



## Full wwPDB EM Validation Report ⓘ

Nov 2, 2022 – 08:14 AM EDT

PDB ID : 5THR  
EMDB ID : EMD-8407  
Title : Cryo-EM structure of a BG505 Env-sCD4-17b-8ANC195 complex  
Authors : Wang, H.; Bjorkman, P.J.  
Deposited on : 2016-09-30  
Resolution : 8.90 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
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) : 2.31.2

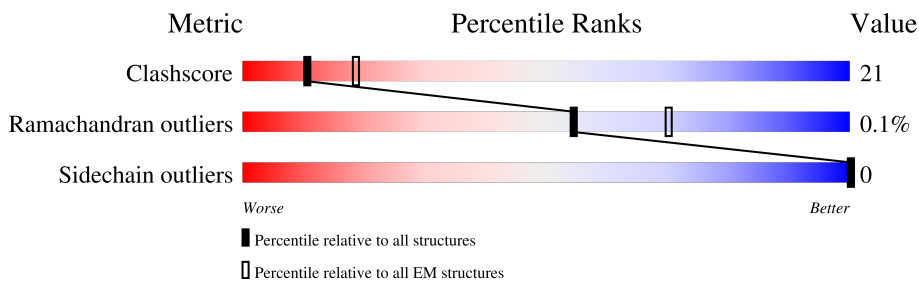
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 8.90 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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	153	<div style="display: flex; justify-content: space-between;"> <span>35%</span> <span>42%</span> <span>31%</span> <span>7%</span> <span>19%</span> </div>
1	B	153	<div style="display: flex; justify-content: space-between;"> <span>31%</span> <span>36%</span> <span>35%</span> <span>7%</span> <span>20%</span> </div>
1	C	153	<div style="display: flex; justify-content: space-between;"> <span>33%</span> <span>38%</span> <span>35%</span> <span>7%</span> <span>20%</span> </div>
2	D	481	<div style="display: flex; justify-content: space-between;"> <span>13%</span> <span>46%</span> <span>29%</span> <span>•</span> <span>24%</span> </div>
2	E	481	<div style="display: flex; justify-content: space-between;"> <span>14%</span> <span>47%</span> <span>29%</span> <span>•</span> <span>24%</span> </div>
2	F	481	<div style="display: flex; justify-content: space-between;"> <span>11%</span> <span>46%</span> <span>29%</span> <span>•</span> <span>24%</span> </div>
3	G	192	<div style="display: flex; justify-content: space-between;"> <span>16%</span> <span>37%</span> <span>14%</span> <span>49%</span> </div>
3	H	192	<div style="display: flex; justify-content: space-between;"> <span>18%</span> <span>38%</span> <span>13%</span> <span>49%</span> </div>

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Mol	Chain	Length	Quality of chain
3	I	192	20% 36% 15% 49%
4	J	214	18% 29% 21% 50%
4	K	214	19% 29% 21% 50%
4	L	214	18% 30% 20% 50%
5	M	229	6% 43% 12% 45%
5	N	229	5% 44% 12% 45%
5	O	229	9% 41% 14% 45%
6	P	244	5% 34% 20% 46%
6	R	244	5% 34% 20% 46%
6	T	244	7% 30% 23% 46%
7	Q	215	7% 32% 18% 50%
7	S	215	7% 30% 20% 50%
7	U	215	6% 31% 19% 50%
8	V	4	50% 50%
8	Y	4	50% 50%
8	b	4	50% 50%
9	W	5	20% 20% 40% 40%
9	X	5	20% 80%
9	Z	5	20% 60% 20%
9	a	5	20% 80%
9	c	5	100%
9	d	5	20% 80%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	NAG	V	1	-	-	X	-
8	NAG	V	2	-	-	X	-
8	BMA	V	3	-	-	X	-
8	MAN	V	4	-	-	X	-

## 2 Entry composition i

There are 9 unique types of molecules in this entry. The entry contains 25071 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 BG505 SOSIP gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	124	983	619	170	188	6	0	0
1	B	123	975	613	169	187	6	0	0
1	C	123	975	613	169	187	6	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	559	PRO	ILE	conflict	UNP Q2N0S6
A	605	CYS	THR	conflict	UNP Q2N0S6
B	559	PRO	ILE	conflict	UNP Q2N0S6
B	605	CYS	THR	conflict	UNP Q2N0S6
C	559	PRO	ILE	conflict	UNP Q2N0S6
C	605	CYS	THR	conflict	UNP Q2N0S6

- Molecule 2 is a protein called BG505 SOSIP gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	364	2845	1792	496	533	24	0	0
2	E	364	2845	1792	496	533	24	0	0
2	F	364	2845	1792	496	533	24	0	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	332	ASN	THR	conflict	UNP Q2N0S6
D	501	CYS	ALA	conflict	UNP Q2N0S6
D	509	ARG	-	expression tag	UNP Q2N0S6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	510	ARG	-	expression tag	UNP Q2N0S6
D	511	ARG	-	expression tag	UNP Q2N0S6
D	512	ARG	-	expression tag	UNP Q2N0S6
D	513	ARG	-	expression tag	UNP Q2N0S6
E	332	ASN	THR	conflict	UNP Q2N0S6
E	501	CYS	ALA	conflict	UNP Q2N0S6
E	509	ARG	-	expression tag	UNP Q2N0S6
E	510	ARG	-	expression tag	UNP Q2N0S6
E	511	ARG	-	expression tag	UNP Q2N0S6
E	512	ARG	-	expression tag	UNP Q2N0S6
E	513	ARG	-	expression tag	UNP Q2N0S6
F	332	ASN	THR	conflict	UNP Q2N0S6
F	501	CYS	ALA	conflict	UNP Q2N0S6
F	509	ARG	-	expression tag	UNP Q2N0S6
F	510	ARG	-	expression tag	UNP Q2N0S6
F	511	ARG	-	expression tag	UNP Q2N0S6
F	512	ARG	-	expression tag	UNP Q2N0S6
F	513	ARG	-	expression tag	UNP Q2N0S6

- Molecule 3 is a protein called T-cell surface glycoprotein CD4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	G	98	786	496	137	151	2	0	0
3	H	98	786	496	137	151	2	0	0
3	I	97	775	487	136	150	2	0	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	183	ILE	-	expression tag	UNP P01730
G	184	ASP	-	expression tag	UNP P01730
G	185	GLY	-	expression tag	UNP P01730
G	186	ARG	-	expression tag	UNP P01730
G	187	HIS	-	expression tag	UNP P01730
G	188	HIS	-	expression tag	UNP P01730
G	189	HIS	-	expression tag	UNP P01730
G	190	HIS	-	expression tag	UNP P01730
G	191	HIS	-	expression tag	UNP P01730
G	192	HIS	-	expression tag	UNP P01730

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Chain	Residue	Modelled	Actual	Comment	Reference
H	183	ILE	-	expression tag	UNP P01730
H	184	ASP	-	expression tag	UNP P01730
H	185	GLY	-	expression tag	UNP P01730
H	186	ARG	-	expression tag	UNP P01730
H	187	HIS	-	expression tag	UNP P01730
H	188	HIS	-	expression tag	UNP P01730
H	189	HIS	-	expression tag	UNP P01730
H	190	HIS	-	expression tag	UNP P01730
H	191	HIS	-	expression tag	UNP P01730
H	192	HIS	-	expression tag	UNP P01730
I	183	ILE	-	expression tag	UNP P01730
I	184	ASP	-	expression tag	UNP P01730
I	185	GLY	-	expression tag	UNP P01730
I	186	ARG	-	expression tag	UNP P01730
I	187	HIS	-	expression tag	UNP P01730
I	188	HIS	-	expression tag	UNP P01730
I	189	HIS	-	expression tag	UNP P01730
I	190	HIS	-	expression tag	UNP P01730
I	191	HIS	-	expression tag	UNP P01730
I	192	HIS	-	expression tag	UNP P01730

- Molecule 4 is a protein called 17b Fab VL domain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	107	Total	C	N	O	S	0	0
			819	512	141	163	3		
4	K	107	Total	C	N	O	S	0	0
			819	512	141	163	3		
4	L	107	Total	C	N	O	S	0	0
			819	512	141	163	3		

- Molecule 5 is a protein called 17b Fab VH domain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	127	Total	C	N	O	S	0	0
			985	621	168	193	3		
5	N	127	Total	C	N	O	S	0	0
			985	621	168	193	3		
5	O	127	Total	C	N	O	S	0	0
			985	621	168	193	3		

- Molecule 6 is a protein called 8ANC195 G52K5 VH domain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	P	131	Total	C	N	O	S	0	0
			980	622	167	188	3		
6	R	131	Total	C	N	O	S	0	0
			980	622	167	188	3		
6	T	131	Total	C	N	O	S	0	0
			980	622	167	188	3		

- Molecule 7 is a protein called 8ANC195 G52K5 VL domain.

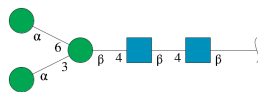
Mol	Chain	Residues	Atoms					AltConf	Trace
7	Q	107	Total	C	N	O	S	0	0
			796	501	135	157	3		
7	S	107	Total	C	N	O	S	0	0
			796	501	135	157	3		
7	U	107	Total	C	N	O	S	0	0
			796	501	135	157	3		

- Molecule 8 is an oligosaccharide called 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
8	V	4	Total	C	N	O	0	0
			50	28	2	20		
8	Y	4	Total	C	N	O	0	0
			50	28	2	20		
8	b	4	Total	C	N	O	0	0
			50	28	2	20		

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



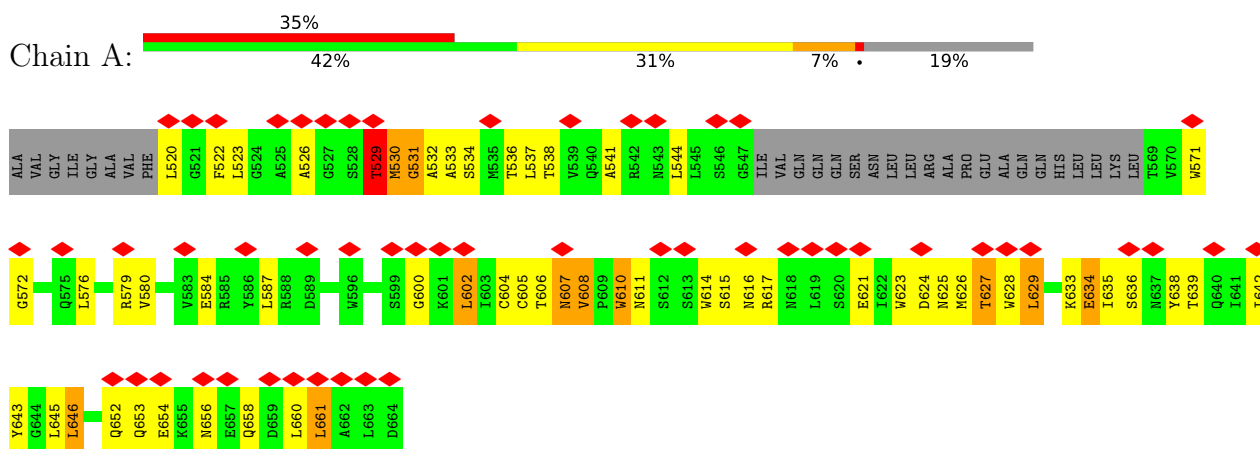


Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	W	5	61	34	2	25	0	0
9	X	5	61	34	2	25	0	0
9	Z	5	61	34	2	25	0	0
9	a	5	61	34	2	25	0	0
9	c	5	61	34	2	25	0	0
9	d	5	61	34	2	25	0	0

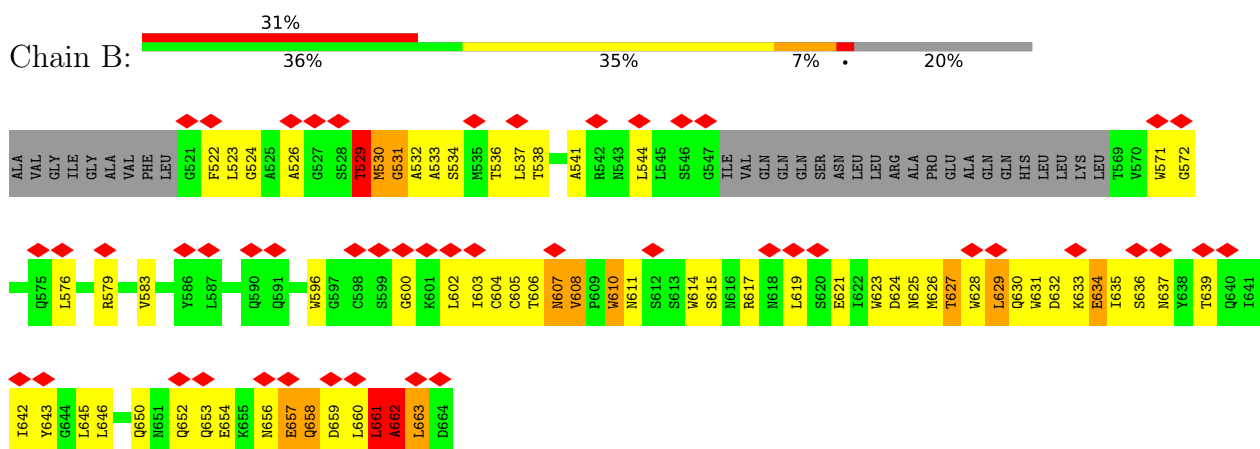
### 3 Residue-property plots [i](#)

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.

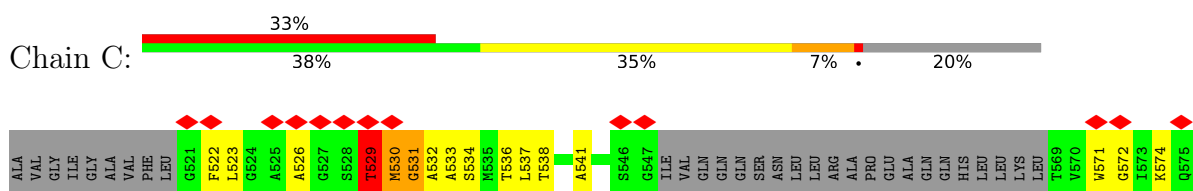
- Molecule 1: BG505 SOSIP gp41



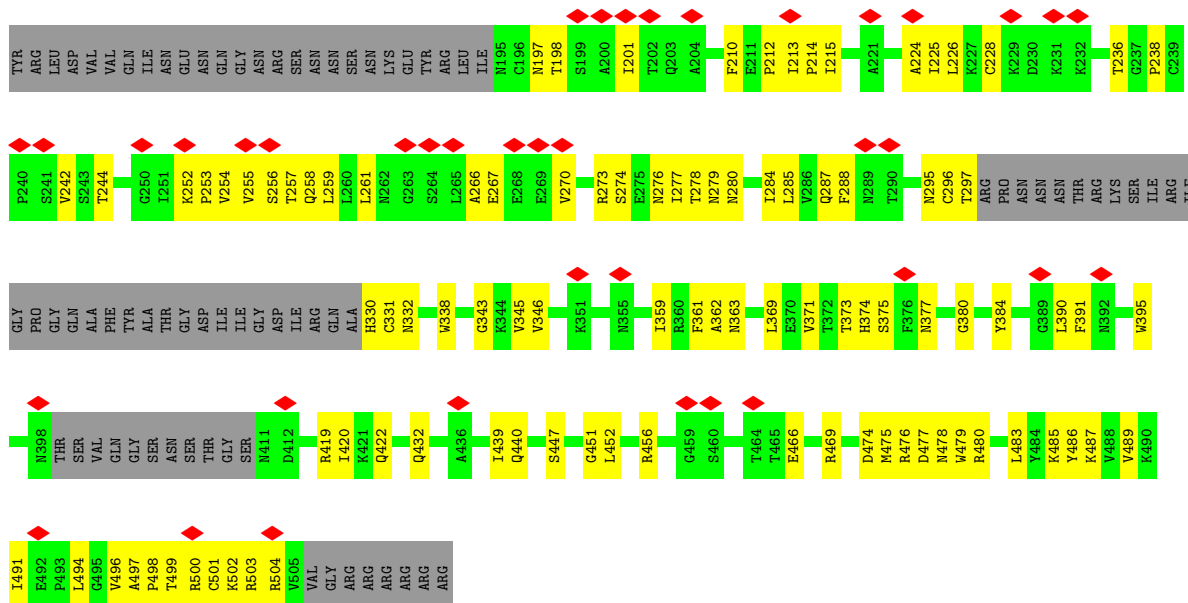
- Molecule 1: BG505 SOSIP gp41



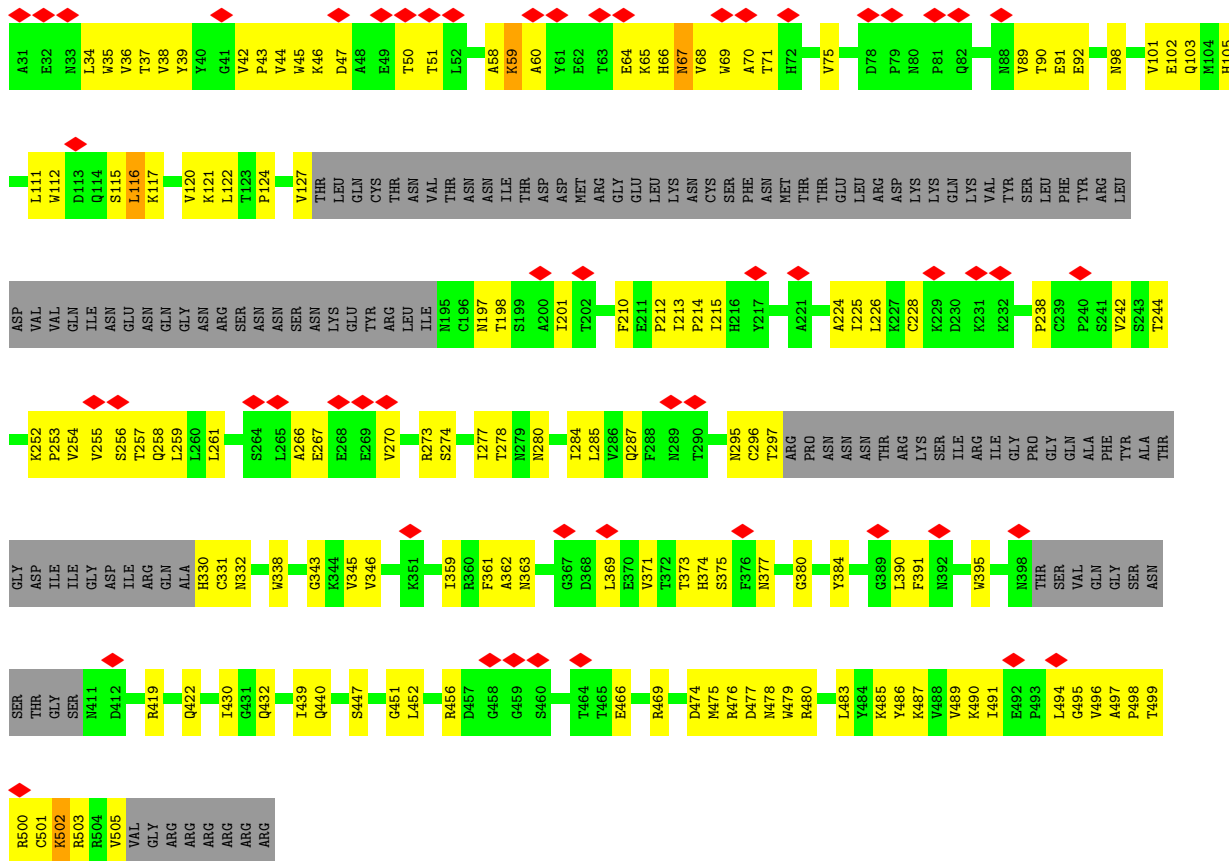
- Molecule 1: BG505 SOSIP gp41







• Molecule 2: BG505 SOSIP gp120

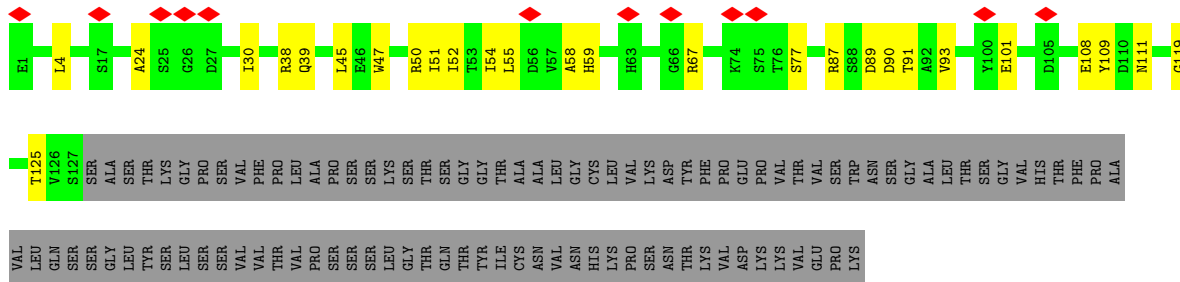
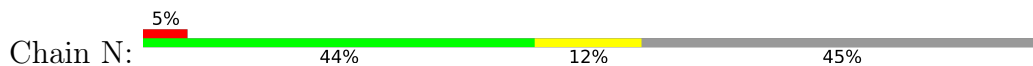


• Molecule 3: T-cell surface glycoprotein CD4

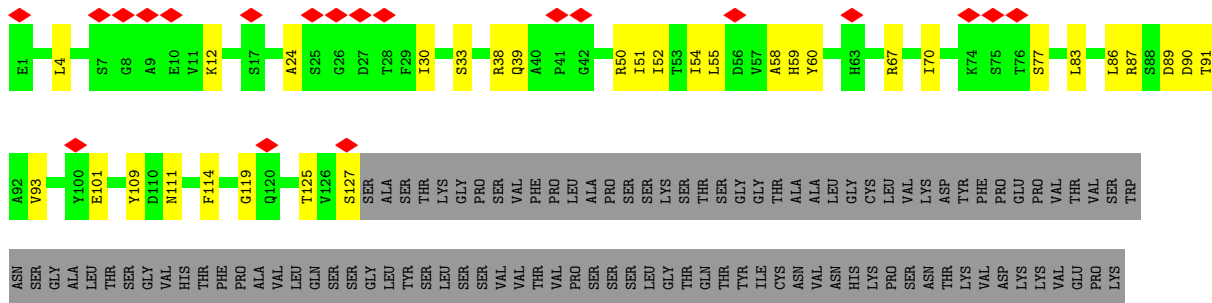
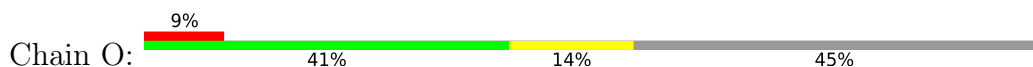




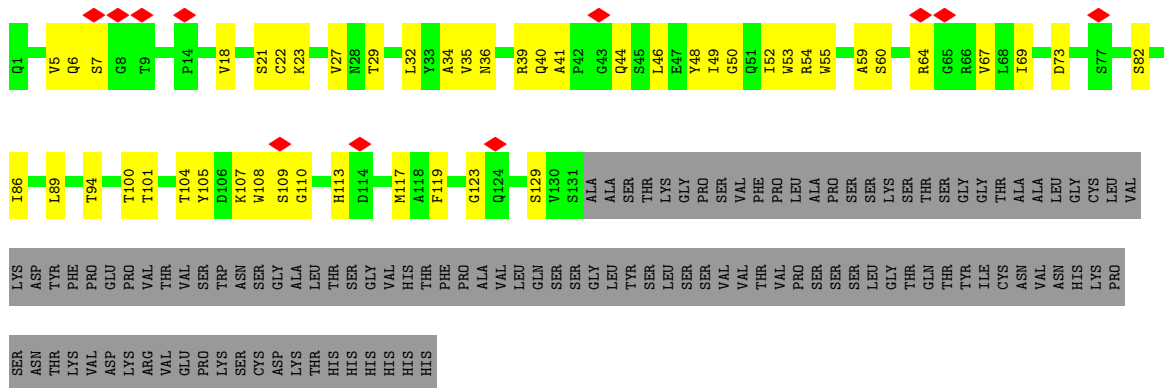
• Molecule 5: 17b Fab VH domain



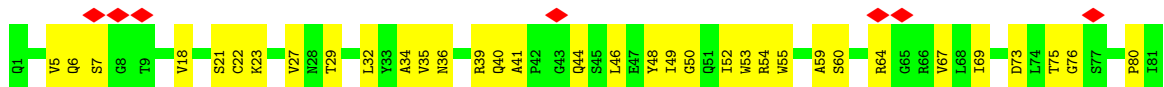
• Molecule 5: 17b Fab VH domain



• Molecule 6: 8ANC195 G52K5 VH domain

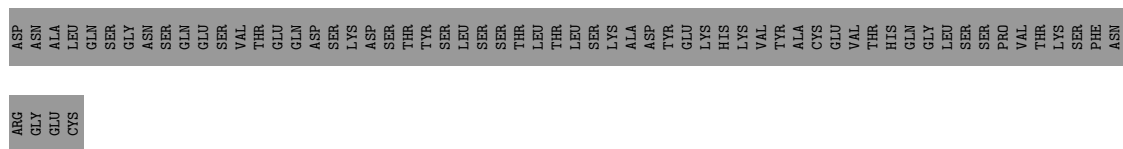


• Molecule 6: 8ANC195 G52K5 VH domain

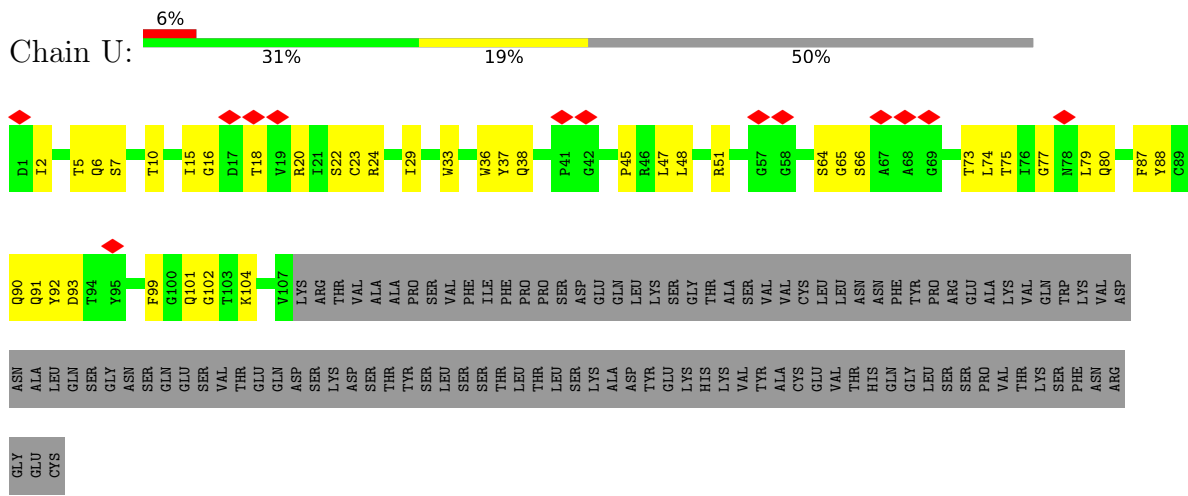








• Molecule 7: 8ANC195 G52K5 VL domain



• Molecule 8: 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



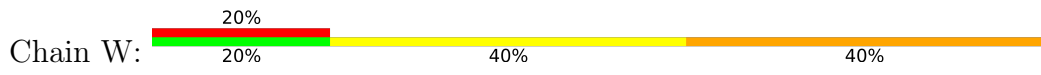
• Molecule 8: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

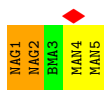


• Molecule 8: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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





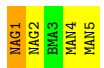
- Molecule 9: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X: 20% 80%



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

Chain Z: 20% 60% 20%



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

Chain a: 20% 80%



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

Chain c: 100%



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

Chain d: 20% 80%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	5175	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 ( $e^-/\text{\AA}^2$ )	35	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.017	Depositor
Minimum map value	-0.008	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0074	Depositor
Map size (Å)	319.8, 319.8, 319.8	wwPDB
Map dimensions	390, 390, 390	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82, 0.82, 0.82	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: NAG, BMA, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.84	3/1000 (0.3%)	1.30	19/1356 (1.4%)
1	B	1.03	8/992 (0.8%)	1.36	19/1345 (1.4%)
1	C	0.80	2/992 (0.2%)	1.31	21/1345 (1.6%)
2	D	0.45	1/2909 (0.0%)	0.76	5/3956 (0.1%)
2	E	0.45	1/2909 (0.0%)	0.76	5/3956 (0.1%)
2	F	0.50	3/2909 (0.1%)	0.78	6/3956 (0.2%)
3	G	0.29	0/797	0.61	0/1069
3	H	0.29	0/797	0.61	0/1069
3	I	0.29	0/785	0.62	0/1053
4	J	0.29	0/838	0.61	0/1139
4	K	0.29	0/838	0.62	0/1139
4	L	0.29	0/838	0.61	0/1139
5	M	0.27	0/1006	0.56	0/1365
5	N	0.27	0/1006	0.56	0/1365
5	O	0.27	0/1006	0.56	0/1365
6	P	0.38	0/1006	0.63	0/1372
6	R	0.38	0/1006	0.63	0/1372
6	T	0.38	0/1006	0.63	0/1372
7	Q	0.34	0/814	0.62	0/1109
7	S	0.34	0/814	0.62	0/1109
7	U	0.34	0/814	0.62	0/1109
All	All	0.47	18/25082 (0.1%)	0.78	75/34060 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	4
All	All	0	13

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	608	VAL	CB-CG2	-15.19	1.21	1.52
1	A	608	VAL	CB-CG2	-15.03	1.21	1.52
1	C	608	VAL	CB-CG2	-14.94	1.21	1.52
1	B	657	GLU	CD-OE2	-8.64	1.16	1.25
1	B	658	GLN	CB-CG	-8.62	1.29	1.52
1	B	661	LEU	CG-CD2	-8.33	1.21	1.51
1	A	634	GLU	CG-CD	-8.30	1.39	1.51
2	F	501	CYS	CB-SG	-7.41	1.69	1.82
1	B	631	TRP	CB-CG	-6.84	1.38	1.50
1	A	602	LEU	CG-CD1	-6.25	1.28	1.51
2	D	67	ASN	CB-CG	5.96	1.64	1.51
2	E	67	ASN	CB-CG	5.96	1.64	1.51
2	F	67	ASN	CB-CG	5.94	1.64	1.51
1	C	631	TRP	CB-CG	-5.85	1.39	1.50
1	B	658	GLN	CG-CD	-5.75	1.37	1.51
1	B	657	GLU	CD-OE1	-5.56	1.19	1.25
1	B	634	GLU	CG-CD	-5.46	1.43	1.51
2	F	502	LYS	CD-CE	5.04	1.63	1.51

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	572	GLY	N-CA-C	12.55	144.47	113.10
1	B	572	GLY	N-CA-C	12.53	144.43	113.10
1	C	572	GLY	N-CA-C	12.53	144.43	113.10
1	C	628	TRP	CA-CB-CG	-9.97	94.75	113.70
1	A	628	TRP	CA-CB-CG	-9.90	94.89	113.70
1	B	529	THR	C-N-CA	9.82	146.26	121.70
1	A	529	THR	C-N-CA	9.81	146.23	121.70
1	C	529	THR	C-N-CA	9.80	146.21	121.70
2	F	68	VAL	C-N-CA	9.72	145.99	121.70
2	E	68	VAL	C-N-CA	9.71	145.98	121.70
2	D	68	VAL	C-N-CA	9.70	145.94	121.70
1	B	628	TRP	CA-CB-CG	-9.60	95.47	113.70
2	F	116	LEU	C-N-CA	9.44	145.29	121.70
2	E	116	LEU	C-N-CA	9.38	145.15	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	116	LEU	C-N-CA	9.38	145.15	121.70
1	A	629	LEU	N-CA-C	8.85	134.88	111.00
1	A	628	TRP	N-CA-C	8.79	134.74	111.00
1	B	661	LEU	N-CA-C	8.75	134.62	111.00
1	B	628	TRP	N-CA-C	8.73	134.56	111.00
1	B	661	LEU	C-N-CA	8.72	143.50	121.70
1	C	628	TRP	N-CA-C	8.62	134.28	111.00
2	F	59	LYS	C-N-CA	7.55	140.58	121.70
2	D	59	LYS	C-N-CA	7.54	140.56	121.70
1	C	629	LEU	N-CA-C	7.54	131.36	111.00
2	E	59	LYS	C-N-CA	7.54	140.54	121.70
1	A	629	LEU	CB-CA-C	-7.45	96.05	110.20
1	B	629	LEU	N-CA-C	7.35	130.84	111.00
1	B	571	TRP	CA-CB-CG	7.07	127.14	113.70
1	C	571	TRP	CA-CB-CG	6.96	126.93	113.70
1	A	571	TRP	CA-CB-CG	6.94	126.89	113.70
2	F	67	ASN	C-N-CA	-6.88	104.49	121.70
2	D	67	ASN	C-N-CA	-6.87	104.52	121.70
2	E	67	ASN	C-N-CA	-6.87	104.53	121.70
1	B	530	MET	N-CA-C	6.83	129.45	111.00
1	A	530	MET	N-CA-C	6.82	129.41	111.00
1	B	660	LEU	N-CA-C	6.82	129.41	111.00
1	C	530	MET	N-CA-C	6.81	129.39	111.00
1	C	629	LEU	CB-CA-C	-6.73	97.41	110.20
1	B	610	TRP	CA-CB-CG	6.72	126.46	113.70
1	A	661	LEU	C-N-CA	6.61	138.23	121.70
1	C	660	LEU	N-CA-C	6.61	128.85	111.00
2	F	501	CYS	CA-CB-SG	-6.57	102.17	114.00
1	B	627	THR	C-N-CA	6.47	137.88	121.70
1	A	627	THR	C-N-CA	6.41	137.73	121.70
1	C	627	THR	C-N-CA	6.41	137.72	121.70
1	B	607	ASN	N-CA-C	6.39	128.25	111.00
1	B	571	TRP	N-CA-C	6.35	128.15	111.00
1	C	571	TRP	N-CA-C	6.34	128.12	111.00
1	A	571	TRP	N-CA-C	6.34	128.11	111.00
1	C	610	TRP	CA-CB-CG	6.33	125.72	113.70
1	A	607	ASN	N-CA-C	6.26	127.89	111.00
1	C	607	ASN	N-CA-C	6.23	127.82	111.00
1	A	660	LEU	N-CA-C	6.18	127.68	111.00
2	D	267	GLU	C-N-CA	6.17	137.12	121.70
2	E	267	GLU	C-N-CA	6.17	137.12	121.70
2	F	267	GLU	C-N-CA	6.16	137.10	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	531	GLY	N-CA-C	6.11	128.37	113.10
1	C	531	GLY	N-CA-C	6.09	128.33	113.10
1	A	610	TRP	CA-CB-CG	6.08	125.26	113.70
1	B	531	GLY	N-CA-C	6.08	128.29	113.10
1	C	661	LEU	C-N-CA	6.07	136.87	121.70
1	B	571	TRP	C-N-CA	-5.95	109.80	122.30
1	C	571	TRP	C-N-CA	-5.94	109.83	122.30
1	A	571	TRP	C-N-CA	-5.92	109.87	122.30
1	C	661	LEU	N-CA-C	5.71	126.41	111.00
1	A	610	TRP	N-CA-C	-5.59	95.92	111.00
1	C	610	TRP	N-CA-C	-5.55	96.00	111.00
1	B	629	LEU	CB-CA-C	-5.48	99.78	110.20
1	B	610	TRP	N-CA-C	-5.46	96.27	111.00
1	B	662	ALA	N-CA-C	5.40	125.57	111.00
1	C	663	LEU	N-CA-C	5.33	125.38	111.00
1	C	601	LYS	C-N-CA	5.25	134.82	121.70
1	A	646	LEU	CA-CB-CG	5.08	126.99	115.30
1	C	646	LEU	CA-CB-CG	5.07	126.97	115.30
1	A	661	LEU	N-CA-C	5.00	124.50	111.00

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	529	THR	Mainchain,Peptide
1	A	661	LEU	Mainchain,Peptide
1	B	529	THR	Mainchain,Peptide
1	B	661	LEU	Mainchain,Peptide
1	B	662	ALA	Peptide
1	C	529	THR	Mainchain,Peptide
1	C	661	LEU	Mainchain,Peptide

## 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	983	0	961	66	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	975	0	950	91	0
1	C	975	0	950	75	0
2	D	2845	0	2786	163	0
2	E	2845	0	2786	122	0
2	F	2845	0	2785	124	0
3	G	786	0	804	23	0
3	H	786	0	804	16	0
3	I	775	0	795	18	0
4	J	819	0	782	33	0
4	K	819	0	782	34	0
4	L	819	0	782	33	0
5	M	985	0	952	19	0
5	N	985	0	952	19	0
5	O	985	0	952	20	0
6	P	980	0	935	54	0
6	R	980	0	935	55	0
6	T	980	0	935	173	0
7	Q	796	0	755	30	0
7	S	796	0	755	33	0
7	U	796	0	755	33	0
8	V	50	0	42	88	0
8	Y	50	0	43	0	0
8	b	50	0	43	0	0
9	W	61	0	52	5	0
9	X	61	0	52	0	0
9	Z	61	0	52	2	0
9	a	61	0	52	0	0
9	c	61	0	52	0	0
9	d	61	0	52	0	0
All	All	25071	0	24333	1028	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 21.

All (1028) 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:T:55:TRP:CG	8:V:2:NAG:H4	1.27	1.68
6:T:70:SER:HB2	8:V:4:MAN:C4	1.10	1.55
6:T:70:SER:CB	8:V:4:MAN:C4	1.77	1.54
6:T:70:SER:HB3	8:V:4:MAN:C3	1.38	1.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:55:TRP:CE3	8:V:3:BMA:H2	1.54	1.41
6:T:55:TRP:CD2	8:V:2:NAG:H61	1.61	1.36
6:T:70:SER:CB	8:V:4:MAN:C3	2.00	1.33
2:D:90:THR:HB	6:T:54:ARG:CZ	1.57	1.33
6:T:55:TRP:CD2	8:V:2:NAG:H4	1.65	1.30
6:T:70:SER:HB3	8:V:4:MAN:O3	1.25	1.29
6:T:55:TRP:CE2	8:V:2:NAG:H61	1.67	1.28
6:T:55:TRP:CG	8:V:2:NAG:C4	2.18	1.27
2:D:90:THR:CB	6:T:54:ARG:NH1	1.99	1.26
6:T:55:TRP:CE2	8:V:2:NAG:C6	2.19	1.25
6:T:55:TRP:CE3	8:V:2:NAG:H61	1.72	1.24
6:T:55:TRP:CZ2	8:V:2:NAG:O6	1.92	1.23
2:D:90:THR:HB	6:T:54:ARG:NH1	1.51	1.20
6:T:55:TRP:CE3	8:V:3:BMA:C2	2.25	1.17
6:T:55:TRP:HE3	8:V:3:BMA:C2	1.56	1.16
6:T:55:TRP:CZ2	8:V:2:NAG:C6	2.30	1.14
2:E:90:THR:HB	6:R:54:ARG:NH1	1.61	1.14
2:D:90:THR:CB	6:T:54:ARG:CZ	2.24	1.14
6:T:70:SER:CA	8:V:4:MAN:O2	1.96	1.12
6:T:55:TRP:CB	8:V:2:NAG:H4	1.79	1.11
1:B:654:GLU:O	1:B:658:GLN:HB2	1.51	1.09
6:T:55:TRP:CZ3	8:V:2:NAG:H61	1.87	1.08
6:T:55:TRP:HB2	8:V:2:NAG:O3	1.53	1.08
6:T:55:TRP:CZ3	8:V:3:BMA:H2	1.87	1.07
6:T:55:TRP:CZ2	8:V:2:NAG:H61	1.88	1.04
2:E:90:THR:HB	6:R:54:ARG:HH12	1.11	1.03
2:D:90:THR:HB	6:T:54:ARG:NH2	1.73	1.02
6:T:55:TRP:CD2	8:V:2:NAG:C6	2.39	1.02
6:T:55:TRP:CH2	8:V:2:NAG:H61	1.94	1.02
6:T:70:SER:HA	8:V:4:MAN:O2	1.57	1.01
2:D:90:THR:CG2	6:T:54:ARG:CZ	2.40	1.00
6:T:55:TRP:CD1	8:V:2:NAG:H2	1.97	0.99
1:B:605:CYS:HB2	2:D:503:ARG:H	1.26	0.99
6:T:55:TRP:CD2	8:V:2:NAG:C4	2.40	0.99
1:A:520:LEU:N	1:A:536:THR:HG1	1.61	0.98
6:T:55:TRP:HB3	8:V:3:BMA:C1	1.94	0.98
6:T:70:SER:HB2	8:V:4:MAN:C5	1.94	0.98
1:B:605:CYS:SG	2:D:502:LYS:N	2.36	0.96
6:T:70:SER:HB3	8:V:4:MAN:C2	1.95	0.96
6:T:55:TRP:O	8:V:3:BMA:H5	1.66	0.95
6:T:70:SER:CB	8:V:4:MAN:C2	2.44	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:90:THR:CB	6:R:54:ARG:NH1	2.31	0.94
6:T:70:SER:HB3	8:V:4:MAN:HO3	1.15	0.93
6:T:73:ASP:OD2	8:V:1:NAG:O3	1.87	0.93
1:A:600:GLY:HA3	2:E:503:ARG:HH12	1.33	0.92
6:T:55:TRP:CH2	8:V:2:NAG:C6	2.51	0.91
2:E:115:SER:OG	2:E:116:LEU:N	2.02	0.90
6:T:55:TRP:CE3	8:V:3:BMA:C1	2.54	0.90
6:T:25:TYR:HD1	9:W:2:NAG:O7	1.56	0.89
1:B:610:TRP:HD1	2:D:34:LEU:HB2	1.37	0.88
6:T:70:SER:CB	8:V:4:MAN:O3	2.13	0.88
2:D:45:TRP:NE1	6:T:108:TRP:CZ2	2.40	0.88
2:F:90:THR:HB	6:P:54:ARG:NH1	1.88	0.88
2:D:90:THR:HG21	6:T:54:ARG:HD3	1.56	0.87
2:D:115:SER:OG	2:D:116:LEU:N	2.02	0.87
6:T:70:SER:CB	8:V:4:MAN:O2	2.22	0.87
2:F:115:SER:OG	2:F:116:LEU:N	2.02	0.87
6:T:52:ILE:HD12	6:T:69:ILE:O	1.76	0.86
2:D:90:THR:OG1	6:T:54:ARG:NH1	2.09	0.85
4:K:4:MET:N	4:K:99:THR:HG1	1.75	0.84
2:D:90:THR:HG21	6:T:54:ARG:CD	2.08	0.83
4:L:4:MET:N	4:L:99:THR:HG1	1.75	0.83
1:A:638:TYR:OH	7:S:51:ARG:NH2	2.10	0.83
2:D:90:THR:HG21	6:T:54:ARG:NE	1.93	0.83
1:B:639:THR:HG22	2:D:496:VAL:HG22	1.60	0.82
1:A:605:CYS:HB3	2:E:35:TRP:HE3	1.44	0.82
1:C:605:CYS:HB2	2:F:502:LYS:HA	1.62	0.82
6:T:55:TRP:HE3	8:V:3:BMA:C1	1.91	0.82
4:J:4:MET:N	4:J:99:THR:HG1	1.77	0.81
6:T:55:TRP:CB	8:V:2:NAG:C4	2.52	0.81
1:C:654:GLU:O	1:C:658:GLN:HB2	1.82	0.80
2:E:60:ALA:HA	2:E:65:LYS:HD3	1.65	0.79
2:F:60:ALA:HA	2:F:65:LYS:HD3	1.64	0.79
6:T:55:TRP:CB	8:V:2:NAG:O3	2.29	0.79
2:F:90:THR:HB	6:P:54:ARG:HH12	1.44	0.79
6:P:52:ILE:HD12	6:P:69:ILE:O	1.83	0.79
2:D:60:ALA:HA	2:D:65:LYS:HD3	1.64	0.78
6:R:52:ILE:HD12	6:R:69:ILE:O	1.83	0.78
2:F:101:VAL:O	2:F:479:TRP:NE1	2.17	0.78
1:B:537:LEU:HD21	2:D:43:PRO:HD2	1.65	0.78
1:C:633:LYS:HD3	6:P:108:TRP:HB3	1.65	0.78
2:D:90:THR:HB	6:T:54:ARG:HH12	1.46	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:634:GLU:OE1	7:S:51:ARG:NE	2.15	0.77
2:D:101:VAL:O	2:D:479:TRP:NE1	2.17	0.77
2:D:90:THR:HG21	6:T:54:ARG:CZ	2.12	0.77
6:T:55:TRP:CD2	8:V:2:NAG:C5	2.66	0.77
1:B:629:LEU:HD22	6:T:107:LYS:HD3	1.66	0.77
2:E:101:VAL:O	2:E:479:TRP:NE1	2.17	0.76
2:E:236:THR:HB	6:R:32:LEU:HD11	1.67	0.76
1:C:614:TRP:HD1	7:Q:30:THR:HG23	1.51	0.76
6:T:53:TRP:NE1	6:T:54:ARG:HG3	1.99	0.76
6:T:25:TYR:HD1	9:W:2:NAG:C7	1.97	0.76
6:T:55:TRP:CD1	8:V:2:NAG:C2	2.67	0.76
1:B:633:LYS:HB2	6:T:108:TRP:HD1	1.51	0.75
1:C:638:TYR:OH	7:Q:51:ARG:NH2	2.18	0.75
6:T:70:SER:HB2	8:V:4:MAN:C3	1.89	0.75
2:F:91:GLU:OE2	2:F:487:LYS:NZ	2.19	0.75
7:Q:6:GLN:H	7:Q:101:GLN:H	1.35	0.75
6:T:55:TRP:CE3	8:V:2:NAG:C6	2.63	0.75
6:R:18:VAL:HB	6:R:89:LEU:HD11	1.69	0.75
1:C:639:THR:HG22	2:F:496:VAL:HG22	1.69	0.74
6:T:55:TRP:HB2	8:V:2:NAG:C3	2.16	0.74
6:T:70:SER:HB3	8:V:4:MAN:O2	1.83	0.74
1:B:659:ASP:HA	1:C:603:ILE:HG21	1.67	0.74
2:E:91:GLU:OE2	2:E:487:LYS:NZ	2.20	0.74
6:T:55:TRP:CZ3	8:V:2:NAG:C6	2.67	0.74
1:A:639:THR:HG22	2:E:496:VAL:HG22	1.69	0.74
7:U:6:GLN:H	7:U:101:GLN:H	1.35	0.74
2:D:91:GLU:OE2	2:D:487:LYS:NZ	2.20	0.74
2:E:90:THR:CG2	6:R:54:ARG:NH1	2.51	0.74
1:B:642:ILE:HG22	1:B:646:LEU:HG	1.70	0.73
2:E:90:THR:O	6:R:54:ARG:NH2	2.22	0.73
4:K:16:GLY:H	4:K:78:LEU:HB3	1.54	0.73
6:P:18:VAL:HB	6:P:89:LEU:HD11	1.69	0.73
7:Q:5:THR:HB	7:Q:24:ARG:HB2	1.70	0.73
6:T:18:VAL:HB	6:T:89:LEU:HD11	1.69	0.73
2:D:90:THR:CB	6:T:54:ARG:HH12	1.99	0.73
7:U:5:THR:HB	7:U:24:ARG:HB2	1.70	0.73
1:A:629:LEU:HD22	6:R:107:LYS:HD3	1.70	0.72
1:A:654:GLU:O	1:A:658:GLN:HB2	1.89	0.72
4:J:16:GLY:H	4:J:78:LEU:HB3	1.54	0.72
7:S:5:THR:HB	7:S:24:ARG:HB2	1.70	0.72
7:S:6:GLN:H	7:S:101:GLN:H	1.35	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:55:TRP:NE1	8:V:2:NAG:O5	2.22	0.72
6:P:53:TRP:NE1	6:P:54:ARG:HG3	2.04	0.72
1:C:605:CYS:HB3	2:F:35:TRP:HE3	1.52	0.72
6:R:53:TRP:NE1	6:R:54:ARG:HG3	2.05	0.72
2:F:111:LEU:O	2:F:115:SER:HB3	1.90	0.72
4:L:16:GLY:H	4:L:78:LEU:HB3	1.54	0.71
1:B:658:GLN:HE22	1:C:601:LYS:N	1.88	0.71
1:C:634:GLU:OE1	7:Q:51:ARG:NE	2.21	0.71
6:T:25:TYR:CD1	9:W:2:NAG:O7	2.43	0.71
2:E:111:LEU:O	2:E:115:SER:HB3	1.90	0.70
6:T:55:TRP:CE2	8:V:2:NAG:C5	2.74	0.70
1:C:629:LEU:HD22	6:P:107:LYS:HD3	1.72	0.70
2:F:359:ILE:HG12	2:F:466:GLU:HB2	1.74	0.70
2:D:359:ILE:HG12	2:D:466:GLU:HB2	1.73	0.70
1:A:658:GLN:O	2:D:501:CYS:SG	2.50	0.70
2:E:359:ILE:HG12	2:E:466:GLU:HB2	1.73	0.70
1:A:614:TRP:HD1	7:S:30:THR:HG23	1.56	0.70
2:D:111:LEU:O	2:D:115:SER:HB3	1.90	0.70
1:A:538:THR:HA	1:A:602:LEU:HD13	1.72	0.69
6:T:55:TRP:CD1	8:V:2:NAG:O5	2.45	0.69
6:T:70:SER:OG	8:V:4:MAN:C4	2.39	0.69
2:F:90:THR:CB	6:P:54:ARG:NH1	2.55	0.69
6:T:70:SER:N	8:V:4:MAN:O2	2.26	0.69
2:F:91:GLU:HB3	2:F:242:VAL:HG21	1.75	0.69
6:P:39:ARG:HB3	6:P:49:ILE:HD11	1.76	0.68
1:B:654:GLU:O	1:B:658:GLN:CB	2.37	0.68
6:R:39:ARG:HB3	6:R:49:ILE:HD11	1.76	0.68
1:A:605:CYS:SG	2:E:502:LYS:N	2.66	0.68
6:T:55:TRP:HD1	8:V:2:NAG:H2	1.57	0.68
1:B:534:SER:O	1:B:538:THR:OG1	2.05	0.68
2:E:91:GLU:HB3	2:E:242:VAL:HG21	1.75	0.68
6:T:39:ARG:HB3	6:T:49:ILE:HD11	1.75	0.68
2:D:280:ASN:O	3:G:29:LYS:NZ	2.24	0.68
6:T:55:TRP:O	8:V:3:BMA:C5	2.42	0.68
2:F:274:SER:HB2	2:F:285:LEU:H	1.59	0.67
1:A:642:ILE:HG22	1:A:646:LEU:HG	1.76	0.67
2:D:274:SER:HB2	2:D:285:LEU:H	1.59	0.67
2:D:91:GLU:HB3	2:D:242:VAL:HG21	1.75	0.67
6:R:22:CYS:HB3	6:R:82:SER:HB3	1.76	0.67
1:A:520:LEU:N	1:A:536:THR:OG1	2.27	0.67
1:C:642:ILE:HG22	1:C:646:LEU:HG	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:22:CYS:HB3	6:T:82:SER:HB3	1.76	0.67
2:D:474:ASP:HA	3:G:40:GLN:HB3	1.77	0.67
2:E:274:SER:HB2	2:E:285:LEU:H	1.59	0.67
6:T:55:TRP:CB	8:V:2:NAG:C3	2.72	0.67
2:D:90:THR:O	6:T:54:ARG:NH2	2.28	0.66
2:F:284:ILE:HD11	2:F:456:ARG:HE	1.61	0.66
6:P:22:CYS:HB3	6:P:82:SER:HB3	1.76	0.66
2:D:284:ILE:HD11	2:D:456:ARG:HE	1.61	0.66
2:F:70:ALA:HB3	2:F:213:ILE:HD11	1.78	0.66
4:L:90:GLN:HE21	4:L:92:ASN:HB3	1.62	0.65
6:T:29:THR:CB	8:V:1:NAG:HN2	2.08	0.65
4:K:90:GLN:HE21	4:K:92:ASN:HB3	1.61	0.65
6:P:7:SER:HB3	6:P:21:SER:H	1.62	0.65
6:T:7:SER:HB3	6:T:21:SER:H	1.62	0.65
2:E:70:ALA:HB3	2:E:213:ILE:HD11	1.78	0.65
2:E:284:ILE:HD11	2:E:456:ARG:HE	1.61	0.65
2:F:363:ASN:OD1	2:F:469:ARG:NH1	2.30	0.65
1:B:633:LYS:HB2	6:T:108:TRP:CD1	2.30	0.65
4:J:90:GLN:HE21	4:J:92:ASN:HB3	1.61	0.65
6:R:7:SER:HB3	6:R:21:SER:H	1.62	0.65
2:E:266:ALA:HA	2:E:273:ARG:HH22	1.62	0.65
6:T:29:THR:OG1	8:V:1:NAG:H3	1.96	0.65
2:D:70:ALA:HB3	2:D:213:ILE:HD11	1.78	0.64
2:D:90:THR:CG2	6:T:54:ARG:NE	2.55	0.64
1:C:616:ASN:ND2	7:Q:28:SER:O	2.26	0.64
2:D:266:ALA:HA	2:D:273:ARG:HH22	1.62	0.64
2:F:266:ALA:HA	2:F:273:ARG:HH22	1.62	0.64
1:B:524:GLY:HA2	2:D:87:GLU:HB3	1.80	0.64
2:D:363:ASN:OD1	2:D:469:ARG:NH1	2.30	0.64
1:B:538:THR:HA	1:B:602:LEU:HD13	1.79	0.64
2:E:363:ASN:OD1	2:E:469:ARG:NH1	2.30	0.64
7:Q:37:TYR:HB2	7:Q:88:TYR:HB2	1.80	0.64
1:B:610:TRP:CD1	2:D:34:LEU:HB2	2.28	0.64
6:T:113:HIS:HD2	7:U:93:ASP:HA	1.62	0.64
1:A:534:SER:O	1:A:538:THR:OG1	2.04	0.63
2:D:92:GLU:HA	2:D:238:PRO:HA	1.80	0.63
1:B:610:TRP:CE3	1:B:642:ILE:HD11	2.34	0.63
6:P:50:GLY:HA3	6:P:59:ALA:HA	1.80	0.63
7:U:37:TYR:HB2	7:U:88:TYR:HB2	1.80	0.63
2:E:111:LEU:O	2:E:115:SER:CB	2.47	0.63
1:B:659:ASP:OD1	1:C:603:ILE:HG12	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:610:TRP:HB3	2:D:34:LEU:O	1.98	0.63
1:C:605:CYS:CB	2:F:502:LYS:HA	2.28	0.63
4:K:37:GLN:HB3	4:K:45:ARG:HB3	1.81	0.63
1:A:658:GLN:NE2	1:B:603:ILE:O	2.31	0.63
2:D:345:VAL:HG21	2:D:452:LEU:HD13	1.81	0.63
1:A:602:LEU:HD23	2:E:39:TYR:CD1	2.33	0.63
1:B:607:ASN:ND2	1:B:653:GLN:OE1	2.32	0.63
2:F:92:GLU:HA	2:F:238:PRO:HA	1.80	0.63
7:S:37:TYR:HB2	7:S:88:TYR:HB2	1.80	0.63
2:F:111:LEU:O	2:F:115:SER:CB	2.47	0.63
2:F:261:LEU:HD11	2:F:447:SER:HB3	1.80	0.63
2:F:345:VAL:HG21	2:F:452:LEU:HD13	1.81	0.62
7:S:38:GLN:HB2	7:S:48:LEU:HD11	1.81	0.62
2:E:92:GLU:HA	2:E:238:PRO:HA	1.80	0.62
6:R:32:LEU:HD22	6:R:105:TYR:HB2	1.80	0.62
2:E:474:ASP:HB3	2:E:477:ASP:HB2	1.82	0.62
7:Q:38:GLN:HB2	7:Q:48:LEU:HD11	1.81	0.62
2:E:261:LEU:HD11	2:E:447:SER:HB3	1.80	0.62
6:R:50:GLY:HA3	6:R:59:ALA:HA	1.80	0.62
6:T:32:LEU:HD22	6:T:105:TYR:HB2	1.80	0.62
4:L:37:GLN:HB3	4:L:45:ARG:HB3	1.81	0.62
6:T:50:GLY:HA3	6:T:59:ALA:HA	1.80	0.62
4:L:23:CYS:HB3	4:L:71:PHE:HB2	1.82	0.62
6:P:32:LEU:HD22	6:P:105:TYR:HB2	1.81	0.62
2:D:111:LEU:O	2:D:115:SER:CB	2.47	0.62
2:D:474:ASP:HB3	2:D:477:ASP:HB2	1.82	0.62
2:D:261:LEU:HD11	2:D:447:SER:HB3	1.80	0.62
2:E:345:VAL:HG21	2:E:452:LEU:HD13	1.81	0.62
6:T:53:TRP:CD1	6:T:54:ARG:HG3	2.34	0.62
1:B:533:ALA:HA	1:B:536:THR:HG22	1.82	0.62
1:C:607:ASN:ND2	1:C:653:GLN:OE1	2.32	0.62
1:C:664:ASP:HB2	2:E:502:LYS:HD2	1.82	0.62
1:A:533:ALA:HA	1:A:536:THR:HG22	1.80	0.62
2:E:280:ASN:HA	2:E:456:ARG:HD2	1.81	0.62
7:U:38:GLN:HB2	7:U:48:LEU:HD11	1.81	0.62
6:P:41:ALA:HB3	6:P:44:GLN:HB2	1.82	0.61
6:T:55:TRP:CE2	8:V:2:NAG:O6	2.34	0.61
2:D:280:ASN:HA	2:D:456:ARG:HD2	1.81	0.61
1:C:606:THR:HB	1:C:646:LEU:HB3	1.82	0.61
4:J:23:CYS:HB3	4:J:71:PHE:HB2	1.82	0.61
1:C:600:GLY:HA3	2:F:503:ARG:HH12	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:633:LYS:HD3	6:T:108:TRP:HB3	1.83	0.61
2:D:287:GLN:HA	2:D:451:GLY:HA2	1.83	0.61
1:C:533:ALA:HA	1:C:536:THR:HG22	1.82	0.61
4:J:37:GLN:HB3	4:J:45:ARG:HB3	1.81	0.61
2:F:474:ASP:HB3	2:F:477:ASP:HB2	1.82	0.61
7:Q:2:ILE:O	7:Q:91:GLN:NE2	2.34	0.61
6:T:40:GLN:HB2	6:T:46:LEU:HG	1.83	0.61
7:Q:6:GLN:HB3	7:Q:102:GLY:H	1.66	0.60
2:D:115:SER:O	2:D:117:LYS:HG3	2.01	0.60
2:E:287:GLN:HA	2:E:451:GLY:HA2	1.83	0.60
6:R:40:GLN:HB2	6:R:46:LEU:HG	1.83	0.60
1:B:617:ARG:NH2	1:B:621:GLU:O	2.35	0.60
2:F:280:ASN:HA	2:F:456:ARG:HD2	1.83	0.60
2:F:287:GLN:HA	2:F:451:GLY:HA2	1.83	0.60
4:K:23:CYS:HB3	4:K:71:PHE:HB2	1.82	0.60
1:B:617:ARG:HG3	2:D:498:PRO:HG2	1.82	0.60
7:S:6:GLN:HB3	7:S:102:GLY:H	1.66	0.60
1:C:617:ARG:NH2	1:C:621:GLU:O	2.35	0.60
2:E:115:SER:O	2:E:117:LYS:HG3	2.01	0.60
6:P:40:GLN:HB2	6:P:46:LEU:HG	1.83	0.60
6:T:70:SER:CB	8:V:4:MAN:HO3	2.03	0.60
1:A:617:ARG:NH2	1:A:621:GLU:O	2.35	0.60
6:T:41:ALA:HB3	6:T:44:GLN:HB2	1.82	0.60
7:U:2:ILE:O	7:U:91:GLN:NE2	2.34	0.60
1:B:523:LEU:HB2	2:D:86:LEU:HD22	1.83	0.60
2:F:115:SER:O	2:F:117:LYS:HG3	2.01	0.60
6:R:41:ALA:HB3	6:R:44:GLN:HB2	1.82	0.60
2:E:276:ASN:OD1	6:R:75:THR:OG1	2.14	0.60
7:U:6:GLN:HB3	7:U:102:GLY:H	1.66	0.59
1:B:605:CYS:HB2	2:D:503:ARG:N	2.09	0.59
6:R:53:TRP:HZ2	6:R:54:ARG:CZ	2.15	0.59
1:B:642:ILE:HG21	2:D:36:VAL:HG22	1.83	0.59
2:E:422:GLN:HG3	5:N:109:TYR:H	1.67	0.59
2:D:228:CYS:HB3	2:D:485:LYS:HB3	1.85	0.59
1:B:610:TRP:HD1	2:D:34:LEU:CB	2.13	0.59
1:B:643:TYR:OH	2:D:495:GLY:O	2.20	0.59
6:P:52:ILE:HD12	6:P:69:ILE:C	2.23	0.59
3:I:37:LEU:HA	3:I:47:GLY:H	1.67	0.59
7:S:2:ILE:O	7:S:91:GLN:NE2	2.34	0.59
1:A:607:ASN:ND2	1:A:653:GLN:OE1	2.36	0.59
1:C:538:THR:HA	1:C:602:LEU:HD13	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:98:ASN:ND2	2:F:483:LEU:O	2.35	0.59
2:F:228:CYS:HB3	2:F:485:LYS:HB3	1.85	0.59
6:T:55:TRP:HE3	8:V:3:BMA:C3	2.14	0.59
2:F:102:GLU:HA	2:F:479:TRP:HZ2	1.68	0.58
2:D:98:ASN:ND2	2:D:483:LEU:O	2.35	0.58
2:E:98:ASN:ND2	2:E:483:LEU:O	2.35	0.58
7:U:16:GLY:N	7:U:79:LEU:O	2.36	0.58
1:B:633:LYS:CD	6:T:108:TRP:HB3	2.34	0.58
1:B:643:TYR:HE2	2:D:494:LEU:HB3	1.69	0.58
1:B:658:GLN:HG2	1:C:603:ILE:O	2.03	0.58
6:P:53:TRP:HZ2	6:P:54:ARG:CZ	2.17	0.58
7:Q:29:ILE:HG21	7:Q:33:TRP:HB2	1.86	0.58
6:T:52:ILE:HD12	6:T:69:ILE:C	2.24	0.58
2:D:45:TRP:HE1	6:T:108:TRP:HZ2	1.41	0.58
4:J:41:GLY:H	5:M:39:GLN:HE22	1.52	0.58
7:U:29:ILE:HG21	7:U:33:TRP:HB2	1.86	0.58
2:E:67:ASN:O	2:E:69:TRP:N	2.34	0.58
1:A:537:LEU:HD22	2:E:42:VAL:HG12	1.86	0.58
7:S:64:SER:OG	7:S:75:THR:O	2.22	0.58
1:A:605:CYS:HB3	2:E:35:TRP:CE3	2.33	0.57
1:C:605:CYS:HB3	2:F:35:TRP:CE3	2.38	0.57
4:J:22:SER:OG	4:J:70:GLU:OE2	2.22	0.57
2:D:102:GLU:HA	2:D:479:TRP:HZ2	1.68	0.57
2:F:37:THR:HG23	2:F:497:ALA:O	2.04	0.57
6:T:55:TRP:CG	8:V:2:NAG:C3	2.86	0.57
2:E:228:CYS:HB3	2:E:485:LYS:HB3	1.85	0.57
2:D:92:GLU:OE1	6:T:105:TYR:N	2.37	0.57
1:C:541:ALA:HB3	1:C:602:LEU:HD11	1.85	0.57
2:E:212:PRO:HD3	2:E:377:ASN:HD22	1.69	0.57
6:R:55:TRP:HZ2	6:R:73:ASP:HB2	1.70	0.57
2:D:212:PRO:HD3	2:D:377:ASN:HD22	1.69	0.57
2:F:212:PRO:HD3	2:F:377:ASN:HD22	1.69	0.57
3:H:30:ASN:HD21	3:H:34:ILE:HD12	1.70	0.57
3:I:30:ASN:HD21	3:I:34:ILE:HD12	1.70	0.57
4:J:44:PRO:O	5:M:118:TRP:NE1	2.38	0.57
6:P:29:THR:OG1	6:P:73:ASP:OD2	2.20	0.57
2:E:102:GLU:HA	2:E:479:TRP:HZ2	1.68	0.57
2:F:277:ILE:HG22	2:F:278:THR:HG23	1.86	0.57
7:U:37:TYR:HB3	7:U:45:PRO:HB3	1.87	0.57
2:D:90:THR:CG2	6:T:54:ARG:NH1	2.63	0.57
6:P:55:TRP:HZ2	6:P:73:ASP:HB2	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S:29:ILE:HG21	7:S:33:TRP:HB2	1.86	0.57
6:T:55:TRP:HZ2	6:T:73:ASP:HB2	1.69	0.57
7:U:6:GLN:HE22	7:U:87:PHE:HB2	1.70	0.57
2:E:277:ILE:HG22	2:E:278:THR:HG23	1.87	0.56
3:G:30:ASN:HD21	3:G:34:ILE:HD12	1.70	0.56
6:T:53:TRP:HZ2	6:T:54:ARG:CZ	2.18	0.56
6:T:70:SER:HA	8:V:4:MAN:C2	2.33	0.56
7:U:64:SER:OG	7:U:75:THR:O	2.22	0.56
6:P:94:THR:HG23	6:P:129:SER:HA	1.88	0.56
7:U:2:ILE:HB	7:U:91:GLN:HE22	1.70	0.56
1:A:606:THR:HB	1:A:646:LEU:HB3	1.86	0.56
7:S:2:ILE:HB	7:S:91:GLN:HE22	1.70	0.56
6:T:72:VAL:HG22	8:V:4:MAN:O6	2.05	0.56
1:A:537:LEU:HD21	2:E:43:PRO:HD2	1.88	0.56
2:D:277:ILE:HG22	2:D:278:THR:HG23	1.87	0.56
2:D:504:ARG:HH21	2:E:504:ARG:HH12	1.52	0.56
6:R:6:GLN:HG3	6:R:123:GLY:HA3	1.88	0.56
1:B:662:ALA:HB1	2:F:502:LYS:HB2	1.85	0.56
2:D:51:THR:HA	2:D:103:GLN:HG3	1.88	0.56
3:H:79:SER:HB2	3:H:97:VAL:HB	1.87	0.56
4:K:22:SER:OG	4:K:70:GLU:OE2	2.22	0.56
1:B:657:GLU:O	1:B:661:LEU:HG	2.06	0.56
2:F:224:ALA:N	2:F:489:VAL:O	2.39	0.56
4:L:22:SER:OG	4:L:70:GLU:OE2	2.22	0.56
6:P:53:TRP:CD1	6:P:54:ARG:HG3	2.40	0.56
7:S:16:GLY:N	7:S:79:LEU:O	2.36	0.56
7:S:37:TYR:HB3	7:S:45:PRO:HB3	1.87	0.56
6:T:94:THR:HG23	6:T:129:SER:HA	1.88	0.56
1:B:605:CYS:SG	2:D:501:CYS:HB3	2.46	0.56
2:F:51:THR:HA	2:F:103:GLN:HG3	1.88	0.56
7:S:6:GLN:HE22	7:S:87:PHE:HB2	1.70	0.56
6:T:6:GLN:HG3	6:T:123:GLY:HA3	1.88	0.56
7:U:7:SER:OG	7:U:24:ARG:NH1	2.39	0.56
7:Q:64:SER:OG	7:Q:75:THR:O	2.22	0.56
2:D:127:VAL:O	2:D:197:ASN:ND2	2.39	0.56
5:M:51:ILE:HD12	5:M:58:ALA:HB2	1.88	0.56
7:Q:37:TYR:HB3	7:Q:45:PRO:HB3	1.87	0.56
6:T:29:THR:OG1	6:T:73:ASP:OD2	2.20	0.56
6:T:55:TRP:CD1	8:V:2:NAG:C1	2.89	0.56
2:F:124:PRO:HB2	3:I:60:SER:HB3	1.87	0.56
4:J:64:GLY:HA2	4:J:73:LEU:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:64:GLY:HA2	4:L:73:LEU:HA	1.88	0.56
5:O:30:ILE:HD12	5:O:54:ILE:HD12	1.88	0.56
5:O:50:ARG:NH1	5:O:111:ASN:OD1	2.39	0.56
5:O:51:ILE:HD12	5:O:58:ALA:HB2	1.89	0.56
7:Q:7:SER:OG	7:Q:24:ARG:NH1	2.39	0.56
6:R:52:ILE:HD12	6:R:69:ILE:C	2.26	0.56
6:R:94:THR:HG23	6:R:129:SER:HA	1.88	0.56
1:A:538:THR:HA	1:A:602:LEU:CD1	2.37	0.55
2:E:224:ALA:N	2:E:489:VAL:O	2.39	0.55
3:G:79:SER:HB2	3:G:97:VAL:HB	1.87	0.55
5:M:30:ILE:HD12	5:M:54:ILE:HD12	1.88	0.55
7:Q:2:ILE:HB	7:Q:91:GLN:HE22	1.70	0.55
6:T:55:TRP:CH2	8:V:2:NAG:O6	2.55	0.55
4:K:64:GLY:HA2	4:K:73:LEU:HA	1.88	0.55
6:P:32:LEU:O	6:P:104:THR:N	2.38	0.55
7:Q:6:GLN:HE22	7:Q:87:PHE:HB2	1.70	0.55
7:S:7:SER:OG	7:S:24:ARG:NH1	2.39	0.55
2:D:67:ASN:O	2:D:69:TRP:N	2.34	0.55
2:E:487:LYS:HZ2	6:R:108:TRP:HH2	1.54	0.55
2:F:67:ASN:O	2:F:69:TRP:N	2.34	0.55
2:F:98:ASN:HD22	2:F:101:VAL:HG23	1.72	0.55
1:B:633:LYS:HG2	1:B:637:ASN:ND2	2.22	0.55
2:F:430:ILE:HG21	3:I:59:ARG:HB3	1.88	0.55
5:N:30:ILE:HD12	5:N:54:ILE:HD12	1.88	0.55
6:R:53:TRP:CD1	6:R:54:ARG:HG3	2.41	0.55
6:T:70:SER:HA	8:V:4:MAN:HO2	1.71	0.55
2:E:127:VAL:O	2:E:197:ASN:ND2	2.39	0.55
2:F:127:VAL:O	2:F:197:ASN:ND2	2.39	0.55
1:B:650:GLN:NE2	2:D:505:VAL:HA	2.22	0.55
2:D:224:ALA:N	2:D:489:VAL:O	2.39	0.55
5:N:51:ILE:HD12	5:N:58:ALA:HB2	1.88	0.55
1:C:662:ALA:O	2:E:502:LYS:HB2	2.07	0.55
5:O:67:ARG:NH2	5:O:90:ASP:OD2	2.40	0.55
7:Q:16:GLY:N	7:Q:79:LEU:O	2.36	0.55
2:D:98:ASN:HD22	2:D:101:VAL:HG23	1.72	0.55
2:E:51:THR:HA	2:E:103:GLN:HG3	1.88	0.55
1:B:606:THR:HB	1:B:646:LEU:HB3	1.89	0.54
2:D:90:THR:HB	6:T:54:ARG:HH22	1.68	0.54
4:L:62:PHE:HD1	4:L:73:LEU:HD21	1.73	0.54
5:N:67:ARG:NH2	5:N:90:ASP:OD2	2.40	0.54
6:P:6:GLN:HG3	6:P:123:GLY:HA3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:50:ARG:NH1	5:N:111:ASN:OD1	2.39	0.54
1:B:600:GLY:HA3	2:D:503:ARG:HH12	1.73	0.54
1:C:534:SER:O	1:C:538:THR:OG1	2.04	0.54
1:C:608:VAL:HG21	1:C:645:LEU:HB3	1.90	0.54
2:D:210:PHE:HB3	2:D:380:GLY:HA2	1.89	0.54
6:T:29:THR:OG1	8:V:1:NAG:N2	2.36	0.54
1:B:643:TYR:CE2	2:D:494:LEU:HB3	2.43	0.54
1:A:608:VAL:HG21	1:A:645:LEU:HB3	1.90	0.54
1:A:636:SER:O	1:A:639:THR:OG1	2.20	0.54
2:F:210:PHE:HB3	2:F:380:GLY:HA2	1.89	0.54
4:K:4:MET:N	4:K:99:THR:OG1	2.40	0.54
7:U:66:SER:OG	7:U:73:THR:OG1	2.24	0.54
2:E:210:PHE:HB3	2:E:380:GLY:HA2	1.89	0.54
2:E:105:HIS:HB2	2:E:479:TRP:CD1	2.43	0.54
4:J:62:PHE:HD1	4:J:73:LEU:HD21	1.73	0.54
4:K:62:PHE:HD1	4:K:73:LEU:HD21	1.72	0.54
7:Q:66:SER:OG	7:Q:73:THR:OG1	2.24	0.54
6:T:69:ILE:C	8:V:4:MAN:O2	2.46	0.54
2:E:98:ASN:HD22	2:E:101:VAL:HG23	1.72	0.54
5:M:67:ARG:NH2	5:M:90:ASP:OD2	2.40	0.54
2:F:64:GLU:HB2	2:F:66:HIS:ND1	2.24	0.53
4:J:33:LEU:HB3	4:J:51:ALA:HB2	1.90	0.53
5:M:50:ARG:NH1	5:M:111:ASN:OD1	2.39	0.53
6:P:36:ASN:HB3	6:P:48:TYR:HE1	1.73	0.53
2:E:90:THR:HG21	6:R:54:ARG:NH1	2.22	0.53
2:F:361:PHE:HB3	2:F:391:PHE:HB3	1.89	0.53
1:A:532:ALA:H	1:A:625:ASN:HA	1.73	0.53
2:D:105:HIS:HB2	2:D:479:TRP:CD1	2.43	0.53
4:K:33:LEU:HB3	4:K:51:ALA:HB2	1.90	0.53
6:R:32:LEU:O	6:R:104:THR:N	2.38	0.53
2:D:361:PHE:HB3	2:D:391:PHE:HB3	1.89	0.53
4:L:4:MET:N	4:L:99:THR:OG1	2.40	0.53
4:L:21:LEU:HD21	4:L:106:LEU:HD11	1.91	0.53
2:E:361:PHE:HB3	2:E:391:PHE:HB3	1.89	0.53
4:J:4:MET:N	4:J:99:THR:OG1	2.41	0.53
6:R:53:TRP:CZ2	6:R:54:ARG:CZ	2.91	0.53
1:C:630:GLN:O	1:C:630:GLN:NE2	2.42	0.53
4:K:15:PRO:HA	4:K:78:LEU:HD22	1.91	0.53
1:C:529:THR:HA	1:C:626:MET:HA	1.90	0.53
2:D:64:GLU:HB2	2:D:66:HIS:ND1	2.24	0.53
1:B:529:THR:HA	1:B:626:MET:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:105:HIS:HB2	2:F:479:TRP:CD1	2.43	0.53
1:C:636:SER:O	1:C:639:THR:OG1	2.20	0.53
1:A:604:CYS:HB3	2:E:37:THR:HA	1.91	0.53
1:B:541:ALA:HB3	1:B:602:LEU:HD11	1.90	0.53
4:J:15:PRO:HA	4:J:78:LEU:HD22	1.91	0.53
6:P:53:TRP:CZ2	6:P:54:ARG:CZ	2.93	0.53
3:H:37:LEU:HA	3:H:47:GLY:H	1.75	0.52
4:J:21:LEU:HD21	4:J:106:LEU:HD11	1.91	0.52
1:A:529:THR:HA	1:A:626:MET:HA	1.90	0.52
1:B:608:VAL:HG21	1:B:645:LEU:HB3	1.90	0.52
2:F:124:PRO:HA	2:F:198:THR:HA	1.91	0.52
6:R:36:ASN:HB3	6:R:48:TYR:HE1	1.73	0.52
6:T:36:ASN:HB3	6:T:48:TYR:HE1	1.73	0.52
2:E:58:ALA:C	2:E:60:ALA:H	2.13	0.52
2:E:64:GLU:HB2	2:E:66:HIS:ND1	2.24	0.52
4:L:15:PRO:HA	4:L:78:LEU:HD22	1.90	0.52
4:L:33:LEU:HB3	4:L:51:ALA:HB2	1.90	0.52
6:T:73:ASP:OD2	8:V:1:NAG:N2	2.42	0.52
2:D:58:ALA:C	2:D:60:ALA:H	2.13	0.52
1:A:532:ALA:H	1:A:625:ASN:CA	2.23	0.52
2:D:439:ILE:HG13	2:D:440:GLN:HG3	1.92	0.52
2:D:469:ARG:HD2	3:G:48:PRO:HG3	1.92	0.52
2:F:58:ALA:C	2:F:60:ALA:H	2.13	0.52
6:T:46:LEU:HB2	7:U:99:PHE:CE2	2.45	0.52
1:B:522:PHE:HE2	2:D:244:THR:HG21	1.74	0.52
2:D:281:ALA:HA	3:G:29:LYS:HE3	1.91	0.52
2:E:92:GLU:HG2	2:E:238:PRO:HB3	1.92	0.52
2:D:124:PRO:HA	2:D:198:THR:HA	1.91	0.52
2:F:439:ILE:HG13	2:F:440:GLN:HG3	1.92	0.52
6:T:32:LEU:O	6:T:104:THR:N	2.38	0.52
6:T:55:TRP:CD1	8:V:2:NAG:C4	2.88	0.52
6:T:70:SER:HB2	8:V:4:MAN:O5	2.09	0.52
1:B:630:GLN:HA	6:T:107:LYS:O	2.10	0.52
1:B:643:TYR:CE1	2:D:38:VAL:HG22	2.44	0.52
2:E:67:ASN:O	2:E:210:PHE:HE1	1.93	0.52
4:K:41:GLY:H	5:N:39:GLN:HE22	1.55	0.52
6:P:52:ILE:HD12	6:P:69:ILE:HG22	1.90	0.52
1:B:544:LEU:HD21	2:D:40:TYR:CE2	2.45	0.52
1:C:532:ALA:H	1:C:625:ASN:HA	1.73	0.52
1:C:537:LEU:HD21	2:F:43:PRO:HD2	1.92	0.52
2:D:92:GLU:HG2	2:D:238:PRO:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:24:ALA:O	5:O:77:SER:OG	2.26	0.52
1:C:532:ALA:H	1:C:625:ASN:CA	2.23	0.51
4:K:21:LEU:HD21	4:K:106:LEU:HD11	1.91	0.51
7:Q:15:ILE:HG23	7:Q:80:GLN:HA	1.92	0.51
1:B:629:LEU:HD12	1:B:629:LEU:H	1.75	0.51
6:T:55:TRP:CG	8:V:2:NAG:H2	2.43	0.51
2:D:256:SER:O	2:D:478:ASN:ND2	2.43	0.51
2:F:67:ASN:O	2:F:210:PHE:HE1	1.93	0.51
1:A:531:GLY:HA3	1:A:624:ASP:N	2.26	0.51
1:A:530:MET:HA	1:A:626:MET:HB2	1.93	0.51
1:B:532:ALA:H	1:B:625:ASN:HA	1.74	0.51
1:B:629:LEU:HD23	6:T:108:TRP:CZ2	2.46	0.51
2:E:439:ILE:HG13	2:E:440:GLN:HG3	1.92	0.51
2:F:256:SER:O	2:F:478:ASN:ND2	2.43	0.51
4:L:28:SER:HA	4:L:69:ALA:HB2	1.93	0.51
6:R:29:THR:OG1	6:R:73:ASP:OD2	2.20	0.51
6:T:25:TYR:CD1	9:W:2:NAG:C7	2.86	0.51
1:C:631:TRP:CE3	6:P:113:HIS:HB2	2.45	0.51
2:E:124:PRO:HA	2:E:198:THR:HA	1.91	0.51
7:S:15:ILE:HG23	7:S:80:GLN:HA	1.92	0.51
6:T:55:TRP:CE2	8:V:2:NAG:O5	2.63	0.51
1:A:605:CYS:HB2	2:E:503:ARG:H	1.76	0.51
2:E:45:TRP:HA	2:E:491:ILE:HB	1.93	0.51
2:E:47:ASP:HA	2:E:489:VAL:HG12	1.93	0.51
3:I:14:LEU:HB3	3:I:93:VAL:HG11	1.93	0.51
6:T:35:VAL:O	6:T:52:ILE:HG22	2.10	0.51
2:D:67:ASN:O	2:D:210:PHE:HE1	1.93	0.51
2:E:90:THR:CG2	6:R:54:ARG:CZ	2.89	0.51
2:E:256:SER:O	2:E:478:ASN:ND2	2.43	0.51
3:I:79:SER:HB2	3:I:97:VAL:HB	1.93	0.51
4:J:28:SER:HA	4:J:69:ALA:HB2	1.93	0.51
6:R:35:VAL:O	6:R:52:ILE:HG22	2.10	0.51
1:B:532:ALA:H	1:B:625:ASN:CA	2.24	0.51
1:B:636:SER:O	1:B:639:THR:OG1	2.18	0.51
3:I:13:GLU:OE2	3:I:58:ARG:NH1	2.38	0.51
1:A:526:ALA:HA	1:A:627:THR:HG21	1.93	0.50
2:D:47:ASP:HA	2:D:489:VAL:HG12	1.93	0.50
5:N:38:ARG:NH2	5:N:89:ASP:O	2.45	0.50
1:B:526:ALA:HA	1:B:627:THR:HG21	1.93	0.50
3:G:37:LEU:HA	3:G:47:GLY:H	1.75	0.50
3:I:75:LYS:H	3:I:78:ASP:HB2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:254:VAL:HG11	2:E:261:LEU:HB3	1.94	0.50
5:M:38:ARG:NH2	5:M:89:ASP:O	2.45	0.50
7:S:20:ARG:HA	7:S:75:THR:HA	1.93	0.50
2:F:45:TRP:HA	2:F:491:ILE:HB	1.92	0.50
1:C:633:LYS:HB2	6:P:108:TRP:HD1	1.76	0.50
6:T:120:SER:HA	7:U:47:LEU:HB2	1.93	0.50
7:U:15:ILE:HG23	7:U:80:GLN:HA	1.92	0.50
4:J:99:THR:HA	5:M:47:TRP:HB2	1.92	0.50
1:B:530:MET:HA	1:B:626:MET:HB2	1.92	0.50
1:B:531:GLY:HA3	1:B:624:ASP:N	2.26	0.50
2:D:69:TRP:HE1	2:D:253:PRO:HG2	1.77	0.50
5:O:38:ARG:NH2	5:O:89:ASP:O	2.45	0.50
1:B:639:THR:HB	2:D:496:VAL:HG13	1.93	0.50
1:C:531:GLY:HA3	1:C:624:ASP:N	2.26	0.50
2:D:254:VAL:HG11	2:D:261:LEU:HB3	1.94	0.50
4:K:28:SER:HA	4:K:69:ALA:HB2	1.93	0.50
6:T:29:THR:OG1	8:V:1:NAG:C3	2.59	0.50
2:F:69:TRP:HE1	2:F:253:PRO:HG2	1.77	0.50
2:F:487:LYS:NZ	6:P:108:TRP:HH2	2.10	0.50
1:C:526:ALA:HA	1:C:627:THR:HG21	1.93	0.49
2:D:474:ASP:N	3:G:40:GLN:HE21	2.10	0.49
2:F:92:GLU:HG2	2:F:238:PRO:HB3	1.93	0.49
2:F:254:VAL:HG11	2:F:261:LEU:HB3	1.94	0.49
1:C:530:MET:HA	1:C:626:MET:HB2	1.93	0.49
6:P:5:VAL:O	6:P:23:LYS:N	2.43	0.49
7:U:20:ARG:HA	7:U:75:THR:HA	1.93	0.49
1:A:604:CYS:H	2:E:37:THR:HG22	1.78	0.49
2:D:45:TRP:HA	2:D:491:ILE:HB	1.93	0.49
2:E:369:LEU:O	2:E:373:THR:OG1	2.23	0.49
3:H:75:LYS:H	3:H:78:ASP:HB2	1.78	0.49
3:G:75:LYS:H	3:G:78:ASP:HB2	1.78	0.49
6:R:67:VAL:HG22	6:R:86:ILE:HG12	1.94	0.49
1:C:631:TRP:CZ3	6:P:113:HIS:HB2	2.48	0.49
2:E:69:TRP:HE1	2:E:253:PRO:HG2	1.77	0.49
7:Q:20:ARG:HA	7:Q:75:THR:HA	1.93	0.49
2:D:102:GLU:HA	2:D:479:TRP:CZ2	2.48	0.49
2:D:422:GLN:HG3	5:M:109:TYR:H	1.77	0.49
3:I:79:SER:OG	3:I:95:LEU:O	2.30	0.49
3:I:83:ILE:HA	3:I:92:GLU:HG3	1.95	0.49
6:R:53:TRP:CZ2	6:R:54:ARG:NE	2.80	0.49
1:B:532:ALA:HB3	1:B:625:ASN:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:643:TYR:OH	2:D:38:VAL:HA	2.12	0.49
2:F:47:ASP:HA	2:F:489:VAL:HG12	1.93	0.49
3:I:9:GLY:N	3:I:74:LEU:O	2.43	0.49
1:C:602:LEU:HA	2:F:39:TYR:CD1	2.48	0.48
6:P:53:TRP:CZ2	6:P:54:ARG:NE	2.81	0.48
2:D:296:CYS:HA	2:D:331:CYS:HA	1.95	0.48
2:F:102:GLU:HA	2:F:479:TRP:CZ2	2.48	0.48
2:F:297:THR:OG1	2:F:330:HIS:NE2	2.45	0.48
3:H:13:GLU:OE2	3:H:58:ARG:NH1	2.38	0.48
2:E:112:TRP:HA	2:E:115:SER:HB3	1.95	0.48
6:P:67:VAL:HG22	6:P:86:ILE:HG12	1.94	0.48
6:T:55:TRP:CG	8:V:2:NAG:C5	2.90	0.48
2:D:92:GLU:OE1	6:T:105:TYR:CA	2.62	0.48
3:I:81:THR:HG22	3:I:92:GLU:HG2	1.93	0.48
1:B:635:ILE:O	1:B:639:THR:HG23	2.13	0.48
2:D:112:TRP:HA	2:D:115:SER:HB3	1.95	0.48
2:D:37:THR:HG23	2:D:497:ALA:O	2.13	0.48
2:F:45:TRP:HE1	6:P:108:TRP:HZ2	1.59	0.48
3:H:3:VAL:HA	3:H:94:GLN:HB3	1.96	0.48
3:H:81:THR:HG22	3:H:92:GLU:HG2	1.95	0.48
3:I:3:VAL:HA	3:I:94:GLN:HB3	1.96	0.48
5:M:24:ALA:O	5:M:77:SER:OG	2.26	0.48
2:E:279:ASN:ND2	9:Z:1:NAG:O5	2.47	0.48
3:G:3:VAL:HA	3:G:94:GLN:HB3	1.96	0.48
3:G:14:LEU:HB3	3:G:93:VAL:HG11	1.96	0.48
6:T:46:LEU:HB2	7:U:99:PHE:CZ	2.48	0.48
6:T:53:TRP:CZ2	6:T:54:ARG:CZ	2.96	0.48
4:K:83:PHE:HA	4:K:106:LEU:HB2	1.96	0.48
6:R:5:VAL:O	6:R:23:LYS:N	2.43	0.48
1:B:576:LEU:HA	1:B:579:ARG:HE	1.79	0.48
1:C:630:GLN:CD	6:P:110:GLY:H	2.17	0.48
1:C:643:TYR:HE2	2:F:494:LEU:HB3	1.79	0.48
2:D:226:LEU:HA	2:D:244:THR:HA	1.96	0.48
2:D:279:ASN:HB2	6:T:76:GLY:HA2	1.96	0.48
6:P:35:VAL:O	6:P:52:ILE:HG22	2.13	0.48
2:D:279:ASN:ND2	9:W:1:NAG:O5	2.46	0.48
6:T:67:VAL:HG22	6:T:86:ILE:HG12	1.94	0.48
1:C:576:LEU:HA	1:C:579:ARG:HE	1.79	0.47
2:E:346:VAL:HG23	2:E:359:ILE:HB	1.96	0.47
2:F:296:CYS:HA	2:F:331:CYS:HA	1.96	0.47
4:L:83:PHE:HA	4:L:106:LEU:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:642:ILE:HG21	2:D:36:VAL:CG2	2.43	0.47
1:C:603:ILE:HA	2:F:37:THR:CG2	2.44	0.47
3:G:81:THR:HG22	3:G:92:GLU:HG2	1.95	0.47
6:P:52:ILE:CD1	6:P:69:ILE:HG22	2.44	0.47
1:C:611:ASN:O	1:C:615:SER:N	2.41	0.47
2:D:297:THR:OG1	2:D:330:HIS:NE2	2.45	0.47
2:E:101:VAL:HG11	2:E:480:ARG:HG2	1.96	0.47
2:F:112:TRP:HA	2:F:115:SER:HB3	1.95	0.47
2:F:226:LEU:HA	2:F:244:THR:HA	1.96	0.47
2:F:346:VAL:HG23	2:F:359:ILE:HB	1.96	0.47
3:G:83:ILE:HA	3:G:92:GLU:HG3	1.96	0.47
4:J:83:PHE:HA	4:J:106:LEU:HB2	1.96	0.47
4:K:47:LEU:HA	4:K:58:VAL:HG21	1.96	0.47
4:L:47:LEU:HA	4:L:58:VAL:HG21	1.96	0.47
4:L:90:GLN:HG2	4:L:92:ASN:H	1.80	0.47
5:M:50:ARG:H	5:M:59:HIS:HB2	1.79	0.47
5:N:50:ARG:H	5:N:59:HIS:HB2	1.79	0.47
6:T:55:TRP:CE3	8:V:2:NAG:H4	2.40	0.47
1:C:532:ALA:HB3	1:C:625:ASN:HA	1.95	0.47
2:D:101:VAL:HG11	2:D:480:ARG:HG2	1.96	0.47
2:E:37:THR:HG23	2:E:497:ALA:O	2.13	0.47
2:F:476:ARG:HA	2:F:479:TRP:HE3	1.80	0.47
3:H:14:LEU:HB3	3:H:93:VAL:HG11	1.96	0.47
1:A:635:ILE:O	1:A:639:THR:HG23	2.15	0.47
2:E:122:LEU:HD12	2:E:432:GLN:HB2	1.96	0.47
2:E:296:CYS:HA	2:E:331:CYS:HA	1.96	0.47
6:T:49:ILE:HG21	6:T:67:VAL:HG11	1.97	0.47
1:A:532:ALA:HB3	1:A:625:ASN:HA	1.95	0.47
1:A:576:LEU:HA	1:A:579:ARG:HE	1.79	0.47
1:B:634:GLU:OE1	7:U:51:ARG:NE	2.47	0.47
2:E:60:ALA:CA	2:E:65:LYS:HD3	2.39	0.47
2:E:102:GLU:HA	2:E:479:TRP:CZ2	2.48	0.47
2:E:487:LYS:NZ	6:R:108:TRP:HH2	2.13	0.47
2:F:122:LEU:HD12	2:F:432:GLN:HB2	1.96	0.47
4:J:47:LEU:HA	4:J:58:VAL:HG21	1.96	0.47
4:K:19:ALA:HB2	4:K:78:LEU:HD12	1.97	0.47
4:K:90:GLN:HG2	4:K:92:ASN:H	1.80	0.47
4:K:99:THR:HA	5:N:47:TRP:HB2	1.96	0.47
6:P:36:ASN:ND2	6:P:117:MET:HG2	2.30	0.47
6:R:49:ILE:HG21	6:R:67:VAL:HG11	1.97	0.47
6:R:52:ILE:HD12	6:R:69:ILE:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S:66:SER:OG	7:S:73:THR:OG1	2.24	0.47
1:C:635:ILE:O	1:C:639:THR:HG23	2.15	0.47
2:E:295:ASN:O	2:E:332:ASN:N	2.45	0.47
4:K:20:THR:O	4:K:21:LEU:HD22	2.15	0.47
1:A:523:LEU:HD21	2:E:45:TRP:HZ3	1.80	0.47
2:D:295:ASN:O	2:D:332:ASN:N	2.46	0.47
2:E:297:THR:OG1	2:E:330:HIS:NE2	2.45	0.47
3:G:9:GLY:N	3:G:74:LEU:O	2.46	0.47
4:K:93:ASN:O	4:K:98:TYR:OH	2.24	0.47
4:L:37:GLN:N	4:L:45:ARG:O	2.48	0.47
4:L:61:ARG:NE	4:L:82:ASP:OD1	2.43	0.47
2:D:346:VAL:HG23	2:D:359:ILE:HB	1.96	0.47
4:J:90:GLN:HG2	4:J:92:ASN:H	1.80	0.47
5:O:4:LEU:HB2	5:O:119:GLY:HA2	1.97	0.47
1:A:658:GLN:HG2	2:D:501:CYS:SG	2.54	0.46
1:B:657:GLU:HB3	1:B:661:LEU:HD21	1.97	0.46
2:D:122:LEU:HD12	2:D:432:GLN:HB2	1.96	0.46
2:D:474:ASP:OD1	2:D:475:MET:N	2.49	0.46
3:H:83:ILE:HA	3:H:92:GLU:HG3	1.96	0.46
4:K:37:GLN:N	4:K:45:ARG:O	2.48	0.46
5:O:87:ARG:N	5:O:90:ASP:OD2	2.48	0.46
2:F:474:ASP:OD1	2:F:475:MET:N	2.48	0.46
3:G:29:LYS:HB2	3:G:83:ILE:HB	1.97	0.46
3:H:29:LYS:HB2	3:H:83:ILE:HB	1.97	0.46
5:O:50:ARG:H	5:O:59:HIS:HB2	1.79	0.46
7:Q:65:GLY:HA2	7:Q:75:THR:H	1.80	0.46
6:R:36:ASN:ND2	6:R:117:MET:HG2	2.30	0.46
1:C:602:LEU:HA	2:F:39:TYR:HD1	1.80	0.46
2:D:60:ALA:CA	2:D:65:LYS:HD3	2.39	0.46
2:E:65:LYS:HA	2:E:65:LYS:HD2	1.79	0.46
2:E:476:ARG:HA	2:E:479:TRP:HE3	1.80	0.46
6:T:27:VAL:HG21	6:T:101:THR:HG21	1.97	0.46
6:T:55:TRP:CE3	8:V:2:NAG:C4	2.95	0.46
7:U:65:GLY:HA2	7:U:75:THR:H	1.80	0.46
1:B:596:TRP:HH2	2:D:494:LEU:HD11	1.78	0.46
2:D:50:THR:OG1	2:D:51:THR:N	2.48	0.46
2:E:226:LEU:HA	2:E:244:THR:HA	1.96	0.46
4:J:20:THR:O	4:J:21:LEU:HD22	2.15	0.46
4:J:61:ARG:NE	4:J:82:ASP:OD1	2.43	0.46
4:L:82:ASP:O	4:L:86:TYR:OH	2.29	0.46
1:A:638:TYR:OH	7:S:31:GLY:HA3	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:4:LEU:HB2	5:M:119:GLY:HA2	1.97	0.46
7:U:37:TYR:HE2	7:U:90:GLN:HB3	1.81	0.46
2:D:69:TRP:HH2	2:D:255:VAL:HG23	1.81	0.46
6:R:48:TYR:HB3	7:S:96:PRO:HB2	1.97	0.46
1:B:662:ALA:CB	2:F:502:LYS:HB2	2.45	0.46
1:C:523:LEU:HB3	2:F:89:VAL:HG21	1.96	0.46
2:D:384:TYR:H	2:D:419:ARG:H	1.63	0.46
2:F:101:VAL:HG11	2:F:480:ARG:HG2	1.96	0.46
4:L:19:ALA:HB2	4:L:78:LEU:HD12	1.97	0.46
1:A:532:ALA:H	1:A:625:ASN:N	2.14	0.46
2:E:384:TYR:H	2:E:419:ARG:H	1.63	0.46
2:F:499:THR:OG1	2:F:500:ARG:N	2.48	0.46
1:C:532:ALA:H	1:C:625:ASN:N	2.14	0.46
2:D:34:LEU:HD13	2:D:498:PRO:HB2	1.97	0.46
2:E:34:LEU:HD13	2:E:498:PRO:HB2	1.97	0.46
2:F:90:THR:HB	6:P:54:ARG:CZ	2.46	0.46
2:F:90:THR:CG2	6:P:54:ARG:NH1	2.79	0.46
4:L:89:GLN:HE21	4:L:98:TYR:HB2	1.81	0.46
5:N:39:GLN:HB3	5:N:93:VAL:HB	1.98	0.46
5:O:12:LYS:O	5:O:127:SER:N	2.39	0.46
6:P:49:ILE:HG21	6:P:67:VAL:HG11	1.97	0.46
6:R:53:TRP:CZ2	6:R:54:ARG:HD2	2.51	0.46
1:A:576:LEU:O	1:A:580:VAL:HG23	2.16	0.46
2:F:50:THR:OG1	2:F:51:THR:N	2.48	0.46
3:I:74:LEU:HD11	3:I:95:LEU:HD21	1.98	0.46
4:J:37:GLN:N	4:J:45:ARG:O	2.48	0.46
4:K:95:PRO:HD2	4:K:97:ARG:HH12	1.81	0.46
4:L:20:THR:O	4:L:21:LEU:HD22	2.15	0.46
5:N:24:ALA:O	5:N:77:SER:OG	2.26	0.46
6:R:27:VAL:HG21	6:R:101:THR:HG21	1.97	0.46
1:C:522:PHE:CE1	2:F:43:PRO:HB3	2.51	0.45
4:J:95:PRO:HD2	4:J:97:ARG:HH12	1.81	0.45
1:C:643:TYR:OH	2:F:495:GLY:O	2.34	0.45
2:D:499:THR:OG1	2:D:500:ARG:N	2.49	0.45
3:H:9:GLY:N	3:H:74:LEU:O	2.46	0.45
4:J:19:ALA:HB2	4:J:78:LEU:HD12	1.97	0.45
5:M:39:GLN:HB3	5:M:93:VAL:HB	1.98	0.45
7:Q:37:TYR:HE2	7:Q:90:GLN:HB3	1.81	0.45
7:S:37:TYR:HE2	7:S:90:GLN:HB3	1.81	0.45
7:S:65:GLY:HA2	7:S:75:THR:H	1.80	0.45
6:T:29:THR:HB	8:V:1:NAG:HN2	1.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:499:THR:OG1	2:E:500:ARG:N	2.49	0.45
6:P:27:VAL:HG21	6:P:101:THR:HG21	1.97	0.45
6:T:36:ASN:ND2	6:T:117:MET:HG2	2.30	0.45
2:D:476:ARG:HA	2:D:479:TRP:HE3	1.80	0.45
2:E:45:TRP:HE1	6:R:108:TRP:HZ2	1.65	0.45
2:E:474:ASP:OD1	2:E:475:MET:N	2.48	0.45
2:F:384:TYR:H	2:F:419:ARG:H	1.63	0.45
4:J:89:GLN:HE21	4:J:98:TYR:HB2	1.81	0.45
4:K:100:PHE:HB2	5:N:45:LEU:HB2	1.97	0.45
7:U:36:TRP:CD2	7:U:74:LEU:HD22	2.51	0.45
1:B:630:GLN:CD	6:T:110:GLY:H	2.20	0.45
2:F:105:HIS:HB2	2:F:479:TRP:CG	2.52	0.45
7:Q:36:TRP:CD2	7:Q:74:LEU:HD22	2.51	0.45
7:S:36:TRP:CD2	7:S:74:LEU:HD22	2.51	0.45
8:V:4:MAN:O6	8:V:4:MAN:O4	2.33	0.45
1:B:629:LEU:HA	1:B:632:ASP:HB2	1.98	0.45
1:C:652:GLN:O	1:C:656:ASN:HB2	2.17	0.45
2:D:105:HIS:HB2	2:D:479:TRP:CG	2.52	0.45
2:E:69:TRP:HH2	2:E:255:VAL:HG23	1.80	0.45
2:F:121:LYS:HB3	2:F:201:ILE:HB	1.99	0.45
2:F:295:ASN:O	2:F:332:ASN:N	2.46	0.45
4:K:89:GLN:HE21	4:K:98:TYR:HB2	1.81	0.45
6:T:52:ILE:CD1	6:T:69:ILE:HG22	2.47	0.45
1:B:604:CYS:SG	2:D:503:ARG:NH2	2.89	0.45
1:B:642:ILE:CG2	2:D:36:VAL:HG22	2.46	0.45
1:C:629:LEU:HD12	1:C:629:LEU:H	1.82	0.45
2:F:69:TRP:HH2	2:F:255:VAL:HG23	1.80	0.45
3:H:79:SER:OG	3:H:95:LEU:O	2.35	0.45
1:B:611:ASN:O	1:B:615:SER:N	2.41	0.45
2:F:34:LEU:HD13	2:F:498:PRO:HB2	1.97	0.45
5:N:4:LEU:HB2	5:N:119:GLY:HA2	1.97	0.45
4:J:35:TRP:CD1	4:J:48:ILE:HB	2.52	0.44
4:K:35:TRP:CD1	4:K:48:ILE:HB	2.52	0.44
4:L:46:LEU:HD11	5:O:114:PHE:HB2	2.00	0.44
5:O:39:GLN:HB3	5:O:93:VAL:HB	1.98	0.44
1:C:650:GLN:NE2	2:F:505:VAL:HA	2.32	0.44
2:E:105:HIS:HB2	2:E:479:TRP:CG	2.52	0.44
2:F:42:VAL:HB	2:F:44:VAL:HG23	2.00	0.44
1:B:532:ALA:H	1:B:625:ASN:N	2.14	0.44
6:P:53:TRP:CZ2	6:P:54:ARG:HD2	2.52	0.44
6:T:5:VAL:O	6:T:23:LYS:N	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:55:TRP:HB3	8:V:2:NAG:C4	2.38	0.44
1:A:652:GLN:O	1:A:656:ASN:HB2	2.17	0.44
1:C:537:LEU:HD22	2:F:42:VAL:HG12	1.99	0.44
1:C:604:CYS:HB3	2:F:37:THR:HA	1.99	0.44
1:C:630:GLN:HE22	6:P:109:SER:N	2.14	0.44
2:D:92:GLU:OE1	6:T:105:TYR:HA	2.18	0.44
3:H:54:ARG:HB3	3:H:71:ILE:HG23	2.00	0.44
6:T:70:SER:HA	8:V:4:MAN:C1	2.47	0.44
1:A:587:LEU:HD11	1:C:587:LEU:HD13	2.00	0.44
2:D:59:LYS:HD3	2:D:59:LYS:HA	1.81	0.44
6:T:69:ILE:O	8:V:4:MAN:O2	2.33	0.44
1:A:534:SER:OG	2:E:497:ALA:HB2	2.18	0.44
2:D:92:GLU:OE2	6:T:31:GLY:O	2.35	0.44
2:D:121:LYS:HB3	2:D:201:ILE:HB	1.99	0.44
2:E:65:LYS:HD2	2:E:71:THR:O	2.18	0.44
2:E:266:ALA:N	2:E:288:PHE:O	2.50	0.44
2:F:65:LYS:HD2	2:F:71:THR:O	2.18	0.44
5:M:87:ARG:N	5:M:90:ASP:OD2	2.48	0.44
1:A:544:LEU:HD21	2:E:40:TYR:CD2	2.53	0.44
1:B:652:GLN:O	1:B:656:ASN:HB2	2.18	0.44
2:D:266:ALA:N	2:D:288:PHE:O	2.50	0.44
6:R:34:ALA:HB1	6:R:53:TRP:HA	2.00	0.44
6:R:52:ILE:CD1	6:R:69:ILE:HG22	2.48	0.44
1:C:638:TYR:OH	7:Q:31:GLY:HA3	2.17	0.44
2:D:65:LYS:HD2	2:D:71:THR:O	2.18	0.44
2:D:70:ALA:HB2	2:D:215:ILE:HD11	2.00	0.44
4:L:35:TRP:CD1	4:L:48:ILE:HB	2.52	0.44
4:L:36:TYR:HB3	4:L:44:PRO:HB3	2.00	0.44
2:D:69:TRP:HB3	2:D:213:ILE:HG12	2.00	0.43
2:E:420:ILE:HB	5:N:108:GLU:HB2	2.00	0.43
2:F:70:ALA:HB2	2:F:215:ILE:HD11	2.00	0.43
3:G:13:GLU:OE2	3:G:58:ARG:NH1	2.38	0.43
4:L:95:PRO:HD2	4:L:97:ARG:HH12	1.81	0.43
5:N:87:ARG:N	5:N:90:ASP:OD2	2.48	0.43
1:A:634:GLU:OE2	6:R:110:GLY:HA2	2.18	0.43
2:D:90:THR:CB	6:T:54:ARG:NH2	2.59	0.43
2:D:277:ILE:H	6:T:75:THR:HG23	1.82	0.43
2:E:50:THR:OG1	2:E:51:THR:N	2.48	0.43
3:I:54:ARG:HB3	3:I:71:ILE:HG23	2.00	0.43
6:P:100:THR:HG21	6:P:119:PHE:HA	2.00	0.43
2:E:42:VAL:HB	2:E:44:VAL:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:120:VAL:HG21	5:O:55:LEU:HD21	2.00	0.43
2:F:503:ARG:HE	2:F:503:ARG:HB3	1.49	0.43
6:T:55:TRP:CG	8:V:2:NAG:C2	2.98	0.43
7:U:38:GLN:HA	7:U:87:PHE:HA	2.01	0.43
1:A:616:ASN:ND2	7:S:28:SER:O	2.46	0.43
1:B:537:LEU:HD22	2:D:42:VAL:HG12	1.99	0.43
7:S:38:GLN:HA	7:S:87:PHE:HA	2.01	0.43
2:F:257:THR:OG1	2:F:375:SER:N	2.52	0.43
3:H:58:ARG:HH11	3:H:61:LEU:HD12	1.84	0.43
4:K:36:TYR:HB3	4:K:44:PRO:HB3	2.00	0.43
1:C:574:LYS:HE2	2:F:75:VAL:HG22	1.99	0.43
2:D:42:VAL:HB	2:D:44:VAL:HG23	2.00	0.43
2:E:346:VAL:HG11	2:E:395:TRP:CG	2.54	0.43
6:P:34:ALA:HB1	6:P:53:TRP:HA	2.00	0.43
1:B:658:GLN:HE22	1:C:600:GLY:C	2.22	0.43
2:E:121:LYS:HB3	2:E:201:ILE:HB	1.99	0.43
2:E:362:ALA:HB3	2:E:469:ARG:HG2	2.01	0.43
4:K:61:ARG:NE	4:K:82:ASP:OD1	2.43	0.43
6:T:55:TRP:CZ2	6:T:73:ASP:HB2	2.53	0.43
6:T:100:THR:HG21	6:T:119:PHE:HA	2.00	0.43
1:B:630:GLN:O	1:B:630:GLN:NE2	2.52	0.43
1:C:643:TYR:CE1	2:F:38:VAL:HG22	2.54	0.43
2:E:270:VAL:HG21	2:E:345:VAL:HG22	2.01	0.43
2:E:384:TYR:HB2	2:E:419:ARG:HB3	2.01	0.43
3:G:54:ARG:HB3	3:G:71:ILE:HG23	2.00	0.43
3:G:58:ARG:HH11	3:G:61:LEU:HD12	1.84	0.43
4:J:36:TYR:HB2	4:J:87:TYR:HB2	2.01	0.43
2:D:343:GLY:HA2	2:D:346:VAL:HG12	2.01	0.43
2:D:457:ASP:HA	3:G:48:PRO:HB2	2.01	0.43
2:D:457:ASP:O	3:G:34:ILE:HG23	2.19	0.43
3:G:74:LEU:HD11	3:G:95:LEU:HD21	2.01	0.43
3:H:50:LYS:O	3:H:54:ARG:NH2	2.52	0.43
4:L:36:TYR:HB2	4:L:87:TYR:HB2	2.01	0.43
1:A:643:TYR:HE2	2:E:494:LEU:HB3	1.84	0.42
7:Q:38:GLN:HA	7:Q:87:PHE:HA	2.01	0.42
6:T:34:ALA:HB1	6:T:53:TRP:HA	2.02	0.42
1:A:633:LYS:HD3	6:R:108:TRP:HB3	2.00	0.42
1:C:604:CYS:H	2:F:37:THR:HG22	1.81	0.42
2:D:369:LEU:O	2:D:373:THR:OG1	2.23	0.42
2:E:257:THR:OG1	2:E:375:SER:N	2.52	0.42
2:F:60:ALA:CA	2:F:65:LYS:HD3	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:69:TRP:HB3	2:F:213:ILE:HG12	2.00	0.42
4:J:36:TYR:HB3	4:J:44:PRO:HB3	2.00	0.42
6:P:36:ASN:HD22	6:P:119:PHE:HE1	1.66	0.42
6:P:55:TRP:CZ2	6:P:73:ASP:HB2	2.54	0.42
6:R:36:ASN:HD22	6:R:119:PHE:HE1	1.66	0.42
1:C:630:GLN:NE2	6:P:110:GLY:N	2.67	0.42
2:D:257:THR:OG1	2:D:375:SER:N	2.52	0.42
2:D:346:VAL:HG11	2:D:395:TRP:CG	2.54	0.42
5:M:12:LYS:O	5:M:127:SER:N	2.39	0.42
6:T:73:ASP:OD2	8:V:1:NAG:C3	2.65	0.42
6:T:113:HIS:CD2	7:U:93:ASP:O	2.72	0.42
1:A:522:PHE:CE1	2:E:43:PRO:HB3	2.55	0.42
1:A:611:ASN:O	1:A:615:SER:N	2.41	0.42
1:B:610:TRP:CD1	2:D:34:LEU:CB	2.96	0.42
2:E:225:ILE:HG22	2:E:486:TYR:CD1	2.55	0.42
2:E:343:GLY:HA2	2:E:346:VAL:HG12	2.01	0.42
2:F:343:GLY:HA2	2:F:346:VAL:HG12	2.01	0.42
3:G:79:SER:OG	3:G:95:LEU:O	2.35	0.42
3:I:58:ARG:HH11	3:I:61:LEU:HD12	1.85	0.42
4:L:93:ASN:O	4:L:98:TYR:OH	2.24	0.42
2:E:69:TRP:HB3	2:E:213:ILE:HG12	2.00	0.42
2:E:70:ALA:HB2	2:E:215:ILE:HD11	2.00	0.42
2:F:362:ALA:HB3	2:F:469:ARG:HG2	2.01	0.42
1:A:537:LEU:HD23	1:A:537:LEU:HA	1.90	0.42
1:A:610:TRP:HD1	2:E:34:LEU:HB2	1.84	0.42
1:B:610:TRP:CE3	1:B:614:TRP:HB3	2.54	0.42
1:B:610:TRP:CZ3	1:B:642:ILE:HD11	2.54	0.42
2:F:225:ILE:HG22	2:F:486:TYR:CD1	2.55	0.42
3:H:74:LEU:HD11	3:H:95:LEU:HD21	2.01	0.42
6:P:36:ASN:ND2	6:P:117:MET:H	2.18	0.42
7:U:7:SER:HB2	7:U:22:SER:HB3	2.02	0.42
1:C:662:ALA:HB1	2:E:501:CYS:O	2.20	0.42
2:F:346:VAL:HG11	2:F:395:TRP:CG	2.54	0.42
2:F:369:LEU:O	2:F:373:THR:OG1	2.23	0.42
7:Q:6:GLN:HA	7:Q:23:CYS:HA	2.02	0.42
7:Q:7:SER:HB2	7:Q:22:SER:HB3	2.02	0.42
6:T:53:TRP:CZ2	6:T:54:ARG:NE	2.88	0.42
1:A:658:GLN:C	2:D:501:CYS:SG	2.98	0.42
3:G:50:LYS:O	3:G:54:ARG:NH2	2.52	0.42
6:R:29:THR:HG23	6:R:32:LEU:H	1.85	0.42
6:T:36:ASN:HD22	6:T:119:PHE:HE1	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:6:GLN:HA	7:U:23:CYS:HA	2.02	0.42
1:B:661:LEU:HD13	1:B:663:LEU:HD12	2.02	0.42
2:D:362:ALA:HB3	2:D:469:ARG:HG2	2.01	0.42
2:F:34:LEU:HD23	2:F:500:ARG:HG3	2.01	0.42
2:F:90:THR:O	6:P:54:ARG:NH2	2.53	0.42
4:K:46:LEU:HD21	4:K:49:TYR:HB3	2.02	0.42
4:L:21:LEU:HD12	4:L:86:TYR:HB2	2.02	0.42
7:S:6:GLN:HA	7:S:23:CYS:HA	2.02	0.42
1:A:584:GLU:OE2	1:B:583:VAL:HG11	2.19	0.41
1:B:619:LEU:HG	2:D:500:ARG:NH2	2.35	0.41
1:B:630:GLN:HE22	6:T:109:SER:N	2.17	0.41
2:D:225:ILE:HG22	2:D:486:TYR:CD1	2.55	0.41
2:D:384:TYR:HB2	2:D:419:ARG:HB3	2.01	0.41
2:E:67:ASN:O	2:E:67:ASN:CG	2.58	0.41
2:F:270:VAL:HG21	2:F:345:VAL:HG22	2.01	0.41
4:K:36:TYR:HB2	4:K:87:TYR:HB2	2.01	0.41
4:L:22:SER:OG	4:L:23:CYS:N	2.53	0.41
1:A:523:LEU:HD11	2:E:45:TRP:CZ3	2.55	0.41
3:I:50:LYS:O	3:I:54:ARG:NH2	2.52	0.41
4:J:46:LEU:HD21	4:J:49:TYR:HB3	2.02	0.41
7:Q:10:THR:HG22	7:Q:104:LYS:HB2	2.03	0.41
6:R:100:THR:HG21	6:R:119:PHE:HA	2.00	0.41
7:S:18:THR:HA	7:S:77:GLY:HA2	2.02	0.41
6:T:29:THR:HG23	6:T:32:LEU:H	1.85	0.41
7:U:10:THR:HG22	7:U:104:LYS:HB2	2.02	0.41
2:F:67:ASN:O	2:F:67:ASN:CG	2.59	0.41
6:R:36:ASN:ND2	6:R:117:MET:H	2.18	0.41
6:T:52:ILE:HD12	6:T:69:ILE:HG22	2.01	0.41
6:T:72:VAL:CG2	8:V:4:MAN:O6	2.67	0.41
1:B:605:CYS:HB3	2:D:35:TRP:HE3	1.84	0.41
2:E:259:LEU:H	2:E:374:HIS:CE1	2.39	0.41
6:R:76:GLY:O	9:Z:1:NAG:O6	2.28	0.41
1:C:529:THR:HG22	1:C:626:MET:HG3	2.02	0.41
2:D:36:VAL:HB	2:D:496:VAL:HB	2.02	0.41
2:D:259:LEU:H	2:D:374:HIS:CE1	2.39	0.41
2:D:270:VAL:HG21	2:D:345:VAL:HG22	2.01	0.41
2:E:214:PRO:HB3	2:E:252:LYS:HG2	2.03	0.41
4:L:46:LEU:HD21	4:L:49:TYR:HB3	2.02	0.41
5:N:50:ARG:O	5:N:59:HIS:ND1	2.42	0.41
6:P:29:THR:HG23	6:P:32:LEU:H	1.85	0.41
7:S:51:ARG:HD2	7:S:51:ARG:HA	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:70:SER:CA	8:V:4:MAN:C2	2.82	0.41
1:B:529:THR:HG22	1:B:626:MET:HG3	2.02	0.41
1:C:639:THR:HB	2:F:496:VAL:HG13	2.02	0.41
2:D:90:THR:O	6:T:107:LYS:NZ	2.54	0.41
6:R:27:VAL:HG12	6:R:80:PRO:HG2	2.03	0.41
2:D:90:THR:HG21	6:T:54:ARG:NH1	2.33	0.41
2:F:36:VAL:HG12	2:F:498:PRO:HA	2.02	0.41
5:M:38:ARG:HD3	5:M:46:GLU:HB2	2.03	0.41
7:Q:51:ARG:HD2	7:Q:51:ARG:HA	1.82	0.41
6:T:36:ASN:ND2	6:T:117:MET:H	2.18	0.41
7:U:18:THR:HA	7:U:77:GLY:HA2	2.02	0.41
1:A:531:GLY:HA3	1:A:623:TRP:HA	2.02	0.41
1:A:532:ALA:CB	1:A:625:ASN:HA	2.51	0.41
1:B:642:ILE:HD13	2:D:36:VAL:HG11	2.02	0.41
2:F:36:VAL:HB	2:F:496:VAL:HB	2.03	0.41
4:J:22:SER:OG	4:J:23:CYS:N	2.53	0.41
1:A:529:THR:HG22	1:A:626:MET:HG3	2.02	0.41
1:A:541:ALA:HB3	1:A:602:LEU:HD11	2.03	0.41
1:A:608:VAL:H	1:A:646:LEU:HD23	1.86	0.41
1:C:608:VAL:H	1:C:646:LEU:HD23	1.86	0.41
2:D:120:VAL:HG21	5:M:55:LEU:HD21	2.03	0.41
2:D:338:TRP:CE2	2:D:390:LEU:HB3	2.56	0.41
2:F:214:PRO:HB3	2:F:252:LYS:HG2	2.03	0.41
2:F:384:TYR:HB2	2:F:419:ARG:HB3	2.02	0.41
4:K:21:LEU:HD12	4:K:86:TYR:HB2	2.02	0.41
4:K:22:SER:OG	4:K:23:CYS:N	2.54	0.41
4:K:29:VAL:HA	4:K:92:ASN:HD22	1.86	0.41
5:N:52:ILE:HG21	5:N:55:LEU:HD13	2.03	0.41
5:N:91:THR:HG23	5:N:125:THR:HA	2.03	0.41
5:O:91:THR:HG23	5:O:125:THR:HA	2.03	0.41
5:O:101:GLU:HB3	5:O:109:TYR:CE1	2.56	0.41
7:S:7:SER:HB2	7:S:22:SER:HB3	2.02	0.41
6:T:46:LEU:HD13	7:U:99:PHE:HE2	1.86	0.41
6:T:60:SER:O	6:T:64:ARG:N	2.54	0.41
6:T:116:VAL:HG12	7:U:92:TYR:HB2	2.03	0.41
6:T:119:PHE:O	7:U:37:TYR:HE1	2.03	0.41
1:C:531:GLY:HA3	1:C:623:TRP:HA	2.02	0.41
4:J:21:LEU:HD12	4:J:86:TYR:HB2	2.02	0.41
4:L:29:VAL:HA	4:L:92:ASN:HD22	1.86	0.41
5:N:101:GLU:HB3	5:N:109:TYR:CE1	2.56	0.41
1:C:532:ALA:CB	1:C:625:ASN:HA	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:643:TYR:HD1	1:C:643:TYR:HA	1.73	0.40
2:E:36:VAL:HB	2:E:496:VAL:HB	2.02	0.40
2:F:46:LYS:N	2:F:490:LYS:O	2.50	0.40
4:J:29:VAL:HG12	4:J:32:ASP:H	1.87	0.40
4:K:29:VAL:HG13	4:K:92:ASN:HB2	2.03	0.40
4:L:20:THR:C	4:L:21:LEU:HD22	2.42	0.40
5:M:91:THR:HG23	5:M:125:THR:HA	2.03	0.40
6:P:60:SER:O	6:P:64:ARG:N	2.54	0.40
7:S:10:THR:HG22	7:S:104:LYS:HB2	2.02	0.40
1:B:531:GLY:HA3	1:B:623:TRP:HA	2.02	0.40
2:D:258:GLN:NE2	2:D:371:VAL:O	2.55	0.40
2:F:59:LYS:HD3	2:F:59:LYS:HA	1.81	0.40
2:F:338:TRP:CE2	2:F:390:LEU:HB3	2.56	0.40
2:F:422:GLN:HG3	5:O:109:TYR:H	1.86	0.40
5:O:52:ILE:HG21	5:O:55:LEU:HD13	2.03	0.40
6:R:60:SER:O	6:R:64:ARG:N	2.54	0.40
1:B:544:LEU:HD21	2:D:40:TYR:HE2	1.84	0.40
2:D:34:LEU:HD23	2:D:500:ARG:HG3	2.04	0.40
2:D:116:LEU:HD21	2:D:208:VAL:HG12	2.04	0.40
2:F:258:GLN:NE2	2:F:371:VAL:O	2.55	0.40
1:A:523:LEU:HD21	2:E:45:TRP:CZ3	2.57	0.40
1:A:638:TYR:CZ	7:S:31:GLY:HA3	2.56	0.40
1:C:523:LEU:HD21	2:F:45:TRP:HZ3	1.86	0.40
2:D:67:ASN:O	2:D:67:ASN:CG	2.58	0.40
2:E:258:GLN:NE2	2:E:371:VAL:O	2.55	0.40
2:E:338:TRP:CE2	2:E:390:LEU:HB3	2.56	0.40
2:F:259:LEU:H	2:F:374:HIS:CE1	2.39	0.40
5:M:101:GLU:HB3	5:M:109:TYR:CE1	2.56	0.40
5:O:33:SER:HA	5:O:52:ILE:HA	2.03	0.40
5:O:83:LEU:HB3	5:O:86:LEU:HD21	2.04	0.40
1:B:523:LEU:HD12	2:D:86:LEU:HD22	2.03	0.40
1:B:596:TRP:CH2	2:D:494:LEU:HD11	2.55	0.40
1:C:643:TYR:OH	2:F:38:VAL:HA	2.21	0.40
3:I:40:GLN:HG2	3:I:45:THR:HG21	2.02	0.40
4:J:29:VAL:HA	4:J:92:ASN:HD22	1.86	0.40
5:O:60:TYR:OH	5:O:70:ILE:N	2.55	0.40
6:P:48:TYR:HB3	7:Q:96:PRO:HB2	2.04	0.40
6:R:52:ILE:HB	6:R:69:ILE:CG2	2.52	0.40
7:S:46:ARG:HH12	7:S:59:VAL:HG22	1.87	0.40
6:T:16:SER:O	6:T:89:LEU:N	2.45	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	120/153 (78%)	103 (86%)	17 (14%)	0	100	100
1	B	119/153 (78%)	102 (86%)	16 (13%)	1 (1%)	19	60
1	C	119/153 (78%)	99 (83%)	19 (16%)	1 (1%)	19	60
2	D	356/481 (74%)	322 (90%)	34 (10%)	0	100	100
2	E	356/481 (74%)	322 (90%)	34 (10%)	0	100	100
2	F	356/481 (74%)	323 (91%)	33 (9%)	0	100	100
3	G	96/192 (50%)	88 (92%)	8 (8%)	0	100	100
3	H	96/192 (50%)	88 (92%)	8 (8%)	0	100	100
3	I	95/192 (50%)	88 (93%)	7 (7%)	0	100	100
4	J	103/214 (48%)	97 (94%)	6 (6%)	0	100	100
4	K	103/214 (48%)	97 (94%)	6 (6%)	0	100	100
4	L	103/214 (48%)	97 (94%)	6 (6%)	0	100	100
5	M	125/229 (55%)	120 (96%)	5 (4%)	0	100	100
5	N	125/229 (55%)	120 (96%)	5 (4%)	0	100	100
5	O	125/229 (55%)	120 (96%)	5 (4%)	0	100	100
6	P	129/244 (53%)	120 (93%)	9 (7%)	0	100	100
6	R	129/244 (53%)	120 (93%)	9 (7%)	0	100	100
6	T	129/244 (53%)	120 (93%)	9 (7%)	0	100	100
7	Q	105/215 (49%)	99 (94%)	6 (6%)	0	100	100
7	S	105/215 (49%)	99 (94%)	6 (6%)	0	100	100
7	U	105/215 (49%)	99 (94%)	6 (6%)	0	100	100
All	All	3099/5184 (60%)	2843 (92%)	254 (8%)	2 (0%)	54	86

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	663	LEU
1	C	663	LEU

### 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	106/129 (82%)	106 (100%)	0	100	100
1	B	105/129 (81%)	105 (100%)	0	100	100
1	C	105/129 (81%)	105 (100%)	0	100	100
2	D	323/428 (76%)	323 (100%)	0	100	100
2	E	323/428 (76%)	323 (100%)	0	100	100
2	F	323/428 (76%)	323 (100%)	0	100	100
3	G	90/173 (52%)	90 (100%)	0	100	100
3	H	90/173 (52%)	90 (100%)	0	100	100
3	I	89/173 (51%)	89 (100%)	0	100	100
4	J	88/184 (48%)	88 (100%)	0	100	100
4	K	88/184 (48%)	88 (100%)	0	100	100
4	L	88/184 (48%)	88 (100%)	0	100	100
5	M	105/193 (54%)	105 (100%)	0	100	100
5	N	105/193 (54%)	105 (100%)	0	100	100
5	O	105/193 (54%)	105 (100%)	0	100	100
6	P	106/210 (50%)	106 (100%)	0	100	100
6	R	106/210 (50%)	106 (100%)	0	100	100
6	T	106/210 (50%)	106 (100%)	0	100	100
7	Q	82/182 (45%)	82 (100%)	0	100	100
7	S	82/182 (45%)	82 (100%)	0	100	100
7	U	82/182 (45%)	82 (100%)	0	100	100
All	All	2697/4497 (60%)	2697 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	607	ASN
1	A	650	GLN
1	B	607	ASN
1	B	637	ASN
1	B	650	GLN
1	B	658	GLN
1	C	607	ASN
1	C	650	GLN
2	D	67	ASN
2	D	98	ASN
2	D	103	GLN
2	D	293	GLN
2	D	339	ASN
2	D	422	GLN
2	D	448	ASN
2	E	67	ASN
2	E	98	ASN
2	E	103	GLN
2	E	293	GLN
2	E	339	ASN
2	E	422	GLN
2	E	448	ASN
2	F	67	ASN
2	F	98	ASN
2	F	103	GLN
2	F	293	GLN
2	F	339	ASN
2	F	422	GLN
2	F	448	ASN
3	G	40	GLN
3	I	40	GLN
4	J	90	GLN
4	K	90	GLN
4	L	90	GLN
6	P	6	GLN
6	P	36	ASN
6	P	112	HIS
6	P	113	HIS
6	R	6	GLN

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Mol	Chain	Res	Type
6	R	36	ASN
6	R	113	HIS
6	T	6	GLN
6	T	36	ASN
6	T	113	HIS
7	U	80	GLN

### 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](#)

42 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
8	NAG	V	1	2,8	14,14,15	0.40	0	17,19,21	0.71	1 (5%)
8	NAG	V	2	8	14,14,15	0.47	0	17,19,21	0.48	0
8	BMA	V	3	8	11,11,12	0.70	0	15,15,17	0.92	0
8	MAN	V	4	8	11,11,12	1.23	2 (18%)	15,15,17	1.68	2 (13%)
9	NAG	W	1	9,2	14,14,15	0.55	0	17,19,21	1.04	1 (5%)
9	NAG	W	2	9	14,14,15	0.29	0	17,19,21	0.64	1 (5%)
9	BMA	W	3	9	11,11,12	0.66	0	15,15,17	0.86	0
9	MAN	W	4	9	11,11,12	0.80	0	15,15,17	0.92	1 (6%)
9	MAN	W	5	9	11,11,12	0.76	0	15,15,17	1.02	2 (13%)
9	NAG	X	1	9,2	14,14,15	0.58	0	17,19,21	1.03	1 (5%)
9	NAG	X	2	9	14,14,15	0.92	1 (7%)	17,19,21	2.06	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	BMA	X	3	9	11,11,12	0.73	0	15,15,17	0.69	0
9	MAN	X	4	9	11,11,12	0.76	0	15,15,17	0.95	2 (13%)
9	MAN	X	5	9	11,11,12	0.79	0	15,15,17	1.10	2 (13%)
8	NAG	Y	1	2,8	14,14,15	0.40	0	17,19,21	0.71	1 (5%)
8	NAG	Y	2	8	14,14,15	0.48	0	17,19,21	0.48	0
8	BMA	Y	3	8	11,11,12	0.72	0	15,15,17	0.92	0
8	MAN	Y	4	8	11,11,12	1.23	2 (18%)	15,15,17	1.68	2 (13%)
9	NAG	Z	1	9,2	14,14,15	0.55	0	17,19,21	1.04	1 (5%)
9	NAG	Z	2	9	14,14,15	0.28	0	17,19,21	0.64	1 (5%)
9	BMA	Z	3	9	11,11,12	0.67	0	15,15,17	0.86	0
9	MAN	Z	4	9	11,11,12	0.79	0	15,15,17	0.91	1 (6%)
9	MAN	Z	5	9	11,11,12	0.76	0	15,15,17	1.02	2 (13%)
9	NAG	a	1	9,2	14,14,15	0.58	0	17,19,21	1.03	1 (5%)
9	NAG	a	2	9	14,14,15	0.92	1 (7%)	17,19,21	2.06	3 (17%)
9	BMA	a	3	9	11,11,12	0.74	0	15,15,17	0.69	0
9	MAN	a	4	9	11,11,12	0.75	0	15,15,17	0.95	2 (13%)
9	MAN	a	5	9	11,11,12	0.78	0	15,15,17	1.10	2 (13%)
8	NAG	b	1	2,8	14,14,15	0.45	0	17,19,21	0.79	1 (5%)
8	NAG	b	2	8	14,14,15	0.42	0	17,19,21	0.46	0
8	BMA	b	3	8	11,11,12	0.80	0	15,15,17	0.85	0
8	MAN	b	4	8	11,11,12	1.41	2 (18%)	15,15,17	1.97	4 (26%)
9	NAG	c	1	9,2	14,14,15	0.65	0	17,19,21	0.81	1 (5%)
9	NAG	c	2	9	14,14,15	0.45	0	17,19,21	0.63	1 (5%)
9	BMA	c	3	9	11,11,12	0.77	0	15,15,17	0.94	1 (6%)
9	MAN	c	4	9	11,11,12	0.79	0	15,15,17	0.98	2 (13%)
9	MAN	c	5	9	11,11,12	0.75	0	15,15,17	0.99	2 (13%)
9	NAG	d	1	9,2	14,14,15	0.39	0	17,19,21	1.06	2 (11%)
9	NAG	d	2	9	14,14,15	0.81	1 (7%)	17,19,21	2.02	3 (17%)
9	BMA	d	3	9	11,11,12	0.74	0	15,15,17	0.77	0
9	MAN	d	4	9	11,11,12	0.75	0	15,15,17	0.97	2 (13%)
9	MAN	d	5	9	11,11,12	0.74	0	15,15,17	1.06	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	V	1	2,8	-	2/6/23/26	0/1/1/1
8	NAG	V	2	8	-	2/6/23/26	0/1/1/1
8	BMA	V	3	8	-	0/2/19/22	0/1/1/1
8	MAN	V	4	8	-	2/2/19/22	0/1/1/1
9	NAG	W	1	9,2	-	1/6/23/26	0/1/1/1
9	NAG	W	2	9	-	2/6/23/26	0/1/1/1
9	BMA	W	3	9	-	0/2/19/22	0/1/1/1
9	MAN	W	4	9	-	1/2/19/22	0/1/1/1
9	MAN	W	5	9	-	0/2/19/22	0/1/1/1
9	NAG	X	1	9,2	-	2/6/23/26	0/1/1/1
9	NAG	X	2	9	-	3/6/23/26	0/1/1/1
9	BMA	X	3	9	-	2/2/19/22	0/1/1/1
9	MAN	X	4	9	-	1/2/19/22	0/1/1/1
9	MAN	X	5	9	-	0/2/19/22	0/1/1/1
8	NAG	Y	1	2,8	-	2/6/23/26	0/1/1/1
8	NAG	Y	2	8	-	2/6/23/26	0/1/1/1
8	BMA	Y	3	8	-	0/2/19/22	0/1/1/1
8	MAN	Y	4	8	-	2/2/19/22	0/1/1/1
9	NAG	Z	1	9,2	-	1/6/23/26	0/1/1/1
9	NAG	Z	2	9	-	2/6/23/26	0/1/1/1
9	BMA	Z	3	9	-	0/2/19/22	0/1/1/1
9	MAN	Z	4	9	-	1/2/19/22	0/1/1/1
9	MAN	Z	5	9	-	0/2/19/22	0/1/1/1
9	NAG	a	1	9,2	-	2/6/23/26	0/1/1/1
9	NAG	a	2	9	-	3/6/23/26	0/1/1/1
9	BMA	a	3	9	-	2/2/19/22	0/1/1/1
9	MAN	a	4	9	-	1/2/19/22	0/1/1/1
9	MAN	a	5	9	-	0/2/19/22	0/1/1/1
8	NAG	b	1	2,8	-	0/6/23/26	0/1/1/1
8	NAG	b	2	8	-	2/6/23/26	0/1/1/1
8	BMA	b	3	8	-	1/2/19/22	0/1/1/1
8	MAN	b	4	8	-	0/2/19/22	0/1/1/1
9	NAG	c	1	9,2	-	2/6/23/26	0/1/1/1
9	NAG	c	2	9	-	1/6/23/26	0/1/1/1
9	BMA	c	3	9	-	0/2/19/22	0/1/1/1
9	MAN	c	4	9	-	1/2/19/22	0/1/1/1
9	MAN	c	5	9	-	0/2/19/22	0/1/1/1
9	NAG	d	1	9,2	-	2/6/23/26	0/1/1/1
9	NAG	d	2	9	-	5/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BMA	d	3	9	-	2/2/19/22	0/1/1/1
9	MAN	d	4	9	-	1/2/19/22	0/1/1/1
9	MAN	d	5	9	-	0/2/19/22	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	b	4	MAN	C1-C2	3.89	1.61	1.52
8	V	4	MAN	C1-C2	3.20	1.59	1.52
8	Y	4	MAN	C1-C2	3.19	1.59	1.52
9	X	2	NAG	C1-C2	2.99	1.56	1.52
9	a	2	NAG	C1-C2	2.98	1.56	1.52
9	d	2	NAG	C1-C2	2.49	1.56	1.52
8	Y	4	MAN	C2-C3	2.31	1.55	1.52
8	V	4	MAN	C2-C3	2.28	1.55	1.52
8	b	4	MAN	C2-C3	2.26	1.55	1.52

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	d	2	NAG	C2-N2-C7	6.79	132.57	122.90
9	a	2	NAG	C2-N2-C7	6.77	132.54	122.90
9	X	2	NAG	C2-N2-C7	6.74	132.50	122.90
8	b	4	MAN	C1-O5-C5	4.37	118.11	112.19
8	b	4	MAN	C1-C2-C3	4.20	114.83	109.67
8	V	4	MAN	C1-C2-C3	3.65	114.16	109.67
8	Y	4	MAN	C1-C2-C3	3.63	114.13	109.67
8	Y	4	MAN	C1-O5-C5	3.58	117.04	112.19
8	V	4	MAN	C1-O5-C5	3.56	117.02	112.19
9	X	1	NAG	C1-O5-C5	3.51	116.95	112.19
9	a	1	NAG	C1-O5-C5	3.51	116.95	112.19
9	d	2	NAG	C1-C2-N2	3.05	115.70	110.49
8	b	4	MAN	O5-C1-C2	2.88	115.22	110.77
9	X	2	NAG	C1-C2-N2	2.86	115.38	110.49
9	X	5	MAN	C1-O5-C5	2.86	116.07	112.19
8	b	1	NAG	C1-O5-C5	2.84	116.04	112.19
9	a	5	MAN	C1-O5-C5	2.84	116.04	112.19
9	a	2	NAG	C1-C2-N2	2.84	115.34	110.49
9	X	2	NAG	C1-O5-C5	2.83	116.03	112.19
9	a	2	NAG	C1-O5-C5	2.83	116.02	112.19
9	Z	1	NAG	C1-O5-C5	2.72	115.88	112.19
9	W	1	NAG	C1-O5-C5	2.70	115.85	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	d	5	MAN	C1-O5-C5	2.64	115.77	112.19
8	Y	1	NAG	C1-O5-C5	2.55	115.65	112.19
8	V	1	NAG	C1-O5-C5	2.54	115.64	112.19
9	Z	5	MAN	C1-O5-C5	2.50	115.58	112.19
9	W	5	MAN	C1-O5-C5	2.50	115.58	112.19
9	d	2	NAG	C1-O5-C5	2.44	115.49	112.19
9	c	5	MAN	C1-O5-C5	2.32	115.34	112.19
9	d	4	MAN	C1-O5-C5	2.29	115.29	112.19
9	d	4	MAN	O2-C2-C3	-2.25	105.63	110.14
9	W	4	MAN	O2-C2-C3	-2.24	105.66	110.14
9	Z	4	MAN	O2-C2-C3	-2.23	105.68	110.14
9	c	5	MAN	O2-C2-C3	-2.22	105.68	110.14
9	Z	5	MAN	O2-C2-C3	-2.22	105.69	110.14
9	X	4	MAN	C1-O5-C5	2.22	115.20	112.19
9	a	4	MAN	C1-O5-C5	2.21	115.19	112.19
9	c	3	BMA	C1-O5-C5	2.21	115.19	112.19
9	a	5	MAN	O2-C2-C3	-2.21	105.71	110.14
9	W	5	MAN	O2-C2-C3	-2.21	105.72	110.14
9	a	4	MAN	O2-C2-C3	-2.20	105.72	110.14
9	X	4	MAN	O2-C2-C3	-2.20	105.74	110.14
9	c	4	MAN	O2-C2-C3	-2.19	105.74	110.14
9	c	4	MAN	C1-O5-C5	2.19	115.16	112.19
9	X	5	MAN	O2-C2-C3	-2.19	105.76	110.14
9	d	5	MAN	O2-C2-C3	-2.18	105.78	110.14
9	Z	2	NAG	C1-O5-C5	2.17	115.13	112.19
9	W	2	NAG	C1-O5-C5	2.16	115.12	112.19
9	d	1	NAG	C1-O5-C5	2.14	115.09	112.19
9	c	1	NAG	C1-O5-C5	2.14	115.09	112.19
9	c	2	NAG	C1-O5-C5	2.08	115.01	112.19
8	b	4	MAN	O2-C2-C3	-2.05	106.03	110.14
9	d	1	NAG	O4-C4-C5	-2.04	104.24	109.30

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	V	1	NAG	O5-C5-C6-O6
8	Y	1	NAG	O5-C5-C6-O6
9	X	3	BMA	O5-C5-C6-O6
9	a	3	BMA	O5-C5-C6-O6
9	c	1	NAG	O5-C5-C6-O6
9	X	3	BMA	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
9	a	3	BMA	C4-C5-C6-O6
8	V	4	MAN	O5-C5-C6-O6
8	Y	4	MAN	O5-C5-C6-O6
8	b	2	NAG	O5-C5-C6-O6
8	V	1	NAG	C4-C5-C6-O6
8	Y	1	NAG	C4-C5-C6-O6
9	d	3	BMA	C4-C5-C6-O6
8	V	4	MAN	C4-C5-C6-O6
8	Y	4	MAN	C4-C5-C6-O6
9	X	1	NAG	C8-C7-N2-C2
9	X	1	NAG	O7-C7-N2-C2
9	X	2	NAG	C8-C7-N2-C2
9	X	2	NAG	O7-C7-N2-C2
9	a	1	NAG	C8-C7-N2-C2
9	a	1	NAG	O7-C7-N2-C2
9	a	2	NAG	C8-C7-N2-C2
9	a	2	NAG	O7-C7-N2-C2
9	d	1	NAG	C8-C7-N2-C2
9	d	1	NAG	O7-C7-N2-C2
9	d	2	NAG	C8-C7-N2-C2
9	d	2	NAG	O7-C7-N2-C2
8	b	2	NAG	C4-C5-C6-O6
9	c	1	NAG	C4-C5-C6-O6
8	V	2	NAG	O5-C5-C6-O6
8	Y	2	NAG	O5-C5-C6-O6
9	W	2	NAG	O5-C5-C6-O6
9	Z	2	NAG	O5-C5-C6-O6
9	d	2	NAG	O5-C5-C6-O6
9	d	3	BMA	O5-C5-C6-O6
9	W	2	NAG	C4-C5-C6-O6
9	Z	2	NAG	C4-C5-C6-O6
9	d	2	NAG	C4-C5-C6-O6
9	W	4	MAN	O5-C5-C6-O6
9	Z	4	MAN	O5-C5-C6-O6
9	c	4	MAN	O5-C5-C6-O6
8	V	2	NAG	C4-C5-C6-O6
8	Y	2	NAG	C4-C5-C6-O6
9	X	4	MAN	O5-C5-C6-O6
9	a	4	MAN	O5-C5-C6-O6
9	d	4	MAN	O5-C5-C6-O6
9	W	1	NAG	O5-C5-C6-O6
9	Z	1	NAG	O5-C5-C6-O6

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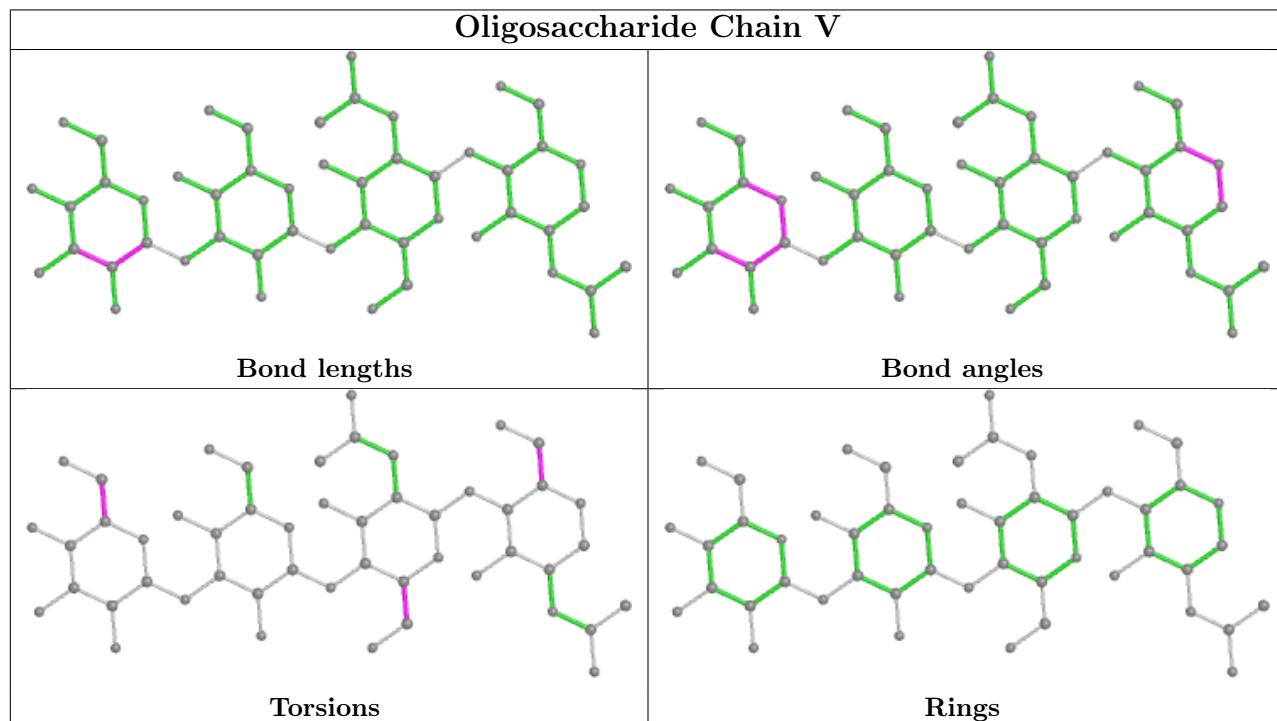
Mol	Chain	Res	Type	Atoms
9	X	2	NAG	C3-C2-N2-C7
9	a	2	NAG	C3-C2-N2-C7
9	d	2	NAG	C3-C2-N2-C7
9	c	2	NAG	O5-C5-C6-O6
8	b	3	BMA	C4-C5-C6-O6

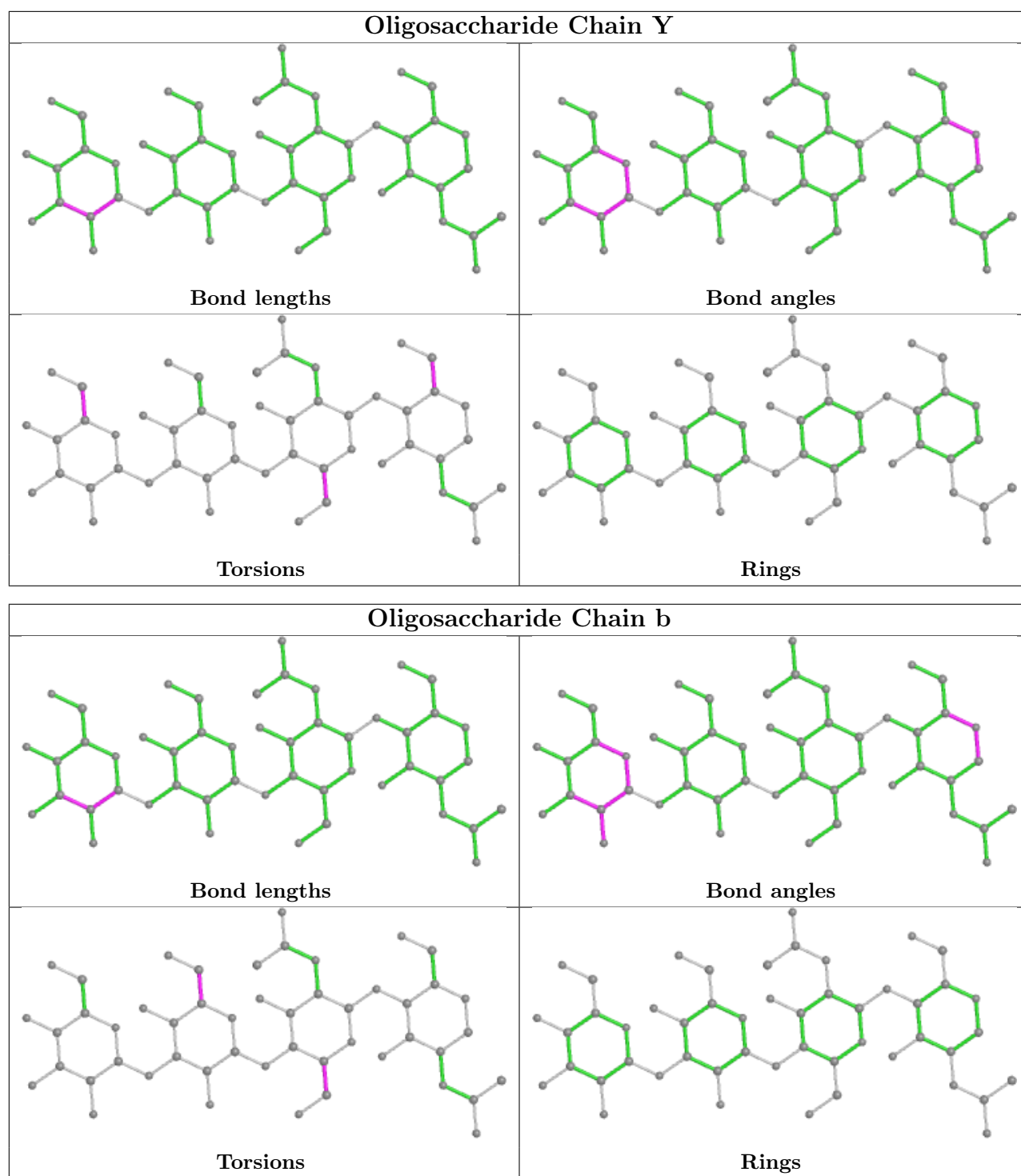
There are no ring outliers.

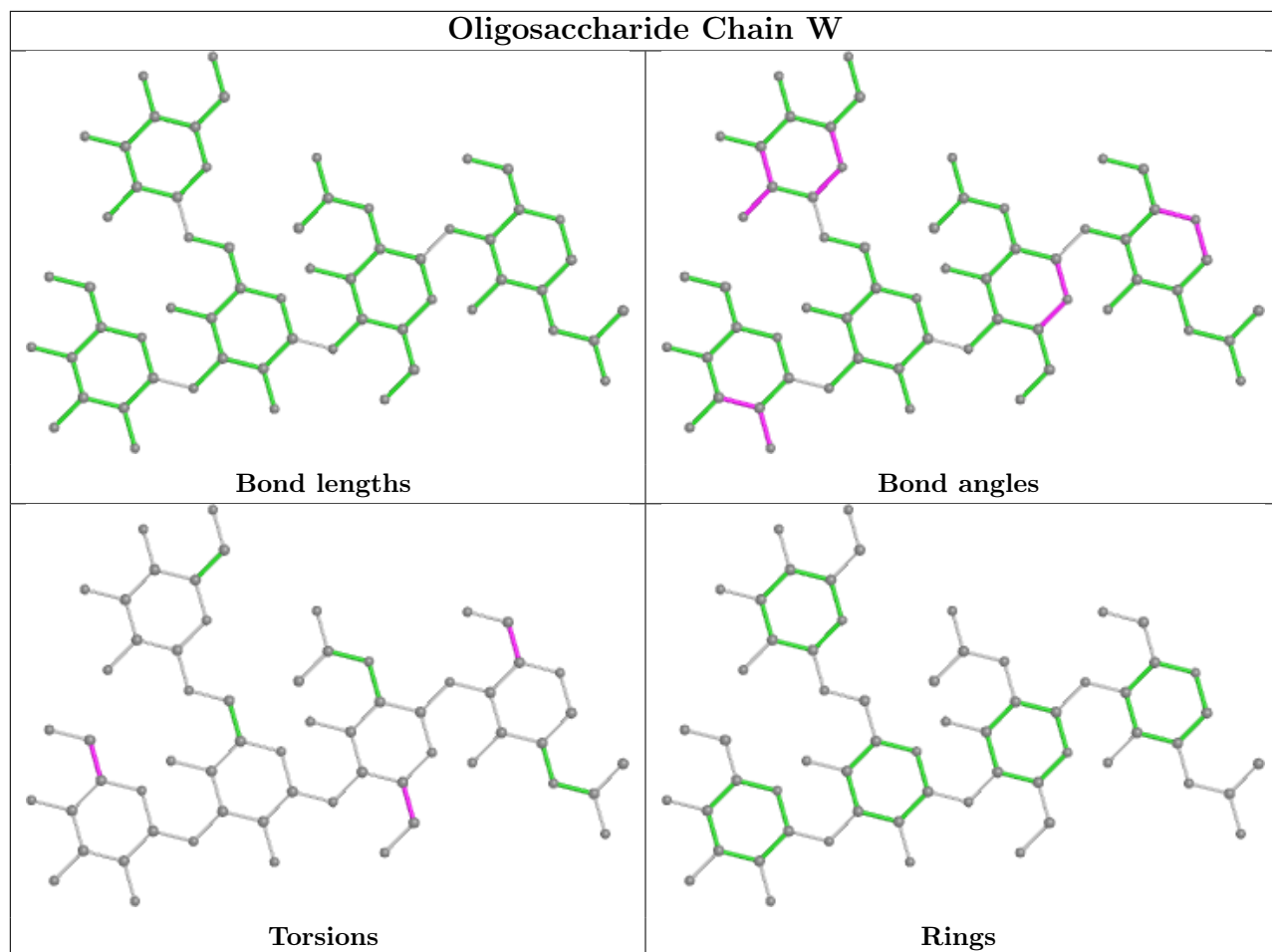
7 monomers are involved in 95 short contacts:

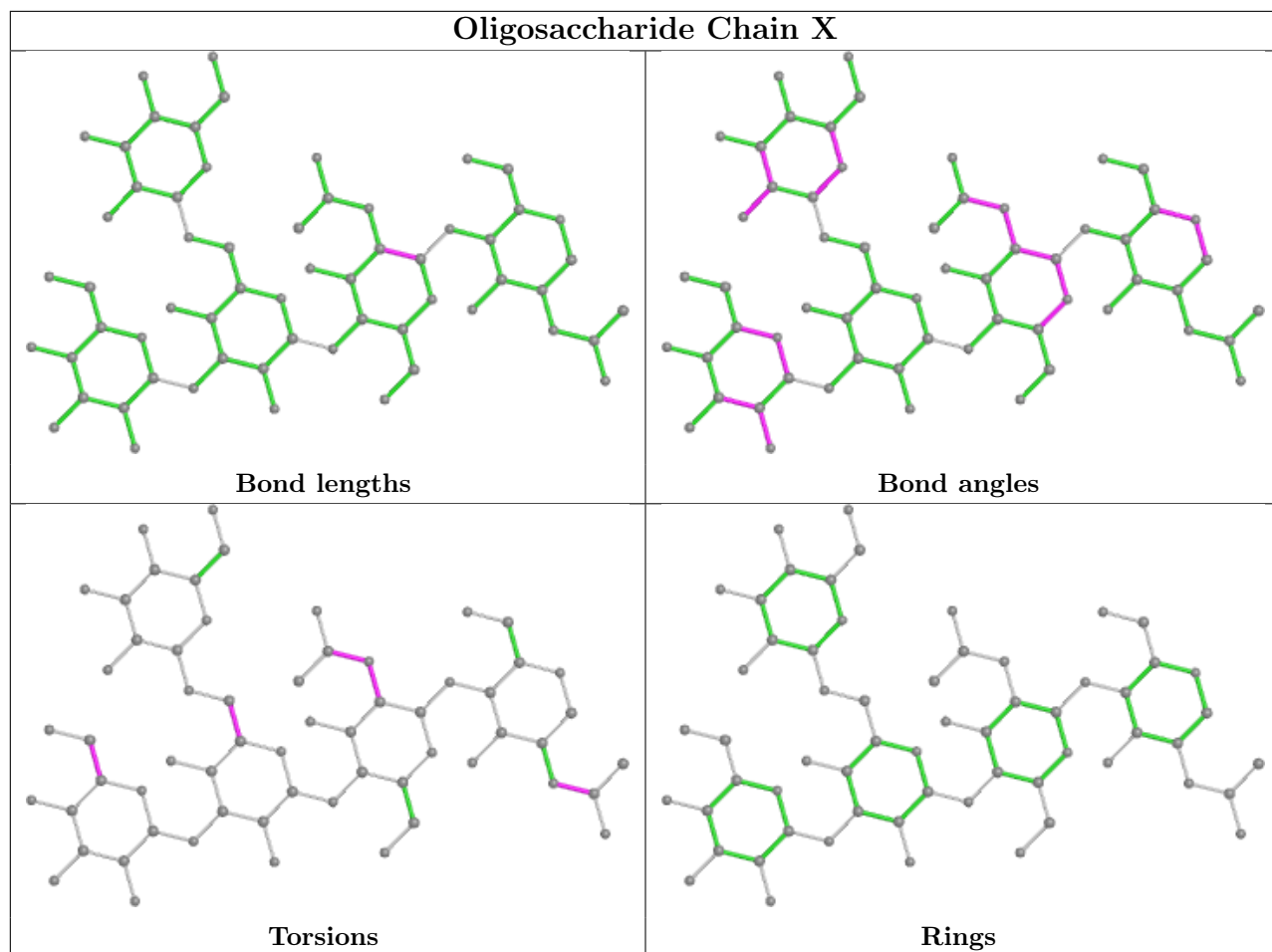
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	Z	1	NAG	2	0
8	V	4	MAN	28	0
8	V	2	NAG	42	0
8	V	3	BMA	10	0
9	W	1	NAG	1	0
8	V	1	NAG	8	0
9	W	2	NAG	4	0

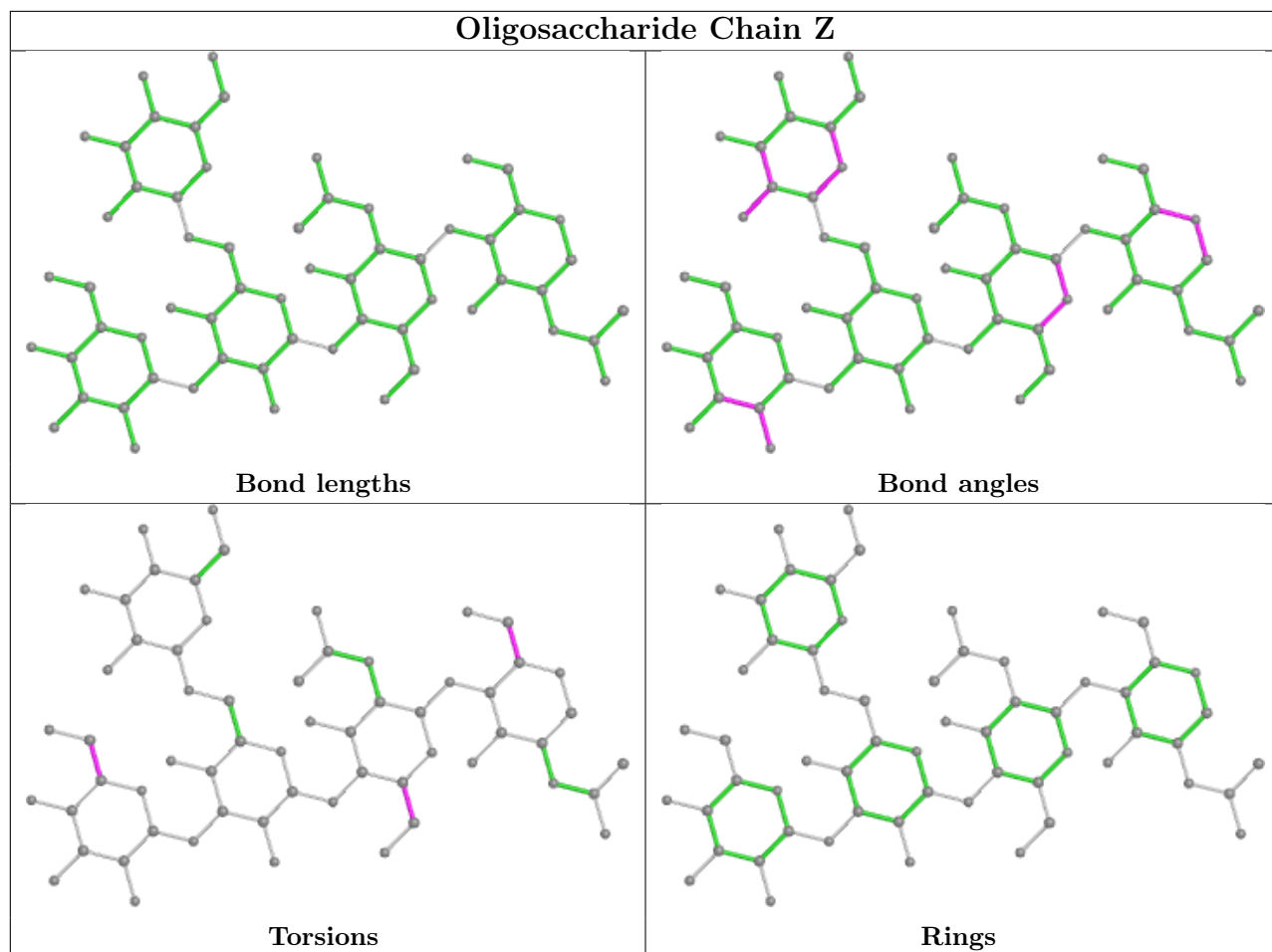
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

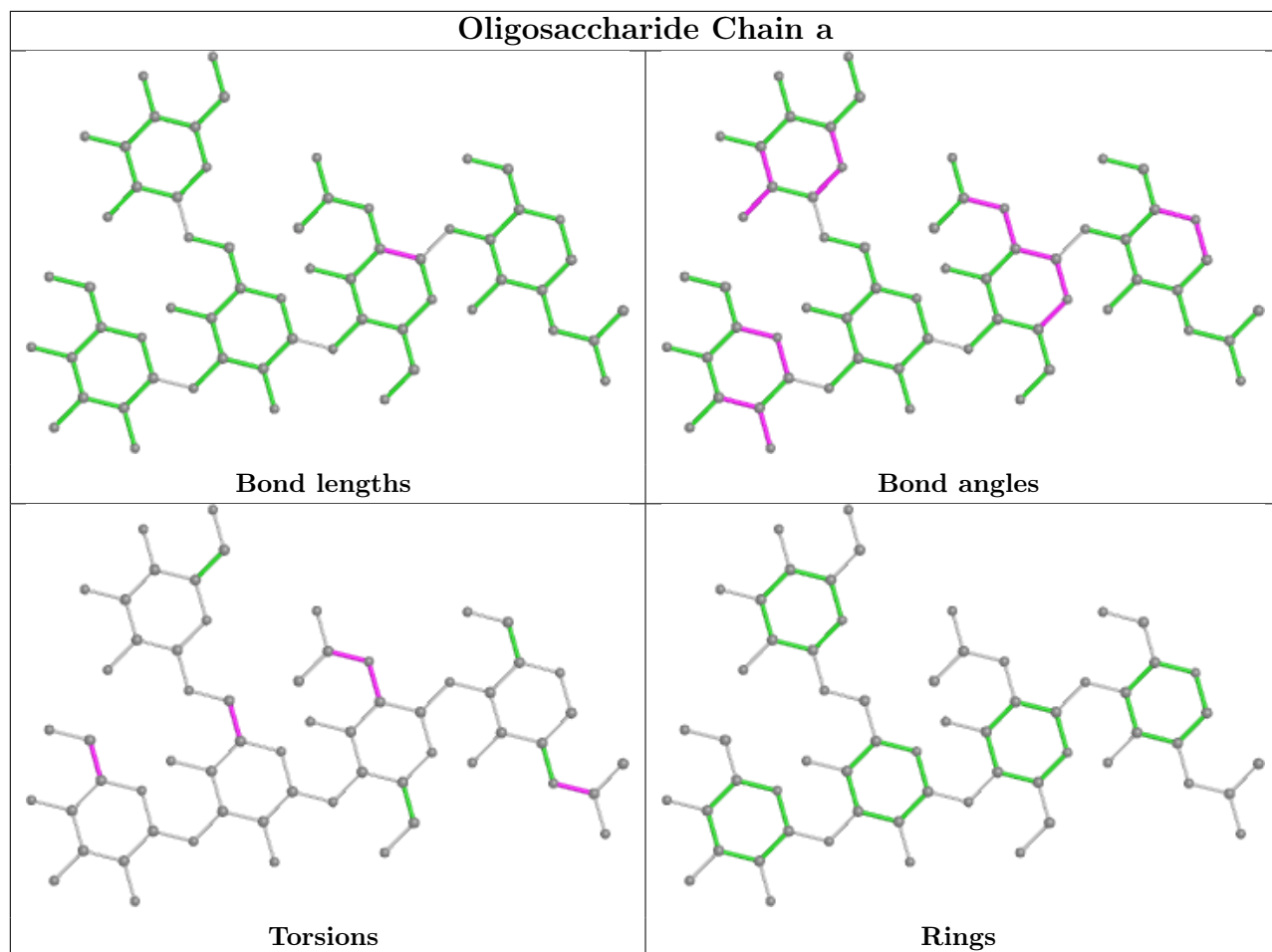




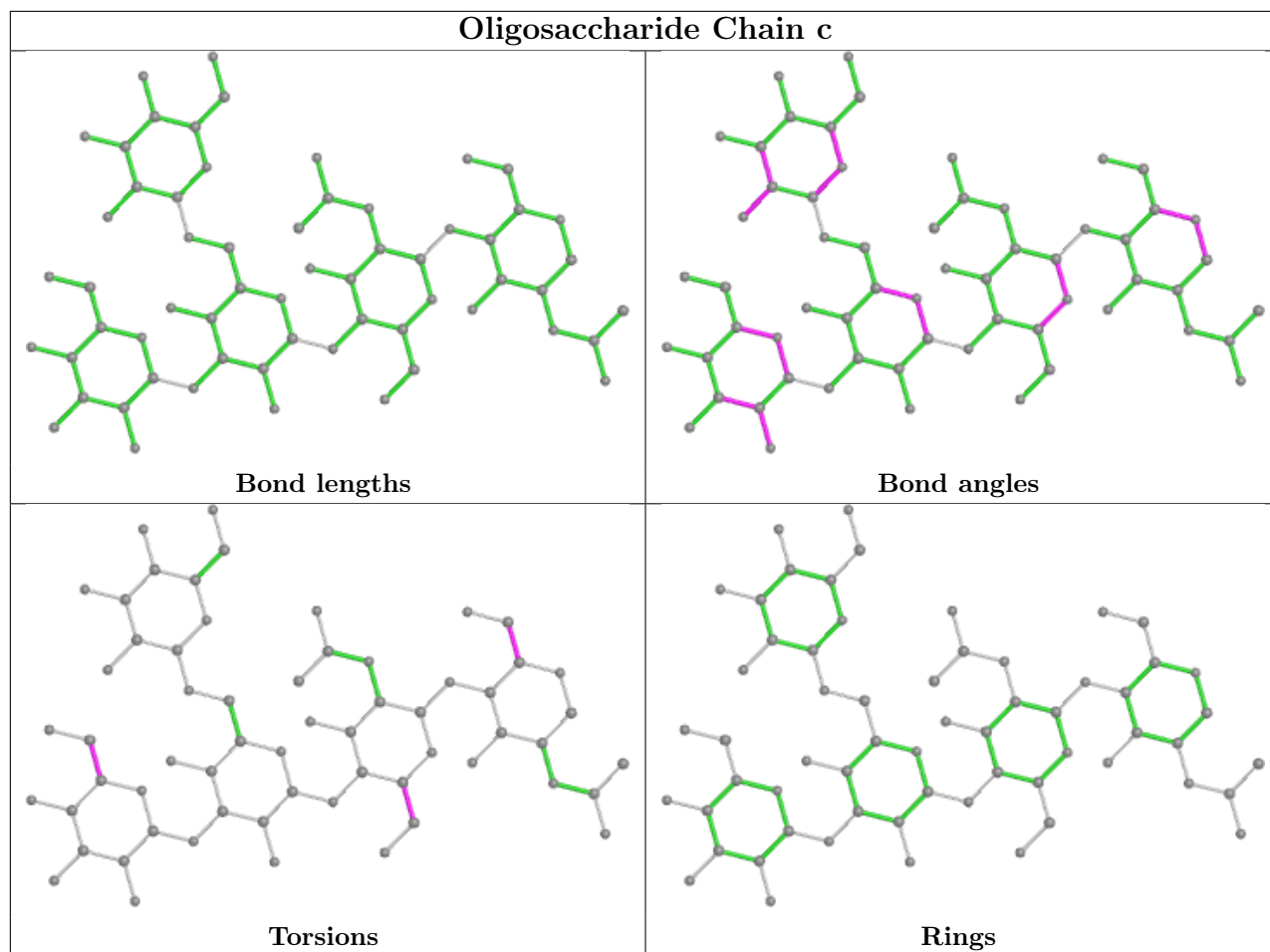


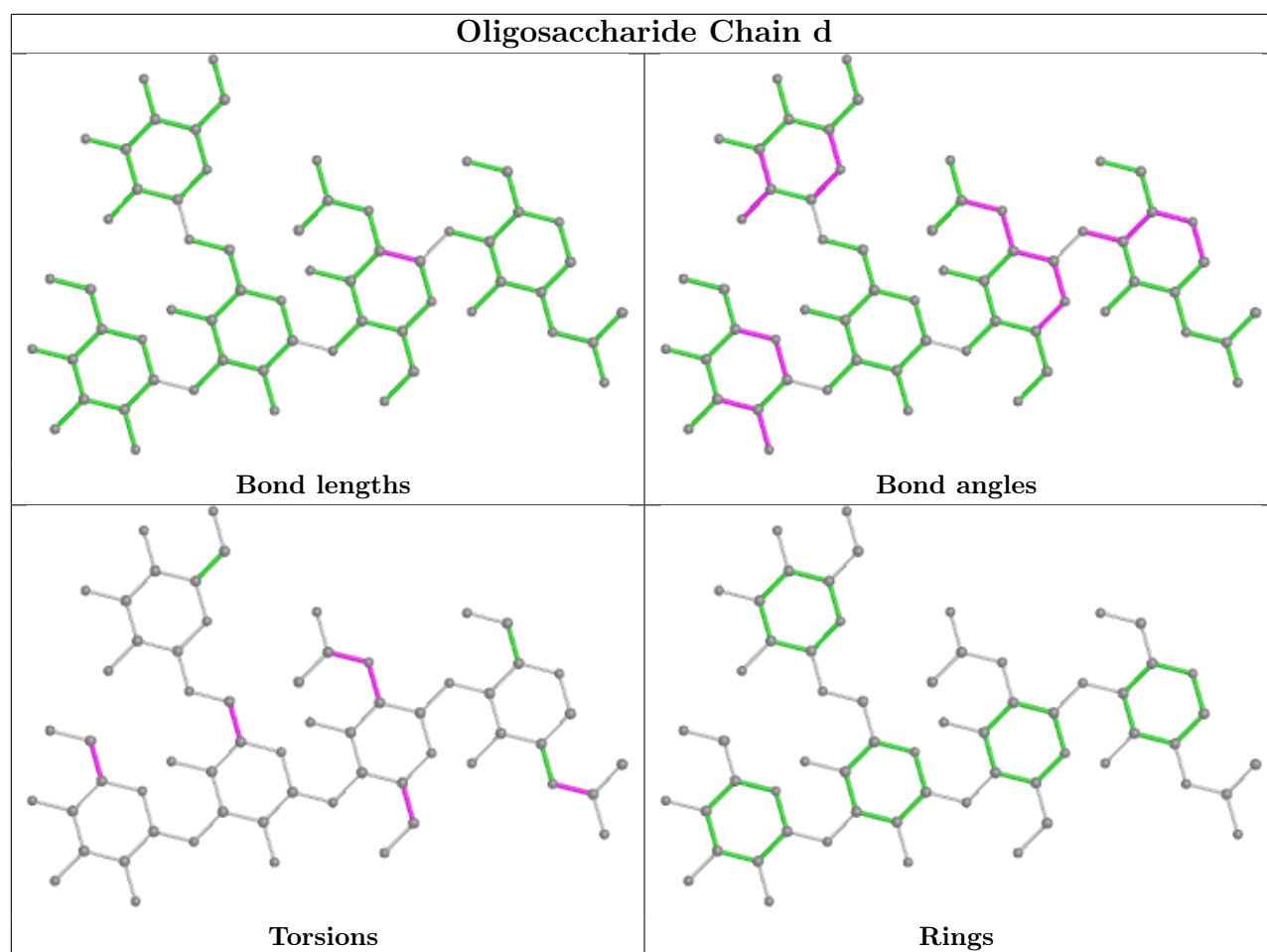












## 5.6 Ligand geometry [i](#)

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.

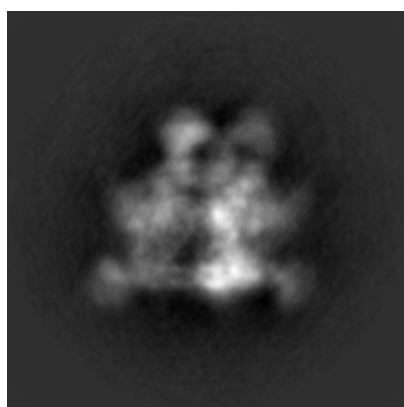
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8407. These allow visual inspection of the internal detail of the map and identification of artifacts.

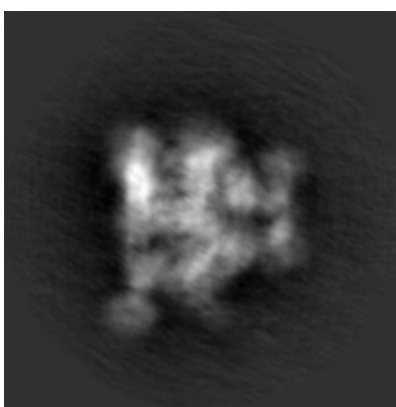
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

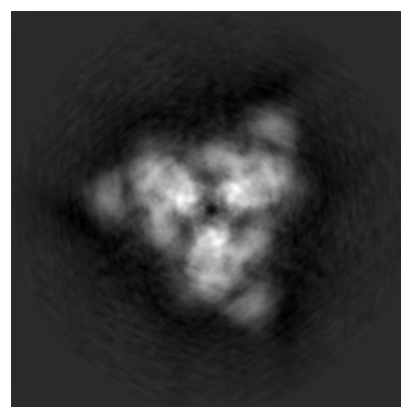
#### 6.1.1 Primary map



X



Y

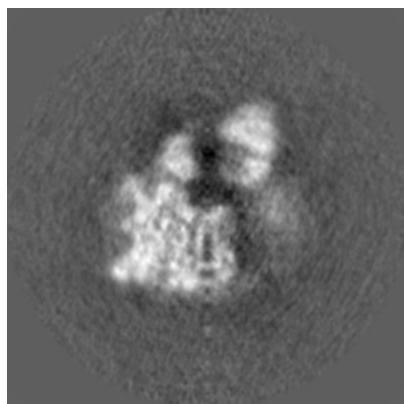


Z

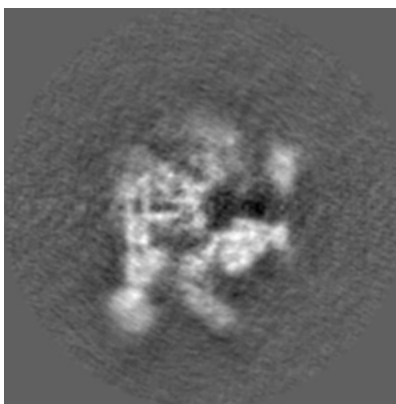
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

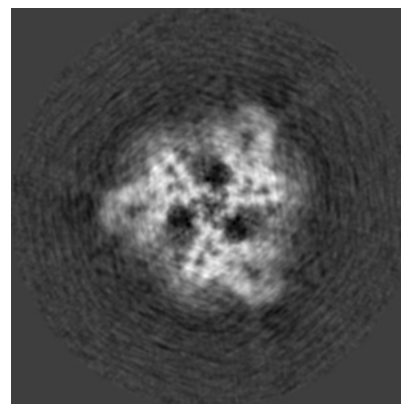
#### 6.2.1 Primary map



X Index: 195



Y Index: 195

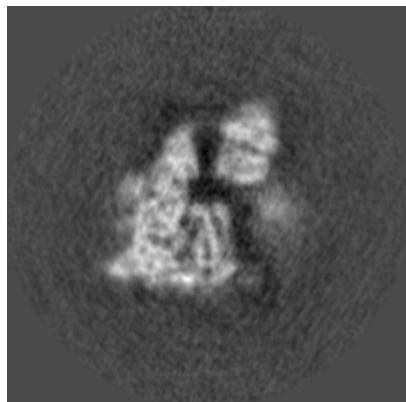


Z Index: 195

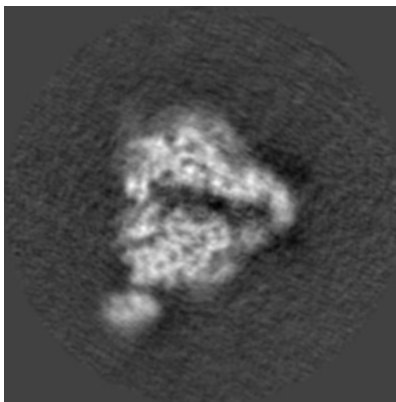
The images above show central slices of the map in three orthogonal directions.

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

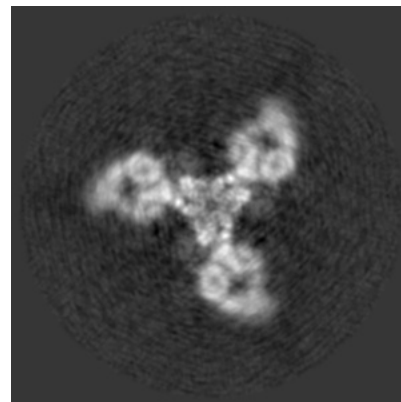
### 6.3.1 Primary map



X Index: 201



Y Index: 219



Z Index: 134

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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0074. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

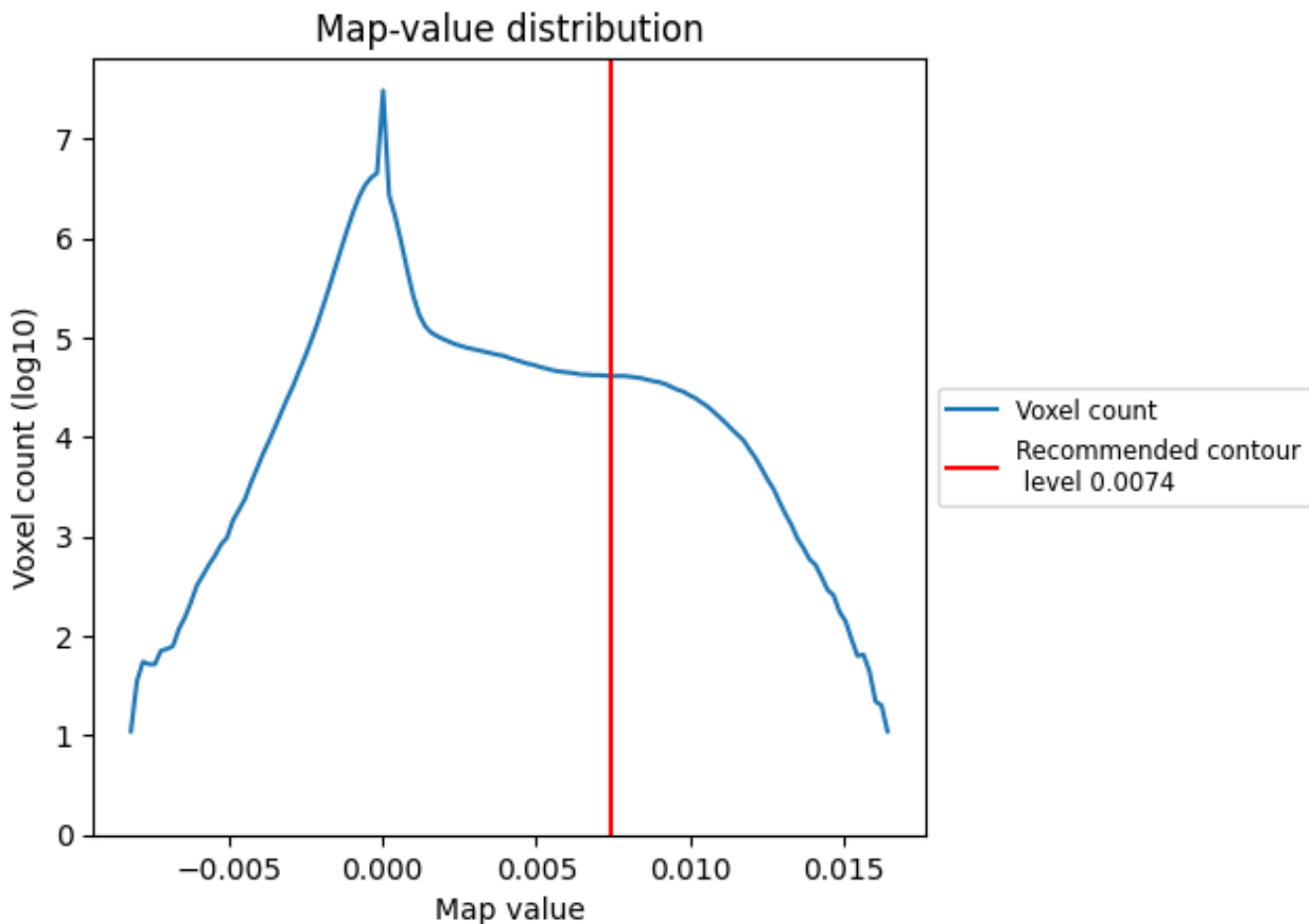
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

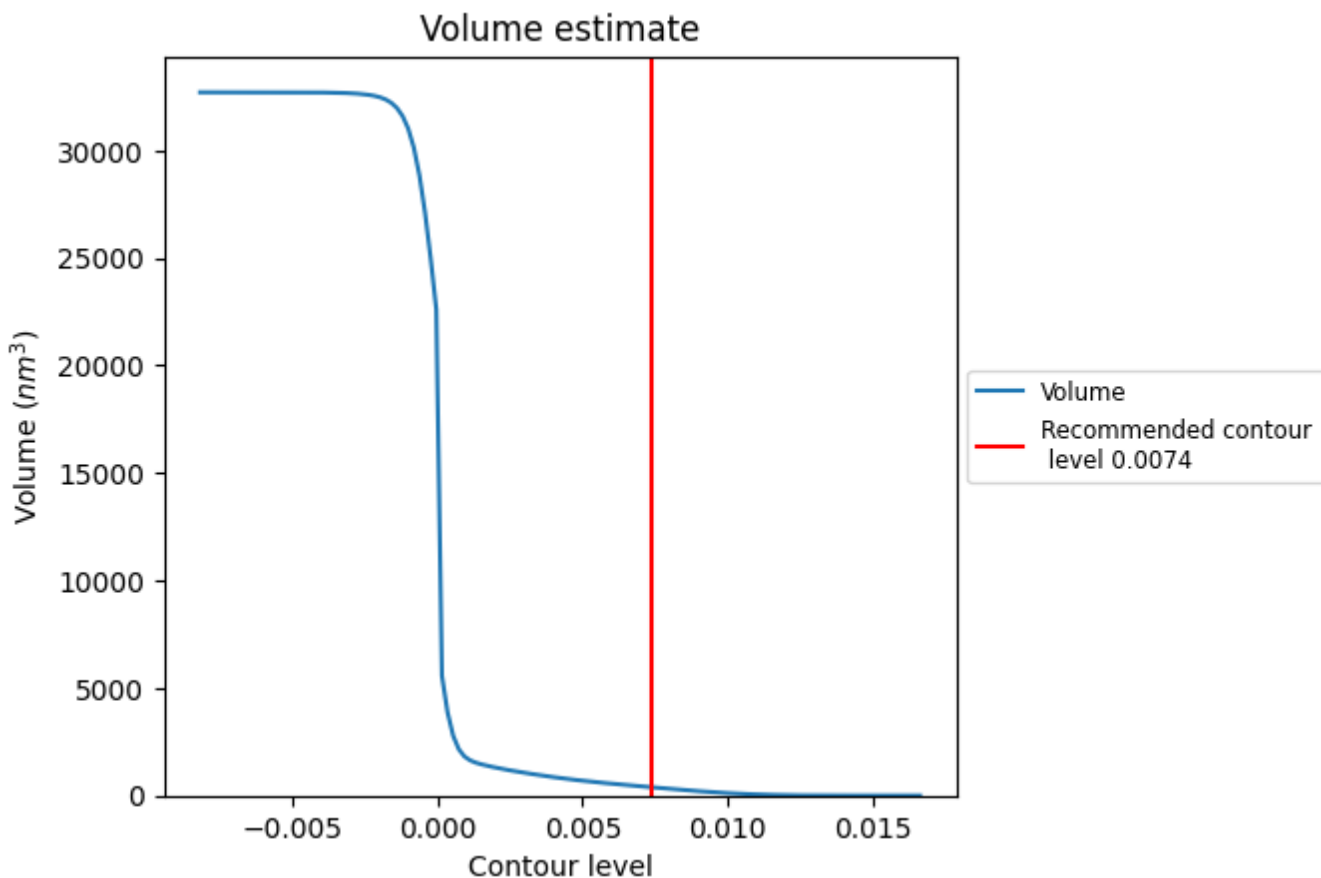
This section contains the results of statistical analysis of the map.

### 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.

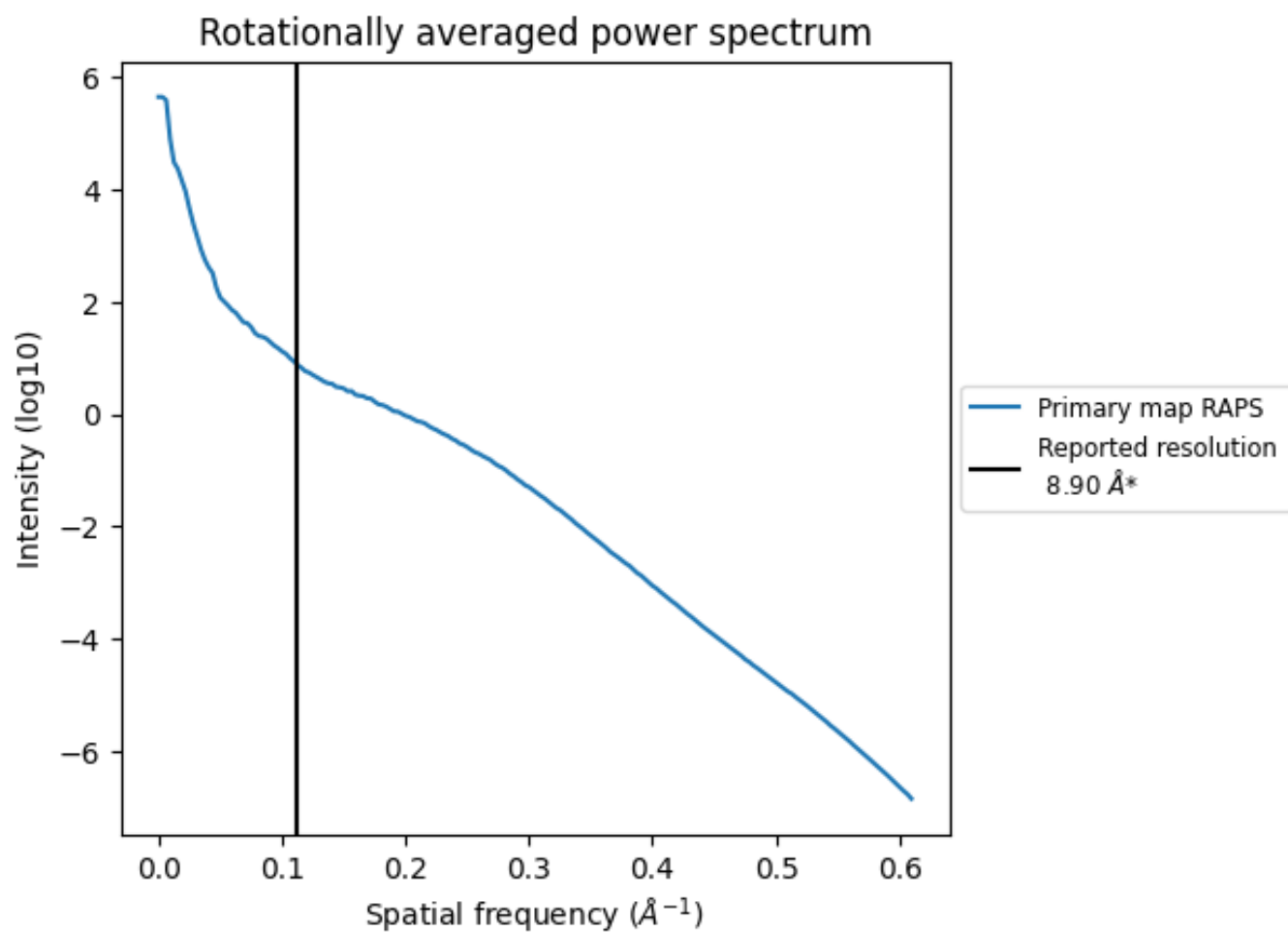
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 384 nm<sup>3</sup>; this corresponds to an approximate mass of 347 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](#)



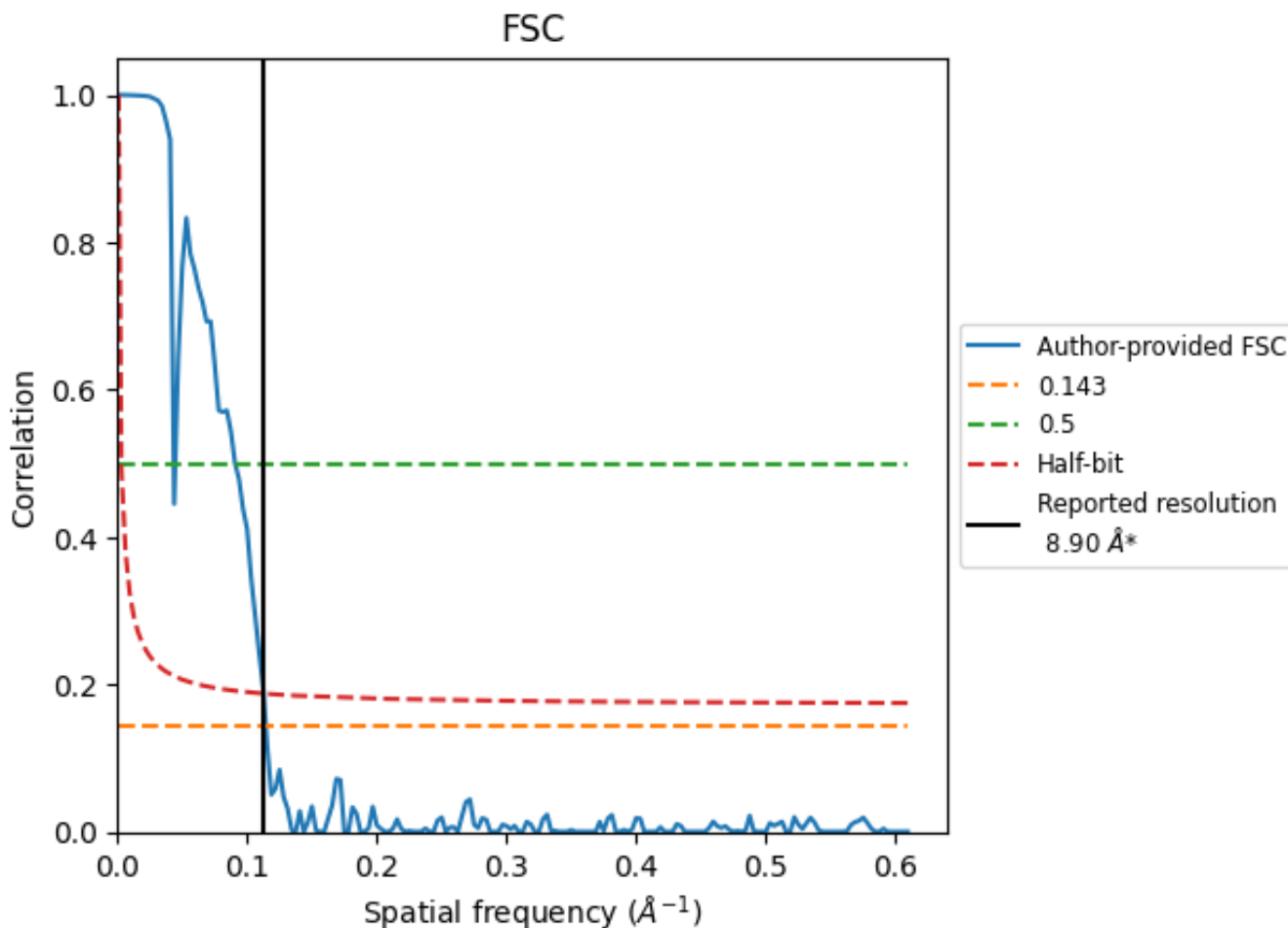
\*Reported resolution corresponds to spatial frequency of 0.112 Å<sup>-1</sup>



## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.112 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

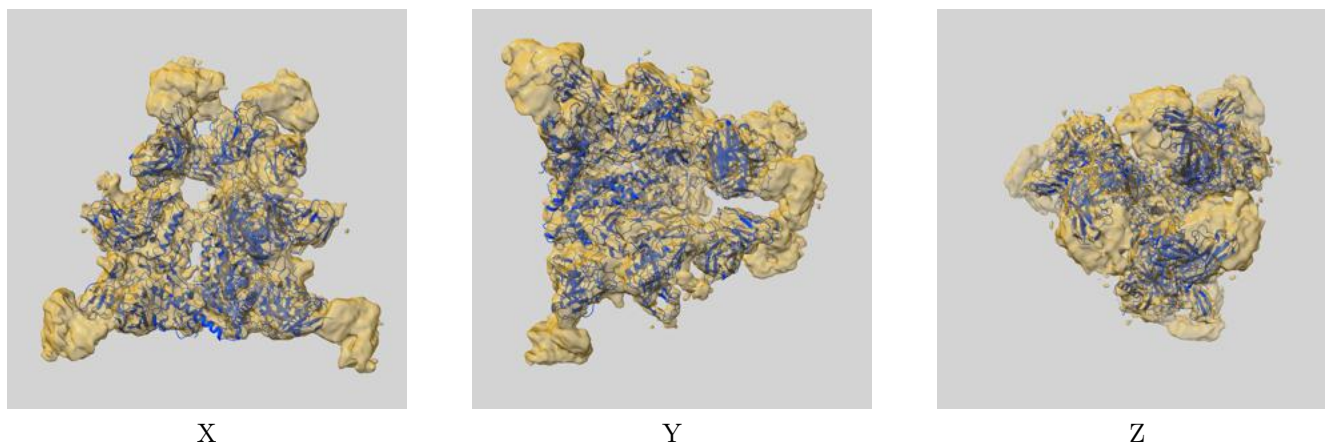
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	8.90	-	-
Author-provided FSC curve	8.73	23.04	8.87
Unmasked-calculated*	-	-	-

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

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

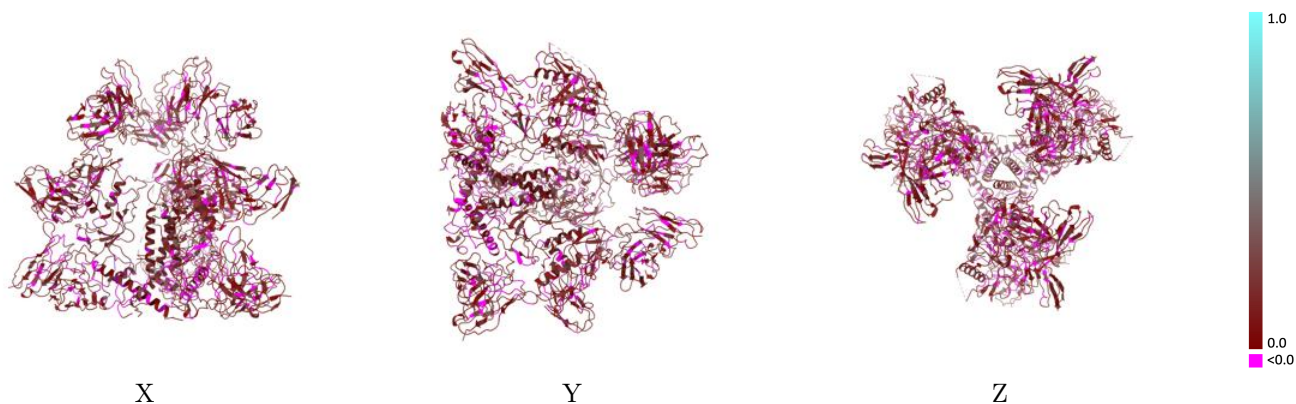
This section contains information regarding the fit between EMDB map EMD-8407 and PDB model 5THR. Per-residue inclusion information can be found in section 3 on page 10.

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



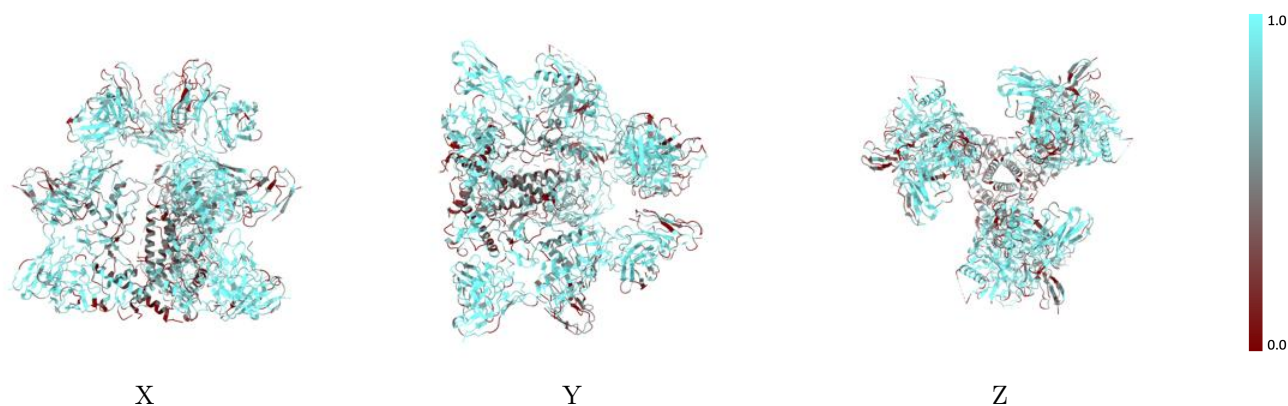
The images above show the 3D surface view of the map at the recommended contour level 0.0074 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



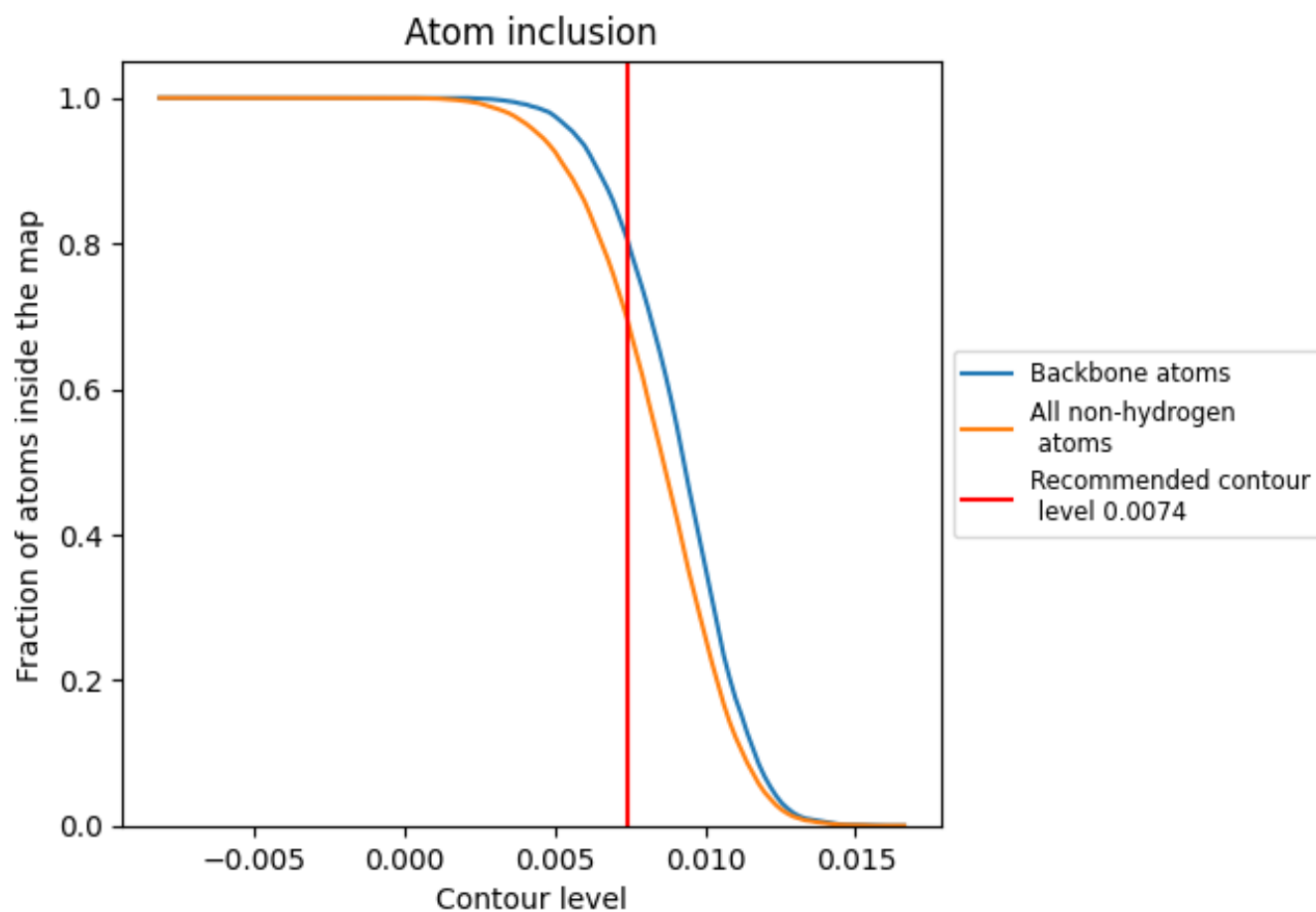
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0074).































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 70% 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 (0.0074) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6961	 0.1200
A	 0.4829	 0.0830
B	 0.5277	 0.0870
C	 0.4974	 0.0840
D	 0.7231	 0.1390
E	 0.7138	 0.1310
F	 0.7166	 0.1310
G	 0.5431	 0.1130
H	 0.5161	 0.1070
I	 0.5052	 0.1100
J	 0.6186	 0.1170
K	 0.6148	 0.1160
L	 0.6173	 0.1150
M	 0.7873	 0.1200
N	 0.7873	 0.1220
O	 0.7645	 0.1240
P	 0.8326	 0.1000
Q	 0.7741	 0.1340
R	 0.8545	 0.1080
S	 0.7818	 0.1230
T	 0.8617	 0.1260
U	 0.7895	 0.1130
V	 0.9200	 0.1700
W	 0.7049	 0.1690
X	 0.8852	 0.2180
Y	 0.8000	 0.1220
Z	 0.8852	 0.2360
a	 0.9016	 0.2200
b	 0.8400	 0.1040
c	 0.8689	 0.2450
d	 0.8852	 0.2540

