



## Full wwPDB EM Validation Report ⓘ

Apr 8, 2026 – 11:51 PM UTC

PDB ID : 9MZS / pdb\_00009mzs  
EMDB ID : EMD-48767  
Title : cryoEM structure of GluK2 bound to BPAM344 and glutamate in the non-active state, composite map  
Authors : Zhou, C.; Tajima, N.  
Deposited on : 2025-01-23  
Resolution : 3.90 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

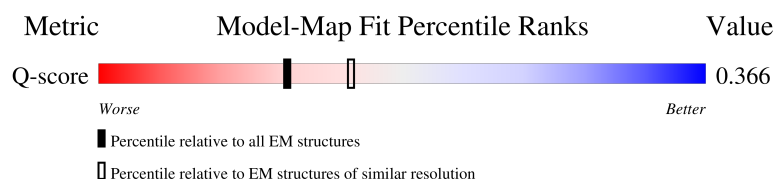
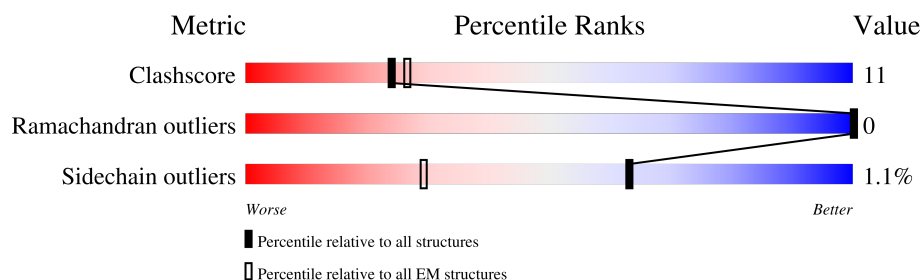
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 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 3.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8855 ( 3.40 - 4.40 )

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

Mol	Chain	Length	Quality of chain
1	A	908	 5% 64% 21% 15%
1	B	908	 5% 62% 22% 15%
1	C	908	 5% 62% 23% 15%
1	D	908	 5% 63% 21% 15%

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Mol	Chain	Length	Quality of chain
2	E	3	 67% 33%
2	F	3	 33% 67%
2	H	3	 67% 33%
2	I	3	 100%
2	N	3	 33% 33% 67%
2	O	3	 33% 67% 33%
3	G	2	 50% 50%
3	J	2	 100%
3	M	2	 50% 50%
4	K	3	 33% 67%
5	L	3	 100%

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 25004 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.

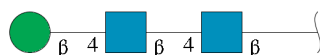
- Molecule 1 is a protein called Glutamate receptor ionotropic, kainate 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	774	Total	C	N	O	S	2	0
			6136	3942	1017	1143	34		
1	B	770	Total	C	N	O	S	1	0
			6097	3915	1013	1135	34		
1	C	775	Total	C	N	O	S	2	0
			6139	3943	1020	1142	34		
1	D	770	Total	C	N	O	S	0	0
			6090	3909	1013	1134	34		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	676	CYS	LYS	conflict	UNP P42260
A	802	CYS	ASN	conflict	UNP P42260
B	676	CYS	LYS	conflict	UNP P42260
B	802	CYS	ASN	conflict	UNP P42260
C	676	CYS	LYS	conflict	UNP P42260
C	802	CYS	ASN	conflict	UNP P42260
D	676	CYS	LYS	conflict	UNP P42260
D	802	CYS	ASN	conflict	UNP P42260

- Molecule 2 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
2	E	3	Total	C	N	O	0	0
			39	22	2	15		
2	F	3	Total	C	N	O	0	0
			39	22	2	15		

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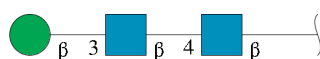
Mol	Chain	Residues	Atoms				AltConf	Trace
2	H	3	Total	C	N	O	0	0
			39	22	2	15		
2	I	3	Total	C	N	O	0	0
			39	22	2	15		
2	N	3	Total	C	N	O	0	0
			39	22	2	15		
2	O	3	Total	C	N	O	0	0
			39	22	2	15		

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



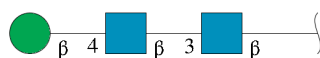
Mol	Chain	Residues	Atoms				AltConf	Trace
3	G	2	Total	C	N	O	0	0
			28	16	2	10		
3	J	2	Total	C	N	O	0	0
			28	16	2	10		
3	M	2	Total	C	N	O	0	0
			28	16	2	10		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
4	K	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose.



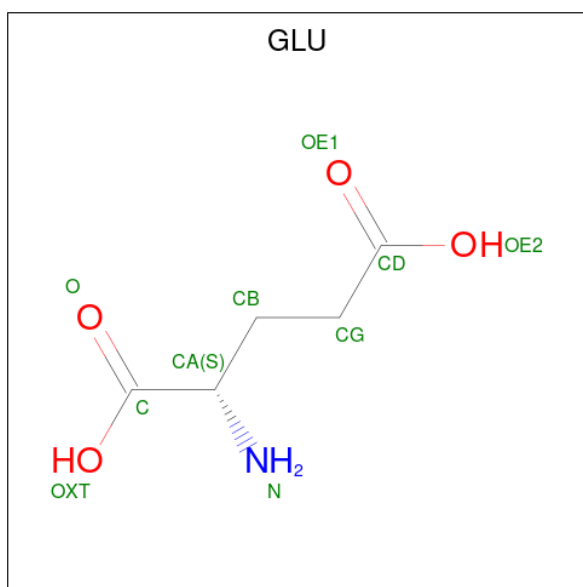
Mol	Chain	Residues	Atoms				AltConf	Trace
5	L	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).



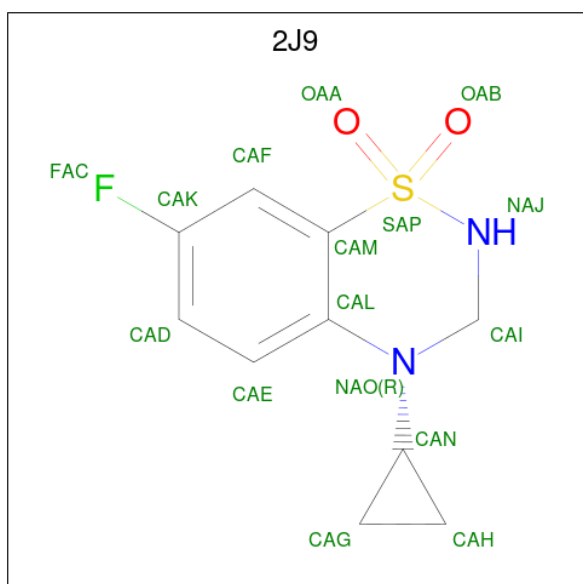
Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 7 is GLUTAMIC ACID (CCD ID: GLU) (formula:  $C_5H_9NO_4$ ).



Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	N	O	0
			10	5	1	4	
7	B	1	Total	C	N	O	0
			10	5	1	4	
7	C	1	Total	C	N	O	0
			10	5	1	4	
7	D	1	Total	C	N	O	0
			10	5	1	4	

- Molecule 8 is 4-cyclopropyl-7-fluoro-3,4-dihydro-2H-1,2,4-benzothiadiazine 1,1-dioxide (CCD ID: 2J9) (formula: C<sub>10</sub>H<sub>11</sub>FN<sub>2</sub>O<sub>2</sub>S).



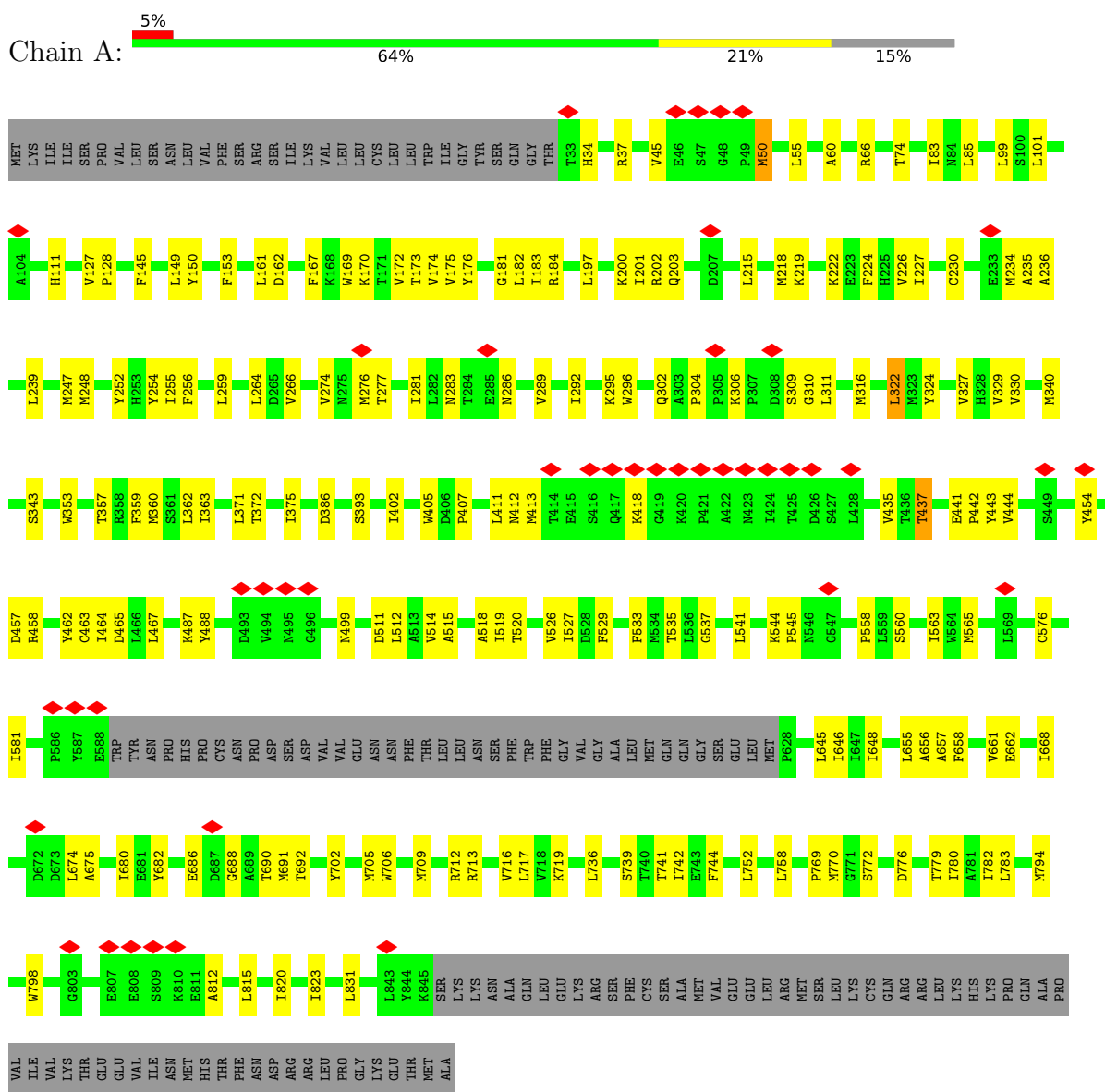
Mol	Chain	Residues	Atoms						AltConf
8	B	1	Total	C	F	N	O	S	0
			16	10	1	2	2	1	
8	C	1	Total	C	F	N	O	S	0
			16	10	1	2	2	1	
8	D	1	Total	C	F	N	O	S	0
			16	10	1	2	2	1	
8	D	1	Total	C	F	N	O	S	0
			16	10	1	2	2	1	



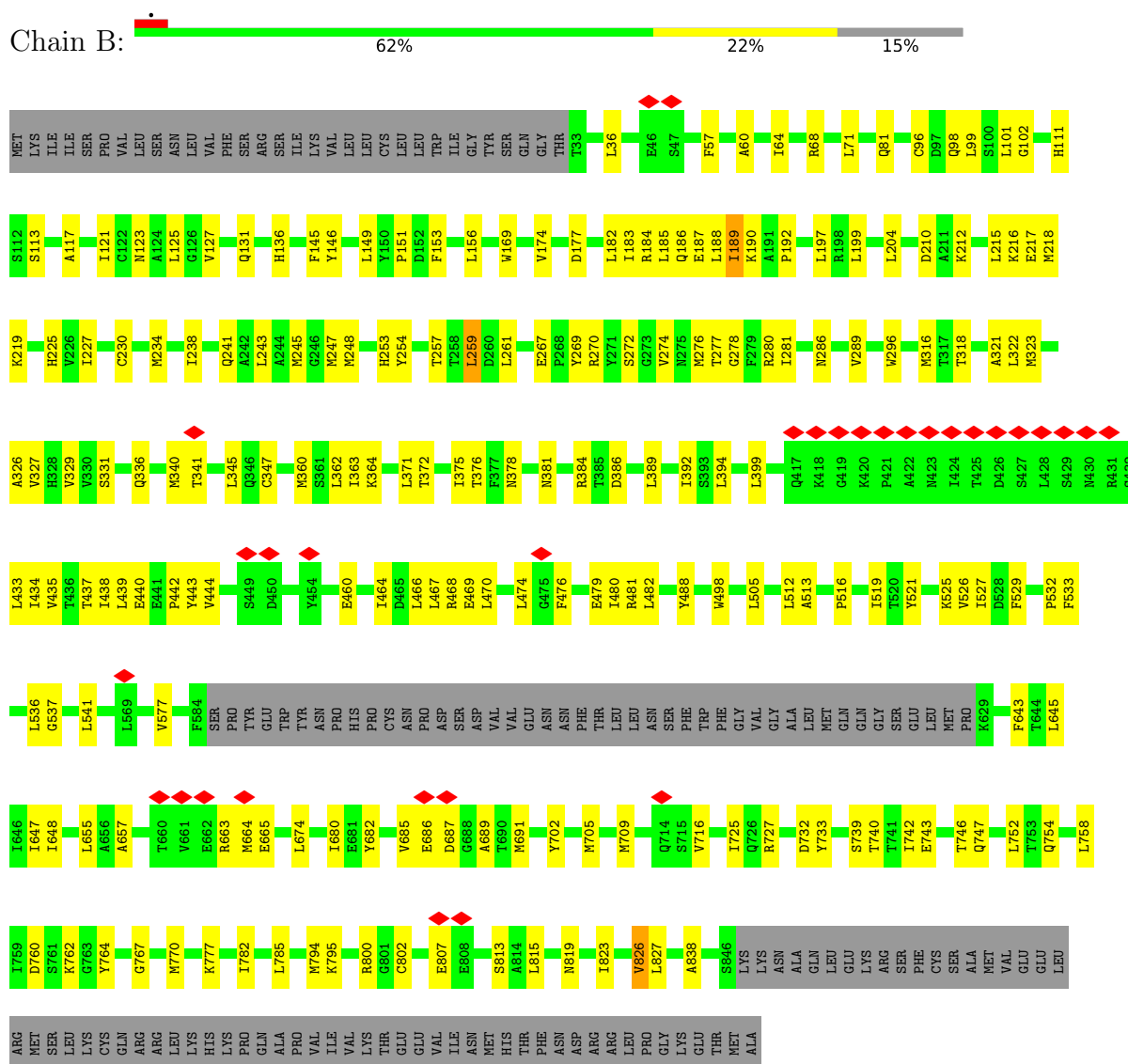
### 3 Residue-property plots

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

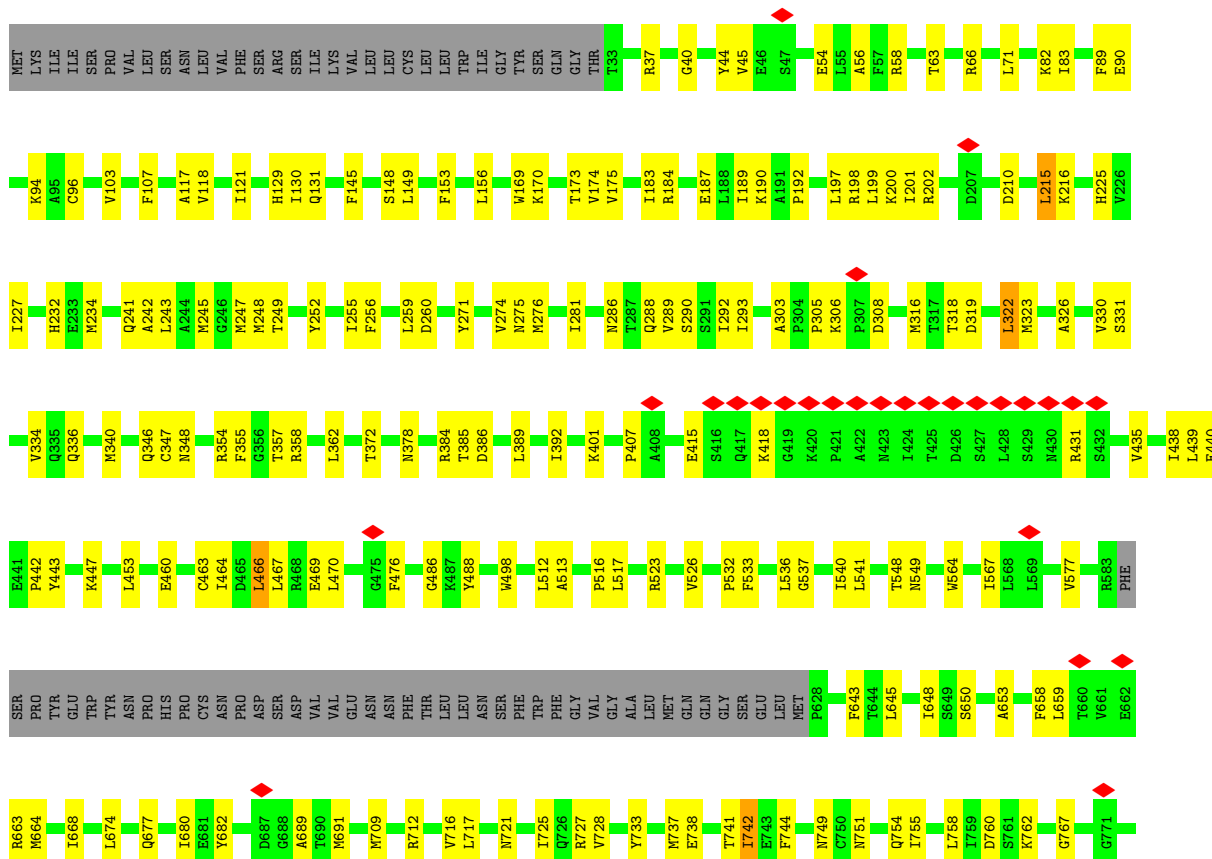
- Molecule 1: Glutamate receptor ionotropic, kainate 2

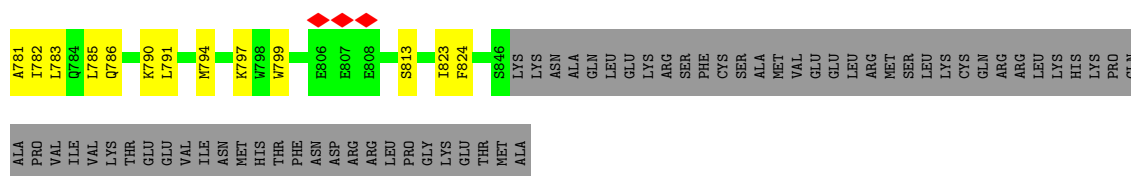


Chain B:



- Molecule 1: Glutamate receptor ionotropic, kainate 2





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

Chain E: 67% 33%



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

Chain F: 33% 67%



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

Chain H: 67% 33%



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

Chain I: 100%



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

Chain N: 33% 33% 67%



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

Chain O: 33% 67% 67%



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

Chain G: 50% 50%



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

Chain J: 100%



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

Chain M: 50% 50%



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

Chain K: 33% 67%



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L: 100%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	127714	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.140	Depositor
Minimum map value	-1.199	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.056	Depositor
Recommended contour level	0.243	Depositor
Map size ( $\text{\AA}$ )	296.8, 296.8, 296.8	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.06, 1.06, 1.06	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: 2J9, BMA, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.11	0/6279	0.34	2/8501 (0.0%)
1	B	0.12	0/6234	0.34	0/8438
1	C	0.13	0/6281	0.31	0/8501
1	D	0.11	0/6224	0.29	0/8425
All	All	0.12	0/25018	0.32	2/33865 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	50	MET	CB-CA-C	9.43	129.49	111.48
1	A	50	MET	N-CA-C	-6.06	101.22	109.95

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6136	0	6133	129	0
1	B	6097	0	6095	145	0
1	C	6139	0	6149	149	0
1	D	6090	0	6089	148	0
2	E	39	0	34	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	39	0	34	0	0
2	H	39	0	34	0	0
2	I	39	0	34	0	0
2	N	39	0	34	0	0
2	O	39	0	34	1	0
3	G	28	0	25	1	0
3	J	28	0	25	0	0
3	M	28	0	25	2	0
4	K	39	0	34	0	0
5	L	39	0	34	0	0
6	A	14	0	13	0	0
6	B	14	0	13	0	0
6	C	14	0	13	0	0
7	A	10	0	5	2	0
7	B	10	0	5	1	0
7	C	10	0	5	1	0
7	D	10	0	5	0	0
8	B	16	0	11	2	0
8	C	16	0	11	1	0
8	D	32	0	22	4	0
All	All	25004	0	24916	537	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 (537) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:527:ILE:HA	1:C:770:MET:HE1	1.65	0.79
1:A:645:LEU:HD21	1:B:648:ILE:HD12	1.64	0.79
1:A:527:ILE:HA	1:A:770:MET:HE1	1.64	0.78
1:B:439:LEU:HD21	1:B:482:LEU:HD13	1.66	0.77
1:A:169:TRP:HE1	1:A:172:VAL:HB	1.47	0.77
1:C:536:LEU:HB2	1:C:763:GLY:H	1.50	0.75
1:C:669:ASP:HA	1:C:755:ILE:HD11	1.67	0.75
1:C:83:ILE:HG22	1:C:85:LEU:H	1.52	0.74
1:C:189:ILE:HG22	1:D:201:ILE:HG13	1.69	0.74
1:C:227:ILE:HG12	1:C:255:ILE:HB	1.68	0.73
1:B:434:ILE:HD11	1:B:481:ARG:HD3	1.70	0.73
1:A:45:VAL:HG11	1:A:50:MET:HG2	1.72	0.72
1:A:292:ILE:HA	1:A:295:LYS:HG2	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:TYR:HB2	1:B:276:MET:HG2	1.71	0.72
1:A:686:GLU:HB3	1:A:719:LYS:HA	1.71	0.71
1:B:183:ILE:HD12	1:B:183:ILE:H	1.56	0.69
1:D:435:VAL:HG12	1:D:512:LEU:HB2	1.74	0.69
1:C:658:PHE:HE1	1:D:813:SER:H	1.41	0.68
1:A:85:LEU:HB3	1:A:111:HIS:HB2	1.74	0.68
1:B:527:ILE:HG13	1:B:529:PHE:HE1	1.58	0.68
1:D:536:LEU:HD11	1:D:762:LYS:HB2	1.76	0.68
1:A:37:ARG:HH12	1:A:101:LEU:HB3	1.58	0.68
1:A:454:TYR:HA	1:A:458:ARG:HD3	1.76	0.67
1:D:210:ASP:HA	1:D:241:GLN:HE22	1.58	0.66
1:B:664:MET:HE3	1:B:665:GLU:O	1.96	0.66
1:B:322:LEU:HD22	1:B:372:THR:HG21	1.77	0.66
1:A:558:PRO:HG2	1:A:655:LEU:HB2	1.78	0.66
1:D:275:ASN:HB3	3:M:1:NAG:HN2	1.60	0.66
1:B:316:MET:HG3	1:B:321:ALA:HB2	1.76	0.65
1:A:541:LEU:HB2	1:A:742:ILE:HD11	1.79	0.65
1:D:281:ILE:HD13	1:D:389:LEU:HD23	1.78	0.65
1:C:163:LEU:HD22	1:C:411:LEU:HD11	1.78	0.65
1:D:340:MET:HA	1:D:340:MET:HE3	1.77	0.65
1:A:276:MET:HE2	1:A:276:MET:HA	1.78	0.65
1:B:101:LEU:HD23	1:B:102:GLY:O	1.97	0.65
1:A:248:MET:HB2	1:A:274:VAL:HG21	1.80	0.64
1:B:36:LEU:HD11	1:B:340:MET:HG3	1.79	0.64
1:C:567:ILE:HD11	1:C:647:ILE:HD12	1.79	0.64
1:C:161:LEU:HD21	1:C:188:LEU:HA	1.80	0.64
1:B:68:ARG:H	3:G:1:NAG:H82	1.63	0.63
1:D:173:THR:HG22	1:D:200:LYS:HB2	1.80	0.63
1:D:340:MET:HE1	1:D:355:PHE:HD2	1.62	0.63
1:B:149:LEU:HD13	1:B:326:ALA:HA	1.80	0.63
1:D:290:SER:HA	1:D:293:ILE:HD12	1.81	0.63
1:A:215:LEU:HD13	1:A:218:MET:HE1	1.81	0.63
1:C:360:MET:HA	1:C:363:ILE:HG12	1.80	0.63
1:C:151:PRO:HB2	1:C:156:LEU:HD21	1.81	0.62
1:A:658:PHE:HE1	1:B:813:SER:H	1.48	0.62
1:D:440:GLU:HG3	1:D:442:PRO:HD2	1.82	0.62
1:A:537:GLY:HA3	1:A:758:LEU:HD22	1.82	0.62
1:B:743:GLU:HA	1:B:746:THR:HG22	1.82	0.62
1:A:99:LEU:HD11	1:A:127:VAL:HG11	1.82	0.62
1:A:283:ASN:HB3	1:A:289:VAL:HG21	1.81	0.62
1:A:526:VAL:HG13	1:A:527:ILE:HG23	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:440:GLU:HG3	1:C:442:PRO:HD2	1.83	0.61
1:D:249:THR:H	1:D:252:TYR:HB2	1.66	0.61
1:C:749:ASN:HB2	1:C:752:LEU:HD12	1.83	0.61
1:B:647:ILE:H	1:B:647:ILE:HD12	1.65	0.61
1:C:677:GLN:HE22	1:C:680:ILE:HG13	1.65	0.61
1:A:281:ILE:HG13	1:A:372:THR:HB	1.82	0.60
1:D:668:ILE:HG12	1:D:674:LEU:HD13	1.82	0.60
1:A:162:ASP:HB3	1:A:411:LEU:HD22	1.82	0.60
1:C:645:LEU:HD11	1:D:648:ILE:HG13	1.82	0.60
1:A:533:PHE:HB3	1:A:782:ILE:HD11	1.84	0.60
1:A:254:TYR:HB2	1:A:276:MET:HE1	1.81	0.60
1:B:689:ALA:H	7:B:1003:GLU:HB3	1.65	0.60
1:D:541:LEU:HB2	1:D:742:ILE:HD11	1.82	0.60
1:B:57:PHE:HB2	1:B:323:MET:HE1	1.84	0.59
1:B:329:VAL:HG21	1:B:375:ILE:HG21	1.84	0.59
1:C:688:GLY:H	1:C:691:MET:HE2	1.67	0.59
1:D:354:ARG:HH11	1:D:354:ARG:HG2	1.68	0.59
1:B:437:THR:HG21	1:B:444:VAL:HG21	1.84	0.59
1:C:126:GLY:HA2	1:C:145:PHE:HE2	1.66	0.59
1:C:138:VAL:HG13	1:C:141:ASN:HB2	1.84	0.59
1:D:292:ILE:HD12	1:D:292:ILE:H	1.68	0.59
1:D:183:ILE:HD12	1:D:183:ILE:H	1.68	0.59
1:A:182:LEU:HB3	1:B:182:LEU:HD23	1.83	0.59
1:A:443:TYR:HB3	1:A:463:CYS:HB2	1.84	0.59
1:D:293:ILE:HG23	1:D:316:MET:HG2	1.85	0.58
1:C:172:VAL:HG12	1:C:197:LEU:HD11	1.86	0.58
1:A:706:TRP:HA	1:A:709:MET:HG3	1.83	0.58
1:B:536:LEU:HD11	1:B:762:LYS:HB2	1.85	0.58
1:B:725:ILE:HD12	1:B:725:ILE:H	1.68	0.58
1:A:183:ILE:HD11	1:B:183:ILE:HD11	1.86	0.58
1:D:659:LEU:HD23	1:D:659:LEU:H	1.69	0.58
1:A:60:ALA:HB1	1:A:327:VAL:HG21	1.86	0.58
1:D:447:LYS:HG3	1:D:453:LEU:HB2	1.85	0.58
1:A:668:ILE:HG23	1:A:674:LEU:HD21	1.86	0.58
1:C:523:ARG:HH21	1:C:689:ALA:HB2	1.66	0.58
1:C:245:MET:HA	1:C:245:MET:HE3	1.86	0.58
1:B:533:PHE:HB3	1:B:782:ILE:HD12	1.84	0.58
1:B:177:ASP:HA	1:B:204:LEU:HB2	1.85	0.57
1:C:248:MET:N	1:C:248:MET:HE2	2.19	0.57
1:C:533:PHE:HD1	1:C:534:MET:HG3	1.69	0.57
1:A:770:MET:N	1:A:770:MET:HE2	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:ALA:HB1	1:B:327:VAL:HG11	1.86	0.57
1:C:686:GLU:HA	1:C:717:LEU:HD12	1.85	0.57
1:D:691:MET:HE1	1:D:717:LEU:HD21	1.86	0.57
1:D:564:TRP:HA	1:D:567:ILE:HD12	1.85	0.57
1:B:371:LEU:HD12	1:B:371:LEU:H	1.69	0.57
1:A:289:VAL:HG13	1:A:371:LEU:HG	1.87	0.57
1:C:201:ILE:HG13	1:D:189:ILE:HG22	1.86	0.57
1:D:197:LEU:HD12	1:D:198:ARG:H	1.70	0.57
1:C:533:PHE:HB3	1:C:782:ILE:HD11	1.86	0.56
1:D:130:ILE:HG21	1:D:326:ALA:HB1	1.87	0.56
1:A:444:VAL:HG12	1:A:464:ILE:HG12	1.88	0.56
1:C:459:PHE:HB2	1:C:480:ILE:HD12	1.86	0.56
1:B:770:MET:HE3	1:B:770:MET:HA	1.87	0.56
1:D:286:ASN:HB3	1:D:289:VAL:HG22	1.88	0.56
1:D:442:PRO:HG2	1:D:741:THR:HG23	1.87	0.56
1:B:375:ILE:HA	1:B:384:ARG:HH12	1.70	0.56
1:C:215:LEU:HA	1:C:218:MET:HG2	1.87	0.56
1:D:438:ILE:HD11	1:D:486:GLY:HA2	1.88	0.56
1:C:259:LEU:HD13	1:C:281:ILE:HB	1.88	0.56
1:C:523:ARG:HE	1:C:689:ALA:HB2	1.72	0.56
1:A:201:ILE:HG22	1:B:190:LYS:HG2	1.88	0.55
1:C:643:PHE:HA	1:D:823:ILE:HD11	1.86	0.55
1:D:537:GLY:HA3	1:D:758:LEU:HG	1.88	0.55
1:D:532:PRO:HG2	8:D:1002:2J9:H11	1.89	0.55
1:B:177:ASP:HB3	1:B:204:LEU:HD12	1.88	0.55
1:C:770:MET:HE2	1:C:770:MET:N	2.21	0.55
1:B:131:GLN:HE22	1:B:146:TYR:HB2	1.71	0.55
1:B:532:PRO:HG2	8:B:1002:2J9:H11	1.87	0.55
1:A:227:ILE:HG12	1:A:255:ILE:HB	1.89	0.55
1:B:185:LEU:HD21	1:B:257:THR:HG21	1.89	0.55
1:B:702:TYR:HA	1:B:705:MET:HB2	1.89	0.55
1:C:121:ILE:HD12	1:C:121:ILE:H	1.71	0.55
1:A:150:TYR:HA	1:A:322:LEU:HD21	1.87	0.55
1:A:286:ASN:HB3	1:A:289:VAL:HG23	1.88	0.55
1:B:742:ILE:HG21	1:B:754:GLN:HB2	1.88	0.55
1:C:516:PRO:HA	1:C:764:TYR:CE2	2.42	0.55
1:C:340:MET:HE1	1:C:355:PHE:CD2	2.41	0.54
1:A:467:LEU:HB2	1:A:514:VAL:HG11	1.89	0.54
1:A:413:MET:N	1:A:413:MET:HE2	2.22	0.54
1:B:187:GLU:HA	1:B:190:LYS:HZ3	1.72	0.54
1:B:657:ALA:HB2	1:C:660:THR:HG22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:VAL:HG12	1:A:227:ILE:HB	1.88	0.54
1:A:442:PRO:HG2	1:A:741:THR:HG23	1.88	0.54
1:B:272:SER:HA	1:D:245:MET:HA	1.88	0.54
1:B:286:ASN:HB3	1:B:289:VAL:HG12	1.89	0.54
1:B:253:HIS:HE1	1:B:277:THR:HG23	1.73	0.54
1:B:438:ILE:HG21	1:B:488:TYR:CZ	2.43	0.54
1:C:737:MET:HE3	1:C:741:THR:HB	1.90	0.54
1:A:646:ILE:HG21	1:B:823:ILE:HD13	1.88	0.53
1:C:135:LYS:HG2	1:C:137:GLN:HE22	1.73	0.53
1:A:675:ALA:HB3	1:B:802:CYS:HB3	1.90	0.53
1:B:440:GLU:HG2	1:B:442:PRO:HD2	1.89	0.53
1:A:815:LEU:HD13	1:A:820:ILE:HD11	1.91	0.53
1:A:340:MET:HE3	1:A:340:MET:HA	1.91	0.53
1:A:779:THR:HA	1:A:782:ILE:HG22	1.90	0.53
1:A:302:GLN:HE22	1:A:304:PRO:HG3	1.74	0.53
1:C:769:PRO:HD2	1:C:772:SER:HB2	1.90	0.53
1:D:790:LYS:O	1:D:794:MET:HG3	2.08	0.53
1:B:296:TRP:CD2	1:B:316:MET:HE1	2.44	0.53
1:B:340:MET:HE3	1:B:340:MET:HA	1.90	0.53
1:B:336:GLN:HG3	1:B:362:LEU:HD13	1.90	0.53
1:A:405:TRP:HD1	1:A:411:LEU:HB3	1.74	0.52
1:A:823:ILE:HD11	1:D:643:PHE:HA	1.90	0.52
1:C:198:ARG:HH21	1:D:198:ARG:HD3	1.74	0.52
1:D:677:GLN:HE22	1:D:680:ILE:H	1.57	0.52
1:A:172:VAL:HG12	1:A:197:LEU:HD21	1.91	0.52
1:A:236:ALA:HB1	1:A:310:GLY:H	1.74	0.52
1:A:145:PHE:HZ	1:A:357:THR:HG22	1.75	0.52
1:D:415:GLU:HA	1:D:418:LYS:HE2	1.91	0.52
1:C:60:ALA:HB1	1:C:327:VAL:HG21	1.91	0.52
1:C:718:VAL:HB	1:C:723:GLU:HB2	1.92	0.52
1:A:128:PRO:HG3	1:A:359:PHE:HD2	1.75	0.52
1:C:224:PHE:CD2	1:C:251:TYR:HB3	2.45	0.52
1:B:216:LYS:HG3	1:B:217:GLU:OE1	2.09	0.52
1:C:489:GLY:HA2	1:C:499:ASN:HB2	1.92	0.52
1:D:275:ASN:HB3	3:M:1:NAG:N2	2.25	0.52
1:A:201:ILE:C	1:A:202:ARG:HD2	2.34	0.51
1:C:192:PRO:HB2	1:D:200:LYS:HG3	1.92	0.51
1:A:215:LEU:HA	1:A:218:MET:HE1	1.92	0.51
1:C:396:GLU:HG3	1:C:397:GLU:HG2	1.92	0.51
1:C:132:THR:HB	1:C:322:LEU:HB3	1.93	0.51
1:D:175:VAL:HG22	1:D:202:ARG:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:656:ALA:HA	1:D:653:ALA:HB1	1.93	0.51
1:A:239:LEU:HD21	1:A:256:PHE:HZ	1.76	0.51
1:A:412:ASN:C	1:A:413:MET:HE2	2.36	0.51
1:D:37:ARG:HB3	1:D:103:VAL:HA	1.92	0.51
1:C:349:ARG:HB2	1:C:351:LYS:HZ2	1.75	0.51
1:C:371:LEU:H	1:C:371:LEU:HD22	1.76	0.51
1:A:488:TYR:CE2	7:A:1002:GLU:HB3	2.46	0.51
1:C:536:LEU:HD13	1:C:738:GLU:HG2	1.93	0.51
1:B:219:LYS:HB2	1:B:247:MET:HE1	1.93	0.50
1:C:156:LEU:O	1:C:160:ILE:HG12	2.11	0.50
1:D:153:PHE:CD2	1:D:184:ARG:HB3	2.46	0.50
1:A:655:LEU:HD21	1:D:650:SER:HA	1.93	0.50
1:A:831:LEU:HD22	1:D:577:VAL:HG21	1.92	0.50
1:A:769:PRO:HD2	1:A:772:SER:HB2	1.94	0.50
1:A:776:ASP:O	1:A:780:ILE:HG12	2.11	0.50
1:C:354:ARG:H	1:C:354:ARG:HD3	1.77	0.50
1:B:71:LEU:HD21	1:B:331:SER:HB2	1.93	0.50
1:C:437:THR:HA	1:C:515:ALA:HB2	1.93	0.50
1:D:248:MET:HB2	1:D:274:VAL:HB	1.94	0.50
1:B:261:LEU:HD12	1:B:278:GLY:HA3	1.93	0.50
1:C:179:SER:HB2	1:D:183:ILE:HG23	1.94	0.50
1:C:682:TYR:CD2	1:C:705:MET:HE1	2.47	0.50
1:C:44:TYR:HA	1:C:82:LYS:HE2	1.94	0.49
1:D:303:ALA:O	1:D:305:PRO:HD3	2.12	0.49
1:A:235:ALA:HB1	1:A:256:PHE:HE2	1.78	0.49
1:C:329:VAL:HG12	1:C:368:TRP:HB3	1.94	0.49
1:B:289:VAL:HG23	1:B:371:LEU:HB3	1.95	0.49
1:D:153:PHE:HB3	1:D:184:ARG:O	2.13	0.49
1:D:749:ASN:HD21	1:D:751:ASN:HB2	1.77	0.49
1:D:169:TRP:CZ3	1:D:225:HIS:HB3	2.47	0.49
1:C:435:VAL:HG23	1:C:480:ILE:HA	1.93	0.49
1:D:742:ILE:HG21	1:D:754:GLN:HB2	1.93	0.49
1:D:392:ILE:HG22	1:D:401:LYS:HA	1.95	0.49
1:A:360:MET:HA	1:A:363:ILE:HD12	1.94	0.49
1:C:205:PRO:HD3	1:C:214:LEU:HD22	1.95	0.49
1:D:83:ILE:HD11	1:D:94:LYS:HG3	1.94	0.49
1:B:149:LEU:O	1:B:322:LEU:HD12	2.13	0.48
1:B:153:PHE:CD2	1:B:184:ARG:HB2	2.47	0.48
1:B:433:LEU:HD12	1:B:476:PHE:CD1	2.48	0.48
1:D:467:LEU:HA	1:D:470:LEU:HD12	1.95	0.48
1:B:153:PHE:HB3	1:B:184:ARG:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:727:ARG:HB3	1:B:733:TYR:HD2	1.78	0.48
1:D:533:PHE:HB3	1:D:782:ILE:HD12	1.95	0.48
1:A:201:ILE:HG13	1:B:189:ILE:HG22	1.94	0.48
1:B:81:GLN:HG2	1:B:98:GLN:NE2	2.28	0.48
1:B:248:MET:HE3	1:B:274:VAL:HG21	1.96	0.48
1:B:466:LEU:O	1:B:470:LEU:HG	2.13	0.48
1:C:536:LEU:HD22	1:C:738:GLU:HB3	1.93	0.48
1:C:685:VAL:HG11	7:C:1003:GLU:HB3	1.95	0.48
1:C:185:LEU:HB3	1:C:188:LEU:HB3	1.94	0.48
1:C:279:PHE:HD2	1:C:389:LEU:HD11	1.77	0.48
1:A:306:LYS:NZ	1:A:311:LEU:HB3	2.29	0.48
1:C:243:LEU:HA	1:C:248:MET:HE3	1.95	0.48
1:C:434:ILE:HB	1:C:510:ALA:HA	1.95	0.48
1:D:153:PHE:HA	1:D:156:LEU:HB2	1.94	0.48
1:B:281:ILE:HG13	1:B:372:THR:HB	1.94	0.48
1:D:118:VAL:HG13	1:D:129:HIS:HE1	1.79	0.48
1:D:247:MET:HE3	1:D:247:MET:O	2.14	0.48
1:A:465:ASP:HB3	1:A:794:MET:HE2	1.94	0.48
1:B:153:PHE:HD2	1:B:184:ARG:HB2	1.79	0.48
1:D:322:LEU:HD13	1:D:372:THR:HG21	1.95	0.48
1:A:435:VAL:HG11	1:A:467:LEU:HD11	1.96	0.48
1:B:674:LEU:HD12	1:B:682:TYR:CD2	2.48	0.48
1:C:364:LYS:HA	1:C:377:PHE:HD2	1.79	0.48
1:D:721:ASN:O	1:D:725:ILE:HG12	2.14	0.48
1:B:823:ILE:O	1:B:826:VAL:HG12	2.14	0.47
1:C:121:ILE:HG13	1:D:89:PHE:HB2	1.96	0.47
1:C:737:MET:HE2	1:C:742:ILE:HD13	1.96	0.47
1:A:181:GLY:HA2	1:A:184:ARG:HB2	1.96	0.47
1:C:267:GLU:HG2	1:C:268:PRO:HD3	1.96	0.47
1:C:439:LEU:HB2	1:C:482:LEU:HD21	1.96	0.47
1:B:743:GLU:O	1:B:747:GLN:HB2	2.14	0.47
1:C:89:PHE:HB2	1:D:121:ILE:HD13	1.96	0.47
1:C:333:ALA:HB1	1:C:363:ILE:HG22	1.97	0.47
1:D:71:LEU:HD11	1:D:334:VAL:HG13	1.95	0.47
1:D:306:LYS:HG3	1:D:308:ASP:OD1	2.15	0.47
1:A:782:ILE:HG23	1:A:783:LEU:HD22	1.96	0.47
1:D:131:GLN:HB2	1:D:148:SER:HB2	1.95	0.47
1:D:442:PRO:HG3	1:D:744:PHE:CE1	2.50	0.47
1:D:728:VAL:HA	1:D:733:TYR:HB3	1.96	0.47
1:B:434:ILE:HG13	1:B:479:GLU:OE2	2.15	0.47
1:C:716:VAL:HG23	1:C:717:LEU:HD22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:549:ASN:HB3	1:D:664:MET:HB3	1.96	0.47
1:A:219:LYS:HG2	1:A:247:MET:HE1	1.96	0.47
1:A:264:LEU:HB3	1:A:266:VAL:HG13	1.96	0.47
1:B:156:LEU:HD12	1:B:156:LEU:H	1.79	0.47
1:B:474:LEU:HD11	1:B:777:LYS:HD2	1.96	0.47
1:D:256:PHE:HE1	1:D:276:MET:HB2	1.79	0.47
1:D:498:TRP:NE1	1:D:526:VAL:HG11	2.29	0.47
1:B:215:LEU:HD13	1:B:218:MET:HE3	1.97	0.47
1:D:56:ALA:HB3	1:D:323:MET:HE1	1.95	0.47
1:D:259:LEU:HB3	1:D:318:THR:HG21	1.96	0.47
1:D:232:HIS:HB3	1:D:260:ASP:HB3	1.97	0.47
1:B:212:LYS:HG3	1:B:245:MET:HE1	1.97	0.47
1:B:360:MET:HG2	1:B:364:LYS:HG3	1.97	0.47
1:C:340:MET:HE1	1:C:355:PHE:HD2	1.80	0.47
1:D:215:LEU:HD12	1:D:247:MET:HG3	1.97	0.47
1:A:688:GLY:H	1:A:691:MET:HE2	1.80	0.46
1:B:815:LEU:HD22	1:B:819:ASN:ND2	2.30	0.46
1:C:777:LYS:HA	1:C:777:LYS:HD2	1.69	0.46
1:D:242:ALA:O	1:D:247:MET:HB2	2.14	0.46
1:B:145:PHE:HA	1:B:360:MET:HE1	1.97	0.46
1:D:431:ARG:HH22	1:D:476:PHE:HA	1.80	0.46
1:D:443:TYR:HB3	1:D:463:CYS:SG	2.55	0.46
1:A:329:VAL:HG11	1:A:375:ILE:HG21	1.97	0.46
1:A:259:LEU:HD13	1:A:281:ILE:HB	1.98	0.46
1:D:346:GLN:OE1	1:D:348:ASN:HB2	2.16	0.46
1:A:393:SER:HB3	1:A:402:ILE:HD12	1.98	0.46
1:A:442:PRO:HG3	1:A:744:PHE:CD2	2.51	0.46
1:B:169:TRP:CZ3	1:B:225:HIS:HB3	2.51	0.46
1:B:261:LEU:HD23	1:B:261:LEU:HA	1.82	0.46
1:B:360:MET:HA	1:B:363:ILE:HD12	1.98	0.46
1:C:536:LEU:HD21	1:C:764:TYR:CE1	2.51	0.46
1:A:520:THR:C	1:D:783:LEU:HD13	2.41	0.46
1:D:466:LEU:O	1:D:470:LEU:HG	2.16	0.46
1:D:523:ARG:HH12	1:D:689:ALA:HB2	1.81	0.46
1:B:210:ASP:HA	1:B:241:GLN:HE22	1.80	0.45
1:C:50:MET:HG3	1:C:54:GLU:HG2	1.97	0.45
1:C:677:GLN:HG2	1:C:679:LYS:HE2	1.98	0.45
1:D:386:ASP:HA	1:D:407:PRO:HG3	1.98	0.45
1:A:544:LYS:H	1:A:752:LEU:HA	1.82	0.45
1:B:519:ILE:HG22	1:C:783:LEU:HD11	1.98	0.45
1:C:533:PHE:CD1	1:C:534:MET:HG3	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:ARG:HH12	2:E:1:NAG:H82	1.80	0.45
1:B:99:LEU:HD11	1:B:127:VAL:HG11	1.99	0.45
1:B:686:GLU:OE2	1:B:687:ASP:HB2	2.16	0.45
1:C:823:ILE:HD12	1:C:823:ILE:HA	1.89	0.45
1:D:785:LEU:HB3	1:D:791:LEU:HG	1.97	0.45
1:B:376:THR:OG1	1:B:386:ASP:HB3	2.17	0.45
1:C:198:ARG:HA	1:D:198:ARG:HH12	1.81	0.45
1:C:281:ILE:HG13	1:C:372:THR:HB	1.97	0.45
1:D:517:LEU:HD11	1:D:523:ARG:HD3	1.97	0.45
1:A:362:LEU:HD12	1:A:362:LEU:H	1.81	0.45
1:C:736:LEU:HD23	1:C:736:LEU:HA	1.67	0.45
1:D:469:GLU:OE1	1:D:785:LEU:HD21	2.16	0.45
1:D:737:MET:SD	1:D:742:ILE:HG12	2.56	0.45
8:B:1002:2J9:H1	1:C:786:GLN:HG2	1.99	0.45
1:C:169:TRP:CZ3	1:C:225:HIS:HB3	2.52	0.45
1:C:437:THR:HB	1:C:444:VAL:HG21	1.98	0.45
1:C:643:PHE:HD1	1:D:823:ILE:HG13	1.81	0.45
1:D:129:HIS:CE1	1:D:131:GLN:HE22	2.34	0.45
1:D:460:GLU:C	1:D:464:ILE:HD12	2.42	0.45
1:D:498:TRP:HE1	1:D:526:VAL:HG11	1.82	0.45
8:D:1002:2J9:H7	8:D:1002:2J9:H3	1.67	0.45
1:D:187:GLU:OE2	1:D:190:LYS:HE2	2.17	0.45
1:D:443:TYR:HE1	1:D:799:TRP:CZ2	2.34	0.45
1:A:316:MET:HE2	1:A:316:MET:HA	1.98	0.45
1:A:175:VAL:HG22	1:A:202:ARG:HB2	1.99	0.45
1:A:292:ILE:HG21	1:A:324:TYR:CE2	2.52	0.45
1:A:411:LEU:HD23	1:A:411:LEU:H	1.82	0.45
1:C:514:VAL:HG23	1:C:766:VAL:HG22	1.98	0.45
1:D:536:LEU:HG	1:D:762:LYS:C	2.42	0.45
1:C:845:LYS:HD3	1:C:848:LYS:HZ3	1.82	0.44
1:B:467:LEU:HD12	1:B:468:ARG:N	2.32	0.44
1:C:160:ILE:HD13	1:C:279:PHE:CE1	2.52	0.44
1:D:40:GLY:HA3	1:D:107:PHE:H	1.82	0.44
1:B:136:HIS:CD2	1:B:183:ILE:HG21	2.52	0.44
1:B:498:TRP:NE1	1:B:526:VAL:HG11	2.33	0.44
1:D:712:ARG:O	1:D:716:VAL:HG22	2.17	0.44
1:B:433:LEU:HD23	1:B:433:LEU:HA	1.79	0.44
1:D:96:CYS:HB2	1:D:347:CYS:HB3	1.48	0.44
1:D:149:LEU:HD11	1:D:322:LEU:O	2.17	0.44
1:B:435:VAL:HG23	1:B:480:ILE:HA	1.98	0.44
1:B:537:GLY:H	1:B:739:SER:HB3	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:411:LEU:HD23	1:C:411:LEU:HA	1.72	0.44
1:C:648:ILE:HD13	1:C:648:ILE:HA	1.81	0.44
1:D:540:ILE:HB	1:D:755:ILE:HG23	2.00	0.44
1:D:674:LEU:HG	1:D:682:TYR:HE2	1.82	0.44
1:A:544:LYS:HG3	1:A:545:PRO:HD2	2.00	0.44
1:A:688:GLY:H	1:A:691:MET:CE	2.30	0.44
1:D:281:ILE:HG13	1:D:372:THR:HB	1.98	0.44
1:A:437:THR:HA	1:A:515:ALA:HB2	2.00	0.44
1:D:536:LEU:HD22	1:D:738:GLU:OE1	2.18	0.44
1:A:167:PHE:HD2	1:A:169:TRP:HZ3	1.66	0.44
1:A:658:PHE:O	1:A:662:GLU:HG2	2.18	0.44
1:B:727:ARG:HB3	1:B:733:TYR:CD2	2.53	0.44
1:C:267:GLU:HA	1:C:270:ARG:HD3	2.00	0.44
1:C:224:PHE:CE2	1:C:251:TYR:HB3	2.53	0.43
1:A:648:ILE:HG13	1:D:645:LEU:HD21	1.98	0.43
1:B:123:ASN:HA	1:B:145:PHE:HB2	2.00	0.43
1:A:519:ILE:HG12	1:A:529:PHE:CD2	2.53	0.43
1:B:189:ILE:HD12	1:B:189:ILE:H	1.83	0.43
1:B:245:MET:HA	1:D:271:TYR:O	2.18	0.43
1:C:537:GLY:HA3	1:C:758:LEU:HG	2.00	0.43
1:C:467:LEU:HD21	1:C:478:TYR:CG	2.52	0.43
1:B:230:CYS:SG	1:B:234:MET:HB3	2.58	0.43
1:C:286:ASN:HB3	1:C:289:VAL:HG22	2.00	0.43
1:C:728:VAL:HA	1:C:733:TYR:HB3	2.01	0.43
8:C:1002:2J9:H7	8:C:1002:2J9:H1	1.79	0.43
1:D:192:PRO:HG3	1:D:199:LEU:HD23	2.01	0.43
2:O:1:NAG:H61	2:O:2:NAG:H83	2.00	0.43
1:A:83:ILE:HD12	1:A:83:ILE:HA	1.95	0.43
1:A:713:ARG:HA	1:A:717:LEU:HD23	2.00	0.43
1:C:324:TYR:CD2	1:C:371:LEU:HD21	2.54	0.43
1:D:443:TYR:CD2	1:D:516:PRO:HG3	2.54	0.43
1:D:781:ALA:O	1:D:785:LEU:HD23	2.19	0.43
1:A:176:TYR:CZ	1:A:203:GLN:HB2	2.53	0.43
1:A:560:SER:O	1:A:563:ILE:HG22	2.19	0.43
1:C:153:PHE:CD2	1:C:184:ARG:HG3	2.54	0.43
1:C:153:PHE:CG	1:C:184:ARG:HG3	2.52	0.43
1:C:318:THR:O	1:C:322:LEU:HB2	2.19	0.43
1:C:677:GLN:HE21	1:C:679:LYS:HB2	1.83	0.43
1:D:727:ARG:HD3	1:D:733:TYR:CZ	2.54	0.43
1:B:267:GLU:HA	1:B:270:ARG:HD3	2.00	0.43
1:B:643:PHE:O	1:B:647:ILE:HD12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:664:MET:HE3	1:B:665:GLU:N	2.34	0.43
1:C:433:LEU:HD11	1:C:774:TYR:CZ	2.54	0.43
1:D:149:LEU:O	1:D:384:ARG:HD3	2.19	0.43
1:D:783:LEU:HD23	1:D:783:LEU:HA	1.77	0.43
1:A:296:TRP:CD2	1:A:316:MET:HE1	2.54	0.43
1:B:151:PRO:HB2	1:B:156:LEU:HD11	2.01	0.43
1:B:389:LEU:HD23	1:B:389:LEU:HA	1.89	0.43
1:C:201:ILE:HD13	1:C:201:ILE:HA	1.84	0.43
1:C:441:GLU:O	1:C:445:LEU:HB3	2.19	0.43
1:D:443:TYR:HD2	1:D:516:PRO:HG3	1.84	0.43
1:A:441:GLU:HB2	1:A:442:PRO:HD3	1.99	0.43
1:A:668:ILE:HD13	1:A:680:ILE:HG21	2.00	0.43
1:B:513:ALA:HB3	1:B:767:GLY:HA3	2.00	0.43
1:C:57:PHE:HD2	1:C:58:ARG:HH22	1.66	0.43
1:C:198:ARG:HA	1:D:198:ARG:HH22	1.84	0.43
1:C:743:GLU:O	1:C:747:GLN:HG2	2.18	0.43
1:D:145:PHE:HZ	1:D:357:THR:HG22	1.84	0.43
1:A:739:SER:HA	1:A:742:ILE:HB	2.01	0.42
1:B:197:LEU:HD23	1:B:197:LEU:HA	1.84	0.42
1:B:577:VAL:HG21	1:C:831:LEU:HD22	2.01	0.42
1:B:680:ILE:HD12	1:B:732:ASP:HB3	2.01	0.42
1:B:537:GLY:HA3	1:B:758:LEU:HG	2.01	0.42
1:C:359:PHE:O	1:C:362:LEU:HG	2.19	0.42
1:D:288:GLN:H	1:D:288:GLN:HG3	1.68	0.42
1:A:230:CYS:SG	1:A:234:MET:HB3	2.60	0.42
1:C:359:PHE:O	1:C:363:ILE:HG23	2.19	0.42
1:C:428:LEU:HB3	1:C:431:ARG:HB3	2.00	0.42
1:C:447:LYS:HA	1:C:460:GLU:HG2	2.00	0.42
1:C:541:LEU:HB2	1:C:742:ILE:HD11	2.02	0.42
1:D:331:SER:HA	1:D:334:VAL:HG12	2.01	0.42
1:B:125:LEU:HD12	1:B:345:LEU:HB3	2.00	0.42
1:B:186:GLN:HG3	1:B:187:GLU:OE2	2.20	0.42
1:C:123:ASN:HA	1:C:145:PHE:HD2	1.83	0.42
1:D:439:LEU:HD23	1:D:439:LEU:HA	1.82	0.42
8:D:1001:2J9:H3	8:D:1001:2J9:H7	1.66	0.42
1:A:565:MET:HE2	1:A:565:MET:HA	2.00	0.42
1:A:674:LEU:HB3	1:A:682:TYR:HE1	1.84	0.42
1:B:316:MET:HE2	1:B:316:MET:HA	2.01	0.42
1:B:685:VAL:O	1:B:691:MET:HE2	2.19	0.42
1:D:170:LYS:HA	1:D:170:LYS:HD2	1.81	0.42
1:D:358:ARG:HH12	1:D:362:LEU:HD21	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:518:ALA:H	7:A:1002:GLU:N	2.17	0.42
1:B:460:GLU:HA	1:B:464:ILE:HG21	2.00	0.42
1:C:538:ILE:HB	1:C:759:ILE:HB	2.00	0.42
1:A:224:PHE:HA	1:A:252:TYR:CE1	2.55	0.42
1:A:690:THR:HG21	1:A:736:LEU:O	2.19	0.42
1:B:57:PHE:CB	1:B:323:MET:HE1	2.49	0.42
1:C:797:LYS:O	1:C:800:ARG:HG2	2.20	0.42
1:A:487:LYS:HE3	1:A:499:ASN:HB2	2.01	0.42
1:B:800:ARG:HE	1:B:802:CYS:HA	1.85	0.42
1:D:742:ILE:HD13	1:D:742:ILE:HA	1.73	0.42
1:A:712:ARG:O	1:A:716:VAL:HG22	2.18	0.42
1:A:812:ALA:HB1	1:D:658:PHE:CZ	2.54	0.42
1:B:174:VAL:HA	1:B:227:ILE:HG23	2.02	0.42
1:B:259:LEU:O	1:B:318:THR:HG21	2.20	0.42
1:B:443:TYR:HD2	1:B:516:PRO:HG3	1.85	0.42
1:B:537:GLY:HA2	1:B:760:ASP:O	2.19	0.42
1:B:655:LEU:O	1:B:655:LEU:HD12	2.20	0.42
1:D:513:ALA:HB3	1:D:767:GLY:HA3	2.02	0.42
1:A:34:HIS:HB2	1:A:74:THR:HG22	2.02	0.42
1:B:111:HIS:NE2	1:B:113:SER:HB3	2.35	0.42
1:C:242:ALA:HB1	1:C:247:MET:HB2	2.01	0.42
1:D:234:MET:HE2	1:D:234:MET:HB2	1.83	0.42
1:B:64:ILE:HD12	1:B:64:ILE:HA	1.86	0.41
1:B:469:GLU:CD	1:B:785:LEU:HD11	2.44	0.41
1:B:505:LEU:HD12	1:B:505:LEU:O	2.20	0.41
1:C:375:ILE:HG12	1:C:384:ARG:HH11	1.84	0.41
1:C:700:SER:HB2	1:D:797:LYS:HB2	2.02	0.41
1:D:548:THR:HA	1:D:663:ARG:HA	2.02	0.41
1:A:702:TYR:HA	1:A:705:MET:HG3	2.02	0.41
1:B:435:VAL:HG12	1:B:512:LEU:HB2	2.02	0.41
1:B:645:LEU:HD23	1:B:645:LEU:HA	1.89	0.41
1:C:498:TRP:HB3	1:C:502:VAL:HB	2.02	0.41
1:D:83:ILE:HD12	1:D:90:GLU:HG2	2.02	0.41
1:D:326:ALA:O	1:D:330:VAL:HG12	2.19	0.41
1:D:537:GLY:HA2	1:D:760:ASP:O	2.20	0.41
1:B:740:THR:HG21	1:B:764:TYR:HE2	1.85	0.41
1:C:323:MET:HE3	1:C:323:MET:HA	2.01	0.41
1:D:438:ILE:HG21	1:D:488:TYR:CE1	2.55	0.41
1:A:386:ASP:HA	1:A:407:PRO:HG2	2.02	0.41
1:A:823:ILE:HG13	1:D:643:PHE:HD1	1.85	0.41
1:B:663:ARG:HH21	1:B:807:GLU:HG2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:336:GLN:HG3	1:D:362:LEU:HD13	2.03	0.41
1:D:378:ASN:HB2	1:D:385:THR:HG22	2.01	0.41
1:B:96:CYS:HB2	1:B:347:CYS:HB3	1.38	0.41
1:B:296:TRP:CE3	1:B:316:MET:HE1	2.55	0.41
1:C:420:LYS:HD2	1:C:420:LYS:HA	1.83	0.41
1:C:581:ILE:HD12	1:C:585:SER:HB2	2.02	0.41
1:C:683:GLY:HA3	1:C:733:TYR:OH	2.20	0.41
1:A:247:MET:HG3	1:A:254:TYR:OH	2.21	0.41
1:B:394:LEU:HA	1:B:399:LEU:HD23	2.03	0.41
1:C:41:ILE:HD11	1:C:118:VAL:HG21	2.02	0.41
1:C:403:GLY:HA3	1:C:413:MET:HA	2.02	0.41
1:C:512:LEU:HD23	1:C:512:LEU:HA	1.93	0.41
1:C:536:LEU:HD23	1:C:536:LEU:HA	1.80	0.41
1:C:785:LEU:HD22	1:C:791:LEU:HG	2.02	0.41
1:D:63:THR:HA	1:D:66:ARG:HG2	2.02	0.41
1:A:173:THR:O	1:A:226:VAL:HA	2.19	0.41
1:B:184:ARG:HG3	1:B:185:LEU:HD12	2.03	0.41
1:B:364:LYS:HE2	1:B:364:LYS:HB3	1.88	0.41
1:B:742:ILE:HD13	1:B:742:ILE:HA	1.93	0.41
1:C:379:LYS:HD3	1:C:379:LYS:HA	1.76	0.41
1:C:559:LEU:HD23	1:C:559:LEU:HA	1.88	0.41
1:C:669:ASP:OD1	1:C:669:ASP:C	2.64	0.41
1:B:243:LEU:HD22	1:B:269:TYR:HE1	1.85	0.41
1:B:795:LYS:HE3	1:B:795:LYS:HB3	1.90	0.41
1:B:827:LEU:HD12	1:B:827:LEU:HA	1.87	0.41
1:C:255:ILE:HG13	1:C:277:THR:HG23	2.02	0.41
1:C:265:ASP:HA	1:C:312:LEU:HD13	2.03	0.41
1:D:44:TYR:HB2	1:D:82:LYS:C	2.46	0.41
1:D:117:ALA:O	1:D:121:ILE:HG12	2.21	0.41
1:D:215:LEU:HD13	1:D:215:LEU:HA	1.90	0.41
1:D:243:LEU:HD12	1:D:243:LEU:HA	1.90	0.41
1:D:319:ASP:OD1	1:D:319:ASP:N	2.53	0.41
1:D:786:GLN:HG3	8:D:1001:2J9:H2	2.02	0.41
1:A:200:LYS:HD3	1:B:192:PRO:HB2	2.02	0.41
1:A:254:TYR:O	1:A:277:THR:HG22	2.21	0.41
1:A:581:ILE:HD13	1:B:838:ALA:HB1	2.02	0.41
1:B:238:ILE:HD13	1:B:238:ILE:HA	1.83	0.41
1:B:378:ASN:HB3	1:B:381:ASN:O	2.21	0.41
1:B:466:LEU:HA	1:B:794:MET:HE1	2.03	0.41
1:C:435:VAL:HG12	1:C:512:LEU:HB3	2.03	0.41
1:C:451:LYS:HG2	1:C:452:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:216:LYS:HB2	1:D:216:LYS:HE2	1.87	0.41
1:A:222:LYS:HE2	1:A:222:LYS:HB2	1.89	0.41
1:A:306:LYS:HD2	1:A:309:SER:HB2	2.03	0.41
1:A:520:THR:HG21	1:A:692:THR:HG21	2.03	0.41
1:B:189:ILE:HA	1:B:199:LEU:HD22	2.02	0.41
1:B:521:TYR:CE1	1:B:525:LYS:HD3	2.55	0.41
1:C:411:LEU:HD13	1:C:413:MET:HE3	2.03	0.41
1:C:702:TYR:HA	1:C:705:MET:HB2	2.03	0.41
1:D:227:ILE:HG23	1:D:255:ILE:HB	2.03	0.41
1:D:438:ILE:HD12	1:D:438:ILE:HA	1.86	0.41
1:A:170:LYS:HA	1:A:170:LYS:HD2	1.72	0.40
1:A:418:LYS:HD2	1:A:418:LYS:HA	1.95	0.40
1:B:280:ARG:HD3	1:B:392:ILE:HD11	2.02	0.40
1:C:405:TRP:CD1	1:C:411:LEU:H	2.39	0.40
1:C:470:LEU:HD13	1:C:778:ILE:HD11	2.03	0.40
1:A:343:SER:HB3	1:A:353:TRP:HE1	1.86	0.40
1:A:435:VAL:HA	1:A:512:LEU:O	2.21	0.40
1:A:462:TYR:HA	1:A:798:TRP:CD1	2.56	0.40
1:C:300:ARG:HH21	1:C:303:ALA:HB2	1.85	0.40
1:C:536:LEU:O	1:C:761:SER:HA	2.21	0.40
1:C:563:ILE:HD11	1:D:824:PHE:HE2	1.85	0.40
1:D:54:GLU:O	1:D:58:ARG:HG2	2.21	0.40
1:D:169:TRP:CE3	1:D:225:HIS:HB3	2.57	0.40
1:A:657:ALA:O	1:A:661:VAL:HG22	2.22	0.40
1:C:420:LYS:HB3	1:C:421:PRO:HD3	2.03	0.40
1:D:316:MET:HE3	1:D:316:MET:HA	2.02	0.40
1:B:117:ALA:O	1:B:121:ILE:HG12	2.21	0.40
1:A:327:VAL:HA	1:A:330:VAL:HG12	2.04	0.40
1:A:511:ASP:O	1:A:769:PRO:HD3	2.21	0.40
1:B:541:LEU:HD13	1:B:742:ILE:HD12	2.03	0.40
1:B:709:MET:HB2	1:B:716:VAL:HG21	2.03	0.40
1:C:58:ARG:HH21	1:C:61:VAL:HG21	1.85	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	772/908 (85%)	735 (95%)	37 (5%)	0	100	100
1	B	767/908 (84%)	728 (95%)	39 (5%)	0	100	100
1	C	773/908 (85%)	737 (95%)	36 (5%)	0	100	100
1	D	766/908 (84%)	738 (96%)	28 (4%)	0	100	100
All	All	3078/3632 (85%)	2938 (96%)	140 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	673/794 (85%)	663 (98%)	10 (2%)	57	70
1	B	668/794 (84%)	662 (99%)	6 (1%)	70	75
1	C	674/794 (85%)	665 (99%)	9 (1%)	61	71
1	D	667/794 (84%)	660 (99%)	7 (1%)	68	75
All	All	2682/3176 (84%)	2650 (99%)	32 (1%)	63	72

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	LEU
1	A	149	LEU
1	A	153	PHE
1	A	161	LEU
1	A	322	LEU
1	A	437	THR
1	A	457	ASP
1	A	535[A]	THR

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Mol	Chain	Res	Type
1	A	535[B]	THR
1	A	576	CYS
1	B	188	LEU
1	B	189	ILE
1	B	259	LEU
1	B	341	THR
1	B	752	LEU
1	B	826	VAL
1	C	127	VAL
1	C	230	CYS
1	C	316	MET
1	C	471[A]	SER
1	C	471[B]	SER
1	C	535[A]	THR
1	C	535[B]	THR
1	C	648	ILE
1	C	815	LEU
1	D	45	VAL
1	D	174	VAL
1	D	215	LEU
1	D	322	LEU
1	D	466	LEU
1	D	709	MET
1	D	742	ILE

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

Mol	Chain	Res	Type
1	A	186	GLN
1	A	232	HIS
1	A	491	GLN
1	A	726	GLN
1	A	751	ASN
1	B	98	GLN
1	B	131	GLN
1	B	203	GLN
1	C	136	HIS
1	C	203	GLN
1	C	253	HIS
1	C	275	ASN
1	D	34	HIS
1	D	129	HIS

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Mol	Chain	Res	Type
1	D	348	ASN
1	D	430	ASN
1	D	508	HIS
1	D	749	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

30 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	$\# Z  > 2$
2	NAG	E	1	2,1	14,14,15	0.68	0	17,19,21	1.21	2 (11%)
2	NAG	E	2	2	14,14,15	0.79	0	17,19,21	2.14	5 (29%)
2	BMA	E	3	2	11,11,12	0.82	0	15,15,17	1.84	3 (20%)
2	NAG	F	1	2,1	14,14,15	0.74	0	17,19,21	1.21	1 (5%)
2	NAG	F	2	2	14,14,15	0.74	0	17,19,21	0.84	0
2	BMA	F	3	2	11,11,12	0.83	0	15,15,17	2.09	4 (26%)
3	NAG	G	1	3,1	14,14,15	0.69	0	17,19,21	0.98	1 (5%)
3	NAG	G	2	3	14,14,15	0.72	0	17,19,21	0.93	0
2	NAG	H	1	2,1	14,14,15	0.74	0	17,19,21	0.90	0
2	NAG	H	2	2	14,14,15	0.70	0	17,19,21	0.83	0
2	BMA	H	3	2	11,11,12	0.85	0	15,15,17	2.15	4 (26%)
2	NAG	I	1	2,1	14,14,15	0.72	0	17,19,21	1.88	3 (17%)
2	NAG	I	2	2	14,14,15	0.73	0	17,19,21	1.31	2 (11%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	BMA	I	3	2	11,11,12	0.85	0	15,15,17	2.09	4 (26%)
3	NAG	J	1	3,1	14,14,15	0.73	0	17,19,21	0.86	0
3	NAG	J	2	3	14,14,15	0.78	0	17,19,21	1.01	0
4	NAG	K	1	4,1	14,14,15	0.74	0	17,19,21	0.97	0
4	NAG	K	2	4	14,14,15	0.68	0	17,19,21	1.22	1 (5%)
4	BMA	K	3	4	11,11,12	0.91	1 (9%)	15,15,17	3.17	7 (46%)
5	NAG	L	1	5,1	14,14,15	0.86	0	17,19,21	1.60	3 (17%)
5	NAG	L	2	5	14,14,15	0.74	0	17,19,21	1.48	2 (11%)
5	BMA	L	3	5	11,11,12	0.89	0	15,15,17	2.22	3 (20%)
3	NAG	M	1	3,1	14,14,15	0.86	0	17,19,21	1.48	3 (17%)
3	NAG	M	2	3	14,14,15	0.74	0	17,19,21	0.99	0
2	NAG	N	1	2,1	14,14,15	0.75	0	17,19,21	0.90	0
2	NAG	N	2	2	14,14,15	0.77	0	17,19,21	1.22	2 (11%)
2	BMA	N	3	2	11,11,12	0.88	0	15,15,17	2.09	3 (20%)
2	NAG	O	1	2,1	14,14,15	0.73	0	17,19,21	0.80	1 (5%)
2	NAG	O	2	2	14,14,15	0.73	0	17,19,21	1.28	2 (11%)
2	BMA	O	3	2	11,11,12	0.84	0	15,15,17	2.16	3 (20%)

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
2	NAG	E	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	BMA	E	3	2	-	1/2/19/22	0/1/1/1
2	NAG	F	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	1/6/23/26	0/1/1/1
2	BMA	F	3	2	-	0/2/19/22	0/1/1/1
3	NAG	G	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1
2	BMA	H	3	2	-	0/2/19/22	0/1/1/1
2	NAG	I	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	2/6/23/26	0/1/1/1
2	BMA	I	3	2	-	0/2/19/22	0/1/1/1
3	NAG	J	1	3,1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	J	2	3	-	0/6/23/26	0/1/1/1
4	NAG	K	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	K	2	4	-	3/6/23/26	0/1/1/1
4	BMA	K	3	4	-	0/2/19/22	0/1/1/1
5	NAG	L	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	L	2	5	-	2/6/23/26	0/1/1/1
5	BMA	L	3	5	-	2/2/19/22	0/1/1/1
3	NAG	M	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	M	2	3	-	2/6/23/26	0/1/1/1
2	NAG	N	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	N	2	2	-	0/6/23/26	0/1/1/1
2	BMA	N	3	2	-	0/2/19/22	0/1/1/1
2	NAG	O	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	O	2	2	-	2/6/23/26	0/1/1/1
2	BMA	O	3	2	-	1/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	3	BMA	C2-C3	2.14	1.55	1.52

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	3	BMA	C1-O5-C5	8.51	123.59	112.19
5	L	3	BMA	C1-O5-C5	6.87	121.40	112.19
2	O	3	BMA	C1-O5-C5	6.69	121.15	112.19
2	H	3	BMA	C1-O5-C5	6.44	120.81	112.19
2	N	3	BMA	C1-O5-C5	6.22	120.52	112.19
2	F	3	BMA	C1-O5-C5	6.16	120.44	112.19
2	I	3	BMA	C1-O5-C5	6.10	120.36	112.19
2	I	1	NAG	C1-O5-C5	5.72	119.86	112.19
2	E	2	NAG	O5-C1-C2	-5.55	102.71	111.29
2	E	3	BMA	C1-O5-C5	5.10	119.02	112.19
4	K	3	BMA	C1-C2-C3	4.87	116.74	109.64
4	K	3	BMA	C2-C3-C4	4.62	118.98	110.86
5	L	1	NAG	C4-C3-C2	4.04	116.93	111.02
3	M	1	NAG	C4-C3-C2	3.96	116.82	111.02
5	L	2	NAG	O5-C1-C2	-3.80	105.42	111.29
2	E	2	NAG	C4-C3-C2	3.74	116.50	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	1	NAG	O4-C4-C5	3.45	117.83	109.32
2	O	2	NAG	C2-N2-C7	3.26	127.26	122.90
4	K	2	NAG	C2-N2-C7	3.19	127.17	122.90
4	K	3	BMA	C3-C4-C5	3.19	116.01	110.23
2	F	1	NAG	C1-O5-C5	3.19	116.46	112.19
2	E	1	NAG	O4-C4-C3	-3.16	102.92	110.38
5	L	1	NAG	C2-N2-C7	3.16	127.14	122.90
2	E	2	NAG	C3-C4-C5	3.15	115.94	110.23
5	L	2	NAG	C4-C3-C2	3.12	115.59	111.02
3	M	1	NAG	C2-N2-C7	3.11	127.07	122.90
2	N	2	NAG	C4-C3-C2	2.98	115.38	111.02
2	I	2	NAG	C2-N2-C7	2.96	126.86	122.90
2	E	2	NAG	O4-C4-C3	-2.94	103.44	110.38
2	E	1	NAG	O5-C1-C2	-2.88	106.83	111.29
2	N	2	NAG	O3-C3-C2	-2.83	103.53	109.40
2	I	3	BMA	C3-C4-C5	2.68	115.09	110.23
2	I	2	NAG	C1-O5-C5	2.68	115.77	112.19
2	F	3	BMA	C3-C4-C5	2.65	115.04	110.23
2	H	3	BMA	C3-C4-C5	2.65	115.03	110.23
5	L	3	BMA	C2-C3-C4	2.60	115.44	110.86
2	N	3	BMA	C2-C3-C4	2.58	115.39	110.86
2	N	3	BMA	C3-C4-C5	2.54	114.84	110.23
2	E	2	NAG	C1-C2-N2	2.44	114.27	110.43
2	H	3	BMA	C2-C3-C4	2.37	115.03	110.86
4	K	3	BMA	O4-C4-C3	-2.34	104.86	110.38
4	K	3	BMA	O3-C3-C2	-2.32	105.32	110.05
3	G	1	NAG	C1-O5-C5	2.32	115.30	112.19
2	I	3	BMA	C2-C3-C4	2.31	114.93	110.86
2	O	2	NAG	C1-O5-C5	2.28	115.24	112.19
2	O	3	BMA	C2-C3-C4	2.28	114.87	110.86
2	I	1	NAG	O5-C5-C6	-2.27	103.24	107.66
2	O	3	BMA	C3-C4-C5	2.26	114.33	110.23
2	F	3	BMA	C2-C3-C4	2.25	114.82	110.86
3	M	1	NAG	O3-C3-C2	-2.25	104.74	109.40
5	L	3	BMA	C3-C4-C5	2.23	114.27	110.23
2	E	3	BMA	C3-C4-C5	2.22	114.26	110.23
5	L	1	NAG	O3-C3-C2	-2.16	104.91	109.40
2	O	1	NAG	O5-C1-C2	-2.13	108.00	111.29
4	K	3	BMA	O5-C1-C2	2.07	115.73	110.79
2	I	3	BMA	O4-C4-C3	-2.05	105.56	110.38
2	H	3	BMA	O4-C4-C3	-2.03	105.59	110.38
2	F	3	BMA	O4-C4-C3	-2.03	105.60	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	3	BMA	C2-C3-C4	2.03	114.42	110.86

There are no chirality outliers.

All (30) torsion outliers are listed below:

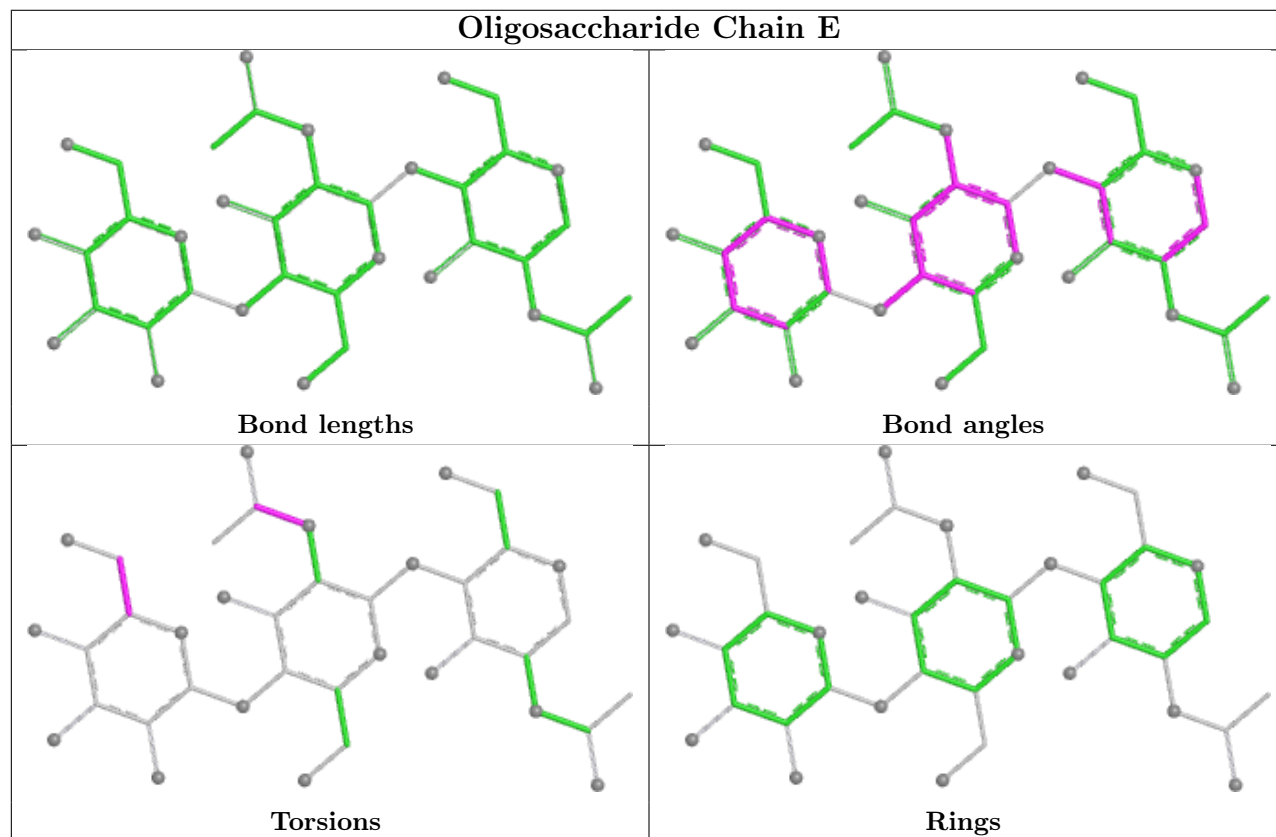
Mol	Chain	Res	Type	Atoms
3	M	2	NAG	C4-C5-C6-O6
3	M	2	NAG	O5-C5-C6-O6
5	L	3	BMA	O5-C5-C6-O6
3	J	1	NAG	O5-C5-C6-O6
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2
2	F	1	NAG	C8-C7-N2-C2
2	F	1	NAG	O7-C7-N2-C2
2	N	1	NAG	C8-C7-N2-C2
2	N	1	NAG	O7-C7-N2-C2
3	G	2	NAG	C8-C7-N2-C2
3	G	2	NAG	O7-C7-N2-C2
5	L	1	NAG	C8-C7-N2-C2
5	L	1	NAG	O7-C7-N2-C2
5	L	2	NAG	C8-C7-N2-C2
5	L	2	NAG	O7-C7-N2-C2
5	L	3	BMA	C4-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
4	K	2	NAG	O5-C5-C6-O6
2	E	3	BMA	O5-C5-C6-O6
3	J	1	NAG	C4-C5-C6-O6
2	I	2	NAG	C1-C2-N2-C7
2	O	2	NAG	C1-C2-N2-C7
4	K	2	NAG	C1-C2-N2-C7
2	I	2	NAG	C3-C2-N2-C7
2	O	2	NAG	C3-C2-N2-C7
3	M	1	NAG	C3-C2-N2-C7
4	K	2	NAG	C3-C2-N2-C7
2	O	3	BMA	O5-C5-C6-O6

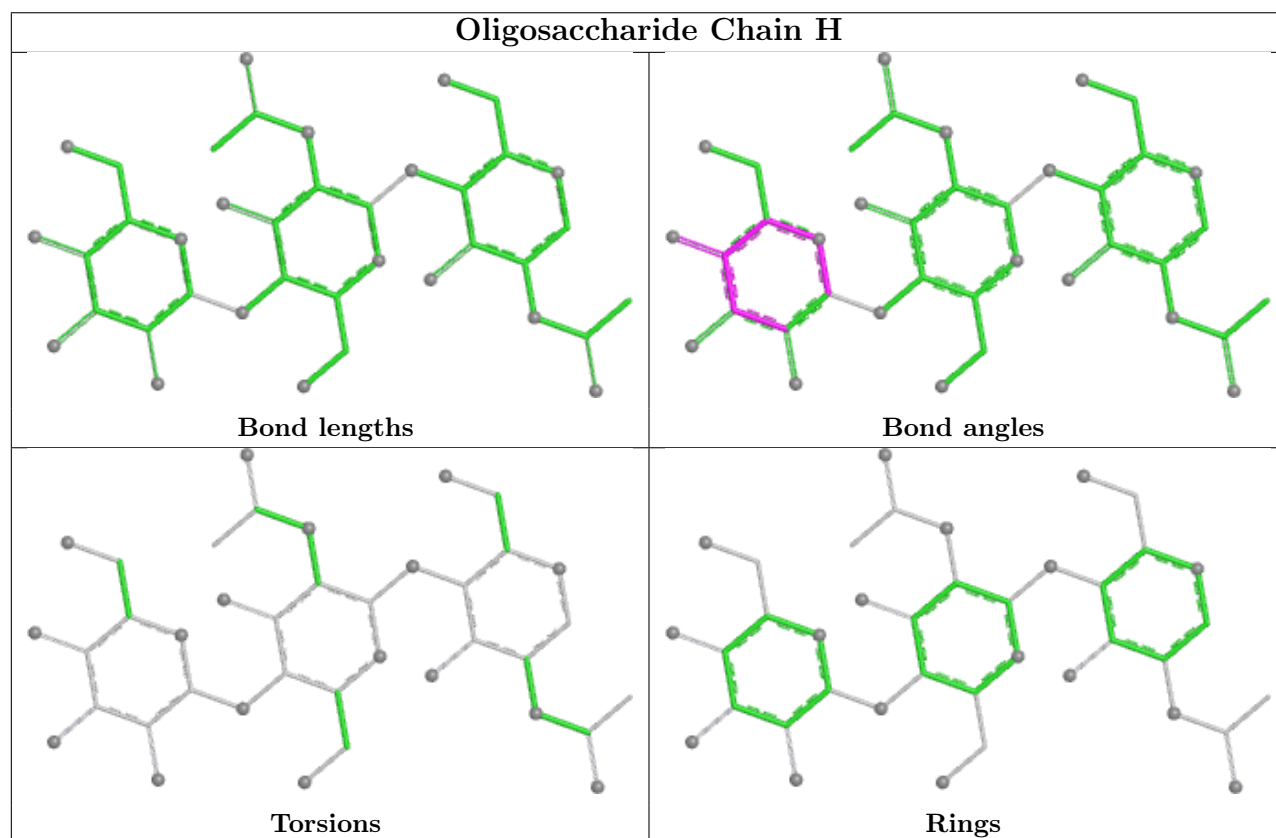
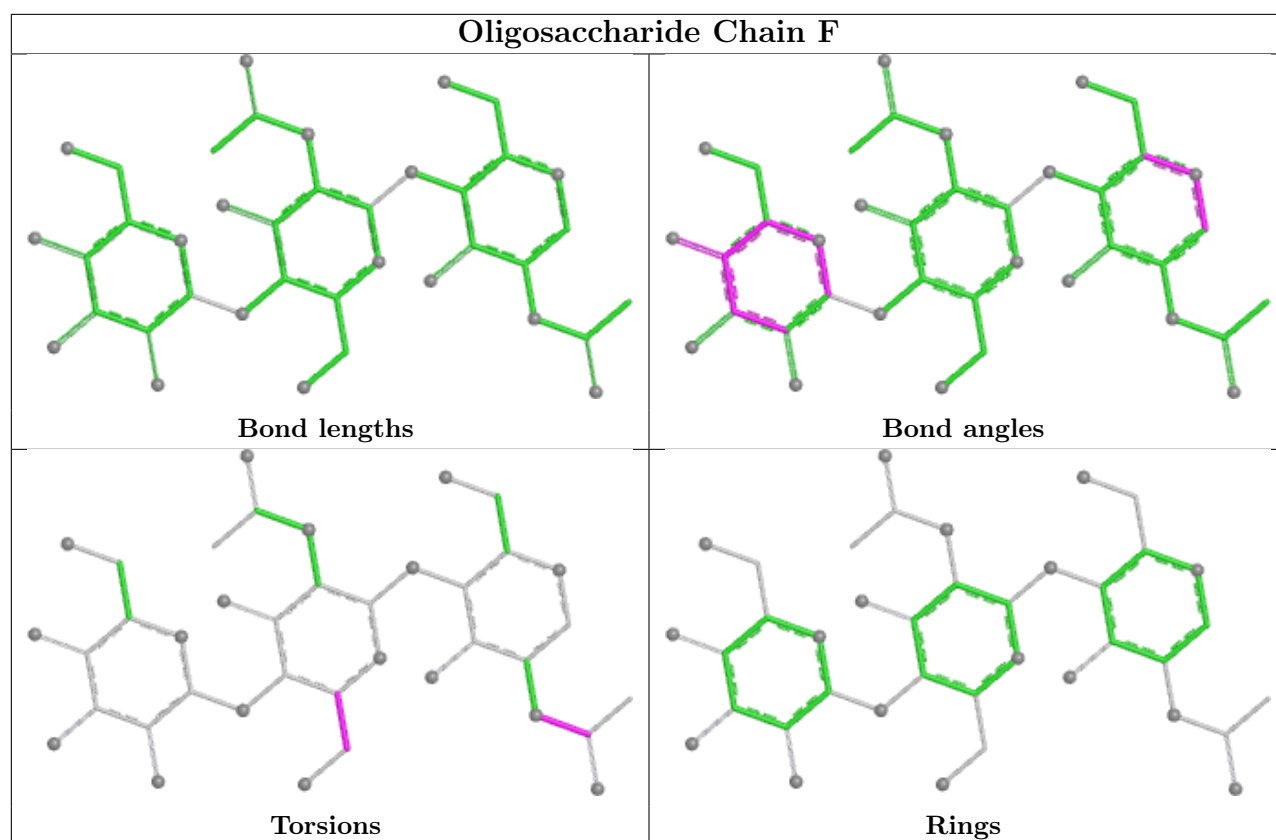
There are no ring outliers.

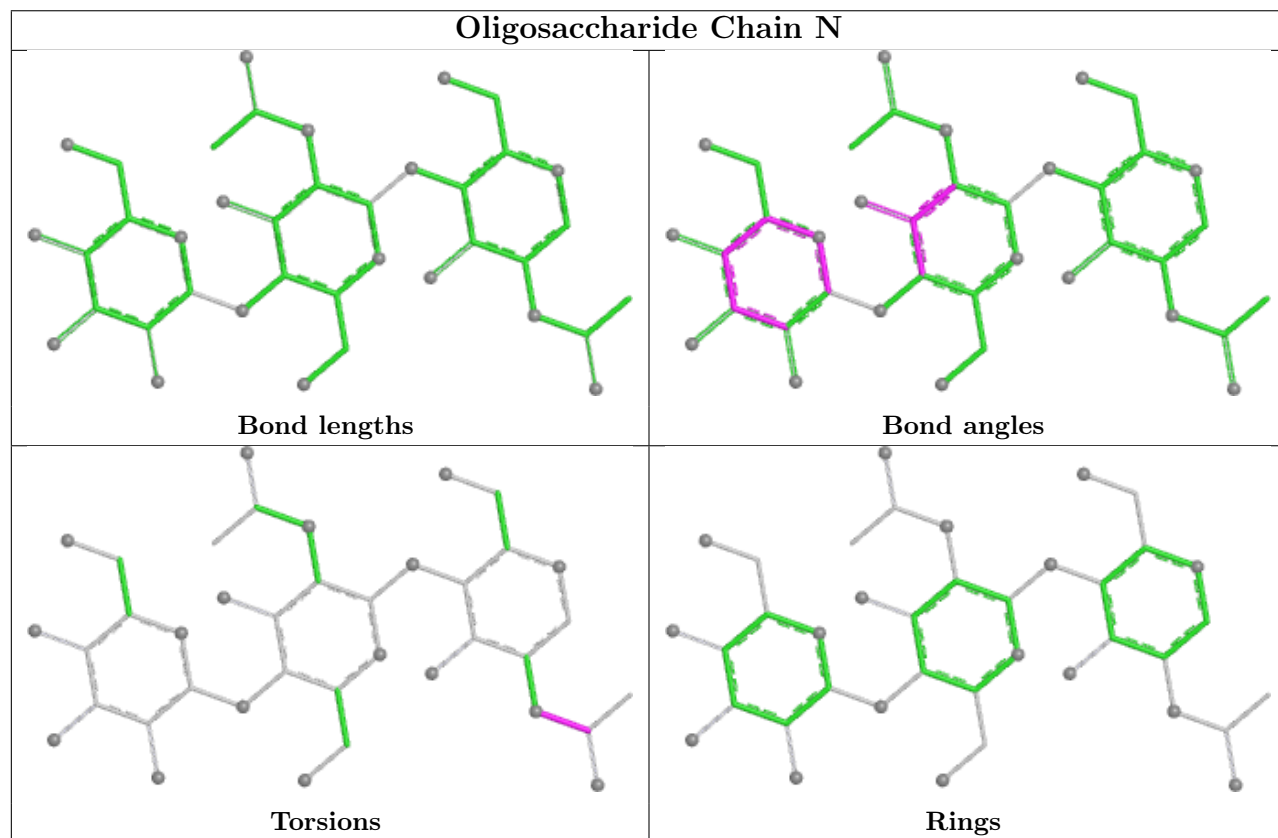
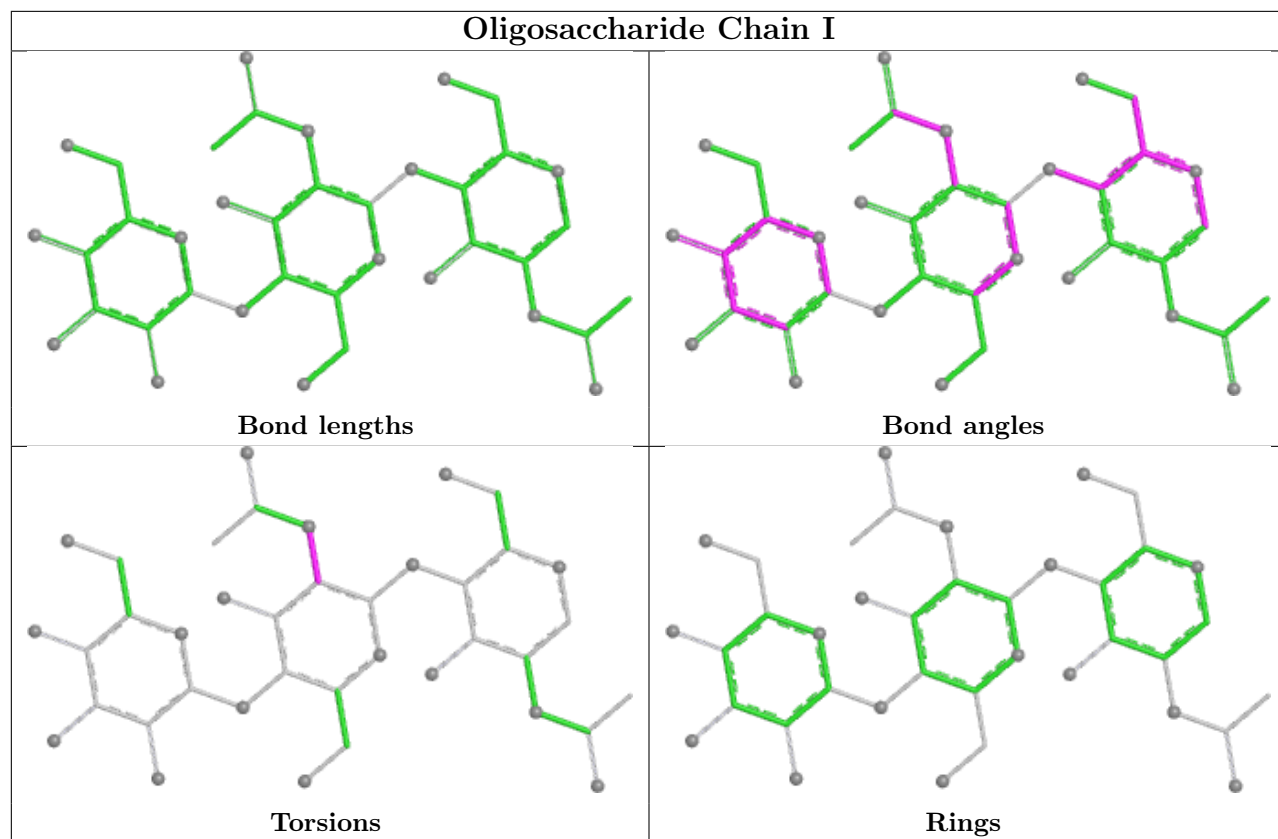
5 monomers are involved in 5 short contacts:

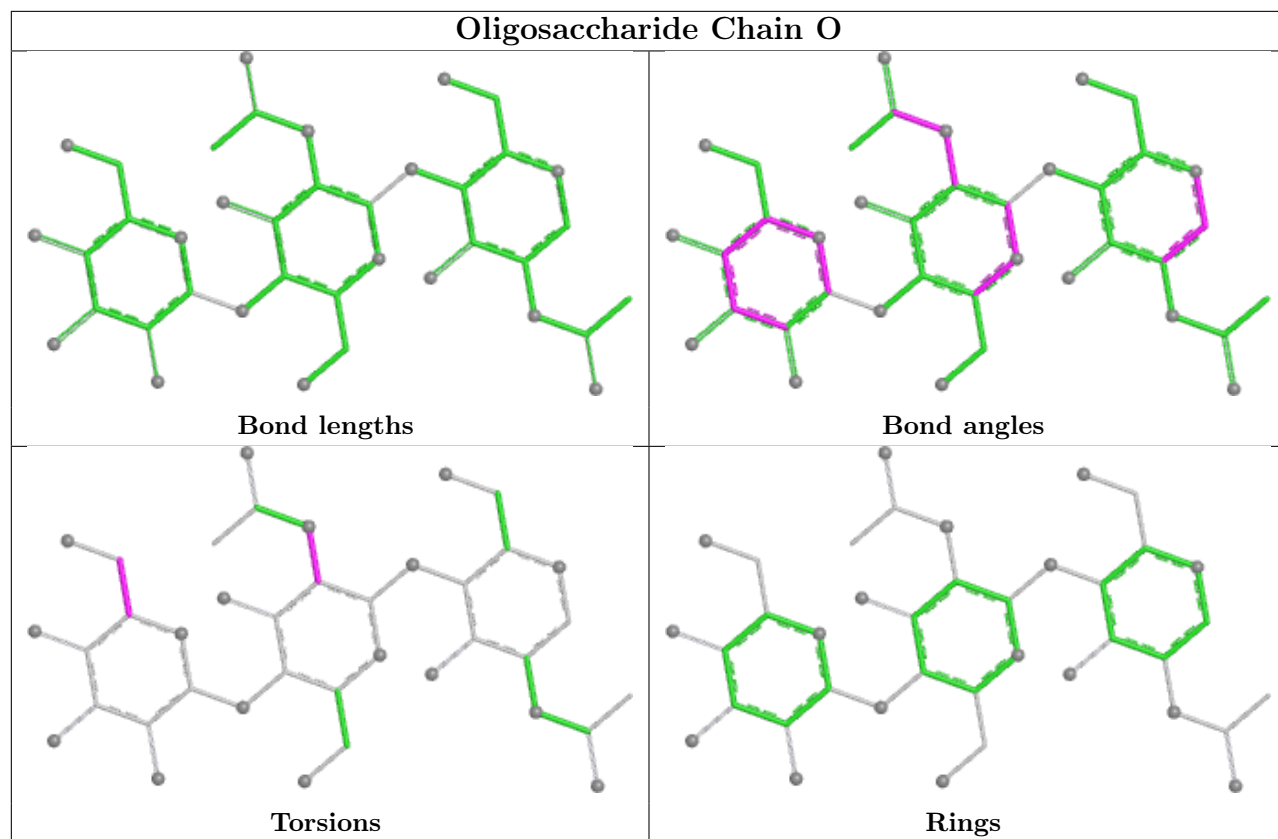
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	1	NAG	1	0
2	O	2	NAG	1	0
3	M	1	NAG	2	0
2	O	1	NAG	1	0
2	E	1	NAG	1	0

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

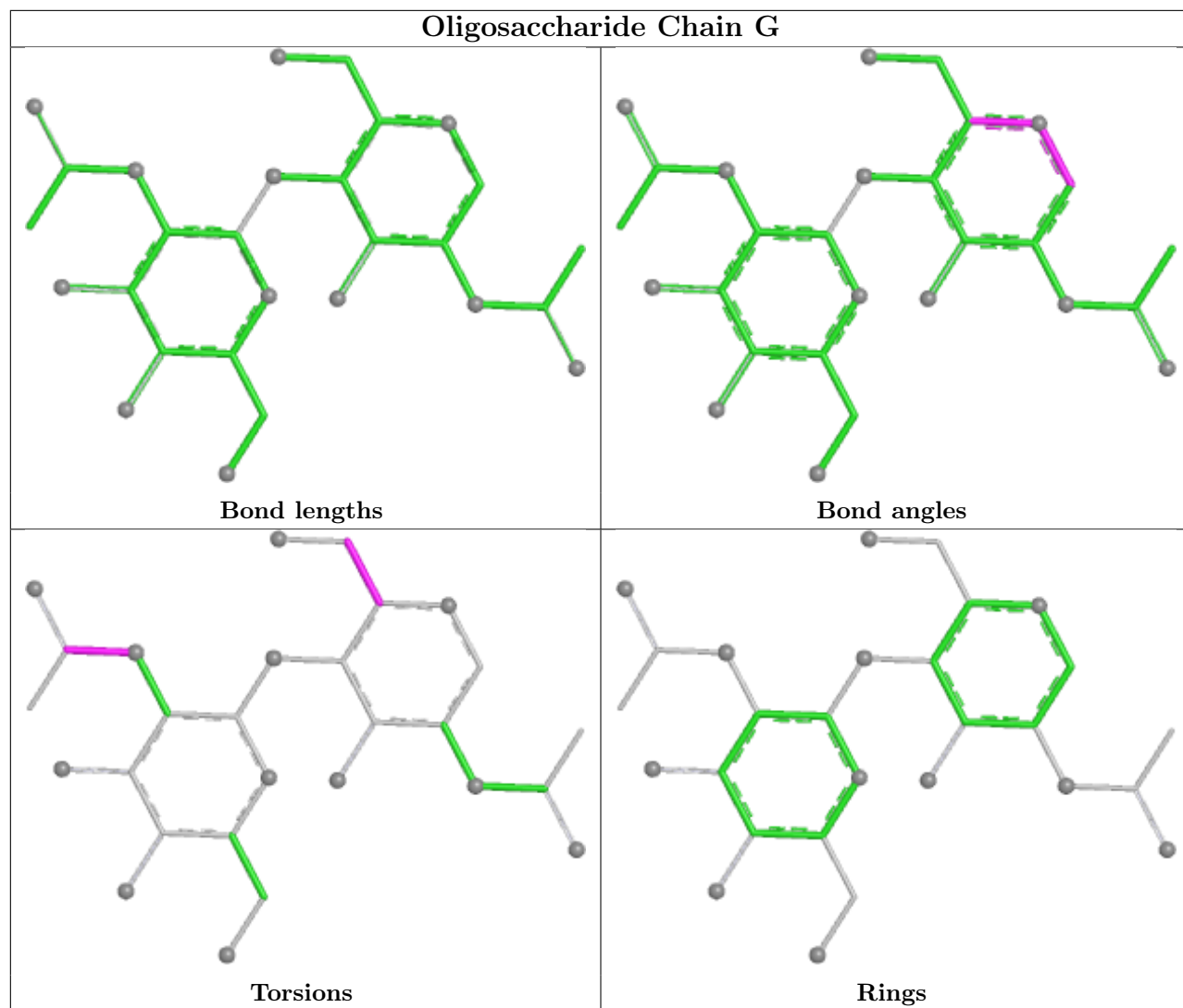


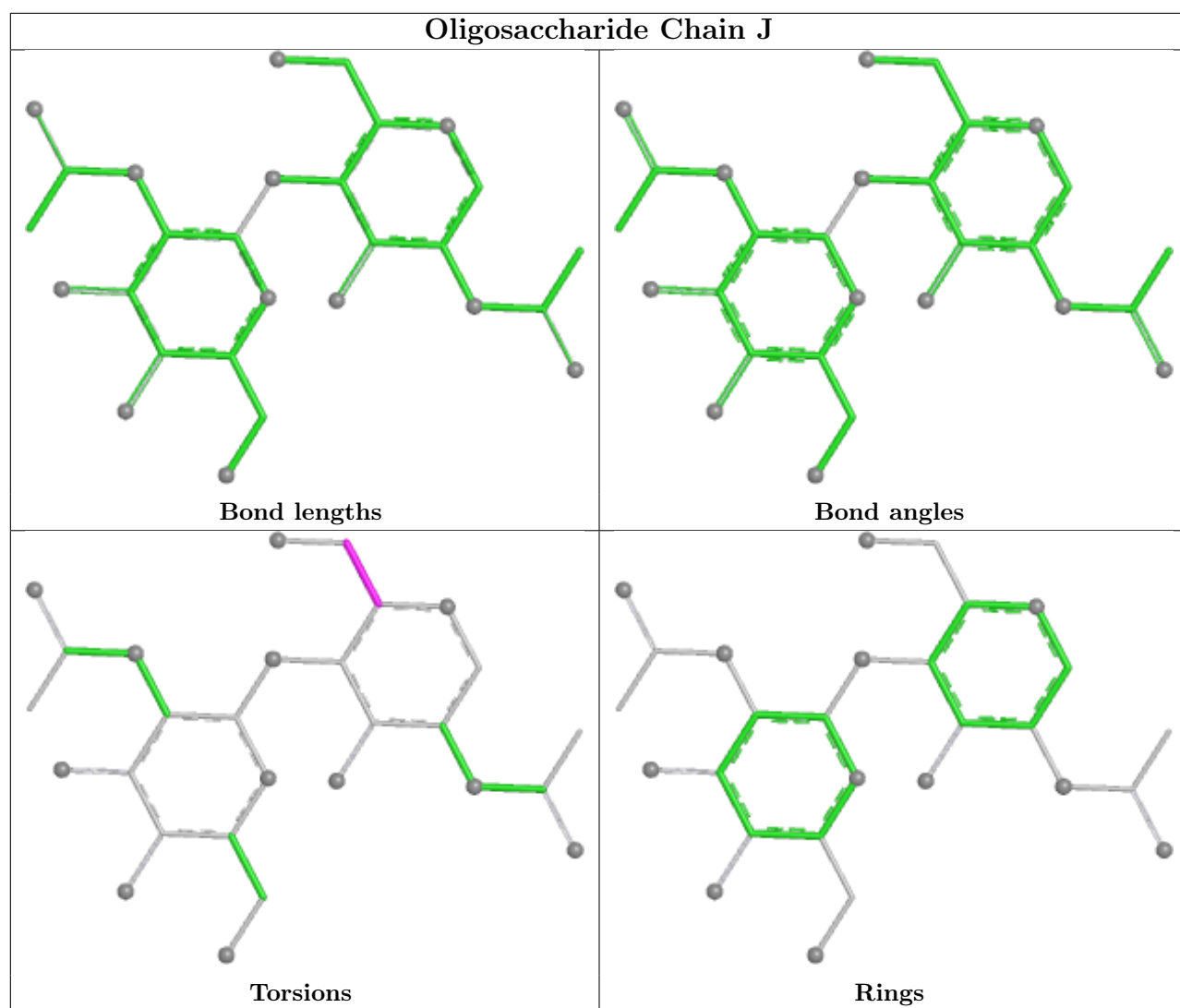


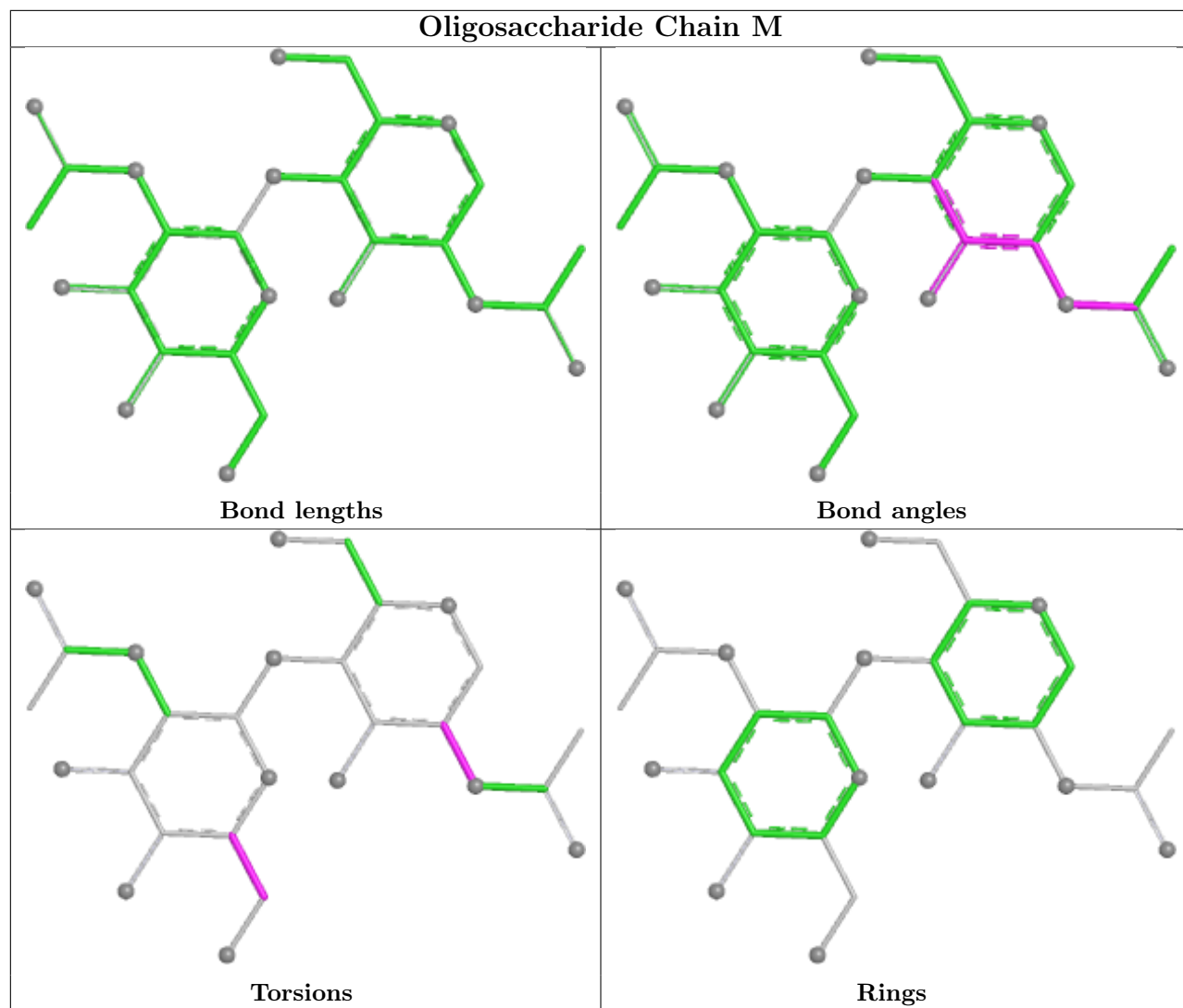


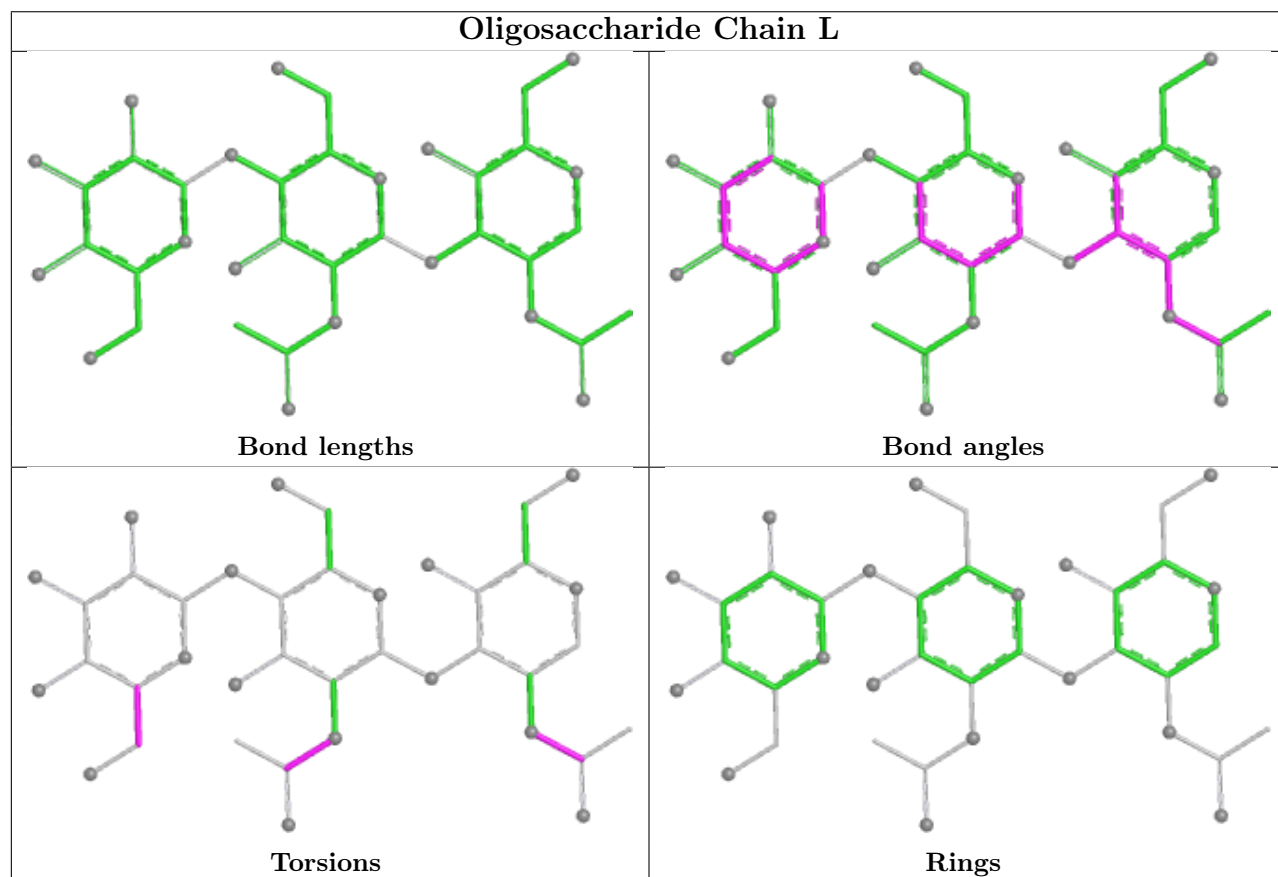
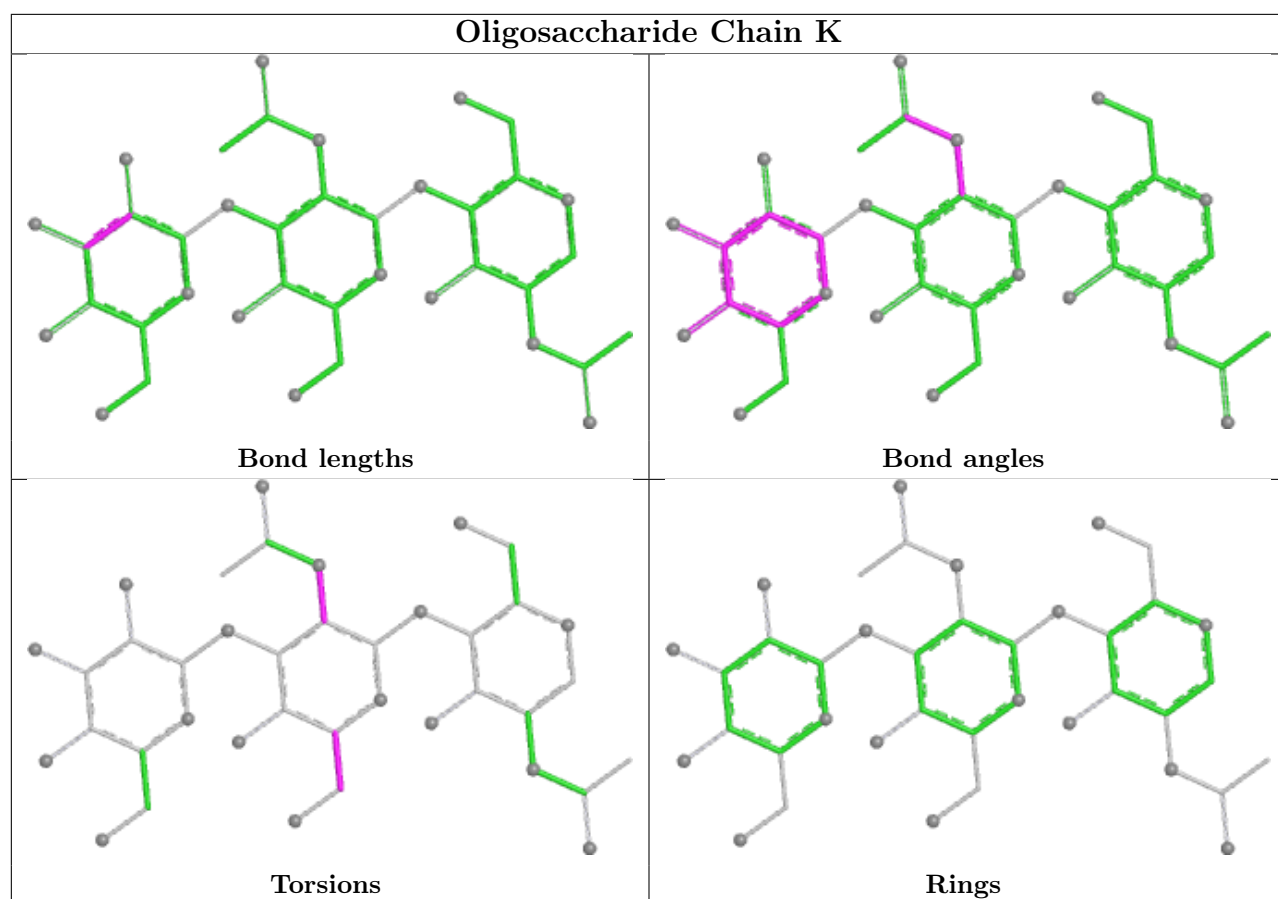












## 5.6 Ligand geometry

11 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
6	NAG	C	1001	1	14,14,15	0.72	0	17,19,21	0.77	0
6	NAG	A	1001	1	14,14,15	0.72	0	17,19,21	0.88	1 (5%)
8	2J9	B	1002	-	17,18,18	1.03	1 (5%)	24,28,28	3.77	3 (12%)
7	GLU	B	1003	-	8,9,9	1.11	1 (12%)	8,11,11	1.14	1 (12%)
6	NAG	B	1001	1	14,14,15	0.70	0	17,19,21	0.78	0
7	GLU	C	1003	-	8,9,9	1.09	1 (12%)	8,11,11	1.13	1 (12%)
7	GLU	A	1002	-	8,9,9	1.08	1 (12%)	8,11,11	1.14	1 (12%)
8	2J9	D	1001	-	17,18,18	1.05	1 (5%)	24,28,28	3.14	3 (12%)
7	GLU	D	1003	-	8,9,9	1.11	1 (12%)	8,11,11	1.19	1 (12%)
8	2J9	C	1002	-	17,18,18	1.07	1 (5%)	24,28,28	3.22	3 (12%)
8	2J9	D	1002	-	17,18,18	1.04	1 (5%)	24,28,28	3.35	3 (12%)

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	C	1001	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1001	1	-	2/6/23/26	0/1/1/1
8	2J9	B	1002	-	-	1/4/22/22	0/3/3/3
7	GLU	B	1003	-	-	0/9/9/9	-
6	NAG	B	1001	1	-	1/6/23/26	0/1/1/1
7	GLU	C	1003	-	-	0/9/9/9	-
7	GLU	A	1002	-	-	1/9/9/9	-
8	2J9	D	1001	-	-	3/4/22/22	0/3/3/3
7	GLU	D	1003	-	-	6/9/9/9	-
8	2J9	C	1002	-	-	1/4/22/22	0/3/3/3
8	2J9	D	1002	-	-	3/4/22/22	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	1002	2J9	CAN-NAO	-2.69	1.43	1.47
8	B	1002	2J9	CAN-NAO	-2.69	1.43	1.47
8	D	1001	2J9	CAN-NAO	-2.66	1.43	1.47
8	D	1002	2J9	CAN-NAO	-2.60	1.43	1.47
7	B	1003	GLU	OXT-C	-2.28	1.23	1.30
7	D	1003	GLU	OXT-C	-2.28	1.23	1.30
7	C	1003	GLU	OXT-C	-2.23	1.23	1.30
7	A	1002	GLU	OXT-C	-2.21	1.23	1.30

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	1002	2J9	CAI-NAO-CAL	17.38	120.45	110.17
8	D	1002	2J9	CAI-NAO-CAL	15.11	119.11	110.17
8	C	1002	2J9	CAI-NAO-CAL	14.53	118.76	110.17
8	D	1001	2J9	CAI-NAO-CAL	14.12	118.52	110.17
8	C	1002	2J9	CAF-CAM-SAP	-4.05	116.59	119.82
8	D	1002	2J9	CAF-CAM-SAP	-4.04	116.60	119.82
8	D	1001	2J9	CAF-CAM-SAP	-3.96	116.67	119.82
8	B	1002	2J9	CAF-CAM-SAP	-3.79	116.80	119.82
8	C	1002	2J9	CAK-CAF-CAM	3.01	118.72	116.92
8	D	1002	2J9	CAK-CAF-CAM	2.88	118.64	116.92
8	D	1001	2J9	CAK-CAF-CAM	2.82	118.61	116.92
8	B	1002	2J9	CAK-CAF-CAM	2.75	118.57	116.92
7	D	1003	GLU	OXT-C-O	-2.67	118.03	124.08
7	B	1003	GLU	OXT-C-O	-2.47	118.47	124.08
7	A	1002	GLU	OXT-C-O	-2.42	118.58	124.08
7	C	1003	GLU	OXT-C-O	-2.40	118.65	124.08
6	A	1001	NAG	C2-N2-C7	2.08	125.69	122.90

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	1003	GLU	O-C-CA-N
8	B	1002	2J9	CAG-CAN-NAO-CAI
8	C	1002	2J9	CAG-CAN-NAO-CAI
8	D	1001	2J9	CAH-CAN-NAO-CAI
8	D	1002	2J9	CAH-CAN-NAO-CAI
6	A	1001	NAG	C8-C7-N2-C2
6	A	1001	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
7	D	1003	GLU	OXT-C-CA-N
8	D	1002	2J9	CAG-CAN-NAO-CAL
8	D	1001	2J9	CAG-CAN-NAO-CAL
6	B	1001	NAG	O5-C5-C6-O6
8	D	1002	2J9	CAH-CAN-NAO-CAL
8	D	1001	2J9	CAH-CAN-NAO-CAL
7	A	1002	GLU	C-CA-CB-CG
7	D	1003	GLU	OE2-CD-CG-CB
7	D	1003	GLU	OE1-CD-CG-CB
7	D	1003	GLU	O-C-CA-CB
7	D	1003	GLU	OXT-C-CA-CB

There are no ring outliers.

7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	1002	2J9	2	0
7	B	1003	GLU	1	0
7	C	1003	GLU	1	0
7	A	1002	GLU	2	0
8	D	1001	2J9	2	0
8	C	1002	2J9	1	0
8	D	1002	2J9	2	0

## 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.

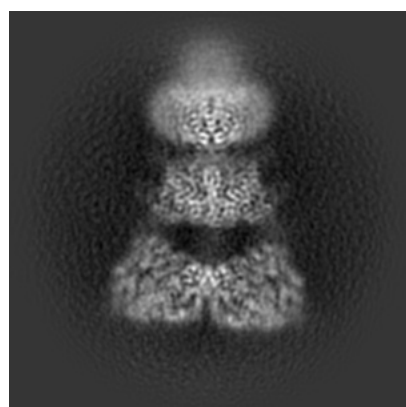
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48767. These allow visual inspection of the internal detail of the map and identification of artifacts.

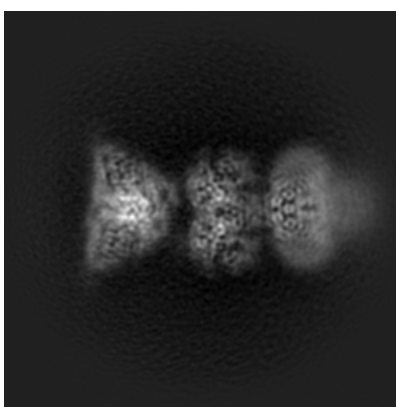
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

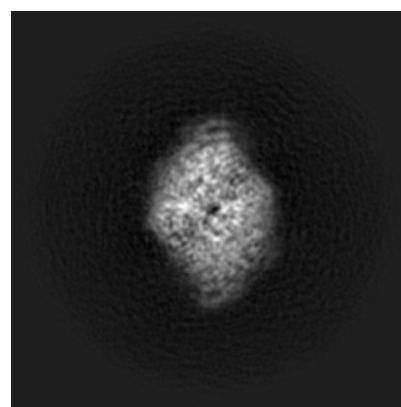
#### 6.1.1 Primary map



X



Y

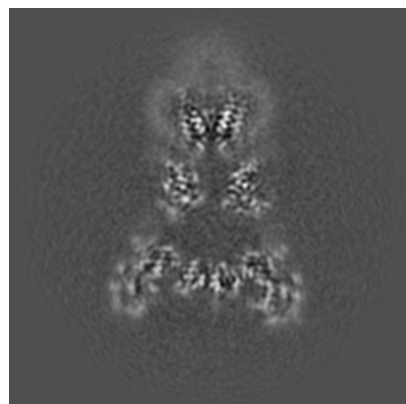


Z

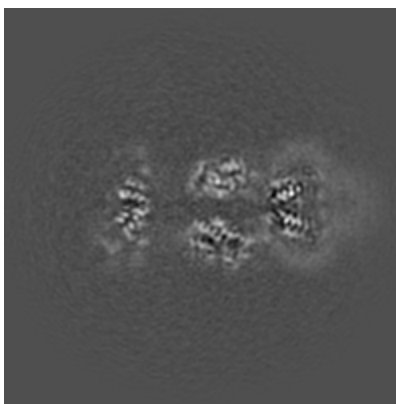
The images above show the map projected in three orthogonal directions.

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

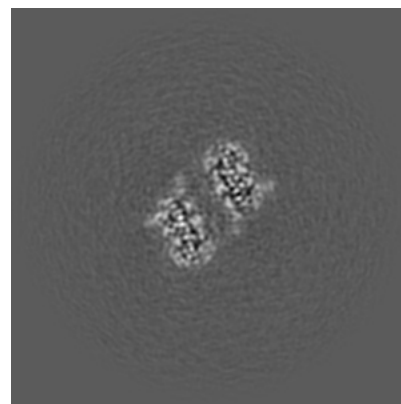
#### 6.2.1 Primary map



X Index: 140



Y Index: 140



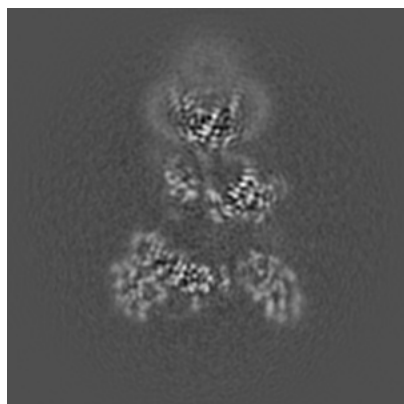
Z Index: 140



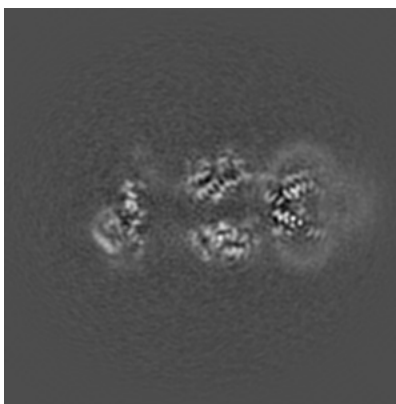
The images above show central slices of the map in three orthogonal directions.

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

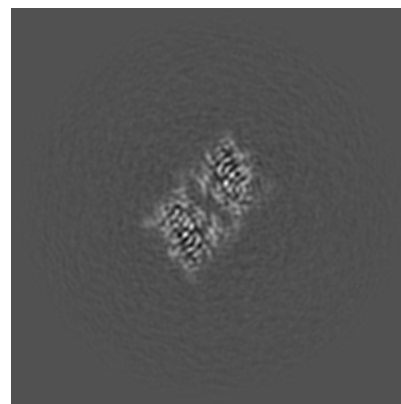
### 6.3.1 Primary map



X Index: 147



Y Index: 143

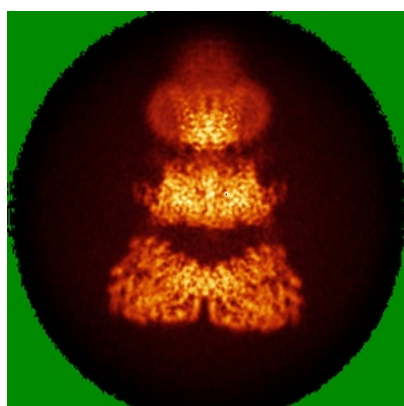


Z Index: 145

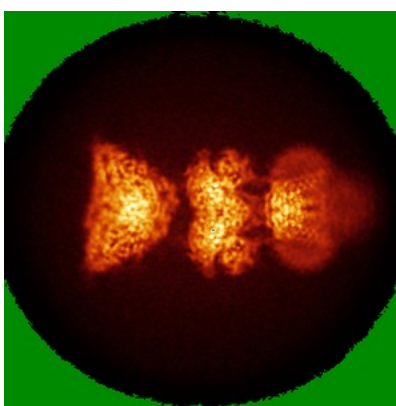
The images above show the largest variance slices of the map in three orthogonal directions.

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

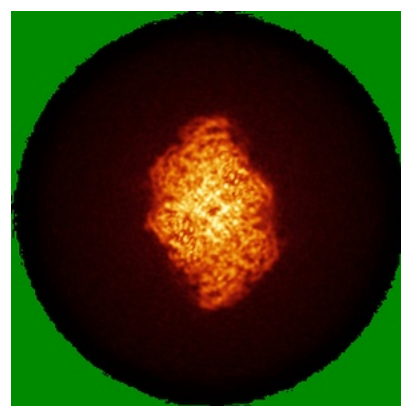
### 6.4.1 Primary map



X



Y

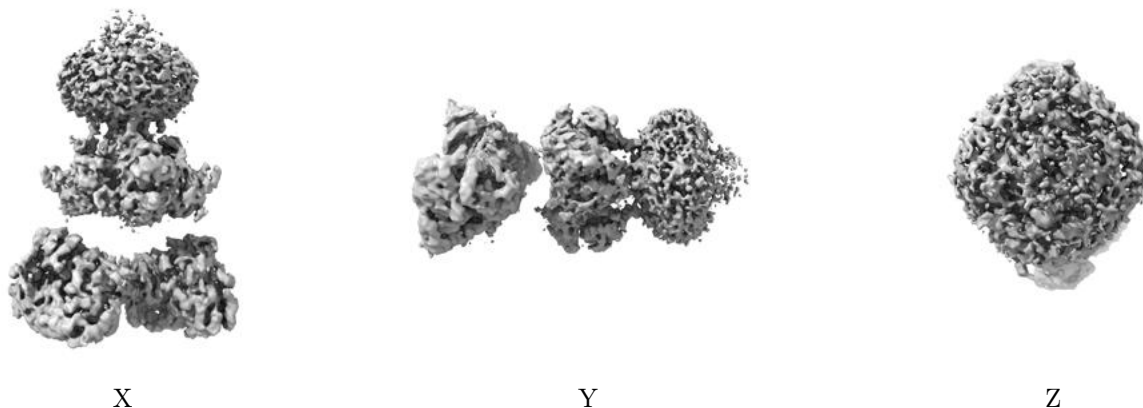


Z

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 0.243. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

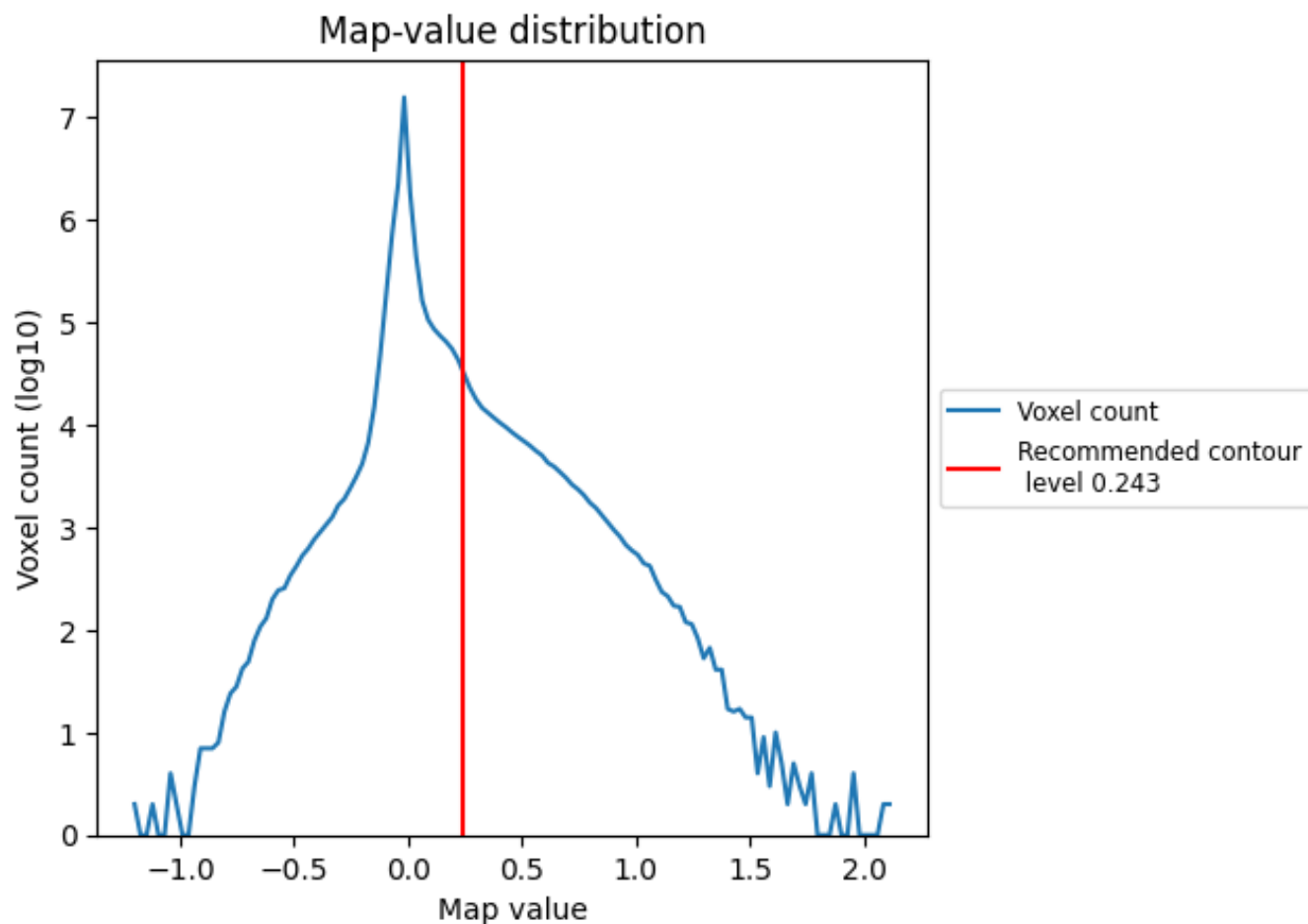
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

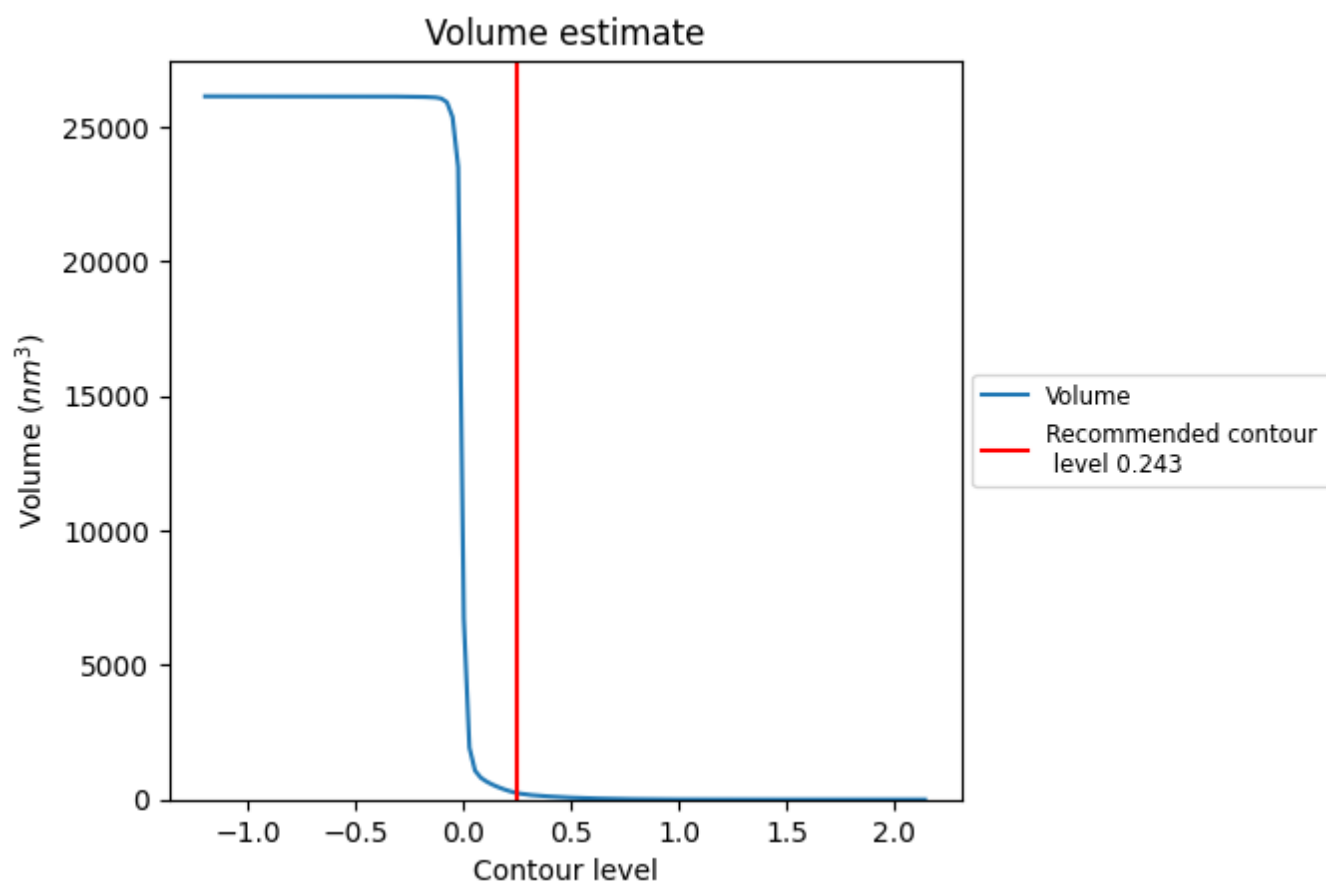
This section contains the results of statistical analysis of the map.

### 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.

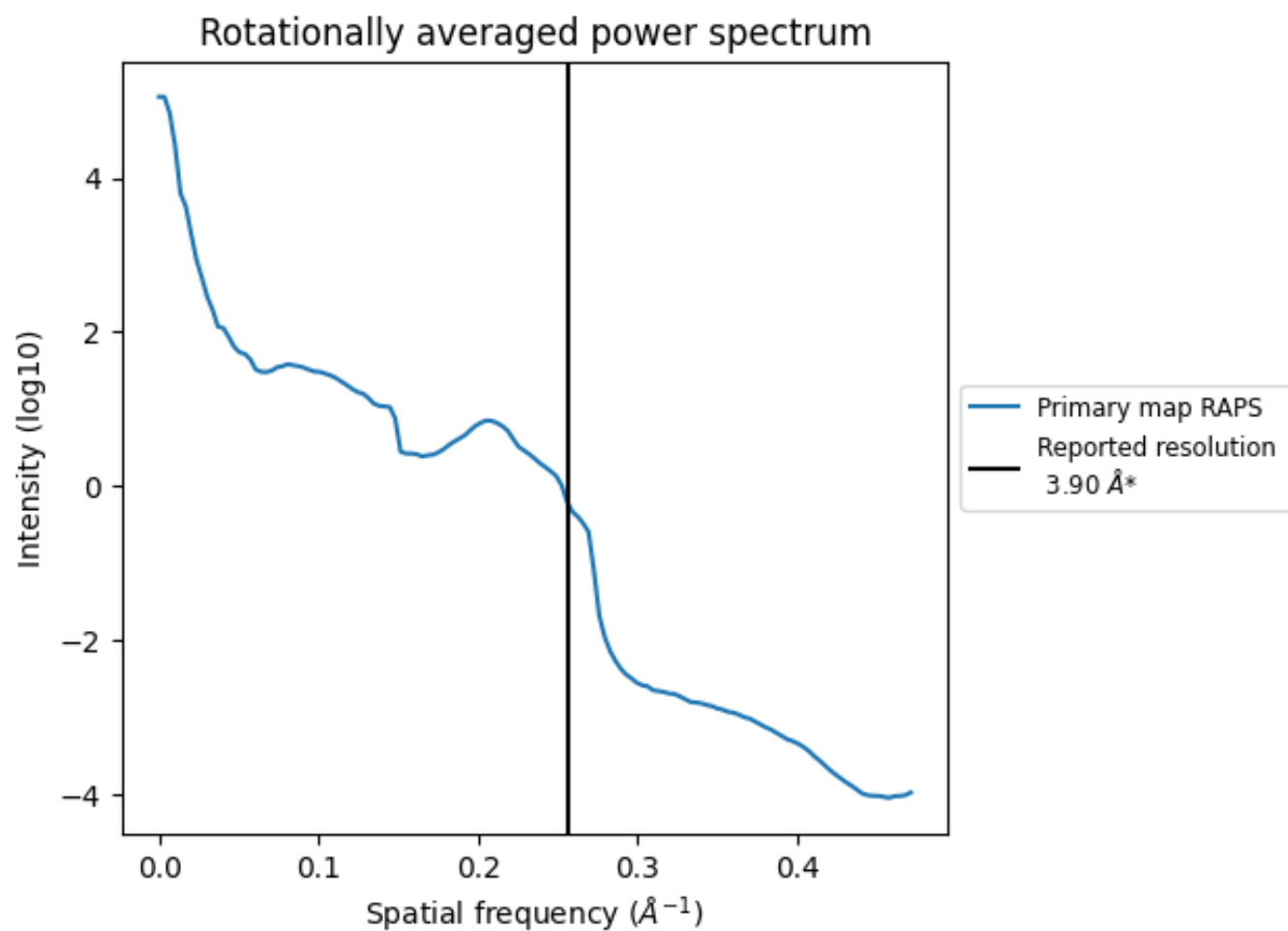
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 252 nm<sup>3</sup>; this corresponds to an approximate mass of 228 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 0.256 Å<sup>-1</sup>

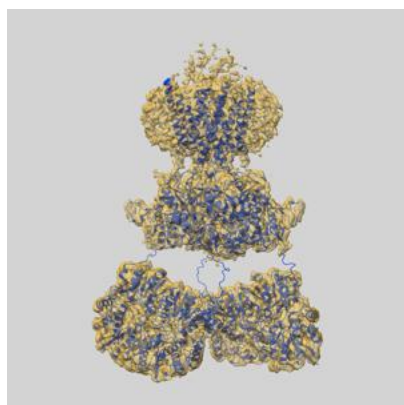
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

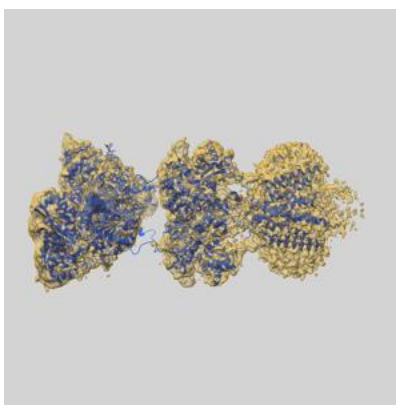
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-48767 and PDB model 9MZS. Per-residue inclusion information can be found in section 3 on page 9.

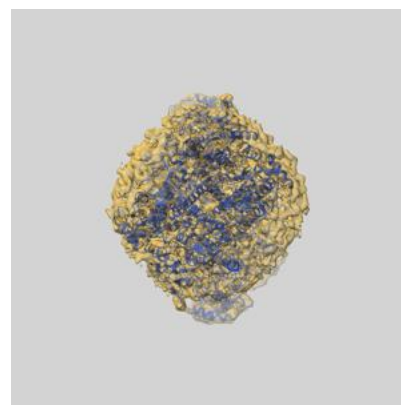
### 9.1 Map-model overlay [i](#)



X



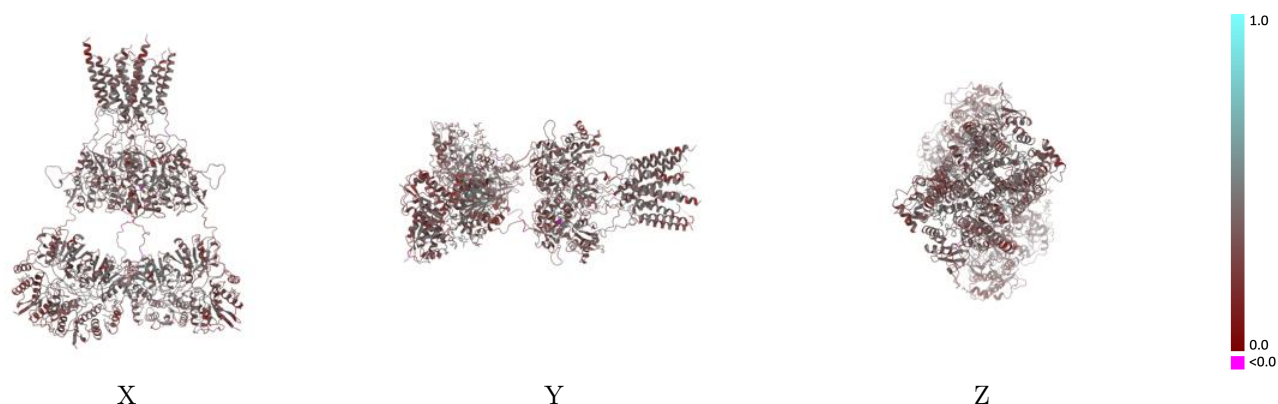
Y



Z

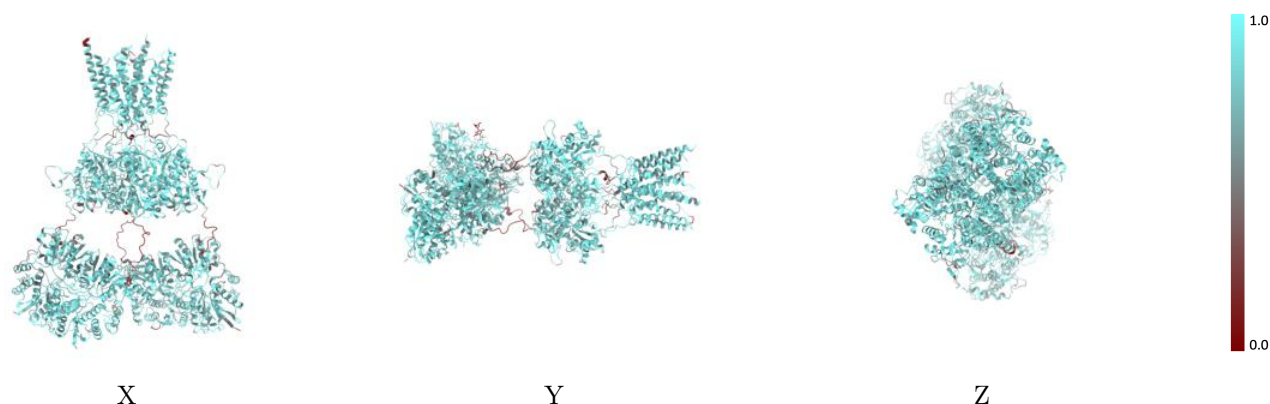
The images above show the 3D surface view of the map at the recommended contour level 0.243 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



The images above show the model with each residue coloured according 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.

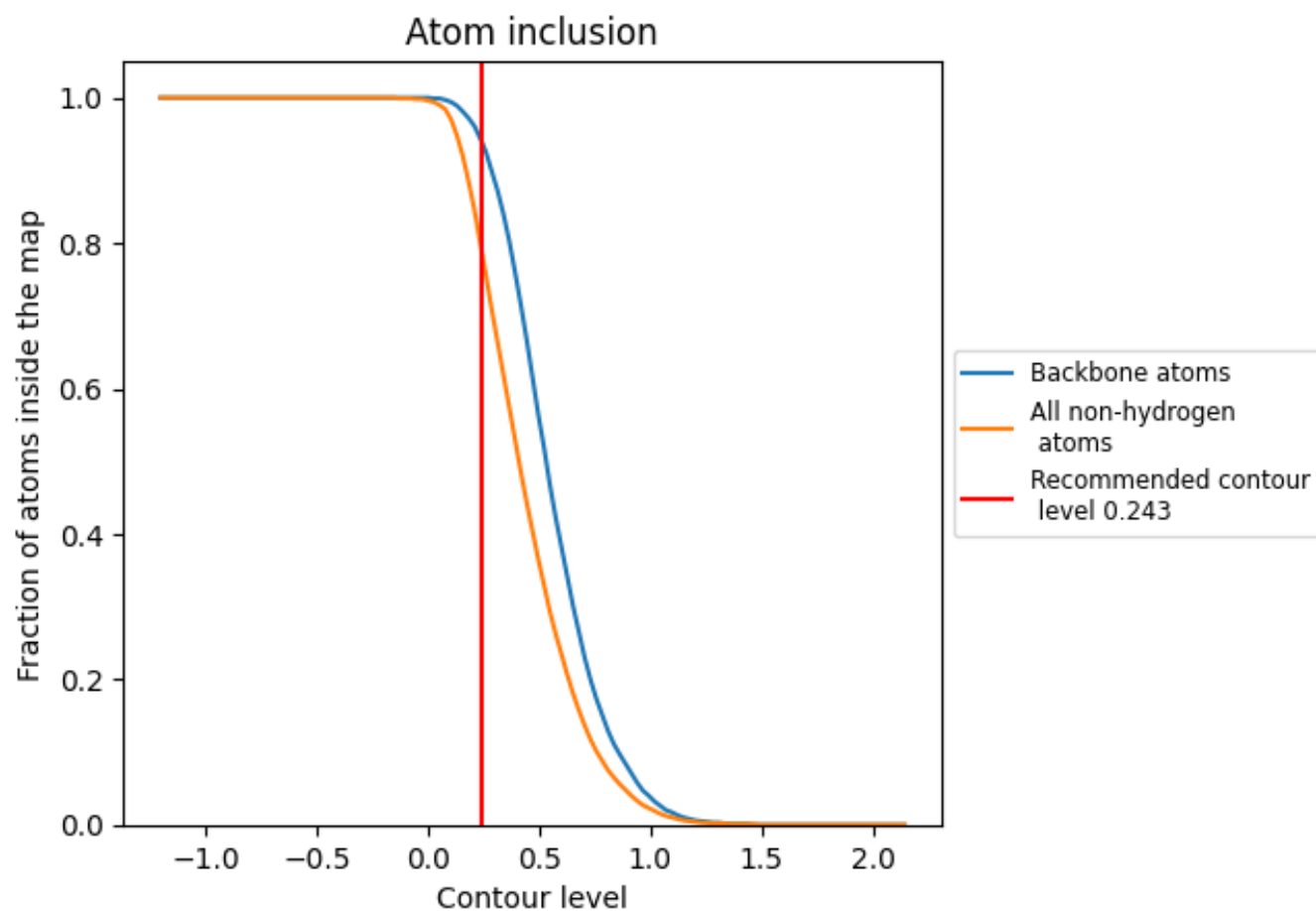
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.243).



































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 79% 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 (0.243) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7880	 0.3660
A	 0.7750	 0.3560
B	 0.8050	 0.3740
C	 0.7660	 0.3580
D	 0.8100	 0.3770
E	 0.6920	 0.3620
F	 0.8720	 0.4090
G	 0.6430	 0.2640
H	 0.8970	 0.4180
I	 0.6670	 0.3640
J	 0.7500	 0.4090
K	 0.9230	 0.4310
L	 0.8460	 0.3360
M	 0.5710	 0.2580
N	 0.6920	 0.3670
O	 0.2820	 0.3080

