



Full wwPDB EM Validation Report ⓘ

Nov 18, 2024 – 12:29 PM JST

PDB ID : 8XZ9
EMDB ID : EMD-38790
Title : BA.2.86 Spike in complex with bovine ACE2 (bound 2 ACE2)
Authors : Yue, C.; Liu, P.
Deposited on : 2024-01-21
Resolution : 3.37 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

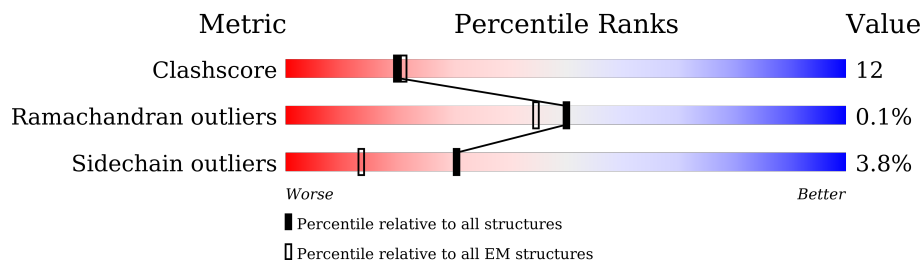
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.37 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.



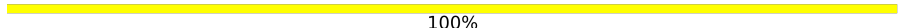
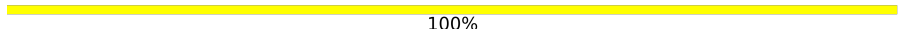

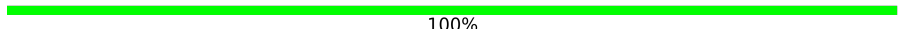
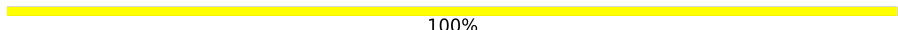
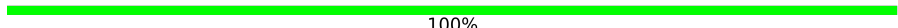


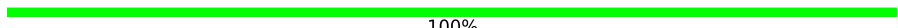

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	596	
1	E	596	
2	B	1120	
2	C	1120	
2	D	1120	
3	F	2	
3	G	2	
3	H	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	I	2	 100%
3	J	2	 100%
3	K	2	 50% 50%
3	M	2	 100%
3	N	2	 100%
3	O	2	 100%
3	P	2	 50% 50%
3	Q	2	 100%
3	R	2	 100%
4	L	2	 50% 50%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 35083 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 Processed angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	596	Total	C	N	O	S	0	0
			4906	3136	815	925	30		
1	E	595	Total	C	N	O	S	0	0
			4897	3131	814	922	30		

- Molecule 2 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1063	Total	C	N	O	S	0	0
			8320	5326	1383	1573	38		
2	C	1063	Total	C	N	O	S	0	0
			8316	5322	1383	1573	38		
2	D	1063	Total	C	N	O	S	0	0
			8316	5322	1383	1573	38		

There are 171 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	23	THR	-	expression tag	UNP P0DTC2
B	24	THR	-	expression tag	UNP P0DTC2
B	25	THR	-	expression tag	UNP P0DTC2
B	26	GLN	-	expression tag	UNP P0DTC2
B	27	SER	-	expression tag	UNP P0DTC2
B	50	LEU	SER	conflict	UNP P0DTC2
B	127	PHE	VAL	conflict	UNP P0DTC2
B	158	GLY	ARG	conflict	UNP P0DTC2
B	?	-	ASN	deletion	UNP P0DTC2
B	212	ILE	LEU	variant	UNP P0DTC2
B	213	GLY	VAL	variant	UNP P0DTC2
B	216	PHE	LEU	conflict	UNP P0DTC2
B	245	ASN	HIS	conflict	UNP P0DTC2
B	264	ASP	ALA	conflict	UNP P0DTC2
B	332	VAL	ILE	conflict	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	339	HIS	GLY	variant	UNP P0DTC2
B	356	THR	LYS	conflict	UNP P0DTC2
B	371	PHE	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	376	ALA	THR	variant	UNP P0DTC2
B	403	LYS	ARG	conflict	UNP P0DTC2
B	405	ASN	ASP	variant	UNP P0DTC2
B	408	SER	ARG	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	445	HIS	VAL	conflict	UNP P0DTC2
B	446	SER	GLY	variant	UNP P0DTC2
B	450	ASP	ASN	conflict	UNP P0DTC2
B	452	TRP	LEU	conflict	UNP P0DTC2
B	460	LYS	ASN	conflict	UNP P0DTC2
B	477	ASN	SER	conflict	UNP P0DTC2
B	478	LYS	THR	conflict	UNP P0DTC2
B	481	LYS	ASN	variant	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	484	LYS	GLU	variant	UNP P0DTC2
B	486	PRO	PHE	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	conflict	UNP P0DTC2
B	554	LYS	GLU	conflict	UNP P0DTC2
B	570	VAL	ALA	conflict	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	621	SER	PRO	conflict	UNP P0DTC2
B	655	TYR	HIS	variant	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	817	PRO	PHE	conflict	UNP P0DTC2
B	892	PRO	ALA	conflict	UNP P0DTC2
B	899	PRO	ALA	conflict	UNP P0DTC2
B	939	PHE	SER	conflict	UNP P0DTC2
B	942	PRO	ALA	conflict	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
B	986	PRO	LYS	variant	UNP P0DTC2
B	987	PRO	VAL	variant	UNP P0DTC2
B	1143	LEU	PRO	conflict	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	23	THR	-	expression tag	UNP P0DTC2
C	24	THR	-	expression tag	UNP P0DTC2
C	25	THR	-	expression tag	UNP P0DTC2
C	26	GLN	-	expression tag	UNP P0DTC2
C	27	SER	-	expression tag	UNP P0DTC2
C	50	LEU	SER	conflict	UNP P0DTC2
C	127	PHE	VAL	conflict	UNP P0DTC2
C	158	GLY	ARG	conflict	UNP P0DTC2
C	?	-	ASN	deletion	UNP P0DTC2
C	212	ILE	LEU	variant	UNP P0DTC2
C	213	GLY	VAL	variant	UNP P0DTC2
C	216	PHE	LEU	conflict	UNP P0DTC2
C	245	ASN	HIS	conflict	UNP P0DTC2
C	264	ASP	ALA	conflict	UNP P0DTC2
C	332	VAL	ILE	conflict	UNP P0DTC2
C	339	HIS	GLY	variant	UNP P0DTC2
C	356	THR	LYS	conflict	UNP P0DTC2
C	371	PHE	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	376	ALA	THR	variant	UNP P0DTC2
C	403	LYS	ARG	conflict	UNP P0DTC2
C	405	ASN	ASP	variant	UNP P0DTC2
C	408	SER	ARG	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	445	HIS	VAL	conflict	UNP P0DTC2
C	446	SER	GLY	variant	UNP P0DTC2
C	450	ASP	ASN	conflict	UNP P0DTC2
C	452	TRP	LEU	conflict	UNP P0DTC2
C	460	LYS	ASN	conflict	UNP P0DTC2
C	477	ASN	SER	conflict	UNP P0DTC2
C	478	LYS	THR	conflict	UNP P0DTC2
C	481	LYS	ASN	variant	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	484	LYS	GLU	variant	UNP P0DTC2
C	486	PRO	PHE	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	conflict	UNP P0DTC2
C	554	LYS	GLU	conflict	UNP P0DTC2
C	570	VAL	ALA	conflict	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	614	GLY	ASP	variant	UNP P0DTC2
C	621	SER	PRO	conflict	UNP P0DTC2
C	655	TYR	HIS	variant	UNP P0DTC2
C	764	LYS	ASN	variant	UNP P0DTC2
C	796	TYR	ASP	variant	UNP P0DTC2
C	817	PRO	PHE	conflict	UNP P0DTC2
C	892	PRO	ALA	conflict	UNP P0DTC2
C	899	PRO	ALA	conflict	UNP P0DTC2
C	939	PHE	SER	conflict	UNP P0DTC2
C	942	PRO	ALA	conflict	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	UNP P0DTC2
C	986	PRO	LYS	variant	UNP P0DTC2
C	987	PRO	VAL	variant	UNP P0DTC2
C	1143	LEU	PRO	conflict	UNP P0DTC2
D	23	THR	-	expression tag	UNP P0DTC2
D	24	THR	-	expression tag	UNP P0DTC2
D	25	THR	-	expression tag	UNP P0DTC2
D	26	GLN	-	expression tag	UNP P0DTC2
D	27	SER	-	expression tag	UNP P0DTC2
D	50	LEU	SER	conflict	UNP P0DTC2
D	127	PHE	VAL	conflict	UNP P0DTC2
D	158	GLY	ARG	conflict	UNP P0DTC2
D	?	-	ASN	deletion	UNP P0DTC2
D	212	ILE	LEU	variant	UNP P0DTC2
D	213	GLY	VAL	variant	UNP P0DTC2
D	216	PHE	LEU	conflict	UNP P0DTC2
D	245	ASN	HIS	conflict	UNP P0DTC2
D	264	ASP	ALA	conflict	UNP P0DTC2
D	332	VAL	ILE	conflict	UNP P0DTC2
D	339	HIS	GLY	variant	UNP P0DTC2
D	356	THR	LYS	conflict	UNP P0DTC2
D	371	PHE	SER	variant	UNP P0DTC2
D	373	PRO	SER	variant	UNP P0DTC2
D	375	PHE	SER	variant	UNP P0DTC2
D	376	ALA	THR	variant	UNP P0DTC2
D	403	LYS	ARG	conflict	UNP P0DTC2
D	405	ASN	ASP	variant	UNP P0DTC2
D	408	SER	ARG	variant	UNP P0DTC2
D	417	ASN	LYS	variant	UNP P0DTC2
D	440	LYS	ASN	variant	UNP P0DTC2
D	445	HIS	VAL	conflict	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	446	SER	GLY	variant	UNP P0DTC2
D	450	ASP	ASN	conflict	UNP P0DTC2
D	452	TRP	LEU	conflict	UNP P0DTC2
D	460	LYS	ASN	conflict	UNP P0DTC2
D	477	ASN	SER	conflict	UNP P0DTC2
D	478	LYS	THR	conflict	UNP P0DTC2
D	481	LYS	ASN	variant	UNP P0DTC2
D	?	-	VAL	deletion	UNP P0DTC2
D	484	LYS	GLU	variant	UNP P0DTC2
D	486	PRO	PHE	variant	UNP P0DTC2
D	498	ARG	GLN	variant	UNP P0DTC2
D	501	TYR	ASN	variant	UNP P0DTC2
D	505	HIS	TYR	conflict	UNP P0DTC2
D	554	LYS	GLU	conflict	UNP P0DTC2
D	570	VAL	ALA	conflict	UNP P0DTC2
D	614	GLY	ASP	variant	UNP P0DTC2
D	621	SER	PRO	conflict	UNP P0DTC2
D	655	TYR	HIS	variant	UNP P0DTC2
D	764	LYS	ASN	variant	UNP P0DTC2
D	796	TYR	ASP	variant	UNP P0DTC2
D	817	PRO	PHE	conflict	UNP P0DTC2
D	892	PRO	ALA	conflict	UNP P0DTC2
D	899	PRO	ALA	conflict	UNP P0DTC2
D	939	PHE	SER	conflict	UNP P0DTC2
D	942	PRO	ALA	conflict	UNP P0DTC2
D	954	HIS	GLN	variant	UNP P0DTC2
D	969	LYS	ASN	variant	UNP P0DTC2
D	986	PRO	LYS	variant	UNP P0DTC2
D	987	PRO	VAL	variant	UNP P0DTC2
D	1143	LEU	PRO	conflict	UNP P0DTC2

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



Mol	Chain	Residues	Atoms			AltConf	Trace	
			Total	C	N			O
3	F	2	25	14	1	10	0	0

Continued on next page...

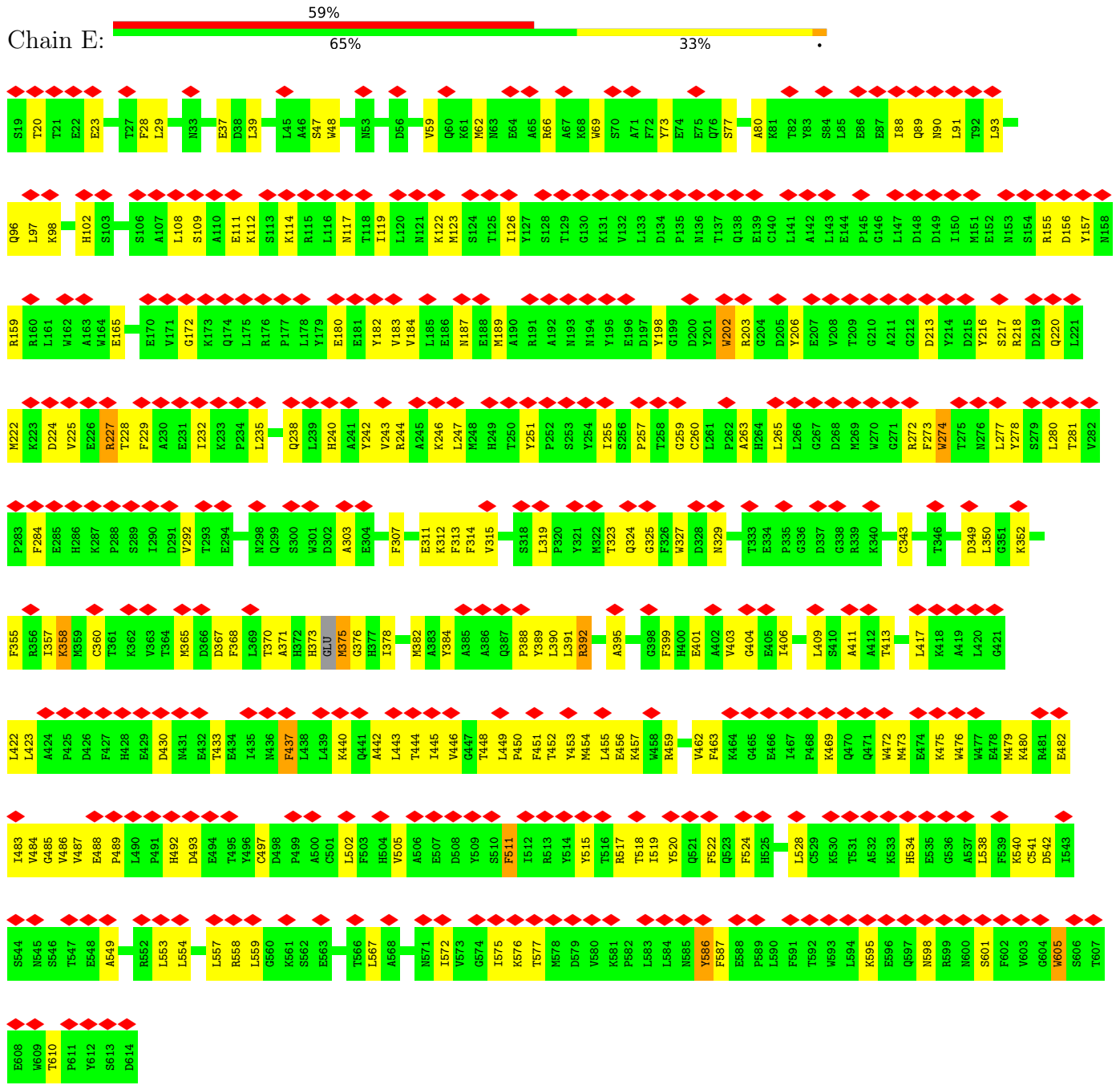
Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	H	2	25	14	1	10	0	0
3	I	2	25	14	1	10	0	0
3	J	2	25	14	1	10	0	0
3	K	2	25	14	1	10	0	0
3	M	2	25	14	1	10	0	0
3	N	2	25	14	1	10	0	0
3	O	2	25	14	1	10	0	0
3	P	2	25	14	1	10	0	0
3	Q	2	25	14	1	10	0	0
3	R	2	25	14	1	10	0	0
3	G	2	25	14	1	10	0	0

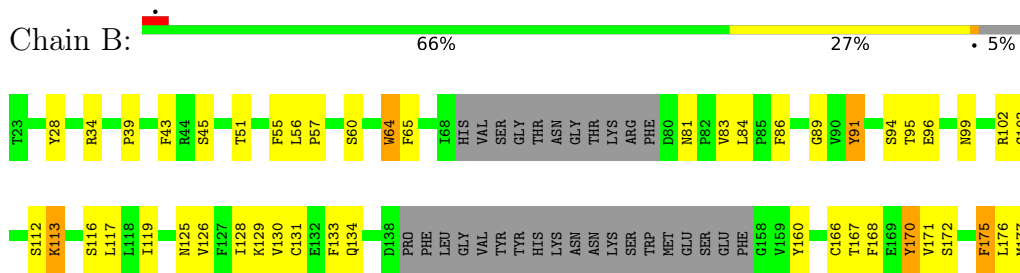
- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

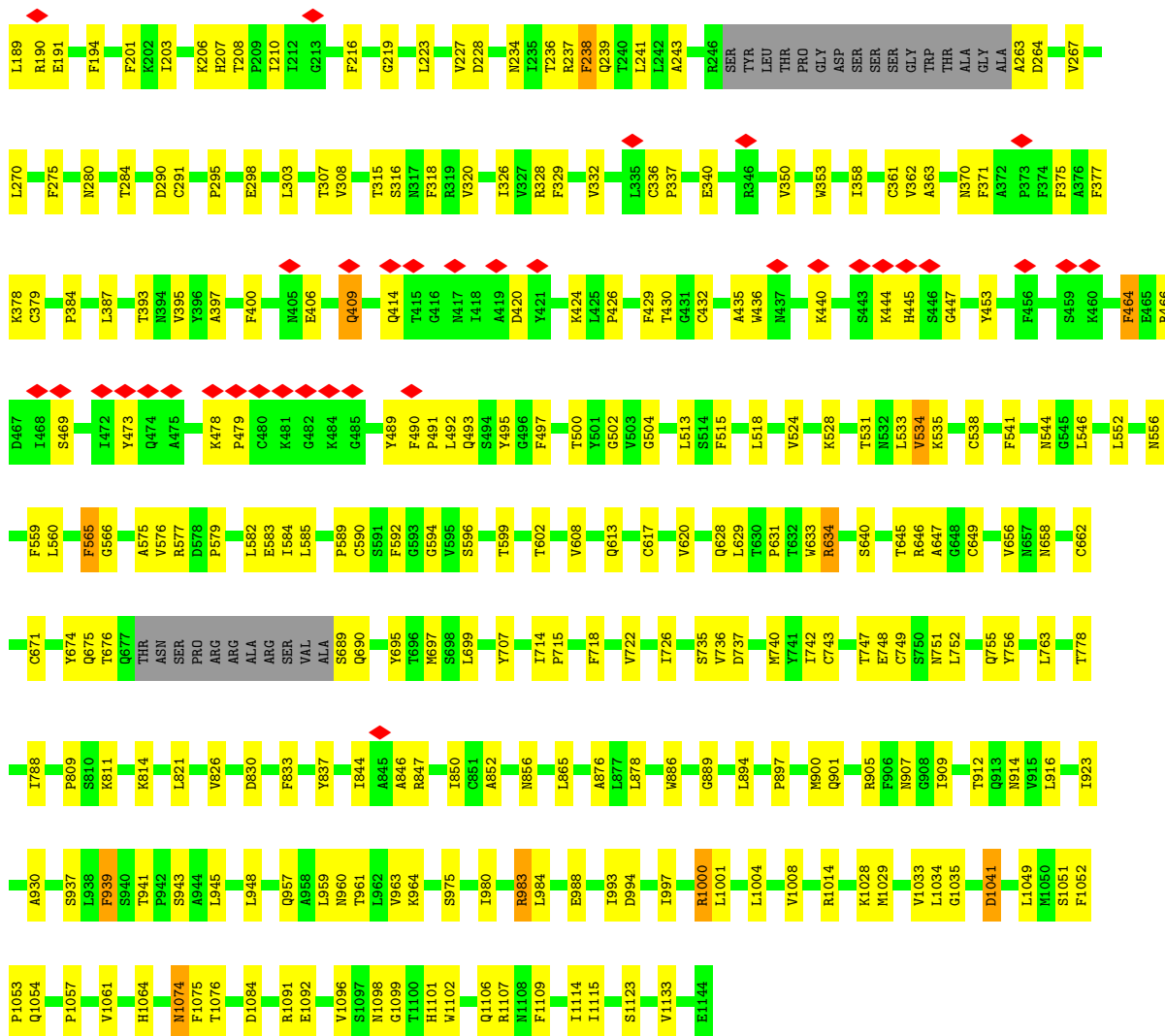


Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	L	2	28	16	2	10	0	0

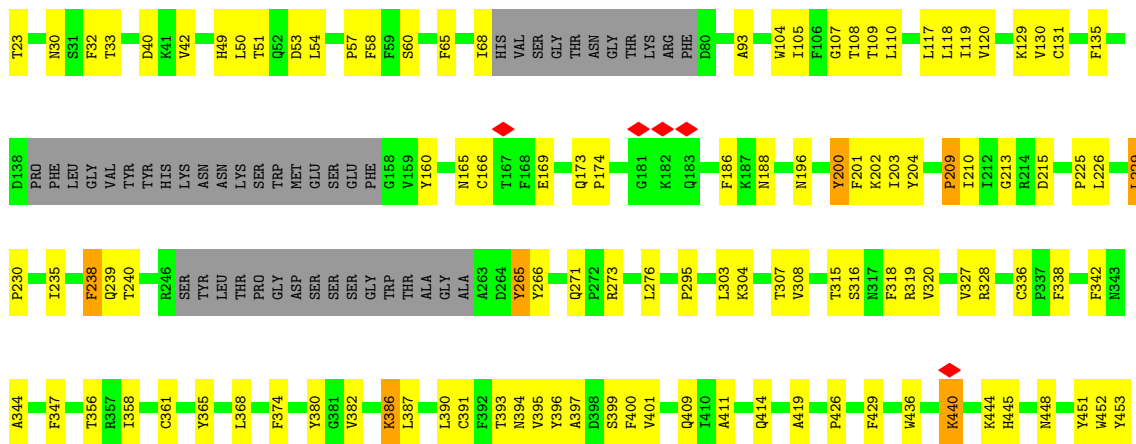


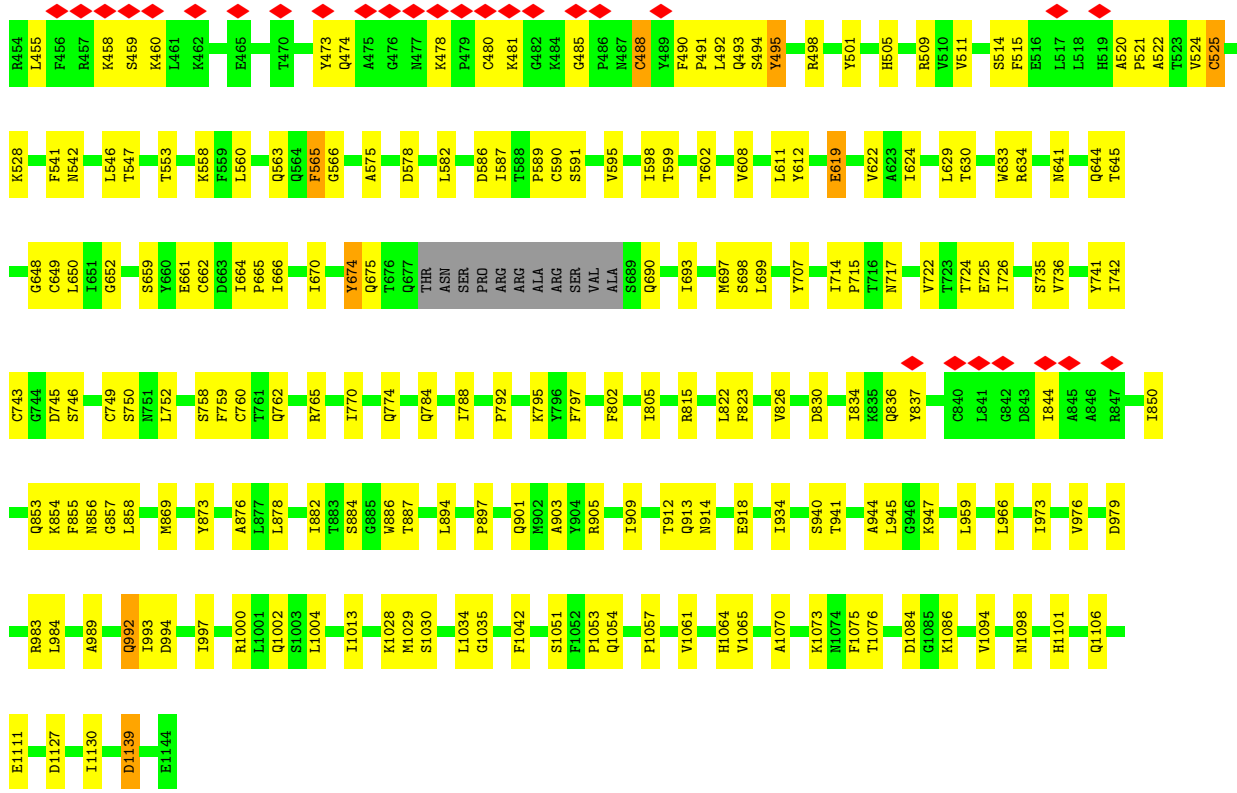
• Molecule 2: Spike glycoprotein



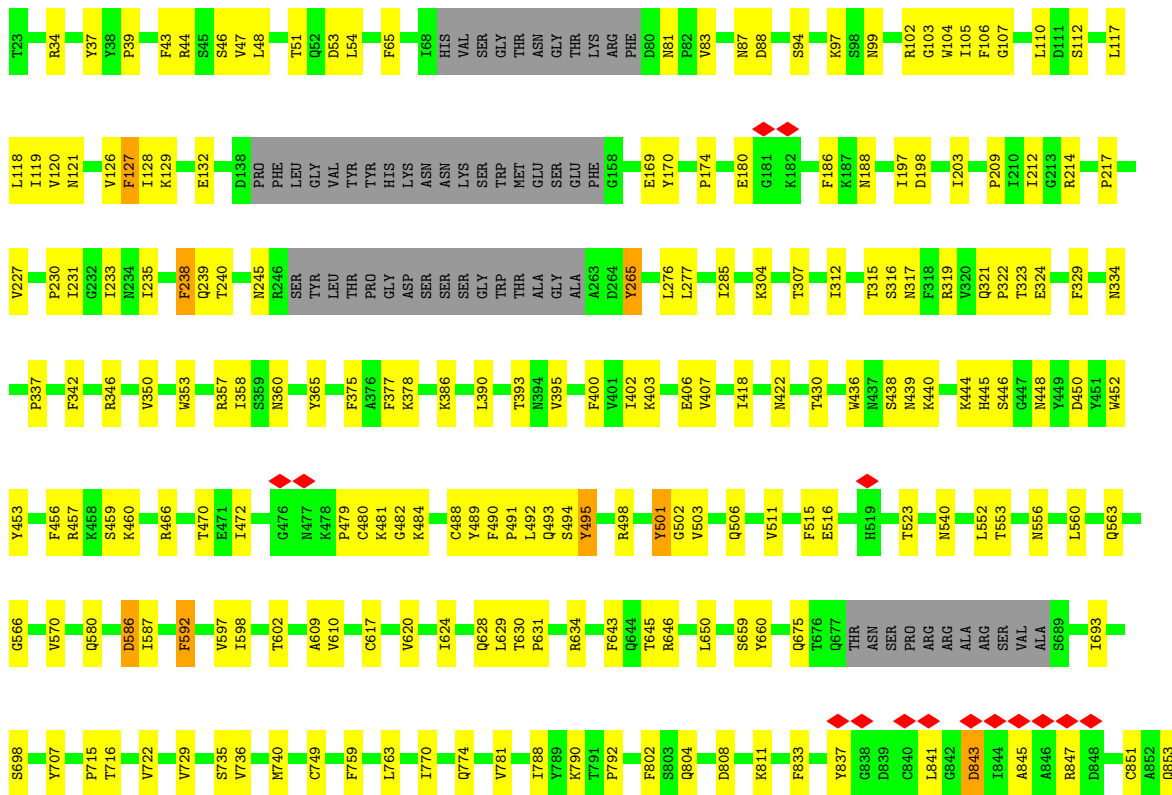


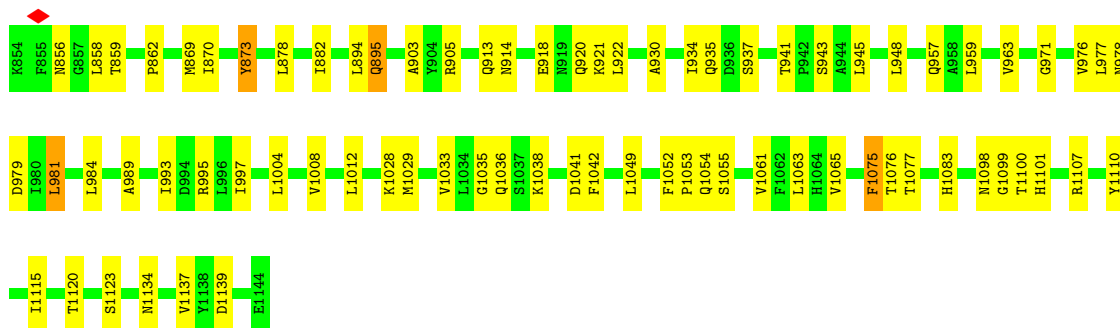
• Molecule 2: Spike glycoprotein





• Molecule 2: Spike glycoprotein





- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 100%

MAG1
BMA2

- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H: 100%

MAG1
BMA2

- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I: 100%

MAG1
BMA2

- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J: 100%

MAG1
BMA2

- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K: 50% 50%

MAG1
BMA2

- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M: 100%

MAG1
BMA2

- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  100%

NA1
NA2

- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  100%

NA1
NA2

- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:  50% 50%

NA1
NA2

- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:  100%

NA1
NA2

- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:  100%

NA1
NA2

- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  100%

NA1
NA2

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

Chain L:  50% 50%

NA1
NA2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	5828	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.398	Depositor
Minimum map value	-1.098	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.066	Depositor
Recommended contour level	0.2	Depositor
Map size (\AA)	360.0, 360.0, 360.0	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.0, 1.0, 1.0	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, 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	0.25	0/5043	0.49	0/6838
1	E	0.25	0/5033	0.49	0/6823
2	B	0.26	0/8520	0.49	0/11597
2	C	0.26	0/8516	0.47	1/11591 (0.0%)
2	D	0.26	0/8516	0.47	0/11591
All	All	0.26	0/35628	0.48	1/48440 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	209	PRO	CA-N-CD	-5.37	103.99	111.50

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	4906	0	4696	139	0
1	E	4897	0	4689	143	0
2	B	8320	0	8123	211	0
2	C	8316	0	8116	209	0
2	D	8316	0	8114	190	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	25	0	22	0	0
3	G	25	0	22	0	0
3	H	25	0	22	0	0
3	I	25	0	22	1	0
3	J	25	0	22	0	0
3	K	25	0	22	1	0
3	M	25	0	22	0	0
3	N	25	0	22	1	0
3	O	25	0	22	0	0
3	P	25	0	22	0	0
3	Q	25	0	22	0	0
3	R	25	0	22	0	0
4	L	28	0	25	1	0
All	All	35083	0	34027	842	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 12.

All (842) 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:C:886:TRP:HB3	2:C:1035:GLY:HA2	1.64	0.78
2:C:474:GLN:NE2	2:C:478:LYS:O	2.17	0.77
1:E:475:LYS:NZ	1:E:479:MET:SD	2.58	0.77
2:B:126:VAL:HG23	2:B:172:SER:H	1.52	0.75
1:A:450:PRO:HB3	1:A:484:VAL:HG21	1.67	0.75
1:E:274:TRP:HB3	1:E:443:LEU:HD22	1.69	0.74
1:A:528:LEU:HB3	1:A:543:ILE:HG21	1.69	0.73
1:E:232:ILE:HG13	1:E:235:LEU:HD12	1.70	0.73
2:D:472:ILE:HG13	2:D:482:GLY:H	1.54	0.73
2:C:391:CYS:HA	2:C:525:CYS:HB3	1.70	0.73
1:A:401:GLU:HB3	1:A:517:ARG:HD2	1.70	0.72
1:A:96:GLN:HG2	1:A:391:LEU:HD11	1.69	0.72
2:B:336:CYS:H	2:B:362:VAL:HG22	1.53	0.72
2:C:173:GLN:HG3	2:C:174:PRO:HD2	1.71	0.72
2:B:206:LYS:HB2	2:B:223:LEU:HA	1.72	0.71
2:C:361:CYS:H	2:C:524:VAL:HG22	1.55	0.71
2:D:984:LEU:HB3	2:D:989:ALA:HB2	1.73	0.71
2:B:189:LEU:HD21	2:B:210:ILE:HG12	1.71	0.71
2:D:976:VAL:HG13	2:D:979:ASP:HB2	1.72	0.71
1:A:203:ARG:HH12	1:A:222:MET:HB2	1.55	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:203:ARG:HH21	1:E:220:GLN:HE21	1.39	0.71
2:D:128:ILE:HB	2:D:170:TYR:HB3	1.74	0.70
1:E:480:LYS:HE3	1:E:486:VAL:HB	1.71	0.70
1:E:88:ILE:HD11	1:E:93:LEU:HB3	1.72	0.70
2:D:895:GLN:H	2:D:895:GLN:HE21	1.39	0.70
2:B:379:CYS:HB3	2:B:432:CYS:HA	1.74	0.69
2:B:112:SER:H	2:B:134:GLN:HE22	1.37	0.69
2:B:350:VAL:HG12	2:B:400:PHE:HD2	1.57	0.69
1:E:39:LEU:HD21	1:E:69:TRP:HA	1.75	0.69
2:C:830:ASP:OD2	2:C:853:GLN:NE2	2.26	0.69
1:E:473:MET:HA	1:E:476:TRP:HB2	1.73	0.68
2:D:126:VAL:HG13	2:D:174:PRO:HA	1.75	0.68
1:A:331:MET:HE2	1:A:335:PRO:HD3	1.74	0.68
2:B:94:SER:HB3	2:B:190:ARG:HB2	1.75	0.68
3:I:1:NAG:H62	3:I:2:BMA:H2	1.76	0.68
2:D:107:GLY:H	2:D:235:ILE:HG23	1.60	0.67
2:B:900:MET:SD	2:D:1077:THR:OG1	2.51	0.67
1:A:75:GLU:HG2	1:A:78:ARG:HH21	1.59	0.67
1:E:180:GLU:O	1:E:184:VAL:HG23	1.95	0.67
1:A:214:TYR:HE2	1:A:564:PRO:HG2	1.60	0.66
2:D:498:ARG:H	2:D:501:TYR:HE1	1.42	0.66
1:E:213:ASP:O	1:E:576:LYS:NZ	2.29	0.66
2:C:108:THR:HG22	2:C:109:THR:HG23	1.77	0.66
1:A:58:ASN:O	1:A:62:MET:HG3	1.95	0.66
1:E:376:GLY:HA3	1:E:404:GLY:HA2	1.78	0.66
1:A:552:ARG:NH1	1:A:572:ILE:O	2.29	0.66
2:C:65:PHE:HB2	2:C:265:TYR:HB3	1.77	0.66
2:B:886:TRP:HB3	2:B:1035:GLY:HA2	1.76	0.66
2:B:393:THR:HB	2:B:518:LEU:HD23	1.78	0.66
2:B:361:CYS:H	2:B:524:VAL:HG22	1.58	0.65
2:D:439:ASN:ND2	2:D:506:GLN:OE1	2.29	0.65
1:A:217:SER:OG	1:A:219:ASP:OD1	2.15	0.65
2:C:724:THR:HB	2:C:934:ILE:HD11	1.77	0.65
1:A:300:SER:O	1:A:305:ARG:NH2	2.28	0.65
1:A:369:LEU:HG	1:A:408:SER:HB3	1.78	0.65
2:B:39:PRO:HG2	2:B:51:THR:HG21	1.78	0.65
2:B:320:VAL:HG13	2:B:628:GLN:HG3	1.78	0.65
2:B:656:VAL:HG23	2:B:695:TYR:HB3	1.78	0.65
1:A:141:LEU:HD21	1:A:147:LEU:HB2	1.79	0.64
1:A:203:ARG:HD2	1:A:218:ARG:HB3	1.79	0.64
1:A:519:ILE:HG23	1:A:520:TYR:HD1	1.63	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:125:ASN:HB3	2:B:171:VAL:HB	1.79	0.64
2:D:323:THR:OG1	2:D:324:GLU:OE1	2.16	0.64
1:A:473:MET:HE3	1:A:473:MET:HA	1.79	0.64
1:E:388:PRO:HD2	1:E:391:LEU:HD12	1.78	0.64
2:B:689:SER:OG	2:B:690:GLN:N	2.30	0.64
2:C:319:ARG:HD3	2:D:740:MET:HE1	1.80	0.64
1:E:449:LEU:HD21	1:E:518:THR:HG21	1.79	0.64
2:B:552:LEU:HD12	2:B:585:LEU:HD13	1.80	0.64
2:C:973:ILE:HD12	2:C:983:ARG:HH21	1.63	0.64
2:B:328:ARG:NH1	2:B:531:THR:O	2.30	0.63
2:B:236:THR:HG1	4:L:1:NAG:HO3	1.45	0.63
2:D:334:ASN:ND2	2:D:360:ASN:O	2.30	0.63
2:B:577:ARG:HD3	2:B:582:LEU:HD13	1.81	0.63
2:C:547:THR:HB	2:D:978:ASN:HD21	1.64	0.63
1:E:479:MET:HA	1:E:482:GLU:HG2	1.80	0.63
1:A:403:VAL:HA	1:A:406:ILE:HG12	1.81	0.63
2:B:303:LEU:HD12	2:B:308:VAL:HG12	1.80	0.63
2:B:699:LEU:HD21	2:C:869:MET:HB3	1.82	0.62
2:B:384:PRO:HD2	2:D:456:PHE:HZ	1.63	0.62
2:D:34:ARG:NH2	2:D:217:PRO:O	2.31	0.62
2:D:103:GLY:HA3	2:D:120:VAL:HA	1.81	0.62
1:A:395:ALA:HB3	1:A:399:PHE:HE2	1.64	0.62
2:C:1098:ASN:OD1	2:C:1101:HIS:N	2.28	0.62
1:E:156:ASP:HB3	1:E:159:ARG:HG2	1.82	0.62
1:A:263:ALA:N	1:A:487:VAL:O	2.28	0.62
2:D:321:GLN:N	2:D:628:GLN:O	2.30	0.62
1:E:172:GLY:HA2	1:E:497:CYS:HB2	1.80	0.62
2:B:983:ARG:HB2	2:D:390:LEU:HD11	1.80	0.61
1:A:41:TYR:OH	2:B:500:THR:OG1	2.18	0.61
2:D:631:PRO:O	2:D:634:ARG:NH1	2.33	0.61
1:A:438:LEU:HD21	1:A:587:PHE:HA	1.83	0.61
2:B:961:THR:HG21	2:C:765:ARG:HH22	1.65	0.61
2:C:396:TYR:HB2	2:C:514:SER:HB3	1.81	0.61
2:D:319:ARG:NH1	2:D:321:GLN:OE1	2.34	0.61
1:E:28:PHE:HE2	1:E:80:ALA:HB2	1.64	0.61
1:E:260:CYS:HB2	1:E:487:VAL:HG23	1.83	0.61
2:D:65:PHE:HB2	2:D:265:TYR:HB3	1.83	0.60
2:B:128:ILE:HG23	2:B:130:VAL:HG23	1.83	0.60
2:B:420:ASP:OD1	2:B:424:LYS:NZ	2.31	0.60
2:C:707:TYR:HB3	2:D:792:PRO:HG3	1.82	0.60
2:C:674:TYR:HB2	2:C:690:GLN:HE21	1.67	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:912:THR:OG1	2:C:1106:GLN:NE2	2.34	0.60
1:A:227:ARG:NH2	1:A:578:MET:O	2.35	0.60
1:E:349:ASP:O	1:E:392:ARG:NH2	2.33	0.60
2:B:980:ILE:HA	2:B:983:ARG:HG2	1.84	0.59
2:D:1053:PRO:O	2:D:1054:GLN:NE2	2.35	0.59
1:A:185:LEU:O	1:A:189:MET:HG2	2.02	0.59
2:B:45:SER:HB3	2:B:846:ALA:HB2	1.83	0.59
1:E:247:LEU:HB3	1:E:255:ILE:HD13	1.83	0.59
1:E:371:ALA:O	1:E:375:MET:HG2	2.02	0.59
1:E:413:THR:OG1	1:E:542:ASP:OD2	2.19	0.59
2:D:659:SER:HB3	2:D:698:SER:HB2	1.84	0.59
1:A:483:ILE:HG22	1:A:484:VAL:HG23	1.85	0.59
2:C:553:THR:HG21	2:D:841:LEU:HB2	1.83	0.59
2:C:715:PRO:HD3	2:D:894:LEU:HD13	1.83	0.59
1:A:119:ILE:HD11	1:A:178:LEU:HD22	1.84	0.59
2:B:707:TYR:HB3	2:C:792:PRO:HG3	1.85	0.59
2:C:1053:PRO:O	2:C:1054:GLN:NE2	2.36	0.59
2:B:444:LYS:NZ	2:B:445:HIS:O	2.34	0.59
2:B:560:LEU:O	2:B:577:ARG:NH2	2.36	0.59
2:B:590:CYS:O	2:C:837:TYR:OH	2.20	0.58
2:B:945:LEU:HD23	2:B:948:LEU:HD12	1.84	0.58
1:E:598:ASN:OD1	1:E:601:SER:OG	2.21	0.58
2:C:210:ILE:HG23	2:C:213:GLY:H	1.68	0.58
2:D:444:LYS:HG2	2:D:448:ASN:HB2	1.85	0.58
2:D:736:VAL:HG22	2:D:858:LEU:HD23	1.83	0.58
2:B:34:ARG:NH2	2:B:219:GLY:O	2.36	0.58
1:E:524:PHE:HD1	1:E:572:ILE:HG21	1.67	0.58
1:E:554:LEU:HA	1:E:557:LEU:HB2	1.84	0.58
2:D:402:ILE:HD12	2:D:406:GLU:HG3	1.84	0.58
2:D:617:CYS:HA	2:D:620:VAL:HG22	1.84	0.58
1:E:203:ARG:O	1:E:203:ARG:NH1	2.26	0.58
2:B:1029:MET:O	2:B:1033:VAL:HB	2.03	0.58
2:C:575:ALA:HA	2:C:586:ASP:HA	1.85	0.58
2:D:1098:ASN:OD1	2:D:1101:HIS:N	2.37	0.58
2:B:736:VAL:HG11	2:B:1004:LEU:HD11	1.86	0.58
2:B:959:LEU:O	2:B:963:VAL:HG23	2.04	0.58
1:E:217:SER:OG	1:E:218:ARG:N	2.37	0.58
2:B:206:LYS:HE3	2:B:208:THR:HB	1.86	0.58
2:D:903:ALA:HB1	2:D:913:GLN:HG3	1.86	0.58
1:A:56:ASP:OD1	1:A:56:ASP:N	2.36	0.57
2:D:808:ASP:HB3	2:D:811:LYS:HG3	1.84	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:393:THR:HA	2:C:522:ALA:HA	1.85	0.57
1:E:47:SER:HB2	1:E:66:ARG:HH22	1.69	0.57
1:E:255:ILE:HD11	1:E:265:LEU:HD13	1.86	0.57
1:E:355:PHE:HB3	1:E:378:ILE:HD11	1.86	0.57
2:B:852:ALA:O	2:B:856:ASN:ND2	2.36	0.57
2:B:84:LEU:HD22	2:B:267:VAL:HG11	1.86	0.57
2:C:546:LEU:HD22	2:C:565:PHE:HE1	1.68	0.57
2:D:119:ILE:HG23	2:D:128:ILE:HG13	1.87	0.57
1:E:528:LEU:HD13	1:E:549:ALA:HB1	1.86	0.57
2:B:914:ASN:ND2	2:D:1123:SER:OG	2.37	0.57
2:C:823:PHE:HD1	2:C:1057:PRO:HG3	1.69	0.57
2:D:457:ARG:NH2	2:D:460:LYS:O	2.37	0.57
1:E:307:PHE:O	1:E:311:GLU:HG2	2.05	0.57
1:A:260:CYS:HB3	1:A:485:GLY:HA2	1.85	0.57
2:B:912:THR:OG1	2:B:1106:GLN:NE2	2.38	0.57
2:C:53:ASP:OD1	2:C:54:LEU:N	2.38	0.57
2:C:358:ILE:HB	2:C:395:VAL:HB	1.87	0.57
2:B:1098:ASN:OD1	2:B:1101:HIS:N	2.31	0.57
2:D:83:VAL:HG22	2:D:239:GLN:HB2	1.87	0.57
1:A:88:ILE:HG23	1:A:93:LEU:HD23	1.87	0.57
1:A:275:THR:HG22	1:A:444:THR:HA	1.86	0.57
2:B:715:PRO:HD3	2:C:894:LEU:HD13	1.86	0.57
2:D:452:TRP:HB3	2:D:492:LEU:HD13	1.87	0.56
1:E:375:MET:O	1:E:378:ILE:HG22	2.05	0.56
2:B:430:THR:OG1	2:B:515:PHE:O	2.22	0.56
2:C:1084:ASP:OD1	2:C:1084:ASP:N	2.39	0.56
2:B:377:PHE:O	2:D:489:TYR:OH	2.15	0.56
2:D:1139:ASP:N	2:D:1139:ASP:OD1	2.38	0.56
1:E:90:ASN:OD1	1:E:91:LEU:N	2.35	0.56
1:E:155:ARG:NH1	1:E:251:TYR:OH	2.35	0.56
1:E:395:ALA:HB3	1:E:399:PHE:HE2	1.71	0.56
2:B:444:LYS:NZ	2:B:447:GLY:O	2.37	0.56
2:C:1139:ASP:OD1	2:C:1139:ASP:N	2.39	0.56
2:D:914:ASN:ND2	2:D:918:GLU:OE2	2.37	0.56
1:A:260:CYS:HB2	1:A:487:VAL:HG23	1.88	0.56
2:B:556:ASN:HB2	2:C:844:ILE:HG12	1.86	0.56
2:C:131:CYS:HB2	2:C:160:TYR:HE2	1.69	0.56
2:D:319:ARG:HB2	2:D:592:PHE:CE1	2.41	0.56
2:D:337:PRO:HG2	2:D:358:ILE:HG12	1.87	0.56
1:E:534:HIS:ND1	1:E:541:CYS:SG	2.74	0.56
2:B:726:ILE:HG12	2:B:1061:VAL:HG22	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:188:ASN:HA	2:D:209:PRO:HA	1.88	0.56
1:E:274:TRP:HD1	1:E:277:LEU:HD12	1.70	0.56
2:D:770:ILE:O	2:D:774:GLN:HG2	2.05	0.56
2:C:356:THR:OG1	2:C:397:ALA:O	2.24	0.56
2:C:624:ILE:HD11	2:C:629:LEU:HD22	1.88	0.56
2:D:450:ASP:OD1	2:D:450:ASP:N	2.39	0.56
2:D:375:PHE:HE2	2:D:407:VAL:HG21	1.71	0.55
1:E:314:PHE:CE2	1:E:375:MET:HB2	2.42	0.55
1:E:437:PHE:HA	1:E:440:LYS:HE3	1.87	0.55
1:A:88:ILE:HD13	1:A:97:LEU:HD22	1.88	0.55
2:B:363:ALA:HB2	2:B:524:VAL:HG12	1.87	0.55
2:D:48:LEU:HD12	2:D:276:LEU:HD21	1.88	0.55
1:A:528:LEU:HD11	1:A:553:LEU:HD21	1.88	0.55
2:B:384:PRO:HA	2:B:387:LEU:HD12	1.88	0.55
1:E:538:LEU:HD23	1:E:586:TYR:HA	1.89	0.55
2:B:633:TRP:O	2:B:634:ARG:NH1	2.39	0.55
2:B:1041:ASP:HB3	2:C:1030:SER:HB3	1.89	0.55
2:C:118:LEU:HD11	2:C:120:VAL:HB	1.87	0.55
2:C:742:ILE:O	2:C:1000:ARG:NH1	2.37	0.55
2:D:833:PHE:HB3	2:D:862:PRO:HB3	1.89	0.55
1:A:35:GLU:HG2	2:B:493:GLN:HE22	1.72	0.55
2:C:40:ASP:N	2:C:40:ASP:OD1	2.40	0.55
2:C:276:LEU:HD11	2:C:304:LYS:HA	1.89	0.55
2:C:303:LEU:HD12	2:C:308:VAL:HG22	1.88	0.55
2:C:411:ALA:HB3	2:C:414:GLN:HG3	1.89	0.55
2:C:675:GLN:HG3	2:C:693:ILE:HD11	1.89	0.55
2:D:312:ILE:HB	2:D:598:ILE:HG22	1.89	0.55
2:B:722:VAL:HG12	2:B:930:ALA:HB1	1.89	0.55
2:C:104:TRP:HD1	2:C:238:PHE:HE1	1.55	0.55
2:B:280:ASN:OD1	2:B:284:THR:OG1	2.25	0.54
2:C:884:SER:O	2:C:887:THR:OG1	2.23	0.54
2:B:596:SER:OG	2:B:613:GLN:OE1	2.25	0.54
2:C:762:GLN:OE1	2:C:765:ARG:NH2	2.41	0.54
2:D:395:VAL:HG22	2:D:515:PHE:CD1	2.42	0.54
1:E:155:ARG:HH12	1:E:280:LEU:HD21	1.71	0.54
2:B:821:LEU:HD21	2:B:939:PHE:HD1	1.72	0.54
2:C:365:TYR:HD2	2:C:368:LEU:HD12	1.72	0.54
1:E:114:LYS:HA	1:E:117:ASN:ND2	2.21	0.54
2:C:590:CYS:O	2:D:837:TYR:OH	2.26	0.54
1:A:259:GLY:HA2	1:A:606:SER:H	1.71	0.54
2:D:570:VAL:HG23	2:D:570:VAL:O	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:735:SER:OG	2:D:859:THR:OG1	2.22	0.54
1:A:458:TRP:HH2	1:A:475:LYS:HB3	1.72	0.54
2:B:370:ASN:OD1	2:B:371:PHE:N	2.40	0.54
2:B:763:LEU:HG	2:B:1008:VAL:HG21	1.88	0.54
2:C:914:ASN:ND2	2:C:1111:GLU:OE1	2.40	0.54
1:A:468:PRO:O	1:A:472:TRP:NE1	2.41	0.54
2:B:176:LEU:HB2	2:B:190:ARG:HH21	1.73	0.54
2:C:1051:SER:OG	2:C:1064:HIS:ND1	2.31	0.54
2:B:177:MET:HE1	2:B:207:HIS:HB2	1.89	0.53
1:E:558:ARG:HG3	1:E:559:LEU:HD12	1.89	0.53
2:C:914:ASN:O	2:C:918:GLU:HG2	2.09	0.53
2:D:905:ARG:NH1	2:D:1035:GLY:O	2.42	0.53
2:D:945:LEU:HD23	2:D:948:LEU:HD12	1.90	0.53
2:B:166:CYS:SG	2:B:167:THR:N	2.81	0.53
2:B:735:SER:O	2:B:735:SER:OG	2.25	0.53
2:B:1084:ASP:N	2:B:1084:ASP:OD1	2.41	0.53
2:C:271:GLN:OE1	2:C:273:ARG:NH1	2.42	0.53
2:C:295:PRO:HB2	2:C:608:VAL:HG21	1.89	0.53
2:D:102:ARG:O	2:D:121:ASN:ND2	2.41	0.53
1:A:203:ARG:NH1	1:A:218:ARG:O	2.39	0.53
1:E:28:PHE:CE2	1:E:80:ALA:HB2	2.43	0.53
1:E:88:ILE:HG21	1:E:97:LEU:HD23	1.90	0.53
2:B:707:TYR:HE1	2:C:897:PRO:HA	1.74	0.53
2:D:117:LEU:HD11	2:D:231:ILE:HG13	1.89	0.53
2:D:804:GLN:NE2	2:D:935:GLN:OE1	2.41	0.53
1:E:401:GLU:HB3	1:E:517:ARG:HD3	1.90	0.53
2:B:473:TYR:HB2	2:B:491:PRO:HG3	1.91	0.53
2:D:856:ASN:HD21	2:D:963:VAL:HG13	1.73	0.53
2:D:457:ARG:NE	2:D:459:SER:O	2.42	0.53
1:A:80:ALA:HB1	1:A:100:LEU:HD21	1.91	0.53
2:B:39:PRO:HG3	2:B:55:PHE:HZ	1.74	0.53
2:C:1130:ILE:HD12	2:D:920:GLN:HG2	1.90	0.53
2:D:353:TRP:O	2:D:466:ARG:NH1	2.42	0.53
2:D:971:GLY:O	2:D:995:ARG:NH1	2.41	0.53
2:B:189:LEU:HB3	2:B:191:GLU:OE1	2.09	0.52
2:B:264:ASP:OD1	2:B:264:ASP:N	2.41	0.52
2:C:984:LEU:HB3	2:C:989:ALA:HB2	1.90	0.52
2:D:937:SER:O	2:D:941:THR:HB	2.10	0.52
1:E:157:TYR:CE2	1:E:265:LEU:HD11	2.44	0.52
1:E:235:LEU:O	1:E:238:GLN:HG2	2.09	0.52
1:E:453:TYR:O	1:E:456:GLU:HG2	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:527:ALA:HB2	1:A:573:VAL:HG22	1.91	0.52
2:D:922:LEU:HD11	3:K:1:NAG:H3	1.91	0.52
1:E:48:TRP:HE1	1:E:350:LEU:HD11	1.75	0.52
2:B:502:GLY:O	2:B:504:GLY:N	2.41	0.52
2:D:722:VAL:HG22	2:D:1065:VAL:HG22	1.92	0.52
2:D:843:ASP:O	2:D:845:ALA:N	2.42	0.52
2:C:129:LYS:HG2	2:C:169:GLU:HA	1.90	0.52
2:D:989:ALA:O	2:D:993:ILE:HG12	2.10	0.52
1:E:502:LEU:HB2	1:E:505:VAL:HG23	1.91	0.52
1:A:372:HIS:ND1	1:A:411:ALA:HB2	2.25	0.52
2:B:748:GLU:O	2:B:752:LEU:HG	2.08	0.52
2:C:714:ILE:HD11	2:C:1094:VAL:HG21	1.91	0.52
1:E:203:ARG:NH2	1:E:217:SER:O	2.43	0.52
1:A:477:TRP:CE3	1:A:480:LYS:HD2	2.45	0.52
2:C:815:ARG:HD2	2:C:823:PHE:HE2	1.75	0.52
2:C:905:ARG:O	2:C:909:ILE:HG23	2.09	0.52
2:D:395:VAL:HG22	2:D:515:PHE:HD1	1.74	0.52
2:C:319:ARG:HH11	2:D:740:MET:HE1	1.75	0.52
2:C:792:PRO:O	2:C:795:LYS:NZ	2.42	0.52
2:D:127:PHE:HE1	2:D:129:LYS:HB2	1.74	0.52
2:D:553:THR:O	2:D:586:ASP:N	2.42	0.52
2:B:267:VAL:HG23	2:B:267:VAL:O	2.10	0.52
2:C:822:LEU:HD22	2:C:945:LEU:HD21	1.91	0.52
2:C:901:GLN:O	2:C:905:ARG:HG2	2.09	0.52
1:E:350:LEU:O	1:E:392:ARG:NH2	2.43	0.52
2:B:617:CYS:HA	2:B:620:VAL:HG12	1.91	0.52
1:A:114:LYS:HA	1:A:117:ASN:ND2	2.26	0.51
2:B:714:ILE:HD12	2:B:1096:VAL:HG11	1.92	0.51
2:B:905:ARG:O	2:B:909:ILE:HG23	2.11	0.51
2:B:1053:PRO:O	2:B:1054:GLN:NE2	2.43	0.51
1:E:450:PRO:O	1:E:454:MET:HG2	2.10	0.51
2:C:393:THR:HG21	2:C:520:ALA:HB3	1.91	0.51
2:C:320:VAL:N	2:C:591:SER:OG	2.44	0.51
2:D:39:PRO:HG2	2:D:51:THR:HG21	1.92	0.51
2:D:105:ILE:HG22	2:D:110:LEU:HD22	1.92	0.51
1:E:469:LYS:HA	1:E:472:TRP:HE1	1.75	0.51
1:A:176:ARG:HG2	1:A:495:THR:HA	1.93	0.51
1:A:180:GLU:HA	1:A:183:VAL:HG12	1.93	0.51
2:B:1051:SER:OG	2:B:1064:HIS:ND1	2.30	0.51
2:C:401:VAL:HG22	2:C:509:ARG:HG2	1.93	0.51
2:C:736:VAL:HG21	2:C:1004:LEU:HD11	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:736:VAL:HG11	2:D:1004:LEU:HD11	1.92	0.51
2:D:749:CYS:SG	2:D:997:ILE:HD11	2.51	0.51
2:B:337:PRO:HB2	2:B:340:GLU:HB2	1.93	0.51
2:B:878:LEU:HD11	2:B:1054:GLN:HE22	1.75	0.51
2:C:661:GLU:N	2:C:661:GLU:OE2	2.44	0.51
2:D:456:PHE:HB2	2:D:491:PRO:HA	1.93	0.51
1:A:563:GLU:HB3	1:A:567:LEU:HD21	1.93	0.51
2:B:307:THR:HA	2:B:602:THR:HG21	1.93	0.51
2:C:826:VAL:HB	2:C:1057:PRO:HG2	1.93	0.51
1:A:395:ALA:HB3	1:A:399:PHE:CE2	2.46	0.51
2:B:83:VAL:HG21	2:B:237:ARG:HH11	1.76	0.51
1:E:417:LEU:HD12	1:E:422:LEU:HD13	1.93	0.51
1:A:219:ASP:OD1	1:A:219:ASP:N	2.41	0.51
2:B:86:PHE:H	2:B:237:ARG:HA	1.76	0.51
2:C:342:PHE:HE1	2:C:511:VAL:HG21	1.75	0.51
1:E:242:TYR:OH	1:E:598:ASN:ND2	2.44	0.51
1:E:373:HIS:HE1	1:E:401:GLU:HA	1.76	0.51
1:A:260:CYS:SG	1:A:605:TRP:HB2	2.51	0.51
2:B:464:PHE:CG	2:B:464:PHE:O	2.63	0.51
2:D:597:VAL:HG22	2:D:610:VAL:HG12	1.93	0.51
1:E:482:GLU:HG3	1:E:483:ILE:HG12	1.91	0.51
2:D:418:ILE:HG13	2:D:422:ASN:HD22	1.75	0.50
2:D:729:VAL:HG11	2:D:781:VAL:HG11	1.92	0.50
2:D:104:TRP:HD1	2:D:238:PHE:HE1	1.60	0.50
2:B:56:LEU:HD12	2:B:57:PRO:HD2	1.94	0.50
2:D:127:PHE:CE1	2:D:129:LYS:HB2	2.46	0.50
1:A:317:ILE:HG23	1:A:319:LEU:HD23	1.92	0.50
2:B:409:GLN:O	2:B:414:GLN:NE2	2.34	0.50
2:C:666:ILE:HD12	2:C:670:ILE:HG22	1.94	0.50
2:D:452:TRP:HZ3	2:D:494:SER:HA	1.76	0.50
1:E:216:TYR:OH	1:E:576:LYS:O	2.20	0.50
1:A:20:THR:OG1	1:A:23:GLU:OE1	2.26	0.50
1:A:183:VAL:HG23	1:A:463:PHE:HD1	1.76	0.50
1:A:264:HIS:CG	1:A:489:PRO:HG2	2.47	0.50
2:B:589:PRO:O	2:C:837:TYR:OH	2.30	0.50
2:B:937:SER:O	2:B:941:THR:OG1	2.21	0.50
2:C:547:THR:HB	2:D:978:ASN:ND2	2.26	0.50
2:C:453:TYR:HE2	2:C:455:LEU:HD11	1.77	0.50
1:A:302:ASP:HB2	1:A:305:ARG:HE	1.76	0.50
2:B:676:THR:HG23	2:B:690:GLN:HG2	1.94	0.50
1:E:244:ARG:NH1	1:E:259:GLY:O	2.45	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:89:GLY:O	2:B:270:LEU:HG	2.12	0.49
2:C:57:PRO:HG3	2:C:273:ARG:HD2	1.93	0.49
1:E:292:VAL:HG21	1:E:417:LEU:HD11	1.94	0.49
1:A:176:ARG:NE	1:A:494:GLU:O	2.40	0.49
1:A:381:ASP:HA	1:A:384:TYR:CE2	2.48	0.49
2:B:901:GLN:O	2:B:905:ARG:HG2	2.12	0.49
1:E:313:PHE:HE2	1:E:411:ALA:HB2	1.76	0.49
1:E:442:ALA:O	1:E:446:VAL:HG22	2.12	0.49
1:A:372:HIS:HD1	1:A:411:ALA:HB2	1.77	0.49
2:C:444:LYS:NZ	2:C:445:HIS:O	2.44	0.49
2:C:546:LEU:HD22	2:C:565:PHE:CE1	2.46	0.49
2:B:599:THR:HB	2:B:608:VAL:HG12	1.94	0.49
2:C:387:LEU:HA	2:C:390:LEU:HD13	1.95	0.49
1:E:456:GLU:HA	1:E:459:ARG:HG2	1.94	0.49
1:A:63:ASN:HA	1:A:66:ARG:HG2	1.94	0.49
2:D:1029:MET:O	2:D:1033:VAL:HB	2.11	0.49
2:C:23:THR:HB	2:C:68:ILE:HB	1.94	0.49
2:C:131:CYS:HA	2:C:166:CYS:HB3	1.93	0.49
2:D:276:LEU:HD11	2:D:304:LYS:HA	1.95	0.49
1:E:184:VAL:HA	1:E:187:ASN:ND2	2.26	0.49
2:B:298:GLU:OE1	2:B:633:TRP:NE1	2.31	0.49
2:B:629:LEU:HG	2:B:631:PRO:HD2	1.94	0.49
2:C:858:LEU:HD13	2:C:959:LEU:HG	1.95	0.49
2:C:1002:GLN:HG2	2:D:759:PHE:HZ	1.77	0.49
2:B:116:SER:O	2:B:117:LEU:HG	2.12	0.49
2:C:474:GLN:NE2	2:C:480:CYS:HB2	2.28	0.49
1:E:122:LYS:O	1:E:126:ILE:HG12	2.13	0.49
1:A:88:ILE:HG22	1:A:94:LYS:HG2	1.94	0.49
1:E:595:LYS:HA	1:E:598:ASN:HB2	1.95	0.49
1:A:187:ASN:O	1:A:191:ARG:HG2	2.13	0.48
2:B:83:VAL:HA	2:B:239:GLN:HG2	1.95	0.48
2:C:394:ASN:N	2:C:394:ASN:OD1	2.45	0.48
2:C:726:ILE:HG12	2:C:1061:VAL:HG22	1.95	0.48
2:D:360:ASN:H	2:D:523:THR:HB	1.77	0.48
1:E:225:VAL:HB	1:E:453:TYR:HE1	1.78	0.48
3:N:1:NAG:H62	3:N:2:BMA:H2	1.94	0.48
2:C:374:PHE:HD1	2:C:436:TRP:HB3	1.77	0.48
2:C:758:SER:O	2:C:758:SER:OG	2.25	0.48
1:A:481:ARG:HG2	1:A:487:VAL:HA	1.94	0.48
2:C:735:SER:O	2:C:735:SER:OG	2.27	0.48
1:E:392:ARG:O	1:E:392:ARG:HG2	2.12	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:290:ASP:OD1	2:B:291:CYS:N	2.45	0.48
1:A:184:VAL:HA	1:A:187:ASN:HD21	1.78	0.48
1:A:481:ARG:HG2	1:A:487:VAL:HG22	1.95	0.48
2:D:895:GLN:HE21	2:D:895:GLN:N	2.10	0.48
1:E:444:THR:HG23	1:E:445:ILE:HG12	1.96	0.48
2:C:856:ASN:ND2	2:C:966:LEU:HD22	2.28	0.48
1:A:246:LYS:HD3	1:A:281:THR:HG22	1.94	0.48
1:A:289:SER:OG	1:A:290:ILE:N	2.46	0.48
2:B:108:THR:OG1	2:B:234:ASN:ND2	2.47	0.48
2:B:1123:SER:HB2	2:C:914:ASN:HD22	1.78	0.48
2:C:200:TYR:HA	2:C:230:PRO:HA	1.96	0.48
1:E:534:HIS:HE1	1:E:540:LYS:HG3	1.78	0.48
1:A:401:GLU:OE1	1:A:517:ARG:NH1	2.47	0.48
2:B:905:ARG:NH1	2:B:1049:LEU:O	2.46	0.48
1:E:246:LYS:HD3	1:E:281:THR:HA	1.94	0.48
1:E:272:ARG:HG2	1:E:448:THR:HG23	1.95	0.48
1:A:60:GLN:HA	1:A:63:ASN:ND2	2.29	0.48
2:B:131:CYS:HB2	2:B:133:PHE:CE1	2.49	0.48
2:B:894:LEU:HD13	2:D:715:PRO:HD3	1.95	0.48
2:C:973:ILE:HG12	2:C:992:GLN:OE1	2.13	0.48
2:C:976:VAL:HB	2:C:979:ASP:HB3	1.96	0.48
2:B:102:ARG:HG3	2:B:243:ALA:HB2	1.96	0.47
2:B:534:VAL:HG23	2:B:535:LYS:N	2.29	0.47
2:B:565:PHE:HB3	2:C:42:VAL:HA	1.96	0.47
2:B:788:ILE:HG23	2:B:876:ALA:HB2	1.95	0.47
1:A:60:GLN:HA	1:A:63:ASN:HD21	1.78	0.47
1:A:235:LEU:HB2	1:A:591:PHE:CE2	2.49	0.47
2:B:43:PHE:H	2:D:566:GLY:HA2	1.79	0.47
2:C:344:ALA:HB3	2:C:347:PHE:HE1	1.80	0.47
2:D:307:THR:HA	2:D:602:THR:HG21	1.96	0.47
2:D:1098:ASN:OD1	2:D:1100:THR:N	2.44	0.47
2:C:319:ARG:H	2:C:630:THR:HB	1.79	0.47
2:C:505:HIS:HB2	1:E:352:LYS:HD3	1.95	0.47
1:A:116:LEU:O	1:A:120:LEU:HG	2.14	0.47
1:A:519:ILE:HG23	1:A:520:TYR:CD1	2.48	0.47
2:B:350:VAL:HG12	2:B:400:PHE:CD2	2.44	0.47
1:A:314:PHE:HE2	1:A:375:MET:HB3	1.79	0.47
1:A:389:TYR:HA	1:A:392:ARG:HD3	1.95	0.47
2:B:844:ILE:HG22	2:D:556:ASN:HD21	1.80	0.47
2:D:853:GLN:HA	2:D:858:LEU:HD12	1.96	0.47
1:E:480:LYS:HA	1:E:480:LYS:HD2	1.63	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:LEU:HD21	1:A:486:VAL:HG22	1.96	0.47
1:A:402:ALA:O	1:A:406:ILE:HG23	2.15	0.47
2:B:64:TRP:HE1	2:B:263:ALA:N	2.12	0.47
2:B:749:CYS:SG	2:B:997:ILE:HD11	2.54	0.47
2:D:598:ILE:HD11	2:D:650:LEU:HD11	1.95	0.47
2:D:1075:PHE:O	2:D:1076:THR:OG1	2.28	0.47
2:B:167:THR:OG1	2:B:168:PHE:N	2.45	0.47
2:C:722:VAL:HG22	2:C:1065:VAL:HG22	1.97	0.47
2:C:726:ILE:HD12	2:C:945:LEU:HA	1.97	0.47
2:D:878:LEU:O	2:D:882:ILE:HG23	2.15	0.47
1:E:89:GLN:NE2	1:E:90:ASN:HB2	2.29	0.47
1:E:313:PHE:CE2	1:E:411:ALA:HB2	2.50	0.47
1:A:304:GLU:HG3	1:A:332:LEU:HD23	1.97	0.47
1:A:314:PHE:HA	1:A:317:ILE:HG22	1.97	0.47
2:B:96:GLU:O	2:B:187:LYS:HA	2.15	0.47
2:B:576:VAL:HG23	2:B:585:LEU:HB2	1.97	0.47
2:C:318:PHE:HB3	2:C:595:VAL:HG23	1.96	0.47
2:C:444:LYS:HE2	2:C:444:LYS:HB2	1.72	0.47
2:C:459:SER:OG	2:C:460:LYS:N	2.47	0.47
2:D:37:TYR:OH	2:D:53:ASP:OD1	2.32	0.47
2:D:106:PHE:HD2	2:D:235:ILE:HG21	1.78	0.47
1:E:48:TRP:NE1	1:E:350:LEU:HD11	2.30	0.47
1:E:343:CYS:HB2	1:E:360:CYS:N	2.30	0.47
1:A:522:PHE:O	1:A:526:GLU:HG2	2.16	0.47
2:B:295:PRO:HB2	2:B:608:VAL:HG21	1.97	0.47
2:B:752:LEU:HA	2:B:755:GLN:HG2	1.97	0.47
2:D:763:LEU:HB3	2:D:1008:VAL:HG21	1.96	0.47
2:D:1098:ASN:OD1	2:D:1099:GLY:N	2.48	0.47
1:E:20:THR:OG1	1:E:23:GLU:OE1	2.32	0.47
1:A:553:LEU:O	1:A:557:LEU:HG	2.15	0.46
2:B:742:ILE:O	2:B:1000:ARG:NH1	2.49	0.46
1:E:73:TYR:O	1:E:77:SER:OG	2.27	0.46
2:C:541:PHE:CZ	2:C:587:ILE:HD13	2.51	0.46
2:D:99:ASN:OD1	2:D:102:ARG:NH1	2.48	0.46
2:D:598:ILE:HG13	2:D:609:ALA:HB3	1.96	0.46
1:E:184:VAL:HA	1:E:187:ASN:HD21	1.79	0.46
1:E:452:THR:OG1	1:E:511:PHE:O	2.31	0.46
2:B:104:TRP:HB2	2:B:119:ILE:HB	1.98	0.46
2:B:993:ILE:O	2:B:997:ILE:HG12	2.15	0.46
2:C:444:LYS:HG2	2:C:448:ASN:HD22	1.81	0.46
1:E:224:ASP:OD1	1:E:227:ARG:NH2	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:870:ILE:HG22	2:D:1055:SER:HB2	1.98	0.46
2:C:426:PRO:HG2	2:C:429:PHE:HB2	1.97	0.46
2:C:451:TYR:HB2	2:C:495:TYR:HB2	1.98	0.46
2:C:659:SER:HB3	2:C:698:SER:HB2	1.98	0.46
2:D:716:THR:HA	2:D:1110:TYR:HB3	1.97	0.46
2:B:358:ILE:HG13	2:B:395:VAL:HB	1.98	0.46
2:C:49:HIS:CE1	2:C:51:THR:HG22	2.50	0.46
2:C:662:CYS:HB2	2:C:697:MET:HE2	1.98	0.46
2:C:878:LEU:O	2:C:882:ILE:HG23	2.16	0.46
1:E:417:LEU:HD23	1:E:423:LEU:HD22	1.98	0.46
1:A:438:LEU:HG	1:A:590:LEU:HD12	1.98	0.46
2:B:897:PRO:HA	2:D:707:TYR:HE1	1.81	0.46
2:C:478:LYS:HD3	2:C:478:LYS:HA	1.68	0.46
2:D:675:GLN:HG3	2:D:693:ILE:HD11	1.97	0.46
1:E:108:LEU:HB3	1:E:112:LYS:HB2	1.97	0.46
1:A:335:PRO:HG2	1:A:339:ARG:HH21	1.81	0.46
1:A:363:VAL:HG23	1:A:363:VAL:O	2.16	0.46
2:B:589:PRO:HB3	2:C:855:PHE:HA	1.97	0.46
2:C:473:TYR:HB2	2:C:491:PRO:HG3	1.97	0.46
2:D:54:LEU:HD23	2:D:88:ASP:HB3	1.98	0.46
2:D:104:TRP:CD1	2:D:238:PHE:HE1	2.34	0.46
2:B:878:LEU:HD21	2:B:1052:PHE:HB3	1.98	0.46
2:D:180:GLU:HA	2:D:186:PHE:HD2	1.80	0.46
2:D:1115:ILE:HG23	2:D:1120:THR:HG21	1.98	0.46
1:E:198:TYR:HB3	1:E:463:PHE:CG	2.51	0.46
2:C:107:GLY:H	2:C:235:ILE:HG23	1.80	0.45
1:E:180:GLU:O	1:E:183:VAL:HG12	2.16	0.45
1:A:549:ALA:O	1:A:553:LEU:HG	2.15	0.45
2:B:95:THR:HG23	2:B:263:ALA:HB1	1.98	0.45
2:C:746:SER:O	2:C:750:SER:OG	2.28	0.45
2:D:342:PHE:HE1	2:D:511:VAL:HG11	1.80	0.45
1:E:358:LYS:H	1:E:358:LYS:HG3	1.63	0.45
1:E:528:LEU:HD11	1:E:553:LEU:HG	1.97	0.45
2:C:1075:PHE:O	2:C:1076:THR:OG1	2.32	0.45
1:A:172:GLY:HA3	1:A:497:CYS:H	1.81	0.45
1:A:290:ILE:HD11	1:A:417:LEU:HD22	1.99	0.45
2:B:113:LYS:N	2:B:134:GLN:OE1	2.46	0.45
2:C:586:ASP:OD1	2:C:586:ASP:N	2.40	0.45
2:C:619:GLU:HA	2:C:622:VAL:HG22	1.98	0.45
2:D:319:ARG:O	2:D:630:THR:OG1	2.34	0.45
1:E:172:GLY:HA3	1:E:497:CYS:H	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:198:TYR:HE1	1:E:202:TRP:HD1	1.63	0.45
1:A:388:PRO:O	1:A:392:ARG:HG3	2.17	0.45
1:A:530:LYS:HZ3	1:A:538:LEU:HD12	1.82	0.45
1:A:546:SER:OG	1:A:549:ALA:HB3	2.17	0.45
2:B:194:PHE:HB3	2:B:201:PHE:CZ	2.52	0.45
2:B:984:LEU:HD13	2:B:988:GLU:HG3	1.98	0.45
1:E:109:SER:OG	1:E:112:LYS:NZ	2.40	0.45
1:E:240:HIS:HA	1:E:243:VAL:HG12	1.99	0.45
2:C:436:TRP:HZ2	2:C:509:ARG:HE	1.63	0.45
2:C:560:LEU:HB2	2:C:563:GLN:HG3	1.97	0.45
2:C:612:TYR:O	2:C:648:GLY:HA3	2.16	0.45
2:D:445:HIS:CE1	2:D:446:SER:HB3	2.51	0.45
1:E:493:ASP:OD1	1:E:493:ASP:N	2.50	0.45
1:A:183:VAL:HG23	1:A:463:PHE:HA	1.99	0.45
1:A:479:MET:HA	1:A:482:GLU:HG2	1.98	0.45
1:A:481:ARG:HB2	1:A:607:THR:HG23	1.99	0.45
2:C:453:TYR:CZ	2:C:493:GLN:HB2	2.52	0.45
1:E:229:PHE:HE2	1:E:457:LYS:HE2	1.81	0.45
1:A:233:LYS:HZ2	1:A:483:ILE:HG23	1.82	0.45
1:A:542:ASP:OD1	1:A:543:ILE:N	2.50	0.45
2:C:452:TRP:CD1	2:C:494:SER:HA	2.52	0.45
2:D:921:LYS:O	2:D:922:LEU:HB3	2.17	0.45
1:A:565:TRP:CE2	1:A:569:LEU:HB2	2.52	0.45
2:B:206:LYS:HG3	2:B:208:THR:HG22	1.99	0.45
2:D:231:ILE:HG22	2:D:233:ILE:HG23	1.99	0.45
2:D:977:LEU:O	2:D:981:LEU:HG	2.17	0.45
1:E:378:ILE:O	1:E:382:MET:HG2	2.17	0.45
1:E:384:TYR:CD1	1:E:392:ARG:HA	2.51	0.45
1:A:61:LYS:O	1:A:64:GLU:HG2	2.18	0.45
2:B:170:TYR:CE2	2:B:227:VAL:HG11	2.53	0.45
2:B:478:LYS:HD2	2:B:479:PRO:HD2	1.98	0.45
2:B:1114:ILE:HD12	2:B:1114:ILE:HA	1.89	0.45
2:D:106:PHE:HB2	2:D:117:LEU:HB3	1.99	0.45
2:D:403:LYS:HG3	2:D:495:TYR:HE1	1.82	0.45
1:E:114:LYS:HA	1:E:117:ASN:HD21	1.82	0.45
1:E:119:ILE:O	1:E:123:MET:HG2	2.16	0.45
1:A:203:ARG:NH2	1:A:222:MET:SD	2.90	0.44
2:B:106:PHE:HD1	2:B:117:LEU:HD11	1.82	0.44
2:B:176:LEU:HD12	2:B:190:ARG:HE	1.82	0.44
2:C:409:GLN:HG2	2:C:419:ALA:HB2	1.99	0.44
2:D:480:CYS:HB3	2:D:488:CYS:HB3	1.64	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:490:PHE:CG	2:D:491:PRO:HD2	2.52	0.44
2:B:103:GLY:O	2:B:241:LEU:N	2.40	0.44
2:D:105:ILE:HG12	2:D:118:LEU:HD13	2.00	0.44
1:E:37:GLU:OE1	1:E:392:ARG:NH1	2.51	0.44
2:C:699:LEU:HD12	2:D:788:ILE:HD11	1.99	0.44
2:C:1028:LYS:NZ	2:C:1042:PHE:O	2.46	0.44
1:E:406:ILE:HA	1:E:409:LEU:HD12	1.98	0.44
1:E:488:GLU:OE2	1:E:492:HIS:ND1	2.50	0.44
1:A:582:PRO:HA	1:A:585:ASN:OD1	2.17	0.44
2:B:778:THR:HG22	2:B:865:LEU:HD12	1.99	0.44
2:C:118:LEU:HD22	2:C:160:TYR:CE1	2.52	0.44
2:C:204:TYR:HA	2:C:225:PRO:HA	1.99	0.44
2:C:741:TYR:CE1	2:C:966:LEU:HD11	2.52	0.44
2:D:393:THR:OG1	2:D:516:GLU:OE1	2.36	0.44
2:B:315:THR:OG1	2:B:316:SER:N	2.51	0.44
2:C:201:PHE:N	2:C:229:LEU:O	2.50	0.44
2:C:215:ASP:OD1	2:C:266:TYR:OH	2.36	0.44
2:D:203:ILE:HB	2:D:227:VAL:HG22	2.00	0.44
2:D:624:ILE:HD11	2:D:629:LEU:HD22	1.99	0.44
2:D:735:SER:OG	2:D:735:SER:O	2.31	0.44
1:E:403:VAL:HA	1:E:406:ILE:HG12	2.00	0.44
2:B:533:LEU:HD12	2:B:533:LEU:O	2.17	0.44
2:C:440:LYS:HE2	2:C:440:LYS:HB2	1.73	0.44
2:C:528:LYS:HA	2:C:528:LYS:HD3	1.74	0.44
2:C:784:GLN:HG2	2:C:1034:LEU:HD11	1.99	0.44
1:A:426:ASP:OD1	1:A:426:ASP:N	2.49	0.44
2:B:592:PHE:CE2	2:C:857:GLY:HA2	2.53	0.44
2:B:811:LYS:HB2	2:B:811:LYS:HE2	1.73	0.44
2:C:315:THR:OG1	2:C:316:SER:N	2.51	0.44
2:C:382:VAL:HG21	2:C:515:PHE:HD2	1.82	0.44
2:D:350:VAL:HG11	2:D:418:ILE:HD11	2.00	0.44
1:E:303:ALA:O	1:E:307:PHE:CD1	2.70	0.44
1:A:236:TYR:CD1	1:A:239:LEU:HD21	2.53	0.43
2:B:889:GLY:HA3	2:B:1034:LEU:HB3	2.00	0.43
2:C:93:ALA:HB3	2:C:266:TYR:HB2	1.98	0.43
2:C:566:GLY:HA2	2:D:43:PHE:HB3	2.00	0.43
1:E:430:ASP:HB2	1:E:433:THR:HG23	2.00	0.43
2:B:743:CYS:HB3	2:B:749:CYS:HB3	1.86	0.43
2:C:836:GLN:HE22	2:C:850:ILE:HD13	1.83	0.43
2:D:94:SER:HB3	2:D:265:TYR:H	1.82	0.43
2:D:112:SER:HA	2:D:132:GLU:HG3	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:560:LEU:H	2:D:563:GLN:HG3	1.83	0.43
2:D:934:ILE:HG13	2:D:935:GLN:N	2.33	0.43
1:E:244:ARG:HH22	1:E:605:TRP:HB3	1.82	0.43
1:A:391:LEU:HD22	1:A:562:SER:HA	1.99	0.43
2:B:91:TYR:O	2:B:267:VAL:HA	2.18	0.43
2:B:99:ASN:HD21	2:B:102:ARG:NE	2.17	0.43
2:B:830:ASP:HB2	2:B:850:ILE:HD12	2.01	0.43
2:C:328:ARG:HD3	2:C:578:ASP:OD1	2.19	0.43
2:C:336:CYS:HB2	2:C:361:CYS:HB3	1.81	0.43
2:C:589:PRO:O	2:D:837:TYR:OH	2.34	0.43
1:A:416:TYR:HB2	1:A:542:ASP:OD2	2.18	0.43
1:A:451:PHE:HA	1:A:454:MET:HB3	1.99	0.43
1:A:452:THR:OG1	1:A:511:PHE:HB3	2.19	0.43
2:B:634:ARG:HA	2:B:634:ARG:HD3	1.77	0.43
2:B:662:CYS:HB2	2:B:671:CYS:HB2	1.31	0.43
2:B:1075:PHE:O	2:B:1076:THR:OG1	2.33	0.43
2:D:470:THR:O	2:D:470:THR:OG1	2.36	0.43
2:D:1054:GLN:HB2	2:D:1061:VAL:HB	1.99	0.43
2:D:1123:SER:OG	2:D:1123:SER:O	2.35	0.43
1:E:319:LEU:HD23	1:E:319:LEU:HA	1.90	0.43
1:A:242:TYR:CE2	1:A:594:LEU:HD21	2.53	0.43
1:A:450:PRO:HA	1:A:453:TYR:CZ	2.54	0.43
2:B:104:TRP:HB3	2:B:106:PHE:CE1	2.54	0.43
2:B:440:LYS:HE2	2:B:440:LYS:HB2	1.84	0.43
2:C:196:ASN:HD22	2:C:235:ILE:HG13	1.84	0.43
2:D:315:THR:OG1	2:D:316:SER:N	2.51	0.43
2:D:472:ILE:HG21	2:D:481:LYS:HA	2.00	0.43
2:D:645:THR:OG1	2:D:646:ARG:N	2.51	0.43
2:D:943:SER:O	2:D:943:SER:OG	2.37	0.43
2:D:978:ASN:OD1	2:D:979:ASP:N	2.52	0.43
1:E:198:TYR:HE1	1:E:202:TRP:CD1	2.36	0.43
1:E:575:ILE:HG13	1:E:577:THR:H	1.84	0.43
2:B:430:THR:O	2:B:515:PHE:N	2.35	0.43
2:B:490:PHE:CE2	2:B:492:LEU:HB2	2.54	0.43
2:B:546:LEU:HD12	2:B:565:PHE:CE1	2.54	0.43
2:C:117:LEU:HA	2:C:130:VAL:HA	2.00	0.43
2:C:634:ARG:HD3	2:C:634:ARG:HA	1.86	0.43
2:D:322:PRO:HG2	2:D:540:ASN:HD21	1.84	0.43
1:A:315:VAL:HG21	1:A:321:TYR:CZ	2.54	0.43
1:A:477:TRP:O	1:A:481:ARG:HG3	2.18	0.43
2:B:329:PHE:CD2	2:B:528:LYS:HB3	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:707:TYR:HE2	2:C:797:PHE:CD2	2.36	0.43
2:C:202:LYS:HB2	2:C:202:LYS:HE3	1.84	0.43
2:C:498:ARG:HB2	2:C:501:TYR:CZ	2.54	0.43
2:C:611:LEU:HB2	2:C:650:LEU:HD13	2.01	0.43
2:C:903:ALA:HB1	2:C:913:GLN:HB3	2.00	0.43
2:D:552:LEU:HD23	2:D:587:ILE:HG12	2.01	0.43
1:A:144:GLU:N	1:A:145:PRO:HD2	2.34	0.43
1:A:186:GLU:HB3	1:A:198:TYR:CG	2.54	0.43
2:B:353:TRP:CZ2	2:B:466:ARG:HG2	2.54	0.43
2:B:897:PRO:HA	2:D:707:TYR:CE1	2.54	0.43
2:B:943:SER:O	2:B:943:SER:OG	2.33	0.43
2:D:978:ASN:O	2:D:981:LEU:HD12	2.18	0.43
1:A:331:MET:HG3	1:A:358:LYS:HE2	2.01	0.43
2:C:598:ILE:HG23	2:C:664:ILE:HG21	2.01	0.43
2:C:699:LEU:HB3	2:D:873:TYR:CZ	2.54	0.43
1:E:165:GLU:OE1	1:E:492:HIS:NE2	2.49	0.43
2:B:559:PHE:HB3	2:B:577:ARG:NH2	2.33	0.42
2:C:752:LEU:HD21	2:C:994:ASP:HB2	2.01	0.42
2:D:847:ARG:HD2	2:D:851:CYS:HB2	2.00	0.42
2:D:1083:HIS:CG	2:D:1137:VAL:HG22	2.53	0.42
1:A:156:ASP:O	1:A:160:ARG:HG3	2.19	0.42
2:C:641:ASN:HB2	2:C:652:GLY:H	1.84	0.42
2:D:277:LEU:HD22	2:D:285:ILE:HD13	2.01	0.42
2:B:747:THR:O	2:B:751:ASN:ND2	2.36	0.42
2:C:743:CYS:HB3	2:C:749:CYS:HB3	1.74	0.42
1:E:357:ILE:HD11	1:E:378:ILE:HD12	2.01	0.42
2:B:176:LEU:HB2	2:B:190:ARG:NH2	2.33	0.42
2:B:594:GLY:O	2:B:613:GLN:N	2.41	0.42
2:B:756:TYR:OH	2:B:994:ASP:OD1	2.30	0.42
2:B:916:LEU:HD12	2:B:923:ILE:HD12	2.02	0.42
2:D:245:ASN:OD1	2:D:245:ASN:N	2.51	0.42
1:E:459:ARG:HA	1:E:462:VAL:HG22	2.02	0.42
1:A:504:HIS:O	1:A:509:TYR:HB2	2.20	0.42
2:B:194:PHE:HD1	2:B:203:ILE:HG12	1.85	0.42
2:B:737:ASP:OD2	2:D:317:ASN:ND2	2.51	0.42
2:C:399:SER:HB3	2:C:511:VAL:HG22	2.02	0.42
2:D:1029:MET:CE	2:D:1053:PRO:HB3	2.49	0.42
1:A:72:PHE:O	1:A:76:GLN:HG2	2.20	0.42
2:B:43:PHE:HE2	2:B:45:SER:HB2	1.84	0.42
2:C:307:THR:HA	2:C:602:THR:HG21	2.01	0.42
2:C:805:ILE:HB	2:C:878:LEU:HD11	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1127:ASP:OD1	2:C:1127:ASP:N	2.53	0.42
1:E:312:LYS:HA	1:E:315:VAL:HG22	2.02	0.42
1:E:451:PHE:O	1:E:455:LEU:HG	2.20	0.42
1:A:260:CYS:HB2	1:A:487:VAL:CG2	2.48	0.42
2:B:1074:ASN:O	2:B:1074:ASN:ND2	2.53	0.42
2:C:226:LEU:HD23	2:C:226:LEU:HA	1.92	0.42
2:C:485:GLY:H	2:C:488:CYS:HB3	1.84	0.42
2:D:502:GLY:O	2:D:506:GLN:HG2	2.19	0.42
2:D:790:LYS:HB3	2:D:790:LYS:HE2	1.87	0.42
2:D:1036:GLN:HE21	2:D:1049:LEU:HA	1.85	0.42
1:E:29:LEU:HD13	1:E:96:GLN:HE21	1.85	0.42
1:E:323:THR:OG1	1:E:324:GLN:N	2.53	0.42
1:A:184:VAL:HA	1:A:187:ASN:ND2	2.35	0.42
2:B:81:ASN:HD21	2:B:241:LEU:HD23	1.84	0.42
2:B:131:CYS:HB3	2:B:166:CYS:HA	2.01	0.42
2:C:823:PHE:CD1	2:C:1057:PRO:HG3	2.53	0.42
2:D:81:ASN:ND2	2:D:240:THR:O	2.47	0.42
2:D:129:LYS:HZ3	2:D:169:GLU:HB2	1.84	0.42
2:D:1052:PHE:HB2	2:D:1063:LEU:HB2	2.02	0.42
1:E:487:VAL:HG11	1:E:610:THR:HA	2.01	0.42
1:A:214:TYR:OH	1:A:567:LEU:N	2.51	0.42
2:C:1029:MET:HE1	2:C:1053:PRO:HB3	2.02	0.42
2:C:1086:LYS:HB2	2:C:1086:LYS:HE3	1.69	0.42
1:E:240:HIS:CE1	1:E:484:VAL:HG13	2.55	0.42
2:B:89:GLY:HA2	2:B:194:PHE:O	2.20	0.42
2:B:375:PHE:H	2:B:436:TRP:HA	1.84	0.42
2:C:674:TYR:HB2	2:C:690:GLN:NE2	2.33	0.42
2:C:725:GLU:OE2	2:C:1028:LYS:HD2	2.19	0.42
2:C:788:ILE:HG23	2:C:876:ALA:HB2	2.01	0.42
2:C:853:GLN:HB2	2:C:858:LEU:HD12	2.02	0.42
2:D:1028:LYS:NZ	2:D:1042:PHE:O	2.51	0.42
1:E:222:MET:HA	1:E:225:VAL:HG22	2.01	0.42
1:E:247:LEU:HD23	1:E:247:LEU:HA	1.80	0.42
1:A:65:ALA:HA	1:A:68:LYS:HD3	2.02	0.41
1:A:503:PHE:N	1:A:503:PHE:CD1	2.88	0.41
2:B:535:LYS:HA	2:B:535:LYS:HD3	1.83	0.41
2:B:544:ASN:HB2	2:B:579:PRO:HG3	2.01	0.41
2:B:960:ASN:OD1	2:B:964:LYS:NZ	2.51	0.41
2:B:1001:LEU:HD23	2:B:1001:LEU:HA	1.83	0.41
2:C:119:ILE:HG22	2:C:119:ILE:O	2.20	0.41
2:D:97:LYS:HD3	2:D:97:LYS:HA	1.89	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:367:ASP:HA	1:E:370:THR:HG22	2.01	0.41
1:E:442:ALA:HA	1:E:587:PHE:HE2	1.84	0.41
2:B:126:VAL:HG21	2:B:170:TYR:CZ	2.55	0.41
2:B:378:LYS:NZ	2:D:484:LYS:HB3	2.35	0.41
2:B:397:ALA:HA	2:B:513:LEU:HA	2.01	0.41
2:B:907:ASN:HD22	2:D:1107:ARG:NH2	2.18	0.41
2:B:1004:LEU:HD12	2:B:1004:LEU:HA	1.86	0.41
2:C:327:VAL:HA	2:C:542:ASN:HB3	2.02	0.41
2:C:344:ALA:HB3	2:C:347:PHE:CE1	2.55	0.41
2:C:386:LYS:HE2	2:C:386:LYS:HB2	1.90	0.41
2:C:490:PHE:CE2	2:C:492:LEU:HB2	2.56	0.41
2:C:582:LEU:HD23	2:C:582:LEU:HA	1.92	0.41
1:E:48:TRP:CD1	1:E:350:LEU:HD21	2.54	0.41
1:E:576:LYS:HE2	1:E:576:LYS:HB3	1.88	0.41
1:A:34:HIS:HA	1:A:37:GLU:OE1	2.20	0.41
2:B:566:GLY:HA3	2:B:575:ALA:HB3	2.02	0.41
2:B:1102:TRP:HB3	2:B:1115:ILE:HD11	2.01	0.41
2:C:203:ILE:HD12	2:C:203:ILE:N	2.35	0.41
2:C:941:THR:HG21	2:C:944:ALA:HB2	2.03	0.41
2:D:44:ARG:HD2	2:D:47:VAL:HG21	2.01	0.41
2:C:558:LYS:HA	2:C:558:LYS:HD3	1.88	0.41
2:D:453:TYR:OH	2:D:493:GLN:NE2	2.38	0.41
1:E:278:TYR:HE1	1:E:443:LEU:HB2	1.85	0.41
1:A:300:SER:O	1:A:300:SER:OG	2.30	0.41
2:B:128:ILE:HD13	2:B:128:ILE:HA	1.86	0.41
2:B:326:ILE:HG13	2:B:541:PHE:HA	2.02	0.41
2:B:592:PHE:HE2	2:C:857:GLY:HA2	1.84	0.41
2:B:646:ARG:HH12	2:C:834:ILE:HD12	1.86	0.41
2:C:599:THR:HB	2:C:608:VAL:HG12	2.02	0.41
2:D:436:TRP:NE1	2:D:438:SER:OG	2.54	0.41
2:D:993:ILE:O	2:D:997:ILE:HG12	2.21	0.41
1:E:520:TYR:HB3	1:E:524:PHE:CZ	2.55	0.41
1:A:610:THR:HG23	1:A:613:SER:HB3	2.03	0.41
2:B:84:LEU:O	2:B:238:PHE:N	2.53	0.41
2:B:375:PHE:N	2:B:435:ALA:O	2.53	0.41
2:B:584:ILE:HD12	2:B:584:ILE:HA	1.84	0.41
2:B:707:TYR:CE1	2:C:897:PRO:HA	2.53	0.41
2:B:1091:ARG:HB3	2:B:1092:GLU:OE1	2.21	0.41
2:C:521:PRO:HB2	2:D:230:PRO:HB2	2.03	0.41
2:C:1029:MET:CE	2:C:1053:PRO:HB3	2.50	0.41
1:E:325:GLY:O	1:E:329:ASN:ND2	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:LEU:HD23	1:A:39:LEU:HA	1.83	0.41
1:A:481:ARG:HA	1:A:486:VAL:H	1.85	0.41
2:B:426:PRO:HG2	2:B:429:PHE:HB2	2.03	0.41
2:B:697:MET:HB3	2:C:869:MET:HE1	2.03	0.41
2:B:826:VAL:HB	2:B:1057:PRO:HG2	2.03	0.41
2:B:901:GLN:HE21	2:B:905:ARG:HH21	1.69	0.41
2:C:1013:ILE:HD13	2:D:1012:LEU:HB3	2.02	0.41
1:E:303:ALA:O	1:E:307:PHE:HD1	2.03	0.41
1:A:55:THR:O	1:A:59:VAL:HG13	2.21	0.41
1:A:236:TYR:HD1	1:A:239:LEU:HD21	1.86	0.41
2:C:644:GLN:NE2	2:C:645:THR:O	2.44	0.41
2:C:854:LYS:HD2	2:C:854:LYS:HA	1.83	0.41
1:A:48:TRP:CD1	1:A:356:ARG:HD3	2.56	0.41
1:A:483:ILE:HD13	1:A:483:ILE:HA	1.94	0.41
1:A:575:ILE:HD11	1:A:579:ASP:HB2	2.03	0.41
2:B:318:PHE:HD2	2:B:629:LEU:HD11	1.86	0.41
2:B:538:CYS:HB3	2:B:590:CYS:SG	2.60	0.41
2:B:645:THR:HG22	2:B:647:ALA:H	1.86	0.41
2:B:1098:ASN:OD1	2:B:1099:GLY:N	2.54	0.41
2:C:188:ASN:HA	2:C:209:PRO:HB3	2.02	0.41
2:C:240:THR:HB	2:C:265:TYR:OH	2.21	0.41
2:C:699:LEU:HB2	2:D:788:ILE:HD11	2.03	0.41
2:D:452:TRP:CZ3	2:D:494:SER:HA	2.55	0.41
2:D:869:MET:HE3	2:D:869:MET:HB2	2.03	0.41
2:D:959:LEU:O	2:D:963:VAL:HG23	2.21	0.41
2:D:976:VAL:CG1	2:D:979:ASP:HB2	2.48	0.41
1:E:59:VAL:O	1:E:62:MET:HG2	2.21	0.41
1:E:91:LEU:HD12	1:E:91:LEU:HA	1.95	0.41
1:E:111:GLU:HA	1:E:114:LYS:HG2	2.03	0.41
1:E:343:CYS:HB2	1:E:360:CYS:H	1.85	0.41
1:A:94:LYS:HE3	1:A:94:LYS:HB3	1.72	0.41
2:B:126:VAL:HG13	2:B:175:PHE:HB2	2.03	0.41
2:B:406:GLU:O	2:B:409:GLN:HG2	2.21	0.41
2:B:1102:TRP:CZ2	2:B:1133:VAL:HG11	2.55	0.41
2:C:105:ILE:HB	2:C:239:GLN:HB3	2.02	0.41
2:C:387:LEU:H	2:C:387:LEU:HD23	1.86	0.41
2:C:802:PHE:CD1	2:C:805:ILE:HD11	2.55	0.41
2:C:830:ASP:HA	2:C:850:ILE:HG12	2.03	0.41
2:D:127:PHE:C	2:D:127:PHE:CD1	2.94	0.41
1:A:186:GLU:HA	1:A:189:MET:HG2	2.03	0.40
2:B:188:ASN:HA	2:B:207:HIS:NE2	2.35	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:458:LYS:HA	2:C:458:LYS:HD3	1.81	0.40
2:C:717:ASN:HB3	2:C:1070:ALA:HB3	2.02	0.40
2:C:993:ILE:O	2:C:997:ILE:HG13	2.21	0.40
2:D:323:THR:OG1	2:D:324:GLU:N	2.55	0.40
2:D:479:PRO:O	2:D:481:LYS:NZ	2.54	0.40
1:E:263:ALA:HB3	1:E:489:PRO:HD3	2.02	0.40
1:A:112:LYS:HA	1:A:115:ARG:HG2	2.02	0.40
2:B:444:LYS:HE2	2:B:444:LYS:HB2	1.88	0.40
2:C:30:ASN:HB3	2:C:32:PHE:CE1	2.56	0.40
2:C:33:THR:HG23	2:C:58:PHE:CZ	2.56	0.40
2:C:50:LEU:HD13	2:C:276:LEU:HD12	2.03	0.40
2:C:770:ILE:O	2:C:774:GLN:HG2	2.21	0.40
2:D:87:ASN:OD1	2:D:87:ASN:N	2.47	0.40
2:D:878:LEU:HD12	2:D:878:LEU:HA	1.88	0.40
2:D:1038:LYS:HB3	2:D:1038:LYS:HE2	1.76	0.40
2:D:1098:ASN:CG	2:D:1101:HIS:H	2.23	0.40
1:E:224:ASP:O	1:E:228:THR:HG23	2.21	0.40
1:E:260:CYS:HB3	1:E:485:GLY:C	2.41	0.40
1:E:422:LEU:H	1:E:422:LEU:HD12	1.86	0.40
1:A:373:HIS:CD2	1:A:404:GLY:HA3	2.56	0.40
1:A:406:ILE:HG21	1:A:524:PHE:HB2	2.03	0.40
1:A:449:LEU:HD12	1:A:518:THR:HG21	2.03	0.40
2:B:589:PRO:HD3	2:C:855:PHE:HB2	2.03	0.40
2:B:809:PRO:HA	2:B:814:LYS:HE3	2.03	0.40
2:C:752:LEU:HD23	2:C:993:ILE:HG22	2.02	0.40
1:A:48:TRP:CZ2	1:A:356:ARG:HB3	2.56	0.40
1:A:65:ALA:O	1:A:68:LYS:HG2	2.21	0.40
1:A:359:MET:HB2	1:A:359:MET:HE2	1.87	0.40
2:B:847:ARG:HE	2:B:847:ARG:HB2	1.61	0.40
2:C:295:PRO:HG3	2:C:633:TRP:CE3	2.56	0.40
2:D:329:PHE:O	2:D:580:GLN:NE2	2.53	0.40
2:D:503:VAL:HA	2:D:506:GLN:HG2	2.02	0.40
2:D:643:PHE:O	2:D:650:LEU:N	2.40	0.40
2:D:905:ARG:HD2	2:D:1049:LEU:O	2.22	0.40
2:D:930:ALA:O	2:D:934:ILE:HG23	2.22	0.40
1:E:469:LYS:HA	1:E:469:LYS:HD3	1.68	0.40
1:E:519:ILE:HG13	1:E:520:TYR:N	2.35	0.40
1:A:236:TYR:HA	1:A:239:LEU:HG	2.02	0.40
1:A:581:LYS:HA	1:A:581:LYS:HD2	1.89	0.40
2:B:718:PHE:HD1	2:B:1109:PHE:HE1	1.70	0.40
2:D:197:ILE:HG12	2:D:198:ASP:OD2	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:96:GLN:HG2	1:E:390:LEU:HB2	2.04	0.40
1:E:553:LEU:HD23	1:E:553:LEU:HA	1.82	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	594/596 (100%)	573 (96%)	21 (4%)	0	100	100
1	E	591/596 (99%)	570 (96%)	21 (4%)	0	100	100
2	B	1053/1120 (94%)	964 (92%)	87 (8%)	2 (0%)	44	72
2	C	1053/1120 (94%)	980 (93%)	73 (7%)	0	100	100
2	D	1053/1120 (94%)	993 (94%)	59 (6%)	1 (0%)	48	77
All	All	4344/4552 (95%)	4080 (94%)	261 (6%)	3 (0%)	50	77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	534	VAL
2	B	332	VAL
2	D	212	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	525/525 (100%)	507 (97%)	18 (3%)	32	58
1	E	524/525 (100%)	499 (95%)	25 (5%)	21	48
2	B	926/975 (95%)	883 (95%)	43 (5%)	23	50
2	C	925/975 (95%)	893 (96%)	32 (4%)	31	57
2	D	925/975 (95%)	897 (97%)	28 (3%)	36	62
All	All	3825/3975 (96%)	3679 (96%)	146 (4%)	30	54

All (146) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LYS
1	A	27	THR
1	A	155	ARG
1	A	198	TYR
1	A	276	ASN
1	A	296	MET
1	A	313	PHE
1	A	314	PHE
1	A	322	MET
1	A	331	MET
1	A	348	TRP
1	A	366	ASP
1	A	380	TYR
1	A	399	PHE
1	A	416	TYR
1	A	441	GLN
1	A	469	LYS
1	A	605	TRP
2	B	28	TYR
2	B	60	SER
2	B	64	TRP
2	B	65	PHE
2	B	91	TYR
2	B	113	LYS
2	B	129	LYS
2	B	160	TYR
2	B	170	TYR
2	B	175	PHE
2	B	182	LYS
2	B	216	PHE
2	B	228	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	238	PHE
2	B	275	PHE
2	B	409	GLN
2	B	453	TYR
2	B	464	PHE
2	B	469	SER
2	B	489	TYR
2	B	495	TYR
2	B	497	PHE
2	B	565	PHE
2	B	583	GLU
2	B	634	ARG
2	B	640	SER
2	B	649	CYS
2	B	658	ASN
2	B	674	TYR
2	B	675	GLN
2	B	740	MET
2	B	833	PHE
2	B	837	TYR
2	B	939	PHE
2	B	957	GLN
2	B	975	SER
2	B	983	ARG
2	B	1000	ARG
2	B	1014	ARG
2	B	1028	LYS
2	B	1041	ASP
2	B	1074	ASN
2	B	1107	ARG
2	C	60	SER
2	C	110	LEU
2	C	135	PHE
2	C	165	ASN
2	C	186	PHE
2	C	200	TYR
2	C	229	LEU
2	C	238	PHE
2	C	265	TYR
2	C	338	PHE
2	C	380	TYR
2	C	386	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	400	PHE
2	C	440	LYS
2	C	481	LYS
2	C	488	CYS
2	C	495	TYR
2	C	525	CYS
2	C	565	PHE
2	C	619	GLU
2	C	649	CYS
2	C	665	PRO
2	C	674	TYR
2	C	745	ASP
2	C	759	PHE
2	C	760	CYS
2	C	873	TYR
2	C	940	SER
2	C	947	LYS
2	C	992	GLN
2	C	1073	LYS
2	C	1139	ASP
2	D	46	SER
2	D	127	PHE
2	D	214	ARG
2	D	238	PHE
2	D	265	TYR
2	D	346	ARG
2	D	357	ARG
2	D	365	TYR
2	D	377	PHE
2	D	378	LYS
2	D	386	LYS
2	D	400	PHE
2	D	430	THR
2	D	440	LYS
2	D	495	TYR
2	D	501	TYR
2	D	586	ASP
2	D	592	PHE
2	D	660	TYR
2	D	802	PHE
2	D	843	ASP
2	D	873	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	895	GLN
2	D	957	GLN
2	D	981	LEU
2	D	1041	ASP
2	D	1075	PHE
2	D	1134	ASN
1	E	98	LYS
1	E	102	HIS
1	E	182	TYR
1	E	189	MET
1	E	202	TRP
1	E	206	TYR
1	E	227	ARG
1	E	257	PRO
1	E	273	PHE
1	E	274	TRP
1	E	284	PHE
1	E	327	TRP
1	E	358	LYS
1	E	365	MET
1	E	368	PHE
1	E	375	MET
1	E	389	TYR
1	E	392	ARG
1	E	437	PHE
1	E	511	PHE
1	E	515	TYR
1	E	522	PHE
1	E	567	LEU
1	E	586	TYR
1	E	605	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	523	GLN
1	A	545	ASN
2	C	165	ASN
2	D	343	ASN
2	D	804	GLN
2	D	957	GLN
2	D	1074	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	220	GLN
1	E	598	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

26 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
3	NAG	F	1	2,3	14,14,15	0.25	0	17,19,21	0.44	0
3	BMA	F	2	3	11,11,12	0.55	0	15,15,17	0.72	0
3	NAG	G	1	2,3	14,14,15	0.56	0	17,19,21	0.61	0
3	BMA	G	2	3	11,11,12	0.54	0	15,15,17	0.92	0
3	NAG	H	1	2,3	14,14,15	0.20	0	17,19,21	0.44	0
3	BMA	H	2	3	11,11,12	0.55	0	15,15,17	0.76	0
3	NAG	I	1	2,3	14,14,15	0.33	0	17,19,21	0.42	0
3	BMA	I	2	3	11,11,12	0.60	0	15,15,17	0.68	0
3	NAG	J	1	2,3	14,14,15	0.84	1 (7%)	17,19,21	0.83	0
3	BMA	J	2	3	11,11,12	0.51	0	15,15,17	0.97	1 (6%)
3	NAG	K	1	2,3	14,14,15	0.19	0	17,19,21	0.43	0
3	BMA	K	2	3	11,11,12	0.58	0	15,15,17	0.77	0
4	NAG	L	1	2,4	14,14,15	0.41	0	17,19,21	0.40	0
4	NAG	L	2	4	14,14,15	0.25	0	17,19,21	0.43	0
3	NAG	M	1	2,3	14,14,15	0.20	0	17,19,21	0.44	0
3	BMA	M	2	3	11,11,12	0.57	0	15,15,17	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	N	1	2,3	14,14,15	0.21	0	17,19,21	0.46	0
3	BMA	N	2	3	11,11,12	0.57	0	15,15,17	0.72	0
3	NAG	O	1	2,3	14,14,15	0.19	0	17,19,21	0.44	0
3	BMA	O	2	3	11,11,12	0.56	0	15,15,17	0.70	0
3	NAG	P	1	2,3	14,14,15	0.66	1 (7%)	17,19,21	0.71	0
3	BMA	P	2	3	11,11,12	0.50	0	15,15,17	0.91	0
3	NAG	Q	1	2,3	14,14,15	0.20	0	17,19,21	0.44	0
3	BMA	Q	2	3	11,11,12	0.52	0	15,15,17	0.77	0
3	NAG	R	1	2,3	14,14,15	0.23	0	17,19,21	0.41	0
3	BMA	R	2	3	11,11,12	0.58	0	15,15,17	0.77	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
3	NAG	F	1	2,3	-	2/6/23/26	0/1/1/1
3	BMA	F	2	3	-	0/2/19/22	0/1/1/1
3	NAG	G	1	2,3	-	2/6/23/26	0/1/1/1
3	BMA	G	2	3	-	0/2/19/22	0/1/1/1
3	NAG	H	1	2,3	-	0/6/23/26	0/1/1/1
3	BMA	H	2	3	-	0/2/19/22	0/1/1/1
3	NAG	I	1	2,3	-	2/6/23/26	0/1/1/1
3	BMA	I	2	3	-	0/2/19/22	0/1/1/1
3	NAG	J	1	2,3	-	2/6/23/26	0/1/1/1
3	BMA	J	2	3	-	0/2/19/22	0/1/1/1
3	NAG	K	1	2,3	-	2/6/23/26	0/1/1/1
3	BMA	K	2	3	-	0/2/19/22	0/1/1/1
4	NAG	L	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	L	2	4	-	1/6/23/26	0/1/1/1
3	NAG	M	1	2,3	-	2/6/23/26	0/1/1/1
3	BMA	M	2	3	-	0/2/19/22	0/1/1/1
3	NAG	N	1	2,3	-	2/6/23/26	0/1/1/1
3	BMA	N	2	3	-	0/2/19/22	0/1/1/1
3	NAG	O	1	2,3	-	2/6/23/26	0/1/1/1
3	BMA	O	2	3	-	0/2/19/22	0/1/1/1
3	NAG	P	1	2,3	-	2/6/23/26	0/1/1/1
3	BMA	P	2	3	-	0/2/19/22	0/1/1/1
3	NAG	Q	1	2,3	-	1/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	Q	2	3	-	0/2/19/22	0/1/1/1
3	NAG	R	1	2,3	-	4/6/23/26	0/1/1/1
3	BMA	R	2	3	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	1	NAG	O5-C1	-2.89	1.39	1.43
3	P	1	NAG	O5-C1	-2.28	1.40	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	2	BMA	C1-O5-C5	2.01	114.92	112.19

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	M	1	NAG	O5-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
4	L	1	NAG	O5-C5-C6-O6
3	J	1	NAG	O5-C5-C6-O6
3	O	1	NAG	O5-C5-C6-O6
3	P	1	NAG	O5-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
3	J	1	NAG	C4-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
4	L	1	NAG	C4-C5-C6-O6
3	R	1	NAG	C8-C7-N2-C2
3	R	1	NAG	O7-C7-N2-C2
3	P	1	NAG	C4-C5-C6-O6
3	K	1	NAG	O5-C5-C6-O6
3	M	1	NAG	C4-C5-C6-O6
3	O	1	NAG	C4-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
3	N	1	NAG	C4-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
3	R	1	NAG	C4-C5-C6-O6
3	N	1	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

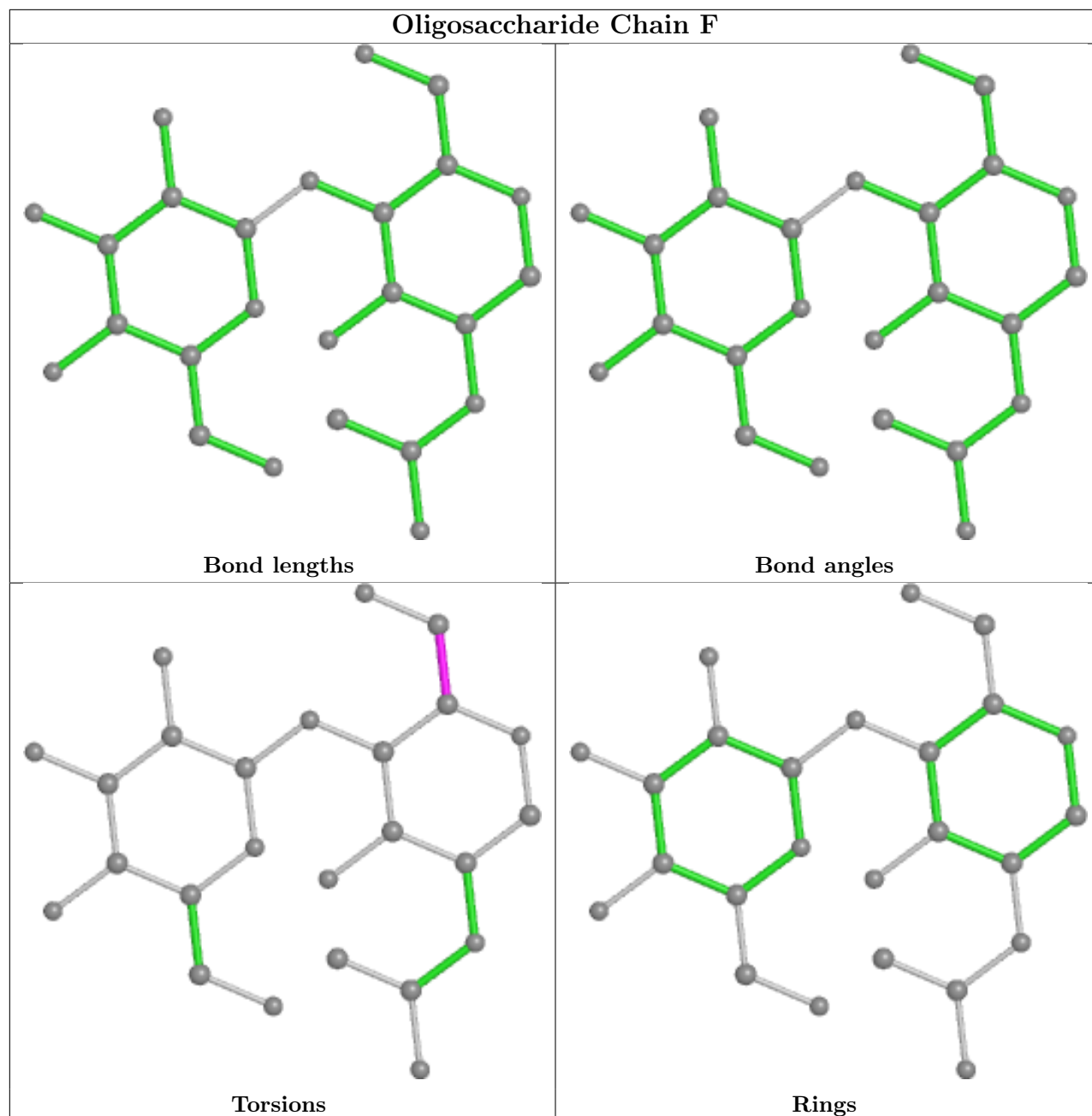
Mol	Chain	Res	Type	Atoms
3	R	1	NAG	O5-C5-C6-O6
3	K	1	NAG	C4-C5-C6-O6
3	Q	1	NAG	O5-C5-C6-O6
4	L	2	NAG	O5-C5-C6-O6

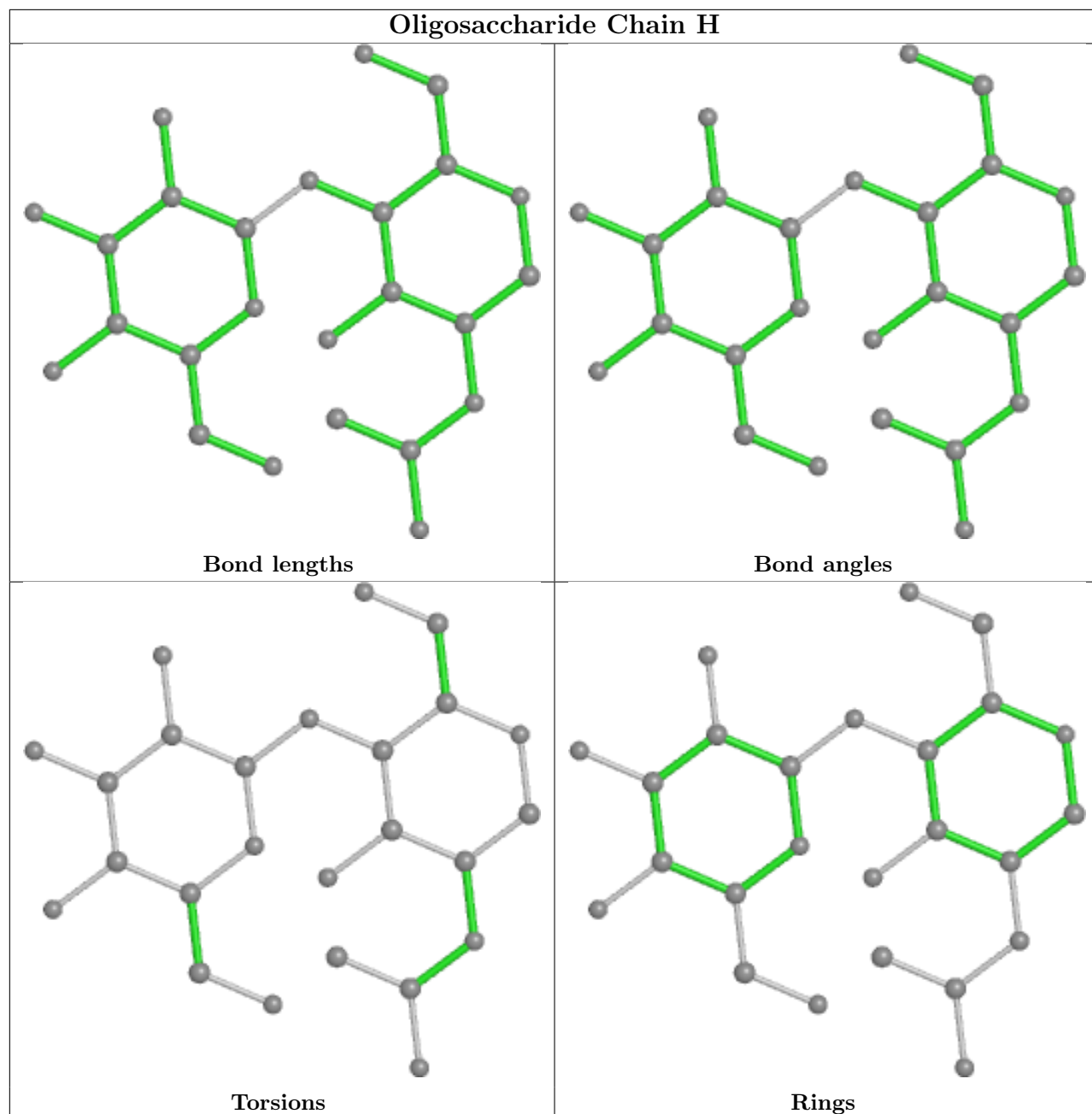
There are no ring outliers.

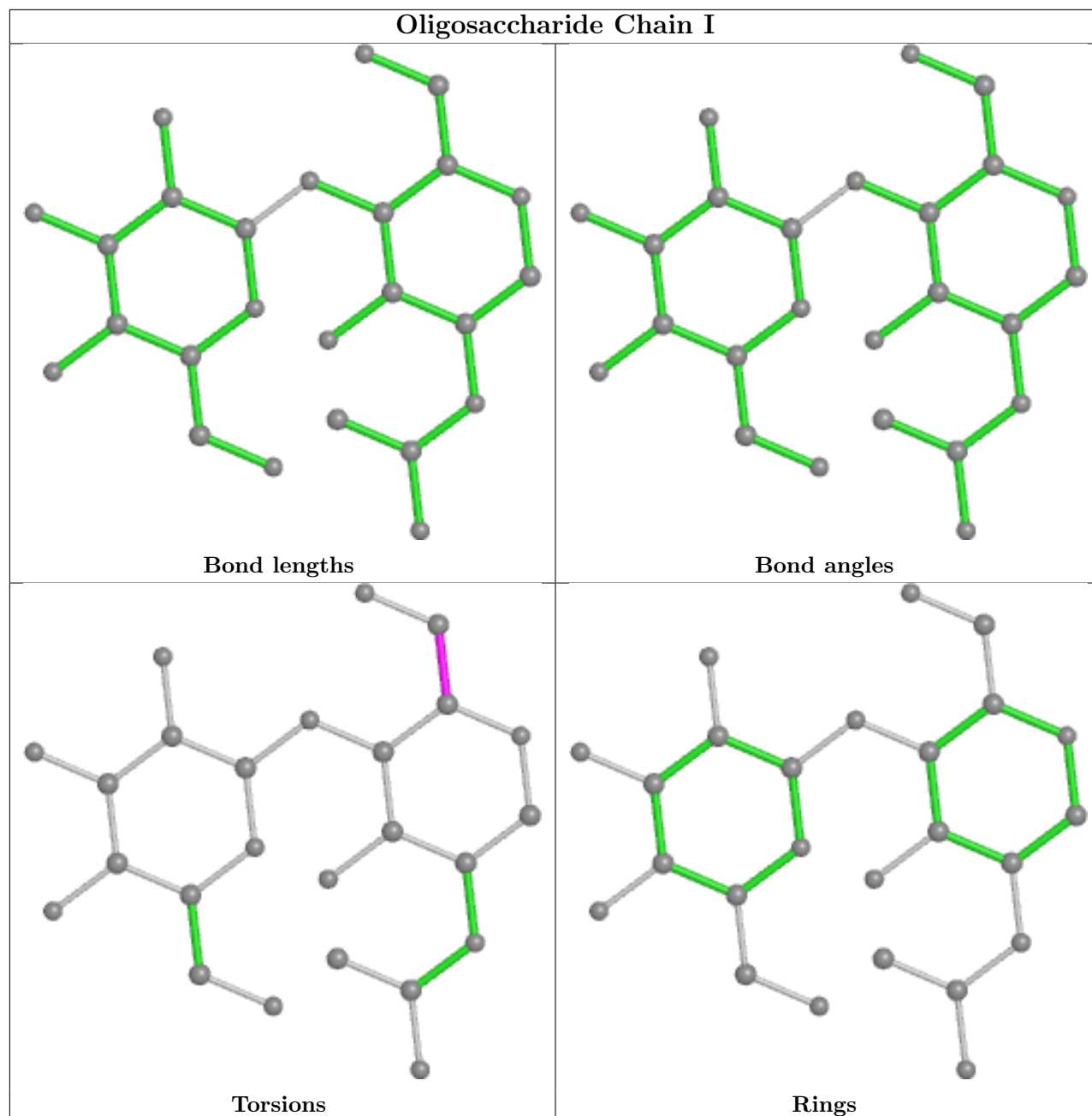
6 monomers are involved in 4 short contacts:

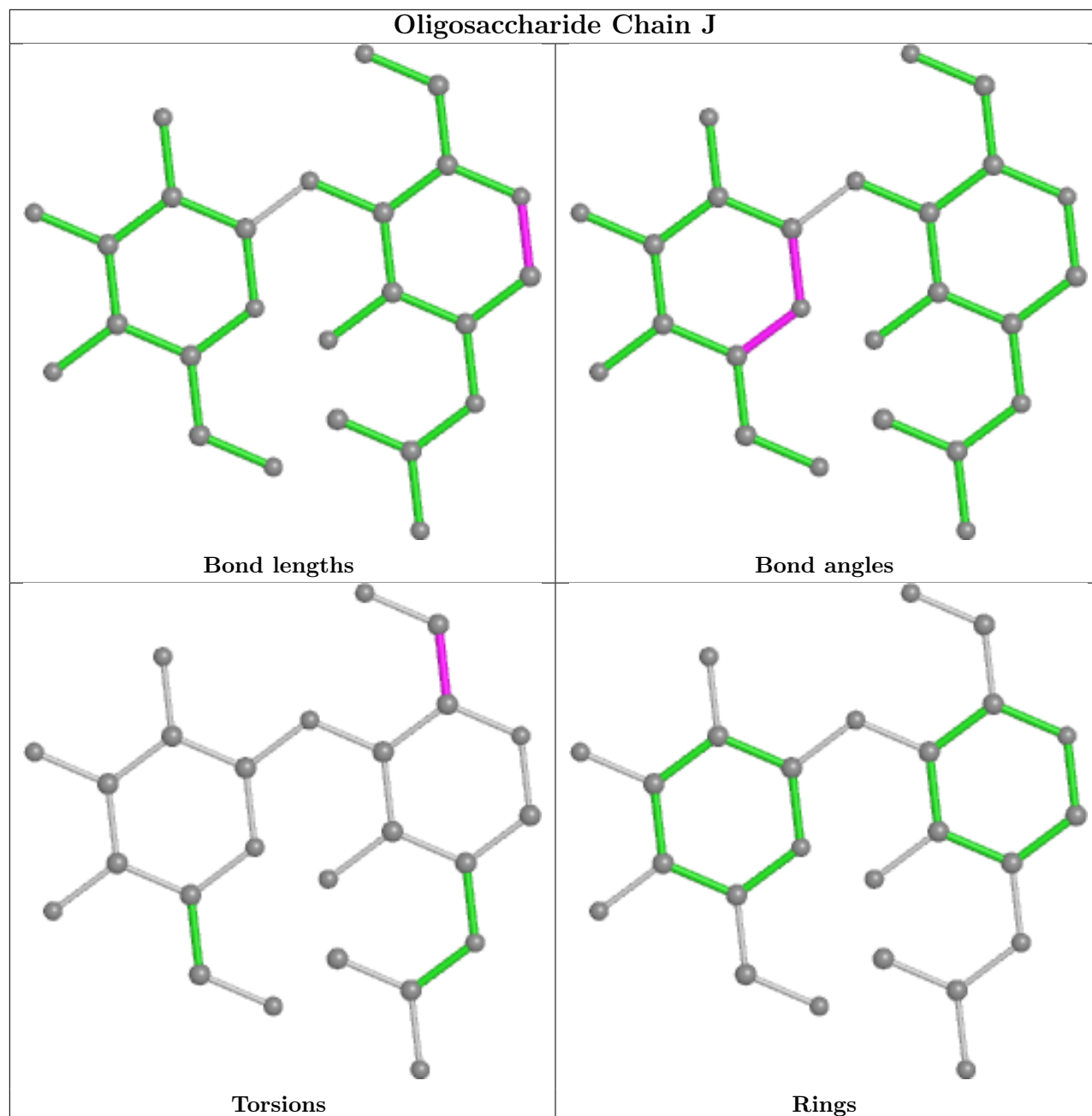
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	1	NAG	1	0
4	L	1	NAG	1	0
3	N	1	NAG	1	0
3	N	2	BMA	1	0
3	I	1	NAG	1	0
3	I	2	BMA	1	0

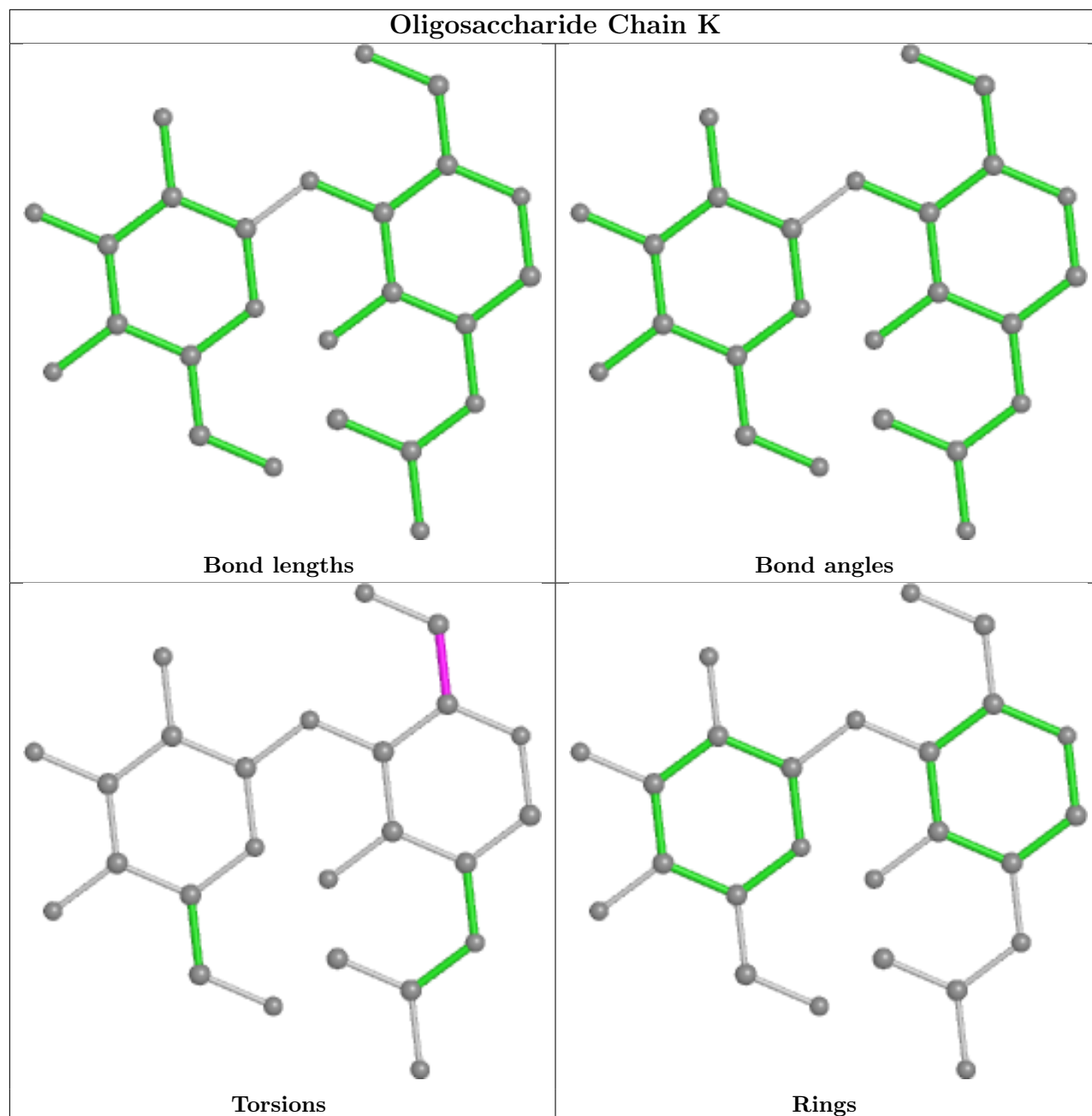
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

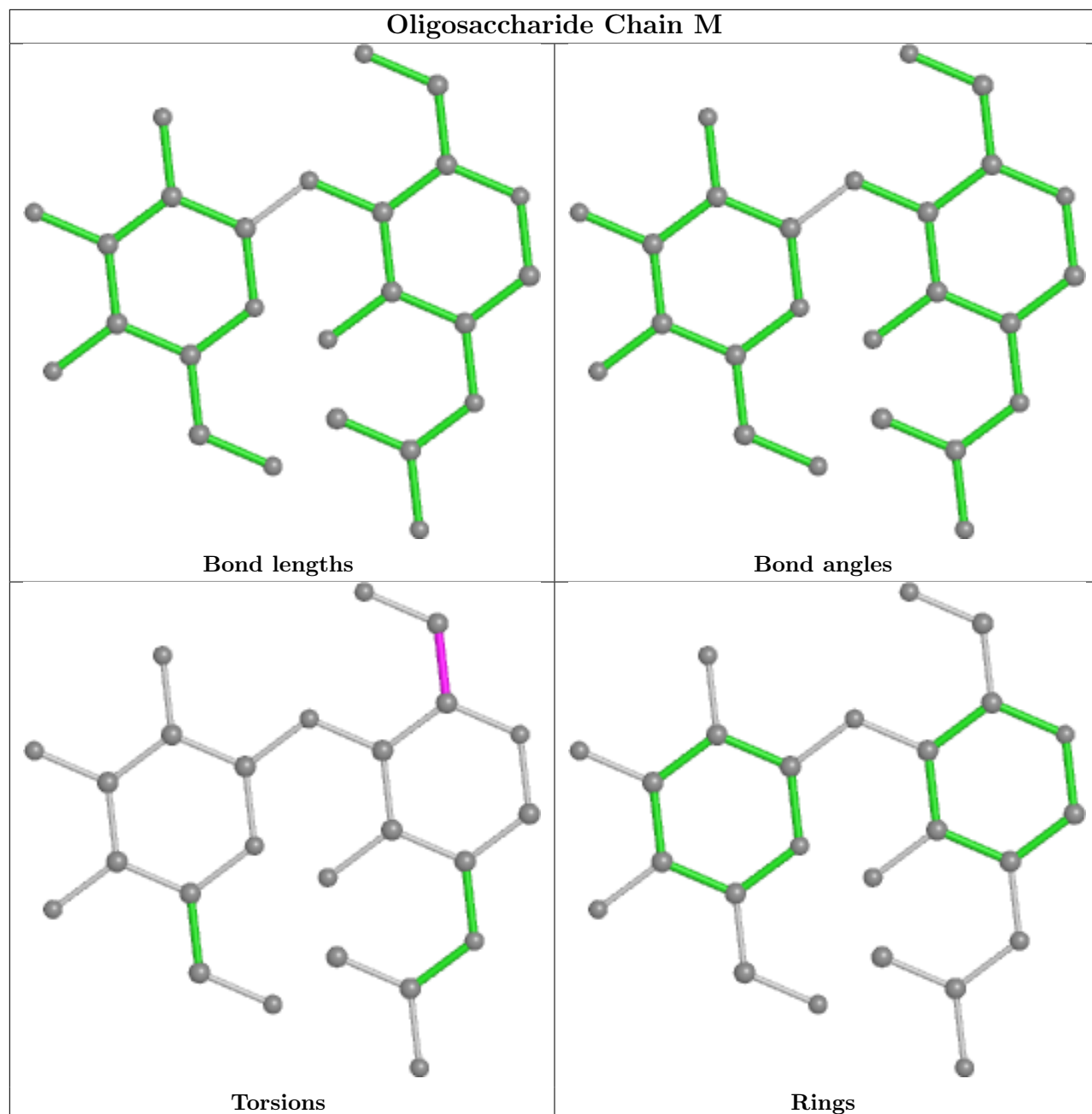


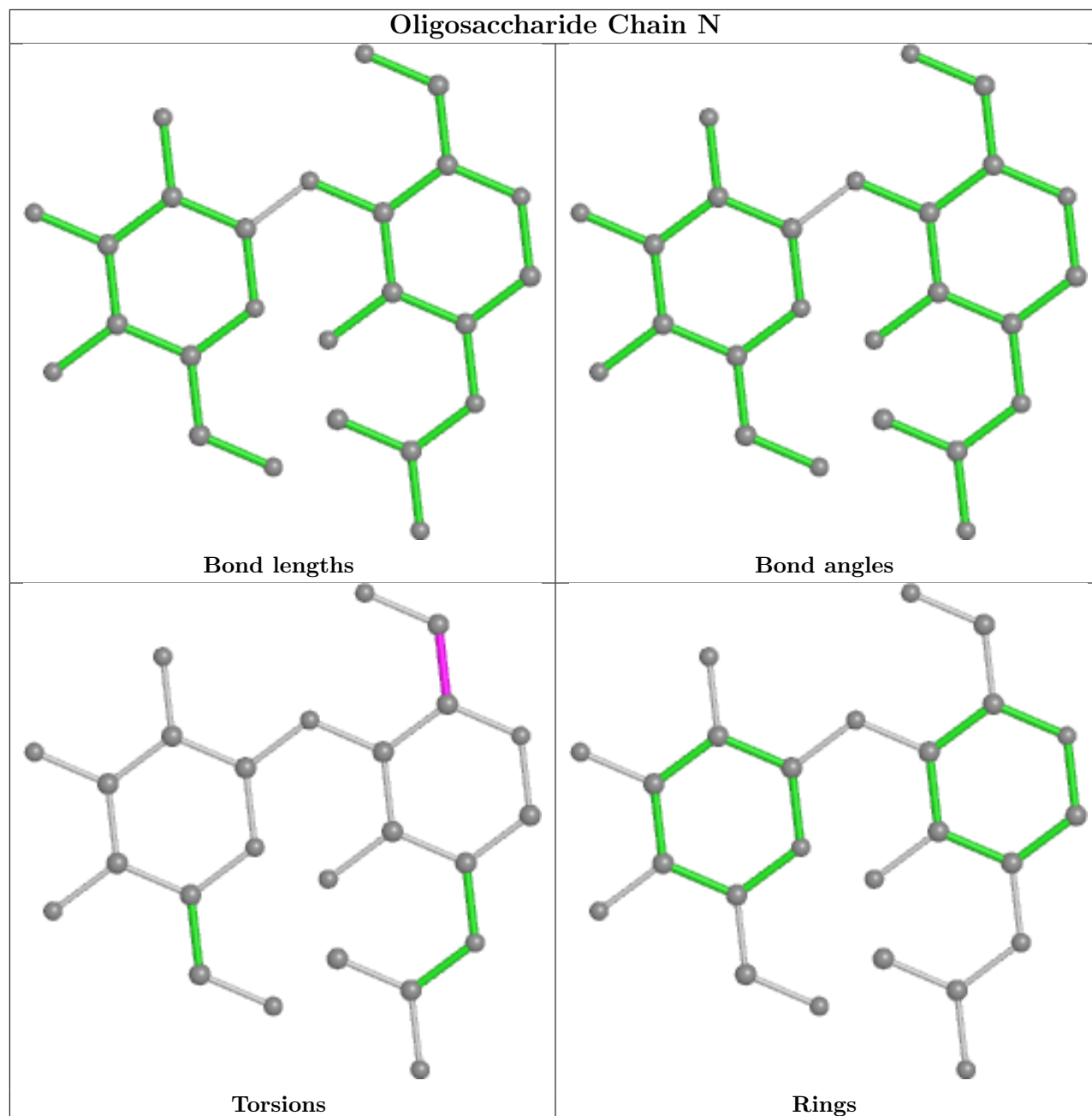


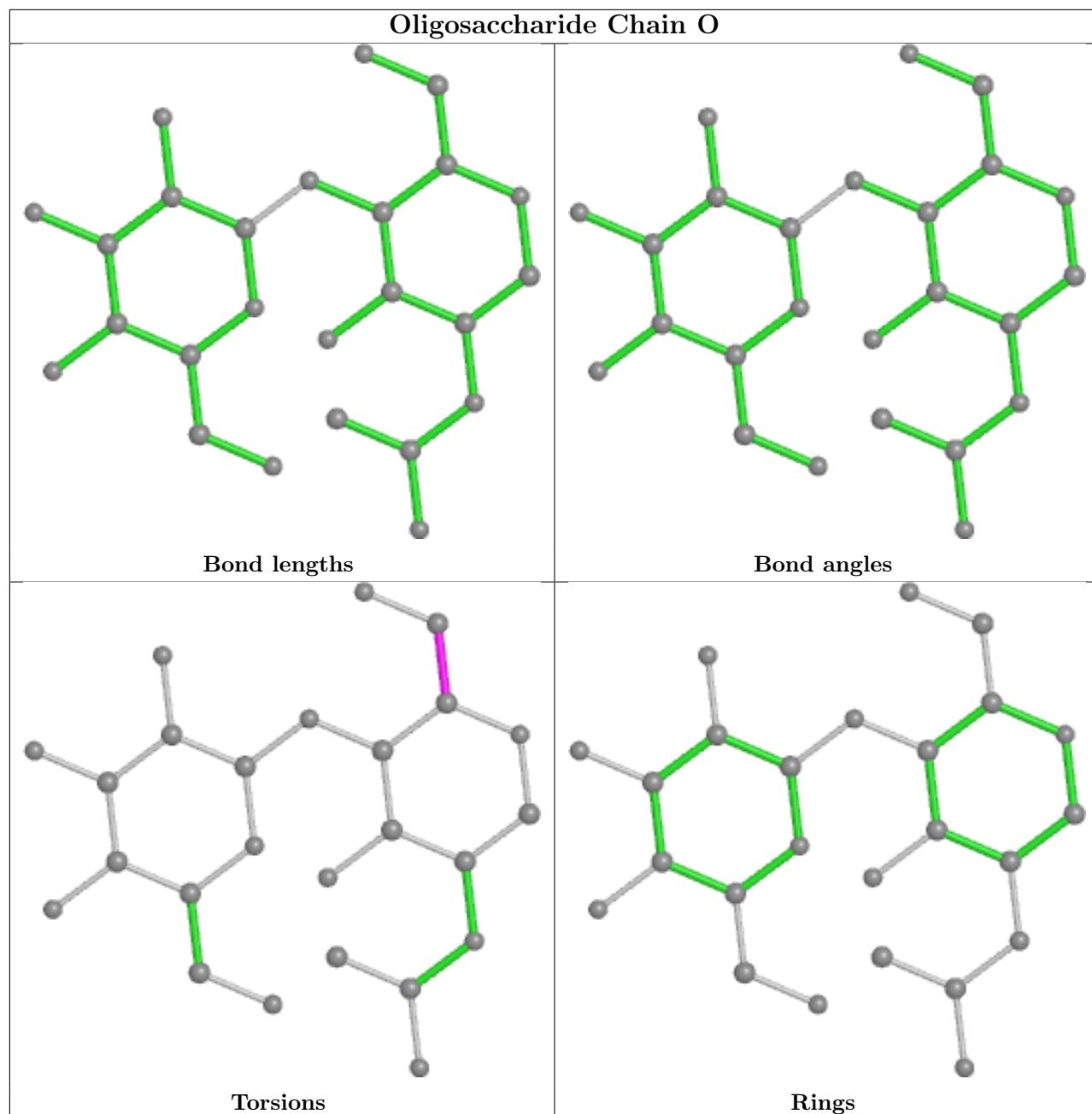


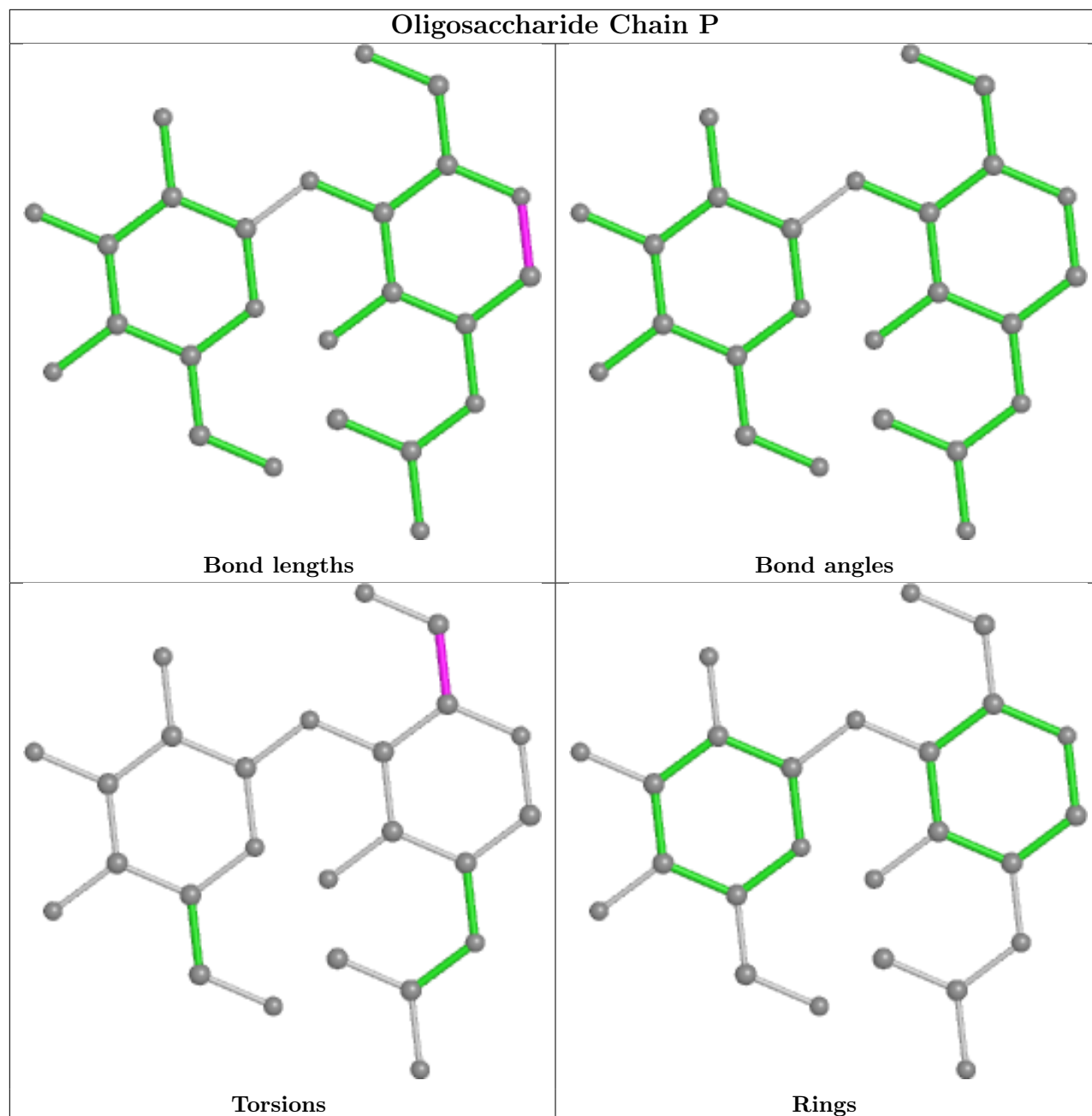


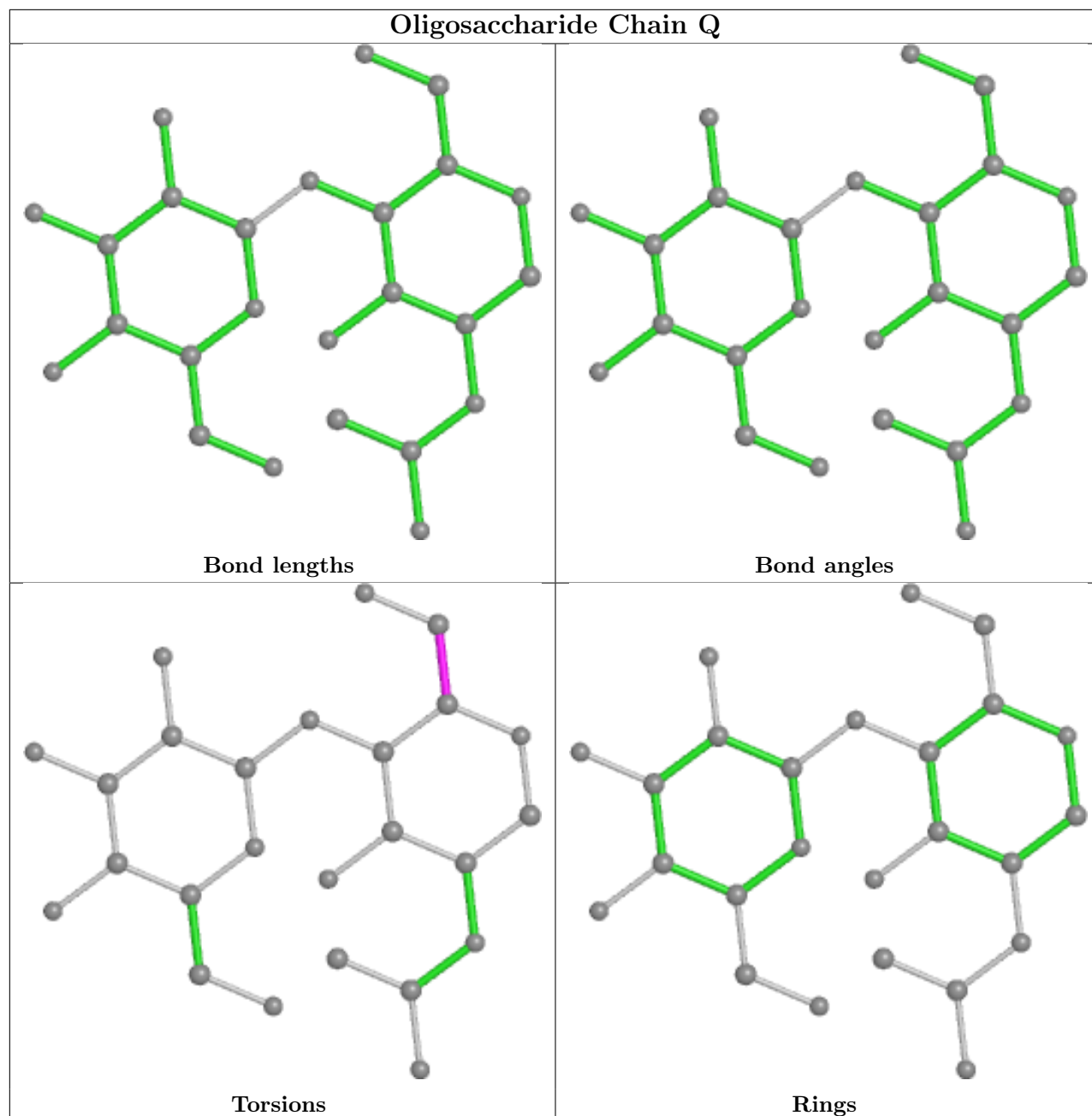


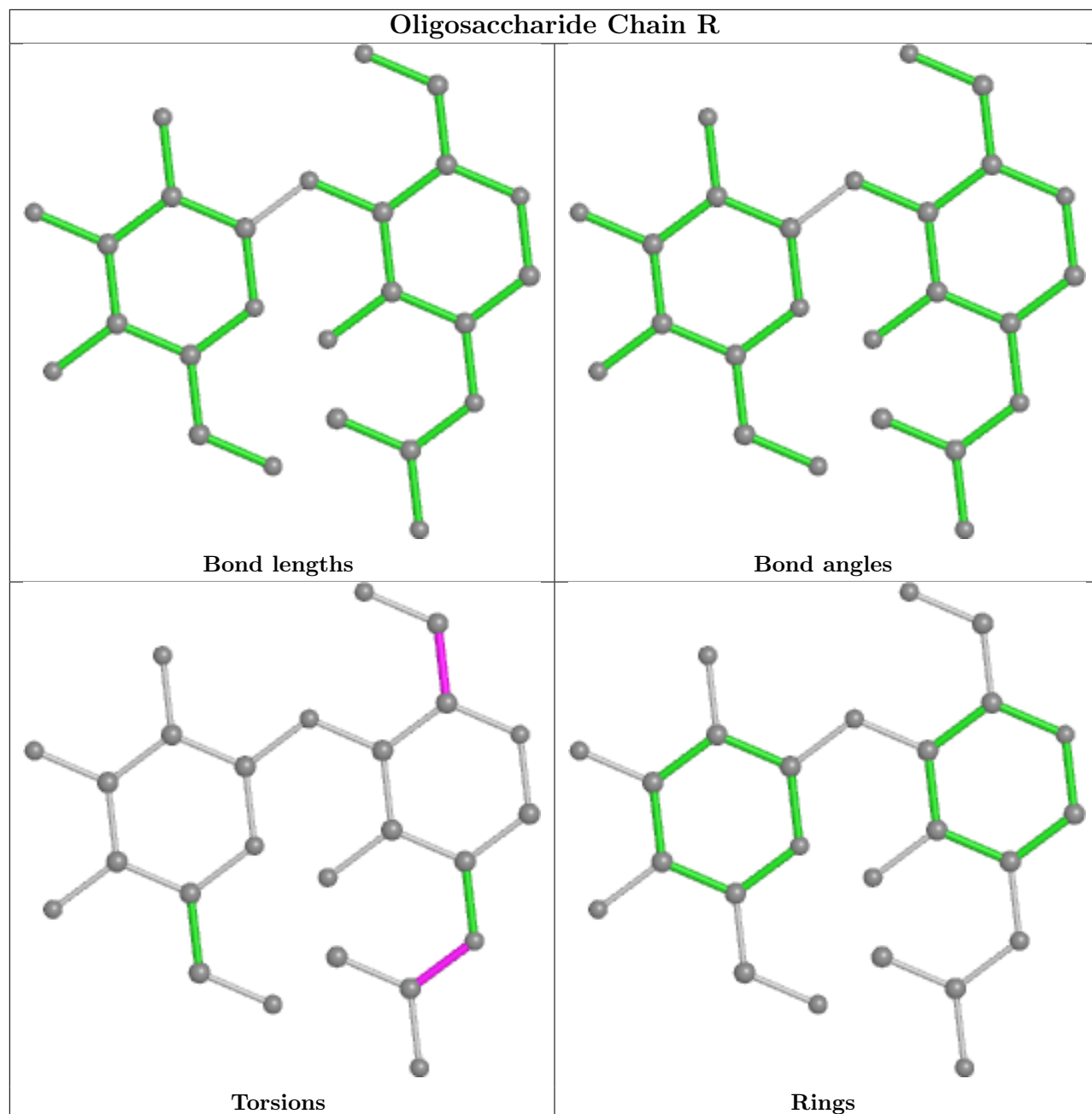


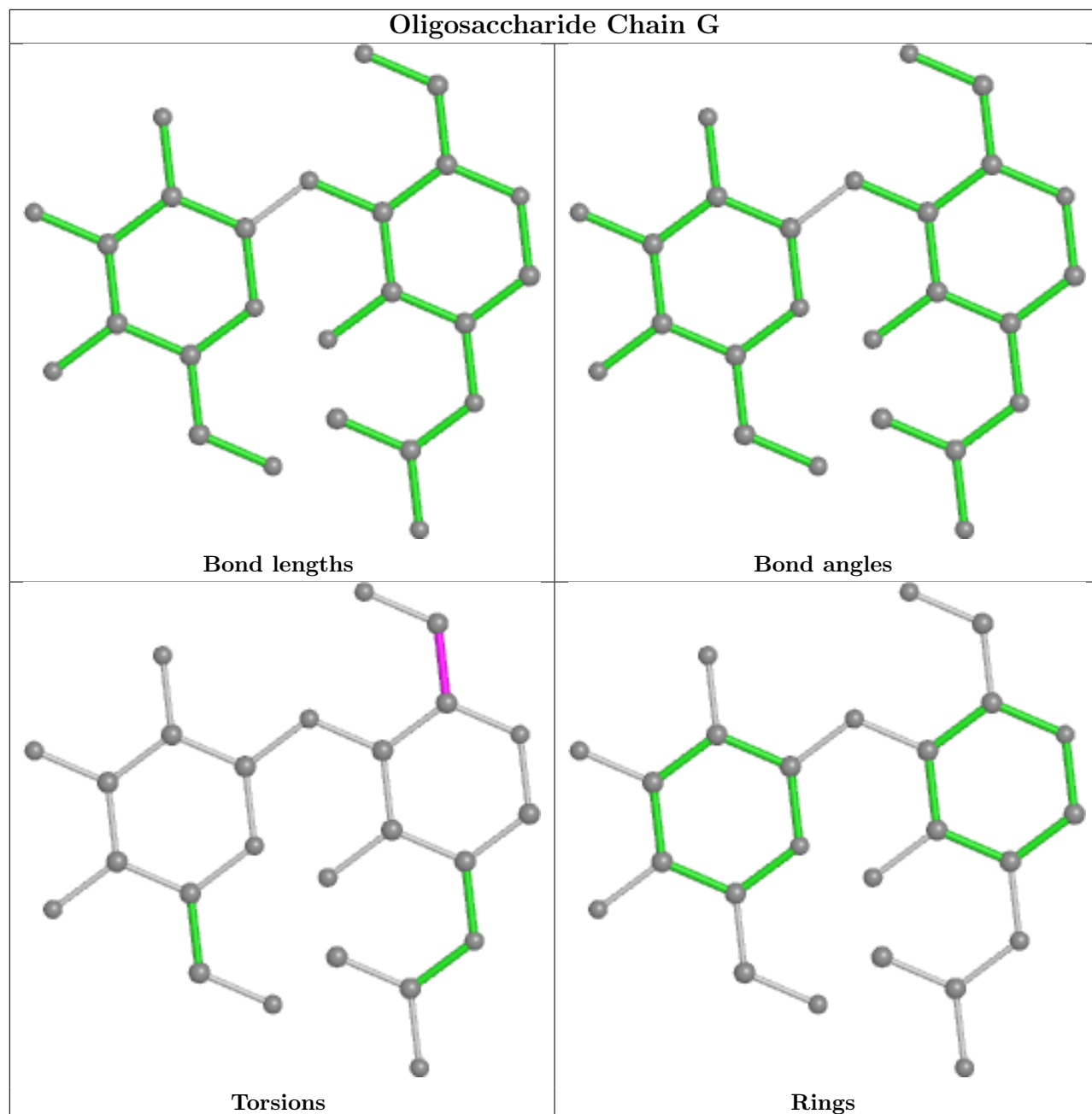


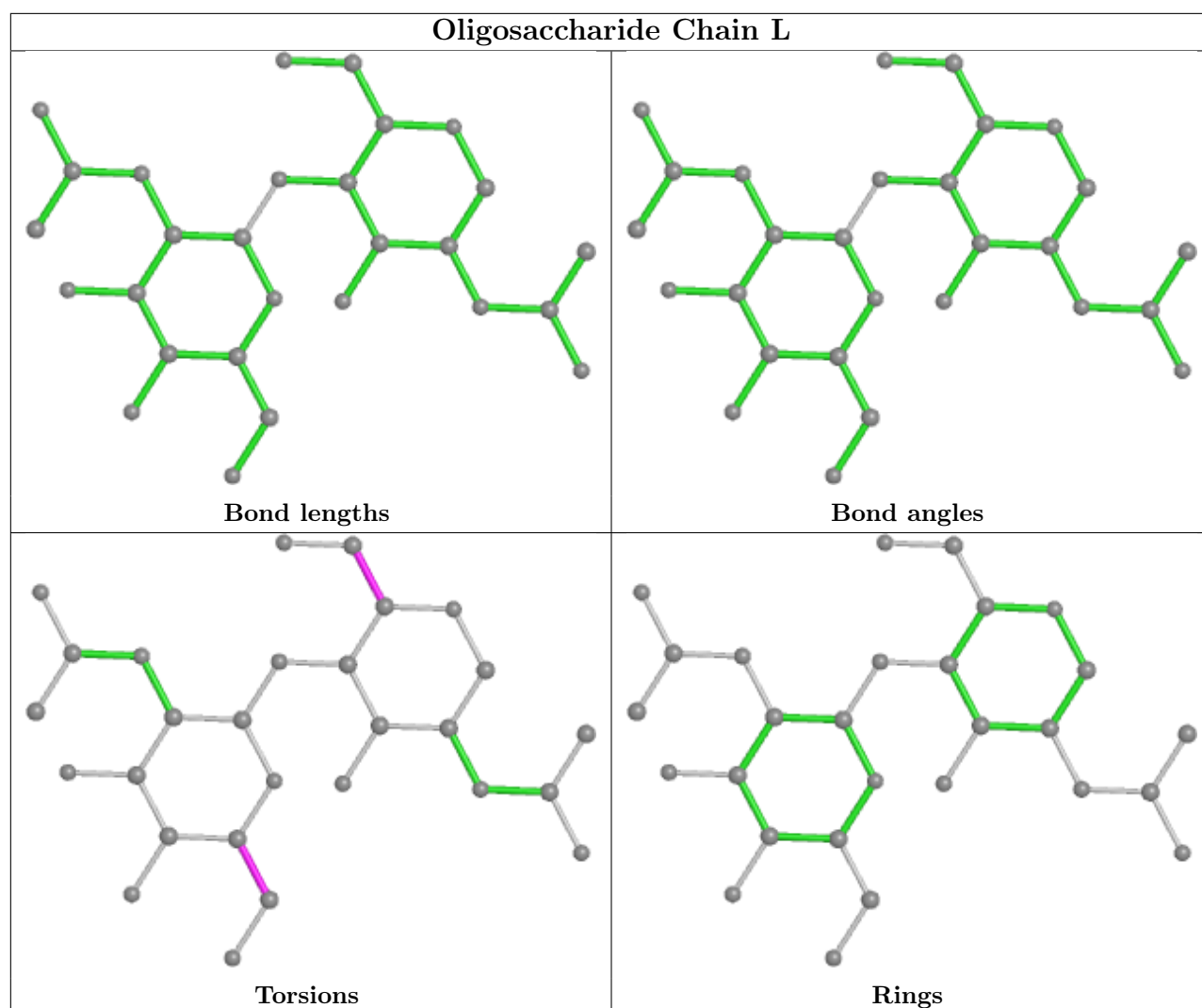












5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.

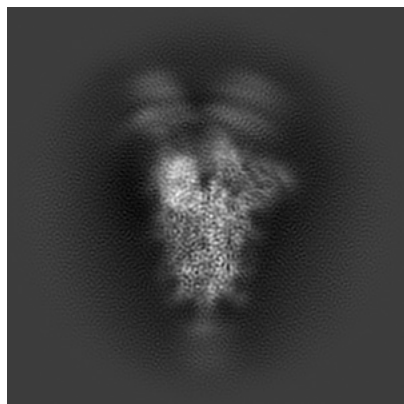
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38790. These allow visual inspection of the internal detail of the map and identification of artifacts.

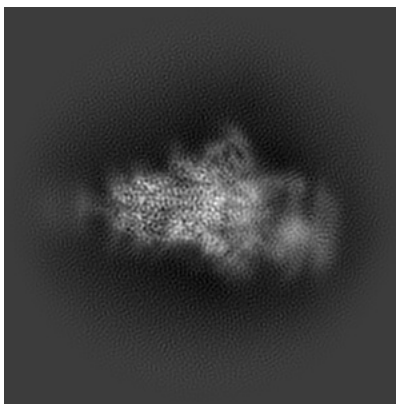
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

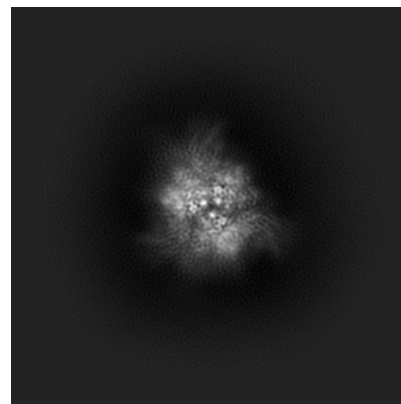
6.1.1 Primary map



X

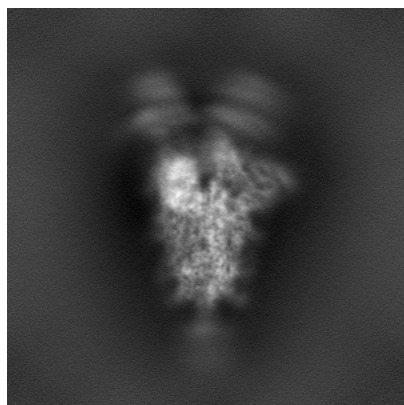


Y

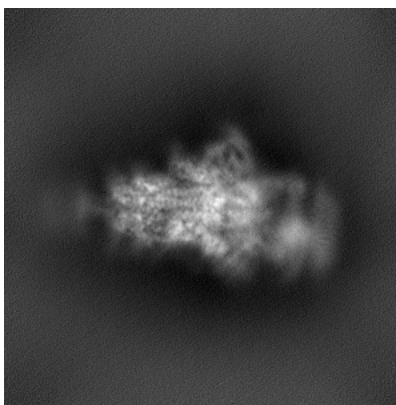


Z

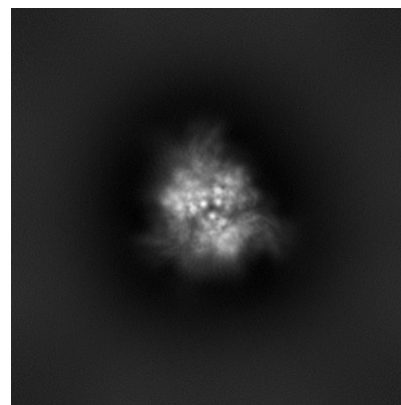
6.1.2 Raw map



X



Y

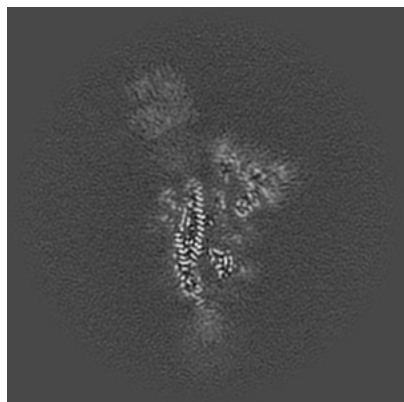


Z

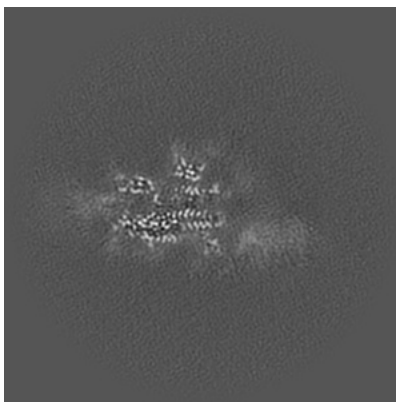
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

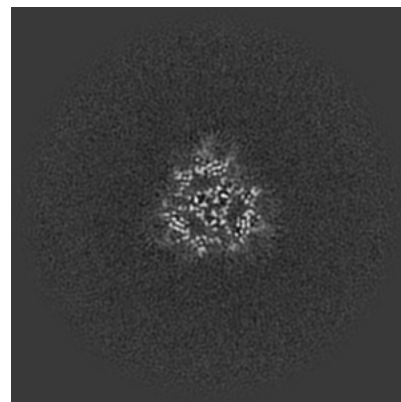
6.2.1 Primary map



X Index: 180

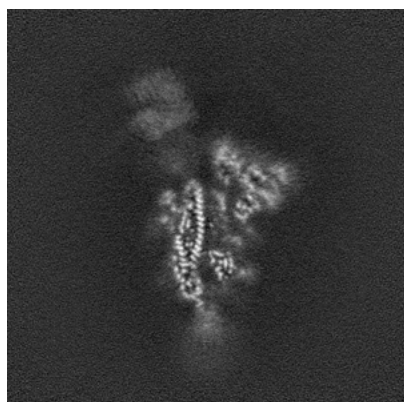


Y Index: 180

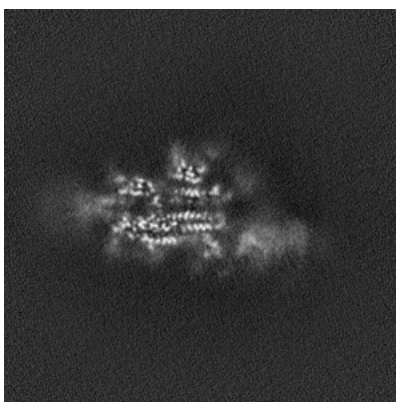


Z Index: 180

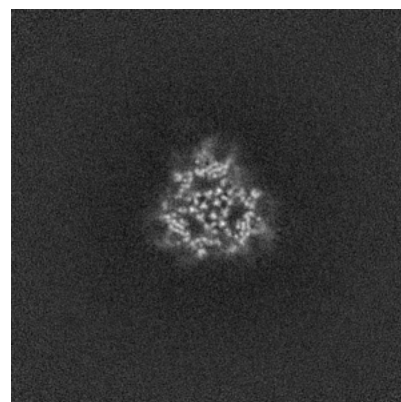
6.2.2 Raw map



X Index: 180



Y Index: 180

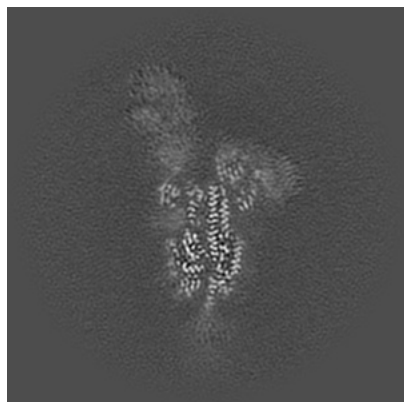


Z Index: 180

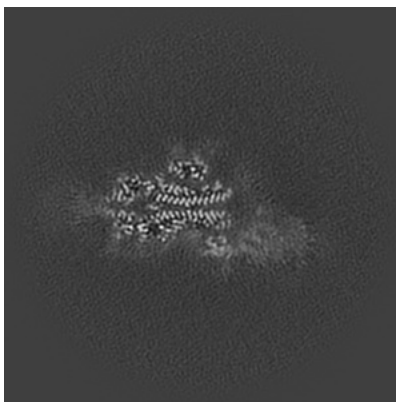
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

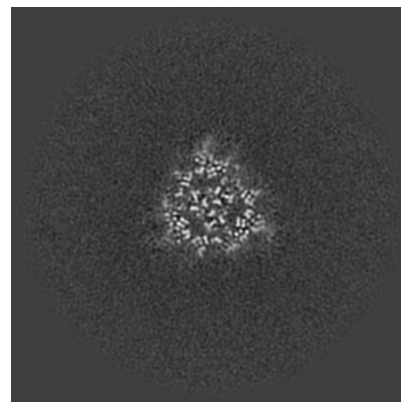
6.3.1 Primary map



X Index: 187

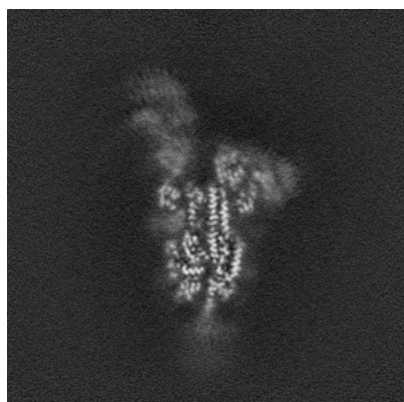


Y Index: 184

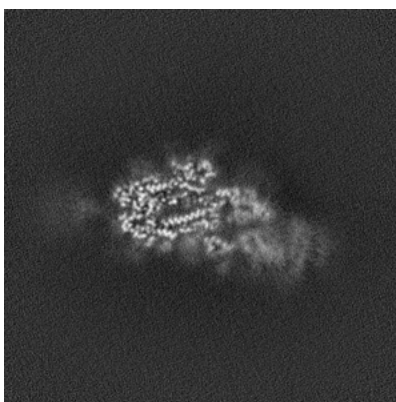


Z Index: 181

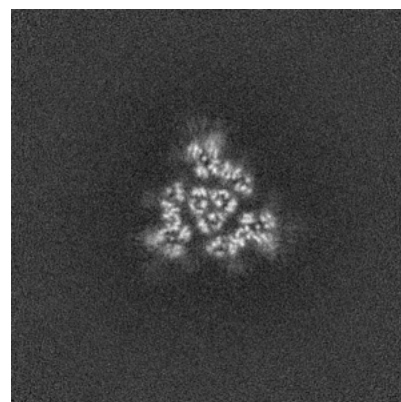
6.3.2 Raw map



X Index: 187



Y Index: 192

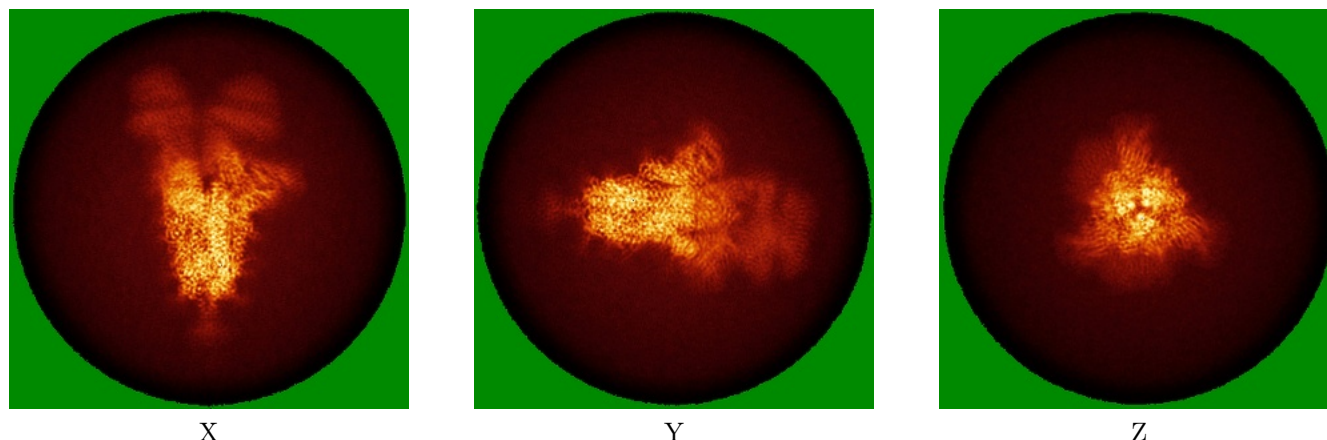


Z Index: 191

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

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

6.4.1 Primary map

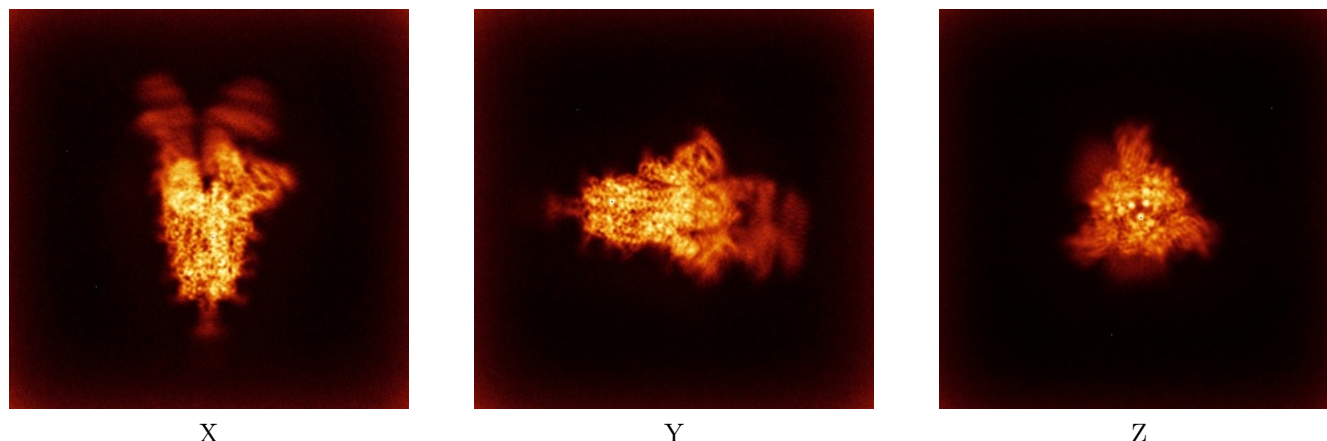


X

Y

Z

6.4.2 Raw map



X

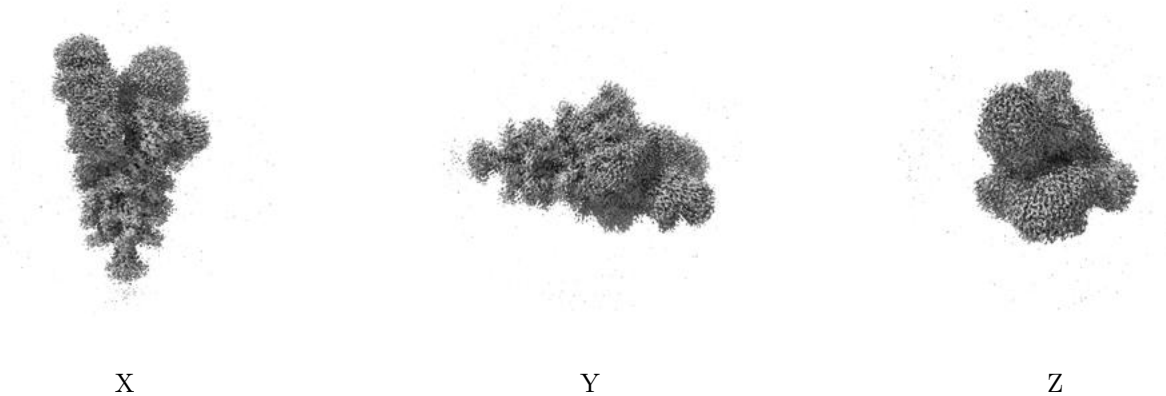
Y

Z

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

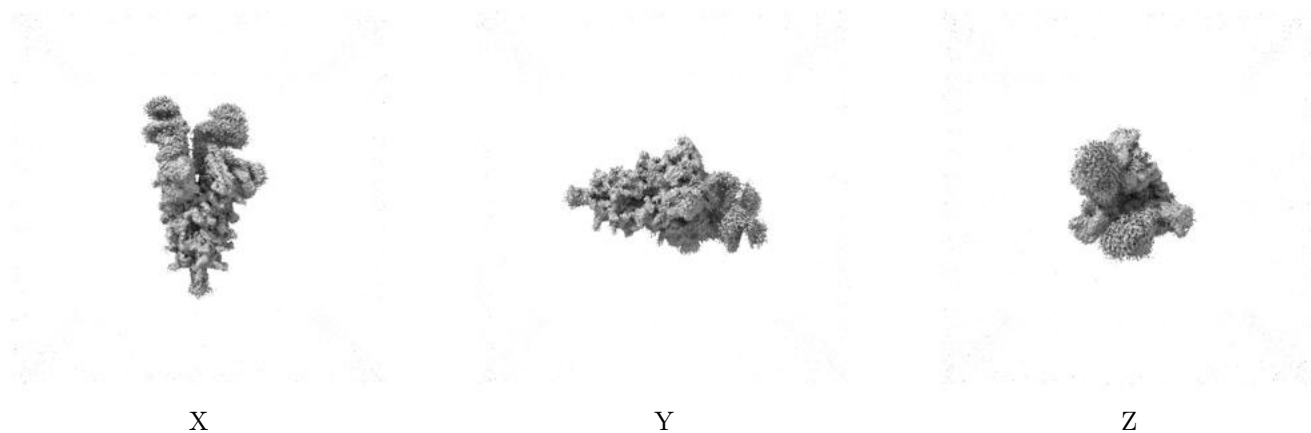
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. 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.

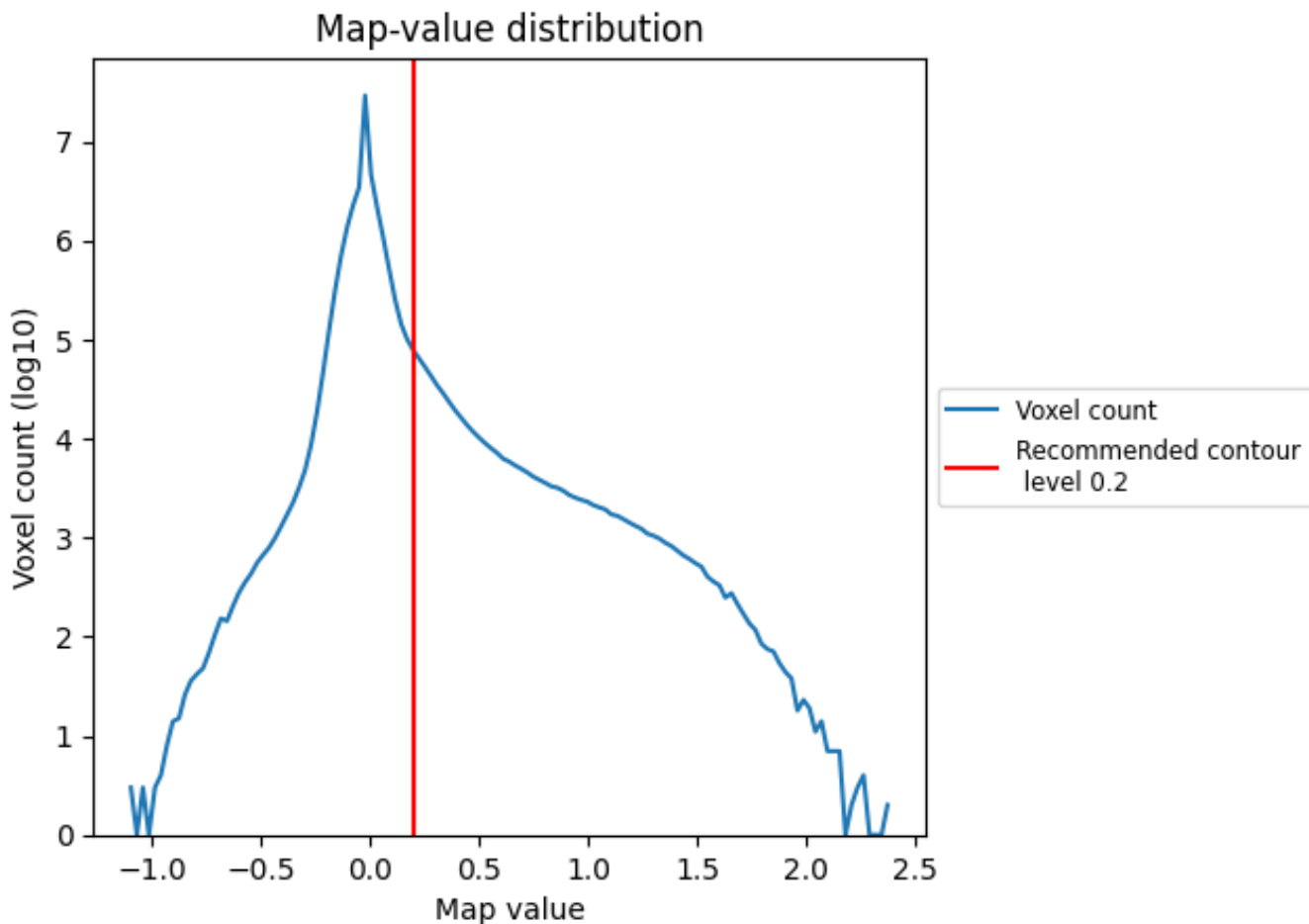
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

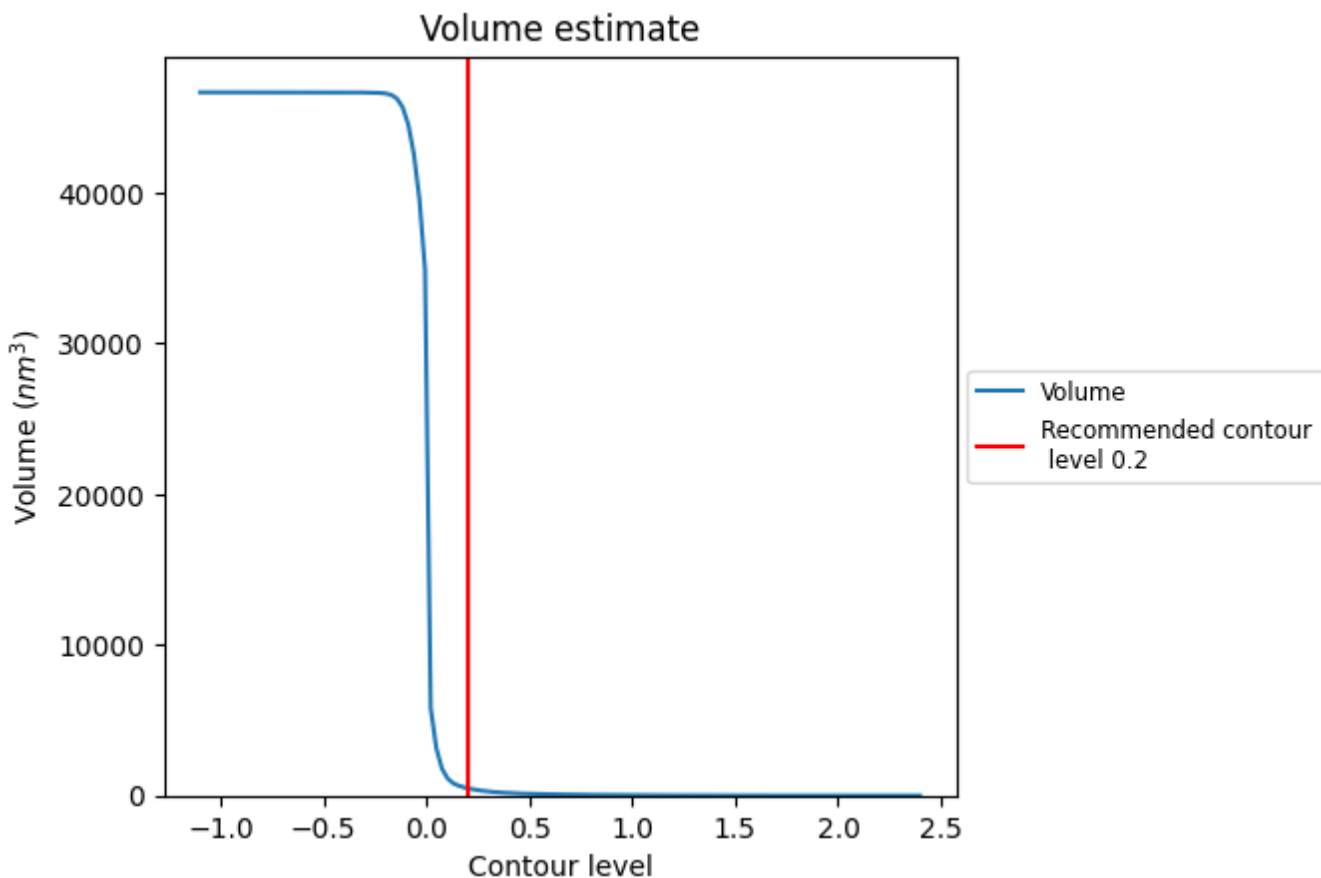
This section contains the results of statistical analysis of the map.

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.

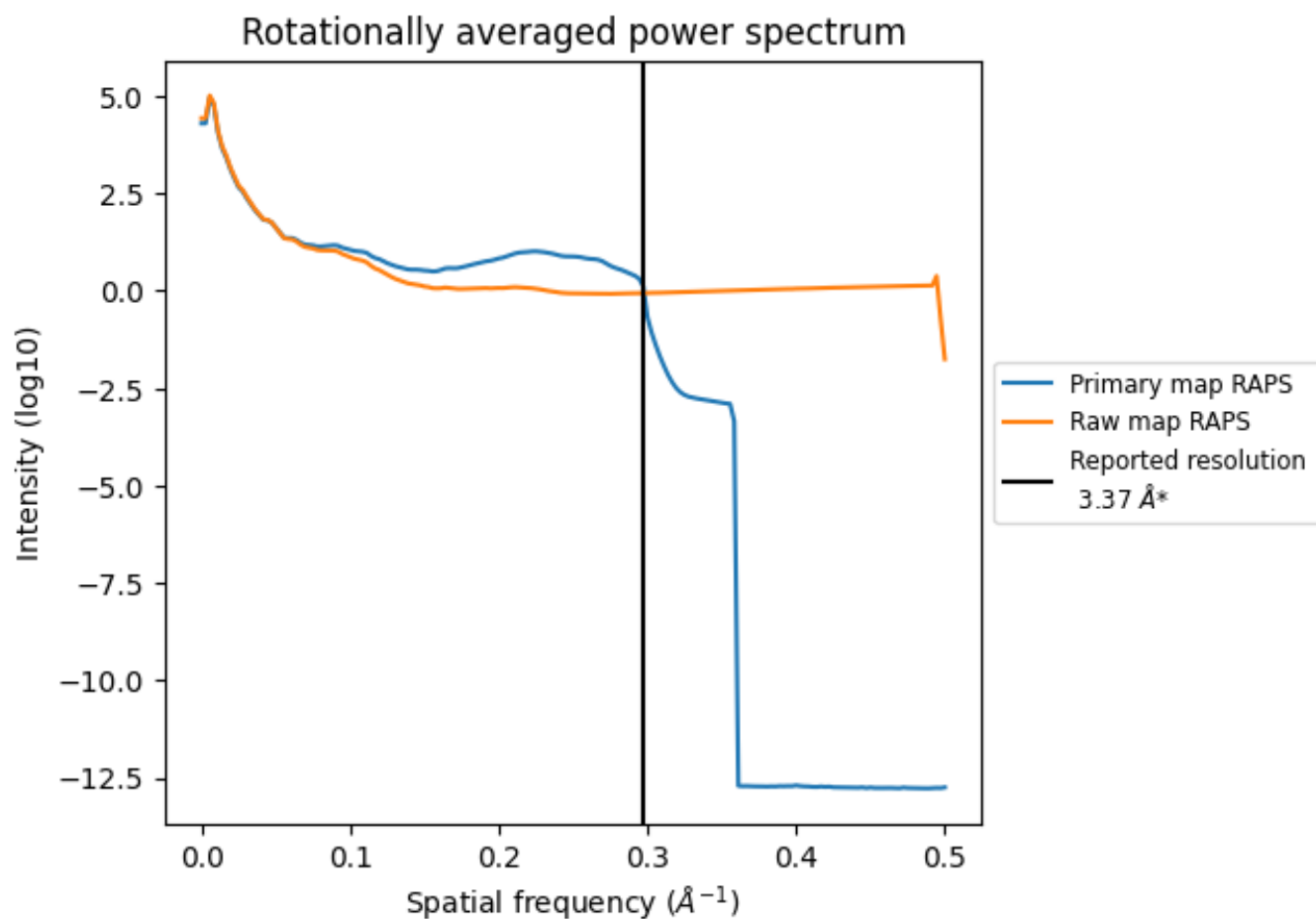
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 492 nm^3 ; this corresponds to an approximate mass of 444 kDa.

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

7.3 Rotationally averaged power spectrum i

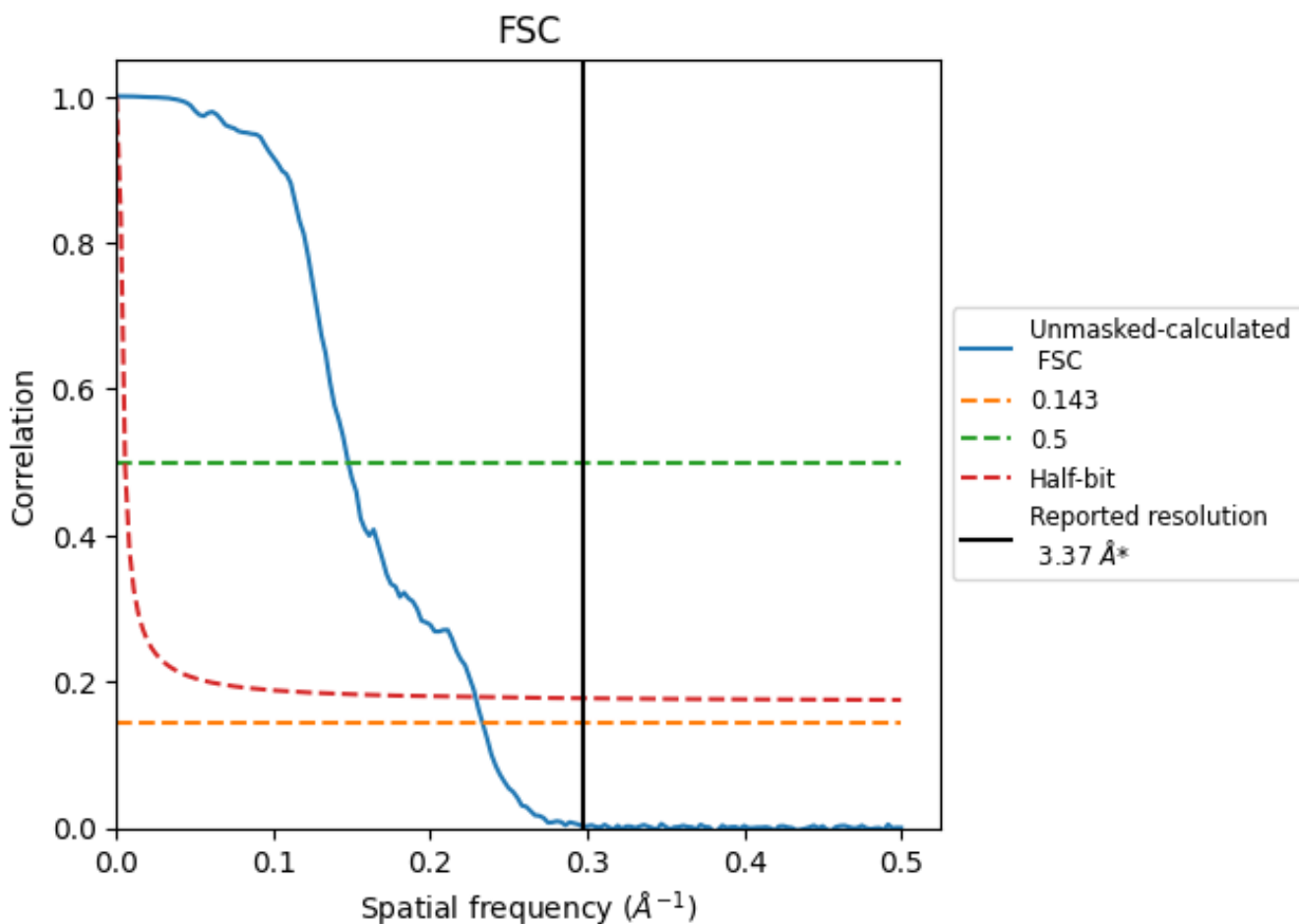


*Reported resolution corresponds to spatial frequency of 0.297 Å⁻¹

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 0.297 Å⁻¹

8.2 Resolution estimates [i](#)

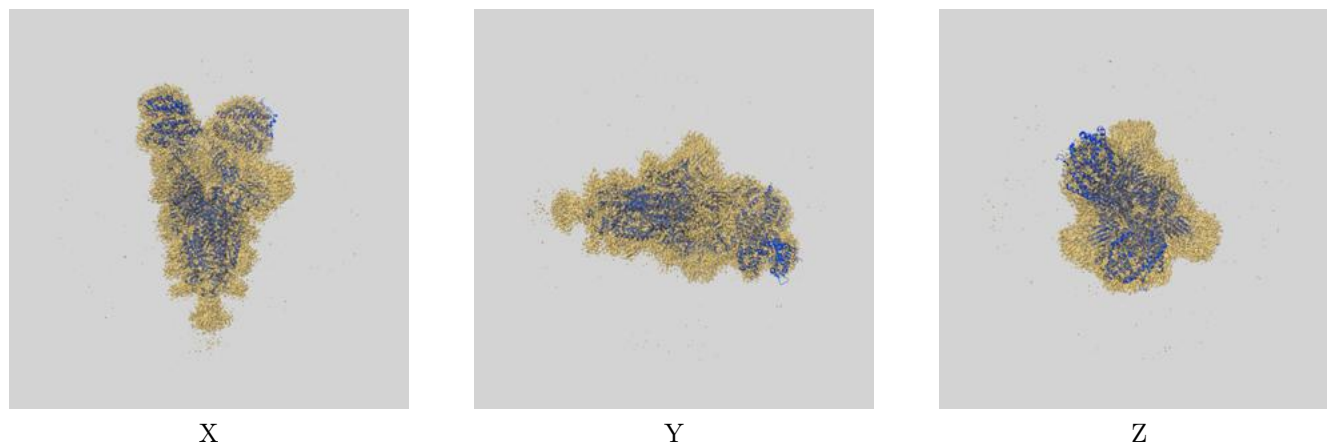
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.37	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.28	6.77	4.37

*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 4.28 differs from the reported value 3.37 by more than 10 %

9 Map-model fit [i](#)

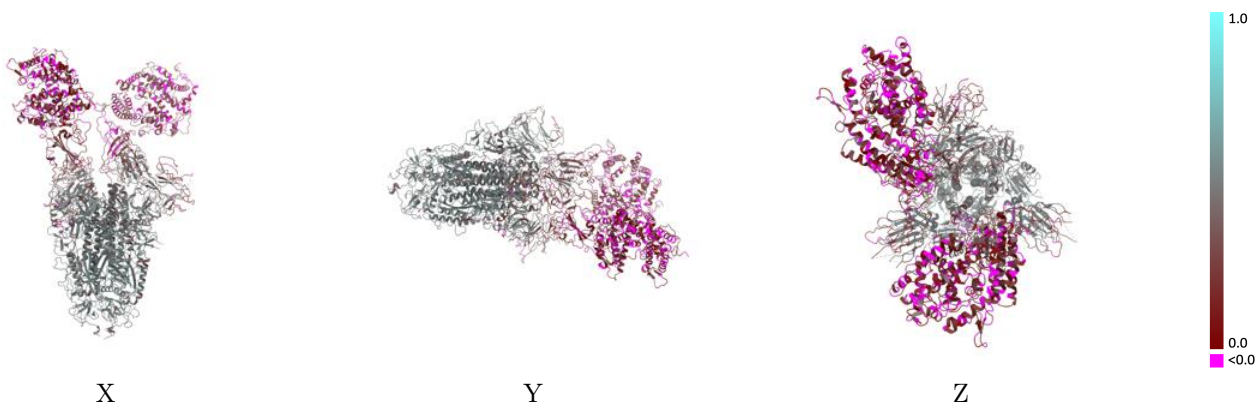
This section contains information regarding the fit between EMDB map EMD-38790 and PDB model 8XZ9. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)



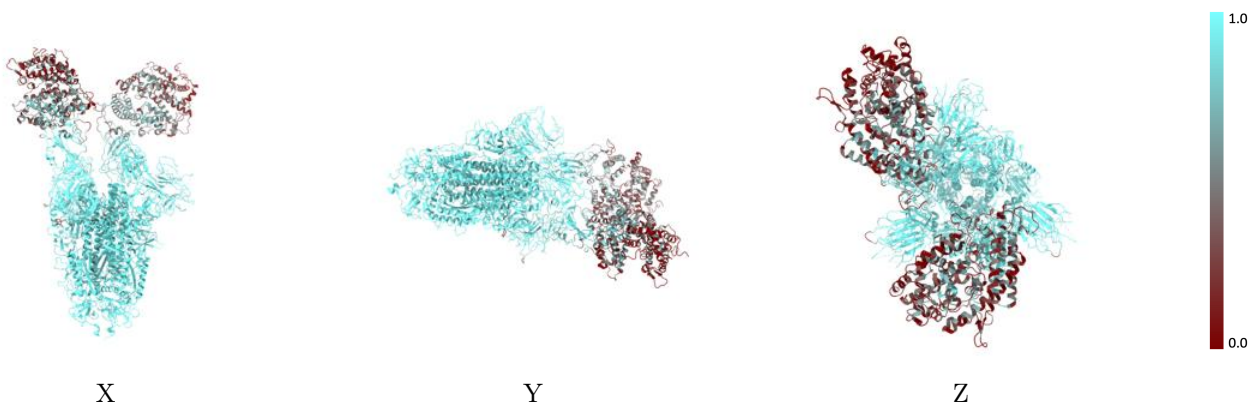
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



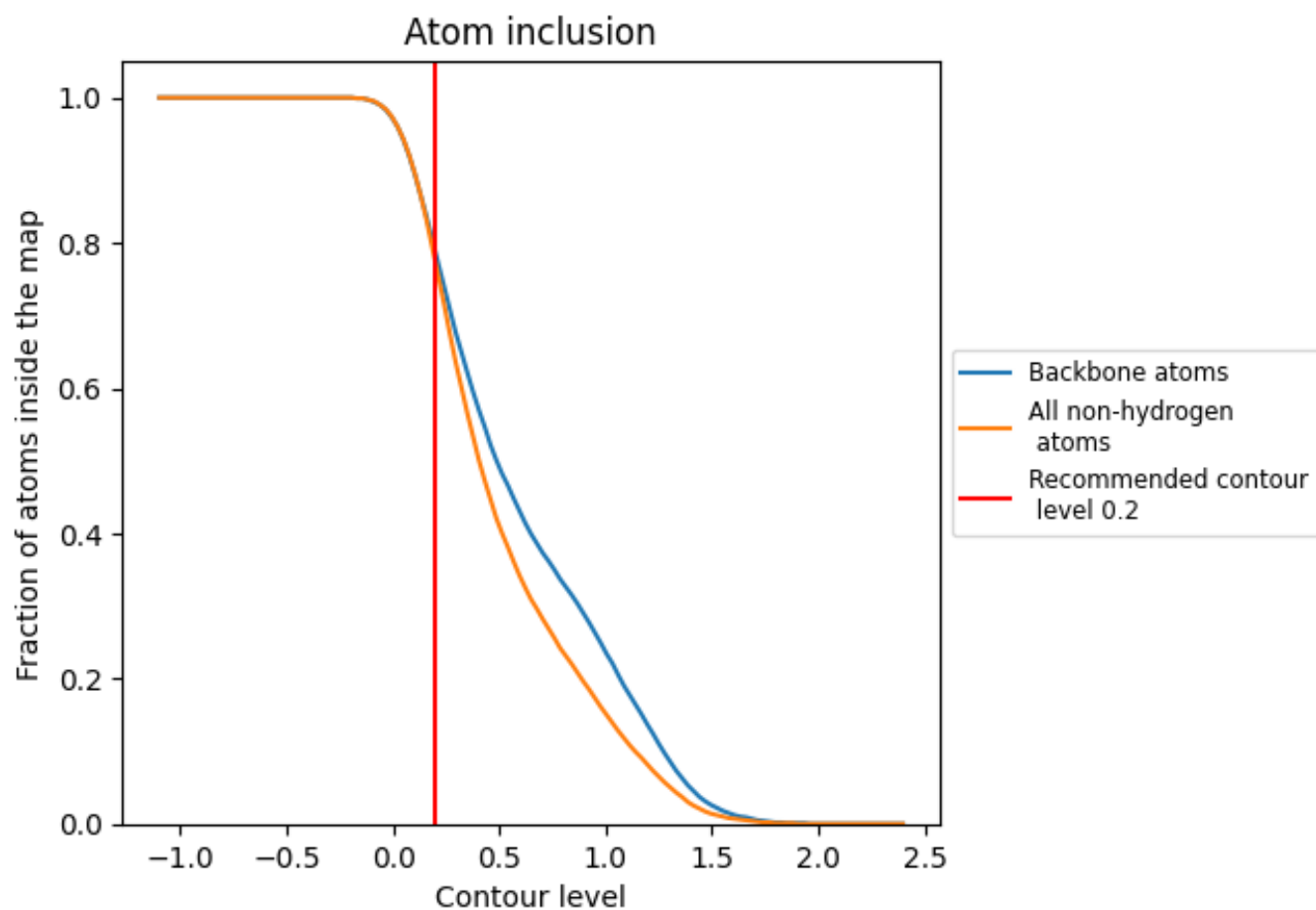
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).







































9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 77% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7730	 0.3250
A	 0.3560	 0.0910
B	 0.9180	 0.3880
C	 0.9230	 0.4070
D	 0.9560	 0.4470
E	 0.3630	 0.1040
F	 0.9600	 0.4060
G	 0.9200	 0.3070
H	 0.9600	 0.4070
I	 0.9200	 0.3820
J	 0.9200	 0.3580
K	 1.0000	 0.4780
L	 0.6790	 0.1230
M	 0.9600	 0.4400
N	 0.9600	 0.4010
O	 0.9600	 0.4660
P	 0.9200	 0.3220
Q	 0.8000	 0.2660
R	 0.8800	 0.4170

