



Full wwPDB EM Validation Report ⓘ

Feb 11, 2023 – 02:45 PM EST

PDB ID : 7TN9
EMDB ID : EMD-26005
Title : Structure of the Inmazeb cocktail and resistance to escape against Ebola virus
Authors : Rayaprolu, V.; Fulton, B.; Rafique, A.; Arturo, E.; Williams, D.; Hariharan, C.; Callaway, H.; Parvate, A.; Schendel, S.L.; Parekh, D.; Hui, S.; Shaffer, K.; Pascal, K.E.; Wloga, E.; Giordano, S.; Copin, R.; Franklin, M.; Boytz, R.M.; Donahue, C.; Davey, R.; Baum, A.; Kyratsous, C.A.; Sapphire, E.O.
Deposited on : 2022-01-20
Resolution : 3.10 Å(reported)
Based on initial model : 5JQ3

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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.32.1

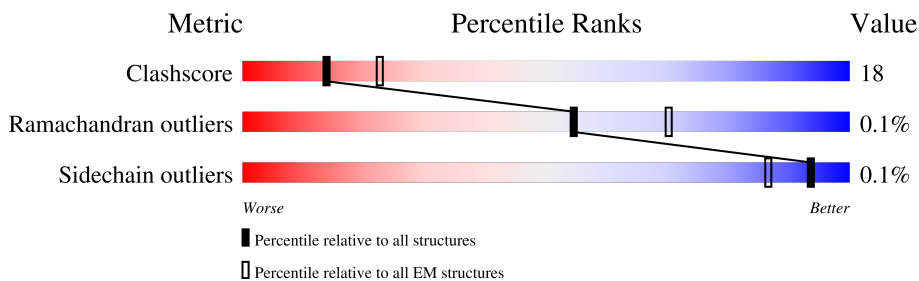
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	217	33% 20% 47%
1	C	217	34% 20% 47%
1	E	217	38% 15% 47%
2	S	321	51% 23% 26%
2	T	321	57% 26% 16%
2	U	321	56% 28% 16%
3	N	213	28% 21% 52%

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Mol	Chain	Length	Quality of chain
3	P	213	31% 16% 53%
3	R	213	37% 12% 51%
4	B	220	39% 12% 49%
4	D	220	37% 14% 49%
4	F	220	31% 20% 49%
5	V	140	54% 24% 21%
5	W	140	46% 32% 21%
5	X	140	50% 26% 24%
6	M	217	28% 25% 47%
6	O	217	32% 21% 47%
6	Q	217	33% 21% 47%
7	G	215	31% 22% 47%
7	I	215	16% 28% 24% 47%
8	H	215	26% 24% 50%
8	J	215	25% 21% 22% 56%
9	K	6	67% 33%
9	L	6	83% 17%
9	Y	6	83% 17%

2 Entry composition i

There are 10 unique types of molecules in this entry. The entry contains 22621 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 REGN3471 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	116	895	570	151	170	4	0	0
1	C	116	895	570	151	170	4	0	0
1	E	116	895	570	151	170	4	0	0

- Molecule 2 is a protein called Envelope glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	T	269	2127	1359	361	402	5	0	0
2	S	237	1872	1205	313	349	5	0	0
2	U	269	2127	1359	361	402	5	0	0

There are 123 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	31	ARG	-	expression tag	UNP Q05320
T	312	ASN	-	expression tag	UNP Q05320
T	313	THR	-	expression tag	UNP Q05320
T	314	HIS	-	expression tag	UNP Q05320
T	315	HIS	-	expression tag	UNP Q05320
T	316	GLN	-	expression tag	UNP Q05320
T	317	ASP	-	expression tag	UNP Q05320
T	318	THR	-	expression tag	UNP Q05320
T	319	GLY	-	expression tag	UNP Q05320
T	320	GLU	-	expression tag	UNP Q05320
T	321	GLU	-	expression tag	UNP Q05320
T	322	SER	-	expression tag	UNP Q05320
T	323	ALA	-	expression tag	UNP Q05320

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Chain	Residue	Modelled	Actual	Comment	Reference
T	324	SER	-	expression tag	UNP Q05320
T	325	SER	-	expression tag	UNP Q05320
T	326	GLY	-	expression tag	UNP Q05320
T	327	LYS	-	expression tag	UNP Q05320
T	328	LEU	-	expression tag	UNP Q05320
T	329	GLY	-	expression tag	UNP Q05320
T	330	LEU	-	expression tag	UNP Q05320
T	331	ILE	-	expression tag	UNP Q05320
T	332	THR	-	expression tag	UNP Q05320
T	333	ASN	-	expression tag	UNP Q05320
T	334	THR	-	expression tag	UNP Q05320
T	335	ILE	-	expression tag	UNP Q05320
T	336	ALA	-	expression tag	UNP Q05320
T	337	GLY	-	expression tag	UNP Q05320
T	338	VAL	-	expression tag	UNP Q05320
T	339	ALA	-	expression tag	UNP Q05320
T	340	GLY	-	expression tag	UNP Q05320
T	341	LEU	-	expression tag	UNP Q05320
T	342	ILE	-	expression tag	UNP Q05320
T	343	THR	-	expression tag	UNP Q05320
T	344	GLY	-	expression tag	UNP Q05320
T	345	GLY	-	expression tag	UNP Q05320
T	346	ARG	-	expression tag	UNP Q05320
T	347	ARG	-	expression tag	UNP Q05320
T	348	THR	-	expression tag	UNP Q05320
T	349	ARG	-	expression tag	UNP Q05320
T	350	ARG	-	expression tag	UNP Q05320
T	351	GLU	-	expression tag	UNP Q05320
S	31	ARG	-	expression tag	UNP Q05320
S	312	ASN	-	expression tag	UNP Q05320
S	313	THR	-	expression tag	UNP Q05320
S	314	HIS	-	expression tag	UNP Q05320
S	315	HIS	-	expression tag	UNP Q05320
S	316	GLN	-	expression tag	UNP Q05320
S	317	ASP	-	expression tag	UNP Q05320
S	318	THR	-	expression tag	UNP Q05320
S	319	GLY	-	expression tag	UNP Q05320
S	320	GLU	-	expression tag	UNP Q05320
S	321	GLU	-	expression tag	UNP Q05320
S	322	SER	-	expression tag	UNP Q05320
S	323	ALA	-	expression tag	UNP Q05320
S	324	SER	-	expression tag	UNP Q05320

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Chain	Residue	Modelled	Actual	Comment	Reference
S	325	SER	-	expression tag	UNP Q05320
S	326	GLY	-	expression tag	UNP Q05320
S	327	LYS	-	expression tag	UNP Q05320
S	328	LEU	-	expression tag	UNP Q05320
S	329	GLY	-	expression tag	UNP Q05320
S	330	LEU	-	expression tag	UNP Q05320
S	331	ILE	-	expression tag	UNP Q05320
S	332	THR	-	expression tag	UNP Q05320
S	333	ASN	-	expression tag	UNP Q05320
S	334	THR	-	expression tag	UNP Q05320
S	335	ILE	-	expression tag	UNP Q05320
S	336	ALA	-	expression tag	UNP Q05320
S	337	GLY	-	expression tag	UNP Q05320
S	338	VAL	-	expression tag	UNP Q05320
S	339	ALA	-	expression tag	UNP Q05320
S	340	GLY	-	expression tag	UNP Q05320
S	341	LEU	-	expression tag	UNP Q05320
S	342	ILE	-	expression tag	UNP Q05320
S	343	THR	-	expression tag	UNP Q05320
S	344	GLY	-	expression tag	UNP Q05320
S	345	GLY	-	expression tag	UNP Q05320
S	346	ARG	-	expression tag	UNP Q05320
S	347	ARG	-	expression tag	UNP Q05320
S	348	THR	-	expression tag	UNP Q05320
S	349	ARG	-	expression tag	UNP Q05320
S	350	ARG	-	expression tag	UNP Q05320
S	351	GLU	-	expression tag	UNP Q05320
U	31	ARG	-	expression tag	UNP Q05320
U	312	ASN	-	expression tag	UNP Q05320
U	313	THR	-	expression tag	UNP Q05320
U	314	HIS	-	expression tag	UNP Q05320
U	315	HIS	-	expression tag	UNP Q05320
U	316	GLN	-	expression tag	UNP Q05320
U	317	ASP	-	expression tag	UNP Q05320
U	318	THR	-	expression tag	UNP Q05320
U	319	GLY	-	expression tag	UNP Q05320
U	320	GLU	-	expression tag	UNP Q05320
U	321	GLU	-	expression tag	UNP Q05320
U	322	SER	-	expression tag	UNP Q05320
U	323	ALA	-	expression tag	UNP Q05320
U	324	SER	-	expression tag	UNP Q05320
U	325	SER	-	expression tag	UNP Q05320

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Chain	Residue	Modelled	Actual	Comment	Reference
U	326	GLY	-	expression tag	UNP Q05320
U	327	LYS	-	expression tag	UNP Q05320
U	328	LEU	-	expression tag	UNP Q05320
U	329	GLY	-	expression tag	UNP Q05320
U	330	LEU	-	expression tag	UNP Q05320
U	331	ILE	-	expression tag	UNP Q05320
U	332	THR	-	expression tag	UNP Q05320
U	333	ASN	-	expression tag	UNP Q05320
U	334	THR	-	expression tag	UNP Q05320
U	335	ILE	-	expression tag	UNP Q05320
U	336	ALA	-	expression tag	UNP Q05320
U	337	GLY	-	expression tag	UNP Q05320
U	338	VAL	-	expression tag	UNP Q05320
U	339	ALA	-	expression tag	UNP Q05320
U	340	GLY	-	expression tag	UNP Q05320
U	341	LEU	-	expression tag	UNP Q05320
U	342	ILE	-	expression tag	UNP Q05320
U	343	THR	-	expression tag	UNP Q05320
U	344	GLY	-	expression tag	UNP Q05320
U	345	GLY	-	expression tag	UNP Q05320
U	346	ARG	-	expression tag	UNP Q05320
U	347	ARG	-	expression tag	UNP Q05320
U	348	THR	-	expression tag	UNP Q05320
U	349	ARG	-	expression tag	UNP Q05320
U	350	ARG	-	expression tag	UNP Q05320
U	351	GLU	-	expression tag	UNP Q05320

- Molecule 3 is a protein called REGN3479 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	R	105	Total	C	N	O	S	0	0
			796	498	132	163	3		
3	N	103	Total	C	N	O	S	0	0
			779	487	130	159	3		
3	P	101	Total	C	N	O	S	0	0
			760	475	125	157	3		

- Molecule 4 is a protein called REGN3471 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	113	Total	C	N	O	S	0	0
			873	552	142	176	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	113	Total	C	N	O	S	0	0
			873	552	142	176	3		
4	D	113	Total	C	N	O	S	0	0
			873	552	142	176	3		

- Molecule 5 is a protein called GP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	W	110	Total	C	N	O	S	0	0
			862	549	151	156	6		
5	V	110	Total	C	N	O	S	0	0
			862	549	151	156	6		
5	X	107	Total	C	N	O	S	0	0
			839	534	147	152	6		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	544	THR	ILE	conflict	UNP Q05320
W	638	ASP	-	expression tag	UNP Q05320
W	639	ASP	-	expression tag	UNP Q05320
W	640	ASP	-	expression tag	UNP Q05320
W	641	ASP	-	expression tag	UNP Q05320
W	642	LYS	-	expression tag	UNP Q05320
V	544	THR	ILE	conflict	UNP Q05320
V	638	ASP	-	expression tag	UNP Q05320
V	639	ASP	-	expression tag	UNP Q05320
V	640	ASP	-	expression tag	UNP Q05320
V	641	ASP	-	expression tag	UNP Q05320
V	642	LYS	-	expression tag	UNP Q05320
X	544	THR	ILE	conflict	UNP Q05320
X	638	ASP	-	expression tag	UNP Q05320
X	639	ASP	-	expression tag	UNP Q05320
X	640	ASP	-	expression tag	UNP Q05320
X	641	ASP	-	expression tag	UNP Q05320
X	642	LYS	-	expression tag	UNP Q05320

- Molecule 6 is a protein called REGN3479 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Q	116	Total	C	N	O	S	0	0
			878	549	152	171	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	M	115	Total	C	N	O	S	0	0
			869	544	151	168	6		
6	O	115	Total	C	N	O	S	0	0
			869	544	151	168	6		

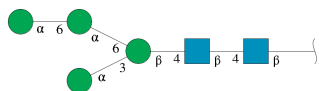
- Molecule 7 is a protein called REGN3470 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	115	Total	C	N	O	S	0	0
			912	577	161	169	5		
7	I	113	Total	C	N	O	S	0	0
			899	569	159	166	5		

- Molecule 8 is a protein called REGN3470 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	107	Total	C	N	O	S	0	0
			810	511	134	162	3		
8	J	95	Total	C	N	O	S	0	0
			728	461	119	145	3		

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).

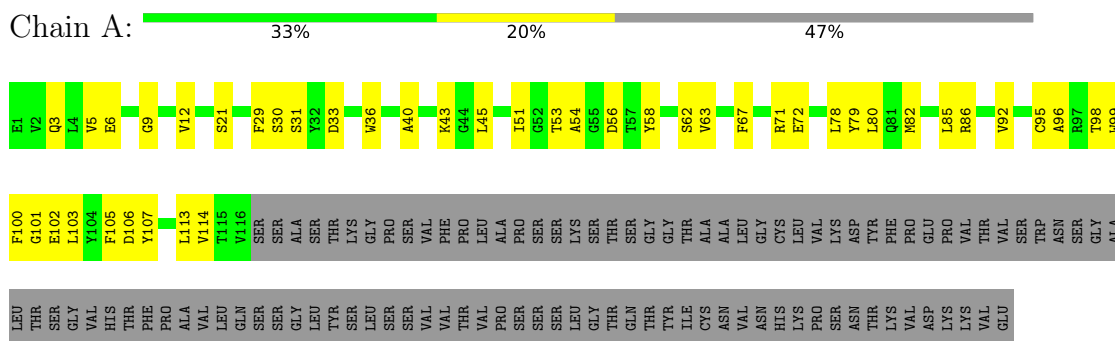


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
10	T	1	Total 14	8	1	5	0
10	T	1	Total 14	8	1	5	0
10	T	1	Total 14	8	1	5	0
10	S	1	Total 14	8	1	5	0
10	S	1	Total 14	8	1	5	0
10	U	1	Total 14	8	1	5	0
10	U	1	Total 14	8	1	5	0
10	U	1	Total 14	8	1	5	0

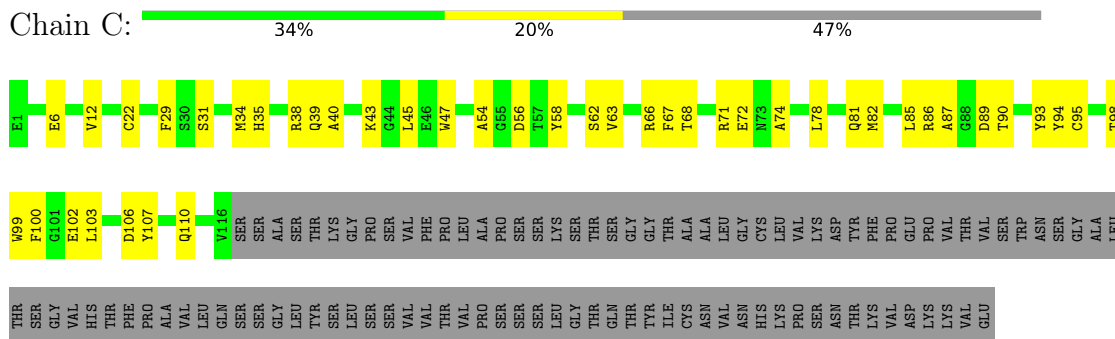
3 Residue-property plots [i](#)

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.

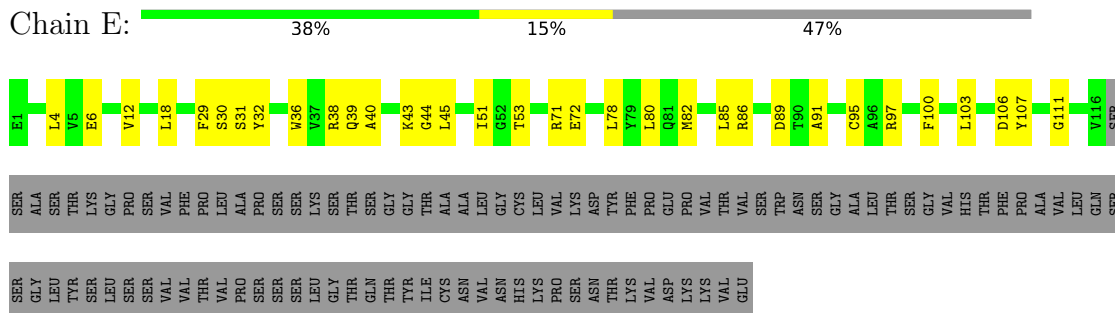
- Molecule 1: REGN3471 heavy chain

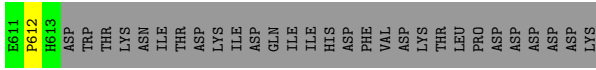


- Molecule 1: REGN3471 heavy chain

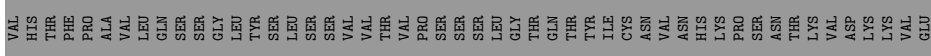
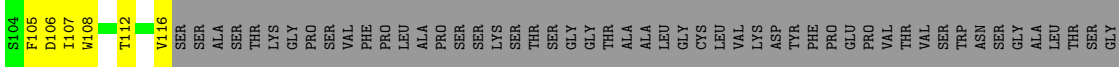
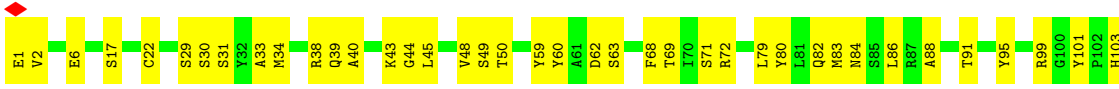
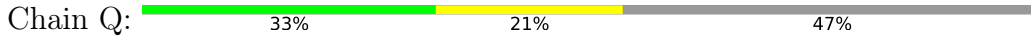


- Molecule 1: REGN3471 heavy chain

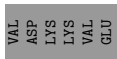
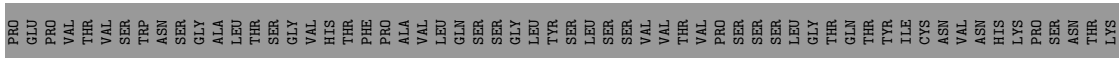
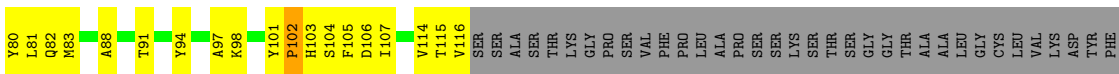
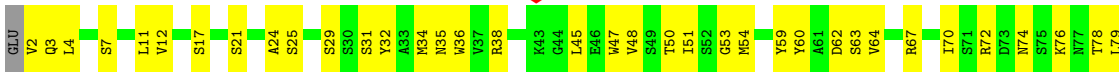
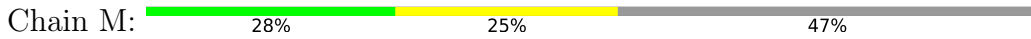




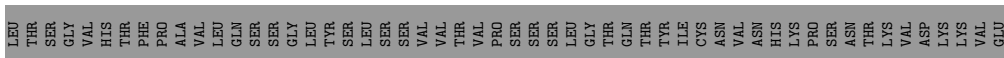
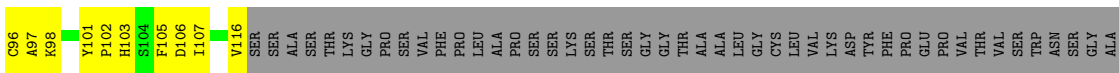
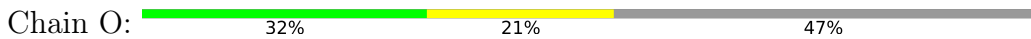
• Molecule 6: REGN3479 heavy chain



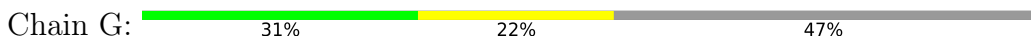
• Molecule 6: REGN3479 heavy chain

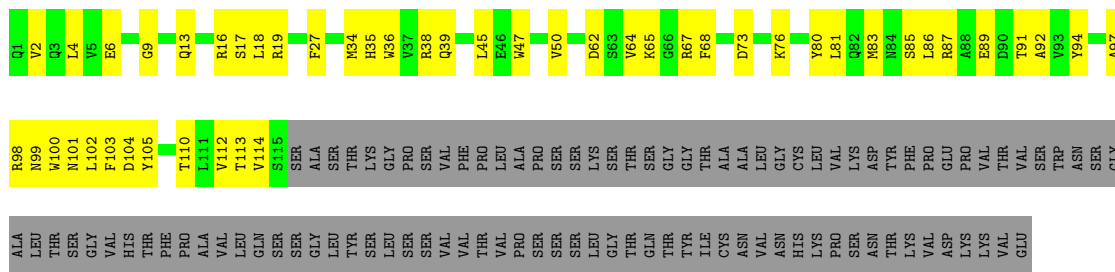


• Molecule 6: REGN3479 heavy chain

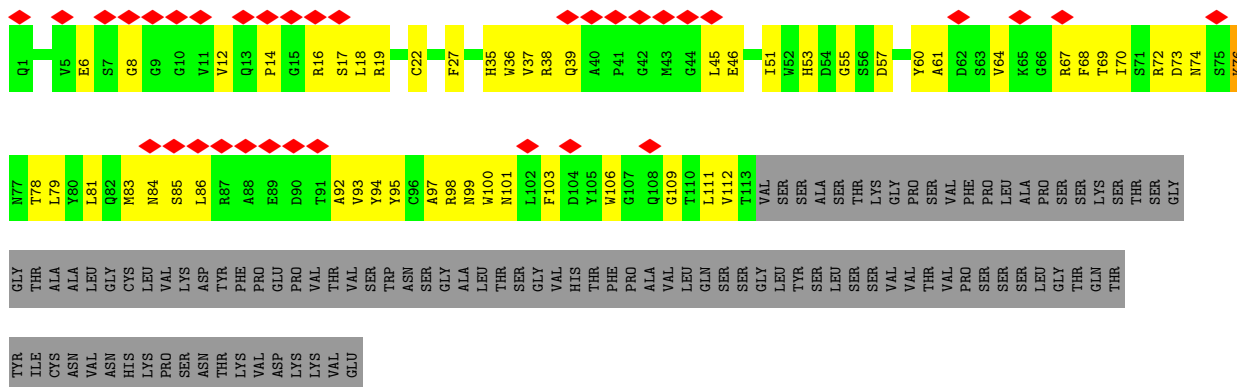
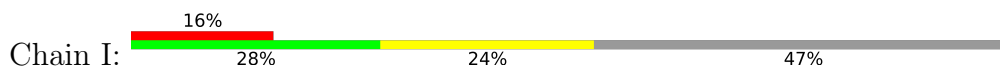


• Molecule 7: REGN3470 heavy chain

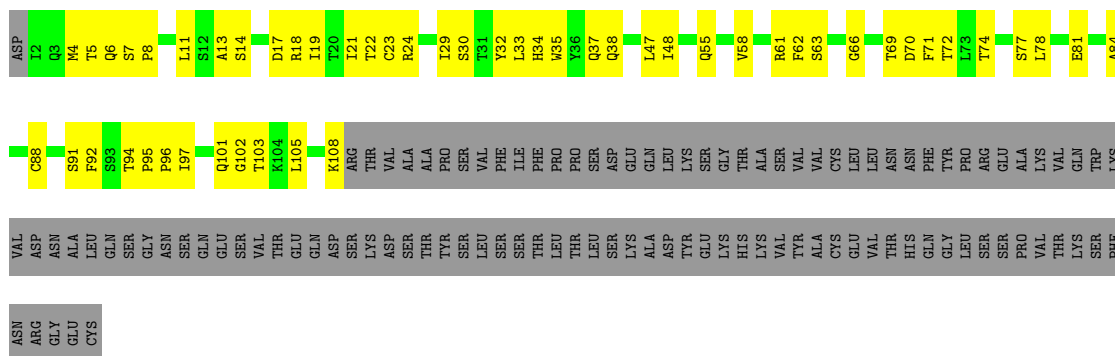
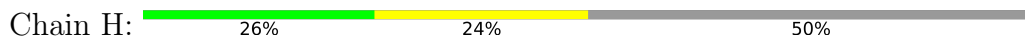




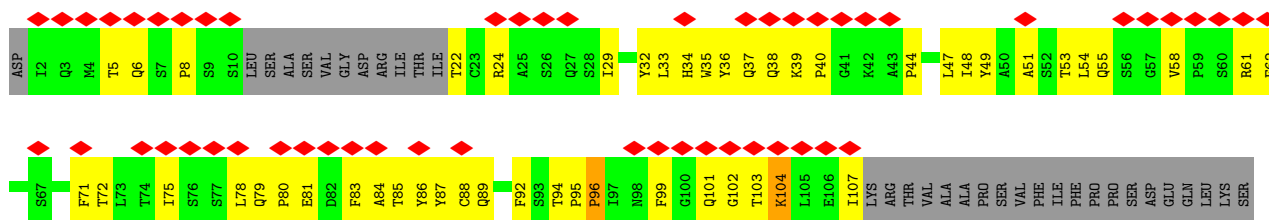
• Molecule 7: REGN3470 heavy chain



• Molecule 8: REGN3470 light chain



• Molecule 8: REGN3470 light chain



GLY THR ALA SER VAL VAL CYS LEU THR ASN ASN PHE TYR PRO ARG SER GLU ALA VAL VAL GLN THR PHE VAL VAL ASP ASN ALA LEU GLN SER SER GLY ASN ASN SER SER GLN GLU VAL THR THR GLU GLN ASP SER LYS ASP SER THR TYR THR LEU SER SER SER SER THR LEU LEU THR THR LYS LYS ALA ASP TYR GLU

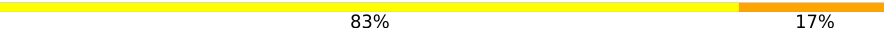
LYS HIS VAL TYR ALA CYS GLU VAL THR HIS ASN GLN GLY LEU SER SER PRO VAL THR LYS SER PHE ASN ARG ARG GLY CYS

- Molecule 9: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  67% 33%


MAG1
MAG2
BMA3
MAN4
MAN5
MAN6

- Molecule 9: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  83% 17%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6

- Molecule 9: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:  83% 17%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	276715	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 ($e^-/\text{\AA}^2$)	52.4	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.718	Depositor
Minimum map value	-0.619	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.030	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	537.8048, 537.8048, 537.8048	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0504, 1.0504, 1.0504	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, MAN, 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	0.44	0/918	0.52	0/1245
1	C	0.41	0/918	0.52	0/1245
1	E	0.43	0/918	0.51	0/1245
2	S	0.38	0/1921	0.49	0/2609
2	T	0.40	0/2179	0.54	2/2958 (0.1%)
2	U	0.40	1/2178 (0.0%)	0.52	1/2955 (0.0%)
3	N	0.29	0/795	0.53	0/1078
3	P	0.31	0/776	0.52	0/1053
3	R	0.34	0/812	0.55	0/1101
4	B	0.40	0/893	0.54	0/1214
4	D	0.41	0/893	0.53	0/1214
4	F	0.42	0/893	0.57	0/1214
5	V	0.37	0/884	0.56	0/1205
5	W	0.42	0/884	0.56	0/1205
5	X	0.40	0/861	0.55	0/1173
6	M	0.32	0/888	0.53	0/1201
6	O	0.32	0/888	0.50	0/1201
6	Q	0.33	0/897	0.51	0/1213
7	G	0.33	0/936	0.50	0/1271
7	I	0.33	0/923	0.59	1/1253 (0.1%)
8	H	0.31	0/829	0.56	0/1126
8	J	0.29	0/746	0.52	0/1012
All	All	0.37	1/22830 (0.0%)	0.53	4/30991 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	U	53	CYS	CB-SG	-5.23	1.73	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	51	LEU	CA-CB-CG	7.78	133.19	115.30
2	U	53	CYS	CA-CB-SG	6.24	125.23	114.00
7	I	76	LYS	CB-CG-CD	5.38	125.59	111.60
2	T	297	LEU	CA-CB-CG	5.22	127.32	115.30

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	895	0	851	35	0
1	C	895	0	851	31	0
1	E	895	0	851	28	0
2	S	1872	0	1810	55	0
2	T	2127	0	2079	77	0
2	U	2127	0	2077	80	0
3	N	779	0	758	33	0
3	P	760	0	734	26	0
3	R	796	0	775	19	0
4	B	873	0	848	19	0
4	D	873	0	848	20	0
4	F	873	0	848	35	0
5	V	862	0	835	38	0
5	W	862	0	836	57	0
5	X	839	0	809	44	0
6	M	869	0	837	57	0
6	O	869	0	837	42	0
6	Q	878	0	846	40	0
7	G	912	0	864	37	0
7	I	899	0	850	51	0
8	H	810	0	789	45	0
8	J	728	0	703	45	0
9	K	72	0	61	7	0
9	L	72	0	61	4	0
9	Y	72	0	61	4	0
10	S	28	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	T	42	0	39	1	0
10	U	42	0	39	0	0
All	All	22621	0	21823	786	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 18.

All (786) 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)
6:O:57:SER:HB3	6:O:59:TYR:HE1	1.31	0.94
2:T:73:ASN:HB3	5:W:508:GLN:HE21	1.34	0.92
7:I:17:SER:HB3	7:I:83:MET:HG3	1.53	0.91
2:S:104:TRP:NE1	5:V:545:GLU:OE1	2.06	0.88
2:S:128:GLY:HA3	5:V:580:ARG:HH22	1.37	0.86
4:B:24:LYS:NZ	4:B:76:GLU:OE1	2.08	0.85
8:H:5:THR:O	8:H:24:ARG:N	2.09	0.84
1:A:86:ARG:HD3	4:F:20:THR:HG21	1.60	0.83
7:I:16:ARG:HE	7:I:17:SER:H	1.22	0.83
5:W:505:VAL:HG22	5:W:560:GLN:HB2	1.62	0.82
2:U:237:ASP:OD1	2:U:238:ASN:N	2.12	0.81
2:U:128:GLY:HA3	5:X:580:ARG:HH12	1.44	0.81
3:N:6:GLN:NE2	3:N:99:GLN:O	2.11	0.81
8:J:36:TYR:HB2	8:J:87:TYR:HB2	1.63	0.81
6:O:52:SER:HB3	6:O:57:SER:HB2	1.62	0.80
6:Q:33:ALA:HB3	6:Q:99:ARG:HD2	1.65	0.79
7:I:36:TRP:HE1	7:I:79:LEU:HD21	1.45	0.79
7:G:13:GLN:H	7:G:16:ARG:HH21	1.31	0.78
1:C:62:SER:N	4:B:76:GLU:OE2	2.18	0.77
5:W:527:ILE:HD13	6:Q:59:TYR:HD1	1.50	0.77
5:W:574:ARG:HH21	5:X:521:GLN:HE22	1.30	0.77
8:H:61:ARG:NH2	8:H:81:GLU:OE2	2.18	0.77
1:E:40:ALA:HB3	1:E:43:LYS:HB3	1.67	0.76
2:T:294:LYS:HE2	2:T:296:ASN:HD22	1.51	0.76
3:N:63:SER:OG	3:N:74:THR:OG1	2.02	0.76
5:V:566:THR:HG21	9:L:1:NAG:H82	1.68	0.76
7:G:87:ARG:NH2	7:G:89:GLU:OE2	2.19	0.74
1:A:82:MET:HB3	1:A:85:LEU:HD21	1.69	0.74
2:S:106:GLU:OE2	2:S:136:ARG:NH2	2.20	0.74
2:T:73:ASN:HB3	5:W:508:GLN:NE2	2.03	0.74
6:M:36:TRP:HE1	6:M:79:LEU:HD22	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:127:ASP:OD1	2:T:128:GLY:N	2.21	0.74
2:S:251:GLN:O	2:S:255:GLN:NE2	2.21	0.73
2:U:85:ARG:NH1	2:U:178:GLU:OE2	2.21	0.73
6:M:29:SER:O	6:M:72:ARG:NH2	2.21	0.73
1:C:6:GLU:OE2	1:C:95:CYS:N	2.17	0.73
3:N:90:GLN:HE21	3:N:96:THR:H	1.35	0.73
2:U:127:ASP:OD2	2:U:128:GLY:N	2.22	0.73
2:T:51:LEU:HB3	5:W:595:GLN:NE2	2.04	0.73
5:W:564:GLU:OE1	6:M:53:GLY:N	2.21	0.73
2:U:68:LEU:HD11	5:X:558:LEU:HG	1.71	0.73
7:I:53:HIS:O	7:I:72:ARG:NH1	2.22	0.73
1:A:45:LEU:HD21	4:B:50:PRO:HG2	1.70	0.72
1:A:40:ALA:HB3	1:A:43:LYS:HB3	1.71	0.72
7:G:39:GLN:HA	7:G:45:LEU:HA	1.70	0.72
7:I:35:HIS:HB2	7:I:97:ALA:HB3	1.70	0.72
8:H:18:ARG:HH12	8:H:74:THR:HB	1.55	0.72
1:C:82:MET:HB3	1:C:85:LEU:HD21	1.72	0.71
7:G:19:ARG:HD2	7:G:80:TYR:HB3	1.71	0.71
5:X:603:ILE:HG13	5:X:610:ILE:HD11	1.72	0.71
1:A:3:GLN:HE22	1:A:5:VAL:HG22	1.55	0.70
3:P:35:TRP:HB2	3:P:48:ILE:HB	1.73	0.70
5:W:513:PRO:O	5:W:555:ILE:HD11	1.90	0.70
1:E:12:VAL:HG11	1:E:18:LEU:HB2	1.73	0.70
2:T:301:ILE:HD12	2:T:306:LEU:HD21	1.74	0.70
3:N:49:TYR:HB2	3:N:53:SER:HB2	1.74	0.70
6:O:2:VAL:N	6:O:25:SER:O	2.23	0.70
1:E:38:ARG:NH1	1:E:89:ASP:OD1	2.24	0.70
1:A:62:SER:N	4:F:76:GLU:OE1	2.25	0.70
8:J:95:PRO:HD2	8:J:96:PRO:HD3	1.73	0.70
8:H:32:TYR:HB3	8:H:91:SER:HB3	1.73	0.69
6:M:91:THR:HB	6:M:116:VAL:HG22	1.75	0.69
6:O:57:SER:HB3	6:O:59:TYR:CE1	2.22	0.69
5:X:566:THR:HG21	9:Y:1:NAG:H82	1.75	0.69
6:O:35:ASN:HD22	6:O:105:PHE:HE1	1.41	0.69
2:S:242:VAL:HG12	2:S:275:TRP:HB2	1.75	0.69
2:T:306:LEU:O	7:G:101:ASN:ND2	2.26	0.69
2:U:81:SER:HA	2:U:84:LYS:HE2	1.75	0.69
3:P:34:ASN:HB2	3:P:89:GLN:HB3	1.74	0.69
2:U:111:LEU:HD12	2:U:170:ILE:HG21	1.74	0.68
2:U:38:ILE:HG21	2:U:193:PHE:HE1	1.56	0.68
6:O:50:THR:HB	6:O:59:TYR:HB2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:W:566:THR:HG21	9:K:1:NAG:H82	1.76	0.68
2:U:282:ASP:OD1	2:U:283:THR:N	2.27	0.68
5:X:596:ARG:NH1	5:X:596:ARG:HB2	2.09	0.68
7:G:35:HIS:HB2	7:G:97:ALA:HB3	1.74	0.67
4:B:2:ILE:HG13	4:B:27:GLN:HB2	1.76	0.67
4:F:50:PRO:HG2	1:E:45:LEU:HD21	1.75	0.67
2:S:271:GLY:N	4:F:62:SER:HG	1.93	0.66
2:U:182:ALA:HB2	5:X:562:ALA:HB2	1.78	0.66
2:T:111:LEU:HD12	2:T:170:ILE:HG21	1.77	0.66
3:R:90:GLN:HE21	3:R:96:THR:H	1.44	0.66
1:E:43:LYS:HG2	1:E:44:GLY:H	1.58	0.66
2:S:86:TRP:NE1	2:S:178:GLU:OE2	2.29	0.66
8:J:6:GLN:HE21	8:J:103:THR:HG23	1.60	0.66
1:C:22:CYS:HB3	1:C:78:LEU:HB3	1.78	0.65
2:T:182:ALA:HB2	5:W:562:ALA:HB2	1.77	0.65
2:S:58:SER:OG	2:S:62:GLN:NE2	2.29	0.65
6:Q:106:ASP:OD1	6:Q:107:ILE:N	2.30	0.65
8:H:37:GLN:HB2	8:H:47:LEU:HD11	1.78	0.65
2:T:48:VAL:O	5:W:595:GLN:NE2	2.30	0.65
2:S:288:TRP:HB3	2:S:292:GLU:HB2	1.79	0.65
3:P:6:GLN:O	3:P:99:GLN:NE2	2.30	0.65
2:S:43:LEU:HD22	5:V:558:LEU:HD23	1.78	0.65
6:Q:62:ASP:OD1	6:Q:63:SER:N	2.30	0.65
8:H:63:SER:O	8:H:74:THR:OG1	2.10	0.65
7:I:16:ARG:NE	7:I:17:SER:H	1.94	0.64
8:J:6:GLN:NE2	8:J:101:GLN:O	2.30	0.64
2:U:120:GLU:OE2	2:U:172:ARG:NH1	2.30	0.64
1:E:12:VAL:HG21	1:E:85:LEU:HD22	1.79	0.64
3:N:90:GLN:NE2	3:N:93:SER:O	2.29	0.64
6:Q:6:GLU:HA	6:Q:22:CYS:HA	1.80	0.64
6:M:2:VAL:N	6:M:25:SER:O	2.31	0.64
6:M:36:TRP:HD1	6:M:70:ILE:HD11	1.61	0.64
6:O:6:GLU:OE2	6:O:96:CYS:N	2.31	0.64
3:N:44:PRO:HG2	6:M:45:LEU:HD21	1.79	0.64
6:M:35:ASN:HD22	6:M:105:PHE:HE1	1.43	0.64
6:Q:40:ALA:HB3	6:Q:43:LYS:HB3	1.81	0.63
6:M:101:TYR:CD2	6:M:102:PRO:HD3	2.33	0.63
8:H:18:ARG:NH1	8:H:19:ILE:O	2.32	0.63
1:A:33:ASP:OD1	1:A:98:THR:OG1	2.17	0.63
5:X:551:GLN:HG3	5:X:554:LEU:H	1.63	0.63
6:M:7:SER:HG	6:M:21:SER:HG	1.41	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:GLU:OE2	1:A:95:CYS:N	2.25	0.62
2:S:291:TRP:CD1	5:V:513:PRO:HD2	2.34	0.62
2:U:154:HIS:NE2	2:U:178:GLU:OE1	2.29	0.62
3:P:90:GLN:NE2	3:P:93:SER:O	2.33	0.62
5:V:513:PRO:O	5:V:555:ILE:HD11	1.99	0.62
4:B:53:LEU:HA	4:B:64:VAL:HG21	1.82	0.62
1:A:9:GLY:HA2	1:A:114:VAL:HG12	1.82	0.62
8:H:78:LEU:HD11	8:H:105:LEU:HD21	1.82	0.61
7:I:99:ASN:HB3	7:I:103:PHE:H	1.65	0.61
3:R:95:LEU:HD21	6:Q:103:HIS:ND1	2.16	0.61
6:O:106:ASP:OD2	6:O:107:ILE:N	2.34	0.61
6:Q:83:MET:HG3	6:Q:86:LEU:HD11	1.81	0.61
6:M:34:MET:HB2	6:M:79:LEU:HD12	1.82	0.61
1:C:40:ALA:HB3	1:C:43:LYS:HB2	1.81	0.61
7:G:99:ASN:HB3	7:G:102:LEU:O	2.01	0.60
8:J:95:PRO:HD2	8:J:96:PRO:CD	2.31	0.60
2:T:293:THR:O	2:T:294:LYS:HG2	2.00	0.60
4:F:97:TYR:HB2	1:E:103:LEU:HB2	1.83	0.60
6:M:101:TYR:HE1	9:K:2:NAG:H61	1.66	0.60
8:J:49:TYR:HE1	8:J:55:GLN:HG3	1.67	0.60
2:T:104:TRP:NE1	5:W:545:GLU:OE2	2.35	0.60
6:M:35:ASN:HD21	6:M:103:HIS:CE1	2.20	0.60
8:H:14:SER:HB3	8:H:17:ASP:HB2	1.84	0.60
6:M:70:ILE:HD12	6:M:81:LEU:HD13	1.84	0.60
3:N:49:TYR:CD2	9:K:5:MAN:H61	2.36	0.60
8:H:4:MET:HG3	8:H:23:CYS:SG	2.42	0.60
7:I:12:VAL:HG21	7:I:18:LEU:HD22	1.82	0.60
2:S:197:HIS:HB3	5:V:546:GLY:HA2	1.83	0.60
7:I:27:PHE:HB2	7:I:98:ARG:HH21	1.67	0.59
6:M:32:TYR:CG	6:M:98:LYS:HD2	2.36	0.59
7:I:36:TRP:NE1	7:I:81:LEU:HB2	2.17	0.59
7:G:103:PHE:HZ	8:H:97:ILE:HD12	1.66	0.59
1:C:39:GLN:HE21	1:C:94:TYR:HE1	1.50	0.59
2:U:291:TRP:HA	2:U:294:LYS:HE2	1.82	0.59
6:M:36:TRP:NE1	6:M:79:LEU:HD22	2.17	0.59
2:U:73:ASN:HB3	5:X:508:GLN:NE2	2.17	0.59
2:U:198:PRO:HG2	5:X:548:MET:HG2	1.85	0.59
3:N:19:VAL:HG12	3:N:78:LEU:HD21	1.83	0.59
2:T:79:VAL:HG13	2:T:80:PRO:HD3	1.84	0.59
2:T:74:GLY:HA3	5:W:510:LYS:HB2	1.84	0.59
6:M:106:ASP:OD1	6:M:107:ILE:N	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:W:504:ILE:HG12	5:W:505:VAL:H	1.67	0.58
5:W:580:ARG:HB3	5:W:582:PHE:CE2	2.38	0.58
7:I:18:LEU:O	7:I:83:MET:HG2	2.02	0.58
3:R:61:ARG:NH1	3:R:82:ASP:OD1	2.36	0.58
6:Q:31:SER:HB2	5:V:507:ALA:H	1.68	0.58
6:M:64:VAL:HG12	6:M:67:ARG:HH11	1.68	0.58
1:C:106:ASP:OD2	1:C:107:TYR:N	2.37	0.58
2:U:128:GLY:H	5:X:580:ARG:HH22	1.50	0.58
3:N:2:ILE:HG22	3:N:27:GLN:HB2	1.85	0.58
7:G:13:GLN:N	7:G:16:ARG:HH21	2.02	0.58
6:M:51:ILE:HD11	6:M:70:ILE:HG12	1.85	0.57
1:E:72:GLU:O	1:E:72:GLU:HG2	2.04	0.57
5:X:517:TYR:CZ	5:X:546:GLY:HA3	2.38	0.57
3:P:95:LEU:HD11	6:O:103:HIS:CD2	2.39	0.57
1:E:29:PHE:O	1:E:71:ARG:NH2	2.38	0.57
4:B:39:LEU:HD13	4:B:77:PHE:CD2	2.40	0.57
1:A:82:MET:HE3	1:A:85:LEU:HD11	1.87	0.57
3:R:14:SER:HA	3:R:105:ILE:HD13	1.87	0.57
1:A:30:SER:O	1:A:53:THR:OG1	2.13	0.57
6:O:72:ARG:HA	6:O:79:LEU:HA	1.87	0.57
6:M:62:ASP:OD1	6:M:63:SER:N	2.38	0.56
2:T:255:GLN:NE2	2:T:301:ILE:O	2.38	0.56
2:U:242:VAL:HG12	2:U:275:TRP:HB2	1.86	0.56
2:T:90:SER:HB2	2:T:150:ASP:H	1.70	0.56
2:U:123:PRO:HG3	2:U:151:PHE:HD1	1.68	0.56
6:Q:31:SER:HB3	5:V:504:ILE:HG23	1.87	0.56
7:I:51:ILE:HG12	7:I:55:GLY:HA2	1.86	0.56
8:J:47:LEU:HA	8:J:58:VAL:HG21	1.86	0.56
1:C:103:LEU:HB2	4:D:97:TYR:HB2	1.87	0.56
8:H:24:ARG:NH2	8:H:70:ASP:OD1	2.38	0.56
5:X:596:ARG:HB2	5:X:596:ARG:HH11	1.70	0.56
1:C:86:ARG:HH22	4:B:78:THR:HG21	1.69	0.56
2:S:115:LYS:HE2	2:S:147:CYS:HB2	1.88	0.56
2:S:218:ILE:HG23	2:S:234:PHE:CE1	2.41	0.56
6:Q:30:SER:HG	5:V:504:ILE:N	2.03	0.56
8:H:21:ILE:HG12	8:H:103:THR:HG21	1.88	0.56
8:H:94:THR:O	8:H:97:ILE:HG23	2.06	0.56
1:A:72:GLU:OE2	1:A:79:TYR:HE2	1.88	0.56
1:A:72:GLU:O	1:A:72:GLU:HG2	2.05	0.56
2:U:57:LEU:HD11	2:U:63:LEU:HG	1.87	0.56
7:G:68:PHE:CD2	7:G:83:MET:HA	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:234:PHE:N	2:S:242:VAL:O	2.37	0.56
6:Q:91:THR:HB	6:Q:116:VAL:HG12	1.88	0.56
7:G:35:HIS:HE2	7:G:100:TRP:HA	1.71	0.56
1:C:31:SER:HB3	1:C:100:PHE:HE1	1.70	0.56
2:S:182:ALA:HB2	5:V:562:ALA:HB2	1.87	0.55
6:O:22:CYS:HB3	6:O:79:LEU:HD11	1.86	0.55
1:A:106:ASP:OD2	1:A:107:TYR:N	2.39	0.55
2:U:117:ASP:O	4:B:102:LEU:HD13	2.05	0.55
7:G:91:THR:HG23	7:G:113:THR:HA	1.88	0.55
2:U:47:ASP:HB3	2:U:50:LYS:HB3	1.89	0.55
7:G:9:GLY:HA2	7:G:112:VAL:HG22	1.87	0.55
3:N:20:THR:HG22	3:N:74:THR:HG22	1.89	0.55
8:H:101:GLN:NE2	8:H:102:GLY:O	2.40	0.55
7:I:16:ARG:HH22	7:I:84:ASN:HA	1.70	0.55
7:I:6:GLU:HG3	7:I:22:CYS:HA	1.89	0.55
2:S:256:LEU:HD21	2:S:277:VAL:HG21	1.88	0.55
3:R:17:ASP:O	3:R:78:LEU:HD23	2.07	0.55
8:H:11:LEU:HB3	8:H:19:ILE:HD11	1.89	0.55
7:I:8:GLY:O	7:I:18:LEU:HD12	2.07	0.55
1:A:31:SER:HB3	1:A:100:PHE:HE1	1.71	0.55
6:O:29:SER:O	6:O:72:ARG:NH2	2.40	0.55
4:F:60:ARG:NH2	4:F:64:VAL:O	2.40	0.54
7:I:61:ALA:HB3	7:I:64:VAL:HG22	1.89	0.54
4:F:45:LYS:HD3	4:F:90:ALA:HB2	1.89	0.54
6:Q:6:GLU:HG2	6:Q:112:THR:HG23	1.88	0.54
8:J:22:THR:N	8:J:71:PHE:O	2.40	0.54
7:G:86:LEU:HD12	7:G:114:VAL:HG22	1.88	0.54
2:U:52:VAL:HG22	2:U:54:ARG:H	1.72	0.54
5:W:521:GLN:HG2	5:W:544:THR:CG2	2.37	0.54
6:M:2:VAL:HG13	6:M:3:GLN:HG2	1.89	0.54
6:M:35:ASN:HD21	6:M:103:HIS:HE1	1.54	0.54
8:H:33:LEU:HD21	8:H:88:CYS:HB2	1.90	0.54
8:H:95:PRO:HB2	8:H:96:PRO:HD3	1.88	0.54
2:S:154:HIS:CE1	2:S:156:GLU:HB2	2.43	0.54
2:U:164:ARG:NH2	5:W:575:ALA:O	2.41	0.54
3:P:35:TRP:CE2	3:P:73:LEU:HB2	2.43	0.54
1:C:35:HIS:HD2	1:C:47:TRP:HE1	1.56	0.54
6:O:36:TRP:NE1	6:O:81:LEU:HB2	2.23	0.54
5:V:611:GLU:OE2	5:X:602:HIS:ND1	2.41	0.54
3:N:37:GLN:HB2	3:N:47:LEU:HD11	1.90	0.54
7:I:36:TRP:NE1	7:I:79:LEU:HD21	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:33:LEU:HB3	8:J:51:ALA:HB2	1.90	0.54
8:J:89:GLN:OE1	8:J:99:PHE:HA	2.07	0.53
4:D:39:LEU:HD13	4:D:77:PHE:CD2	2.44	0.53
3:N:51:ALA:HB1	3:N:66:GLY:HA3	1.89	0.53
8:J:29:ILE:HG23	8:J:92:PHE:HB2	1.90	0.53
2:U:120:GLU:OE2	2:U:172:ARG:HD3	2.08	0.53
6:Q:6:GLU:OE1	6:Q:6:GLU:N	2.39	0.53
6:M:48:VAL:HG23	6:M:64:VAL:HG21	1.90	0.53
2:T:49:ASP:OD1	2:T:50:LYS:N	2.41	0.53
2:S:162:TYR:CE2	2:S:176:PHE:HB3	2.44	0.53
7:G:34:MET:SD	7:G:98:ARG:HA	2.48	0.53
8:H:17:ASP:OD1	8:H:18:ARG:N	2.41	0.53
3:P:2:ILE:HD13	3:P:93:SER:HB2	1.90	0.53
1:C:38:ARG:NH1	1:C:93:TYR:OH	2.40	0.53
5:W:521:GLN:HG3	5:W:542:ILE:O	2.08	0.53
6:M:101:TYR:HD2	6:M:102:PRO:HD3	1.73	0.53
7:G:64:VAL:HB	7:G:68:PHE:HD1	1.74	0.53
5:V:521:GLN:HA	5:V:544:THR:OG1	2.09	0.53
4:D:53:LEU:HA	4:D:64:VAL:HG21	1.90	0.53
4:F:96:GLN:HE21	4:F:103:THR:H	1.56	0.53
5:V:583:SER:O	5:V:587:ARG:HG3	2.09	0.53
2:U:38:ILE:HB	2:U:187:PRO:HD3	1.90	0.53
2:S:57:LEU:HB3	5:X:594:LEU:HD22	1.90	0.53
2:U:78:ASP:OD1	2:U:81:SER:HB3	2.08	0.53
5:W:587:ARG:HA	5:W:590:ILE:HG12	1.91	0.53
8:J:37:GLN:HB3	8:J:47:LEU:HD11	1.90	0.53
1:C:68:THR:HG23	1:C:81:GLN:HB3	1.90	0.53
3:P:90:GLN:HE21	3:P:96:THR:HB	1.74	0.52
1:A:101:GLY:O	2:U:143:GLY:HA2	2.09	0.52
2:U:191:LYS:HB3	2:U:195:SER:HB3	1.92	0.52
6:M:12:VAL:O	6:M:116:VAL:HA	2.09	0.52
6:O:67:ARG:NH2	6:O:90:ASP:OD1	2.37	0.52
5:V:521:GLN:NE2	5:X:574:ARG:HD2	2.24	0.52
8:J:36:TYR:HE2	8:J:89:GLN:HB2	1.74	0.52
3:R:6:GLN:OE1	3:R:101:THR:HG23	2.09	0.52
7:G:104:ASP:OD1	7:G:105:TYR:N	2.43	0.52
2:T:196:SER:O	2:T:198:PRO:HD3	2.09	0.52
8:J:39:LYS:HD3	8:J:40:PRO:HD2	1.91	0.52
2:U:263:SER:HB3	8:J:32:TYR:CE1	2.45	0.52
6:Q:68:PHE:CE1	6:Q:83:MET:HB2	2.45	0.52
2:T:98:ASN:ND2	5:W:582:PHE:HD1	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:249:THR:HG21	2:T:286:GLY:HA3	1.90	0.52
8:H:34:HIS:HE1	8:H:91:SER:HB2	1.74	0.52
1:A:29:PHE:O	1:A:71:ARG:NH2	2.43	0.52
2:T:116:PRO:HD2	1:C:58:TYR:CE2	2.44	0.52
2:U:45:VAL:HG21	6:O:56:GLY:HA3	1.90	0.52
3:N:11:LEU:HD11	3:N:19:VAL:HG21	1.92	0.52
3:N:34:ASN:OD1	3:N:89:GLN:HB3	2.10	0.52
2:T:291:TRP:CD1	5:W:513:PRO:HD2	2.44	0.52
4:F:53:LEU:HA	4:F:64:VAL:HG11	1.92	0.52
1:E:86:ARG:HH22	4:D:78:THR:HG21	1.74	0.52
2:S:63:LEU:HB3	5:V:585:LEU:HD22	1.92	0.52
4:B:20:THR:HG22	4:B:80:THR:HG22	1.92	0.52
2:S:104:TRP:CZ2	2:S:134:ARG:HD2	2.45	0.52
7:G:38:ARG:HD3	7:G:94:TYR:CZ	2.44	0.52
3:P:63:SER:OG	3:P:74:THR:HG23	2.10	0.52
8:J:49:TYR:HB2	8:J:53:THR:HG23	1.91	0.52
2:T:154:HIS:CE1	2:T:156:GLU:HB2	2.45	0.51
6:O:97:ALA:HB1	6:O:105:PHE:HB3	1.92	0.51
6:O:101:TYR:CD1	9:Y:2:NAG:H4	2.45	0.51
8:J:83:PHE:CG	8:J:107:ILE:HG12	2.45	0.51
2:T:154:HIS:ND1	2:T:156:GLU:HB2	2.25	0.51
6:M:35:ASN:N	6:M:97:ALA:O	2.35	0.51
8:H:61:ARG:HD2	8:H:77:SER:O	2.11	0.51
2:T:51:LEU:HB3	5:W:595:GLN:HE21	1.74	0.51
8:H:22:THR:HG23	8:H:72:THR:HG22	1.92	0.51
7:I:14:PRO:HA	7:I:86:LEU:HD22	1.93	0.51
1:C:72:GLU:OE2	1:C:74:ALA:HB3	2.10	0.51
2:U:156:GLU:HG2	9:Y:2:NAG:H62	1.93	0.51
1:E:6:GLU:OE2	1:E:95:CYS:N	2.28	0.51
3:R:29:ILE:N	3:R:68:GLY:O	2.41	0.51
6:M:4:LEU:HD23	6:M:24:ALA:HA	1.92	0.51
8:J:79:GLN:HB3	8:J:80:PRO:HD2	1.93	0.51
2:U:98:ASN:HB2	5:X:582:PHE:CD1	2.46	0.51
3:P:7:SER:HB3	3:P:8:PRO:HD3	1.92	0.51
8:J:80:PRO:HA	8:J:83:PHE:CD2	2.45	0.51
4:D:38:TYR:HB2	4:D:98:TYR:HB2	1.92	0.51
5:W:550:ASN:OD1	5:W:551:GLN:N	2.44	0.51
8:J:85:THR:HB	8:J:102:GLY:HA3	1.91	0.51
4:F:67:ARG:NH2	4:F:88:ASP:OD2	2.41	0.51
7:G:39:GLN:O	7:G:92:ALA:HB1	2.11	0.51
7:G:98:ARG:HD2	7:G:98:ARG:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:TRP:NE1	1:A:80:LEU:HB2	2.26	0.51
5:V:521:GLN:HE21	5:X:574:ARG:HD2	1.74	0.51
2:S:196:SER:O	2:S:198:PRO:HD3	2.11	0.51
3:P:92:TYR:O	5:V:528:GLY:HA3	2.10	0.51
6:O:102:PRO:HA	5:V:529:LEU:HD11	1.93	0.51
4:D:3:VAL:HG12	4:D:26:SER:HB3	1.93	0.51
2:S:234:PHE:HB3	2:S:242:VAL:HG23	1.93	0.50
7:I:64:VAL:HA	7:I:67:ARG:NH1	2.26	0.50
1:A:58:TYR:HB3	2:U:117:ASP:OD1	2.11	0.50
2:S:114:LYS:O	2:S:144:THR:HA	2.11	0.50
8:J:34:HIS:N	8:J:89:GLN:O	2.40	0.50
2:S:37:VAL:HG23	2:S:46:SER:HB2	1.93	0.50
5:W:521:GLN:HG2	5:W:544:THR:HG23	1.93	0.50
8:H:55:GLN:HB3	8:H:58:VAL:HG13	1.93	0.50
6:O:59:TYR:HD2	5:V:527:ILE:CD1	2.24	0.50
8:J:37:GLN:HE21	8:J:84:ALA:HB3	1.76	0.50
1:E:30:SER:O	1:E:53:THR:HG23	2.10	0.50
1:E:38:ARG:HG3	1:E:91:ALA:HB3	1.93	0.50
1:A:29:PHE:HZ	1:A:78:LEU:HB2	1.75	0.50
2:S:247:ARG:HH11	2:S:279:PRO:HD2	1.76	0.50
3:N:61:ARG:NH2	3:N:82:ASP:OD2	2.32	0.50
7:G:68:PHE:HD2	7:G:83:MET:HA	1.76	0.50
8:H:13:ALA:O	8:H:108:LYS:N	2.43	0.50
6:O:35:ASN:ND2	6:O:105:PHE:HE1	2.06	0.50
2:S:156:GLU:HG2	9:L:2:NAG:H62	1.94	0.50
3:R:81:GLU:OE2	3:R:81:GLU:N	2.36	0.50
6:O:8:GLY:O	6:O:18:LEU:HD21	2.11	0.50
5:W:517:TYR:CZ	5:W:546:GLY:HA3	2.47	0.50
1:A:92:VAL:HG22	1:A:113:LEU:HD13	1.94	0.50
2:U:281:ILE:HG21	2:U:301:ILE:HD12	1.93	0.50
6:O:32:TYR:HD1	6:O:98:LYS:HD3	1.76	0.50
2:T:94:PRO:HB3	2:T:169:VAL:HG21	1.94	0.50
2:S:96:VAL:HG22	2:S:167:SER:HB2	1.93	0.50
2:U:104:TRP:NE1	5:X:545:GLU:OE1	2.41	0.50
7:I:100:TRP:HD1	7:I:101:ASN:OD1	1.95	0.50
2:S:232:TYR:HB2	2:S:244:LEU:HB2	1.92	0.49
3:N:50:ALA:HB2	6:M:102:PRO:HG3	1.94	0.49
3:N:95:LEU:HD21	6:M:103:HIS:ND1	2.28	0.49
8:J:95:PRO:CD	8:J:96:PRO:HD3	2.42	0.49
7:G:4:LEU:HD21	7:G:27:PHE:HE2	1.78	0.49
8:H:30:SER:H	8:H:92:PHE:HE2	1.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:37:VAL:HB	7:I:95:TYR:HB2	1.94	0.49
6:M:76:LYS:HB2	6:M:78:THR:HG22	1.94	0.49
7:G:67:ARG:HB3	7:G:85:SER:HB3	1.94	0.49
8:H:6:GLN:HA	8:H:23:CYS:HA	1.94	0.49
7:I:37:VAL:HG11	7:I:45:LEU:HD22	1.93	0.49
4:B:43:GLN:HB2	4:B:53:LEU:HD11	1.93	0.49
2:T:77:THR:OG1	2:T:107:ASN:ND2	2.45	0.49
2:T:311:VAL:O	2:T:312:ASN:HB3	2.12	0.49
2:U:255:GLN:OE1	2:U:301:ILE:HB	2.12	0.49
6:Q:79:LEU:HD23	6:Q:79:LEU:H	1.77	0.49
4:F:38:TYR:HD1	4:F:97:TYR:CE2	2.29	0.49
6:M:101:TYR:CZ	9:K:3:BMA:H3	2.48	0.49
1:C:39:GLN:HB2	1:C:45:LEU:HD13	1.94	0.49
2:T:258:GLU:HA	10:T:603:NAG:H82	1.94	0.49
6:M:83:MET:HE1	6:M:114:VAL:HG21	1.95	0.49
3:R:38:GLN:NE2	6:Q:39:GLN:HE22	2.11	0.49
2:T:164:ARG:NH1	5:V:575:ALA:O	2.45	0.49
3:R:94:THR:HG23	3:R:96:THR:HG23	1.95	0.49
4:F:2:ILE:HG13	4:F:27:GLN:HB2	1.93	0.49
4:D:43:GLN:HB2	4:D:53:LEU:HD11	1.94	0.49
2:T:146:PRO:HG3	1:C:56:ASP:OD2	2.13	0.49
2:S:88:PHE:HB3	2:S:149:GLY:H	1.77	0.49
2:U:86:TRP:HZ3	2:U:111:LEU:HD21	1.76	0.49
5:W:527:ILE:HD13	6:Q:59:TYR:CD1	2.40	0.49
7:G:100:TRP:HE1	8:H:94:THR:HG21	1.77	0.49
7:I:39:GLN:O	7:I:92:ALA:HB1	2.13	0.49
2:T:193:PHE:HE1	5:W:554:LEU:HD21	1.77	0.49
6:Q:105:PHE:O	6:Q:108:TRP:NE1	2.45	0.49
8:J:78:LEU:HD23	8:J:83:PHE:HE1	1.77	0.49
1:E:31:SER:HB3	1:E:100:PHE:HE1	1.78	0.49
5:W:507:ALA:H	6:M:31:SER:HB2	1.77	0.48
6:Q:99:ARG:NH1	6:Q:103:HIS:HD2	2.12	0.48
2:T:240:THR:OG1	2:T:266:ARG:HB2	2.13	0.48
5:W:507:ALA:HB2	6:M:31:SER:HB2	1.94	0.48
7:G:38:ARG:NH1	7:G:94:TYR:OH	2.46	0.48
1:A:102:GLU:HG2	2:U:221:GLN:HE22	1.78	0.48
2:T:163:ASP:OD2	5:W:543:TYR:OH	2.31	0.48
1:E:106:ASP:OD1	1:E:107:TYR:N	2.46	0.48
2:T:68:LEU:HD11	5:W:558:LEU:HG	1.96	0.48
2:S:197:HIS:O	2:S:197:HIS:ND1	2.47	0.48
2:T:252:PHE:HD2	2:T:301:ILE:HD11	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:24:LYS:HG3	4:F:76:GLU:HB3	1.96	0.48
3:P:38:GLN:OE1	6:O:39:GLN:NE2	2.46	0.48
5:V:562:ALA:HA	5:V:565:THR:HG22	1.96	0.48
7:I:94:TYR:O	7:I:109:GLY:HA2	2.13	0.48
1:E:51:ILE:HG21	1:E:78:LEU:HD11	1.94	0.48
7:G:6:GLU:HB3	7:G:110:THR:HB	1.95	0.48
6:O:40:ALA:HB3	6:O:43:LYS:HB2	1.95	0.48
7:I:68:PHE:CE1	7:I:83:MET:HB2	2.49	0.48
8:J:36:TYR:O	8:J:87:TYR:N	2.41	0.48
1:E:32:TYR:CD1	1:E:97:ARG:HD3	2.48	0.48
3:R:45:LYS:NZ	3:R:58:VAL:HG22	2.29	0.48
7:G:36:TRP:NE1	7:G:81:LEU:HB2	2.29	0.48
2:T:252:PHE:CE2	2:T:279:PRO:HG3	2.49	0.48
3:R:93:SER:O	3:R:94:THR:HG22	2.14	0.48
6:O:91:THR:HG22	6:O:116:VAL:H	1.79	0.48
2:S:234:PHE:CE2	2:S:236:VAL:HG12	2.49	0.47
3:P:95:LEU:HD21	6:O:103:HIS:CD2	2.49	0.47
5:X:603:ILE:H	5:X:603:ILE:HD12	1.79	0.47
7:I:16:ARG:HE	7:I:17:SER:N	2.00	0.47
7:I:67:ARG:HB2	7:I:85:SER:H	1.80	0.47
4:B:89:VAL:HG23	4:B:110:VAL:O	2.14	0.47
2:T:79:VAL:CG1	2:T:80:PRO:HD3	2.43	0.47
7:I:16:ARG:NH2	7:I:84:ASN:HA	2.29	0.47
7:I:38:ARG:O	7:I:46:GLU:HG2	2.14	0.47
6:Q:69:THR:HG23	6:Q:82:GLN:HB3	1.97	0.47
2:T:114:LYS:O	2:T:144:THR:HA	2.15	0.47
2:S:191:LYS:O	2:S:195:SER:HB2	2.15	0.47
2:U:132:PHE:HD2	2:U:135:CYS:SG	2.37	0.47
4:F:31:TYR:HB2	4:F:38:TYR:HE2	1.78	0.47
5:W:562:ALA:HA	5:W:565:THR:HG22	1.95	0.47
7:G:17:SER:HA	7:G:83:MET:O	2.14	0.47
5:X:584:ILE:H	5:X:584:ILE:HD12	1.80	0.47
4:B:61:GLU:HB3	4:B:64:VAL:HG23	1.95	0.47
7:I:19:ARG:HG2	7:I:19:ARG:HH11	1.79	0.47
2:T:242:VAL:HG11	2:T:256:LEU:HD21	1.97	0.47
2:U:154:HIS:CE1	2:U:156:GLU:HB2	2.49	0.47
2:U:282:ASP:OD1	2:U:283:THR:HG23	2.15	0.47
6:Q:72:ARG:HA	6:Q:79:LEU:HA	1.96	0.47
8:H:7:SER:HB2	8:H:8:PRO:HD3	1.95	0.47
6:O:32:TYR:CE2	5:X:507:ALA:HA	2.50	0.47
2:T:131:GLY:O	2:T:163:ASP:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:61:GLU:O	4:F:64:VAL:HG22	2.14	0.47
6:M:98:LYS:HB3	6:M:107:ILE:HG22	1.95	0.47
7:I:76:LYS:NZ	7:I:78:THR:HG21	2.30	0.47
4:B:24:LYS:HZ3	4:B:76:GLU:HB3	1.79	0.47
2:U:73:ASN:HB3	5:X:508:GLN:HE21	1.80	0.47
4:F:97:TYR:HA	4:F:102:LEU:HD22	1.96	0.47
8:H:47:LEU:HA	8:H:58:VAL:HG11	1.96	0.47
6:O:47:TRP:CZ3	5:V:527:ILE:HG13	2.50	0.47
1:C:29:PHE:O	1:C:71:ARG:NH2	2.47	0.47
2:S:123:PRO:HG3	2:S:151:PHE:CD2	2.50	0.47
2:U:249:THR:HG23	2:U:252:PHE:H	1.79	0.47
2:U:291:TRP:HD1	2:U:295:LYS:HZ1	1.63	0.47
4:F:43:GLN:HB2	4:F:53:LEU:HD11	1.96	0.47
5:W:507:ALA:CB	6:M:31:SER:HB2	2.45	0.47
1:A:96:ALA:HB1	1:A:105:PHE:HB3	1.96	0.47
1:A:103:LEU:HD23	1:A:103:LEU:HA	1.74	0.47
2:U:63:LEU:HB3	5:X:585:LEU:HD22	1.97	0.47
2:U:304:GLU:OE2	8:J:32:TYR:HA	2.15	0.47
8:H:66:GLY:HA3	8:H:71:PHE:HA	1.96	0.47
7:I:18:LEU:H	7:I:18:LEU:HD23	1.78	0.47
6:M:60:TYR:OH	6:M:70:ILE:N	2.36	0.46
6:M:88:ALA:HA	6:M:116:VAL:HG21	1.97	0.46
8:J:35:TRP:CZ3	8:J:88:CYS:HB3	2.51	0.46
7:G:62:ASP:O	7:G:65:LYS:HG2	2.14	0.46
8:J:8:PRO:HB2	8:J:103:THR:HB	1.97	0.46
2:T:292:GLU:HG3	5:W:510:LYS:NZ	2.31	0.46
8:H:61:ARG:HG3	8:H:62:PHE:HD1	1.81	0.46
5:V:530:ALA:HA	5:V:535:PHE:O	2.16	0.46
8:J:33:LEU:HD21	8:J:88:CYS:HB2	1.97	0.46
5:W:563:ASN:O	5:W:566:THR:HG22	2.15	0.46
5:W:607:ASP:OD1	5:W:608:CYS:N	2.48	0.46
6:M:3:GLN:HB2	6:M:25:SER:HB2	1.97	0.46
8:H:5:THR:HB	8:H:24:ARG:HB3	1.96	0.46
7:I:70:ILE:HD11	7:I:79:LEU:HD21	1.97	0.46
8:J:6:GLN:NE2	8:J:86:TYR:O	2.49	0.46
1:E:36:TRP:HE1	1:E:78:LEU:CD2	2.29	0.46
2:T:51:LEU:HD12	2:T:51:LEU:O	2.16	0.46
2:T:85:ARG:HH22	2:T:178:GLU:CD	2.19	0.46
2:T:98:ASN:HD22	5:W:582:PHE:HD1	1.64	0.46
2:T:294:LYS:HG3	2:T:296:ASN:ND2	2.30	0.46
2:U:234:PHE:HB3	2:U:242:VAL:HG23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:34:ASN:HD22	6:M:104:SER:HB2	1.80	0.46
4:F:19:ALA:HB2	4:F:84:LEU:HD12	1.97	0.46
4:F:61:GLU:HB3	4:F:64:VAL:HG13	1.98	0.46
8:H:47:LEU:HD13	8:H:62:PHE:HD2	1.81	0.46
8:J:5:THR:OG1	8:J:24:ARG:NE	2.49	0.46
8:J:38:GLN:HB2	8:J:44:PRO:HG3	1.98	0.46
4:B:7:SER:HB2	4:B:22:ASN:HB2	1.97	0.46
2:S:142:SER:O	2:S:221:GLN:HA	2.16	0.46
3:N:17:ASP:O	3:N:78:LEU:HD23	2.15	0.46
5:W:514:ASN:OD1	5:W:549:HIS:HB2	2.15	0.46
3:P:46:LEU:HB2	6:O:105:PHE:O	2.16	0.46
6:O:4:LEU:HD22	6:O:22:CYS:SG	2.56	0.46
8:J:61:ARG:NH1	8:J:81:GLU:OE2	2.40	0.46
4:D:61:GLU:HB3	4:D:64:VAL:HG23	1.97	0.46
2:S:49:ASP:OD1	2:S:50:LYS:N	2.49	0.46
2:U:252:PHE:CZ	2:U:279:PRO:HG3	2.51	0.46
3:N:49:TYR:CE2	3:N:55:GLN:HA	2.51	0.46
6:Q:29:SER:O	6:Q:72:ARG:NH1	2.47	0.46
2:T:156:GLU:OE2	9:K:2:NAG:H62	2.17	0.45
8:J:37:GLN:CB	8:J:47:LEU:HD11	2.45	0.45
4:B:3:VAL:HG22	4:B:26:SER:HB3	1.98	0.45
2:S:71:GLU:OE2	2:S:106:GLU:N	2.39	0.45
2:S:77:THR:O	2:S:109:TYR:OH	2.20	0.45
4:F:89:VAL:O	4:F:89:VAL:HG23	2.17	0.45
2:U:114:LYS:O	2:U:144:THR:HA	2.16	0.45
2:U:162:TYR:CE1	2:U:176:PHE:HB3	2.50	0.45
6:Q:71:SER:O	6:Q:80:TYR:N	2.42	0.45
8:H:29:ILE:HB	8:H:71:PHE:HE2	1.81	0.45
1:C:87:ALA:O	1:C:90:THR:HG22	2.16	0.45
2:U:254:LEU:O	2:U:257:ASN:HB3	2.16	0.45
6:Q:99:ARG:HH11	6:Q:103:HIS:HD2	1.63	0.45
7:I:22:CYS:HB3	7:I:79:LEU:HD22	1.97	0.45
5:W:527:ILE:HD11	6:Q:103:HIS:NE2	2.31	0.45
1:A:12:VAL:HG21	1:A:85:LEU:HD12	1.99	0.45
5:W:505:VAL:HG12	5:W:505:VAL:O	2.16	0.45
6:M:17:SER:HB3	6:M:82:GLN:NE2	2.32	0.45
6:M:51:ILE:HD13	6:M:79:LEU:HD11	1.99	0.45
1:C:66:ARG:NH1	1:C:89:ASP:OD2	2.41	0.45
1:A:63:VAL:HB	1:A:67:PHE:CG	2.51	0.45
1:A:99:TRP:CZ2	2:U:272:LYS:HD2	2.52	0.45
2:U:89:ARG:NH1	5:V:536:GLY:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:83:PHE:O	3:N:103:LEU:HB2	2.16	0.45
6:M:38:ARG:HD3	6:M:94:TYR:CZ	2.51	0.45
6:O:36:TRP:CD1	6:O:81:LEU:HB2	2.51	0.45
5:V:513:PRO:HA	5:V:552:ASP:OD2	2.16	0.45
2:T:245:GLU:OE1	2:T:247:ARG:NH1	2.50	0.45
2:U:255:GLN:O	2:U:259:THR:HG23	2.17	0.45
3:R:2:ILE:HD11	3:R:27:GLN:NE2	2.31	0.45
2:S:57:LEU:HD21	2:S:63:LEU:HD11	1.99	0.45
3:N:84:ALA:HA	3:N:102:ARG:HH12	1.82	0.45
6:M:11:LEU:HD13	6:M:115:THR:OG1	2.17	0.45
8:H:24:ARG:NH2	8:H:69:THR:OG1	2.40	0.45
7:I:93:VAL:HA	7:I:111:LEU:HA	1.98	0.45
1:A:21:SER:HB3	1:A:79:TYR:CE1	2.52	0.45
2:T:134:ARG:NH1	5:W:543:TYR:HB2	2.31	0.45
2:S:51:LEU:O	2:S:51:LEU:HD23	2.17	0.45
2:S:85:ARG:NH1	2:S:178:GLU:OE1	2.48	0.45
2:S:198:PRO:HB2	5:V:550:ASN:HD21	1.82	0.45
6:M:35:ASN:ND2	6:M:103:HIS:HE1	2.15	0.45
7:I:73:ASP:OD2	7:I:73:ASP:N	2.50	0.45
2:S:123:PRO:HG3	2:S:151:PHE:HD2	1.81	0.44
2:U:33:ILE:HD12	2:U:33:ILE:H	1.81	0.44
6:O:74:ASN:OD1	6:O:75:SER:N	2.50	0.44
4:D:86:ALA:O	4:D:89:VAL:HG12	2.17	0.44
2:T:115:LYS:HD2	2:T:119:SER:HB2	1.99	0.44
2:T:182:ALA:HB2	5:W:562:ALA:CB	2.47	0.44
2:U:97:VAL:HG23	5:X:573:LEU:HD11	1.98	0.44
5:V:585:LEU:HD23	5:V:585:LEU:HA	1.79	0.44
5:X:609:CYS:O	5:X:609:CYS:SG	2.75	0.44
7:I:100:TRP:HE1	8:J:94:THR:HB	1.82	0.44
8:J:37:GLN:HE22	8:J:39:LYS:HB2	1.82	0.44
1:C:110:GLN:NE2	4:D:49:PRO:HD3	2.32	0.44
7:G:35:HIS:NE2	7:G:100:TRP:HA	2.31	0.44
8:H:38:GLN:O	8:H:84:ALA:HB1	2.18	0.44
3:P:6:GLN:NE2	3:P:88:CYS:SG	2.89	0.44
3:P:78:LEU:HD12	3:P:79:GLN:H	1.83	0.44
2:U:192:ASP:OD1	2:U:193:PHE:N	2.50	0.44
3:N:21:ILE:HD13	3:N:101:THR:HG21	1.99	0.44
7:I:60:TYR:CZ	7:I:69:THR:HA	2.52	0.44
2:U:194:PHE:HA	5:X:517:TYR:CE2	2.52	0.44
3:N:2:ILE:HD11	3:N:90:GLN:OE1	2.18	0.44
6:Q:50:THR:HG22	6:Q:59:TYR:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:6:GLN:HE22	8:J:102:GLY:HA2	1.83	0.44
3:N:18:ARG:HA	3:N:18:ARG:NE	2.32	0.44
8:H:55:GLN:O	8:H:58:VAL:HG22	2.17	0.44
6:O:62:ASP:OD1	6:O:63:SER:N	2.51	0.44
1:E:4:LEU:HD23	1:E:95:CYS:SG	2.58	0.44
3:R:95:LEU:HD21	6:Q:103:HIS:HD1	1.83	0.44
3:N:35:TRP:HB2	3:N:48:ILE:HG12	1.98	0.44
4:F:20:THR:HG23	4:F:78:THR:HG23	1.99	0.44
8:J:84:ALA:O	8:J:104:LYS:HA	2.18	0.44
4:B:86:ALA:HA	4:B:112:ILE:HG13	1.99	0.44
1:A:98:THR:HB	1:A:102:GLU:O	2.17	0.44
2:T:87:GLY:O	2:T:153:PHE:N	2.33	0.44
6:M:59:TYR:HB3	5:X:527:ILE:HD12	1.99	0.44
6:M:101:TYR:HE1	9:K:2:NAG:C6	2.30	0.44
6:M:101:TYR:H	9:K:5:MAN:H62	1.82	0.44
2:T:199:LEU:HD12	5:W:549:HIS:NE2	2.33	0.43
6:Q:39:GLN:HB2	6:Q:45:LEU:HD23	1.99	0.43
6:O:34:MET:HB3	6:O:79:LEU:HD22	2.00	0.43
1:E:31:SER:HB3	1:E:100:PHE:CE1	2.52	0.43
1:E:39:GLN:O	1:E:91:ALA:HB1	2.18	0.43
4:D:7:SER:HB2	4:D:8:PRO:HD3	1.99	0.43
2:T:88:PHE:CE2	2:T:152:ALA:HB2	2.53	0.43
3:R:39:LYS:HD3	3:R:84:ALA:HB2	1.99	0.43
5:W:513:PRO:HA	5:W:552:ASP:OD1	2.18	0.43
6:Q:1:GLU:HG2	6:Q:2:VAL:N	2.33	0.43
1:C:63:VAL:HB	1:C:67:PHE:CG	2.53	0.43
1:A:33:ASP:HA	1:A:71:ARG:HH12	1.83	0.43
4:F:39:LEU:HD13	4:F:77:PHE:CD2	2.52	0.43
7:G:99:ASN:OD1	7:G:100:TRP:N	2.52	0.43
1:A:51:ILE:HD12	1:A:56:ASP:O	2.18	0.43
3:R:45:LYS:HZ1	3:R:58:VAL:HG22	1.83	0.43
4:F:6:GLN:NE2	4:F:94:CYS:H	2.17	0.43
5:W:522:ASP:OD1	5:W:525:ALA:HB3	2.19	0.43
3:P:93:SER:HA	5:V:528:GLY:HA3	2.00	0.43
3:P:99:GLN:HG2	3:P:100:GLY:N	2.33	0.43
5:V:563:ASN:O	5:V:566:THR:HG22	2.18	0.43
7:I:36:TRP:CD2	7:I:81:LEU:HD22	2.54	0.43
8:J:47:LEU:O	8:J:54:LEU:HD12	2.18	0.43
8:H:13:ALA:HB1	8:H:17:ASP:HB3	1.99	0.43
5:V:554:LEU:O	5:V:558:LEU:HG	2.18	0.43
2:T:193:PHE:CE1	5:W:548:MET:HE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:234:PHE:HB2	2:S:244:LEU:HD21	2.01	0.43
2:S:245:GLU:HG3	2:S:247:ARG:NH2	2.34	0.43
2:U:71:GLU:HG3	2:U:77:THR:HG21	1.99	0.43
2:U:126:PRO:HD2	2:U:129:ILE:HG13	2.01	0.43
2:U:162:TYR:OH	2:U:170:ILE:HA	2.18	0.43
3:N:33:LEU:O	3:N:51:ALA:N	2.47	0.43
3:N:90:GLN:NE2	3:N:96:THR:H	2.09	0.43
8:H:13:ALA:HB2	8:H:19:ILE:HD12	2.00	0.43
2:T:126:PRO:HB2	5:W:580:ARG:NH2	2.33	0.43
2:T:154:HIS:NE2	2:T:178:GLU:OE1	2.41	0.43
1:A:54:ALA:HB3	2:U:146:PRO:HG2	1.99	0.43
3:R:2:ILE:HD11	3:R:27:GLN:HE21	1.83	0.43
2:T:296:ASN:O	2:T:297:LEU:HG	2.19	0.43
4:F:13:VAL:O	4:F:112:ILE:HA	2.19	0.43
6:M:53:GLY:O	6:M:72:ARG:NH2	2.51	0.43
3:P:23:CYS:HB2	3:P:35:TRP:CH2	2.54	0.43
3:P:55:GLN:NE2	3:P:56:SER:H	2.15	0.43
4:D:11:LEU:O	4:D:11:LEU:HD23	2.19	0.43
2:T:37:VAL:HG23	2:T:46:SER:HB2	2.01	0.43
2:T:134:ARG:HA	2:T:134:ARG:HD3	1.84	0.43
6:Q:101:TYR:CD1	9:L:2:NAG:H4	2.54	0.43
6:O:59:TYR:OH	5:X:567:GLN:HG2	2.18	0.43
1:C:12:VAL:HG11	1:C:85:LEU:HD12	2.01	0.43
1:E:86:ARG:H	1:E:86:ARG:HG2	1.74	0.43
3:N:38:GLN:HE22	6:M:45:LEU:HD11	1.84	0.42
4:F:60:ARG:HH21	4:F:65:PRO:C	2.22	0.42
7:I:39:GLN:C	7:I:92:ALA:HB1	2.40	0.42
1:E:6:GLU:OE1	1:E:111:GLY:HA2	2.19	0.42
1:E:43:LYS:HG2	1:E:44:GLY:N	2.30	0.42
2:U:198:PRO:HG2	5:X:548:MET:HA	2.01	0.42
7:G:102:LEU:HB3	8:H:34:HIS:CD2	2.54	0.42
6:O:13:GLN:H	6:O:13:GLN:CD	2.22	0.42
2:T:142:SER:O	2:T:221:GLN:HA	2.19	0.42
2:U:234:PHE:CE2	2:U:236:VAL:HG12	2.54	0.42
6:M:36:TRP:CD1	6:M:70:ILE:HD11	2.46	0.42
5:X:562:ALA:O	5:X:565:THR:HG22	2.19	0.42
8:J:22:THR:N	8:J:72:THR:HA	2.33	0.42
1:C:86:ARG:HG2	1:C:89:ASP:OD1	2.19	0.42
4:B:21:ILE:HG12	4:B:108:THR:HG21	2.01	0.42
1:A:58:TYR:HB3	2:U:117:ASP:CG	2.39	0.42
2:T:63:LEU:HB3	5:W:585:LEU:HD22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:290:PHE:O	2:T:295:LYS:HG2	2.20	0.42
2:S:164:ARG:HE	2:S:164:ARG:HB2	1.63	0.42
2:S:186:LEU:HD23	2:S:186:LEU:HA	1.83	0.42
4:F:7:SER:HB2	4:F:8:PRO:HD3	2.01	0.42
6:M:59:TYR:HB3	5:X:527:ILE:CD1	2.50	0.42
3:P:5:THR:OG1	3:P:24:ARG:NH1	2.52	0.42
1:C:98:THR:HB	1:C:102:GLU:O	2.20	0.42
2:T:57:LEU:HA	2:T:62:GLN:OE1	2.19	0.42
2:U:62:GLN:HE21	2:U:62:GLN:HB3	1.73	0.42
4:F:45:LYS:HB2	4:F:48:GLN:HB2	2.01	0.42
5:W:504:ILE:HG23	5:W:506:ASN:H	1.85	0.42
7:G:2:VAL:HB	7:G:105:TYR:CE1	2.54	0.42
3:P:18:ARG:HH12	3:P:20:THR:N	2.18	0.42
7:I:38:ARG:CG	7:I:92:ALA:HB3	2.49	0.42
4:D:89:VAL:HG23	4:D:110:VAL:O	2.19	0.42
2:T:162:TYR:OH	2:T:170:ILE:HA	2.19	0.42
5:W:515:LEU:HB2	5:W:555:ILE:HD12	2.01	0.42
6:Q:34:MET:CB	6:Q:79:LEU:HD13	2.49	0.42
6:Q:39:GLN:HE21	6:Q:95:TYR:HE1	1.67	0.42
5:V:596:ARG:HB2	5:V:597:TRP:CD1	2.54	0.42
7:I:17:SER:CB	7:I:83:MET:HG3	2.36	0.42
4:D:14:SER:HA	4:D:113:LYS:H	1.84	0.42
6:Q:88:ALA:O	6:Q:91:THR:HG22	2.20	0.42
6:O:59:TYR:HD2	5:V:527:ILE:HD13	1.85	0.42
2:U:265:LYS:HB3	2:U:268:ASN:OD1	2.19	0.42
3:R:19:VAL:HB	3:R:78:LEU:HD21	2.01	0.42
4:F:6:GLN:OE1	4:F:108:THR:HG23	2.19	0.42
8:H:47:LEU:HB2	8:H:48:ILE:HD12	2.01	0.42
2:U:240:THR:HG21	2:U:266:ARG:HG2	2.01	0.42
3:N:91:SER:O	5:X:529:LEU:N	2.44	0.42
6:M:79:LEU:HD23	6:M:80:TYR:N	2.34	0.42
5:X:513:PRO:HB2	5:X:552:ASP:OD1	2.20	0.42
1:E:29:PHE:HZ	1:E:78:LEU:HB2	1.85	0.42
4:D:55:TYR:HD2	4:D:56:TRP:CD1	2.37	0.42
2:T:43:LEU:HB2	5:W:554:LEU:HD12	2.02	0.42
3:N:61:ARG:NH2	3:N:79:GLN:OE1	2.52	0.42
5:W:507:ALA:HA	6:M:32:TYR:CE1	2.55	0.42
6:O:32:TYR:HA	5:X:507:ALA:HB2	2.01	0.42
1:C:35:HIS:HD2	1:C:47:TRP:NE1	2.16	0.42
2:T:300:LYS:HD2	2:T:300:LYS:HA	1.86	0.41
6:Q:17:SER:HB2	6:Q:84:ASN:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:6:GLN:HE22	3:P:87:TYR:HA	1.85	0.41
6:O:71:SER:O	6:O:80:TYR:N	2.40	0.41
2:U:104:TRP:CH2	2:U:134:ARG:HD2	2.55	0.41
2:U:291:TRP:CD1	2:U:292:GLU:HG3	2.55	0.41
4:F:36:LYS:NZ	4:F:56:TRP:CE2	2.88	0.41
6:Q:39:GLN:HG3	6:Q:44:GLY:O	2.20	0.41
4:B:69:SER:OG	4:B:80:THR:OG1	2.35	0.41
2:S:89:ARG:HD2	5:W:534:TYR:O	2.20	0.41
2:S:290:PHE:CE1	2:S:291:TRP:HE3	2.38	0.41
7:G:73:ASP:OD2	7:G:76:LYS:HD3	2.21	0.41
8:J:6:GLN:OE1	8:J:87:TYR:HA	2.20	0.41
1:C:34:MET:HB3	1:C:78:LEU:HD22	2.00	0.41
2:T:123:PRO:HG3	2:T:151:PHE:HD2	1.85	0.41
2:U:49:ASP:OD1	2:U:50:LYS:N	2.53	0.41
2:U:89:ARG:HD2	5:V:534:TYR:O	2.19	0.41
2:U:186:LEU:HD11	2:U:194:PHE:HD1	1.86	0.41
6:Q:30:SER:HB3	5:V:504:ILE:HG22	2.03	0.41
8:H:23:CYS:HB2	8:H:35:TRP:CH2	2.56	0.41
7:I:36:TRP:CD1	7:I:70:ILE:HD13	2.55	0.41
7:I:79:LEU:C	7:I:79:LEU:HD23	2.41	0.41
7:I:103:PHE:HB3	7:I:106:TRP:NE1	2.35	0.41
2:T:48:VAL:HG23	2:T:49:ASP:N	2.35	0.41
2:T:256:LEU:HD11	2:T:308:PHE:HE2	1.85	0.41
4:F:6:GLN:HA	4:F:22:ASN:O	2.21	0.41
5:X:591:ASP:O	5:X:595:GLN:HG2	2.20	0.41
7:I:60:TYR:CE1	7:I:70:ILE:HG22	2.56	0.41
1:C:99:TRP:CG	1:C:100:PHE:N	2.89	0.41
1:E:43:LYS:CG	1:E:44:GLY:H	2.31	0.41
4:D:95:GLN:HE21	4:D:97:TYR:HB3	1.86	0.41
1:A:36:TRP:NE1	1:A:78:LEU:HD21	2.36	0.41
2:S:126:PRO:HD2	2:S:129:ILE:HG13	2.02	0.41
2:S:127:ASP:N	2:S:127:ASP:OD1	2.52	0.41
2:U:291:TRP:NE1	2:U:292:GLU:HG3	2.36	0.41
3:N:92:TYR:O	5:X:528:GLY:HA3	2.21	0.41
6:M:35:ASN:OD1	6:M:50:THR:OG1	2.36	0.41
5:X:569:LEU:HD12	5:X:569:LEU:HA	1.84	0.41
4:D:13:VAL:HG11	4:D:19:ALA:HB2	2.02	0.41
1:A:105:PHE:N	4:B:42:TYR:OH	2.52	0.41
2:T:133:PRO:HB3	5:W:543:TYR:CE1	2.56	0.41
2:T:184:LEU:HD23	2:T:184:LEU:HA	1.84	0.41
2:S:94:PRO:HB3	2:S:169:VAL:HG11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:4:MET:HE2	3:N:23:CYS:SG	2.61	0.41
6:M:47:TRP:CH2	5:X:527:ILE:HG13	2.56	0.41
8:H:34:HIS:CE1	8:H:91:SER:HB2	2.54	0.41
5:X:610:ILE:O	5:X:612:PRO:HD3	2.21	0.41
8:J:62:PHE:HA	8:J:75:ILE:HD12	2.02	0.41
2:T:146:PRO:HG2	1:C:54:ALA:HB3	2.02	0.41
2:T:152:ALA:O	2:T:169:VAL:HA	2.20	0.41
2:T:301:ILE:O	2:T:301:ILE:HG13	2.19	0.41
5:W:608:CYS:SG	5:W:610:ILE:HG12	2.61	0.41
7:G:38:ARG:HG3	7:G:92:ALA:HB3	2.02	0.41
7:I:37:VAL:O	7:I:95:TYR:N	2.40	0.41
2:U:198:PRO:HD2	5:X:547:LEU:O	2.20	0.41
5:W:585:LEU:HD23	5:W:585:LEU:HA	1.80	0.41
6:M:54:MET:HA	6:M:74:ASN:HD21	1.86	0.41
7:G:18:LEU:O	7:G:83:MET:HB2	2.20	0.41
7:G:47:TRP:HZ2	7:G:50:VAL:HG12	1.85	0.41
7:I:92:ALA:O	7:I:112:VAL:N	2.48	0.41
4:D:101:PRO:O	4:D:103:THR:HG23	2.21	0.41
2:T:96:VAL:HG12	2:T:167:SER:HB2	2.02	0.41
3:R:33:LEU:HD23	3:R:34:ASN:N	2.36	0.41
4:F:95:GLN:HG2	4:F:96:GLN:N	2.36	0.41
5:V:515:LEU:CD2	5:V:517:TYR:HB3	2.51	0.41
1:C:103:LEU:HD12	4:D:102:LEU:HD11	2.03	0.41
2:U:182:ALA:HB2	5:X:562:ALA:CB	2.49	0.40
4:F:11:LEU:HD11	4:F:20:THR:O	2.22	0.40
4:F:44:GLN:O	4:F:90:ALA:HB1	2.21	0.40
8:H:94:THR:CG2	8:H:95:PRO:HD3	2.51	0.40
1:E:82:MET:HE3	1:E:85:LEU:HD21	2.03	0.40
2:S:132:PHE:HD2	2:S:135:CYS:SG	2.44	0.40
2:U:99:TYR:HD2	2:U:101:ALA:O	2.04	0.40
6:Q:101:TYR:CZ	9:L:3:BMA:H3	2.57	0.40
6:O:39:GLN:HB3	6:O:95:TYR:HE1	1.86	0.40
7:I:45:LEU:HD11	8:J:44:PRO:HG2	2.02	0.40
8:J:47:LEU:HB3	8:J:48:ILE:HD12	2.02	0.40
8:J:61:ARG:HH22	8:J:79:GLN:CD	2.25	0.40
1:C:12:VAL:HG11	1:C:85:LEU:CD1	2.52	0.40
2:U:123:PRO:HG3	2:U:151:PHE:CD1	2.52	0.40
4:F:1:ASP:HB2	4:F:101:PRO:HG3	2.04	0.40
6:Q:38:ARG:HG2	6:Q:48:VAL:HG22	2.04	0.40
6:Q:49:SER:OG	6:Q:60:TYR:HD1	2.05	0.40
8:H:22:THR:HA	8:H:72:THR:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:51:ILE:HD12	7:I:70:ILE:HG23	2.02	0.40
1:E:36:TRP:NE1	1:E:80:LEU:HB2	2.36	0.40
2:S:37:VAL:HG22	2:S:185:ILE:HD12	2.02	0.40
2:U:309:THR:OG1	7:I:57:ASP:OD2	2.25	0.40
5:W:601:CYS:HB2	5:W:608:CYS:HB2	1.44	0.40
6:O:101:TYR:H	9:Y:5:MAN:H62	1.87	0.40
5:V:610:ILE:O	5:V:610:ILE:HG13	2.22	0.40
5:X:584:ILE:O	5:X:588:LYS:HG2	2.22	0.40
2:T:112:GLU:HB2	2:T:142:SER:HA	2.04	0.40
2:U:57:LEU:HD12	2:U:62:GLN:HB2	2.04	0.40
4:F:60:ARG:NH2	4:F:64:VAL:HG23	2.37	0.40
3:P:36:TYR:HB2	3:P:87:TYR:HB2	2.04	0.40
3:P:45:LYS:HE3	3:P:45:LYS:HB2	1.90	0.40
3:P:94:THR:HA	5:V:527:ILE:HB	2.03	0.40
6:O:32:TYR:HD1	6:O:98:LYS:CD	2.35	0.40
5:X:562:ALA:HA	5:X:565:THR:HG22	2.03	0.40
4:D:2:ILE:HD13	4:D:99:SER:HB3	2.04	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	114/217 (52%)	113 (99%)	1 (1%)	0	100	100
1	C	114/217 (52%)	111 (97%)	3 (3%)	0	100	100
1	E	114/217 (52%)	111 (97%)	3 (3%)	0	100	100
2	S	229/321 (71%)	225 (98%)	4 (2%)	0	100	100
2	T	265/321 (83%)	260 (98%)	5 (2%)	0	100	100
2	U	264/321 (82%)	257 (97%)	7 (3%)	0	100	100
3	N	101/213 (47%)	97 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	P	99/213 (46%)	98 (99%)	1 (1%)	0	100	100
3	R	103/213 (48%)	99 (96%)	4 (4%)	0	100	100
4	B	111/220 (50%)	106 (96%)	5 (4%)	0	100	100
4	D	111/220 (50%)	105 (95%)	6 (5%)	0	100	100
4	F	111/220 (50%)	105 (95%)	6 (5%)	0	100	100
5	V	108/140 (77%)	106 (98%)	2 (2%)	0	100	100
5	W	108/140 (77%)	106 (98%)	2 (2%)	0	100	100
5	X	105/140 (75%)	102 (97%)	3 (3%)	0	100	100
6	M	113/217 (52%)	110 (97%)	2 (2%)	1 (1%)	17	52
6	O	113/217 (52%)	109 (96%)	4 (4%)	0	100	100
6	Q	114/217 (52%)	113 (99%)	1 (1%)	0	100	100
7	G	113/215 (53%)	110 (97%)	3 (3%)	0	100	100
7	I	111/215 (52%)	109 (98%)	2 (2%)	0	100	100
8	H	105/215 (49%)	99 (94%)	6 (6%)	0	100	100
8	J	91/215 (42%)	89 (98%)	1 (1%)	1 (1%)	14	46
All	All	2817/4844 (58%)	2740 (97%)	75 (3%)	2 (0%)	54	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	M	102	PRO
8	J	96	PRO

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	91/178 (51%)	91 (100%)	0	100	100
1	C	91/178 (51%)	91 (100%)	0	100	100
1	E	91/178 (51%)	91 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	S	201/273 (74%)	201 (100%)	0	100	100
2	T	232/273 (85%)	232 (100%)	0	100	100
2	U	232/273 (85%)	232 (100%)	0	100	100
3	N	89/188 (47%)	89 (100%)	0	100	100
3	P	87/188 (46%)	87 (100%)	0	100	100
3	R	91/188 (48%)	91 (100%)	0	100	100
4	B	98/194 (50%)	98 (100%)	0	100	100
4	D	98/194 (50%)	98 (100%)	0	100	100
4	F	98/194 (50%)	98 (100%)	0	100	100
5	V	90/119 (76%)	90 (100%)	0	100	100
5	W	90/119 (76%)	89 (99%)	1 (1%)	73	89
5	X	87/119 (73%)	87 (100%)	0	100	100
6	M	92/180 (51%)	92 (100%)	0	100	100
6	O	92/180 (51%)	92 (100%)	0	100	100
6	Q	93/180 (52%)	93 (100%)	0	100	100
7	G	95/181 (52%)	95 (100%)	0	100	100
7	I	93/181 (51%)	92 (99%)	1 (1%)	73	89
8	H	92/190 (48%)	92 (100%)	0	100	100
8	J	83/190 (44%)	82 (99%)	1 (1%)	71	88
All	All	2406/4138 (58%)	2403 (100%)	3 (0%)	93	98

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	W	601	CYS
7	I	74	ASN
8	J	104	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
2	T	98	ASN
2	T	296	ASN

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Mol	Chain	Res	Type
2	S	62	GLN
2	S	255	GLN
3	R	38	GLN
5	W	595	GLN
6	M	103	HIS
8	H	34	HIS
3	P	38	GLN
6	O	39	GLN
5	V	521	GLN
5	V	567	GLN
5	X	521	GLN
8	J	6	GLN
8	J	37	GLN
1	C	35	HIS
1	E	35	HIS

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](#)

18 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	$\# Z > 2$
9	NAG	K	1	9,5	14,14,15	0.47	0	17,19,21	0.68	0
9	NAG	K	2	9	14,14,15	0.29	0	17,19,21	0.54	0
9	BMA	K	3	9	11,11,12	0.87	0	15,15,17	1.26	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	MAN	K	4	9	11,11,12	1.11	1 (9%)	15,15,17	2.64	6 (40%)
9	MAN	K	5	9	11,11,12	0.67	0	15,15,17	0.94	1 (6%)
9	MAN	K	6	9	11,11,12	0.90	1 (9%)	15,15,17	1.01	1 (6%)
9	NAG	L	1	9,5	14,14,15	0.40	0	17,19,21	0.52	0
9	NAG	L	2	9	14,14,15	0.18	0	17,19,21	0.46	0
9	BMA	L	3	9	11,11,12	0.69	0	15,15,17	1.08	1 (6%)
9	MAN	L	4	9	11,11,12	0.63	0	15,15,17	1.06	2 (13%)
9	MAN	L	5	9	11,11,12	0.77	0	15,15,17	0.91	1 (6%)
9	MAN	L	6	9	11,11,12	0.82	1 (9%)	15,15,17	0.89	1 (6%)
9	NAG	Y	1	9,5	14,14,15	0.45	0	17,19,21	0.45	0
9	NAG	Y	2	9	14,14,15	0.46	0	17,19,21	0.41	0
9	BMA	Y	3	9	11,11,12	0.67	0	15,15,17	1.23	3 (20%)
9	MAN	Y	4	9	11,11,12	0.79	1 (9%)	15,15,17	1.14	2 (13%)
9	MAN	Y	5	9	11,11,12	1.05	1 (9%)	15,15,17	0.89	1 (6%)
9	MAN	Y	6	9	11,11,12	0.81	1 (9%)	15,15,17	0.94	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	K	1	9,5	-	0/6/23/26	0/1/1/1
9	NAG	K	2	9	-	2/6/23/26	0/1/1/1
9	BMA	K	3	9	-	2/2/19/22	0/1/1/1
9	MAN	K	4	9	-	2/2/19/22	0/1/1/1
9	MAN	K	5	9	-	1/2/19/22	0/1/1/1
9	MAN	K	6	9	-	0/2/19/22	0/1/1/1
9	NAG	L	1	9,5	-	0/6/23/26	0/1/1/1
9	NAG	L	2	9	-	2/6/23/26	0/1/1/1
9	BMA	L	3	9	-	2/2/19/22	0/1/1/1
9	MAN	L	4	9	-	1/2/19/22	1/1/1/1
9	MAN	L	5	9	-	2/2/19/22	0/1/1/1
9	MAN	L	6	9	-	0/2/19/22	0/1/1/1
9	NAG	Y	1	9,5	-	1/6/23/26	0/1/1/1
9	NAG	Y	2	9	-	2/6/23/26	0/1/1/1
9	BMA	Y	3	9	-	0/2/19/22	0/1/1/1
9	MAN	Y	4	9	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	MAN	Y	5	9	-	1/2/19/22	0/1/1/1
9	MAN	Y	6	9	-	2/2/19/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	Y	5	MAN	O5-C1	-3.28	1.38	1.43
9	K	4	MAN	C1-C2	2.86	1.58	1.52
9	K	6	MAN	O5-C1	-2.45	1.39	1.43
9	L	6	MAN	O5-C1	-2.40	1.39	1.43
9	Y	4	MAN	C1-C2	2.33	1.57	1.52
9	Y	6	MAN	O5-C1	-2.10	1.40	1.43

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	K	4	MAN	C1-O5-C5	6.10	120.46	112.19
9	K	4	MAN	C1-C2-C3	4.12	114.73	109.67
9	K	4	MAN	O5-C5-C6	4.06	113.58	107.20
9	K	3	BMA	C1-C2-C3	-3.32	105.58	109.67
9	K	4	MAN	O5-C5-C4	2.89	117.86	110.83
9	K	4	MAN	O5-C1-C2	2.86	115.18	110.77
9	K	4	MAN	O2-C2-C3	-2.79	104.56	110.14
9	Y	6	MAN	O2-C2-C3	-2.57	104.99	110.14
9	K	6	MAN	O2-C2-C3	-2.48	105.17	110.14
9	Y	4	MAN	O2-C2-C3	-2.46	105.20	110.14
9	L	6	MAN	O2-C2-C3	-2.42	105.28	110.14
9	K	5	MAN	O2-C2-C3	-2.37	105.38	110.14
9	L	4	MAN	C1-O5-C5	2.37	115.40	112.19
9	L	5	MAN	O2-C2-C3	-2.36	105.41	110.14
9	L	4	MAN	O2-C2-C3	-2.34	105.45	110.14
9	Y	3	BMA	O5-C5-C6	2.32	110.84	107.20
9	Y	3	BMA	C1-O5-C5	2.31	115.33	112.19
9	Y	5	MAN	O2-C2-C3	-2.29	105.55	110.14
9	Y	3	BMA	O5-C5-C4	-2.25	105.35	110.83
9	Y	4	MAN	C1-O5-C5	2.15	115.10	112.19
9	K	3	BMA	O3-C3-C4	2.08	115.16	110.35
9	L	3	BMA	C1-O5-C5	2.06	114.98	112.19

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	L	2	NAG	O5-C5-C6-O6
9	K	2	NAG	O5-C5-C6-O6
9	Y	2	NAG	O5-C5-C6-O6
9	K	2	NAG	C4-C5-C6-O6
9	K	4	MAN	O5-C5-C6-O6
9	L	2	NAG	C4-C5-C6-O6
9	K	3	BMA	C4-C5-C6-O6
9	Y	2	NAG	C4-C5-C6-O6
9	L	5	MAN	O5-C5-C6-O6
9	L	4	MAN	O5-C5-C6-O6
9	L	5	MAN	C4-C5-C6-O6
9	K	3	BMA	O5-C5-C6-O6
9	K	4	MAN	C4-C5-C6-O6
9	L	3	BMA	C4-C5-C6-O6
9	Y	5	MAN	O5-C5-C6-O6
9	Y	1	NAG	O5-C5-C6-O6
9	Y	6	MAN	O5-C5-C6-O6
9	K	5	MAN	C4-C5-C6-O6
9	L	3	BMA	O5-C5-C6-O6
9	Y	6	MAN	C4-C5-C6-O6

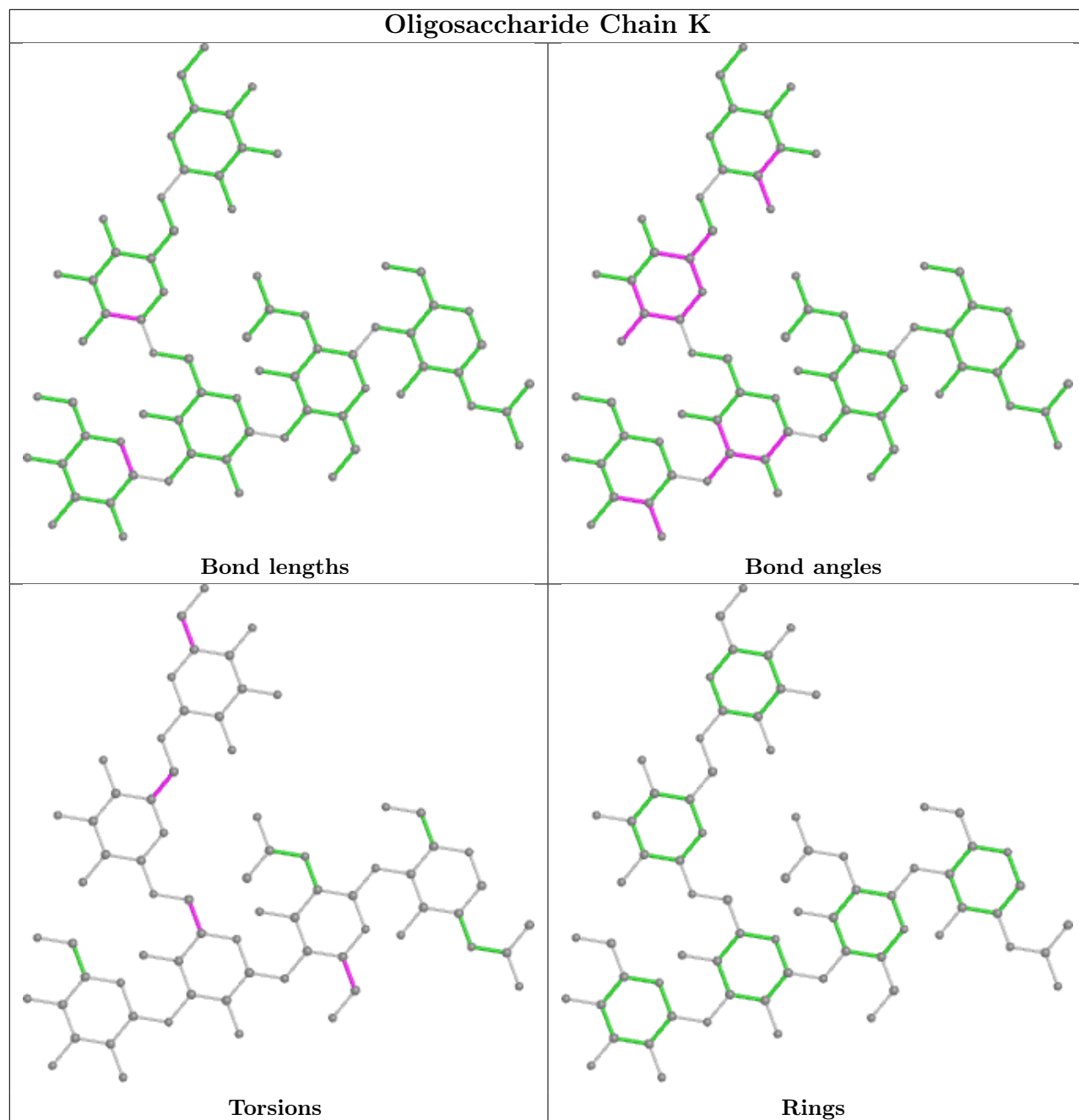
All (1) ring outliers are listed below:

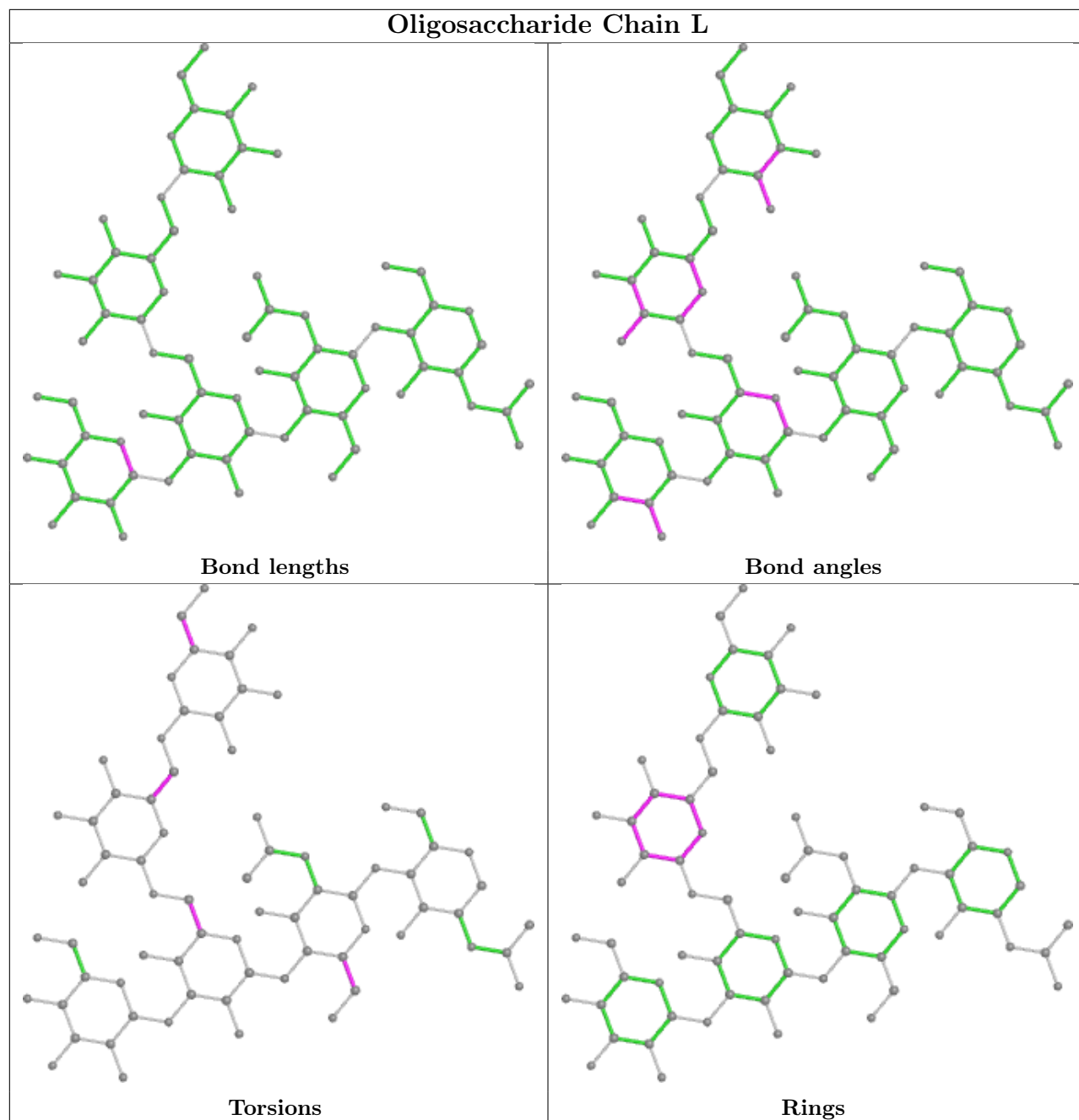
Mol	Chain	Res	Type	Atoms
9	L	4	MAN	C1-C2-C3-C4-C5-O5

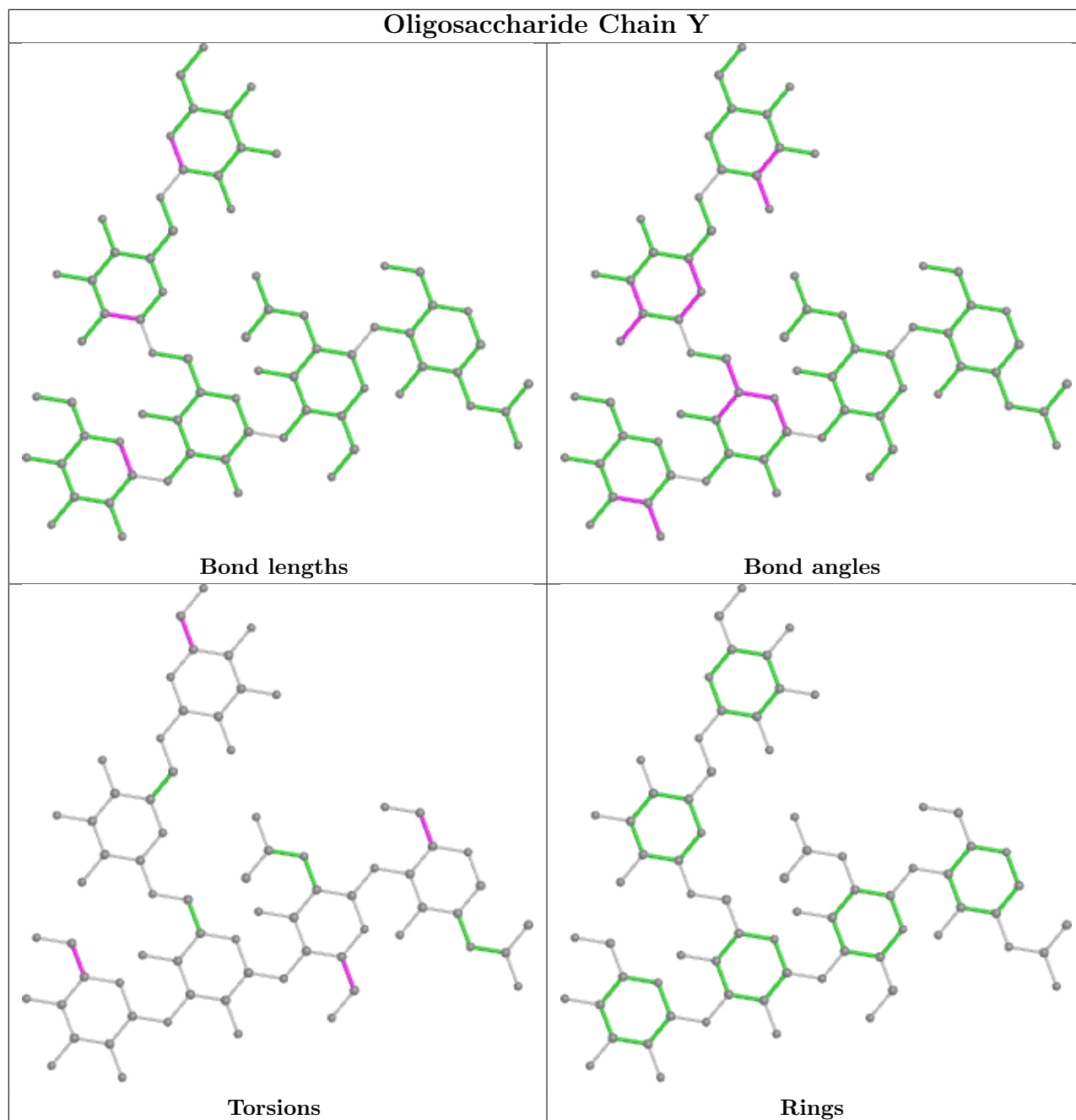
10 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	L	3	BMA	1	0
9	L	1	NAG	1	0
9	L	2	NAG	2	0
9	K	3	BMA	1	0
9	Y	2	NAG	2	0
9	K	2	NAG	3	0
9	K	1	NAG	1	0
9	Y	1	NAG	1	0
9	K	5	MAN	2	0
9	Y	5	MAN	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](#)

8 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
10	NAG	T	602	2	14,14,15	0.34	0	17,19,21	0.45	0
10	NAG	U	601	2	14,14,15	0.25	0	17,19,21	0.38	0
10	NAG	T	603	2	14,14,15	0.58	0	17,19,21	0.47	0
10	NAG	S	402	2	14,14,15	0.29	0	17,19,21	0.40	0
10	NAG	S	401	2	14,14,15	0.21	0	17,19,21	0.38	0
10	NAG	U	603	2	14,14,15	0.26	0	17,19,21	0.51	0
10	NAG	T	601	2	14,14,15	0.20	0	17,19,21	0.53	0
10	NAG	U	602	2	14,14,15	0.22	0	17,19,21	0.50	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	T	602	2	-	0/6/23/26	0/1/1/1
10	NAG	U	601	2	-	2/6/23/26	0/1/1/1
10	NAG	T	603	2	-	2/6/23/26	0/1/1/1
10	NAG	S	402	2	-	0/6/23/26	0/1/1/1
10	NAG	S	401	2	-	0/6/23/26	0/1/1/1
10	NAG	U	603	2	-	2/6/23/26	0/1/1/1
10	NAG	T	601	2	-	2/6/23/26	0/1/1/1
10	NAG	U	602	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

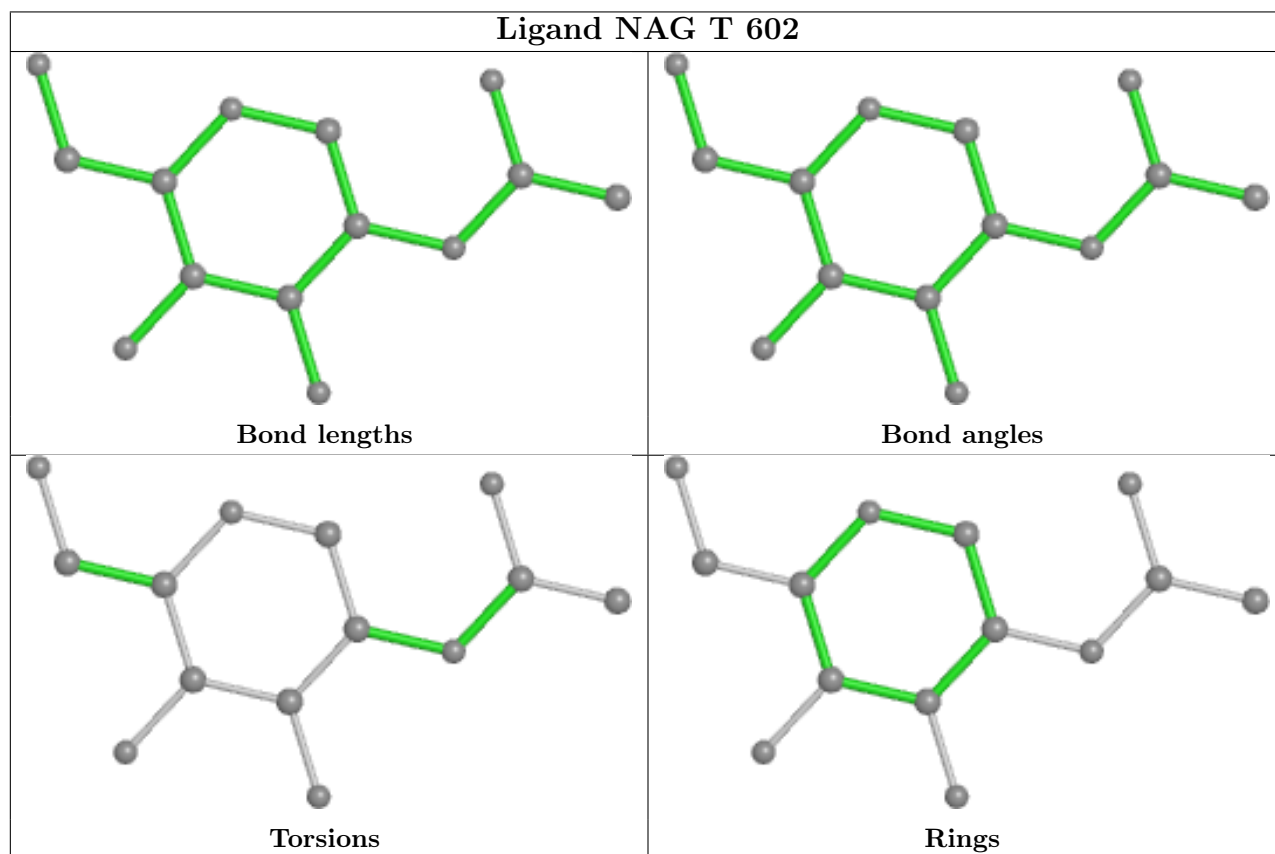
Mol	Chain	Res	Type	Atoms
10	T	601	NAG	C4-C5-C6-O6
10	T	601	NAG	O5-C5-C6-O6
10	T	603	NAG	C1-C2-N2-C7
10	U	601	NAG	C4-C5-C6-O6
10	U	603	NAG	O5-C5-C6-O6
10	U	601	NAG	O5-C5-C6-O6
10	T	603	NAG	C3-C2-N2-C7
10	U	603	NAG	C3-C2-N2-C7

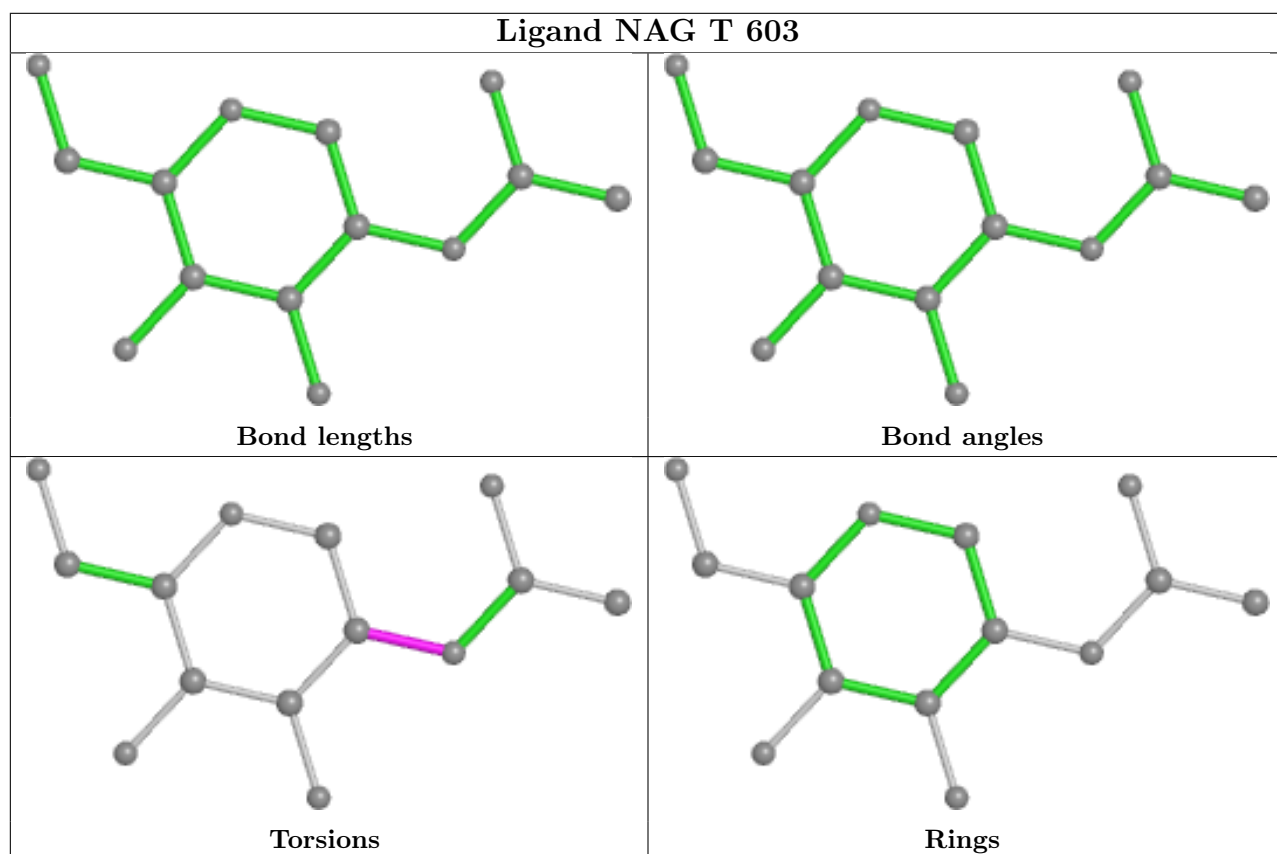
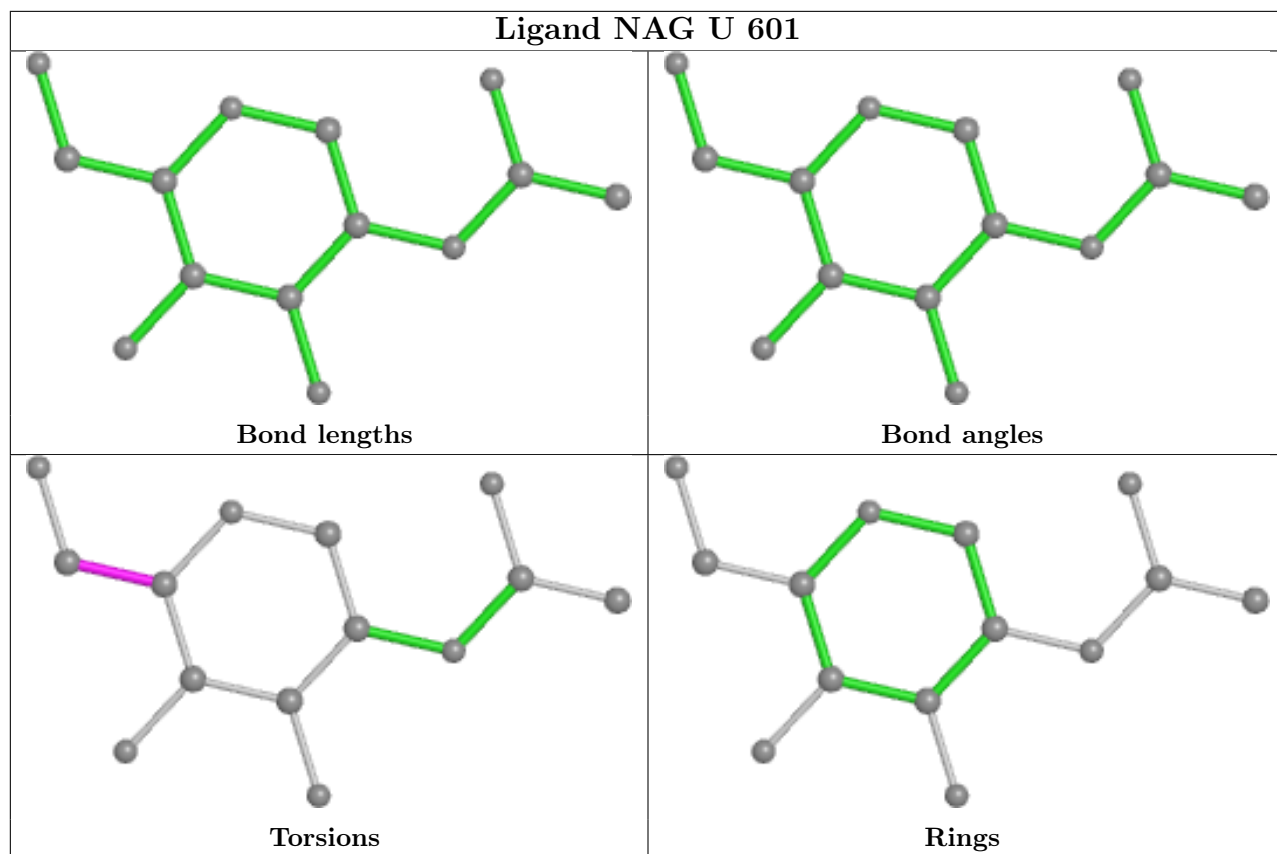
There are no ring outliers.

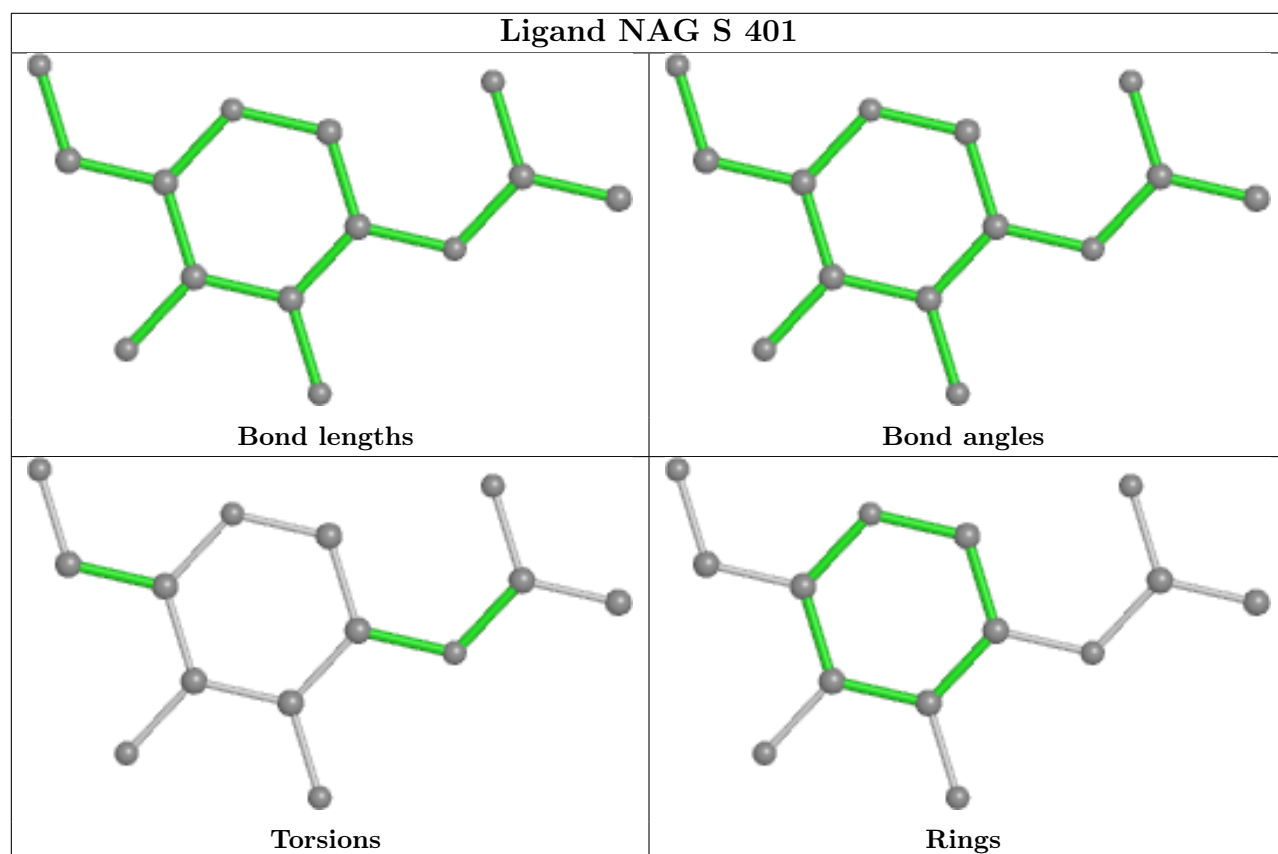
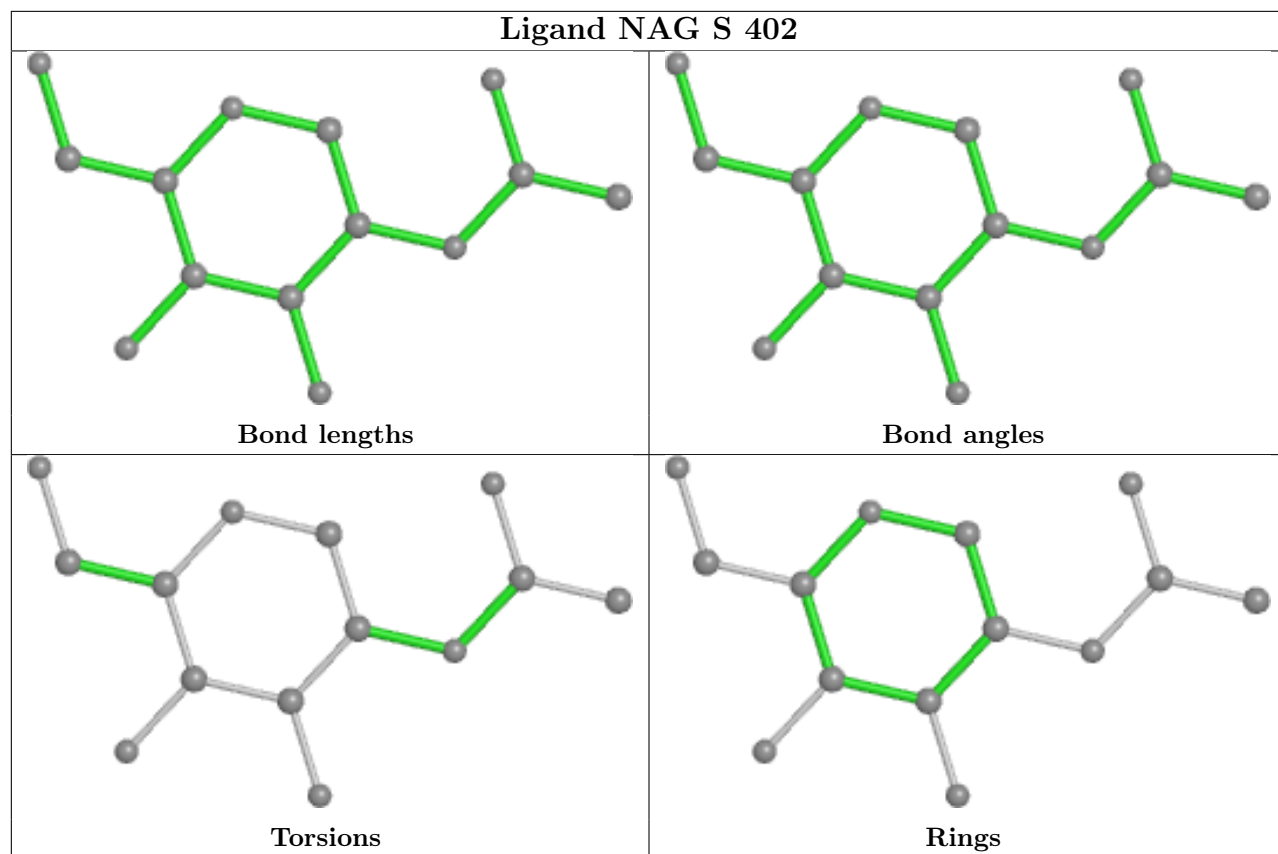
1 monomer is involved in 1 short contact:

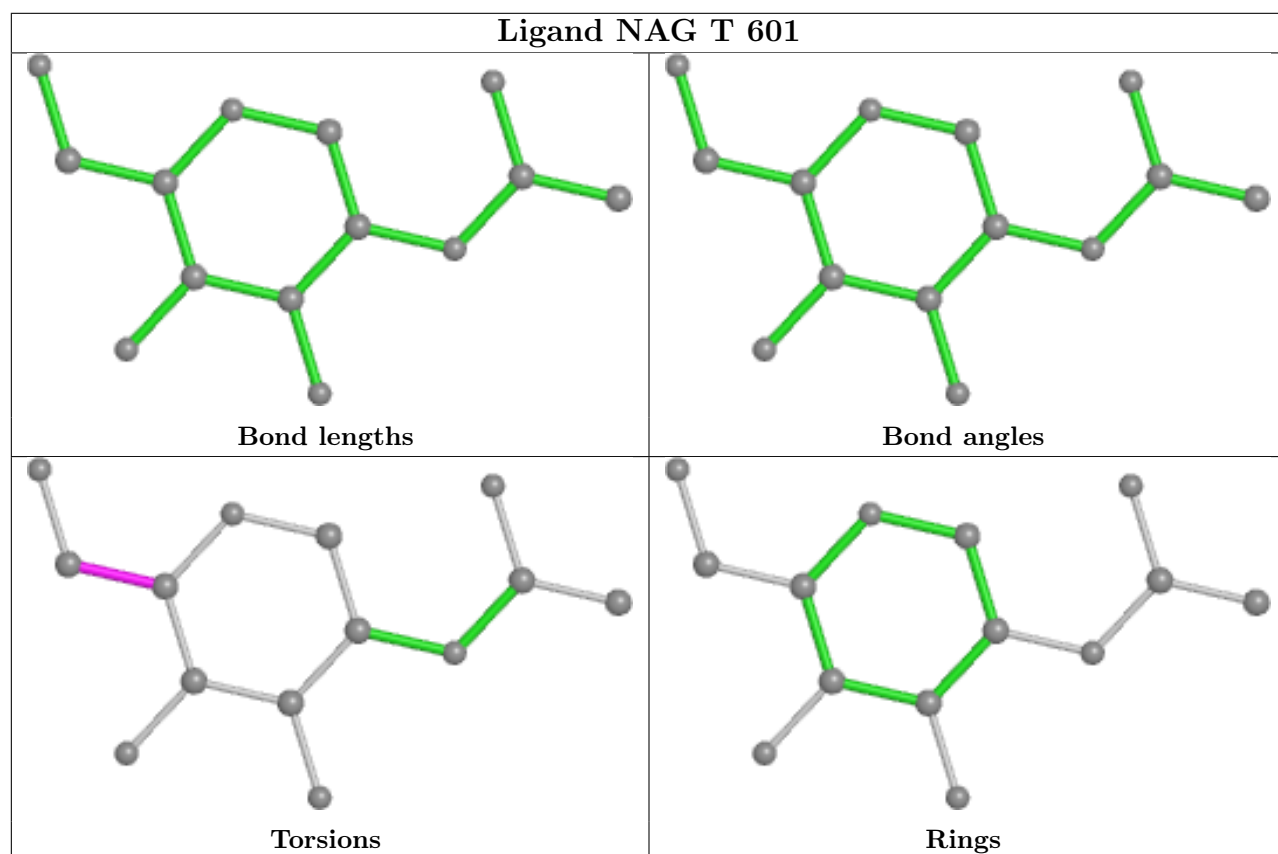
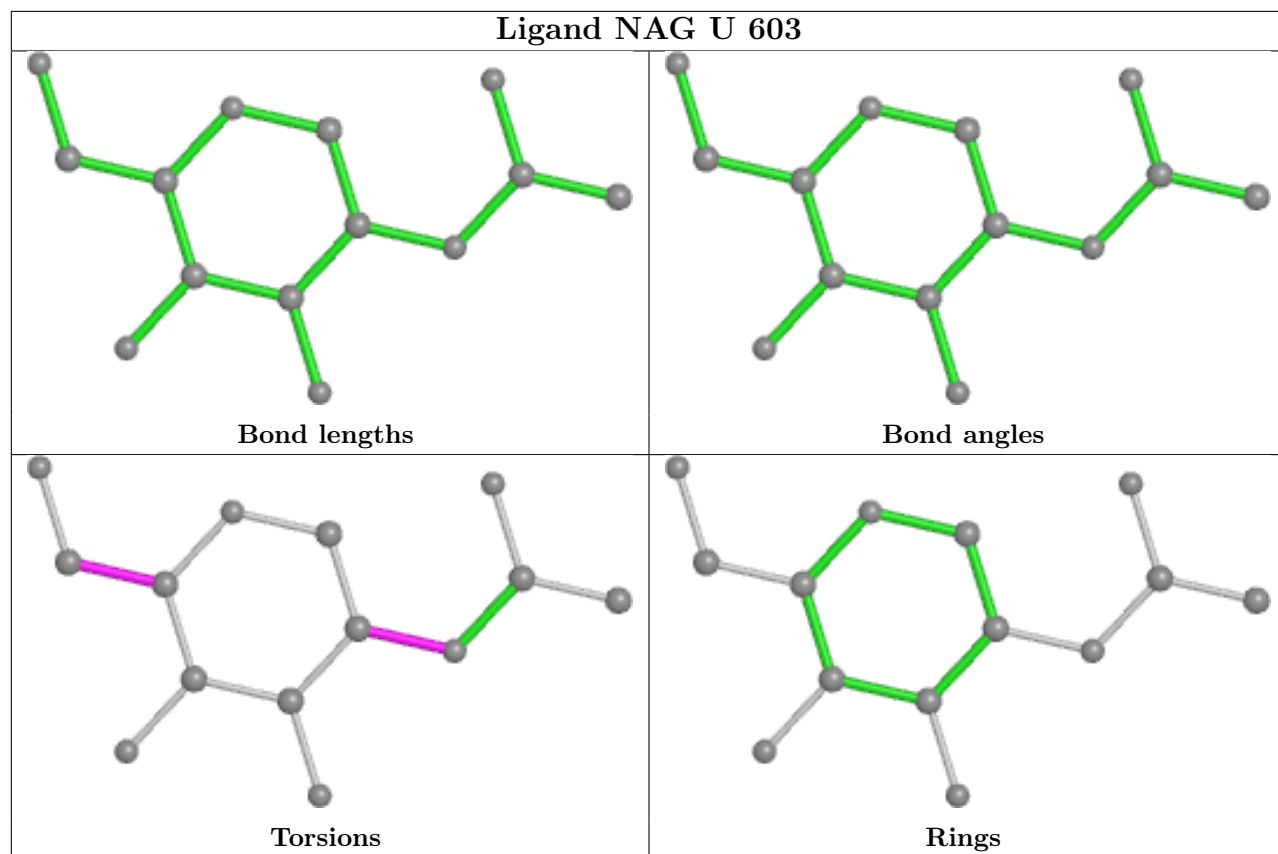
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	T	603	NAG	1	0

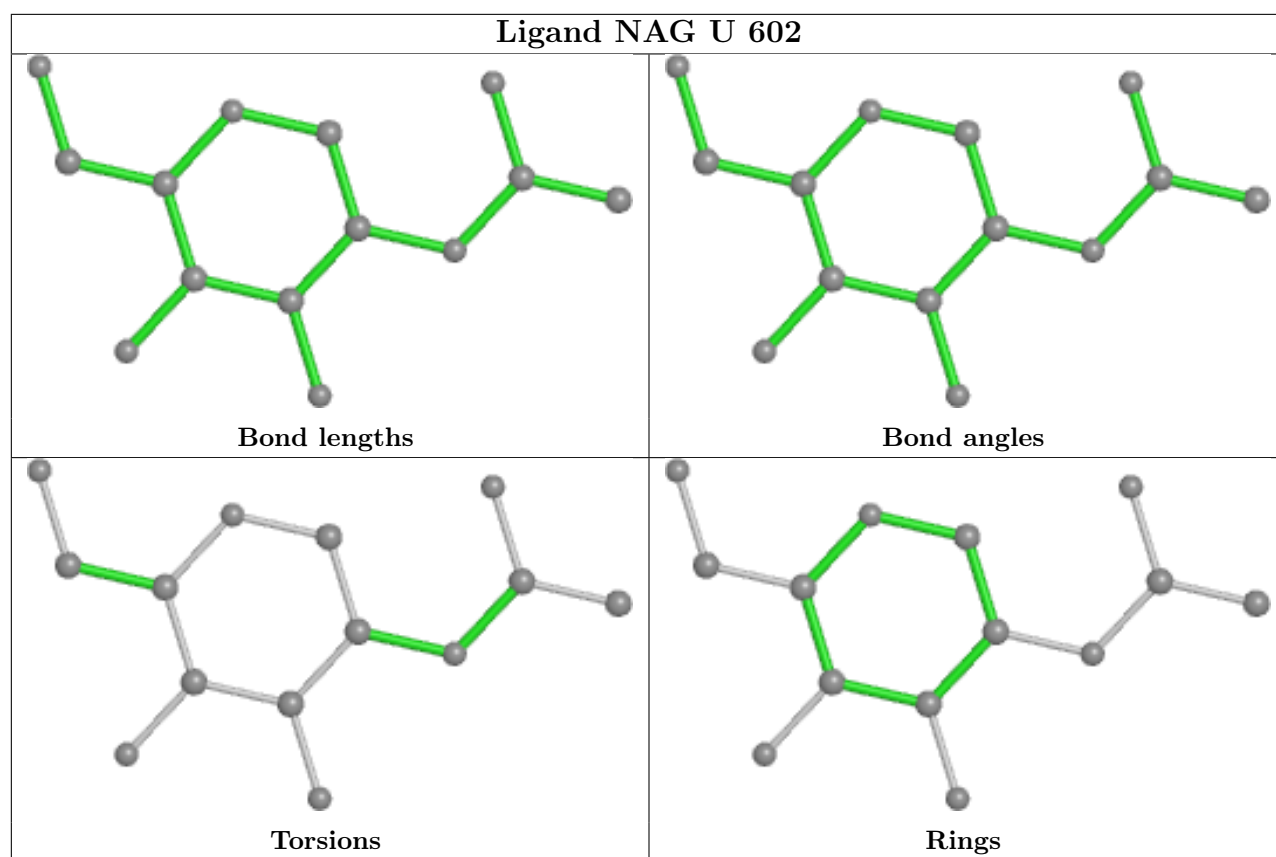
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	U	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	U	311:VAL	C	312:ASN	N	3.22

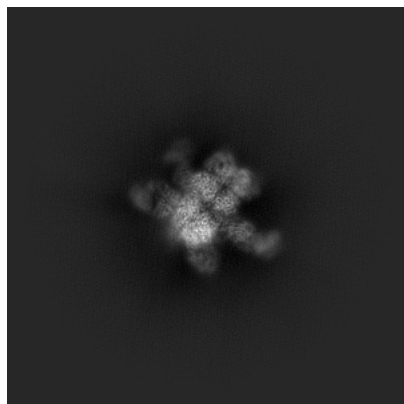
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26005. These allow visual inspection of the internal detail of the map and identification of artifacts.

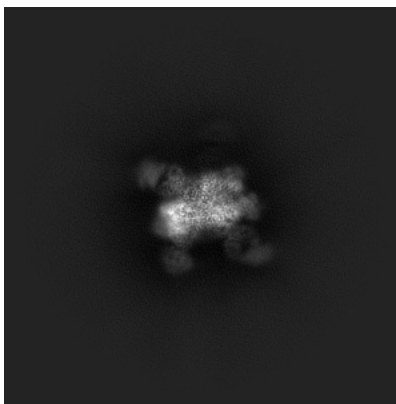
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

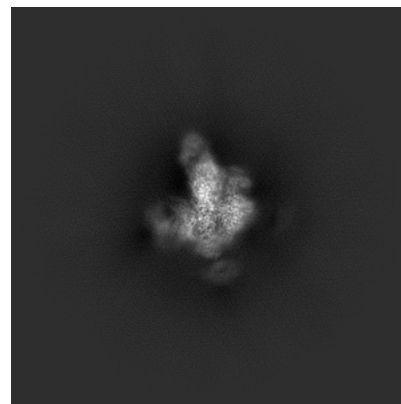
6.1.1 Primary map



X

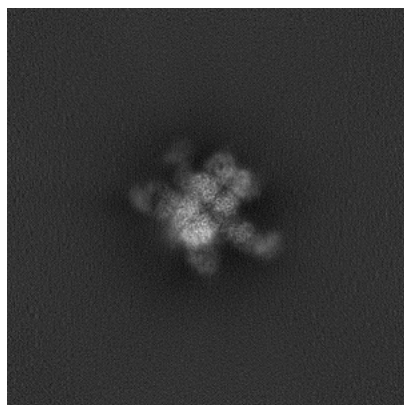


Y

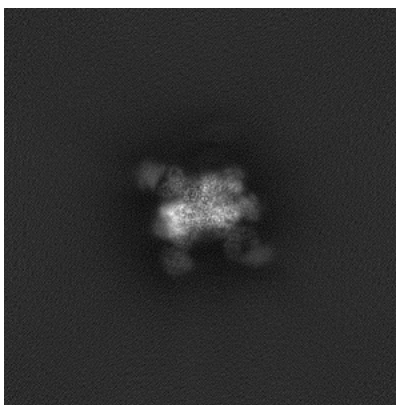


Z

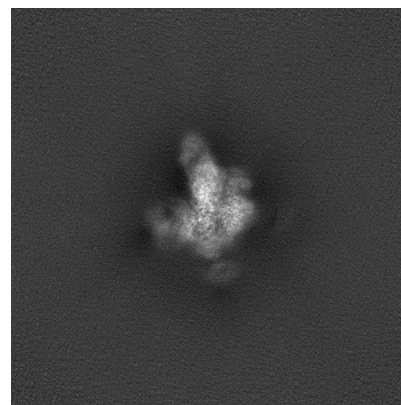
6.1.2 Raw map



X



Y

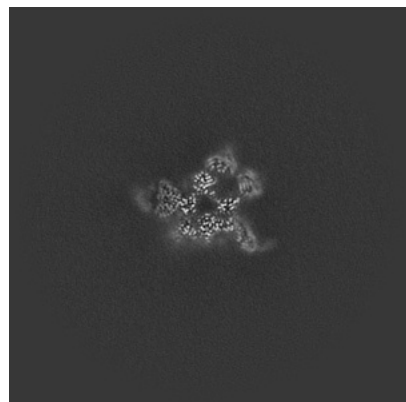


Z

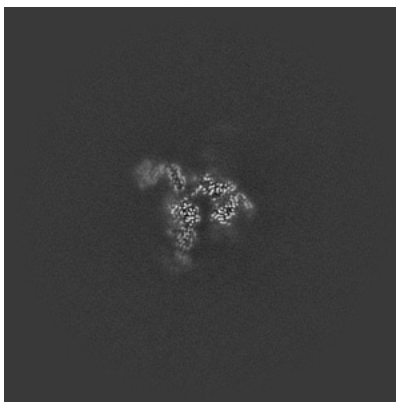
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

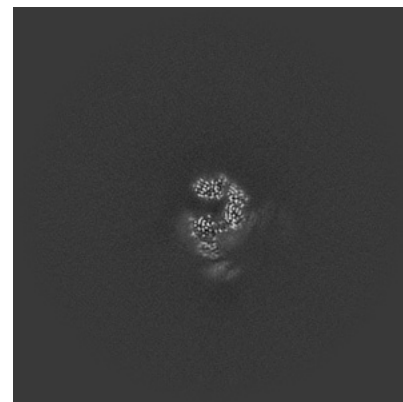
6.2.1 Primary map



X Index: 256

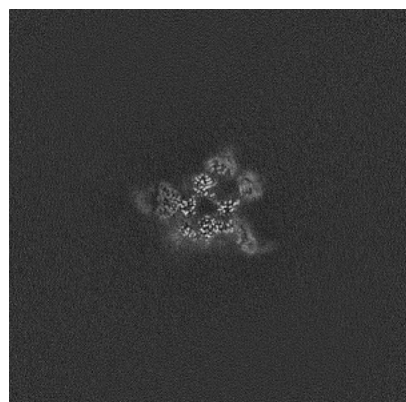


Y Index: 256

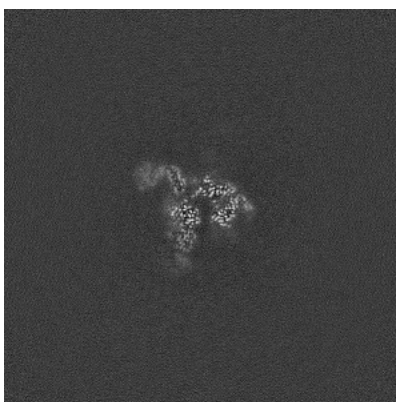


Z Index: 256

6.2.2 Raw map



X Index: 256



Y Index: 256

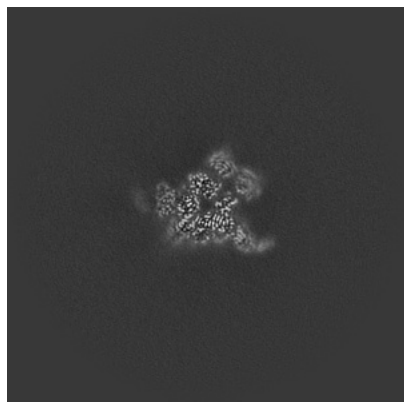


Z Index: 256

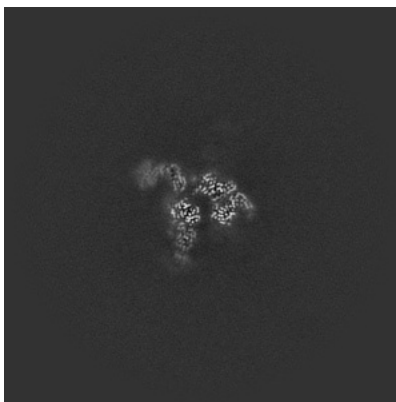
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 251

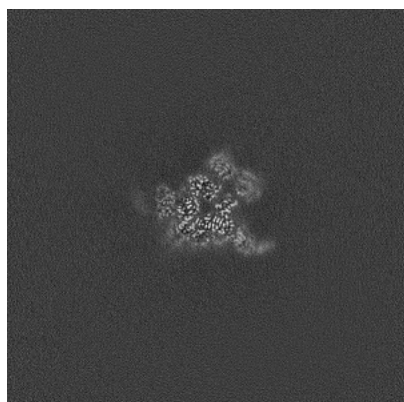


Y Index: 257

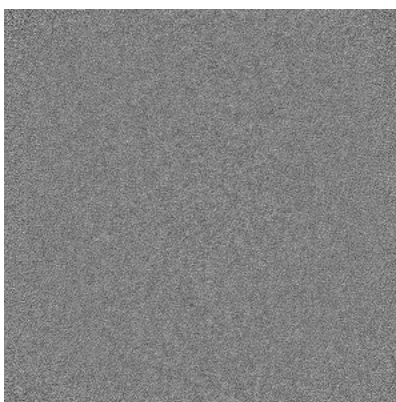


Z Index: 226

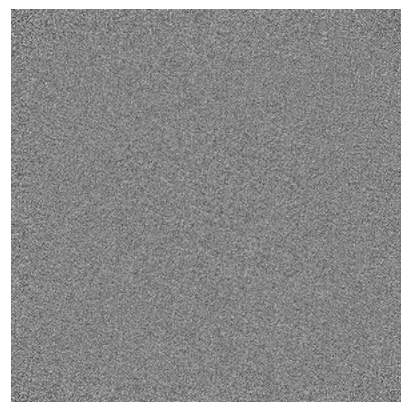
6.3.2 Raw map



X Index: 251



Y Index: 0

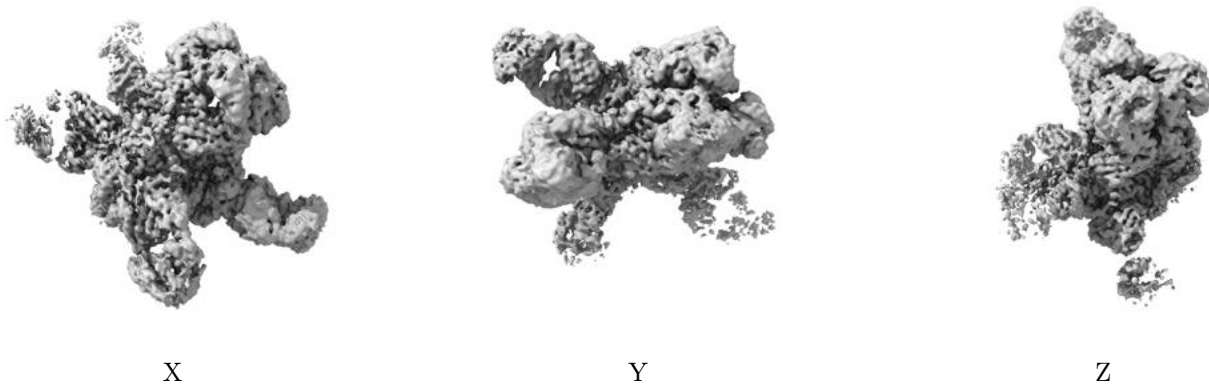


Z Index: 0

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

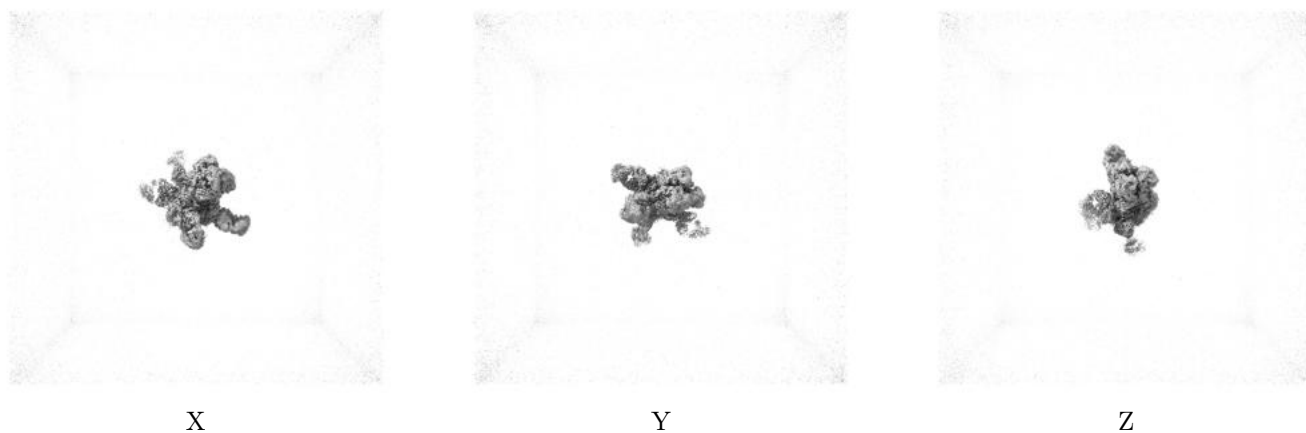
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

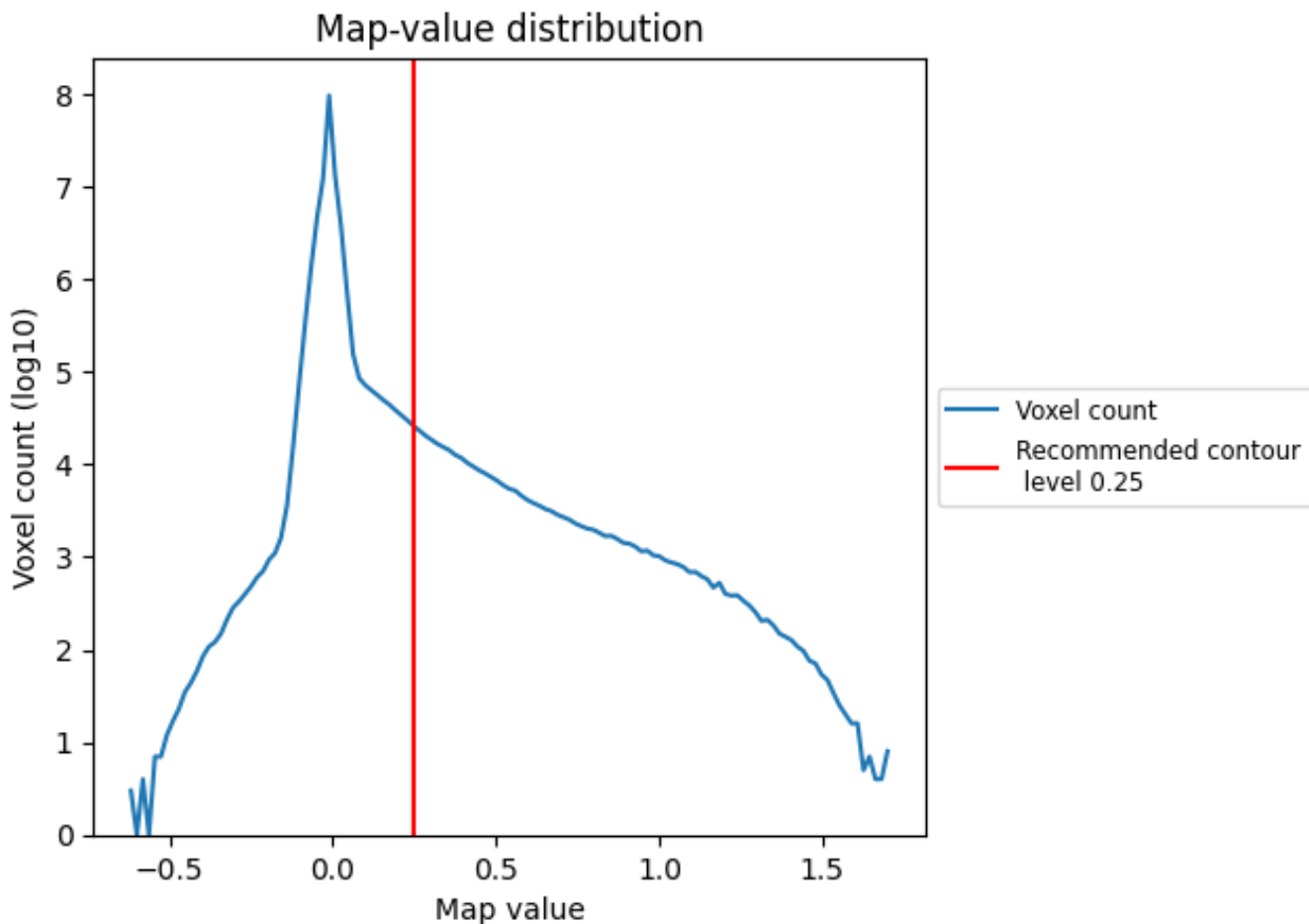
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

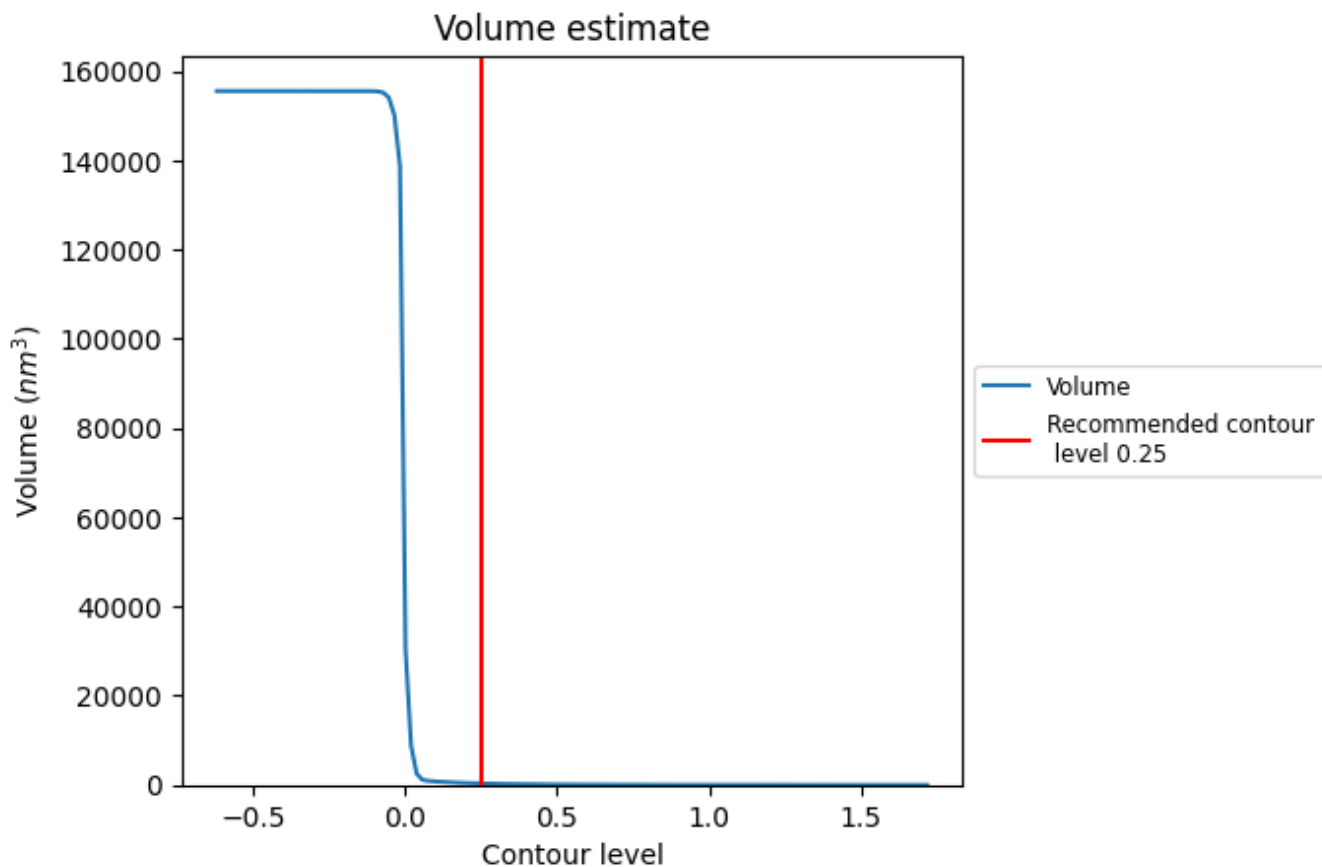
This section contains the results of statistical analysis of the map.

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.

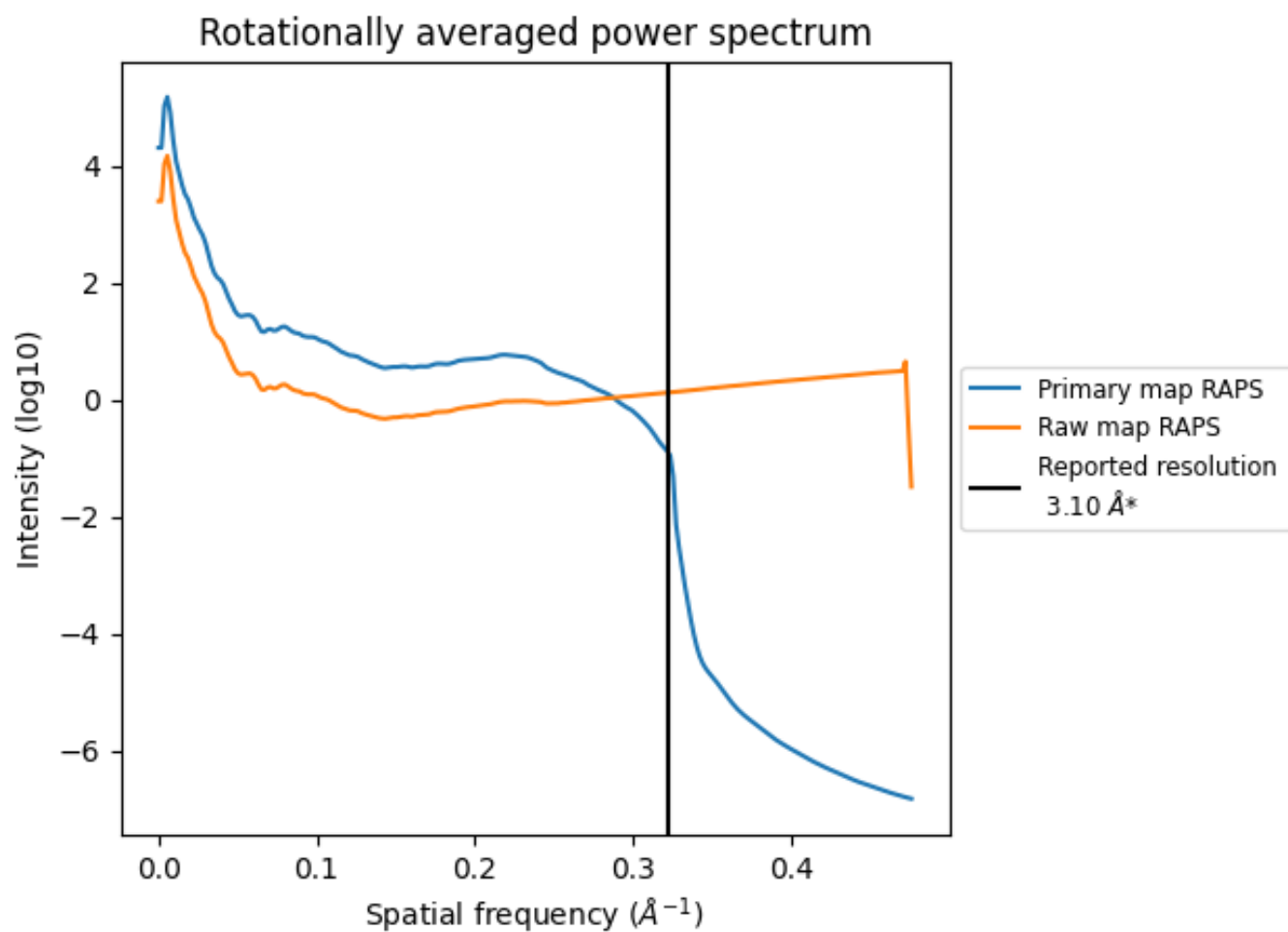
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 332 nm³; this corresponds to an approximate mass of 300 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

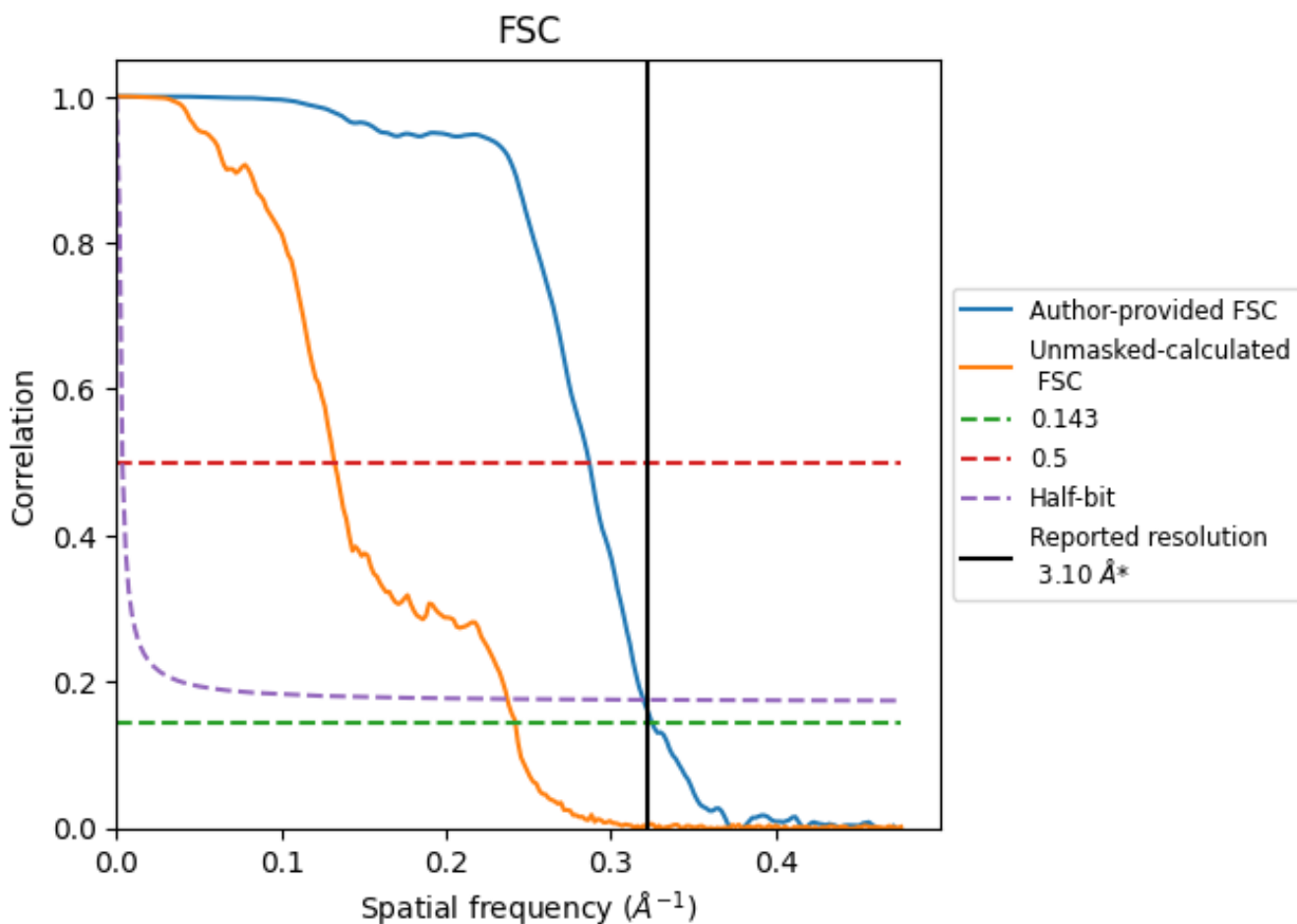


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 0.323 \AA^{-1}

8.2 Resolution estimates [i](#)

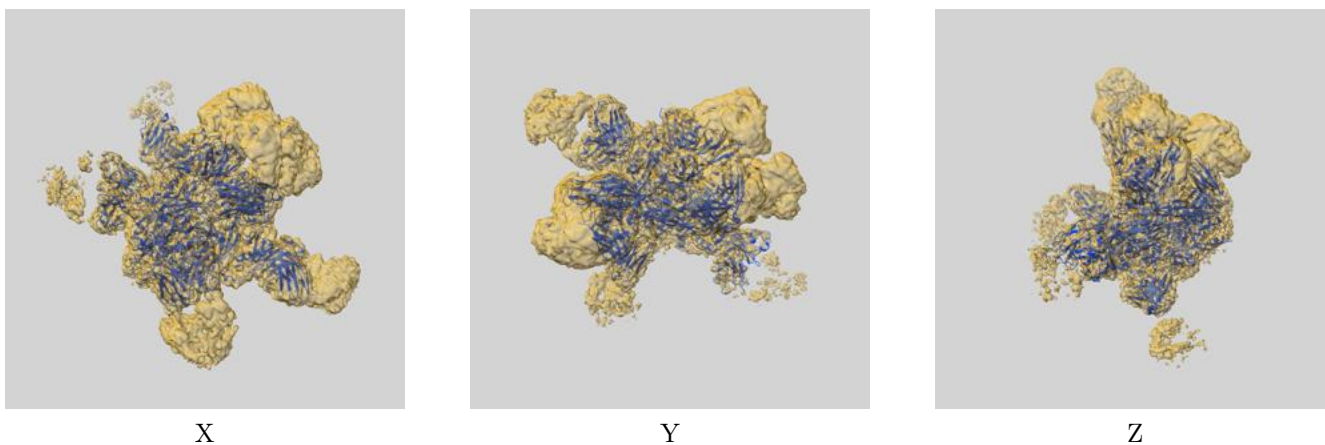
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.08	3.49	3.13
Unmasked-calculated*	4.13	7.56	4.22

*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 4.13 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

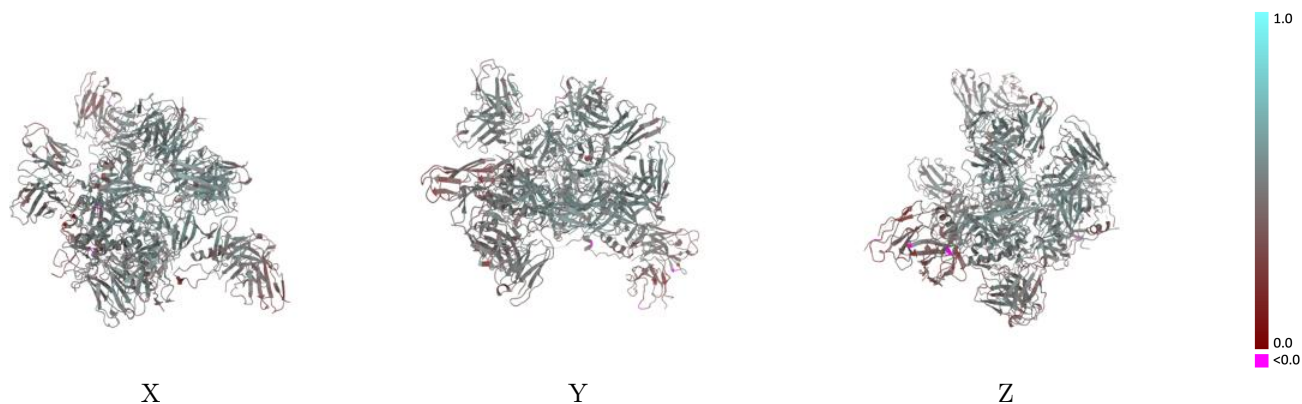
This section contains information regarding the fit between EMDB map EMD-26005 and PDB model 7TN9. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



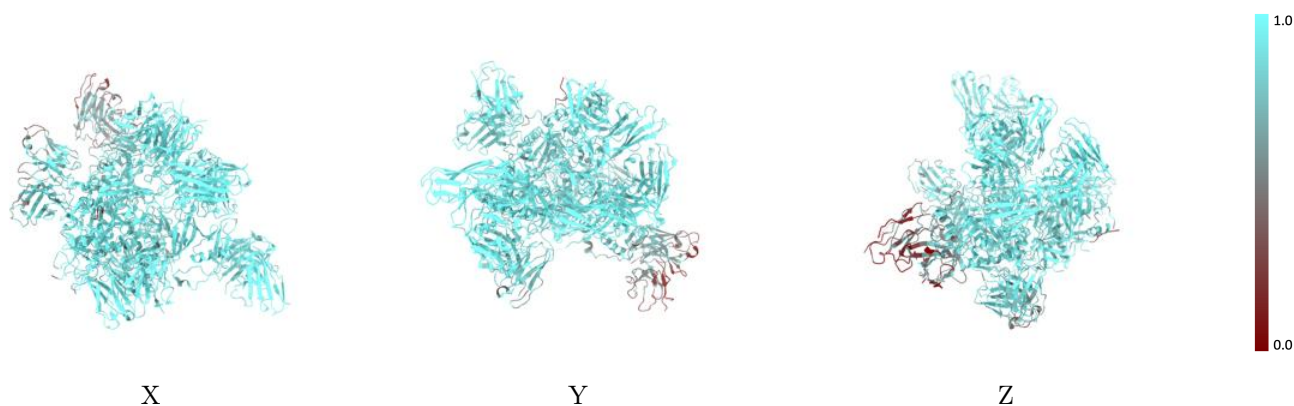
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



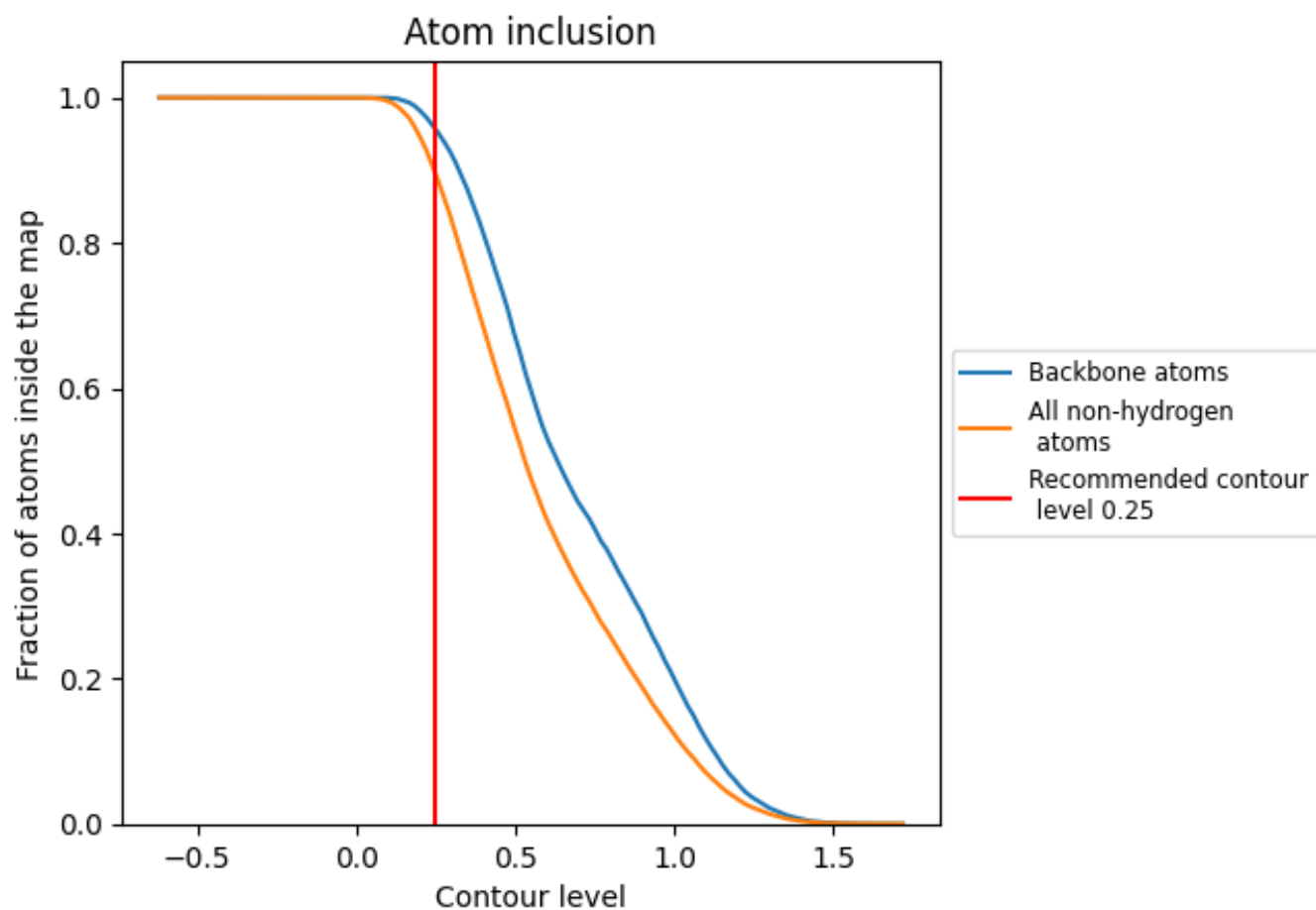
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.25).





















































9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 89% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8941	 0.4750
A	 0.9713	 0.5190
B	 0.9650	 0.5160
C	 0.9782	 0.5260
D	 0.9627	 0.5050
E	 0.9770	 0.5200
F	 0.9603	 0.5100
G	 0.9740	 0.4660
H	 0.9624	 0.4130
I	 0.5682	 0.3860
J	 0.3538	 0.3470
K	 0.9583	 0.4830
L	 0.9861	 0.5110
M	 0.8701	 0.4620
N	 0.8183	 0.4610
O	 0.8512	 0.4560
P	 0.7794	 0.4490
Q	 0.9544	 0.4850
R	 0.9348	 0.4820
S	 0.9082	 0.4920
T	 0.9544	 0.4920
U	 0.8866	 0.4830
V	 0.9291	 0.4540
W	 0.9362	 0.4640
X	 0.9611	 0.4690
Y	 0.9583	 0.5060

