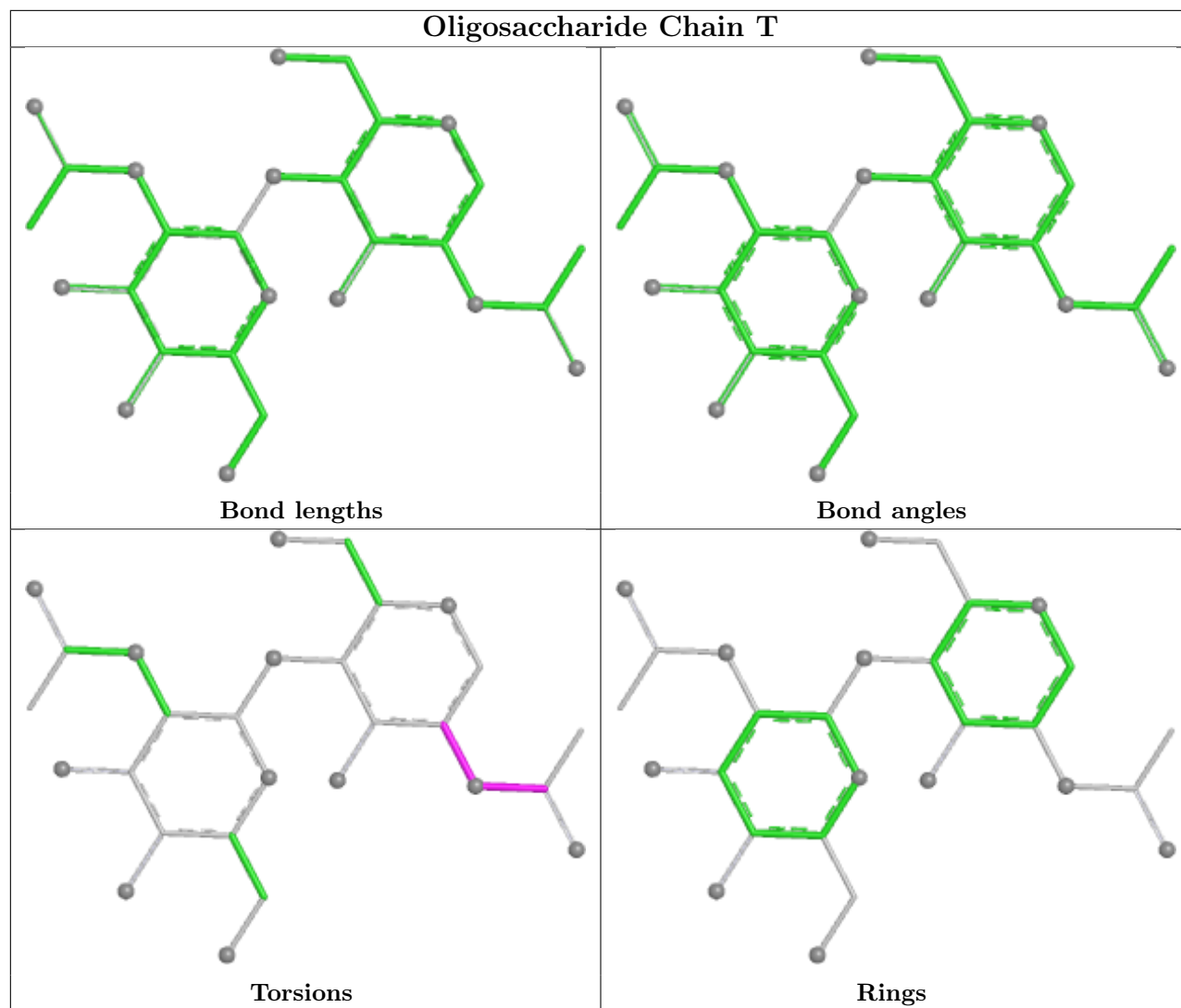
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	S	1	NAG	2	0
16	X	1	NAG	9	0
18	Y	2	NAG	2	0
18	c	4	BMA	1	0
17	W	2	NAG	1	0
17	Q	1	NAG	1	0
17	U	1	NAG	7	0
16	S	2	NAG	2	0
19	Z	5	BMA	1	0
18	Y	1	NAG	3	0
17	U	3	BMA	1	0
17	W	1	NAG	3	0
16	T	1	NAG	1	0
19	Z	1	NAG	13	0
15	O	4	BMA	1	0
16	V	1	NAG	2	0
18	Y	3	BMA	1	0
18	c	3	BMA	1	0
18	c	2	NAG	11	0
19	Z	2	NAG	4	0
17	R	1	NAG	3	0
17	b	1	NAG	4	0
17	U	2	NAG	6	0
15	O	5	BMA	1	0
16	a	1	NAG	3	0
18	c	1	NAG	9	0
16	P	1	NAG	1	0

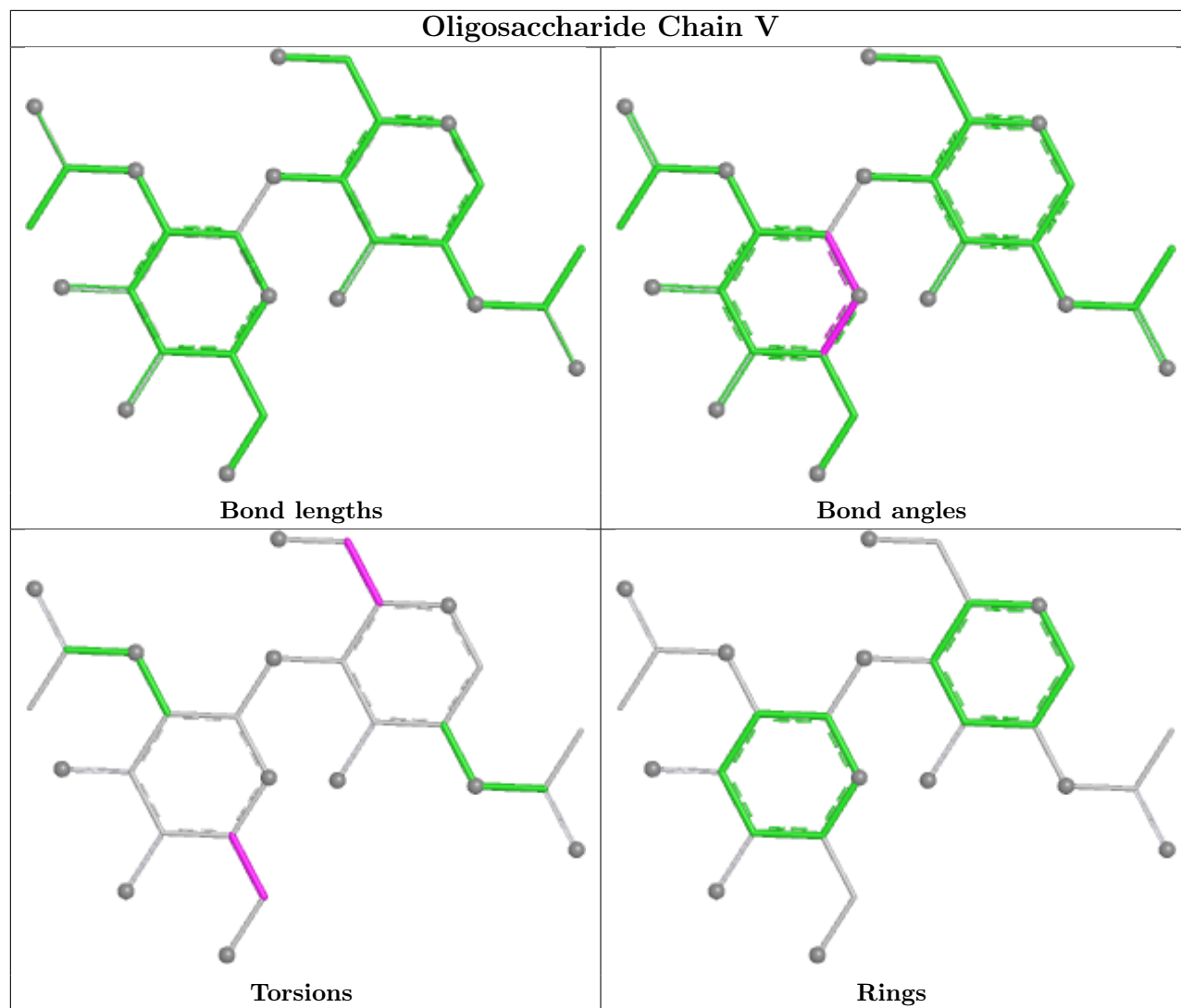
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

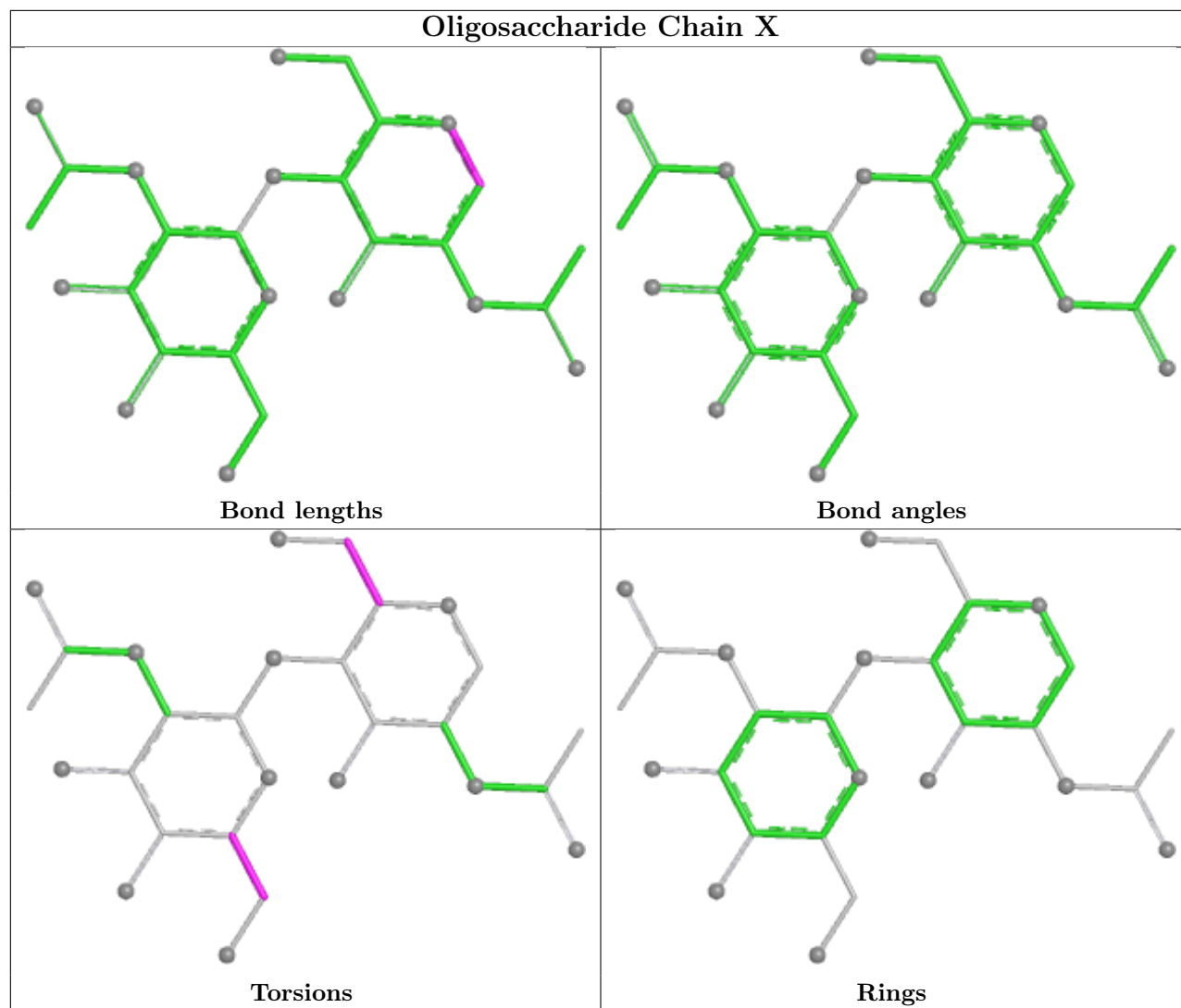


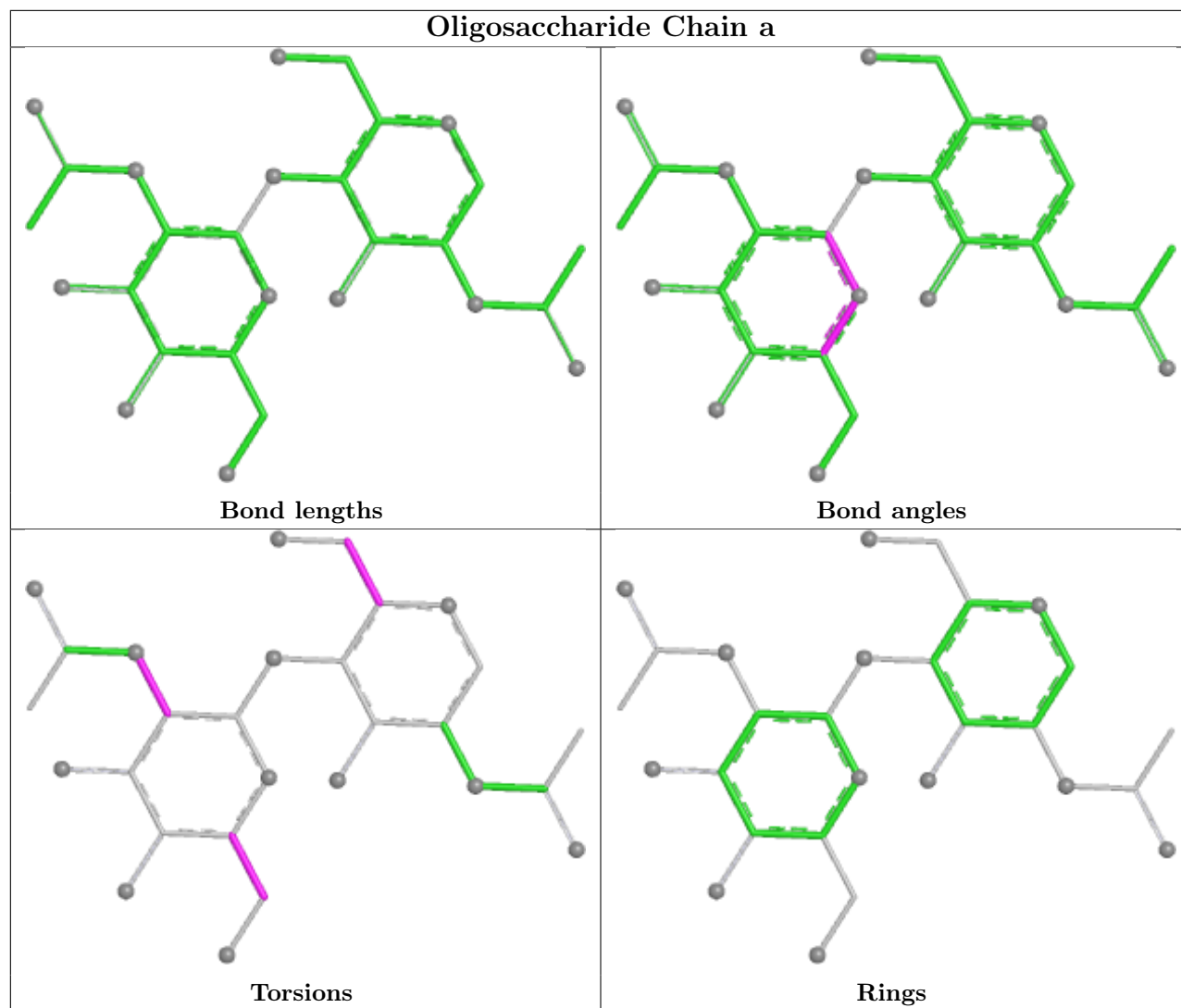


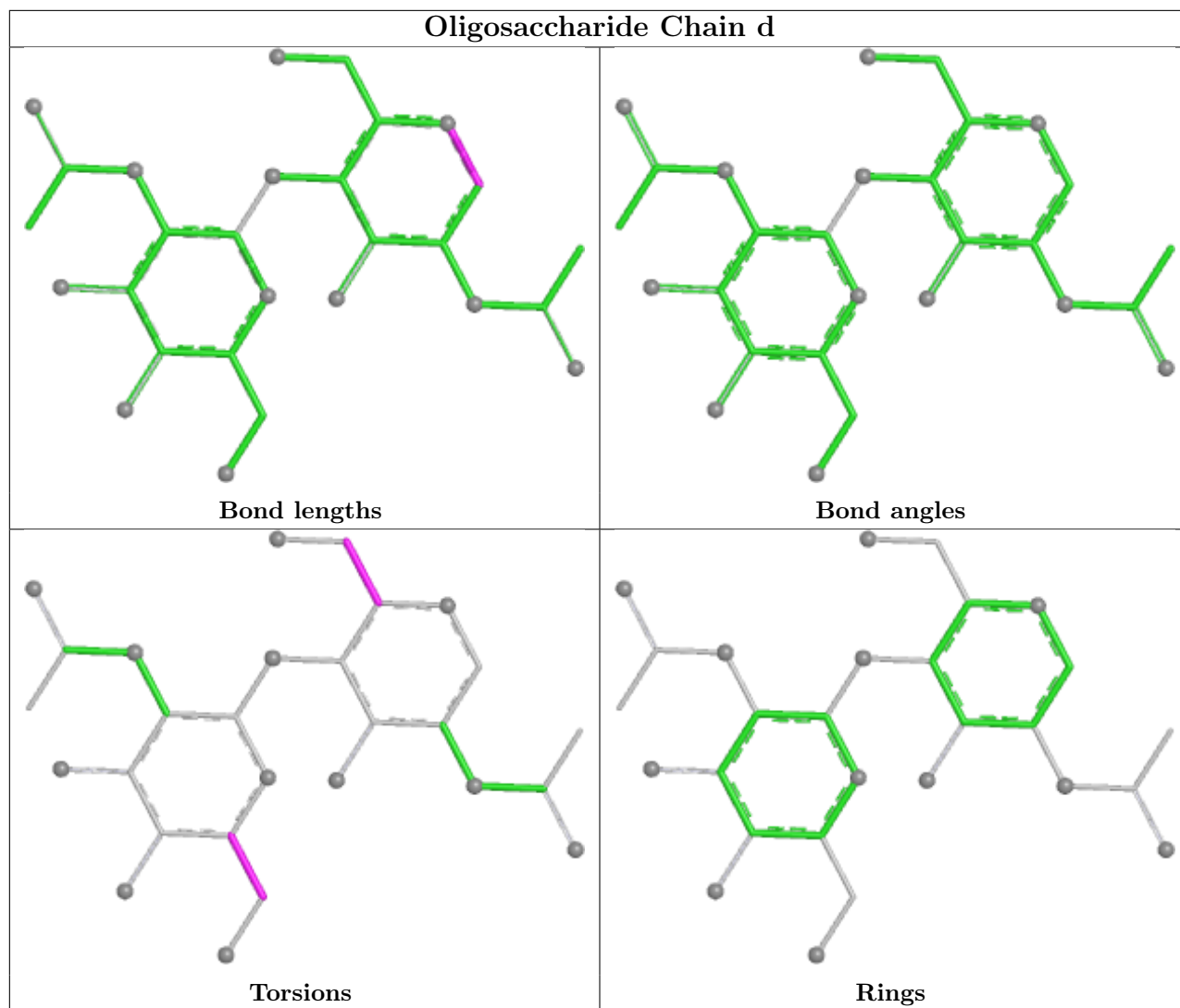


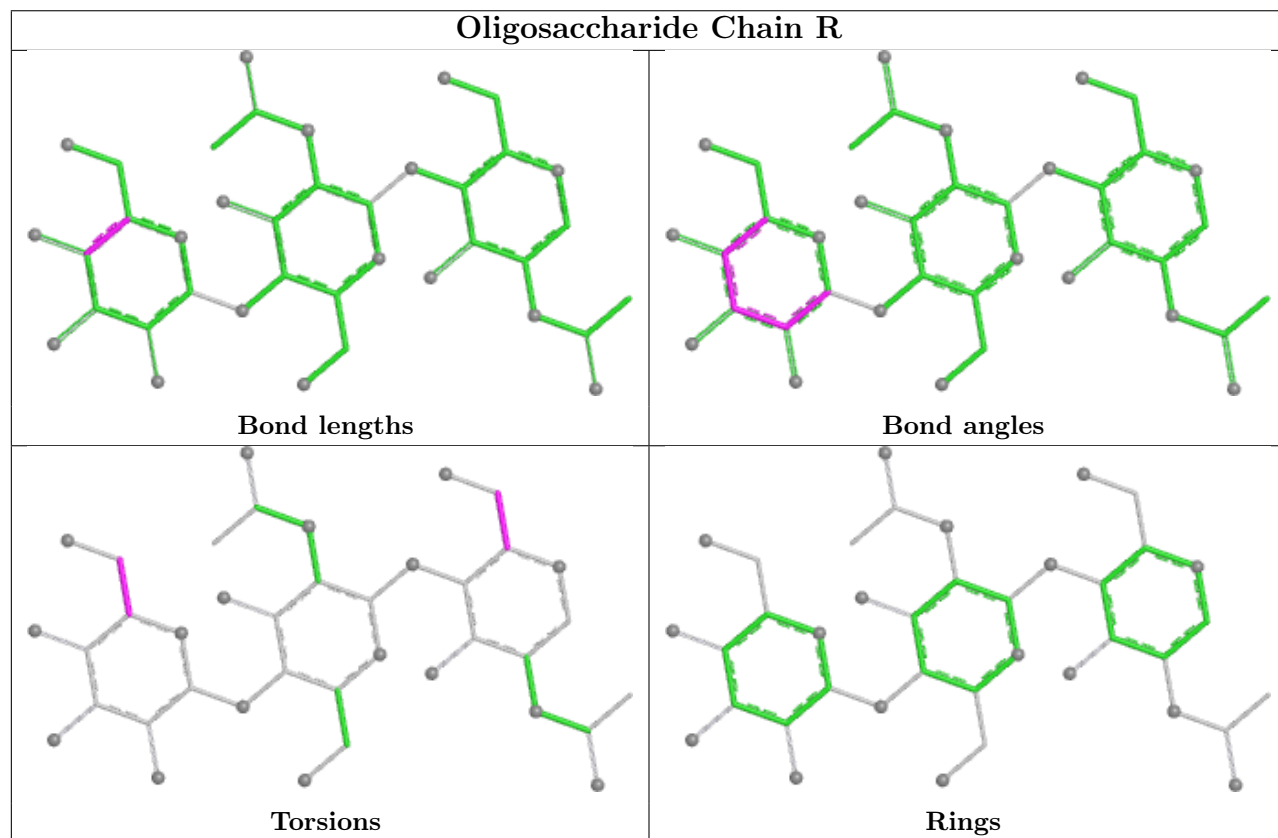
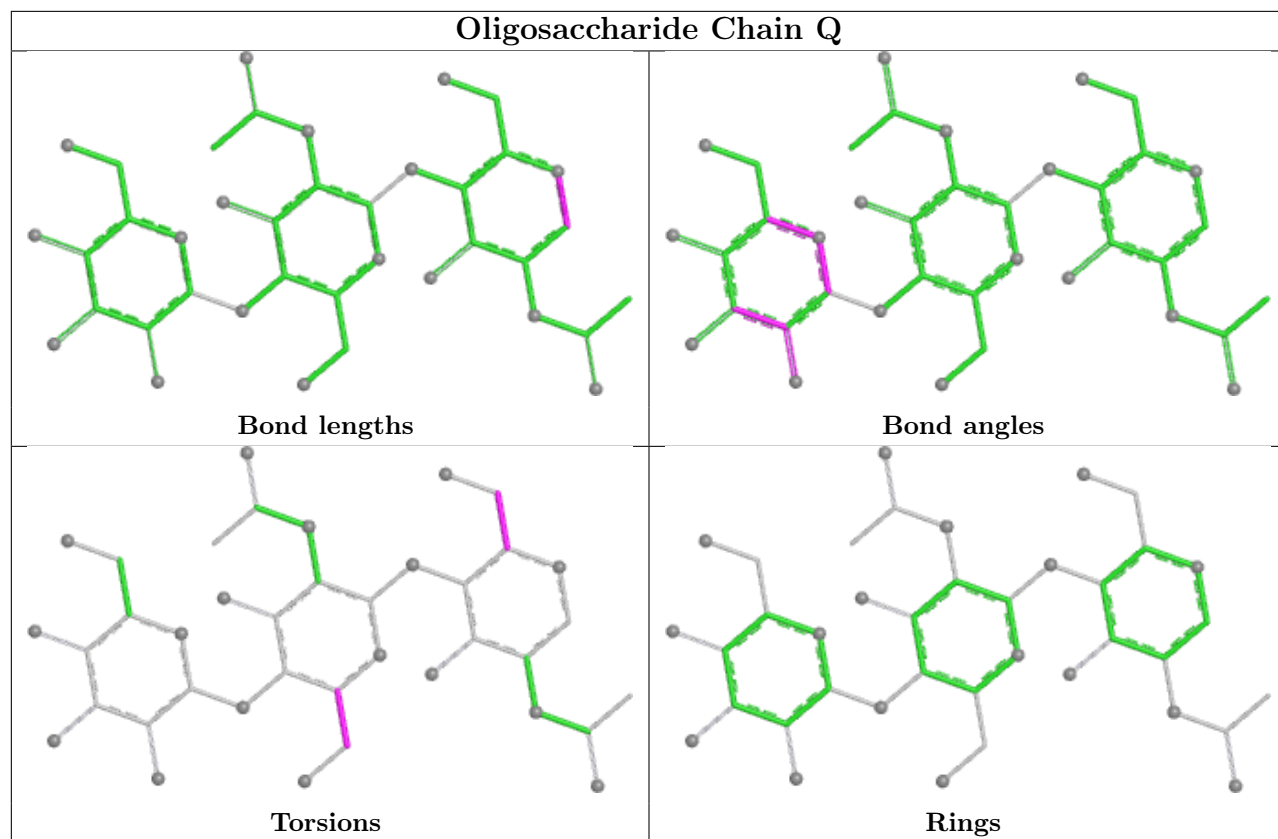


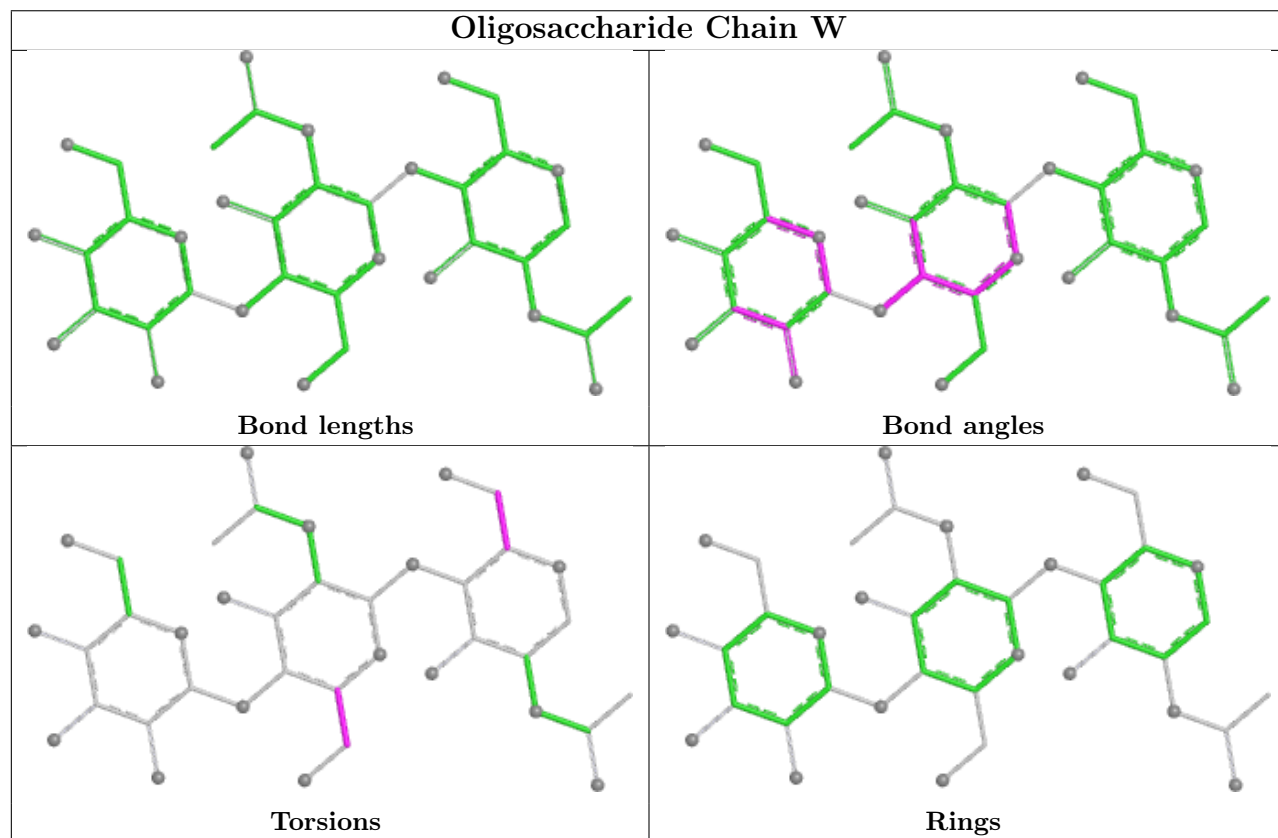
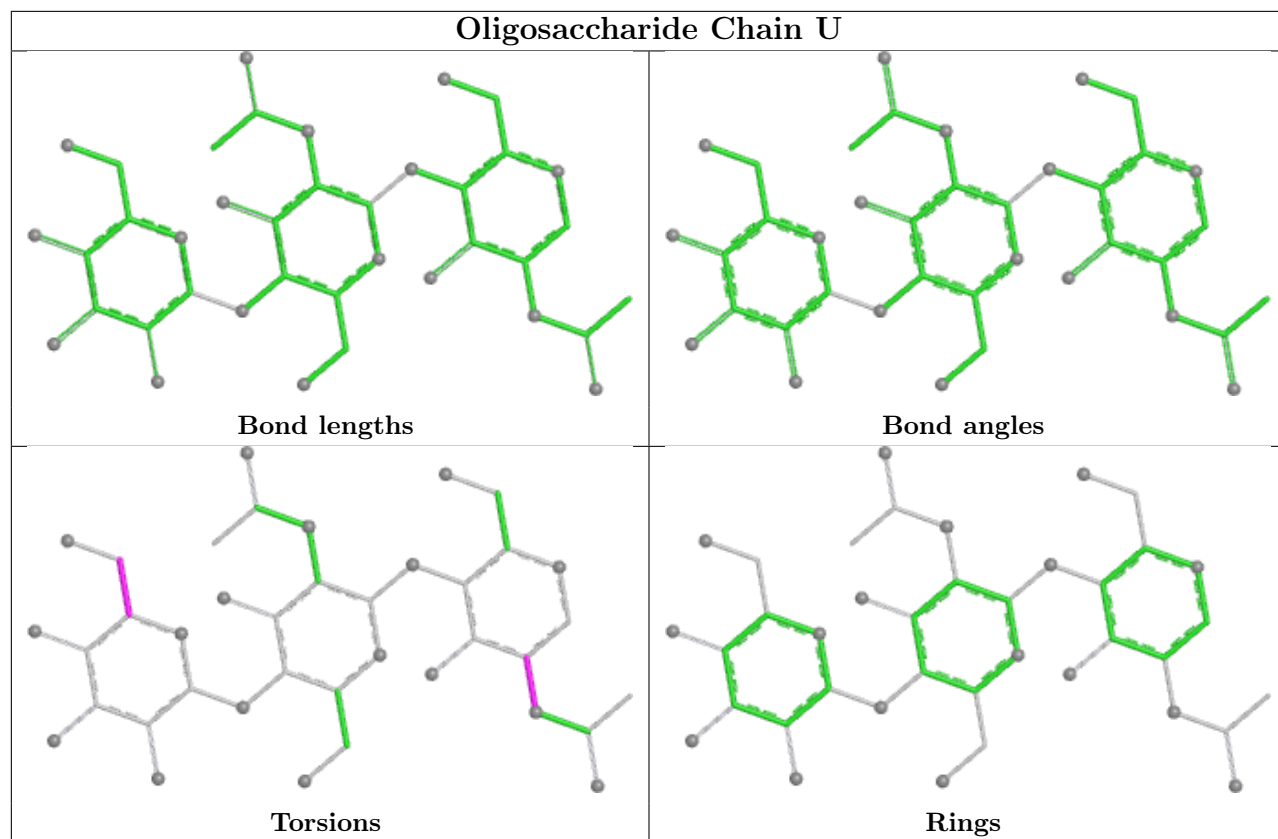


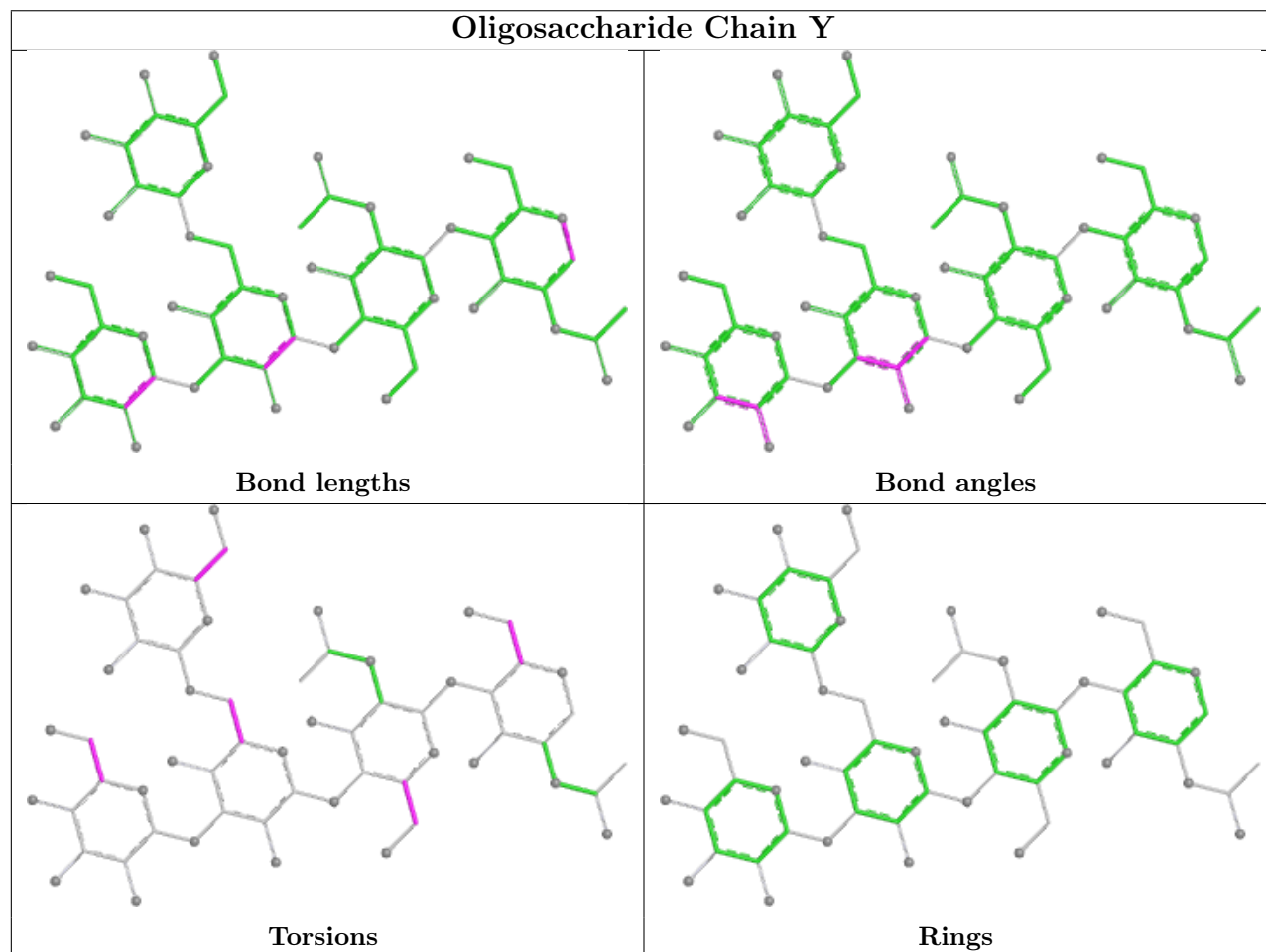
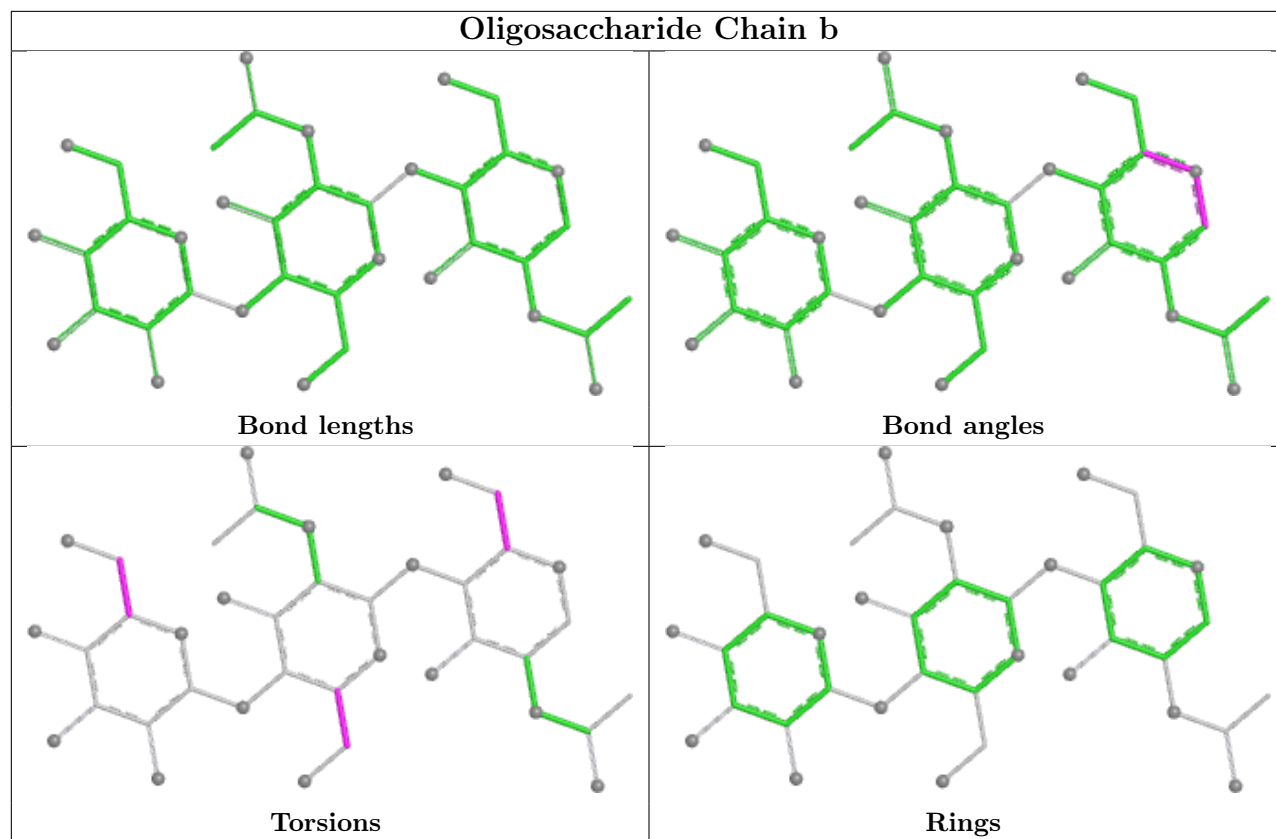


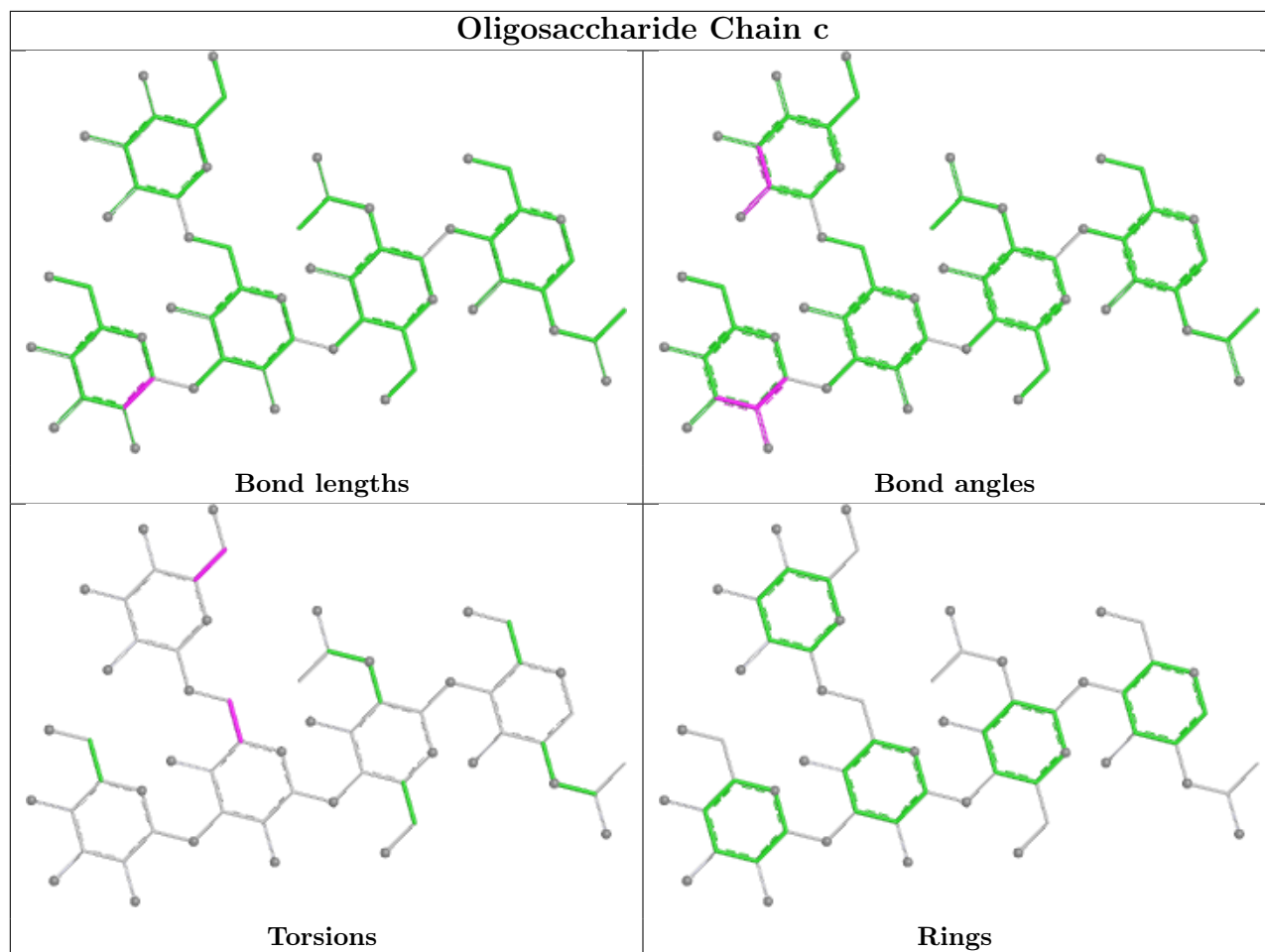


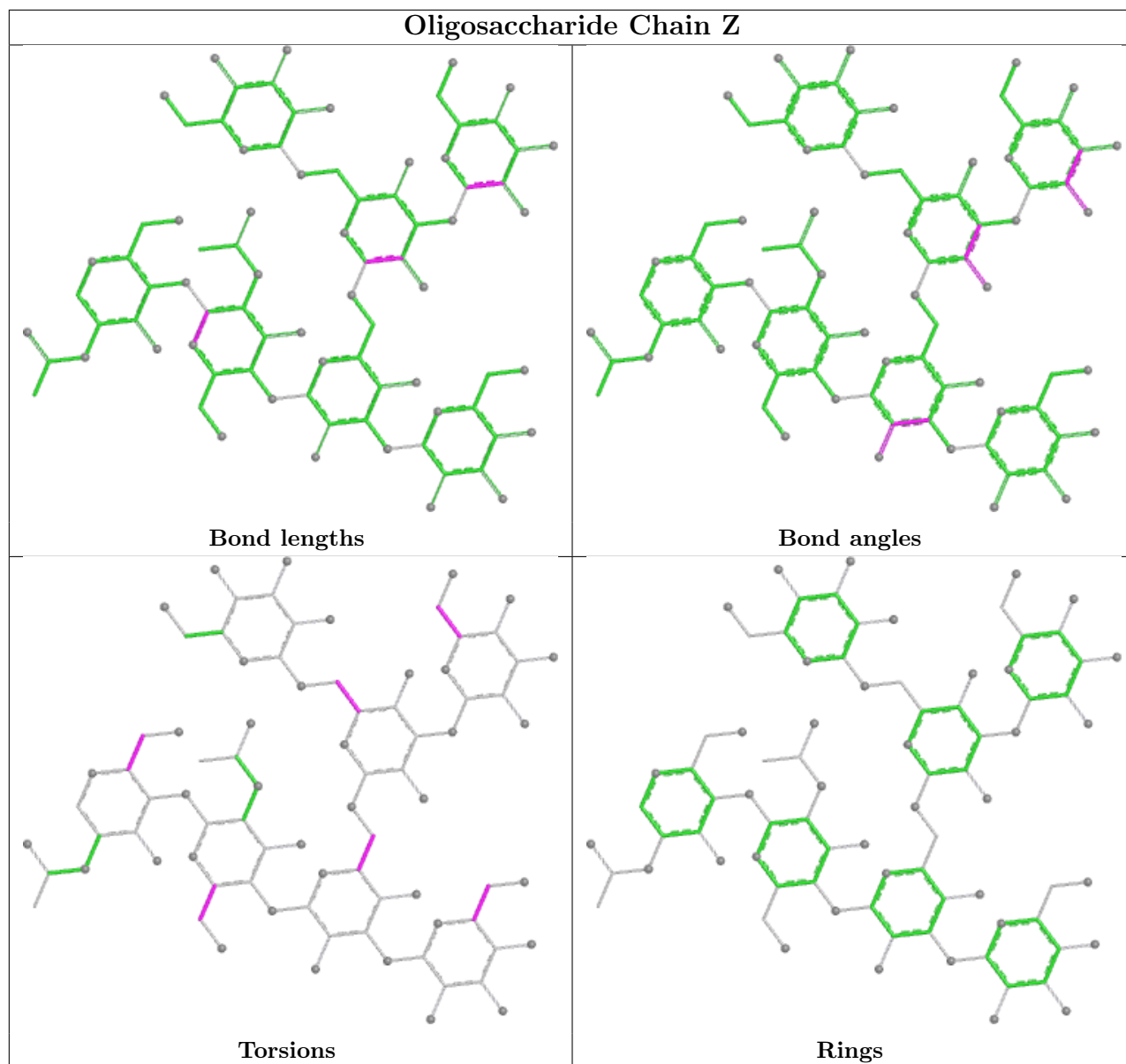












5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	9Z9	A	703	-	44,44,44	0.73	1 (2%)	64,68,68	1.50	12 (18%)
22	NAG	E	1201	5	14,14,15	0.48	0	17,19,21	0.42	0
22	NAG	G	901	7	14,14,15	0.45	0	17,19,21	0.51	0
22	NAG	G	902	7	14,14,15	0.19	0	17,19,21	0.42	0
22	NAG	G	903	7	14,14,15	0.51	0	17,19,21	0.82	1 (5%)
22	NAG	F	1201	-	14,14,15	0.26	0	17,19,21	0.34	0
22	NAG	E	1203	5	14,14,15	0.22	0	17,19,21	0.47	0
22	NAG	E	1204	5	14,14,15	0.33	0	17,19,21	0.44	0
22	NAG	E	1202	5	14,14,15	0.30	0	17,19,21	0.41	0
22	NAG	H	1001	-	14,14,15	0.44	0	17,19,21	0.51	0
21	9Z9	A	704	-	44,44,44	0.73	1 (2%)	64,68,68	1.50	12 (18%)
21	9Z9	A	702	-	44,44,44	0.74	1 (2%)	64,68,68	1.51	11 (17%)

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
21	9Z9	A	703	-	-	0/12/100/100	0/6/6/6
22	NAG	E	1201	5	-	0/6/23/26	0/1/1/1
22	NAG	G	901	7	-	2/6/23/26	0/1/1/1
22	NAG	G	902	7	-	2/6/23/26	0/1/1/1
22	NAG	G	903	7	-	2/6/23/26	0/1/1/1
22	NAG	F	1201	-	-	1/6/23/26	0/1/1/1
22	NAG	E	1203	5	-	2/6/23/26	0/1/1/1
22	NAG	E	1204	5	-	0/6/23/26	0/1/1/1
22	NAG	E	1202	5	-	0/6/23/26	0/1/1/1
22	NAG	H	1001	-	-	2/6/23/26	0/1/1/1
21	9Z9	A	704	-	-	0/12/100/100	0/6/6/6
21	9Z9	A	702	-	-	0/12/100/100	0/6/6/6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	703	9Z9	C11-C08	-2.37	1.52	1.56
21	A	702	9Z9	C11-C08	-2.31	1.52	1.56
21	A	704	9Z9	C11-C08	-2.30	1.52	1.56

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	704	9Z9	C02-C06-C07	-4.62	107.85	114.41
21	A	702	9Z9	C02-C06-C07	-4.61	107.87	114.41
21	A	703	9Z9	C02-C06-C07	-4.57	107.93	114.41
21	A	704	9Z9	C02-C03-C74	-3.71	109.52	120.50
21	A	703	9Z9	C02-C03-C74	-3.70	109.56	120.50
21	A	702	9Z9	C02-C03-C74	-3.69	109.57	120.50
21	A	702	9Z9	C09-C10-C02	-3.32	107.14	112.74
21	A	703	9Z9	C09-C10-C02	-3.31	107.16	112.74
21	A	704	9Z9	C09-C10-C02	-3.30	107.18	112.74
21	A	702	9Z9	C12-C11-C08	-3.11	108.17	111.66
21	A	703	9Z9	C76-C73-C74	-3.11	110.03	115.66
21	A	704	9Z9	C76-C73-C74	-3.09	110.06	115.66
21	A	703	9Z9	C12-C11-C08	-3.08	108.21	111.66
21	A	702	9Z9	C76-C73-C74	-3.06	110.12	115.66
21	A	704	9Z9	C12-C11-C08	-3.05	108.24	111.66
22	G	903	NAG	C1-O5-C5	2.88	116.04	112.19
21	A	702	9Z9	C75-C74-C73	-2.79	110.44	114.94
21	A	704	9Z9	C75-C74-C73	-2.76	110.48	114.94
21	A	703	9Z9	C75-C74-C73	-2.72	110.55	114.94
21	A	704	9Z9	C09-C08-C11	-2.60	109.88	113.08
21	A	703	9Z9	C09-C08-C11	-2.58	109.90	113.08
21	A	703	9Z9	C08-C11-C13	2.57	113.41	109.65
21	A	702	9Z9	C09-C08-C11	-2.56	109.93	113.08
21	A	702	9Z9	C08-C11-C13	2.52	113.34	109.65
21	A	703	9Z9	C07-C15-C14	-2.51	109.28	112.76
21	A	704	9Z9	C07-C15-C14	-2.51	109.28	112.76
21	A	702	9Z9	C07-C15-C14	-2.50	109.30	112.76
21	A	704	9Z9	C08-C11-C13	2.50	113.31	109.65
21	A	702	9Z9	O80-C79-C78	-2.25	109.28	112.17
21	A	704	9Z9	O80-C79-C78	-2.23	109.30	112.17
21	A	703	9Z9	O80-C79-C78	-2.18	109.37	112.17
21	A	702	9Z9	C17-C16-C13	-2.17	108.25	111.45
21	A	704	9Z9	C17-C16-C13	-2.14	108.29	111.45
21	A	703	9Z9	C17-C16-C13	-2.08	108.38	111.45
21	A	703	9Z9	C75-C74-C03	-2.00	110.49	114.50
21	A	704	9Z9	C75-C74-C03	-2.00	110.50	114.50

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	G	903	NAG	C4-C5-C6-O6
22	G	901	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

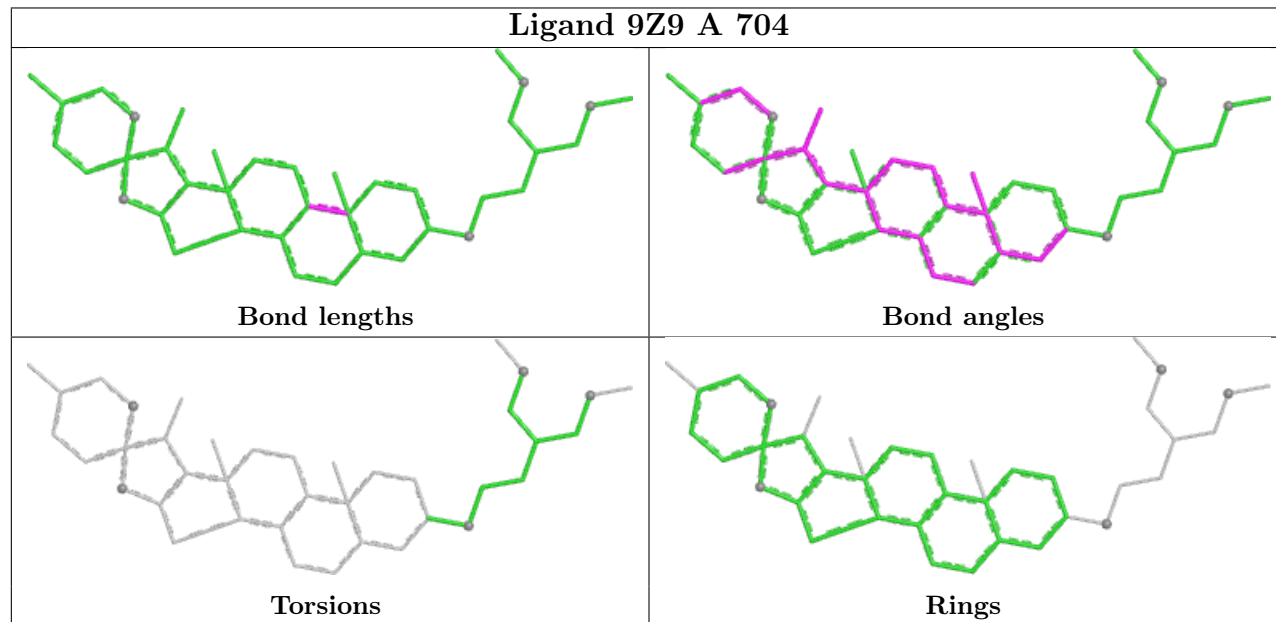
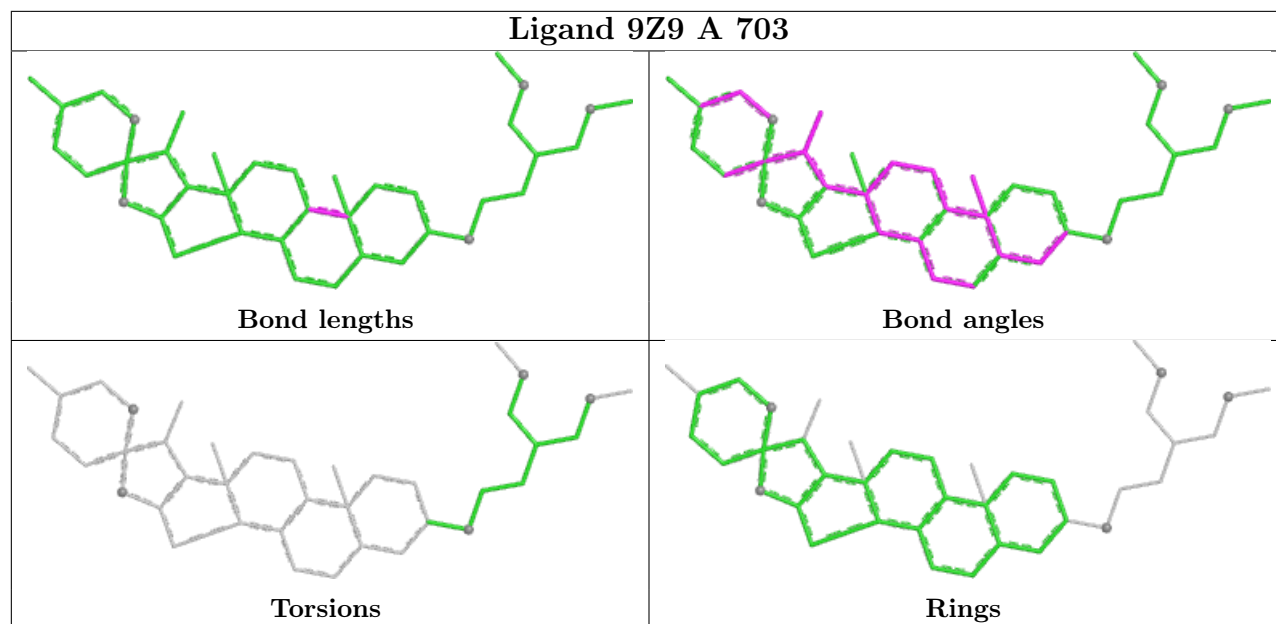
Mol	Chain	Res	Type	Atoms
22	G	903	NAG	O5-C5-C6-O6
22	G	902	NAG	O5-C5-C6-O6
22	G	901	NAG	C4-C5-C6-O6
22	G	902	NAG	C4-C5-C6-O6
22	E	1203	NAG	C4-C5-C6-O6
22	F	1201	NAG	O5-C5-C6-O6
22	H	1001	NAG	C4-C5-C6-O6
22	E	1203	NAG	O5-C5-C6-O6
22	H	1001	NAG	O5-C5-C6-O6

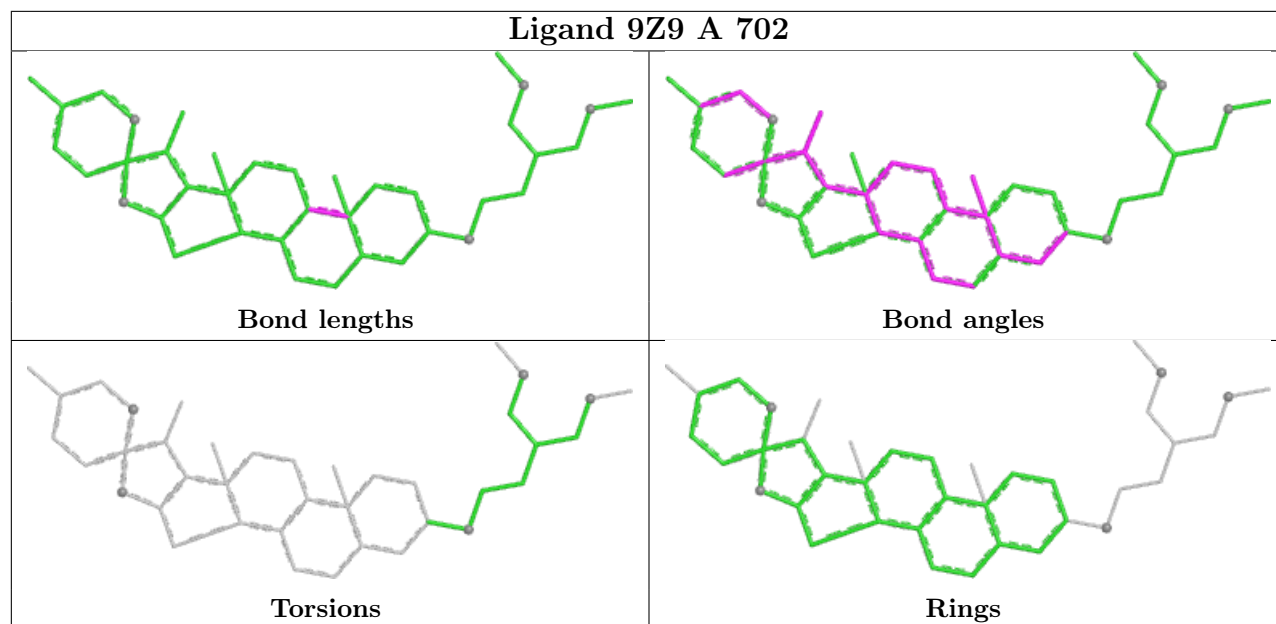
There are no ring outliers.

10 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A	703	9Z9	9	0
22	G	901	NAG	1	0
22	G	902	NAG	1	0
22	G	903	NAG	1	0
22	F	1201	NAG	2	0
22	E	1204	NAG	1	0
22	E	1202	NAG	1	0
22	H	1001	NAG	1	0
21	A	704	9Z9	6	0
21	A	702	9Z9	11	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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.

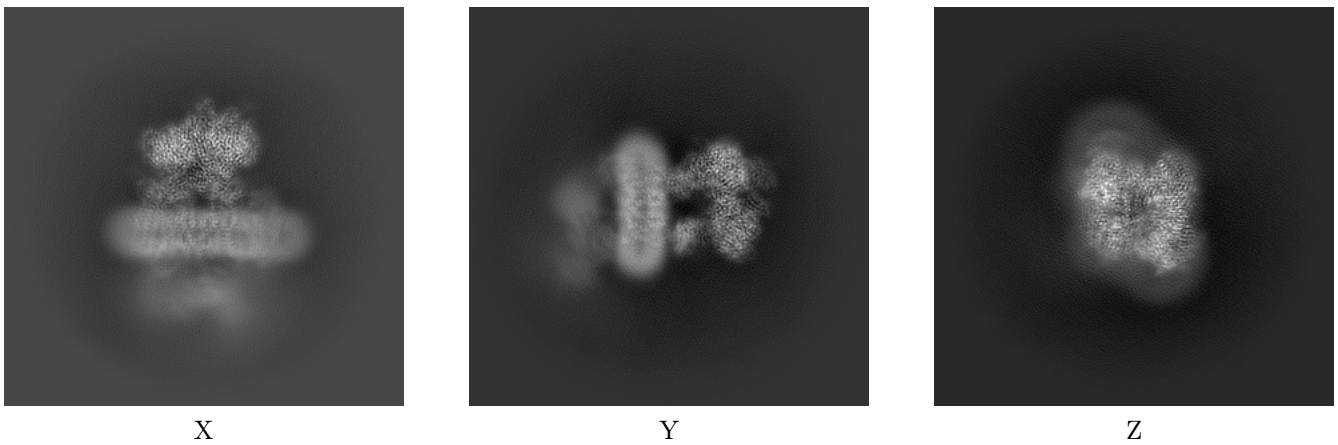
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31076. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

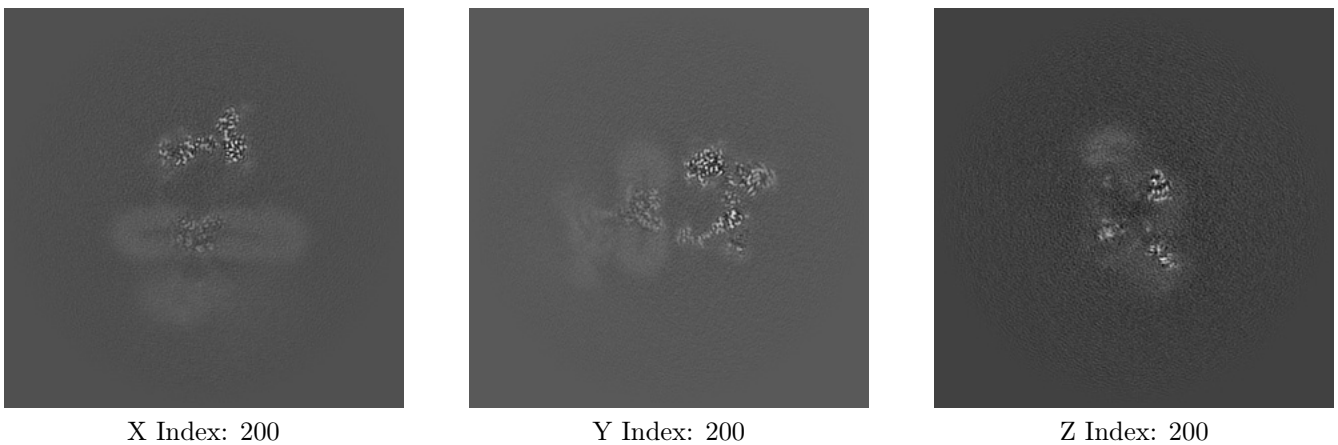
6.1.1 Primary map



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

6.2 Central slices [i](#)

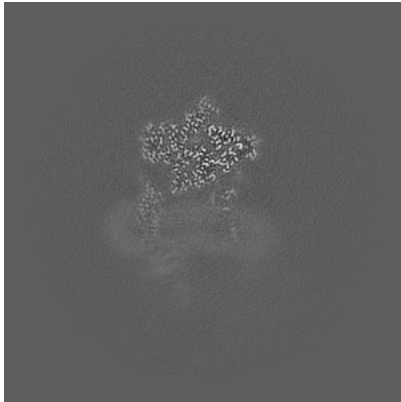
6.2.1 Primary map



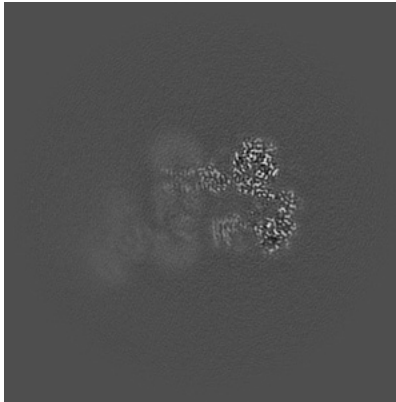
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

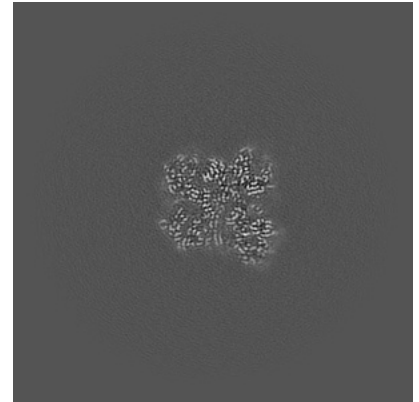
6.3.1 Primary map



X Index: 235



Y Index: 218

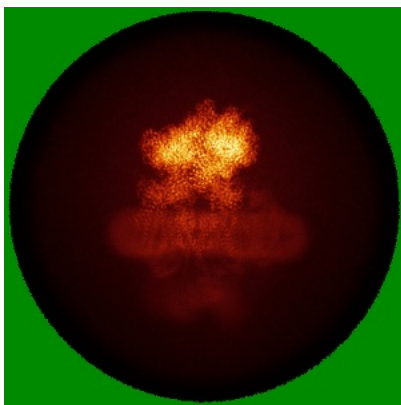


Z Index: 260

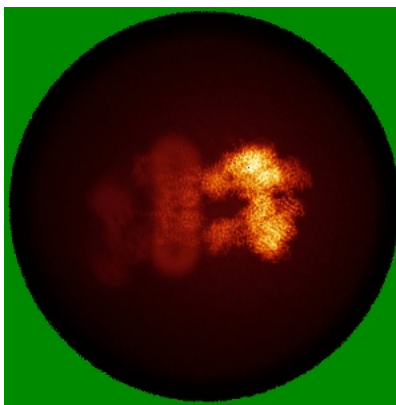
The images above show the largest variance slices of the map in three orthogonal directions.

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

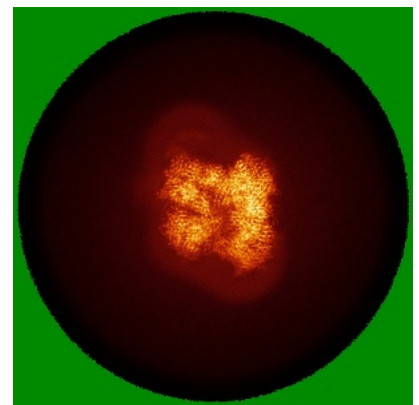
6.4.1 Primary map



X



Y

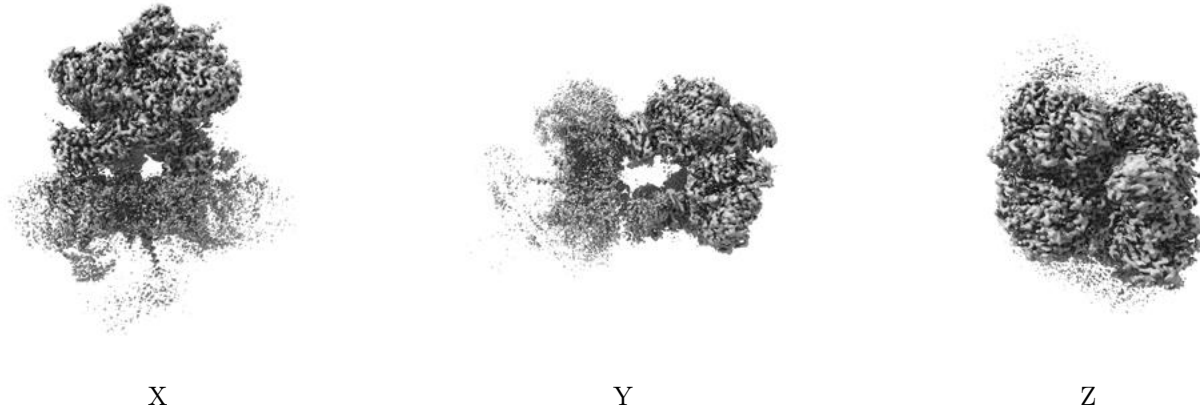


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

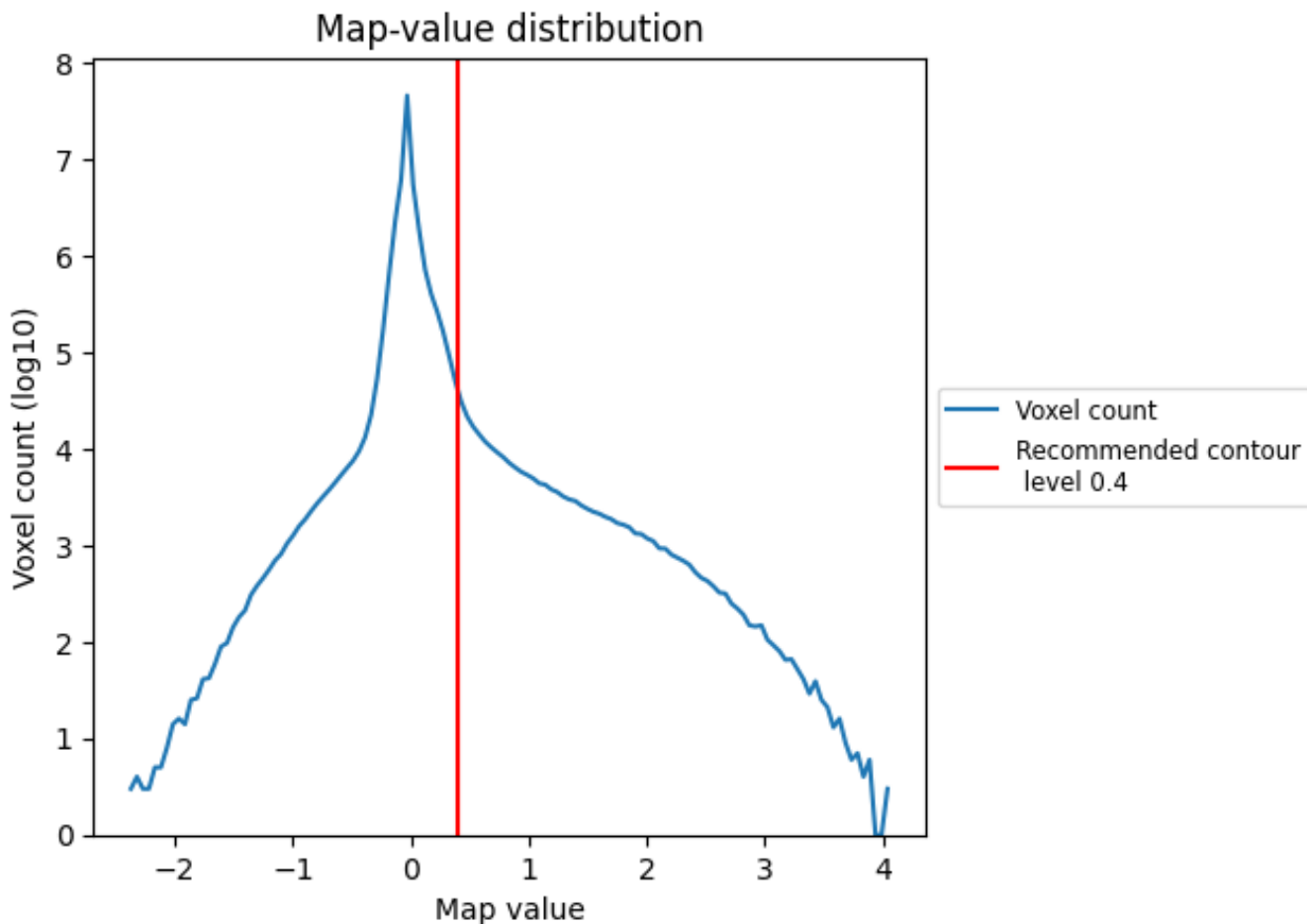
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

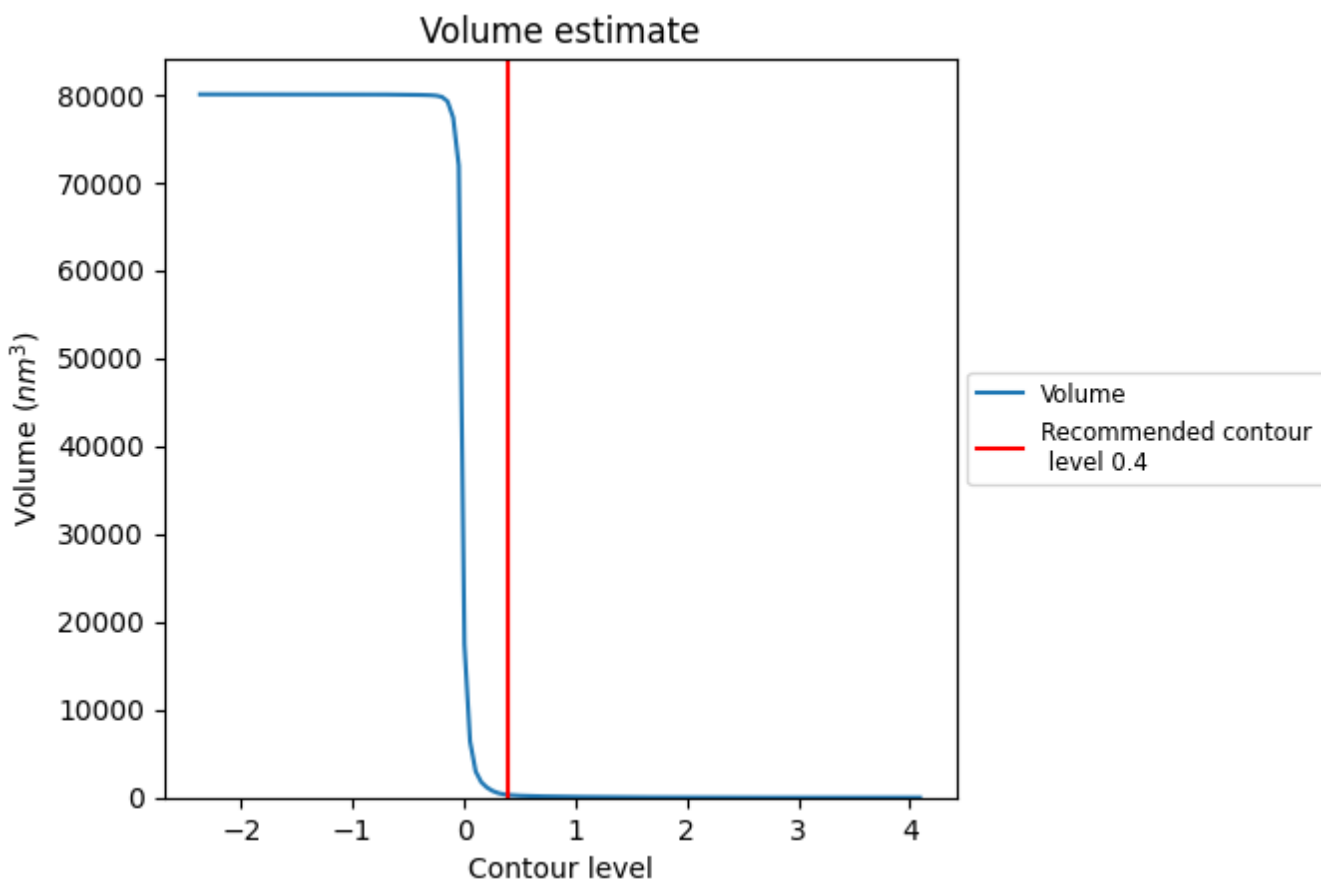
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

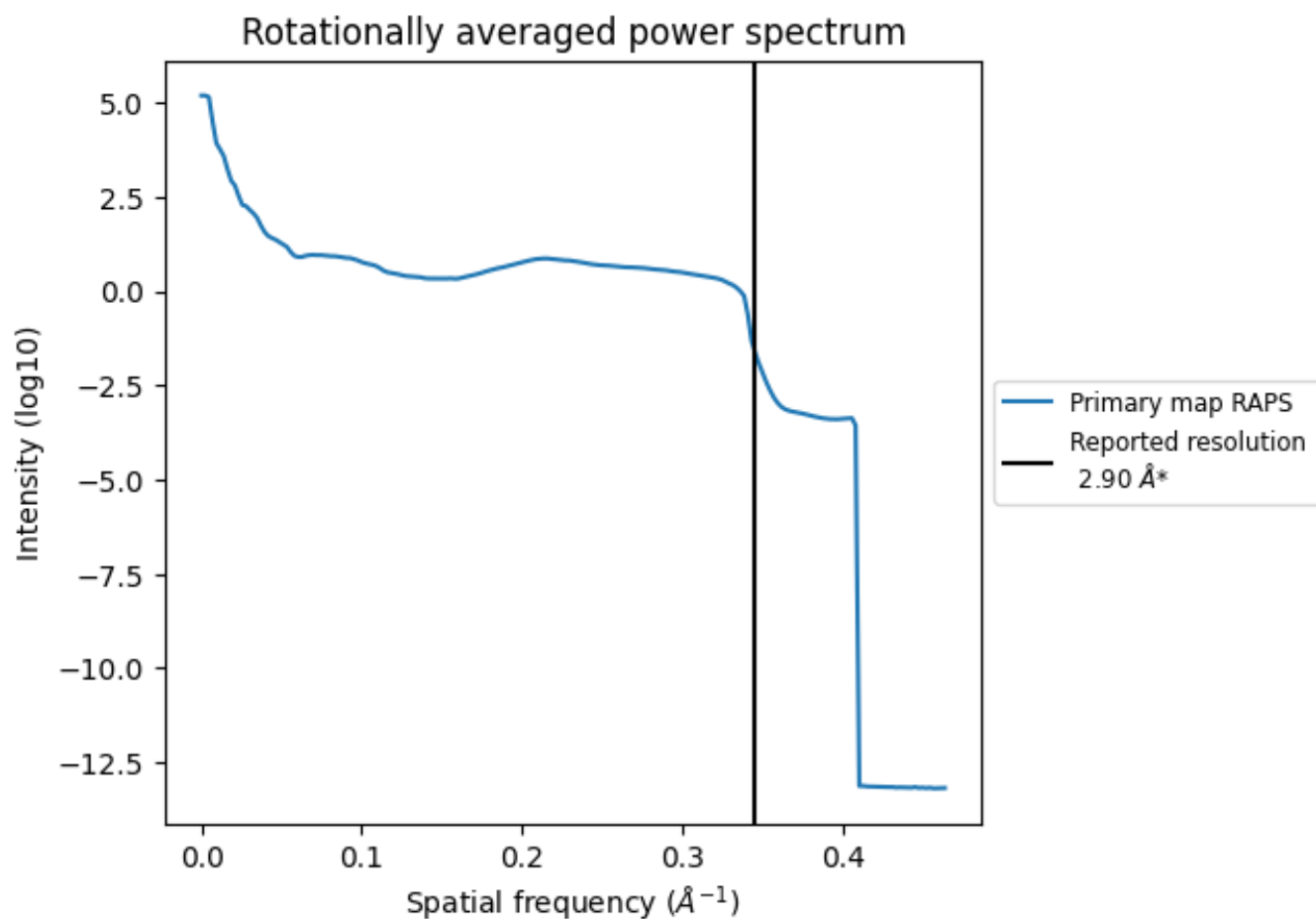
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 295 nm^3 ; this corresponds to an approximate mass of 266 kDa.

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

7.3 Rotationally averaged power spectrum i



*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

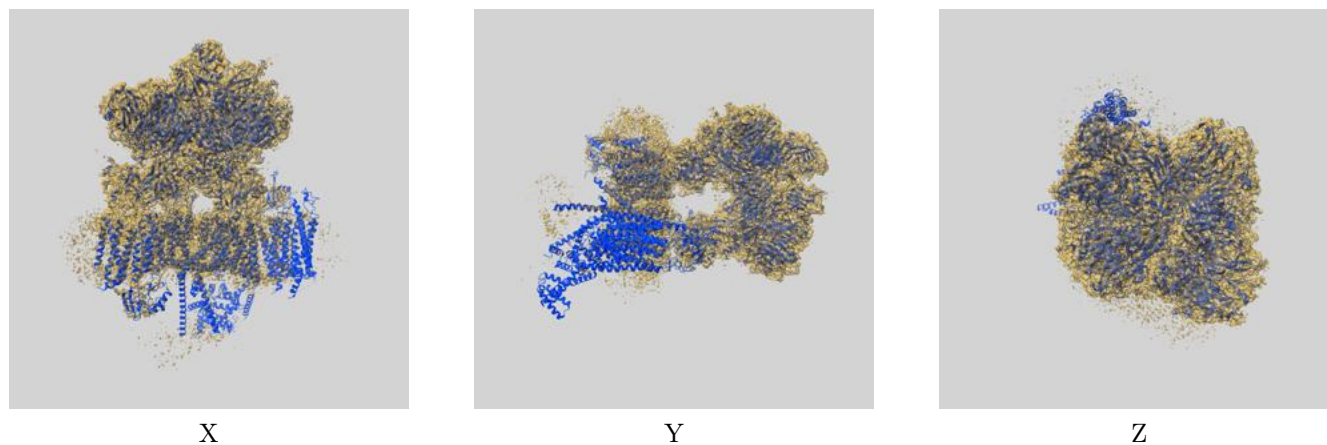
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

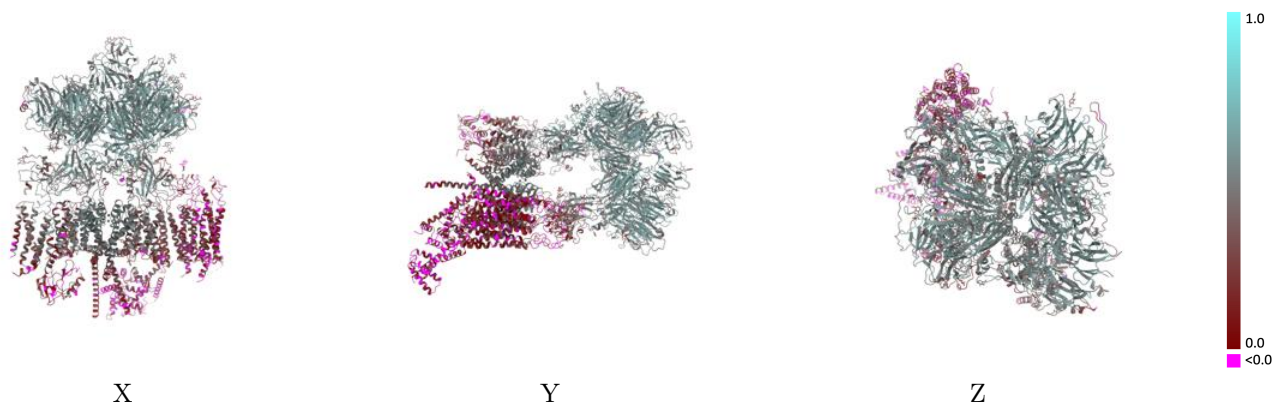
This section contains information regarding the fit between EMDB map EMD-31076 and PDB model 7EEB. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



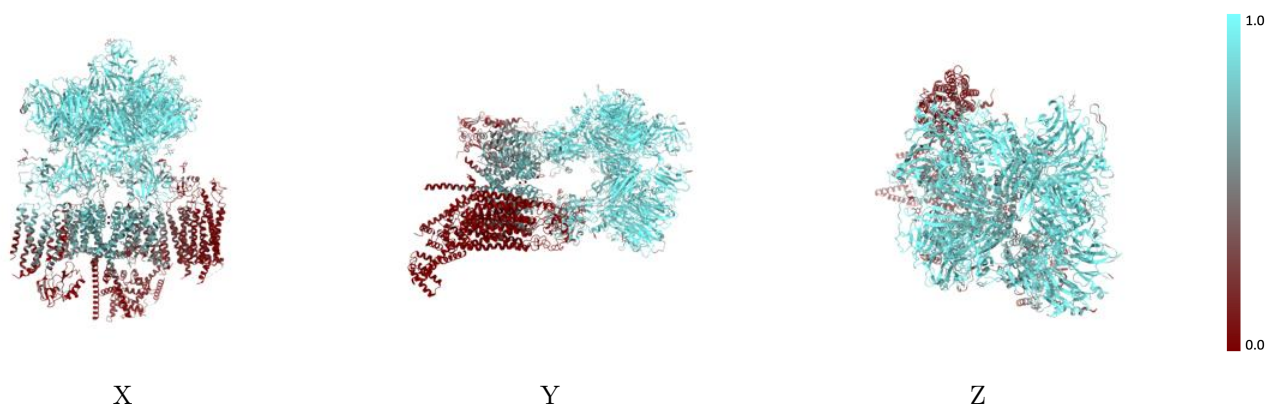
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



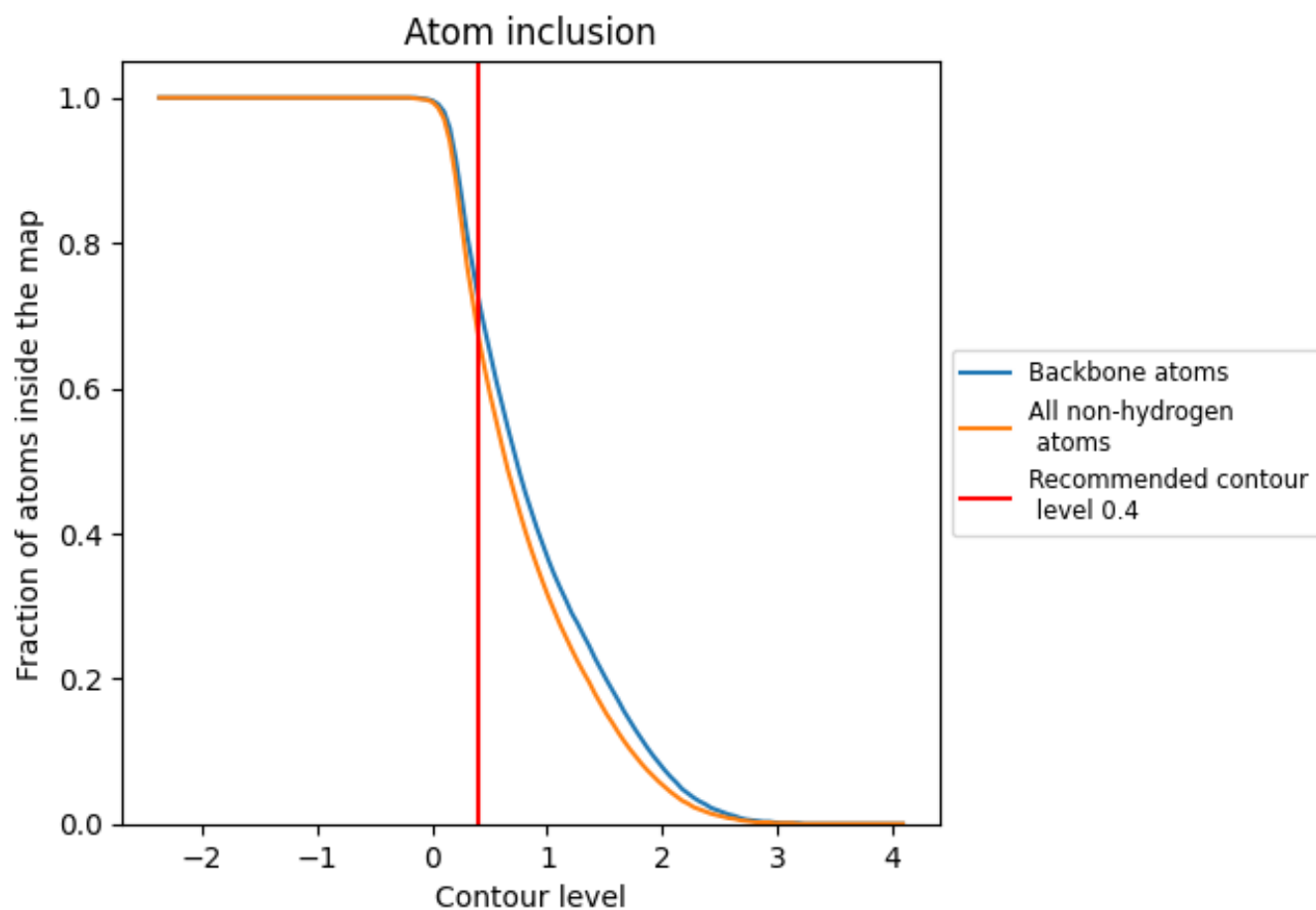
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.4).































































9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 67% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6740	 0.4260
A	 0.6040	 0.4150
B	 0.4950	 0.3700
C	 0.5530	 0.3920
D	 0.6310	 0.4380
E	 0.8540	 0.5060
F	 0.8960	 0.5400
G	 0.8250	 0.4800
H	 0.8440	 0.5020
I	 0.0070	 0.0540
J	 0.1340	 0.1840
K	 0.0040	 0.0140
L	 0.0450	 0.1190
M	 0.5040	 0.3680
N	 0.3570	 0.2590
O	 0.7590	 0.4420
P	 0.6430	 0.4570
Q	 0.9230	 0.5490
R	 0.8210	 0.5000
S	 0.8570	 0.5240
T	 0.6430	 0.4020
U	 0.6150	 0.3200
V	 0.6430	 0.4160
W	 0.6670	 0.4570
X	 0.8570	 0.4790
Y	 0.6720	 0.4120
Z	 0.8680	 0.4550
a	 0.5000	 0.3700
b	 0.4620	 0.2670
c	 0.7700	 0.4710
d	 0.0000	 0.0460

