



# Full wwPDB EM Validation Report ⓘ

Nov 26, 2025 – 02:49 PM EST

PDB ID : 9CF5 / pdb\_00009cf5  
EMDB ID : EMD-45530  
Title : STRUCTURE OF CD4 MIMETIC CJF-III-288 IN COMPLEX WITH BG505  
SOSIP.664 HIV-1ENV TRIMER AND 17B FAB  
Authors : Niu, L.; Tolbert, W.D.; Pazgier, M.  
Deposited on : 2024-06-27  
Resolution : 3.50 Å(reported)  
Based on initial model : 7LOK

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev129  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.46

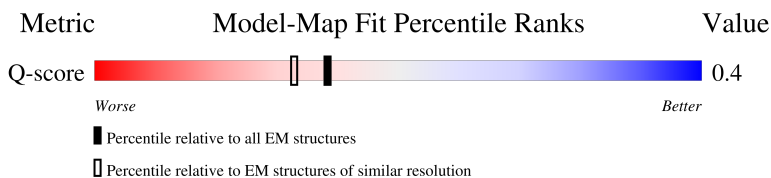
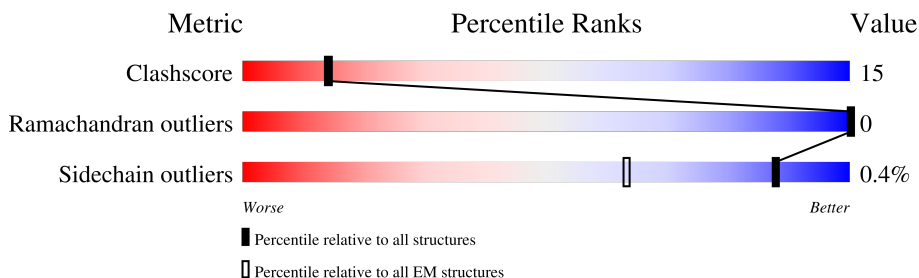
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.50 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.







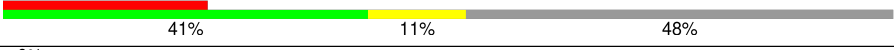
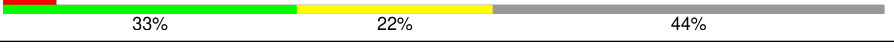
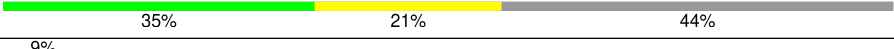
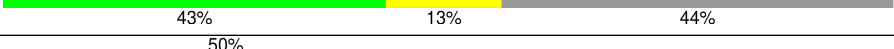
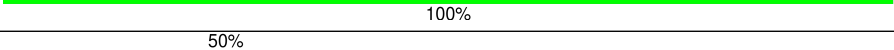
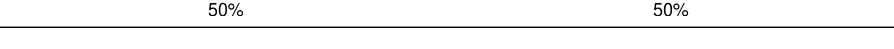
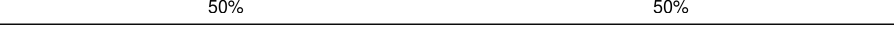
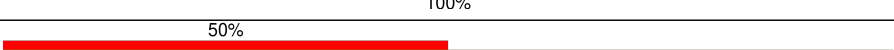




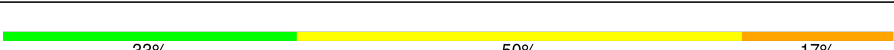



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	13950 ( 3.00 - 4.00 )

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

Mol	Chain	Length	Quality of chain
1	A	479	
1	C	479	
1	E	479	
2	B	153	

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Mol	Chain	Length	Quality of chain
2	D	153	
2	F	153	
3	G	214	
3	I	214	
3	K	214	
4	H	230	
4	J	230	
4	L	230	
5	M	2	
5	P	2	
5	Q	2	
5	R	2	
5	T	2	
5	U	2	
5	V	2	
5	W	2	
5	X	2	
6	N	6	
7	O	7	
7	S	7	

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 18048 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 Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	364	Total	C	N	O	S	0	0
			2848	1794	499	531	24		
1	C	365	Total	C	N	O	S	0	0
			2862	1803	503	532	24		
1	E	364	Total	C	N	O	S	0	0
			2851	1797	499	531	24		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	332	ASN	THR	engineered mutation	UNP Q2N0S6
A	501	CYS	ALA	engineered mutation	UNP Q2N0S6
A	509	ARG	GLU	engineered mutation	UNP Q2N0S6
A	510	ARG	LYS	engineered mutation	UNP Q2N0S6
A	512	ARG	-	insertion	UNP Q2N0S6
A	513	ARG	-	insertion	UNP Q2N0S6
C	332	ASN	THR	engineered mutation	UNP Q2N0S6
C	501	CYS	ALA	engineered mutation	UNP Q2N0S6
C	509	ARG	GLU	engineered mutation	UNP Q2N0S6
C	510	ARG	LYS	engineered mutation	UNP Q2N0S6
C	512	ARG	-	insertion	UNP Q2N0S6
C	513	ARG	-	insertion	UNP Q2N0S6
E	332	ASN	THR	engineered mutation	UNP Q2N0S6
E	501	CYS	ALA	engineered mutation	UNP Q2N0S6
E	509	ARG	GLU	engineered mutation	UNP Q2N0S6
E	510	ARG	LYS	engineered mutation	UNP Q2N0S6
E	512	ARG	-	insertion	UNP Q2N0S6
E	513	ARG	-	insertion	UNP Q2N0S6

- Molecule 2 is a protein called Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	134	Total	C	N	O	S	0	0
			1049	666	185	192	6		
2	D	120	Total	C	N	O	S	0	0
			964	611	166	181	6		
2	F	126	Total	C	N	O	S	0	0
			980	625	170	179	6		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	engineered mutation	UNP Q2N0S6
B	605	CYS	THR	engineered mutation	UNP Q2N0S6
D	559	PRO	ILE	engineered mutation	UNP Q2N0S6
D	605	CYS	THR	engineered mutation	UNP Q2N0S6
F	559	PRO	ILE	engineered mutation	UNP Q2N0S6
F	605	CYS	THR	engineered mutation	UNP Q2N0S6

- Molecule 3 is a protein called 17b Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	111	Total	C	N	O	S	0	0
			850	532	149	166	3		
3	I	111	Total	C	N	O	S	0	0
			853	533	149	168	3		
3	G	111	Total	C	N	O	S	0	0
			853	533	149	168	3		

- Molecule 4 is a protein called 17b Fab heavy chain.

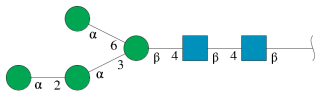
Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	128	Total	C	N	O	S	0	0
			991	624	169	195	3		
4	J	128	Total	C	N	O	S	0	0
			991	624	169	195	3		
4	H	128	Total	C	N	O	S	0	0
			991	624	169	195	3		

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



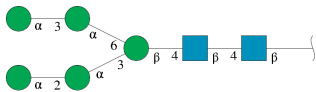
Mol	Chain	Residues	Atoms				AltConf	Trace
5	M	2	Total	C	N	O	0	0
			28	16	2	10		
5	W	2	Total	C	N	O	0	0
			28	16	2	10		
5	X	2	Total	C	N	O	0	0
			28	16	2	10		
5	P	2	Total	C	N	O	0	0
			28	16	2	10		
5	Q	2	Total	C	N	O	0	0
			28	16	2	10		
5	R	2	Total	C	N	O	0	0
			28	16	2	10		
5	T	2	Total	C	N	O	0	0
			28	16	2	10		
5	U	2	Total	C	N	O	0	0
			28	16	2	10		
5	V	2	Total	C	N	O	0	0
			28	16	2	10		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
6	N	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

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

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

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

- Molecule 9 is propyl (2R,3S)-2-(carbamimidamidomethyl)-3-[2-(4-chloro-3-fluoroanilino)(oxo)acetamido]-6-[(methylamino)methyl]-2,3-dihydro-1H-indole-1-carboxylate (CCD ID: Y26) (formula: C<sub>24</sub>H<sub>29</sub>ClFN<sub>7</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



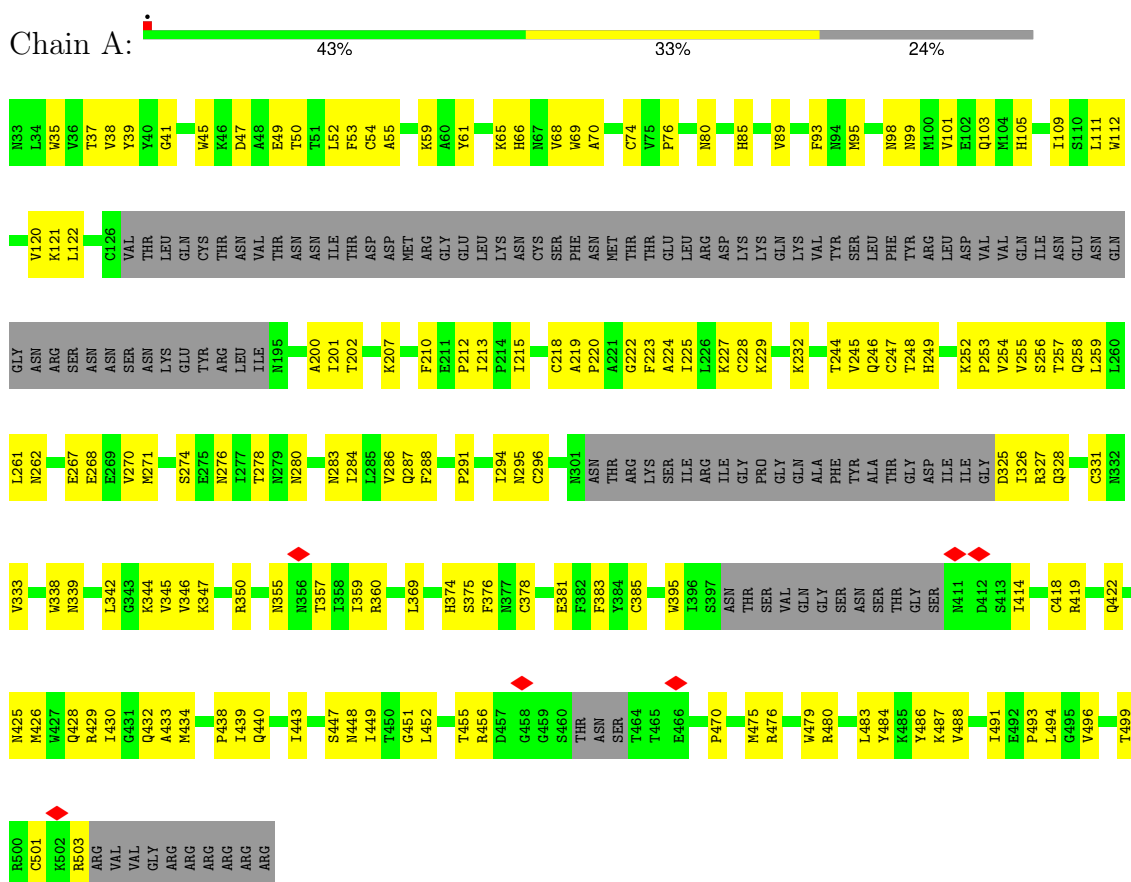


Mol	Chain	Residues	Atoms						AltConf
9	A	1	Total 37	C 24	Cl 1	F 1	N 7	O 4	0
9	C	1	Total 37	C 24	Cl 1	F 1	N 7	O 4	0
9	E	1	Total 37	C 24	Cl 1	F 1	N 7	O 4	0

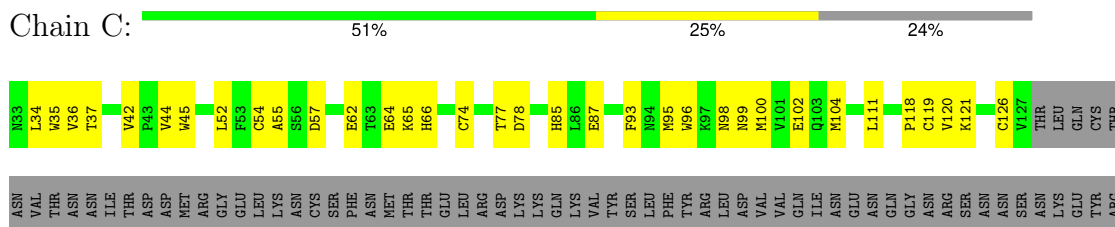
### 3 Residue-property plots

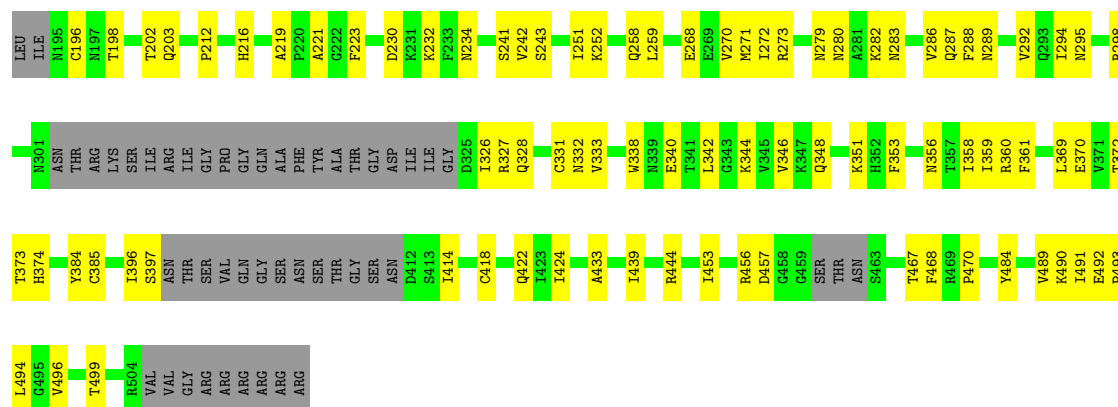
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

#### • Molecule 1: Envelope glycoprotein gp120



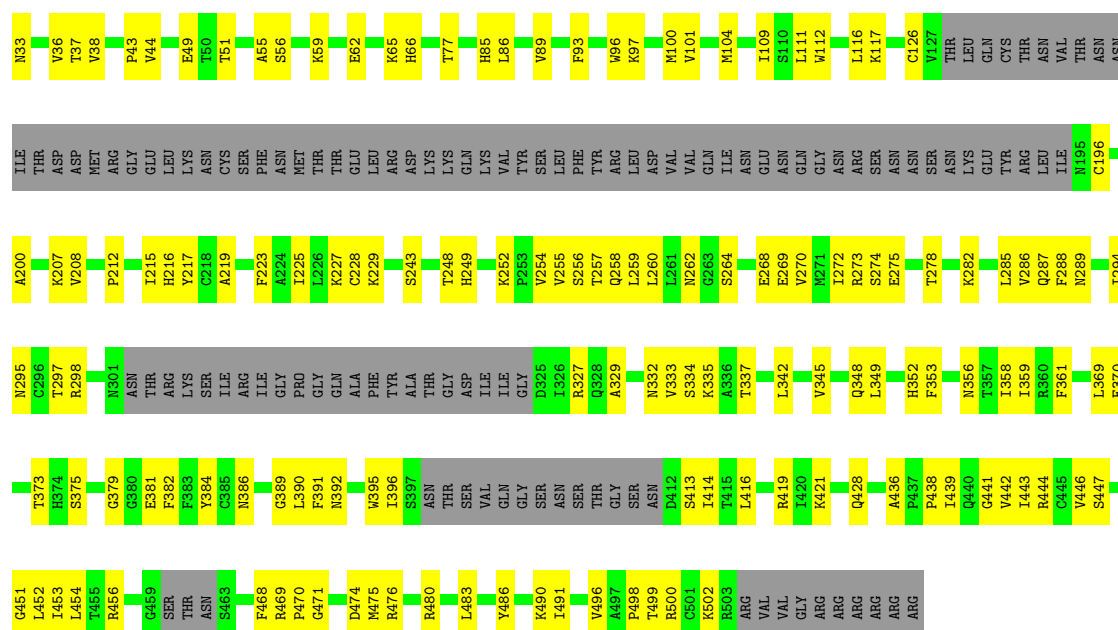
#### • Molecule 1: Envelope glycoprotein gp120





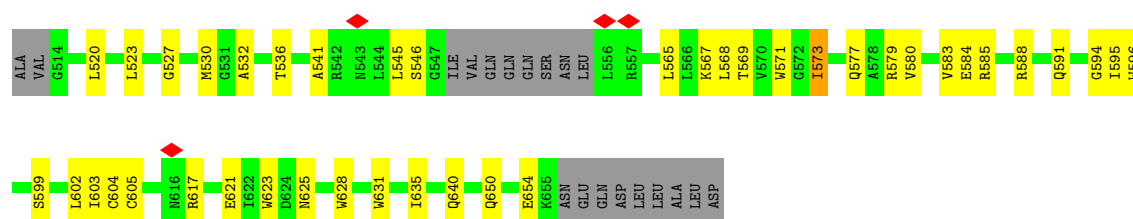
• Molecule 1: Envelope glycoprotein gp120

Chain E: 46% 30% 24%



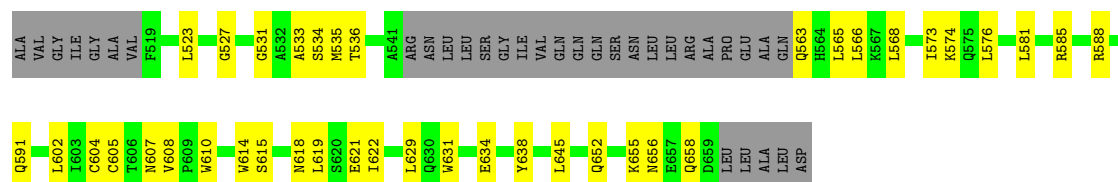
• Molecule 2: Envelope glycoprotein gp41

Chain B: 61% 26% 12%

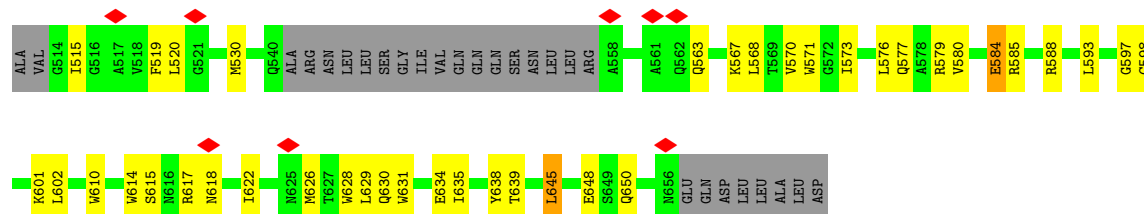


• Molecule 2: Envelope glycoprotein gp41

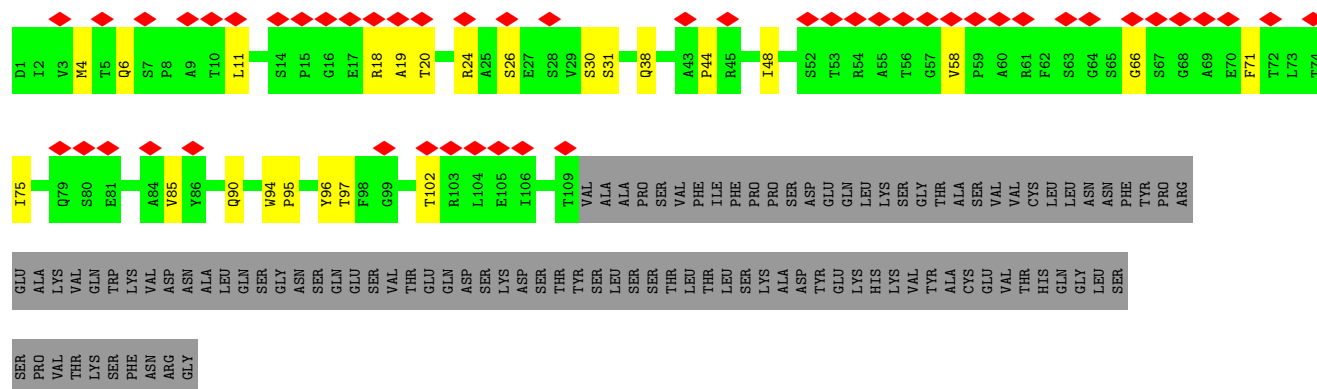
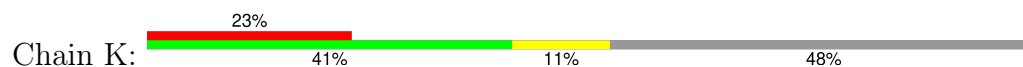
Chain D: 53% 25% 22%



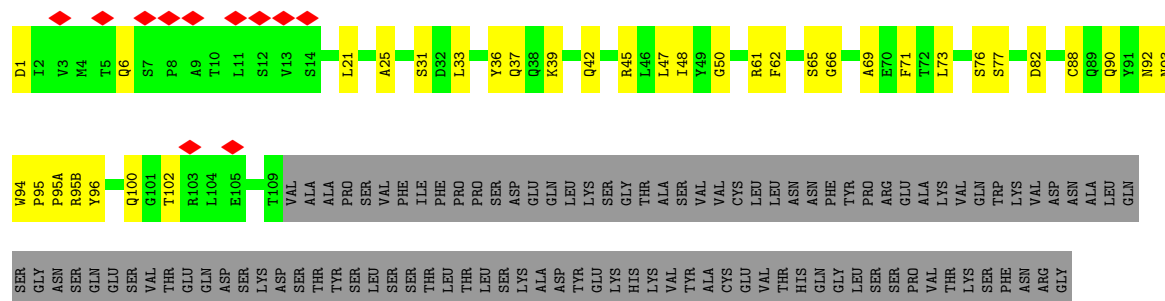
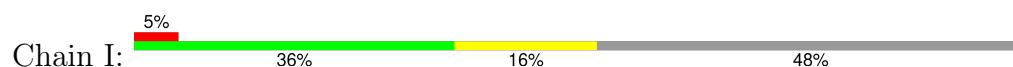
• Molecule 2: Envelope glycoprotein gp41



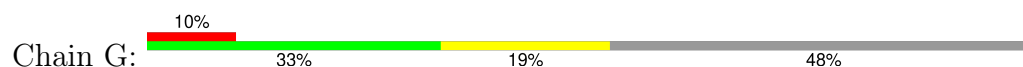
• Molecule 3: 17b Fab light chain



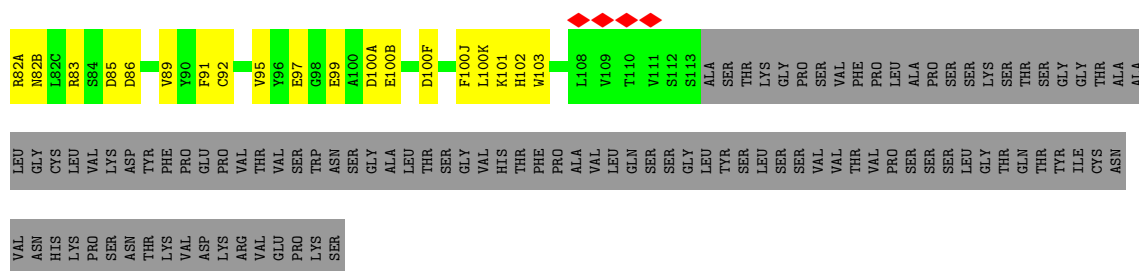
• Molecule 3: 17b Fab light chain



• Molecule 3: 17b Fab light chain







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



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



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



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

Chain R:  100%

NAG1  
NAG2

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

Chain T:  50% 50%

NAG1  
NAG2

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

Chain U:  50% 50%

NAG1  
NAG2

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

Chain V:  100%

NAG1  
NAG2

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

Chain N:  33% 50% 17%

NAG1  
NAG2  
MAN3  
MAN4  
MAN5  
MAN6  
MAN7

- Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  43% 57%

NAG1  
NAG2  
MAN3  
MAN4  
MAN5  
MAN6  
MAN7

- Molecule 7:  $\alpha$ -D-mannopyranose-(1-2)- $\alpha$ -D-mannopyranose-(1-3)-[ $\alpha$ -D-mannopyranose-(1-3)- $\alpha$ -D-mannopyranose-(1-6)] $\beta$ -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose

Chain S:  14% 86%

MAG1	MAG2	EMAG3	MAN4	MAN5	MAN6	MAN7
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## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	1087694	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 ( $e^-/\text{\AA}^2$ )	54.2	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.310	Depositor
Minimum map value	-0.832	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.0659	Depositor
Map size (Å)	332.80002, 332.80002, 332.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.832, 0.832, 0.832	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, BMA, Y26, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.16	0/2912	0.35	0/3957
1	C	0.21	0/2926	0.42	1/3976 (0.0%)
1	E	0.21	0/2915	0.43	1/3962 (0.0%)
2	B	0.17	0/1069	0.39	0/1450
2	D	0.16	0/983	0.30	0/1332
2	F	0.19	0/1000	0.42	0/1358
3	G	0.11	0/873	0.30	0/1187
3	I	0.14	0/873	0.34	0/1187
3	K	0.08	0/870	0.23	0/1183
4	H	0.14	0/1012	0.38	0/1373
4	J	0.17	0/1012	0.38	0/1373
4	L	0.11	0/1012	0.31	0/1373
All	All	0.17	0/17457	0.38	2/23711 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	326	ILE	N-CA-C	-5.50	108.48	113.71
1	E	43	PRO	CA-N-CD	-5.07	104.90	112.00

There are no chirality outliers.

There are no planarity outliers.

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

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2848	0	2775	124	0
1	C	2862	0	2799	86	0
1	E	2851	0	2786	107	0
2	B	1049	0	1034	38	0
2	D	964	0	937	35	0
2	F	980	0	958	31	0
3	G	853	0	825	31	0
3	I	853	0	825	27	0
3	K	850	0	823	14	0
4	H	991	0	957	39	0
4	J	991	0	957	36	0
4	L	991	0	957	21	0
5	M	28	0	25	0	0
5	P	28	0	25	1	0
5	Q	28	0	25	0	0
5	R	28	0	25	2	0
5	T	28	0	25	1	0
5	U	28	0	25	0	0
5	V	28	0	25	0	0
5	W	28	0	25	1	0
5	X	28	0	25	1	0
6	N	72	0	61	2	0
7	O	83	0	70	0	0
7	S	83	0	70	3	0
8	A	98	0	91	7	0
8	B	14	0	13	0	0
8	C	112	0	104	2	0
8	D	28	0	26	0	0
8	E	112	0	104	3	0
9	A	37	0	0	1	0
9	C	37	0	0	0	0
9	E	37	0	0	1	0
All	All	18048	0	17397	544	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 15.

All (544) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:385:CYS:HA	1:C:418:CYS:HB3	1.49	0.91
1:A:342:LEU:HA	1:A:345:VAL:HG12	1.59	0.84
4:L:35:THR:HB	4:L:100(K):LEU:HD21	1.65	0.79
1:A:218:CYS:HA	1:A:247:CYS:HB2	1.65	0.78
3:G:34:ALA:HB3	3:G:89:GLN:HB3	1.64	0.78
1:E:207:LYS:HE3	1:E:436:ALA:HB3	1.67	0.76
1:E:55:ALA:HB1	1:E:77:THR:HA	1.66	0.76
1:A:291:PRO:HG3	8:A:607:NAG:H82	1.68	0.76
4:H:23:LYS:NZ	4:H:75:THR:O	2.19	0.75
4:L:2:VAL:HG11	4:L:27:ASP:HB2	1.68	0.73
1:A:101:VAL:HG23	1:A:479:TRP:HB2	1.71	0.72
1:C:358:ILE:HD12	1:C:396:ILE:HG12	1.70	0.72
1:E:101:VAL:HG21	1:E:480:ARG:HG2	1.72	0.71
1:A:355:ASN:HB2	8:A:604:NAG:N2	2.05	0.71
1:C:385:CYS:HA	1:C:418:CYS:CB	2.21	0.70
1:E:421:LYS:NZ	4:H:100(B):GLU:O	2.24	0.70
1:A:355:ASN:H	8:A:604:NAG:H82	1.55	0.70
4:L:4:LEU:O	4:L:105:GLN:NE2	2.25	0.70
3:K:4:MET:HE1	3:K:26:SER:H	1.57	0.69
1:E:264:SER:O	1:E:287:GLN:NE2	2.26	0.69
1:E:100:MET:HE1	1:E:248:THR:HG21	1.74	0.69
1:A:50:THR:O	1:A:103:GLN:NE2	2.25	0.68
3:G:54:ARG:NH2	3:G:62:PHE:O	2.26	0.68
3:I:90:GLN:HE22	3:I:93:ASN:HD22	1.40	0.67
1:E:272:ILE:HD12	1:E:286:VAL:HG22	1.76	0.67
3:K:90:GLN:HE21	3:K:97:THR:HG22	1.58	0.67
1:C:118:PRO:HG2	1:C:121:LYS:HB2	1.77	0.67
4:H:37:VAL:HG12	4:H:91:PHE:HB2	1.76	0.67
1:A:491:ILE:HG23	1:A:493:PRO:HD3	1.77	0.66
4:J:19:LYS:HD2	4:J:79:TYR:HB3	1.77	0.66
4:J:33:SER:OG	4:J:50:ARG:NH1	2.28	0.66
1:A:338:TRP:O	1:A:342:LEU:HD23	1.96	0.66
1:C:279:ASN:OD1	1:C:282:LYS:N	2.29	0.65
3:G:4:MET:SD	3:G:4:MET:N	2.69	0.65
4:J:20:VAL:HG21	4:J:107:THR:HG21	1.78	0.65
3:I:33:LEU:HD11	3:I:88:CYS:HB2	1.78	0.65
1:C:44:VAL:HG23	1:C:492:GLU:HG3	1.79	0.64
1:A:54:CYS:SG	1:A:55:ALA:N	2.70	0.64
1:E:254:VAL:HG21	1:E:262:ASN:HB2	1.79	0.64
8:A:605:NAG:H3	5:X:1:NAG:H3	1.79	0.64
3:G:54:ARG:NH1	3:G:58:VAL:O	2.31	0.64
1:C:298:ARG:NH2	1:C:439:ILE:O	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:640:GLN:N	2:B:640:GLN:OE1	2.30	0.63
1:E:391:PHE:HD2	1:E:470:PRO:HG2	1.63	0.63
4:H:82(A):ARG:O	4:H:82(B):ASN:ND2	2.31	0.63
4:L:72:ASP:O	4:L:76:SER:HA	1.99	0.63
1:A:98:ASN:ND2	1:A:486:TYR:O	2.31	0.63
4:H:71:ALA:HB2	4:H:78:VAL:HG13	1.81	0.62
4:H:48:MET:HE1	4:H:80:LEU:HD21	1.82	0.62
2:B:541:ALA:HA	2:B:545:LEU:HD13	1.82	0.62
4:J:50:ARG:NH2	4:J:100(G):ASN:OD1	2.33	0.61
1:C:295:ASN:HB2	1:C:444:ARG:HH12	1.65	0.61
1:C:259:LEU:HB2	1:C:374:HIS:CE1	2.36	0.61
1:A:105:HIS:O	1:A:109:ILE:HG23	2.01	0.61
3:I:37:GLN:OE1	3:I:45:ARG:NH2	2.34	0.61
4:H:31:ARG:NH1	4:H:100(A):ASP:OD1	2.34	0.61
2:B:617:ARG:NH2	2:B:621:GLU:O	2.34	0.61
1:E:219:ALA:HB2	1:E:225:ILE:HG13	1.83	0.60
2:D:535:MET:SD	2:D:535:MET:N	2.74	0.60
4:H:100(A):ASP:OD1	4:H:100(A):ASP:N	2.34	0.60
1:E:93:PHE:CE1	1:E:228:CYS:HB2	2.37	0.59
1:E:361:PHE:HE1	1:E:468:PHE:HB2	1.67	0.59
1:A:52:LEU:HB2	1:A:219:ALA:HA	1.85	0.59
1:A:121:LYS:O	1:A:200:ALA:HA	2.03	0.59
8:A:601:NAG:HN2	8:A:602:NAG:H81	1.68	0.59
1:C:292:VAL:HG11	1:C:338:TRP:HE3	1.66	0.59
8:C:604:NAG:H3	8:C:604:NAG:H83	1.84	0.59
1:A:256:SER:H	1:A:475:MET:HE1	1.65	0.59
2:D:614:TRP:HA	2:D:638:TYR:CE2	2.38	0.59
4:L:23:LYS:HE2	4:L:23:LYS:HA	1.85	0.59
4:J:2:VAL:HG12	4:J:26:GLY:HA3	1.85	0.59
3:G:36:TYR:HB2	3:G:87:TYR:HB2	1.85	0.59
4:H:83:ARG:HD2	4:H:85:ASP:H	1.68	0.59
2:B:541:ALA:HB1	2:D:591:GLN:HE22	1.68	0.58
3:K:19:ALA:HB3	3:K:75:ILE:HD11	1.84	0.58
4:J:87:THR:HG22	4:J:110:THR:HA	1.85	0.58
4:J:83:ARG:HH12	4:J:85:ASP:HB3	1.69	0.58
1:A:503:ARG:NH1	2:B:605:CYS:SG	2.77	0.58
1:C:294:ILE:HD11	1:C:331:CYS:HB3	1.86	0.58
1:E:273:ARG:NH2	1:E:287:GLN:OE1	2.30	0.58
1:E:447:SER:OG	7:S:1:NAG:O7	2.21	0.58
3:G:6:GLN:OE1	3:G:101:GLY:N	2.33	0.58
4:H:31:ARG:HH11	4:H:99:GLU:HA	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:GLN:HB3	1:A:374:HIS:HA	1.84	0.58
1:C:55:ALA:HB1	1:C:77:THR:HA	1.86	0.58
1:C:360:ARG:O	1:C:467:THR:HA	2.04	0.58
8:A:603:NAG:H83	8:A:603:NAG:H3	1.86	0.57
4:L:48:MET:HA	4:L:60:ALA:HB2	1.86	0.57
1:E:496:VAL:O	2:F:631:TRP:NE1	2.30	0.57
8:E:604:NAG:H83	8:E:604:NAG:H3	1.85	0.57
1:A:327:ARG:HG3	1:A:438:PRO:HG3	1.85	0.57
1:A:339:ASN:HB3	8:A:603:NAG:H82	1.86	0.57
4:H:6:GLU:HA	4:H:23:LYS:HB3	1.86	0.57
1:E:112:TRP:CZ2	1:E:255:VAL:HG21	2.39	0.57
1:C:87:GLU:HG2	8:C:601:NAG:H82	1.86	0.57
2:D:608:VAL:HG21	2:D:645:LEU:HD11	1.86	0.57
1:E:349:LEU:HD22	1:E:468:PHE:CE2	2.40	0.57
1:E:389:GLY:HA2	8:E:607:NAG:H61	1.87	0.57
2:F:614:TRP:HB3	2:F:638:TYR:CG	2.40	0.57
3:I:95(B):ARG:HG2	4:J:61:PRO:HD3	1.86	0.57
2:F:519:PHE:HE2	2:F:585:ARG:HD3	1.70	0.57
3:I:25:ALA:HB3	3:I:69:ALA:HA	1.85	0.57
2:F:593:LEU:HB3	2:F:598:CYS:O	2.05	0.57
1:A:39:TYR:HE1	2:B:603:ILE:HG23	1.68	0.57
1:E:100:MET:HE2	1:E:483:LEU:HD22	1.87	0.56
1:C:342:LEU:HG	1:C:361:PHE:HE2	1.70	0.56
2:F:597:GLY:HA2	2:F:650:GLN:HE22	1.68	0.56
1:A:374:HIS:HD2	1:A:385:CYS:HB2	1.70	0.56
2:D:602:LEU:HD12	2:D:602:LEU:H	1.68	0.56
4:J:23:LYS:NZ	4:J:75:THR:O	2.38	0.56
4:J:97:GLU:HG3	4:J:100(E):TYR:CZ	2.40	0.56
4:H:33:SER:HB3	4:H:97:GLU:HG3	1.87	0.56
4:J:31:ARG:NH2	4:J:100(A):ASP:OD1	2.33	0.56
1:A:258:GLN:HE22	1:A:470:PRO:HG2	1.69	0.56
1:A:207:LYS:HG3	1:A:439:ILE:HD11	1.85	0.56
1:A:47:ASP:OD2	1:A:487:LYS:NZ	2.37	0.56
3:I:31:SER:O	3:I:31:SER:OG	2.24	0.56
3:I:95(A):PRO:HG2	4:J:58:HIS:HB2	1.88	0.56
1:A:385:CYS:N	1:A:418:CYS:SG	2.79	0.56
5:W:1:NAG:H83	5:W:1:NAG:H3	1.88	0.55
1:A:50:THR:HB	1:A:223:PHE:HE2	1.71	0.55
1:C:373:THR:HG22	5:R:1:NAG:H83	1.89	0.55
1:E:38:VAL:HG12	1:E:38:VAL:O	2.06	0.55
1:E:359:ILE:HG22	1:E:395:TRP:HB2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:573:ILE:HG13	2:F:573:ILE:HD12	1.88	0.55
1:E:275:GLU:HB3	1:E:282:LYS:HB3	1.88	0.55
4:H:39:GLN:HB3	4:H:89:VAL:HG13	1.88	0.55
3:G:61:ARG:NH1	3:G:82:ASP:OD2	2.40	0.55
1:C:280:ASN:ND2	1:C:457:ASP:O	2.40	0.55
1:A:344:LYS:O	1:A:347:LYS:HG2	2.07	0.54
3:I:1:ASP:OD2	4:J:62:HIS:ND1	2.40	0.54
3:I:6:GLN:CD	3:I:100:GLN:HE22	2.15	0.54
1:E:298:ARG:NH2	1:E:441:GLY:O	2.34	0.54
1:C:77:THR:OG1	1:C:78:ASP:N	2.40	0.54
1:C:85:HIS:HD1	1:C:243:SER:HG	1.53	0.54
1:A:256:SER:N	1:A:475:MET:HE1	2.22	0.54
3:I:37:GLN:OE1	3:I:39:LYS:NZ	2.34	0.54
4:H:4:LEU:HD21	4:H:102:HIS:CE1	2.42	0.54
1:A:225:ILE:HG12	1:A:488:VAL:HG12	1.89	0.54
1:A:232:LYS:O	1:A:232:LYS:HG3	2.06	0.54
1:A:252:LYS:HE3	1:A:262:ASN:HB3	1.90	0.54
1:A:333:VAL:HG12	1:A:414:ILE:HB	1.90	0.54
1:A:207:LYS:HE2	1:A:439:ILE:HD11	1.90	0.54
1:E:498:PRO:HG2	2:F:622:ILE:HG21	1.89	0.54
3:G:95(B):ARG:NH1	4:H:59:TYR:O	2.40	0.54
1:C:98:ASN:OD1	1:C:99:ASN:N	2.40	0.54
2:F:635:ILE:O	2:F:639:THR:OG1	2.25	0.54
3:I:42:GLN:N	3:I:42:GLN:OE1	2.41	0.54
1:C:370:GLU:OE2	1:C:384:TYR:OH	2.23	0.53
1:C:45:TRP:HB2	1:C:489:VAL:HB	1.89	0.53
3:G:38:GLN:H	3:G:85:VAL:HG12	1.73	0.53
2:B:568:LEU:HD21	2:D:574:LYS:HE2	1.91	0.53
1:C:496:VAL:O	2:D:631:TRP:NE1	2.33	0.53
3:K:66:GLY:HA3	3:K:71:PHE:HA	1.91	0.53
4:L:95:VAL:HG21	4:L:100(H):ASN:HB2	1.91	0.53
1:C:234:ASN:ND2	1:C:234:ASN:O	2.42	0.53
4:H:83:ARG:HE	4:H:86:ASP:H	1.55	0.53
1:A:246:GLN:HB2	2:B:520:LEU:HD11	1.90	0.53
1:E:369:LEU:O	1:E:373:THR:OG1	2.26	0.53
1:C:45:TRP:CE2	2:D:629:LEU:HD21	2.44	0.52
4:J:99:GLU:O	4:J:99:GLU:HG3	2.09	0.52
1:A:37:THR:HG21	1:A:499:THR:HB	1.91	0.52
1:A:66:HIS:CD2	1:A:212:PRO:HA	2.44	0.52
1:C:333:VAL:HG13	1:C:414:ILE:HG23	1.91	0.52
1:C:34:LEU:HB3	2:D:610:TRP:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:361:PHE:O	1:E:392:ASN:HA	2.10	0.52
2:F:630:GLN:N	2:F:630:GLN:OE1	2.41	0.52
1:A:381:GLU:OE1	1:A:443:ILE:HD13	2.09	0.52
1:C:223:PHE:CE1	1:C:490:LYS:HB3	2.45	0.52
4:J:97:GLU:N	4:J:97:GLU:OE1	2.43	0.52
1:E:248:THR:HB	1:E:486:TYR:CZ	2.45	0.52
3:K:4:MET:HE2	3:K:4:MET:HA	1.91	0.52
1:E:278:THR:O	5:T:1:NAG:O6	2.27	0.52
1:E:44:VAL:HG23	2:F:629:LEU:HA	1.90	0.52
1:E:295:ASN:OD1	1:E:332:ASN:HB3	2.09	0.52
4:H:16:SER:OG	4:H:17:SER:N	2.41	0.52
2:B:595:ILE:HG13	2:B:596:TRP:CD1	2.45	0.52
4:L:37:VAL:HA	4:L:48:MET:HE1	1.92	0.52
1:C:126:CYS:HB3	1:C:196:CYS:HA	1.90	0.52
3:G:49:TYR:HE1	3:G:55:ALA:HA	1.74	0.52
1:A:65:LYS:HA	1:A:68:VAL:HG12	1.92	0.52
1:C:37:THR:HG21	1:C:499:THR:HG22	1.91	0.51
1:E:101:VAL:HA	1:E:483:LEU:HD12	1.92	0.51
2:F:634:GLU:OE1	2:F:634:GLU:N	2.40	0.51
3:G:81:GLU:OE2	3:G:81:GLU:N	2.34	0.51
1:A:385:CYS:HA	1:A:418:CYS:HA	1.92	0.51
3:I:47:LEU:C	3:I:48:ILE:HD13	2.35	0.51
1:E:269:GLU:OE1	1:E:348:GLN:NE2	2.43	0.51
5:P:1:NAG:H4	5:P:2:NAG:N2	2.25	0.51
3:K:85:VAL:HG23	3:K:102:THR:H	1.75	0.51
1:A:483:LEU:HD23	1:A:486:TYR:HD2	1.75	0.51
1:A:202:THR:HG21	4:L:58:HIS:HE1	1.76	0.51
1:E:342:LEU:HD11	1:E:361:PHE:CD2	2.45	0.51
1:A:434:MET:HE1	4:L:100(E):TYR:CE1	2.46	0.51
1:A:246:GLN:O	1:A:246:GLN:NE2	2.44	0.51
1:C:327:ARG:HH21	1:C:422:GLN:HE22	1.59	0.51
3:I:31:SER:OG	3:I:50:GLY:O	2.29	0.51
1:A:270:VAL:HA	1:A:287:GLN:O	2.10	0.51
1:E:381:GLU:HG3	1:E:443:ILE:HD13	1.92	0.51
2:F:615:SER:O	2:F:617:ARG:NE	2.44	0.51
1:A:296:CYS:HA	1:A:331:CYS:HA	1.93	0.51
2:B:545:LEU:HD22	2:D:591:GLN:NE2	2.26	0.51
2:B:584:GLU:O	2:B:588:ARG:HG3	2.11	0.51
1:E:59:LYS:HB2	1:E:62:GLU:HG3	1.92	0.51
1:C:340:GLU:O	1:C:344:LYS:HG3	2.11	0.50
2:D:534:SER:OG	2:D:535:MET:SD	2.66	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:212:PRO:O	1:E:252:LYS:HE3	2.12	0.50
2:B:565:LEU:HD11	2:D:566:LEU:HD11	1.92	0.50
2:F:570:VAL:HA	2:F:573:ILE:HG22	1.93	0.50
4:H:95:VAL:HG23	4:H:100(K):LEU:HD13	1.94	0.50
1:C:66:HIS:CE1	1:C:111:LEU:HD21	2.47	0.50
1:C:422:GLN:NE2	4:J:100(E):TYR:O	2.44	0.50
1:E:227:LYS:HG2	1:E:229:LYS:HG2	1.93	0.50
1:A:50:THR:HB	1:A:223:PHE:CE2	2.47	0.50
1:C:258:GLN:HG2	1:C:470:PRO:HB2	1.93	0.50
4:J:40:ALA:HB3	4:J:43:GLN:HB3	1.93	0.50
3:G:54:ARG:HD3	3:G:55:ALA:N	2.26	0.50
1:A:224:ALA:HB1	1:A:244:THR:HG23	1.93	0.49
4:H:100(J):PHE:CD1	4:H:100(J):PHE:C	2.90	0.49
1:A:120:VAL:HA	1:A:201:ILE:O	2.11	0.49
4:J:12:LYS:HZ2	4:J:18:VAL:HA	1.77	0.49
1:E:66:HIS:CE1	1:E:111:LEU:HD21	2.48	0.49
1:E:452:LEU:HD23	1:E:454:LEU:HD21	1.94	0.49
1:A:369:LEU:HD23	1:A:369:LEU:H	1.77	0.49
2:B:594:GLY:HA2	2:B:599:SER:HB2	1.94	0.49
1:C:230:ASP:N	1:C:241:SER:OG	2.46	0.49
1:E:456:ARG:HA	1:E:468:PHE:HD1	1.77	0.49
3:G:86:TYR:HB2	3:G:102:THR:OG1	2.12	0.49
4:L:53:ILE:HD12	4:L:53:ILE:H	1.78	0.49
1:E:361:PHE:CE1	1:E:468:PHE:HB2	2.46	0.49
1:A:35:TRP:CD1	1:A:501:CYS:H	2.30	0.49
2:B:580:VAL:HG23	2:F:579:ARG:NH2	2.28	0.49
1:C:272:ILE:HD12	1:C:286:VAL:HG22	1.94	0.49
1:E:342:LEU:HD11	1:E:361:PHE:HD2	1.78	0.49
1:C:118:PRO:HB3	1:C:433:ALA:HB1	1.95	0.49
3:G:96:TYR:HD2	4:H:47:TRP:CD1	2.30	0.49
1:A:80:ASN:OD1	1:A:80:ASN:N	2.46	0.49
1:C:270:VAL:HG12	1:C:288:PHE:HA	1.95	0.49
1:A:93:PHE:CE2	1:A:228:CYS:HB2	2.48	0.49
1:A:350:ARG:NH1	1:A:357:THR:O	2.46	0.49
1:E:33:ASN:OD1	1:E:500:ARG:NH1	2.36	0.49
1:A:89:VAL:HB	2:B:527:GLY:HA3	1.95	0.48
1:A:422:GLN:OE1	4:L:100(E):TYR:N	2.43	0.48
1:E:49:GLU:OE2	1:E:49:GLU:N	2.34	0.48
1:E:258:GLN:OE1	1:E:471:GLY:N	2.38	0.48
3:K:38:GLN:HA	3:K:44:PRO:HG3	1.96	0.48
2:D:619:LEU:HA	2:D:622:ILE:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:474:ASP:OD2	1:E:476:ARG:NH1	2.46	0.48
3:G:91:TYR:HB3	3:G:96:TYR:HD1	1.77	0.48
3:G:105:GLU:OE2	3:G:106:ILE:N	2.46	0.48
1:A:215:ILE:HD12	1:A:253:PRO:HG3	1.96	0.48
1:C:295:ASN:OD1	1:C:332:ASN:HB3	2.14	0.48
3:I:61:ARG:NH1	3:I:82:ASP:OD2	2.47	0.48
3:K:30:SER:OG	3:K:31:SER:N	2.38	0.48
1:A:267:GLU:H	1:A:267:GLU:CD	2.20	0.48
2:B:573:ILE:O	2:B:577:GLN:HG3	2.14	0.48
2:D:638:TYR:N	2:D:638:TYR:CD1	2.81	0.48
1:A:41:GLY:N	1:A:493:PRO:O	2.47	0.47
2:B:532:ALA:O	2:B:536:THR:HG22	2.15	0.47
2:D:615:SER:OG	2:D:634:GLU:OE1	2.30	0.47
2:F:580:VAL:HG12	2:F:584:GLU:OE2	2.14	0.47
1:C:95:MET:HE1	1:C:273:ARG:HB3	1.97	0.47
4:H:18:VAL:HG12	4:H:82:LEU:HB2	1.96	0.47
1:A:426:MET:HE2	1:A:429:ARG:HB2	1.96	0.47
1:C:52:LEU:HD23	1:C:219:ALA:HA	1.96	0.47
4:H:34:PHE:HD2	4:H:78:VAL:HG21	1.79	0.47
1:A:328:GLN:HG3	1:A:419:ARG:HH11	1.80	0.47
1:E:56:SER:HB3	1:E:215:ILE:HG12	1.94	0.47
4:J:47:TRP:CZ2	4:J:50:ARG:HB2	2.50	0.47
2:B:546:SER:O	2:B:546:SER:OG	2.32	0.47
1:C:95:MET:HE2	1:C:96:TRP:CZ2	2.50	0.47
4:J:87:THR:HG22	4:J:111:VAL:H	1.79	0.47
1:E:256:SER:OG	1:E:257:THR:N	2.45	0.47
1:A:248:THR:OG1	1:A:249:HIS:N	2.48	0.47
1:E:117:LYS:HA	1:E:117:LYS:HD3	1.77	0.47
1:A:112:TRP:CZ2	1:A:255:VAL:HG21	2.50	0.47
1:E:109:ILE:HG12	1:E:428:GLN:HG2	1.96	0.47
2:F:568:LEU:HA	2:F:571:TRP:CE3	2.50	0.47
1:A:257:THR:OG1	1:A:375:SER:OG	2.33	0.47
1:A:383:PHE:HB3	1:A:418:CYS:SG	2.55	0.47
1:E:288:PHE:CE1	1:E:452:LEU:HD11	2.50	0.47
1:A:59:LYS:HB3	1:A:61:TYR:CE2	2.49	0.46
1:A:93:PHE:HE2	1:A:228:CYS:HB2	1.79	0.46
4:L:2:VAL:HG22	4:L:102:HIS:HE1	1.79	0.46
1:E:295:ASN:HB3	1:E:446:VAL:HG12	1.97	0.46
1:E:348:GLN:O	1:E:352:HIS:ND1	2.28	0.46
1:A:271:MET:HE2	1:A:271:MET:HA	1.96	0.46
1:C:45:TRP:HZ3	2:D:523:LEU:HG	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55:ALA:HB3	1:C:216:HIS:HB2	1.96	0.46
3:I:36:TYR:OH	4:J:100(K):LEU:N	2.48	0.46
1:E:126:CYS:HA	1:E:196:CYS:HA	1.96	0.46
4:H:37:VAL:HG11	4:H:103:TRP:HZ3	1.79	0.46
1:A:98:ASN:O	1:A:101:VAL:HG12	2.16	0.46
1:E:216:HIS:HB3	1:E:249:HIS:O	2.16	0.46
4:J:18:VAL:HG12	4:J:82:LEU:HB3	1.98	0.46
4:J:36:TRP:HE1	4:J:78:VAL:HG22	1.81	0.46
1:A:66:HIS:NE2	1:A:210:PHE:HE1	2.13	0.46
3:I:90:GLN:OE1	3:I:92:ASN:N	2.37	0.46
4:J:100:ALA:HA	4:J:100(D):GLU:O	2.16	0.46
4:J:100(J):PHE:O	4:J:100(K):LEU:HD23	2.16	0.46
1:A:218:CYS:CA	1:A:247:CYS:HB2	2.31	0.46
2:F:568:LEU:HD13	2:F:571:TRP:HE3	1.81	0.46
2:F:584:GLU:O	2:F:588:ARG:HG3	2.15	0.46
4:H:4:LEU:HD11	4:H:102:HIS:NE2	2.31	0.46
1:A:121:LYS:HE2	1:A:121:LYS:HB3	1.79	0.46
1:A:346:VAL:HG11	1:A:395:TRP:CE2	2.51	0.46
4:H:19:LYS:HD2	4:H:19:LYS:HA	1.73	0.46
1:A:85:HIS:CE1	1:A:229:LYS:HD2	2.51	0.46
1:A:359:ILE:O	1:A:360:ARG:NE	2.49	0.46
4:L:89:VAL:HB	4:L:108:LEU:HG	1.98	0.46
1:C:270:VAL:HG23	1:C:348:GLN:HG3	1.98	0.46
1:E:93:PHE:HE1	1:E:228:CYS:HB2	1.80	0.46
1:E:100:MET:HG2	1:E:483:LEU:HD13	1.97	0.46
1:E:270:VAL:HG21	1:E:345:VAL:HA	1.97	0.46
1:E:491:ILE:HD13	2:F:520:LEU:HB2	1.98	0.46
1:A:294:ILE:HD12	1:A:449:ILE:HD11	1.98	0.45
1:C:327:ARG:HD3	4:J:100(D):GLU:OE1	2.15	0.45
1:E:51:THR:O	1:E:51:THR:OG1	2.34	0.45
1:E:386:ASN:O	1:E:416:LEU:HD23	2.15	0.45
2:B:577:GLN:HA	2:B:580:VAL:HG22	1.98	0.45
2:B:591:GLN:HG2	2:F:515:ILE:HD11	1.98	0.45
2:D:652:GLN:OE1	2:D:655:LYS:NZ	2.28	0.45
1:E:86:LEU:HB2	1:E:89:VAL:HG11	1.97	0.45
1:E:104:MET:SD	1:E:217:TYR:OH	2.63	0.45
1:A:360:ARG:HE	1:A:395:TRP:HD1	1.64	0.45
4:J:38:ARG:HB2	4:J:90:TYR:CD1	2.51	0.45
1:E:358:ILE:HG23	1:E:396:ILE:HG12	1.98	0.45
2:B:625:ASN:OD1	2:B:625:ASN:N	2.48	0.45
3:K:48:ILE:HD11	3:K:58:VAL:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:48:MET:SD	4:L:48:MET:N	2.78	0.45
4:H:1:GLU:HG2	4:H:2:VAL:HG12	1.96	0.45
1:C:212:PRO:HB2	1:C:252:LYS:HG2	1.98	0.45
2:B:588:ARG:O	2:B:591:GLN:HG3	2.17	0.45
1:C:198:THR:O	1:C:198:THR:OG1	2.31	0.45
3:G:24:ARG:HA	3:G:24:ARG:NE	2.32	0.45
1:A:259:LEU:HD12	1:A:374:HIS:CE1	2.51	0.45
1:E:256:SER:OG	1:E:259:LEU:O	2.30	0.45
1:A:261:LEU:HD23	1:A:447:SER:OG	2.17	0.45
1:C:120:VAL:HG12	1:C:120:VAL:O	2.17	0.45
3:I:39:LYS:HG3	3:I:42:GLN:HE22	1.82	0.45
1:A:112:TRP:HZ2	1:A:255:VAL:HG21	1.82	0.45
1:A:426:MET:HG3	1:A:433:ALA:HB2	1.97	0.45
3:I:65:SER:OG	3:I:66:GLY:N	2.50	0.45
3:I:95:PRO:O	3:I:95(B):ARG:N	2.48	0.45
1:E:502:LYS:HD2	1:E:502:LYS:HA	1.80	0.45
1:C:119:CYS:O	1:C:202:THR:HA	2.17	0.45
1:E:260:LEU:HD12	1:E:451:GLY:HA3	1.99	0.45
1:E:390:LEU:HD12	1:E:416:LEU:HD21	1.97	0.45
1:A:39:TYR:CE1	2:B:603:ILE:HG23	2.51	0.44
1:A:476:ARG:HB3	1:A:480:ARG:NH2	2.32	0.44
2:B:595:ILE:HG22	2:F:602:LEU:HD13	1.98	0.44
4:H:83:ARG:HE	4:H:86:ASP:N	2.13	0.44
1:A:45:TRP:HH2	1:A:89:VAL:HG21	1.81	0.44
1:E:268:GLU:C	1:E:289:ASN:HD21	2.25	0.44
1:E:288:PHE:CZ	1:E:452:LEU:HD11	2.52	0.44
4:H:4:LEU:HA	4:H:24:ALA:HA	1.98	0.44
4:H:52:ILE:HB	4:H:56:VAL:HG12	1.99	0.44
4:J:83:ARG:HH22	4:J:85:ASP:CB	2.30	0.44
1:E:334:SER:HB3	1:E:337:THR:OG1	2.18	0.44
1:A:95:MET:HG3	1:A:484:TYR:HA	1.99	0.44
1:E:255:VAL:HG13	1:E:475:MET:HE3	2.00	0.44
3:G:19:ALA:H	3:G:75:ILE:HD11	1.82	0.44
3:G:54:ARG:NH2	3:G:59:PRO:O	2.49	0.44
1:C:456:ARG:HG2	1:C:468:PHE:HE1	1.83	0.44
3:I:33:LEU:HD23	3:I:71:PHE:CG	2.53	0.44
1:A:428:GLN:HG2	1:A:429:ARG:HG3	1.99	0.44
1:A:494:LEU:HD23	1:A:494:LEU:HA	1.84	0.44
2:B:530:MET:HB2	2:B:623:TRP:HA	1.99	0.44
1:C:232:LYS:HG3	1:C:232:LYS:O	2.17	0.44
1:A:49:GLU:HG2	1:A:99:ASN:HD21	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:ARG:O	1:A:419:ARG:NH1	2.51	0.44
4:L:12:LYS:HG2	4:L:18:VAL:HG12	1.98	0.44
1:E:358:ILE:HD12	1:E:396:ILE:HG23	1.98	0.44
1:E:446:VAL:O	7:S:1:NAG:H5	2.17	0.44
4:H:30:ILE:HD12	4:H:73:LYS:HG2	2.00	0.44
1:A:286:VAL:O	1:A:451:GLY:HA2	2.17	0.44
1:C:36:VAL:HG12	2:D:608:VAL:HG13	2.00	0.44
1:C:346:VAL:HB	1:C:359:ILE:HD11	1.99	0.44
4:J:38:ARG:NE	4:J:46:GLU:OE1	2.36	0.44
4:J:59:TYR:HE1	4:J:69:ILE:HG13	1.81	0.44
1:A:342:LEU:HA	1:A:345:VAL:CG1	2.41	0.43
1:E:116:LEU:HD23	1:E:116:LEU:HA	1.78	0.43
4:H:81:GLU:OE1	4:H:82(A):ARG:NH1	2.50	0.43
1:C:353:PHE:CZ	1:C:456:ARG:HD3	2.53	0.43
4:L:36:TRP:HE1	4:L:69:ILE:HG12	1.82	0.43
1:C:93:PHE:HE2	1:C:242:VAL:HG12	1.83	0.43
1:E:65:LYS:HG2	1:E:208:VAL:HG11	1.99	0.43
2:F:530:MET:HG3	2:F:628:TRP:CE2	2.53	0.43
1:A:280:ASN:HA	1:A:456:ARG:HG3	2.00	0.43
1:C:298:ARG:HB2	1:C:328:GLN:O	2.19	0.43
2:D:656:ASN:OD1	2:D:656:ASN:C	2.62	0.43
1:A:244:THR:HG21	2:B:523:LEU:HD12	2.01	0.43
2:B:579:ARG:O	2:B:583:VAL:HG23	2.18	0.43
4:J:4:LEU:HD11	4:J:102:HIS:HB3	1.99	0.43
1:E:332:ASN:HD21	1:E:413:SER:HB3	1.83	0.43
1:A:53:PHE:HE1	1:A:220:PRO:HA	1.84	0.43
1:C:45:TRP:CZ2	2:D:629:LEU:HD21	2.54	0.43
1:E:391:PHE:HD2	1:E:470:PRO:CG	2.31	0.43
3:G:27:GLU:N	3:G:27:GLU:OE1	2.51	0.43
4:H:68:THR:HG22	4:H:81:GLU:HB3	1.99	0.43
1:A:425:ASN:OD1	1:A:432:GLN:NE2	2.49	0.43
2:D:585:ARG:HA	2:D:588:ARG:HB3	2.00	0.43
3:I:39:LYS:CG	3:I:42:GLN:HE22	2.32	0.43
1:E:297:THR:HA	1:E:443:ILE:O	2.18	0.43
1:A:344:LYS:HD3	1:A:347:LYS:HD3	1.99	0.43
3:K:94:TRP:CE3	3:K:95:PRO:HA	2.54	0.43
1:C:273:ARG:HH12	1:C:287:GLN:NE2	2.16	0.43
3:I:93:ASN:HD21	3:I:96:TYR:HA	1.84	0.43
1:E:96:TRP:HH2	1:E:285:LEU:HD12	1.84	0.43
2:F:598:CYS:HB2	2:F:601:LYS:HE3	2.01	0.43
1:A:37:THR:O	1:A:496:VAL:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:ASP:OD1	1:A:325:ASP:N	2.51	0.43
1:E:375:SER:O	9:E:609:Y26:F22	2.26	0.43
2:B:617:ARG:HE	2:B:617:ARG:HB3	1.58	0.43
1:C:42:VAL:HG12	1:C:493:PRO:O	2.18	0.43
1:C:491:ILE:H	1:C:491:ILE:HD12	1.84	0.43
4:J:54:LEU:HD23	4:J:54:LEU:O	2.19	0.43
2:F:573:ILE:O	2:F:577:GLN:HG3	2.19	0.43
2:F:645:LEU:O	2:F:648:GLU:HG3	2.19	0.43
3:G:56:THR:N	4:H:101:LYS:HZ1	2.16	0.43
1:C:369:LEU:HA	1:C:372:THR:HG22	2.00	0.42
2:D:573:ILE:O	2:D:576:LEU:N	2.52	0.42
2:D:604:CYS:SG	2:D:605:CYS:N	2.92	0.42
1:E:37:THR:HG21	1:E:499:THR:HB	2.00	0.42
4:H:48:MET:CE	4:H:67:VAL:HG21	2.49	0.42
1:A:38:VAL:HG13	2:B:604:CYS:HB3	2.01	0.42
1:A:440:GLN:O	6:N:5:MAN:O6	2.28	0.42
1:C:104:MET:HE1	1:C:251:ILE:HG22	2.01	0.42
1:E:257:THR:C	1:E:259:LEU:H	2.27	0.42
1:E:419:ARG:HG3	1:E:421:LYS:HE3	2.00	0.42
1:A:207:LYS:HA	1:A:207:LYS:HD2	1.59	0.42
1:A:283:ASN:OD1	1:A:455:THR:OG1	2.33	0.42
1:C:102:GLU:H	1:C:102:GLU:HG2	1.63	0.42
2:D:568:LEU:HD23	2:D:568:LEU:HA	1.81	0.42
1:E:223:PHE:CE2	1:E:490:LYS:HB2	2.54	0.42
1:A:274:SER:OG	1:A:284:ILE:HA	2.20	0.42
1:C:35:TRP:HE1	2:D:607:ASN:HA	1.84	0.42
1:C:65:LYS:HD3	1:C:65:LYS:HA	1.83	0.42
1:E:93:PHE:CD1	1:E:228:CYS:HB2	2.54	0.42
1:E:419:ARG:H	1:E:419:ARG:HG2	1.46	0.42
3:G:61:ARG:HE	3:G:75:ILE:HG22	1.84	0.42
1:A:288:PHE:HZ	1:A:452:LEU:HG	1.84	0.42
4:J:36:TRP:CD1	4:J:69:ILE:HD13	2.54	0.42
1:E:116:LEU:HD13	1:E:382:PHE:HZ	1.84	0.42
3:G:33:LEU:HB3	3:G:51:ALA:HB2	2.02	0.42
1:A:39:TYR:HD2	2:B:628:TRP:CH2	2.37	0.42
1:A:428:GLN:OE1	1:A:428:GLN:N	2.52	0.42
1:A:451:GLY:O	1:A:452:LEU:HD23	2.20	0.42
3:K:6:GLN:OE1	3:K:24:ARG:N	2.52	0.42
1:C:118:PRO:CG	1:C:121:LYS:HB2	2.46	0.42
4:J:39:GLN:HB2	4:J:45:LEU:HD23	2.02	0.42
1:E:349:LEU:O	1:E:353:PHE:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:356:ASN:ND2	1:E:356:ASN:O	2.52	0.42
3:G:95(A):PRO:O	3:G:95(B):ARG:HD3	2.20	0.42
2:B:631:TRP:CZ2	2:B:635:ILE:HD11	2.55	0.42
1:C:87:GLU:O	2:D:527:GLY:HA3	2.19	0.42
1:C:121:LYS:HE2	1:C:121:LYS:HB3	1.71	0.42
1:C:283:ASN:OD1	1:C:453:ILE:HG23	2.19	0.42
1:A:70:ALA:O	1:A:74:CYS:HB2	2.20	0.42
1:A:342:LEU:HD13	1:A:345:VAL:HG11	2.01	0.42
1:A:430:ILE:HG23	9:A:608:Y26:N13	2.35	0.42
2:B:567:LYS:HB3	2:B:567:LYS:HE2	1.83	0.42
3:K:11:LEU:HD12	3:K:11:LEU:HA	1.83	0.42
3:K:18:ARG:HH11	3:K:20:THR:HG22	1.85	0.42
2:D:533:ALA:HA	2:D:536:THR:HG22	2.01	0.42
1:E:36:VAL:HG12	2:F:610:TRP:CE3	2.55	0.42
4:L:13:LYS:HE2	4:L:13:LYS:HB2	1.89	0.42
2:D:563:GLN:HG3	2:D:565:LEU:H	1.85	0.42
1:A:76:PRO:HD3	2:B:571:TRP:CD2	2.55	0.42
1:A:376:PHE:CD1	1:A:376:PHE:C	2.98	0.42
2:B:602:LEU:HD12	2:B:602:LEU:H	1.84	0.42
3:I:21:LEU:HD23	3:I:102:THR:HG21	2.01	0.42
1:A:256:SER:OG	1:A:376:PHE:HB3	2.21	0.41
1:C:271:MET:HE3	1:C:272:ILE:H	1.86	0.41
2:D:618:ASN:OD1	2:D:621:GLU:HB3	2.20	0.41
2:B:650:GLN:O	2:B:654:GLU:HG2	2.20	0.41
1:E:274:SER:OG	8:E:602:NAG:O7	2.32	0.41
1:E:327:ARG:HG3	1:E:438:PRO:HG2	2.01	0.41
3:G:10:THR:OG1	3:G:103:ARG:O	2.33	0.41
1:A:254:VAL:HG11	1:A:261:LEU:O	2.20	0.41
1:C:54:CYS:HB2	1:C:74:CYS:HB2	1.82	0.41
1:C:287:GLN:HE21	1:C:287:GLN:HB2	1.61	0.41
2:F:622:ILE:HA	2:F:626:MET:HG2	2.02	0.41
4:H:67:VAL:HG23	4:H:81:GLU:O	2.19	0.41
1:A:69:TRP:CE3	1:A:111:LEU:HD12	2.55	0.41
1:C:37:THR:HB	2:D:605:CYS:HB3	2.03	0.41
2:D:655:LYS:HA	2:D:658:GLN:HB3	2.02	0.41
3:I:94:TRP:HA	3:I:95:PRO:C	2.45	0.41
1:C:95:MET:SD	1:C:484:TYR:HB2	2.61	0.41
1:C:203:GLN:O	3:I:94:TRP:NE1	2.52	0.41
1:C:351:LYS:HE3	1:C:351:LYS:HB2	1.85	0.41
3:I:76:SER:OG	3:I:77:SER:N	2.53	0.41
4:J:95:VAL:HG21	4:J:100(J):PHE:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:200:ALA:HB1	4:H:56:VAL:HG23	2.03	0.41
3:G:46:LEU:HD21	3:G:49:TYR:HB3	2.01	0.41
1:A:267:GLU:HG2	1:A:268:GLU:N	2.36	0.41
1:A:222:GLY:HA3	2:B:585:ARG:NH1	2.36	0.41
4:L:23:LYS:NZ	4:L:77:THR:HA	2.36	0.41
2:F:568:LEU:O	2:F:568:LEU:HD12	2.20	0.41
3:G:54:ARG:HH12	3:G:60:ALA:HA	1.85	0.41
3:G:94:TRP:HA	3:G:95:PRO:C	2.46	0.41
1:E:65:LYS:HA	1:E:65:LYS:HD3	1.54	0.41
1:A:276:ASN:OD1	1:A:278:THR:OG1	2.34	0.41
1:A:295:ASN:N	1:A:295:ASN:OD1	2.52	0.41
2:B:569:THR:O	2:B:573:ILE:HD12	2.20	0.41
1:C:494:LEU:HD12	1:C:494:LEU:HA	1.84	0.41
3:I:62:PHE:CD1	3:I:73:LEU:HD11	2.55	0.41
4:J:84:SER:O	4:J:87:THR:HG23	2.21	0.41
1:E:335:LYS:HE2	1:E:414:ILE:HB	2.02	0.41
1:E:379:GLY:N	7:S:2:NAG:O6	2.54	0.41
3:G:95(A):PRO:HB2	3:G:96:TYR:CZ	2.56	0.41
4:L:36:TRP:HZ2	4:L:78:VAL:HG11	1.86	0.41
1:C:493:PRO:HG2	2:D:585:ARG:NH1	2.36	0.41
2:D:531:GLY:O	2:D:534:SER:OG	2.39	0.41
1:E:327:ARG:NH2	4:H:100(F):ASP:OD1	2.54	0.41
2:F:618:ASN:O	2:F:622:ILE:HG12	2.20	0.41
5:R:1:NAG:H61	5:R:2:NAG:N2	2.36	0.41
3:K:96:TYR:HB2	4:L:47:TRP:CE3	2.56	0.40
1:E:207:LYS:HZ3	1:E:439:ILE:HG23	1.86	0.40
1:A:342:LEU:O	1:A:346:VAL:HG22	2.22	0.40
1:A:378:CYS:SG	6:N:2:NAG:O6	2.77	0.40
1:E:85:HIS:HA	1:E:243:SER:HA	2.03	0.40
1:E:260:LEU:HD21	1:E:453:ILE:HD11	2.03	0.40
1:E:469:ARG:HA	1:E:470:PRO:HD3	1.87	0.40
1:A:376:PHE:CE1	1:A:383:PHE:HB2	2.56	0.40
1:C:221:ALA:HB1	2:D:581:LEU:HD13	2.03	0.40
1:C:268:GLU:C	1:C:289:ASN:HD21	2.29	0.40
1:C:356:ASN:OD1	1:C:397:SER:OG	2.27	0.40
1:E:298:ARG:HB2	1:E:329:ALA:HB2	2.03	0.40
3:G:30:SER:HA	3:G:71:PHE:CE1	2.57	0.40
2:B:577:GLN:HG2	2:F:576:LEU:HD21	2.02	0.40
1:C:62:GLU:HG3	1:C:64:GLU:HB3	2.02	0.40
1:C:100:MET:HE2	1:C:100:MET:HB3	1.93	0.40
1:E:294:ILE:HA	1:E:333:VAL:HG12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:442:VAL:HG12	1:E:444:ARG:HG2	2.04	0.40
2:F:563:GLN:O	2:F:567:LYS:HG2	2.21	0.40
3:G:96:TYR:OH	4:H:50:ARG:HD2	2.21	0.40
1:A:213:ILE:O	1:A:253:PRO:HD2	2.22	0.40
1:A:227:LYS:HE3	1:A:245:VAL:HG21	2.04	0.40
1:A:326:ILE:HA	1:A:326:ILE:HD12	1.87	0.40
1:C:490:LYS:HE2	1:C:490:LYS:HB2	1.86	0.40
1:E:97:LYS:O	1:E:97:LYS:HD3	2.22	0.40
1:E:370:GLU:HG3	1:E:384:TYR:CE2	2.56	0.40
4:H:36:TRP:CH2	4:H:92:CYS:HB2	2.57	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	354/479 (74%)	335 (95%)	19 (5%)	0	100	100
1	C	355/479 (74%)	320 (90%)	35 (10%)	0	100	100
1	E	354/479 (74%)	308 (87%)	46 (13%)	0	100	100
2	B	130/153 (85%)	121 (93%)	9 (7%)	0	100	100
2	D	116/153 (76%)	113 (97%)	3 (3%)	0	100	100
2	F	122/153 (80%)	109 (89%)	13 (11%)	0	100	100
3	G	109/214 (51%)	104 (95%)	5 (5%)	0	100	100
3	I	109/214 (51%)	102 (94%)	7 (6%)	0	100	100
3	K	109/214 (51%)	100 (92%)	9 (8%)	0	100	100
4	H	126/230 (55%)	118 (94%)	8 (6%)	0	100	100
4	J	126/230 (55%)	119 (94%)	7 (6%)	0	100	100
4	L	126/230 (55%)	122 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2136/3228 (66%)	1971 (92%)	165 (8%)	0	100	100

There are no Ramachandran outliers to report.

### 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	322/427 (75%)	320 (99%)	2 (1%)	84	91
1	C	324/427 (76%)	322 (99%)	2 (1%)	84	91
1	E	323/427 (76%)	323 (100%)	0	100	100
2	B	110/129 (85%)	109 (99%)	1 (1%)	75	86
2	D	104/129 (81%)	104 (100%)	0	100	100
2	F	102/129 (79%)	100 (98%)	2 (2%)	50	72
3	G	92/184 (50%)	92 (100%)	0	100	100
3	I	92/184 (50%)	92 (100%)	0	100	100
3	K	91/184 (50%)	91 (100%)	0	100	100
4	H	106/194 (55%)	106 (100%)	0	100	100
4	J	106/194 (55%)	106 (100%)	0	100	100
4	L	106/194 (55%)	105 (99%)	1 (1%)	75	86
All	All	1878/2802 (67%)	1870 (100%)	8 (0%)	88	95

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	LEU
1	A	448	ASN
2	B	573	ILE
4	L	70	THR
1	C	57	ASP
1	C	424	ILE

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Mol	Chain	Res	Type
2	F	584	GLU
2	F	645	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	328	GLN
1	A	330	HIS
1	A	374	HIS
2	B	590	GLN
3	K	79	GLN
3	K	90	GLN
4	L	100(H)	ASN
1	C	33	ASN
1	C	99	ASN
1	C	287	GLN
1	C	352	HIS
1	C	422	GLN
1	C	425	ASN
1	C	432	GLN
2	D	591	GLN
2	D	630	GLN
2	D	658	GLN
3	I	93	ASN
3	I	100	GLN
4	J	39	GLN
1	E	66	HIS
1	E	425	ASN
4	H	43	GLN
4	H	82(B)	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 ⓘ

38 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
5	NAG	M	1	5,1	14,14,15	0.20	0	17,19,21	0.49	0
5	NAG	M	2	5	14,14,15	0.25	0	17,19,21	0.42	0
6	NAG	N	1	6,1	14,14,15	0.16	0	17,19,21	0.49	0
6	NAG	N	2	6	14,14,15	0.23	0	17,19,21	0.38	0
6	BMA	N	3	6	11,11,12	0.58	0	15,15,17	0.76	0
6	MAN	N	4	6	11,11,12	0.61	0	15,15,17	1.02	2 (13%)
6	MAN	N	5	6	11,11,12	0.65	0	15,15,17	0.88	1 (6%)
6	MAN	N	6	6	11,11,12	0.81	0	15,15,17	1.25	2 (13%)
7	NAG	O	1	7,1	14,14,15	0.29	0	17,19,21	0.66	0
7	NAG	O	2	7	14,14,15	0.23	0	17,19,21	0.42	0
7	BMA	O	3	7	11,11,12	0.63	0	15,15,17	0.82	0
7	MAN	O	4	7	11,11,12	0.53	0	15,15,17	1.21	2 (13%)
7	MAN	O	5	7	11,11,12	0.58	0	15,15,17	0.89	1 (6%)
7	MAN	O	6	7	11,11,12	0.85	0	15,15,17	0.91	1 (6%)
7	MAN	O	7	7	11,11,12	0.85	0	15,15,17	1.12	2 (13%)
5	NAG	P	1	5,1	14,14,15	0.28	0	17,19,21	0.58	0
5	NAG	P	2	5	14,14,15	0.52	0	17,19,21	0.69	1 (5%)
5	NAG	Q	1	5,1	14,14,15	0.92	1 (7%)	17,19,21	1.27	1 (5%)
5	NAG	Q	2	5	14,14,15	0.28	0	17,19,21	0.48	0
5	NAG	R	1	5,1	14,14,15	0.29	0	17,19,21	0.58	0
5	NAG	R	2	5	14,14,15	0.22	0	17,19,21	0.49	0
7	NAG	S	1	7,1	14,14,15	0.19	0	17,19,21	0.77	0
7	NAG	S	2	7	14,14,15	0.28	0	17,19,21	0.43	0
7	BMA	S	3	7	11,11,12	0.58	0	15,15,17	0.89	0
7	MAN	S	4	7	11,11,12	0.55	0	15,15,17	1.20	2 (13%)
7	MAN	S	5	7	11,11,12	0.72	0	15,15,17	1.23	2 (13%)
7	MAN	S	6	7	11,11,12	0.79	1 (9%)	15,15,17	1.20	2 (13%)
7	MAN	S	7	7	11,11,12	0.80	0	15,15,17	1.26	2 (13%)
5	NAG	T	1	5,1	14,14,15	0.20	0	17,19,21	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	T	2	5	14,14,15	0.24	0	17,19,21	0.45	0
5	NAG	U	1	5,1	14,14,15	0.23	0	17,19,21	0.47	0
5	NAG	U	2	5	14,14,15	1.04	1 (7%)	17,19,21	1.17	1 (5%)
5	NAG	V	1	5,1	14,14,15	0.18	0	17,19,21	0.58	0
5	NAG	V	2	5	14,14,15	0.37	0	17,19,21	0.46	0
5	NAG	W	1	5,1	14,14,15	0.44	0	17,19,21	1.35	2 (11%)
5	NAG	W	2	5	14,14,15	0.22	0	17,19,21	0.45	0
5	NAG	X	1	5,1	14,14,15	0.27	0	17,19,21	0.48	0
5	NAG	X	2	5	14,14,15	0.26	0	17,19,21	0.53	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	M	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	M	2	5	-	1/6/23/26	0/1/1/1
6	NAG	N	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	N	2	6	-	2/6/23/26	0/1/1/1
6	BMA	N	3	6	-	2/2/19/22	0/1/1/1
6	MAN	N	4	6	-	0/2/19/22	0/1/1/1
6	MAN	N	5	6	-	2/2/19/22	0/1/1/1
6	MAN	N	6	6	-	2/2/19/22	0/1/1/1
7	NAG	O	1	7,1	-	4/6/23/26	0/1/1/1
7	NAG	O	2	7	-	2/6/23/26	0/1/1/1
7	BMA	O	3	7	-	0/2/19/22	0/1/1/1
7	MAN	O	4	7	-	2/2/19/22	0/1/1/1
7	MAN	O	5	7	-	2/2/19/22	0/1/1/1
7	MAN	O	6	7	-	1/2/19/22	0/1/1/1
7	MAN	O	7	7	-	1/2/19/22	1/1/1/1
5	NAG	P	1	5,1	-	3/6/23/26	0/1/1/1
5	NAG	P	2	5	-	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	-	1/6/23/26	0/1/1/1
5	NAG	R	1	5,1	-	4/6/23/26	0/1/1/1
5	NAG	R	2	5	-	0/6/23/26	0/1/1/1
7	NAG	S	1	7,1	-	4/6/23/26	0/1/1/1
7	NAG	S	2	7	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BMA	S	3	7	-	2/2/19/22	0/1/1/1
7	MAN	S	4	7	-	2/2/19/22	0/1/1/1
7	MAN	S	5	7	-	1/2/19/22	1/1/1/1
7	MAN	S	6	7	-	2/2/19/22	1/1/1/1
7	MAN	S	7	7	-	1/2/19/22	1/1/1/1
5	NAG	T	1	5,1	-	4/6/23/26	0/1/1/1
5	NAG	T	2	5	-	2/6/23/26	0/1/1/1
5	NAG	U	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	U	2	5	-	1/6/23/26	0/1/1/1
5	NAG	V	1	5,1	-	4/6/23/26	0/1/1/1
5	NAG	V	2	5	-	2/6/23/26	0/1/1/1
5	NAG	W	1	5,1	-	6/6/23/26	0/1/1/1
5	NAG	W	2	5	-	1/6/23/26	0/1/1/1
5	NAG	X	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	X	2	5	-	4/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	U	2	NAG	O5-C1	3.48	1.49	1.43
5	Q	1	NAG	O5-C1	3.26	1.49	1.43
7	S	6	MAN	C1-C2	2.01	1.57	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Q	1	NAG	C1-O5-C5	4.98	118.86	112.19
5	W	1	NAG	C2-N2-C7	4.57	129.02	122.90
5	U	2	NAG	C1-O5-C5	4.56	118.30	112.19
7	S	7	MAN	C1-O5-C5	3.84	117.33	112.19
7	S	5	MAN	C1-O5-C5	3.82	117.30	112.19
6	N	6	MAN	C1-O5-C5	3.47	116.83	112.19
7	S	6	MAN	C1-O5-C5	3.43	116.78	112.19
7	O	4	MAN	C1-O5-C5	3.34	116.66	112.19
7	S	4	MAN	C1-O5-C5	3.25	116.54	112.19
7	O	7	MAN	C1-O5-C5	3.19	116.47	112.19
7	S	4	MAN	O2-C2-C3	-2.69	104.58	110.15
6	N	4	MAN	O2-C2-C3	-2.66	104.64	110.15
7	O	4	MAN	O2-C2-C3	-2.44	105.10	110.15
5	P	2	NAG	C1-O5-C5	2.40	115.40	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	N	4	MAN	C1-O5-C5	2.28	115.25	112.19
5	W	1	NAG	C1-C2-N2	2.26	114.00	110.43
7	O	5	MAN	O2-C2-C3	-2.23	105.52	110.15
6	N	6	MAN	O2-C2-C3	-2.18	105.63	110.15
6	N	5	MAN	O2-C2-C3	-2.18	105.64	110.15
7	S	6	MAN	O2-C2-C3	-2.16	105.67	110.15
7	O	6	MAN	O2-C2-C3	-2.15	105.69	110.15
7	O	7	MAN	O2-C2-C3	-2.15	105.70	110.15
7	S	5	MAN	O2-C2-C3	-2.15	105.70	110.15
7	S	7	MAN	O2-C2-C3	-2.09	105.82	110.15

There are no chirality outliers.

All (77) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	V	2	NAG	C4-C5-C6-O6
7	S	3	BMA	O5-C5-C6-O6
7	S	4	MAN	C4-C5-C6-O6
5	P	2	NAG	O5-C5-C6-O6
5	T	1	NAG	O5-C5-C6-O6
5	V	2	NAG	O5-C5-C6-O6
6	N	3	BMA	C4-C5-C6-O6
6	N	1	NAG	O5-C5-C6-O6
5	P	2	NAG	C4-C5-C6-O6
7	O	1	NAG	O5-C5-C6-O6
7	O	4	MAN	O5-C5-C6-O6
7	S	4	MAN	O5-C5-C6-O6
5	T	1	NAG	C4-C5-C6-O6
7	O	2	NAG	C4-C5-C6-O6
5	X	2	NAG	O5-C5-C6-O6
5	Q	1	NAG	O5-C5-C6-O6
5	T	2	NAG	O5-C5-C6-O6
7	S	1	NAG	C4-C5-C6-O6
7	S	3	BMA	C4-C5-C6-O6
5	V	1	NAG	O5-C5-C6-O6
6	N	3	BMA	O5-C5-C6-O6
7	O	4	MAN	C4-C5-C6-O6
5	V	1	NAG	C4-C5-C6-O6
6	N	1	NAG	C4-C5-C6-O6
7	O	1	NAG	C4-C5-C6-O6
5	X	2	NAG	C4-C5-C6-O6
5	M	1	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
5	M	1	NAG	O7-C7-N2-C2
5	W	1	NAG	C8-C7-N2-C2
5	W	1	NAG	O7-C7-N2-C2
6	N	2	NAG	C8-C7-N2-C2
6	N	2	NAG	O7-C7-N2-C2
5	X	1	NAG	O5-C5-C6-O6
5	Q	2	NAG	O5-C5-C6-O6
6	N	5	MAN	O5-C5-C6-O6
7	S	1	NAG	O5-C5-C6-O6
7	O	2	NAG	O5-C5-C6-O6
6	N	5	MAN	C4-C5-C6-O6
5	Q	1	NAG	C4-C5-C6-O6
5	U	2	NAG	O5-C5-C6-O6
7	O	5	MAN	O5-C5-C6-O6
5	R	1	NAG	O5-C5-C6-O6
6	N	6	MAN	O5-C5-C6-O6
5	R	1	NAG	C4-C5-C6-O6
6	N	6	MAN	C4-C5-C6-O6
5	W	2	NAG	O5-C5-C6-O6
7	O	6	MAN	O5-C5-C6-O6
7	O	7	MAN	O5-C5-C6-O6
5	T	2	NAG	C4-C5-C6-O6
5	X	1	NAG	C4-C5-C6-O6
5	M	2	NAG	O5-C5-C6-O6
7	S	7	MAN	O5-C5-C6-O6
5	P	1	NAG	O5-C5-C6-O6
7	S	5	MAN	O5-C5-C6-O6
5	X	2	NAG	C1-C2-N2-C7
5	T	1	NAG	C1-C2-N2-C7
5	V	1	NAG	C1-C2-N2-C7
7	S	1	NAG	C1-C2-N2-C7
5	P	1	NAG	C3-C2-N2-C7
5	R	1	NAG	C3-C2-N2-C7
7	O	1	NAG	C3-C2-N2-C7
7	S	1	NAG	C3-C2-N2-C7
7	S	2	NAG	O5-C5-C6-O6
5	W	1	NAG	C4-C5-C6-O6
7	O	5	MAN	C4-C5-C6-O6
5	W	1	NAG	C1-C2-N2-C7
5	P	1	NAG	C1-C2-N2-C7
5	R	1	NAG	C1-C2-N2-C7
7	O	1	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
7	S	6	MAN	C4-C5-C6-O6
5	W	1	NAG	C3-C2-N2-C7
5	X	2	NAG	C3-C2-N2-C7
5	T	1	NAG	C3-C2-N2-C7
5	V	1	NAG	C3-C2-N2-C7
7	S	6	MAN	O5-C5-C6-O6
5	U	1	NAG	C4-C5-C6-O6
5	W	1	NAG	O5-C5-C6-O6

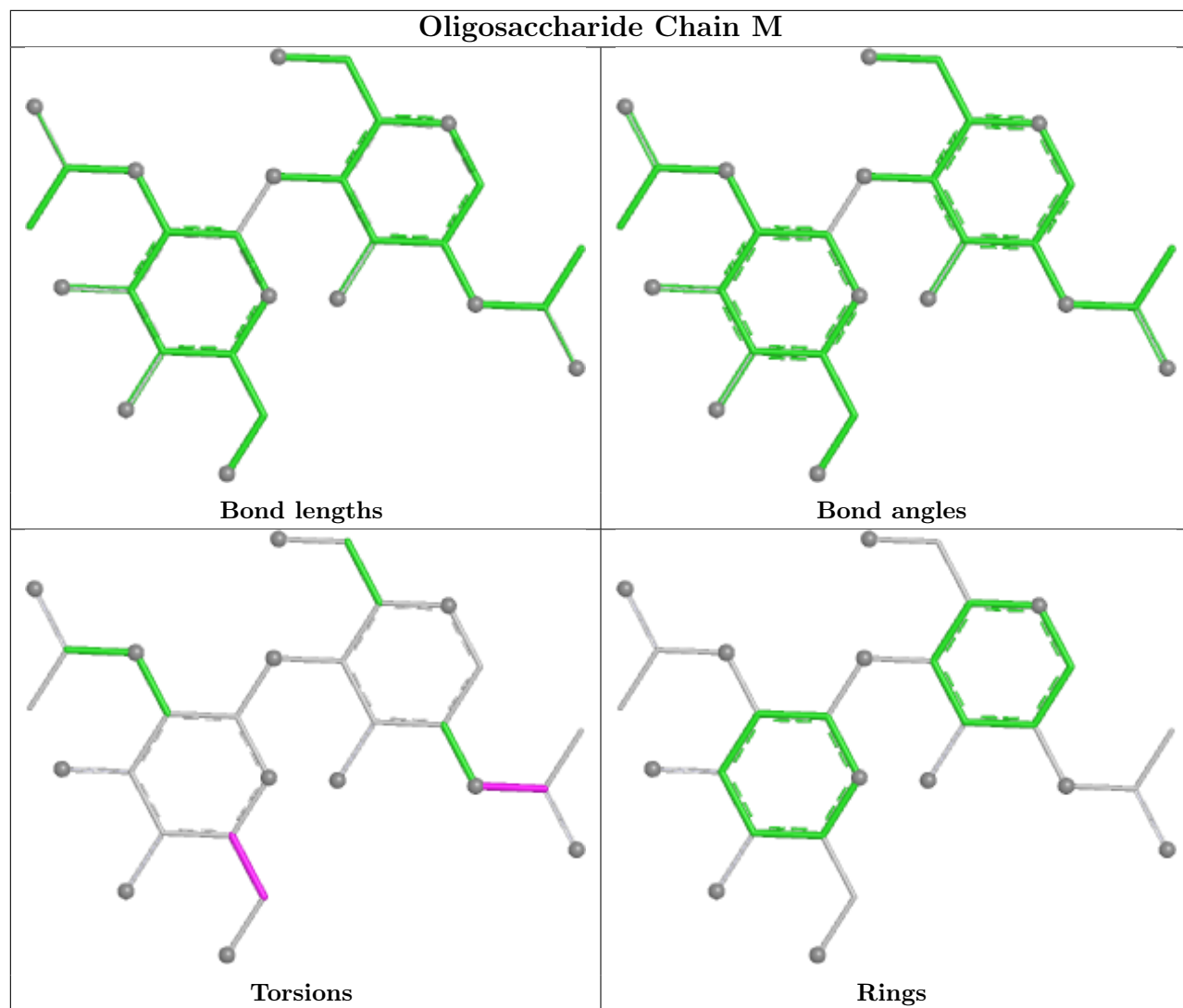
All (4) ring outliers are listed below:

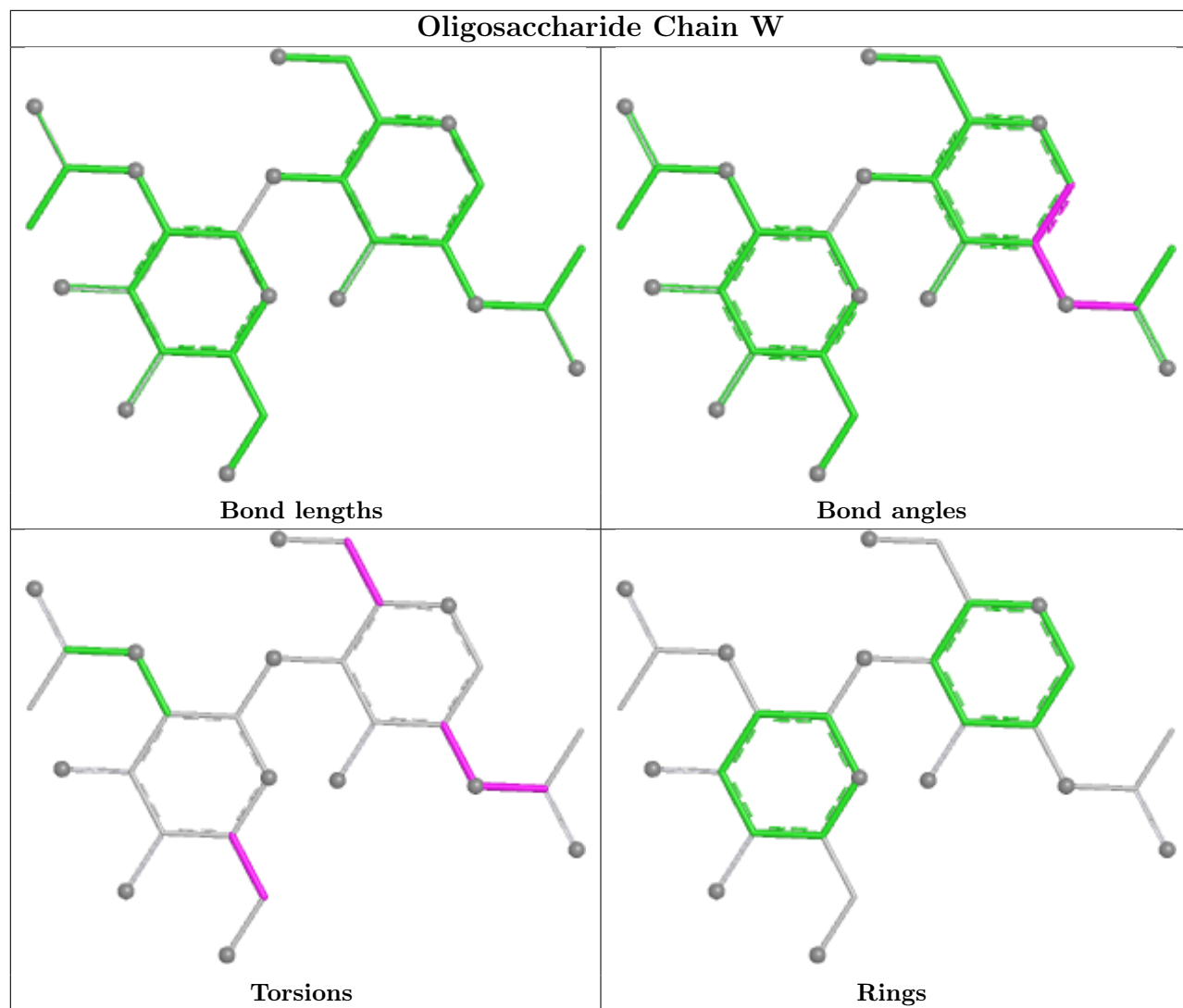
Mol	Chain	Res	Type	Atoms
7	S	6	MAN	C1-C2-C3-C4-C5-O5
7	S	5	MAN	C1-C2-C3-C4-C5-O5
7	S	7	MAN	C1-C2-C3-C4-C5-O5
7	O	7	MAN	C1-C2-C3-C4-C5-O5

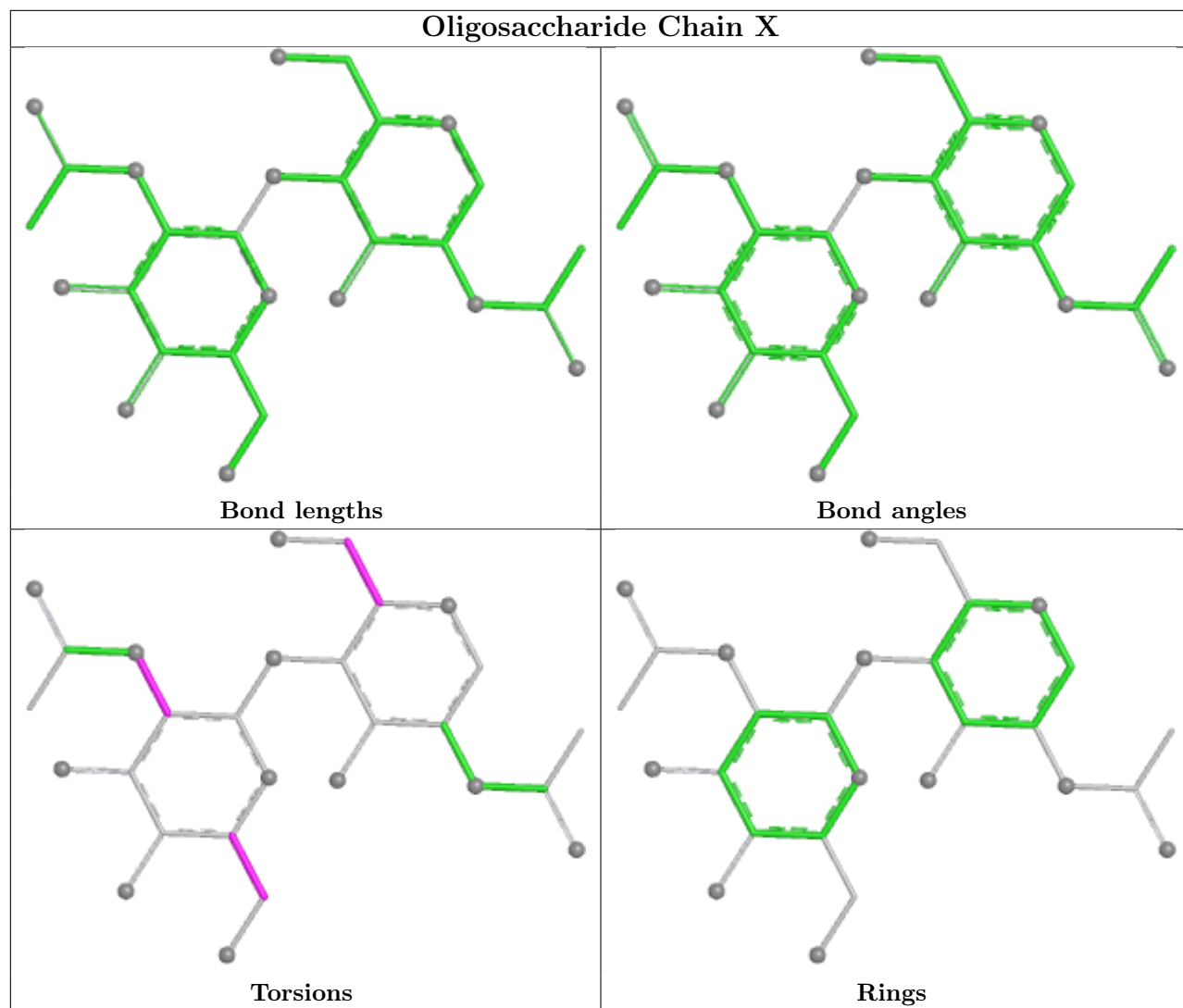
11 monomers are involved in 11 short contacts:

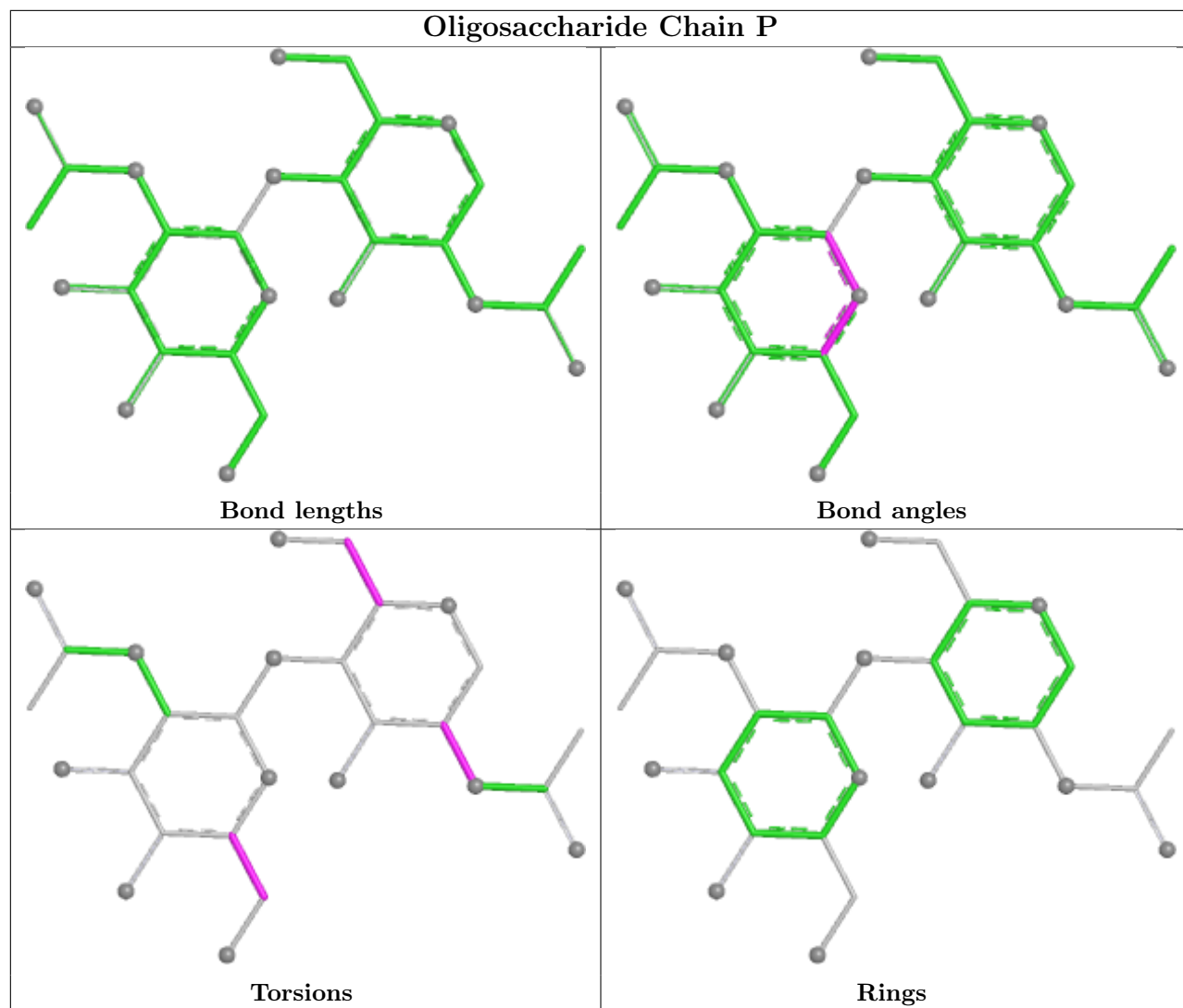
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	R	2	NAG	1	0
6	N	5	MAN	1	0
7	S	2	NAG	1	0
5	W	1	NAG	1	0
5	P	2	NAG	1	0
5	P	1	NAG	1	0
6	N	2	NAG	1	0
7	S	1	NAG	2	0
5	T	1	NAG	1	0
5	X	1	NAG	1	0
5	R	1	NAG	2	0

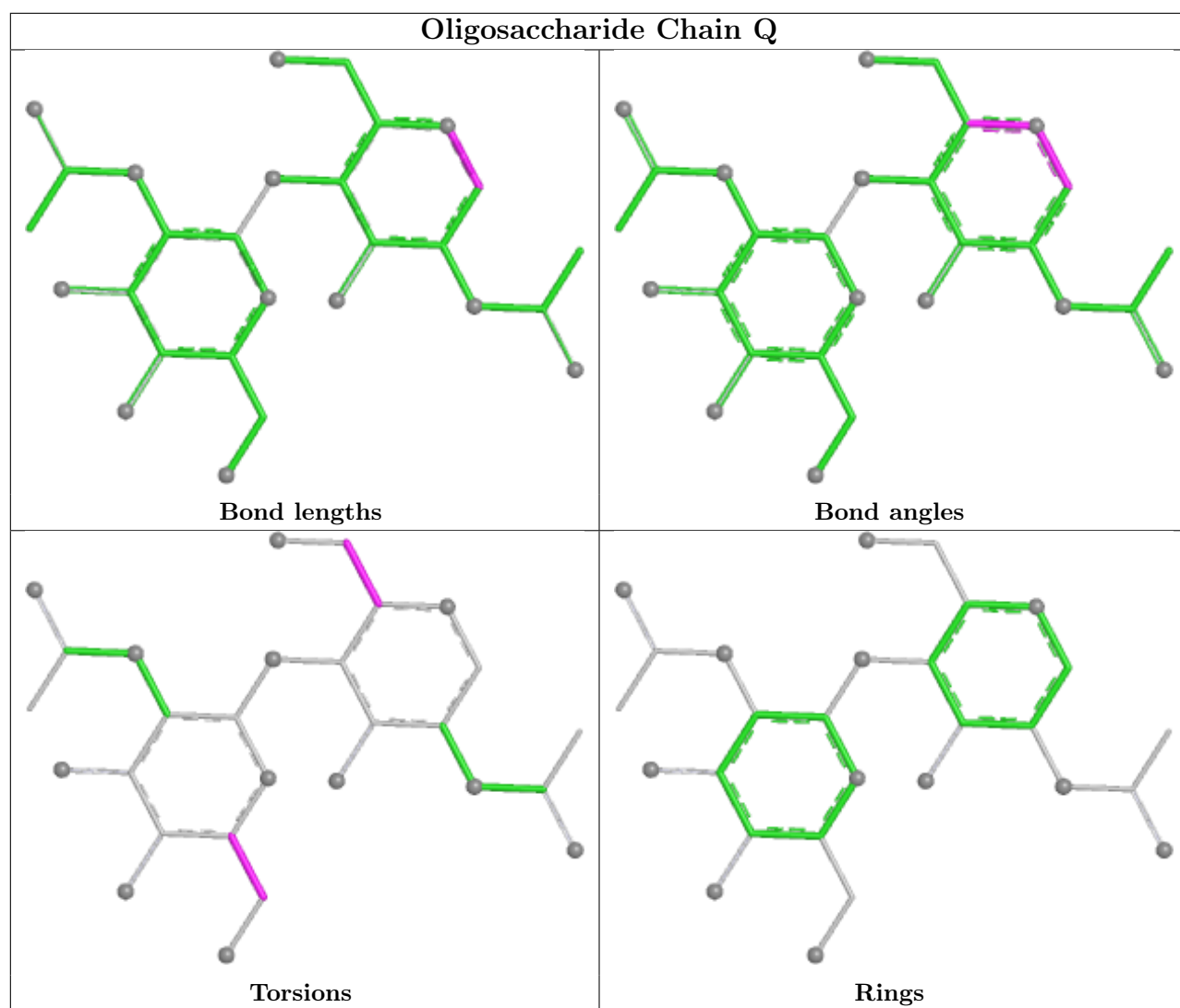
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

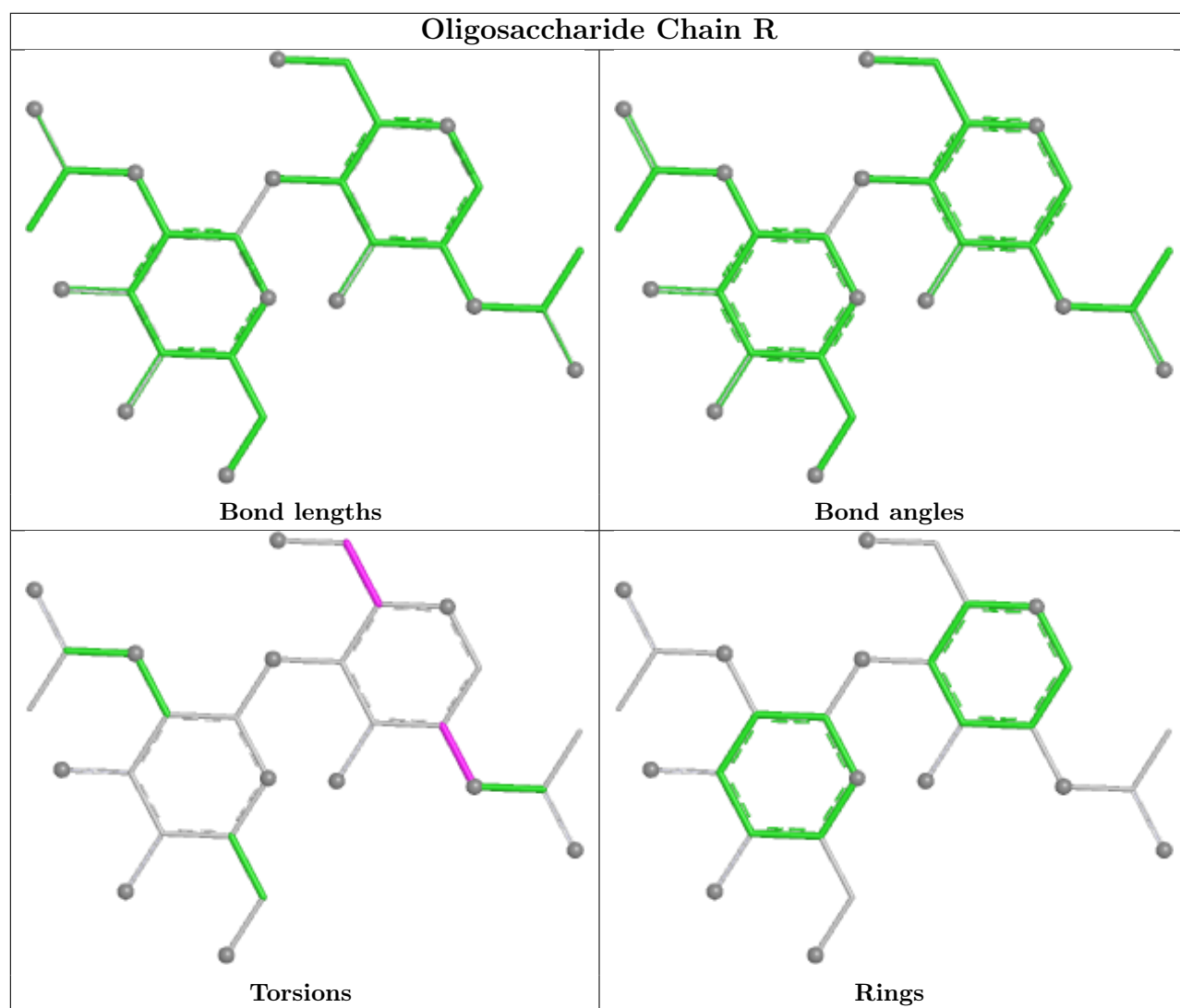


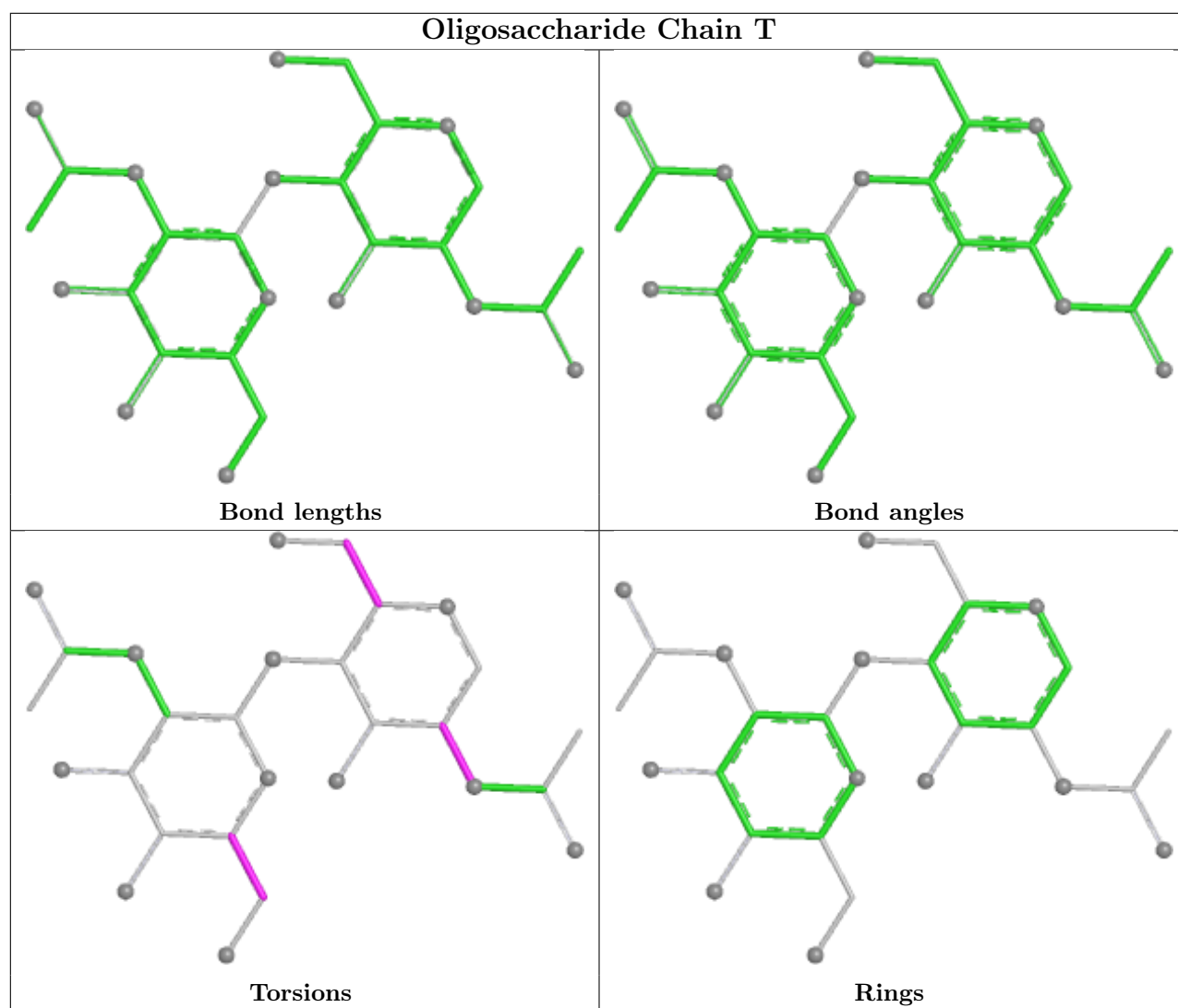




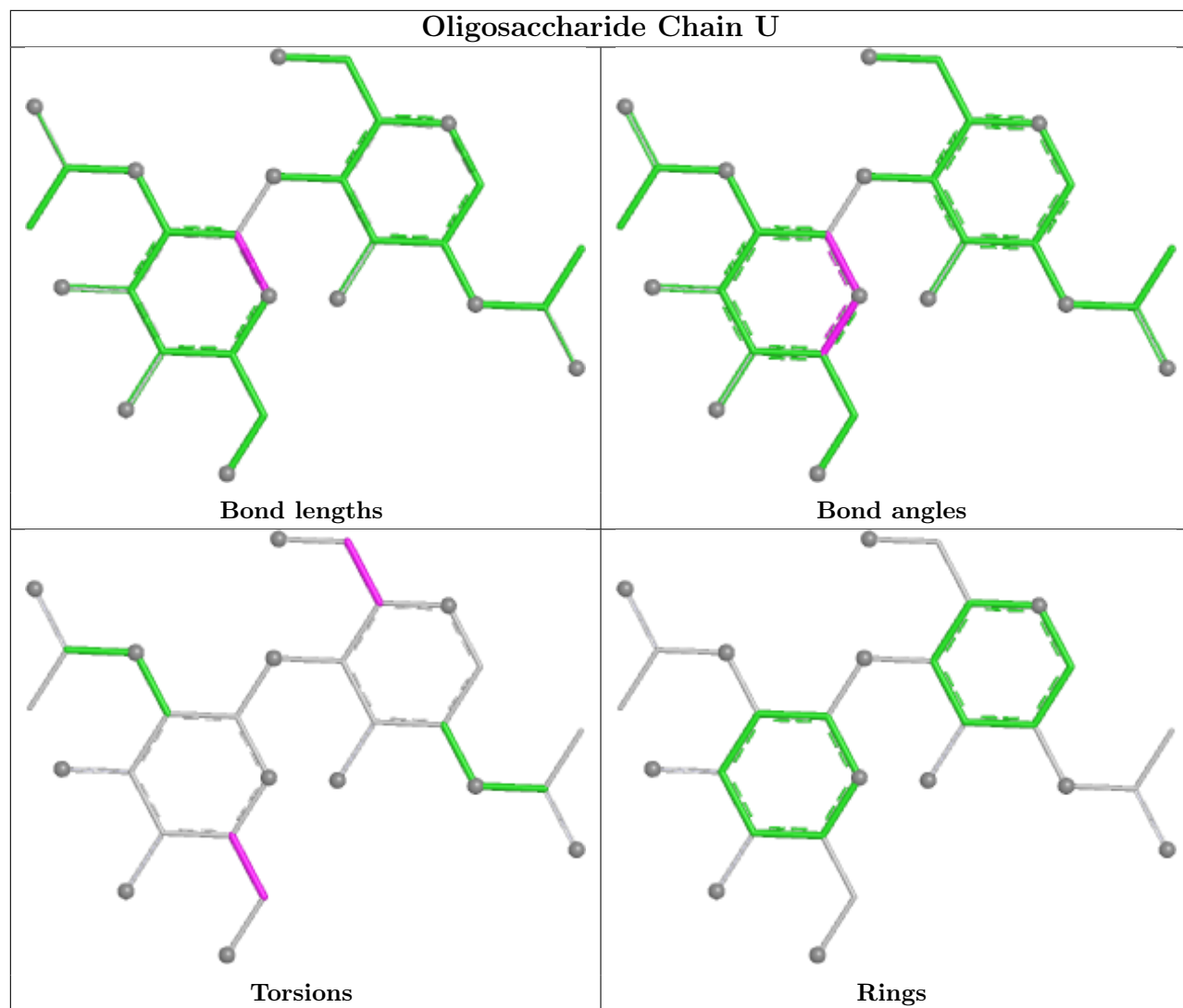


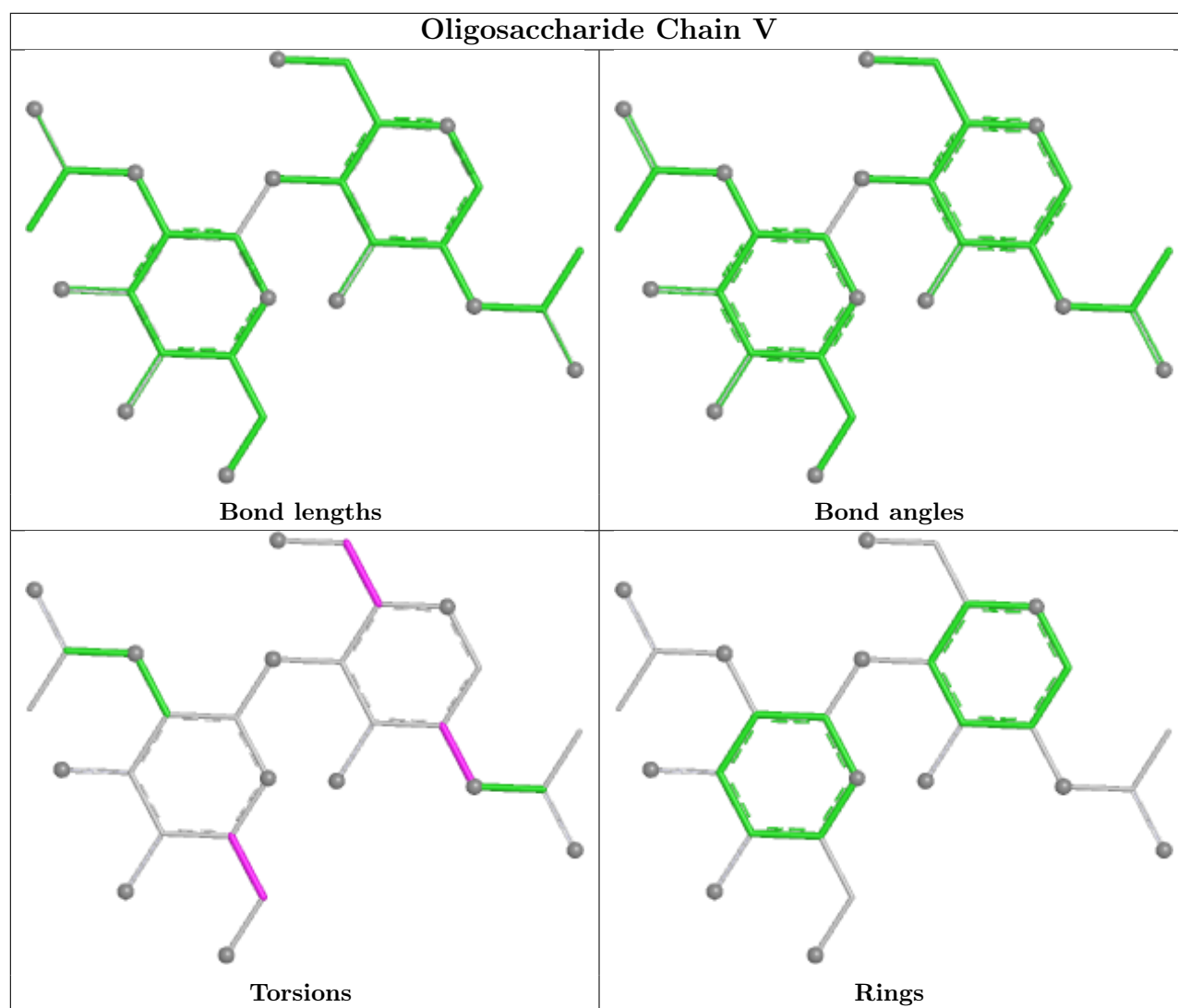


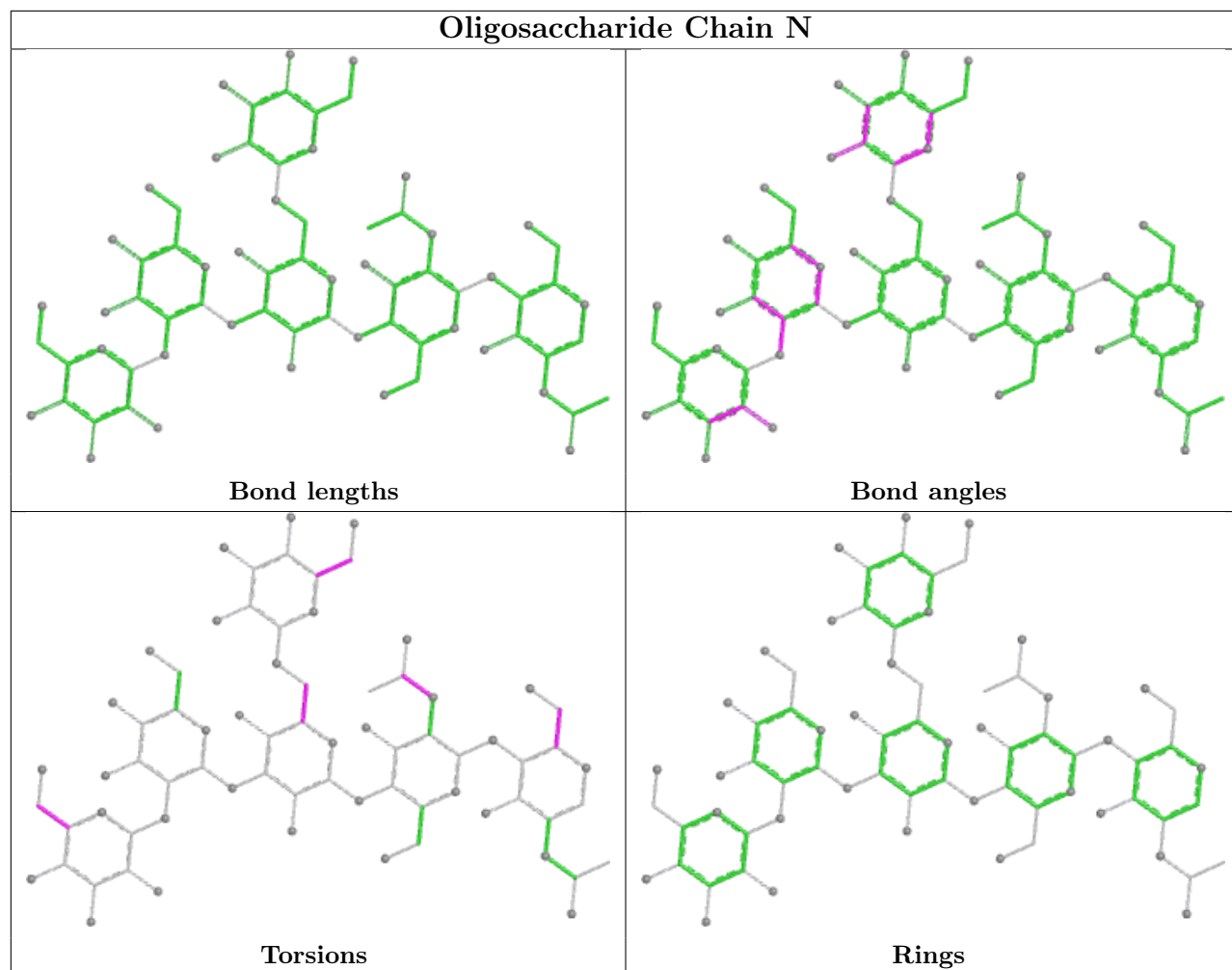


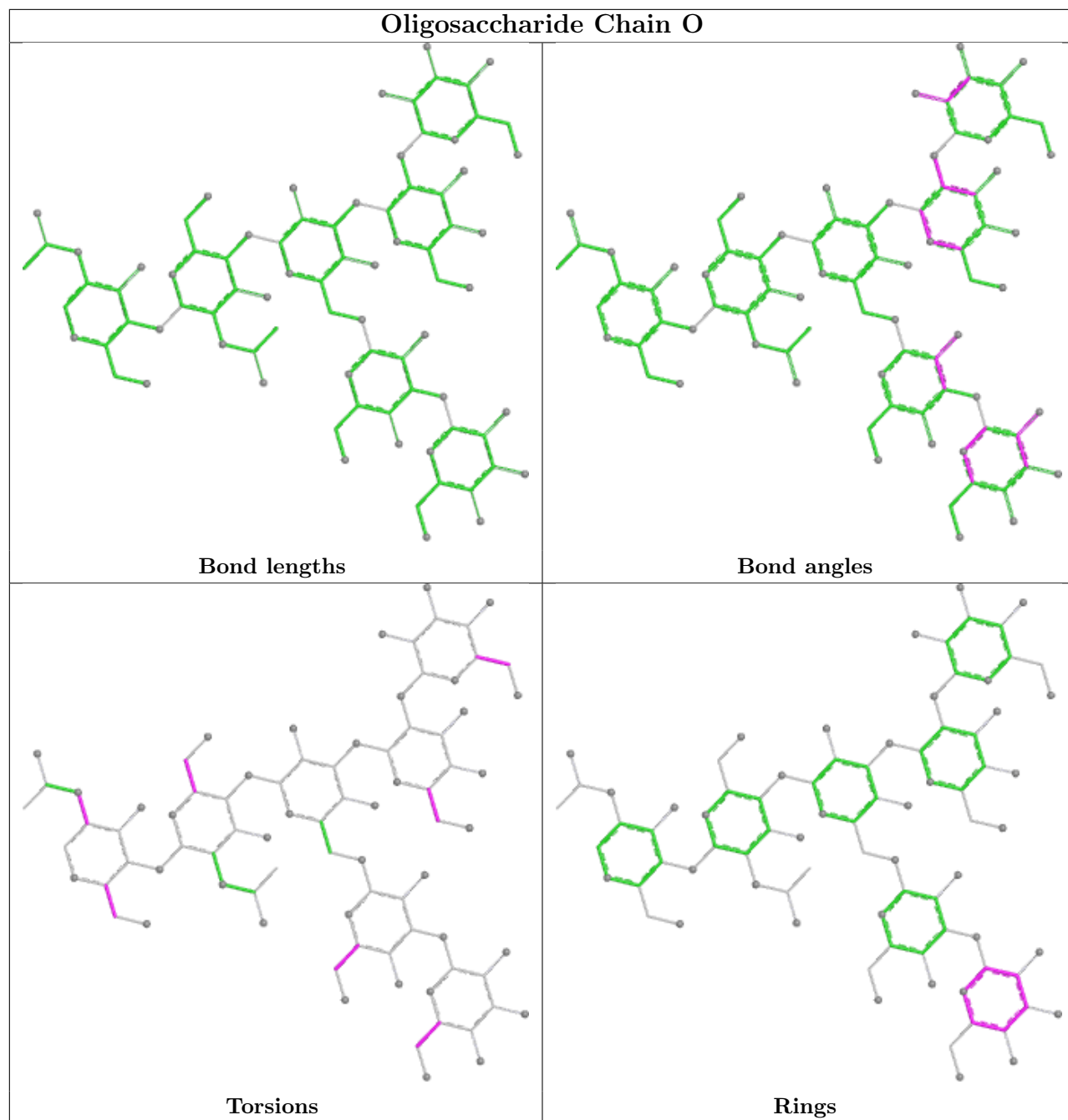


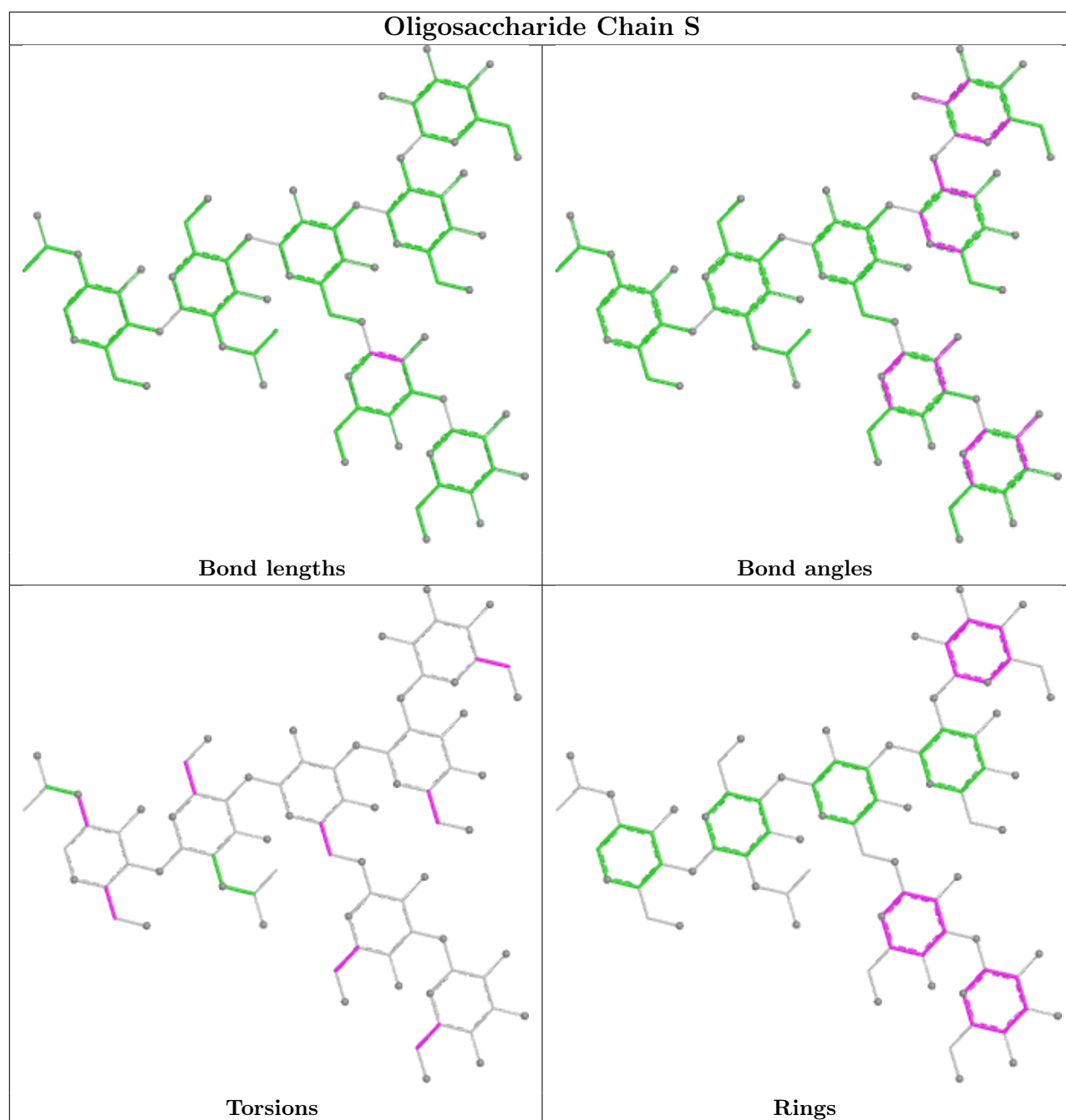












## 5.6 Ligand geometry [i](#)

29 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
8	NAG	A	607	1	14,14,15	0.27	0	17,19,21	0.45	0
8	NAG	C	607	1	14,14,15	0.30	0	17,19,21	0.38	0
8	NAG	A	605	1	14,14,15	0.22	0	17,19,21	0.39	0
9	Y26	A	608	-	38,39,39	2.52	13 (34%)	48,54,54	1.75	8 (16%)
8	NAG	D	701	2	14,14,15	0.21	0	17,19,21	0.40	0
8	NAG	C	604	1	14,14,15	0.52	0	17,19,21	1.40	3 (17%)
8	NAG	E	608	1	14,14,15	0.23	0	17,19,21	0.49	0
8	NAG	E	602	1	14,14,15	0.78	1 (7%)	17,19,21	1.00	1 (5%)
8	NAG	C	605	1	14,14,15	0.26	0	17,19,21	0.55	0
8	NAG	A	604	1	14,14,15	0.69	1 (7%)	17,19,21	0.59	0
9	Y26	E	609	-	38,39,39	2.56	13 (34%)	48,54,54	1.81	8 (16%)
8	NAG	E	603	1	14,14,15	0.16	0	17,19,21	0.46	0
8	NAG	E	605	1	14,14,15	0.86	1 (7%)	17,19,21	1.06	1 (5%)
9	Y26	C	609	-	38,39,39	2.55	11 (28%)	48,54,54	1.87	11 (22%)
8	NAG	A	601	1	14,14,15	0.23	0	17,19,21	0.48	0
8	NAG	C	603	1	14,14,15	0.20	0	17,19,21	0.51	0
8	NAG	C	601	1	14,14,15	0.24	0	17,19,21	0.47	0
8	NAG	E	604	1	14,14,15	0.50	0	17,19,21	1.37	2 (11%)
8	NAG	A	602	1	14,14,15	0.25	0	17,19,21	0.44	0
8	NAG	A	606	1	14,14,15	0.28	0	17,19,21	0.56	0
8	NAG	D	702	2	14,14,15	0.20	0	17,19,21	0.45	0
8	NAG	A	603	1	14,14,15	0.46	0	17,19,21	1.34	2 (11%)
8	NAG	E	606	1	14,14,15	0.23	0	17,19,21	0.43	0
8	NAG	E	607	1	14,14,15	0.18	0	17,19,21	0.46	0
8	NAG	E	601	1	14,14,15	0.25	0	17,19,21	0.42	0
8	NAG	C	608	1	14,14,15	0.21	0	17,19,21	0.53	0
8	NAG	C	606	1	14,14,15	0.37	0	17,19,21	0.63	1 (5%)
8	NAG	B	701	2	14,14,15	0.26	0	17,19,21	0.42	0
8	NAG	C	602	1	14,14,15	0.33	0	17,19,21	0.61	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	A	607	1	-	0/6/23/26	0/1/1/1
8	NAG	C	607	1	-	2/6/23/26	0/1/1/1
8	NAG	A	605	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	Y26	A	608	-	-	11/28/44/44	0/3/3/3
8	NAG	D	701	2	-	2/6/23/26	0/1/1/1
8	NAG	C	604	1	-	6/6/23/26	0/1/1/1
8	NAG	E	608	1	-	0/6/23/26	0/1/1/1
8	NAG	E	602	1	-	2/6/23/26	0/1/1/1
8	NAG	C	605	1	-	4/6/23/26	0/1/1/1
8	NAG	A	604	1	-	2/6/23/26	0/1/1/1
9	Y26	E	609	-	-	11/28/44/44	0/3/3/3
8	NAG	E	603	1	-	1/6/23/26	0/1/1/1
8	NAG	E	605	1	-	4/6/23/26	0/1/1/1
9	Y26	C	609	-	-	9/28/44/44	0/3/3/3
8	NAG	A	601	1	-	2/6/23/26	0/1/1/1
8	NAG	C	603	1	-	0/6/23/26	0/1/1/1
8	NAG	C	601	1	-	2/6/23/26	0/1/1/1
8	NAG	E	604	1	-	4/6/23/26	0/1/1/1
8	NAG	A	602	1	-	2/6/23/26	0/1/1/1
8	NAG	A	606	1	-	4/6/23/26	0/1/1/1
8	NAG	D	702	2	-	2/6/23/26	0/1/1/1
8	NAG	A	603	1	-	5/6/23/26	0/1/1/1
8	NAG	E	606	1	-	2/6/23/26	0/1/1/1
8	NAG	E	607	1	-	1/6/23/26	0/1/1/1
8	NAG	E	601	1	-	2/6/23/26	0/1/1/1
8	NAG	C	608	1	-	0/6/23/26	0/1/1/1
8	NAG	C	606	1	-	0/6/23/26	0/1/1/1
8	NAG	B	701	2	-	1/6/23/26	0/1/1/1
8	NAG	C	602	1	-	4/6/23/26	0/1/1/1

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	609	Y26	C14-C08	-6.90	1.47	1.55
9	E	609	Y26	C11-N10	6.53	1.45	1.33
9	E	609	Y26	C14-C08	-6.48	1.48	1.55
9	A	608	Y26	C11-N10	6.37	1.45	1.33
9	C	609	Y26	C11-N10	6.12	1.45	1.33
9	A	608	Y26	C14-C08	-6.12	1.48	1.55
9	A	608	Y26	C02-N07	5.55	1.45	1.37
9	A	608	Y26	C16-N15	5.53	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	609	Y26	C02-N07	5.53	1.45	1.37
9	E	609	Y26	C02-N07	5.53	1.45	1.37
9	E	609	Y26	C16-N15	5.51	1.45	1.34
9	C	609	Y26	C16-N15	5.21	1.45	1.34
9	E	609	Y26	C17-N18	4.87	1.45	1.35
9	A	608	Y26	C17-N18	4.86	1.45	1.35
9	C	609	Y26	C17-N18	4.75	1.45	1.35
9	C	609	Y26	C29-N07	4.59	1.49	1.40
9	A	608	Y26	C29-N07	4.57	1.49	1.40
9	E	609	Y26	C29-N07	4.44	1.49	1.40
9	C	609	Y26	O03-C02	2.99	1.40	1.34
9	A	608	Y26	O03-C02	2.83	1.40	1.34
9	E	609	Y26	O03-C02	2.79	1.40	1.34
9	E	609	Y26	O28-C16	-2.75	1.18	1.23
9	C	609	Y26	O28-C16	-2.73	1.18	1.23
9	C	609	Y26	O27-C17	-2.69	1.18	1.23
9	E	609	Y26	O27-C17	-2.68	1.18	1.23
8	E	605	NAG	O5-C1	2.62	1.48	1.43
9	A	608	Y26	O27-C17	-2.61	1.18	1.23
9	A	608	Y26	O28-C16	-2.50	1.18	1.23
8	E	602	NAG	O5-C1	2.49	1.47	1.43
9	C	609	Y26	C11-N13	-2.43	1.25	1.34
9	A	608	Y26	C11-N13	-2.41	1.25	1.34
9	E	609	Y26	C11-N13	-2.39	1.25	1.34
9	C	609	Y26	C08-N07	-2.34	1.45	1.47
8	A	604	NAG	C1-C2	2.31	1.55	1.52
9	E	609	Y26	C08-N07	-2.23	1.45	1.47
9	E	609	Y26	C19-N18	2.20	1.46	1.41
9	A	608	Y26	C23-CL24	2.15	1.78	1.73
9	A	608	Y26	C19-N18	2.08	1.45	1.41
9	E	609	Y26	C23-CL24	2.03	1.78	1.73
9	A	608	Y26	C08-N07	-2.01	1.45	1.47

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	609	Y26	C08-C14-N15	-7.11	107.24	115.01
9	E	609	Y26	O03-C02-N07	6.57	120.39	111.04
9	A	608	Y26	O03-C02-N07	6.37	120.10	111.04
9	C	609	Y26	O03-C02-N07	6.22	119.89	111.04
9	E	609	Y26	C08-C14-N15	-5.47	109.03	115.01
9	A	608	Y26	C08-C14-N15	-4.79	109.78	115.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	603	NAG	C2-N2-C7	4.57	129.02	122.90
8	C	604	NAG	C2-N2-C7	4.53	128.97	122.90
8	E	604	NAG	C2-N2-C7	4.51	128.94	122.90
9	A	608	Y26	C16-C17-N18	3.96	118.94	112.25
8	E	605	NAG	C1-O5-C5	3.91	117.42	112.19
8	E	602	NAG	C1-O5-C5	3.84	117.33	112.19
9	E	609	Y26	C17-C16-N15	3.75	122.71	113.73
9	C	609	Y26	C17-C16-N15	3.04	121.03	113.73
9	E	609	Y26	O03-C02-O01	-2.88	119.75	124.76
9	C	609	Y26	C16-C17-N18	2.76	116.91	112.25
9	E	609	Y26	C29-N07-C08	-2.72	106.77	109.75
9	E	609	Y26	C16-C17-N18	2.65	116.73	112.25
9	C	609	Y26	C29-N07-C08	-2.65	106.85	109.75
9	A	608	Y26	O03-C02-O01	-2.64	120.17	124.76
9	A	608	Y26	C17-C16-N15	2.64	120.05	113.73
9	C	609	Y26	O01-C02-N07	-2.62	119.71	123.99
9	A	608	Y26	O01-C02-N07	-2.61	119.73	123.99
9	A	608	Y26	C19-N18-C17	-2.54	122.95	127.45
9	E	609	Y26	O01-C02-N07	-2.53	119.86	123.99
9	C	609	Y26	O03-C02-O01	-2.51	120.40	124.76
9	E	609	Y26	O28-C16-N15	-2.46	118.76	123.09
9	C	609	Y26	C37-C29-N07	2.28	132.59	128.59
8	E	604	NAG	C1-C2-N2	2.22	113.93	110.43
8	C	604	NAG	C1-C2-N2	2.18	113.87	110.43
8	A	603	NAG	C1-C2-N2	2.17	113.85	110.43
8	C	604	NAG	C1-O5-C5	2.17	115.09	112.19
9	C	609	Y26	C30-C14-N15	-2.14	108.53	114.77
9	A	608	Y26	C30-C14-N15	-2.10	108.62	114.77
9	C	609	Y26	O28-C16-N15	-2.07	119.45	123.09
8	C	602	NAG	C1-O5-C5	2.07	114.95	112.19
9	C	609	Y26	C37-C29-C30	-2.06	119.22	121.93
8	C	606	NAG	C1-O5-C5	2.01	114.87	112.19

There are no chirality outliers.

All (87) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	608	Y26	O01-C02-N07-C29
9	A	608	Y26	O03-C02-N07-C29
9	A	608	Y26	C33-C34-N35-C36
9	C	609	Y26	O01-C02-N07-C08
9	C	609	Y26	O01-C02-N07-C29

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Mol	Chain	Res	Type	Atoms
9	C	609	Y26	O03-C02-N07-C08
9	C	609	Y26	O03-C02-N07-C29
9	C	609	Y26	C14-C08-C09-N10
9	C	609	Y26	C33-C34-N35-C36
9	E	609	Y26	O01-C02-N07-C08
9	E	609	Y26	O03-C02-N07-C08
9	E	609	Y26	C14-C08-C09-N10
9	E	609	Y26	C33-C34-N35-C36
8	C	602	NAG	C4-C5-C6-O6
8	A	602	NAG	O5-C5-C6-O6
8	C	601	NAG	O5-C5-C6-O6
8	C	602	NAG	O5-C5-C6-O6
8	C	605	NAG	C4-C5-C6-O6
8	A	601	NAG	O5-C5-C6-O6
8	D	702	NAG	O5-C5-C6-O6
8	A	605	NAG	O5-C5-C6-O6
8	A	602	NAG	C4-C5-C6-O6
8	C	601	NAG	C4-C5-C6-O6
8	D	701	NAG	O5-C5-C6-O6
8	C	604	NAG	O5-C5-C6-O6
8	C	605	NAG	O5-C5-C6-O6
8	E	606	NAG	O5-C5-C6-O6
8	D	702	NAG	C4-C5-C6-O6
8	C	604	NAG	C4-C5-C6-O6
8	E	606	NAG	C4-C5-C6-O6
8	C	607	NAG	O5-C5-C6-O6
8	A	601	NAG	C4-C5-C6-O6
8	A	603	NAG	C8-C7-N2-C2
8	A	603	NAG	O7-C7-N2-C2
8	C	602	NAG	C8-C7-N2-C2
8	C	602	NAG	O7-C7-N2-C2
8	C	604	NAG	C8-C7-N2-C2
8	C	604	NAG	O7-C7-N2-C2
8	E	602	NAG	C8-C7-N2-C2
8	E	602	NAG	O7-C7-N2-C2
8	E	604	NAG	C8-C7-N2-C2
8	E	604	NAG	O7-C7-N2-C2
8	E	605	NAG	O5-C5-C6-O6
8	A	606	NAG	O5-C5-C6-O6
8	E	601	NAG	O5-C5-C6-O6
9	E	609	Y26	N07-C02-O03-C04
8	D	701	NAG	C4-C5-C6-O6

*Continued on next page...*

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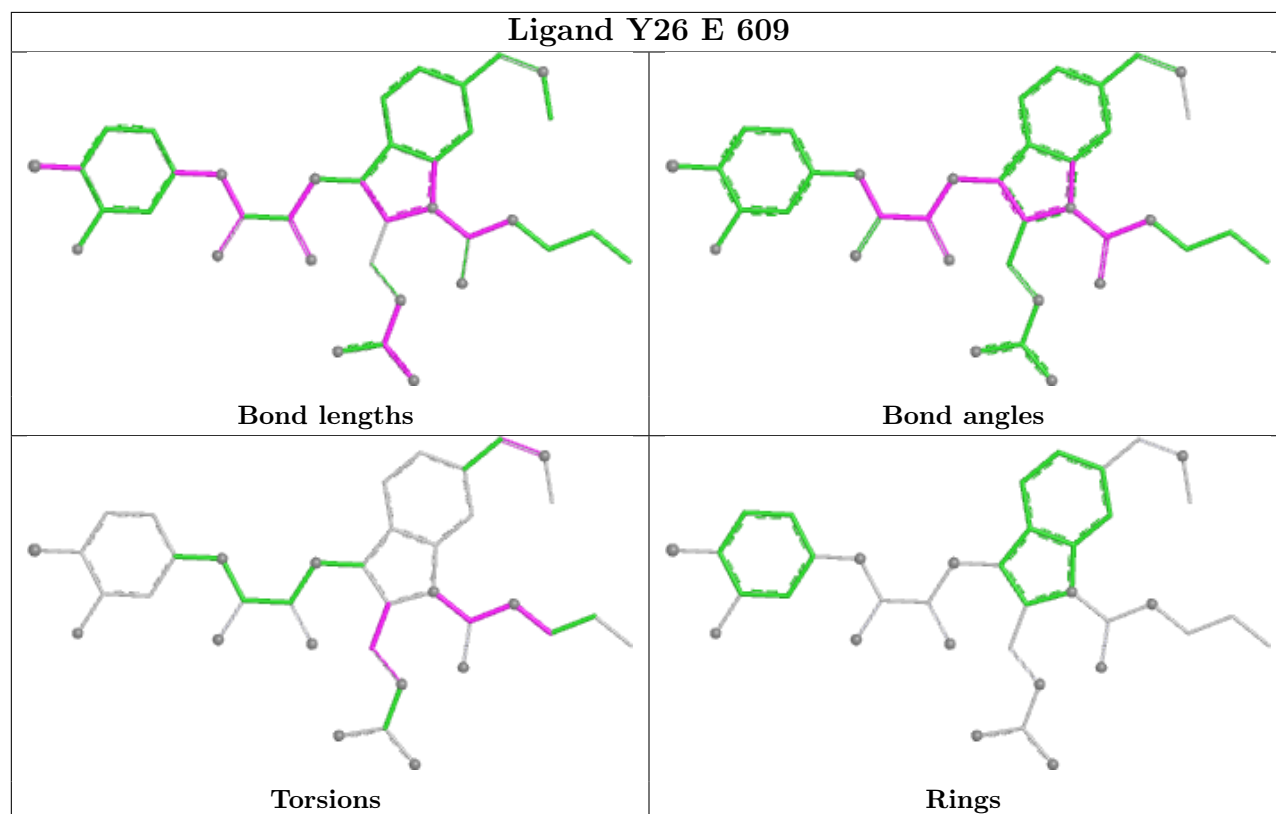
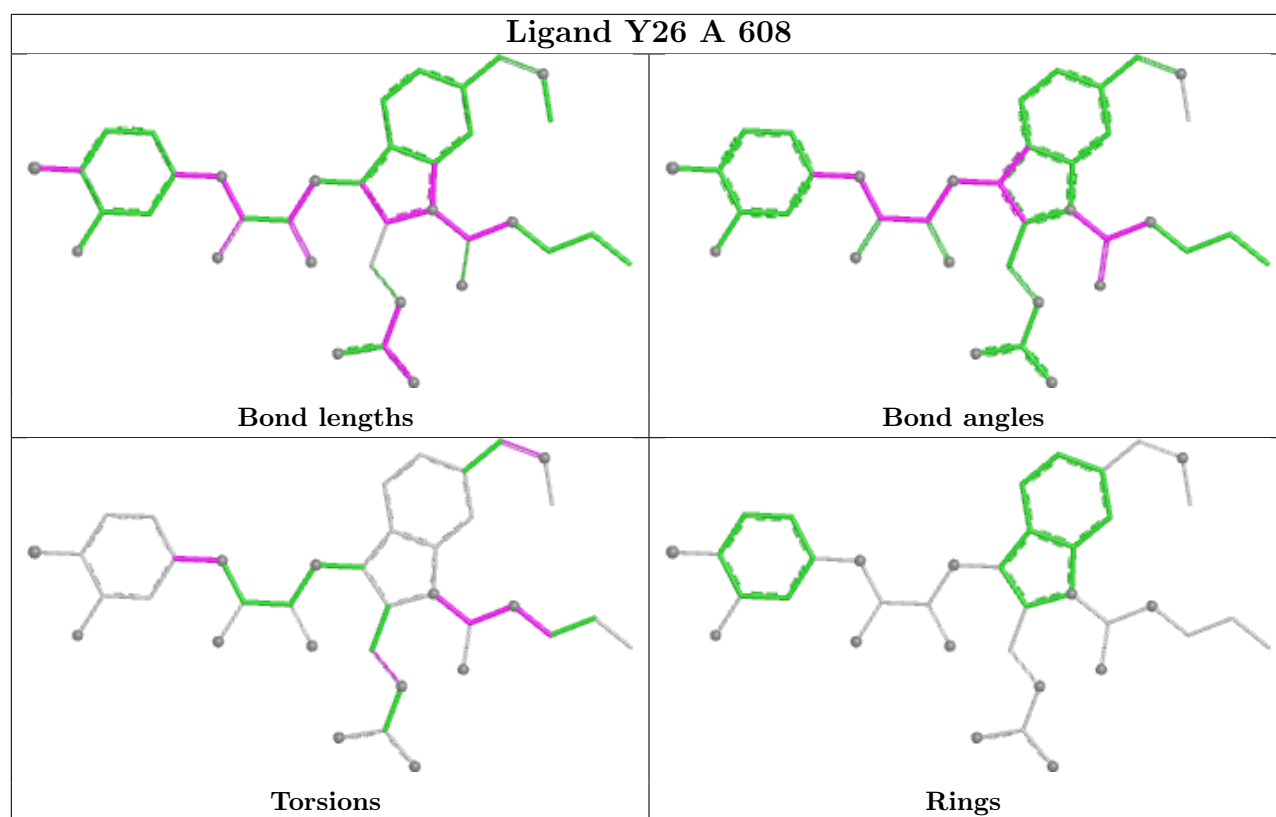
Mol	Chain	Res	Type	Atoms
8	A	605	NAG	C4-C5-C6-O6
8	E	607	NAG	O5-C5-C6-O6
9	E	609	Y26	O01-C02-O03-C04
8	B	701	NAG	O5-C5-C6-O6
9	E	609	Y26	O01-C02-N07-C29
9	E	609	Y26	O03-C02-N07-C29
8	E	603	NAG	O5-C5-C6-O6
9	A	608	Y26	O01-C02-N07-C08
9	A	608	Y26	O03-C02-N07-C08
9	C	609	Y26	N07-C08-C09-N10
9	C	609	Y26	C08-C09-N10-C11
9	A	608	Y26	C05-C04-O03-C02
9	C	609	Y26	C05-C04-O03-C02
9	E	609	Y26	C05-C04-O03-C02
8	E	601	NAG	C4-C5-C6-O6
8	A	606	NAG	C1-C2-N2-C7
8	C	605	NAG	C1-C2-N2-C7
8	E	605	NAG	C1-C2-N2-C7
9	E	609	Y26	C08-C09-N10-C11
8	E	605	NAG	C4-C5-C6-O6
8	A	604	NAG	C4-C5-C6-O6
9	A	608	Y26	C08-C09-N10-C11
8	A	603	NAG	C4-C5-C6-O6
9	A	608	Y26	N07-C02-O03-C04
8	A	606	NAG	C3-C2-N2-C7
8	C	604	NAG	C3-C2-N2-C7
8	C	605	NAG	C3-C2-N2-C7
8	E	605	NAG	C3-C2-N2-C7
9	E	609	Y26	N07-C08-C09-N10
8	C	607	NAG	C4-C5-C6-O6
9	A	608	Y26	O01-C02-O03-C04
8	A	606	NAG	C4-C5-C6-O6
8	A	603	NAG	C1-C2-N2-C7
8	C	604	NAG	C1-C2-N2-C7
8	E	604	NAG	C1-C2-N2-C7
8	A	603	NAG	C3-C2-N2-C7
8	E	604	NAG	C3-C2-N2-C7
9	A	608	Y26	C26-C19-N18-C17
9	A	608	Y26	C20-C19-N18-C17
8	A	604	NAG	O5-C5-C6-O6

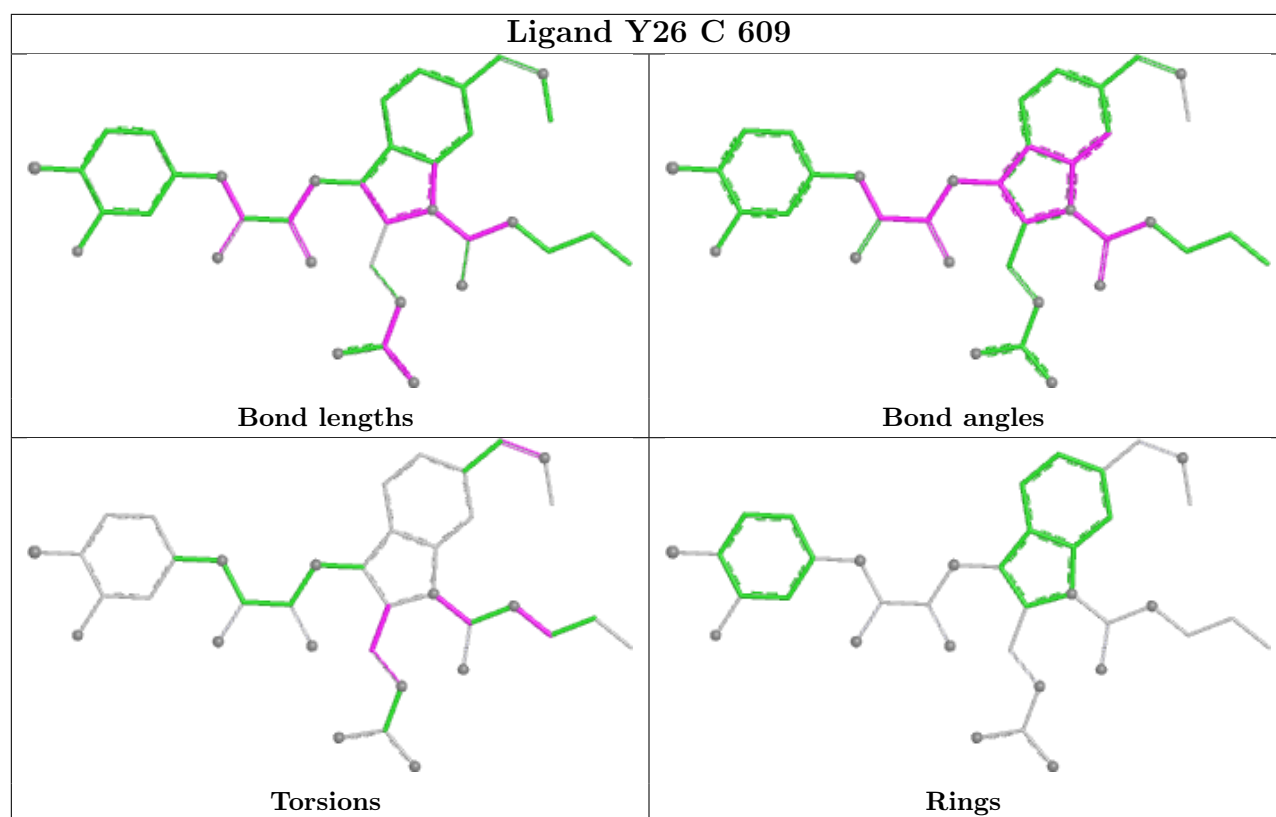
There are no ring outliers.

13 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	607	NAG	1	0
8	A	605	NAG	1	0
9	A	608	Y26	1	0
8	C	604	NAG	1	0
8	E	602	NAG	1	0
8	A	604	NAG	2	0
9	E	609	Y26	1	0
8	A	601	NAG	1	0
8	C	601	NAG	1	0
8	E	604	NAG	1	0
8	A	602	NAG	1	0
8	A	603	NAG	2	0
8	E	607	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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

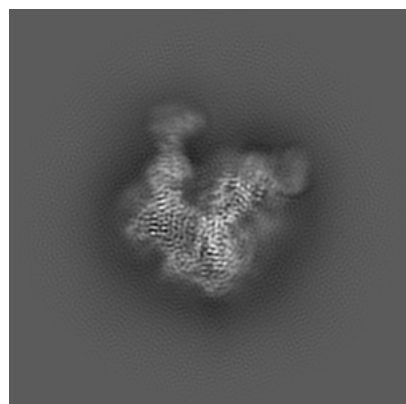
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45530. These allow visual inspection of the internal detail of the map and identification of artifacts.

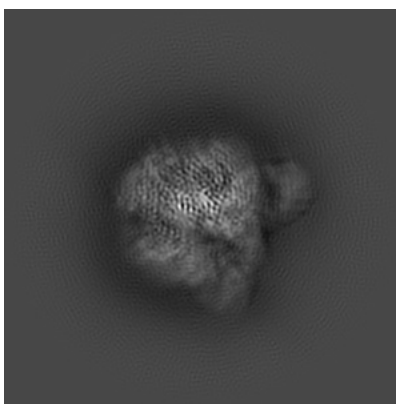
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

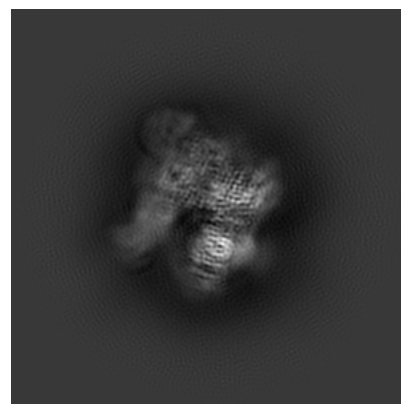
#### 6.1.1 Primary map



X

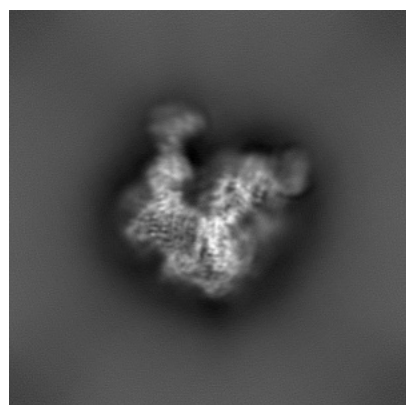


Y

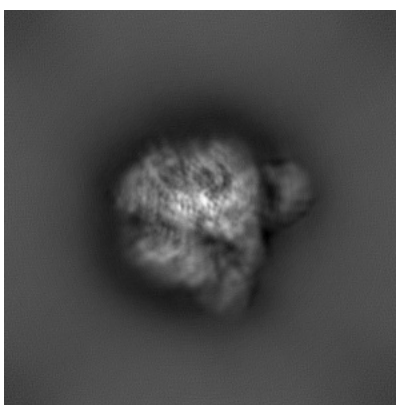


Z

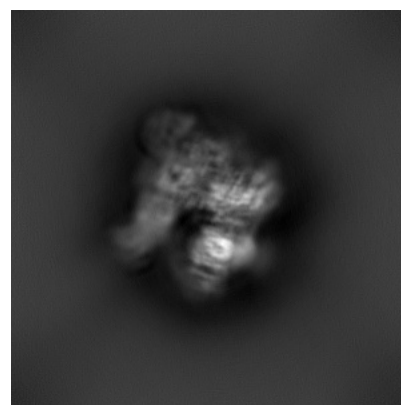
#### 6.1.2 Raw map



X



Y

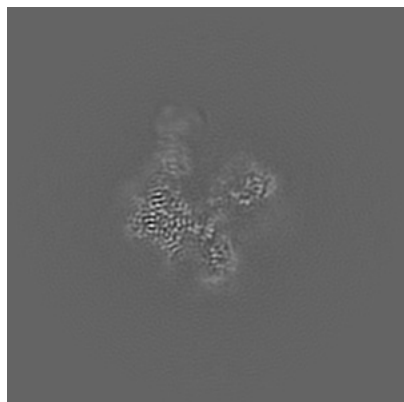


Z

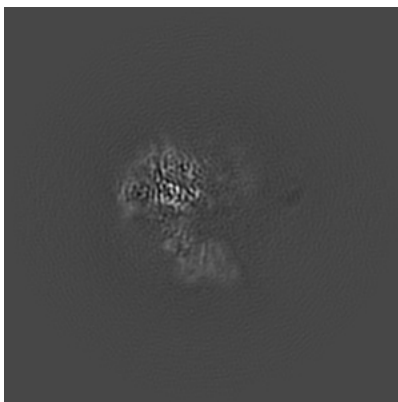
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

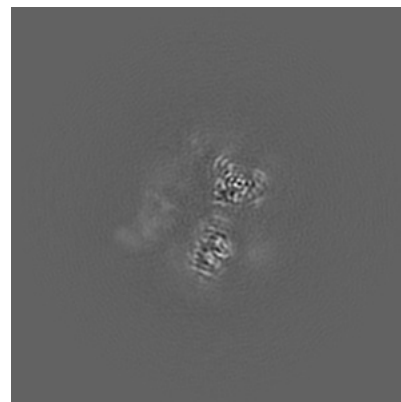
### 6.2.1 Primary map



X Index: 200

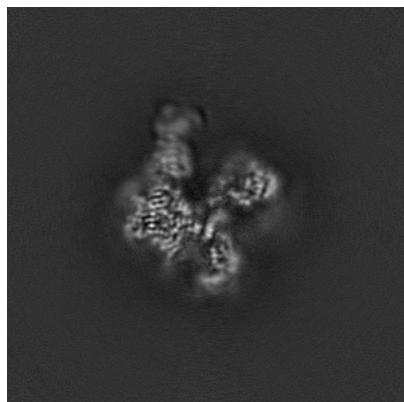


Y Index: 200

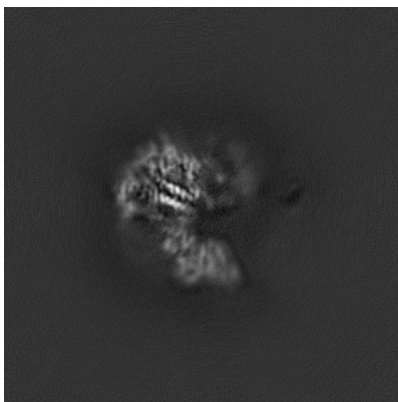


Z Index: 200

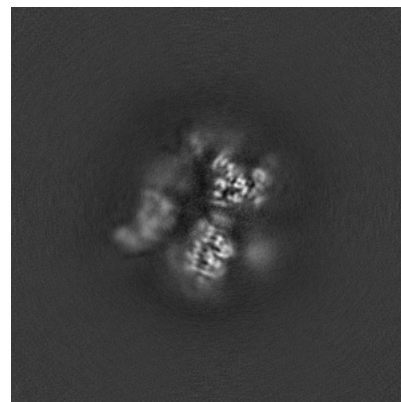
### 6.2.2 Raw map



X Index: 200



Y Index: 200



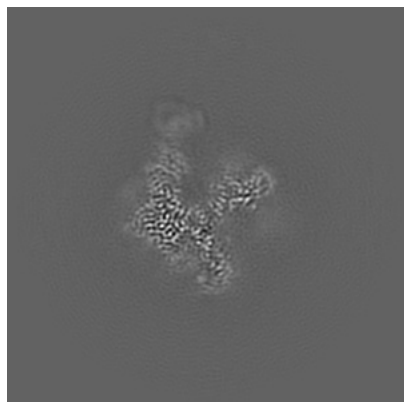
Z Index: 200

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

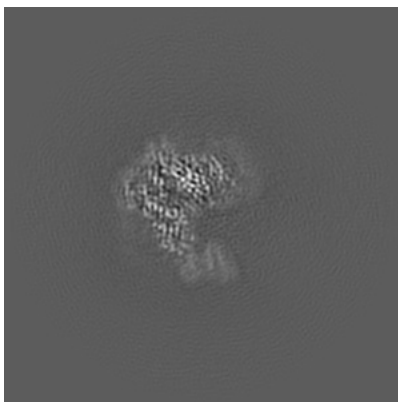


## 6.3 Largest variance slices [i](#)

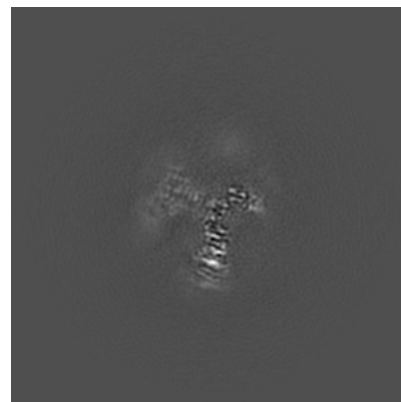
### 6.3.1 Primary map



X Index: 206

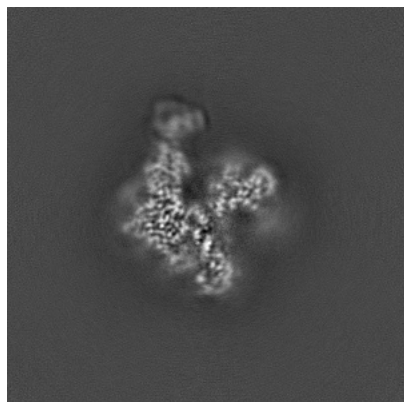


Y Index: 207

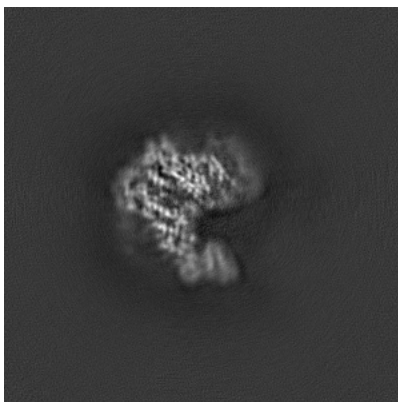


Z Index: 181

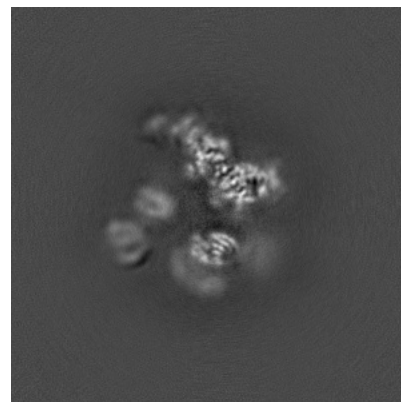
### 6.3.2 Raw map



X Index: 207



Y Index: 207

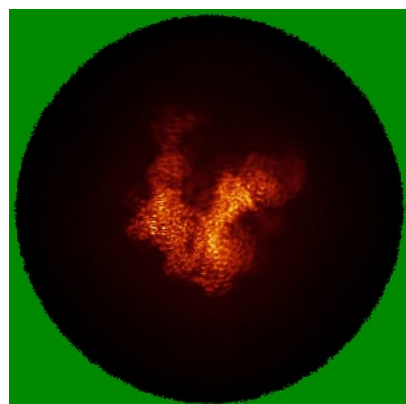


Z Index: 216

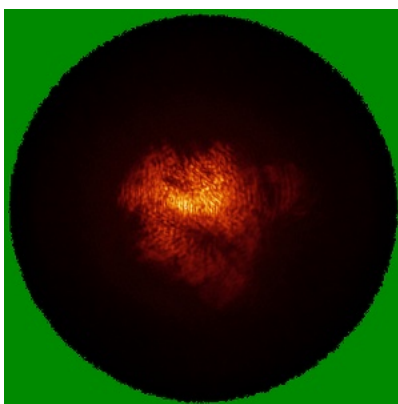
The images above show the largest variance slices of the map in three orthogonal directions.

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

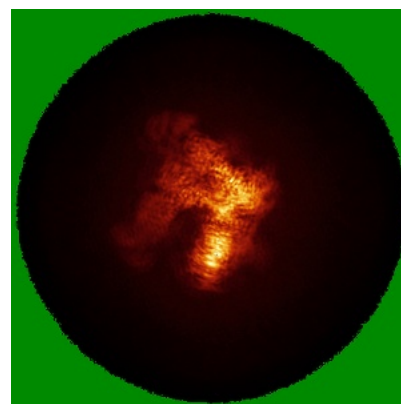
### 6.4.1 Primary map



X

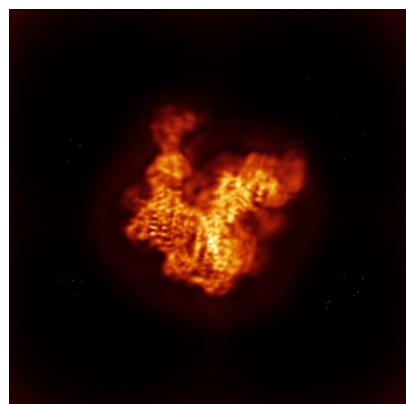


Y

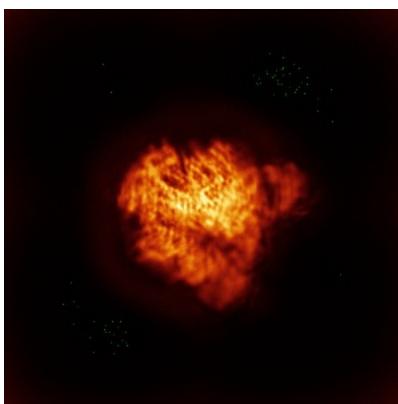


Z

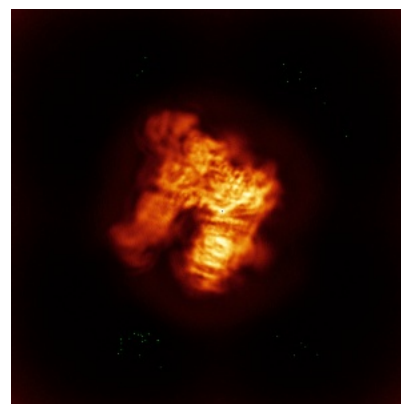
### 6.4.2 Raw map



X



Y

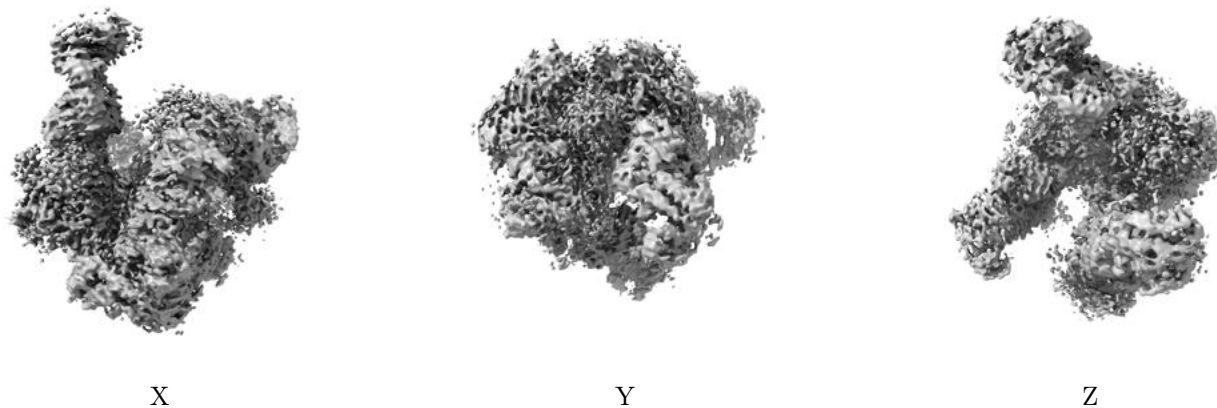


Z

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

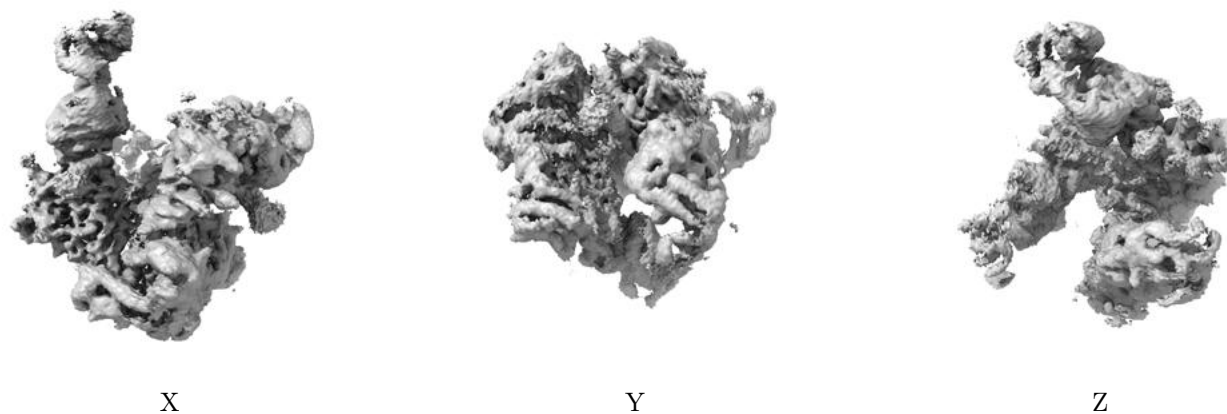
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0659. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

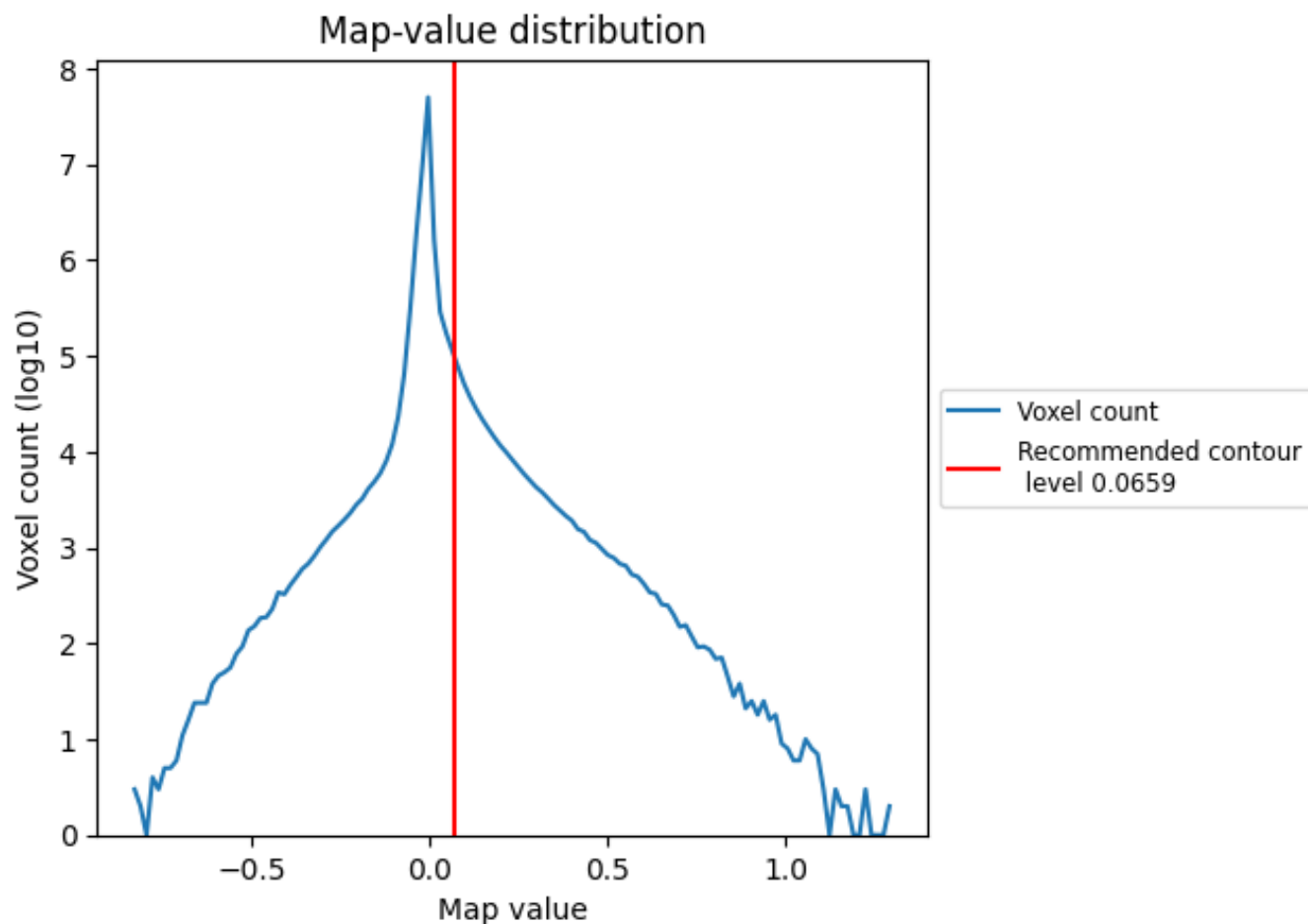
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

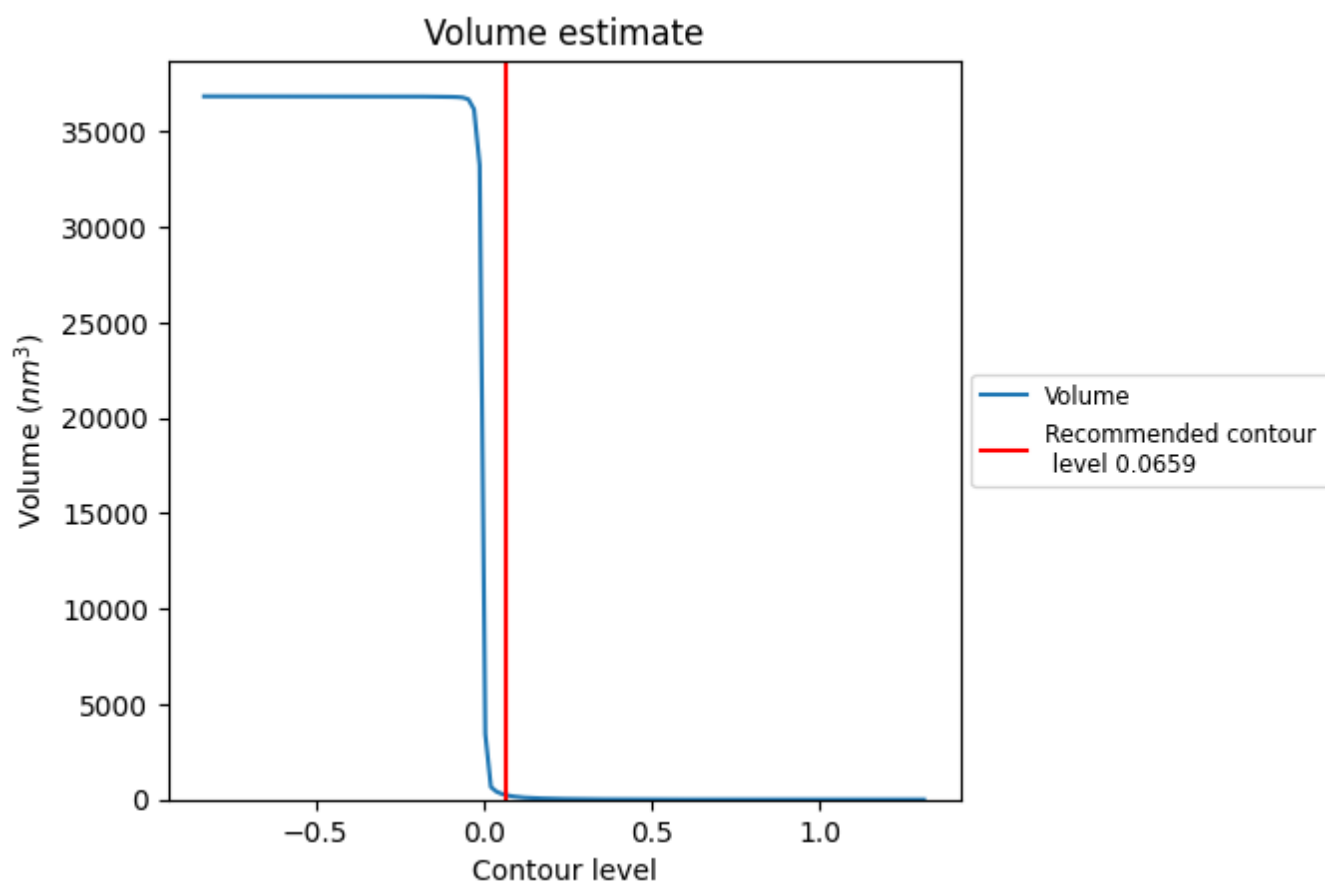
This section contains the results of statistical analysis of the map.

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



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

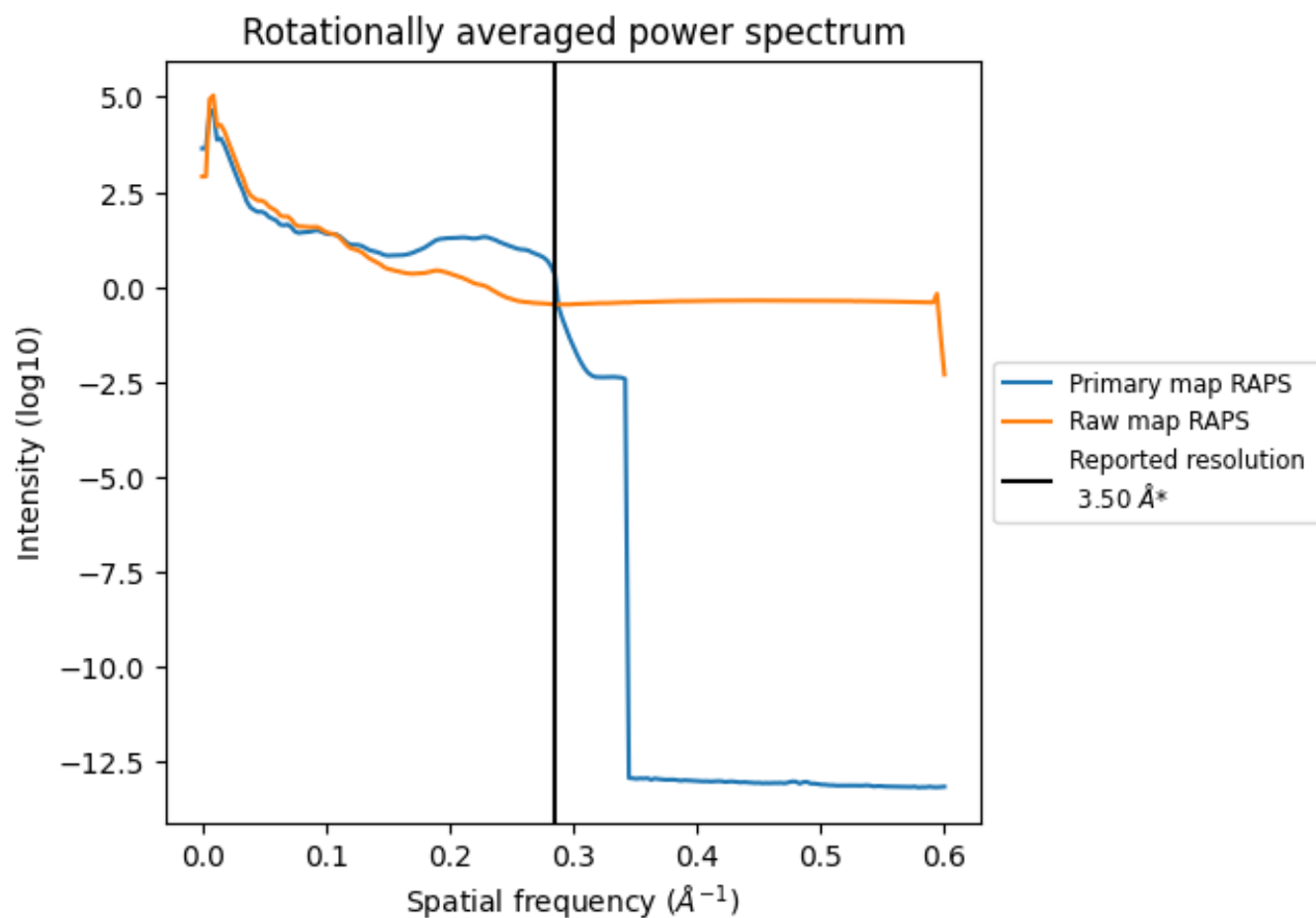
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 241 nm<sup>3</sup>; this corresponds to an approximate mass of 218 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 ⓘ

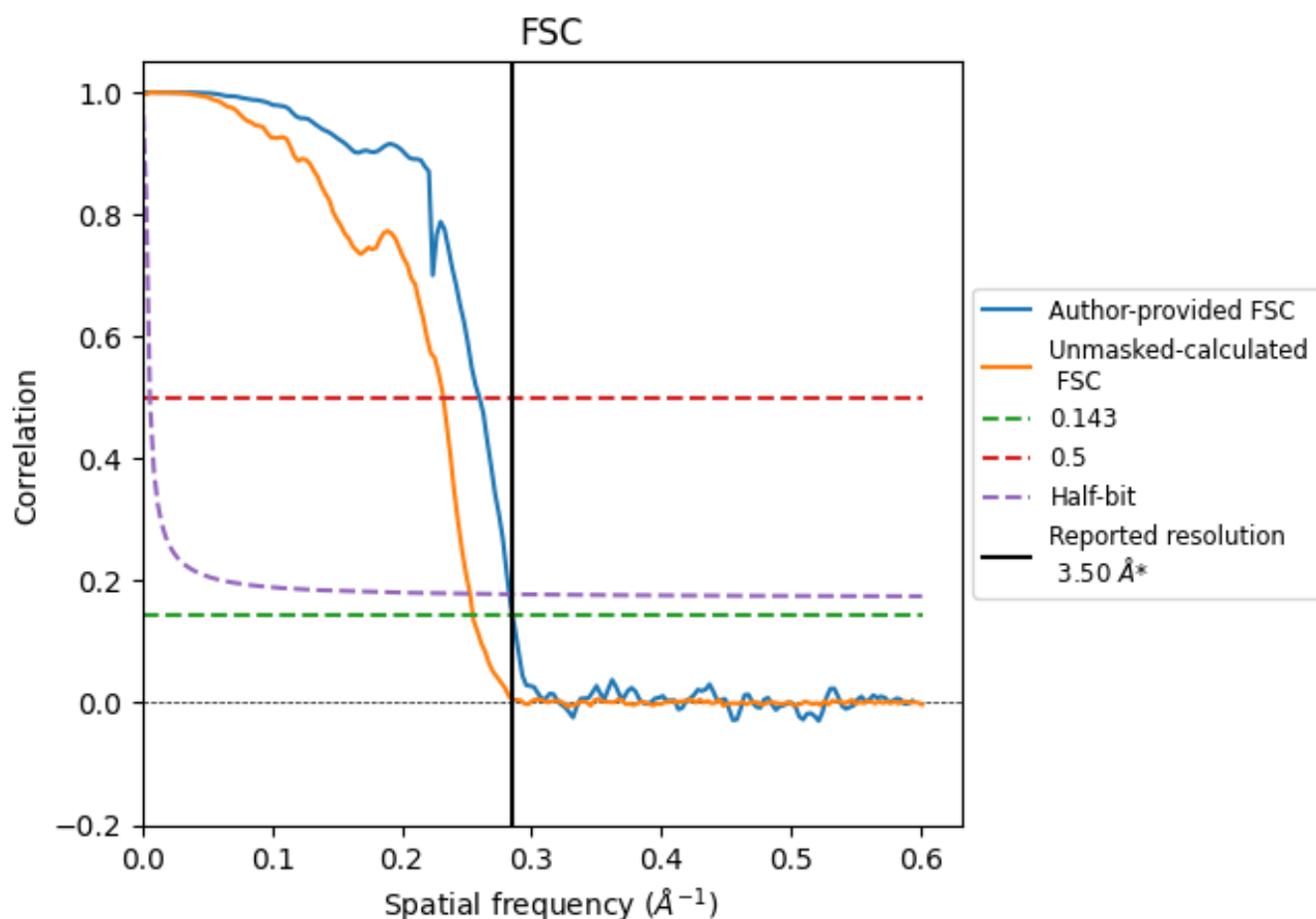


\*Reported resolution corresponds to spatial frequency of 0.286 Å<sup>-1</sup>

## 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 0.286 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.51	3.85	3.53
Unmasked-calculated*	3.92	4.31	3.96

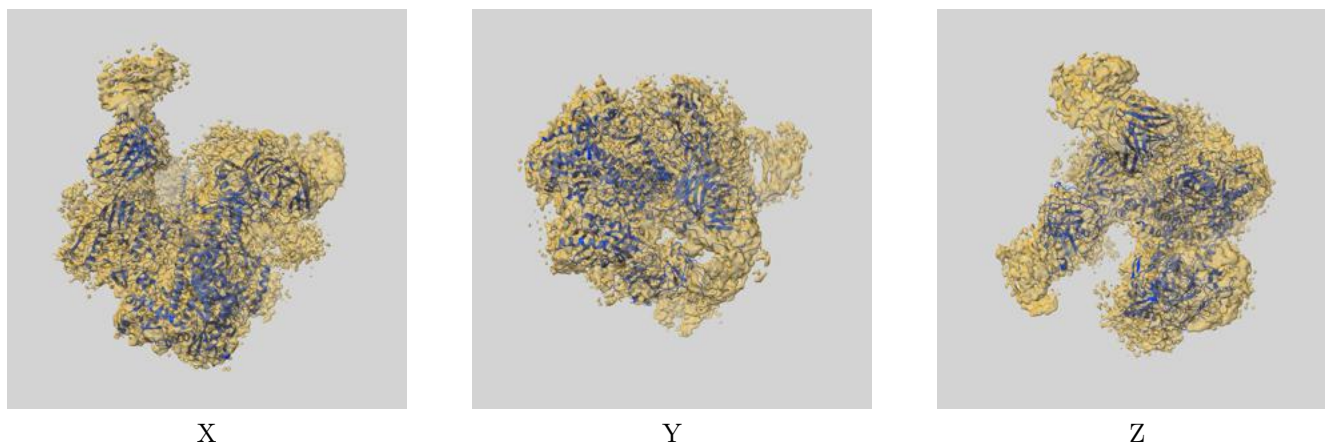
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.92 differs from the reported value 3.5 by more than 10 %



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

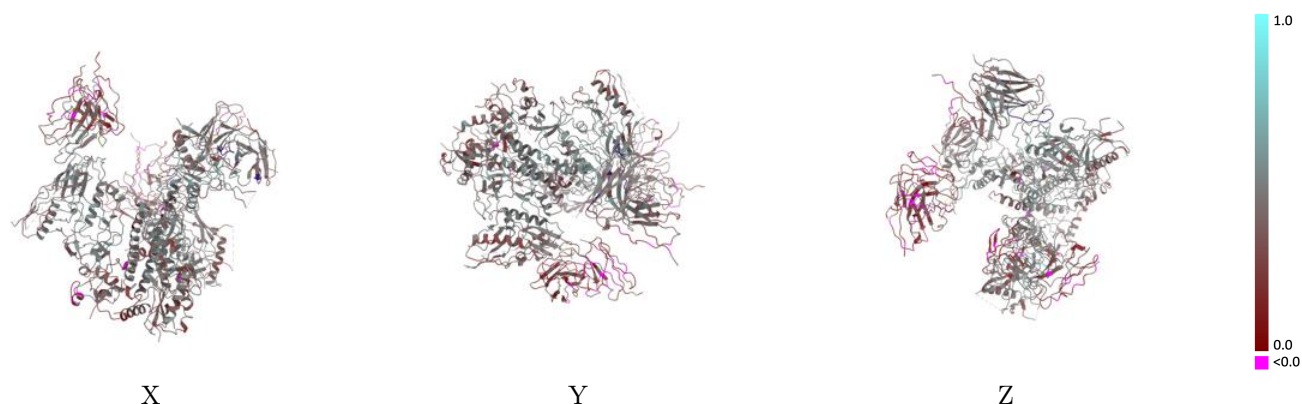
This section contains information regarding the fit between EMDB map EMD-45530 and PDB model 9CF5. Per-residue inclusion information can be found in section [3](#) on page [10](#).

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



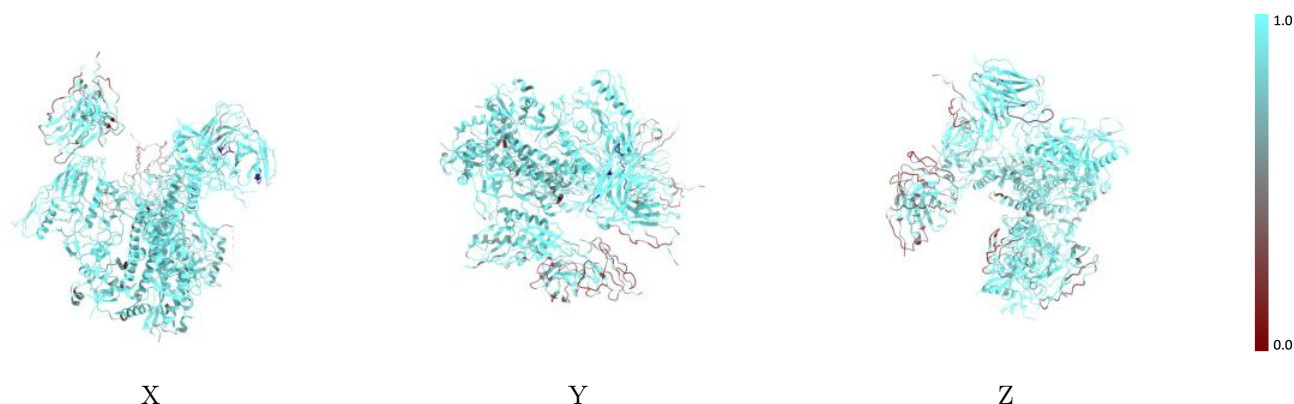
The images above show the 3D surface view of the map at the recommended contour level 0.0659 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



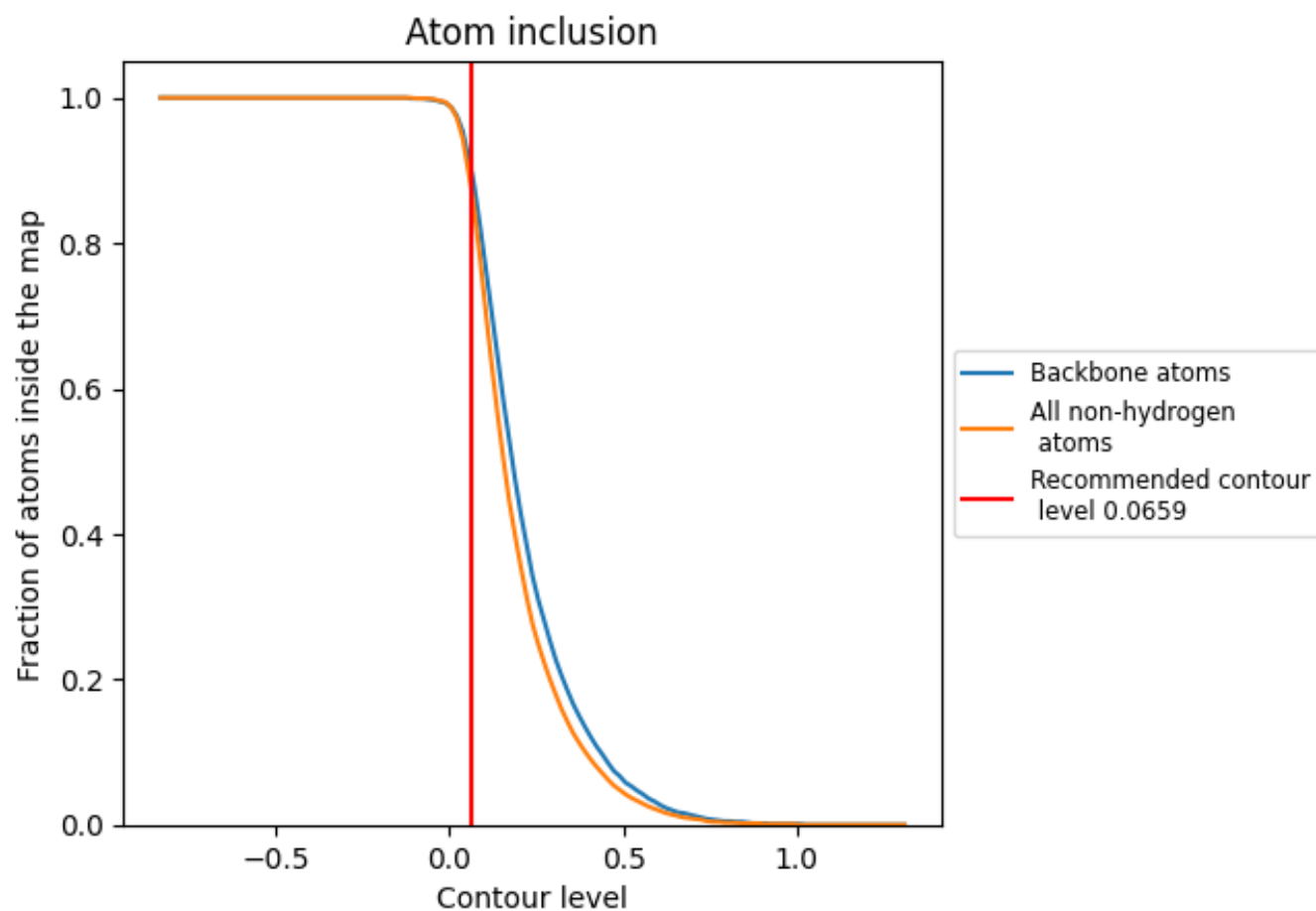
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0659).



















































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 87% 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 (0.0659) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8660	 0.4000
A	 0.8970	 0.4270
B	 0.8620	 0.4010
C	 0.9460	 0.4750
D	 0.9280	 0.4280
E	 0.9290	 0.4580
F	 0.8480	 0.3690
G	 0.7300	 0.2810
H	 0.8240	 0.3260
I	 0.8350	 0.3700
J	 0.9560	 0.4430
K	 0.5190	 0.2120
L	 0.7370	 0.2540
M	 0.5710	 0.2740
N	 0.8470	 0.4260
O	 0.9400	 0.4930
P	 0.4290	 0.0640
Q	 0.6790	 0.2640
R	 0.9640	 0.4160
S	 0.8190	 0.4010
T	 0.5710	 0.3050
U	 0.7860	 0.2710
V	 0.8570	 0.3620
W	 0.5000	 0.3430
X	 0.6790	 0.2850

