



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 08:12 AM UTC

PDB ID : 5JNX / pdb_00005jnx
EMDB ID : EMD-8169
Title : The 6.6 Å cryo-EM structure of the full-length human NPC1 in complex with the cleaved glycoprotein of Ebola virus
Authors : Gong, X.; Qian, H.W.; Zhou, X.H.; Wu, J.P.; Wan, T.; Shi, Y.; Gao, F.; Zhou, Q.; Yan, N.
Deposited on : 2016-05-01
Resolution : 6.56 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

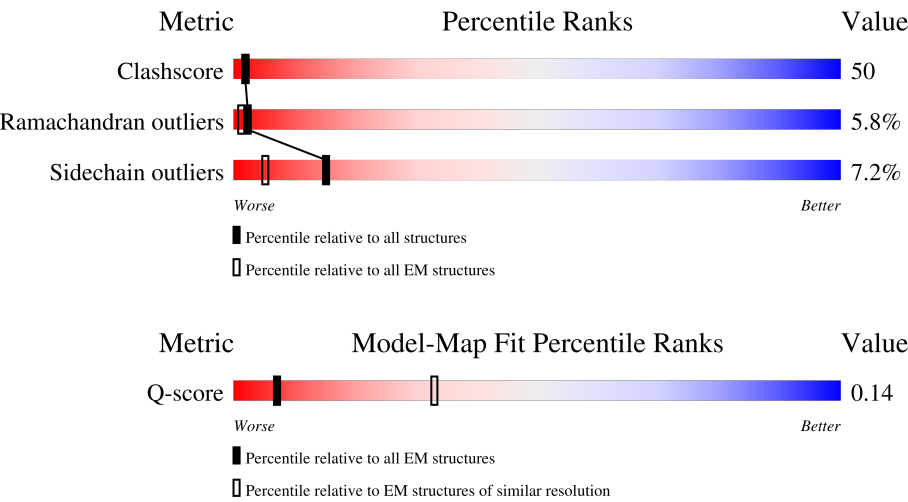
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13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

1 Overall quality at a glance i

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

The reported resolution of this entry is 6.56 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	501 (6.07 - 7.06)

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	1278	
2	C	158	
2	E	158	
2	G	158	

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Mol	Chain	Length	Quality of chain
3	D	130	
3	F	130	
3	H	130	
4	B	2	
4	I	2	
4	K	2	
4	M	2	
4	N	2	
4	O	2	
4	P	2	
5	J	3	
6	L	4	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	J	1	-	-	X	-
5	NAG	J	2	-	-	X	-
6	NAG	L	1	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13749 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 Niemann-Pick C1 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1133	Total	C	N	O	S	1	0
			7695	4862	1315	1476	42		

- Molecule 2 is a protein called Envelope glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	158	Total	C	N	O	S	0	0
			1194	757	209	223	5		
2	E	158	Total	C	N	O	S	0	0
			1194	757	209	223	5		
2	G	158	Total	C	N	O	S	0	0
			1194	757	209	223	5		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	31	ARG	-	expression tag	UNP P87666
C	42	VAL	THR	engineered mutation	UNP P87666
E	31	ARG	-	expression tag	UNP P87666
E	42	VAL	THR	engineered mutation	UNP P87666
G	31	ARG	-	expression tag	UNP P87666
G	42	VAL	THR	engineered mutation	UNP P87666

- Molecule 3 is a protein called Envelope glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	87	Total	C	N	O	S	0	0
			687	441	121	122	3		
3	F	87	Total	C	N	O	S	0	0
			687	441	121	122	3		
3	H	87	Total	C	N	O	S	0	0
			687	441	121	122	3		

There are 18 discrepancies between the modelled and reference sequences:

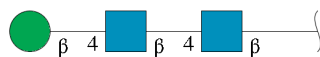
Chain	Residue	Modelled	Actual	Comment	Reference
D	633	HIS	-	expression tag	UNP P87666
D	634	HIS	-	expression tag	UNP P87666
D	635	HIS	-	expression tag	UNP P87666
D	636	HIS	-	expression tag	UNP P87666
D	637	HIS	-	expression tag	UNP P87666
D	638	HIS	-	expression tag	UNP P87666
F	633	HIS	-	expression tag	UNP P87666
F	634	HIS	-	expression tag	UNP P87666
F	635	HIS	-	expression tag	UNP P87666
F	636	HIS	-	expression tag	UNP P87666
F	637	HIS	-	expression tag	UNP P87666
F	638	HIS	-	expression tag	UNP P87666
H	633	HIS	-	expression tag	UNP P87666
H	634	HIS	-	expression tag	UNP P87666
H	635	HIS	-	expression tag	UNP P87666
H	636	HIS	-	expression tag	UNP P87666
H	637	HIS	-	expression tag	UNP P87666
H	638	HIS	-	expression tag	UNP P87666

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



Mol	Chain	Residues	Atoms				AltConf	Trace
4	B	2	Total	C	N	O	0	0
			28	16	2	10		
4	I	2	Total	C	N	O	0	0
			28	16	2	10		
4	K	2	Total	C	N	O	0	0
			28	16	2	10		
4	M	2	Total	C	N	O	0	0
			28	16	2	10		
4	N	2	Total	C	N	O	0	0
			28	16	2	10		
4	O	2	Total	C	N	O	0	0
			28	16	2	10		
4	P	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 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.



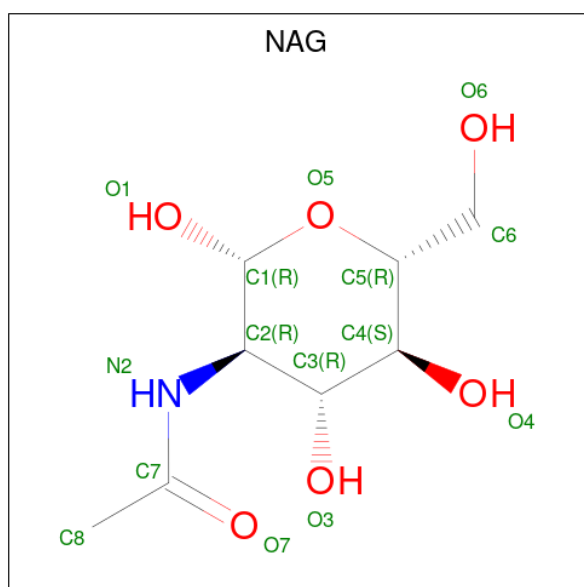
Mol	Chain	Residues	Atoms				AltConf	Trace
5	J	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 6 is an oligosaccharide called alpha-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.

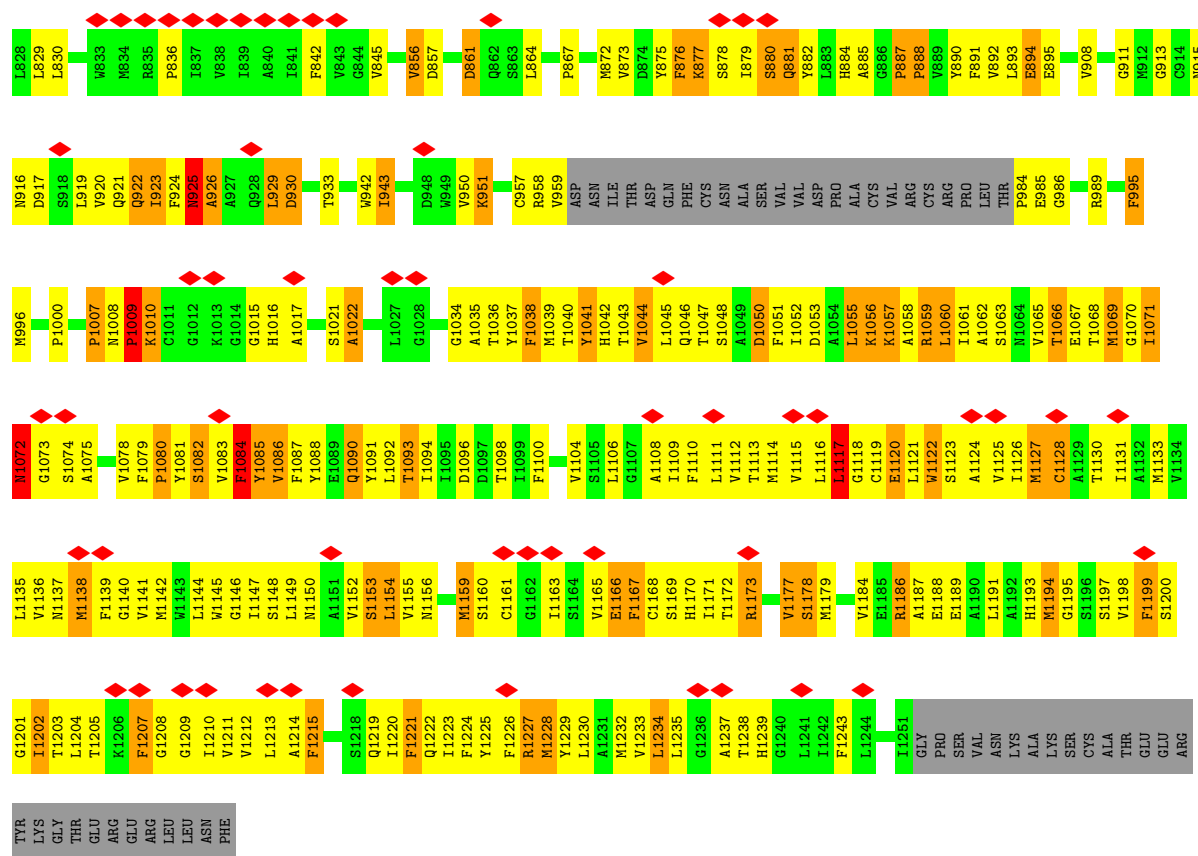


Mol	Chain	Residues	Atoms				AltConf	Trace
6	L	4	Total	C	N	O	0	0
			50	28	2	20		

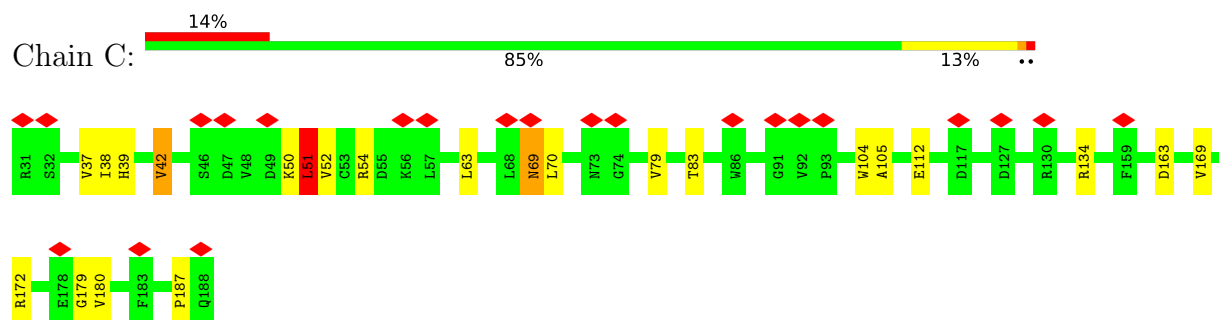
- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



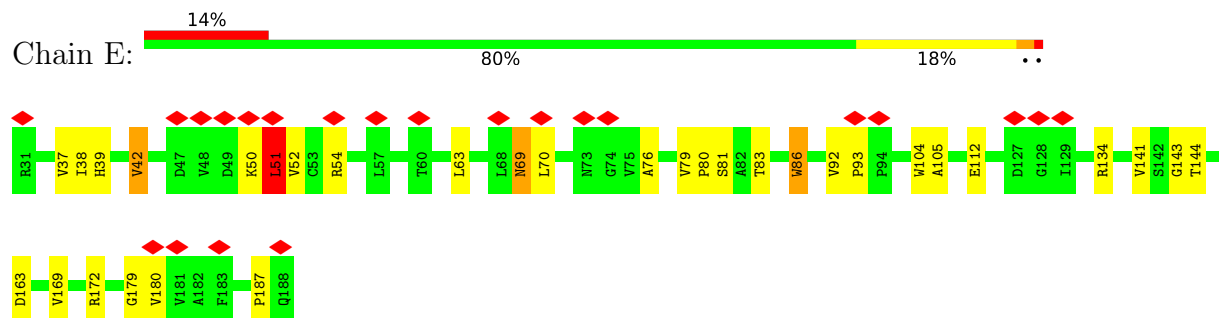
Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	



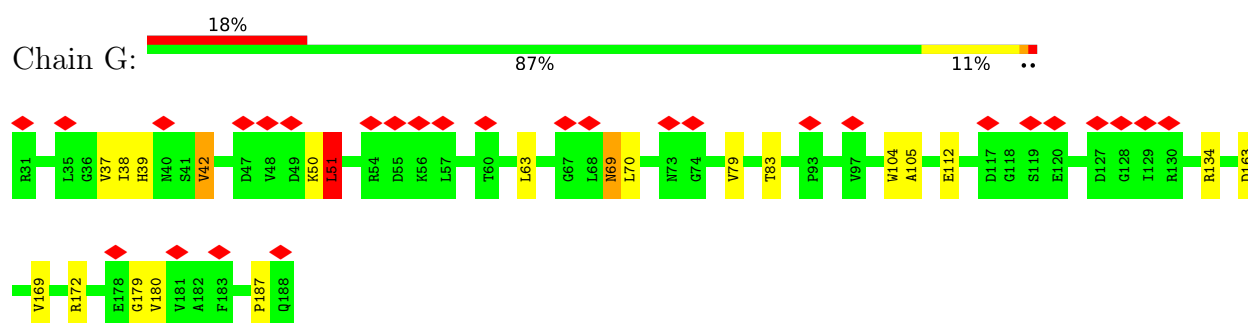
• Molecule 2: Envelope glycoprotein



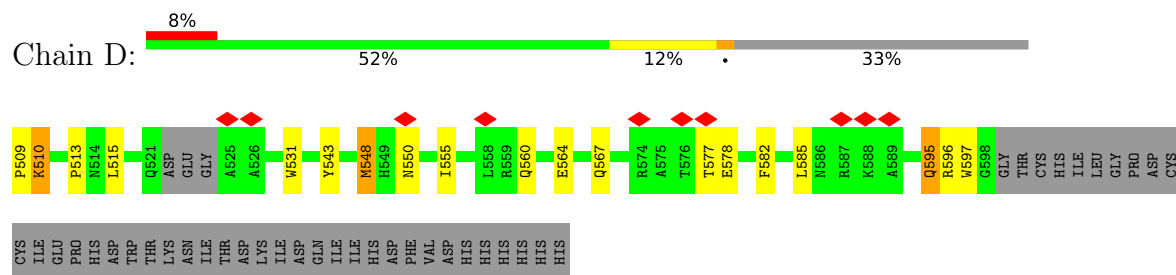
• Molecule 2: Envelope glycoprotein



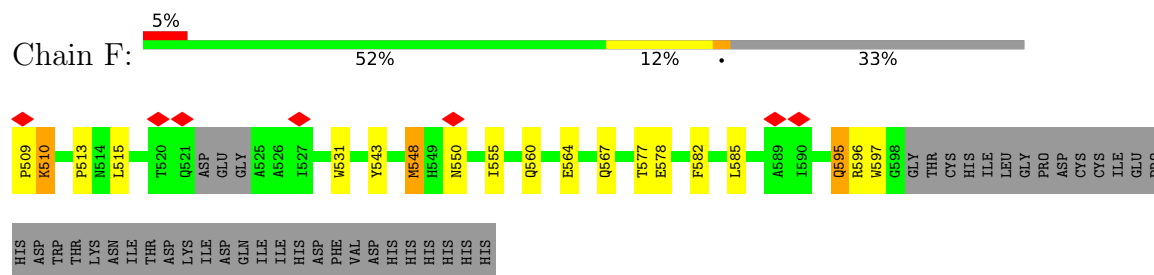
• Molecule 2: Envelope glycoprotein



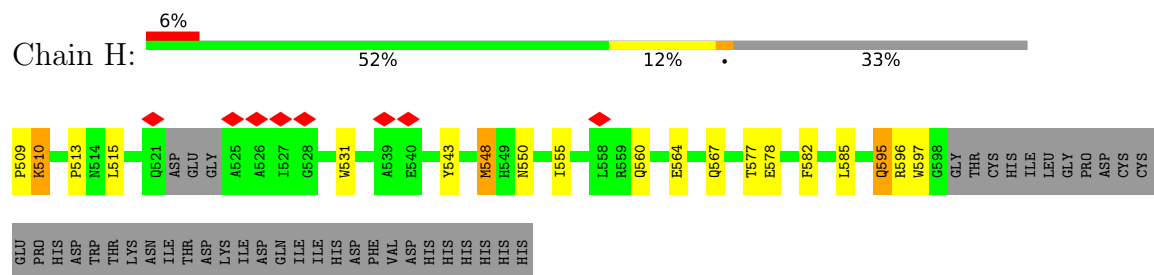
- Molecule 3: Envelope glycoprotein



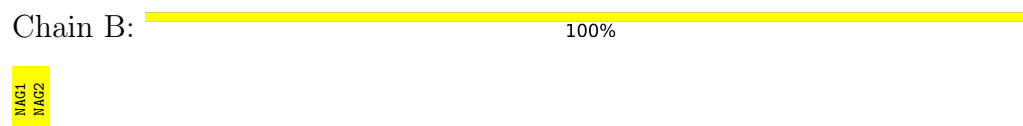
- Molecule 3: Envelope glycoprotein



- Molecule 3: Envelope glycoprotein



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



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



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



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



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



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



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

Chain J:  100%

MAG1
MAG2
BMA3

- Molecule 6: alpha-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

Chain L:  100%

MAG1
MAG2
BMA3
MAN4

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	50223	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)	1700	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	38270	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.090	Depositor
Minimum map value	-0.042	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	334.47424, 334.47424, 334.47424	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.30654, 1.30654, 1.30654	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.64	20/7843 (0.3%)	0.97	55/10748 (0.5%)
2	C	0.55	1/1223 (0.1%)	0.86	0/1664
2	E	0.58	2/1223 (0.2%)	0.85	0/1664
2	G	0.55	1/1223 (0.1%)	0.85	0/1664
3	D	0.54	0/702	1.01	1/952 (0.1%)
3	F	0.54	0/702	1.01	1/952 (0.1%)
3	H	0.54	0/702	1.01	2/952 (0.2%)
All	All	0.60	24/13618 (0.2%)	0.95	59/18596 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
2	C	0	1
2	E	0	1
2	G	0	1
All	All	0	5

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	469	LEU	C-N	-9.33	1.22	1.33
1	A	1060	LEU	C-N	8.59	1.44	1.33
1	A	881	GLN	C-N	-8.29	1.22	1.33
1	A	884	HIS	C-N	-7.96	1.23	1.33
1	A	429	VAL	C-N	-7.63	1.23	1.33
2	E	42	VAL	CA-CB	7.19	1.61	1.53
2	C	42	VAL	CA-CB	7.05	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	42	VAL	CA-CB	6.97	1.61	1.53
1	A	602	SER	N-CA	6.53	1.54	1.45
1	A	252	GLN	C-N	6.38	1.40	1.33
1	A	254	PRO	C-N	6.31	1.40	1.33
1	A	253	PRO	C-N	6.26	1.40	1.33
1	A	671	SER	CA-C	5.94	1.60	1.52
1	A	602	SER	CA-C	5.58	1.59	1.52
2	E	86	TRP	C-N	5.35	1.40	1.33
1	A	166	PRO	N-CD	5.29	1.55	1.47
1	A	424	PRO	N-CD	5.08	1.54	1.47
1	A	254	PRO	N-CD	5.08	1.54	1.47
1	A	249	PRO	N-CD	5.07	1.54	1.47
1	A	401	PRO	N-CD	5.06	1.54	1.47
1	A	251	PRO	N-CD	5.05	1.54	1.47
1	A	422	PRO	N-CD	5.04	1.54	1.47
1	A	255	PRO	N-CD	5.03	1.54	1.47
1	A	253	PRO	N-CD	5.03	1.54	1.47

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	881	GLN	N-CA-C	10.41	123.54	108.86
1	A	995	PHE	N-CA-C	10.38	121.93	108.34
1	A	429	VAL	O-C-N	-8.86	111.00	121.10
1	A	602	SER	CB-CA-C	-8.61	91.12	110.07
1	A	996	MET	CA-C-N	-8.60	105.12	121.54
1	A	996	MET	C-N-CA	-8.60	105.12	121.54
1	A	755	PRO	CA-N-CD	-8.58	99.99	112.00
1	A	671	SER	N-CA-C	8.47	121.37	107.73
1	A	248	GLY	C-N-CD	8.46	139.21	120.60
1	A	603	PHE	N-CA-C	8.42	123.57	109.76
1	A	423	TYR	C-N-CD	8.41	139.11	120.60
1	A	887	PRO	N-CA-CB	8.37	111.20	103.08
1	A	363	ALA	N-CA-C	7.00	118.80	111.03
1	A	254	PRO	CA-C-N	-6.98	113.19	120.38
1	A	254	PRO	C-N-CA	-6.98	113.19	120.38
1	A	1009	PRO	N-CA-CB	6.91	110.50	103.25
1	A	252	GLN	CA-C-N	-6.89	113.28	120.38
1	A	252	GLN	C-N-CA	-6.89	113.28	120.38
1	A	253	PRO	CA-C-N	-6.88	113.30	120.38
1	A	253	PRO	C-N-CA	-6.88	113.30	120.38
1	A	377	PRO	N-CA-CB	6.85	110.44	103.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	752	SER	N-CA-C	6.85	119.76	111.40
1	A	733	PRO	N-CA-CB	6.82	110.41	103.25
1	A	1007	PRO	N-CA-CB	6.82	110.41	103.25
1	A	836	PRO	N-CA-CB	6.80	111.06	103.44
1	A	888	PRO	N-CA-CB	6.79	110.38	103.25
1	A	350	PRO	N-CA-CB	6.76	110.35	103.25
1	A	1000	PRO	N-CA-CB	6.66	110.41	103.15
1	A	867	PRO	N-CA-CB	6.66	110.41	103.15
1	A	827	PRO	N-CA-CB	6.53	110.44	103.52
1	A	602	SER	N-CA-C	6.01	118.32	109.24
1	A	469	LEU	O-C-N	5.84	130.42	122.82
1	A	752	SER	CB-CA-C	-5.69	101.24	110.79
1	A	165	ALA	CA-C-N	-5.47	113.00	119.84
1	A	165	ALA	C-N-CA	-5.47	113.00	119.84
3	F	510	LYS	N-CA-C	5.39	118.78	111.17
3	D	510	LYS	N-CA-C	5.38	118.76	111.17
3	H	510	LYS	N-CA-C	5.38	118.76	111.17
1	A	363	ALA	CB-CA-C	-5.38	102.61	110.95
1	A	256	PRO	CA-N-CD	-5.26	104.64	112.00
1	A	690	ILE	CA-C-N	-5.22	113.32	119.84
1	A	690	ILE	C-N-CA	-5.22	113.32	119.84
1	A	383	ALA	CA-C-N	-5.22	113.32	119.84
1	A	383	ALA	C-N-CA	-5.22	113.32	119.84
1	A	400	GLY	CA-C-N	-5.21	113.33	119.84
1	A	400	GLY	C-N-CA	-5.21	113.33	119.84
1	A	421	GLN	CA-C-N	-5.17	113.38	119.84
1	A	421	GLN	C-N-CA	-5.17	113.38	119.84
1	A	469	LEU	CA-C-N	-5.15	115.88	123.30
1	A	469	LEU	C-N-CA	-5.15	115.88	123.30
1	A	259	PRO	CA-N-CD	-5.08	104.88	112.00
1	A	256	PRO	CA-C-N	-5.08	113.50	119.84
1	A	256	PRO	C-N-CA	-5.08	113.50	119.84
3	H	510	LYS	CA-C-O	-5.07	116.39	122.27
1	A	470	ALA	CA-C-N	5.06	124.85	119.28
1	A	470	ALA	C-N-CA	5.06	124.85	119.28
1	A	925	ASN	CA-C-N	5.05	131.19	121.54
1	A	925	ASN	C-N-CA	5.05	131.19	121.54
1	A	257	PRO	CA-N-CD	-5.03	104.95	112.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	602	SER	Peptide
1	A	603	PHE	Peptide
2	C	69	ASN	Sidechain
2	E	69	ASN	Sidechain
2	G	69	ASN	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7695	0	6477	1163	0
2	C	1194	0	1153	18	0
2	E	1194	0	1153	71	0
2	G	1194	0	1153	17	0
3	D	687	0	679	20	0
3	F	687	0	679	21	0
3	H	687	0	679	18	0
4	B	28	0	25	0	0
4	I	28	0	25	2	0
4	K	28	0	25	4	0
4	M	28	0	25	3	0
4	N	28	0	25	1	0
4	O	28	0	25	2	0
4	P	28	0	25	1	0
5	J	39	0	34	17	0
6	L	50	0	43	9	0
7	A	126	0	117	8	0
All	All	13749	0	12342	1286	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 50.

All (1286) 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:724:LEU:HD22	1:A:1170:HIS:CE1	1.29	1.62
1:A:656:LEU:CD1	1:A:685:ILE:HG13	1.17	1.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1138:MET:HE2	1:A:1232:MET:CB	1.20	1.59
1:A:656:LEU:HD11	1:A:685:ILE:CG1	1.31	1.58
1:A:598:ASN:HD21	4:K:1:NAG:C1	0.99	1.57
1:A:693:LEU:HD11	1:A:763:PHE:CE2	1.41	1.53
1:A:185:ASN:HD21	4:M:1:NAG:C1	1.24	1.51
1:A:403:PHE:CE2	1:A:566:PRO:HB3	1.46	1.50
1:A:503:PHE:CZ	2:E:86:TRP:HE3	1.30	1.49
1:A:684:LEU:CD2	1:A:728:LEU:HD13	1.45	1.46
1:A:70:ASN:HD21	7:A:1317:NAG:C1	1.26	1.46
1:A:656:LEU:CD1	1:A:685:ILE:CG1	1.85	1.45
1:A:659:ALA:HA	1:A:662:LEU:CD2	1.46	1.44
1:A:693:LEU:CD1	1:A:763:PHE:HE2	1.30	1.44
1:A:503:PHE:CZ	2:E:86:TRP:CE3	2.05	1.44
1:A:631:MET:CE	1:A:1204:LEU:O	1.64	1.42
1:A:693:LEU:HD11	1:A:763:PHE:CD2	1.52	1.42
1:A:1133:MET:HG2	1:A:1239:HIS:NE2	1.12	1.41
1:A:1133:MET:HG2	1:A:1239:HIS:CD2	1.52	1.40
1:A:693:LEU:CD1	1:A:763:PHE:CE2	2.03	1.39
1:A:688:GLU:CG	1:A:724:LEU:HD23	1.52	1.39
1:A:1178:SER:CB	1:A:1186:ARG:HH11	1.35	1.38
1:A:1133:MET:HE2	1:A:1239:HIS:ND1	1.04	1.36
1:A:503:PHE:CE2	2:E:86:TRP:HE3	1.41	1.36
1:A:684:LEU:HD21	1:A:728:LEU:CD1	1.51	1.36
1:A:1142:MET:HA	1:A:1147:ILE:CB	1.57	1.35
1:A:684:LEU:HD21	1:A:728:LEU:CD2	1.55	1.34
1:A:856:VAL:CB	1:A:1091:TYR:HE2	1.41	1.32
1:A:523:LEU:HD11	1:A:1016:HIS:CB	1.58	1.31
1:A:401:PRO:HD3	1:A:571:TYR:CE1	1.65	1.30
1:A:686:VAL:CG1	1:A:690:ILE:HD11	1.61	1.30
1:A:724:LEU:CD2	1:A:1170:HIS:CE1	2.13	1.30
1:A:1084:PHE:CE1	1:A:1085:TYR:CD1	2.20	1.29
1:A:723:GLN:OE1	1:A:1169:SER:HB2	1.20	1.28
1:A:751:LEU:O	1:A:755:PRO:HG3	1.29	1.28
1:A:1138:MET:CE	1:A:1232:MET:HB2	1.63	1.27
1:A:452:ASN:HD21	7:A:1323:NAG:C1	1.45	1.27
1:A:923:ILE:O	1:A:1042:HIS:CB	1.83	1.27
1:A:401:PRO:HG3	1:A:571:TYR:CD1	1.68	1.26
1:A:688:GLU:O	1:A:691:PRO:HD2	1.19	1.26
1:A:1133:MET:CE	1:A:1239:HIS:ND1	1.96	1.26
1:A:648:LEU:HB3	1:A:763:PHE:CE1	1.70	1.26
1:A:686:VAL:HG12	1:A:690:ILE:CD1	1.62	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1142:MET:HE3	1:A:1148:SER:O	1.11	1.25
1:A:503:PHE:CE2	2:E:86:TRP:CE3	2.18	1.25
1:A:162:ASP:OD2	1:A:244:SER:CB	1.86	1.24
1:A:1070:GLY:O	1:A:1071:ILE:CG1	1.83	1.24
1:A:688:GLU:O	1:A:691:PRO:CD	1.86	1.23
1:A:688:GLU:HG2	1:A:1170:HIS:NE2	1.54	1.22
1:A:1138:MET:CE	1:A:1232:MET:CB	2.15	1.22
1:A:882:TYR:CB	1:A:1082:SER:HB3	1.70	1.22
1:A:1055:LEU:HD23	1:A:1085:TYR:CZ	1.73	1.22
1:A:162:ASP:OD2	1:A:244:SER:HB3	1.04	1.22
1:A:659:ALA:CA	1:A:662:LEU:HD23	1.66	1.22
1:A:915:ASN:CB	1:A:920:VAL:HA	1.68	1.21
1:A:478:ASN:HD21	6:L:1:NAG:C1	1.52	1.21
1:A:856:VAL:O	1:A:1048:SER:CB	1.89	1.21
1:A:406:GLU:OE1	1:A:583:TRP:HZ3	1.17	1.20
1:A:684:LEU:HD21	1:A:728:LEU:CG	1.70	1.20
1:A:724:LEU:HD22	1:A:1170:HIS:NE2	1.54	1.20
1:A:926:ALA:O	1:A:1040:THR:HG22	1.34	1.20
1:A:684:LEU:CD2	1:A:728:LEU:CD1	2.09	1.19
1:A:1133:MET:HE2	1:A:1239:HIS:CG	1.76	1.19
1:A:503:PHE:CB	2:E:83:THR:HG21	1.48	1.19
1:A:1133:MET:CG	1:A:1239:HIS:CD2	2.26	1.19
1:A:1127:MET:CE	1:A:1168:CYS:HB3	1.74	1.18
1:A:1142:MET:CA	1:A:1147:ILE:CB	2.22	1.18
1:A:1108:ALA:O	1:A:1112:VAL:HG23	1.43	1.18
1:A:1084:PHE:CE1	1:A:1085:TYR:HD1	1.59	1.17
1:A:250:LYS:HB3	1:A:251:PRO:CD	1.70	1.17
1:A:421:GLN:OE1	2:E:144:THR:HG22	1.45	1.17
1:A:732:ALA:CB	1:A:749:GLY:HA3	1.75	1.17
1:A:1009:PRO:HA	1:A:1016:HIS:O	1.44	1.17
1:A:656:LEU:HD13	1:A:685:ILE:HG13	1.26	1.16
1:A:923:ILE:O	1:A:1042:HIS:HB2	1.33	1.16
1:A:924:PHE:H	1:A:925:ASN:CB	1.56	1.16
1:A:1133:MET:CG	1:A:1239:HIS:NE2	2.08	1.16
1:A:1138:MET:HE1	1:A:1232:MET:HA	1.23	1.16
1:A:730:GLU:CG	1:A:1108:ALA:HB1	1.76	1.15
1:A:755:PRO:HD2	1:A:756:ALA:H	1.06	1.15
1:A:1138:MET:CE	1:A:1232:MET:HA	1.76	1.15
1:A:507:ALA:HB1	1:A:529:LEU:HG	1.28	1.15
1:A:656:LEU:HD13	1:A:685:ILE:CG1	1.74	1.15
1:A:1071:ILE:O	1:A:1072:ASN:O	1.65	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1142:MET:CE	1:A:1148:SER:O	1.93	1.15
1:A:1178:SER:CB	1:A:1186:ARG:CD	2.25	1.15
1:A:676:SER:HB3	1:A:1225:TYR:OH	1.41	1.15
1:A:724:LEU:CD1	1:A:1166:GLU:HG2	1.77	1.15
1:A:767:ALA:O	1:A:771:ASP:CB	1.94	1.15
1:A:1133:MET:HG2	1:A:1239:HIS:CE1	1.81	1.15
1:A:959:VAL:CB	1:A:984:PRO:N	2.10	1.14
1:A:1178:SER:CB	1:A:1186:ARG:HD2	1.76	1.14
2:E:76:ALA:HB1	2:E:81:SER:CB	1.78	1.13
1:A:1071:ILE:CG2	1:A:1072:ASN:H	1.62	1.13
1:A:1138:MET:HE2	1:A:1232:MET:CA	1.76	1.13
1:A:688:GLU:HG3	1:A:724:LEU:HD23	1.29	1.13
1:A:631:MET:SD	1:A:1208:GLY:CA	2.36	1.13
1:A:656:LEU:HD11	1:A:685:ILE:CB	1.77	1.12
1:A:684:LEU:CD2	1:A:728:LEU:HD22	1.79	1.12
1:A:856:VAL:O	1:A:1048:SER:HB3	1.44	1.13
1:A:1140:GLY:O	1:A:1144:LEU:CB	1.97	1.12
1:A:135:ASN:HD21	7:A:1322:NAG:C1	1.50	1.12
1:A:879:ILE:CA	1:A:1043:THR:HG21	1.79	1.12
1:A:1062:ALA:HB1	1:A:1078:VAL:HB	1.18	1.12
1:A:1070:GLY:O	1:A:1071:ILE:HG13	0.95	1.12
1:A:684:LEU:HD23	1:A:728:LEU:HD13	1.14	1.12
1:A:752:SER:O	1:A:755:PRO:HD2	1.46	1.12
1:A:656:LEU:CB	1:A:682:LEU:HD11	1.79	1.11
1:A:1098:THR:HG22	1:A:1154:LEU:HD21	1.22	1.11
1:A:406:GLU:OE1	1:A:583:TRP:CZ3	2.03	1.11
1:A:915:ASN:CA	1:A:920:VAL:HA	1.81	1.10
1:A:1046:GLN:CB	1:A:1050:ASP:OD2	1.98	1.10
1:A:403:PHE:CD2	1:A:566:PRO:HB3	1.87	1.10
1:A:635:ILE:HG23	1:A:690:ILE:HD13	1.14	1.10
1:A:688:GLU:C	1:A:691:PRO:CD	2.23	1.10
1:A:752:SER:O	1:A:755:PRO:CD	1.99	1.10
1:A:1127:MET:HA	1:A:1127:MET:HE3	1.17	1.10
1:A:1178:SER:CB	1:A:1186:ARG:NH1	2.15	1.09
1:A:401:PRO:HG3	1:A:571:TYR:HD1	1.01	1.09
1:A:856:VAL:CB	1:A:1091:TYR:CE2	2.34	1.09
3:F:510:LYS:NZ	4:O:1:NAG:O6	1.86	1.09
1:A:680:LEU:HB3	1:A:1229:TYR:OH	1.51	1.09
1:A:504:PHE:HE2	2:E:79:VAL:CG1	1.63	1.09
1:A:720:LEU:HD22	1:A:1170:HIS:HA	1.28	1.09
1:A:724:LEU:HD11	1:A:1166:GLU:CG	1.81	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:510:LYS:NZ	4:N:1:NAG:O6	1.86	1.08
5:J:2:NAG:H62	5:J:3:BMA:C2	1.82	1.08
1:A:631:MET:HE1	1:A:1204:LEU:C	1.77	1.08
1:A:929:LEU:CB	1:A:1038:PHE:CD2	2.37	1.08
1:A:228:ASP:CB	1:A:246:VAL:HG13	1.84	1.07
1:A:365:SER:HA	1:A:662:LEU:HB3	1.30	1.07
1:A:607:ARG:HG2	1:A:611:ASP:CG	1.79	1.07
1:A:659:ALA:HA	1:A:662:LEU:HD23	1.13	1.07
1:A:659:ALA:C	1:A:662:LEU:HD23	1.77	1.07
1:A:1142:MET:O	1:A:1147:ILE:CB	2.02	1.07
3:H:510:LYS:NZ	4:P:1:NAG:O6	1.86	1.07
1:A:1071:ILE:HG22	1:A:1072:ASN:N	1.61	1.07
1:A:730:GLU:HG3	1:A:1108:ALA:CB	1.82	1.07
1:A:687:ILE:O	1:A:691:PRO:HD3	1.53	1.06
1:A:879:ILE:C	1:A:1043:THR:CG2	2.28	1.06
1:A:693:LEU:HD12	1:A:763:PHE:HE2	1.18	1.06
1:A:1062:ALA:HB1	1:A:1078:VAL:CB	1.86	1.06
1:A:403:PHE:HE2	1:A:566:PRO:CB	1.67	1.06
1:A:915:ASN:HA	1:A:920:VAL:HA	1.38	1.06
1:A:503:PHE:HE1	2:E:83:THR:O	1.36	1.06
1:A:923:ILE:C	1:A:1042:HIS:HB3	1.80	1.05
1:A:1138:MET:CE	1:A:1232:MET:CA	2.31	1.05
1:A:688:GLU:HG2	1:A:724:LEU:HD23	1.32	1.05
1:A:879:ILE:C	1:A:1043:THR:HG22	1.81	1.05
1:A:879:ILE:N	1:A:1043:THR:HG21	1.71	1.05
1:A:196:LYS:HG3	1:A:204:THR:OG1	1.54	1.05
1:A:631:MET:HE1	1:A:1204:LEU:O	0.88	1.05
1:A:685:ILE:O	1:A:689:VAL:HG23	1.56	1.05
1:A:635:ILE:HG23	1:A:690:ILE:CD1	1.86	1.04
1:A:635:ILE:CG2	1:A:690:ILE:CD1	2.35	1.04
1:A:1133:MET:CE	1:A:1239:HIS:CG	2.39	1.04
1:A:503:PHE:CD2	2:E:83:THR:HG22	1.60	1.04
1:A:686:VAL:CG1	1:A:690:ILE:CD1	2.27	1.04
1:A:717:GLY:O	1:A:721:ASP:HB2	1.58	1.04
1:A:1065:VAL:O	1:A:1068:THR:HG22	1.56	1.04
1:A:688:GLU:C	1:A:691:PRO:HD3	1.82	1.04
1:A:403:PHE:CE2	1:A:566:PRO:CB	2.40	1.03
1:A:1156:ASN:HB3	1:A:1228:MET:CE	1.87	1.03
1:A:1046:GLN:HB3	1:A:1050:ASP:OD2	1.59	1.03
1:A:656:LEU:HB2	1:A:682:LEU:CD1	1.88	1.03
1:A:688:GLU:HG2	1:A:724:LEU:CD2	1.87	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:732:ALA:CB	1:A:749:GLY:CA	2.35	1.03
1:A:751:LEU:O	1:A:755:PRO:CG	2.05	1.03
1:A:732:ALA:HB3	1:A:749:GLY:HA3	1.40	1.03
1:A:250:LYS:HB3	1:A:251:PRO:HD3	1.38	1.02
1:A:635:ILE:HG21	1:A:690:ILE:HD11	1.40	1.02
1:A:684:LEU:CD2	1:A:728:LEU:CD2	2.33	1.02
1:A:523:LEU:CD1	1:A:1016:HIS:CB	2.36	1.02
1:A:1194:MET:HE3	1:A:1194:MET:HA	1.39	1.02
5:J:2:NAG:C6	5:J:3:BMA:H2	1.90	1.02
1:A:879:ILE:CA	1:A:1043:THR:CG2	2.38	1.02
1:A:922:GLN:O	1:A:1042:HIS:ND1	1.93	1.02
1:A:924:PHE:N	1:A:925:ASN:CB	2.22	1.02
2:E:76:ALA:CB	2:E:81:SER:HB2	1.89	1.02
1:A:631:MET:SD	1:A:1208:GLY:N	2.32	1.02
1:A:1084:PHE:CE1	1:A:1085:TYR:CE1	2.47	1.01
1:A:659:ALA:CA	1:A:662:LEU:CD2	2.28	1.01
1:A:723:GLN:OE1	1:A:1169:SER:CB	2.08	1.01
1:A:1127:MET:HE1	1:A:1168:CYS:HB3	1.38	1.01
1:A:401:PRO:HB2	1:A:569:ASN:ND2	1.75	1.01
1:A:688:GLU:CG	1:A:724:LEU:CD2	2.38	1.01
3:D:595:GLN:HE21	3:D:595:GLN:HA	1.25	1.00
1:A:337:ARG:HA	1:A:718:GLU:HG3	1.41	1.00
1:A:504:PHE:CE2	2:E:79:VAL:HG11	1.97	1.00
1:A:752:SER:C	1:A:755:PRO:CD	2.34	1.00
1:A:1138:MET:HE3	1:A:1138:MET:HA	1.40	1.00
1:A:648:LEU:HD12	1:A:763:PHE:CD1	1.95	1.00
1:A:401:PRO:CD	1:A:571:TYR:CE1	2.44	0.99
1:A:929:LEU:CB	1:A:1038:PHE:CE2	2.45	0.99
1:A:503:PHE:HB2	2:E:83:THR:HG21	1.44	0.99
3:H:595:GLN:HE21	3:H:595:GLN:HA	1.25	0.99
1:A:1062:ALA:HA	1:A:1078:VAL:HG21	1.44	0.99
1:A:1045:LEU:HA	1:A:1051:PHE:HZ	1.27	0.99
1:A:676:SER:OG	1:A:1226:PHE:CE2	2.15	0.98
1:A:1142:MET:C	1:A:1147:ILE:CB	2.35	0.98
1:A:504:PHE:HE2	2:E:79:VAL:HG11	1.24	0.98
1:A:724:LEU:HD22	1:A:1170:HIS:HE1	1.21	0.98
1:A:1209:GLY:HA3	1:A:1230:LEU:HD13	1.43	0.98
3:F:595:GLN:HE21	3:F:595:GLN:HA	1.25	0.98
5:J:2:NAG:H62	5:J:3:BMA:H2	0.99	0.98
1:A:402:PHE:O	1:A:403:PHE:HB3	1.63	0.98
1:A:686:VAL:HG12	1:A:690:ILE:HD12	1.42	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1138:MET:HE2	1:A:1232:MET:HB3	1.46	0.98
1:A:135:ASN:HD22	7:A:1322:NAG:C1	1.66	0.97
1:A:684:LEU:CD1	1:A:1166:GLU:HG3	1.93	0.97
2:E:76:ALA:HB1	2:E:81:SER:HB2	0.99	0.97
1:A:635:ILE:CG2	1:A:690:ILE:HD13	1.94	0.97
1:A:1156:ASN:ND2	1:A:1228:MET:HE3	1.79	0.97
1:A:1071:ILE:HG22	1:A:1072:ASN:H	0.83	0.97
1:A:656:LEU:HB2	1:A:682:LEU:HD11	0.98	0.97
1:A:720:LEU:O	1:A:723:GLN:NE2	1.98	0.97
1:A:459:ASN:HD21	7:A:1324:NAG:C1	1.66	0.97
1:A:1062:ALA:CB	1:A:1078:VAL:HB	1.95	0.97
1:A:607:ARG:O	1:A:611:ASP:N	1.98	0.96
1:A:680:LEU:CB	1:A:1229:TYR:OH	2.13	0.96
1:A:677:TYR:O	1:A:681:PRO:CB	2.12	0.96
1:A:724:LEU:CD2	1:A:1170:HIS:NE2	2.22	0.96
1:A:1045:LEU:HA	1:A:1051:PHE:CZ	1.99	0.96
1:A:1062:ALA:CA	1:A:1078:VAL:HG21	1.95	0.96
1:A:1085:TYR:O	1:A:1087:PHE:N	1.97	0.96
1:A:1055:LEU:HD23	1:A:1085:TYR:OH	1.66	0.96
1:A:506:TYR:CE1	2:E:80:PRO:HG3	2.00	0.96
1:A:557:ASN:HD22	5:J:1:NAG:C1	1.79	0.96
1:A:591:VAL:CG1	1:A:603:PHE:CE1	2.49	0.96
1:A:503:PHE:CE1	2:E:83:THR:O	2.18	0.95
1:A:503:PHE:HB3	2:E:83:THR:HG21	1.48	0.95
1:A:732:ALA:HB1	1:A:749:GLY:HA3	1.45	0.95
1:A:607:ARG:HG2	1:A:611:ASP:OD2	1.64	0.95
1:A:686:VAL:O	1:A:690:ILE:HG13	1.65	0.95
1:A:1127:MET:CE	1:A:1127:MET:HA	1.94	0.95
1:A:557:ASN:HD21	5:J:1:NAG:C1	1.72	0.95
1:A:685:ILE:O	1:A:689:VAL:CG2	2.15	0.95
1:A:718:GLU:O	1:A:722:GLN:HB2	1.67	0.95
1:A:401:PRO:CG	1:A:571:TYR:CD1	2.49	0.95
1:A:659:ALA:O	1:A:662:LEU:HD23	1.66	0.95
1:A:365:SER:HA	1:A:662:LEU:CB	1.95	0.95
1:A:653:LYS:O	1:A:682:LEU:HD21	1.65	0.95
1:A:692:PHE:CE1	1:A:713:GLU:HA	2.02	0.95
1:A:1156:ASN:CG	1:A:1228:MET:HE3	1.93	0.94
1:A:241:GLN:NE2	1:A:518:ARG:HH22	1.64	0.94
1:A:656:LEU:CD1	1:A:685:ILE:HG12	1.93	0.94
1:A:635:ILE:CG2	1:A:690:ILE:HD11	1.98	0.94
1:A:943:ILE:CB	1:A:1010:LYS:O	2.15	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:879:ILE:O	1:A:1043:THR:CG2	2.14	0.94
1:A:1156:ASN:HB3	1:A:1228:MET:HE1	1.47	0.94
1:A:398:HIS:HB3	1:A:399:PHE:CE1	2.02	0.94
1:A:1110:PHE:O	1:A:1114:MET:HG2	1.67	0.94
1:A:591:VAL:HG11	1:A:603:PHE:CE1	2.02	0.93
1:A:1046:GLN:CG	1:A:1050:ASP:OD2	2.16	0.93
1:A:421:GLN:OE1	2:E:144:THR:CG2	2.15	0.93
1:A:688:GLU:HG2	1:A:1170:HIS:CE1	2.03	0.93
1:A:503:PHE:HZ	2:E:86:TRP:CE3	1.72	0.93
1:A:729:GLY:O	1:A:733:PRO:CB	2.17	0.93
1:A:1135:LEU:HD21	1:A:1161:CYS:SG	2.08	0.93
1:A:1229:TYR:O	1:A:1233:VAL:HG23	1.69	0.93
1:A:507:ALA:HB1	1:A:529:LEU:CG	1.99	0.92
1:A:1084:PHE:CZ	1:A:1085:TYR:HE1	1.87	0.92
1:A:241:GLN:HE22	1:A:518:ARG:NH2	1.68	0.92
1:A:923:ILE:O	1:A:1042:HIS:HB3	1.63	0.92
2:E:76:ALA:CB	2:E:81:SER:CB	2.46	0.92
1:A:752:SER:C	1:A:755:PRO:HD3	1.93	0.92
1:A:1084:PHE:CZ	1:A:1085:TYR:CE1	2.57	0.92
1:A:1130:THR:HG21	1:A:1168:CYS:SG	2.08	0.92
1:A:371:VAL:O	1:A:373:VAL:N	2.01	0.92
1:A:494:VAL:HA	1:A:497:HIS:CE1	2.06	0.91
1:A:228:ASP:HB3	1:A:246:VAL:HG13	1.48	0.91
1:A:1046:GLN:HG2	1:A:1050:ASP:OD2	1.71	0.91
1:A:879:ILE:O	1:A:1043:THR:HG22	1.71	0.91
1:A:1171:ILE:HG23	1:A:1191:LEU:CD2	2.00	0.91
1:A:724:LEU:O	1:A:728:LEU:HG	1.70	0.91
1:A:885:ALA:O	1:A:1079:PHE:O	1.89	0.91
1:A:1059:ARG:HG3	1:A:1059:ARG:HH11	1.36	0.91
1:A:680:LEU:CG	1:A:1229:TYR:OH	2.16	0.91
1:A:678:ILE:HG12	1:A:748:LEU:HD21	1.51	0.90
1:A:724:LEU:CD2	1:A:1170:HIS:HE1	1.74	0.90
1:A:396:ASP:O	1:A:400:GLY:N	2.04	0.90
1:A:1070:GLY:C	1:A:1071:ILE:HG13	1.97	0.90
1:A:656:LEU:HB3	1:A:751:LEU:HD21	1.54	0.90
1:A:1141:VAL:O	1:A:1147:ILE:CB	2.19	0.90
1:A:1156:ASN:CB	1:A:1228:MET:HE3	2.00	0.90
1:A:684:LEU:HD21	1:A:728:LEU:HD22	1.40	0.90
1:A:620:ASP:O	1:A:623:THR:OG1	1.88	0.89
1:A:732:ALA:HB3	1:A:749:GLY:CA	1.98	0.89
1:A:924:PHE:CB	1:A:1041:TYR:O	2.20	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:631:MET:HG3	1:A:1208:GLY:HA3	1.54	0.89
1:A:915:ASN:CB	1:A:920:VAL:CA	2.51	0.89
1:A:591:VAL:HG12	1:A:603:PHE:CZ	2.08	0.89
1:A:1082:SER:HB2	1:A:1084:PHE:CD1	2.08	0.89
1:A:401:PRO:HB2	1:A:569:ASN:HD21	1.30	0.89
1:A:504:PHE:CE2	2:E:79:VAL:CG1	2.53	0.89
1:A:641:HIS:O	1:A:642:MET:O	1.89	0.89
1:A:506:TYR:OH	2:E:80:PRO:HA	1.73	0.88
1:A:680:LEU:HG	1:A:1229:TYR:OH	1.70	0.88
1:A:1098:THR:HG22	1:A:1154:LEU:CD2	2.03	0.88
1:A:228:ASP:HA	1:A:246:VAL:CG1	2.03	0.88
1:A:659:ALA:HA	1:A:662:LEU:HD22	1.54	0.88
1:A:1082:SER:O	1:A:1084:PHE:N	2.05	0.88
1:A:632:PHE:HZ	1:A:650:VAL:HG23	1.39	0.88
1:A:631:MET:SD	1:A:1208:GLY:HA2	2.14	0.88
1:A:755:PRO:HD2	1:A:756:ALA:N	1.84	0.88
1:A:1178:SER:CB	1:A:1186:ARG:HD3	2.04	0.88
1:A:504:PHE:HZ	2:E:141:VAL:HG21	1.39	0.87
1:A:544:TRP:HD1	1:A:545:LEU:N	1.72	0.87
1:A:1009:PRO:CA	1:A:1016:HIS:O	2.22	0.87
1:A:1127:MET:CE	1:A:1168:CYS:CB	2.52	0.87
1:A:929:LEU:CB	1:A:1038:PHE:HD2	1.81	0.87
1:A:1138:MET:HE2	1:A:1232:MET:HB2	0.88	0.87
1:A:507:ALA:CB	1:A:529:LEU:HG	2.05	0.87
1:A:879:ILE:HA	1:A:1043:THR:CG2	2.04	0.87
1:A:459:ASN:HD22	7:A:1324:NAG:C1	1.87	0.87
1:A:755:PRO:CD	1:A:756:ALA:H	1.88	0.87
1:A:523:LEU:HD11	1:A:1016:HIS:CA	2.04	0.86
1:A:1085:TYR:O	1:A:1088:TYR:N	2.06	0.86
1:A:684:LEU:HD11	1:A:728:LEU:CD2	2.05	0.86
1:A:692:PHE:HZ	1:A:713:GLU:CB	1.86	0.86
1:A:692:PHE:CZ	1:A:713:GLU:HA	2.10	0.86
1:A:650:VAL:O	1:A:654:VAL:HG23	1.74	0.86
1:A:384:PRO:HA	1:A:389:ARG:HG3	1.58	0.85
1:A:401:PRO:HD3	1:A:571:TYR:HE1	1.08	0.85
3:D:595:GLN:HA	3:D:595:GLN:NE2	1.92	0.85
3:F:595:GLN:HA	3:F:595:GLN:NE2	1.92	0.85
1:A:688:GLU:CG	1:A:1170:HIS:NE2	2.39	0.85
1:A:441:HIS:CE1	1:A:495:LEU:HD23	2.12	0.85
1:A:894:GLU:CB	1:A:995:PHE:CB	2.55	0.84
1:A:402:PHE:O	1:A:403:PHE:CB	2.25	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:720:LEU:HD22	1:A:1170:HIS:CA	2.06	0.84
1:A:1062:ALA:CB	1:A:1078:VAL:CB	2.52	0.84
1:A:656:LEU:CD1	1:A:682:LEU:HD12	2.07	0.84
1:A:1133:MET:CG	1:A:1239:HIS:CE1	2.53	0.84
1:A:959:VAL:C	1:A:984:PRO:N	2.36	0.84
1:A:196:LYS:CG	1:A:204:THR:OG1	2.25	0.84
1:A:1055:LEU:HD22	1:A:1055:LEU:O	1.78	0.84
1:A:1084:PHE:HE1	1:A:1085:TYR:CD1	1.88	0.84
2:C:39:HIS:HB2	2:C:42:VAL:HG22	1.60	0.84
1:A:167:SER:O	1:A:168:SER:OG	1.96	0.83
1:A:228:ASP:CB	1:A:246:VAL:CG1	2.56	0.83
1:A:631:MET:CE	1:A:1204:LEU:C	2.44	0.83
1:A:684:LEU:HG	1:A:1166:GLU:HG3	1.61	0.83
1:A:693:LEU:CD1	1:A:763:PHE:CD2	2.48	0.83
1:A:1133:MET:HE2	1:A:1239:HIS:CE1	2.09	0.83
1:A:1167:PHE:CE2	1:A:1237:ALA:HA	2.13	0.83
1:A:1082:SER:HB2	1:A:1084:PHE:CE1	2.14	0.83
2:G:39:HIS:HB2	2:G:42:VAL:HG22	1.60	0.83
3:H:595:GLN:HA	3:H:595:GLN:NE2	1.92	0.83
1:A:732:ALA:HB1	1:A:749:GLY:CA	2.02	0.83
1:A:1068:THR:HG23	1:A:1069:MET:H	1.44	0.83
1:A:656:LEU:CB	1:A:682:LEU:CD1	2.53	0.82
1:A:1133:MET:SD	1:A:1239:HIS:CE1	2.71	0.82
1:A:1209:GLY:O	1:A:1213:LEU:N	2.11	0.82
1:A:856:VAL:C	1:A:1048:SER:CB	2.53	0.82
1:A:926:ALA:O	1:A:1040:THR:CG2	2.23	0.82
1:A:241:GLN:HE22	1:A:518:ARG:HH22	0.85	0.82
1:A:631:MET:CG	1:A:1208:GLY:HA3	2.10	0.82
1:A:856:VAL:O	1:A:1048:SER:HB2	1.75	0.82
1:A:591:VAL:CG1	1:A:603:PHE:CZ	2.63	0.82
1:A:686:VAL:HG13	1:A:690:ILE:HD11	1.62	0.82
1:A:1127:MET:HE2	1:A:1168:CYS:CB	2.08	0.82
1:A:1210:ILE:HG13	1:A:1214:ALA:HB3	1.61	0.82
1:A:401:PRO:HB2	1:A:569:ASN:CG	2.03	0.81
1:A:684:LEU:CG	1:A:1166:GLU:HG3	2.10	0.81
2:E:39:HIS:HB2	2:E:42:VAL:HG22	1.60	0.81
1:A:228:ASP:HA	1:A:246:VAL:HG11	1.61	0.81
1:A:503:PHE:HE2	2:E:86:TRP:CE3	1.97	0.81
1:A:656:LEU:HD13	1:A:685:ILE:HG12	1.56	0.81
1:A:396:ASP:HA	1:A:400:GLY:CA	2.11	0.81
1:A:1202:ILE:HG21	1:A:1237:ALA:HB1	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:720:LEU:O	1:A:723:GLN:HG3	1.79	0.81
1:A:879:ILE:C	1:A:1043:THR:HG21	2.00	0.81
1:A:676:SER:OG	1:A:1226:PHE:HE2	1.60	0.81
1:A:959:VAL:C	1:A:984:PRO:CB	2.54	0.81
1:A:1135:LEU:O	1:A:1139:PHE:HD2	1.64	0.81
1:A:421:GLN:HG2	2:E:143:GLY:HA2	1.60	0.81
1:A:693:LEU:HD11	1:A:763:PHE:HD2	1.36	0.81
1:A:396:ASP:HA	1:A:400:GLY:HA2	1.63	0.80
1:A:1140:GLY:O	1:A:1144:LEU:N	2.13	0.80
1:A:631:MET:HE2	1:A:1204:LEU:O	1.81	0.80
1:A:1108:ALA:O	1:A:1112:VAL:CG2	2.28	0.80
1:A:1229:TYR:CE1	1:A:1233:VAL:HG21	2.15	0.80
1:A:678:ILE:CG1	1:A:748:LEU:HD21	2.11	0.80
1:A:648:LEU:CB	1:A:763:PHE:CE1	2.60	0.80
1:A:985:GLU:CB	1:A:986:GLY:HA2	2.11	0.80
1:A:1127:MET:HE2	1:A:1168:CYS:HB3	1.62	0.80
1:A:1142:MET:CE	1:A:1153:SER:OG	2.30	0.80
1:A:628:TYR:OH	1:A:653:LYS:HD2	1.82	0.80
1:A:1171:ILE:CG2	1:A:1191:LEU:CD2	2.59	0.80
1:A:1229:TYR:CD1	1:A:1233:VAL:HG21	2.15	0.80
1:A:1209:GLY:HA3	1:A:1230:LEU:CD1	2.10	0.80
1:A:503:PHE:CE2	2:E:86:TRP:CZ3	2.69	0.80
1:A:608:SER:O	1:A:612:GLU:HB2	1.82	0.80
1:A:503:PHE:CZ	2:E:86:TRP:HB2	2.17	0.79
5:J:1:NAG:H62	5:J:2:NAG:C8	2.12	0.79
1:A:607:ARG:CG	1:A:611:ASP:CG	2.53	0.79
1:A:633:LEU:O	1:A:636:SER:OG	1.99	0.79
1:A:648:LEU:HB3	1:A:763:PHE:CZ	2.17	0.79
1:A:687:ILE:O	1:A:691:PRO:CD	2.28	0.79
1:A:503:PHE:CZ	2:E:83:THR:HA	2.15	0.79
1:A:504:PHE:HE2	2:E:79:VAL:HG12	1.46	0.79
1:A:404:ARG:HD2	1:A:567:VAL:CG2	2.12	0.79
1:A:648:LEU:HD11	1:A:763:PHE:HA	1.64	0.79
1:A:381:TRP:HD1	1:A:382:SER:N	1.80	0.79
1:A:584:GLU:OE2	1:A:606:GLU:HB2	1.82	0.79
1:A:580:ALA:O	1:A:584:GLU:HG3	1.83	0.79
1:A:401:PRO:CB	1:A:569:ASN:HD21	1.96	0.79
1:A:472:LEU:HD21	1:A:1017:ALA:CB	2.13	0.78
1:A:1142:MET:HE3	1:A:1148:SER:C	2.06	0.78
1:A:185:ASN:HD22	4:M:1:NAG:C1	1.93	0.78
1:A:730:GLU:HG2	1:A:1112:VAL:CG2	2.13	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1171:ILE:HG23	1:A:1191:LEU:HD23	1.63	0.78
1:A:659:ALA:O	1:A:662:LEU:CD2	2.31	0.78
1:A:720:LEU:CD2	1:A:1170:HIS:HA	2.11	0.78
1:A:1142:MET:HE2	1:A:1153:SER:OG	1.84	0.78
6:L:1:NAG:H62	6:L:2:NAG:HN2	1.47	0.78
1:A:337:ARG:HA	1:A:718:GLU:CG	2.12	0.78
1:A:635:ILE:HG21	1:A:690:ILE:CD1	2.09	0.78
1:A:409:ILE:HG21	1:A:872:MET:CB	2.14	0.78
1:A:1110:PHE:HE2	1:A:1124:ALA:HB1	1.48	0.78
1:A:228:ASP:CA	1:A:246:VAL:HG13	2.14	0.78
1:A:1184:VAL:O	1:A:1184:VAL:HG12	1.84	0.78
1:A:632:PHE:CZ	1:A:650:VAL:HG23	2.19	0.78
1:A:1051:PHE:HB3	1:A:1084:PHE:HD2	1.49	0.77
1:A:653:LYS:C	1:A:653:LYS:HE3	2.09	0.77
1:A:629:ALA:O	1:A:633:LEU:HG	1.84	0.77
1:A:1021:SER:O	1:A:1022:ALA:CB	2.31	0.77
1:A:752:SER:HA	1:A:755:PRO:CG	2.15	0.77
1:A:1201:GLY:O	1:A:1205:THR:HG23	1.84	0.77
1:A:544:TRP:CD1	1:A:545:LEU:N	2.53	0.76
1:A:688:GLU:OE1	1:A:721:ASP:OD1	2.02	0.76
1:A:1114:MET:HE1	1:A:1124:ALA:HB2	1.67	0.76
1:A:381:TRP:O	1:A:740:PHE:CB	2.33	0.76
1:A:684:LEU:CD1	1:A:728:LEU:HD22	2.15	0.76
1:A:1135:LEU:O	1:A:1139:PHE:CD2	2.38	0.76
1:A:631:MET:CG	1:A:1208:GLY:CA	2.64	0.76
1:A:1156:ASN:CB	1:A:1228:MET:CE	2.57	0.76
1:A:494:VAL:HA	1:A:497:HIS:ND1	2.01	0.76
1:A:503:PHE:HZ	2:E:86:TRP:HB2	1.48	0.76
1:A:630:ILE:O	1:A:634:TYR:CD2	2.39	0.76
1:A:503:PHE:CD2	2:E:83:THR:CG2	2.28	0.75
1:A:1127:MET:CE	1:A:1130:THR:HG21	2.16	0.75
1:A:720:LEU:C	1:A:723:GLN:HE21	1.93	0.75
1:A:506:TYR:OH	2:E:80:PRO:CA	2.34	0.75
1:A:656:LEU:HD11	1:A:685:ILE:HG13	0.78	0.75
1:A:1138:MET:SD	1:A:1232:MET:HB2	2.27	0.75
1:A:1194:MET:HA	1:A:1194:MET:CE	2.15	0.75
1:A:856:VAL:C	1:A:1048:SER:HB3	2.11	0.75
1:A:1199:PHE:O	1:A:1203:THR:CG2	2.34	0.75
1:A:396:ASP:CA	1:A:400:GLY:HA2	2.17	0.74
1:A:726:ARG:HB3	1:A:1112:VAL:CG1	2.16	0.74
1:A:441:HIS:NE2	1:A:496:ASP:OD1	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:LYS:HB3	1:A:251:PRO:HD2	1.68	0.74
1:A:407:GLN:HB3	1:A:604:THR:HG21	1.67	0.74
1:A:515:TYR:CE1	1:A:526:THR:CG2	2.70	0.74
1:A:684:LEU:HD11	1:A:728:LEU:HD21	1.68	0.74
1:A:688:GLU:C	1:A:691:PRO:HD2	1.97	0.74
1:A:185:ASN:ND2	4:M:1:NAG:O5	2.20	0.74
1:A:730:GLU:HG3	1:A:1108:ALA:HB1	0.87	0.74
1:A:873:VAL:CB	1:A:1045:LEU:HD13	2.17	0.74
1:A:1045:LEU:CA	1:A:1051:PHE:CZ	2.70	0.74
1:A:1084:PHE:CD1	1:A:1085:TYR:HD1	2.06	0.74
1:A:1045:LEU:CA	1:A:1051:PHE:HZ	2.00	0.74
1:A:881:GLN:CB	1:A:1041:TYR:HB2	2.17	0.74
1:A:726:ARG:HB3	1:A:1112:VAL:HG11	1.68	0.74
1:A:1055:LEU:HD23	1:A:1085:TYR:CE2	2.23	0.74
5:J:1:NAG:C1	5:J:1:NAG:H82	2.18	0.74
1:A:503:PHE:CE2	2:E:83:THR:HG22	2.22	0.74
2:E:70:LEU:HD13	2:E:179:GLY:HA2	1.70	0.74
1:A:656:LEU:HD11	1:A:685:ILE:CG2	2.18	0.73
1:A:720:LEU:HB3	1:A:1170:HIS:HD2	1.52	0.73
1:A:1127:MET:O	1:A:1130:THR:OG1	2.06	0.73
1:A:621:VAL:O	1:A:625:VAL:HG23	1.87	0.73
1:A:368:LEU:O	1:A:665:LEU:CB	2.36	0.73
1:A:676:SER:CB	1:A:1225:TYR:OH	2.30	0.73
1:A:1065:VAL:O	1:A:1068:THR:CG2	2.36	0.73
1:A:228:ASP:CA	1:A:246:VAL:CG1	2.67	0.73
1:A:401:PRO:CB	1:A:569:ASN:OD1	2.36	0.73
1:A:1062:ALA:O	1:A:1066:THR:OG1	2.06	0.73
1:A:1203:THR:HG23	1:A:1204:LEU:N	2.03	0.73
1:A:504:PHE:CZ	2:E:141:VAL:HG21	2.23	0.73
1:A:984:PRO:O	1:A:989:ARG:N	2.21	0.73
1:A:1210:ILE:CD1	1:A:1214:ALA:HB2	2.19	0.73
1:A:1068:THR:HG23	1:A:1069:MET:N	2.03	0.73
1:A:1122:TRP:O	1:A:1126:ILE:HG13	1.89	0.72
1:A:915:ASN:HA	1:A:920:VAL:CA	2.17	0.72
2:G:70:LEU:HD13	2:G:179:GLY:HA2	1.70	0.72
1:A:108:PHE:HE1	1:A:194:PHE:HE1	1.37	0.72
1:A:259:PRO:O	1:A:260:TRP:CB	2.37	0.72
1:A:684:LEU:HD23	1:A:728:LEU:CD1	1.96	0.72
2:C:70:LEU:HD13	2:C:179:GLY:HA2	1.70	0.72
1:A:158:ASN:CG	7:A:1303:NAG:C1	2.60	0.72
1:A:1138:MET:O	1:A:1142:MET:HG2	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:676:SER:HB3	1:A:1225:TYR:CZ	2.23	0.72
1:A:878:SER:C	1:A:1043:THR:HG21	2.13	0.72
5:J:1:NAG:C6	5:J:2:NAG:C8	2.68	0.72
1:A:544:TRP:CZ2	1:A:1041:TYR:HE1	2.07	0.72
1:A:684:LEU:HD11	1:A:1166:GLU:HG3	1.71	0.72
1:A:386:SER:O	1:A:390:LEU:HD12	1.90	0.71
1:A:751:LEU:C	1:A:751:LEU:HD23	2.15	0.71
1:A:1062:ALA:HB2	1:A:1078:VAL:HG11	1.70	0.71
1:A:632:PHE:CZ	1:A:650:VAL:CG2	2.72	0.71
1:A:1131:ILE:O	1:A:1135:LEU:HG	1.90	0.71
1:A:1211:VAL:O	1:A:1215:PHE:CB	2.38	0.71
1:A:1124:ALA:O	1:A:1128:CYS:HB2	1.91	0.71
1:A:693:LEU:HD12	1:A:763:PHE:CE2	2.01	0.71
1:A:631:MET:SD	1:A:1208:GLY:HA3	2.30	0.71
1:A:929:LEU:CB	1:A:1038:PHE:HE2	1.98	0.71
1:A:1161:CYS:O	1:A:1165:VAL:HG23	1.91	0.71
1:A:1228:MET:HG3	1:A:1229:TYR:N	2.04	0.71
1:A:692:PHE:HE1	1:A:713:GLU:HA	1.53	0.71
1:A:703:PHE:C	1:A:708:ALA:HB2	2.15	0.71
1:A:1062:ALA:HB1	1:A:1078:VAL:CG2	2.20	0.71
1:A:1133:MET:HG3	1:A:1239:HIS:CD2	2.23	0.71
1:A:503:PHE:CE1	2:E:83:THR:C	2.51	0.71
1:A:689:VAL:HG21	1:A:759:THR:HG21	1.72	0.71
1:A:754:MET:N	1:A:755:PRO:HD3	2.05	0.71
1:A:403:PHE:HE2	1:A:566:PRO:HB3	0.94	0.70
1:A:1098:THR:CG2	1:A:1154:LEU:HD21	2.13	0.70
1:A:1051:PHE:HB3	1:A:1084:PHE:CD2	2.25	0.70
1:A:404:ARG:HD2	1:A:567:VAL:HG23	1.72	0.70
1:A:591:VAL:HB	1:A:603:PHE:HE1	1.55	0.70
1:A:503:PHE:HZ	2:E:86:TRP:CD2	2.10	0.70
1:A:684:LEU:CD1	1:A:728:LEU:CD2	2.70	0.70
6:L:1:NAG:H62	6:L:2:NAG:N2	2.06	0.70
1:A:506:TYR:HB3	1:A:528:LEU:HD13	1.74	0.70
1:A:824:SER:CB	1:A:1188:GLU:OE1	2.40	0.70
1:A:228:ASP:HA	1:A:246:VAL:HG13	1.74	0.70
1:A:406:GLU:OE2	1:A:567:VAL:CG1	2.40	0.70
1:A:591:VAL:HB	1:A:603:PHE:CE1	2.27	0.69
1:A:684:LEU:HD21	1:A:728:LEU:HD11	1.69	0.69
1:A:722:GLN:HE21	1:A:1116:LEU:HD11	1.57	0.69
2:E:76:ALA:CB	2:E:81:SER:HB3	2.22	0.69
1:A:506:TYR:CZ	2:E:80:PRO:HG3	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:39:HIS:HD2	2:E:42:VAL:HG21	1.58	0.69
1:A:730:GLU:HG2	1:A:1112:VAL:HG21	1.73	0.69
1:A:704:ILE:HA	1:A:708:ALA:HB3	1.75	0.69
1:A:1106:LEU:CD2	1:A:1131:ILE:HD13	2.22	0.69
1:A:751:LEU:O	1:A:755:PRO:CD	2.41	0.69
1:A:1130:THR:CG2	1:A:1168:CYS:SG	2.79	0.69
2:C:39:HIS:HD2	2:C:42:VAL:HG21	1.58	0.69
1:A:607:ARG:HG2	1:A:611:ASP:OD1	1.93	0.69
1:A:692:PHE:CZ	1:A:713:GLU:CA	2.76	0.69
1:A:755:PRO:CD	1:A:756:ALA:N	2.51	0.69
1:A:1127:MET:HE1	1:A:1168:CYS:CB	2.19	0.69
1:A:1203:THR:CG2	1:A:1204:LEU:N	2.55	0.69
1:A:1046:GLN:HB3	1:A:1050:ASP:CG	2.18	0.69
1:A:752:SER:O	1:A:755:PRO:CG	2.41	0.68
1:A:924:PHE:CA	1:A:925:ASN:CB	2.71	0.68
4:I:2:NAG:O7	4:I:2:NAG:O3	2.11	0.68
6:L:2:NAG:H4	6:L:3:BMA:O2	1.93	0.68
1:A:662:LEU:HG	1:A:663:ILE:N	2.07	0.68
1:A:1047:THR:HG22	1:A:1048:SER:N	2.09	0.68
1:A:1160:SER:HB2	1:A:1232:MET:SD	2.34	0.68
1:A:108:PHE:CE1	1:A:194:PHE:HE1	2.12	0.68
1:A:1009:PRO:O	1:A:1010:LYS:O	2.11	0.68
1:A:1133:MET:CG	1:A:1239:HIS:CG	2.77	0.68
1:A:630:ILE:HG22	1:A:634:TYR:HE2	1.59	0.68
1:A:704:ILE:HA	1:A:708:ALA:CB	2.24	0.68
5:J:1:NAG:C6	5:J:2:NAG:H82	2.24	0.68
1:A:648:LEU:CD1	1:A:763:PHE:CD1	2.74	0.68
1:A:1110:PHE:O	1:A:1114:MET:CG	2.39	0.68
1:A:1133:MET:HG2	1:A:1239:HIS:HE2	1.51	0.68
1:A:544:TRP:CZ2	1:A:1041:TYR:CE1	2.82	0.67
1:A:1110:PHE:CE2	1:A:1124:ALA:HB1	2.29	0.67
6:L:1:NAG:C6	6:L:2:NAG:C1	2.73	0.67
1:A:762:LEU:O	1:A:766:LEU:HG	1.95	0.67
1:A:653:LYS:HB2	1:A:682:LEU:HD23	1.75	0.67
2:G:39:HIS:HD2	2:G:42:VAL:HG21	1.57	0.67
3:H:509:PRO:HB2	3:H:510:LYS:HG3	1.77	0.67
1:A:656:LEU:CG	1:A:685:ILE:HG13	2.18	0.67
1:A:1133:MET:HG2	1:A:1239:HIS:CG	2.24	0.67
1:A:1046:GLN:O	1:A:1047:THR:OG1	2.06	0.67
1:A:1062:ALA:HB2	1:A:1078:VAL:CG1	2.24	0.67
1:A:635:ILE:HG13	1:A:1204:LEU:HD13	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1059:ARG:HG3	1:A:1059:ARG:NH1	2.09	0.67
1:A:401:PRO:HG3	1:A:571:TYR:CE1	2.29	0.67
1:A:656:LEU:HD13	1:A:682:LEU:HD12	1.75	0.67
1:A:401:PRO:HB2	1:A:569:ASN:OD1	1.94	0.67
1:A:950:VAL:O	1:A:951:LYS:CB	2.43	0.67
1:A:1080:PRO:HG2	1:A:1085:TYR:CE2	2.30	0.67
1:A:1085:TYR:O	1:A:1086:VAL:C	2.37	0.67
1:A:627:SER:OG	1:A:1212:VAL:CG2	2.43	0.67
1:A:1159:MET:HE1	1:A:1163:ILE:HD11	1.77	0.67
1:A:399:PHE:HE2	1:A:1022:ALA:HA	1.60	0.66
1:A:407:GLN:HB3	1:A:604:THR:CG2	2.24	0.66
1:A:688:GLU:CB	1:A:724:LEU:HD23	2.25	0.66
1:A:1022:ALA:O	1:A:1035:ALA:N	2.27	0.66
3:D:509:PRO:HB2	3:D:510:LYS:HG3	1.77	0.66
1:A:691:PRO:HD2	1:A:692:PHE:H	1.60	0.66
1:A:630:ILE:O	1:A:634:TYR:HD2	1.79	0.66
1:A:1135:LEU:HB3	1:A:1139:PHE:HE2	1.59	0.66
1:A:690:ILE:O	1:A:694:VAL:HG23	1.96	0.66
1:A:1138:MET:CE	1:A:1138:MET:HA	2.22	0.66
3:F:595:GLN:HE21	3:F:595:GLN:CA	2.05	0.66
3:H:595:GLN:HE21	3:H:595:GLN:CA	2.05	0.66
1:A:506:TYR:OH	2:E:80:PRO:CB	2.44	0.66
3:D:595:GLN:HE21	3:D:595:GLN:CA	2.05	0.66
1:A:250:LYS:CB	1:A:251:PRO:CD	2.60	0.66
1:A:611:ASP:O	1:A:615:ARG:HB2	1.96	0.66
1:A:685:ILE:HD13	1:A:685:ILE:N	2.09	0.65
1:A:1229:TYR:O	1:A:1233:VAL:CG2	2.43	0.65
3:F:509:PRO:HB2	3:F:510:LYS:HG3	1.77	0.65
1:A:472:LEU:HD22	1:A:538:GLY:HA3	1.78	0.65
1:A:692:PHE:HZ	1:A:713:GLU:CA	2.08	0.65
1:A:723:GLN:NE2	1:A:724:LEU:HB2	2.12	0.65
1:A:1114:MET:CE	1:A:1124:ALA:HB2	2.27	0.65
1:A:1167:PHE:CE2	1:A:1237:ALA:CA	2.79	0.65
1:A:724:LEU:HD11	1:A:1166:GLU:HG2	0.84	0.65
1:A:1082:SER:O	1:A:1084:PHE:HD1	1.79	0.65
1:A:1213:LEU:C	1:A:1227:ARG:HH21	2.03	0.65
5:J:1:NAG:O6	5:J:2:NAG:C8	2.45	0.65
1:A:656:LEU:HD12	1:A:682:LEU:HD12	1.77	0.65
1:A:879:ILE:O	1:A:1043:THR:HG21	1.92	0.65
1:A:591:VAL:CB	1:A:603:PHE:CE1	2.80	0.65
1:A:757:VAL:O	1:A:760:PHE:HB2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:640:GLY:O	1:A:642:MET:N	2.30	0.65
1:A:423:TYR:CE1	1:A:424:PRO:HB3	2.32	0.64
1:A:1207:PHE:O	1:A:1210:ILE:HG22	1.97	0.64
1:A:1210:ILE:HG23	1:A:1211:VAL:N	2.11	0.64
1:A:1084:PHE:HZ	1:A:1085:TYR:HE1	1.38	0.64
1:A:1133:MET:HE3	1:A:1239:HIS:HB2	1.79	0.64
1:A:363:ALA:O	1:A:367:GLY:N	2.27	0.64
1:A:474:PRO:O	1:A:476:ASN:N	2.30	0.64
1:A:627:SER:OG	1:A:1212:VAL:HG22	1.96	0.64
1:A:674:VAL:O	1:A:678:ILE:CD1	2.46	0.64
1:A:692:PHE:CZ	1:A:713:GLU:CB	2.76	0.64
1:A:1046:GLN:CG	1:A:1050:ASP:CG	2.70	0.64
1:A:1156:ASN:HD22	1:A:1228:MET:HE3	1.61	0.64
1:A:384:PRO:O	1:A:385:SER:OG	2.14	0.64
1:A:407:GLN:O	1:A:604:THR:OG1	2.16	0.64
1:A:686:VAL:O	1:A:690:ILE:N	2.30	0.64
1:A:1137:ASN:HB3	1:A:1235:LEU:HD13	1.80	0.64
1:A:1145:TRP:O	1:A:1147:ILE:N	2.31	0.64
1:A:653:LYS:HA	1:A:682:LEU:HG	1.80	0.64
2:E:76:ALA:HB2	2:E:81:SER:HB3	1.80	0.64
1:A:723:GLN:HG2	1:A:1173:ARG:HG3	1.79	0.64
1:A:401:PRO:CG	1:A:571:TYR:CE1	2.79	0.64
1:A:618:ASP:O	1:A:621:VAL:HG23	1.96	0.64
1:A:395:PHE:CD2	1:A:1081:TYR:HD2	2.15	0.63
1:A:1080:PRO:HG2	1:A:1085:TYR:HE2	1.62	0.63
1:A:664:VAL:CG1	1:A:669:ALA:HB3	2.28	0.63
1:A:1142:MET:HE1	1:A:1153:SER:OG	1.98	0.63
1:A:674:VAL:O	1:A:678:ILE:HG13	1.97	0.63
1:A:1138:MET:HE3	1:A:1138:MET:CA	2.21	0.63
1:A:403:PHE:HE2	1:A:566:PRO:CG	2.11	0.63
1:A:396:ASP:C	1:A:400:GLY:H	2.06	0.63
1:A:401:PRO:CD	1:A:571:TYR:HE1	1.96	0.63
1:A:1062:ALA:CB	1:A:1078:VAL:HG11	2.29	0.63
1:A:630:ILE:CG2	1:A:634:TYR:HE2	2.12	0.63
1:A:1055:LEU:HD22	1:A:1055:LEU:C	2.24	0.63
1:A:1142:MET:CE	1:A:1148:SER:C	2.71	0.63
1:A:1229:TYR:CD1	1:A:1233:VAL:CG2	2.82	0.63
1:A:1062:ALA:CB	1:A:1078:VAL:CG1	2.77	0.62
1:A:252:GLN:O	1:A:254:PRO:HD3	1.99	0.62
1:A:1045:LEU:N	1:A:1051:PHE:CZ	2.67	0.62
1:A:167:SER:C	1:A:168:SER:HG	2.01	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:ASP:HB2	1:A:246:VAL:CG1	2.29	0.62
1:A:1177:VAL:O	1:A:1186:ARG:NH1	2.32	0.62
1:A:250:LYS:CB	1:A:251:PRO:HD3	2.24	0.62
1:A:630:ILE:HA	1:A:633:LEU:HD12	1.81	0.62
1:A:684:LEU:HD22	1:A:728:LEU:HD22	1.75	0.62
1:A:754:MET:N	1:A:755:PRO:CD	2.62	0.62
1:A:1046:GLN:HG2	1:A:1050:ASP:CG	2.25	0.62
1:A:607:ARG:O	1:A:611:ASP:HB2	1.99	0.62
1:A:1085:TYR:C	1:A:1087:PHE:N	2.57	0.62
1:A:885:ALA:O	1:A:1079:PHE:HB2	1.99	0.62
1:A:680:LEU:O	1:A:683:THR:HG22	2.00	0.62
1:A:381:TRP:CD1	1:A:382:SER:N	2.64	0.62
1:A:591:VAL:CB	1:A:603:PHE:HE1	2.12	0.62
1:A:631:MET:SD	1:A:1207:PHE:C	2.83	0.62
1:A:678:ILE:HG12	1:A:748:LEU:CD2	2.27	0.62
1:A:1210:ILE:HG13	1:A:1214:ALA:CB	2.30	0.62
1:A:686:VAL:HG11	1:A:690:ILE:HD11	1.73	0.61
1:A:724:LEU:CD1	1:A:1166:GLU:HA	2.29	0.61
1:A:252:GLN:C	1:A:254:PRO:HD3	2.25	0.61
1:A:684:LEU:HD21	1:A:728:LEU:HD21	1.72	0.61
1:A:723:GLN:CD	1:A:1169:SER:HB2	2.17	0.61
1:A:1171:ILE:HA	1:A:1194:MET:HG2	1.81	0.61
1:A:1199:PHE:O	1:A:1203:THR:HG22	2.00	0.61
1:A:631:MET:CE	1:A:1208:GLY:N	2.63	0.61
1:A:431:PHE:CE2	1:A:510:HIS:HD2	2.18	0.61
1:A:751:LEU:C	1:A:755:PRO:HG3	2.20	0.61
1:A:875:TYR:O	1:A:876:PHE:O	2.18	0.61
1:A:659:ALA:HA	1:A:662:LEU:HD21	1.71	0.61
1:A:622:PHE:O	1:A:626:ILE:HG13	2.01	0.61
1:A:1055:LEU:C	1:A:1055:LEU:HD13	2.25	0.61
1:A:1092:LEU:HD13	1:A:1093:THR:N	2.15	0.61
1:A:752:SER:CA	1:A:755:PRO:CG	2.78	0.61
1:A:752:SER:HA	1:A:755:PRO:HG3	1.82	0.61
5:J:1:NAG:H62	5:J:2:NAG:H82	1.80	0.61
1:A:724:LEU:HD21	1:A:1166:GLU:CD	2.26	0.60
1:A:881:GLN:CB	1:A:1041:TYR:CB	2.79	0.60
1:A:1186:ARG:HG3	1:A:1187:ALA:N	2.15	0.60
1:A:1194:MET:O	1:A:1198:VAL:HG23	2.00	0.60
1:A:337:ARG:CA	1:A:718:GLU:HG3	2.23	0.60
1:A:724:LEU:HD13	1:A:1166:GLU:HA	1.82	0.60
1:A:1156:ASN:HB3	1:A:1228:MET:HE3	1.60	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:723:GLN:O	1:A:727:VAL:HG23	2.01	0.60
1:A:663:ILE:HD13	1:A:750:ALA:HB1	1.84	0.60
1:A:1140:GLY:O	1:A:1144:LEU:CA	2.49	0.60
1:A:732:ALA:HB3	1:A:749:GLY:HA2	1.81	0.60
5:J:1:NAG:O6	5:J:2:NAG:H82	2.02	0.60
1:A:607:ARG:CG	1:A:611:ASP:OD1	2.50	0.60
1:A:656:LEU:HA	1:A:751:LEU:HG	1.84	0.60
1:A:163:VAL:HA	1:A:242:ASP:O	2.01	0.60
1:A:386:SER:O	1:A:390:LEU:HB2	2.01	0.60
1:A:764:ALA:O	1:A:768:VAL:HG23	2.02	0.60
1:A:1046:GLN:HB3	1:A:1050:ASP:CB	2.32	0.60
1:A:1115:VAL:O	1:A:1115:VAL:HG12	2.02	0.60
1:A:635:ILE:CG1	1:A:1204:LEU:HD13	2.31	0.59
1:A:648:LEU:HD12	1:A:763:PHE:HD1	1.65	0.59
1:A:691:PRO:O	1:A:695:LEU:HG	2.02	0.59
1:A:373:VAL:O	1:A:375:THR:N	2.35	0.59
1:A:924:PHE:CB	1:A:925:ASN:CA	2.80	0.59
1:A:1091:TYR:HA	1:A:1094:ILE:CG1	2.31	0.59
1:A:1021:SER:O	1:A:1022:ALA:HB3	2.01	0.59
1:A:1191:LEU:O	1:A:1195:GLY:N	2.36	0.59
1:A:1055:LEU:HD13	1:A:1056:LYS:N	2.17	0.59
1:A:406:GLU:OE2	1:A:567:VAL:HG13	2.01	0.59
1:A:1209:GLY:O	1:A:1212:VAL:N	2.35	0.59
1:A:122:ASN:ND2	1:A:217[B]:MET:CE	2.66	0.59
1:A:395:PHE:CD2	1:A:1081:TYR:CD2	2.91	0.59
1:A:1106:LEU:HD23	1:A:1131:ILE:HD13	1.84	0.59
1:A:1112:VAL:HA	1:A:1115:VAL:HG23	1.85	0.59
1:A:1149:LEU:HA	1:A:1153:SER:CB	2.33	0.59
1:A:1229:TYR:HD1	1:A:1233:VAL:CG2	2.16	0.59
1:A:1239:HIS:CE1	1:A:1243:PHE:CB	2.86	0.59
1:A:1070:GLY:O	1:A:1071:ILE:CB	2.50	0.58
1:A:382:SER:HB3	1:A:1086:VAL:O	2.03	0.58
1:A:985:GLU:HA	1:A:989:ARG:H	1.68	0.58
1:A:1082:SER:CB	1:A:1084:PHE:CE1	2.86	0.58
2:E:39:HIS:CD2	2:E:42:VAL:HG21	2.38	0.58
1:A:476:ASN:OD1	1:A:478:ASN:HB2	2.02	0.58
1:A:504:PHE:CE2	2:E:79:VAL:HG12	2.29	0.58
1:A:942:TRP:O	1:A:943:ILE:CB	2.50	0.58
1:A:649:LEU:O	1:A:652:SER:N	2.35	0.58
1:A:656:LEU:CD1	1:A:682:LEU:CD1	2.80	0.58
1:A:733:PRO:C	1:A:735:MET:H	2.10	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1080:PRO:HB2	1:A:1085:TYR:CZ	2.37	0.58
1:A:515:TYR:CE1	1:A:526:THR:HG23	2.38	0.58
1:A:686:VAL:O	1:A:690:ILE:CG1	2.44	0.58
1:A:752:SER:HA	1:A:755:PRO:HG2	1.84	0.58
1:A:598:ASN:HD21	4:K:1:NAG:C2	2.04	0.58
1:A:637:LEU:HA	1:A:641:HIS:HA	1.84	0.58
1:A:879:ILE:HA	1:A:1043:THR:HG23	1.85	0.58
1:A:1133:MET:CE	1:A:1239:HIS:CE1	2.74	0.58
1:A:347:VAL:C	1:A:349:ASN:H	2.12	0.58
1:A:915:ASN:CB	1:A:919:LEU:C	2.77	0.58
1:A:1084:PHE:HE1	1:A:1085:TYR:CE1	2.08	0.58
1:A:720:LEU:O	1:A:723:GLN:CG	2.51	0.58
1:A:724:LEU:HD21	1:A:1170:HIS:HE1	1.66	0.58
1:A:1210:ILE:HD12	1:A:1214:ALA:HB2	1.84	0.58
1:A:122:ASN:CG	1:A:217[B]:MET:HE1	2.29	0.57
1:A:402:PHE:O	1:A:403:PHE:CD1	2.57	0.57
1:A:664:VAL:HG13	1:A:669:ALA:HB3	1.85	0.57
1:A:503:PHE:CZ	2:E:86:TRP:CD2	2.81	0.57
1:A:557:ASN:ND2	5:J:1:NAG:O5	2.38	0.57
1:A:478:ASN:CG	6:L:1:NAG:C1	2.78	0.57
1:A:252:GLN:H	1:A:253:PRO:HD3	1.69	0.57
1:A:421:GLN:CG	2:E:143:GLY:HA2	2.32	0.57
1:A:656:LEU:HB3	1:A:751:LEU:CD2	2.31	0.57
1:A:1202:ILE:HG21	1:A:1237:ALA:CB	2.34	0.57
1:A:1203:THR:CG2	1:A:1204:LEU:H	2.18	0.57
1:A:1068:THR:CG2	1:A:1069:MET:H	2.17	0.57
1:A:635:ILE:HG22	1:A:649:LEU:HD11	1.86	0.57
1:A:686:VAL:HG12	1:A:690:ILE:CG1	2.34	0.57
1:A:824:SER:CB	1:A:1188:GLU:CD	2.77	0.57
6:L:2:NAG:O3	6:L:3:BMA:H2	2.03	0.57
1:A:1110:PHE:HD2	1:A:1128:CYS:HG	1.52	0.57
1:A:396:ASP:HA	1:A:400:GLY:N	2.20	0.57
1:A:656:LEU:HD12	1:A:682:LEU:CD1	2.34	0.57
1:A:824:SER:HA	1:A:1188:GLU:CD	2.30	0.57
1:A:1106:LEU:HD22	1:A:1131:ILE:HD13	1.87	0.57
1:A:241:GLN:NE2	1:A:518:ARG:NH2	2.38	0.57
1:A:257:PRO:O	1:A:258:ALA:HB2	2.05	0.57
1:A:655:SER:HB2	1:A:758:HIS:CD2	2.40	0.57
1:A:857:ASP:HA	1:A:1048:SER:HB3	1.87	0.57
1:A:1062:ALA:CB	1:A:1078:VAL:HG21	2.35	0.57
1:A:479:CYS:O	1:A:537:PHE:HB3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:757:VAL:HA	1:A:760:PHE:HD2	1.70	0.56
2:C:39:HIS:CD2	2:C:42:VAL:HG21	2.38	0.56
1:A:1055:LEU:CD2	1:A:1085:TYR:OH	2.47	0.56
1:A:676:SER:CB	1:A:1225:TYR:CZ	2.87	0.56
1:A:688:GLU:O	1:A:691:PRO:CG	2.51	0.56
1:A:1059:ARG:HH11	1:A:1059:ARG:CG	2.14	0.56
1:A:403:PHE:CD2	1:A:566:PRO:CB	2.77	0.56
1:A:752:SER:O	1:A:755:PRO:HG2	2.03	0.56
1:A:916:ASN:N	1:A:919:LEU:O	2.23	0.56
2:G:39:HIS:CD2	2:G:42:VAL:HG21	2.38	0.56
1:A:648:LEU:CD1	1:A:763:PHE:HA	2.33	0.56
1:A:393:GLU:O	1:A:396:ASP:HB2	2.06	0.56
1:A:752:SER:C	1:A:755:PRO:CG	2.78	0.56
1:A:845:VAL:CB	1:A:1136:VAL:HG12	2.36	0.56
1:A:1062:ALA:CB	1:A:1078:VAL:CG2	2.82	0.56
5:J:1:NAG:C6	5:J:2:NAG:H83	2.36	0.56
1:A:474:PRO:C	1:A:476:ASN:N	2.62	0.56
1:A:491:SER:OG	1:A:494:VAL:HG23	2.06	0.56
1:A:656:LEU:HD11	1:A:685:ILE:HG21	1.87	0.56
1:A:724:LEU:HD23	1:A:1170:HIS:NE2	2.17	0.56
1:A:441:HIS:CE1	1:A:496:ASP:OD1	2.59	0.56
1:A:650:VAL:O	1:A:654:VAL:CG2	2.52	0.56
1:A:923:ILE:C	1:A:1042:HIS:CB	2.50	0.56
1:A:1048:SER:HA	1:A:1088:TYR:CE2	2.41	0.56
1:A:1071:ILE:C	1:A:1072:ASN:O	2.43	0.56
1:A:1117:LEU:CD2	1:A:1123:SER:HB3	2.36	0.56
1:A:1229:TYR:HE1	1:A:1233:VAL:HG21	1.70	0.56
5:J:1:NAG:H62	5:J:2:NAG:N2	2.21	0.56
1:A:409:ILE:CG2	1:A:872:MET:CB	2.83	0.55
2:G:69:ASN:HD21	2:G:105:ALA:HB2	1.72	0.55
1:A:92:GLN:HE22	1:A:526:THR:HB	1.71	0.55
1:A:1133:MET:HE3	1:A:1239:HIS:CG	2.35	0.55
1:A:371:VAL:C	1:A:373:VAL:N	2.64	0.55
1:A:627:SER:O	1:A:631:MET:HG2	2.07	0.55
1:A:924:PHE:CB	1:A:925:ASN:HA	2.36	0.55
1:A:1200:SER:O	1:A:1203:THR:HG22	2.07	0.55
1:A:1184:VAL:O	1:A:1184:VAL:CG1	2.53	0.55
2:G:112:GLU:OE2	2:G:172:ARG:HG3	2.07	0.55
1:A:504:PHE:HZ	2:E:141:VAL:CG2	2.16	0.55
1:A:674:VAL:O	1:A:678:ILE:HD12	2.06	0.55
1:A:856:VAL:C	1:A:1048:SER:OG	2.49	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1048:SER:O	1:A:1052:ILE:HD12	2.06	0.55
1:A:252:GLN:N	1:A:253:PRO:HD3	2.22	0.55
1:A:371:VAL:C	1:A:373:VAL:H	2.08	0.55
1:A:753:VAL:O	1:A:757:VAL:HG13	2.07	0.55
1:A:754:MET:O	1:A:757:VAL:HG22	2.07	0.55
1:A:191:GLU:OE2	1:A:195:ASN:ND2	2.39	0.55
1:A:402:PHE:C	1:A:403:PHE:HD1	2.15	0.55
1:A:407:GLN:O	1:A:604:THR:N	2.40	0.55
1:A:1167:PHE:HE2	1:A:1237:ALA:CA	2.19	0.55
1:A:1228:MET:HG3	1:A:1229:TYR:H	1.71	0.55
1:A:398:HIS:HB3	1:A:399:PHE:CD1	2.42	0.55
2:E:112:GLU:OE2	2:E:172:ARG:HG3	2.07	0.55
1:A:185:ASN:ND2	1:A:188:ASN:ND2	2.55	0.54
1:A:431:PHE:CZ	1:A:510:HIS:HD2	2.25	0.54
1:A:444:LEU:HD23	1:A:492:HIS:CG	2.42	0.54
1:A:732:ALA:HB1	1:A:749:GLY:N	2.22	0.54
1:A:164:GLU:OE1	1:A:241:GLN:O	2.26	0.54
1:A:762:LEU:O	1:A:766:LEU:CG	2.55	0.54
1:A:1167:PHE:CE2	1:A:1237:ALA:HB2	2.43	0.54
2:C:69:ASN:HD21	2:C:105:ALA:HB2	1.71	0.54
1:A:1062:ALA:C	1:A:1078:VAL:HG21	2.32	0.54
1:A:1100:PHE:O	1:A:1104:VAL:HG23	2.07	0.54
2:E:163:ASP:OD1	3:F:543:TYR:OH	2.24	0.54
1:A:122:ASN:ND2	1:A:217[B]:MET:HE1	2.23	0.54
1:A:723:GLN:HE22	1:A:724:LEU:HB2	1.70	0.54
1:A:1135:LEU:CD2	1:A:1161:CYS:SG	2.92	0.54
1:A:1224:PHE:HA	1:A:1227:ARG:HB2	1.88	0.54
1:A:166:PRO:O	1:A:167:SER:OG	2.17	0.54
1:A:1091:TYR:HA	1:A:1094:ILE:HG13	1.90	0.54
1:A:1109:ILE:O	1:A:1113:THR:HG23	2.07	0.54
1:A:337:ARG:HA	1:A:718:GLU:CD	2.32	0.54
1:A:664:VAL:CG2	1:A:747:PHE:CB	2.85	0.54
1:A:684:LEU:CD2	1:A:728:LEU:HD11	2.27	0.54
1:A:1127:MET:HE1	1:A:1130:THR:HG21	1.87	0.54
2:C:112:GLU:OE2	2:C:172:ARG:HG3	2.07	0.54
1:A:653:LYS:C	1:A:682:LEU:HD21	2.30	0.54
1:A:653:LYS:HG3	1:A:654:VAL:N	2.23	0.54
1:A:704:ILE:CA	1:A:708:ALA:HB3	2.38	0.54
1:A:631:MET:CG	1:A:1208:GLY:HA2	2.37	0.54
1:A:398:HIS:CB	1:A:399:PHE:CE1	2.86	0.54
1:A:1133:MET:CE	1:A:1239:HIS:CB	2.86	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:649:LEU:HD22	1:A:686:VAL:HG13	1.90	0.53
1:A:674:VAL:O	1:A:678:ILE:CG1	2.56	0.53
1:A:523:LEU:CD1	1:A:1016:HIS:N	2.70	0.53
1:A:882:TYR:CB	1:A:1082:SER:CB	2.64	0.53
1:A:758:HIS:ND1	1:A:762:LEU:HD12	2.23	0.53
2:E:69:ASN:HD21	2:E:105:ALA:HB2	1.72	0.53
1:A:503:PHE:HZ	2:E:86:TRP:CB	2.19	0.53
1:A:632:PHE:CZ	1:A:650:VAL:HG22	2.44	0.53
1:A:1137:ASN:HB3	1:A:1235:LEU:CD1	2.37	0.53
1:A:1167:PHE:CE2	1:A:1237:ALA:CB	2.91	0.53
1:A:406:GLU:OE2	1:A:567:VAL:HG11	2.08	0.53
1:A:396:ASP:CB	1:A:400:GLY:HA2	2.38	0.53
1:A:398:HIS:C	1:A:399:PHE:CG	2.86	0.53
1:A:402:PHE:C	1:A:403:PHE:CD1	2.87	0.53
2:C:39:HIS:CD2	2:C:42:VAL:CG2	2.92	0.53
1:A:544:TRP:HZ2	1:A:1041:TYR:CE1	2.26	0.53
1:A:861:ASP:CB	1:A:1219:GLN:CB	2.87	0.53
1:A:1167:PHE:HE2	1:A:1237:ALA:HB2	1.74	0.53
6:L:1:NAG:H61	6:L:2:NAG:C1	2.38	0.53
1:A:635:ILE:HG22	1:A:649:LEU:CD1	2.39	0.53
1:A:344:SER:O	1:A:348:ARG:N	2.41	0.53
1:A:381:TRP:CD1	1:A:381:TRP:C	2.85	0.53
1:A:684:LEU:CG	1:A:728:LEU:HD22	2.38	0.53
1:A:924:PHE:CB	1:A:925:ASN:CB	2.87	0.53
1:A:1234:LEU:O	1:A:1238:THR:HG23	2.09	0.53
1:A:93:PHE:CE1	1:A:175:LEU:HD13	2.44	0.52
1:A:688:GLU:HA	1:A:691:PRO:HG3	1.91	0.52
1:A:758:HIS:O	1:A:762:LEU:HB2	2.09	0.52
1:A:1092:LEU:C	1:A:1094:ILE:H	2.16	0.52
1:A:381:TRP:HD1	1:A:382:SER:H	1.55	0.52
1:A:402:PHE:O	1:A:403:PHE:CG	2.63	0.52
1:A:1021:SER:O	1:A:1022:ALA:HB2	2.08	0.52
1:A:1171:ILE:HG23	1:A:1191:LEU:HD22	1.90	0.52
1:A:1081:TYR:C	1:A:1081:TYR:CD1	2.86	0.52
1:A:1084:PHE:CD1	1:A:1085:TYR:N	2.78	0.52
1:A:1138:MET:SD	1:A:1138:MET:N	2.83	0.52
1:A:1210:ILE:O	1:A:1214:ALA:N	2.43	0.52
1:A:1210:ILE:CG2	1:A:1211:VAL:N	2.73	0.52
2:C:69:ASN:ND2	2:C:105:ALA:HB2	2.25	0.52
1:A:1068:THR:CG2	1:A:1069:MET:N	2.73	0.52
2:E:39:HIS:CD2	2:E:42:VAL:CG2	2.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:691:PRO:CD	1:A:692:PHE:H	2.21	0.52
3:F:595:GLN:HG3	3:F:596:ARG:NH1	2.25	0.52
1:A:506:TYR:HH	2:E:80:PRO:HA	1.71	0.52
1:A:685:ILE:O	1:A:689:VAL:CB	2.58	0.52
1:A:690:ILE:N	1:A:691:PRO:CD	2.73	0.52
1:A:1239:HIS:NE2	1:A:1243:PHE:CB	2.73	0.52
2:G:39:HIS:CD2	2:G:42:VAL:CG2	2.92	0.52
1:A:387:GLN:O	1:A:391:GLU:HB2	2.10	0.52
1:A:399:PHE:CE2	1:A:1022:ALA:HA	2.45	0.52
1:A:656:LEU:HB3	1:A:751:LEU:HD11	1.91	0.52
1:A:1047:THR:HG22	1:A:1048:SER:H	1.75	0.52
2:E:69:ASN:ND2	2:E:105:ALA:HB2	2.25	0.52
1:A:1239:HIS:O	1:A:1243:PHE:N	2.32	0.51
1:A:114:SER:O	1:A:117:GLN:HG3	2.11	0.51
1:A:915:ASN:CB	1:A:919:LEU:O	2.59	0.51
1:A:1234:LEU:O	1:A:1234:LEU:HD22	2.09	0.51
1:A:923:ILE:CA	1:A:1042:HIS:HB3	2.41	0.51
1:A:523:LEU:CD1	1:A:1015:GLY:C	2.83	0.51
1:A:627:SER:CB	1:A:1211:VAL:HB	2.40	0.51
1:A:751:LEU:O	1:A:751:LEU:HD23	2.11	0.51
1:A:758:HIS:C	1:A:760:PHE:H	2.18	0.51
1:A:1047:THR:CG2	1:A:1048:SER:N	2.73	0.51
1:A:1080:PRO:HB2	1:A:1085:TYR:OH	2.10	0.51
1:A:1193:HIS:O	1:A:1194:MET:HE3	2.10	0.51
3:F:515:LEU:HB3	3:F:548:MET:HB2	1.93	0.51
3:H:595:GLN:HG3	3:H:596:ARG:NH1	2.25	0.51
1:A:1133:MET:CE	1:A:1239:HIS:HB2	2.41	0.51
1:A:515:TYR:CE1	1:A:526:THR:HG22	2.45	0.51
1:A:1121:LEU:O	1:A:1125:VAL:HB	2.11	0.51
1:A:915:ASN:CB	1:A:920:VAL:N	2.73	0.51
1:A:1117:LEU:HD13	1:A:1173:ARG:HD3	1.93	0.51
1:A:1223:ILE:O	1:A:1227:ARG:HG2	2.11	0.51
3:D:515:LEU:HB3	3:D:548:MET:HB2	1.93	0.51
1:A:135:ASN:ND2	7:A:1322:NAG:O5	2.21	0.51
1:A:695:LEU:HD11	1:A:1194:MET:HE1	1.92	0.51
3:D:595:GLN:HG3	3:D:596:ARG:NH1	2.25	0.51
1:A:377:PRO:CB	1:A:378:VAL:HA	2.39	0.51
1:A:381:TRP:C	1:A:383:ALA:H	2.19	0.51
1:A:1044:VAL:HB	1:A:1051:PHE:CE1	2.45	0.51
1:A:1120:GLU:O	1:A:1124:ALA:HB3	2.10	0.51
2:G:69:ASN:ND2	2:G:105:ALA:HB2	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:723:GLN:NE2	1:A:724:LEU:N	2.59	0.51
1:A:1111:LEU:O	1:A:1115:VAL:HG23	2.11	0.51
1:A:1119:CYS:CB	1:A:1122:TRP:CB	2.89	0.51
3:H:515:LEU:HB3	3:H:548:MET:HB2	1.93	0.51
1:A:648:LEU:CB	1:A:763:PHE:CZ	2.93	0.50
1:A:683:THR:HG23	1:A:684:LEU:N	2.25	0.50
1:A:1209:GLY:CA	1:A:1230:LEU:HD13	2.30	0.50
1:A:1133:MET:HE3	1:A:1239:HIS:CB	2.42	0.50
1:A:524:ASN:HD22	4:I:1:NAG:C1	2.02	0.50
1:A:168:SER:C	1:A:170:ASP:H	2.20	0.50
1:A:382:SER:O	1:A:383:ALA:HB3	2.12	0.50
1:A:1090:GLN:C	1:A:1092:LEU:H	2.19	0.50
1:A:423:TYR:CG	1:A:424:PRO:HA	2.47	0.50
1:A:474:PRO:C	1:A:476:ASN:H	2.18	0.50
1:A:584:GLU:OE2	1:A:606:GLU:CB	2.56	0.50
1:A:641:HIS:C	1:A:642:MET:O	2.55	0.50
1:A:423:TYR:CZ	1:A:424:PRO:HB3	2.46	0.50
1:A:732:ALA:CB	1:A:749:GLY:HA2	2.31	0.50
1:A:885:ALA:O	1:A:1079:PHE:C	2.53	0.50
1:A:1115:VAL:C	1:A:1116:LEU:HG	2.36	0.50
1:A:1178:SER:CB	1:A:1186:ARG:CZ	2.89	0.50
1:A:122:ASN:CG	1:A:217[B]:MET:CE	2.85	0.50
1:A:382:SER:HA	1:A:1090:GLN:HG3	1.93	0.50
1:A:680:LEU:HB3	1:A:1229:TYR:HH	1.73	0.50
1:A:753:VAL:C	1:A:755:PRO:CD	2.85	0.50
1:A:523:LEU:HD11	1:A:1016:HIS:N	2.25	0.50
1:A:1229:TYR:HD1	1:A:1233:VAL:HG21	1.69	0.50
1:A:688:GLU:CB	1:A:724:LEU:CD2	2.89	0.49
1:A:719:THR:O	1:A:723:GLN:HG3	2.12	0.49
1:A:749:GLY:O	1:A:752:SER:CB	2.60	0.49
1:A:1115:VAL:O	1:A:1116:LEU:HG	2.12	0.49
1:A:656:LEU:CA	1:A:751:LEU:HG	2.42	0.49
1:A:676:SER:OG	1:A:1225:TYR:CE1	2.65	0.49
1:A:1063:SER:O	1:A:1067:GLU:HB2	2.10	0.49
1:A:659:ALA:O	1:A:663:ILE:HG13	2.12	0.49
1:A:1044:VAL:O	1:A:1045:LEU:C	2.56	0.49
1:A:108:PHE:HE1	1:A:194:PHE:CE1	2.26	0.49
1:A:686:VAL:CG1	1:A:690:ILE:CG1	2.90	0.49
1:A:729:GLY:O	1:A:733:PRO:N	2.45	0.49
1:A:1071:ILE:CG2	1:A:1072:ASN:N	2.34	0.49
1:A:1166:GLU:O	1:A:1169:SER:OG	2.29	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:PHE:CZ	1:A:510:HIS:CD2	3.00	0.49
1:A:506:TYR:OH	2:E:80:PRO:HB3	2.12	0.49
1:A:713:GLU:C	1:A:715:LEU:H	2.21	0.49
1:A:720:LEU:C	1:A:723:GLN:HG3	2.38	0.49
1:A:1167:PHE:CD2	1:A:1237:ALA:HA	2.47	0.49
1:A:663:ILE:HD11	1:A:754:MET:HG3	1.93	0.49
2:E:38:ILE:HG13	2:E:187:PRO:HD3	1.95	0.49
1:A:1152:VAL:HG11	1:A:1225:TYR:HD2	1.77	0.49
1:A:506:TYR:CZ	2:E:80:PRO:HB3	2.48	0.49
1:A:611:ASP:O	1:A:615:ARG:CB	2.60	0.49
1:A:631:MET:CE	1:A:1208:GLY:H	2.26	0.49
1:A:1091:TYR:HA	1:A:1094:ILE:HG12	1.94	0.49
1:A:1093:THR:O	1:A:1093:THR:HG22	2.13	0.49
1:A:1153:SER:HA	1:A:1156:ASN:HB2	1.94	0.49
3:F:510:LYS:NZ	4:O:1:NAG:HO6	2.08	0.49
5:J:1:NAG:O6	5:J:2:NAG:H83	2.12	0.49
1:A:885:ALA:O	1:A:1079:PHE:CA	2.61	0.49
1:A:1223:ILE:O	1:A:1227:ARG:CG	2.61	0.49
1:A:726:ARG:HB3	1:A:1112:VAL:HG13	1.94	0.49
1:A:1194:MET:HE3	1:A:1194:MET:CA	2.28	0.49
2:C:39:HIS:CB	2:C:42:VAL:HG22	2.40	0.49
1:A:627:SER:HB3	1:A:1211:VAL:HB	1.93	0.48
1:A:959:VAL:CA	1:A:984:PRO:N	2.74	0.48
2:C:51:LEU:HD12	2:C:51:LEU:HA	1.68	0.48
1:A:724:LEU:O	1:A:728:LEU:CG	2.53	0.48
1:A:1210:ILE:HG23	1:A:1211:VAL:H	1.76	0.48
1:A:404:ARG:HG3	1:A:567:VAL:O	2.13	0.48
1:A:618:ASP:O	1:A:621:VAL:CG2	2.60	0.48
1:A:893:LEU:O	1:A:894:GLU:C	2.55	0.48
1:A:1059:ARG:NH1	1:A:1059:ARG:CG	2.73	0.48
1:A:352:CYS:O	1:A:353:VAL:C	2.56	0.48
1:A:720:LEU:HD21	1:A:1170:HIS:O	2.13	0.48
1:A:985:GLU:CB	1:A:989:ARG:CB	2.91	0.48
1:A:1167:PHE:HE2	1:A:1237:ALA:CB	2.27	0.48
2:C:163:ASP:OD1	3:D:543:TYR:OH	2.24	0.48
1:A:35:TYR:CZ	1:A:38:LYS:HD2	2.48	0.48
1:A:228:ASP:CG	1:A:245:ILE:HG21	2.39	0.48
1:A:684:LEU:HG	1:A:1166:GLU:CG	2.38	0.48
1:A:544:TRP:O	1:A:879:ILE:CB	2.62	0.48
1:A:1063:SER:O	1:A:1067:GLU:CB	2.62	0.48
1:A:472:LEU:HB3	1:A:476:ASN:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:PRO:CB	1:A:569:ASN:CG	2.79	0.48
1:A:444:LEU:HD23	1:A:492:HIS:CE1	2.49	0.48
1:A:653:LYS:O	1:A:653:LYS:HE3	2.13	0.48
1:A:1063:SER:O	1:A:1067:GLU:HG3	2.14	0.48
2:G:163:ASP:OD1	3:H:543:TYR:OH	2.24	0.48
1:A:1045:LEU:HD23	1:A:1051:PHE:HZ	1.79	0.47
1:A:1085:TYR:C	1:A:1087:PHE:H	2.22	0.47
1:A:915:ASN:HA	1:A:921:GLN:N	2.29	0.47
2:G:38:ILE:HG13	2:G:187:PRO:HD3	1.95	0.47
1:A:688:GLU:HB2	1:A:724:LEU:CD2	2.44	0.47
1:A:704:ILE:CA	1:A:708:ALA:CB	2.92	0.47
1:A:911:GLY:C	1:A:913:GLY:H	2.22	0.47
1:A:687:ILE:C	1:A:691:PRO:HD3	2.35	0.47
1:A:878:SER:C	1:A:1043:THR:CG2	2.86	0.47
1:A:1130:THR:HA	1:A:1133:MET:HB3	1.95	0.47
1:A:1210:ILE:CD1	1:A:1214:ALA:CB	2.91	0.47
1:A:252:GLN:N	1:A:253:PRO:CD	2.78	0.47
1:A:637:LEU:O	1:A:638:ALA:C	2.57	0.47
1:A:653:LYS:C	1:A:653:LYS:CE	2.86	0.47
1:A:684:LEU:CD2	1:A:728:LEU:CG	2.57	0.47
1:A:704:ILE:N	1:A:708:ALA:HB2	2.29	0.47
1:A:1046:GLN:CB	1:A:1050:ASP:CG	2.80	0.47
1:A:1127:MET:CE	1:A:1130:THR:CG2	2.92	0.47
2:C:104:TRP:CZ2	2:C:134:ARG:HD2	2.50	0.47
2:E:104:TRP:CZ2	2:E:134:ARG:HD2	2.50	0.47
1:A:437:ILE:HD13	1:A:509:TYR:CD1	2.50	0.47
2:G:104:TRP:CZ2	2:G:134:ARG:HD2	2.50	0.47
1:A:1232:MET:HG3	1:A:1233:VAL:N	2.29	0.47
2:C:38:ILE:HG13	2:C:187:PRO:HD3	1.95	0.47
3:F:595:GLN:NE2	3:F:595:GLN:CA	2.72	0.47
1:A:421:GLN:HB3	1:A:426:GLY:HA2	1.96	0.47
3:D:548:MET:HE3	3:D:548:MET:HB3	1.74	0.47
1:A:656:LEU:CD1	1:A:685:ILE:CB	2.62	0.46
1:A:1048:SER:O	1:A:1052:ILE:CD1	2.63	0.46
1:A:616:GLU:O	1:A:618:ASP:N	2.48	0.46
1:A:688:GLU:HA	1:A:691:PRO:CG	2.45	0.46
1:A:1222:GLN:C	1:A:1224:PHE:N	2.72	0.46
2:E:37:VAL:HG21	2:E:51:LEU:HD11	1.97	0.46
1:A:648:LEU:CG	1:A:763:PHE:CD1	2.98	0.46
2:G:37:VAL:HG21	2:G:51:LEU:HD11	1.97	0.46
1:A:507:ALA:CB	1:A:529:LEU:CG	2.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:632:PHE:HE1	1:A:649:LEU:CB	2.28	0.46
1:A:635:ILE:HG12	1:A:1204:LEU:CD1	2.45	0.46
1:A:649:LEU:O	1:A:650:VAL:C	2.57	0.46
1:A:880:SER:O	1:A:1043:THR:HG22	2.15	0.46
1:A:372:ARG:C	1:A:374:THR:H	2.23	0.46
1:A:503:PHE:HZ	2:E:86:TRP:CG	2.33	0.46
1:A:544:TRP:CD1	1:A:544:TRP:C	2.92	0.46
1:A:690:ILE:O	1:A:690:ILE:HG22	2.14	0.46
1:A:1210:ILE:CG2	1:A:1211:VAL:H	2.29	0.46
1:A:544:TRP:CD1	1:A:545:LEU:H	2.30	0.46
1:A:656:LEU:CD2	1:A:685:ILE:HG13	2.45	0.46
1:A:824:SER:HA	1:A:1188:GLU:OE2	2.16	0.46
1:A:1046:GLN:C	1:A:1047:THR:HG1	2.08	0.46
1:A:736:PHE:O	1:A:737:LEU:O	2.34	0.46
1:A:162:ASP:OD2	1:A:244:SER:OG	2.33	0.46
1:A:598:ASN:ND2	4:K:1:NAG:C2	2.70	0.46
1:A:1084:PHE:CZ	1:A:1085:TYR:CD1	2.84	0.46
1:A:1141:VAL:C	1:A:1147:ILE:CB	2.89	0.46
1:A:1220:ILE:O	1:A:1221:PHE:C	2.59	0.46
1:A:656:LEU:HB3	1:A:682:LEU:CD1	2.42	0.46
1:A:656:LEU:HD22	1:A:751:LEU:CD2	2.46	0.46
1:A:688:GLU:CA	1:A:691:PRO:HD3	2.45	0.46
1:A:1131:ILE:O	1:A:1135:LEU:CG	2.63	0.46
1:A:673:GLY:C	1:A:675:PHE:H	2.23	0.46
2:C:37:VAL:HG21	2:C:51:LEU:HD11	1.97	0.46
3:H:560:GLN:O	3:H:564:GLU:HG3	2.16	0.46
1:A:476:ASN:HA	6:L:1:NAG:H82	1.98	0.45
1:A:656:LEU:CB	1:A:751:LEU:HD11	2.44	0.45
1:A:985:GLU:HA	1:A:989:ARG:CB	2.46	0.45
1:A:1062:ALA:O	1:A:1078:VAL:HG21	2.15	0.45
1:A:635:ILE:HG21	1:A:686:VAL:CG1	2.46	0.45
1:A:676:SER:CB	1:A:1225:TYR:CE1	2.99	0.45
1:A:758:HIS:C	1:A:760:PHE:N	2.74	0.45
1:A:484:VAL:HG11	1:A:547:LEU:HD21	1.98	0.45
1:A:635:ILE:HG21	1:A:686:VAL:HG11	1.97	0.45
1:A:38:LYS:HB3	1:A:202:PRO:HB3	1.97	0.45
1:A:165:ALA:O	1:A:167:SER:N	2.50	0.45
1:A:401:PRO:CG	1:A:569:ASN:OD1	2.64	0.45
1:A:1159:MET:HE1	1:A:1163:ILE:CD1	2.43	0.45
1:A:1202:ILE:O	1:A:1205:THR:OG1	2.21	0.45
1:A:1229:TYR:HD1	1:A:1229:TYR:C	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:TYR:CZ	2:E:80:PRO:CG	2.99	0.45
1:A:1149:LEU:HA	1:A:1153:SER:HB2	1.97	0.45
1:A:1228:MET:O	1:A:1229:TYR:C	2.58	0.45
1:A:474:PRO:O	1:A:475:TYR:C	2.60	0.45
1:A:1229:TYR:CD1	1:A:1229:TYR:C	2.93	0.45
3:D:560:GLN:O	3:D:564:GLU:HG3	2.16	0.45
1:A:396:ASP:CA	1:A:400:GLY:H	2.30	0.45
1:A:401:PRO:CB	1:A:569:ASN:ND2	2.58	0.45
1:A:421:GLN:H	1:A:421:GLN:CD	2.20	0.45
1:A:1009:PRO:C	1:A:1010:LYS:O	2.59	0.45
1:A:1034:GLY:HA2	1:A:1035:ALA:HA	1.69	0.45
1:A:1043:THR:C	1:A:1044:VAL:HG23	2.42	0.45
1:A:398:HIS:C	1:A:399:PHE:CD1	2.95	0.45
1:A:723:GLN:HG2	1:A:1173:ARG:CG	2.46	0.45
1:A:733:PRO:C	1:A:735:MET:N	2.73	0.45
1:A:1047:THR:CG2	1:A:1048:SER:H	2.30	0.45
1:A:1127:MET:HE3	1:A:1130:THR:CG2	2.46	0.45
3:F:560:GLN:O	3:F:564:GLU:HG3	2.16	0.45
1:A:732:ALA:O	1:A:746:PHE:HA	2.17	0.45
1:A:238:CYS:O	1:A:246:VAL:HG21	2.17	0.44
1:A:1127:MET:HE2	1:A:1168:CYS:HB2	1.98	0.44
1:A:627:SER:CB	1:A:1212:VAL:HG23	2.47	0.44
1:A:653:LYS:HG3	1:A:654:VAL:H	1.82	0.44
1:A:751:LEU:O	1:A:755:PRO:HD3	2.17	0.44
1:A:1053:ASP:O	1:A:1057:LYS:HD2	2.18	0.44
1:A:1225:TYR:HD1	1:A:1226:PHE:CG	2.35	0.44
2:G:39:HIS:CB	2:G:42:VAL:HG22	2.39	0.44
1:A:91:LEU:HD13	1:A:101:PHE:CZ	2.52	0.44
1:A:382:SER:OG	1:A:1086:VAL:HG13	2.17	0.44
1:A:598:ASN:CG	4:K:1:NAG:C1	2.77	0.44
1:A:246:VAL:HG23	1:A:246:VAL:O	2.18	0.44
1:A:472:LEU:HD21	1:A:1017:ALA:HB1	1.96	0.44
1:A:607:ARG:C	1:A:611:ASP:HB2	2.43	0.44
1:A:750:ALA:C	1:A:752:SER:N	2.75	0.44
2:E:51:LEU:HD12	2:E:51:LEU:HA	1.68	0.44
1:A:384:PRO:HA	1:A:389:ARG:CG	2.38	0.44
1:A:688:GLU:HB2	1:A:724:LEU:HD21	1.98	0.44
1:A:1080:PRO:O	1:A:1085:TYR:CE2	2.71	0.44
2:C:79:VAL:O	2:C:83:THR:HG23	2.17	0.44
1:A:682:LEU:HD12	1:A:682:LEU:HA	1.77	0.44
1:A:683:THR:CG2	1:A:684:LEU:N	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:930:ASP:O	1:A:933:THR:N	2.50	0.44
1:A:381:TRP:C	1:A:383:ALA:N	2.74	0.44
1:A:649:LEU:CD2	1:A:686:VAL:HG13	2.47	0.44
1:A:653:LYS:HA	1:A:682:LEU:CG	2.47	0.44
1:A:396:ASP:HA	1:A:400:GLY:H	1.80	0.44
1:A:404:ARG:HH11	1:A:404:ARG:CG	2.30	0.44
1:A:632:PHE:HE1	1:A:649:LEU:HB3	1.83	0.44
1:A:1090:GLN:C	1:A:1092:LEU:N	2.76	0.44
1:A:27:TRP:NE1	1:A:117:GLN:HE22	2.16	0.43
1:A:690:ILE:N	1:A:691:PRO:HD3	2.32	0.43
1:A:421:GLN:OE1	1:A:421:GLN:N	2.39	0.43
1:A:444:LEU:HD23	1:A:492:HIS:CD2	2.53	0.43
1:A:690:ILE:O	1:A:694:VAL:CG2	2.64	0.43
1:A:1090:GLN:O	1:A:1094:ILE:HG12	2.19	0.43
1:A:1222:GLN:C	1:A:1224:PHE:H	2.26	0.43
1:A:691:PRO:HB3	1:A:1197:SER:HB2	2.00	0.43
1:A:723:GLN:OE1	1:A:1169:SER:CA	2.63	0.43
1:A:734:SER:C	1:A:736:PHE:H	2.25	0.43
2:E:79:VAL:O	2:E:83:THR:HG23	2.17	0.43
2:G:70:LEU:HD11	2:G:180:VAL:HG22	2.00	0.43
1:A:66:PHE:HB3	1:A:73:LEU:HD21	2.00	0.43
1:A:627:SER:CB	1:A:1212:VAL:CG2	2.96	0.43
1:A:875:TYR:C	1:A:876:PHE:O	2.60	0.43
1:A:876:PHE:O	1:A:877:LYS:CB	2.67	0.43
1:A:1117:LEU:HD23	1:A:1123:SER:HB3	2.00	0.43
2:G:79:VAL:O	2:G:83:THR:HG23	2.17	0.43
1:A:885:ALA:O	1:A:1079:PHE:CB	2.65	0.43
1:A:1092:LEU:HD13	1:A:1092:LEU:C	2.44	0.43
1:A:648:LEU:O	1:A:649:LEU:C	2.62	0.43
1:A:1202:ILE:O	1:A:1203:THR:C	2.61	0.43
1:A:684:LEU:HD12	1:A:1166:GLU:HG3	1.94	0.43
1:A:1045:LEU:HD23	1:A:1051:PHE:CZ	2.54	0.43
1:A:1117:LEU:HD11	1:A:1173:ARG:HH11	1.84	0.43
1:A:1213:LEU:O	1:A:1227:ARG:NH2	2.41	0.43
1:A:421:GLN:CD	1:A:421:GLN:N	2.76	0.43
1:A:1094:ILE:O	1:A:1098:THR:HG23	2.18	0.43
1:A:364:CYS:O	1:A:662:LEU:HB2	2.18	0.43
1:A:720:LEU:O	1:A:723:GLN:CD	2.60	0.43
1:A:1048:SER:O	1:A:1052:ILE:HG13	2.18	0.43
1:A:1059:ARG:HA	1:A:1059:ARG:HD3	1.75	0.43
1:A:1140:GLY:C	1:A:1144:LEU:CB	2.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:ARG:HH11	1:A:404:ARG:CB	2.32	0.43
2:C:70:LEU:HD11	2:C:180:VAL:HG22	2.00	0.43
2:E:70:LEU:HD11	2:E:180:VAL:HG22	2.00	0.43
1:A:116:ARG:HE	1:A:116:ARG:HB3	1.32	0.42
1:A:196:LYS:HG3	1:A:196:LYS:H	1.53	0.42
2:G:63:LEU:HB3	3:H:585:LEU:HD22	2.01	0.42
1:A:239:SER:O	1:A:243:CYS:HB3	2.20	0.42
1:A:523:LEU:CG	1:A:1016:HIS:CB	2.96	0.42
1:A:622:PHE:O	1:A:626:ILE:CG1	2.67	0.42
1:A:635:ILE:CG1	1:A:1204:LEU:CD1	2.98	0.42
1:A:726:ARG:CB	1:A:1112:VAL:HG11	2.45	0.42
1:A:1117:LEU:HB3	1:A:1118:GLY:H	1.70	0.42
1:A:1198:VAL:O	1:A:1202:ILE:HB	2.18	0.42
3:F:582:PHE:HE2	3:H:577:THR:HG23	1.85	0.42
1:A:656:LEU:HD22	1:A:751:LEU:O	2.19	0.42
1:A:684:LEU:CG	1:A:728:LEU:CD2	2.95	0.42
1:A:726:ARG:NE	1:A:726:ARG:HA	2.35	0.42
3:F:548:MET:HE3	3:F:548:MET:HB3	1.74	0.42
1:A:730:GLU:HG2	1:A:1112:VAL:HG23	1.99	0.42
1:A:1100:PHE:CE1	1:A:1104:VAL:CG2	3.02	0.42
1:A:1159:MET:HE3	1:A:1159:MET:HB3	1.79	0.42
3:D:577:THR:HG23	3:H:582:PHE:HE2	1.85	0.42
1:A:1160:SER:HB2	1:A:1232:MET:CE	2.50	0.42
1:A:1199:PHE:O	1:A:1203:THR:HB	2.20	0.42
3:D:582:PHE:HE2	3:F:577:THR:HG23	1.85	0.42
2:E:63:LEU:HB3	3:F:585:LEU:HD22	2.01	0.42
5:J:1:NAG:C1	5:J:1:NAG:C8	2.86	0.42
1:A:507:ALA:CB	1:A:529:LEU:CD2	2.98	0.42
1:A:1093:THR:HG22	1:A:1096:ASP:HB2	2.01	0.42
1:A:656:LEU:CD2	1:A:751:LEU:O	2.67	0.42
1:A:659:ALA:CA	1:A:662:LEU:HD21	2.36	0.42
1:A:685:ILE:O	1:A:689:VAL:HB	2.19	0.42
1:A:749:GLY:O	1:A:752:SER:HB2	2.18	0.42
1:A:1063:SER:O	1:A:1067:GLU:CG	2.67	0.42
1:A:637:LEU:O	1:A:638:ALA:O	2.37	0.42
1:A:668:VAL:O	1:A:669:ALA:HB2	2.20	0.42
1:A:1202:ILE:CG2	1:A:1237:ALA:CB	2.98	0.42
1:A:396:ASP:O	1:A:399:PHE:N	2.50	0.41
1:A:824:SER:CA	1:A:1188:GLU:CD	2.93	0.41
1:A:908:VAL:HG13	1:A:926:ALA:HA	2.02	0.41
1:A:1058:ALA:HA	1:A:1061:ILE:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1227:ARG:HA	1:A:1227:ARG:HD3	1.78	0.41
2:E:39:HIS:CB	2:E:42:VAL:HG22	2.40	0.41
1:A:506:TYR:CZ	2:E:80:PRO:CB	3.03	0.41
1:A:653:LYS:HA	1:A:682:LEU:CD2	2.50	0.41
1:A:673:GLY:C	1:A:675:PHE:N	2.78	0.41
1:A:691:PRO:CD	1:A:692:PHE:N	2.83	0.41
1:A:1060:LEU:O	1:A:1063:SER:OG	2.25	0.41
1:A:1210:ILE:HD11	1:A:1214:ALA:HB2	2.01	0.41
2:G:51:LEU:HA	2:G:51:LEU:HD12	1.68	0.41
1:A:370:PHE:O	1:A:371:VAL:CB	2.67	0.41
1:A:842:PHE:O	1:A:1136:VAL:HG11	2.21	0.41
2:E:52:VAL:C	2:E:54:ARG:H	2.29	0.41
1:A:509:TYR:CZ	1:A:510:HIS:CE1	3.08	0.41
1:A:399:PHE:CD1	1:A:399:PHE:N	2.88	0.41
1:A:926:ALA:C	1:A:1040:THR:HG22	2.29	0.41
3:D:582:PHE:CE2	3:F:578:GLU:HB3	2.56	0.41
1:A:1225:TYR:HD1	1:A:1226:PHE:CD1	2.39	0.41
3:D:567:GLN:HG3	3:H:531:TRP:CG	2.56	0.41
1:A:131:ASP:HA	1:A:132:PRO:HD2	1.93	0.41
1:A:885:ALA:O	1:A:1079:PHE:N	2.54	0.41
1:A:1112:VAL:HA	1:A:1115:VAL:CG2	2.49	0.41
2:C:63:LEU:HB3	3:D:585:LEU:HD22	2.01	0.41
3:D:513:PRO:O	3:D:555:ILE:HD13	2.21	0.41
3:D:578:GLU:HB3	3:H:582:PHE:CZ	2.56	0.41
1:A:635:ILE:HG12	1:A:1204:LEU:HD12	2.02	0.41
1:A:648:LEU:CG	1:A:763:PHE:CE1	3.03	0.41
1:A:767:ALA:O	1:A:771:ASP:N	2.52	0.41
1:A:1048:SER:O	1:A:1052:ILE:CG1	2.69	0.41
1:A:1152:VAL:O	1:A:1155:VAL:N	2.54	0.41
3:D:578:GLU:HB3	3:H:582:PHE:CE2	2.56	0.41
3:D:582:PHE:CZ	3:F:578:GLU:HB3	2.56	0.41
3:F:582:PHE:CE2	3:H:578:GLU:HB3	2.56	0.41
1:A:684:LEU:HD11	1:A:1166:GLU:CG	2.47	0.41
2:C:52:VAL:C	2:C:54:ARG:H	2.28	0.41
3:F:531:TRP:CG	3:H:567:GLN:HG3	2.56	0.41
3:H:513:PRO:O	3:H:555:ILE:HD13	2.21	0.41
1:A:202:PRO:HG2	1:A:203:PHE:CE2	2.55	0.40
1:A:515:TYR:HE1	1:A:526:THR:CG2	2.28	0.40
1:A:893:LEU:O	1:A:895:GLU:N	2.54	0.40
1:A:1154:LEU:HA	1:A:1154:LEU:HD23	1.78	0.40
1:A:1220:ILE:HA	1:A:1223:ILE:CB	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:92:VAL:HA	2:E:93:PRO:HD3	1.92	0.40
1:A:1082:SER:C	1:A:1084:PHE:N	2.74	0.40
1:A:885:ALA:N	1:A:1079:PHE:O	2.51	0.40
1:A:1156:ASN:HD22	1:A:1228:MET:CE	2.30	0.40
1:A:1222:GLN:O	1:A:1224:PHE:N	2.54	0.40
3:D:531:TRP:CG	3:F:567:GLN:HG3	2.56	0.40
3:F:513:PRO:O	3:F:555:ILE:HD13	2.21	0.40
1:A:639:LEU:C	1:A:641:HIS:N	2.78	0.40
1:A:915:ASN:HA	1:A:921:GLN:H	1.87	0.40
1:A:923:ILE:CB	1:A:925:ASN:CB	2.99	0.40
1:A:1199:PHE:O	1:A:1203:THR:HG21	2.19	0.40
1:A:384:PRO:C	1:A:385:SER:HG	2.19	0.40
1:A:1065:VAL:C	1:A:1068:THR:HG22	2.37	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	1126/1278 (88%)	897 (80%)	135 (12%)	94 (8%)	0	9
2	C	156/158 (99%)	142 (91%)	12 (8%)	2 (1%)	9	42
2	E	156/158 (99%)	141 (90%)	13 (8%)	2 (1%)	9	42
2	G	156/158 (99%)	142 (91%)	12 (8%)	2 (1%)	9	42
3	D	83/130 (64%)	77 (93%)	4 (5%)	2 (2%)	4	27
3	F	83/130 (64%)	77 (93%)	4 (5%)	2 (2%)	4	27
3	H	83/130 (64%)	77 (93%)	4 (5%)	2 (2%)	4	27
All	All	1843/2142 (86%)	1553 (84%)	184 (10%)	106 (6%)	2	13

All (106) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	250	LYS
1	A	256	PRO
1	A	350	PRO
1	A	372	ARG
1	A	374	THR
1	A	376	ASN
1	A	403	PHE
1	A	638	ALA
1	A	639	LEU
1	A	642	MET
1	A	700	ASP
1	A	706	VAL
1	A	737	LEU
1	A	739	SER
1	A	829	LEU
1	A	856	VAL
1	A	864	LEU
1	A	876	PHE
1	A	922	GLN
1	A	929	LEU
1	A	930	ASP
1	A	943	ILE
1	A	951	LYS
1	A	957	CYS
1	A	958	ARG
1	A	1007	PRO
1	A	1008	ASN
1	A	1009	PRO
1	A	1010	LYS
1	A	1044	VAL
1	A	1071	ILE
1	A	1072	ASN
1	A	1083	VAL
1	A	1085	TYR
1	A	1086	VAL
1	A	1122	TRP
1	A	1146	GLY
1	A	260	TRP
1	A	475	TYR
1	A	605	ALA
1	A	606	GLU
1	A	617	SER
1	A	641	HIS

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Mol	Chain	Res	Type
1	A	760	PHE
1	A	830	LEU
1	A	888	PRO
1	A	923	ILE
1	A	1022	ALA
1	A	1073	GLY
1	A	1075	ALA
1	A	1177	VAL
1	A	1179	MET
1	A	1215	PHE
2	C	50	LYS
2	C	51	LEU
3	D	597	TRP
2	E	50	LYS
2	E	51	LEU
3	F	597	TRP
2	G	50	LYS
2	G	51	LEU
3	H	597	TRP
1	A	168	SER
1	A	498	LYS
1	A	668	VAL
1	A	861	ASP
1	A	877	LYS
1	A	890	TYR
1	A	894	GLU
1	A	1178	SER
1	A	1221	PHE
1	A	252	GLN
1	A	348	ARG
1	A	691	PRO
1	A	734	SER
1	A	745	ALA
1	A	891	PHE
1	A	917	ASP
1	A	926	ALA
1	A	1084	PHE
1	A	1093	THR
1	A	1120	GLU
1	A	1150	ASN
1	A	1167	PHE
3	D	550	ASN

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Mol	Chain	Res	Type
3	F	550	ASN
3	H	550	ASN
1	A	258	ALA
1	A	353	VAL
1	A	371	VAL
1	A	384	PRO
1	A	703	PHE
1	A	733	PRO
1	A	925	ASN
1	A	1117	LEU
1	A	253	PRO
1	A	259	PRO
1	A	401	PRO
1	A	880	SER
1	A	887	PRO
1	A	1080	PRO
1	A	166	PRO
1	A	892	VAL
1	A	1202	ILE
1	A	349	ASN
1	A	257	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	643/1109 (58%)	567 (88%)	76 (12%)	5	18
2	C	126/130 (97%)	124 (98%)	2 (2%)	55	70
2	E	126/130 (97%)	124 (98%)	2 (2%)	55	70
2	G	126/130 (97%)	124 (98%)	2 (2%)	55	70
3	D	70/111 (63%)	68 (97%)	2 (3%)	37	58
3	F	70/111 (63%)	68 (97%)	2 (3%)	37	58
3	H	70/111 (63%)	68 (97%)	2 (3%)	37	58
All	All	1231/1832 (67%)	1143 (93%)	88 (7%)	15	35

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	87	LEU
1	A	91	LEU
1	A	105	LEU
1	A	116	ARG
1	A	164	GLU
1	A	196	LYS
1	A	250	LYS
1	A	252	GLN
1	A	381	TRP
1	A	389	ARG
1	A	394	TYR
1	A	398	HIS
1	A	399	PHE
1	A	404	ARG
1	A	406	GLU
1	A	439	ILE
1	A	472	LEU
1	A	495	LEU
1	A	518	ARG
1	A	526	THR
1	A	592	LYS
1	A	602	SER
1	A	607	ARG
1	A	612	GLU
1	A	648	LEU
1	A	653	LYS
1	A	662	LEU
1	A	676	SER
1	A	680	LEU
1	A	682	LEU
1	A	684	LEU
1	A	685	ILE
1	A	688	GLU
1	A	718	GLU
1	A	719	THR
1	A	722	GLN
1	A	730	GLU
1	A	751	LEU
1	A	758	HIS
1	A	760	PHE
1	A	1036	THR

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Mol	Chain	Res	Type
1	A	1037	TYR
1	A	1038	PHE
1	A	1039	MET
1	A	1041	TYR
1	A	1050	ASP
1	A	1055	LEU
1	A	1056	LYS
1	A	1057	LYS
1	A	1059	ARG
1	A	1066	THR
1	A	1069	MET
1	A	1072	ASN
1	A	1074	SER
1	A	1082	SER
1	A	1084	PHE
1	A	1090	GLN
1	A	1117	LEU
1	A	1127	MET
1	A	1128	CYS
1	A	1138	MET
1	A	1153	SER
1	A	1154	LEU
1	A	1159	MET
1	A	1166	GLU
1	A	1172	THR
1	A	1173	ARG
1	A	1186	ARG
1	A	1189	GLU
1	A	1194	MET
1	A	1199	PHE
1	A	1207	PHE
1	A	1227	ARG
1	A	1228	MET
1	A	1234	LEU
2	C	51	LEU
2	C	169	VAL
3	D	548	MET
3	D	595	GLN
2	E	51	LEU
2	E	169	VAL
3	F	548	MET
3	F	595	GLN

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Mol	Chain	Res	Type
2	G	51	LEU
2	G	169	VAL
3	H	548	MET
3	H	595	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	70	ASN
1	A	92	GLN
1	A	135	ASN
1	A	154	ASN
1	A	185	ASN
1	A	200	GLN
1	A	241	GLN
1	A	452	ASN
1	A	459	ASN
1	A	465	GLN
1	A	478	ASN
1	A	510	HIS
1	A	554	ASN
1	A	598	ASN
1	A	722	GLN
1	A	1072	ASN
2	C	39	HIS
2	C	69	ASN
3	D	549	HIS
3	D	595	GLN
2	E	39	HIS
2	E	69	ASN
3	F	595	GLN
2	G	39	HIS
2	G	69	ASN
3	H	549	HIS
3	H	595	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

21 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	B	1	4,1	14,14,15	0.67	0	17,19,21	1.11	1 (5%)
4	NAG	B	2	4	14,14,15	0.55	0	17,19,21	0.74	1 (5%)
4	NAG	I	1	4,1	14,14,15	0.48	0	17,19,21	1.47	3 (17%)
4	NAG	I	2	4	14,14,15	0.29	0	17,19,21	0.57	0
5	NAG	J	1	5,1	14,14,15	0.31	0	17,19,21	0.48	0
5	NAG	J	2	5	14,14,15	0.29	0	17,19,21	0.56	0
5	BMA	J	3	5	11,11,12	0.26	0	15,15,17	0.52	0
4	NAG	K	1	4,1	14,14,15	0.36	0	17,19,21	1.56	3 (17%)
4	NAG	K	2	4	14,14,15	0.68	1 (7%)	17,19,21	1.06	1 (5%)
6	NAG	L	1	1,6	14,14,15	0.28	0	17,19,21	0.56	0
6	NAG	L	2	6	14,14,15	0.27	0	17,19,21	0.78	0
6	BMA	L	3	6	11,11,12	0.28	0	15,15,17	0.64	0
6	MAN	L	4	6	11,11,12	0.35	0	15,15,17	1.02	1 (6%)
4	NAG	M	1	4,1	14,14,15	0.41	0	17,19,21	1.15	2 (11%)
4	NAG	M	2	4	14,14,15	0.42	0	17,19,21	1.15	2 (11%)
4	NAG	N	1	3,4	14,14,15	0.71	1 (7%)	17,19,21	1.01	1 (5%)
4	NAG	N	2	4	14,14,15	0.30	0	17,19,21	0.56	0
4	NAG	O	1	3,4	14,14,15	0.72	1 (7%)	17,19,21	1.01	1 (5%)
4	NAG	O	2	4	14,14,15	0.30	0	17,19,21	0.58	0
4	NAG	P	1	3,4	14,14,15	0.71	1 (7%)	17,19,21	1.00	1 (5%)
4	NAG	P	2	4	14,14,15	0.30	0	17,19,21	0.57	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
4	NAG	B	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	B	2	4	-	0/6/23/26	0/1/1/1
4	NAG	I	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	I	2	4	-	3/6/23/26	0/1/1/1
5	NAG	J	1	5,1	-	5/6/23/26	0/1/1/1
5	NAG	J	2	5	-	2/6/23/26	0/1/1/1
5	BMA	J	3	5	-	2/2/19/22	0/1/1/1
4	NAG	K	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	K	2	4	-	1/6/23/26	0/1/1/1
6	NAG	L	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	L	2	6	-	0/6/23/26	0/1/1/1
6	BMA	L	3	6	-	0/2/19/22	0/1/1/1
6	MAN	L	4	6	-	2/2/19/22	0/1/1/1
4	NAG	M	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	M	2	4	-	0/6/23/26	0/1/1/1
4	NAG	N	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	N	2	4	-	4/6/23/26	0/1/1/1
4	NAG	O	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	O	2	4	-	4/6/23/26	0/1/1/1
4	NAG	P	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	P	2	4	-	4/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	O	1	NAG	C2-N2	2.09	1.49	1.46
4	P	1	NAG	C2-N2	2.08	1.49	1.46
4	K	2	NAG	C1-C2	2.07	1.55	1.52
4	N	1	NAG	C2-N2	2.05	1.49	1.46

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	1	NAG	O5-C1-C2	-4.37	104.53	111.29
4	K	1	NAG	C1-O5-C5	3.47	116.83	112.19
4	K	1	NAG	O4-C4-C3	-3.24	102.75	110.38
4	N	1	NAG	O5-C1-C2	-3.10	106.50	111.29
4	P	1	NAG	O5-C1-C2	-3.09	106.50	111.29
4	O	1	NAG	O5-C1-C2	-3.08	106.52	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	4	MAN	C1-C2-C3	2.94	113.93	109.64
4	K	2	NAG	C4-C3-C2	2.84	115.18	111.02
4	I	1	NAG	C4-C3-C2	2.70	114.98	111.02
4	B	1	NAG	O5-C1-C2	-2.58	107.31	111.29
4	K	1	NAG	O5-C1-C2	-2.53	107.37	111.29
4	M	1	NAG	C8-C7-N2	2.35	120.02	116.12
4	M	2	NAG	C8-C7-N2	2.33	119.99	116.12
4	I	1	NAG	C1-O5-C5	2.24	115.19	112.19
4	B	2	NAG	C1-O5-C5	2.20	115.14	112.19
4	M	2	NAG	C2-N2-C7	-2.17	119.99	122.90
4	M	1	NAG	C2-N2-C7	-2.16	120.00	122.90

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	J	1	NAG	C1-C2-N2-C7
5	J	1	NAG	C8-C7-N2-C2
5	J	1	NAG	O7-C7-N2-C2
5	J	2	NAG	C8-C7-N2-C2
5	J	2	NAG	O7-C7-N2-C2
4	I	2	NAG	O5-C5-C6-O6
6	L	4	MAN	O5-C5-C6-O6
4	I	2	NAG	C4-C5-C6-O6
4	I	1	NAG	O5-C5-C6-O6
6	L	4	MAN	C4-C5-C6-O6
4	N	2	NAG	C8-C7-N2-C2
4	N	2	NAG	O7-C7-N2-C2
4	O	2	NAG	C8-C7-N2-C2
4	O	2	NAG	O7-C7-N2-C2
4	P	2	NAG	C8-C7-N2-C2
4	P	2	NAG	O7-C7-N2-C2
5	J	3	BMA	O5-C5-C6-O6
6	L	1	NAG	O5-C5-C6-O6
4	N	2	NAG	O5-C5-C6-O6
4	O	2	NAG	O5-C5-C6-O6
4	P	2	NAG	O5-C5-C6-O6
5	J	3	BMA	C4-C5-C6-O6
4	N	2	NAG	C4-C5-C6-O6
4	O	2	NAG	C4-C5-C6-O6
4	P	2	NAG	C4-C5-C6-O6
5	J	1	NAG	C4-C5-C6-O6

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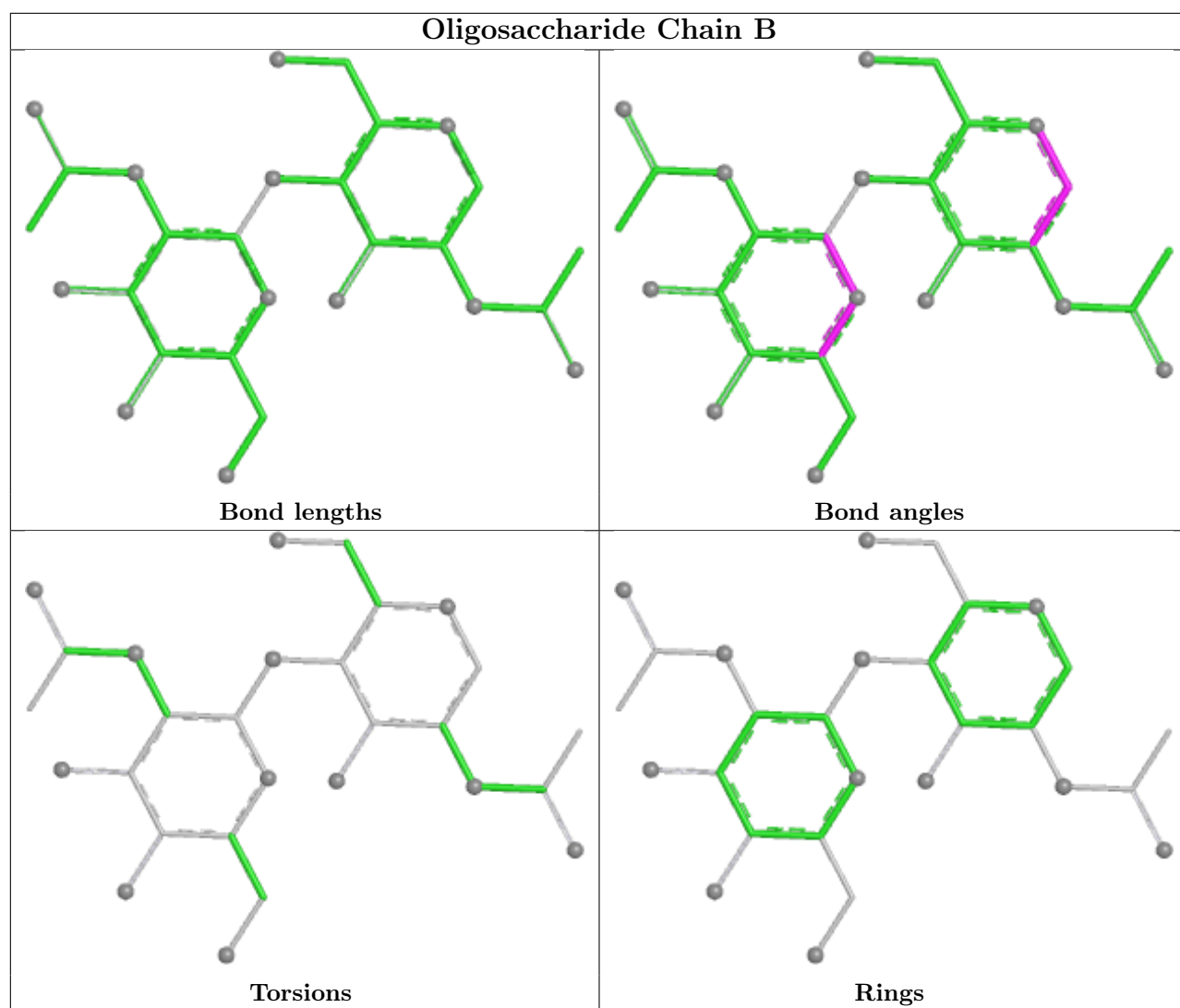
Mol	Chain	Res	Type	Atoms
5	J	1	NAG	O5-C5-C6-O6
4	I	1	NAG	C4-C5-C6-O6
6	L	1	NAG	C4-C5-C6-O6
4	I	2	NAG	C3-C2-N2-C7
4	K	2	NAG	C3-C2-N2-C7

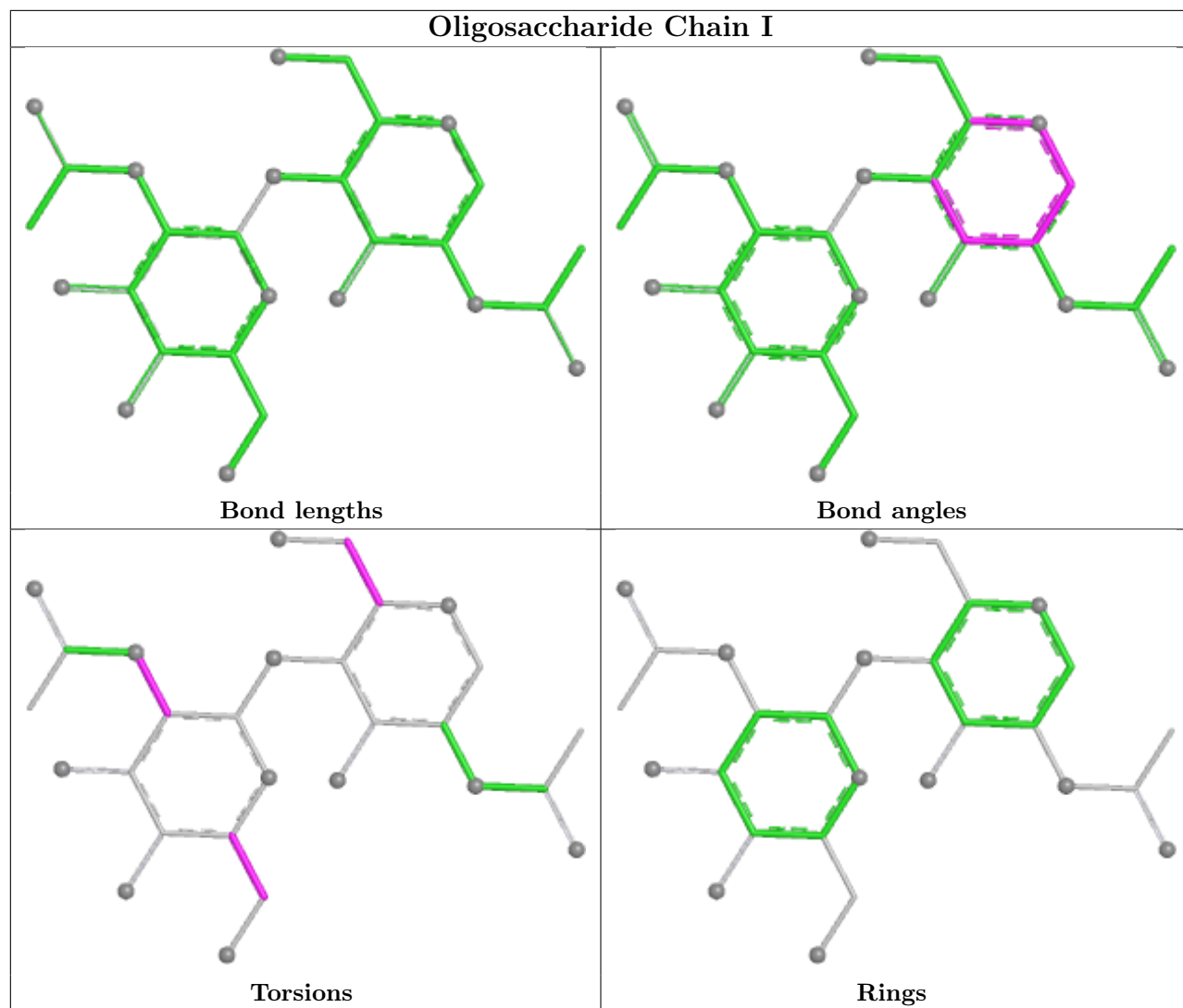
There are no ring outliers.

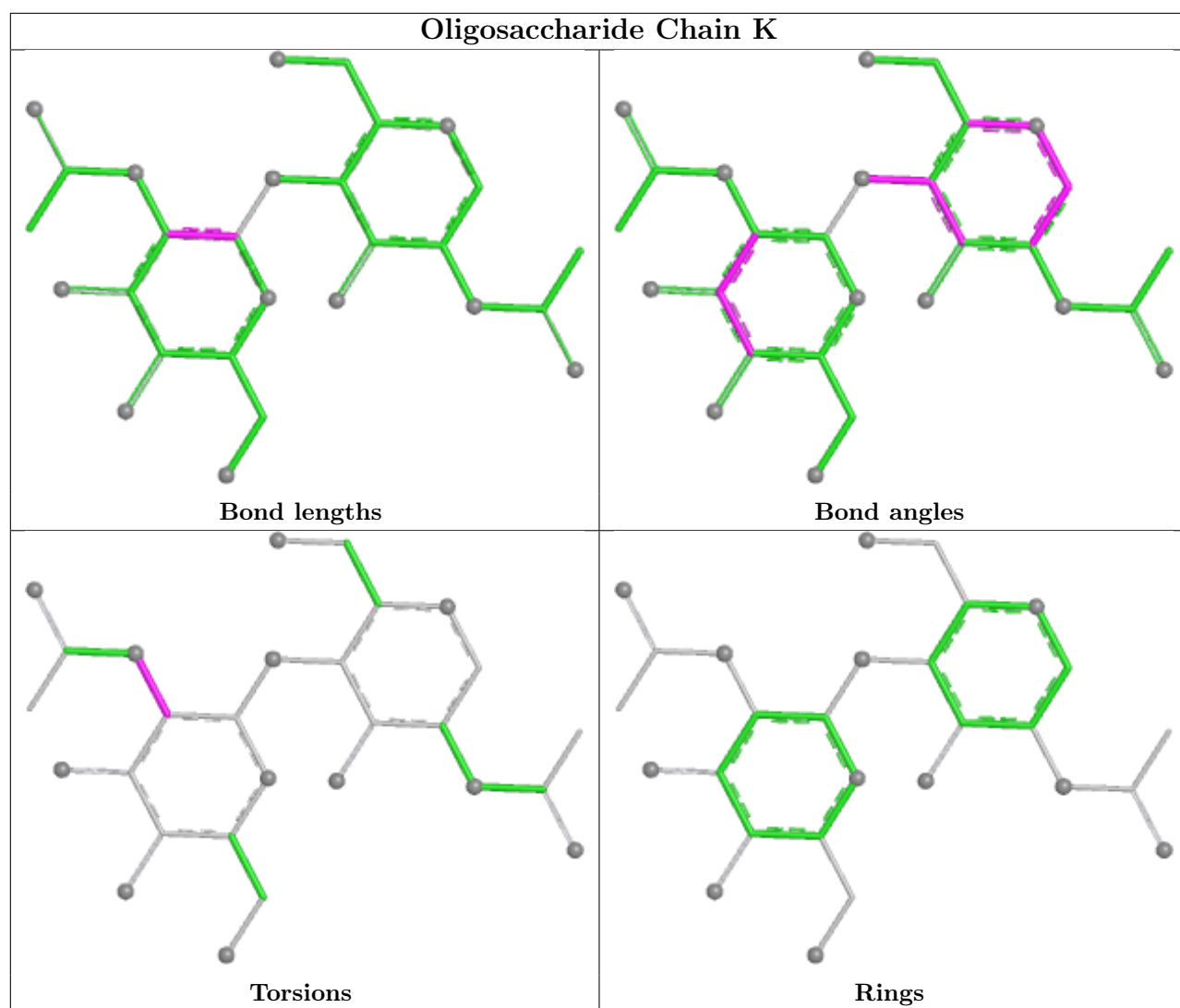
13 monomers are involved in 39 short contacts:

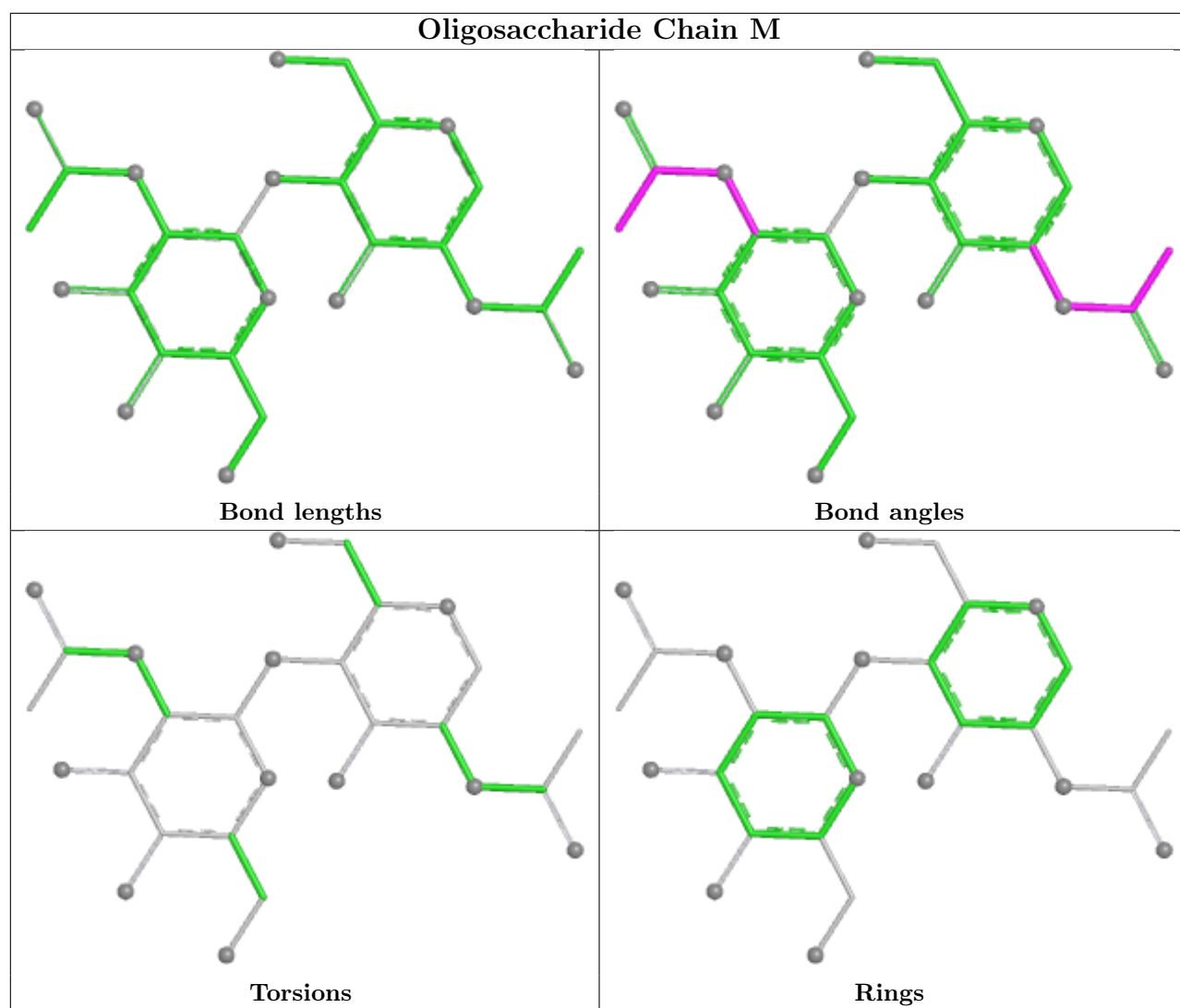
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L	2	NAG	6	0
5	J	1	NAG	14	0
5	J	2	NAG	12	0
6	L	1	NAG	7	0
4	O	1	NAG	2	0
4	N	1	NAG	1	0
4	I	2	NAG	1	0
5	J	3	BMA	3	0
4	K	1	NAG	4	0
6	L	3	BMA	2	0
4	M	1	NAG	3	0
4	P	1	NAG	1	0
4	I	1	NAG	1	0

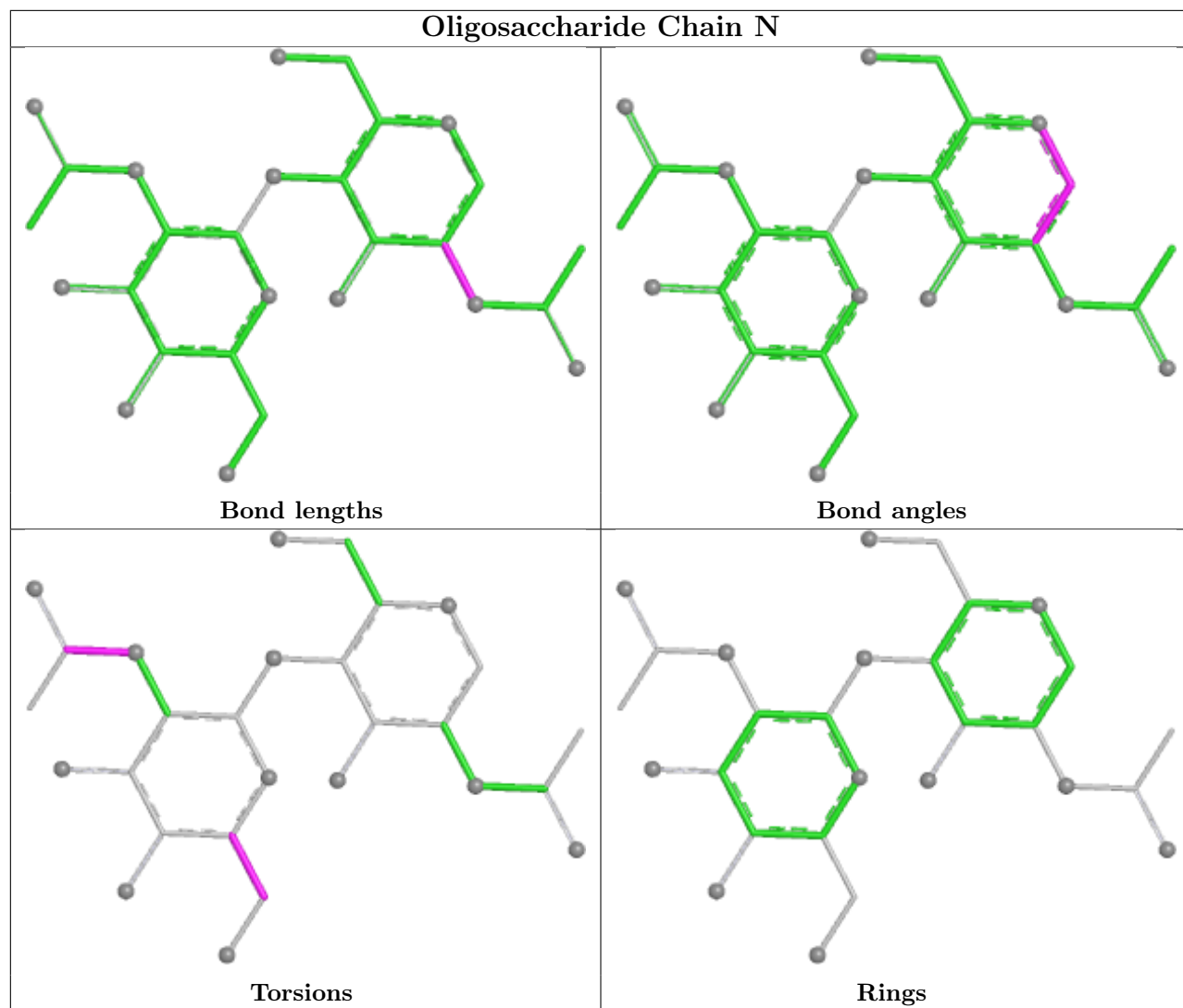
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

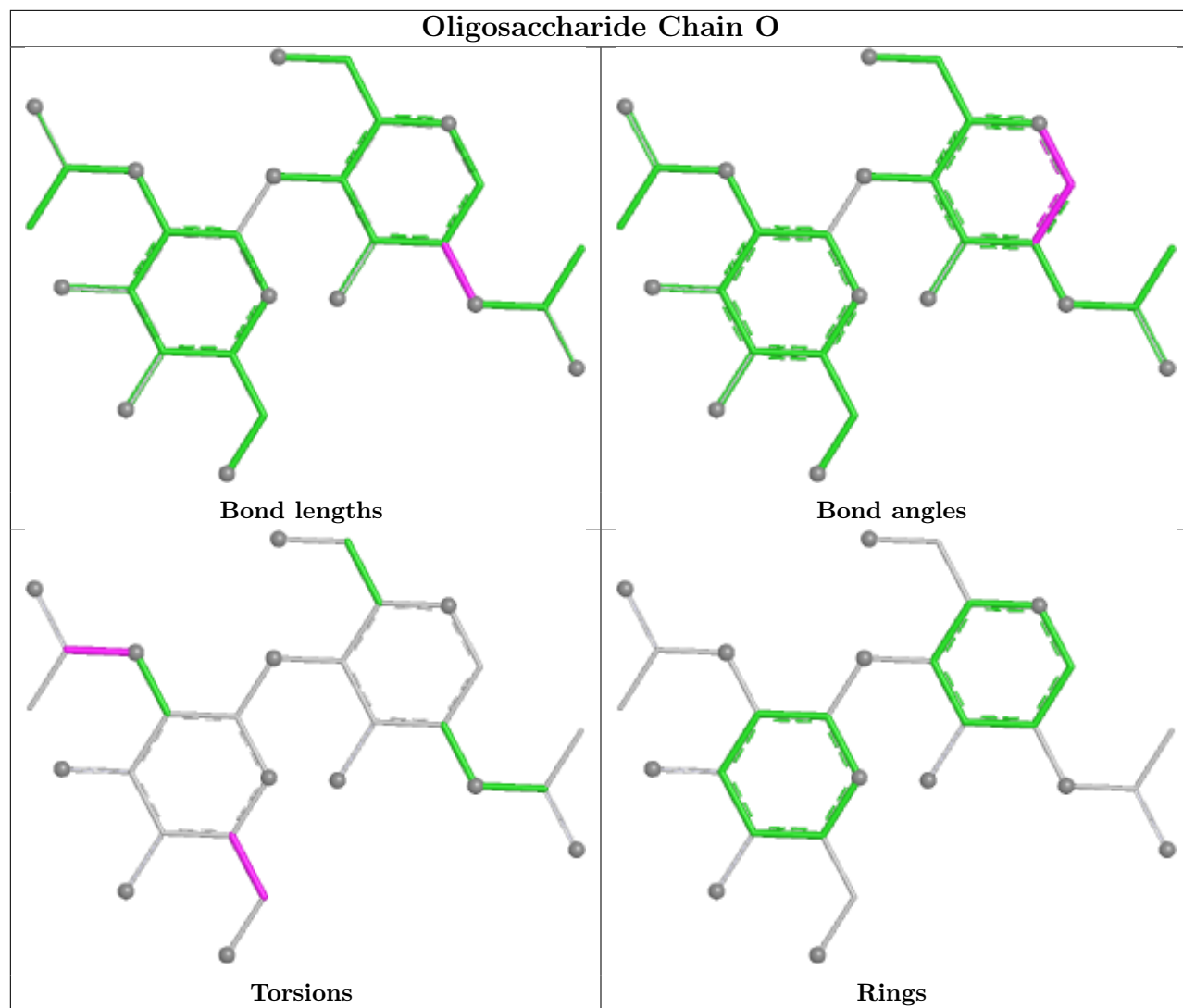


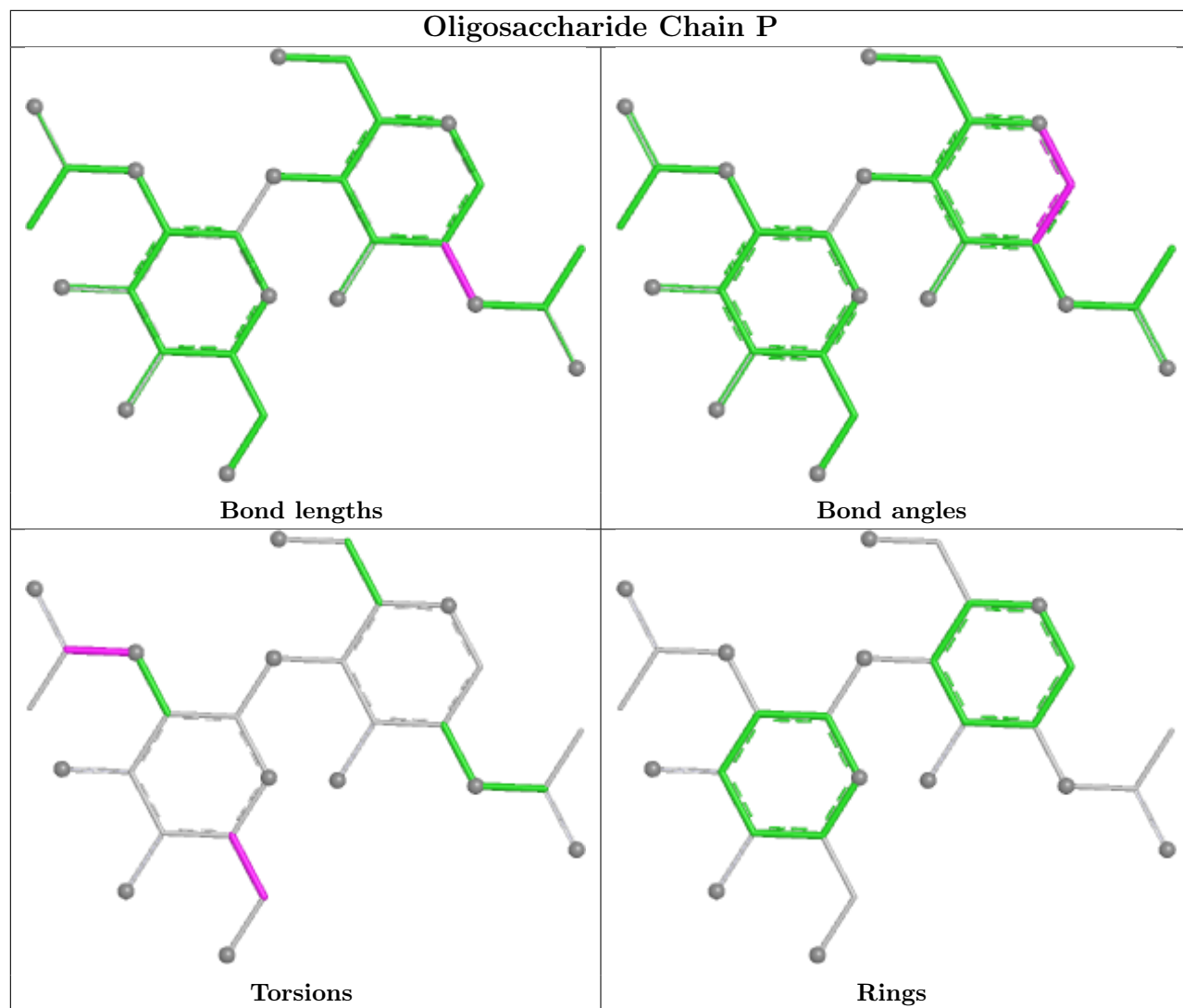


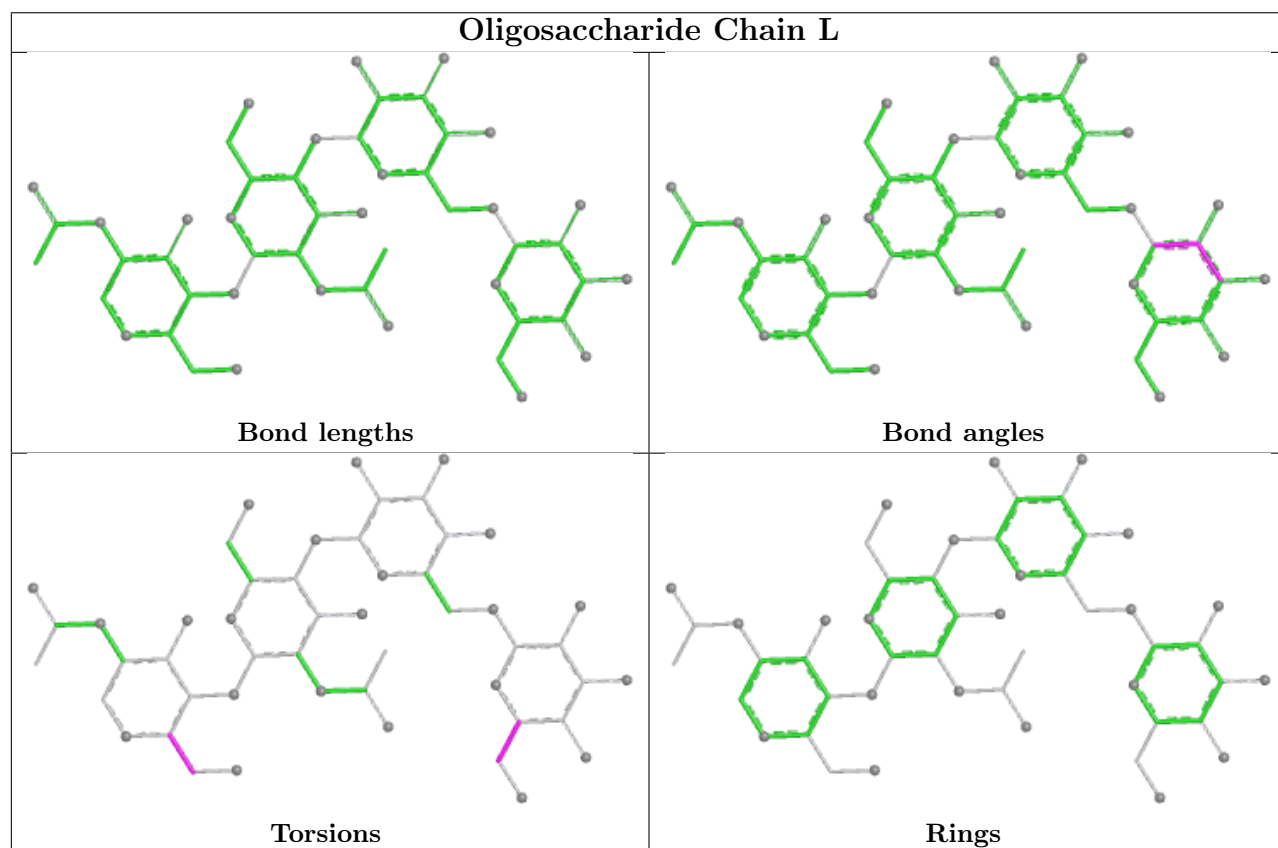
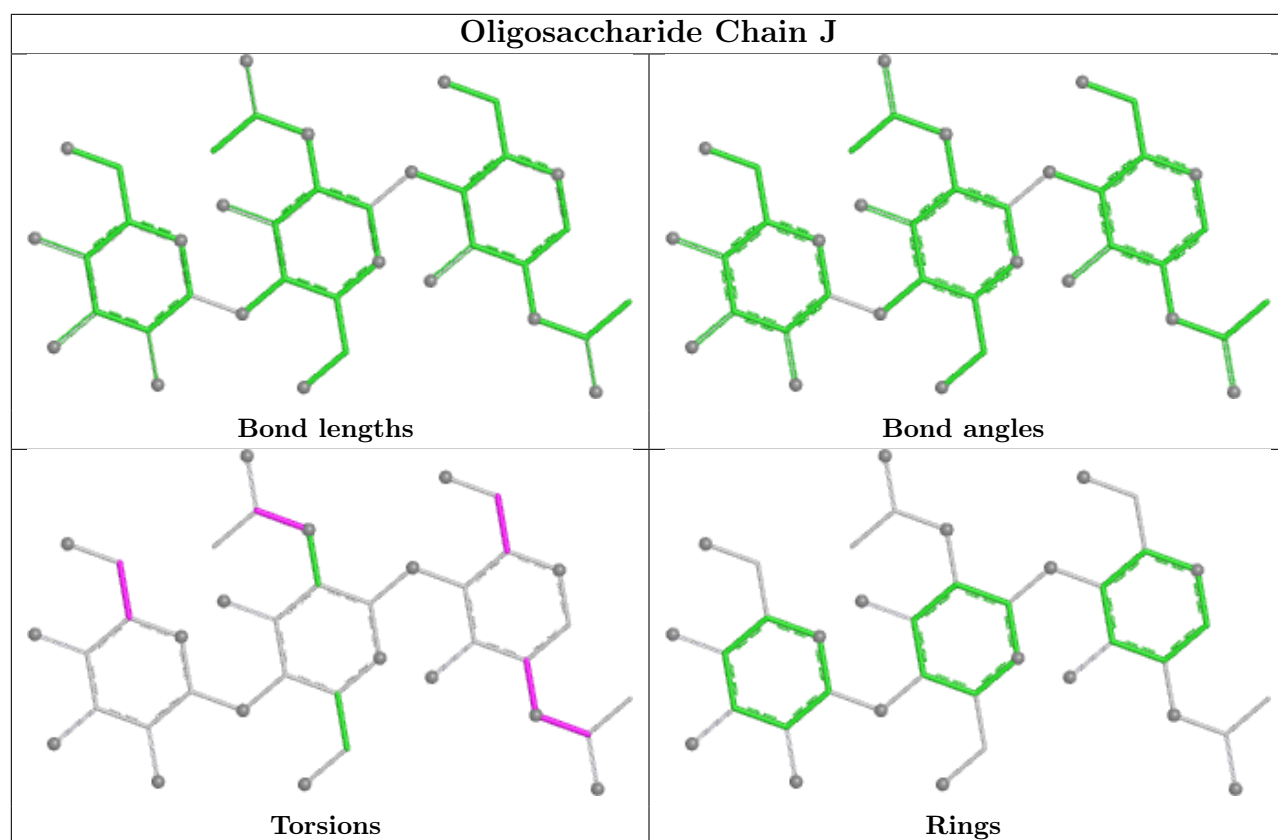












5.6 Ligand geometry

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	NAG	A	1317	1	14,14,15	0.29	0	17,19,21	0.56	0
7	NAG	A	1316	1	14,14,15	0.43	0	17,19,21	1.15	2 (11%)
7	NAG	A	1321	-	14,14,15	0.30	0	17,19,21	0.56	0
7	NAG	A	1324	1	14,14,15	0.44	0	17,19,21	1.17	2 (11%)
7	NAG	A	1323	1	14,14,15	0.28	0	17,19,21	0.56	0
7	NAG	A	1303	1	14,14,15	0.30	0	17,19,21	0.55	0
7	NAG	A	1309	1	14,14,15	0.51	0	17,19,21	1.15	2 (11%)
7	NAG	A	1322	1	14,14,15	0.30	0	17,19,21	0.56	0
7	NAG	A	1320	1	14,14,15	0.30	0	17,19,21	0.56	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	A	1317	1	-	0/6/23/26	0/1/1/1
7	NAG	A	1316	1	-	0/6/23/26	0/1/1/1
7	NAG	A	1321	-	-	0/6/23/26	0/1/1/1
7	NAG	A	1324	1	-	0/6/23/26	0/1/1/1
7	NAG	A	1323	1	-	4/6/23/26	0/1/1/1
7	NAG	A	1303	1	-	5/6/23/26	0/1/1/1
7	NAG	A	1309	1	-	0/6/23/26	0/1/1/1
7	NAG	A	1322	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1320	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1324	NAG	C8-C7-N2	2.32	119.97	116.12
7	A	1316	NAG	C8-C7-N2	2.30	119.94	116.12
7	A	1324	NAG	C2-N2-C7	-2.21	119.94	122.90
7	A	1316	NAG	C2-N2-C7	-2.17	120.00	122.90
7	A	1309	NAG	C1-C2-N2	-2.11	107.11	110.43
7	A	1309	NAG	C8-C7-N2	-2.03	112.75	116.12

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1303	NAG	C8-C7-N2-C2
7	A	1303	NAG	O7-C7-N2-C2
7	A	1322	NAG	C8-C7-N2-C2
7	A	1322	NAG	O7-C7-N2-C2
7	A	1323	NAG	C8-C7-N2-C2
7	A	1323	NAG	O7-C7-N2-C2
7	A	1323	NAG	O5-C5-C6-O6
7	A	1303	NAG	O5-C5-C6-O6
7	A	1323	NAG	C4-C5-C6-O6
7	A	1303	NAG	C4-C5-C6-O6
7	A	1303	NAG	C3-C2-N2-C7

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1317	NAG	1	0
7	A	1324	NAG	2	0
7	A	1323	NAG	1	0
7	A	1303	NAG	1	0
7	A	1322	NAG	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

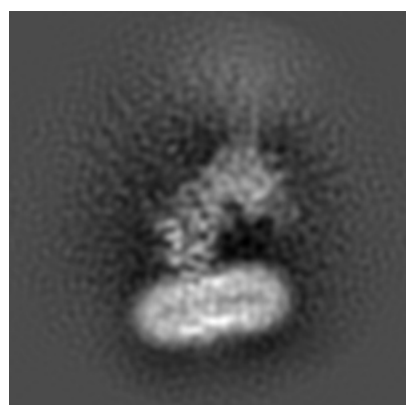
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8169. These allow visual inspection of the internal detail of the map and identification of artifacts.

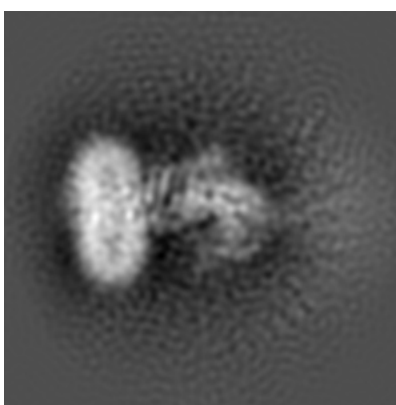
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

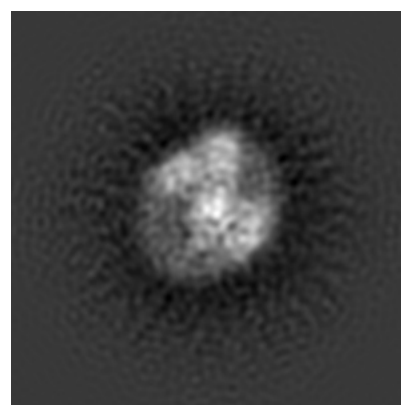
6.1.1 Primary map



X



Y

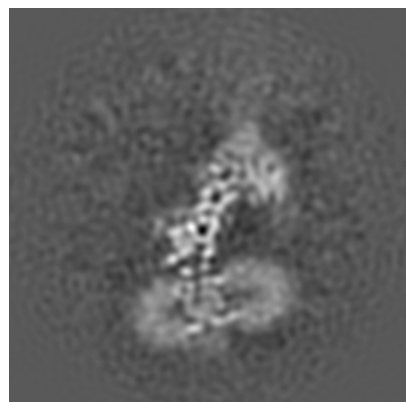


Z

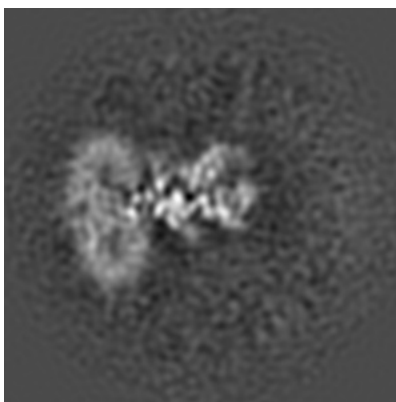
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

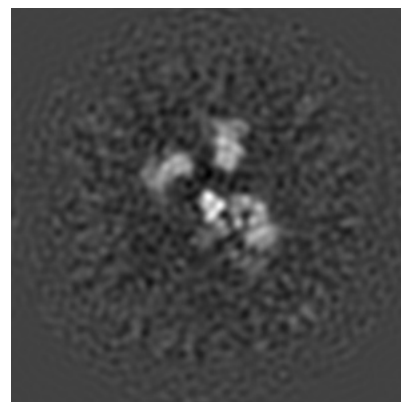
6.2.1 Primary map



X Index: 128



Y Index: 128

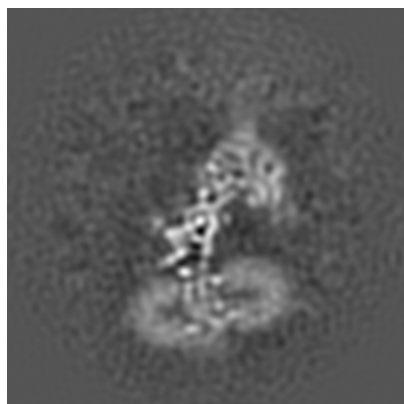


Z Index: 128

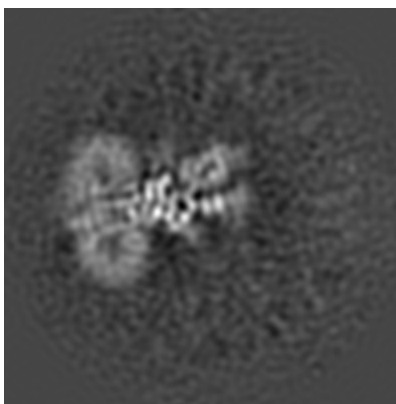
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

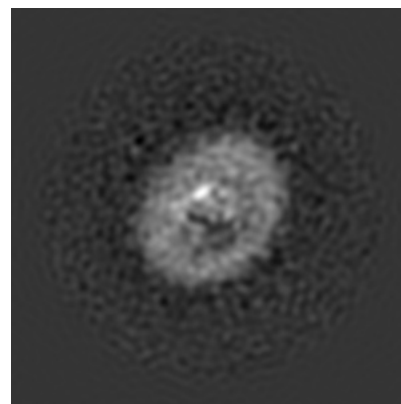
6.3.1 Primary map



X Index: 130



Y Index: 125

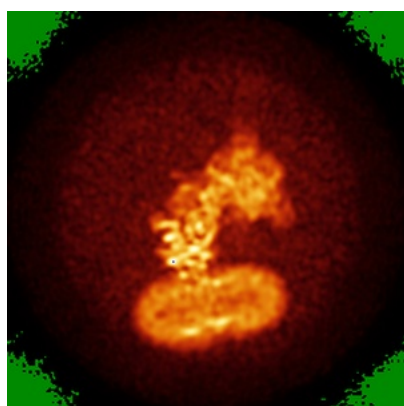


Z Index: 57

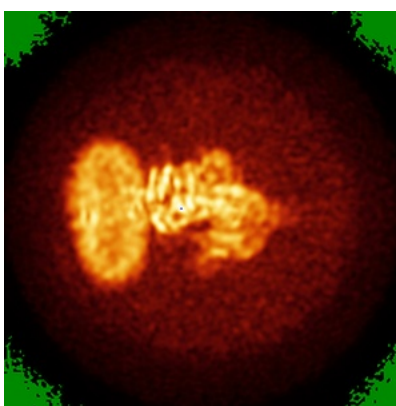
The images above show the largest variance slices of the map in three orthogonal directions.

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

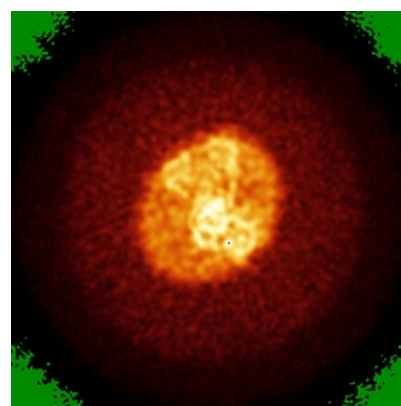
6.4.1 Primary map



X



Y

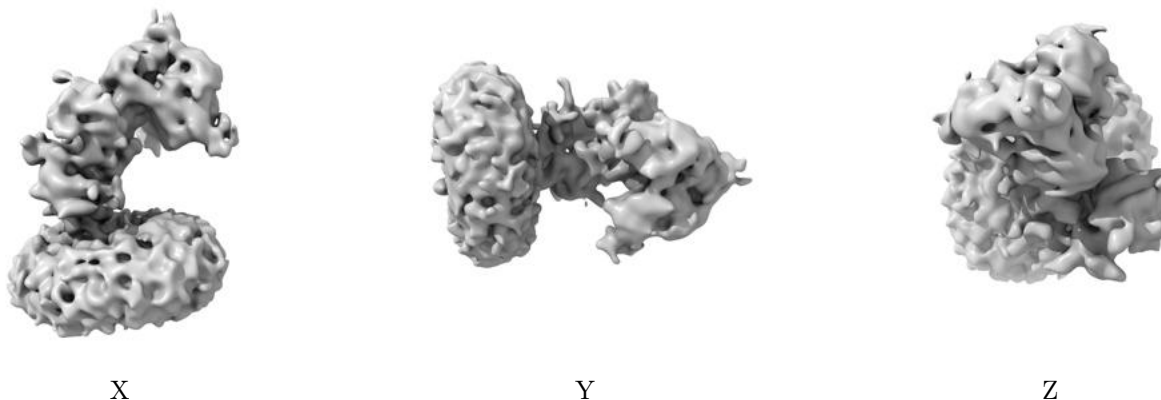


Z

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 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

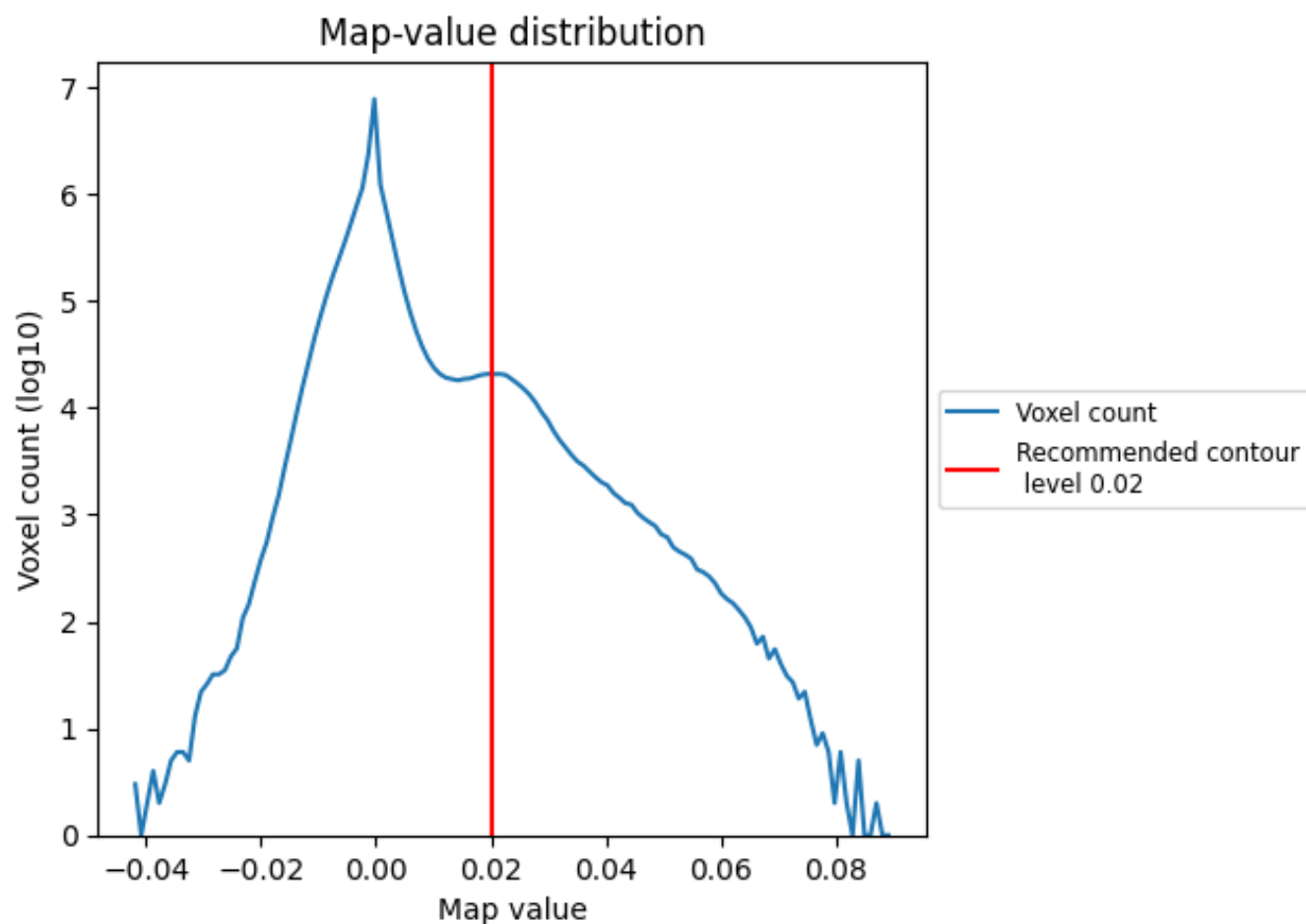
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

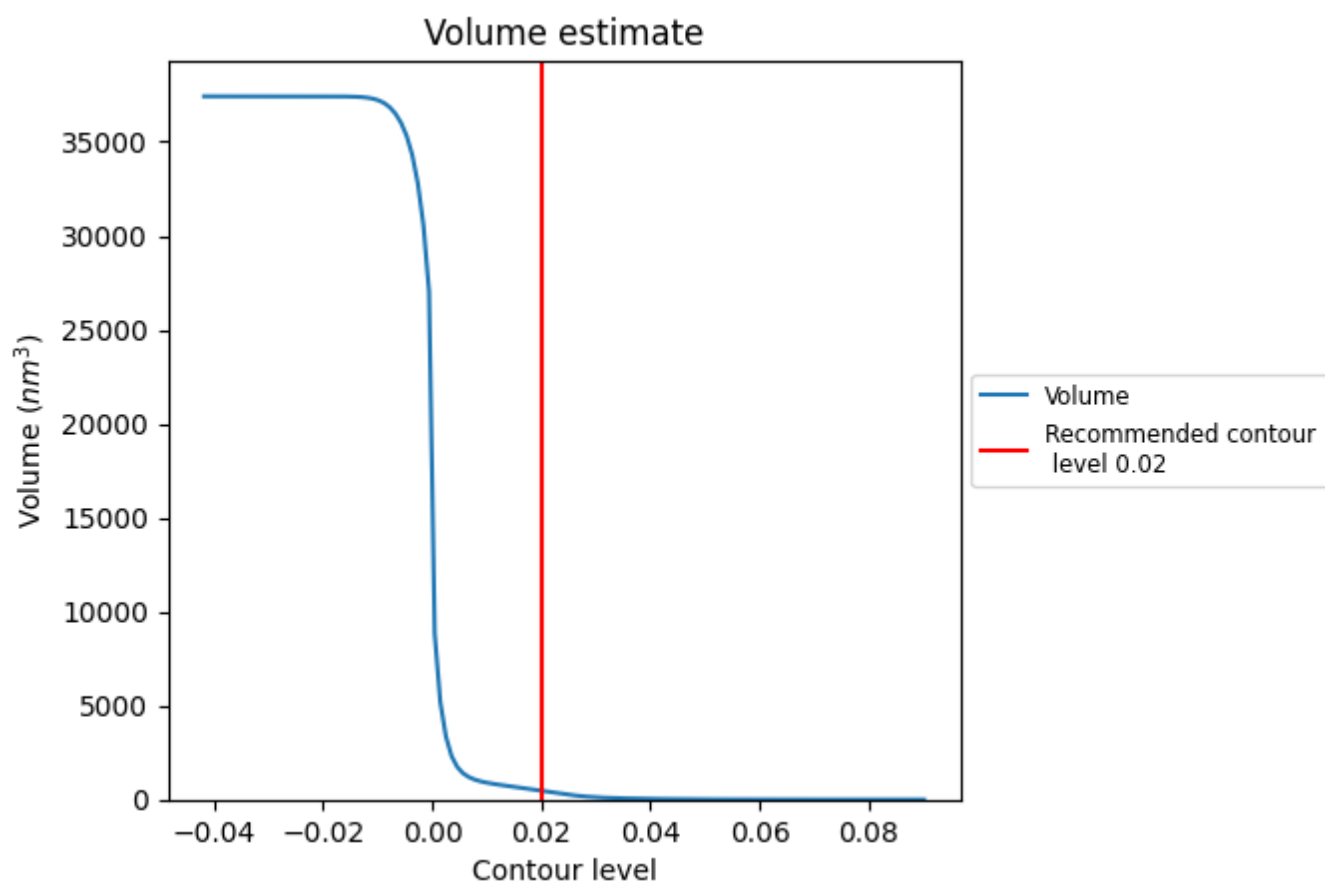
This section contains the results of statistical analysis of the map.

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.

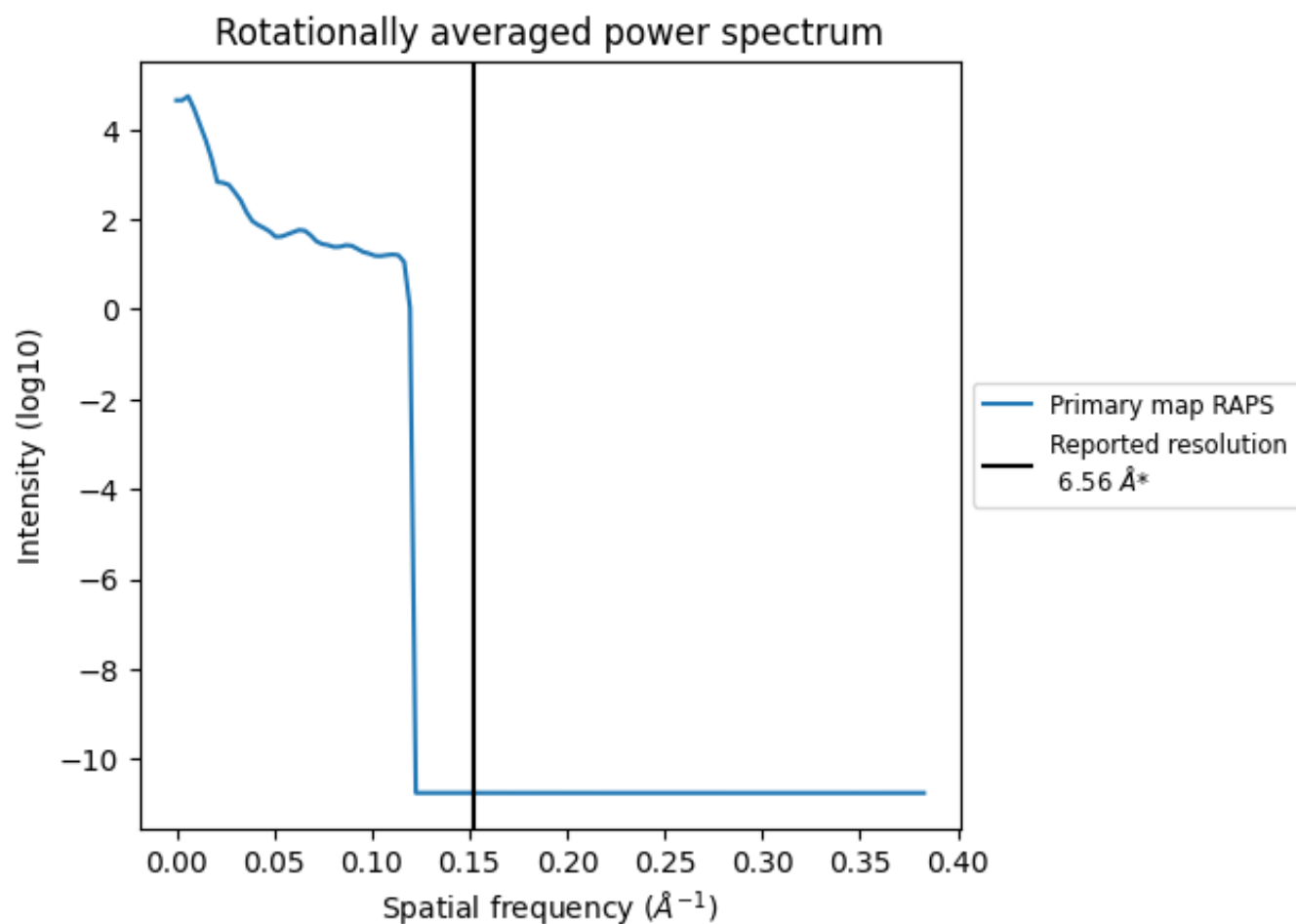
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 471 nm³; this corresponds to an approximate mass of 425 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

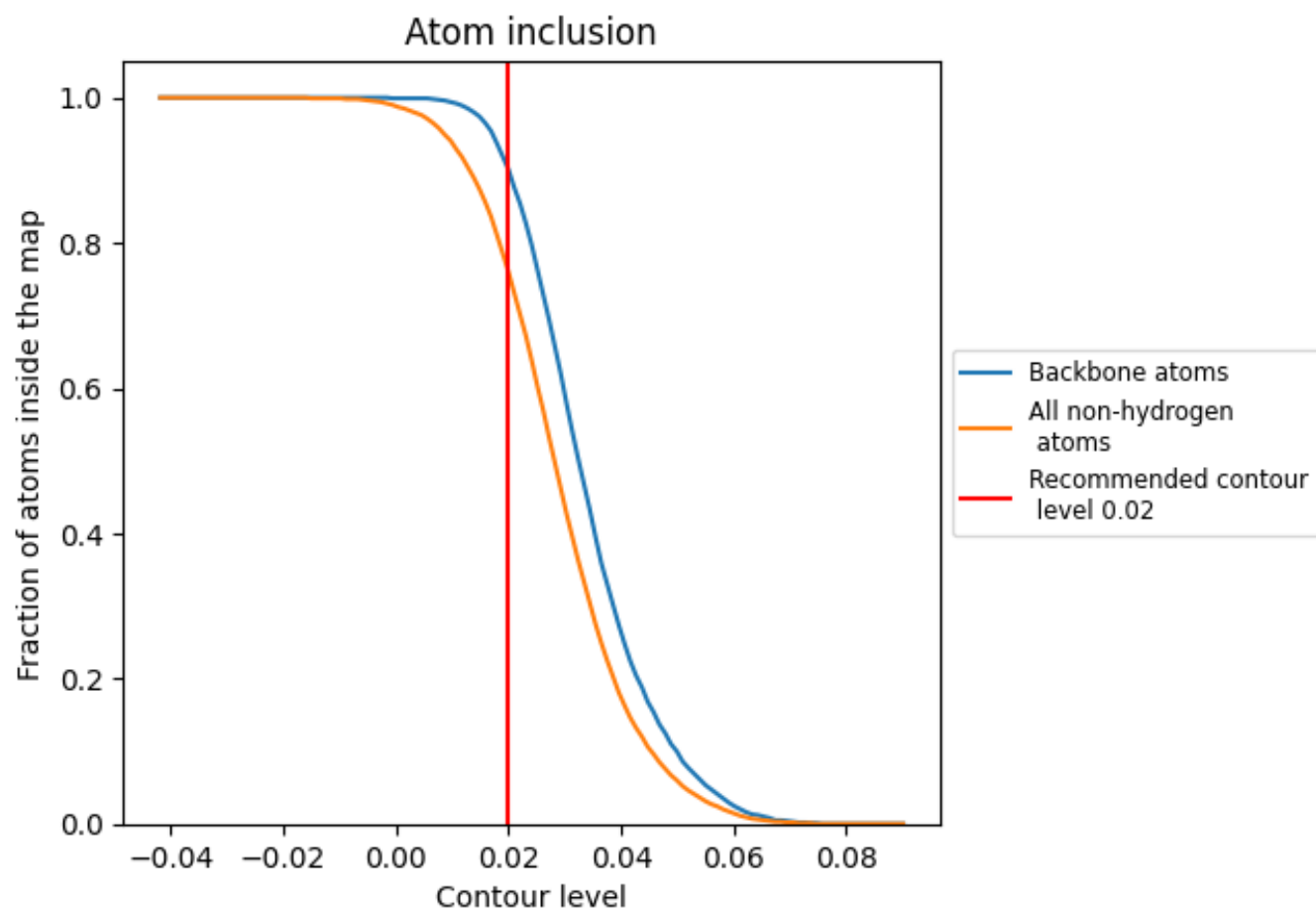


*Reported resolution corresponds to spatial frequency of 0.152 $\text{\AA}^{-1}$

8 Fourier-Shell correlation

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

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 76% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7600	 0.1400
A	 0.7690	 0.1550
B	 0.8210	 0.1610
C	 0.7490	 0.1050
D	 0.7890	 0.1200
E	 0.7250	 0.1120
F	 0.7780	 0.1470
G	 0.7530	 0.1110
H	 0.7900	 0.1460
I	 0.3210	 0.0630
J	 0.8460	 0.1830
K	 0.8210	 0.2580
L	 0.7800	 0.2320
M	 0.0710	 0.1200
N	 0.2140	 0.0730
O	 0.1070	 0.0200
P	 0.7140	 0.1440

