



Full wwPDB EM Validation Report ⓘ

Mar 4, 2026 – 07:20 PM UTC

PDB ID : 9IZ9 / pdb_00009iz9
EMDB ID : EMD-61026
Title : VLP structure of Chikungunya virus complexed with C37 Fab, 2f block.
Authors : Han, X.; Ji, C.; Wang, F.; Tian, S.; Gao, F.G.; Yan, J.
Deposited on : 2024-08-01
Resolution : 3.30 Å(reported)
Based on initial models : 8FCG, 6JO8

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

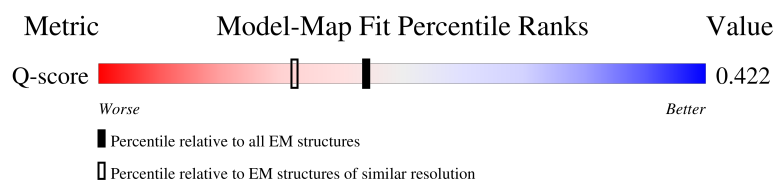
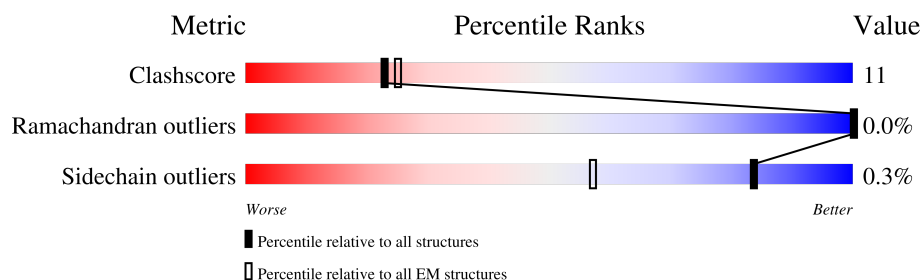
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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

Mol	Chain	Length	Quality of chain
1	M	265	71% 63% 22% 14%
1	O	265	79% 64% 22% 14%
1	Q	265	45% 59% 27% 14%
1	S	265	49% 71% 15% 14%

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Mol	Chain	Length	Quality of chain
2	N	241	
2	P	241	
2	R	241	
2	T	241	
3	A	439	
3	B	439	
3	C	439	
3	D	439	
4	E	419	
4	F	419	
4	G	419	
4	H	419	
5	I	151	
5	J	151	
5	K	151	
5	L	151	
6	U	4	
6	V	4	
6	X	4	
7	W	5	
8	Y	5	
8	c	5	
8	e	5	
9	Z	3	
9	b	3	

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Mol	Chain	Length	Quality of chain
9	d	3	100%
10	a	4	100%
11	f	4	50%25%25%

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 45105 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 C37 Fab, Heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	S	228	Total	C	N	O	S	0	0
			1715	1084	286	340	5		
1	Q	228	Total	C	N	O	S	0	0
			1715	1084	286	340	5		
1	O	228	Total	C	N	O	S	0	0
			1715	1084	286	340	5		
1	M	228	Total	C	N	O	S	0	0
			1715	1084	286	340	5		

- Molecule 2 is a protein called C37 Fab, Light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	T	212	Total	C	N	O	S	0	0
			1634	1020	281	328	5		
2	R	212	Total	C	N	O	S	0	0
			1634	1020	281	328	5		
2	P	212	Total	C	N	O	S	0	0
			1634	1020	281	328	5		
2	N	212	Total	C	N	O	S	0	0
			1634	1020	281	328	5		

- Molecule 3 is a protein called CHIKV E1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	439	Total	C	N	O	S	0	0
			3325	2107	558	634	26		
3	B	439	Total	C	N	O	S	0	0
			3325	2107	558	634	26		
3	C	439	Total	C	N	O	S	0	0
			3325	2107	558	634	26		
3	D	439	Total	C	N	O	S	0	0
			3325	2107	558	634	26		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	211	LYS	GLU	conflict	UNP A0A286S4J4
B	211	LYS	GLU	conflict	UNP A0A286S4J4
C	211	LYS	GLU	conflict	UNP A0A286S4J4
D	211	LYS	GLU	conflict	UNP A0A286S4J4

- Molecule 4 is a protein called Structural polyprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	412	Total	C	N	O	S	0	0
			3230	2031	573	598	28		
4	F	419	Total	C	N	O	S	0	0
			3282	2062	584	607	29		
4	G	419	Total	C	N	O	S	0	0
			3282	2062	584	607	29		
4	H	417	Total	C	N	O	S	0	0
			3263	2049	581	604	29		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	60	ASP	GLY	conflict	UNP D7R9A2
E	211	THR	ILE	conflict	UNP D7R9A2
E	312	MET	THR	conflict	UNP D7R9A2
F	60	ASP	GLY	conflict	UNP D7R9A2
F	211	THR	ILE	conflict	UNP D7R9A2
F	312	MET	THR	conflict	UNP D7R9A2
G	60	ASP	GLY	conflict	UNP D7R9A2
G	211	THR	ILE	conflict	UNP D7R9A2
G	312	MET	THR	conflict	UNP D7R9A2
H	60	ASP	GLY	conflict	UNP D7R9A2
H	211	THR	ILE	conflict	UNP D7R9A2
H	312	MET	THR	conflict	UNP D7R9A2

- Molecule 5 is a protein called CHIKV capsid protein.

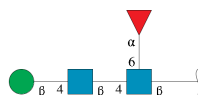
Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	151	Total	C	N	O	S	0	0
			1156	730	204	217	5		
5	J	151	Total	C	N	O	S	0	0
			1156	730	204	217	5		
5	K	151	Total	C	N	O	S	0	0
			1156	730	204	217	5		

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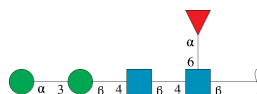
Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	151	Total	C	N	O	S	0	0
			1156	730	204	217	5		

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



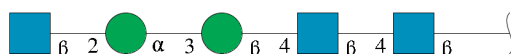
Mol	Chain	Residues	Atoms				AltConf	Trace
6	U	4	Total	C	N	O	0	0
			49	28	2	19		
6	V	4	Total	C	N	O	0	0
			49	28	2	19		
6	X	4	Total	C	N	O	0	0
			49	28	2	19		

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



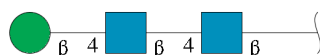
Mol	Chain	Residues	Atoms				AltConf	Trace
7	W	5	Total	C	N	O	0	0
			60	34	2	24		

- Molecule 8 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-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	Y	5	Total	C	N	O	0	0
			64	36	3	25		
8	c	5	Total	C	N	O	0	0
			64	36	3	25		
8	e	5	Total	C	N	O	0	0
			64	36	3	25		

- Molecule 9 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
9	Z	3	Total	C	N	O	0	0
			39	22	2	15		
9	b	3	Total	C	N	O	0	0
			39	22	2	15		
9	d	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 10 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.



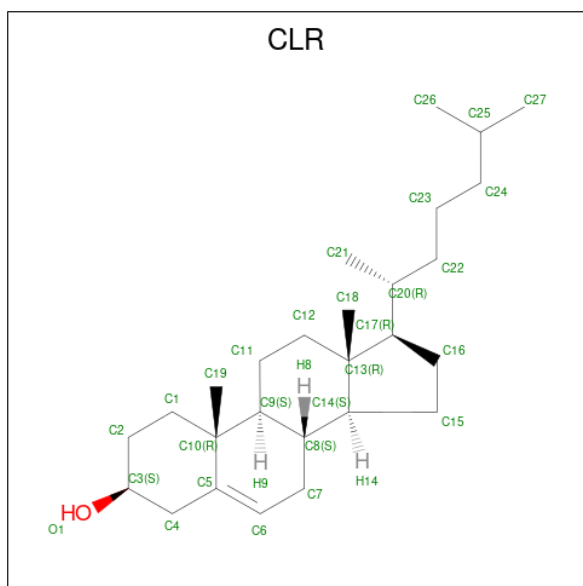
Mol	Chain	Residues	Atoms				AltConf	Trace
10	a	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 11 is an oligosaccharide called 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
11	f	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 12 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$).

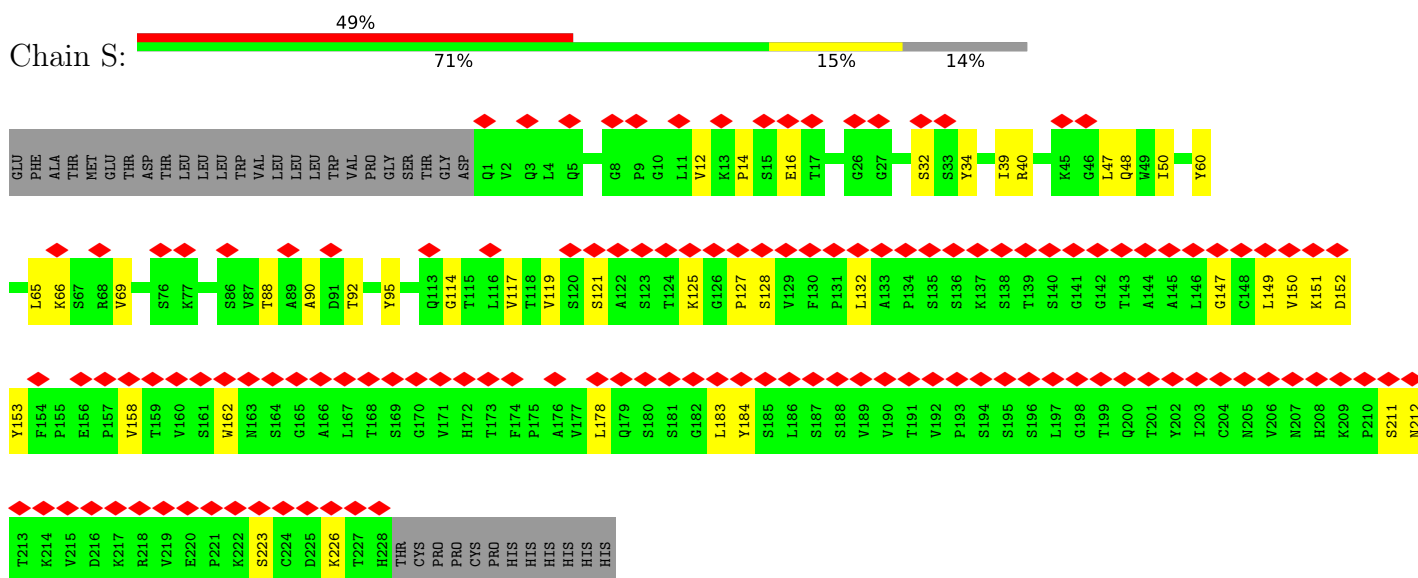


Mol	Chain	Residues	Atoms			AltConf
12	B	1	Total	C	O	0
			28	27	1	
12	D	1	Total	C	O	0
			28	27	1	
12	E	1	Total	C	O	0
			28	27	1	
12	G	1	Total	C	O	0
			28	27	1	

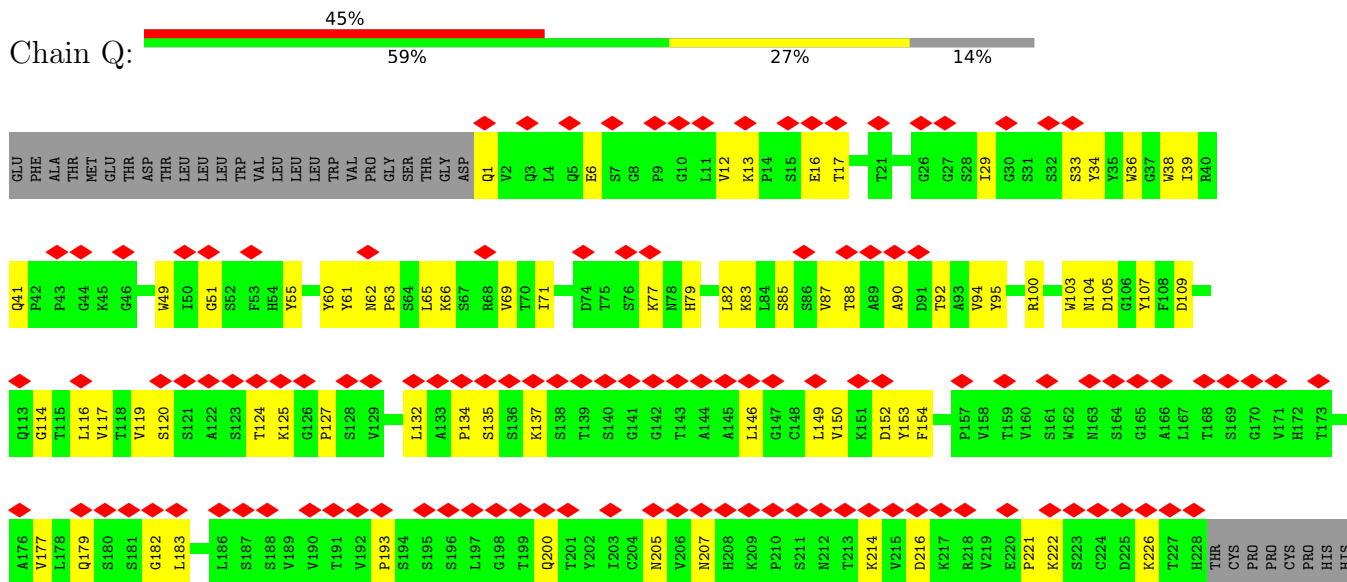
3 Residue-property plots [i](#)

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: C37 Fab, Heavy chain



- Molecule 1: C37 Fab, Heavy chain



HIS
HIS
HIS
HIS

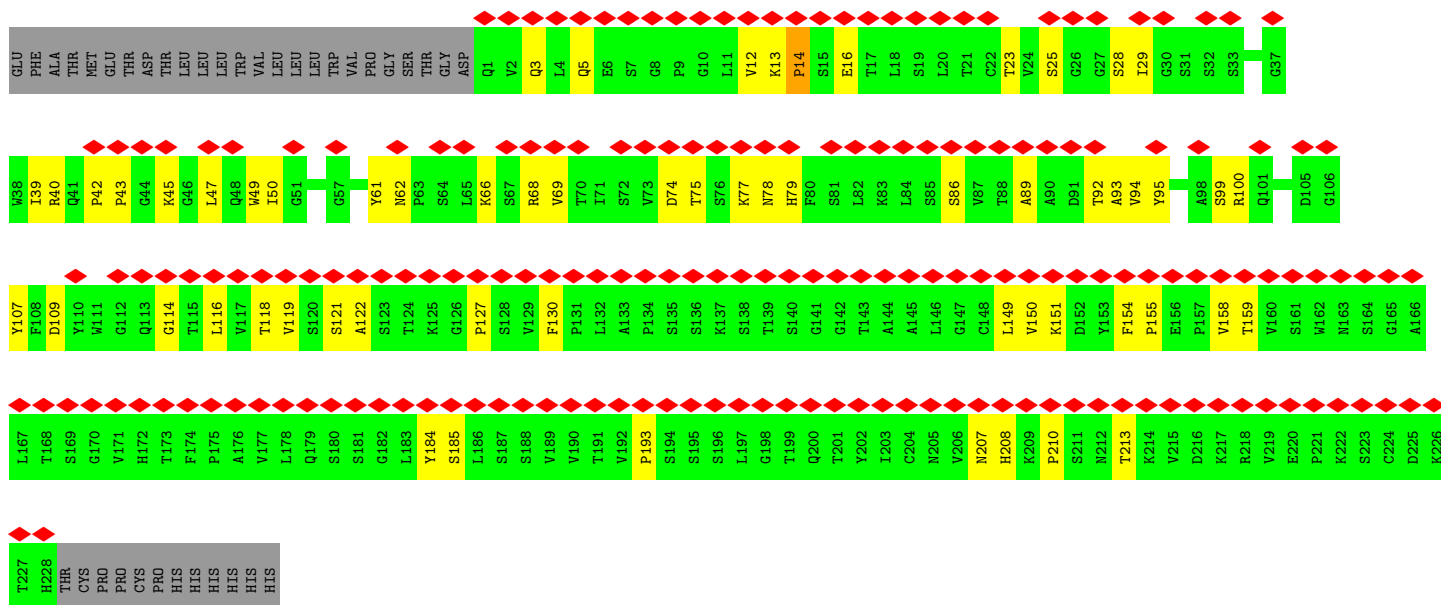
• Molecule 1: C37 Fab, Heavy chain

Chain O: 

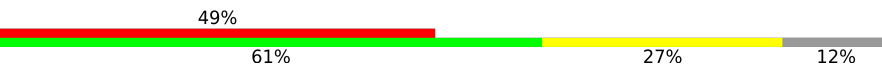


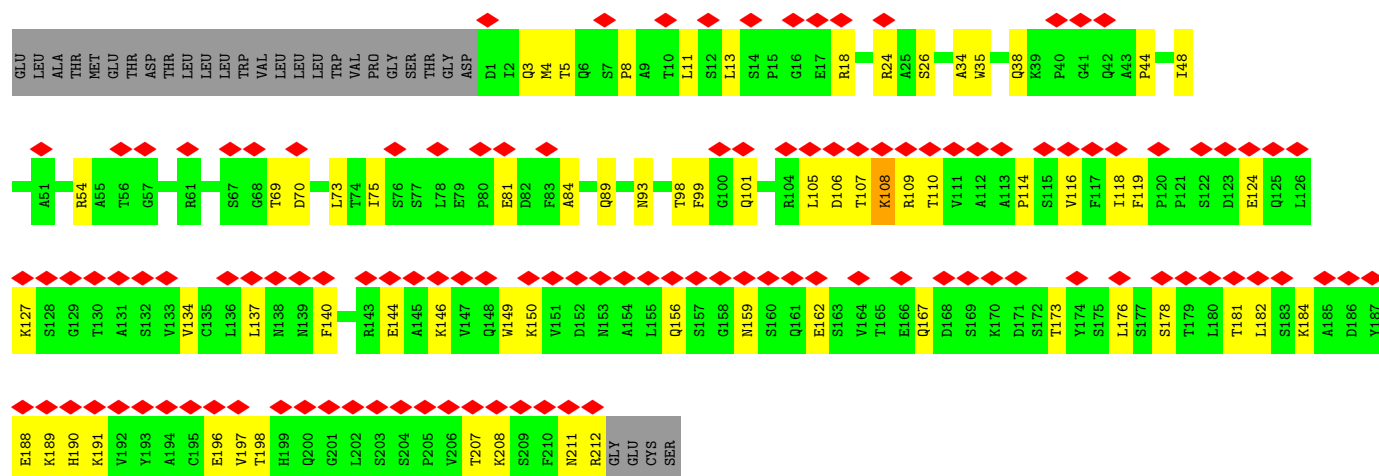
• Molecule 1: C37 Fab, Heavy chain

Chain M: 

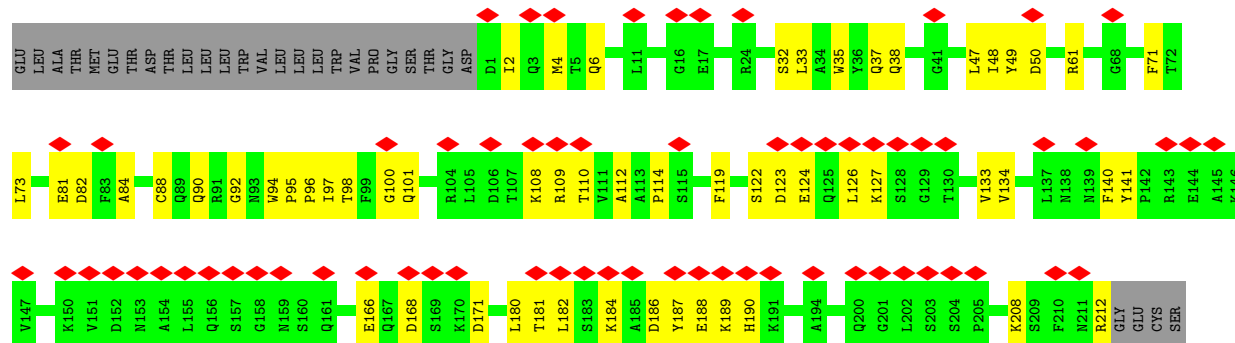


• Molecule 2: C37 Fab, Light chain

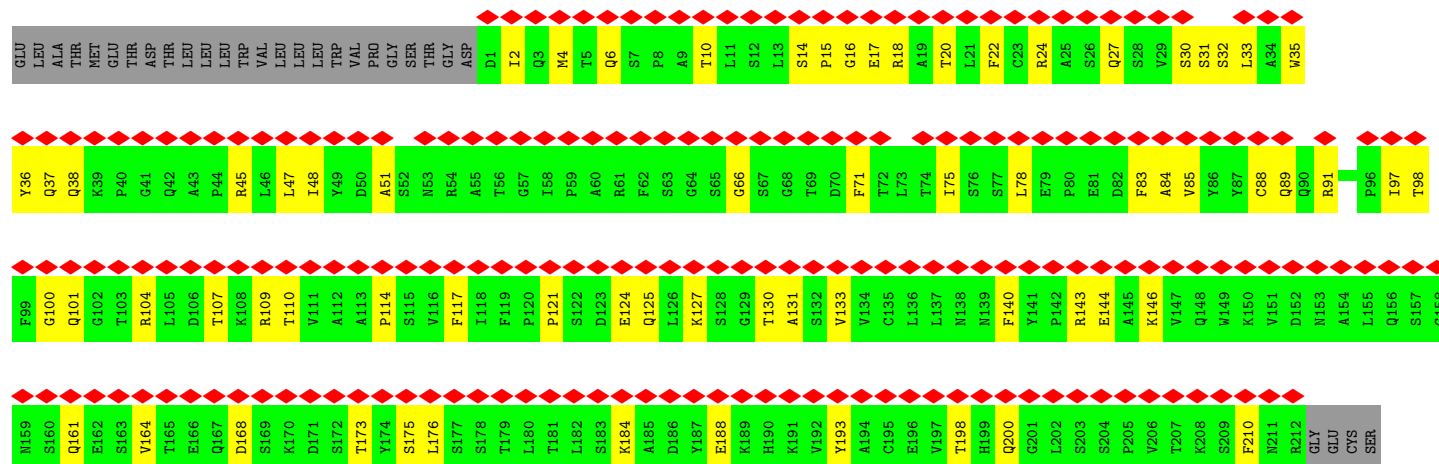
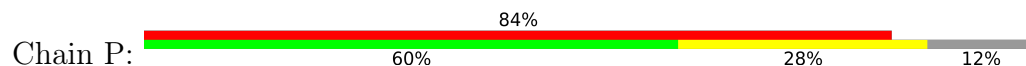
Chain T: 



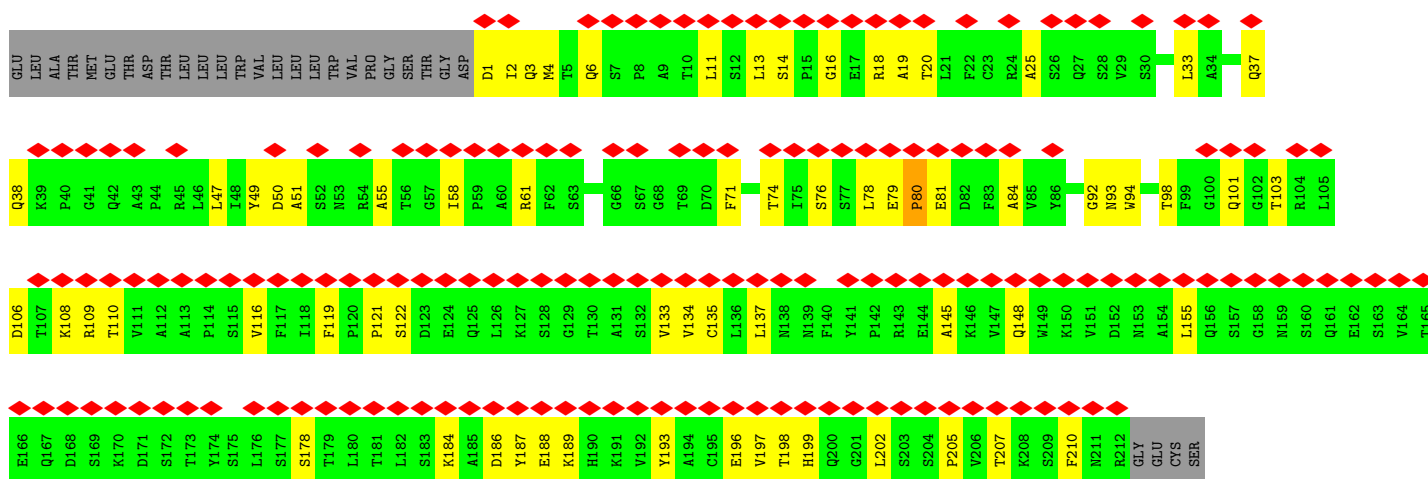
• Molecule 2: C37 Fab, Light chain



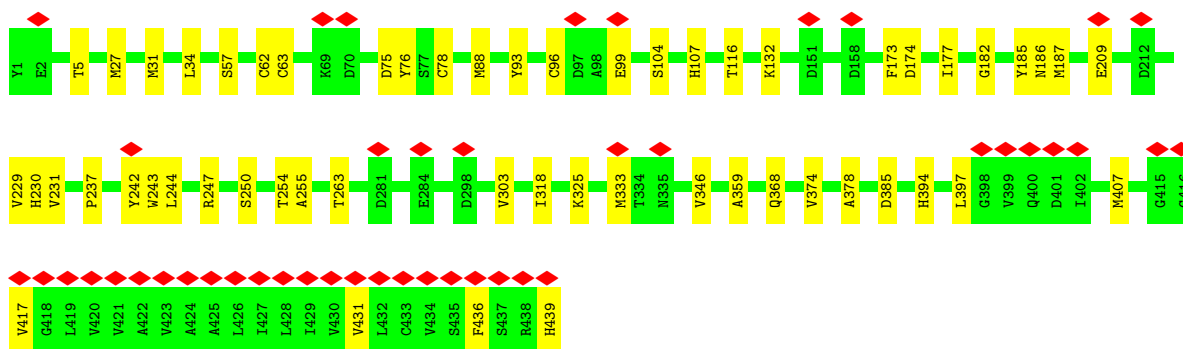
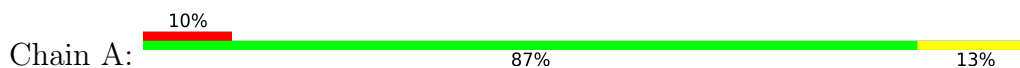
• Molecule 2: C37 Fab, Light chain



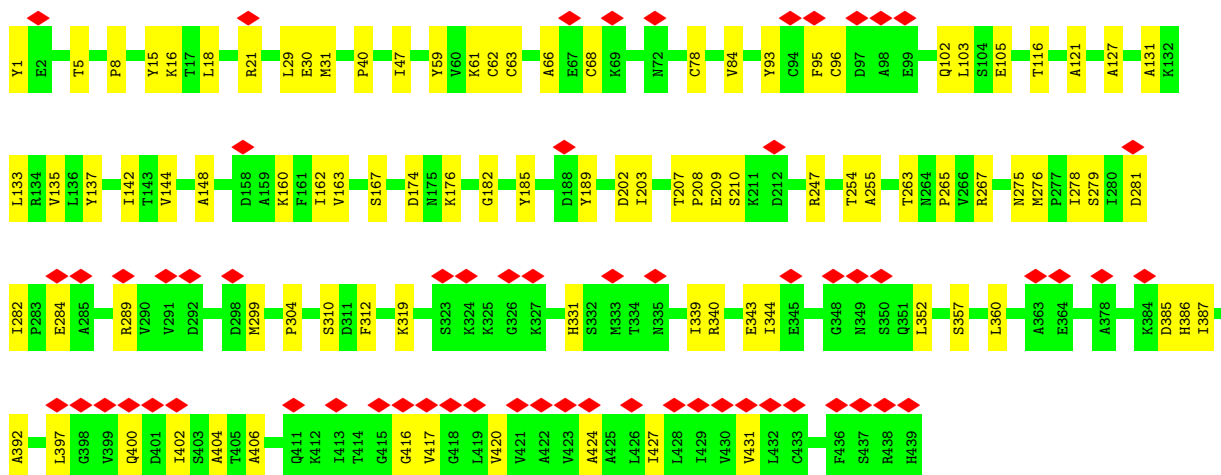
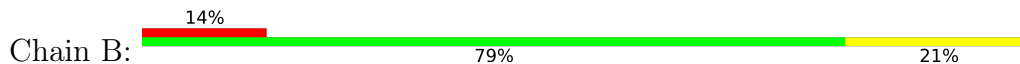
• Molecule 2: C37 Fab, Light chain



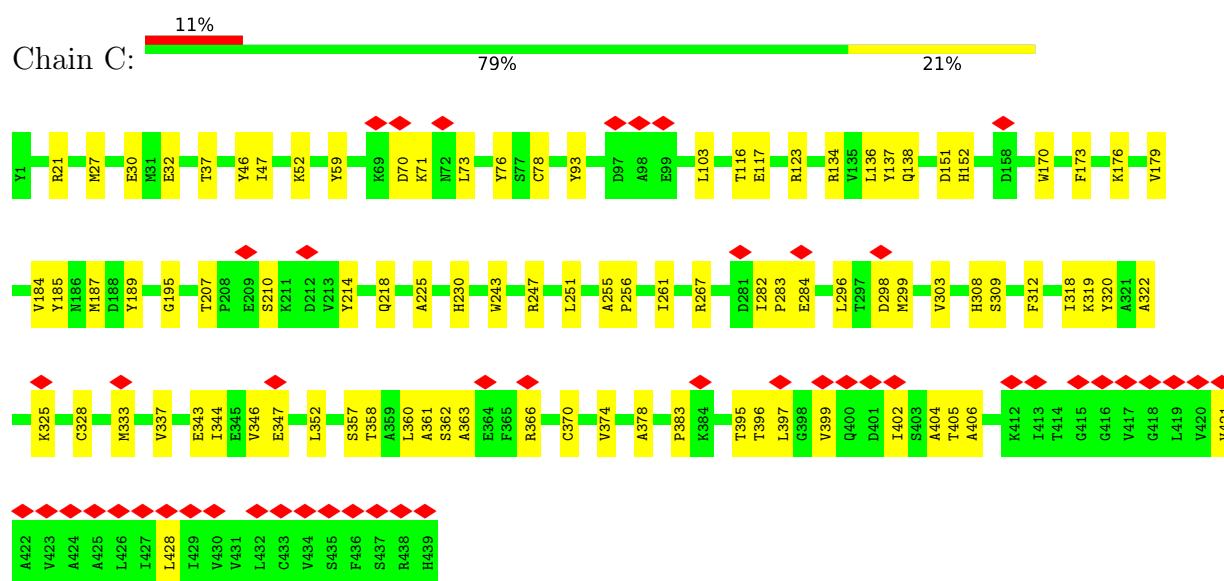
• Molecule 3: CHIKV E1



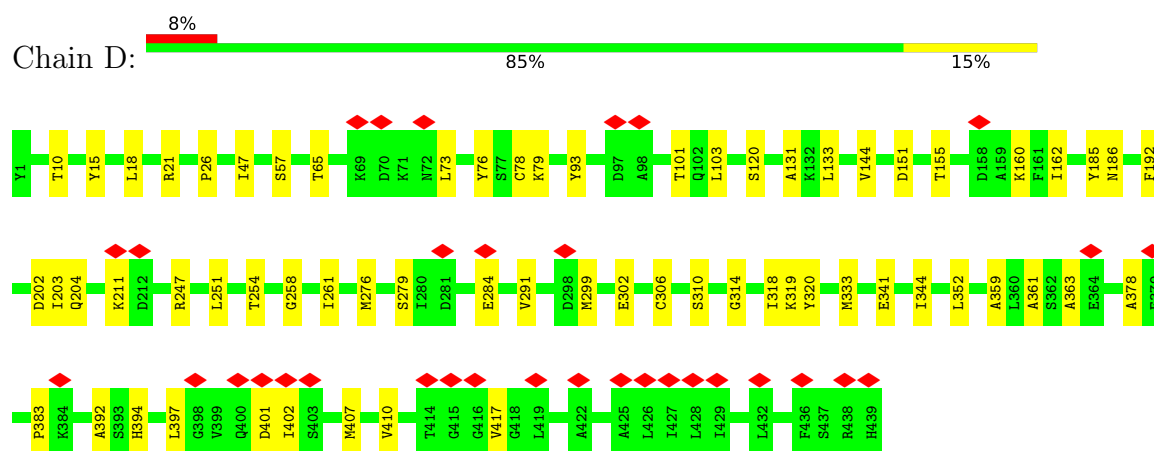
• Molecule 3: CHIKV E1



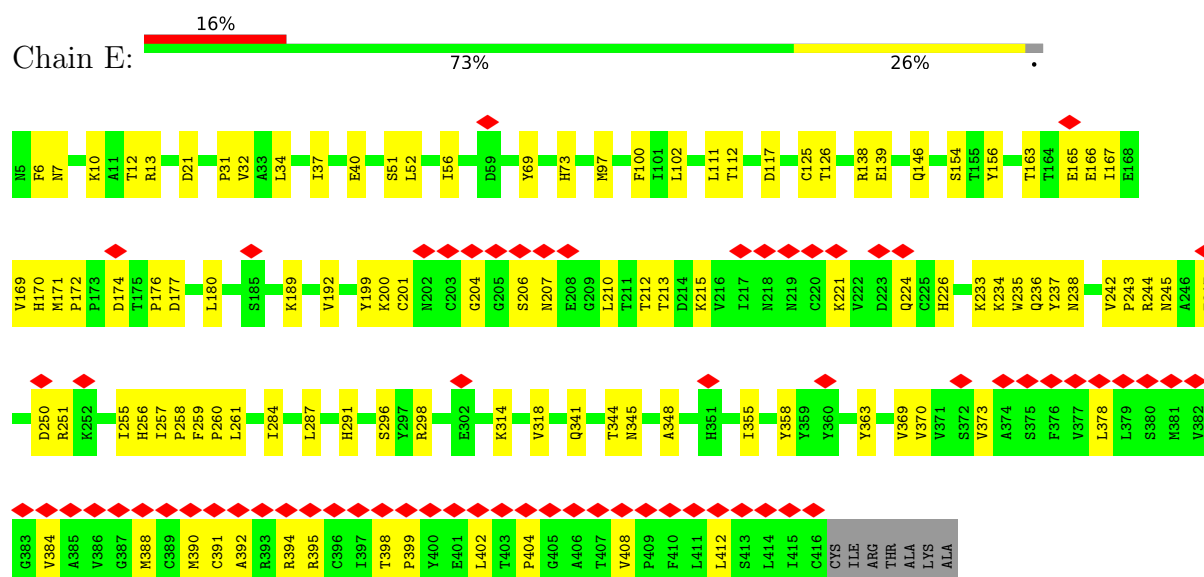
• Molecule 3: CHIKV E1



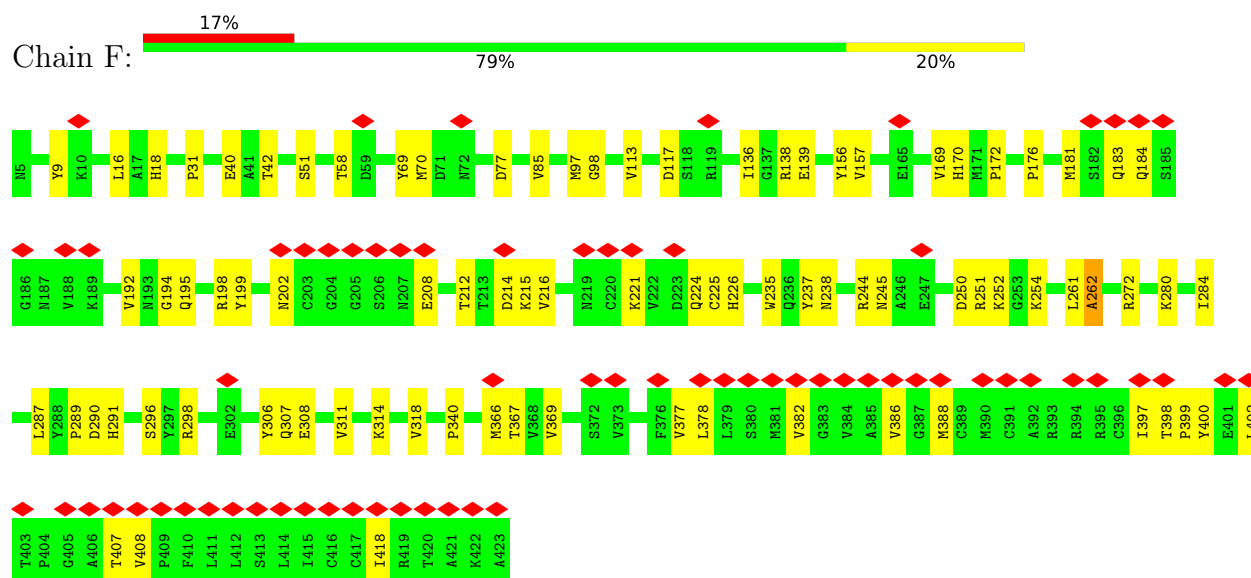
• Molecule 3: CHIKV E1



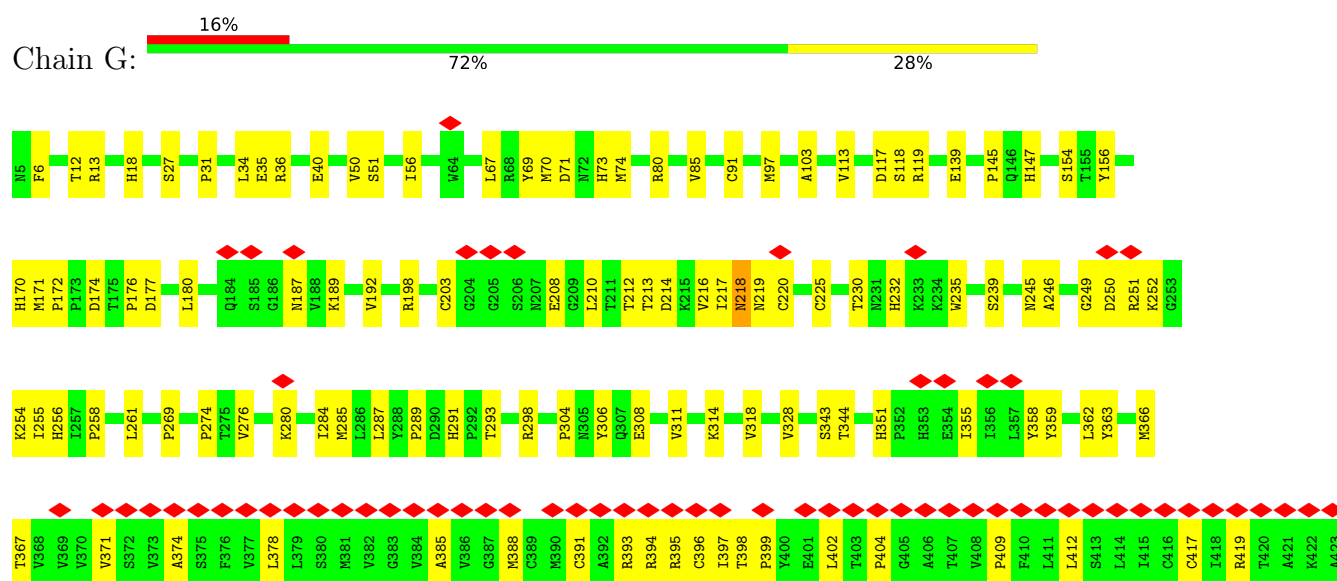
• Molecule 4: Structural polypeptide



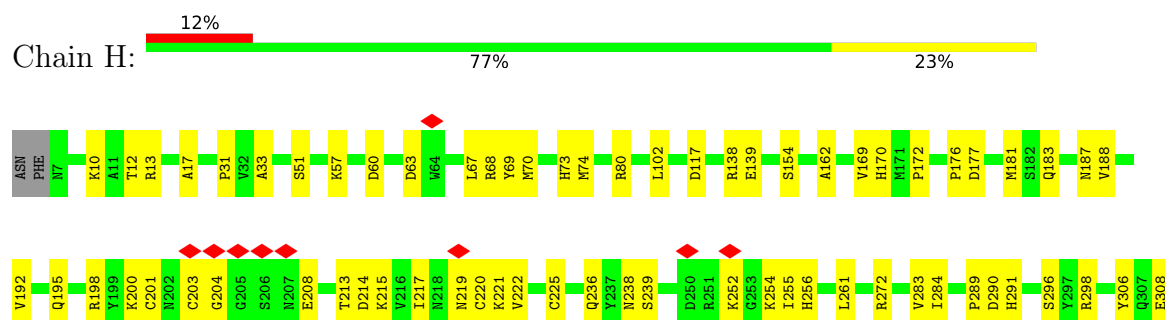
- Molecule 4: Structural polypeptide

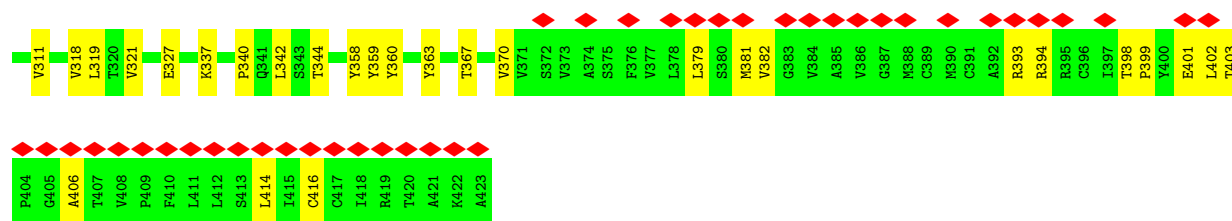


- Molecule 4: Structural polypeptide



- Molecule 4: Structural polypeptide

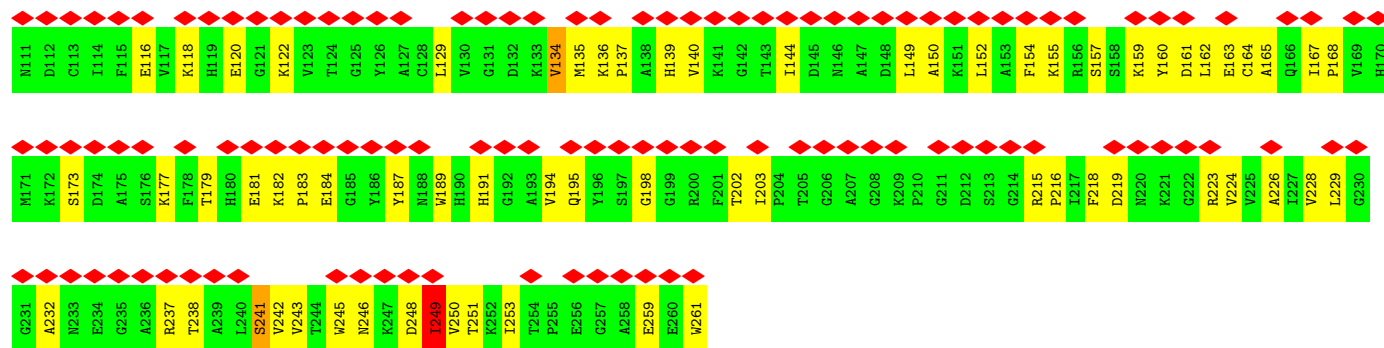
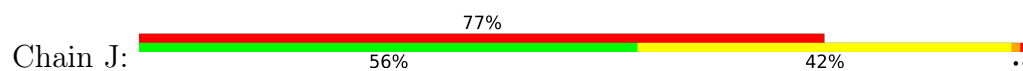




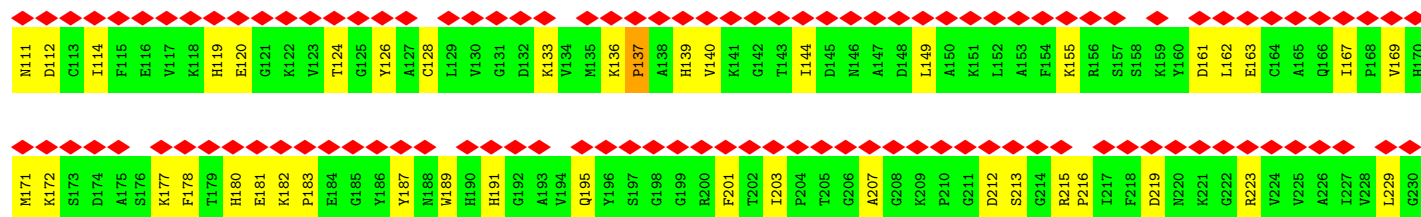
• Molecule 5: CHIKV capsid protein

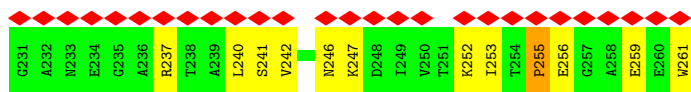


• Molecule 5: CHIKV capsid protein

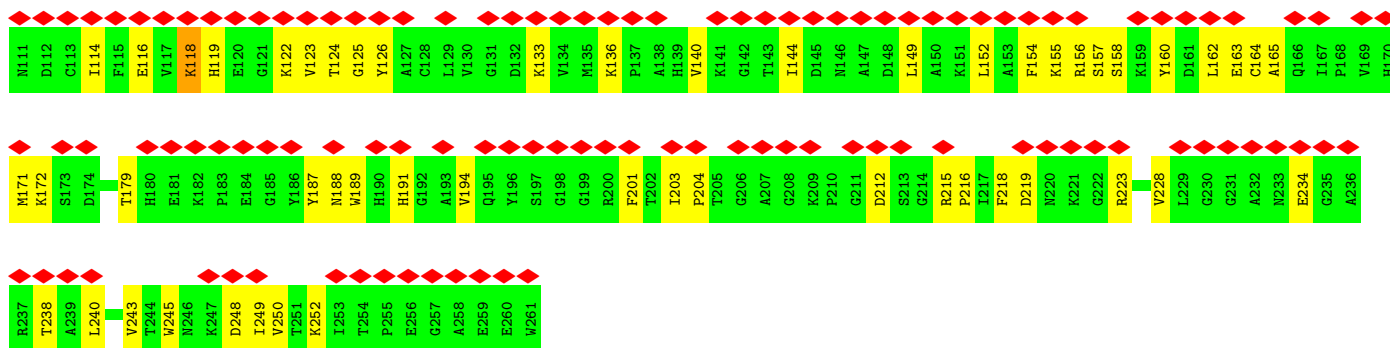


• Molecule 5: CHIKV capsid protein





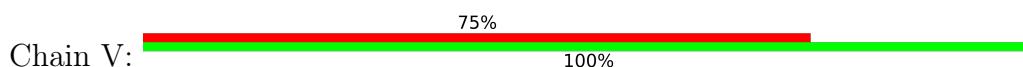
• Molecule 5: CHIKV capsid protein



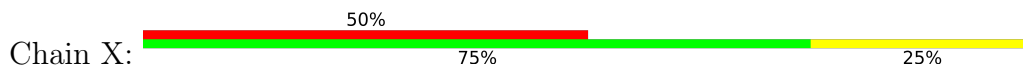
• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



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

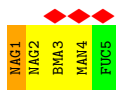


• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

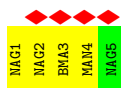
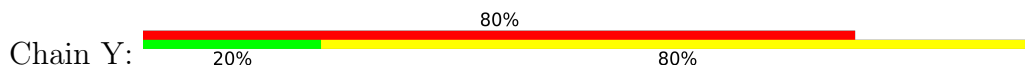


• Molecule 7: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

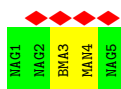
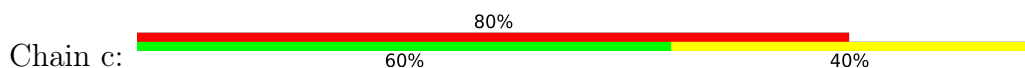




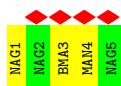
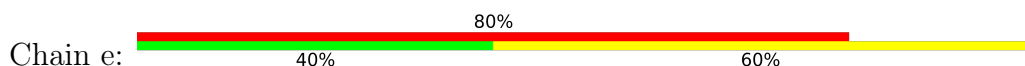
- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



- Molecule 9: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



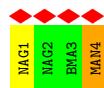
- Molecule 9: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d: 



- Molecule 10: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a: 



- Molecule 11: 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 f: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	559411	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.696	Depositor
Minimum map value	-0.348	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.135	Depositor
Map size ($\text{\AA}$)	501.6, 501.6, 501.6	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.32, 1.32, 1.32	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	M	0.17	0/1763	0.47	2/2409 (0.1%)
1	O	0.13	0/1763	0.37	0/2409
1	Q	0.28	1/1763 (0.1%)	0.64	6/2409 (0.2%)
1	S	0.17	0/1763	0.43	0/2409
2	N	0.16	0/1671	0.45	1/2272 (0.0%)
2	P	0.16	0/1671	0.38	0/2272
2	R	0.15	0/1671	0.41	0/2272
2	T	0.17	0/1671	0.53	2/2272 (0.1%)
3	A	0.16	0/3407	0.35	0/4649
3	B	0.16	0/3407	0.37	0/4649
3	C	0.18	0/3407	0.41	0/4649
3	D	0.23	0/3407	0.42	0/4649
4	E	0.19	0/3317	0.41	0/4521
4	F	0.17	0/3369	0.43	0/4589
4	G	0.26	0/3369	0.49	6/4589 (0.1%)
4	H	0.18	0/3349	0.42	0/4562
5	I	0.28	0/1184	0.75	6/1599 (0.4%)
5	J	0.23	0/1184	0.53	0/1599
5	K	0.22	0/1184	0.60	3/1599 (0.2%)
5	L	0.27	0/1184	0.58	1/1599 (0.1%)
All	All	0.20	1/45504 (0.0%)	0.45	27/61977 (0.0%)

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
4	F	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Q	193	PRO	CG-CD	-5.61	1.31	1.50

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	193	PRO	CA-N-CD	-13.15	93.58	112.00
5	I	246	ASN	N-CA-C	-10.31	96.92	110.53
2	N	80	PRO	CA-N-CD	-9.84	98.23	112.00
2	T	108	LYS	CA-C-N	9.04	137.97	121.70
2	T	108	LYS	C-N-CA	9.04	137.97	121.70
5	I	204	PRO	CA-N-CD	-8.41	100.23	112.00
1	Q	193	PRO	N-CD-CG	-8.13	91.01	103.20
5	I	128	CYS	N-CA-C	7.87	119.96	108.86
5	K	137	PRO	CA-N-CD	-7.79	101.10	112.00
5	I	245	TRP	N-CA-C	7.42	120.58	108.26
4	G	203	CYS	N-CA-C	7.06	117.34	108.45
1	Q	221	PRO	CA-N-CD	-6.84	102.43	112.00
4	G	218	ASN	N-CA-C	6.67	119.82	108.67
1	Q	221	PRO	N-CD-CG	-6.61	93.29	103.20
1	M	193	PRO	CA-N-CD	-6.21	103.30	112.00
1	Q	104	ASN	N-CA-C	6.12	119.87	111.54
5	I	128	CYS	N-CA-CB	-5.62	101.93	111.31
4	G	220	CYS	N-CA-C	5.52	117.85	110.35
5	K	255	PRO	CA-N-CD	-5.47	104.34	112.00
4	G	219	ASN	N-CA-C	5.43	119.00	112.38
4	G	218	ASN	CB-CA-C	-5.40	109.89	117.23
5	K	112	ASP	CB-CA-C	-5.18	110.19	117.23
1	M	14	PRO	CA-N-CD	-5.16	104.78	112.00
1	Q	193	PRO	CA-CB-CG	-5.13	94.75	104.50
5	L	188	ASN	N-CA-C	5.10	117.29	109.07
5	I	249	ILE	N-CA-C	5.09	117.34	108.95
4	G	225	CYS	N-CA-C	5.06	117.97	110.48

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	F	262	ALA	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	M	1715	0	1664	45	0
1	O	1715	0	1664	42	0
1	Q	1715	0	1664	53	0
1	S	1715	0	1664	28	0
2	N	1634	0	1584	43	0
2	P	1634	0	1584	52	0
2	R	1634	0	1584	50	0
2	T	1634	0	1584	50	0
3	A	3325	0	3253	44	0
3	B	3325	0	3253	66	0
3	C	3325	0	3252	67	0
3	D	3325	0	3253	51	0
4	E	3230	0	3161	80	0
4	F	3282	0	3220	69	0
4	G	3282	0	3220	94	0
4	H	3263	0	3205	70	0
5	I	1156	0	1133	42	0
5	J	1156	0	1135	52	0
5	K	1156	0	1135	40	0
5	L	1156	0	1135	49	0
6	U	49	0	43	0	0
6	V	49	0	43	0	0
6	X	49	0	43	0	0
7	W	60	0	52	1	0
8	Y	64	0	55	1	0
8	c	64	0	55	0	0
8	e	64	0	55	0	0
9	Z	39	0	34	1	0
9	b	39	0	34	1	0
9	d	39	0	34	0	0
10	a	50	0	43	1	0
11	f	50	0	43	0	0
12	B	28	0	42	4	0
12	D	28	0	43	3	0
12	E	28	0	42	4	0
12	G	28	0	40	9	0
All	All	45105	0	44048	1002	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 11.

All (1002) 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)
5:I:178:PHE:HB2	5:I:245:TRP:HH2	1.19	1.05
5:I:178:PHE:HB2	5:I:245:TRP:CH2	1.95	1.00
4:G:171:MET:HB3	4:G:245:ASN:HD22	1.33	0.91
4:H:201:CYS:HB3	4:H:225:CYS:HA	1.53	0.91
4:F:192:VAL:HG12	4:F:194:GLY:H	1.39	0.86
2:P:6:GLN:H	2:P:101:GLN:HE22	1.26	0.82
5:L:156:ARG:HH21	5:L:158:SER:HB2	1.47	0.80
4:E:12:THR:HG21	4:E:255:ILE:HD11	1.64	0.80
4:H:360:TYR:HA	4:H:367:THR:HG21	1.64	0.79
4:E:34:LEU:HD23	4:E:37:ILE:HD11	1.63	0.79
5:J:139:HIS:NE2	5:J:261:TRP:O	2.15	0.78
1:M:77:LYS:HD2	1:M:79:HIS:HD2	1.49	0.78
4:G:285:MET:HE1	4:G:328:VAL:HG11	1.67	0.77
1:Q:205:ASN:ND2	1:Q:216:ASP:OD1	2.18	0.76
2:R:109:ARG:HH21	2:R:112:ALA:HB2	1.51	0.76
1:M:28:SER:HA	1:M:78:ASN:HD21	1.49	0.76
3:B:16:LYS:NZ	3:B:339:ILE:O	2.19	0.76
3:B:21:ARG:HH12	3:B:284:GLU:HG3	1.52	0.75
4:F:170:HIS:HB2	4:F:250:ASP:HB2	1.69	0.75
5:K:246:ASN:OD1	5:K:247:LYS:N	2.20	0.74
2:P:15:PRO:HD3	2:P:107:THR:HG23	1.68	0.74
1:O:218:ARG:HE	1:O:220:GLU:HG3	1.51	0.74
4:E:154:SER:HB3	4:E:261:LEU:HD21	1.68	0.74
2:T:5:THR:HA	2:T:101:GLN:HE22	1.51	0.74
5:J:118:LYS:NZ	5:J:120:GLU:O	2.21	0.74
1:O:172:HIS:HE2	2:P:175:SER:HG	1.23	0.73
3:B:63:CYS:N	3:B:96:CYS:SG	2.61	0.73
3:D:186:ASN:HD21	3:D:251:LEU:HD11	1.53	0.73
2:N:18:ARG:NH1	2:N:20:THR:OG1	2.21	0.73
3:D:299:MET:HA	3:D:319:LYS:O	1.89	0.72
2:T:114:PRO:HB3	2:T:140:PHE:HB3	1.71	0.72
5:J:229:LEU:HD11	5:J:243:VAL:HG23	1.72	0.72
2:T:137:LEU:HD21	2:T:197:VAL:HG11	1.69	0.71
3:B:95:PHE:HD2	4:F:226:HIS:HB2	1.55	0.70
3:C:344:ILE:HG21	3:C:352:LEU:HD12	1.71	0.70
5:K:139:HIS:HE1	5:K:229:LEU:HD12	1.57	0.70
4:G:171:MET:HB3	4:G:245:ASN:ND2	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:162:ILE:HG22	3:B:279:SER:HB2	1.72	0.69
2:T:150:LYS:HE3	2:T:150:LYS:HA	1.74	0.69
4:F:407:THR:OG1	5:J:248:ASP:OD2	2.10	0.69
4:H:12:THR:HG21	4:H:255:ILE:HD11	1.74	0.69
2:T:124:GLU:HA	2:T:127:LYS:HE3	1.75	0.69
3:B:16:LYS:HE3	3:B:30:GLU:HG3	1.75	0.69
3:A:229:VAL:HG21	4:E:243:PRO:HG3	1.74	0.69
4:E:97:MET:HE3	4:E:258:PRO:HB3	1.74	0.69
3:C:360:LEU:HD11	3:C:402:ILE:HD11	1.74	0.68
4:H:154:SER:HB3	4:H:261:LEU:HD11	1.75	0.68
2:R:126:LEU:HD22	2:R:184:LYS:HZ1	1.58	0.68
4:H:401:GLU:O	5:L:133:LYS:NZ	2.26	0.68
2:N:6:GLN:H	2:N:101:GLN:HE22	1.42	0.68
3:C:225:ALA:H	3:C:230:HIS:HE1	1.42	0.68
4:G:35:GLU:OE1	4:G:239:SER:OG	2.11	0.68
4:G:374:ALA:O	4:G:378:LEU:HG	1.94	0.68
5:I:190:HIS:HB3	5:I:215:ARG:HD3	1.76	0.67
4:E:169:VAL:HG11	4:E:255:ILE:HD12	1.77	0.67
8:Y:1:NAG:H61	8:Y:2:NAG:HN2	1.59	0.67
4:G:198:ARG:NH1	1:Q:60:TYR:OH	2.27	0.67
2:N:109:ARG:NH1	2:N:110:THR:O	2.28	0.67
3:C:395:THR:HG23	3:C:396:THR:HG22	1.75	0.67
1:Q:49:TRP:HZ3	2:R:96:PRO:HA	1.59	0.67
3:D:211:LYS:HA	3:D:211:LYS:HE2	1.77	0.67
4:G:12:THR:HG21	4:G:255:ILE:HD11	1.75	0.67
3:C:299:MET:HA	3:C:319:LYS:O	1.95	0.67
4:E:402:LEU:HD22	5:I:162:LEU:HD22	1.76	0.67
3:C:308:HIS:O	3:C:308:HIS:ND1	2.27	0.66
4:H:73:HIS:NE2	4:H:177:ASP:OD1	2.26	0.66
5:J:241:SER:HA	5:J:253:ILE:O	1.94	0.66
2:R:37:GLN:HB2	2:R:47:LEU:HD11	1.76	0.66
4:H:403:THR:O	5:L:133:LYS:NZ	2.25	0.66
2:R:81:GLU:OE1	2:R:81:GLU:N	2.28	0.66
4:H:284:ILE:HG12	4:H:318:VAL:HG22	1.78	0.66
1:Q:92:THR:HA	1:Q:117:VAL:O	1.95	0.66
3:A:417:VAL:HG21	4:E:378:LEU:HD22	1.78	0.65
3:D:131:ALA:HB2	3:D:276:MET:HE1	1.78	0.65
1:S:127:PRO:HA	1:S:153:TYR:HB3	1.78	0.65
4:E:169:VAL:HG12	4:E:237:TYR:HA	1.79	0.65
3:D:251:LEU:HB3	3:D:261:ILE:HG13	1.78	0.65
2:N:116:VAL:HG22	2:N:137:LEU:HG	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:73:HIS:NE2	4:E:177:ASP:OD2	2.27	0.65
3:C:399:VAL:HA	12:G:501:CLR:H6	1.79	0.65
4:G:252:LYS:HE2	4:G:254:LYS:HE2	1.79	0.65
1:Q:95:TYR:O	1:Q:114:GLY:HA2	1.96	0.65
3:B:160:LYS:HB3	3:B:281:ASP:HB3	1.77	0.65
3:A:397:LEU:HD11	12:E:501:CLR:H112	1.79	0.64
4:F:221:LYS:HG3	4:F:224:GLN:HE21	1.62	0.64
5:L:162:LEU:HD12	5:L:243:VAL:HG11	1.78	0.64
4:G:245:ASN:OD1	4:G:246:ALA:N	2.30	0.64
3:C:256:PRO:HB3	4:G:304:PRO:HD3	1.79	0.64
3:B:360:LEU:HD23	3:B:402:ILE:HG22	1.78	0.64
2:T:119:PHE:HB2	2:T:134:VAL:HB	1.80	0.64
3:A:5:THR:HG21	3:A:31:MET:HE1	1.80	0.63
4:E:244:ARG:NH2	4:E:247:GLU:O	2.30	0.63
2:N:4:MET:HB3	2:N:25:ALA:HA	1.79	0.63
2:T:4:MET:HE3	2:T:4:MET:HA	1.80	0.63
3:C:255:ALA:O	4:G:298:ARG:NH1	2.30	0.63
4:F:284:ILE:HG12	4:F:318:VAL:HG12	1.80	0.63
5:J:179:THR:HG22	5:J:181:GLU:H	1.63	0.63
2:P:10:THR:HG23	2:P:104:ARG:HB2	1.79	0.63
3:D:73:LEU:HB2	3:D:76:TYR:HB2	1.81	0.63
2:T:4:MET:HG2	2:T:98:THR:HG22	1.79	0.63
5:I:205:THR:OG1	5:I:233:ASN:OD1	2.16	0.63
1:O:92:THR:HA	1:O:117:VAL:O	1.98	0.63
1:M:42:PRO:HB2	1:M:45:LYS:HD3	1.81	0.63
2:T:162:GLU:OE2	2:T:162:GLU:N	2.32	0.63
2:P:37:GLN:HB2	2:P:47:LEU:HD11	1.80	0.63
2:N:14:SER:H	2:N:108:LYS:HE3	1.63	0.63
2:N:119:PHE:HB2	2:N:134:VAL:HB	1.81	0.63
4:H:399:PRO:HB2	5:L:249:ILE:HD11	1.79	0.63
2:R:4:MET:HE2	2:R:4:MET:HA	1.81	0.62
3:A:187:MET:HE1	3:A:243:TRP:HE1	1.63	0.62
3:D:10:THR:OG1	3:D:15:TYR:OH	2.16	0.62
1:O:49:TRP:CG	2:P:97:ILE:HG22	2.34	0.62
3:B:95:PHE:CD2	4:F:226:HIS:HB2	2.34	0.62
4:H:169:VAL:HG21	4:H:255:ILE:HD12	1.81	0.62
5:L:189:TRP:CE3	5:L:191:HIS:HB2	2.35	0.62
1:S:211:SER:O	1:S:212:ASN:ND2	2.32	0.62
3:A:57:SER:OG	4:E:238:ASN:OD1	2.13	0.62
3:A:63:CYS:N	3:A:96:CYS:SG	2.72	0.62
5:L:154:PHE:CE2	5:L:163:GLU:HG3	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:303:VAL:HG21	3:C:378:ALA:HB2	1.82	0.62
4:G:74:MET:HA	4:G:74:MET:HE3	1.80	0.62
4:H:13:ARG:HH11	4:H:70:MET:HE3	1.65	0.62
3:C:93:TYR:HA	4:G:176:PRO:HG2	1.81	0.62
1:M:66:LYS:HA	1:M:69:VAL:HG12	1.82	0.62
4:G:97:MET:HE3	4:G:258:PRO:HB3	1.80	0.62
5:I:139:HIS:O	5:I:141:LYS:NZ	2.31	0.62
4:H:187:ASN:OD1	4:H:219:ASN:N	2.33	0.61
4:H:403:THR:HG22	5:L:250:VAL:HG13	1.81	0.61
5:K:256:GLU:N	5:K:256:GLU:OE1	2.32	0.61
4:G:40:GLU:OE1	4:G:156:TYR:OH	2.16	0.61
5:I:212:ASP:HB3	5:I:215:ARG:HH21	1.65	0.61
4:H:12:THR:O	4:H:68:ARG:NH2	2.33	0.61
1:O:123:SER:HB2	1:O:155:PRO:HD3	1.81	0.61
3:B:59:TYR:HB3	3:B:103:LEU:HB3	1.81	0.61
4:G:284:ILE:HG12	4:G:318:VAL:HG22	1.81	0.61
3:A:242:TYR:CE1	4:G:314:LYS:HB2	2.35	0.61
3:B:148:ALA:HA	3:B:163:VAL:HG23	1.82	0.61
3:C:117:GLU:OE2	4:G:154:SER:OG	2.17	0.61
4:H:200:LYS:HG3	4:H:208:GLU:HB3	1.83	0.61
5:J:182:LYS:NZ	5:J:245:TRP:O	2.29	0.61
2:R:184:LYS:HE2	2:R:184:LYS:HA	1.82	0.61
3:C:184:VAL:HG23	3:C:251:LEU:HD12	1.82	0.61
3:B:131:ALA:HB2	3:B:276:MET:HE1	1.83	0.60
1:Q:95:TYR:O	1:Q:114:GLY:CA	2.49	0.60
1:M:61:TYR:HB2	1:M:66:LYS:HB3	1.81	0.60
3:C:179:VAL:HG22	3:C:184:VAL:HG12	1.84	0.60
1:M:95:TYR:O	1:M:114:GLY:CA	2.49	0.60
3:D:402:ILE:HG13	4:H:359:TYR:HE1	1.65	0.60
5:J:129:LEU:HD22	5:J:134:VAL:HG12	1.82	0.60
1:M:150:VAL:O	1:M:185:SER:HA	2.01	0.60
2:T:35:TRP:CZ3	2:T:73:LEU:HB2	2.36	0.60
3:C:363:ALA:HB3	3:C:378:ALA:HB3	1.84	0.60
4:F:408:VAL:HG11	4:F:418:ILE:HD11	1.84	0.60
2:N:18:ARG:HH11	2:N:74:THR:HG23	1.65	0.60
4:F:400:TYR:HD1	4:F:408:VAL:HG22	1.67	0.60
4:E:210:LEU:HD21	2:N:94:TRP:CE2	2.37	0.60
5:J:152:LEU:HD11	5:J:168:PRO:HD3	1.82	0.60
2:T:109:ARG:HG2	2:T:110:THR:N	2.17	0.59
4:E:37:ILE:HD12	4:E:111:LEU:HD23	1.83	0.59
1:S:50:ILE:HG23	1:S:65:LEU:HD12	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:405:THR:HG22	3:C:406:ALA:H	1.66	0.59
5:I:113:CYS:SG	5:I:216:PRO:HG3	2.42	0.59
1:M:39:ILE:HA	1:M:50:ILE:HG12	1.85	0.59
4:F:184:GLN:O	4:F:184:GLN:HG2	2.01	0.59
4:H:74:MET:SD	4:H:195:GLN:NE2	2.75	0.59
3:A:62:CYS:HB2	3:A:96:CYS:HB3	1.85	0.59
4:H:272:ARG:NH1	4:H:290:ASP:OD1	2.36	0.59
3:B:427:ILE:O	3:B:431:VAL:HG23	2.03	0.59
1:Q:77:LYS:HG2	1:Q:79:HIS:HD2	1.66	0.59
4:F:208:GLU:OE1	4:F:208:GLU:N	2.27	0.59
1:O:111:TRP:HH2	2:P:36:TYR:HE2	1.49	0.59
2:T:4:MET:O	2:T:101:GLN:NE2	2.36	0.59
5:K:119:HIS:HB3	5:K:124:THR:HG21	1.84	0.59
2:T:106:ASP:OD2	2:T:167:GLN:NE2	2.35	0.58
4:H:402:LEU:HD23	5:L:164:CYS:SG	2.42	0.58
2:R:49:TYR:HD1	2:R:50:ASP:HB2	1.67	0.58
3:A:230:HIS:CE1	4:G:147:HIS:HB2	2.39	0.58
4:E:165:GLU:HB3	4:E:257:ILE:HB	1.86	0.58
1:M:150:VAL:HG11	1:M:158:VAL:HG11	1.85	0.58
3:D:333:MET:HE2	3:D:333:MET:HA	1.86	0.58
1:O:179:GLN:HE22	2:P:161:GLN:HE22	1.52	0.58
4:H:139:GLU:OE1	4:H:291:HIS:NE2	2.33	0.58
1:S:223:SER:HA	1:S:226:LYS:HG3	1.86	0.58
2:T:144:GLU:OE2	2:T:144:GLU:N	2.27	0.58
5:K:136:LYS:NZ	5:K:140:VAL:O	2.36	0.58
5:L:162:LEU:HD23	5:L:163:GLU:H	1.68	0.58
1:M:89:ALA:HA	1:M:119:VAL:HB	1.86	0.58
2:N:187:TYR:O	2:N:193:TYR:OH	2.21	0.58
4:E:404:PRO:HA	5:I:133:LYS:HE2	1.85	0.57
5:I:189:TRP:NE1	5:I:191:HIS:O	2.37	0.57
3:D:363:ALA:HB3	3:D:378:ALA:HB3	1.85	0.57
5:J:187:TYR:HB2	5:J:194:VAL:HG23	1.86	0.57
4:F:40:GLU:OE1	4:F:156:TYR:OH	2.19	0.57
3:D:402:ILE:O	4:H:359:TYR:OH	2.08	0.57
4:F:208:GLU:H	4:F:208:GLU:CD	2.13	0.57
1:S:39:ILE:HG21	1:S:47:LEU:HD12	1.85	0.57
5:K:139:HIS:CE1	5:K:229:LEU:HD12	2.37	0.57
5:L:136:LYS:HG2	5:L:163:GLU:HB3	1.86	0.57
3:D:21:ARG:NH1	3:D:284:GLU:OE2	2.38	0.57
4:F:139:GLU:OE1	4:F:291:HIS:NE2	2.27	0.57
1:Q:29:ILE:HD12	1:Q:29:ILE:H	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:190:HIS:O	2:R:212:ARG:NH1	2.37	0.57
2:P:30:SER:OG	2:P:31:SER:N	2.37	0.57
3:D:344:ILE:HG21	3:D:352:LEU:HD12	1.87	0.57
4:G:280:LYS:NZ	4:G:343:SER:O	2.33	0.57
4:G:393:ARG:O	4:G:397:ILE:HG12	2.04	0.57
3:A:237:PRO:HB2	4:G:314:LYS:NZ	2.20	0.57
3:C:325:LYS:HD3	3:C:347:GLU:HB2	1.87	0.57
12:D:501:CLR:H121	4:H:370:VAL:HG11	1.87	0.57
3:D:18:LEU:HD11	3:D:26:PRO:HB3	1.86	0.56
4:G:363:TYR:HB2	12:G:501:CLR:H112	1.87	0.56
4:E:369:VAL:O	4:E:373:VAL:HG13	2.05	0.56
4:G:367:THR:O	4:G:371:VAL:HG12	2.04	0.56
4:H:183:GLN:HG3	4:H:222:VAL:HB	1.88	0.56
5:I:228:VAL:HA	5:I:242:VAL:HG12	1.87	0.56
2:T:11:LEU:HB3	2:T:13:LEU:HD11	1.86	0.56
1:M:68:ARG:NH1	1:M:86:SER:O	2.38	0.56
5:K:137:PRO:HD2	5:K:137:PRO:O	2.06	0.56
1:O:138:SER:HA	2:P:117:PHE:CD1	2.41	0.56
1:M:47:LEU:HD23	1:M:47:LEU:H	1.69	0.56
1:S:50:ILE:HD12	1:S:50:ILE:H	1.71	0.56
4:F:183:GLN:HE22	4:F:221:LYS:NZ	2.04	0.56
5:I:216:PRO:HG2	5:I:218:PHE:HE1	1.70	0.56
5:K:177:LYS:NZ	5:K:178:PHE:H	2.04	0.56
4:G:344:THR:HG21	4:G:358:TYR:CD1	2.40	0.56
4:G:177:ASP:HB3	4:G:180:LEU:HG	1.86	0.56
3:D:186:ASN:ND2	3:D:251:LEU:HD11	2.20	0.56
4:E:31:PRO:O	4:E:51:SER:OG	2.24	0.56
4:F:58:THR:OG1	4:F:77:ASP:OD2	2.22	0.56
3:B:397:LEU:HD13	12:B:501:CLR:H192	1.87	0.56
5:I:229:LEU:HD21	5:I:243:VAL:HG13	1.87	0.56
2:N:196:GLU:OE2	2:N:207:THR:OG1	2.24	0.55
1:O:95:TYR:O	1:O:114:GLY:CA	2.54	0.55
3:A:230:HIS:HE1	4:G:147:HIS:HB2	1.69	0.55
4:H:393:ARG:NH1	4:H:416:CYS:O	2.39	0.55
5:L:156:ARG:HD2	5:L:157:SER:N	2.22	0.55
2:P:18:ARG:NH1	2:P:20:THR:OG1	2.37	0.55
3:C:333:MET:HE2	3:C:333:MET:HA	1.89	0.55
3:D:78:CYS:SG	3:D:79:LYS:N	2.79	0.55
1:O:95:TYR:O	1:O:114:GLY:HA3	2.07	0.55
4:G:171:MET:HE1	4:G:251:ARG:NE	2.22	0.55
1:O:176:ALA:HB2	1:O:186:LEU:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:33:LEU:O	2:P:51:ALA:N	2.40	0.55
4:G:189:LYS:HE2	4:G:214:ASP:HB3	1.88	0.55
5:J:184:GLU:OE1	5:J:198:GLY:N	2.39	0.55
4:E:245:ASN:ND2	4:E:250:ASP:OD2	2.39	0.55
4:H:67:LEU:HD23	4:H:80:ARG:HA	1.89	0.55
1:M:159:THR:HG23	1:M:207:ASN:HB2	1.88	0.55
3:A:431:VAL:HG21	4:E:392:ALA:HB1	1.88	0.55
3:B:1:TYR:N	3:B:282:ILE:O	2.39	0.55
1:Q:38:TRP:CG	1:Q:82:LEU:HD22	2.42	0.55
4:F:198:ARG:HH22	1:O:54:HIS:CD2	2.25	0.55
4:G:71:ASP:OD2	4:G:119:ARG:NH2	2.35	0.55
1:O:34:TYR:HB2	1:O:100:ARG:O	2.07	0.54
3:D:407:MET:HA	3:D:410:VAL:HG12	1.89	0.54
4:G:232:HIS:O	4:G:251:ARG:NH1	2.39	0.54
3:C:78:CYS:SG	3:C:103:LEU:HD11	2.48	0.54
3:D:341:GLU:N	3:D:341:GLU:OE1	2.40	0.54
4:H:363:TYR:O	4:H:367:THR:HG22	2.08	0.54
4:E:32:VAL:HG22	4:E:52:LEU:HG	1.89	0.54
4:F:16:LEU:HD13	4:F:70:MET:HG2	1.89	0.54
1:Q:29:ILE:HG23	1:Q:36:TRP:HE1	1.72	0.54
4:E:384:VAL:O	4:E:388:MET:HG2	2.07	0.54
5:J:135:MET:HB3	5:J:162:LEU:HD21	1.90	0.54
3:A:187:MET:HE1	3:A:243:TRP:NE1	2.22	0.54
4:G:69:TYR:OH	4:G:117:ASP:OD1	2.14	0.54
2:T:146:LYS:HB3	2:T:198:THR:OG1	2.07	0.54
3:B:207:THR:HG22	3:B:210:SER:HB2	1.90	0.54
4:E:363:TYR:CD2	12:E:501:CLR:H111	2.43	0.54
5:J:202:THR:HG23	5:J:237:ARG:HH21	1.72	0.54
2:T:38:GLN:O	2:T:84:ALA:HB1	2.08	0.54
3:A:209:GLU:OE1	3:A:209:GLU:N	2.40	0.54
3:B:18:LEU:HD22	3:B:331:HIS:ND1	2.23	0.54
3:B:343:GLU:C	3:B:344:ILE:HD13	2.33	0.54
4:F:9:TYR:HE2	4:F:97:MET:HE3	1.73	0.54
4:G:355:ILE:HD12	4:G:355:ILE:H	1.73	0.54
4:H:57:LYS:HZ2	4:H:63:ASP:HB2	1.71	0.54
5:I:128:CYS:SG	5:I:129:LEU:N	2.81	0.54
3:C:187:MET:HE1	3:C:243:TRP:NE1	2.23	0.53
4:E:165:GLU:O	4:E:256:HIS:HA	2.07	0.53
5:I:204:PRO:HD2	5:I:204:PRO:O	2.08	0.53
4:H:327:GLU:OE1	4:H:337:LYS:NZ	2.41	0.53
2:R:35:TRP:HB2	2:R:48:ILE:HB	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:359:ALA:HB2	3:A:394:HIS:CE1	2.43	0.53
4:F:235:TRP:CE2	4:F:252:LYS:HD2	2.44	0.53
4:H:289:PRO:HG3	4:H:311:VAL:HG12	1.90	0.53
2:P:144:GLU:OE1	2:P:144:GLU:N	2.25	0.53
5:L:162:LEU:HD23	5:L:163:GLU:N	2.23	0.53
3:A:174:ASP:OD1	3:A:186:ASN:ND2	2.41	0.53
3:B:163:VAL:HG12	3:B:278:ILE:HD12	1.90	0.53
4:G:31:PRO:O	4:G:51:SER:OG	2.26	0.53
5:L:179:THR:HG21	5:L:223:ARG:HH21	1.73	0.53
3:D:162:ILE:HB	3:D:279:SER:OG	2.09	0.53
4:G:198:ARG:HH21	4:G:230:THR:HG21	1.73	0.53
5:L:203:ILE:HD12	5:L:240:LEU:HD13	1.89	0.53
1:M:5:GLN:HB2	1:M:23:THR:HG22	1.90	0.53
4:F:192:VAL:HG11	4:F:212:THR:O	2.09	0.53
2:R:32:SER:O	2:R:32:SER:OG	2.26	0.53
2:P:33:LEU:HA	2:P:89:GLN:O	2.09	0.53
4:G:289:PRO:HG3	4:G:311:VAL:HG12	1.90	0.53
5:J:177:LYS:HB3	5:J:223:ARG:HG2	1.91	0.53
4:H:192:VAL:HG12	4:H:214:ASP:OD1	2.09	0.53
5:I:232:ALA:HB2	5:I:258:ALA:HA	1.91	0.53
4:G:404:PRO:HA	5:K:133:LYS:HE3	1.89	0.52
4:H:10:LYS:HA	4:H:60:ASP:OD1	2.09	0.52
2:T:189:LYS:HG2	2:T:190:HIS:CD2	2.44	0.52
3:C:312:PHE:HA	3:C:357:SER:HB2	1.92	0.52
4:F:31:PRO:O	4:F:51:SER:OG	2.26	0.52
4:H:138:ARG:NH2	4:H:296:SER:OG	2.40	0.52
1:Q:17:THR:HG22	1:Q:85:SER:HA	1.90	0.52
2:P:4:MET:SD	2:P:4:MET:N	2.83	0.52
2:T:184:LYS:O	2:T:188:GLU:HG2	2.10	0.52
5:K:139:HIS:CD2	5:K:140:VAL:HG23	2.45	0.52
1:O:6:GLU:OE1	1:O:113:GLN:N	2.43	0.52
5:I:215:ARG:O	5:I:228:VAL:HG12	2.10	0.52
2:P:101:GLN:OE1	2:P:101:GLN:N	2.38	0.52
5:J:164:CYS:SG	5:J:165:ALA:N	2.83	0.52
1:M:99:SER:O	1:M:109:ASP:N	2.39	0.52
1:M:95:TYR:O	1:M:114:GLY:HA2	2.09	0.52
3:B:93:TYR:HA	4:F:176:PRO:HG3	1.91	0.52
4:H:17:ALA:HB3	4:H:33:ALA:HB3	1.91	0.52
5:L:234:GLU:HB3	5:L:238:THR:HA	1.91	0.52
3:B:137:TYR:OH	3:B:282:ILE:HG23	2.10	0.51
1:O:149:LEU:HD11	1:O:185:SER:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:116:THR:HB	4:F:261:LEU:HD23	1.91	0.51
3:C:136:LEU:HD11	7:W:1:NAG:H82	1.92	0.51
5:K:259:GLU:OE2	5:K:259:GLU:N	2.39	0.51
1:Q:49:TRP:O	1:Q:62:ASN:ND2	2.42	0.51
1:S:150:VAL:HG11	1:S:158:VAL:HG21	1.92	0.51
2:T:106:ASP:OD2	2:T:107:THR:N	2.44	0.51
3:B:385:ASP:OD1	3:B:386:HIS:N	2.44	0.51
3:C:73:LEU:HB2	3:C:76:TYR:HB2	1.93	0.51
4:H:172:PRO:HB3	4:H:236:GLN:CD	2.36	0.51
5:I:206:GLY:O	5:I:209:LYS:NZ	2.44	0.51
1:S:92:THR:HA	1:S:117:VAL:O	2.09	0.51
2:T:116:VAL:HB	2:T:208:LYS:HZ1	1.73	0.51
2:P:33:LEU:HD21	2:P:88:CYS:HB2	1.93	0.51
1:S:47:LEU:HD21	2:T:99:PHE:CD1	2.45	0.51
3:A:385:ASP:O	4:E:341:GLN:NE2	2.42	0.51
3:B:310:SER:HB3	3:B:392:ALA:HA	1.93	0.51
3:D:155:THR:HG22	3:D:160:LYS:HG3	1.92	0.51
5:J:120:GLU:HG3	5:J:122:LYS:H	1.74	0.51
2:N:1:ASP:OD2	2:N:2:ILE:N	2.42	0.51
2:N:11:LEU:O	2:N:106:ASP:N	2.37	0.51
3:D:186:ASN:HD22	3:D:186:ASN:N	2.08	0.51
3:D:320:TYR:HE2	3:D:352:LEU:HB3	1.75	0.51
4:E:245:ASN:HD22	4:E:250:ASP:CG	2.19	0.51
5:K:181:GLU:OE1	5:K:181:GLU:N	2.31	0.51
2:R:90:GLN:O	2:R:97:ILE:HG13	2.10	0.51
2:T:149:TRP:NE1	2:T:178:SER:OG	2.37	0.51
4:E:345:ASN:OD1	9:Z:1:NAG:N2	2.44	0.51
4:F:69:TYR:OH	4:F:117:ASP:OD1	2.12	0.51
4:G:366:MET:HB2	12:G:501:CLR:H111	1.93	0.51
2:N:61:ARG:NH2	2:N:81:GLU:OE1	2.44	0.51
2:T:191:LYS:HG3	2:T:211:ASN:OD1	2.11	0.51
4:G:85:VAL:HG22	4:G:113:VAL:HG22	1.92	0.51
1:O:150:VAL:O	1:O:185:SER:HA	2.11	0.51
3:A:88:MET:HG3	4:E:176:PRO:HD2	1.93	0.50
3:C:309:SER:HB3	3:C:383:PRO:HB3	1.94	0.50
3:C:318:ILE:HB	3:C:352:LEU:HD21	1.93	0.50
3:C:428:LEU:HD22	4:G:388:MET:HB3	1.92	0.50
4:G:172:PRO:HD3	4:G:235:TRP:HA	1.92	0.50
5:L:215:ARG:O	5:L:228:VAL:HG12	2.10	0.50
2:R:90:GLN:HE21	2:R:98:THR:H	1.59	0.50
1:M:77:LYS:HZ3	1:M:79:HIS:HB3	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:3:GLN:HB2	2:T:26:SER:HB3	1.93	0.50
2:T:48:ILE:HD13	2:T:54:ARG:HA	1.93	0.50
3:A:242:TYR:CD1	4:G:314:LYS:HE3	2.46	0.50
3:C:299:MET:HE3	3:C:374:VAL:HG13	1.92	0.50
1:O:222:LYS:HG3	1:O:224:CYS:H	1.75	0.50
3:A:57:SER:HB3	4:E:242:VAL:O	2.11	0.50
3:A:237:PRO:HB2	4:G:314:LYS:HZ3	1.76	0.50
3:C:21:ARG:NH2	3:C:284:GLU:OE2	2.45	0.50
5:K:128:CYS:HB3	5:K:216:PRO:HG3	1.93	0.50
5:K:213:SER:OG	5:K:229:LEU:O	2.29	0.50
4:E:7:ASN:HA	4:E:10:LYS:NZ	2.26	0.50
4:G:287:LEU:O	4:G:314:LYS:HA	2.12	0.50
2:R:208:LYS:HE3	2:R:208:LYS:HA	1.93	0.50
2:N:198:THR:HG22	2:N:205:PRO:HB3	1.92	0.50
4:F:245:ASN:ND2	4:F:250:ASP:OD2	2.43	0.50
4:G:73:HIS:NE2	4:G:177:ASP:OD2	2.35	0.50
5:L:194:VAL:HG12	5:L:203:ILE:HG12	1.93	0.50
1:O:131:PRO:HB3	1:O:219:VAL:HG22	1.94	0.50
2:P:168:ASP:N	2:P:173:THR:O	2.44	0.50
2:T:35:TRP:CE3	2:T:73:LEU:HB2	2.47	0.50
3:A:63:CYS:HA	3:A:99:GLU:OE2	2.12	0.50
4:E:69:TYR:CZ	4:E:117:ASP:HB2	2.46	0.50
4:E:170:HIS:HB3	4:E:251:ARG:HB2	1.94	0.50
2:P:144:GLU:HG2	2:P:200:GLN:HE22	1.77	0.50
2:T:34:ALA:C	2:T:35:TRP:HD1	2.20	0.50
5:I:127:ALA:HB2	5:I:136:LYS:HB3	1.93	0.50
5:K:126:TYR:HE2	5:K:212:ASP:HA	1.77	0.50
5:K:219:ASP:OD1	5:K:223:ARG:NH1	2.45	0.50
1:M:127:PRO:HD2	1:M:213:THR:OG1	2.12	0.50
3:A:255:ALA:O	4:E:298:ARG:NH1	2.44	0.50
3:C:318:ILE:HD13	3:C:374:VAL:HG21	1.94	0.50
4:G:6:PHE:CE2	4:G:97:MET:HG2	2.47	0.50
4:G:67:LEU:HD23	4:G:80:ARG:HA	1.94	0.50
4:H:204:GLY:N	4:H:220:CYS:SG	2.85	0.50
5:L:116:GLU:HA	5:L:126:TYR:CD1	2.47	0.50
5:L:154:PHE:HE2	5:L:163:GLU:HG3	1.77	0.50
2:P:121:PRO:HD3	2:P:133:VAL:HG22	1.94	0.50
1:S:60:TYR:OH	4:H:198:ARG:NH1	2.36	0.49
4:H:31:PRO:O	4:H:51:SER:OG	2.30	0.49
1:S:32:SER:H	1:S:34:TYR:HE1	1.61	0.49
4:F:289:PRO:HG3	4:F:311:VAL:HG12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:366:MET:HA	4:F:369:VAL:HG12	1.93	0.49
4:G:250:ASP:OD1	4:G:251:ARG:N	2.45	0.49
4:G:274:PRO:HB3	4:G:287:LEU:HD23	1.93	0.49
5:I:136:LYS:NZ	5:I:163:GLU:OE1	2.26	0.49
1:M:12:VAL:HG23	1:M:119:VAL:HG13	1.92	0.49
1:M:43:PRO:HD3	1:M:93:ALA:HA	1.94	0.49
3:C:184:VAL:HG22	3:C:261:ILE:HG21	1.93	0.49
4:F:398:THR:O	4:F:402:LEU:HG	2.12	0.49
1:O:172:HIS:NE2	2:P:175:SER:OG	2.23	0.49
2:P:88:CYS:O	2:P:100:GLY:N	2.45	0.49
2:T:101:GLN:CD	2:T:101:GLN:H	2.19	0.49
3:B:417:VAL:HG21	4:F:378:LEU:HD13	1.94	0.49
4:E:13:ARG:HD3	4:E:234:LYS:HB2	1.95	0.49
4:F:402:LEU:HD22	5:J:164:CYS:HB3	1.95	0.49
4:H:192:VAL:HG11	4:H:213:THR:HA	1.94	0.49
2:T:11:LEU:HB2	2:T:105:LEU:HD12	1.94	0.49
3:B:312:PHE:CD2	3:B:340:ARG:HD3	2.48	0.49
5:K:203:ILE:HD12	5:K:207:ALA:HB3	1.93	0.49
1:Q:16:GLU:O	1:Q:87:VAL:HG23	2.13	0.49
2:R:182:LEU:HB3	2:R:186:ASP:HB2	1.94	0.49
1:O:77:LYS:HE3	1:O:79:HIS:CD2	2.47	0.49
2:T:8:PRO:HG2	2:T:11:LEU:HG	1.95	0.49
5:L:187:TYR:HD2	5:L:219:ASP:HA	1.77	0.49
2:N:19:ALA:HB2	2:N:78:LEU:HD11	1.94	0.49
4:G:212:THR:HG22	2:R:92:GLY:HA2	1.95	0.49
5:L:119:HIS:HB2	5:L:124:THR:HG23	1.95	0.49
2:R:35:TRP:CZ3	2:R:88:CYS:HB3	2.47	0.49
3:B:95:PHE:HZ	4:F:224:GLN:HA	1.76	0.48
4:E:390:MET:N	4:E:390:MET:HE2	2.28	0.48
5:I:179:THR:HG22	5:I:181:GLU:HG3	1.94	0.48
1:O:150:VAL:HG11	1:O:158:VAL:HG21	1.95	0.48
3:D:320:TYR:HD2	3:D:352:LEU:HD22	1.78	0.48
4:E:215:LYS:HE2	2:N:93:ASN:HD21	1.78	0.48
4:G:251:ARG:NH2	1:Q:103:TRP:HA	2.27	0.48
5:J:187:TYR:HB3	5:J:218:PHE:O	2.13	0.48
5:L:144:ILE:HG21	5:L:149:LEU:HB2	1.94	0.48
2:P:38:GLN:O	2:P:84:ALA:HB1	2.13	0.48
2:N:16:GLY:N	2:N:78:LEU:O	2.43	0.48
3:C:173:PHE:HE1	3:C:184:VAL:HG21	1.78	0.48
3:D:258:GLY:HA2	4:H:298:ARG:HH21	1.78	0.48
5:I:118:LYS:NZ	5:I:145:ASP:HB3	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:134:PRO:HD3	1:Q:146:LEU:HB3	1.94	0.48
2:N:148:GLN:HB3	2:N:155:LEU:HD11	1.94	0.48
2:T:109:ARG:HH22	2:T:173:THR:HG22	1.78	0.48
3:B:18:LEU:HD22	3:B:331:HIS:CE1	2.49	0.48
3:C:70:ASP:OD2	3:C:71:LYS:N	2.47	0.48
2:P:124:GLU:HA	2:P:127:LYS:HE2	1.95	0.48
3:A:93:TYR:HA	4:E:176:PRO:HG2	1.96	0.48
5:I:203:ILE:HD12	5:I:207:ALA:HB3	1.94	0.48
2:R:4:MET:HG3	2:R:100:GLY:HA2	1.96	0.48
2:R:124:GLU:H	2:R:124:GLU:CD	2.21	0.48
2:P:168:ASP:HB3	2:P:173:THR:H	1.79	0.48
3:B:176:LYS:HD3	3:B:189:TYR:CE1	2.49	0.48
1:M:155:PRO:HD2	1:M:210:PRO:HB2	1.96	0.48
4:F:202:ASN:OD1	4:F:224:GLN:HB2	2.13	0.48
4:G:13:ARG:CZ	4:G:70:MET:HE1	2.43	0.48
4:G:367:THR:HA	12:G:501:CLR:H183	1.95	0.48
5:J:182:LYS:HZ1	5:J:245:TRP:H	1.62	0.48
1:Q:39:ILE:HD13	1:Q:49:TRP:HA	1.96	0.48
4:E:177:ASP:HB3	4:E:180:LEU:HG	1.95	0.48
4:F:272:ARG:NH1	4:F:290:ASP:OD1	2.46	0.48
4:H:69:TYR:OH	4:H:117:ASP:OD1	2.31	0.48
5:J:134:VAL:HG13	5:J:167:ILE:HG12	1.96	0.48
2:R:127:LYS:HD3	2:R:127:LYS:N	2.28	0.48
2:N:135:CYS:HB3	2:N:178:SER:HB3	1.95	0.48
5:J:195:GLN:OE1	5:J:237:ARG:NH2	2.46	0.48
5:K:180:HIS:O	5:K:182:LYS:NZ	2.47	0.48
4:E:40:GLU:OE1	4:E:156:TYR:OH	2.24	0.47
4:E:210:LEU:HD23	4:E:210:LEU:H	1.79	0.47
5:L:152:LEU:HD22	5:L:165:ALA:HB1	1.96	0.47
2:N:18:ARG:HG3	2:N:76:SER:HA	1.94	0.47
3:B:68:CYS:HB3	3:B:103:LEU:HD11	1.97	0.47
3:C:318:ILE:HB	3:C:352:LEU:CD2	2.44	0.47
2:N:145:ALA:HB2	2:N:199:HIS:HD2	1.78	0.47
3:A:318:ILE:HD13	3:A:374:VAL:HG21	1.95	0.47
4:F:192:VAL:HG13	4:F:195:GLN:O	2.14	0.47
5:J:187:TYR:HD2	5:J:219:ASP:HA	1.78	0.47
5:L:171:MET:HE1	5:L:172:LYS:HE3	1.96	0.47
2:R:114:PRO:HB3	2:R:140:PHE:HB3	1.94	0.47
2:R:187:TYR:O	2:R:212:ARG:NH1	2.47	0.47
1:S:132:LEU:HD22	1:S:149:LEU:HD21	1.95	0.47
2:T:109:ARG:HG2	2:T:110:THR:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:185:TYR:C	3:D:186:ASN:HD22	2.22	0.47
4:G:393:ARG:CZ	4:G:417:CYS:HB2	2.44	0.47
1:Q:65:LEU:O	1:Q:69:VAL:HG12	2.15	0.47
2:R:126:LEU:HB3	2:R:184:LYS:HZ2	1.79	0.47
3:A:76:TYR:OH	3:A:78:CYS:SG	2.64	0.47
3:B:167:SER:OG	3:B:275:ASN:N	2.43	0.47
3:C:138:GLN:OE1	3:C:138:GLN:HA	2.15	0.47
4:E:166:GLU:N	4:E:166:GLU:OE2	2.48	0.47
5:K:126:TYR:OH	5:K:215:ARG:NH2	2.48	0.47
5:L:201:PHE:HB2	5:L:240:LEU:HB3	1.96	0.47
1:O:50:ILE:HD12	1:O:50:ILE:H	1.78	0.47
1:O:50:ILE:HG22	1:O:69:VAL:HG11	1.97	0.47
2:T:18:ARG:HA	2:T:75:ILE:O	2.15	0.47
2:T:191:LYS:HD2	2:T:212:ARG:HB3	1.97	0.47
3:C:337:VAL:HG22	3:C:358:THR:HB	1.97	0.47
4:G:363:TYR:HB3	12:G:501:CLR:H11	1.96	0.47
4:H:252:LYS:HB3	4:H:254:LYS:NZ	2.30	0.47
5:J:259:GLU:OE1	5:J:259:GLU:N	2.35	0.47
1:Q:132:LEU:HD11	1:Q:149:LEU:HG	1.97	0.47
2:R:166:GLU:H	2:R:166:GLU:CD	2.20	0.47
2:P:37:GLN:O	2:P:45:ARG:N	2.33	0.47
2:P:75:ILE:HG21	2:P:78:LEU:HD23	1.95	0.47
2:N:184:LYS:NZ	2:N:188:GLU:OE1	2.30	0.47
1:S:50:ILE:HG22	1:S:69:VAL:HG21	1.97	0.47
1:Q:124:THR:HG22	1:Q:154:PHE:HD1	1.79	0.47
3:B:304:PRO:HG2	3:D:291:VAL:HG12	1.97	0.47
4:G:170:HIS:CD2	4:G:249:GLY:HA3	2.50	0.47
4:G:359:TYR:HD2	12:G:501:CLR:H122	1.78	0.47
4:G:394:ARG:HG3	4:G:395:ARG:N	2.29	0.47
5:K:246:ASN:OD1	5:K:247:LYS:HE2	2.15	0.47
1:Q:207:ASN:OD1	1:Q:214:LYS:HG2	2.14	0.47
1:M:40:ARG:HG2	1:M:50:ILE:HD11	1.97	0.47
2:T:81:GLU:OE1	2:T:81:GLU:N	2.47	0.47
3:B:424:ALA:HB1	4:F:388:MET:HE1	1.96	0.47
3:C:296:LEU:HG	3:C:370:CYS:HB2	1.97	0.47
12:E:501:CLR:H222	12:E:501:CLR:H162	1.52	0.47
5:J:154:PHE:HB3	5:J:163:GLU:HB3	1.97	0.47
2:P:36:TYR:HE1	2:P:89:GLN:NE2	2.12	0.47
3:B:135:VAL:HB	3:B:142:ILE:HG22	1.96	0.46
3:B:162:ILE:CG2	3:B:279:SER:HB2	2.43	0.46
4:E:6:PHE:CD2	4:E:56:ILE:HD11	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:127:PRO:HB2	1:Q:150:VAL:HG23	1.96	0.46
1:S:153:TYR:CE1	1:S:184:TYR:HB2	2.50	0.46
4:E:394:ARG:HH12	4:E:395:ARG:HH21	1.63	0.46
4:F:199:TYR:HA	4:F:226:HIS:O	2.15	0.46
4:G:398:THR:O	4:G:402:LEU:HG	2.14	0.46
5:K:201:PHE:CD1	5:K:242:VAL:HG11	2.50	0.46
5:L:119:HIS:HB2	5:L:124:THR:CG2	2.45	0.46
5:L:156:ARG:NH2	5:L:158:SER:HB2	2.24	0.46
1:Q:100:ARG:NH1	1:Q:109:ASP:OD1	2.40	0.46
1:O:33:SER:HA	1:O:55:TYR:CE1	2.50	0.46
3:C:176:LYS:NZ	3:D:151:ASP:OD1	2.28	0.46
4:E:139:GLU:OE1	4:E:291:HIS:NE2	2.45	0.46
1:S:88:THR:HG23	1:S:90:ALA:H	1.80	0.46
3:C:37:THR:HG23	3:C:267:ARG:HB3	1.98	0.46
5:I:179:THR:CG2	5:I:181:GLU:HG3	2.45	0.46
5:L:155:LYS:HB2	5:L:155:LYS:NZ	2.30	0.46
3:B:404:ALA:C	3:B:406:ALA:H	2.24	0.46
4:F:172:PRO:HD3	4:F:235:TRP:HA	1.97	0.46
2:R:33:LEU:HD13	2:R:71:PHE:CD1	2.50	0.46
2:R:109:ARG:HG2	2:R:110:THR:N	2.30	0.46
3:B:121:ALA:HB1	3:B:189:TYR:CD2	2.51	0.46
3:D:401:ASP:OD2	3:D:401:ASP:N	2.49	0.46
2:R:35:TRP:CE2	2:R:73:LEU:HB2	2.51	0.46
2:R:184:LYS:O	2:R:188:GLU:HG3	2.16	0.46
1:O:135:SER:N	1:O:138:SER:OG	2.36	0.46
2:N:37:GLN:HB2	2:N:47:LEU:HD22	1.97	0.46
4:E:100:PHE:CZ	4:E:257:ILE:HG12	2.51	0.46
4:G:117:ASP:OD1	4:G:118:SER:N	2.46	0.46
2:R:61:ARG:NH2	2:R:82:ASP:OD2	2.44	0.46
1:M:74:ASP:OD1	1:M:74:ASP:N	2.48	0.46
3:A:333:MET:HE1	3:A:368:GLN:HB2	1.98	0.46
3:B:299:MET:HA	3:B:319:LYS:O	2.16	0.46
3:B:416:GLY:O	3:B:420:VAL:HG13	2.15	0.46
3:D:202:ASP:OD2	3:D:203:ILE:N	2.48	0.46
5:L:125:GLY:HA3	5:L:140:VAL:HG11	1.98	0.46
2:R:2:ILE:HG21	2:R:90:GLN:NE2	2.30	0.46
3:B:255:ALA:O	4:F:298:ARG:NH1	2.49	0.46
5:I:134:VAL:HG13	5:I:167:ILE:HG12	1.98	0.46
5:L:189:TRP:HB2	5:L:194:VAL:HG13	1.98	0.46
1:Q:34:TYR:HE1	1:Q:36:TRP:CH2	2.34	0.46
2:P:36:TYR:CE1	2:P:89:GLN:NE2	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:254:THR:HG22	4:F:306:TYR:CG	2.51	0.45
3:C:151:ASP:OD1	3:C:152:HIS:N	2.40	0.45
4:H:169:VAL:HG13	4:H:236:GLN:C	2.42	0.45
5:K:144:ILE:HG21	5:K:149:LEU:HB2	1.97	0.45
1:Q:135:SER:HB2	1:Q:137:LYS:HE3	1.98	0.45
3:D:320:TYR:CD2	3:D:352:LEU:HD22	2.52	0.45
4:H:162:ALA:HA	4:H:256:HIS:CD2	2.50	0.45
1:Q:12:VAL:HG13	1:Q:119:VAL:HG22	1.97	0.45
1:Q:127:PRO:HB3	1:Q:153:TYR:HB3	1.97	0.45
2:P:184:LYS:NZ	2:P:188:GLU:OE2	2.48	0.45
2:N:50:ASP:OD1	2:N:50:ASP:O	2.34	0.45
2:N:121:PRO:HD3	2:N:133:VAL:HG22	1.98	0.45
1:S:178:LEU:HD13	1:S:184:TYR:CD1	2.51	0.45
3:B:387:ILE:HD13	4:F:340:PRO:HA	1.97	0.45
4:F:221:LYS:HG3	4:F:224:GLN:NE2	2.31	0.45
5:I:117:VAL:C	5:I:118:LYS:HD3	2.42	0.45
5:J:245:TRP:NE1	5:J:250:VAL:HG12	2.31	0.45
1:Q:61:TYR:CE1	1:Q:71:ILE:HG13	2.51	0.45
2:P:193:TYR:HB2	2:P:210:PHE:CE1	2.51	0.45
3:C:296:LEU:HD22	3:C:322:ALA:HA	1.99	0.45
4:E:213:THR:HG23	2:N:92:GLY:O	2.16	0.45
5:K:255:PRO:HD2	5:K:255:PRO:O	2.17	0.45
1:Q:94:VAL:HG12	1:Q:116:LEU:HD22	1.98	0.45
1:Q:177:VAL:O	1:Q:179:GLN:NE2	2.49	0.45
3:B:47:ILE:HG13	3:B:208:PRO:HD3	1.97	0.45
5:J:183:PRO:O	5:J:187:TYR:OH	2.20	0.45
4:E:102:LEU:HD22	4:E:259:PHE:CG	2.52	0.45
4:E:210:LEU:HD21	2:N:94:TRP:CZ2	2.52	0.45
4:G:216:VAL:HG12	4:G:218:ASN:H	1.80	0.45
5:K:139:HIS:HD1	5:K:161:ASP:CG	2.25	0.45
5:L:212:ASP:OD1	5:L:215:ARG:NH1	2.50	0.45
1:Q:107:TYR:CE2	2:R:49:TYR:HB2	2.52	0.45
1:O:29:ILE:HG21	1:O:75:THR:HG22	1.97	0.45
3:A:62:CYS:HB2	3:A:96:CYS:CB	2.46	0.45
3:C:397:LEU:HD13	4:G:363:TYR:HE1	1.81	0.45
12:D:501:CLR:H161	4:H:359:TYR:CD2	2.52	0.45
4:E:284:ILE:HG12	4:E:318:VAL:HG22	1.99	0.45
5:I:114:ILE:HG23	5:I:126:TYR:CE2	2.52	0.45
5:J:215:ARG:NH1	5:J:215:ARG:HG2	2.32	0.45
5:K:201:PHE:HD1	5:K:242:VAL:HG11	1.81	0.45
1:Q:120:SER:HB2	1:Q:182:GLY:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:14:PRO:HD2	1:S:121:SER:HB2	1.99	0.45
4:G:34:LEU:HD12	4:G:50:VAL:HG12	1.98	0.45
5:J:155:LYS:O	5:J:163:GLU:HA	2.16	0.45
1:O:160:VAL:HG11	1:O:188:SER:HB3	1.99	0.45
2:N:80:PRO:HD2	2:N:81:GLU:N	2.31	0.45
3:A:75:ASP:O	3:A:107:HIS:HA	2.17	0.45
3:A:104:SER:HB2	3:A:231:VAL:HG13	1.97	0.45
12:B:501:CLR:H222	12:B:501:CLR:H162	1.68	0.45
3:C:46:TYR:O	3:C:47:ILE:HD13	2.17	0.45
4:E:235:TRP:CD1	4:E:235:TRP:N	2.85	0.45
4:E:370:VAL:HG11	12:E:501:CLR:H151	1.98	0.45
4:E:391:CYS:O	4:E:394:ARG:HG2	2.17	0.45
5:J:194:VAL:HG12	5:J:203:ILE:CG2	2.47	0.45
1:Q:6:GLU:OE1	1:Q:6:GLU:N	2.49	0.45
2:P:2:ILE:HD11	2:P:27:GLN:HB2	1.99	0.45
1:M:39:ILE:HG22	1:M:49:TRP:HD1	1.82	0.45
2:N:3:GLN:HA	2:N:98:THR:HG21	1.97	0.45
3:A:116:THR:HB	4:E:261:LEU:HD22	1.98	0.45
3:C:296:LEU:HD21	3:C:346:VAL:HG21	1.98	0.45
4:G:396:CYS:C	4:G:397:ILE:HD13	2.42	0.45
1:Q:63:PRO:HD2	2:R:96:PRO:HB3	1.99	0.45
1:Q:63:PRO:HA	1:Q:66:LYS:HD2	1.97	0.45
5:J:139:HIS:CE1	5:J:140:VAL:HG13	2.52	0.44
5:L:114:ILE:HD13	5:L:114:ILE:HA	1.81	0.44
1:M:49:TRP:O	1:M:62:ASN:ND2	2.43	0.44
3:A:436:PHE:O	3:A:439:HIS:NE2	2.51	0.44
3:B:62:CYS:HB2	3:B:96:CYS:SG	2.57	0.44
4:E:199:TYR:HA	4:E:226:HIS:O	2.18	0.44
4:G:91:CYS:SG	4:G:103:ALA:HB1	2.57	0.44
4:G:251:ARG:HH21	1:Q:103:TRP:HA	1.82	0.44
2:R:119:PHE:HB2	2:R:134:VAL:HB	1.98	0.44
2:P:6:GLN:H	2:P:101:GLN:NE2	2.05	0.44
2:N:79:GLU:HB3	2:N:80:PRO:HD3	1.99	0.44
2:T:38:GLN:HB2	2:T:44:PRO:HB3	1.99	0.44
3:D:310:SER:HB3	3:D:392:ALA:HA	1.99	0.44
2:P:146:LYS:HB3	2:P:198:THR:HB	1.99	0.44
3:B:133:LEU:HB3	3:B:144:VAL:HG22	1.99	0.44
4:H:181:MET:HB3	4:H:222:VAL:HG23	1.99	0.44
2:T:89:GLN:HB2	2:T:99:PHE:CE1	2.51	0.44
4:E:201:CYS:HB2	4:E:207:ASN:OD1	2.16	0.44
4:F:58:THR:HG1	4:F:77:ASP:CG	2.23	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:280:LYS:HB2	9:b:1:NAG:H83	2.00	0.44
5:L:116:GLU:CD	5:L:116:GLU:H	2.26	0.44
1:Q:29:ILE:HG23	1:Q:36:TRP:NE1	2.33	0.44
1:S:128:SER:HB2	1:S:151:LYS:O	2.17	0.44
3:D:133:LEU:HB3	3:D:144:VAL:HG23	1.98	0.44
4:E:112:THR:HA	4:E:125:CYS:O	2.17	0.44
4:E:408:VAL:HG23	4:E:412:LEU:HD23	1.99	0.44
5:J:134:VAL:CG1	5:J:167:ILE:HG12	2.48	0.44
5:J:181:GLU:OE2	5:J:183:PRO:HD3	2.17	0.44
5:K:171:MET:HE1	5:K:172:LYS:NZ	2.32	0.44
4:F:9:TYR:CZ	4:F:98:GLY:HA3	2.53	0.44
4:F:306:TYR:OH	4:F:308:GLU:OE1	2.24	0.44
4:G:276:VAL:HG22	4:G:285:MET:HG2	2.00	0.44
5:K:223:ARG:HB2	5:K:223:ARG:HH11	1.82	0.44
5:L:118:LYS:HE3	5:L:118:LYS:HB3	1.72	0.44
5:L:156:ARG:HA	5:L:163:GLU:OE2	2.17	0.44
1:Q:88:THR:HG23	1:Q:90:ALA:H	1.82	0.44
2:R:6:GLN:H	2:R:101:GLN:HE22	1.65	0.44
2:R:133:VAL:HG13	2:R:180:LEU:HB3	1.99	0.44
1:M:94:VAL:HG22	1:M:116:LEU:HB2	1.99	0.44
2:N:33:LEU:HD13	2:N:71:PHE:CD1	2.53	0.44
1:S:178:LEU:HD13	1:S:184:TYR:HD1	1.83	0.44
3:C:176:LYS:HB3	3:C:189:TYR:CE2	2.53	0.44
3:C:195:GLY:H	3:C:214:TYR:HE2	1.66	0.44
3:C:361:ALA:HB3	3:C:404:ALA:HB2	2.00	0.44
4:E:112:THR:HG22	4:E:126:THR:HG23	1.99	0.44
4:E:167:ILE:HG23	4:E:257:ILE:HD11	1.99	0.44
4:G:6:PHE:HB3	4:G:56:ILE:HD11	1.99	0.44
4:H:74:MET:HE3	4:H:74:MET:HB3	1.90	0.44
4:H:170:HIS:CE1	4:H:238:ASN:HB3	2.53	0.44
1:Q:125:LYS:NZ	1:Q:152:ASP:O	2.51	0.44
2:R:188:GLU:HA	2:R:212:ARG:HH12	1.83	0.44
1:S:65:LEU:O	1:S:69:VAL:HG12	2.18	0.44
3:B:400:GLN:HG3	3:B:400:GLN:O	2.18	0.44
3:C:328:CYS:SG	3:C:370:CYS:N	2.91	0.44
4:E:192:VAL:HG21	4:E:212:THR:O	2.18	0.44
4:E:398:THR:OG1	4:E:399:PRO:HD3	2.17	0.44
4:G:139:GLU:HG2	4:G:293:THR:HG23	2.00	0.44
4:G:171:MET:HE2	4:G:171:MET:HB2	1.71	0.44
4:G:362:LEU:HD23	4:G:362:LEU:HA	1.70	0.44
5:K:189:TRP:CZ2	5:K:191:HIS:HB2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:126:LEU:HD22	2:R:184:LYS:NZ	2.29	0.44
1:O:143:THR:HG22	1:O:191:THR:HG22	2.00	0.44
2:P:164:VAL:HG22	2:P:176:LEU:HD12	2.00	0.44
3:A:244:LEU:HA	3:A:247:ARG:HG3	2.00	0.43
5:I:127:ALA:CB	5:I:136:LYS:HB3	2.48	0.43
5:J:116:GLU:N	5:J:116:GLU:CD	2.76	0.43
5:J:149:LEU:HA	5:J:152:LEU:HG	2.00	0.43
2:N:6:GLN:NE2	2:N:103:THR:HG23	2.32	0.43
3:C:30:GLU:OE2	3:C:134:ARG:NH2	2.42	0.43
3:D:185:TYR:OH	3:D:247:ARG:HD2	2.19	0.43
4:H:208:GLU:OE1	4:H:208:GLU:N	2.51	0.43
5:J:116:GLU:CD	5:J:116:GLU:H	2.27	0.43
1:O:159:THR:HB	1:O:207:ASN:HB2	2.00	0.43
1:M:3:GLN:HB2	1:M:25:SER:OG	2.18	0.43
3:A:34:LEU:HD12	3:A:132:LYS:HG2	2.00	0.43
3:D:383:PRO:HD2	4:H:342:LEU:O	2.18	0.43
4:E:204:GLY:O	4:E:206:SER:N	2.45	0.43
5:L:187:TYR:HB2	5:L:194:VAL:CG2	2.48	0.43
1:M:13:LYS:HB2	1:M:16:GLU:OE2	2.18	0.43
1:M:100:ARG:HB2	1:M:107:TYR:O	2.18	0.43
3:C:185:TYR:OH	3:C:247:ARG:HD2	2.17	0.43
4:F:138:ARG:NH2	4:F:296:SER:OG	2.51	0.43
5:J:215:ARG:HG2	5:J:215:ARG:HH11	1.82	0.43
5:K:195:GLN:OE1	5:K:237:ARG:NH2	2.49	0.43
1:M:92:THR:HG23	1:M:118:THR:HA	2.00	0.43
2:T:156:GLN:OE1	2:T:159:ASN:ND2	2.52	0.43
3:C:32:GLU:OE1	3:C:134:ARG:NH2	2.41	0.43
3:C:137:TYR:OH	3:C:283:PRO:HD2	2.18	0.43
4:E:233:LYS:HB2	4:E:233:LYS:HE2	1.79	0.43
4:G:187:ASN:HA	4:G:218:ASN:O	2.18	0.43
4:H:394:ARG:O	4:H:398:THR:HG23	2.18	0.43
5:I:195:GLN:OE1	5:I:195:GLN:HA	2.18	0.43
1:Q:49:TRP:CE3	2:R:97:ILE:HG22	2.54	0.43
1:O:209:LYS:HD2	1:O:209:LYS:N	2.33	0.43
4:F:181:MET:HE1	4:F:225:CYS:C	2.43	0.43
5:K:111:ASN:O	5:K:114:ILE:HG12	2.17	0.43
1:Q:49:TRP:HE1	1:Q:51:GLY:C	2.26	0.43
1:Q:120:SER:O	1:Q:182:GLY:HA3	2.19	0.43
3:A:254:THR:O	3:A:254:THR:OG1	2.33	0.43
3:C:225:ALA:H	3:C:230:HIS:CE1	2.30	0.43
4:E:172:PRO:HB3	4:E:236:GLN:CD	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:232:ALA:O	5:J:238:THR:HA	2.18	0.43
1:Q:33:SER:HB3	1:Q:55:TYR:CE1	2.53	0.43
2:P:114:PRO:HA	2:P:140:PHE:HB3	2.00	0.43
1:S:152:ASP:HA	1:S:183:LEU:HB3	1.99	0.43
3:B:40:PRO:HA	3:B:127:ALA:HA	2.01	0.43
4:G:174:ASP:O	4:G:176:PRO:HD3	2.19	0.43
4:G:359:TYR:CD2	12:G:501:CLR:H17	2.53	0.43
4:G:402:LEU:HD22	5:K:162:LEU:HD23	2.01	0.43
5:I:168:PRO:HB2	5:I:170:HIS:CE1	2.54	0.43
5:J:189:TRP:CZ2	5:J:191:HIS:HB2	2.53	0.43
5:J:245:TRP:CD1	5:J:250:VAL:HG12	2.54	0.43
5:L:136:LYS:NZ	5:L:140:VAL:O	2.47	0.43
1:Q:154:PHE:HB2	1:Q:183:LEU:HD13	2.01	0.43
2:P:109:ARG:HG2	2:P:110:THR:H	1.83	0.43
2:N:137:LEU:HD11	2:N:197:VAL:HG21	2.00	0.43
2:T:11:LEU:O	2:T:106:ASP:N	2.42	0.43
3:D:47:ILE:HD13	3:D:47:ILE:HA	1.85	0.43
4:G:306:TYR:OH	4:G:308:GLU:OE1	2.24	0.43
4:G:398:THR:OG1	4:G:399:PRO:HD3	2.19	0.43
4:H:192:VAL:HG23	4:H:195:GLN:O	2.18	0.43
3:A:173:PHE:HB3	3:A:177:ILE:HD11	2.00	0.43
3:C:52:LYS:HG3	4:G:36:ARG:HH12	1.82	0.43
4:G:391:CYS:HA	4:G:394:ARG:HG2	2.00	0.43
4:H:344:THR:HG21	4:H:358:TYR:CD2	2.54	0.43
4:H:403:THR:OG1	4:H:406:ALA:HB3	2.17	0.43
5:I:213:SER:HB2	5:I:261:TRP:HB2	2.00	0.43
5:J:157:SER:O	5:J:161:ASP:N	2.52	0.43
5:K:241:SER:HB3	5:K:255:PRO:HD3	2.00	0.43
1:M:14:PRO:HD3	1:M:119:VAL:HG12	2.01	0.43
2:N:193:TYR:HB2	2:N:210:PHE:CE1	2.54	0.43
3:C:333:MET:HB2	3:C:366:ARG:HB2	2.01	0.42
4:F:397:ILE:HD11	4:F:418:ILE:HD13	2.00	0.42
4:G:417:CYS:HA	4:G:419:ARG:HE	1.83	0.42
4:H:13:ARG:NH1	4:H:70:MET:HE3	2.30	0.42
1:M:3:GLN:HB2	1:M:25:SER:HG	1.84	0.42
1:M:149:LEU:HD11	1:M:185:SER:HB2	2.00	0.42
2:N:186:ASP:HA	2:N:189:LYS:HG2	2.01	0.42
4:F:170:HIS:ND1	4:F:238:ASN:HB3	2.34	0.42
5:K:119:HIS:CD2	5:K:120:GLU:HG3	2.53	0.42
4:F:254:LYS:HD2	4:F:254:LYS:C	2.44	0.42
5:J:215:ARG:O	5:J:228:VAL:HG22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:122:SER:O	2:R:126:LEU:HG	2.20	0.42
1:M:77:LYS:HD3	1:M:77:LYS:O	2.19	0.42
1:M:155:PRO:O	1:M:208:HIS:NE2	2.34	0.42
1:S:12:VAL:O	1:S:119:VAL:HA	2.19	0.42
3:B:182:GLY:HA2	3:B:263:THR:OG1	2.20	0.42
3:C:170:TRP:CZ2	3:C:256:PRO:HG2	2.54	0.42
4:E:102:LEU:HD12	4:E:102:LEU:HA	1.86	0.42
4:E:171:MET:HE2	4:E:171:MET:HB2	1.97	0.42
4:H:188:VAL:HG22	4:H:217:ILE:HB	2.02	0.42
1:Q:222:LYS:O	1:Q:226:LYS:HG3	2.19	0.42
2:R:49:TYR:CD1	2:R:50:ASP:HB2	2.52	0.42
3:D:47:ILE:HD13	3:D:120:SER:HA	2.00	0.42
3:D:192:PHE:HA	3:D:204:GLN:OE1	2.20	0.42
12:D:501:CLR:H8	12:D:501:CLR:H182	1.75	0.42
4:F:212:THR:HG21	2:P:32:SER:OG	2.20	0.42
1:S:66:LYS:HB2	1:S:66:LYS:HE3	1.61	0.42
2:T:196:GLU:OE2	2:T:207:THR:OG1	2.27	0.42
3:B:397:LEU:HD13	12:B:501:CLR:C19	2.50	0.42
4:E:165:GLU:OE1	4:E:165:GLU:HA	2.19	0.42
4:E:344:THR:HG21	4:E:358:TYR:CD1	2.54	0.42
4:F:42:THR:HB	4:F:136:ILE:HD11	2.02	0.42
4:H:306:TYR:OH	4:H:308:GLU:OE1	2.24	0.42
5:K:201:PHE:HB2	5:K:240:LEU:HB2	2.01	0.42
5:L:179:THR:OG1	5:L:223:ARG:NE	2.53	0.42
1:Q:41:GLN:O	1:Q:94:VAL:HG22	2.19	0.42
2:R:123:ASP:HB3	2:R:127:LYS:NZ	2.35	0.42
2:T:181:THR:O	2:T:182:LEU:HD23	2.20	0.42
3:B:8:PRO:HD2	3:B:15:TYR:CE1	2.55	0.42
3:B:289:ARG:HD2	3:B:289:ARG:HA	1.71	0.42
4:G:18:HIS:CE1	4:G:27:SER:HB2	2.54	0.42
4:G:145:PRO:HG3	4:G:269:PRO:HB3	2.01	0.42
5:L:118:LYS:HG2	5:L:123:VAL:HG22	2.00	0.42
1:Q:77:LYS:HE2	1:Q:77:LYS:HB3	1.75	0.42
2:T:190:HIS:O	2:T:212:ARG:NE	2.44	0.42
3:B:18:LEU:HD12	3:B:18:LEU:HA	1.86	0.42
3:B:312:PHE:HA	3:B:357:SER:HB2	2.02	0.42
3:C:343:GLU:OE1	3:C:343:GLU:C	2.63	0.42
3:D:254:THR:HG22	4:H:306:TYR:CG	2.55	0.42
3:D:407:MET:HA	3:D:410:VAL:CG1	2.49	0.42
4:F:251:ARG:HD2	4:F:251:ARG:HA	1.86	0.42
4:F:307:GLN:OE1	4:F:307:GLN:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:379:LEU:O	4:H:382:VAL:HG12	2.19	0.42
4:H:414:LEU:HD23	4:H:414:LEU:HA	1.92	0.42
5:I:182:LYS:NZ	5:I:196:TYR:OH	2.42	0.42
5:I:196:TYR:OH	5:I:199:GLY:HA2	2.19	0.42
1:M:29:ILE:HG21	1:M:75:THR:HA	2.02	0.42
3:C:70:ASP:OD2	3:C:70:ASP:C	2.62	0.42
4:G:192:VAL:HG11	4:G:213:THR:HA	2.01	0.42
5:K:155:LYS:O	5:K:163:GLU:HA	2.20	0.42
5:K:183:PRO:O	5:K:187:TYR:OH	2.28	0.42
3:C:123:ARG:HH12	3:C:176:LYS:HE2	1.85	0.42
3:C:218:GLN:O	3:C:218:GLN:HG3	2.20	0.42
3:D:359:ALA:HB2	3:D:394:HIS:CE1	2.55	0.42
4:E:146:GLN:OE1	4:F:18:HIS:ND1	2.39	0.42
4:E:174:ASP:O	4:E:176:PRO:HD3	2.20	0.42
4:E:200:LYS:HB3	4:E:200:LYS:HE2	1.60	0.42
4:F:400:TYR:CD1	4:F:408:VAL:HG22	2.52	0.42
5:L:189:TRP:C	5:L:191:HIS:H	2.28	0.42
1:M:95:TYR:O	1:M:114:GLY:HA3	2.19	0.42
2:N:55:ALA:HB3	2:N:58:ILE:HD12	2.01	0.42
2:T:118:ILE:HB	2:T:208:LYS:HD2	2.01	0.41
3:D:21:ARG:NH2	3:D:284:GLU:OE1	2.53	0.41
4:F:287:LEU:O	4:F:314:LYS:HA	2.20	0.41
4:G:139:GLU:OE1	4:G:291:HIS:NE2	2.45	0.41
5:I:203:ILE:HB	5:I:204:PRO:HD3	2.02	0.41
5:K:167:ILE:O	5:K:169:VAL:N	2.52	0.41
1:O:80:PHE:CZ	1:O:97:CYS:HB2	2.55	0.41
2:P:35:TRP:HB2	2:P:48:ILE:HB	2.00	0.41
3:B:105:GLU:OE2	4:F:244:ARG:NH1	2.52	0.41
3:B:265:PRO:O	3:B:267:ARG:HD3	2.20	0.41
12:B:501:CLR:H161	4:F:367:THR:HA	2.02	0.41
4:E:348:ALA:HA	4:E:355:ILE:HD13	2.01	0.41
4:H:403:THR:HG21	5:L:248:ASP:O	2.20	0.41
5:K:252:LYS:C	5:K:253:ILE:HD13	2.45	0.41
1:O:221:PRO:O	1:O:226:LYS:HE3	2.20	0.41
3:A:250:SER:O	3:A:254:THR:HG22	2.20	0.41
3:B:5:THR:HG21	3:B:31:MET:HE1	2.02	0.41
3:B:424:ALA:CB	4:F:388:MET:HE1	2.50	0.41
3:D:361:ALA:H	3:D:402:ILE:HD12	1.85	0.41
4:E:235:TRP:CZ3	4:E:251:ARG:HG3	2.55	0.41
4:G:210:LEU:HD13	2:R:94:TRP:CZ2	2.55	0.41
4:G:409:PRO:HD2	4:G:412:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:156:ARG:HH22	5:I:158:SER:N	2.17	0.41
5:J:246:ASN:OD1	5:J:246:ASN:C	2.62	0.41
5:L:122:LYS:NZ	5:L:123:VAL:O	2.51	0.41
5:L:160:TYR:HA	5:L:252:LYS:HE2	2.01	0.41
5:L:189:TRP:HB2	5:L:194:VAL:CG1	2.51	0.41
5:L:203:ILE:HG22	5:L:204:PRO:O	2.20	0.41
1:Q:200:GLN:OE1	1:Q:200:GLN:HA	2.20	0.41
2:T:13:LEU:N	2:T:106:ASP:O	2.47	0.41
2:T:24:ARG:HA	2:T:69:THR:O	2.20	0.41
3:A:27:MET:HE3	3:A:27:MET:HB3	1.80	0.41
3:B:209:GLU:OE2	3:B:209:GLU:N	2.53	0.41
3:D:306:CYS:HA	3:D:314:GLY:HA2	2.02	0.41
4:G:363:TYR:CB	12:G:501:CLR:H112	2.49	0.41
5:J:187:TYR:HB2	5:J:194:VAL:CG2	2.49	0.41
2:R:49:TYR:CD1	2:R:49:TYR:C	2.98	0.41
2:R:108:LYS:HA	2:R:141:TYR:OH	2.20	0.41
2:P:32:SER:HB3	2:P:91:ARG:HG2	2.02	0.41
1:M:39:ILE:HG22	1:M:49:TRP:HA	2.01	0.41
3:A:325:LYS:HA	3:A:346:VAL:O	2.21	0.41
3:C:298:ASP:OD1	3:C:298:ASP:O	2.39	0.41
4:F:398:THR:OG1	4:F:399:PRO:HD3	2.20	0.41
4:H:283:VAL:HG13	4:H:319:LEU:HB2	2.01	0.41
5:J:144:ILE:HG23	5:J:150:ALA:HA	2.02	0.41
5:J:216:PRO:HB3	5:J:224:VAL:HG13	2.02	0.41
5:K:136:LYS:HG2	5:K:137:PRO:HD3	2.03	0.41
2:R:168:ASP:HB3	2:R:171:ASP:OD1	2.20	0.41
2:P:15:PRO:HG3	2:P:83:PHE:CZ	2.56	0.41
3:A:185:TYR:OH	3:A:247:ARG:HD2	2.20	0.41
3:B:84:VAL:HG21	3:B:102:GLN:HB2	2.02	0.41
3:C:360:LEU:HD12	3:C:362:SER:O	2.21	0.41
3:C:421:VAL:HG22	4:G:385:ALA:HB2	2.02	0.41
4:F:169:VAL:HG12	4:F:237:TYR:HA	2.01	0.41
4:H:203:CYS:SG	4:H:221:LYS:N	2.89	0.41
5:I:246:ASN:O	5:I:247:LYS:C	2.63	0.41
5:J:226:ALA:HB1	5:J:242:VAL:CG2	2.50	0.41
1:Q:49:TRP:HH2	2:R:95:PRO:HB3	1.84	0.41
2:R:133:VAL:CG1	2:R:180:LEU:HB3	2.50	0.41
1:O:130:PHE:CD2	2:P:125:GLN:HG3	2.55	0.41
2:T:108:LYS:HA	2:T:108:LYS:HD3	1.96	0.41
3:D:318:ILE:HB	3:D:352:LEU:CD2	2.50	0.41
3:D:397:LEU:HD11	3:D:402:ILE:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:382:VAL:O	4:F:386:VAL:HG22	2.20	0.41
5:I:213:SER:HB2	5:I:261:TRP:CB	2.51	0.41
5:J:177:LYS:O	5:J:224:VAL:HG23	2.20	0.41
1:Q:13:LYS:HB2	1:Q:16:GLU:OE1	2.20	0.41
1:O:12:VAL:HG23	1:O:119:VAL:HG13	2.03	0.41
1:O:111:TRP:CH2	2:P:36:TYR:HE2	2.34	0.41
2:P:2:ILE:O	2:P:98:THR:HG21	2.21	0.41
2:P:130:THR:OG1	2:P:131:ALA:N	2.53	0.41
1:S:147:GLY:HA2	1:S:162:TRP:CZ2	2.56	0.41
3:A:407:MET:O	3:A:407:MET:HG2	2.20	0.41
3:B:61:LYS:HB2	3:B:66:ALA:HB2	2.01	0.41
3:C:207:THR:HG22	3:C:210:SER:HB2	2.03	0.41
3:C:320:TYR:HE1	3:C:322:ALA:HB2	1.85	0.41
4:G:97:MET:HE1	4:G:256:HIS:CE1	2.56	0.41
4:G:393:ARG:NH1	4:G:417:CYS:HB2	2.36	0.41
1:S:95:TYR:O	1:S:114:GLY:HA2	2.21	0.41
1:S:125:LYS:HG2	1:S:152:ASP:OD1	2.20	0.41
2:T:137:LEU:HB2	2:T:176:LEU:HB2	2.03	0.41
3:A:303:VAL:HB	3:A:378:ALA:HB2	2.03	0.41
3:B:78:CYS:SG	3:B:103:LEU:HD11	2.61	0.41
3:B:344:ILE:HG13	3:B:352:LEU:HD13	2.03	0.41
3:C:27:MET:HE1	3:C:282:ILE:HG21	2.03	0.41
3:D:57:SER:OG	4:H:239:SER:O	2.35	0.41
3:D:65:THR:HA	3:D:101:THR:HG21	2.01	0.41
3:D:397:LEU:H	3:D:397:LEU:HD23	1.85	0.41
4:E:21:ASP:HB3	4:E:126:THR:HB	2.02	0.41
4:F:214:ASP:OD2	4:F:215:LYS:N	2.54	0.41
4:F:377:VAL:HG12	4:F:378:LEU:HD23	2.03	0.41
4:G:366:MET:HE2	12:G:501:CLR:H42	2.02	0.41
4:H:321:VAL:HG12	4:H:340:PRO:HD3	2.03	0.41
5:I:125:GLY:HA3	5:I:140:VAL:HG11	2.01	0.41
5:J:136:LYS:HE2	5:J:137:PRO:O	2.21	0.41
5:J:173:SER:N	5:L:234:GLU:OE2	2.54	0.41
5:K:261:TRP:CD1	5:K:261:TRP:N	2.87	0.41
1:Q:61:TYR:HE1	1:Q:71:ILE:HG13	1.86	0.41
1:Q:222:LYS:HD3	1:Q:222:LYS:HA	1.93	0.41
2:R:38:GLN:O	2:R:84:ALA:HB1	2.21	0.41
2:R:189:LYS:HB3	2:R:189:LYS:HE3	1.78	0.41
1:O:134:PRO:HD2	1:O:221:PRO:HA	2.03	0.41
2:P:22:PHE:HB3	2:P:24:ARG:NH1	2.36	0.41
2:P:66:GLY:HA3	2:P:71:PHE:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:38:GLN:O	2:N:84:ALA:HB1	2.21	0.41
2:N:199:HIS:HB3	2:N:202:LEU:HD12	2.01	0.41
10:a:4:MAN:O6	10:a:4:MAN:O4	2.26	0.41
3:D:93:TYR:HA	4:H:176:PRO:HG2	2.03	0.41
1:O:4:LEU:HB3	1:O:97:CYS:SG	2.61	0.41
1:M:122:ALA:O	1:M:154:PHE:HB3	2.21	0.41
1:M:151:LYS:HD3	1:M:185:SER:HB3	2.03	0.41
2:N:11:LEU:HG	2:N:13:LEU:HD23	2.02	0.41
3:B:174:ASP:OD2	3:B:174:ASP:N	2.45	0.40
3:C:59:TYR:HB3	3:C:103:LEU:HB3	2.03	0.40
3:C:116:THR:HB	4:G:261:LEU:HD23	2.03	0.40
4:E:163:THR:HG21	4:E:260:PRO:HB3	2.03	0.40
4:F:85:VAL:HG22	4:F:113:VAL:HG22	2.04	0.40
4:F:215:LYS:HG2	4:F:216:VAL:N	2.35	0.40
4:G:35:GLU:OE2	4:G:35:GLU:HA	2.21	0.40
4:H:296:SER:HB2	4:H:306:TYR:CE1	2.56	0.40
5:J:159:LYS:HE2	5:J:160:TYR:CE1	2.56	0.40
2:R:181:THR:C	2:R:182:LEU:HD22	2.47	0.40
1:O:50:ILE:HD12	1:O:50:ILE:N	2.36	0.40
1:O:179:GLN:HE22	2:P:161:GLN:NE2	2.17	0.40
2:T:70:ASP:OD2	2:T:70:ASP:N	2.54	0.40
2:T:93:ASN:OD1	4:H:215:LYS:HD2	2.22	0.40
4:G:351:HIS:O	4:G:355:ILE:HD12	2.21	0.40
4:H:181:MET:HE1	4:H:225:CYS:HB2	2.03	0.40
5:I:181:GLU:OE2	5:I:183:PRO:HD3	2.21	0.40
5:I:182:LYS:HD2	5:I:196:TYR:CE2	2.57	0.40
5:J:249:ILE:HA	5:J:249:ILE:HD12	1.68	0.40
1:Q:83:LYS:HA	1:Q:83:LYS:HD3	1.68	0.40
1:O:34:TYR:HE1	1:O:36:TRP:CZ2	2.39	0.40
2:P:14:SER:HB3	2:P:17:GLU:OE1	2.21	0.40
2:N:49:TYR:C	2:N:51:ALA:H	2.29	0.40
2:N:196:GLU:OE1	2:N:197:VAL:N	2.54	0.40
1:S:40:ARG:O	1:S:48:GLN:N	2.38	0.40
3:A:182:GLY:HA2	3:A:263:THR:OG1	2.22	0.40
4:E:138:ARG:NH2	4:E:296:SER:OG	2.54	0.40
4:E:171:MET:O	4:E:245:ASN:ND2	2.40	0.40
4:E:287:LEU:O	4:E:314:LYS:HA	2.22	0.40
4:H:102:LEU:HD23	4:H:102:LEU:HA	1.87	0.40
5:I:130:VAL:HG11	5:I:135:MET:HE1	2.04	0.40
5:L:172:LYS:HZ2	5:L:172:LYS:HG3	1.61	0.40
5:L:216:PRO:HG2	5:L:218:PHE:HE2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:41:GLN:HB2	1:O:47:LEU:HD12	2.02	0.40
1:O:146:LEU:HD11	1:O:202:TYR:CD2	2.57	0.40
2:P:16:GLY:N	2:P:78:LEU:O	2.45	0.40
1:M:130:PHE:CE1	2:N:122:SER:HB2	2.56	0.40
1:S:14:PRO:CD	1:S:121:SER:HB2	2.50	0.40
3:D:302:GLU:HA	3:D:302:GLU:OE1	2.21	0.40
3:D:417:VAL:HG12	4:H:381:MET:HE2	2.03	0.40
5:J:167:ILE:H	5:J:167:ILE:HG13	1.73	0.40
1:Q:1:GLN:OE1	1:Q:1:GLN:N	2.44	0.40
2:P:143:ARG:HE	2:P:164:VAL:HG11	1.85	0.40
1:M:130:PHE:HB3	1:M:149:LEU:HB3	2.04	0.40
1:M:155:PRO:HD2	1:M:208:HIS:HE1	1.86	0.40
3:B:29:LEU:HD23	3:B:29:LEU:HA	1.89	0.40
3:B:185:TYR:OH	3:B:247:ARG:HD2	2.20	0.40
3:B:202:ASP:OD2	3:B:203:ILE:N	2.54	0.40
4:E:52:LEU:HD23	4:E:52:LEU:HA	1.88	0.40
4:E:221:LYS:HG2	4:E:224:GLN:OE1	2.22	0.40
4:F:157:VAL:HG13	4:F:262:ALA:HB3	2.02	0.40
5:I:130:VAL:O	5:I:131:GLY:C	2.63	0.40
2:P:38:GLN:HB3	2:P:85:VAL:HG13	2.02	0.40
1:M:121:SER:HB3	1:M:154:PHE:CE1	2.56	0.40
1:M:154:PHE:HE2	1:M:184:TYR:HE1	1.68	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	226/265 (85%)	217 (96%)	9 (4%)	0	100	100
1	O	226/265 (85%)	219 (97%)	7 (3%)	0	100	100
1	Q	226/265 (85%)	217 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	S	226/265 (85%)	217 (96%)	9 (4%)	0	100	100
2	N	210/241 (87%)	202 (96%)	8 (4%)	0	100	100
2	P	210/241 (87%)	204 (97%)	6 (3%)	0	100	100
2	R	210/241 (87%)	207 (99%)	3 (1%)	0	100	100
2	T	210/241 (87%)	204 (97%)	6 (3%)	0	100	100
3	A	437/439 (100%)	428 (98%)	9 (2%)	0	100	100
3	B	437/439 (100%)	425 (97%)	12 (3%)	0	100	100
3	C	437/439 (100%)	422 (97%)	15 (3%)	0	100	100
3	D	437/439 (100%)	426 (98%)	11 (2%)	0	100	100
4	E	410/419 (98%)	396 (97%)	14 (3%)	0	100	100
4	F	417/419 (100%)	401 (96%)	16 (4%)	0	100	100
4	G	417/419 (100%)	405 (97%)	12 (3%)	0	100	100
4	H	415/419 (99%)	403 (97%)	12 (3%)	0	100	100
5	I	149/151 (99%)	147 (99%)	1 (1%)	1 (1%)	18	49
5	J	149/151 (99%)	141 (95%)	7 (5%)	1 (1%)	18	49
5	K	149/151 (99%)	144 (97%)	5 (3%)	0	100	100
5	L	149/151 (99%)	144 (97%)	5 (3%)	0	100	100
All	All	5747/6060 (95%)	5569 (97%)	176 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	J	249	ILE
5	I	131	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	197/231 (85%)	197 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O	197/231 (85%)	197 (100%)	0	100	100
1	Q	197/231 (85%)	196 (100%)	1 (0%)	81	83
1	S	197/231 (85%)	196 (100%)	1 (0%)	81	83
2	N	184/209 (88%)	184 (100%)	0	100	100
2	P	184/209 (88%)	184 (100%)	0	100	100
2	R	184/209 (88%)	184 (100%)	0	100	100
2	T	184/209 (88%)	184 (100%)	0	100	100
3	A	366/366 (100%)	366 (100%)	0	100	100
3	B	366/366 (100%)	366 (100%)	0	100	100
3	C	366/366 (100%)	366 (100%)	0	100	100
3	D	366/366 (100%)	365 (100%)	1 (0%)	86	86
4	E	364/369 (99%)	363 (100%)	1 (0%)	86	86
4	F	369/369 (100%)	369 (100%)	0	100	100
4	G	369/369 (100%)	367 (100%)	2 (0%)	81	83
4	H	367/369 (100%)	367 (100%)	0	100	100
5	I	120/120 (100%)	117 (98%)	3 (2%)	42	64
5	J	120/120 (100%)	116 (97%)	4 (3%)	33	59
5	K	120/120 (100%)	120 (100%)	0	100	100
5	L	120/120 (100%)	118 (98%)	2 (2%)	53	71
All	All	4937/5180 (95%)	4922 (100%)	15 (0%)	84	86

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	16	GLU
3	D	103	LEU
4	E	189	LYS
4	G	208	GLU
4	G	217	ILE
5	I	130	VAL
5	I	245	TRP
5	I	248	ASP
5	J	134	VAL
5	J	241	SER
5	J	249	ILE

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Mol	Chain	Res	Type
5	J	251	THR
5	L	118	LYS
5	L	245	TRP
1	Q	105	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	S	212	ASN
2	T	93	ASN
2	T	200	GLN
3	A	125	HIS
3	A	331	HIS
3	B	3	HIS
3	B	235	GLN
3	B	349	ASN
3	D	3	HIS
3	D	138	GLN
3	D	186	ASN
4	E	29	HIS
4	F	146	GLN
4	F	183	GLN
4	F	218	ASN
4	G	127	HIS
4	G	146	GLN
4	G	147	HIS
4	G	207	ASN
4	G	313	HIS
4	H	18	HIS
4	H	123	HIS
4	H	131	HIS
5	J	190	HIS
5	L	139	HIS
5	L	190	HIS
1	Q	179	GLN
2	R	42	GLN
1	O	102	ASN
1	O	179	GLN
1	O	228	HIS
2	P	89	GLN
2	P	156	GLN
2	P	167	GLN

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Mol	Chain	Res	Type
1	M	3	GLN
2	N	138	ASN
2	N	167	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

49 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
6	NAG	U	1	6,3	14,14,15	0.27	0	17,19,21	0.51	0
6	NAG	U	2	6	14,14,15	0.20	0	17,19,21	0.40	0
6	BMA	U	3	6	11,11,12	0.54	0	15,15,17	0.74	0
6	FUC	U	4	6	10,10,11	0.61	0	14,14,16	0.75	0
6	NAG	V	1	6,3	14,14,15	0.26	0	17,19,21	0.47	0
6	NAG	V	2	6	14,14,15	0.24	0	17,19,21	0.39	0
6	BMA	V	3	6	11,11,12	0.55	0	15,15,17	0.69	0
6	FUC	V	4	6	10,10,11	0.72	0	14,14,16	0.84	0
7	NAG	W	1	3,7	14,14,15	0.22	0	17,19,21	1.55	1 (5%)
7	NAG	W	2	7	14,14,15	0.94	1 (7%)	17,19,21	0.98	1 (5%)
7	BMA	W	3	7	11,11,12	0.74	0	15,15,17	1.19	2 (13%)
7	MAN	W	4	7	11,11,12	0.89	0	15,15,17	1.06	2 (13%)
7	FUC	W	5	7	10,10,11	0.65	0	14,14,16	0.72	0
6	NAG	X	1	6,3	14,14,15	0.25	0	17,19,21	0.56	0
6	NAG	X	2	6	14,14,15	0.18	0	17,19,21	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	BMA	X	3	6	11,11,12	0.54	0	15,15,17	0.80	0
6	FUC	X	4	6	10,10,11	0.89	0	14,14,16	1.01	1 (7%)
8	NAG	Y	1	4,8	14,14,15	0.23	0	17,19,21	0.51	0
8	NAG	Y	2	8	14,14,15	0.20	0	17,19,21	0.45	0
8	BMA	Y	3	8	11,11,12	1.07	1 (9%)	15,15,17	0.99	1 (6%)
8	MAN	Y	4	8	11,11,12	0.63	0	15,15,17	1.05	2 (13%)
8	NAG	Y	5	8	14,14,15	0.25	0	17,19,21	0.45	0
9	NAG	Z	1	4,9	14,14,15	0.99	1 (7%)	17,19,21	0.61	0
9	NAG	Z	2	9	14,14,15	0.18	0	17,19,21	0.36	0
9	BMA	Z	3	9	11,11,12	0.53	0	15,15,17	0.76	0
10	NAG	a	1	4,10	14,14,15	0.68	1 (7%)	17,19,21	0.96	1 (5%)
10	NAG	a	2	10	14,14,15	0.39	0	17,19,21	0.43	0
10	BMA	a	3	10	11,11,12	0.52	0	15,15,17	0.82	0
10	MAN	a	4	10	11,11,12	0.78	0	15,15,17	1.27	2 (13%)
9	NAG	b	1	4,9	14,14,15	0.56	0	17,19,21	0.73	1 (5%)
9	NAG	b	2	9	14,14,15	0.29	0	17,19,21	0.39	0
9	BMA	b	3	9	11,11,12	0.64	0	15,15,17	0.84	0
8	NAG	c	1	4,8	14,14,15	0.28	0	17,19,21	0.55	0
8	NAG	c	2	8	14,14,15	0.28	0	17,19,21	0.48	0
8	BMA	c	3	8	11,11,12	0.99	1 (9%)	15,15,17	0.83	0
8	MAN	c	4	8	11,11,12	0.66	0	15,15,17	1.26	2 (13%)
8	NAG	c	5	8	14,14,15	0.32	0	17,19,21	0.40	0
9	NAG	d	1	4,9	14,14,15	0.34	0	17,19,21	0.55	0
9	NAG	d	2	9	14,14,15	0.22	0	17,19,21	0.38	0
9	BMA	d	3	9	11,11,12	0.54	0	15,15,17	0.72	0
8	NAG	e	1	4,8	14,14,15	0.42	0	17,19,21	0.70	1 (5%)
8	NAG	e	2	8	14,14,15	0.27	0	17,19,21	0.48	0
8	BMA	e	3	8	11,11,12	0.98	1 (9%)	15,15,17	0.92	1 (6%)
8	MAN	e	4	8	11,11,12	0.60	0	15,15,17	1.15	2 (13%)
8	NAG	e	5	8	14,14,15	0.23	0	17,19,21	0.47	0
11	NAG	f	1	4,11	14,14,15	0.20	0	17,19,21	0.45	0
11	NAG	f	2	11	14,14,15	0.22	0	17,19,21	0.41	0
11	BMA	f	3	11	11,11,12	0.53	0	15,15,17	0.78	0
11	MAN	f	4	11	11,11,12	0.67	0	15,15,17	1.12	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
6	NAG	U	1	6,3	-	0/6/23/26	0/1/1/1
6	NAG	U	2	6	-	2/6/23/26	0/1/1/1
6	BMA	U	3	6	-	0/2/19/22	0/1/1/1
6	FUC	U	4	6	-	-	0/1/1/1
6	NAG	V	1	6,3	-	2/6/23/26	0/1/1/1
6	NAG	V	2	6	-	4/6/23/26	0/1/1/1
6	BMA	V	3	6	-	0/2/19/22	0/1/1/1
6	FUC	V	4	6	-	-	0/1/1/1
7	NAG	W	1	3,7	-	0/6/23/26	0/1/1/1
7	NAG	W	2	7	-	1/6/23/26	0/1/1/1
7	BMA	W	3	7	-	0/2/19/22	0/1/1/1
7	MAN	W	4	7	-	2/2/19/22	1/1/1/1
7	FUC	W	5	7	-	-	0/1/1/1
6	NAG	X	1	6,3	-	2/6/23/26	0/1/1/1
6	NAG	X	2	6	-	3/6/23/26	0/1/1/1
6	BMA	X	3	6	-	1/2/19/22	0/1/1/1
6	FUC	X	4	6	-	-	0/1/1/1
8	NAG	Y	1	4,8	-	2/6/23/26	0/1/1/1
8	NAG	Y	2	8	-	0/6/23/26	0/1/1/1
8	BMA	Y	3	8	-	1/2/19/22	0/1/1/1
8	MAN	Y	4	8	-	1/2/19/22	0/1/1/1
8	NAG	Y	5	8	-	2/6/23/26	0/1/1/1
9	NAG	Z	1	4,9	-	2/6/23/26	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
10	NAG	a	1	4,10	-	4/6/23/26	0/1/1/1
10	NAG	a	2	10	-	2/6/23/26	0/1/1/1
10	BMA	a	3	10	-	2/2/19/22	0/1/1/1
10	MAN	a	4	10	-	2/2/19/22	0/1/1/1
9	NAG	b	1	4,9	-	3/6/23/26	0/1/1/1
9	NAG	b	2	9	-	2/6/23/26	0/1/1/1
9	BMA	b	3	9	-	0/2/19/22	0/1/1/1
8	NAG	c	1	4,8	-	2/6/23/26	0/1/1/1
8	NAG	c	2	8	-	2/6/23/26	0/1/1/1
8	BMA	c	3	8	-	1/2/19/22	0/1/1/1
8	MAN	c	4	8	-	2/2/19/22	0/1/1/1
8	NAG	c	5	8	-	1/6/23/26	0/1/1/1
9	NAG	d	1	4,9	-	0/6/23/26	0/1/1/1
9	NAG	d	2	9	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BMA	d	3	9	-	0/2/19/22	0/1/1/1
8	NAG	e	1	4,8	-	0/6/23/26	0/1/1/1
8	NAG	e	2	8	-	0/6/23/26	0/1/1/1
8	BMA	e	3	8	-	1/2/19/22	0/1/1/1
8	MAN	e	4	8	-	0/2/19/22	0/1/1/1
8	NAG	e	5	8	-	1/6/23/26	0/1/1/1
11	NAG	f	1	4,11	-	2/6/23/26	0/1/1/1
11	NAG	f	2	11	-	2/6/23/26	0/1/1/1
11	BMA	f	3	11	-	2/2/19/22	0/1/1/1
11	MAN	f	4	11	-	1/2/19/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	Z	1	NAG	C1-C2	3.34	1.56	1.52
7	W	2	NAG	O5-C1	3.14	1.49	1.43
8	Y	3	BMA	C1-C2	2.81	1.58	1.52
8	c	3	BMA	C1-C2	2.78	1.58	1.52
8	e	3	BMA	C1-C2	2.74	1.58	1.52
10	a	1	NAG	O5-C1	-2.30	1.39	1.43

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	W	1	NAG	C1-O5-C5	5.59	119.67	112.19
7	W	2	NAG	C1-O5-C5	3.71	117.16	112.19
10	a	4	MAN	C1-O5-C5	3.68	117.11	112.19
8	c	4	MAN	C1-O5-C5	3.54	116.93	112.19
11	f	4	MAN	C1-O5-C5	3.04	116.26	112.19
8	e	4	MAN	C1-O5-C5	3.04	116.25	112.19
7	W	4	MAN	C1-O5-C5	2.91	116.08	112.19
8	e	4	MAN	O2-C2-C3	-2.83	104.28	110.15
8	c	4	MAN	O2-C2-C3	-2.75	104.45	110.15
7	W	3	BMA	C1-C2-C3	2.74	113.64	109.64
8	Y	4	MAN	O2-C2-C3	-2.59	104.78	110.15
8	Y	4	MAN	C1-O5-C5	2.52	115.57	112.19
8	e	1	NAG	C1-O5-C5	2.27	115.23	112.19
7	W	3	BMA	C1-O5-C5	2.24	115.18	112.19
11	f	4	MAN	O2-C2-C3	-2.20	105.58	110.15
8	Y	3	BMA	C1-C2-C3	2.14	112.76	109.64
10	a	4	MAN	O2-C2-C3	-2.10	105.81	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	W	4	MAN	O2-C2-C3	-2.07	105.85	110.15
9	b	1	NAG	C1-O5-C5	2.04	114.92	112.19
10	a	1	NAG	C2-N2-C7	2.03	125.61	122.90
8	e	3	BMA	O2-C2-C3	-2.02	105.96	110.15
6	X	4	FUC	C1-O5-C5	2.00	117.68	112.97

There are no chirality outliers.

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	Y	5	NAG	C4-C5-C6-O6
6	U	2	NAG	O5-C5-C6-O6
10	a	1	NAG	O5-C5-C6-O6
6	X	1	NAG	O5-C5-C6-O6
11	f	2	NAG	O5-C5-C6-O6
8	Y	5	NAG	O5-C5-C6-O6
9	b	2	NAG	O5-C5-C6-O6
6	V	1	NAG	O5-C5-C6-O6
6	X	2	NAG	O5-C5-C6-O6
10	a	4	MAN	O5-C5-C6-O6
6	U	2	NAG	C4-C5-C6-O6
6	V	2	NAG	O5-C5-C6-O6
10	a	1	NAG	C4-C5-C6-O6
9	Z	1	NAG	O5-C5-C6-O6
9	Z	2	NAG	O5-C5-C6-O6
9	b	1	NAG	O5-C5-C6-O6
8	Y	1	NAG	O5-C5-C6-O6
6	X	1	NAG	C4-C5-C6-O6
9	b	2	NAG	C4-C5-C6-O6
11	f	2	NAG	C4-C5-C6-O6
10	a	3	BMA	O5-C5-C6-O6
8	Y	1	NAG	C4-C5-C6-O6
9	Z	2	NAG	C4-C5-C6-O6
11	f	3	BMA	O5-C5-C6-O6
6	V	1	NAG	C4-C5-C6-O6
6	X	2	NAG	C4-C5-C6-O6
10	a	4	MAN	C4-C5-C6-O6
8	c	4	MAN	O5-C5-C6-O6
9	b	1	NAG	C4-C5-C6-O6
9	Z	1	NAG	C4-C5-C6-O6
6	V	2	NAG	C8-C7-N2-C2
6	V	2	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
11	f	1	NAG	O5-C5-C6-O6
8	c	4	MAN	C4-C5-C6-O6
11	f	3	BMA	C4-C5-C6-O6
11	f	1	NAG	C4-C5-C6-O6
6	V	2	NAG	C4-C5-C6-O6
8	c	2	NAG	O5-C5-C6-O6
8	c	2	NAG	C4-C5-C6-O6
10	a	2	NAG	C4-C5-C6-O6
8	c	1	NAG	O5-C5-C6-O6
10	a	3	BMA	C4-C5-C6-O6
8	e	5	NAG	O5-C5-C6-O6
7	W	4	MAN	C4-C5-C6-O6
6	X	3	BMA	O5-C5-C6-O6
7	W	2	NAG	O5-C5-C6-O6
8	Y	4	MAN	O5-C5-C6-O6
8	e	3	BMA	O5-C5-C6-O6
8	c	5	NAG	O5-C5-C6-O6
8	c	3	BMA	O5-C5-C6-O6
10	a	2	NAG	O5-C5-C6-O6
11	f	4	MAN	O5-C5-C6-O6
8	Y	3	BMA	O5-C5-C6-O6
10	a	1	NAG	C1-C2-N2-C7
9	d	2	NAG	C4-C5-C6-O6
7	W	4	MAN	O5-C5-C6-O6
10	a	1	NAG	C3-C2-N2-C7
9	d	2	NAG	O5-C5-C6-O6
6	X	2	NAG	C1-C2-N2-C7
9	b	1	NAG	C1-C2-N2-C7
8	c	1	NAG	C4-C5-C6-O6

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	W	4	MAN	C1-C2-C3-C4-C5-O5

6 monomers are involved in 5 short contacts:

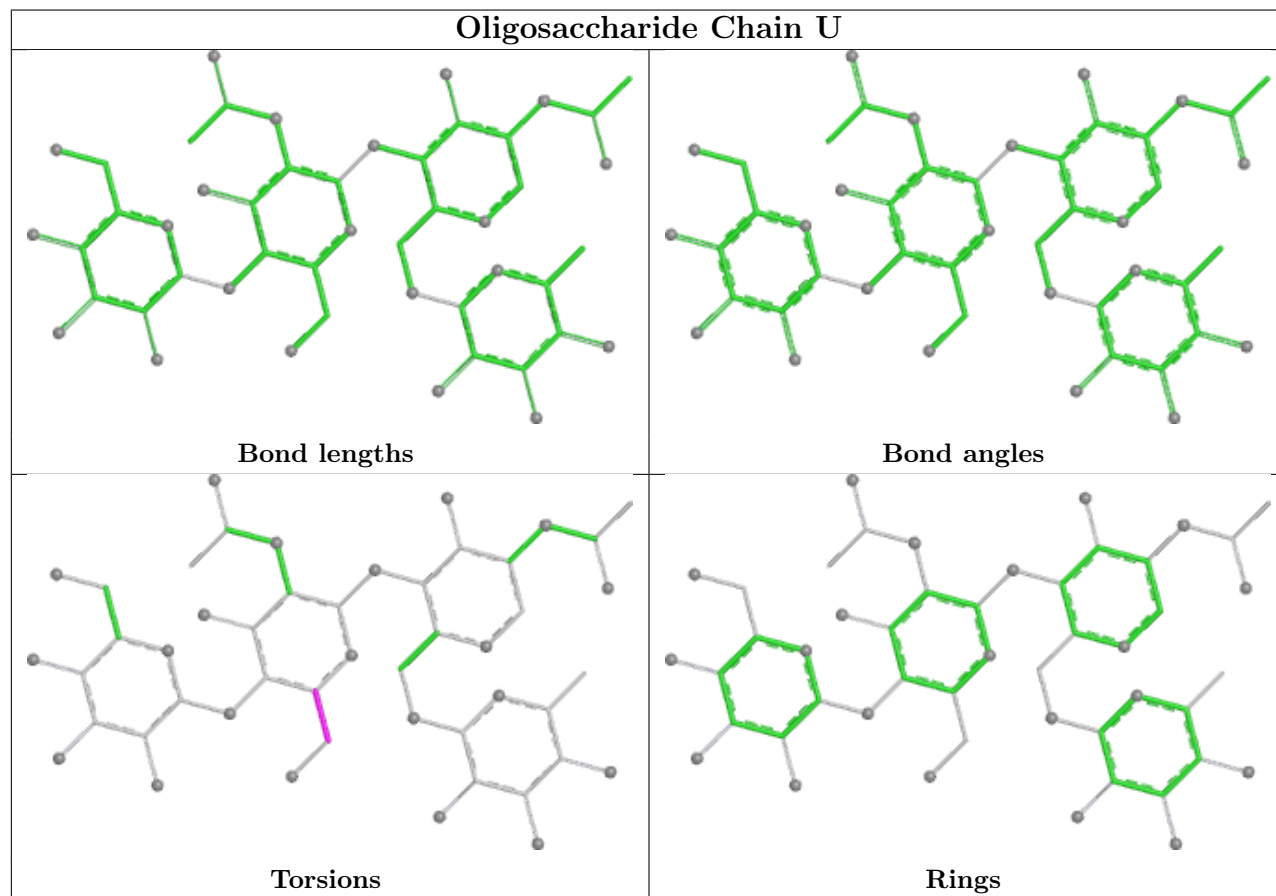
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	a	4	MAN	1	0
8	Y	2	NAG	1	0
7	W	1	NAG	1	0
9	Z	1	NAG	1	0

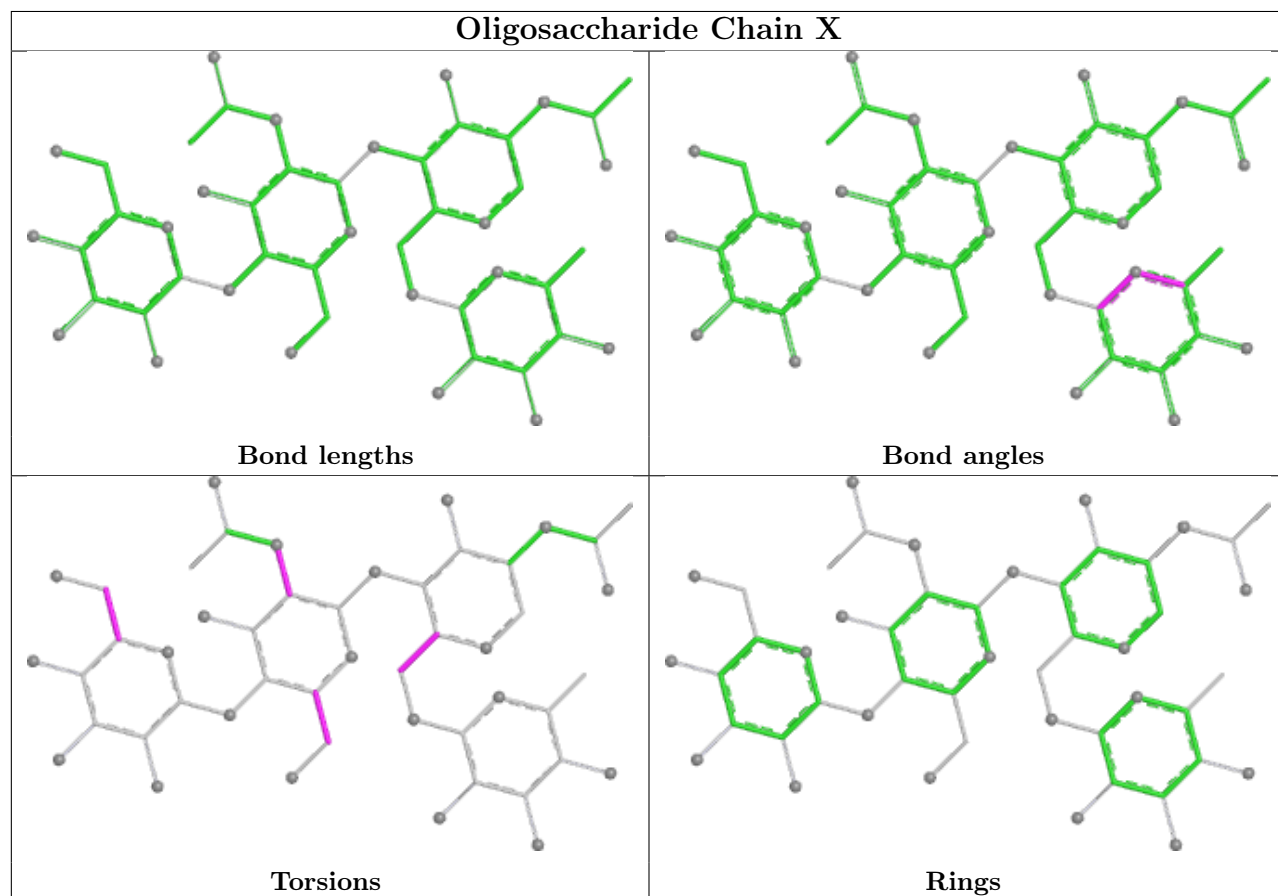
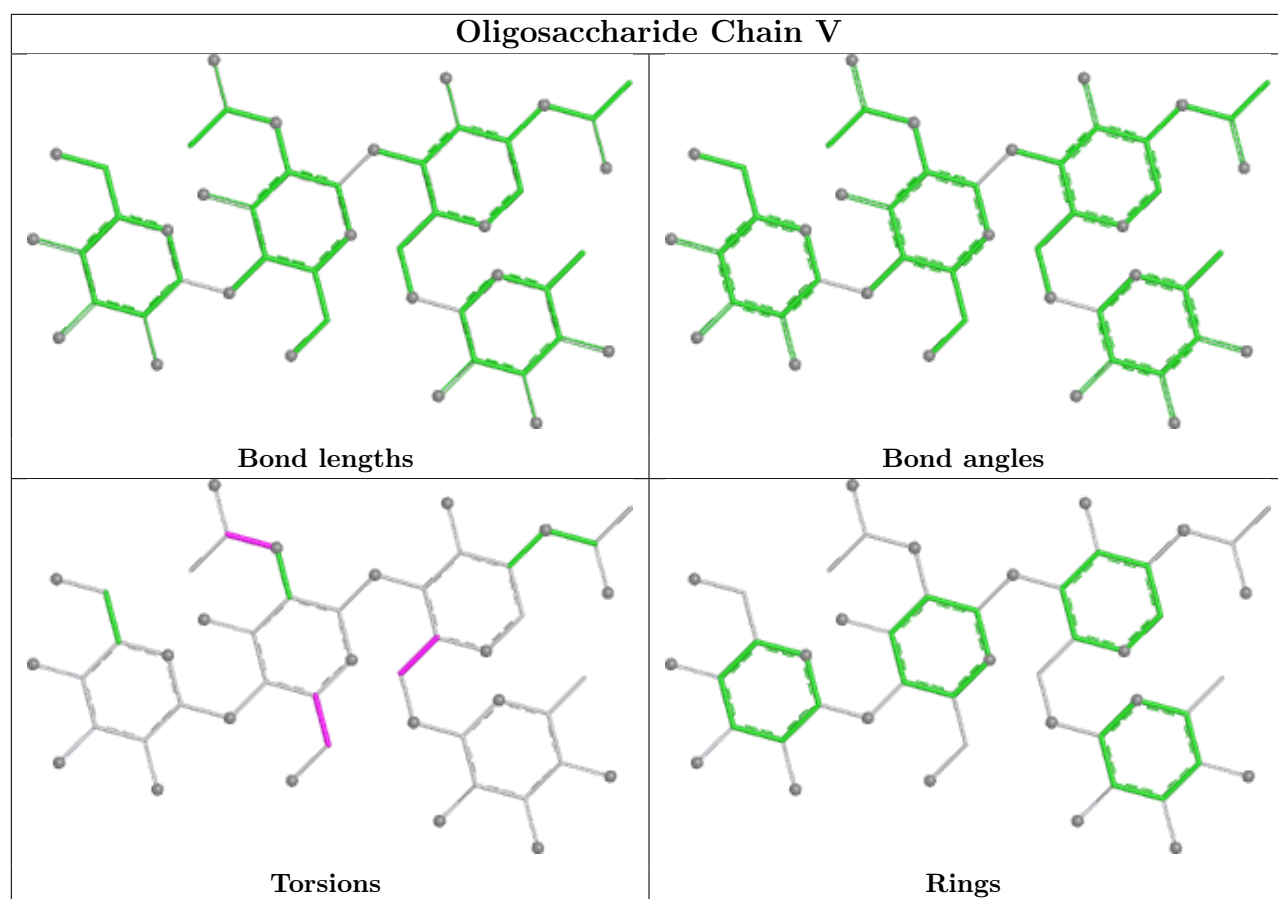
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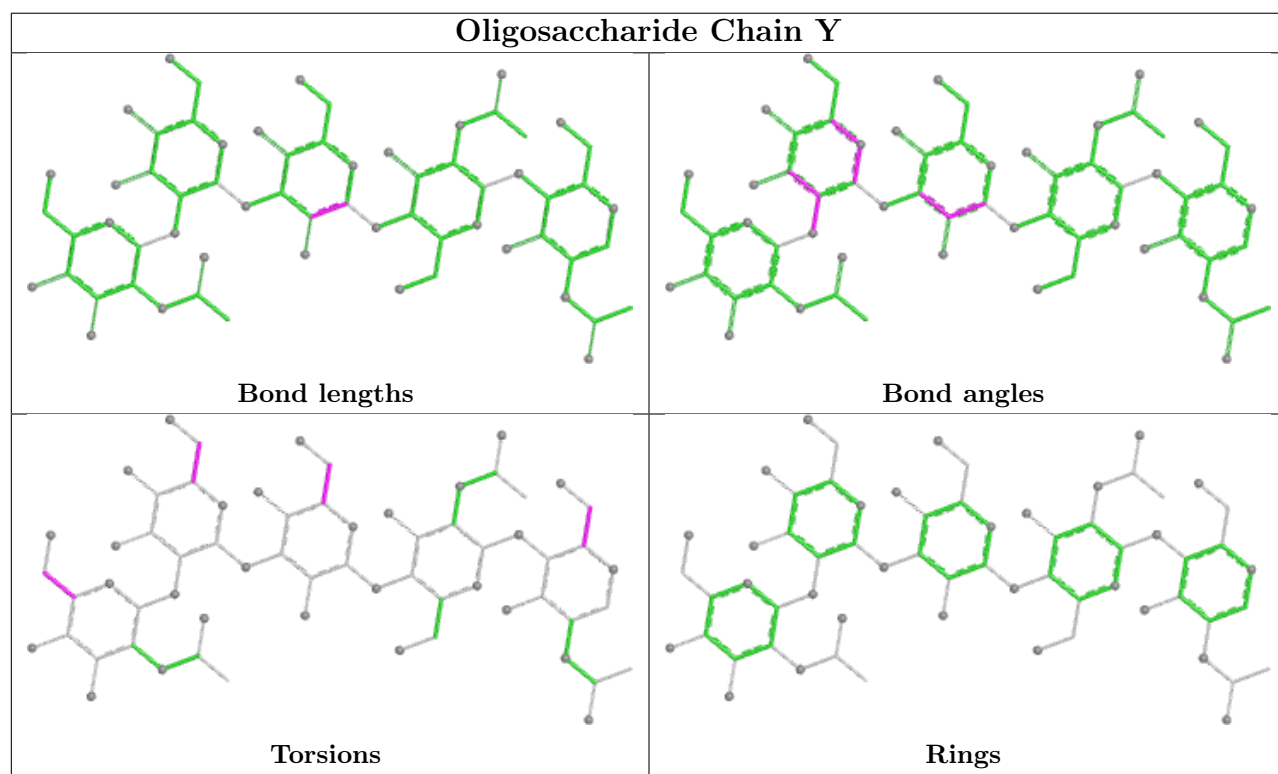
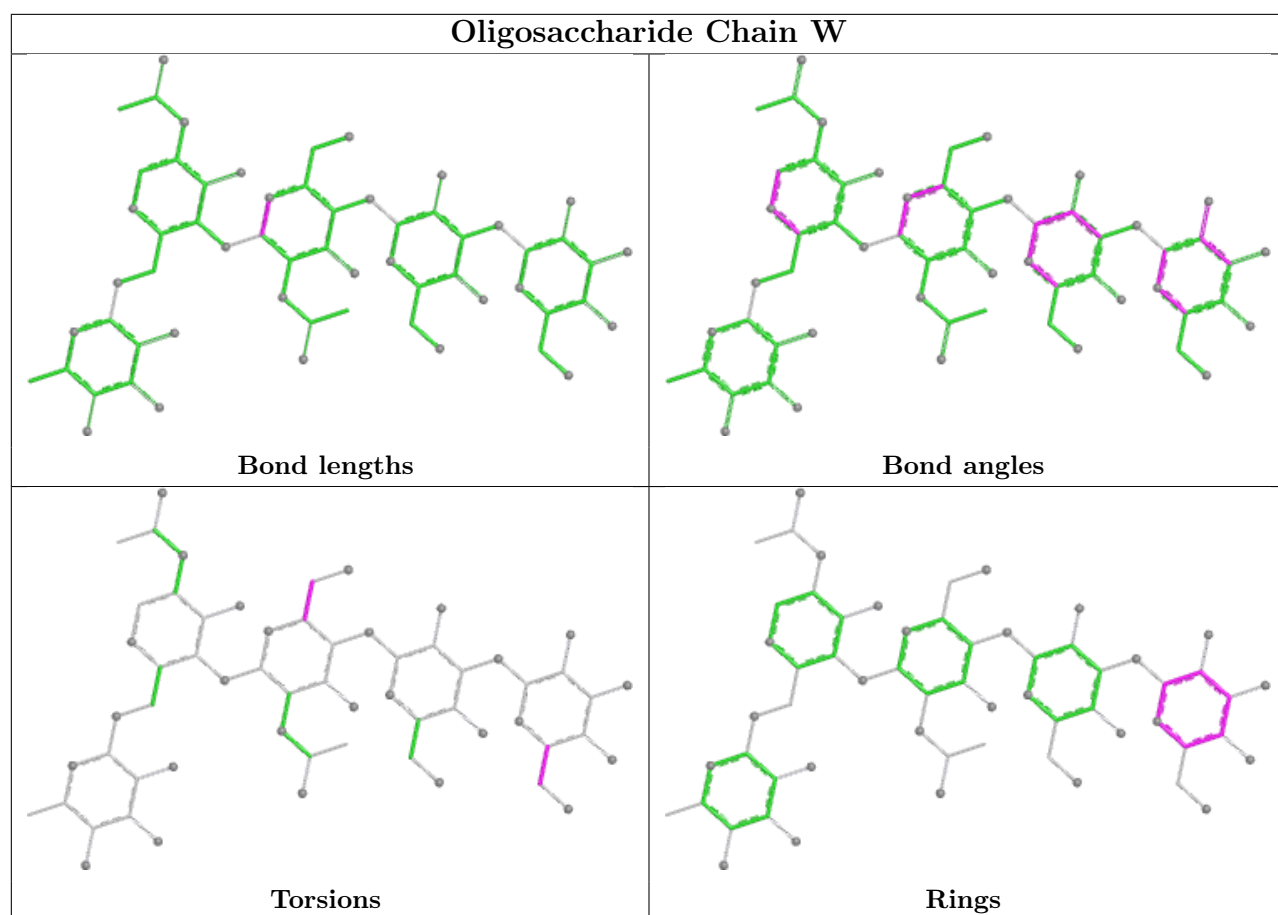
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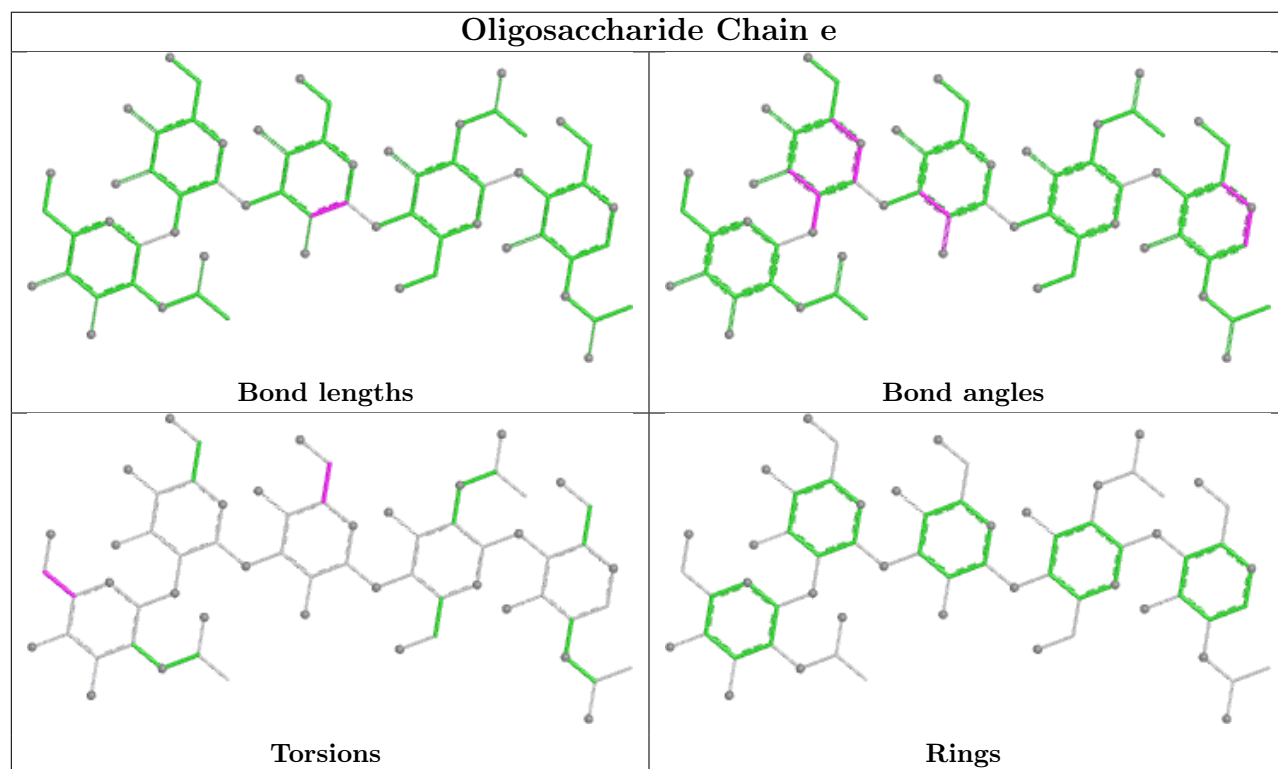
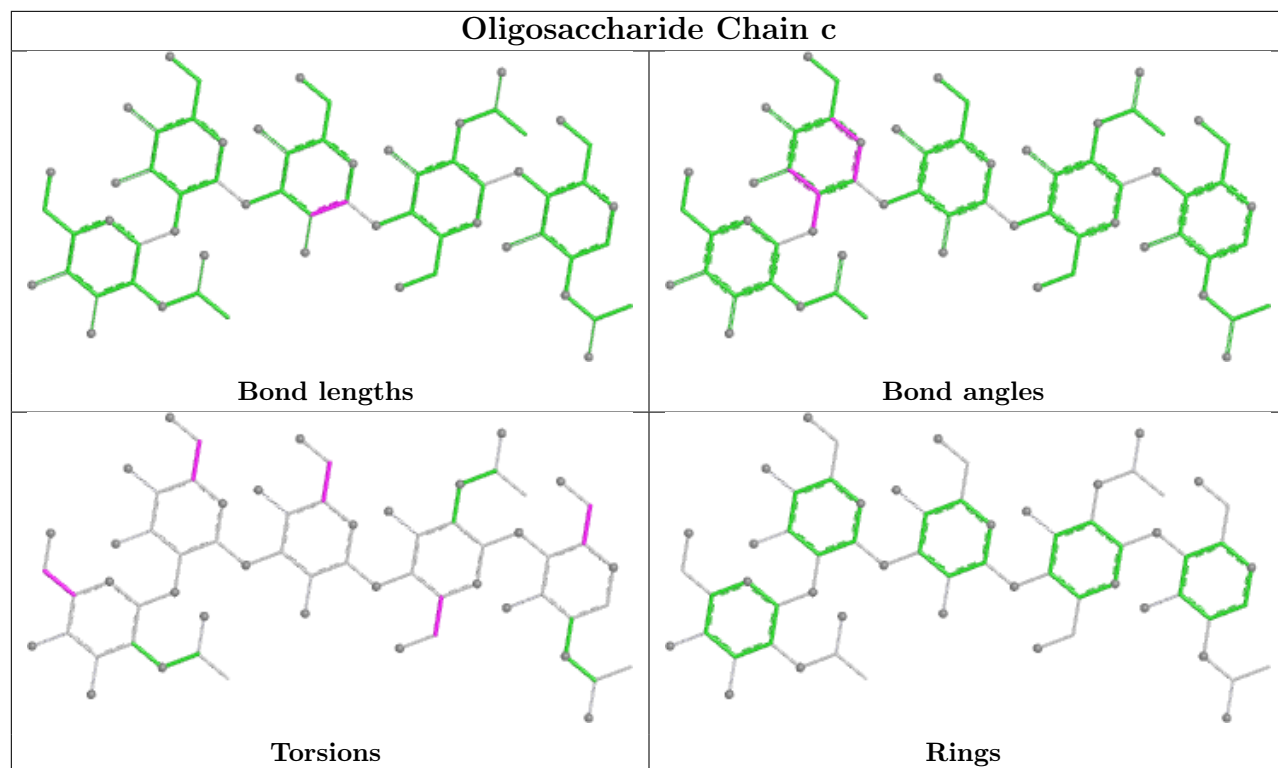
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	b	1	NAG	1	0
8	Y	1	NAG	1	0

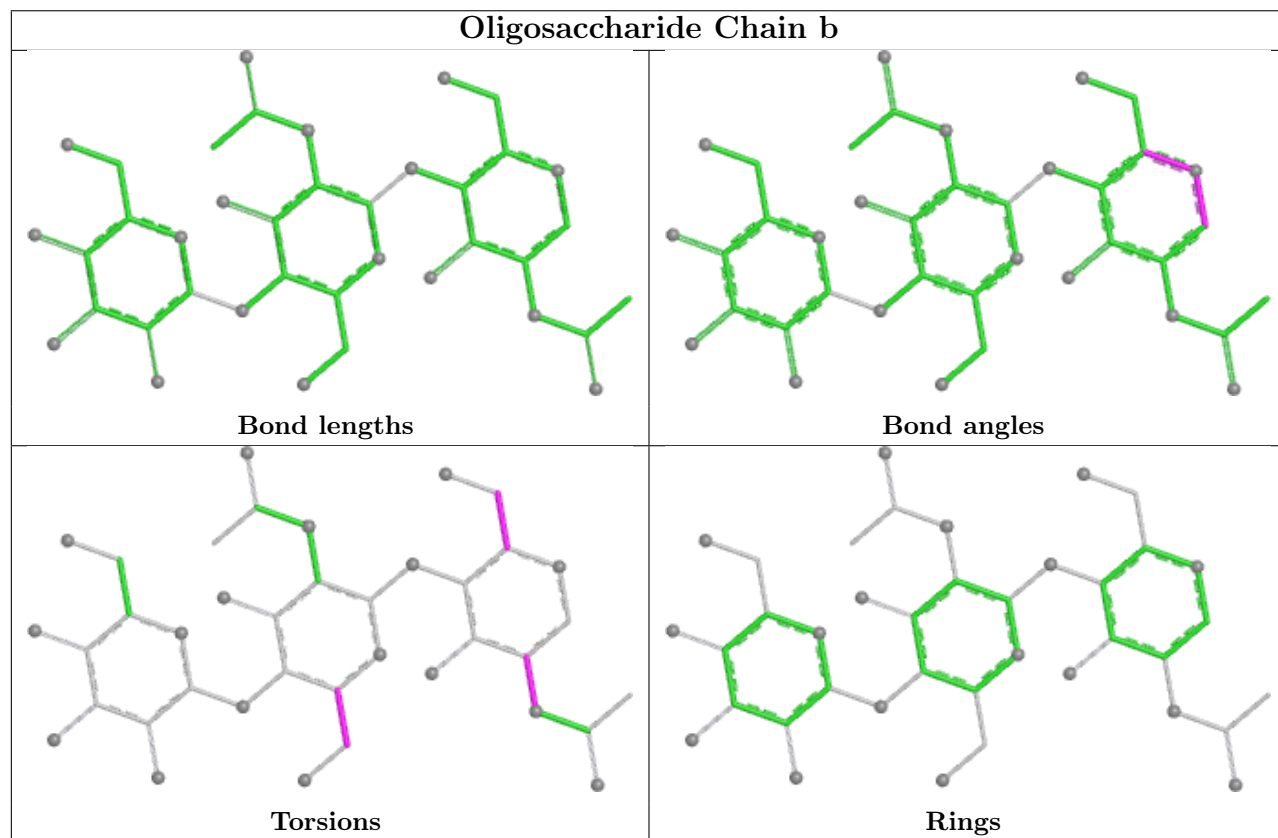
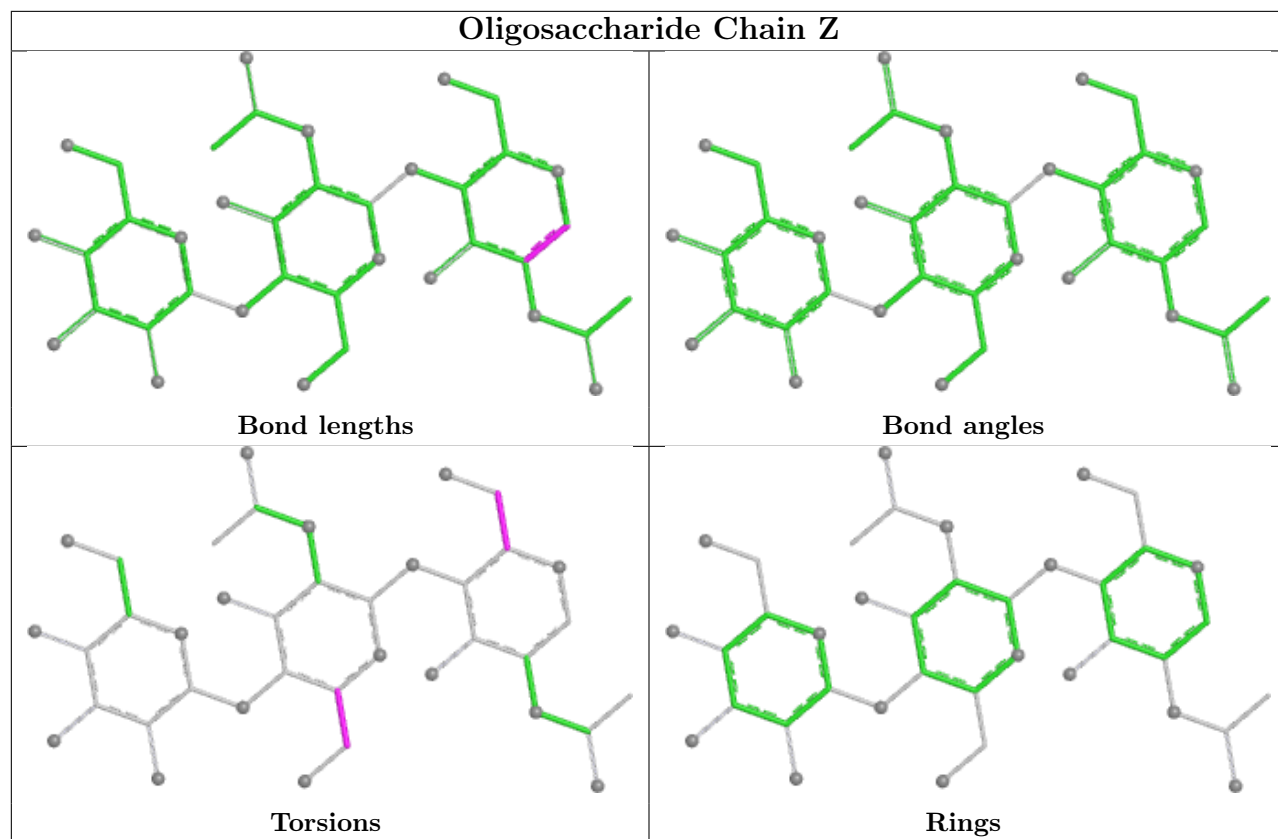
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

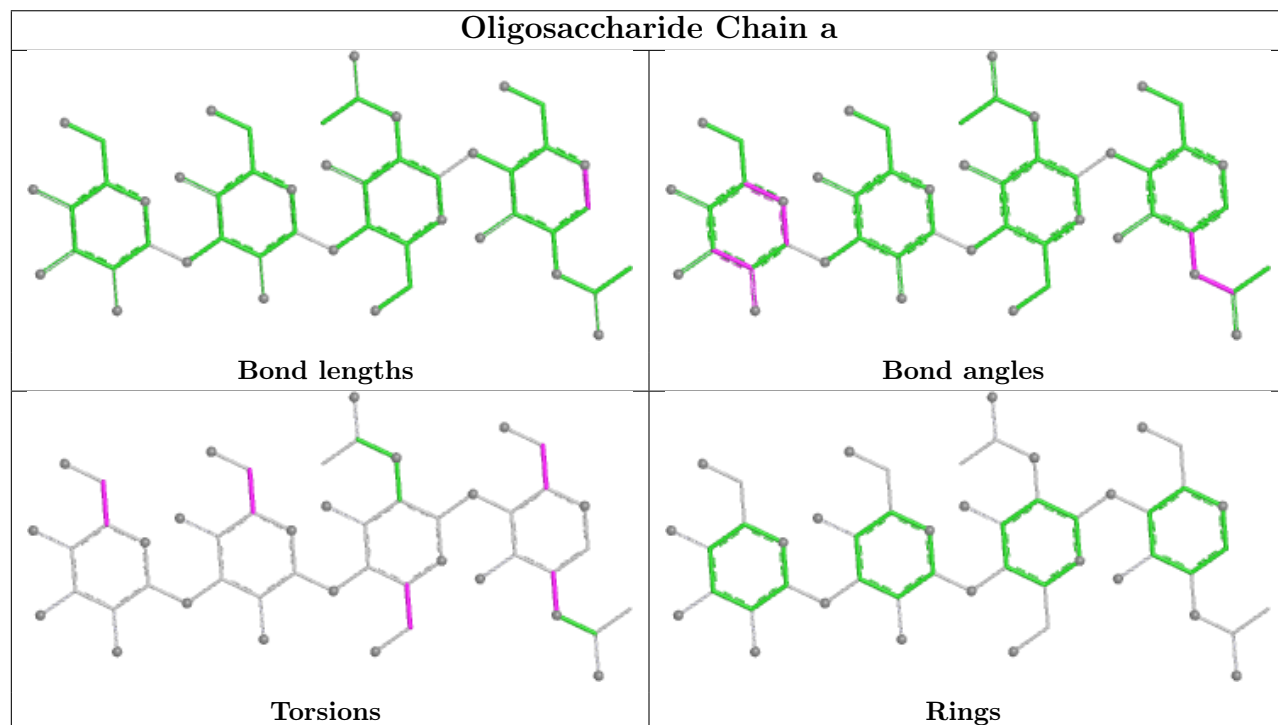
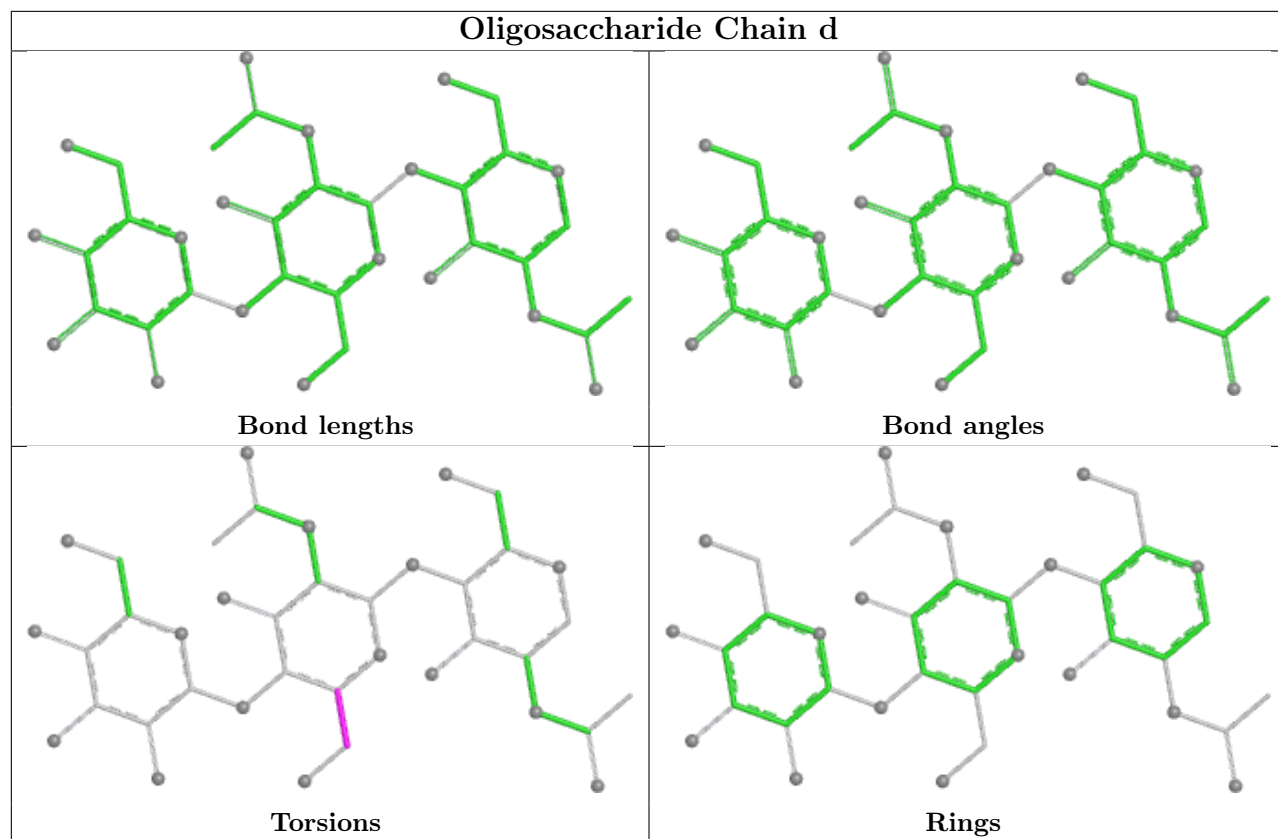


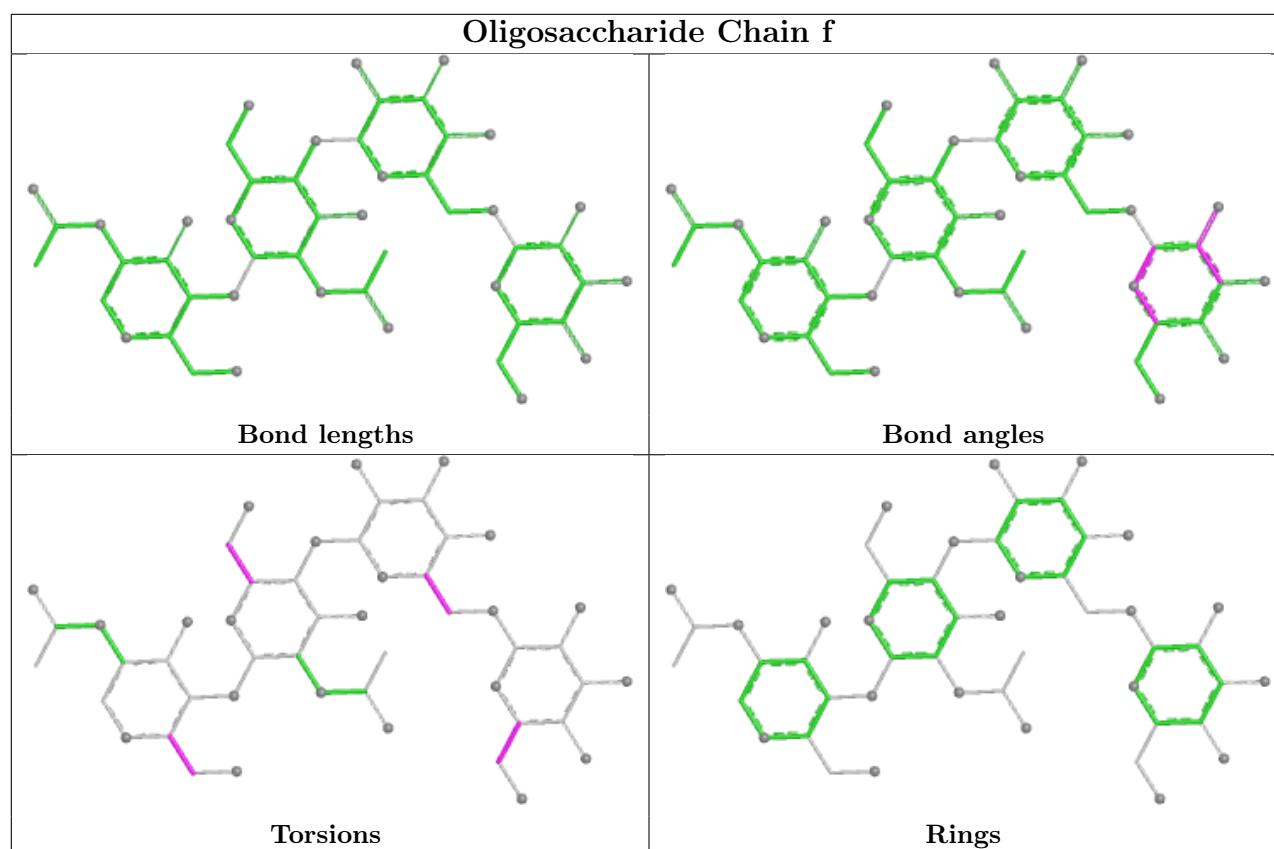












5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
12	CLR	E	501	-	31,31,31	0.49	0	48,48,48	1.04	3 (6%)
12	CLR	D	501	-	31,31,31	0.37	0	48,48,48	1.99	12 (25%)
12	CLR	B	501	-	31,31,31	0.44	0	48,48,48	1.67	8 (16%)
12	CLR	G	501	-	31,31,31	0.44	0	48,48,48	1.11	5 (10%)

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
12	CLR	E	501	-	-	8/10/68/68	0/4/4/4
12	CLR	D	501	-	-	0/10/68/68	0/4/4/4
12	CLR	B	501	-	-	6/10/68/68	0/4/4/4
12	CLR	G	501	-	-	3/10/68/68	0/4/4/4

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	D	501	CLR	C15-C14-C13	5.15	109.89	103.84
12	D	501	CLR	C16-C17-C13	-5.13	97.81	103.84
12	D	501	CLR	C13-C14-C8	-4.99	107.33	114.41
12	B	501	CLR	C8-C7-C6	-4.75	106.18	112.76
12	D	501	CLR	C12-C13-C14	-4.50	100.51	107.25
12	B	501	CLR	C10-C9-C8	-4.29	106.44	112.71
12	B	501	CLR	C14-C8-C9	3.70	113.92	109.09
12	D	501	CLR	C16-C15-C14	-3.35	98.59	105.14
12	D	501	CLR	C15-C14-C8	3.31	124.39	119.10
12	D	501	CLR	C12-C11-C9	3.21	118.60	113.14
12	D	501	CLR	C7-C8-C14	3.14	115.38	110.93
12	E	501	CLR	C12-C13-C14	-3.07	102.66	107.25
12	D	501	CLR	C14-C8-C9	-2.98	105.19	109.09
12	G	501	CLR	C17-C13-C14	2.98	103.51	100.10
12	G	501	CLR	C12-C13-C14	-2.96	102.82	107.25
12	B	501	CLR	C13-C14-C8	2.86	118.47	114.41
12	B	501	CLR	C15-C14-C13	-2.86	100.48	103.84
12	D	501	CLR	C12-C13-C17	2.72	120.61	116.60
12	B	501	CLR	C7-C8-C14	2.69	114.73	110.93
12	E	501	CLR	C17-C13-C14	2.67	103.17	100.10
12	E	501	CLR	C12-C11-C9	2.54	117.45	113.14
12	B	501	CLR	C19-C10-C9	-2.53	108.82	111.66
12	G	501	CLR	C19-C10-C9	2.52	114.48	111.66
12	G	501	CLR	C11-C9-C10	2.22	115.82	113.08
12	D	501	CLR	C7-C8-C9	2.20	112.26	109.72
12	D	501	CLR	C18-C13-C17	-2.14	107.79	111.68
12	G	501	CLR	C12-C11-C9	2.13	116.76	113.14
12	B	501	CLR	C11-C9-C8	2.02	114.60	111.78

There are no chirality outliers.

All (17) torsion outliers are listed below:

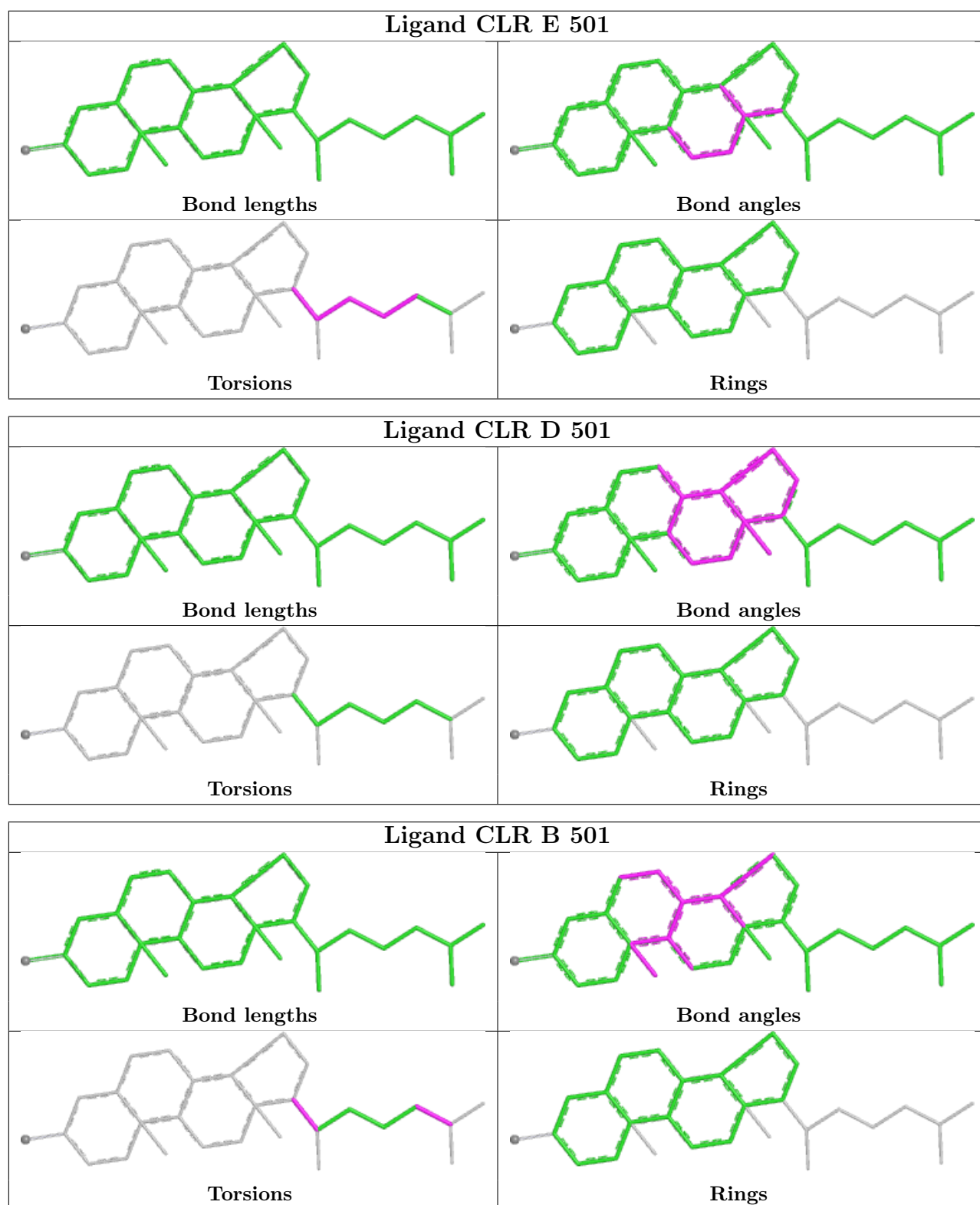
Mol	Chain	Res	Type	Atoms
12	B	501	CLR	C13-C17-C20-C22
12	G	501	CLR	C21-C20-C22-C23
12	B	501	CLR	C13-C17-C20-C21
12	E	501	CLR	C13-C17-C20-C21
12	E	501	CLR	C13-C17-C20-C22
12	G	501	CLR	C17-C20-C22-C23
12	E	501	CLR	C16-C17-C20-C21
12	E	501	CLR	C16-C17-C20-C22
12	B	501	CLR	C16-C17-C20-C21
12	E	501	CLR	C22-C23-C24-C25
12	E	501	CLR	C17-C20-C22-C23
12	E	501	CLR	C21-C20-C22-C23
12	B	501	CLR	C16-C17-C20-C22
12	G	501	CLR	C20-C22-C23-C24
12	B	501	CLR	C23-C24-C25-C27
12	B	501	CLR	C23-C24-C25-C26
12	E	501	CLR	C20-C22-C23-C24

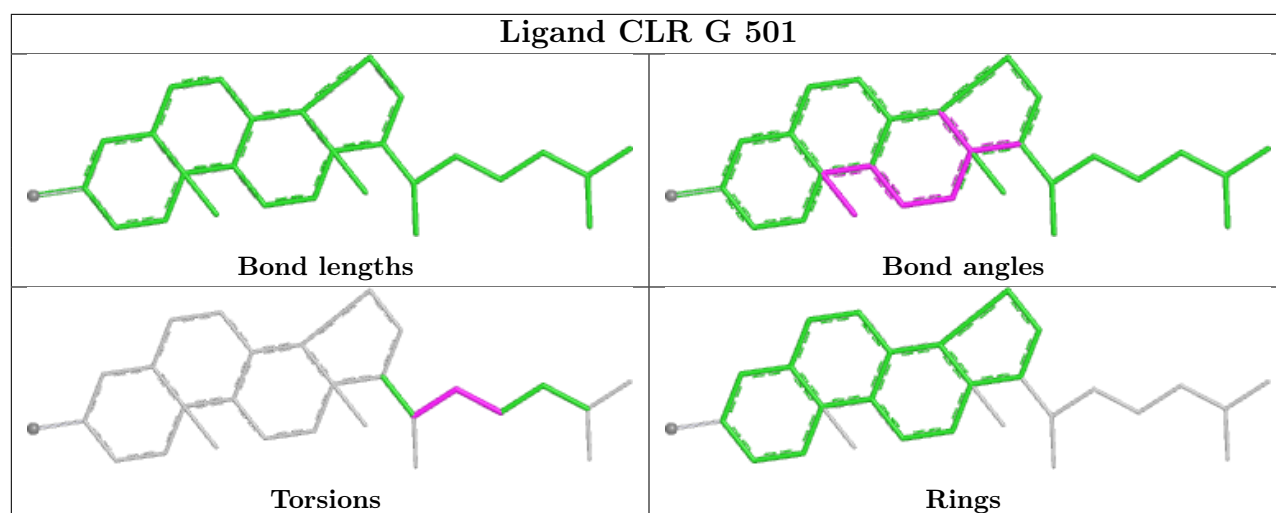
There are no ring outliers.

4 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	E	501	CLR	4	0
12	D	501	CLR	3	0
12	B	501	CLR	4	0
12	G	501	CLR	9	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

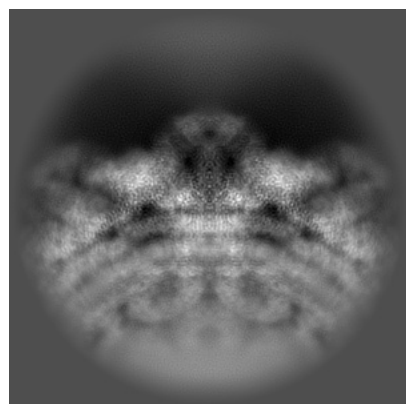
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61026. These allow visual inspection of the internal detail of the map and identification of artifacts.

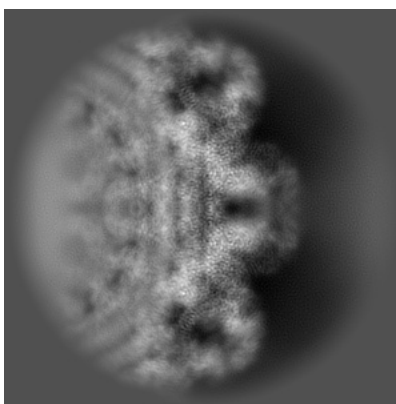
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

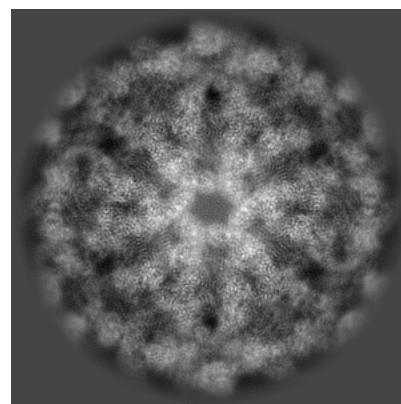
6.1.1 Primary map



X

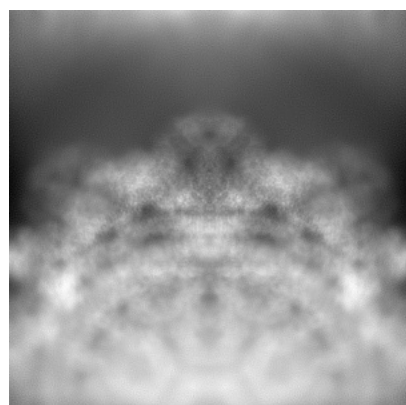


Y

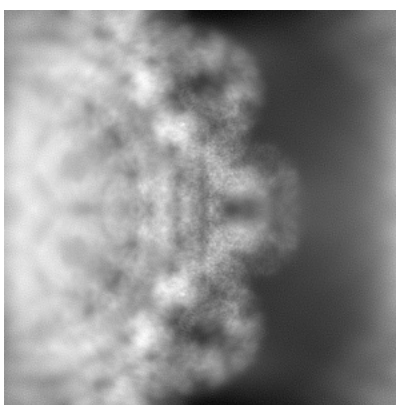


Z

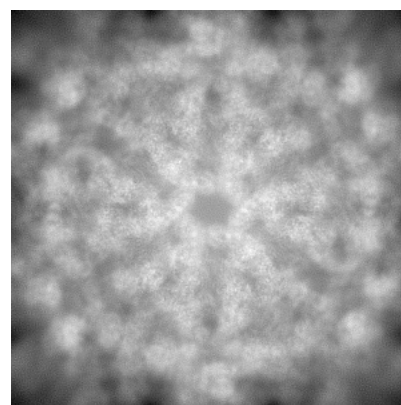
6.1.2 Raw map



X



Y

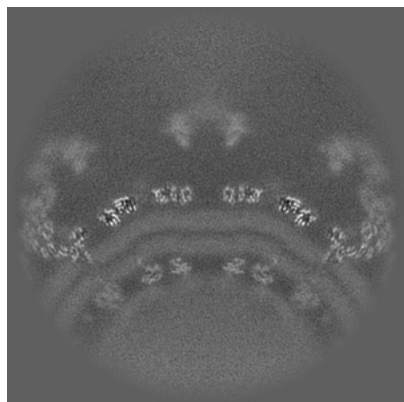


Z

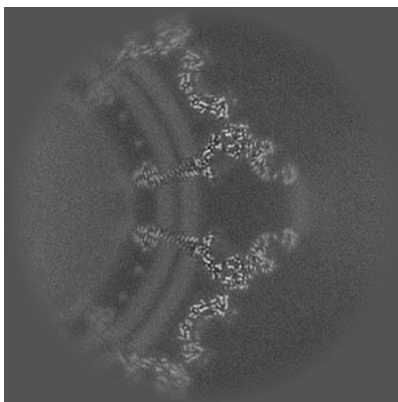
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

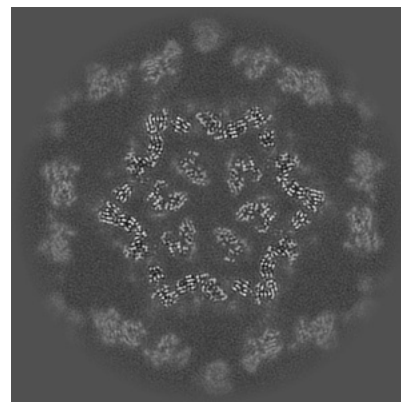
6.2.1 Primary map



X Index: 190

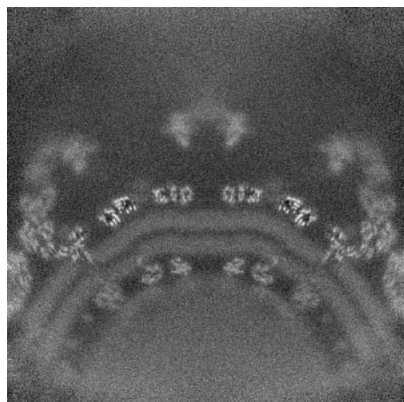


Y Index: 190

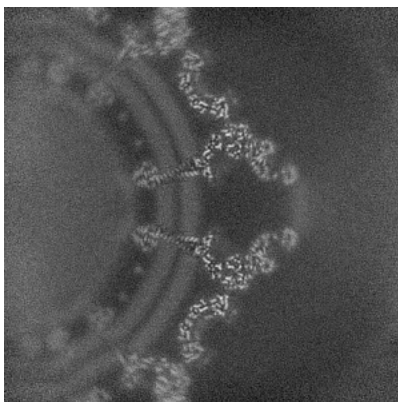


Z Index: 190

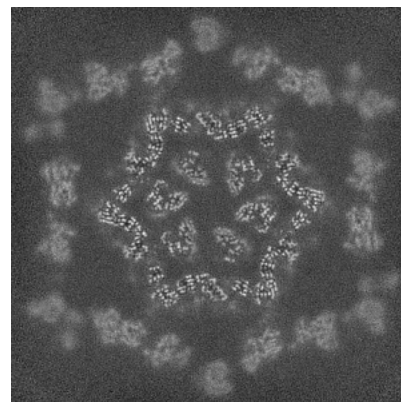
6.2.2 Raw map



X Index: 190



Y Index: 190

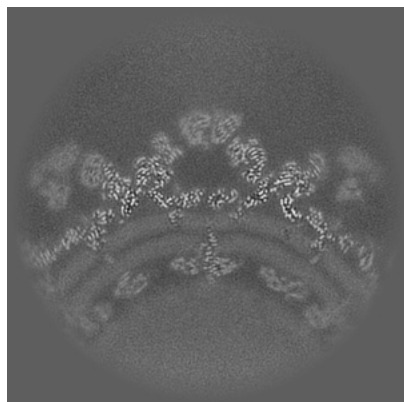


Z Index: 190

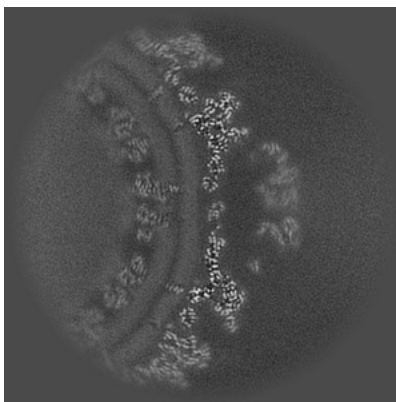
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

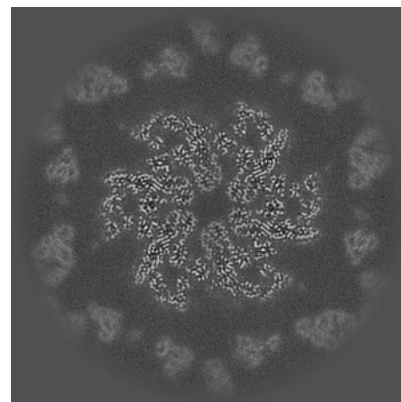
6.3.1 Primary map



X Index: 164

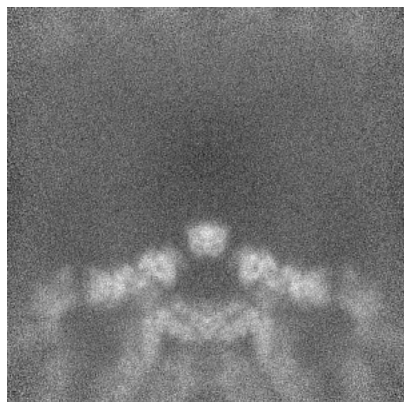


Y Index: 208

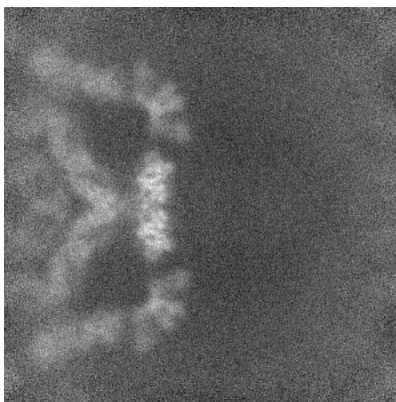


Z Index: 199

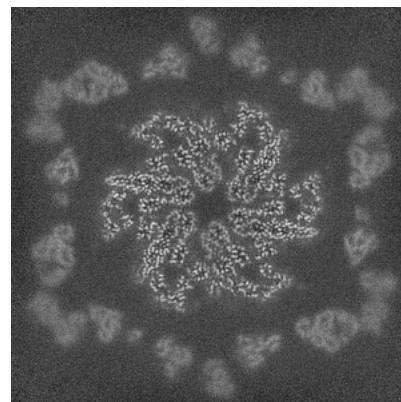
6.3.2 Raw map



X Index: 0



Y Index: 0

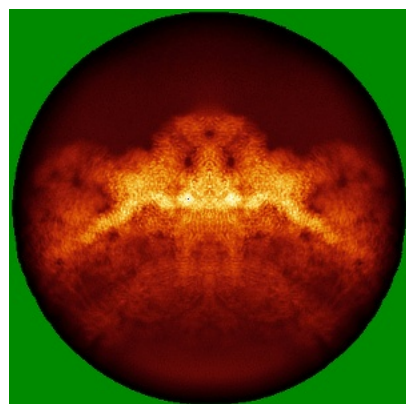


Z Index: 198

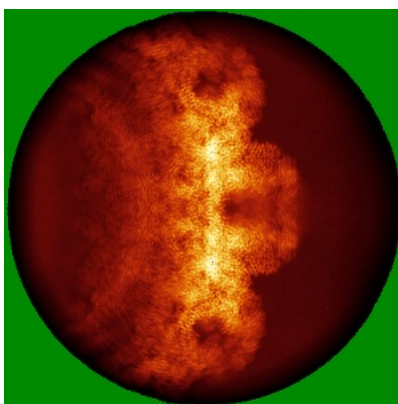
The images above show the largest variance slices of the map in three orthogonal directions.

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

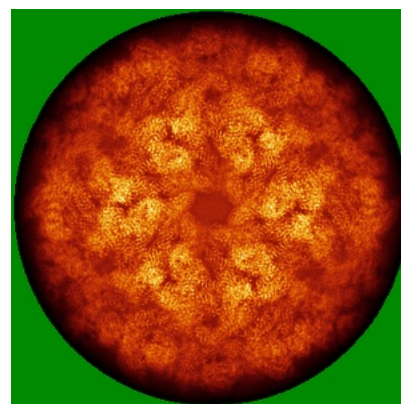
6.4.1 Primary map



X

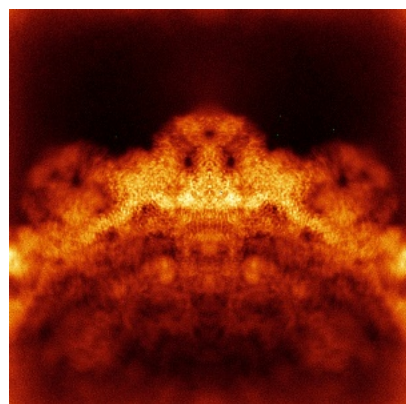


Y

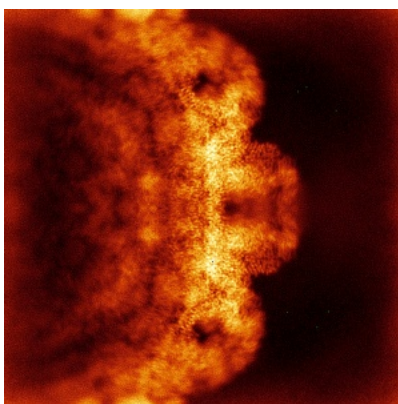


Z

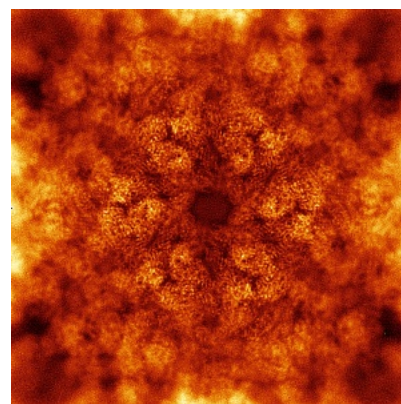
6.4.2 Raw map



X



Y

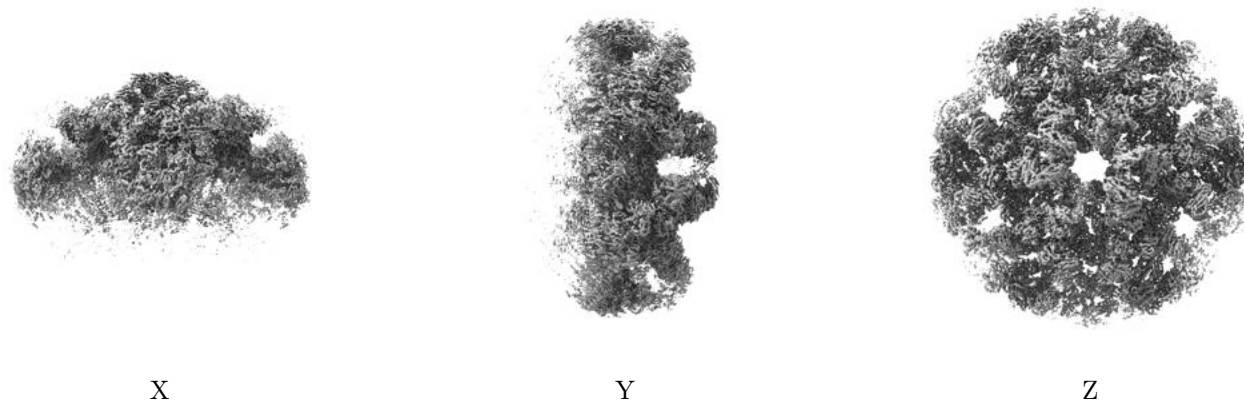


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.135. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

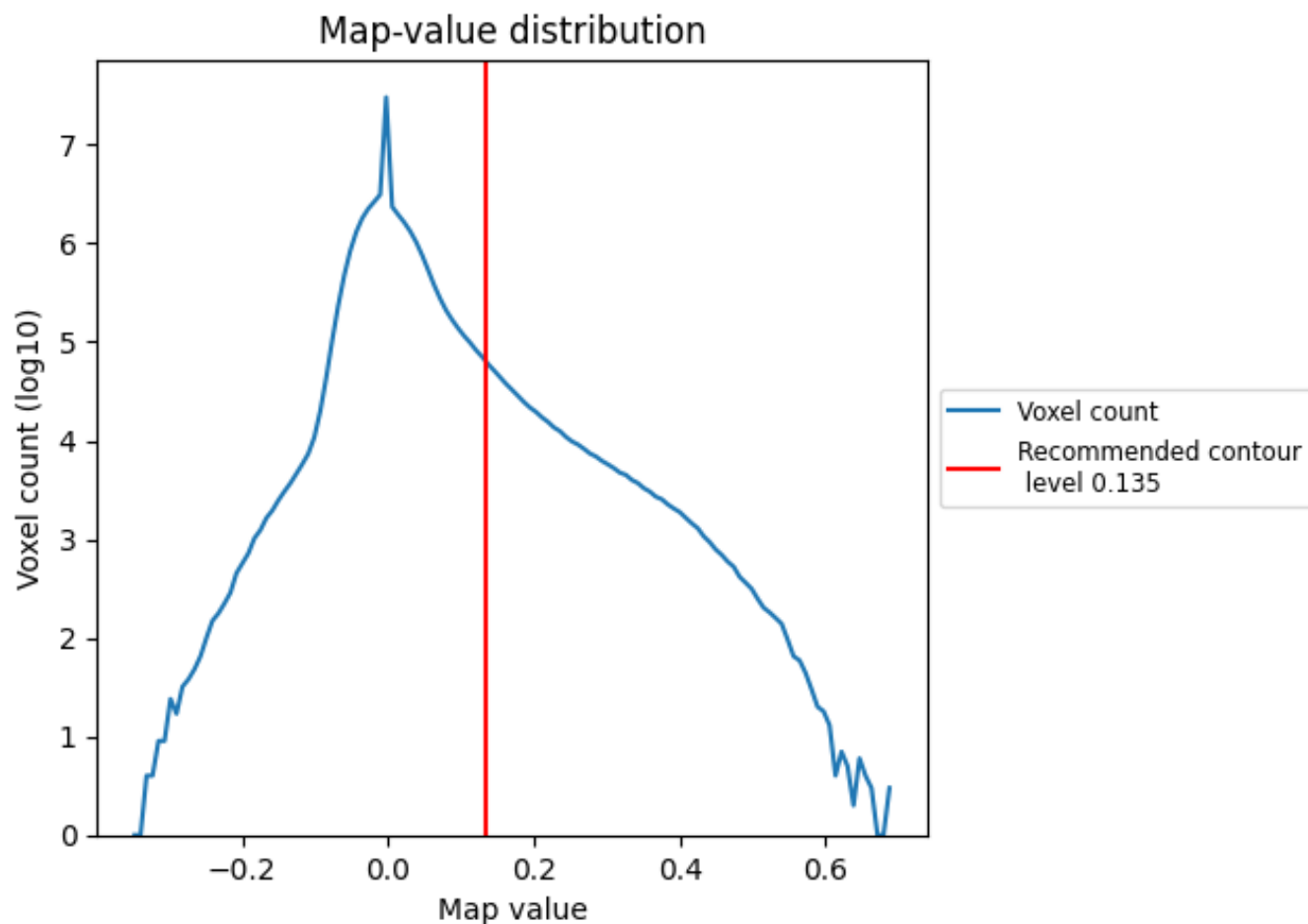
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

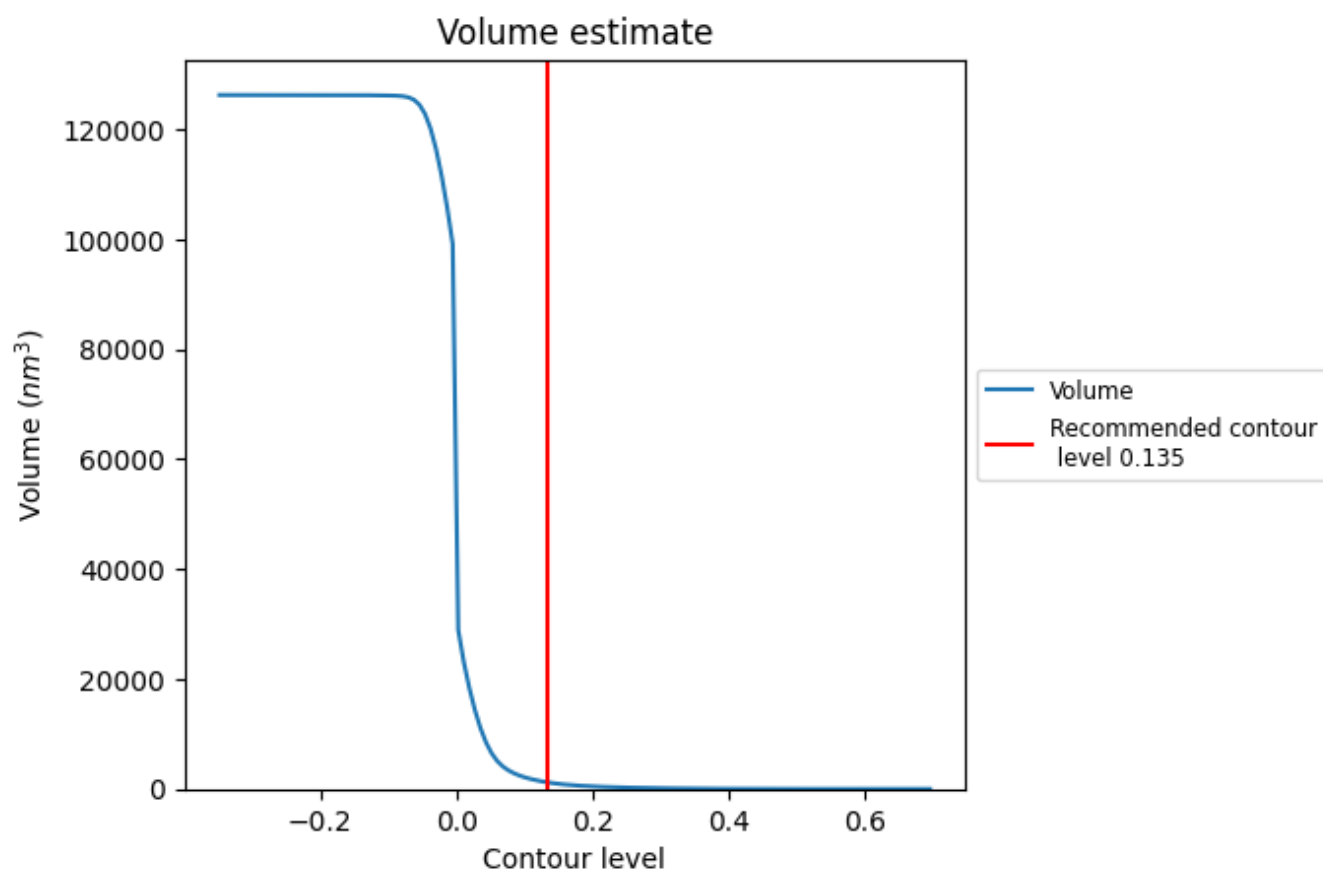
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

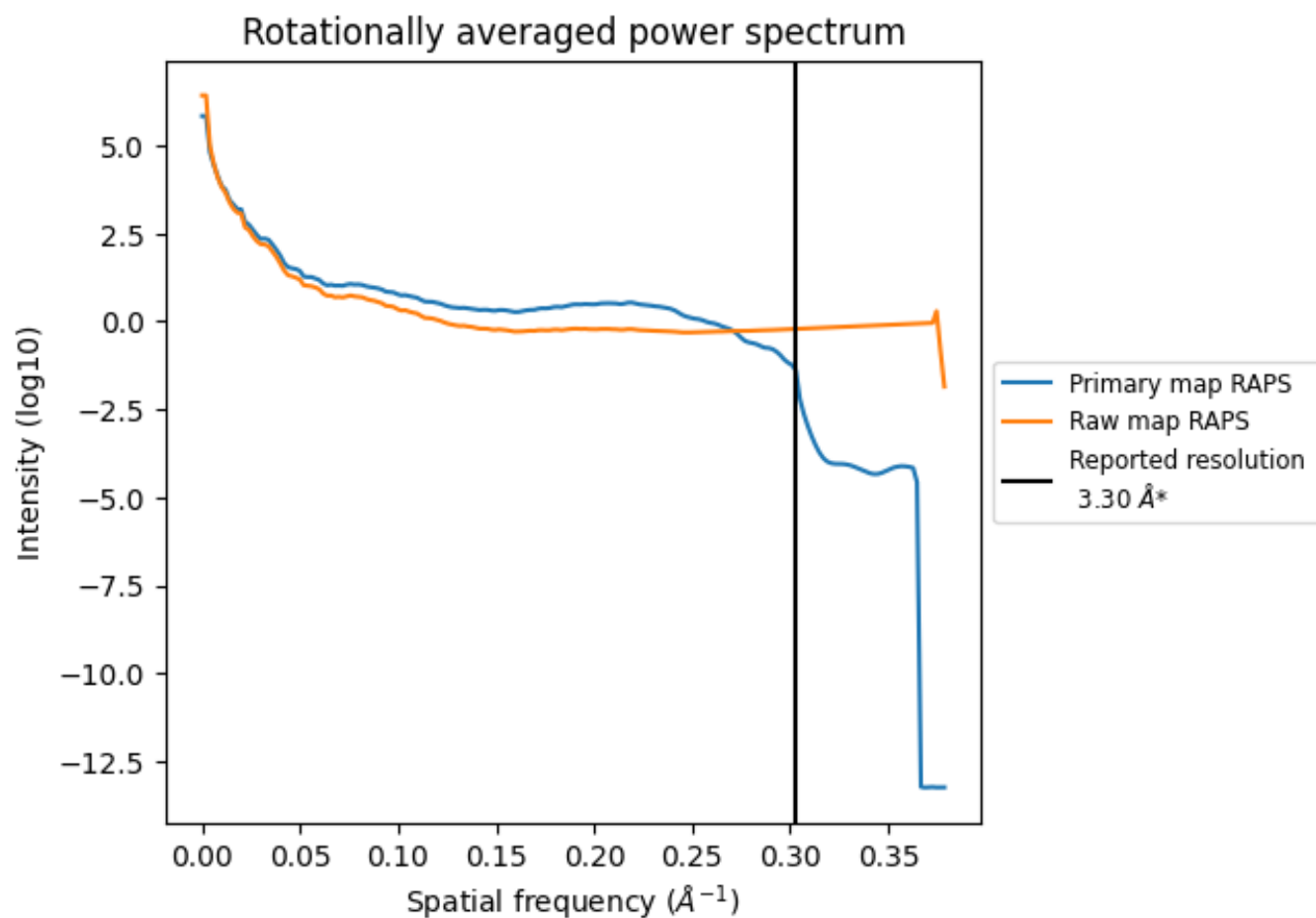
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1182 nm³; this corresponds to an approximate mass of 1068 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

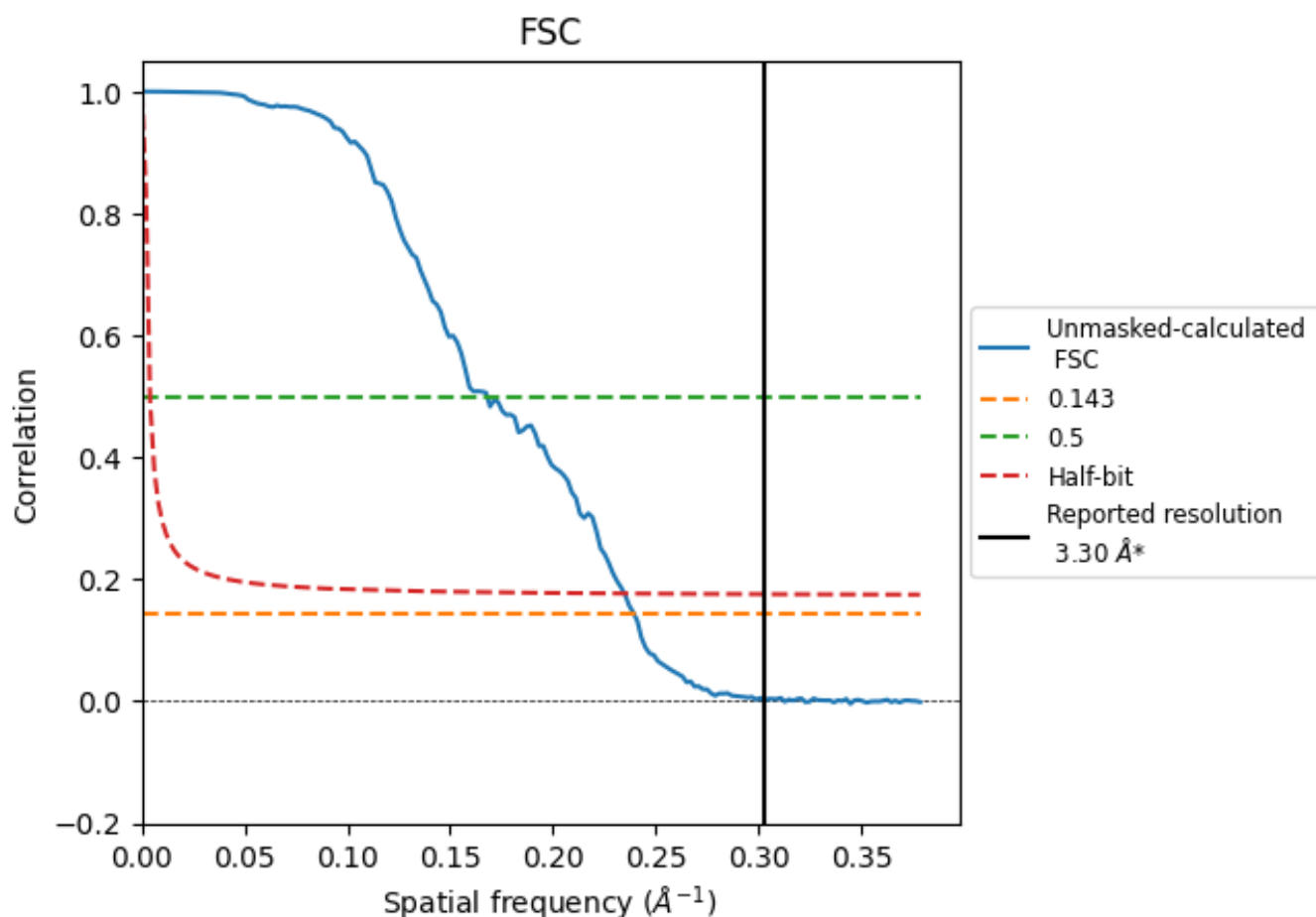


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.303 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

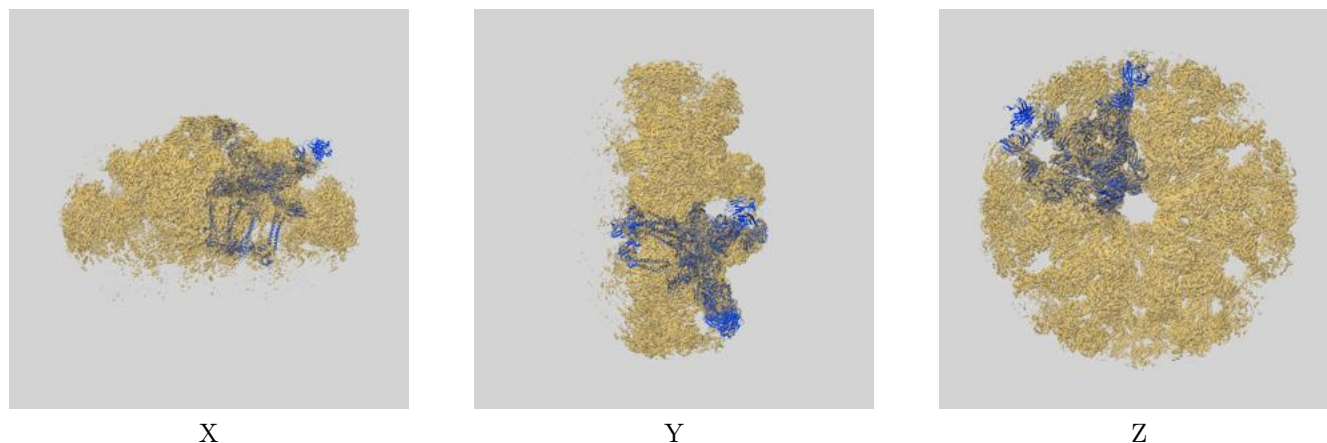
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.17	5.95	4.26

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.17 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-61026 and PDB model 9IZ9. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



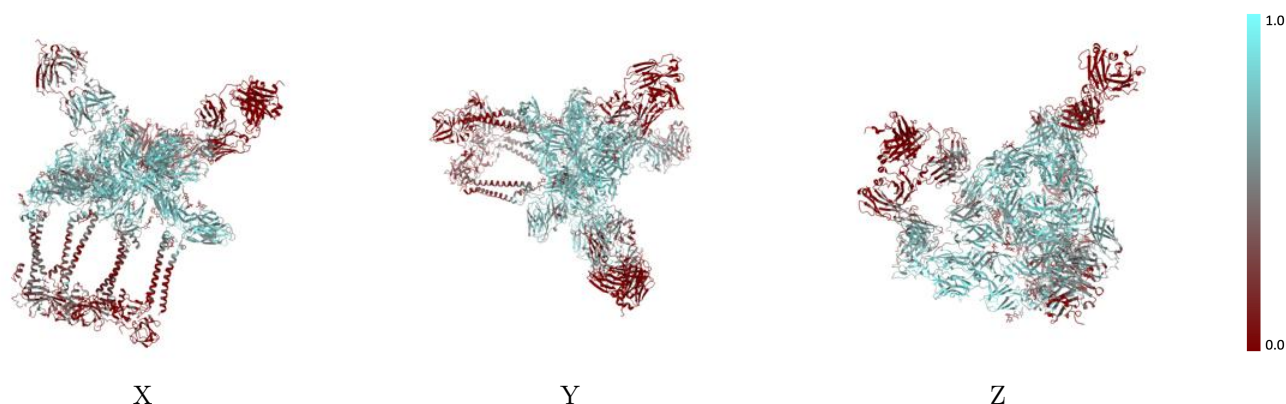
The images above show the 3D surface view of the map at the recommended contour level 0.135 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



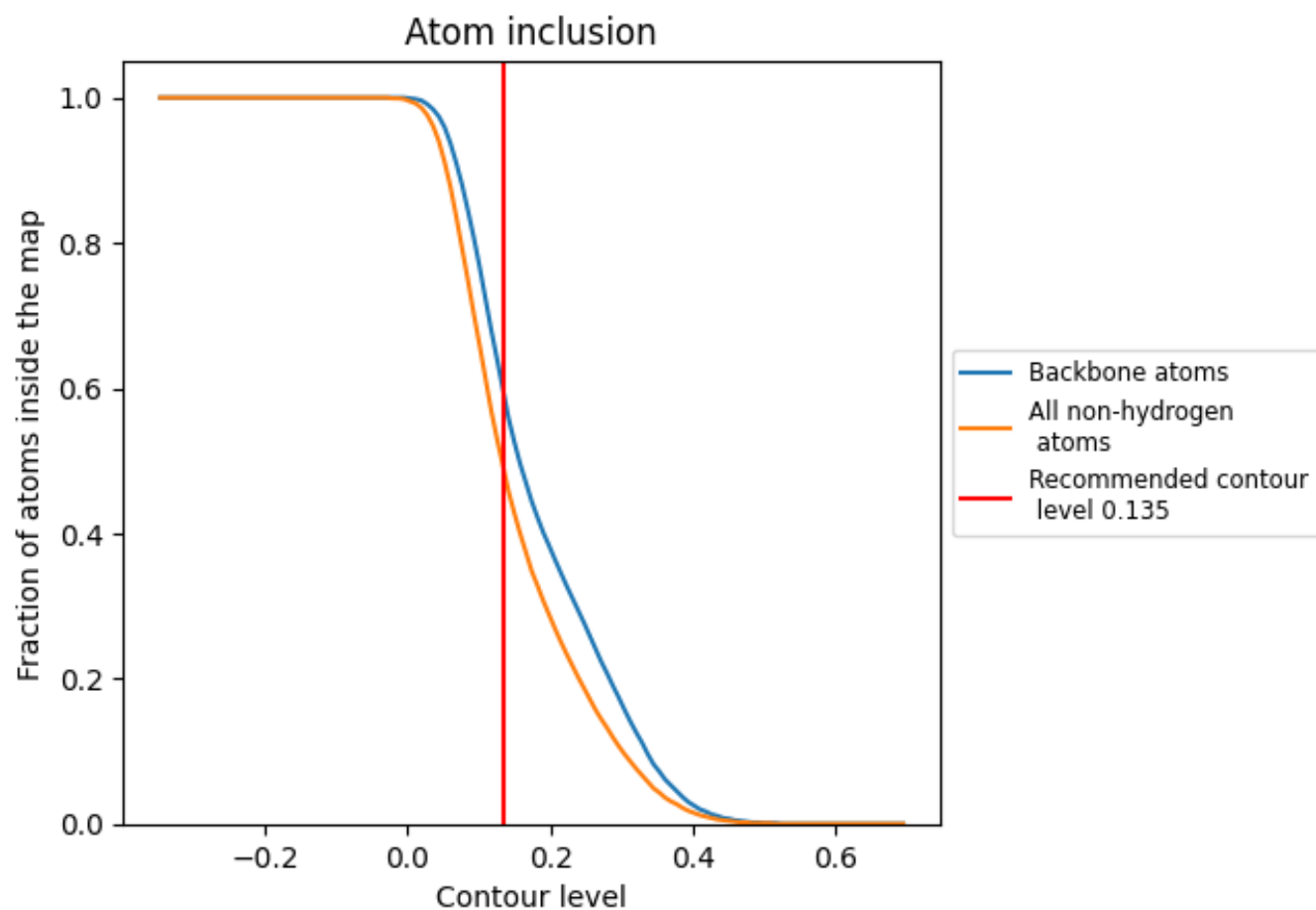
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.135).

9.4 Atom inclusion [i](#)



At the recommended contour level, 59% of all backbone atoms, 49% 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 (0.135) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4870	0.4220
A	0.6630	0.4930
B	0.6220	0.4920
C	0.6760	0.5030
D	0.6900	0.5110
E	0.6350	0.4860
F	0.6370	0.4820
G	0.6480	0.4860
H	0.6840	0.5010
I	0.0740	0.3440
J	0.2490	0.4090
K	0.1310	0.3750
L	0.2600	0.4150
M	0.1780	0.2020
N	0.1870	0.2680
O	0.1050	0.2580
P	0.0720	0.2650
Q	0.4140	0.3090
R	0.4950	0.4160
S	0.3450	0.3300
T	0.3510	0.2990
U	0.4290	0.4950
V	0.3060	0.4440
W	0.2670	0.3890
X	0.4080	0.4820
Y	0.1250	0.3620
Z	0.3330	0.4850
a	0.1200	0.3350
b	0.2310	0.4300
c	0.1410	0.4350
d	0.1540	0.4840
e	0.1880	0.4160
f	0.2200	0.4270

