



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 12:59 PM UTC

PDB ID : 6WZT / pdb_00006wzt
EMDB ID : EMD-21973
Title : CryoEM structure of influenza hemagglutinin A/Victoria/361/2011 in complex with cyno antibody 3B10
Authors : Qiu, Y.; Zhou, Y.; Darricarrere, N.
Deposited on : 2020-05-14
Resolution : 4.70 Å(reported)

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

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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:

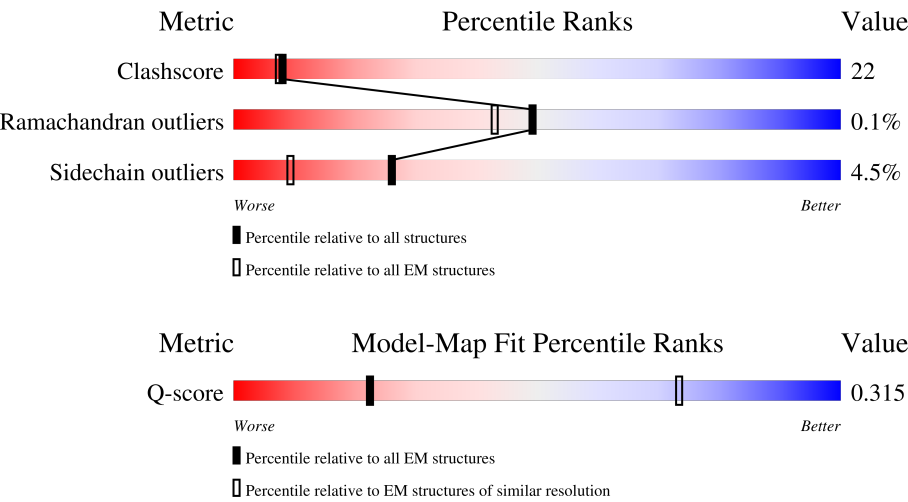
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 4.70 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	1989 (4.20 - 5.20)

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	503	69%26%..
1	B	503	69%27%..
1	C	503	69%27%..
2	E	233	42% 59%33%..

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Mol	Chain	Length	Quality of chain
2	G	233	
2	H	233	
3	D	214	
3	F	214	
3	L	214	
4	I	2	
4	M	2	
4	P	2	
4	S	2	
4	V	2	
4	Y	2	
5	J	3	
5	K	3	
5	N	3	
5	O	3	
5	Q	3	
5	R	3	
5	T	3	
5	U	3	
5	W	3	
5	X	3	
5	Z	3	
5	a	3	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 22368 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	494	Total	C	N	O	S	0	0
			3916	2449	695	754	18		
1	B	494	Total	C	N	O	S	0	0
			3916	2449	695	754	18		
1	C	494	Total	C	N	O	S	0	0
			3916	2449	695	754	18		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	98	PHE	TYR	conflict	UNP A0A075EV12
B	98	PHE	TYR	conflict	UNP A0A075EV12
C	98	PHE	TYR	conflict	UNP A0A075EV12

- Molecule 2 is a protein called Cyno antibody heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	225	Total	C	N	O	S	0	0
			1691	1073	279	333	6		
2	E	225	Total	C	N	O	S	0	0
			1691	1073	279	333	6		
2	G	225	Total	C	N	O	S	0	0
			1691	1073	279	333	6		

- Molecule 3 is a protein called Cyno antibody light chain.

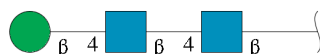
Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	214	Total	C	N	O	S	0	0
			1623	1011	272	334	6		
3	D	214	Total	C	N	O	S	0	0
			1623	1011	272	334	6		
3	F	214	Total	C	N	O	S	0	0
			1623	1011	272	334	6		

- 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	I	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	P	2	Total	C	N	O	0	0
			28	16	2	10		
4	S	2	Total	C	N	O	0	0
			28	16	2	10		
4	V	2	Total	C	N	O	0	0
			28	16	2	10		
4	Y	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.



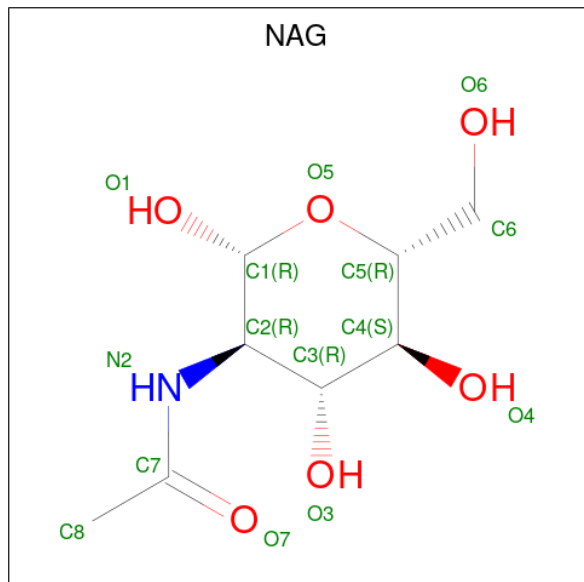
Mol	Chain	Residues	Atoms				AltConf	Trace
5	J	3	Total	C	N	O	0	0
			39	22	2	15		
5	K	3	Total	C	N	O	0	0
			39	22	2	15		
5	N	3	Total	C	N	O	0	0
			39	22	2	15		
5	O	3	Total	C	N	O	0	0
			39	22	2	15		
5	Q	3	Total	C	N	O	0	0
			39	22	2	15		
5	R	3	Total	C	N	O	0	0
			39	22	2	15		
5	T	3	Total	C	N	O	0	0
			39	22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

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Mol	Chain	Residues	Atoms				AltConf	Trace
5	U	3	Total	C	N	O	0	0
			39	22	2	15		
5	W	3	Total	C	N	O	0	0
			39	22	2	15		
5	X	3	Total	C	N	O	0	0
			39	22	2	15		
5	Z	3	Total	C	N	O	0	0
			39	22	2	15		
5	a	3	Total	C	N	O	0	0
			39	22	2	15		

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

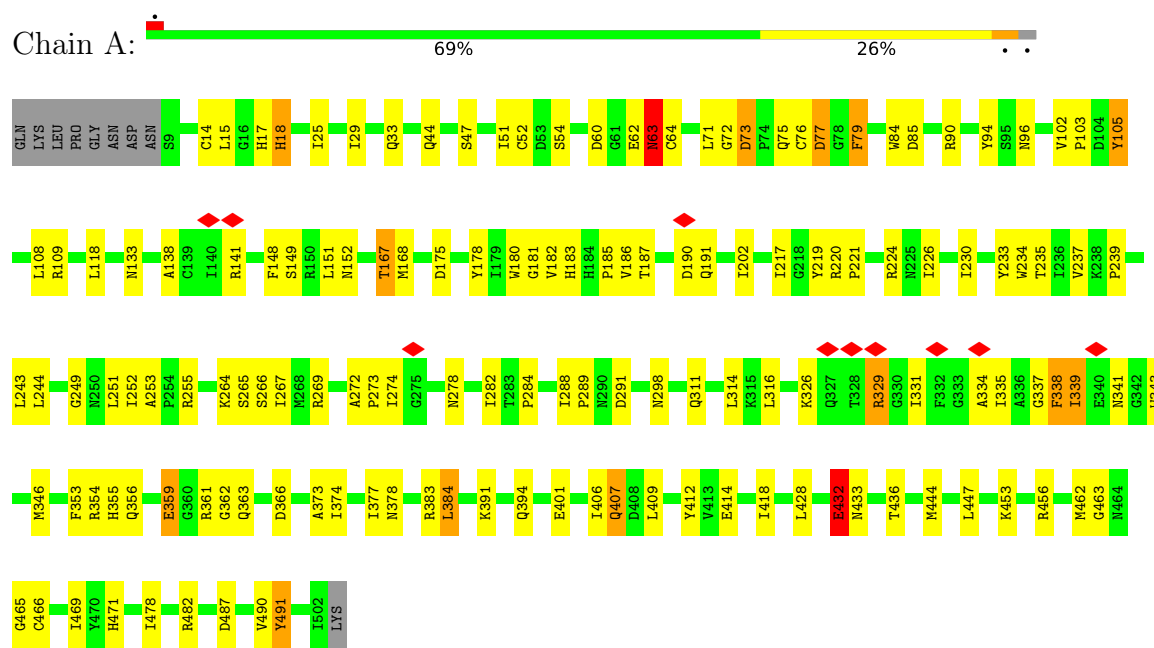


Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	

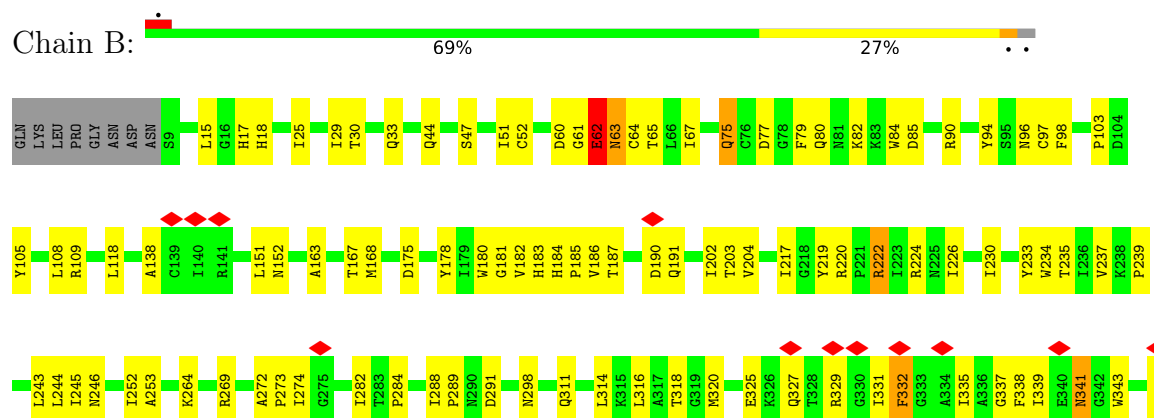
3 Residue-property plots

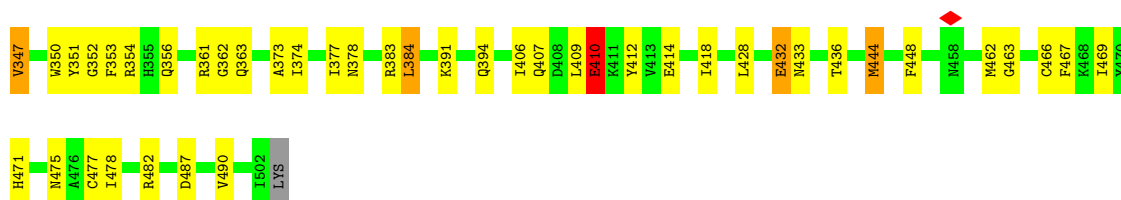
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Hemagglutinin

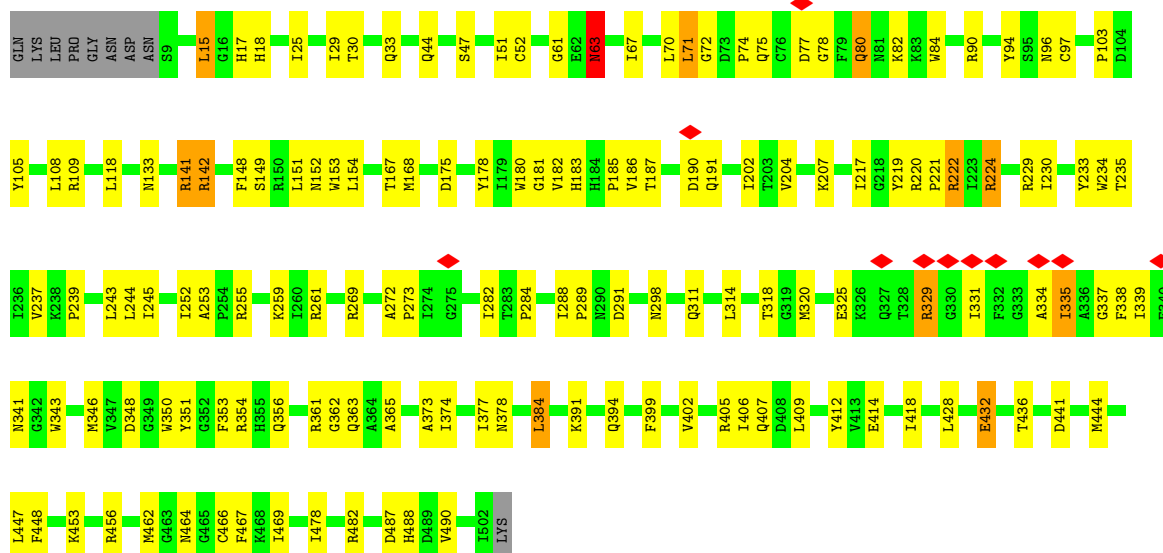


• Molecule 1: Hemagglutinin

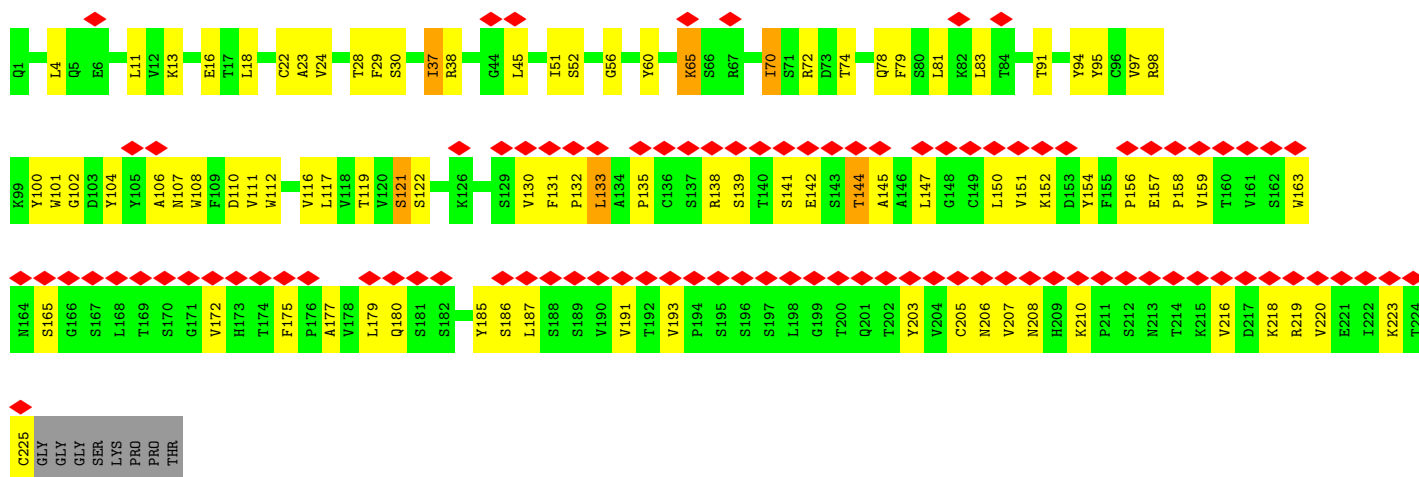
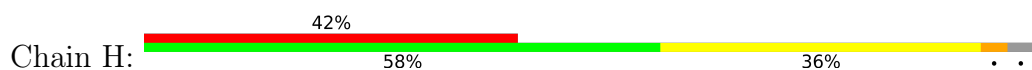




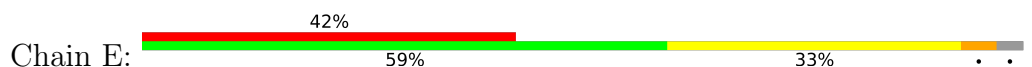
• Molecule 1: Hemagglutinin

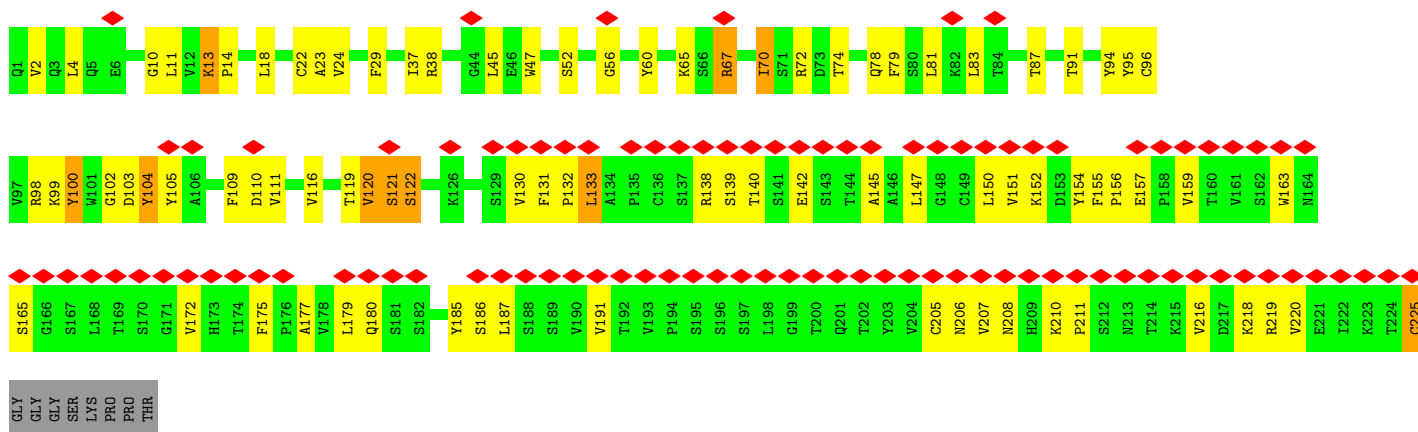


• Molecule 2: Cyno antibody heavy chain

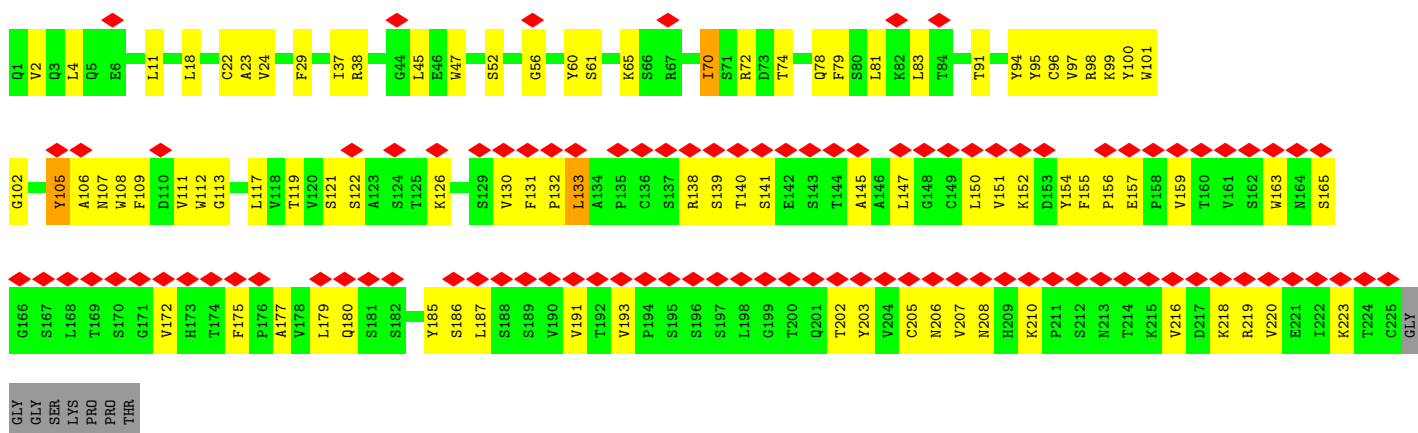
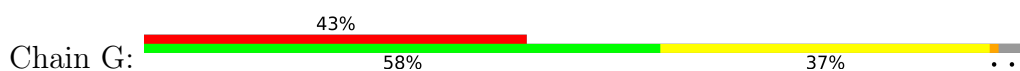


• Molecule 2: Cyno antibody heavy chain

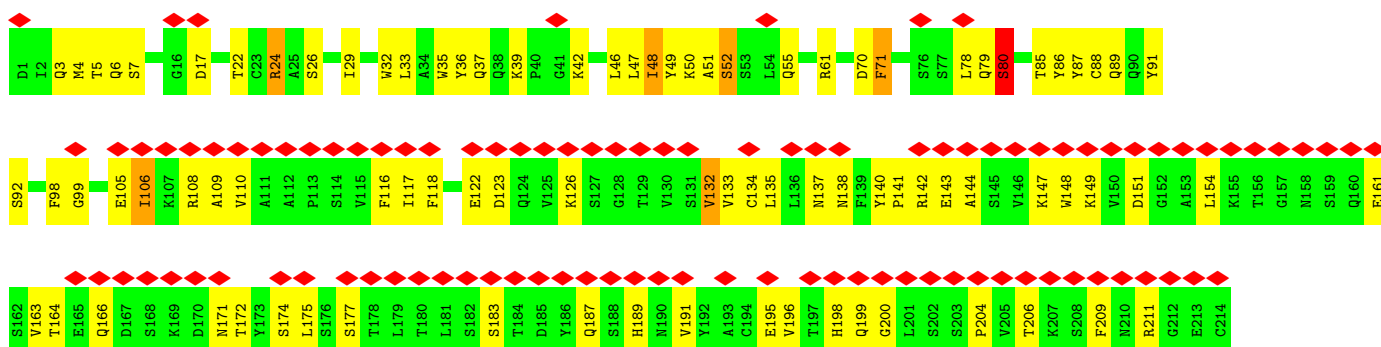




• Molecule 2: Cyno antibody heavy chain

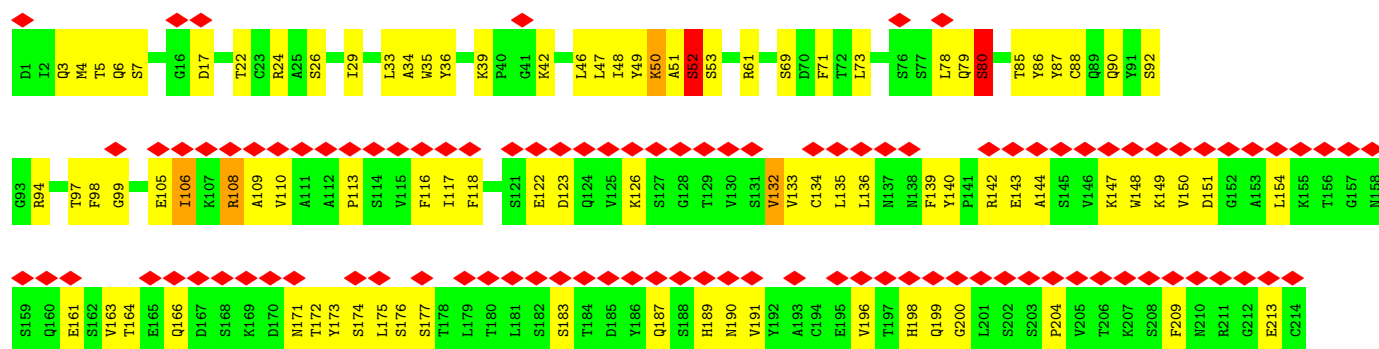


• Molecule 3: Cyno antibody light chain

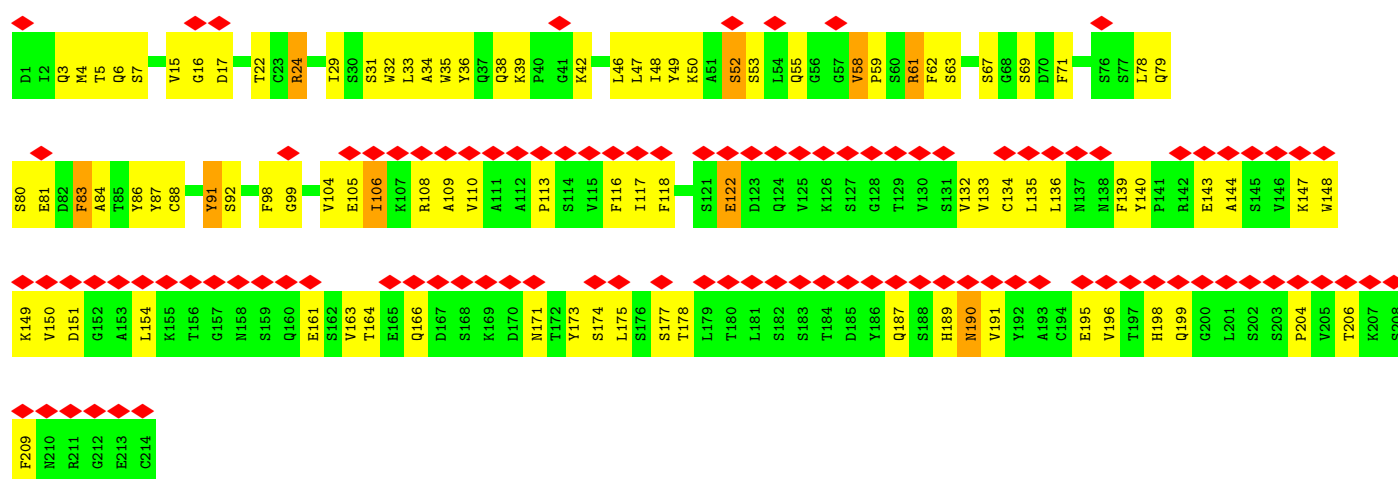


• Molecule 3: Cyno antibody light chain





• Molecule 3: Cyno antibody light chain

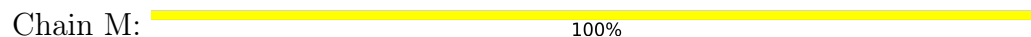


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



MAG1
MAG2

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



MAG1
MAG2

• 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

Chain S:



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

Chain V:



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

Chain Y:



- 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:



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

Chain K:



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

Chain N:



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

Chain O: 100%



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

Chain Q: 100%



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

Chain R: 33% 100%



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

Chain T: 33% 67%



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

Chain U: 67% 33%

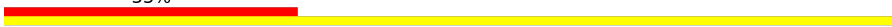


- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W: 33% 67%

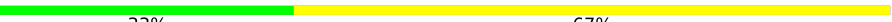


- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:  33% 100%

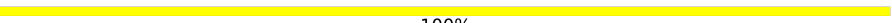


- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:  33% 67%



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

Chain a:  100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	114332	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 ($e^-/\text{\AA}^2$)	42	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.055	Depositor
Minimum map value	-0.029	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	265.0, 265.0, 265.0	wwPDB
Map dimensions	250, 250, 250	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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

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	0.67	4/3997 (0.1%)	1.13	11/5411 (0.2%)
1	B	0.52	0/3997	1.12	10/5411 (0.2%)
1	C	0.52	0/3997	1.11	8/5411 (0.1%)
2	E	0.77	4/1737 (0.2%)	1.06	6/2375 (0.3%)
2	G	0.63	3/1737 (0.2%)	1.00	0/2375
2	H	0.65	3/1737 (0.2%)	0.97	1/2375 (0.0%)
3	D	0.92	3/1658 (0.2%)	1.06	3/2251 (0.1%)
3	F	0.75	4/1658 (0.2%)	1.11	4/2251 (0.2%)
3	L	0.67	3/1658 (0.2%)	1.05	2/2251 (0.1%)
All	All	0.66	24/22176 (0.1%)	1.09	45/30111 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	80	SER	CB-OG	25.02	1.92	1.42
1	A	77	ASP	CG-OD1	19.45	1.62	1.25
2	E	121	SER	CA-CB	-13.25	1.33	1.53
2	E	122	SER	CA-CB	-13.04	1.31	1.53
3	F	52	SER	CA-CB	-12.02	1.33	1.53
1	A	141	ARG	CZ-NH2	11.88	1.48	1.33
1	A	77	ASP	CG-OD2	9.57	1.43	1.25
2	H	225	CYS	C-O	8.64	1.40	1.23
2	G	121	SER	CA-CB	-8.12	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	121	SER	CA-CB	-7.25	1.42	1.52
2	E	67	ARG	CZ-NH1	-7.08	1.22	1.32
3	L	80	SER	CB-OG	6.77	1.55	1.42
2	H	122	SER	CA-CB	-6.62	1.43	1.53
3	L	52	SER	CB-OG	-6.60	1.28	1.42
1	A	141	ARG	CD-NE	6.45	1.55	1.46
2	G	122	SER	CB-OG	6.31	1.54	1.42
2	E	225	CYS	C-O	-6.21	1.11	1.23
3	D	108	ARG	CZ-NH2	6.20	1.41	1.33
2	G	122	SER	CA-CB	-6.07	1.42	1.53
3	F	81	GLU	CD-OE1	-6.02	1.14	1.25
3	L	189	HIS	CG-ND1	-5.93	1.31	1.38
3	F	63	SER	CB-OG	-5.68	1.30	1.42
3	F	122	GLU	CD-OE1	-5.49	1.15	1.25
3	D	52	SER	CA-CB	-5.47	1.44	1.53

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	329	ARG	NE-CZ-NH1	-9.80	111.70	121.50
2	E	121	SER	CB-CA-C	-8.64	97.85	111.51
1	A	141	ARG	NE-CZ-NH2	-8.63	111.43	119.20
1	B	224	ARG	NE-CZ-NH2	-8.14	111.88	119.20
1	B	97	CYS	CA-CB-SG	-7.85	96.34	114.40
1	C	97	CYS	CA-CB-SG	-7.63	96.86	114.40
1	C	291	ASP	CA-CB-CG	7.61	120.21	112.60
1	C	80	GLN	OE1-CD-NE2	7.08	129.68	122.60
1	A	141	ARG	CB-CG-CD	-7.08	95.02	111.30
3	L	52	SER	CB-CA-C	-7.01	102.10	111.63
1	B	64	CYS	CB-CA-C	-6.66	95.46	109.38
1	B	222	ARG	CB-CG-CD	-6.62	96.07	111.30
2	H	219	ARG	NE-CZ-NH1	-6.50	115.00	121.50
3	F	61	ARG	NE-CZ-NH1	-6.25	115.25	121.50
1	C	222	ARG	CB-CG-CD	-6.25	96.94	111.30
1	B	410	GLU	CB-CA-C	-6.04	100.58	110.85
3	F	61	ARG	NE-CZ-NH2	6.03	124.63	119.20
1	A	291	ASP	CA-CB-CG	5.92	118.52	112.60
1	A	141	ARG	NH1-CZ-NH2	5.89	126.96	119.30
1	C	432	GLU	CB-CG-CD	5.84	122.52	112.60
3	L	24	ARG	NE-CZ-NH1	-5.81	115.69	121.50
3	D	190	ASN	OD1-CG-ND2	5.79	128.39	122.60
1	A	63	ASN	N-CA-CB	5.77	120.24	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	52	SER	CA-CB-OG	-5.76	99.57	111.10
2	E	219	ARG	NH1-CZ-NH2	5.76	126.79	119.30
1	B	64	CYS	N-CA-C	5.61	118.37	109.50
1	C	291	ASP	CB-CA-C	5.59	120.93	110.70
3	D	3	GLN	OE1-CD-NE2	-5.53	117.07	122.60
3	F	24	ARG	CG-CD-NE	5.40	123.88	112.00
2	E	121	SER	CA-C-N	-5.36	113.26	120.87
2	E	121	SER	C-N-CA	-5.36	113.26	120.87
1	B	62	GLU	CB-CA-C	5.29	120.95	110.42
2	E	67	ARG	CG-CD-NE	-5.28	100.39	112.00
1	B	63	ASN	CA-C-N	-5.20	114.52	122.62
1	B	63	ASN	C-N-CA	-5.20	114.52	122.62
1	A	77	ASP	CB-CA-C	-5.19	101.42	110.09
1	A	63	ASN	CB-CA-C	5.18	120.74	110.42
1	A	329	ARG	CB-CG-CD	5.18	123.22	111.30
1	A	432	GLU	CB-CG-CD	5.18	121.41	112.60
2	E	219	ARG	NE-CZ-NH2	-5.15	114.56	119.20
1	B	291	ASP	CA-CB-CG	5.10	117.70	112.60
1	A	77	ASP	CB-CG-OD1	-5.10	106.67	118.40
1	C	142	ARG	NE-CZ-NH1	-5.08	116.42	121.50
1	A	338	PHE	CA-CB-CG	5.06	118.86	113.80
3	D	50	LYS	CB-CA-C	-5.05	110.77	116.63

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	77	ASP	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	3916	0	3800	147	0
1	B	3916	0	3801	138	0
1	C	3916	0	3801	152	0
2	E	1691	0	1653	79	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	1691	0	1653	117	0
2	H	1691	0	1653	102	0
3	D	1623	0	1570	96	0
3	F	1623	0	1570	132	0
3	L	1623	0	1570	112	0
4	I	28	0	25	0	0
4	M	28	0	25	0	0
4	P	28	0	25	0	0
4	S	28	0	25	1	0
4	V	28	0	25	0	0
4	Y	28	0	25	0	0
5	J	39	0	34	1	0
5	K	39	0	34	0	0
5	N	39	0	34	5	0
5	O	39	0	34	0	0
5	Q	39	0	34	0	0
5	R	39	0	34	0	0
5	T	39	0	34	2	0
5	U	39	0	34	1	0
5	W	39	0	34	1	0
5	X	39	0	34	0	0
5	Z	39	0	34	0	0
5	a	39	0	34	0	0
6	A	14	0	13	4	0
6	B	14	0	13	0	0
6	C	14	0	13	0	0
All	All	22368	0	21668	974	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 22.

All (974) 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)
2:G:37:ILE:HG21	2:G:112:TRP:CZ3	1.37	1.56
1:C:329:ARG:CD	1:C:335:ILE:HG23	1.43	1.47
2:G:97:VAL:CG1	2:G:112:TRP:CE3	2.01	1.41
1:B:329:ARG:NH2	1:B:335:ILE:HD11	1.30	1.40
1:C:351:TYR:CE1	1:C:444:MET:SD	2.16	1.38
1:B:18:HIS:CE1	1:B:350:TRP:HA	1.60	1.37
2:G:37:ILE:CG2	2:G:112:TRP:HZ3	1.36	1.35

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:ARG:NH2	1:B:335:ILE:CD1	1.89	1.35
2:G:97:VAL:HG11	2:G:112:TRP:CE3	1.57	1.34
3:F:17:ASP:HB3	3:F:78:LEU:CD2	1.61	1.31
2:H:108:TRP:CE3	3:L:91:TYR:CD1	2.19	1.30
1:C:329:ARG:NE	1:C:335:ILE:CG2	1.97	1.28
1:C:351:TYR:CD1	1:C:444:MET:SD	2.27	1.27
2:G:97:VAL:HG11	2:G:112:TRP:CZ3	1.69	1.26
3:F:83:PHE:CE1	3:F:104:VAL:O	1.88	1.25
1:C:363:GLN:NE2	2:G:105:TYR:OH	1.73	1.18
3:F:17:ASP:HB3	3:F:78:LEU:HD21	1.24	1.18
3:F:17:ASP:N	3:F:78:LEU:HG	1.59	1.17
3:D:80:SER:CB	3:D:80:SER:OG	1.92	1.16
2:G:107:ASN:HB3	3:F:49:TYR:HB2	1.25	1.16
3:F:17:ASP:CB	3:F:78:LEU:HD21	1.79	1.13
1:A:329:ARG:NH2	2:H:30:SER:O	1.82	1.12
1:C:329:ARG:CD	1:C:335:ILE:CG2	2.26	1.11
1:C:329:ARG:NE	1:C:335:ILE:HG22	1.64	1.11
1:C:224:ARG:HB3	1:C:224:ARG:HH11	0.95	1.11
1:C:224:ARG:HH11	1:C:224:ARG:CB	1.62	1.11
1:C:18:HIS:NE2	1:C:350:TRP:HA	1.66	1.09
1:C:224:ARG:HB3	1:C:224:ARG:NH1	1.66	1.09
2:G:107:ASN:HB2	3:F:49:TYR:HB3	1.34	1.08
1:A:326:LYS:HG2	2:H:28:THR:HG21	1.30	1.08
1:C:329:ARG:HD3	1:C:335:ILE:HG23	1.28	1.08
1:C:18:HIS:CD2	1:C:350:TRP:HA	1.89	1.07
2:G:107:ASN:HB3	3:F:49:TYR:CB	1.86	1.06
1:C:329:ARG:HE	1:C:335:ILE:HG22	1.19	1.05
2:H:108:TRP:HE3	3:L:91:TYR:CE1	1.75	1.04
3:F:84:ALA:O	3:F:86:TYR:CD1	2.09	1.04
3:F:17:ASP:H	3:F:78:LEU:CG	1.70	1.04
1:B:18:HIS:CE1	1:B:350:TRP:CA	2.41	1.03
3:F:83:PHE:CD1	3:F:104:VAL:O	2.12	1.03
1:A:224:ARG:HH11	1:A:224:ARG:HB3	1.24	1.03
1:C:329:ARG:NE	1:C:335:ILE:HG23	1.65	1.02
1:C:337:GLY:HA2	1:C:343:TRP:HE1	1.20	1.02
3:F:15:VAL:HA	3:F:78:LEU:CD1	1.90	1.02
3:F:80:SER:HB2	3:F:106:ILE:HD13	1.41	1.02
3:F:15:VAL:CA	3:F:78:LEU:CD1	2.37	1.02
2:G:202:THR:HB	2:G:219:ARG:HD2	1.42	1.01
1:C:351:TYR:HE1	1:C:444:MET:SD	1.77	1.00
1:C:75:GLN:CD	1:C:96:ASN:HD21	1.69	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:107:ASN:CB	3:F:49:TYR:HB3	1.91	1.00
3:F:80:SER:HA	3:F:106:ILE:HD11	1.43	1.00
3:F:132:VAL:HG12	3:F:148:TRP:CZ2	1.96	0.99
2:G:37:ILE:HD13	2:G:112:TRP:CH2	1.99	0.98
2:E:133:LEU:HD11	3:D:118:PHE:HB3	1.44	0.97
2:G:107:ASN:CB	3:F:49:TYR:CB	2.41	0.97
3:F:17:ASP:HB3	3:F:78:LEU:HD23	1.45	0.97
1:A:237:VAL:HG13	1:A:243:LEU:CD1	1.94	0.97
3:F:46:LEU:HD23	3:F:55:GLN:OE1	1.65	0.97
3:F:15:VAL:CA	3:F:78:LEU:HD11	1.87	0.96
2:H:133:LEU:HD11	3:L:118:PHE:HB3	1.45	0.96
3:D:29:ILE:HG23	3:D:92:SER:HB2	1.44	0.96
2:H:135:PRO:HD3	2:H:147:LEU:HD23	1.48	0.96
3:F:83:PHE:HE1	3:F:104:VAL:O	1.31	0.96
3:F:132:VAL:CG1	3:F:148:TRP:CZ2	2.50	0.94
3:F:15:VAL:C	3:F:78:LEU:HD11	1.92	0.94
1:B:222:ARG:HH21	5:N:2:NAG:H3	1.33	0.94
1:A:237:VAL:CG1	1:A:243:LEU:CD1	2.46	0.94
2:H:108:TRP:CE3	3:L:91:TYR:CE1	2.52	0.93
1:B:329:ARG:CZ	1:B:335:ILE:CD1	2.47	0.93
2:E:121:SER:OG	2:E:121:SER:O	1.78	0.93
1:C:329:ARG:HD3	1:C:335:ILE:CG2	1.96	0.93
2:G:97:VAL:CG1	2:G:112:TRP:CD2	2.51	0.93
2:H:106:ALA:HB3	3:L:50:LYS:CE	1.99	0.92
2:G:47:TRP:HD1	2:G:109:PHE:HZ	1.15	0.92
1:B:329:ARG:HH22	1:B:335:ILE:HD11	1.34	0.92
3:D:29:ILE:CG2	3:D:92:SER:HB2	1.98	0.92
3:F:15:VAL:HA	3:F:78:LEU:HD12	1.47	0.92
2:H:223:LYS:HD2	3:L:122:GLU:OE1	1.70	0.92
2:G:97:VAL:HG13	2:G:112:TRP:CE3	2.00	0.92
3:F:31:SER:O	3:F:50:LYS:HG3	1.69	0.92
1:B:18:HIS:HE1	1:B:350:TRP:HA	1.35	0.92
1:A:224:ARG:HB3	1:A:224:ARG:NH1	1.86	0.91
2:H:108:TRP:CE3	3:L:91:TYR:HD1	1.73	0.91
2:H:147:LEU:CD1	2:H:203:TYR:HD2	1.85	0.90
1:B:339:ILE:HG12	1:B:444:MET:HE3	1.52	0.90
1:C:363:GLN:HB3	2:G:105:TYR:CE2	2.06	0.90
1:A:224:ARG:HH11	1:A:224:ARG:CB	1.85	0.90
1:C:18:HIS:HE2	1:C:350:TRP:HA	1.31	0.89
3:F:80:SER:HB2	3:F:106:ILE:CD1	2.03	0.89
1:B:337:GLY:HA3	1:B:343:TRP:HE1	1.35	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:17:ASP:CB	3:F:78:LEU:CD2	2.41	0.89
3:F:106:ILE:HD12	3:F:171:ASN:HB2	1.55	0.88
3:F:5:THR:HB	3:F:24:ARG:HB2	1.53	0.88
3:D:51:ALA:O	3:D:52:SER:HB3	1.71	0.88
3:D:29:ILE:HG23	3:D:92:SER:CB	2.03	0.87
2:H:37:ILE:HD11	2:H:45:LEU:HD12	1.55	0.87
1:B:329:ARG:HH21	1:B:335:ILE:CD1	1.80	0.87
1:B:329:ARG:CZ	1:B:335:ILE:HD11	2.04	0.87
3:F:143:GLU:HB3	3:F:199:GLN:HB2	1.57	0.86
1:A:462:MET:HB2	1:A:466:CYS:HB2	1.54	0.86
1:A:237:VAL:CG1	1:A:243:LEU:HD13	2.05	0.86
3:D:143:GLU:HB3	3:D:199:GLN:HB2	1.57	0.85
2:G:60:TYR:HB2	2:G:65:LYS:HG2	1.59	0.85
3:F:17:ASP:H	3:F:78:LEU:HG	0.76	0.85
3:D:29:ILE:CG2	3:D:92:SER:CB	2.54	0.85
2:G:97:VAL:HG11	2:G:112:TRP:CD2	2.11	0.85
3:L:29:ILE:CG2	3:L:92:SER:CB	2.55	0.85
1:A:237:VAL:CG2	1:A:243:LEU:HD13	2.08	0.84
2:G:37:ILE:HD11	2:G:45:LEU:HD12	1.59	0.84
3:D:118:PHE:HD2	3:D:133:VAL:HB	1.43	0.84
1:B:406:ILE:O	1:B:409:LEU:HG	1.77	0.84
3:F:29:ILE:CG2	3:F:92:SER:HB2	2.06	0.84
1:C:220:ARG:NH1	1:C:229:ARG:HB2	1.93	0.83
3:F:46:LEU:CD2	3:F:55:GLN:OE1	2.27	0.83
3:F:29:ILE:CG2	3:F:92:SER:CB	2.56	0.83
3:L:29:ILE:CG2	3:L:92:SER:HB2	2.09	0.82
3:F:84:ALA:O	3:F:86:TYR:CE1	2.31	0.82
1:C:351:TYR:HD1	1:C:444:MET:SD	1.99	0.82
3:L:70:ASP:C	3:L:71:PHE:HD1	1.87	0.82
1:B:18:HIS:HE1	1:B:350:TRP:CA	1.87	0.82
1:C:462:MET:HB2	1:C:466:CYS:HB2	1.61	0.82
2:H:147:LEU:CD1	2:H:203:TYR:CD2	2.63	0.82
2:G:37:ILE:HG21	2:G:112:TRP:CH2	2.13	0.82
1:C:399:PHE:HB3	1:C:407:GLN:NE2	1.93	0.82
3:F:132:VAL:CG1	3:F:148:TRP:HZ2	1.90	0.82
2:G:102:GLY:HA3	2:G:105:TYR:HD2	1.42	0.81
2:H:147:LEU:HD11	2:H:203:TYR:HD2	1.46	0.81
3:L:144:ALA:HB2	3:L:198:HIS:HD2	1.46	0.81
2:H:106:ALA:HB3	3:L:50:LYS:HE3	1.61	0.81
1:A:17:HIS:O	1:A:343:TRP:HB2	1.81	0.81
2:H:133:LEU:CD2	3:L:118:PHE:HD2	1.93	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:84:ALA:O	3:F:86:TYR:HD1	1.61	0.81
1:A:326:LYS:HZ2	6:A:601:NAG:H83	1.46	0.81
3:F:80:SER:CA	3:F:106:ILE:HD11	2.11	0.81
1:B:462:MET:HB2	1:B:466:CYS:HB2	1.60	0.80
3:L:29:ILE:HG23	3:L:92:SER:CB	2.11	0.80
3:D:33:LEU:HD22	3:D:71:PHE:CD2	2.17	0.80
3:F:33:LEU:HD22	3:F:71:PHE:CD2	2.17	0.80
2:E:104:TYR:O	2:E:104:TYR:CD1	2.34	0.79
1:A:237:VAL:HG22	1:A:243:LEU:CD1	2.12	0.79
1:B:329:ARG:HH21	1:B:335:ILE:HD12	1.45	0.79
1:C:356:GLN:HG2	1:C:361:ARG:HG2	1.63	0.79
2:G:117:LEU:CD2	2:G:119:THR:HG23	2.12	0.79
3:F:78:LEU:HD12	3:F:78:LEU:O	1.83	0.79
2:E:104:TYR:O	2:E:104:TYR:HD1	1.63	0.79
1:A:406:ILE:O	1:A:409:LEU:HG	1.83	0.79
2:H:108:TRP:CZ3	3:L:91:TYR:HD1	2.01	0.79
3:L:61:ARG:NH2	3:L:79:GLN:OE1	2.16	0.79
3:F:29:ILE:HG21	3:F:92:SER:CB	2.13	0.79
1:A:237:VAL:CG2	1:A:243:LEU:CD1	2.60	0.78
3:F:17:ASP:HB2	3:F:78:LEU:HD21	1.64	0.78
1:B:362:GLY:HA2	2:E:102:GLY:HA2	1.66	0.78
3:D:5:THR:HB	3:D:24:ARG:HB2	1.65	0.78
1:C:363:GLN:HB3	2:G:105:TYR:HE2	1.45	0.78
2:G:133:LEU:HD11	3:F:118:PHE:HB3	1.63	0.78
1:C:406:ILE:O	1:C:409:LEU:HG	1.83	0.78
3:D:106:ILE:HD12	3:D:171:ASN:HB2	1.67	0.77
1:A:237:VAL:HG22	1:A:243:LEU:CD2	2.14	0.77
3:L:36:TYR:HE2	3:L:89:GLN:OE1	1.67	0.77
2:G:97:VAL:HG12	2:G:112:TRP:CD2	2.19	0.77
2:H:108:TRP:HB2	3:L:91:TYR:CZ	2.20	0.76
3:F:84:ALA:H	3:F:86:TYR:HE1	1.32	0.76
3:L:61:ARG:HH12	3:L:79:GLN:HG3	1.48	0.76
3:D:61:ARG:NH2	3:D:79:GLN:OE1	2.18	0.76
1:B:346:MET:CE	1:B:352:GLY:HA3	2.16	0.76
1:C:399:PHE:CB	1:C:407:GLN:HE21	1.97	0.76
1:A:362:GLY:HA2	2:H:102:GLY:HA2	1.67	0.76
3:D:150:VAL:HG11	3:D:189:HIS:HB3	1.67	0.76
2:G:91:THR:HG23	2:G:119:THR:HA	1.67	0.76
3:L:36:TYR:HD1	3:L:46:LEU:HA	1.49	0.76
1:C:329:ARG:HD2	1:C:335:ILE:HG23	1.59	0.76
1:A:337:GLY:HA2	1:A:343:TRP:HE1	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:GLN:HE22	1:B:289:PRO:HB2	1.50	0.76
3:D:118:PHE:CD2	3:D:133:VAL:HB	2.20	0.76
1:A:237:VAL:HG13	1:A:243:LEU:HD11	1.69	0.75
2:E:37:ILE:HD11	2:E:45:LEU:HD12	1.66	0.75
3:F:29:ILE:HG23	3:F:92:SER:CB	2.16	0.75
1:C:354:ARG:CZ	2:G:101:TRP:CZ2	2.70	0.75
1:A:326:LYS:NZ	6:A:601:NAG:H83	2.02	0.75
1:C:325:GLU:OE1	1:C:329:ARG:NH2	2.19	0.75
1:C:362:GLY:HA2	2:G:102:GLY:HA2	1.67	0.75
3:D:151:ASP:HB2	3:D:191:VAL:HB	1.66	0.75
2:G:99:LYS:HG2	2:G:108:TRP:CD1	2.22	0.75
1:B:151:LEU:HD23	1:B:252:ILE:HG21	1.68	0.75
1:A:44:GLN:HE22	1:A:289:PRO:HB2	1.52	0.75
2:G:47:TRP:CD1	2:G:109:PHE:HZ	2.04	0.75
1:A:151:LEU:HD23	1:A:252:ILE:HG21	1.67	0.75
2:H:147:LEU:HD11	2:H:203:TYR:CD2	2.21	0.75
2:G:97:VAL:CG1	2:G:112:TRP:CZ3	2.49	0.75
2:G:99:LYS:CG	2:G:108:TRP:CD1	2.70	0.74
3:D:61:ARG:HH12	3:D:79:GLN:HG3	1.51	0.74
1:C:44:GLN:HE22	1:C:289:PRO:HB2	1.51	0.74
1:C:151:LEU:HD23	1:C:252:ILE:HG21	1.67	0.74
3:F:38:GLN:O	3:F:84:ALA:HB1	1.87	0.74
2:H:106:ALA:HB3	3:L:50:LYS:HE2	1.70	0.74
2:G:97:VAL:HG12	2:G:112:TRP:CE3	2.20	0.73
3:F:80:SER:HA	3:F:106:ILE:CD1	2.16	0.73
1:B:329:ARG:NH2	1:B:335:ILE:HD12	1.97	0.73
3:L:29:ILE:HG21	3:L:92:SER:CB	2.18	0.73
2:H:91:THR:HG23	2:H:119:THR:HA	1.69	0.73
3:L:144:ALA:HA	3:L:198:HIS:HA	1.70	0.73
1:A:401:GLU:O	1:A:407:GLN:NE2	2.17	0.73
3:F:132:VAL:HG11	3:F:148:TRP:HZ2	1.53	0.73
2:G:102:GLY:HA3	2:G:105:TYR:CD2	2.24	0.72
2:H:133:LEU:HD22	3:L:118:PHE:HD2	1.54	0.72
3:D:17:ASP:HB3	3:D:78:LEU:HD12	1.72	0.72
3:L:106:ILE:HD12	3:L:171:ASN:HB2	1.70	0.72
1:C:329:ARG:HD3	1:C:335:ILE:HA	1.72	0.72
2:G:37:ILE:CG2	2:G:112:TRP:CZ3	2.28	0.72
3:F:29:ILE:HG23	3:F:92:SER:HB2	1.71	0.72
2:H:180:GLN:HE22	2:H:186:SER:HB3	1.54	0.72
3:D:36:TYR:HD1	3:D:46:LEU:HA	1.55	0.72
3:F:80:SER:CB	3:F:106:ILE:CD1	2.67	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:HIS:HE2	1:C:350:TRP:CD1	2.07	0.71
2:H:52:SER:HB3	2:H:56:GLY:H	1.56	0.71
3:L:61:ARG:HH12	3:L:79:GLN:CG	2.03	0.71
1:B:329:ARG:HG2	1:B:332:PHE:H	1.54	0.71
2:E:38:ARG:HB2	2:E:94:TYR:HE1	1.55	0.71
2:G:38:ARG:HB2	2:G:94:TYR:HE1	1.56	0.71
2:E:37:ILE:HG23	2:E:95:TYR:HB2	1.73	0.71
2:G:52:SER:HB3	2:G:56:GLY:H	1.56	0.71
3:L:5:THR:HB	3:L:24:ARG:HB2	1.73	0.71
1:A:75:GLN:O	1:A:76:CYS:SG	2.49	0.70
2:E:52:SER:HB3	2:E:56:GLY:H	1.56	0.70
2:E:180:GLN:HE22	2:E:186:SER:HB3	1.55	0.70
1:B:337:GLY:HA3	1:B:343:TRP:NE1	2.07	0.70
1:A:326:LYS:HG2	2:H:28:THR:CG2	2.18	0.70
1:B:18:HIS:HE1	1:B:350:TRP:CB	2.05	0.69
2:G:180:GLN:HE22	2:G:186:SER:HB3	1.55	0.69
1:A:335:ILE:HG12	2:H:101:TRP:CZ2	2.25	0.69
2:H:37:ILE:HG23	2:H:95:TYR:HB2	1.73	0.69
3:F:36:TYR:HD1	3:F:46:LEU:HA	1.58	0.69
1:C:363:GLN:OE1	2:G:101:TRP:CZ2	2.44	0.69
2:E:175:PHE:CE1	3:D:164:THR:HG23	2.27	0.69
2:E:216:VAL:HG12	2:E:218:LYS:HB2	1.74	0.69
3:F:29:ILE:HG21	3:F:92:SER:HB2	1.73	0.69
1:A:237:VAL:HG11	1:A:243:LEU:HD13	1.73	0.68
3:D:61:ARG:NH1	3:D:79:GLN:HG3	2.08	0.68
2:G:23:ALA:HA	2:G:78:GLN:OE1	1.94	0.68
2:E:122:SER:HB3	2:E:155:PHE:HE1	1.59	0.68
3:L:110:VAL:HG22	3:L:140:TYR:HD2	1.58	0.68
1:C:399:PHE:CB	1:C:407:GLN:NE2	2.54	0.68
2:G:216:VAL:HG12	2:G:218:LYS:HB2	1.75	0.68
3:F:83:PHE:HA	3:F:86:TYR:OH	1.93	0.68
2:H:216:VAL:HG12	2:H:218:LYS:HB2	1.76	0.68
2:G:37:ILE:HG23	2:G:95:TYR:HB2	1.74	0.68
3:L:61:ARG:NH1	3:L:79:GLN:HG3	2.08	0.68
1:A:235:THR:HG22	1:A:243:LEU:HD21	1.76	0.68
1:C:402:VAL:HA	1:C:407:GLN:OE1	1.93	0.68
3:D:61:ARG:HH12	3:D:79:GLN:CG	2.05	0.68
3:L:151:ASP:HB2	3:L:191:VAL:HB	1.76	0.68
3:D:29:ILE:HG21	3:D:92:SER:CB	2.24	0.68
1:B:346:MET:HE1	1:B:352:GLY:HA3	1.75	0.67
1:C:329:ARG:HD3	1:C:335:ILE:CA	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:202:THR:CB	2:G:219:ARG:HD2	2.21	0.67
2:H:38:ARG:HB2	2:H:94:TYR:HE1	1.60	0.67
3:L:29:ILE:HG21	3:L:92:SER:HB3	1.76	0.67
1:C:75:GLN:CD	1:C:96:ASN:ND2	2.50	0.67
3:L:29:ILE:HG23	3:L:92:SER:HB2	1.72	0.67
3:D:113:PRO:HB3	3:D:139:PHE:HB3	1.76	0.67
3:D:116:PHE:HB2	3:D:135:LEU:HB3	1.76	0.67
1:C:18:HIS:CD2	1:C:350:TRP:CA	2.75	0.67
1:C:325:GLU:OE1	1:C:329:ARG:CZ	2.43	0.67
3:F:151:ASP:HB2	3:F:191:VAL:HB	1.75	0.67
2:G:61:SER:O	2:G:65:LYS:HG3	1.95	0.67
1:A:329:ARG:HG3	1:A:331:ILE:H	1.60	0.67
2:G:37:ILE:HD13	2:G:112:TRP:HH2	1.56	0.67
2:G:117:LEU:HD21	2:G:119:THR:HG23	1.75	0.67
3:D:144:ALA:HB2	3:D:198:HIS:HD2	1.60	0.67
2:H:175:PHE:HE1	3:L:174:SER:O	1.77	0.67
1:B:329:ARG:CZ	1:B:335:ILE:HD13	2.24	0.66
3:F:132:VAL:HG11	3:F:148:TRP:CZ2	2.25	0.66
1:C:220:ARG:HH11	1:C:229:ARG:HB2	1.60	0.66
3:F:15:VAL:C	3:F:78:LEU:CD1	2.63	0.66
1:B:346:MET:HE1	1:B:351:TYR:C	2.20	0.66
2:H:23:ALA:HA	2:H:78:GLN:OE1	1.95	0.66
3:F:29:ILE:HG21	3:F:92:SER:HB3	1.78	0.66
1:A:237:VAL:HG22	1:A:243:LEU:HD11	1.78	0.66
1:C:17:HIS:HB3	1:C:444:MET:CE	2.26	0.66
3:D:33:LEU:HD22	3:D:71:PHE:HD2	1.58	0.65
1:C:67:ILE:HG13	1:C:105:TYR:HE1	1.60	0.65
1:C:222:ARG:HH21	5:T:2:NAG:H3	1.61	0.65
2:E:133:LEU:HD21	3:D:118:PHE:HD1	1.60	0.65
1:C:337:GLY:HA2	1:C:343:TRP:NE1	2.04	0.65
3:D:183:SER:O	3:D:187:GLN:HG3	1.97	0.65
1:A:337:GLY:CA	1:A:343:TRP:HE1	2.10	0.65
2:G:109:PHE:HB3	2:G:112:TRP:CZ2	2.31	0.65
3:L:17:ASP:HB3	3:L:78:LEU:HD12	1.78	0.65
2:E:23:ALA:HA	2:E:78:GLN:OE1	1.96	0.65
3:D:106:ILE:H	3:D:171:ASN:CG	2.05	0.65
1:C:17:HIS:O	1:C:343:TRP:HB2	1.97	0.65
3:F:52:SER:OG	3:F:53:SER:N	2.29	0.65
1:C:220:ARG:HH11	1:C:229:ARG:CG	2.09	0.64
3:F:106:ILE:H	3:F:171:ASN:CG	2.04	0.64
3:F:150:VAL:HG11	3:F:189:HIS:HB3	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:HIS:O	1:B:343:TRP:HB2	1.97	0.64
3:L:49:TYR:HE1	3:L:55:GLN:HB2	1.63	0.64
1:B:335:ILE:HG13	1:B:354:ARG:HH11	1.62	0.64
3:L:106:ILE:H	3:L:171:ASN:CG	2.05	0.64
3:D:52:SER:O	3:D:52:SER:OG	2.13	0.64
2:G:131:PHE:HB2	2:G:150:LEU:HB3	1.80	0.64
3:F:38:GLN:C	3:F:84:ALA:HB1	2.21	0.64
1:A:487:ASP:OD2	1:A:490:VAL:HG23	1.97	0.64
2:H:133:LEU:HD21	3:L:118:PHE:HD2	1.63	0.64
1:A:237:VAL:HG21	1:A:243:LEU:HD13	1.77	0.64
1:B:67:ILE:HG13	1:B:105:TYR:HE1	1.61	0.64
1:A:237:VAL:HG22	1:A:243:LEU:HD21	1.79	0.63
3:F:80:SER:CB	3:F:106:ILE:HD11	2.28	0.63
3:L:33:LEU:HD22	3:L:71:PHE:HD2	1.64	0.63
1:B:346:MET:HE1	1:B:352:GLY:CA	2.28	0.63
3:D:47:LEU:HD23	3:D:73:LEU:HD11	1.79	0.63
1:B:325:GLU:O	1:B:325:GLU:HG3	1.97	0.63
2:E:29:PHE:HZ	2:E:72:ARG:HB2	1.63	0.63
1:A:64:CYS:SG	1:A:73:ASP:OD2	2.56	0.63
2:H:131:PHE:HB2	2:H:150:LEU:HB3	1.81	0.63
2:H:135:PRO:HD3	2:H:147:LEU:CD2	2.25	0.63
1:A:237:VAL:CG2	1:A:243:LEU:CD2	2.77	0.63
3:L:166:GLN:HB3	3:L:171:ASN:HA	1.81	0.63
3:D:33:LEU:HD11	3:D:88:CYS:HB2	1.80	0.63
3:F:33:LEU:HD22	3:F:71:PHE:HD2	1.62	0.63
2:H:117:LEU:HD21	2:H:119:THR:HG23	1.81	0.63
3:L:140:TYR:HA	3:L:172:THR:HG22	1.81	0.63
2:G:60:TYR:O	2:G:65:LYS:HE2	1.97	0.63
3:L:110:VAL:HA	3:L:140:TYR:HB3	1.81	0.62
3:L:116:PHE:HB2	3:L:135:LEU:HB3	1.80	0.62
3:L:144:ALA:HB2	3:L:198:HIS:CD2	2.33	0.62
1:B:346:MET:HG2	1:B:363:GLN:CD	2.24	0.62
2:E:131:PHE:HB2	2:E:150:LEU:HB3	1.81	0.62
2:H:180:GLN:NE2	2:H:186:SER:HB3	2.14	0.62
3:D:144:ALA:HA	3:D:198:HIS:HA	1.80	0.62
1:B:353:PHE:HE2	1:B:482:ARG:HG3	1.65	0.62
1:A:167:THR:HG22	5:N:1:NAG:H81	1.82	0.62
3:D:29:ILE:HG21	3:D:92:SER:HB3	1.81	0.62
2:G:29:PHE:HZ	2:G:72:ARG:HB2	1.64	0.62
3:D:166:GLN:HB3	3:D:171:ASN:HA	1.80	0.61
1:B:346:MET:HE1	1:B:352:GLY:N	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:SER:OG	1:A:278:ASN:HA	2.01	0.61
2:E:133:LEU:HD21	3:D:118:PHE:CD1	2.36	0.61
2:G:11:LEU:HA	2:G:119:THR:O	2.00	0.61
3:F:166:GLN:HB3	3:F:171:ASN:HA	1.81	0.61
1:B:152:ASN:ND2	4:S:1:NAG:O7	2.31	0.61
1:C:331:ILE:O	1:C:361:ARG:NH2	2.28	0.61
2:G:47:TRP:HD1	2:G:109:PHE:CZ	2.07	0.61
1:A:462:MET:HB2	1:A:466:CYS:CB	2.30	0.61
1:C:335:ILE:HG22	1:C:335:ILE:O	2.00	0.61
3:F:147:LYS:HG3	3:F:195:GLU:HB2	1.83	0.61
2:G:180:GLN:NE2	2:G:186:SER:HB3	2.16	0.61
2:H:29:PHE:HZ	2:H:72:ARG:HB2	1.65	0.60
3:D:34:ALA:O	3:D:88:CYS:HA	2.00	0.60
3:F:132:VAL:HG12	3:F:148:TRP:CH2	2.35	0.60
1:A:15:LEU:HD11	1:A:447:LEU:CD2	2.31	0.60
3:L:142:ARG:O	3:L:142:ARG:HG2	2.01	0.60
2:E:175:PHE:CE2	3:D:176:SER:HB2	2.36	0.60
2:E:180:GLN:NE2	2:E:186:SER:HB3	2.15	0.60
3:D:140:TYR:HB2	3:D:172:THR:HG22	1.82	0.60
2:G:109:PHE:CB	2:G:112:TRP:CZ2	2.84	0.60
3:F:32:TRP:HB2	3:F:92:SER:HB2	1.82	0.60
1:B:75:GLN:O	1:B:75:GLN:HG3	2.00	0.60
1:B:222:ARG:NH2	5:N:2:NAG:H3	2.12	0.60
1:A:237:VAL:CG2	1:A:243:LEU:HD22	2.31	0.60
2:H:60:TYR:HE1	2:H:70:ILE:HG23	1.65	0.60
1:B:351:TYR:CE1	1:B:444:MET:HG2	2.36	0.60
2:G:175:PHE:HE1	3:F:174:SER:O	1.85	0.60
1:A:335:ILE:HG21	1:A:354:ARG:NH1	2.17	0.60
1:A:79:PHE:HD1	1:A:79:PHE:H	1.49	0.59
1:A:79:PHE:N	1:A:79:PHE:CD1	2.69	0.59
1:A:84:TRP:HZ3	1:A:118:LEU:HG	1.67	0.59
3:L:147:LYS:HG3	3:L:195:GLU:HB2	1.83	0.59
1:B:353:PHE:CE2	1:B:482:ARG:HG3	2.36	0.59
2:G:97:VAL:HG11	2:G:112:TRP:CH2	2.30	0.59
2:G:99:LYS:HG2	2:G:100:TYR:H	1.67	0.59
2:H:133:LEU:CD1	3:L:118:PHE:HB3	2.27	0.59
1:C:219:TYR:OH	5:T:1:NAG:H4	2.02	0.59
1:A:103:PRO:HG2	1:A:233:TYR:HE1	1.66	0.59
2:E:91:THR:HG23	2:E:119:THR:HA	1.84	0.59
2:E:175:PHE:CD2	3:D:176:SER:HB2	2.38	0.59
1:C:354:ARG:NH2	2:G:101:TRP:CZ2	2.71	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:175:PHE:CE1	3:L:164:THR:HG23	2.37	0.58
1:C:348:ASP:OD2	1:C:365:ALA:HB2	2.03	0.58
1:A:384:LEU:HD11	1:A:428:LEU:HD21	1.84	0.58
1:B:384:LEU:HD11	1:B:428:LEU:HD21	1.85	0.58
1:B:18:HIS:ND1	1:B:350:TRP:HA	2.14	0.58
2:E:120:VAL:O	2:E:121:SER:HB3	2.02	0.58
3:F:105:GLU:HB2	3:F:171:ASN:OD1	2.03	0.58
1:B:346:MET:HG2	1:B:363:GLN:OE1	2.04	0.58
2:H:13:LYS:HB2	2:H:16:GLU:HG3	1.84	0.58
2:H:141:SER:HB3	2:H:144:THR:HG22	1.85	0.58
3:L:105:GLU:HB2	3:L:171:ASN:OD1	2.04	0.58
1:C:142:ARG:NH1	1:C:142:ARG:HG2	2.17	0.58
3:F:33:LEU:HG	3:F:34:ALA:N	2.18	0.58
1:A:311:GLN:HG2	1:A:314:LEU:HD21	1.86	0.57
1:A:335:ILE:HG22	1:A:335:ILE:O	2.04	0.57
1:A:85:ASP:O	1:A:265:SER:HA	2.04	0.57
2:G:60:TYR:HE1	2:G:70:ILE:HG23	1.70	0.57
1:A:334:ALA:HB2	1:A:356:GLN:HB2	1.87	0.57
1:B:346:MET:CG	1:B:363:GLN:OE1	2.53	0.57
2:E:133:LEU:CD1	3:D:118:PHE:HB3	2.26	0.57
3:D:105:GLU:HB2	3:D:171:ASN:OD1	2.04	0.57
2:H:104:TYR:O	2:H:104:TYR:CD1	2.58	0.57
2:H:133:LEU:HD21	3:L:118:PHE:CD2	2.39	0.57
2:E:179:LEU:HB2	2:E:185:TYR:HE1	1.69	0.57
1:C:456:ARG:HG3	1:C:488:HIS:CD2	2.40	0.57
1:A:167:THR:HG22	5:N:1:NAG:C8	2.34	0.57
1:B:347:VAL:N	2:E:100:TYR:OH	2.37	0.57
2:E:38:ARG:HB2	2:E:94:TYR:CE1	2.39	0.57
1:C:311:GLN:HG2	1:C:314:LEU:HD21	1.86	0.57
2:E:175:PHE:HE2	3:D:176:SER:CB	2.17	0.56
2:G:109:PHE:HB3	2:G:112:TRP:CE2	2.40	0.56
1:B:356:GLN:HG2	1:B:361:ARG:HG2	1.87	0.56
1:B:163:ALA:HB1	5:U:1:NAG:O3	2.05	0.56
2:G:29:PHE:CZ	2:G:72:ARG:HB2	2.40	0.56
3:F:110:VAL:HA	3:F:140:TYR:HB3	1.86	0.56
1:C:18:HIS:HE2	1:C:350:TRP:CG	2.22	0.56
1:C:220:ARG:HH11	1:C:229:ARG:CB	2.17	0.56
2:G:106:ALA:HB2	3:F:32:TRP:CZ3	2.41	0.56
1:B:311:GLN:HG2	1:B:314:LEU:HD21	1.86	0.56
1:C:384:LEU:HD11	1:C:428:LEU:HD21	1.86	0.56
1:A:490:VAL:HG12	1:A:491:TYR:CD1	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:29:PHE:CZ	2:E:72:ARG:HB2	2.41	0.56
1:A:326:LYS:NZ	6:A:601:NAG:C8	2.68	0.56
3:F:6:GLN:NE2	3:F:86:TYR:O	2.36	0.56
2:H:108:TRP:HB2	3:L:91:TYR:CE1	2.41	0.56
1:B:77:ASP:O	1:B:80:GLN:HG3	2.06	0.56
1:C:343:TRP:HB3	1:C:354:ARG:HH21	1.70	0.56
1:B:244:LEU:HD21	1:C:221:PRO:N	2.21	0.56
3:D:33:LEU:HG	3:D:34:ALA:N	2.19	0.55
3:F:80:SER:CA	3:F:106:ILE:CD1	2.79	0.55
1:A:47:SER:HA	1:A:288:ILE:HG22	1.89	0.55
1:C:487:ASP:OD2	1:C:490:VAL:HG23	2.06	0.55
2:G:163:TRP:CH2	2:G:205:CYS:HB3	2.41	0.55
3:F:144:ALA:HA	3:F:198:HIS:HA	1.87	0.55
2:H:29:PHE:CZ	2:H:72:ARG:HB2	2.41	0.55
2:G:107:ASN:N	3:F:91:TYR:CE2	2.73	0.55
2:H:121:SER:O	2:H:121:SER:OG	2.15	0.55
3:L:116:PHE:HE2	3:L:137:ASN:HB2	1.70	0.55
1:B:51:ILE:HG12	1:B:282:ILE:HD11	1.89	0.55
2:H:108:TRP:HE3	3:L:91:TYR:HE1	1.46	0.55
3:L:36:TYR:CE2	3:L:89:GLN:OE1	2.55	0.55
2:G:102:GLY:CA	2:G:105:TYR:HD2	2.18	0.55
3:L:70:ASP:C	3:L:71:PHE:CD1	2.77	0.55
3:L:142:ARG:O	3:L:142:ARG:CG	2.54	0.55
3:D:47:LEU:CD2	3:D:73:LEU:HD11	2.36	0.55
3:D:161:GLU:HB2	3:D:175:LEU:HD11	1.89	0.55
3:L:6:GLN:NE2	3:L:86:TYR:O	2.37	0.55
3:L:118:PHE:HD1	3:L:133:VAL:O	1.90	0.55
1:B:471:HIS:HE1	1:B:477:CYS:SG	2.30	0.55
2:G:179:LEU:HB2	2:G:185:TYR:HE1	1.72	0.55
1:B:18:HIS:ND1	1:B:350:TRP:O	2.39	0.55
2:E:208:ASN:HB3	2:E:210:LYS:HE2	1.87	0.55
1:C:224:ARG:CB	1:C:224:ARG:NH1	2.44	0.55
3:L:134:CYS:HB2	3:L:148:TRP:HZ3	1.72	0.55
1:B:335:ILE:HG13	1:B:354:ARG:NH1	2.21	0.55
2:E:163:TRP:CH2	2:E:205:CYS:HB3	2.42	0.55
3:F:83:PHE:HD1	3:F:104:VAL:O	1.84	0.55
2:H:18:LEU:HB3	2:H:83:LEU:HB3	1.89	0.55
2:H:163:TRP:CH2	2:H:205:CYS:HB3	2.42	0.55
1:B:363:GLN:NE2	2:E:100:TYR:HE2	2.05	0.55
3:D:29:ILE:CG2	3:D:92:SER:HB3	2.33	0.55
1:C:75:GLN:OE1	1:C:96:ASN:ND2	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:154:TYR:HE2	2:E:157:GLU:HA	1.72	0.54
2:E:2:VAL:HG21	2:E:98:ARG:HH21	1.72	0.54
2:G:18:LEU:HB3	2:G:83:LEU:HB3	1.88	0.54
1:C:47:SER:HA	1:C:288:ILE:HG22	1.90	0.54
1:C:187:THR:C	1:C:217:ILE:HD11	2.33	0.54
2:H:108:TRP:HE3	3:L:91:TYR:CD1	1.82	0.54
2:G:38:ARG:HB2	2:G:94:TYR:CE1	2.41	0.54
3:F:110:VAL:HG22	3:F:140:TYR:HD2	1.72	0.54
2:H:138:ARG:HD3	3:L:209:PHE:HB3	1.88	0.54
2:H:147:LEU:HD13	2:H:203:TYR:HD2	1.70	0.54
3:L:183:SER:O	3:L:187:GLN:HG3	2.08	0.54
3:D:6:GLN:NE2	3:D:86:TYR:O	2.39	0.54
3:F:34:ALA:O	3:F:88:CYS:HA	2.08	0.54
1:A:335:ILE:HD11	2:H:101:TRP:NE1	2.23	0.54
1:A:373:ALA:O	1:A:377:ILE:HG12	2.08	0.54
2:H:11:LEU:HB3	2:H:156:PRO:HG3	1.89	0.54
3:L:32:TRP:HB2	3:L:92:SER:HB2	1.89	0.54
1:B:47:SER:HA	1:B:288:ILE:HG22	1.89	0.54
2:E:11:LEU:HB3	2:E:156:PRO:HG3	1.89	0.54
1:C:17:HIS:HB3	1:C:444:MET:HE2	1.89	0.54
3:F:118:PHE:HD2	3:F:133:VAL:HB	1.72	0.54
1:B:67:ILE:HG13	1:B:105:TYR:CE1	2.42	0.54
1:B:407:GLN:HG3	1:C:405:ARG:HH22	1.73	0.54
1:B:448:PHE:HE1	1:B:467:PHE:CZ	2.26	0.54
3:F:61:ARG:NH1	3:F:79:GLN:OE1	2.41	0.54
1:A:471:HIS:CE1	1:A:491:TYR:HD2	2.25	0.54
1:B:63:ASN:HB3	1:B:75:GLN:NE2	2.23	0.54
2:E:175:PHE:CD1	3:D:164:THR:HG23	2.43	0.54
1:A:187:THR:C	1:A:217:ILE:HD11	2.32	0.53
3:L:36:TYR:CD1	3:L:46:LEU:HA	2.37	0.53
3:D:196:VAL:O	3:D:204:PRO:HA	2.08	0.53
2:G:60:TYR:O	2:G:65:LYS:CE	2.57	0.53
2:G:154:TYR:HE2	2:G:157:GLU:HA	1.73	0.53
2:H:147:LEU:HB2	2:H:191:VAL:HG13	1.90	0.53
1:B:363:GLN:HE22	2:E:100:TYR:HE2	1.55	0.53
2:E:165:SER:H	2:E:206:ASN:ND2	2.05	0.53
3:F:161:GLU:HB2	3:F:175:LEU:HD11	1.89	0.53
2:H:179:LEU:HB2	2:H:185:TYR:HE1	1.72	0.53
2:G:193:VAL:HG21	2:G:203:TYR:HE2	1.73	0.53
2:H:154:TYR:HE2	2:H:157:GLU:HA	1.73	0.53
2:G:208:ASN:HB3	2:G:210:LYS:HE2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:33:LEU:HD11	3:F:88:CYS:HB2	1.90	0.53
2:H:142:GLU:CD	2:H:142:GLU:H	2.16	0.53
3:L:161:GLU:HB2	3:L:175:LEU:HD11	1.89	0.53
3:L:196:VAL:O	3:L:204:PRO:HA	2.09	0.53
1:B:373:ALA:O	1:B:377:ILE:HG12	2.08	0.53
1:B:487:ASP:OD2	1:B:490:VAL:HG23	2.08	0.53
2:G:11:LEU:HB3	2:G:156:PRO:HG3	1.90	0.53
3:F:116:PHE:HB2	3:F:135:LEU:HB3	1.90	0.53
1:A:94:TYR:CE2	1:A:96:ASN:HB3	2.43	0.53
2:H:117:LEU:HD22	2:H:158:PRO:HD3	1.89	0.53
1:C:51:ILE:HG12	1:C:282:ILE:HD11	1.90	0.53
1:C:343:TRP:HE3	1:C:346:MET:SD	2.31	0.53
3:F:134:CYS:HB2	3:F:148:TRP:HZ3	1.72	0.53
1:A:51:ILE:HG12	1:A:282:ILE:HD11	1.89	0.53
1:B:318:THR:O	1:B:350:TRP:HH2	1.92	0.53
2:E:18:LEU:HB3	2:E:83:LEU:HB3	1.89	0.53
1:A:356:GLN:HG2	1:A:361:ARG:HG2	1.90	0.53
2:H:133:LEU:CD2	3:L:118:PHE:CD2	2.84	0.53
2:H:177:ALA:HA	2:H:187:LEU:HB3	1.91	0.53
1:C:329:ARG:CZ	1:C:335:ILE:CG2	2.79	0.53
2:G:131:PHE:CD2	2:G:150:LEU:HD23	2.44	0.53
3:F:58:VAL:HG13	3:F:62:PHE:HD2	1.73	0.53
2:G:165:SER:H	2:G:206:ASN:ND2	2.06	0.52
3:F:196:VAL:O	3:F:204:PRO:HA	2.09	0.52
2:H:208:ASN:HB3	2:H:210:LYS:HE2	1.90	0.52
3:L:108:ARG:HG2	3:L:109:ALA:N	2.24	0.52
1:B:187:THR:C	1:B:217:ILE:HD11	2.33	0.52
3:D:61:ARG:NH1	3:D:79:GLN:CG	2.68	0.52
3:D:134:CYS:HB2	3:D:148:TRP:HZ3	1.73	0.52
1:B:79:PHE:HA	1:B:82:LYS:HD2	1.91	0.52
1:B:75:GLN:CD	1:B:96:ASN:HD21	2.18	0.52
1:C:373:ALA:O	1:C:377:ILE:HG12	2.10	0.52
1:A:72:GLY:H	1:A:148:PHE:HD1	1.56	0.52
2:H:107:ASN:HD22	3:L:50:LYS:HE3	1.74	0.52
3:L:110:VAL:HG22	3:L:140:TYR:CD2	2.42	0.52
1:C:462:MET:HB2	1:C:466:CYS:CB	2.36	0.52
1:C:363:GLN:NE2	2:G:105:TYR:HH	1.99	0.52
2:G:177:ALA:HA	2:G:187:LEU:HB3	1.90	0.52
2:E:177:ALA:HA	2:E:187:LEU:HB3	1.90	0.52
2:H:165:SER:H	2:H:206:ASN:ND2	2.07	0.52
1:B:63:ASN:HB3	1:B:75:GLN:HE21	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:TYR:HE1	1:B:444:MET:HG2	1.74	0.52
1:B:407:GLN:HA	1:B:410:GLU:OE1	2.10	0.52
1:A:462:MET:CB	1:A:466:CYS:HB2	2.33	0.52
2:E:175:PHE:CE2	3:D:176:SER:CB	2.93	0.52
1:C:77:ASP:HA	1:C:80:GLN:NE2	2.25	0.52
1:A:237:VAL:HG21	1:A:243:LEU:HD22	1.92	0.52
1:C:74:PRO:HB3	1:C:141:ARG:HD2	1.92	0.52
2:G:72:ARG:HA	2:G:79:PHE:HA	1.92	0.52
2:G:132:PRO:HB3	2:G:220:VAL:HG22	1.92	0.52
2:G:151:VAL:HG11	2:G:159:VAL:HG11	1.91	0.52
1:A:186:VAL:HG23	1:A:219:TYR:HA	1.93	0.51
2:H:132:PRO:HB3	2:H:220:VAL:HG22	1.92	0.51
1:C:374:ILE:HG13	1:C:378:ASN:OD1	2.10	0.51
3:F:17:ASP:CA	3:F:78:LEU:HG	2.39	0.51
1:A:326:LYS:HE2	2:H:28:THR:CG2	2.39	0.51
1:A:374:ILE:HG13	1:A:378:ASN:OD1	2.10	0.51
1:A:62:GLU:O	1:A:63:ASN:CG	2.54	0.51
2:H:151:VAL:HG11	2:H:159:VAL:HG11	1.91	0.51
3:D:108:ARG:HG2	3:D:109:ALA:N	2.25	0.51
1:B:94:TYR:CE2	1:B:96:ASN:HB3	2.45	0.51
1:B:374:ILE:HG13	1:B:378:ASN:OD1	2.10	0.51
2:E:151:VAL:HG11	2:E:159:VAL:HG11	1.92	0.51
1:C:84:TRP:HZ3	1:C:118:LEU:HG	1.75	0.51
1:C:354:ARG:CZ	2:G:101:TRP:HZ2	2.23	0.51
1:C:183:HIS:HA	1:C:230:ILE:HD13	1.93	0.51
2:G:175:PHE:CE1	3:F:164:THR:HG23	2.46	0.51
1:A:15:LEU:HD11	1:A:447:LEU:HD22	1.92	0.51
1:A:471:HIS:CG	1:A:491:TYR:HD2	2.29	0.51
1:B:284:PRO:HD2	1:B:298:ASN:HD22	1.76	0.51
1:C:67:ILE:HG13	1:C:105:TYR:CE1	2.43	0.51
1:C:478:ILE:HG22	1:C:482:ARG:NH2	2.25	0.51
1:B:84:TRP:HZ3	1:B:118:LEU:HG	1.75	0.51
1:B:204:VAL:HG12	1:B:245:ILE:HG12	1.93	0.51
1:B:478:ILE:HG22	1:B:482:ARG:NH2	2.25	0.51
1:C:18:HIS:HB3	1:C:346:MET:CB	2.41	0.51
1:C:94:TYR:CE2	1:C:96:ASN:HB3	2.46	0.51
1:B:183:HIS:HA	1:B:230:ILE:HD13	1.93	0.51
1:C:185:PRO:HG3	1:C:191:GLN:OE1	2.11	0.51
1:C:318:THR:O	1:C:350:TRP:HH2	1.94	0.51
1:C:399:PHE:HB2	1:C:407:GLN:HE21	1.75	0.51
3:F:190:ASN:N	3:F:190:ASN:OD1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:7:SER:O	3:D:22:THR:N	2.40	0.50
3:D:36:TYR:CD1	3:D:46:LEU:HA	2.41	0.50
1:C:25:ILE:HD11	1:C:33:GLN:HB3	1.93	0.50
1:A:478:ILE:HG22	1:A:482:ARG:NH2	2.27	0.50
2:E:138:ARG:HD3	3:D:209:PHE:HB3	1.93	0.50
1:A:235:THR:CG2	1:A:243:LEU:HD21	2.41	0.50
1:B:394:GLN:HG3	1:C:412:TYR:HE2	1.77	0.50
3:F:47:LEU:O	3:F:48:ILE:HG13	2.11	0.50
1:A:338:PHE:HD1	1:A:339:ILE:H	1.60	0.50
1:B:185:PRO:HG3	1:B:191:GLN:OE1	2.11	0.50
1:C:462:MET:CB	1:C:466:CYS:HB2	2.37	0.50
2:G:2:VAL:HG21	2:G:98:ARG:HH21	1.77	0.50
1:A:185:PRO:HG3	1:A:191:GLN:OE1	2.11	0.50
3:L:29:ILE:HG21	3:L:92:SER:HB2	1.83	0.50
3:D:122:GLU:HG2	3:D:126:LYS:HE2	1.92	0.50
1:A:412:TYR:HE2	1:C:394:GLN:HG3	1.77	0.50
1:B:462:MET:CB	1:B:466:CYS:HB2	2.38	0.50
2:E:72:ARG:HA	2:E:79:PHE:HA	1.92	0.50
2:E:132:PRO:HB3	2:E:220:VAL:HG22	1.92	0.49
2:H:11:LEU:HA	2:H:119:THR:O	2.11	0.49
3:L:29:ILE:CG2	3:L:92:SER:HB3	2.35	0.49
1:B:25:ILE:HD11	1:B:33:GLN:HB3	1.93	0.49
3:D:108:ARG:HG2	3:D:109:ALA:H	1.77	0.49
3:F:31:SER:O	3:F:50:LYS:HE3	2.13	0.49
1:C:329:ARG:HD3	1:C:335:ILE:CB	2.42	0.49
3:L:51:ALA:O	3:L:52:SER:HB3	2.11	0.49
3:L:141:PRO:O	3:L:142:ARG:HB3	2.12	0.49
3:D:144:ALA:HB2	3:D:198:HIS:CD2	2.45	0.49
1:A:394:GLN:HG3	1:B:412:TYR:HE2	1.77	0.49
3:L:80:SER:HA	3:L:106:ILE:HD11	1.95	0.49
2:G:106:ALA:HB2	3:F:32:TRP:CE3	2.47	0.49
3:F:83:PHE:HD1	3:F:104:VAL:HG23	1.77	0.49
1:A:183:HIS:HA	1:A:230:ILE:HD13	1.94	0.49
1:A:284:PRO:HD2	1:A:298:ASN:HD22	1.77	0.49
2:E:122:SER:HB3	2:E:155:PHE:CE1	2.44	0.49
1:B:62:GLU:HA	1:B:90:ARG:HG3	1.94	0.49
2:G:99:LYS:HG3	2:G:108:TRP:CD1	2.45	0.49
2:G:117:LEU:HD21	2:G:119:THR:CG2	2.41	0.49
3:F:16:GLY:N	3:F:78:LEU:CD1	2.75	0.49
3:F:108:ARG:HG2	3:F:109:ALA:N	2.28	0.49
2:H:72:ARG:HA	2:H:79:PHE:HA	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:130:VAL:HG22	2:E:207:VAL:HG21	1.96	0.48
3:F:80:SER:CB	3:F:106:ILE:HD13	2.26	0.48
1:A:72:GLY:N	1:A:148:PHE:HD1	2.11	0.48
2:G:138:ARG:HD3	3:F:209:PHE:HB3	1.94	0.48
1:A:221:PRO:N	1:C:244:LEU:HD21	2.28	0.48
3:L:35:TRP:HB2	3:L:48:ILE:HG22	1.95	0.48
1:B:327:GLN:CD	1:B:327:GLN:H	2.22	0.48
1:B:448:PHE:CE1	1:B:467:PHE:CZ	3.02	0.48
3:D:198:HIS:CE1	3:D:200:GLY:HA3	2.49	0.48
3:F:84:ALA:N	3:F:86:TYR:CE1	2.81	0.48
1:B:219:TYR:OH	5:N:1:NAG:H4	2.13	0.48
1:A:25:ILE:HD11	1:A:33:GLN:HB3	1.94	0.48
3:L:88:CYS:O	3:L:99:GLY:N	2.47	0.48
3:D:29:ILE:HG21	3:D:92:SER:HB2	1.86	0.48
1:C:284:PRO:HD2	1:C:298:ASN:HD22	1.79	0.48
2:G:140:THR:HA	2:G:145:ALA:HA	1.94	0.48
1:A:72:GLY:HA3	1:A:149:SER:OG	2.13	0.48
1:A:73:ASP:OD1	1:A:73:ASP:N	2.28	0.48
3:L:118:PHE:HD1	3:L:133:VAL:C	2.22	0.48
2:G:223:LYS:HB2	3:F:122:GLU:OE2	2.14	0.48
3:F:59:PRO:HD2	3:F:62:PHE:CE2	2.49	0.48
3:F:88:CYS:O	3:F:99:GLY:N	2.47	0.48
3:D:140:TYR:O	3:D:173:TYR:HE2	1.96	0.48
3:D:150:VAL:CG1	3:D:189:HIS:HB3	2.40	0.48
1:C:391:LYS:HB3	1:C:394:GLN:OE1	2.13	0.48
3:L:71:PHE:CD1	3:L:71:PHE:N	2.82	0.48
1:B:391:LYS:HB3	1:B:394:GLN:OE1	2.13	0.48
2:E:140:THR:HA	2:E:145:ALA:HA	1.95	0.48
3:F:35:TRP:HA	3:F:87:TYR:O	2.14	0.48
3:F:195:GLU:HG3	3:F:206:THR:HG23	1.94	0.48
1:A:331:ILE:HG22	1:A:331:ILE:O	2.14	0.48
3:L:132:VAL:HB	3:L:148:TRP:CZ2	2.49	0.48
3:D:35:TRP:HA	3:D:87:TYR:O	2.13	0.48
1:A:391:LYS:HB3	1:A:394:GLN:OE1	2.14	0.47
3:D:136:LEU:HD21	3:D:196:VAL:HG13	1.94	0.47
1:C:61:GLY:C	1:C:63:ASN:H	2.22	0.47
2:G:99:LYS:HG2	2:G:100:TYR:N	2.29	0.47
2:H:130:VAL:HG22	2:H:207:VAL:HG21	1.95	0.47
3:L:61:ARG:NH1	3:L:79:GLN:CG	2.70	0.47
1:C:456:ARG:HH11	1:C:488:HIS:CE1	2.32	0.47
2:G:130:VAL:HG22	2:G:207:VAL:HG21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:TRP:CZ3	1:A:118:LEU:HG	2.47	0.47
1:A:353:PHE:HE1	1:A:366:ASP:HB2	1.80	0.47
1:B:18:HIS:CE1	1:B:350:TRP:C	2.92	0.47
1:C:353:PHE:HE2	1:C:482:ARG:HA	1.78	0.47
2:G:99:LYS:HG3	2:G:108:TRP:CG	2.49	0.47
1:B:331:ILE:O	1:B:331:ILE:HG22	2.13	0.47
1:B:343:TRP:HB3	1:B:354:ARG:HH21	1.79	0.47
1:A:90:ARG:HH22	1:A:273:PRO:HA	1.78	0.47
1:A:105:TYR:CD1	1:A:105:TYR:C	2.92	0.47
1:A:326:LYS:HE2	2:H:28:THR:HG22	1.95	0.47
3:L:198:HIS:CE1	3:L:200:GLY:HA3	2.49	0.47
2:E:60:TYR:HE2	2:E:70:ILE:HG23	1.79	0.47
1:A:109:ARG:HH12	1:A:269:ARG:HH11	1.63	0.47
3:L:36:TYR:HE1	3:L:46:LEU:HD12	1.79	0.47
3:L:195:GLU:HG3	3:L:206:THR:HG23	1.96	0.47
3:D:88:CYS:O	3:D:99:GLY:N	2.48	0.47
1:C:75:GLN:NE2	1:C:96:ASN:ND2	2.62	0.47
2:G:105:TYR:HD1	2:G:106:ALA:H	1.63	0.47
3:F:150:VAL:CG1	3:F:189:HIS:HB3	2.44	0.47
2:H:141:SER:N	2:H:144:THR:O	2.48	0.47
3:L:71:PHE:HD1	3:L:71:PHE:N	2.11	0.47
1:C:175:ASP:OD1	1:C:239:PRO:HD3	2.15	0.47
1:C:339:ILE:CD1	1:C:448:PHE:CD2	2.99	0.46
1:A:490:VAL:HG12	1:A:491:TYR:CE1	2.51	0.46
3:L:143:GLU:HB3	3:L:199:GLN:HB2	1.98	0.46
3:D:90:GLN:HG3	3:D:97:THR:H	1.79	0.46
3:F:29:ILE:HD13	3:F:92:SER:HB3	1.98	0.46
2:H:107:ASN:ND2	3:L:50:LYS:HE3	2.31	0.46
1:B:90:ARG:HH22	1:B:273:PRO:HA	1.81	0.46
1:B:428:LEU:O	1:B:432:GLU:HG2	2.16	0.46
2:H:106:ALA:CB	3:L:50:LYS:HG3	2.45	0.46
1:C:18:HIS:HE2	1:C:350:TRP:CA	2.14	0.46
1:C:78:GLY:O	1:C:82:LYS:NZ	2.38	0.46
1:A:471:HIS:CE1	1:A:491:TYR:CD2	3.04	0.46
1:C:18:HIS:HB3	1:C:346:MET:HB2	1.96	0.46
1:C:339:ILE:HD11	1:C:448:PHE:CD2	2.51	0.46
1:C:363:GLN:HB3	2:G:105:TYR:CZ	2.46	0.46
1:C:456:ARG:HG3	1:C:488:HIS:CG	2.50	0.46
1:A:414:GLU:HG2	1:A:418:ILE:HD11	1.97	0.46
3:F:113:PRO:HB3	3:F:139:PHE:HB3	1.97	0.46
1:A:175:ASP:OD1	1:A:239:PRO:HD3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:VAL:CB	1:A:243:LEU:HD13	2.46	0.46
3:L:52:SER:O	3:L:52:SER:OG	2.17	0.46
1:B:90:ARG:HH12	1:B:272:ALA:C	2.24	0.46
2:E:150:LEU:HD21	2:E:152:LYS:HD2	1.97	0.46
3:D:61:ARG:HH12	3:D:79:GLN:CB	2.28	0.46
3:D:136:LEU:O	3:D:174:SER:HA	2.16	0.46
1:C:109:ARG:HH12	1:C:269:ARG:HH11	1.63	0.46
1:A:102:VAL:HB	1:A:105:TYR:HB2	1.98	0.46
2:E:154:TYR:CE2	2:E:157:GLU:HA	2.51	0.46
3:L:33:LEU:HD21	3:L:88:CYS:HB2	1.98	0.45
1:B:462:MET:HB2	1:B:466:CYS:CB	2.38	0.45
2:E:175:PHE:CE1	3:D:164:THR:CG2	2.98	0.45
1:C:142:ARG:CG	1:C:142:ARG:HH11	2.28	0.45
1:C:338:PHE:HB3	1:C:341:ASN:HB2	1.98	0.45
2:G:172:VAL:HG22	2:G:191:VAL:HG23	1.98	0.45
1:A:338:PHE:HB3	1:A:341:ASN:HB2	1.99	0.45
2:H:98:ARG:HB3	2:H:110:ASP:OD1	2.16	0.45
3:D:47:LEU:HD23	3:D:73:LEU:CD1	2.45	0.45
3:D:161:GLU:HA	3:D:177:SER:HA	1.99	0.45
1:A:326:LYS:CG	2:H:28:THR:HG21	2.22	0.45
2:H:138:ARG:CD	3:L:209:PHE:HB3	2.46	0.45
2:G:175:PHE:CE1	3:F:174:SER:O	2.69	0.45
1:B:109:ARG:HH12	1:B:269:ARG:HH11	1.63	0.45
1:B:448:PHE:CE1	1:B:467:PHE:HZ	2.34	0.45
3:D:132:VAL:HB	3:D:148:TRP:CZ2	2.50	0.45
1:C:90:ARG:HH22	1:C:273:PRO:HA	1.81	0.45
2:G:60:TYR:CB	2:G:65:LYS:HG2	2.39	0.45
3:F:118:PHE:CD2	3:F:133:VAL:HB	2.51	0.45
1:A:428:LEU:O	1:A:432:GLU:HG2	2.16	0.45
2:H:150:LEU:HD21	2:H:152:LYS:HD2	1.97	0.45
1:B:175:ASP:OD1	1:B:239:PRO:HD3	2.16	0.45
3:D:142:ARG:O	3:D:142:ARG:HG3	2.16	0.45
2:G:99:LYS:HD3	2:G:108:TRP:CE2	2.51	0.45
3:F:24:ARG:HA	3:F:24:ARG:HD3	1.74	0.45
1:A:338:PHE:HB3	1:A:341:ASN:H	1.82	0.45
2:H:154:TYR:CE2	2:H:157:GLU:HA	2.52	0.45
1:B:85:ASP:OD1	1:B:264:LYS:HE3	2.16	0.45
2:E:72:ARG:NH1	2:E:74:THR:OG1	2.48	0.45
2:E:121:SER:O	2:E:122:SER:C	2.58	0.45
1:B:329:ARG:HG3	1:B:332:PHE:HB2	1.99	0.45
1:B:414:GLU:HG2	1:B:418:ILE:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:TRP:HB3	1:A:354:ARG:NH2	2.32	0.45
3:L:117:ILE:HG13	3:L:148:TRP:HH2	1.80	0.45
1:B:168:MET:HG2	1:B:178:TYR:OH	2.17	0.45
1:B:316:LEU:HA	1:B:433:ASN:HD21	1.81	0.45
2:E:60:TYR:CE2	2:E:70:ILE:HG23	2.51	0.45
1:C:90:ARG:HH12	1:C:272:ALA:C	2.24	0.45
2:G:60:TYR:CE1	2:G:70:ILE:HG23	2.49	0.45
2:E:175:PHE:HE2	3:D:176:SER:HG	1.63	0.45
3:D:61:ARG:HH22	3:D:79:GLN:HB2	1.82	0.45
1:C:220:ARG:HH12	1:C:229:ARG:HB2	1.76	0.45
1:C:343:TRP:HB3	1:C:354:ARG:NH2	2.32	0.45
2:H:142:GLU:CD	2:H:142:GLU:N	2.74	0.45
1:B:335:ILE:O	1:B:335:ILE:CG2	2.65	0.45
1:C:353:PHE:CE2	1:C:482:ARG:HG3	2.52	0.45
1:C:414:GLU:HG2	1:C:418:ILE:HD11	1.98	0.45
2:G:72:ARG:NH1	2:G:74:THR:OG1	2.48	0.45
1:A:463:GLY:HA2	1:C:453:LYS:HG2	1.98	0.44
1:B:338:PHE:HB3	1:B:341:ASN:HB2	1.98	0.44
1:A:62:GLU:O	1:A:62:GLU:CD	2.60	0.44
2:E:47:TRP:HD1	2:E:109:PHE:HZ	1.65	0.44
3:F:17:ASP:N	3:F:78:LEU:CG	2.50	0.44
3:F:147:LYS:HD3	3:F:149:LYS:HE3	2.00	0.44
1:B:343:TRP:HB3	1:B:354:ARG:NH2	2.32	0.44
3:D:117:ILE:HG13	3:D:148:TRP:HH2	1.82	0.44
2:G:152:LYS:HA	2:G:186:SER:HB2	2.00	0.44
2:H:97:VAL:HG12	2:H:112:TRP:HA	2.00	0.44
2:H:133:LEU:HD22	3:L:118:PHE:CD2	2.44	0.44
3:L:7:SER:O	3:L:22:THR:N	2.40	0.44
3:L:140:TYR:CA	3:L:172:THR:HG22	2.46	0.44
3:F:143:GLU:CB	3:F:199:GLN:HB2	2.39	0.44
1:A:90:ARG:HH12	1:A:272:ALA:C	2.25	0.44
1:A:237:VAL:CB	1:A:243:LEU:CD1	2.95	0.44
1:C:168:MET:HG2	1:C:178:TYR:OH	2.17	0.44
3:F:7:SER:O	3:F:22:THR:N	2.40	0.44
1:A:17:HIS:HB3	1:A:444:MET:HE2	1.99	0.44
1:C:84:TRP:CZ3	1:C:118:LEU:HG	2.53	0.44
3:F:47:LEU:C	3:F:48:ILE:HG13	2.41	0.44
1:A:316:LEU:HA	1:A:433:ASN:HD21	1.82	0.44
3:L:61:ARG:HH12	3:L:79:GLN:CB	2.30	0.44
1:B:84:TRP:CZ3	1:B:118:LEU:HG	2.52	0.44
1:B:203:THR:OG1	1:B:246:ASN:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:346:MET:HG3	1:B:363:GLN:OE1	2.17	0.44
1:C:133:ASN:OD1	1:C:255:ARG:NH2	2.49	0.44
1:C:338:PHE:HD1	1:C:339:ILE:H	1.66	0.44
2:G:154:TYR:CE2	2:G:157:GLU:HA	2.52	0.44
3:F:161:GLU:HA	3:F:177:SER:HA	2.00	0.44
1:A:490:VAL:HG12	1:A:491:TYR:HD1	1.81	0.44
2:E:104:TYR:HD1	2:E:104:TYR:C	2.25	0.44
3:D:147:LYS:HD3	3:D:149:LYS:HE3	1.99	0.44
1:C:72:GLY:HA3	1:C:149:SER:OG	2.18	0.44
1:C:448:PHE:HE1	1:C:467:PHE:CZ	2.36	0.44
3:F:163:VAL:HB	3:F:175:LEU:HD13	2.00	0.44
3:D:4:MET:SD	3:D:90:GLN:HB3	2.58	0.44
2:E:172:VAL:HG22	2:E:191:VAL:HG23	1.99	0.43
1:C:339:ILE:CD1	1:C:448:PHE:HD2	2.31	0.43
1:A:168:MET:HG2	1:A:178:TYR:OH	2.18	0.43
1:A:187:THR:H	1:A:190:ASP:HB3	1.83	0.43
1:A:266:SER:OG	1:A:267:ILE:N	2.51	0.43
1:A:490:VAL:C	1:A:491:TYR:HD1	2.26	0.43
3:L:4:MET:HB2	3:L:98:PHE:O	2.19	0.43
2:E:103:ASP:O	3:D:94:ARG:NH1	2.51	0.43
2:E:138:ARG:CD	3:D:209:PHE:HB3	2.48	0.43
3:F:39:LYS:HB3	3:F:42:LYS:HB2	2.00	0.43
1:A:335:ILE:CG1	2:H:101:TRP:CZ2	2.97	0.43
2:H:172:VAL:HG22	2:H:191:VAL:HG23	1.99	0.43
3:L:147:LYS:HD3	3:L:149:LYS:HE3	2.00	0.43
2:E:151:VAL:HG11	2:E:159:VAL:HG21	2.00	0.43
1:C:354:ARG:NH1	2:G:101:TRP:CE2	2.87	0.43
3:F:133:VAL:HG22	3:F:178:THR:HA	2.00	0.43
1:A:244:LEU:HD12	1:A:244:LEU:O	2.18	0.43
3:L:39:LYS:HB3	3:L:42:LYS:HB2	2.01	0.43
3:L:163:VAL:HB	3:L:175:LEU:HD13	2.00	0.43
3:L:187:GLN:HA	3:L:211:ARG:NH2	2.33	0.43
3:D:4:MET:HB2	3:D:98:PHE:O	2.19	0.43
3:F:4:MET:HB2	3:F:98:PHE:O	2.18	0.43
1:B:325:GLU:O	1:B:325:GLU:CG	2.67	0.43
2:E:151:VAL:O	2:E:186:SER:HA	2.19	0.43
1:C:237:VAL:CG2	1:C:243:LEU:HD12	2.48	0.43
1:A:359:GLU:OE2	1:A:359:GLU:HA	2.17	0.43
1:A:465:GLY:H	1:C:453:LYS:NZ	2.16	0.43
2:H:152:LYS:HA	2:H:186:SER:HB2	2.01	0.43
3:L:80:SER:HA	3:L:106:ILE:CD1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:161:GLU:HA	3:L:177:SER:HA	2.00	0.43
1:B:18:HIS:HE1	1:B:350:TRP:CG	2.36	0.43
1:B:94:TYR:CD2	1:B:96:ASN:HB3	2.53	0.43
1:B:184:HIS:CD2	1:B:220:ARG:HH12	2.37	0.43
1:B:187:THR:H	1:B:190:ASP:HB3	1.84	0.43
3:D:39:LYS:HB3	3:D:42:LYS:HB2	1.99	0.43
1:C:94:TYR:CD2	1:C:96:ASN:HB3	2.53	0.43
1:A:453:LYS:HG2	1:B:463:GLY:HA2	2.00	0.43
2:H:175:PHE:CE1	3:L:174:SER:O	2.64	0.43
1:B:320:MET:HE2	1:B:320:MET:HB2	1.87	0.43
1:C:103:PRO:HG2	1:C:233:TYR:HE1	1.83	0.43
1:C:187:THR:H	1:C:190:ASP:HB3	1.84	0.43
2:H:65:LYS:HB2	2:H:65:LYS:HE3	1.52	0.43
1:B:180:TRP:HZ3	1:B:235:THR:N	2.17	0.43
3:D:209:PHE:HB2	3:D:213:GLU:OE1	2.19	0.43
3:D:49:TYR:HD1	3:D:50:LYS:HB2	1.84	0.43
1:C:320:MET:HE2	1:C:320:MET:HB2	1.86	0.43
3:F:36:TYR:HE1	3:F:46:LEU:HD12	1.84	0.43
1:B:152:ASN:HB3	1:B:253:ALA:HB3	2.01	0.43
2:E:14:PRO:HG3	2:E:121:SER:HA	2.01	0.43
3:D:110:VAL:HG22	3:D:140:TYR:HD2	1.84	0.43
2:G:79:PHE:HZ	2:G:96:CYS:HB2	1.84	0.43
2:G:138:ARG:CD	3:F:209:PHE:HB3	2.49	0.43
2:H:147:LEU:HD12	2:H:193:VAL:HG21	2.00	0.42
2:G:151:VAL:HG11	2:G:159:VAL:HG21	2.01	0.42
1:A:180:TRP:HB2	1:A:252:ILE:O	2.19	0.42
2:H:147:LEU:HD13	2:H:203:TYR:CD2	2.50	0.42
3:L:149:LYS:HG2	3:L:154:LEU:HD12	2.02	0.42
1:B:18:HIS:CE1	1:B:350:TRP:O	2.72	0.42
2:E:4:LEU:HB3	2:E:22:CYS:SG	2.59	0.42
2:E:70:ILE:HG22	2:E:81:LEU:HD13	2.01	0.42
2:E:79:PHE:HZ	2:E:96:CYS:HB2	1.84	0.42
2:E:175:PHE:HE2	3:D:176:SER:OG	2.02	0.42
3:D:163:VAL:HB	3:D:175:LEU:HD13	2.01	0.42
5:J:1:NAG:H4	5:J:2:NAG:H2	1.83	0.42
1:A:335:ILE:HG21	1:A:354:ARG:HH11	1.84	0.42
1:A:456:ARG:NH2	1:B:462:MET:HA	2.34	0.42
2:H:106:ALA:CB	3:L:50:LYS:CG	2.97	0.42
2:H:151:VAL:O	2:H:186:SER:HA	2.20	0.42
2:E:13:LYS:HA	2:E:13:LYS:HD2	1.76	0.42
1:C:441:ASP:O	1:C:444:MET:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:97:VAL:HG13	2:G:112:TRP:HE3	1.72	0.42
3:F:24:ARG:HH11	3:F:24:ARG:HD2	1.65	0.42
1:A:72:GLY:HA3	1:A:149:SER:CB	2.50	0.42
2:H:4:LEU:HB3	2:H:22:CYS:SG	2.59	0.42
2:H:60:TYR:CE1	2:H:70:ILE:HG23	2.50	0.42
2:H:151:VAL:HG11	2:H:159:VAL:HG21	2.02	0.42
2:G:4:LEU:HB3	2:G:22:CYS:SG	2.59	0.42
1:A:354:ARG:HG2	1:A:363:GLN:HG3	2.02	0.42
3:F:136:LEU:O	3:F:174:SER:HA	2.19	0.42
1:A:71:LEU:HB3	1:A:148:PHE:CD1	2.54	0.42
1:A:133:ASN:OD1	1:A:255:ARG:NH2	2.48	0.42
1:B:18:HIS:CE1	1:B:350:TRP:CG	3.07	0.42
1:C:180:TRP:HB2	1:C:252:ILE:O	2.19	0.42
2:G:151:VAL:O	2:G:186:SER:HA	2.19	0.42
1:A:54:SER:OG	1:A:278:ASN:CA	2.67	0.42
3:L:32:TRP:HZ3	3:L:50:LYS:HE2	1.84	0.42
1:B:181:GLY:H	1:B:252:ILE:HB	1.85	0.42
2:E:10:GLY:O	2:E:119:THR:N	2.53	0.42
1:A:237:VAL:HG13	1:A:243:LEU:HD12	1.94	0.42
1:B:103:PRO:HG2	1:B:233:TYR:HE1	1.85	0.42
2:E:87:THR:O	2:E:120:VAL:HG21	2.20	0.42
2:E:133:LEU:CD2	3:D:118:PHE:CD1	3.01	0.42
3:D:123:ASP:HA	3:D:126:LYS:HE3	2.02	0.42
3:D:163:VAL:HA	3:D:175:LEU:HA	2.02	0.42
1:C:71:LEU:HB3	1:C:148:PHE:CE1	2.55	0.42
1:C:180:TRP:HZ3	1:C:235:THR:N	2.18	0.42
2:G:117:LEU:HD23	2:G:119:THR:HG23	1.97	0.42
1:A:180:TRP:HZ3	1:A:235:THR:N	2.18	0.41
2:E:152:LYS:HA	2:E:186:SER:HB2	2.02	0.41
1:C:152:ASN:HB3	1:C:253:ALA:HB3	2.02	0.41
1:C:181:GLY:H	1:C:252:ILE:HB	1.85	0.41
3:F:29:ILE:CG2	3:F:92:SER:HB3	2.40	0.41
1:A:181:GLY:H	1:A:252:ILE:HB	1.86	0.41
1:A:221:PRO:HB2	1:C:207:LYS:HE3	2.01	0.41
2:E:109:PHE:N	2:E:109:PHE:CD1	2.87	0.41
1:C:204:VAL:HG12	1:C:245:ILE:HG12	2.02	0.41
5:W:1:NAG:H4	5:W:2:NAG:H2	1.78	0.41
1:A:138:ALA:HB2	1:A:226:ILE:HD11	2.03	0.41
1:A:152:ASN:HB3	1:A:253:ALA:HB3	2.02	0.41
2:H:70:ILE:HG22	2:H:81:LEU:HD13	2.02	0.41
1:A:326:LYS:HZ1	6:A:601:NAG:C8	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:ARG:HH22	1:B:29:ILE:HD12	1.85	0.41
2:H:145:ALA:N	2:H:193:VAL:O	2.51	0.41
3:L:29:ILE:HG23	3:L:92:SER:OG	2.21	0.41
2:E:11:LEU:HA	2:E:119:THR:O	2.20	0.41
1:C:464:ASN:OD1	1:C:466:CYS:SG	2.78	0.41
3:F:149:LYS:HG2	3:F:154:LEU:HD12	2.02	0.41
1:B:383:ARG:HH22	1:C:29:ILE:HD12	1.84	0.41
2:E:175:PHE:CD1	3:D:164:THR:CG2	3.03	0.41
1:C:108:LEU:HB2	1:C:234:TRP:CD1	2.56	0.41
1:C:186:VAL:HG23	1:C:219:TYR:HA	2.02	0.41
2:G:109:PHE:CD2	2:G:112:TRP:CZ2	3.08	0.41
2:G:126:LYS:N	2:G:155:PHE:O	2.45	0.41
1:A:249:GLY:C	1:A:251:LEU:H	2.29	0.41
1:B:60:ASP:HB2	1:B:274:ILE:HD11	2.03	0.41
1:B:186:VAL:HG23	1:B:219:TYR:HA	2.02	0.41
2:H:175:PHE:CD1	3:L:164:THR:HG23	2.56	0.41
2:G:70:ILE:HG22	2:G:81:LEU:HD13	2.02	0.41
3:F:163:VAL:HA	3:F:175:LEU:HA	2.02	0.41
1:A:220:ARG:HB3	1:A:221:PRO:HD2	2.03	0.41
1:A:471:HIS:CD2	1:A:491:TYR:HD2	2.39	0.41
3:L:163:VAL:HA	3:L:175:LEU:HA	2.02	0.41
1:B:108:LEU:HB2	1:B:234:TRP:CD1	2.56	0.41
1:B:272:ALA:HA	1:B:273:PRO:HD3	1.96	0.41
1:B:346:MET:HG2	1:B:363:GLN:NE2	2.36	0.41
1:B:475:ASN:HB3	2:E:104:TYR:HE2	1.86	0.41
3:D:149:LYS:HG2	3:D:154:LEU:HD12	2.02	0.41
1:A:108:LEU:HB2	1:A:234:TRP:CD1	2.56	0.41
1:A:491:TYR:CD1	1:A:491:TYR:N	2.87	0.41
2:H:72:ARG:NH1	2:H:74:THR:OG1	2.47	0.41
3:L:35:TRP:HA	3:L:87:TYR:O	2.21	0.41
3:L:123:ASP:HA	3:L:126:LYS:HE3	2.03	0.41
1:B:138:ALA:HB2	1:B:226:ILE:HD11	2.03	0.41
1:C:15:LEU:HD11	1:C:447:LEU:CD2	2.51	0.41
1:C:334:ALA:O	1:C:335:ILE:C	2.62	0.41
2:G:37:ILE:CD1	2:G:112:TRP:HH2	2.28	0.41
3:F:117:ILE:HG13	3:F:148:TRP:HH2	1.86	0.41
1:A:94:TYR:CD2	1:A:96:ASN:HB3	2.56	0.41
1:A:471:HIS:CG	1:A:491:TYR:CD2	3.08	0.41
1:B:18:HIS:HD1	1:B:350:TRP:C	2.28	0.41
1:B:180:TRP:HB2	1:B:252:ILE:O	2.21	0.41
2:E:210:LYS:N	2:E:211:PRO:HD2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:155:PHE:HA	2:G:156:PRO:HA	1.87	0.41
1:A:18:HIS:HB2	1:A:346:MET:HB3	2.03	0.40
1:B:18:HIS:ND1	1:B:350:TRP:C	2.79	0.40
1:B:60:ASP:O	1:B:79:PHE:HZ	2.04	0.40
2:E:99:LYS:HB2	2:E:99:LYS:HE3	1.88	0.40
3:F:46:LEU:HD22	3:F:55:GLN:CD	2.47	0.40
1:A:60:ASP:HB2	1:A:274:ILE:HD11	2.02	0.40
1:A:237:VAL:CG1	1:A:243:LEU:HD11	2.35	0.40
2:H:151:VAL:CG1	2:H:159:VAL:HG11	2.52	0.40
1:B:237:VAL:CG2	1:B:243:LEU:HD12	2.52	0.40
1:C:71:LEU:HB3	1:C:148:PHE:CD1	2.57	0.40
3:F:140:TYR:O	3:F:173:TYR:HE2	2.04	0.40
1:A:14:CYS:SG	1:A:337:GLY:O	2.79	0.40
1:A:355:HIS:HB2	1:A:478:ILE:HD12	2.03	0.40
1:B:61:GLY:O	1:B:63:ASN:N	2.54	0.40
1:B:98:PHE:HE2	1:B:230:ILE:HG12	1.87	0.40
1:C:153:TRP:HD1	1:C:154:LEU:N	2.20	0.40
1:C:428:LEU:O	1:C:432:GLU:HG3	2.21	0.40
3:F:46:LEU:HD22	3:F:55:GLN:OE1	2.19	0.40
2:G:4:LEU:HB2	2:G:113:GLY:HA2	2.04	0.40
2:H:51:ILE:HB	2:H:70:ILE:HD11	2.04	0.40
3:L:37:GLN:HB2	3:L:47:LEU:HD12	2.04	0.40
3:D:48:ILE:CG2	3:D:52:SER:HA	2.52	0.40
1:C:259:LYS:HD3	1:C:261:ARG:NH2	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	492/503 (98%)	464 (94%)	27 (6%)	1 (0%)	43 78

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	492/503 (98%)	469 (95%)	22 (4%)	1 (0%)	43	78
1	C	492/503 (98%)	468 (95%)	23 (5%)	1 (0%)	43	78
2	E	223/233 (96%)	211 (95%)	12 (5%)	0	100	100
2	G	223/233 (96%)	215 (96%)	8 (4%)	0	100	100
2	H	223/233 (96%)	215 (96%)	8 (4%)	0	100	100
3	D	212/214 (99%)	203 (96%)	8 (4%)	1 (0%)	24	63
3	F	212/214 (99%)	205 (97%)	7 (3%)	0	100	100
3	L	212/214 (99%)	205 (97%)	7 (3%)	0	100	100
All	All	2781/2850 (98%)	2655 (96%)	122 (4%)	4 (0%)	49	83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
3	D	52	SER
1	C	63	ASN
1	B	62	GLU

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	432/440 (98%)	414 (96%)	18 (4%)	26	49
1	B	432/440 (98%)	415 (96%)	17 (4%)	28	50
1	C	432/440 (98%)	417 (96%)	15 (4%)	32	54
2	E	193/198 (98%)	176 (91%)	17 (9%)	9	29
2	G	193/198 (98%)	185 (96%)	8 (4%)	27	49
2	H	193/198 (98%)	183 (95%)	10 (5%)	21	43
3	D	187/187 (100%)	180 (96%)	7 (4%)	30	51
3	F	187/187 (100%)	178 (95%)	9 (5%)	23	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	L	187/187 (100%)	178 (95%)	9 (5%)	23	45
All	All	2436/2475 (98%)	2326 (96%)	110 (4%)	26	47

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	29	ILE
1	A	52	CYS
1	A	73	ASP
1	A	79	PHE
1	A	105	TYR
1	A	167	THR
1	A	182	VAL
1	A	202	ILE
1	A	264	LYS
1	A	339	ILE
1	A	359	GLU
1	A	384	LEU
1	A	407	GLN
1	A	432	GLU
1	A	436	THR
1	A	469	ILE
1	A	491	TYR
2	H	24	VAL
2	H	37	ILE
2	H	65	LYS
2	H	70	ILE
2	H	100	TYR
2	H	111	VAL
2	H	116	VAL
2	H	133	LEU
2	H	139	SER
2	H	144	THR
3	L	3	GLN
3	L	26	SER
3	L	48	ILE
3	L	71	PHE
3	L	80	SER
3	L	85	THR
3	L	106	ILE
3	L	132	VAL

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Mol	Chain	Res	Type
3	L	138	ASN
1	B	15	LEU
1	B	30	THR
1	B	52	CYS
1	B	65	THR
1	B	75	GLN
1	B	167	THR
1	B	182	VAL
1	B	202	ILE
1	B	332	PHE
1	B	341	ASN
1	B	347	VAL
1	B	384	LEU
1	B	410	GLU
1	B	432	GLU
1	B	436	THR
1	B	444	MET
1	B	469	ILE
2	E	13	LYS
2	E	24	VAL
2	E	65	LYS
2	E	67	ARG
2	E	70	ILE
2	E	100	TYR
2	E	104	TYR
2	E	105	TYR
2	E	110	ASP
2	E	111	VAL
2	E	116	VAL
2	E	120	VAL
2	E	133	LEU
2	E	139	SER
2	E	142	GLU
2	E	147	LEU
2	E	225	CYS
3	D	26	SER
3	D	53	SER
3	D	69	SER
3	D	80	SER
3	D	85	THR
3	D	106	ILE
3	D	132	VAL

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Mol	Chain	Res	Type
1	C	15	LEU
1	C	30	THR
1	C	52	CYS
1	C	63	ASN
1	C	70	LEU
1	C	71	LEU
1	C	141	ARG
1	C	167	THR
1	C	182	VAL
1	C	202	ILE
1	C	224	ARG
1	C	335	ILE
1	C	384	LEU
1	C	436	THR
1	C	469	ILE
2	G	24	VAL
2	G	70	ILE
2	G	105	TYR
2	G	111	VAL
2	G	133	LEU
2	G	139	SER
2	G	141	SER
2	G	147	LEU
3	F	3	GLN
3	F	58	VAL
3	F	67	SER
3	F	69	SER
3	F	83	PHE
3	F	91	TYR
3	F	106	ILE
3	F	187	GLN
3	F	190	ASN

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

Mol	Chain	Res	Type
1	A	44	GLN
1	A	290	ASN
1	A	433	ASN
1	A	445	ASN
1	A	475	ASN
2	H	39	GLN

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Mol	Chain	Res	Type
2	H	107	ASN
2	H	180	GLN
2	H	206	ASN
3	L	38	GLN
3	L	138	ASN
3	L	189	HIS
3	L	198	HIS
1	B	44	GLN
1	B	225	ASN
1	B	278	ASN
1	B	290	ASN
1	B	389	ASN
1	B	433	ASN
1	B	475	ASN
2	E	39	GLN
2	E	107	ASN
2	E	180	GLN
2	E	206	ASN
3	D	38	GLN
3	D	138	ASN
3	D	198	HIS
3	D	210	ASN
1	C	44	GLN
1	C	80	GLN
1	C	96	ASN
1	C	278	ASN
1	C	290	ASN
1	C	355	HIS
1	C	363	GLN
1	C	445	ASN
1	C	475	ASN
2	G	39	GLN
2	G	180	GLN
2	G	206	ASN
3	F	38	GLN
3	F	138	ASN

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 ⓘ

48 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	I	1	4,1	14,14,15	0.52	0	17,19,21	1.32	2 (11%)
4	NAG	I	2	4	14,14,15	0.73	0	17,19,21	1.61	2 (11%)
5	NAG	J	1	5,1	14,14,15	0.53	0	17,19,21	1.39	2 (11%)
5	NAG	J	2	5	14,14,15	0.94	1 (7%)	17,19,21	2.12	3 (17%)
5	BMA	J	3	5	11,11,12	0.62	0	15,15,17	0.91	0
5	NAG	K	1	5,1	14,14,15	0.81	1 (7%)	17,19,21	1.49	3 (17%)
5	NAG	K	2	5	14,14,15	0.55	0	17,19,21	1.95	3 (17%)
5	BMA	K	3	5	11,11,12	0.62	0	15,15,17	0.89	2 (13%)
4	NAG	M	1	4,1	14,14,15	0.81	0	17,19,21	1.88	3 (17%)
4	NAG	M	2	4	14,14,15	0.57	0	17,19,21	1.09	2 (11%)
5	NAG	N	1	5,1	14,14,15	0.64	0	17,19,21	1.88	5 (29%)
5	NAG	N	2	5	14,14,15	0.53	0	17,19,21	1.23	2 (11%)
5	BMA	N	3	5	11,11,12	0.61	0	15,15,17	1.62	1 (6%)
5	NAG	O	1	5,1	14,14,15	0.46	0	17,19,21	1.30	2 (11%)
5	NAG	O	2	5	14,14,15	0.65	0	17,19,21	2.35	4 (23%)
5	BMA	O	3	5	11,11,12	0.55	0	15,15,17	1.17	1 (6%)
4	NAG	P	1	4,1	14,14,15	0.53	0	17,19,21	1.04	1 (5%)
4	NAG	P	2	4	14,14,15	0.57	0	17,19,21	1.39	2 (11%)
5	NAG	Q	1	5,1	14,14,15	0.52	0	17,19,21	1.26	2 (11%)
5	NAG	Q	2	5	14,14,15	0.93	1 (7%)	17,19,21	2.06	4 (23%)
5	BMA	Q	3	5	11,11,12	0.60	0	15,15,17	0.97	1 (6%)
5	NAG	R	1	5,1	14,14,15	0.58	0	17,19,21	1.19	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	R	2	5	14,14,15	0.53	0	17,19,21	1.77	2 (11%)
5	BMA	R	3	5	11,11,12	0.60	0	15,15,17	0.93	1 (6%)
4	NAG	S	1	4,1	14,14,15	0.79	0	17,19,21	1.94	4 (23%)
4	NAG	S	2	4	14,14,15	0.57	0	17,19,21	1.06	2 (11%)
5	NAG	T	1	5,1	14,14,15	0.84	1 (7%)	17,19,21	1.78	5 (29%)
5	NAG	T	2	5	14,14,15	0.52	0	17,19,21	1.51	2 (11%)
5	BMA	T	3	5	11,11,12	0.67	0	15,15,17	1.21	2 (13%)
5	NAG	U	1	5,1	14,14,15	0.44	0	17,19,21	1.36	2 (11%)
5	NAG	U	2	5	14,14,15	0.73	0	17,19,21	2.14	4 (23%)
5	BMA	U	3	5	11,11,12	0.56	0	15,15,17	1.31	1 (6%)
4	NAG	V	1	4,1	14,14,15	0.56	0	17,19,21	1.23	2 (11%)
4	NAG	V	2	4	14,14,15	0.60	0	17,19,21	1.39	3 (17%)
5	NAG	W	1	5,1	14,14,15	0.51	0	17,19,21	1.36	3 (17%)
5	NAG	W	2	5	14,14,15	0.94	1 (7%)	17,19,21	2.16	4 (23%)
5	BMA	W	3	5	11,11,12	0.59	0	15,15,17	0.91	0
5	NAG	X	1	5,1	14,14,15	0.51	0	17,19,21	1.31	2 (11%)
5	NAG	X	2	5	14,14,15	0.54	0	17,19,21	1.83	3 (17%)
5	BMA	X	3	5	11,11,12	0.60	0	15,15,17	0.90	1 (6%)
4	NAG	Y	1	4,1	14,14,15	0.80	0	17,19,21	1.90	3 (17%)
4	NAG	Y	2	4	14,14,15	0.56	0	17,19,21	1.02	2 (11%)
5	NAG	Z	1	5,1	14,14,15	0.73	0	17,19,21	1.69	3 (17%)
5	NAG	Z	2	5	14,14,15	0.51	0	17,19,21	1.48	2 (11%)
5	BMA	Z	3	5	11,11,12	0.61	0	15,15,17	0.90	0
5	NAG	a	1	5,1	14,14,15	0.48	0	17,19,21	1.33	2 (11%)
5	NAG	a	2	5	14,14,15	0.68	0	17,19,21	2.14	4 (23%)
5	BMA	a	3	5	11,11,12	0.59	0	15,15,17	1.04	1 (6%)

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	I	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	I	2	4	-	3/6/23/26	0/1/1/1
5	NAG	J	1	5,1	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	J	2	5	-	2/6/23/26	0/1/1/1
5	BMA	J	3	5	-	0/2/19/22	0/1/1/1
5	NAG	K	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	K	2	5	-	2/6/23/26	0/1/1/1
5	BMA	K	3	5	-	0/2/19/22	0/1/1/1
4	NAG	M	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	M	2	4	-	0/6/23/26	0/1/1/1
5	NAG	N	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	N	2	5	-	0/6/23/26	0/1/1/1
5	BMA	N	3	5	-	1/2/19/22	0/1/1/1
5	NAG	O	1	5,1	-	4/6/23/26	0/1/1/1
5	NAG	O	2	5	-	5/6/23/26	0/1/1/1
5	BMA	O	3	5	-	1/2/19/22	0/1/1/1
4	NAG	P	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	P	2	4	-	2/6/23/26	0/1/1/1
5	NAG	Q	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	Q	2	5	-	2/6/23/26	0/1/1/1
5	BMA	Q	3	5	-	0/2/19/22	0/1/1/1
5	NAG	R	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	R	2	5	-	2/6/23/26	0/1/1/1
5	BMA	R	3	5	-	0/2/19/22	0/1/1/1
4	NAG	S	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	S	2	4	-	0/6/23/26	0/1/1/1
5	NAG	T	1	5,1	-	4/6/23/26	0/1/1/1
5	NAG	T	2	5	-	0/6/23/26	0/1/1/1
5	BMA	T	3	5	-	2/2/19/22	0/1/1/1
5	NAG	U	1	5,1	-	4/6/23/26	0/1/1/1
5	NAG	U	2	5	-	4/6/23/26	0/1/1/1
5	BMA	U	3	5	-	2/2/19/22	0/1/1/1
4	NAG	V	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	V	2	4	-	2/6/23/26	0/1/1/1
5	NAG	W	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	W	2	5	-	2/6/23/26	0/1/1/1
5	BMA	W	3	5	-	0/2/19/22	0/1/1/1
5	NAG	X	1	5,1	-	4/6/23/26	0/1/1/1
5	NAG	X	2	5	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BMA	X	3	5	-	0/2/19/22	0/1/1/1
4	NAG	Y	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	Y	2	4	-	0/6/23/26	0/1/1/1
5	NAG	Z	1	5,1	-	4/6/23/26	0/1/1/1
5	NAG	Z	2	5	-	3/6/23/26	0/1/1/1
5	BMA	Z	3	5	-	1/2/19/22	0/1/1/1
5	NAG	a	1	5,1	-	4/6/23/26	0/1/1/1
5	NAG	a	2	5	-	5/6/23/26	0/1/1/1
5	BMA	a	3	5	-	2/2/19/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	2	NAG	C1-C2	2.76	1.56	1.52
5	Q	2	NAG	C1-C2	2.75	1.56	1.52
5	W	2	NAG	C1-C2	2.68	1.56	1.52
5	K	1	NAG	C1-C2	2.37	1.55	1.52
5	T	1	NAG	C2-N2	-2.06	1.42	1.46

All (109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	O	2	NAG	C1-O5-C5	7.46	122.18	112.19
5	a	2	NAG	C1-O5-C5	6.49	120.88	112.19
5	K	2	NAG	C1-O5-C5	6.49	120.88	112.19
5	W	2	NAG	C1-O5-C5	5.94	120.15	112.19
5	X	2	NAG	C1-O5-C5	5.88	120.07	112.19
5	R	2	NAG	C1-O5-C5	5.83	120.00	112.19
5	J	2	NAG	C1-O5-C5	5.60	119.70	112.19
5	Q	2	NAG	C1-O5-C5	5.49	119.54	112.19
5	N	3	BMA	C1-O5-C5	5.38	119.40	112.19
4	I	2	NAG	C1-O5-C5	5.26	119.23	112.19
5	U	2	NAG	C1-O5-C5	5.07	118.98	112.19
5	Z	2	NAG	C1-O5-C5	4.98	118.86	112.19
5	Q	2	NAG	C2-N2-C7	4.82	129.37	122.90
5	Z	1	NAG	C4-C3-C2	4.81	118.06	111.02
5	J	2	NAG	C2-N2-C7	4.77	129.30	122.90
5	U	2	NAG	C2-N2-C7	4.75	129.27	122.90
4	S	1	NAG	C1-O5-C5	4.71	118.50	112.19
5	W	2	NAG	C2-N2-C7	4.69	129.18	122.90
4	M	1	NAG	C2-N2-C7	4.54	128.99	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	1	NAG	C4-C3-C2	4.49	117.60	111.02
4	Y	1	NAG	C2-N2-C7	4.46	128.88	122.90
4	Y	1	NAG	C1-O5-C5	4.46	118.16	112.19
4	P	2	NAG	C1-O5-C5	4.38	118.05	112.19
4	M	1	NAG	C1-O5-C5	4.37	118.05	112.19
5	T	2	NAG	C4-C3-C2	4.33	117.36	111.02
5	U	3	BMA	C1-O5-C5	4.27	117.90	112.19
5	O	2	NAG	C2-N2-C7	4.13	128.43	122.90
4	I	1	NAG	C4-C3-C2	4.12	117.05	111.02
5	a	2	NAG	C2-N2-C7	4.11	128.40	122.90
5	O	3	BMA	C1-O5-C5	4.07	117.65	112.19
5	T	1	NAG	C8-C7-N2	-4.05	109.40	116.12
4	V	2	NAG	C1-O5-C5	4.04	117.60	112.19
5	R	1	NAG	C1-O5-C5	3.78	117.25	112.19
5	K	1	NAG	C2-N2-C7	3.62	127.75	122.90
5	a	1	NAG	C1-O5-C5	3.55	116.94	112.19
5	X	1	NAG	C1-O5-C5	3.53	116.91	112.19
4	S	1	NAG	C8-C7-N2	3.51	121.95	116.12
5	K	1	NAG	C1-O5-C5	3.49	116.86	112.19
5	N	1	NAG	C8-C7-N2	-3.43	110.43	116.12
4	S	1	NAG	C2-N2-C7	3.34	127.38	122.90
4	V	1	NAG	C4-C3-C2	3.32	115.89	111.02
5	J	1	NAG	C2-N2-C7	3.31	127.33	122.90
5	T	1	NAG	C4-C3-C2	3.29	115.84	111.02
5	N	2	NAG	C4-C3-C2	3.24	115.76	111.02
5	O	1	NAG	C1-O5-C5	3.22	116.51	112.19
5	U	1	NAG	C1-O5-C5	3.18	116.44	112.19
5	W	1	NAG	C2-N2-C7	3.17	127.15	122.90
5	X	2	NAG	C2-N2-C7	3.11	127.06	122.90
5	T	2	NAG	C1-O5-C5	2.98	116.19	112.19
5	U	2	NAG	O5-C1-C2	2.97	115.89	111.29
5	Z	1	NAG	O5-C1-C2	2.94	115.84	111.29
5	a	3	BMA	C1-O5-C5	2.94	116.12	112.19
5	X	1	NAG	C2-N2-C7	2.92	126.81	122.90
5	W	2	NAG	O4-C4-C5	2.83	116.30	109.32
5	U	2	NAG	O4-C4-C5	2.79	116.20	109.32
4	P	1	NAG	C4-C3-C2	2.78	115.09	111.02
4	Y	1	NAG	C8-C7-N2	2.76	120.69	116.12
5	T	1	NAG	O7-C7-N2	2.75	126.84	121.98
5	O	2	NAG	O5-C1-C2	2.73	115.51	111.29
5	T	1	NAG	C3-C4-C5	2.73	115.18	110.23
5	T	3	BMA	C1-O5-C5	2.70	115.81	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	2	NAG	C2-N2-C7	2.68	126.49	122.90
4	I	2	NAG	C4-C3-C2	2.66	114.92	111.02
4	S	2	NAG	C4-C3-C2	2.65	114.91	111.02
5	J	2	NAG	O4-C4-C5	2.59	115.69	109.32
5	Q	1	NAG	C2-N2-C7	2.58	126.36	122.90
4	M	2	NAG	C4-C3-C2	2.57	114.78	111.02
4	M	1	NAG	C8-C7-N2	2.54	120.33	116.12
4	I	1	NAG	C3-C4-C5	2.52	114.80	110.23
4	V	2	NAG	C4-C3-C2	2.50	114.69	111.02
5	R	3	BMA	C1-O5-C5	2.47	115.50	112.19
4	Y	2	NAG	C4-C3-C2	2.45	114.61	111.02
5	N	1	NAG	C3-C4-C5	2.41	114.60	110.23
5	W	2	NAG	C1-C2-N2	2.39	114.19	110.43
5	Z	1	NAG	C2-N2-C7	2.36	126.06	122.90
5	Z	2	NAG	C4-C3-C2	2.32	114.42	111.02
5	a	2	NAG	O4-C4-C5	2.29	114.96	109.32
5	K	2	NAG	C2-N2-C7	2.28	125.95	122.90
5	T	1	NAG	O4-C4-C3	-2.27	105.03	110.38
5	O	2	NAG	O4-C4-C5	2.26	114.89	109.32
5	X	3	BMA	C1-O5-C5	2.25	115.20	112.19
4	M	2	NAG	C2-N2-C7	2.25	125.91	122.90
5	Q	1	NAG	O5-C1-C2	2.24	114.76	111.29
5	N	1	NAG	O7-C7-N2	2.23	125.92	121.98
5	O	1	NAG	C8-C7-N2	2.21	119.78	116.12
4	V	1	NAG	C3-C4-C5	2.20	114.22	110.23
5	N	1	NAG	C2-N2-C7	2.20	125.84	122.90
5	X	2	NAG	C8-C7-N2	2.19	119.75	116.12
4	Y	2	NAG	C2-N2-C7	2.18	125.83	122.90
5	Q	2	NAG	O4-C4-C5	2.17	114.66	109.32
5	Q	3	BMA	C1-O5-C5	2.16	115.08	112.19
5	U	1	NAG	C4-C3-C2	2.13	114.14	111.02
4	S	1	NAG	O7-C7-C8	-2.12	118.28	122.05
5	K	2	NAG	C4-C3-C2	-2.11	107.92	111.02
5	Q	2	NAG	C1-C2-N2	2.11	113.76	110.43
5	T	3	BMA	C1-C2-C3	2.10	112.71	109.64
5	W	1	NAG	C8-C7-N2	2.10	119.60	116.12
5	J	1	NAG	C8-C7-N2	2.09	119.59	116.12
5	W	1	NAG	C4-C3-C2	2.08	114.07	111.02
5	a	1	NAG	C8-C7-N2	2.08	119.57	116.12
5	a	2	NAG	C4-C3-C2	2.08	114.06	111.02
4	S	2	NAG	C2-N2-C7	2.08	125.68	122.90
4	V	2	NAG	C2-N2-C7	2.08	125.68	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	2	NAG	C2-N2-C7	2.07	125.68	122.90
5	K	3	BMA	C2-C3-C4	2.05	114.47	110.86
5	R	1	NAG	C2-N2-C7	2.05	125.64	122.90
5	N	2	NAG	C2-N2-C7	2.04	125.63	122.90
5	K	1	NAG	C8-C7-N2	2.03	119.49	116.12
5	K	3	BMA	C1-O5-C5	2.02	114.89	112.19

There are no chirality outliers.

All (103) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	I	1	NAG	O7-C7-N2-C2
4	I	2	NAG	C8-C7-N2-C2
4	I	2	NAG	O7-C7-N2-C2
4	M	1	NAG	C8-C7-N2-C2
4	M	1	NAG	O7-C7-N2-C2
4	S	1	NAG	C8-C7-N2-C2
4	S	1	NAG	O7-C7-N2-C2
4	Y	1	NAG	C8-C7-N2-C2
4	Y	1	NAG	O7-C7-N2-C2
5	K	1	NAG	C8-C7-N2-C2
5	K	1	NAG	O7-C7-N2-C2
5	K	2	NAG	C8-C7-N2-C2
5	K	2	NAG	O7-C7-N2-C2
5	Q	1	NAG	C8-C7-N2-C2
5	Q	1	NAG	O7-C7-N2-C2
5	R	1	NAG	C8-C7-N2-C2
5	R	1	NAG	O7-C7-N2-C2
5	R	2	NAG	C8-C7-N2-C2
5	R	2	NAG	O7-C7-N2-C2
5	U	1	NAG	C8-C7-N2-C2
5	U	1	NAG	O7-C7-N2-C2
5	X	1	NAG	C8-C7-N2-C2
5	X	1	NAG	O7-C7-N2-C2
5	Z	1	NAG	O7-C7-N2-C2
5	Z	2	NAG	C8-C7-N2-C2
5	Z	2	NAG	O7-C7-N2-C2
5	a	1	NAG	C8-C7-N2-C2
5	a	1	NAG	O7-C7-N2-C2
5	U	2	NAG	C4-C5-C6-O6
4	I	1	NAG	C8-C7-N2-C2
5	Z	1	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
5	T	1	NAG	O5-C5-C6-O6
4	P	1	NAG	O5-C5-C6-O6
5	Z	1	NAG	O5-C5-C6-O6
5	N	1	NAG	O5-C5-C6-O6
5	X	1	NAG	O5-C5-C6-O6
4	V	2	NAG	O5-C5-C6-O6
5	a	3	BMA	O5-C5-C6-O6
4	P	2	NAG	O5-C5-C6-O6
5	O	1	NAG	O5-C5-C6-O6
5	T	1	NAG	C4-C5-C6-O6
4	I	1	NAG	O5-C5-C6-O6
5	O	2	NAG	O5-C5-C6-O6
5	T	3	BMA	C4-C5-C6-O6
5	a	1	NAG	O5-C5-C6-O6
5	a	2	NAG	O5-C5-C6-O6
4	V	1	NAG	O5-C5-C6-O6
5	U	2	NAG	O5-C5-C6-O6
5	O	2	NAG	C8-C7-N2-C2
5	Z	1	NAG	C4-C5-C6-O6
5	U	1	NAG	O5-C5-C6-O6
4	P	1	NAG	C4-C5-C6-O6
5	N	1	NAG	C4-C5-C6-O6
5	X	1	NAG	C4-C5-C6-O6
4	V	1	NAG	C4-C5-C6-O6
5	U	1	NAG	C4-C5-C6-O6
5	O	2	NAG	O7-C7-N2-C2
5	a	3	BMA	C4-C5-C6-O6
5	J	1	NAG	C8-C7-N2-C2
5	J	1	NAG	O7-C7-N2-C2
5	O	1	NAG	C8-C7-N2-C2
5	O	1	NAG	O7-C7-N2-C2
5	T	1	NAG	C8-C7-N2-C2
5	T	1	NAG	O7-C7-N2-C2
5	W	1	NAG	C8-C7-N2-C2
5	W	1	NAG	O7-C7-N2-C2
5	X	2	NAG	C8-C7-N2-C2
5	X	2	NAG	O7-C7-N2-C2
5	a	2	NAG	C8-C7-N2-C2
5	a	2	NAG	O7-C7-N2-C2
4	S	1	NAG	O5-C5-C6-O6
5	T	3	BMA	O5-C5-C6-O6
4	I	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	V	2	NAG	C4-C5-C6-O6
5	U	3	BMA	O5-C5-C6-O6
5	O	2	NAG	C4-C5-C6-O6
5	a	2	NAG	C4-C5-C6-O6
4	P	2	NAG	C4-C5-C6-O6
4	P	1	NAG	C8-C7-N2-C2
4	P	1	NAG	O7-C7-N2-C2
4	M	1	NAG	O5-C5-C6-O6
5	O	1	NAG	C4-C5-C6-O6
5	a	1	NAG	C4-C5-C6-O6
5	N	3	BMA	O5-C5-C6-O6
5	Z	2	NAG	O5-C5-C6-O6
5	O	2	NAG	C3-C2-N2-C7
5	a	2	NAG	C3-C2-N2-C7
5	O	3	BMA	O5-C5-C6-O6
4	Y	1	NAG	O5-C5-C6-O6
5	J	2	NAG	C1-C2-N2-C7
5	Q	2	NAG	C1-C2-N2-C7
5	W	2	NAG	C1-C2-N2-C7
4	I	2	NAG	C4-C5-C6-O6
4	M	1	NAG	C3-C2-N2-C7
4	S	1	NAG	C4-C5-C6-O6
5	J	1	NAG	C4-C5-C6-O6
5	U	2	NAG	C1-C2-N2-C7
5	J	2	NAG	C3-C2-N2-C7
5	Q	2	NAG	C3-C2-N2-C7
5	U	2	NAG	C3-C2-N2-C7
5	W	2	NAG	C3-C2-N2-C7
5	U	3	BMA	C4-C5-C6-O6
5	Z	3	BMA	C4-C5-C6-O6

There are no ring outliers.

10 monomers are involved in 11 short contacts:

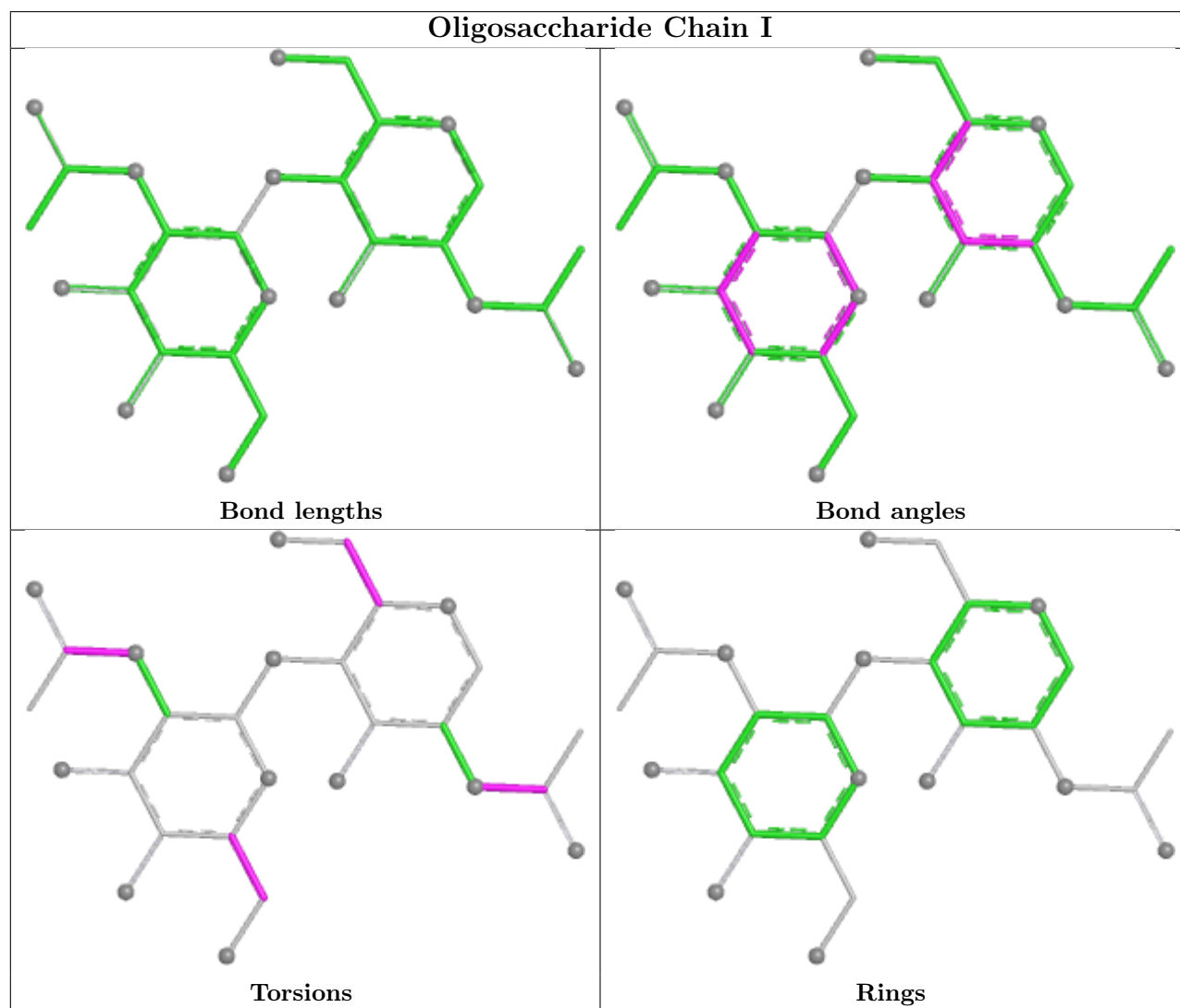
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	J	2	NAG	1	0
5	N	2	NAG	2	0
5	U	1	NAG	1	0
4	S	1	NAG	1	0
5	T	1	NAG	1	0
5	J	1	NAG	1	0
5	T	2	NAG	1	0

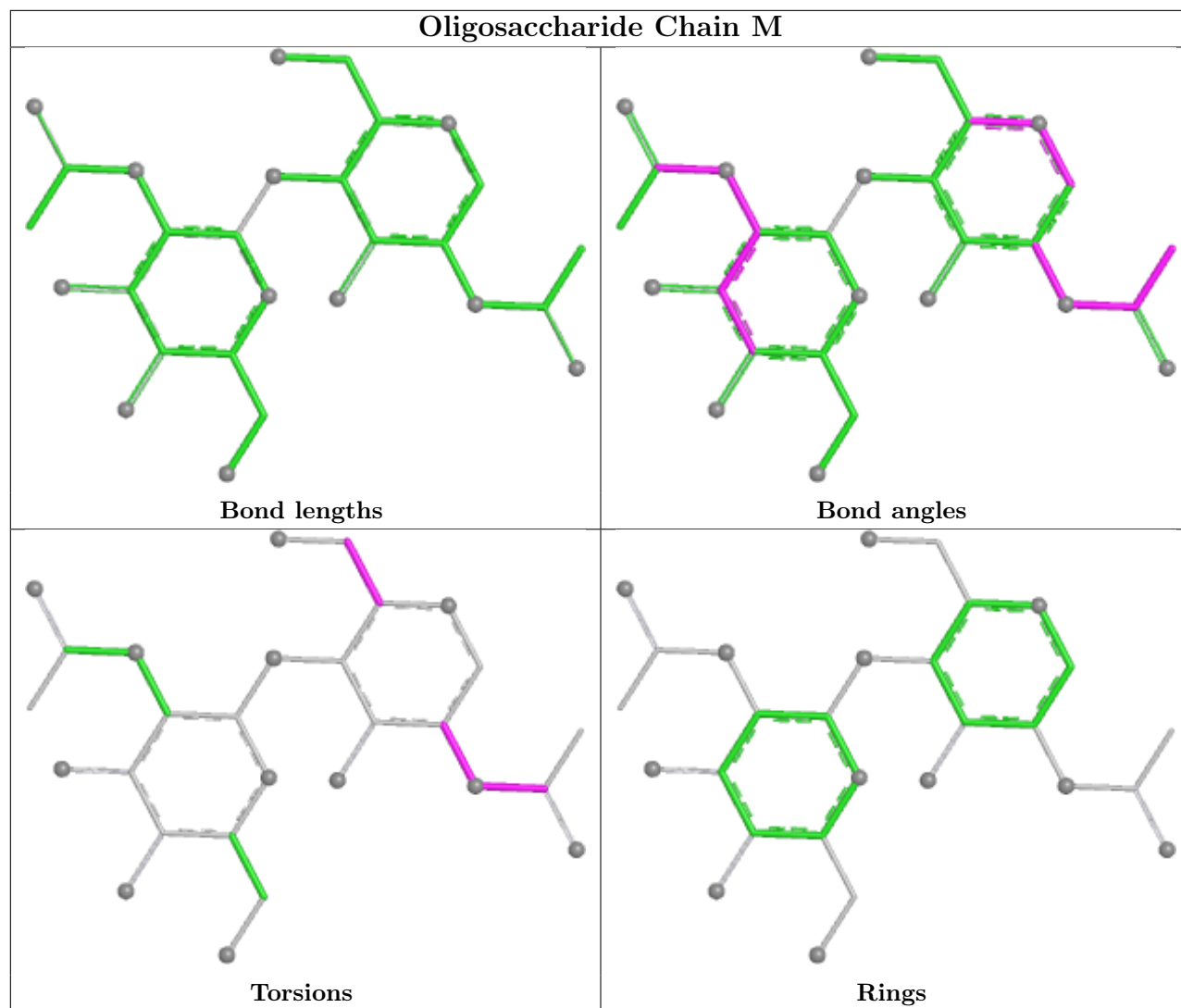
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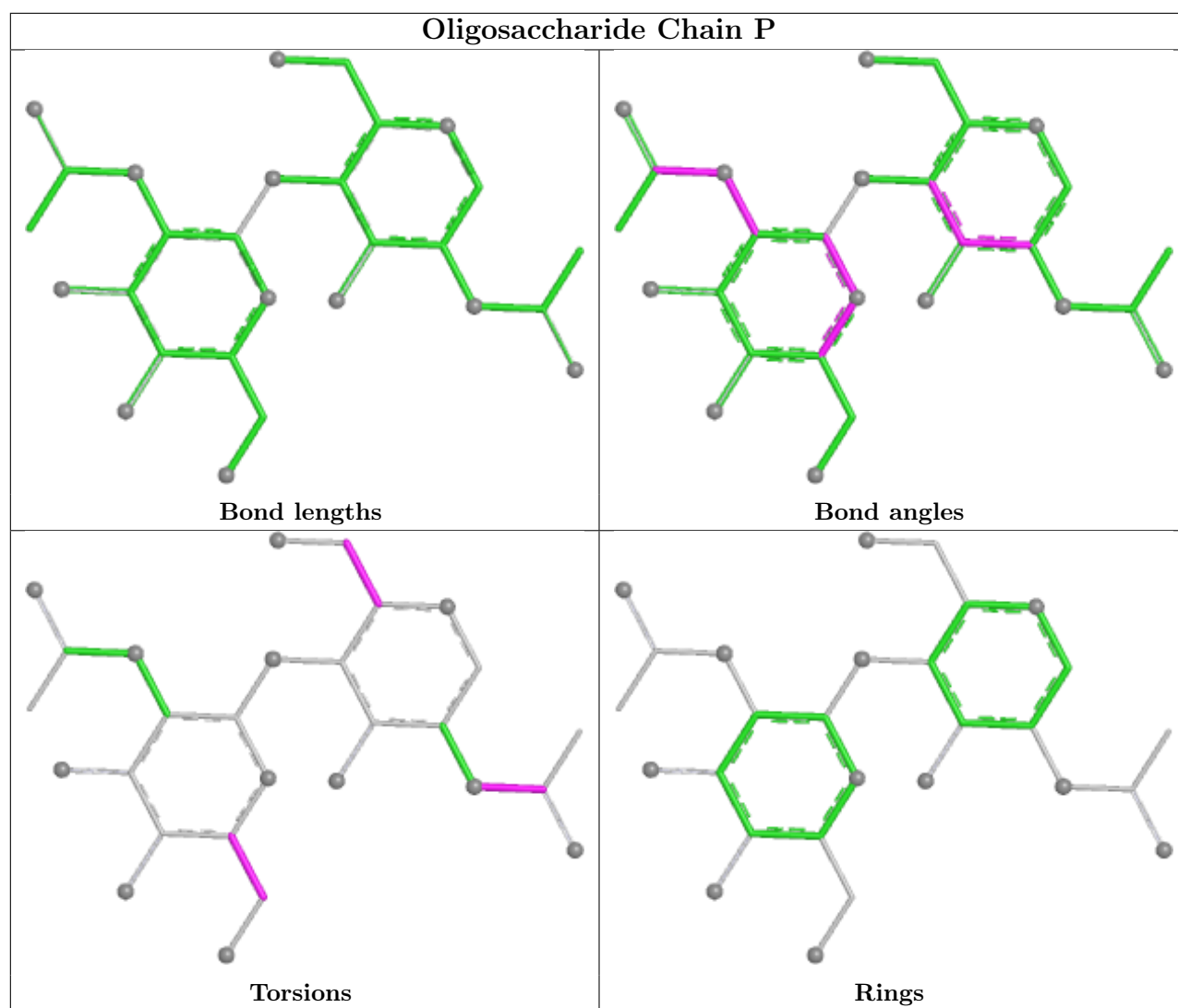
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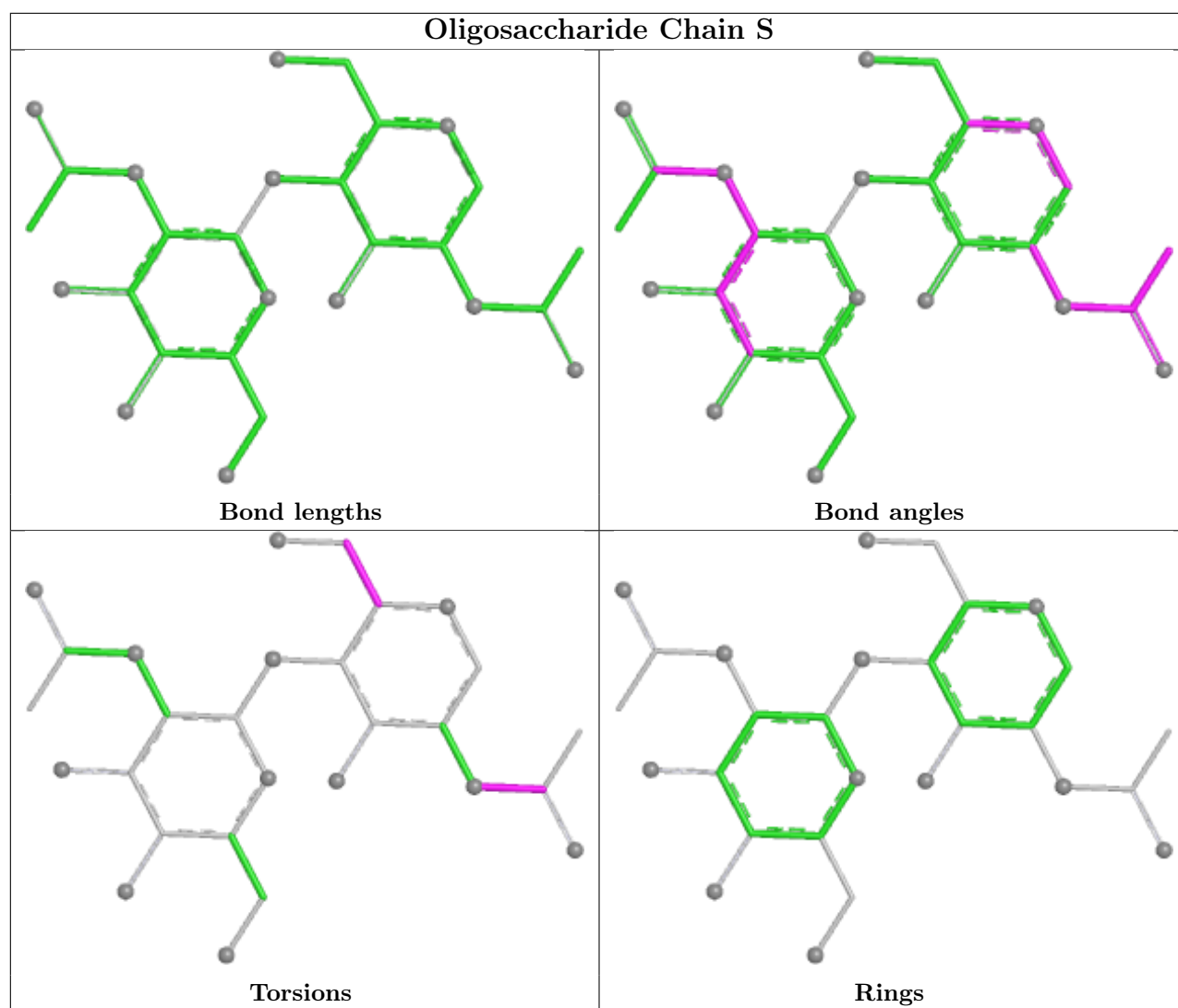
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	N	1	NAG	3	0
5	W	2	NAG	1	0
5	W	1	NAG	1	0

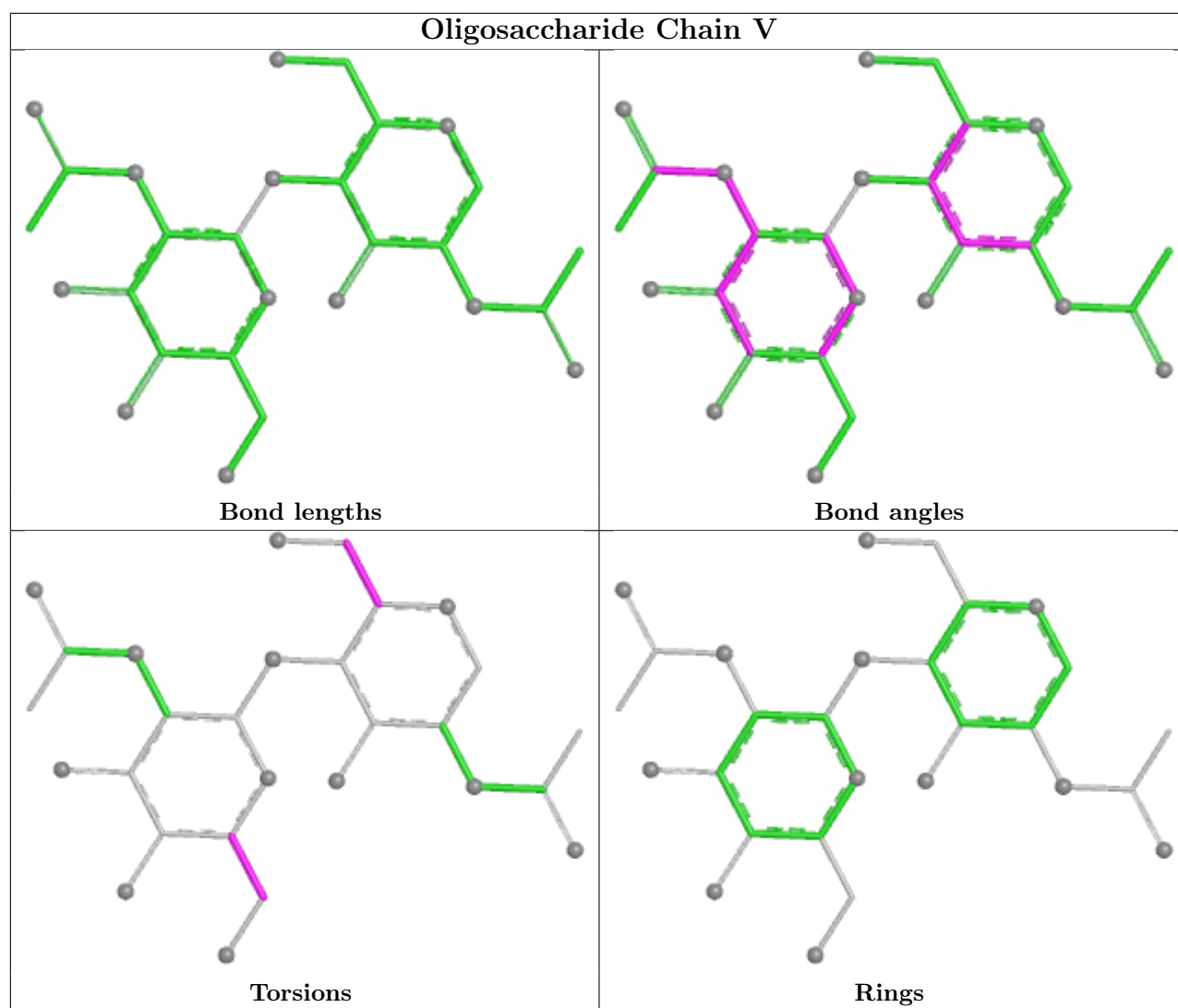
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

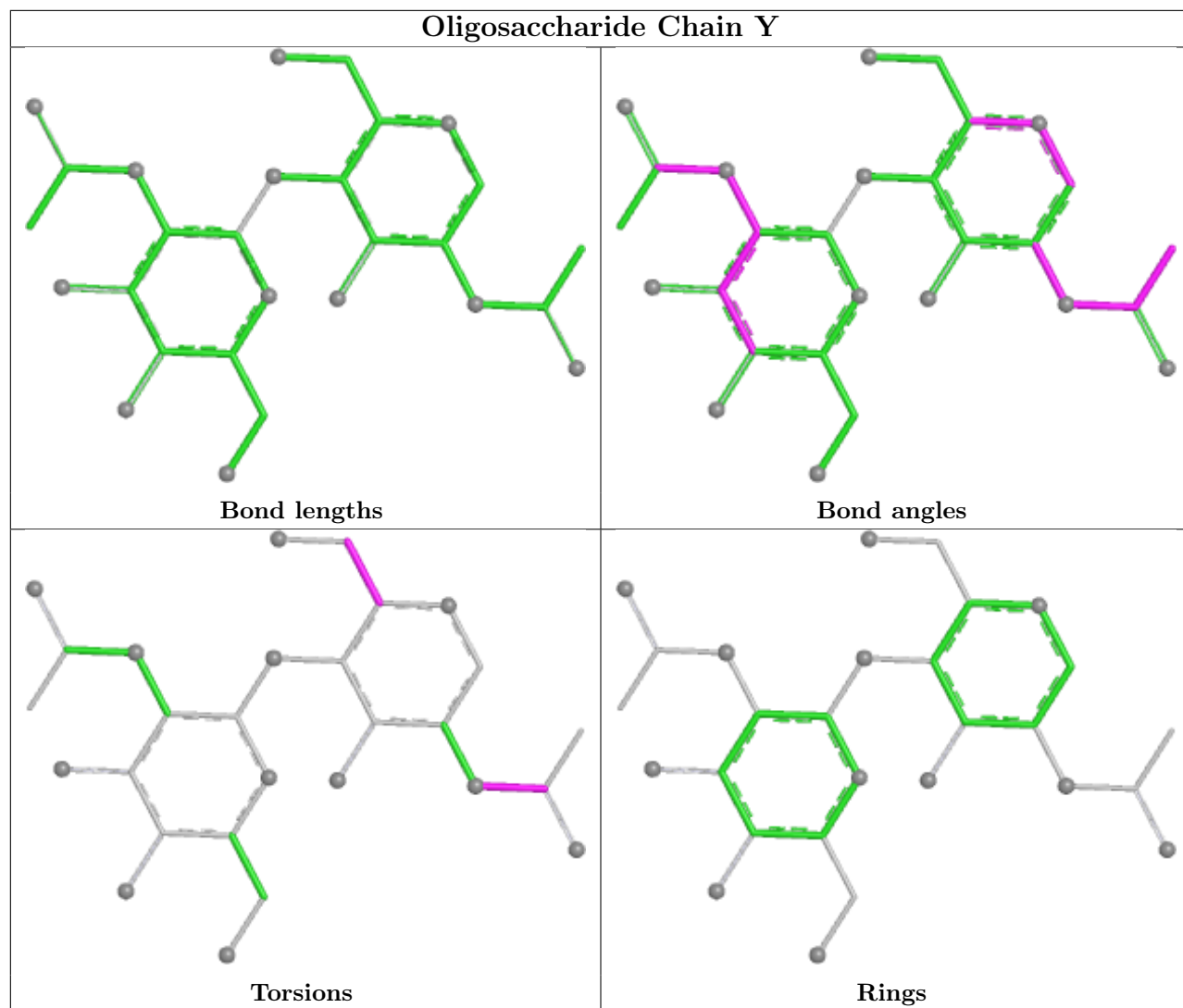


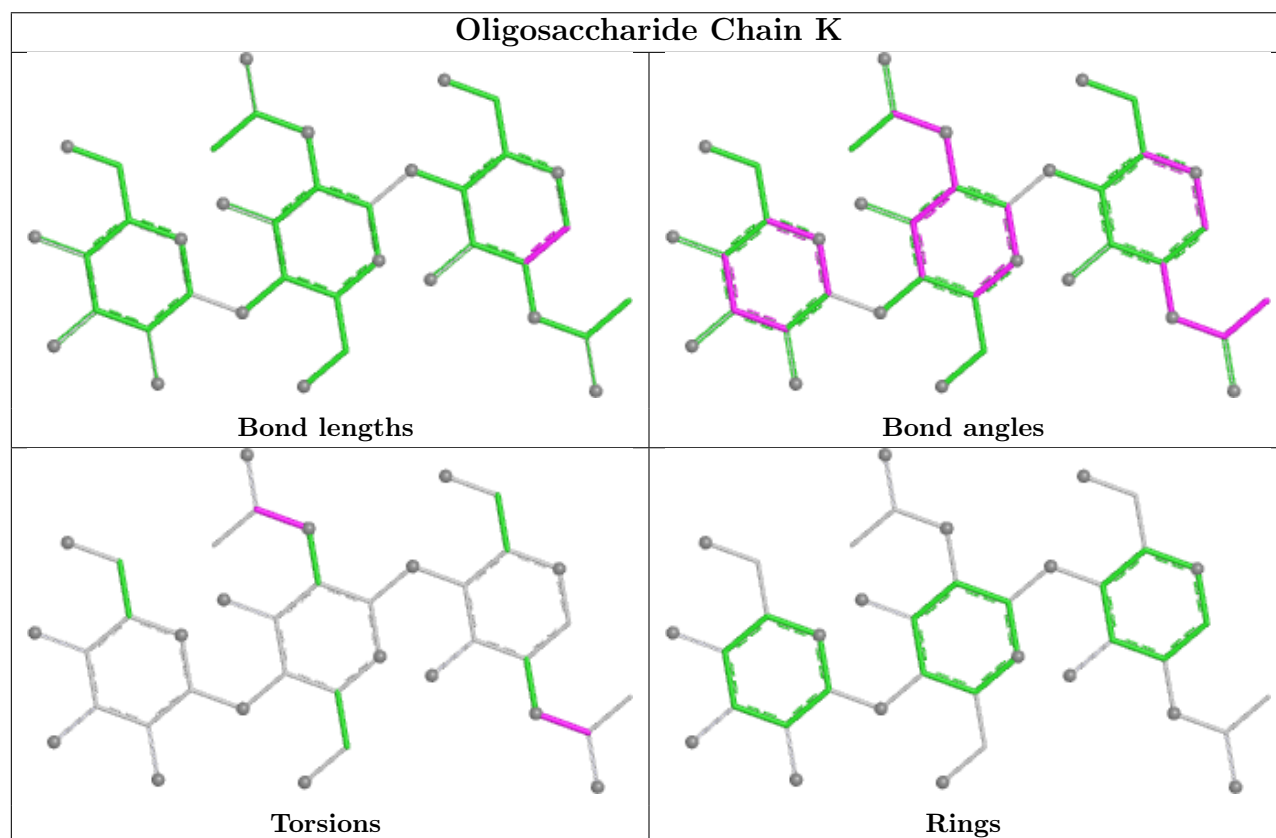
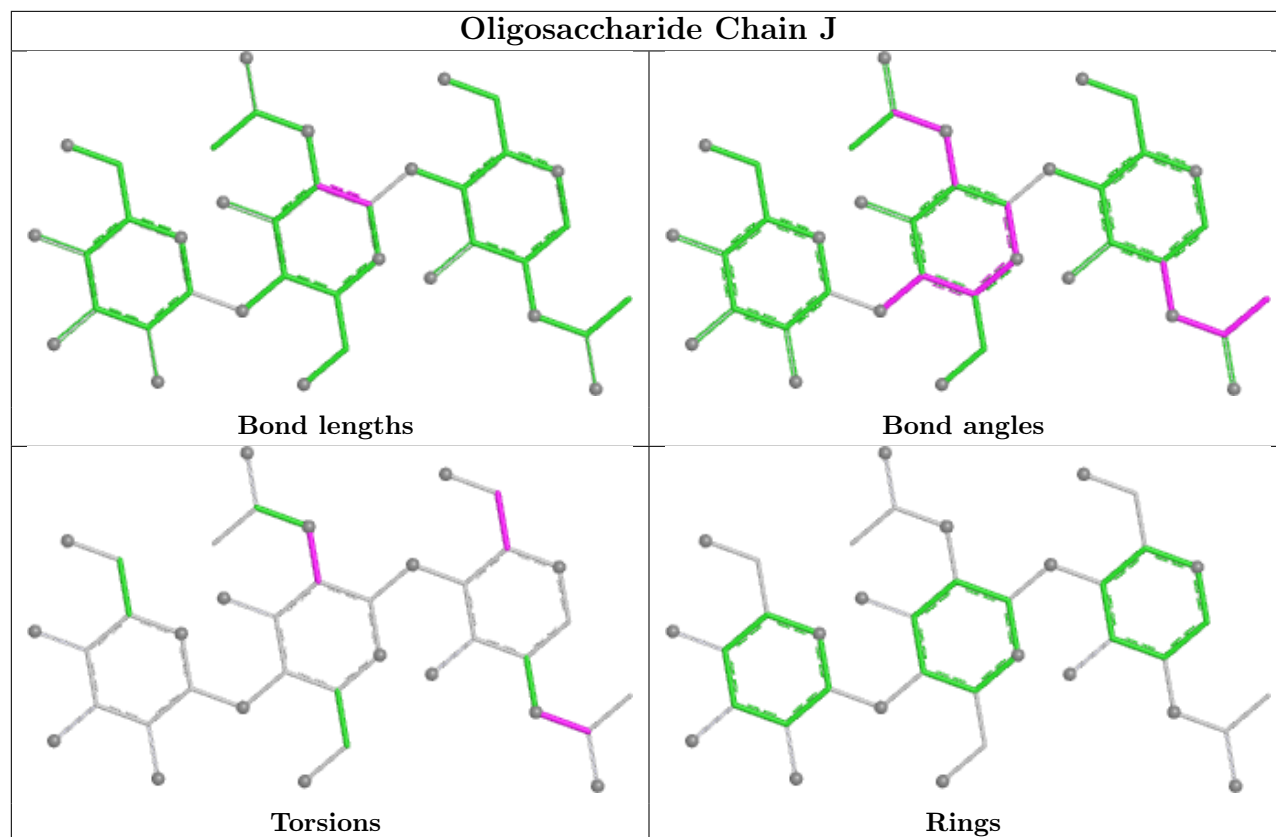


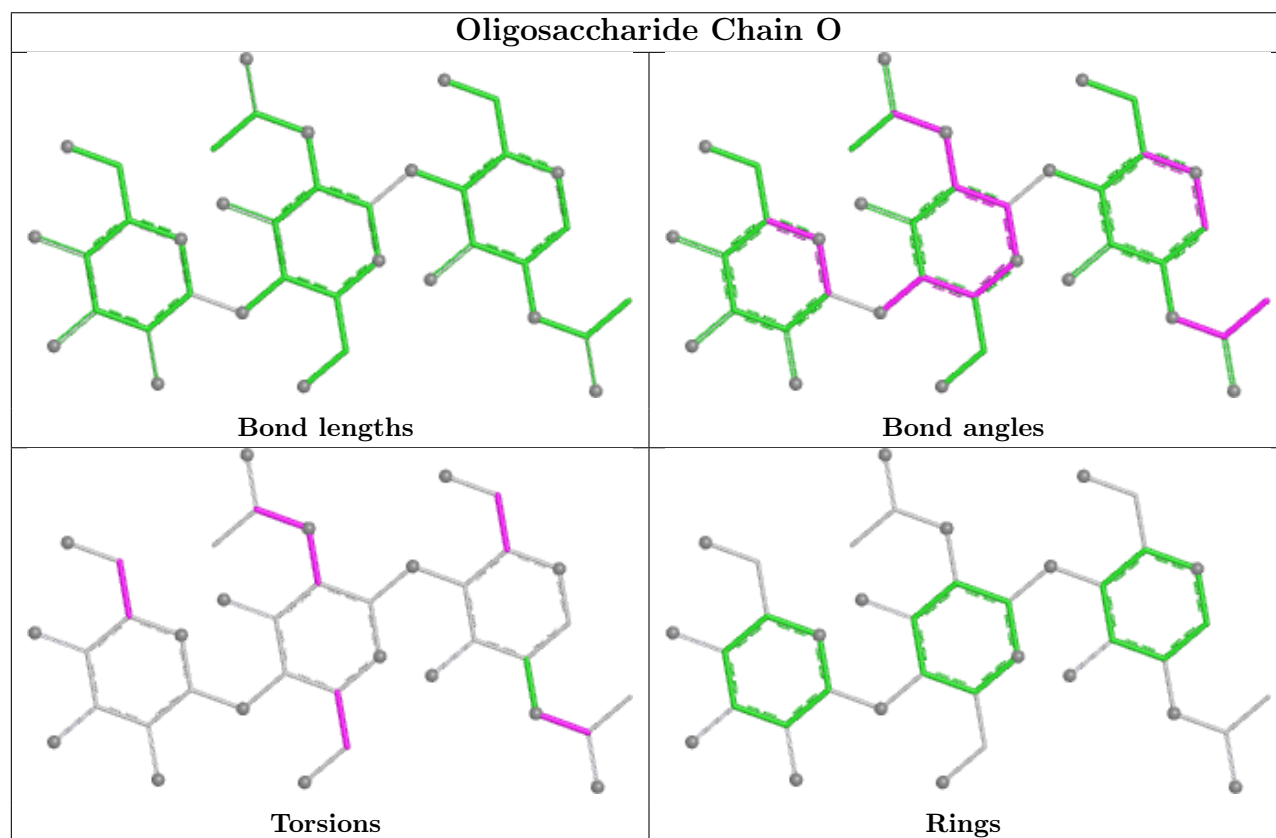
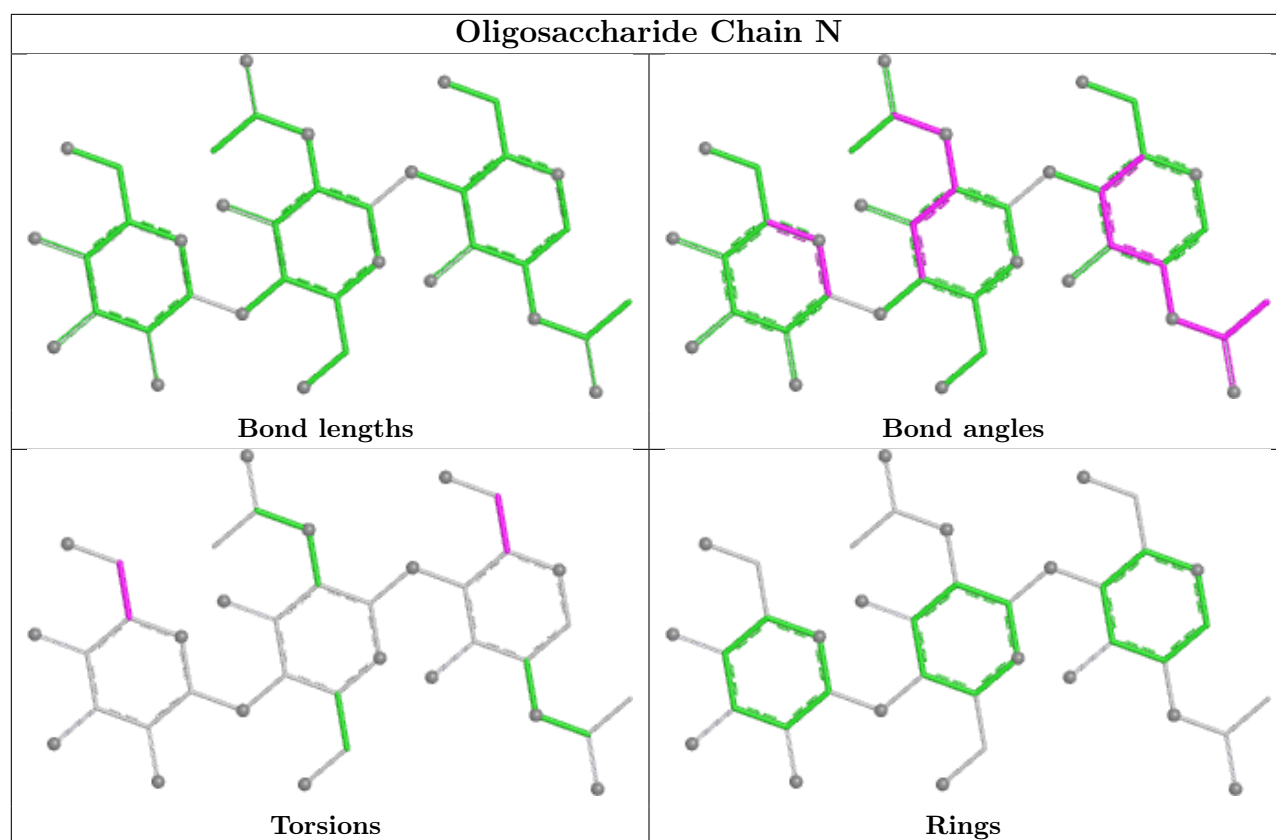


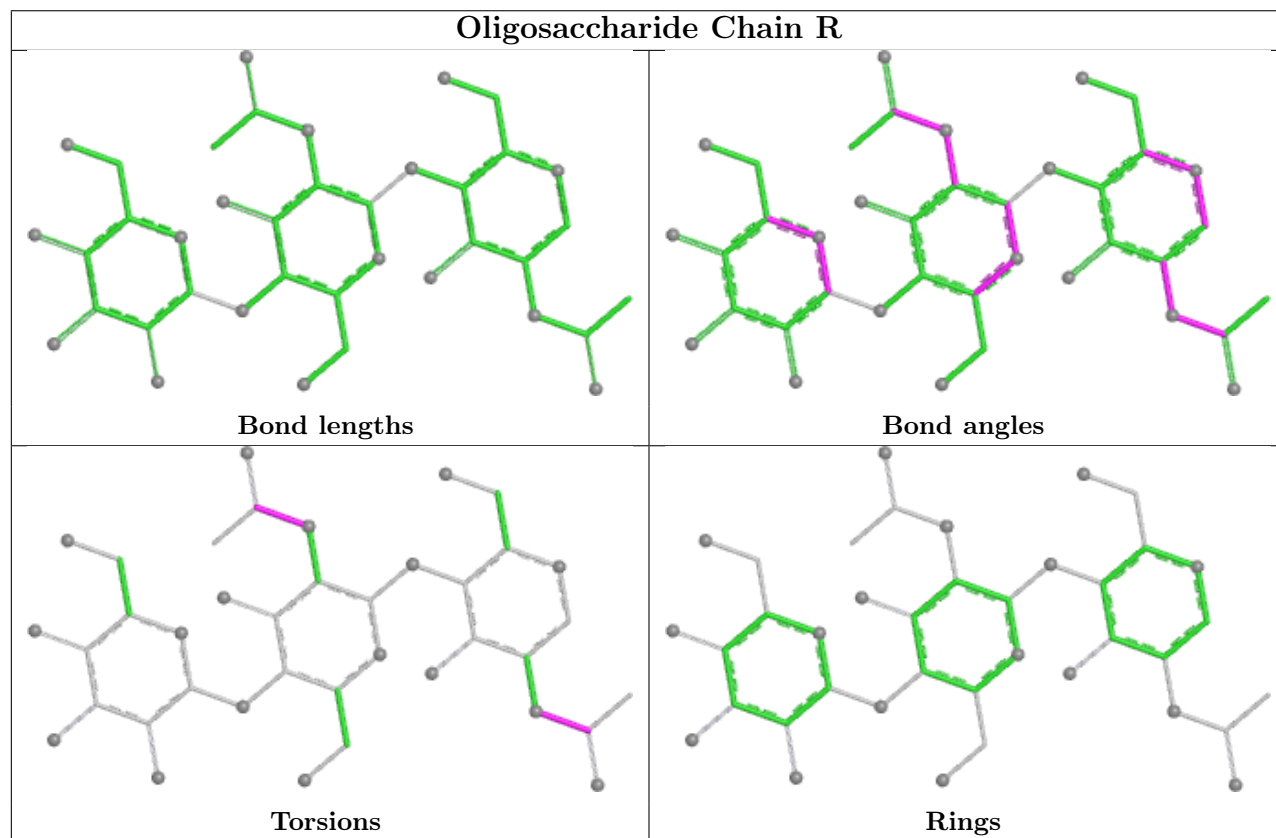
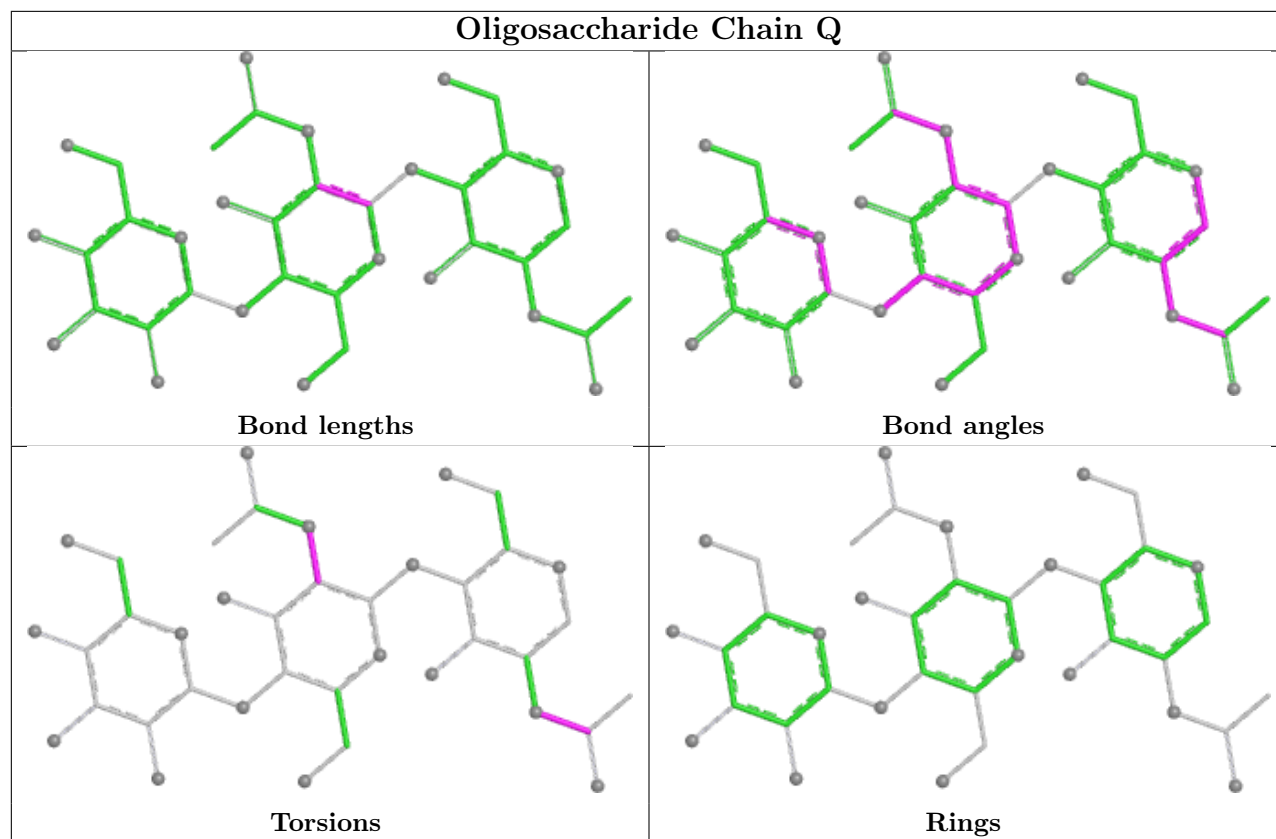


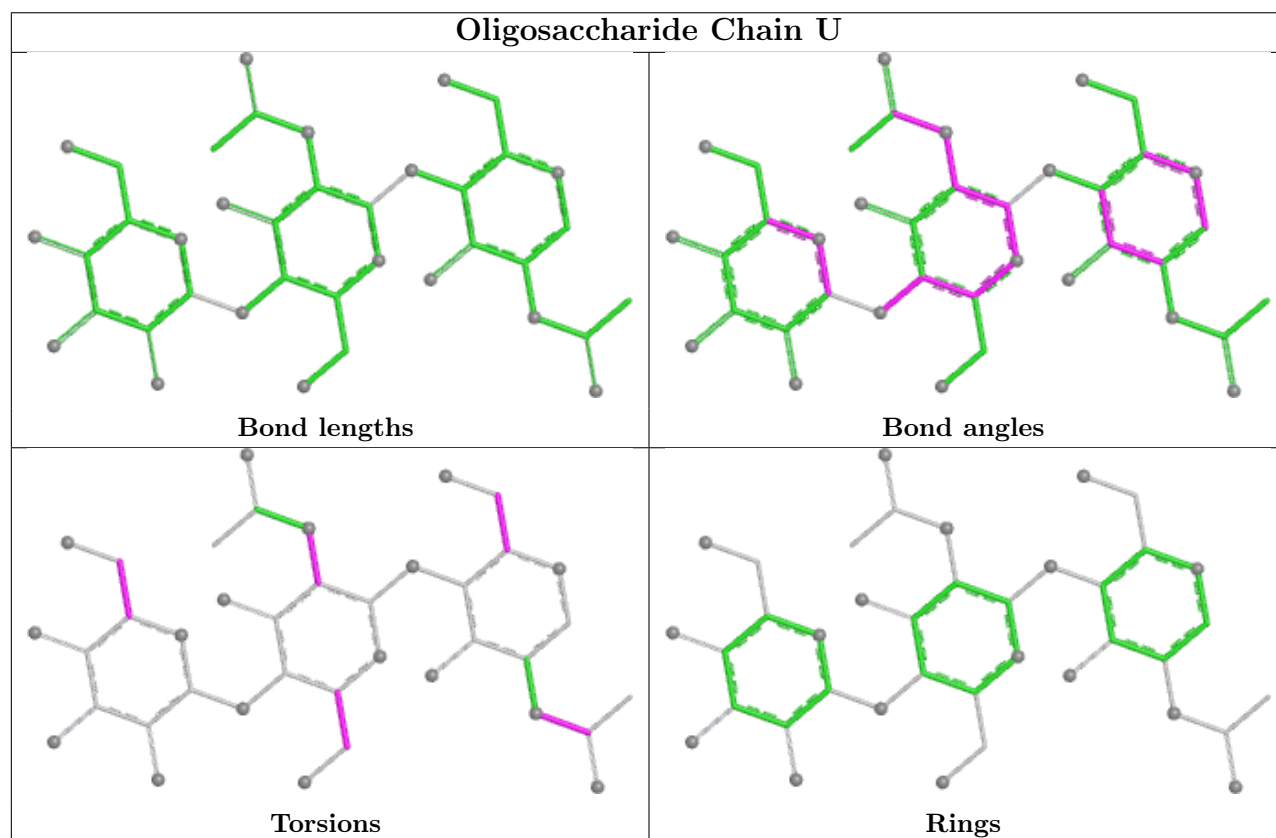
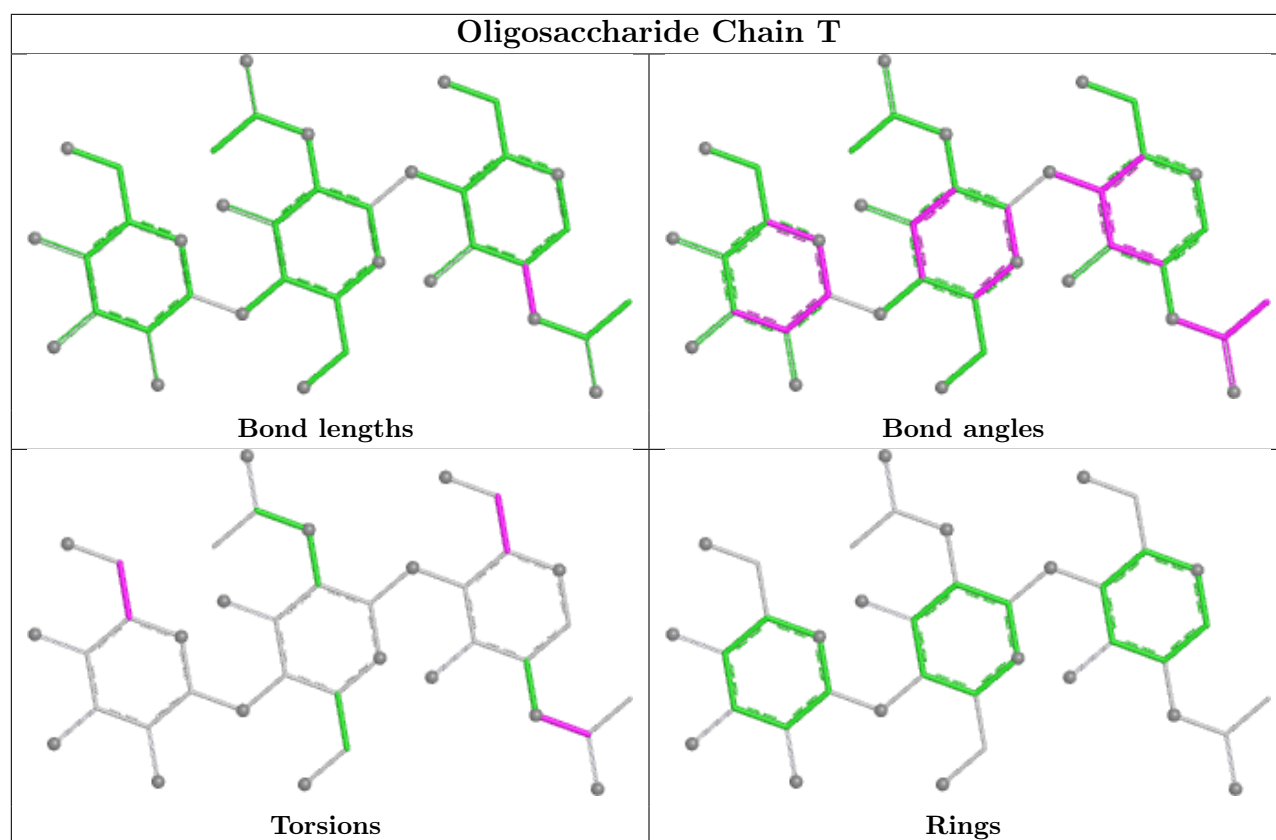


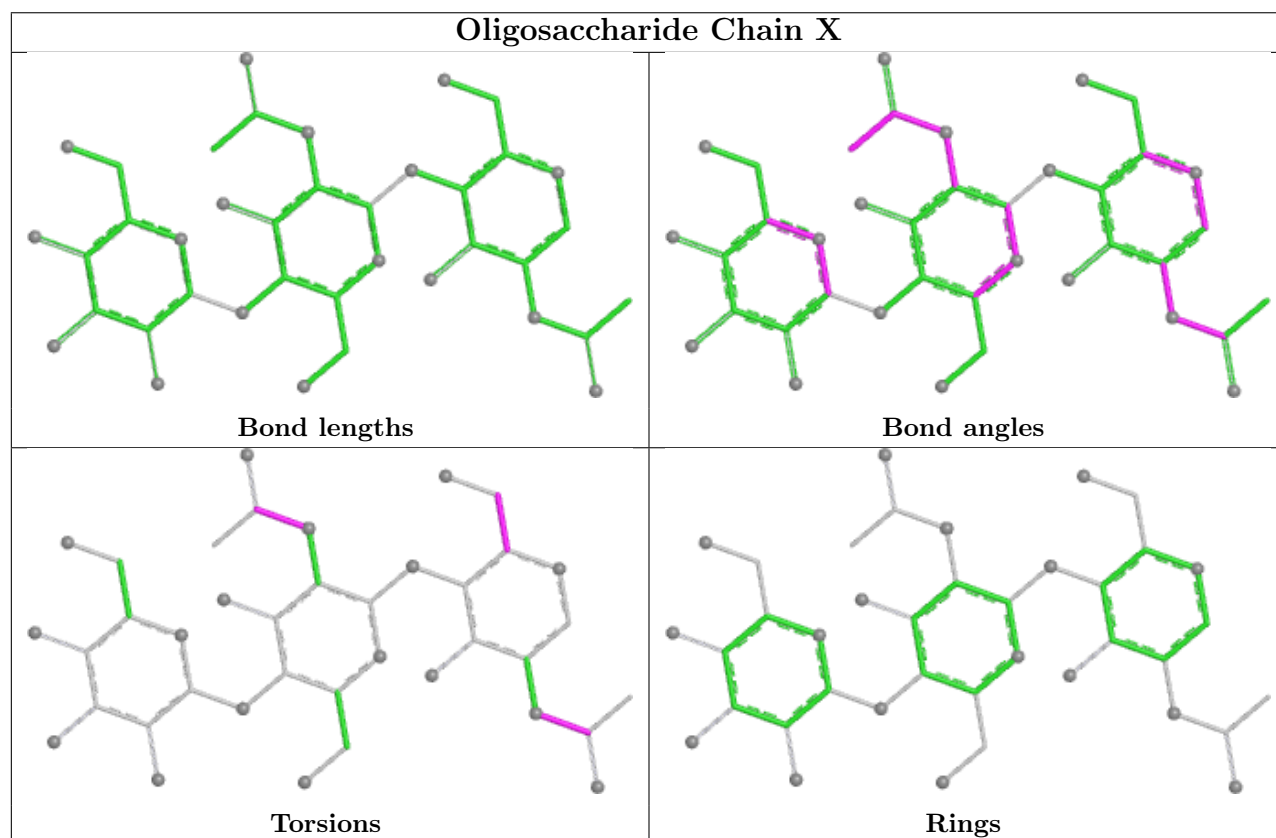
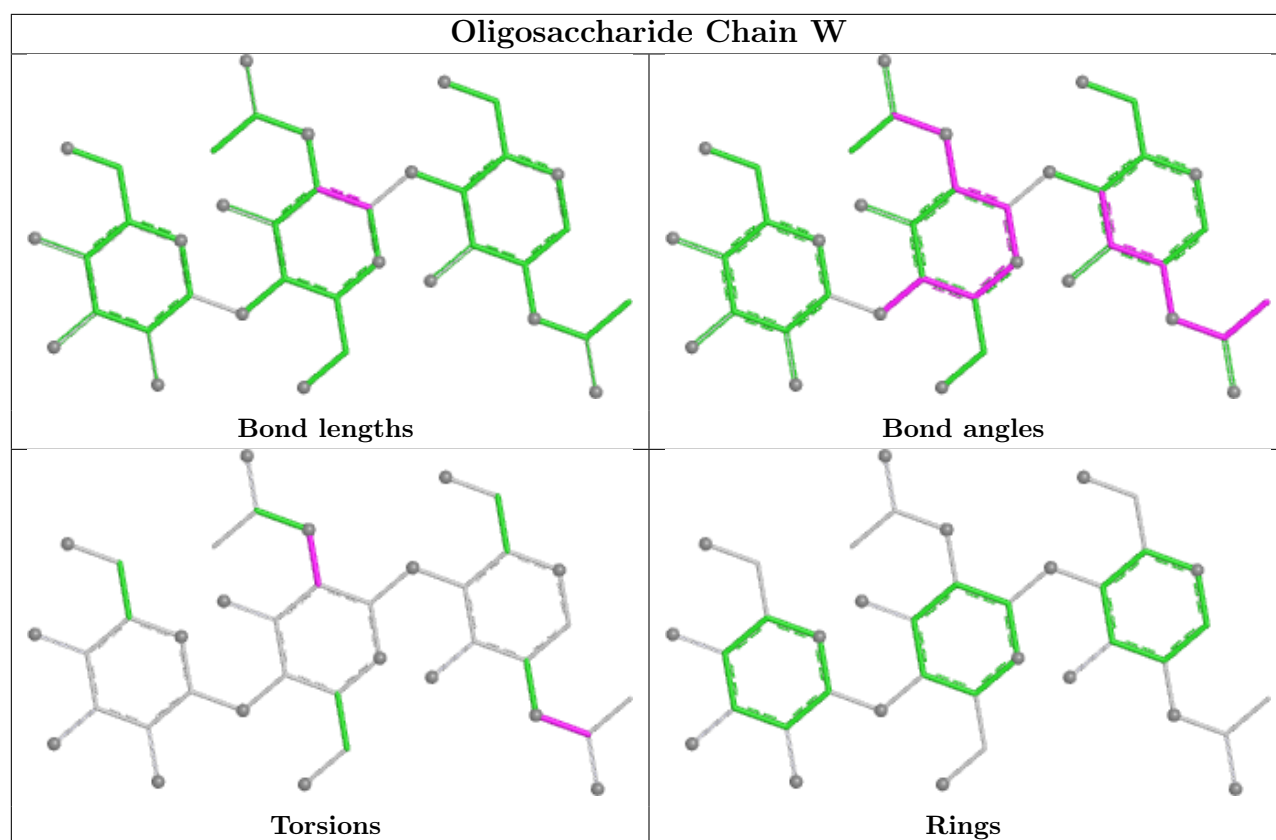


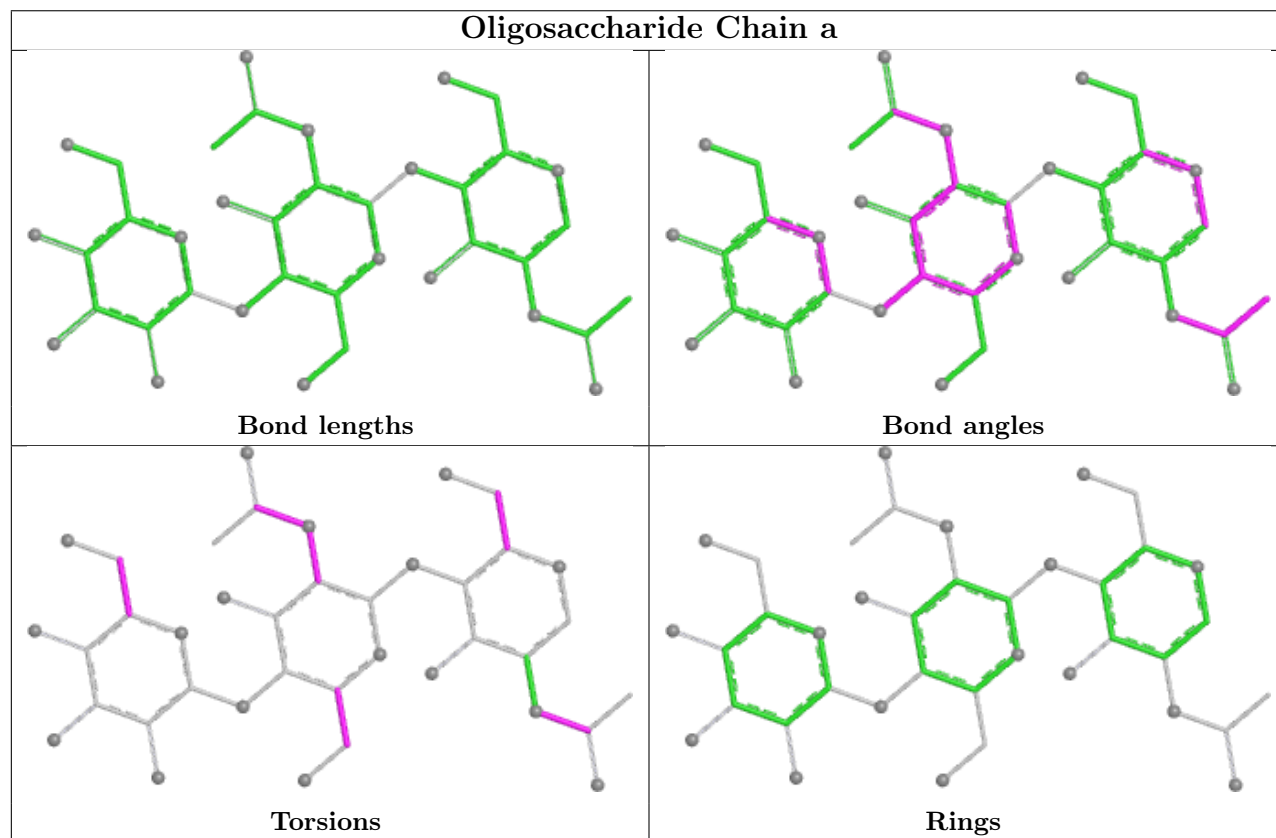
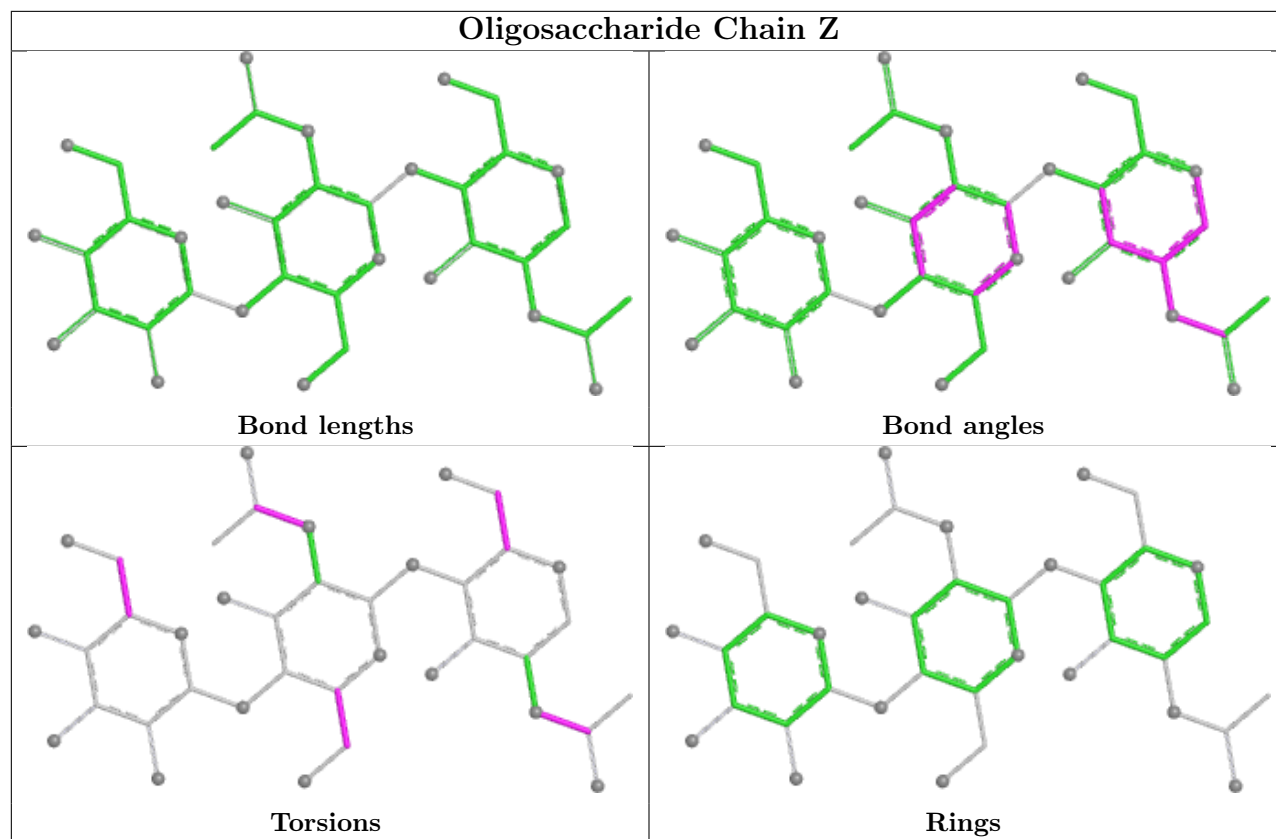












5.6 Ligand geometry

3 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
6	NAG	A	601	1	14,14,15	0.27	0	17,19,21	0.65	0
6	NAG	B	601	1	14,14,15	0.85	1 (7%)	17,19,21	1.36	2 (11%)
6	NAG	C	601	1	14,14,15	0.83	1 (7%)	17,19,21	1.34	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	601	1	-	0/6/23/26	0/1/1/1
6	NAG	B	601	1	-	2/6/23/26	0/1/1/1
6	NAG	C	601	1	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	601	NAG	C1-C2	2.81	1.56	1.52
6	C	601	NAG	C1-C2	2.75	1.56	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	601	NAG	C1-O5-C5	3.87	117.37	112.19
6	B	601	NAG	C1-O5-C5	3.62	117.04	112.19
6	B	601	NAG	C2-N2-C7	2.42	126.15	122.90
6	C	601	NAG	C2-N2-C7	2.09	125.71	122.90

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	601	NAG	C4-C5-C6-O6
6	B	601	NAG	C4-C5-C6-O6
6	C	601	NAG	O5-C5-C6-O6
6	B	601	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	601	NAG	4	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.

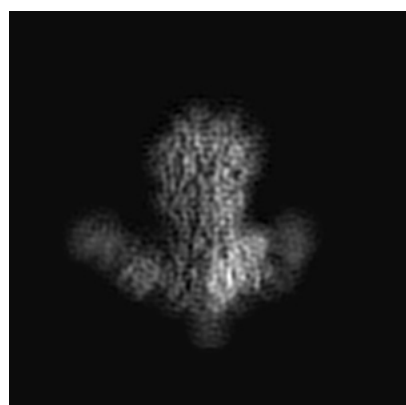
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21973. These allow visual inspection of the internal detail of the map and identification of artifacts.

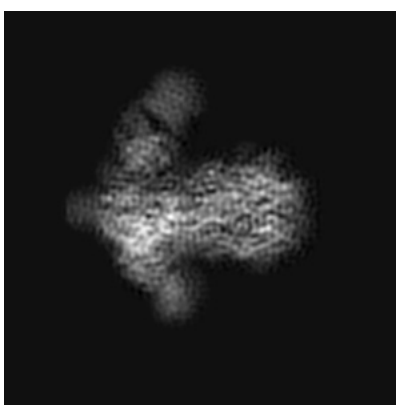
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

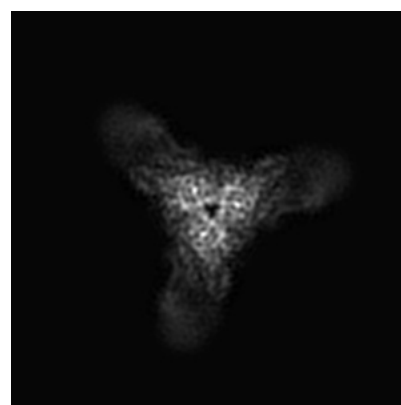
6.1.1 Primary map



X



Y

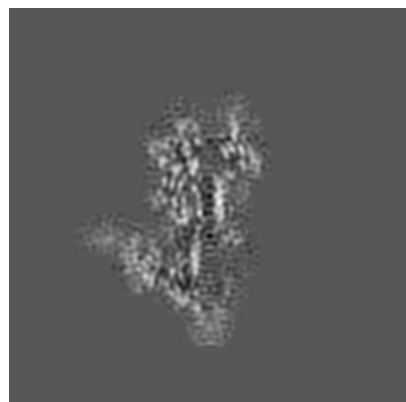


Z

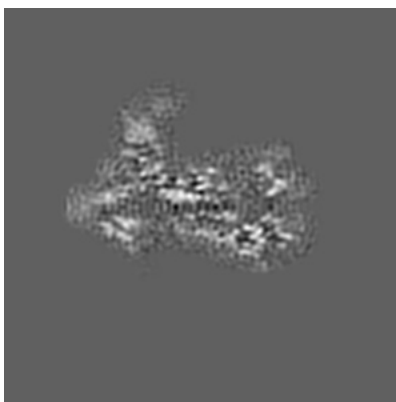
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 125



Y Index: 125

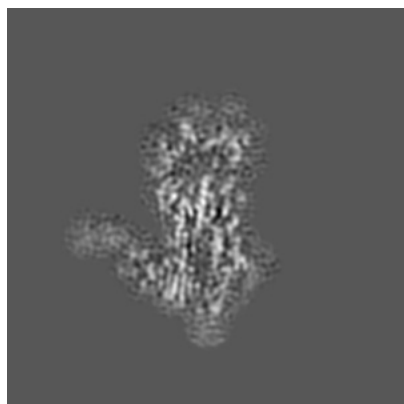


Z Index: 125

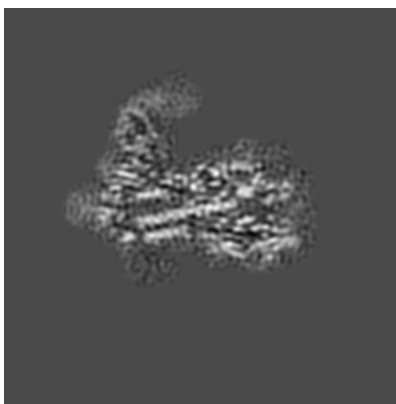
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

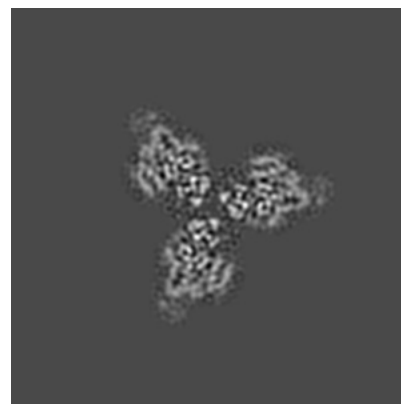
6.3.1 Primary map



X Index: 119



Y Index: 130

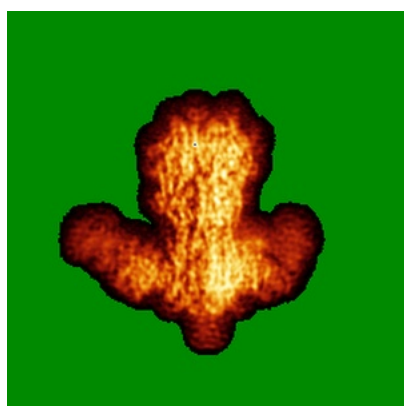


Z Index: 86

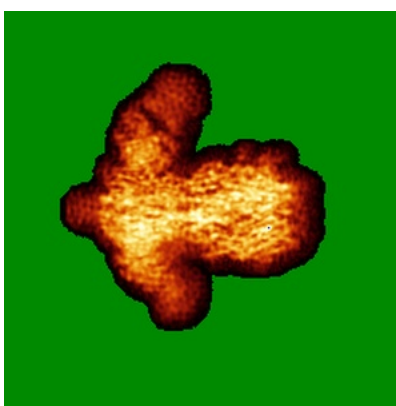
The images above show the largest variance slices of the map in three orthogonal directions.

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

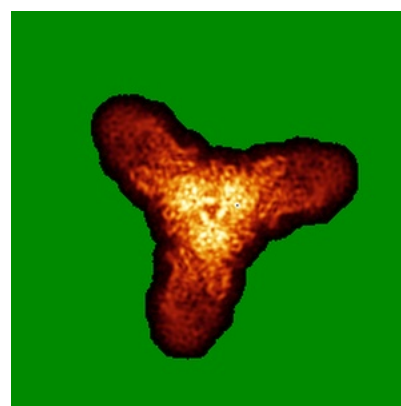
6.4.1 Primary map



X



Y

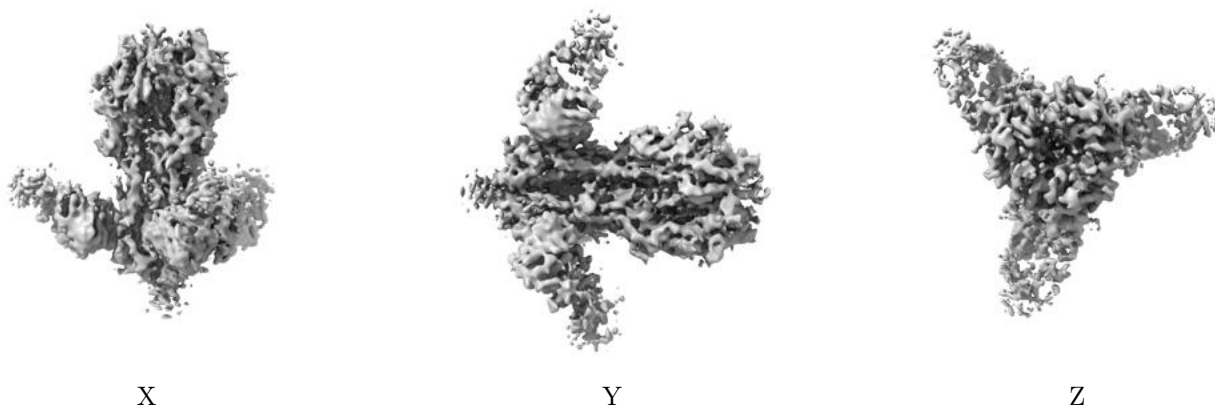


Z

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

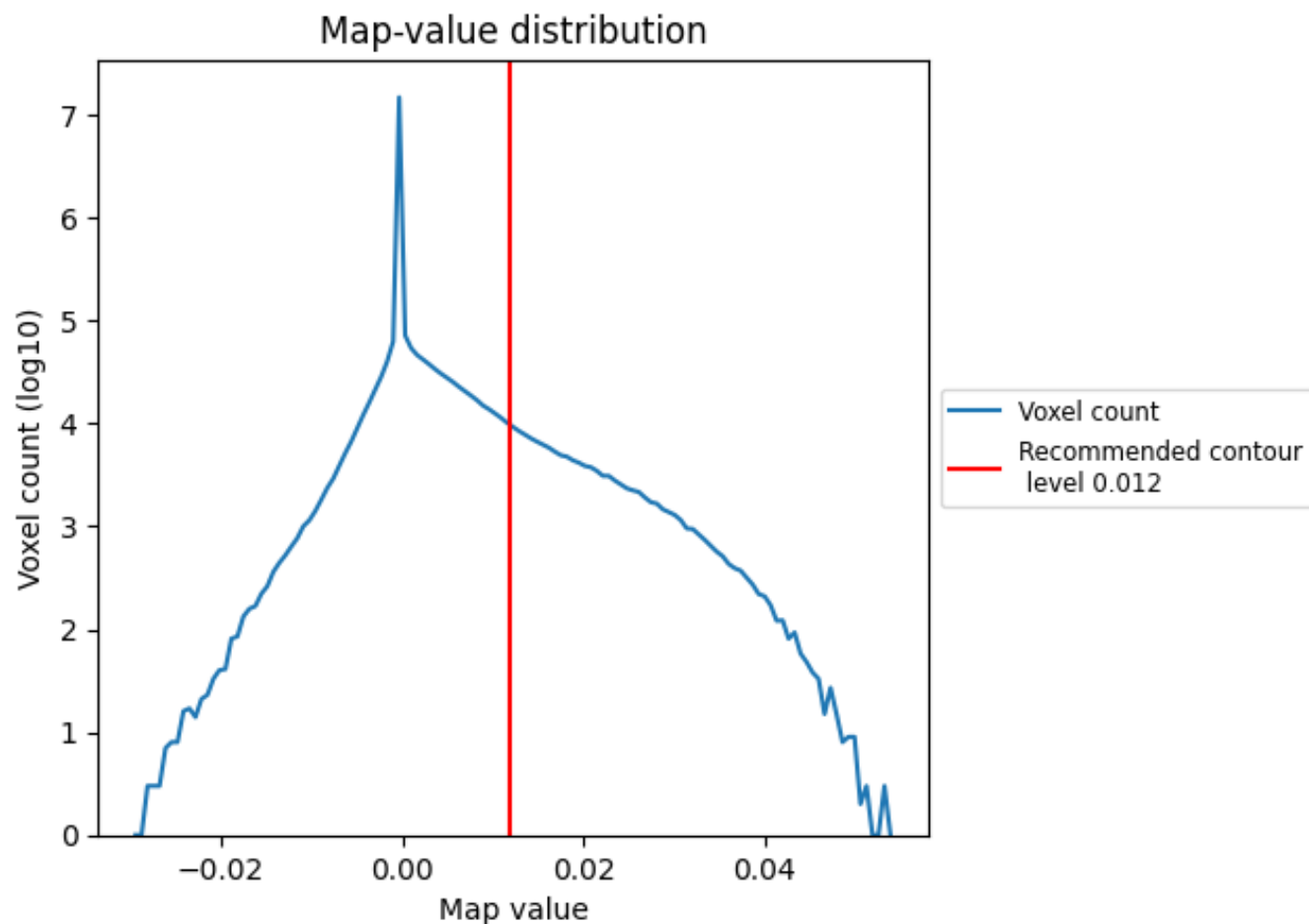
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

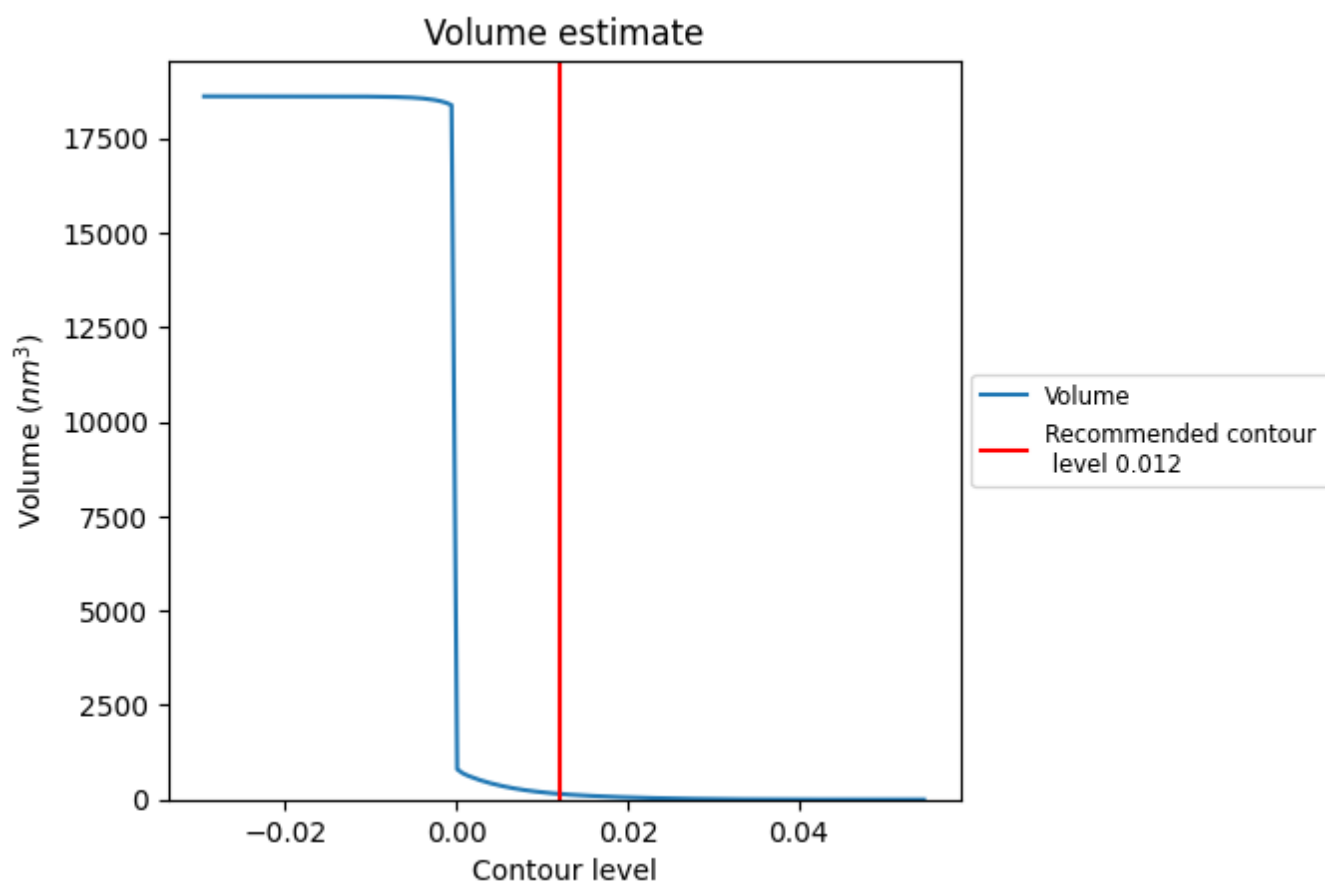
This section contains the results of statistical analysis of the map.

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.

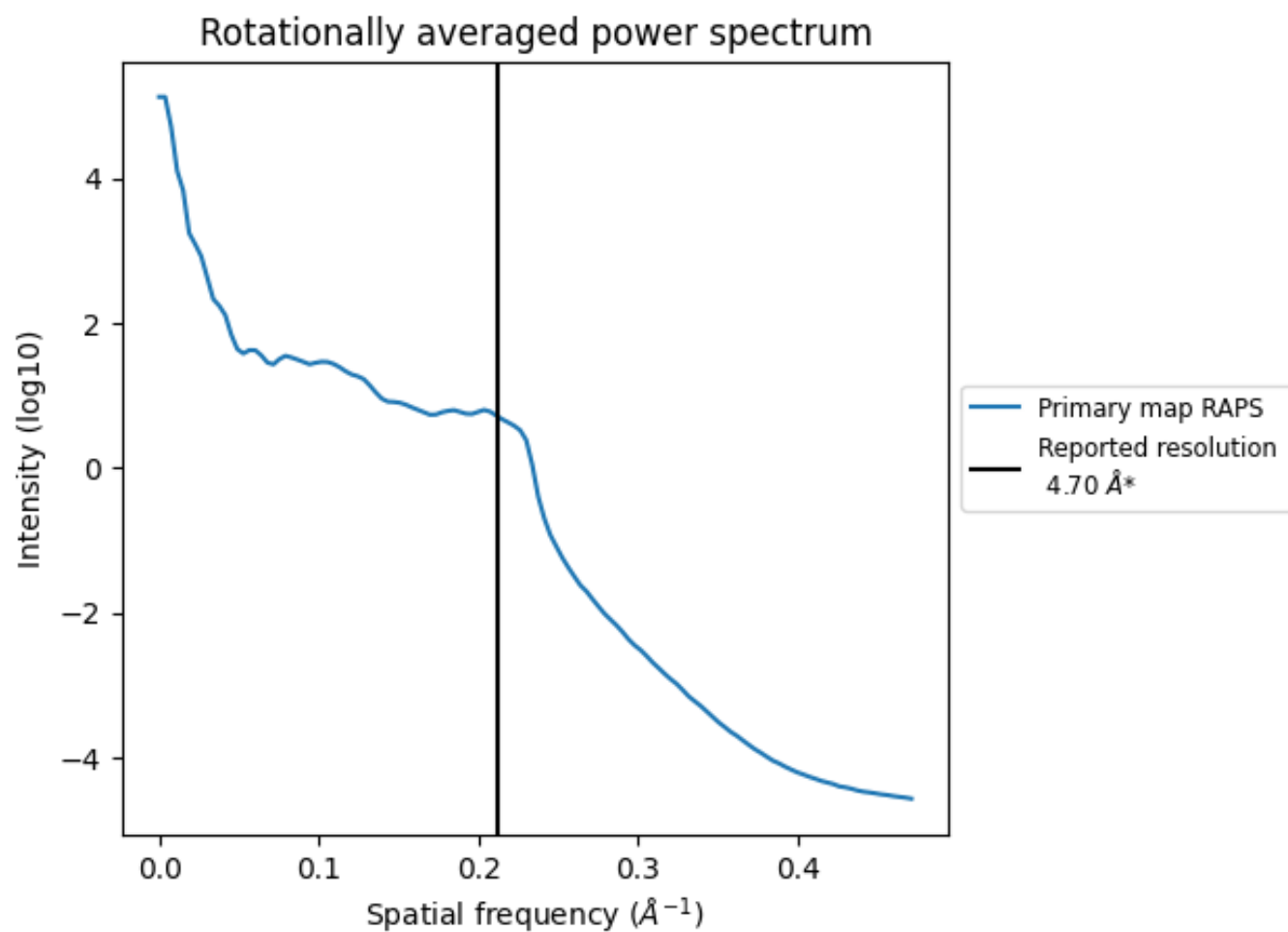
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 151 nm^3 ; this corresponds to an approximate mass of 136 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 ⓘ

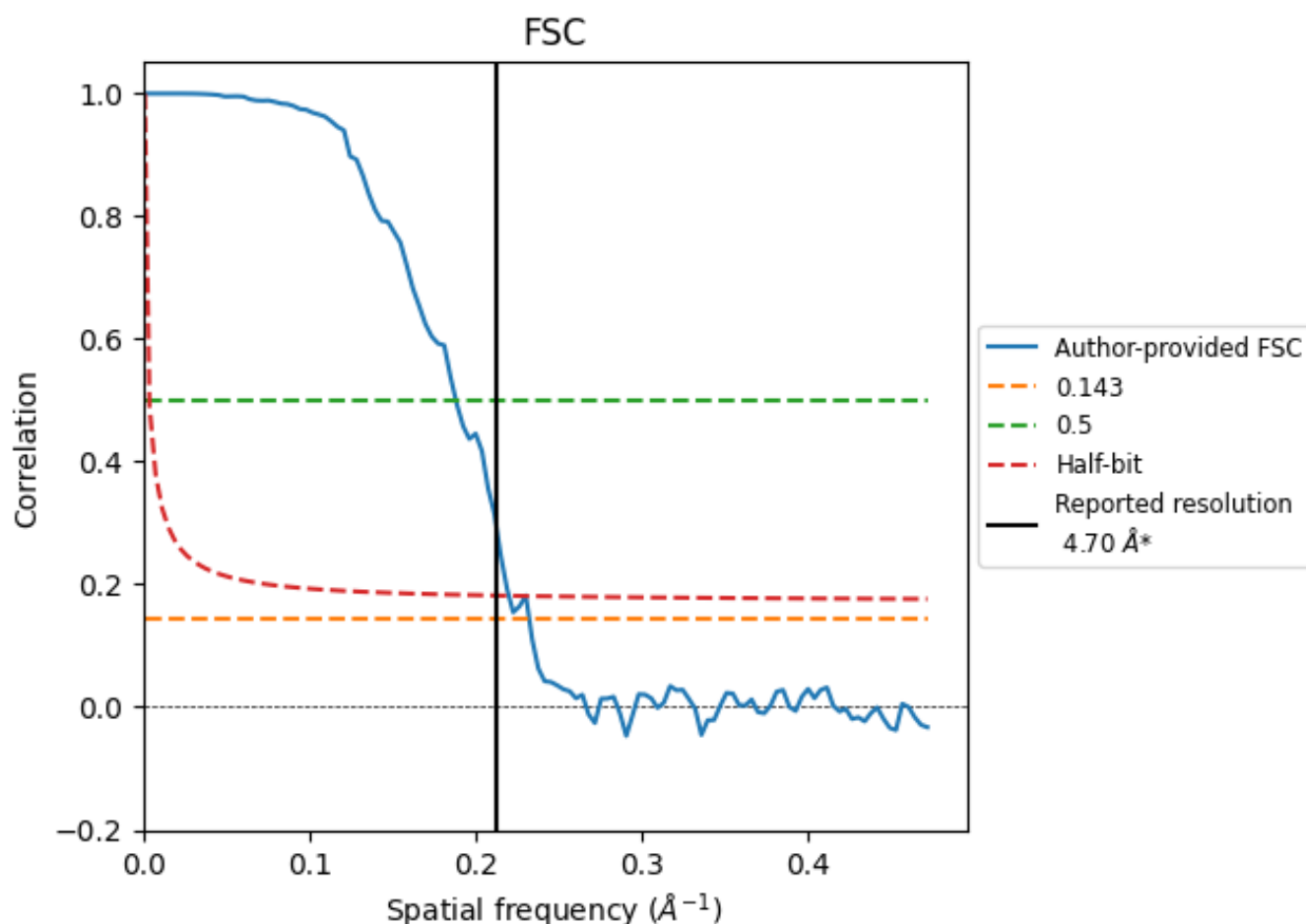


*Reported resolution corresponds to spatial frequency of 0.213 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.213 Å⁻¹

8.2 Resolution estimates [i](#)

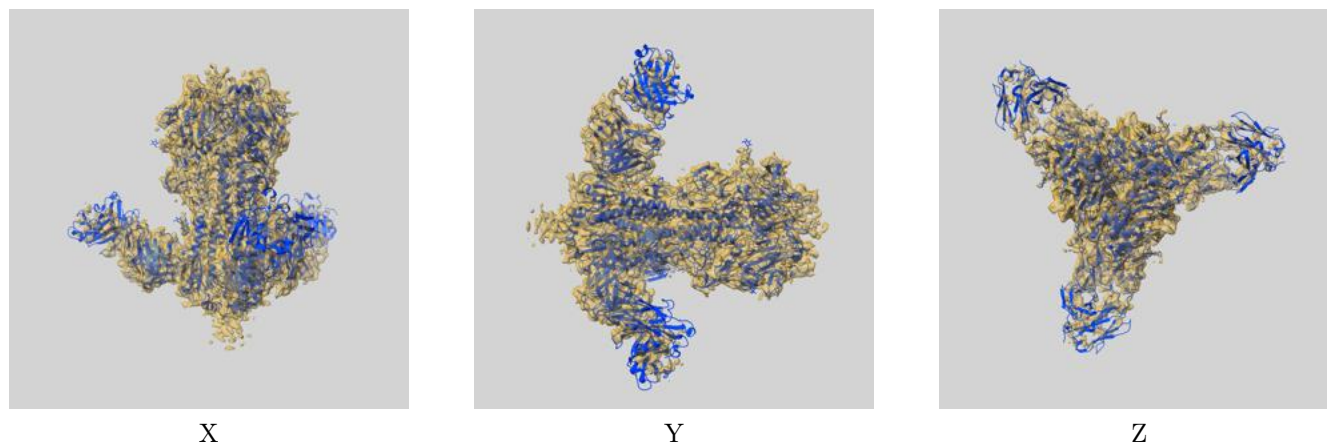
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.70	-	-
Author-provided FSC curve	4.31	5.32	4.55
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

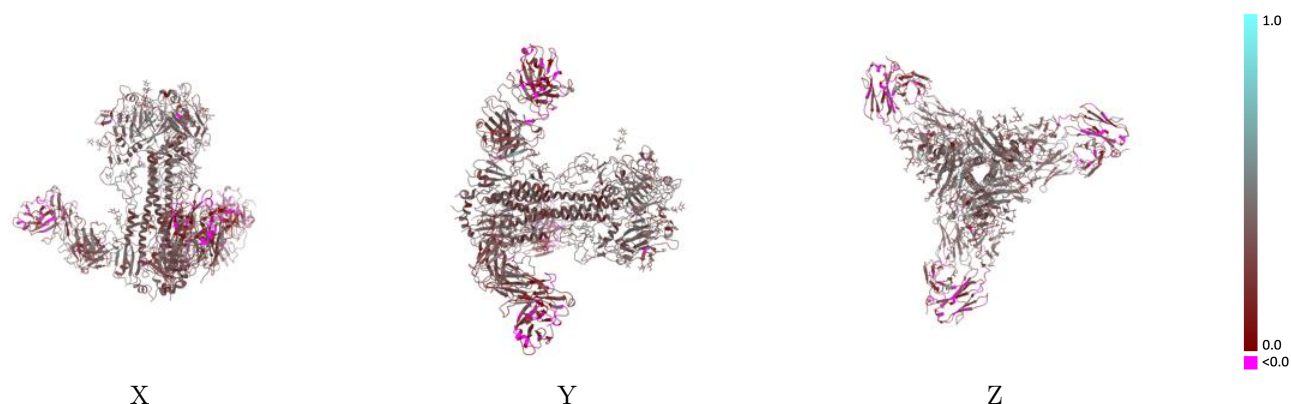
This section contains information regarding the fit between EMDB map EMD-21973 and PDB model 6WZT. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



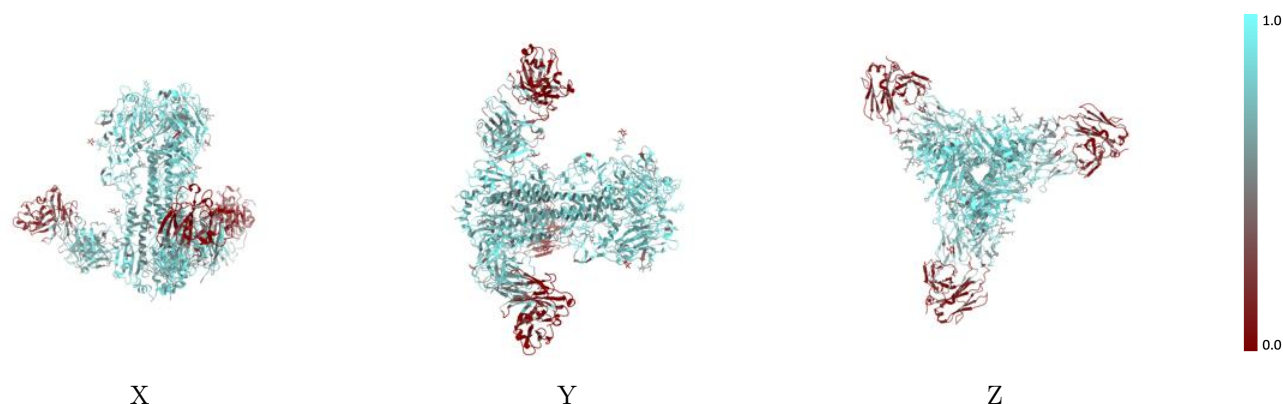
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



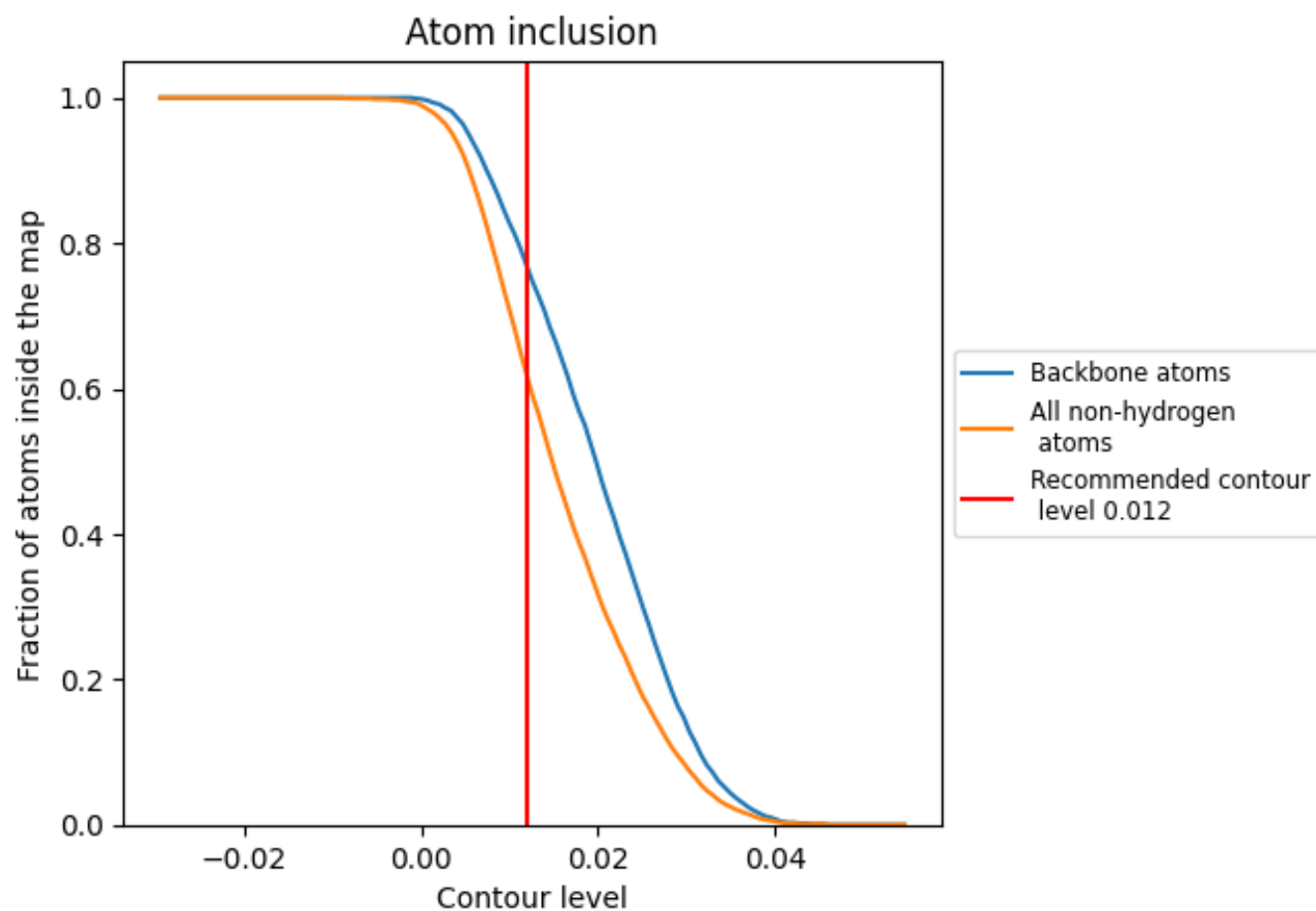
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.012).

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 62% 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 (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6160	 0.3150
A	 0.7760	 0.3690
B	 0.7740	 0.3730
C	 0.7710	 0.3710
D	 0.4040	 0.2340
E	 0.4530	 0.2590
F	 0.3980	 0.2300
G	 0.4520	 0.2600
H	 0.4510	 0.2560
I	 0.5710	 0.3450
J	 0.6410	 0.4010
K	 0.5130	 0.3720
L	 0.4050	 0.2370
M	 0.5000	 0.3270
N	 0.7690	 0.3100
O	 0.8210	 0.3870
P	 0.4290	 0.2500
Q	 0.6150	 0.3980
R	 0.5380	 0.3990
S	 0.5000	 0.3300
T	 0.7950	 0.3750
U	 0.7950	 0.3530
V	 0.4640	 0.2660
W	 0.6150	 0.4040
X	 0.5380	 0.3840
Y	 0.5000	 0.3230
Z	 0.7690	 0.2950
a	 0.7950	 0.3940

