



## Full wwPDB EM Validation Report ⓘ

Oct 28, 2024 – 04:28 AM EDT

PDB ID : 8EOI  
EMDB ID : EMD-28376  
Title : Structure of a human EMC:human Cav1.2 channel complex in GDN detergent  
Authors : Chen, Z.; Mondal, A.; Abderemane-Ali, F.; Minor, D.L.  
Deposited on : 2022-10-03  
Resolution : 3.40 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.dev113  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

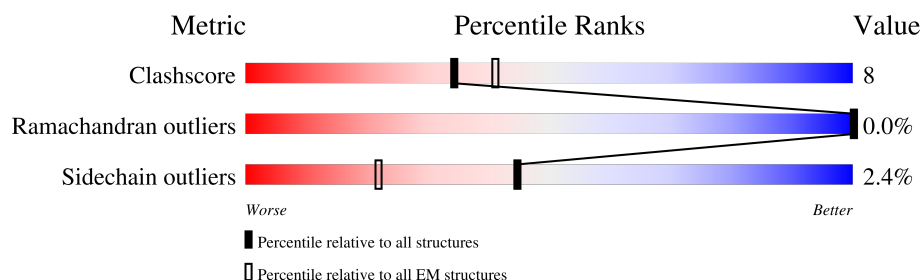
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.40 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	973	
2	B	291	
3	C	258	
4	E	101	
5	F	100	
6	G	116	
7	H	208	
8	I	157	

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Mol	Chain	Length	Quality of chain
9	K	1550	<div><div></div><div>17%</div><div>51%</div><div>20%</div><div>28%</div></div>
10	J	324	<div><div></div><div>29%</div><div>65%</div><div>27%</div><div>9%</div></div>
11	D	170	<div><div></div><div>19%</div><div>5%</div><div>74%</div></div>
12	L	2	<div><div></div><div>100%</div></div>
12	M	2	<div><div></div><div>100%</div></div>
12	N	2	<div><div></div><div>50%</div><div>50%</div></div>

## 2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 28721 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 ER membrane protein complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	936	Total	C	N	O	S	0	0
			7444	4780	1272	1367	25		

- Molecule 2 is a protein called ER membrane protein complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	291	Total	C	N	O	S	0	0
			2403	1509	425	455	14		

- Molecule 3 is a protein called ER membrane protein complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	218	Total	C	N	O	S	0	0
			1777	1161	287	323	6		

- Molecule 4 is a protein called ER membrane protein complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	101	Total	C	N	O	S	0	0
			806	522	140	141	3		

- Molecule 5 is a protein called ER membrane protein complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	100	Total	C	N	O	S	0	0
			781	526	127	126	2		

- Molecule 6 is a protein called ER membrane protein complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	116	Total	C	N	O	S	0	0
			929	600	161	166	2		

- Molecule 7 is a protein called ER membrane protein complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	193	Total	C	N	O	S	0	0
			1543	974	269	288	12		

- Molecule 8 is a protein called ER membrane protein complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	150	Total	C	N	O	S	0	0
			1150	713	210	225	2		

- Molecule 9 is a protein called Voltage-dependent L-type calcium channel subunit alpha-1C.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	1116	Total	C	N	O	S	0	0
			9024	5952	1483	1527	62		

- Molecule 10 is a protein called Voltage-dependent L-type calcium channel subunit beta-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	296	Total	C	N	O	S	0	0
			2364	1494	422	438	10		

- Molecule 11 is a protein called ER membrane protein complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	D	45	Total	C	N	O	S	0	0
			363	241	58	63	1		

- Molecule 12 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
12	L	2	Total	C	N	O	0	0
			28	16	2	10		
12	M	2	Total	C	N	O	0	0
			28	16	2	10		

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

- Molecule 13 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

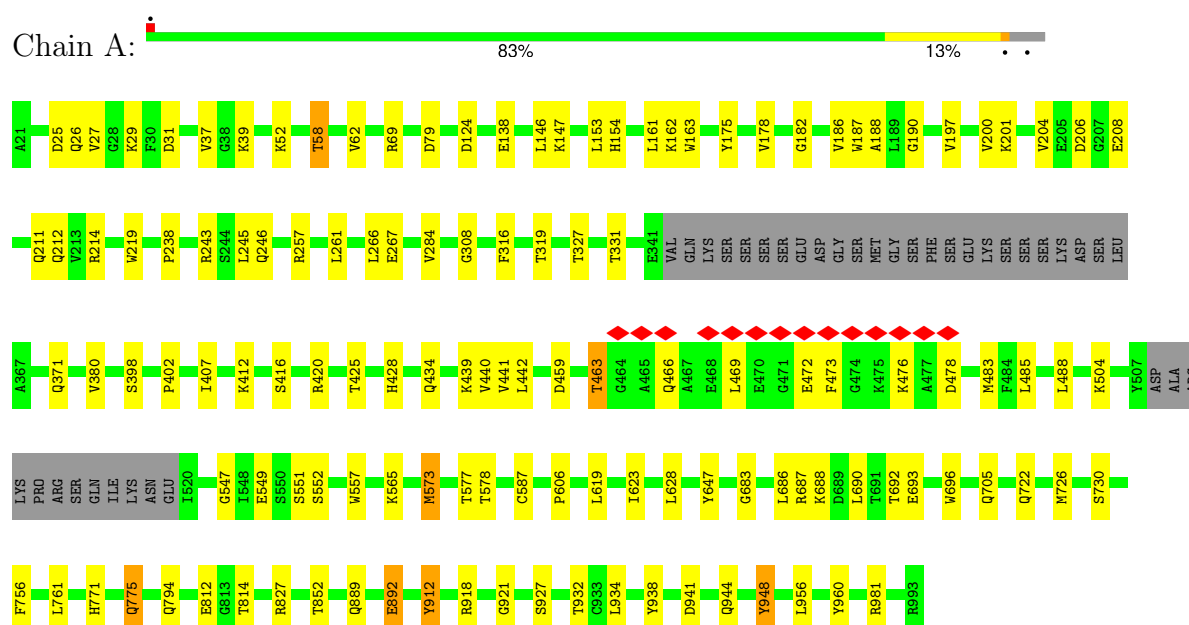
- Molecule 14 is (3beta,14beta,17beta,25R)-3-[4-methoxy-3-(methoxymethyl)butoxy]spirost-5-en (three-letter code: 9Z9) (formula: C<sub>34</sub>H<sub>56</sub>O<sub>5</sub>).



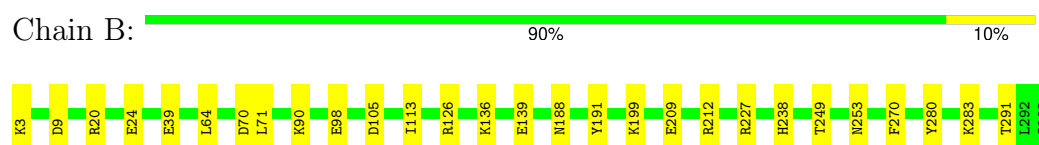
### 3 Residue-property plots

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.

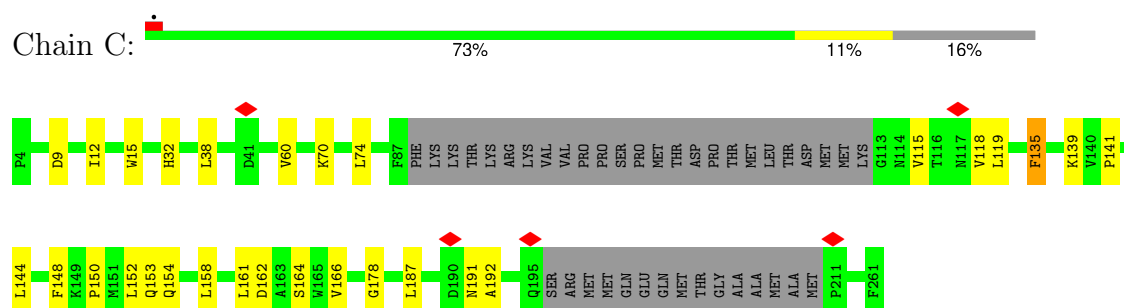
#### • Molecule 1: ER membrane protein complex subunit 1



#### • Molecule 2: ER membrane protein complex subunit 2

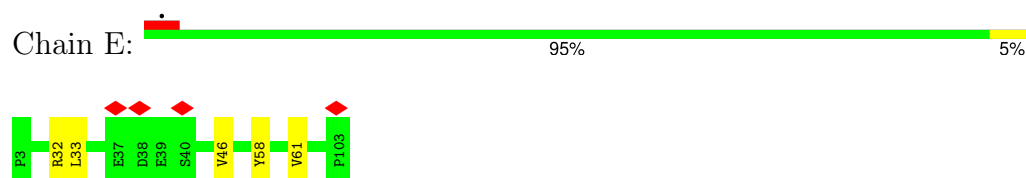


#### • Molecule 3: ER membrane protein complex subunit 3

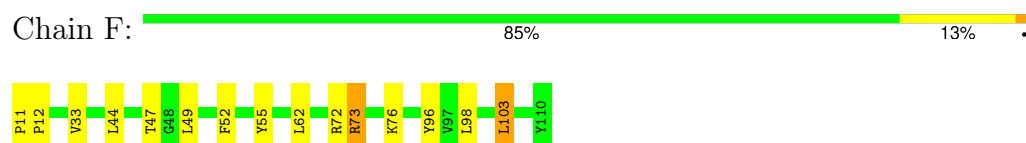




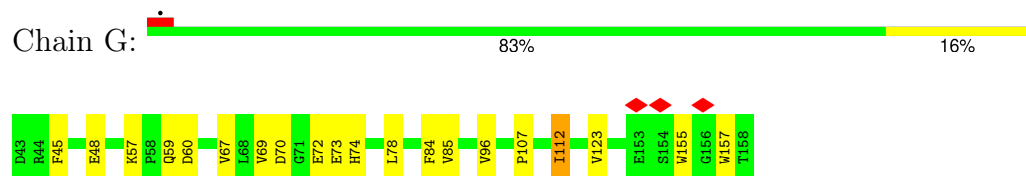
- Molecule 4: ER membrane protein complex subunit 5



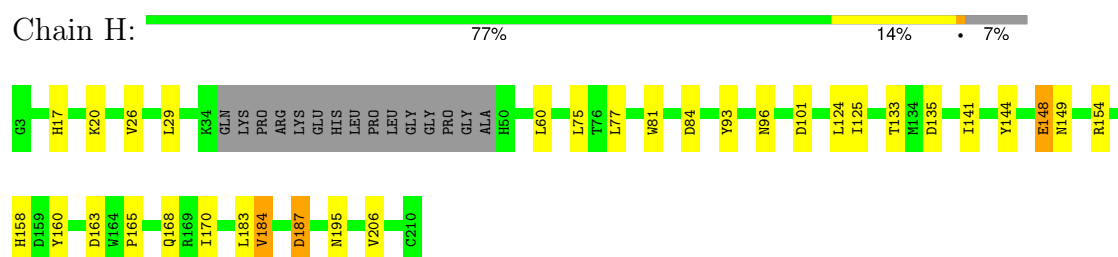
- Molecule 5: ER membrane protein complex subunit 6



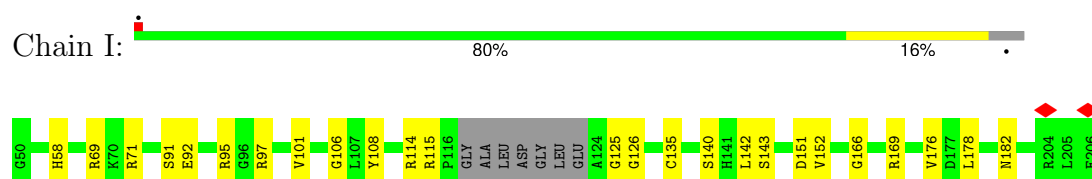
- Molecule 6: ER membrane protein complex subunit 7



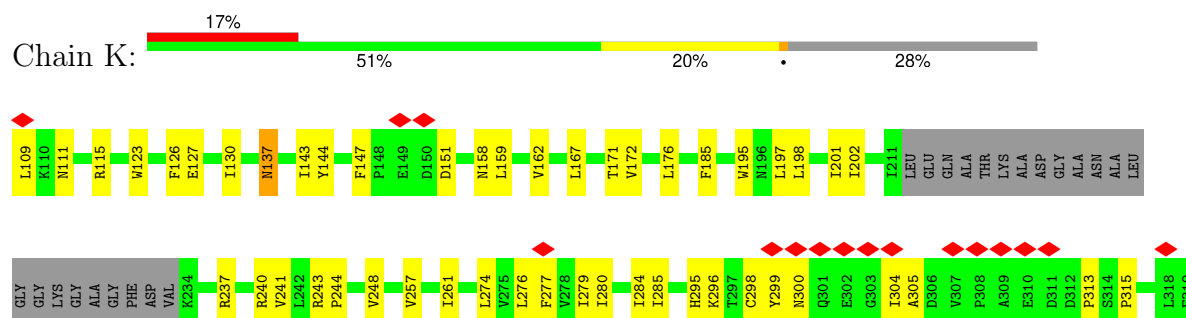
- Molecule 7: ER membrane protein complex subunit 8

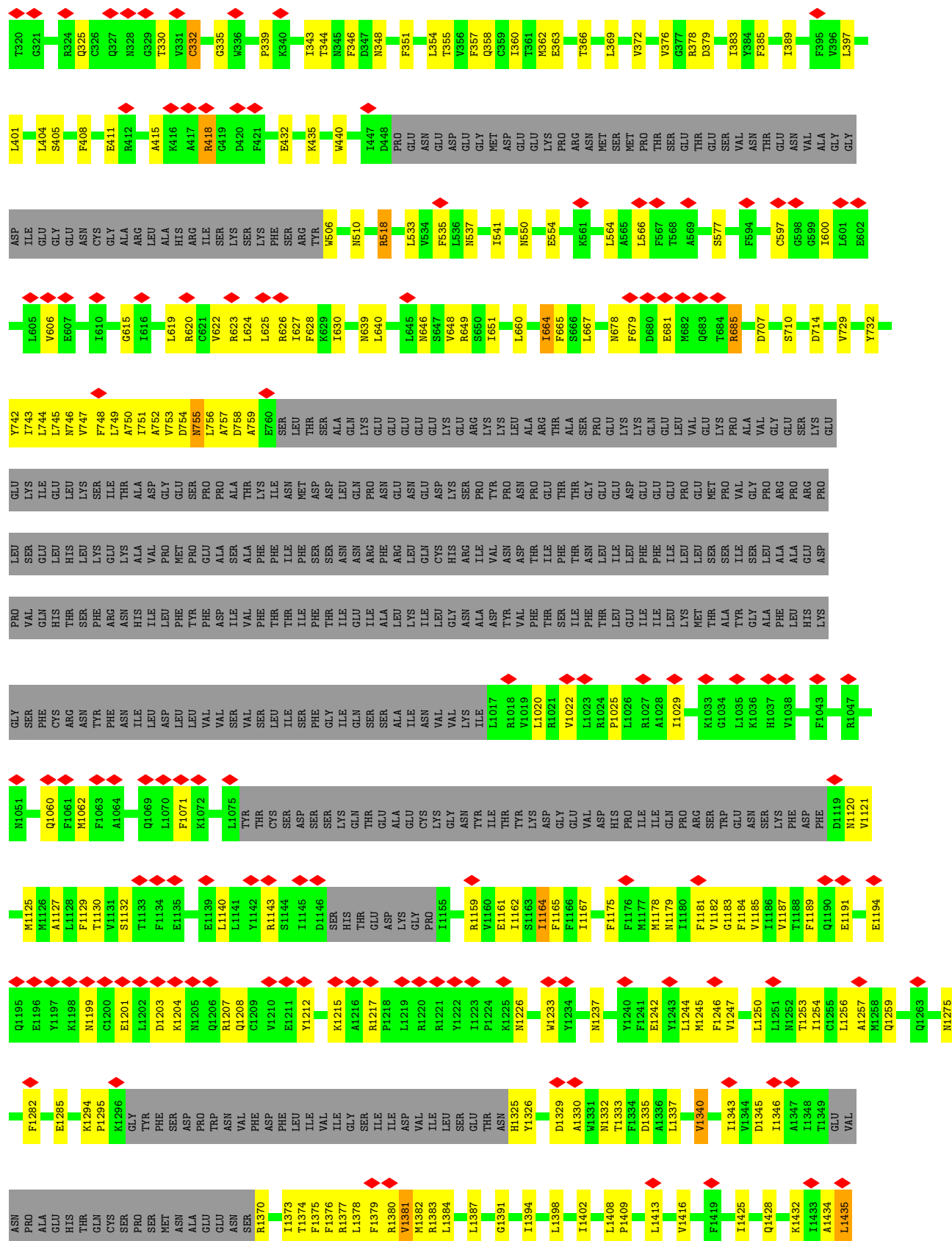


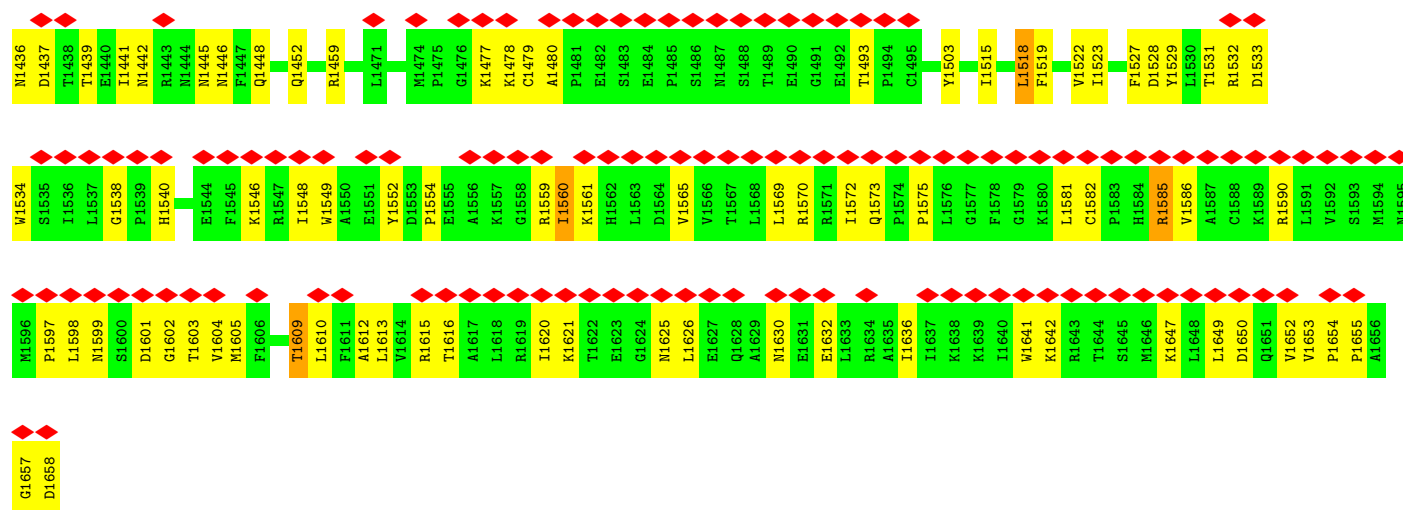
- Molecule 8: ER membrane protein complex subunit 10



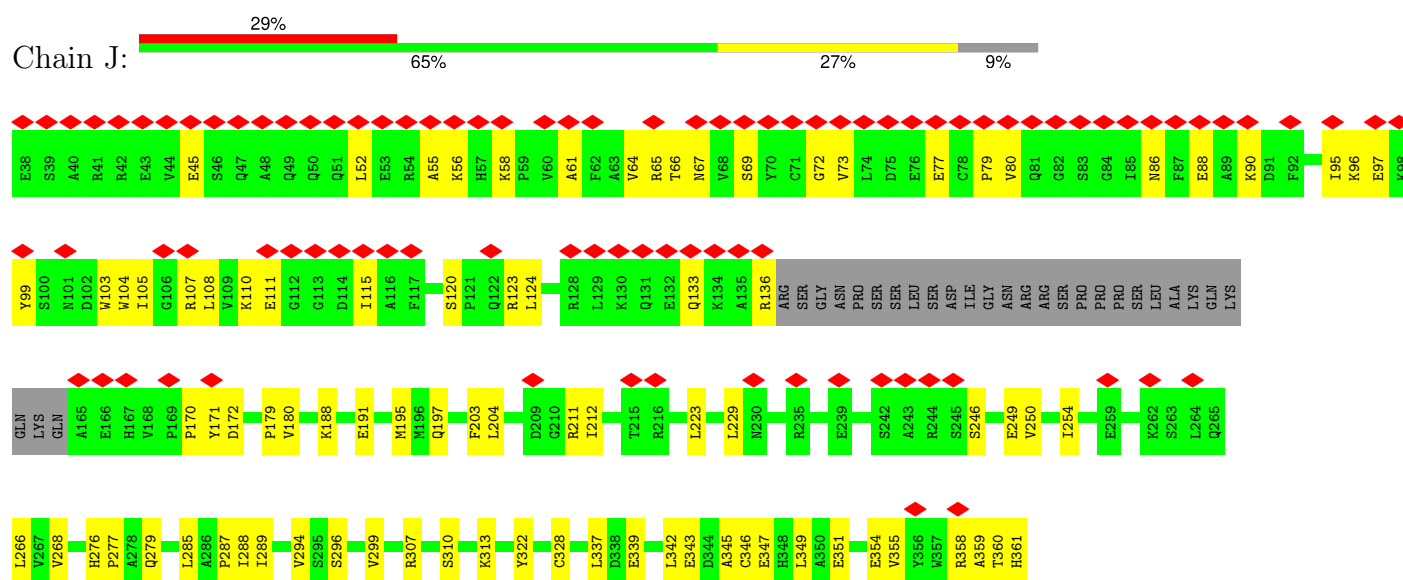
- Molecule 9: Voltage-dependent L-type calcium channel subunit alpha-1C



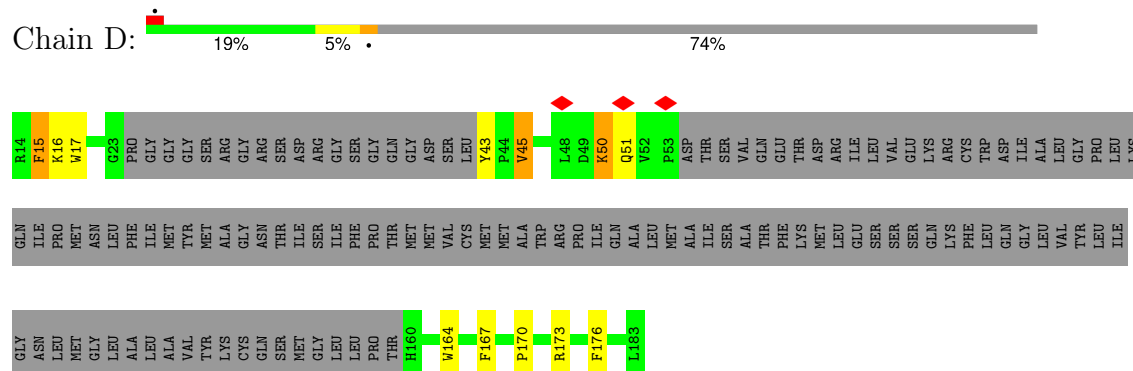




• Molecule 10: Voltage-dependent L-type calcium channel subunit beta-3



• Molecule 11: ER membrane protein complex subunit 4



• Molecule 12: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  100%

HA01  
HA02

- Molecule 12: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  100%

HA01  
HA02

- Molecule 12: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  50% 50%

HA01  
HA02

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	487067	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	46	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	33.490	Depositor
Minimum map value	-11.478	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	5.93	Depositor
Map size ( $\text{\AA}$ )	372.504, 372.504, 372.504	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.8466, 0.8466, 0.8466	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, 9Z9

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.25	0/7615	0.50	0/10346
2	B	0.25	0/2447	0.44	0/3288
3	C	0.24	0/1819	0.45	0/2464
4	E	0.25	0/827	0.45	0/1118
5	F	0.26	0/803	0.45	0/1089
6	G	0.25	0/956	0.53	0/1298
7	H	0.24	0/1583	0.45	0/2156
8	I	0.23	0/1170	0.52	0/1589
9	K	0.25	0/9237	0.46	0/12522
10	J	0.24	0/2408	0.47	0/3252
11	D	0.25	0/374	0.52	0/504
All	All	0.24	0/29239	0.47	0/39626

There are no bond length outliers.

There are no bond angle outliers.

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	7444	0	7495	78	0
2	B	2403	0	2355	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1777	0	1783	18	0
4	E	806	0	803	3	0
5	F	781	0	810	10	0
6	G	929	0	928	9	0
7	H	1543	0	1477	20	0
8	I	1150	0	1124	12	0
9	K	9024	0	9261	229	0
10	J	2364	0	2400	61	0
11	D	363	0	349	6	0
12	L	28	0	25	0	0
12	M	28	0	25	0	0
12	N	28	0	25	1	0
13	A	14	0	13	0	0
14	K	39	0	0	0	0
All	All	28721	0	28873	452	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 8.

All (452) 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)
3:C:32:HIS:HB2	3:C:192:ALA:HB2	1.67	0.75
6:G:155:TRP:NE1	6:G:157:TRP:O	2.23	0.71
9:K:1329:ASP:HB3	9:K:1332:ASN:HB2	1.71	0.71
1:A:243:ARG:NH2	1:A:266:LEU:O	2.24	0.70
9:K:1253:THR:O	9:K:1257:ALA:N	2.25	0.70
9:K:1653:VAL:O	9:K:1657:GLY:N	2.26	0.68
9:K:1199:ASN:ND2	9:K:1203:ASP:O	2.27	0.68
3:C:178:GLY:HA3	5:F:98:LEU:HD13	1.76	0.68
9:K:1548:ILE:O	9:K:1552:TYR:N	2.20	0.67
9:K:1376:PHE:O	9:K:1379:PHE:HB2	1.95	0.67
9:K:623:ARG:HE	9:K:626:ARG:HG3	1.60	0.66
9:K:625:LEU:O	9:K:628:PHE:HB2	1.95	0.66
9:K:746:ASN:O	9:K:750:ALA:N	2.27	0.66
9:K:751:ILE:O	9:K:755:ASN:N	2.23	0.66
1:A:200:VAL:HG12	1:A:212:GLN:HG2	1.78	0.66
9:K:1178:MET:O	9:K:1182:VAL:N	2.24	0.66
6:G:69:VAL:HB	6:G:74:HIS:HB2	1.79	0.65
9:K:1441:ILE:HA	9:K:1445:ASN:HD22	1.61	0.65
9:K:1199:ASN:HD21	9:K:1204:LYS:HA	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:141:PRO:O	5:F:47:THR:OG1	2.14	0.65
9:K:646:ASN:OD1	9:K:649:ARG:NH2	2.30	0.65
9:K:1029:ILE:HD13	9:K:1413:LEU:HD23	1.79	0.64
9:K:1626:LEU:O	9:K:1630:ASN:CB	2.46	0.64
9:K:678:ASN:O	9:K:685:ARG:NH2	2.32	0.63
2:B:249:THR:O	2:B:253:ASN:ND2	2.30	0.63
9:K:1129:PHE:HA	9:K:1132:SER:HB2	1.80	0.63
9:K:750:ALA:O	9:K:754:ASP:N	2.27	0.63
10:J:77:GLU:OE1	10:J:123:ARG:NH2	2.31	0.63
9:K:1370:ARG:O	9:K:1374:THR:OG1	2.17	0.62
3:C:32:HIS:HD2	3:C:191:ASN:HB3	1.64	0.62
9:K:1549:TRP:HZ2	9:K:1572:ILE:HG23	1.64	0.62
9:K:1528:ASP:O	9:K:1532:ARG:NE	2.28	0.62
1:A:466:GLN:HB3	4:E:33:LEU:HD21	1.82	0.62
9:K:1599:ASN:HD21	9:K:1655:PRO:HB3	1.64	0.61
11:D:173:ARG:HH21	11:D:176:PHE:HA	1.65	0.61
9:K:1125:MET:SD	9:K:1125:MET:N	2.71	0.61
9:K:752:ALA:HA	9:K:755:ASN:HB3	1.83	0.61
3:C:150:PRO:O	3:C:154:GLN:NE2	2.33	0.60
9:K:1585:ARG:H	9:K:1590:ARG:HH21	1.48	0.60
9:K:1181:PHE:O	9:K:1185:VAL:N	2.32	0.60
9:K:747:VAL:O	9:K:751:ILE:N	2.32	0.60
9:K:752:ALA:O	9:K:756:LEU:N	2.27	0.60
7:H:96:ASN:ND2	7:H:101:ASP:OD2	2.34	0.60
9:K:408:PHE:HA	9:K:411:GLU:HG2	1.83	0.60
1:A:37:VAL:HB	1:A:58:THR:HG21	1.82	0.60
9:K:298:CYS:SG	9:K:325:GLN:NE2	2.75	0.60
9:K:415:ALA:O	9:K:418:ARG:NH1	2.34	0.60
9:K:1379:PHE:HA	9:K:1382:MET:HB3	1.84	0.60
9:K:1182:VAL:O	9:K:1185:VAL:HB	2.01	0.60
9:K:1275:ASN:OD1	9:K:1380:ARG:NH2	2.32	0.59
3:C:152:LEU:HD23	3:C:166:VAL:HG12	1.84	0.59
10:J:180:VAL:HB	10:J:268:VAL:HG12	1.82	0.59
9:K:564:LEU:HD13	9:K:600:ILE:HG13	1.84	0.59
9:K:749:LEU:O	9:K:753:VAL:N	2.33	0.59
9:K:1175:PHE:O	9:K:1179:ASN:N	2.31	0.59
9:K:137:ASN:OD1	9:K:243:ARG:NH1	2.35	0.59
9:K:167:LEU:HD12	9:K:201:ILE:HG22	1.83	0.59
9:K:1581:LEU:HB3	9:K:1585:ARG:HA	1.85	0.59
9:K:742:TYR:O	9:K:746:ASN:N	2.28	0.58
10:J:69:SER:HA	10:J:88:GLU:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:1253:THR:HA	9:K:1256:LEU:HG	1.84	0.58
9:K:1559:ARG:NH2	9:K:1605:MET:SD	2.76	0.58
9:K:1020:LEU:HD23	9:K:1020:LEU:H	1.69	0.58
10:J:65:ARG:NH2	10:J:172:ASP:OD2	2.35	0.58
9:K:1533:ASP:HB3	9:K:1538:GLY:HA2	1.86	0.58
7:H:184:VAL:HG21	7:H:195:ASN:HB3	1.85	0.58
9:K:743:ILE:O	9:K:747:VAL:N	2.30	0.57
5:F:33:VAL:HG11	5:F:62:LEU:HD22	1.85	0.57
9:K:1442:ASN:H	9:K:1445:ASN:HB3	1.67	0.57
9:K:167:LEU:HD21	9:K:202:ILE:HD13	1.85	0.57
9:K:401:LEU:HD13	9:K:1523:ILE:HG22	1.86	0.57
9:K:745:LEU:O	9:K:749:LEU:N	2.31	0.57
9:K:1140:LEU:HD23	9:K:1143:ARG:HH12	1.69	0.57
7:H:20:LYS:NZ	7:H:183:LEU:O	2.32	0.57
9:K:378:ARG:NH1	9:K:379:ASP:OD2	2.38	0.56
10:J:96:LYS:HD3	10:J:107:ARG:HG2	1.87	0.56
10:J:337:LEU:HD21	10:J:349:LEU:HB2	1.86	0.56
3:C:158:LEU:HD12	3:C:161:LEU:HD22	1.87	0.56
12:N:1:NAG:H3	12:N:1:NAG:H83	1.87	0.56
1:A:463:THR:HG23	1:A:466:GLN:HB2	1.86	0.56
9:K:1435:LEU:HD23	9:K:1435:LEU:H	1.71	0.56
9:K:1570:ARG:HB2	9:K:1582:CYS:HB2	1.87	0.56
9:K:1599:ASN:HB2	9:K:1603:THR:HB	1.86	0.56
1:A:687:ARG:HH21	1:A:693:GLU:HB3	1.69	0.56
5:F:73:ARG:HG3	5:F:76:LYS:HE2	1.88	0.56
2:B:98:GLU:OE2	2:B:126:ARG:NH2	2.38	0.56
9:K:754:ASP:O	9:K:758:ASP:N	2.37	0.56
9:K:1626:LEU:O	9:K:1630:ASN:HB2	2.06	0.56
9:K:755:ASN:O	9:K:759:ALA:N	2.39	0.56
9:K:1127:ALA:O	9:K:1130:THR:OG1	2.17	0.56
9:K:1561:LYS:HD2	9:K:1601:ASP:HB3	1.86	0.56
9:K:1432:LYS:HB3	9:K:1480:ALA:HB3	1.87	0.56
9:K:1532:ARG:HH22	9:K:1540:HIS:HB2	1.71	0.55
1:A:981:ARG:HD3	9:K:123:TRP:CE2	2.41	0.55
9:K:1233:TRP:HD1	9:K:1237:ASN:HB2	1.71	0.55
1:A:316:PHE:HB3	1:A:319:THR:HG21	1.89	0.55
10:J:310:SER:O	10:J:313:LYS:NZ	2.39	0.55
9:K:506:TRP:O	9:K:510:ASN:ND2	2.40	0.55
9:K:1226:ASN:HB2	9:K:1294:LYS:HD3	1.89	0.55
9:K:660:LEU:O	9:K:664:ILE:HG22	2.06	0.55
9:K:1529:TYR:O	9:K:1534:TRP:NE1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:726:MET:SD	1:A:730:SER:OG	2.58	0.55
9:K:1613:LEU:O	9:K:1616:THR:OG1	2.22	0.55
10:J:276:HIS:NE2	10:J:328:CYS:SG	2.80	0.54
9:K:1384:LEU:HA	9:K:1387:LEU:HD13	1.89	0.54
9:K:1615:ARG:HG2	9:K:1620:ILE:HD11	1.89	0.54
10:J:67:ASN:HA	10:J:90:LYS:H	1.72	0.54
10:J:120:SER:O	10:J:124:LEU:N	2.32	0.54
1:A:138:GLU:HA	1:A:284:VAL:HG11	1.88	0.54
2:B:90:LYS:HB3	2:B:113:ILE:HD11	1.88	0.54
9:K:1071:PHE:HB2	9:K:1159:ARG:HD2	1.90	0.54
1:A:960:TYR:HE2	3:C:15:TRP:HB3	1.72	0.54
9:K:1528:ASP:OD1	9:K:1528:ASP:N	2.41	0.54
1:A:371:GLN:NE2	1:A:398:SER:O	2.41	0.54
9:K:746:ASN:HA	9:K:749:LEU:HB3	1.88	0.54
8:I:114:ARG:NH2	8:I:125:GLY:O	2.41	0.54
9:K:300:ASN:N	9:K:304:ILE:O	2.34	0.54
9:K:1164:ILE:O	9:K:1167:ILE:HB	2.06	0.54
9:K:1256:LEU:HA	9:K:1259:GLN:HG2	1.89	0.54
9:K:325:GLN:HE22	9:K:332:CYS:HB3	1.73	0.54
9:K:348:ASN:O	9:K:351:PHE:N	2.34	0.54
9:K:1515:ILE:HA	9:K:1518:LEU:HD23	1.90	0.54
7:H:170:ILE:HG21	7:H:206:VAL:HG23	1.90	0.53
1:A:476:LYS:NZ	1:A:478:ASP:O	2.34	0.53
1:A:459:ASP:OD1	1:A:459:ASP:N	2.42	0.53
9:K:344:THR:HG1	9:K:355:THR:HG1	1.56	0.53
10:J:72:GLY:N	10:J:86:ASN:OD1	2.41	0.53
1:A:79:ASP:O	1:A:918:ARG:NH2	2.42	0.53
2:B:227:ARG:NH2	7:H:187:ASP:OD1	2.35	0.53
9:K:1478:LYS:HE3	9:K:1493:THR:HG22	1.90	0.53
1:A:927:SER:HB3	1:A:934:LEU:HG	1.91	0.53
6:G:48:GLU:HG2	6:G:85:VAL:HG22	1.91	0.53
8:I:92:GLU:OE1	8:I:95:ARG:NH1	2.41	0.53
10:J:58:LYS:HD3	10:J:97:GLU:HB3	1.91	0.53
10:J:64:VAL:HG13	10:J:171:TYR:HA	1.91	0.53
8:I:142:LEU:HD11	8:I:178:LEU:HG	1.90	0.53
9:K:296:LYS:HB3	9:K:315:PRO:HB3	1.90	0.53
10:J:254:ILE:HD12	10:J:285:LEU:HD21	1.89	0.53
6:G:78:LEU:HD23	6:G:84:PHE:HB3	1.91	0.52
6:G:107:PRO:HG2	6:G:123:VAL:HG11	1.90	0.52
1:A:439:LYS:NZ	1:A:441:VAL:O	2.43	0.52
1:A:478:ASP:OD1	1:A:478:ASP:N	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:753:VAL:O	9:K:757:ALA:N	2.36	0.52
9:K:679:PHE:HB2	9:K:681:GLU:HG2	1.91	0.52
9:K:1343:ILE:HA	9:K:1346:ILE:HG12	1.92	0.52
9:K:339:PRO:HB3	9:K:344:THR:HG22	1.91	0.52
2:B:3:LYS:N	2:B:39:GLU:OE1	2.43	0.51
9:K:1560:ILE:HG13	9:K:1604:VAL:HB	1.93	0.51
1:A:549:GLU:HG2	1:A:551:SER:H	1.74	0.51
10:J:61:ALA:N	10:J:95:ILE:O	2.42	0.51
9:K:1179:ASN:HA	9:K:1182:VAL:HB	1.92	0.51
9:K:1187:VAL:O	9:K:1191:GLU:N	2.39	0.51
9:K:1282:PHE:O	9:K:1285:GLU:HG3	2.11	0.51
9:K:1605:MET:O	9:K:1609:THR:OG1	2.28	0.51
1:A:402:PRO:HA	1:A:425:THR:HA	1.92	0.51
9:K:541:ILE:HG21	9:K:623:ARG:HG3	1.91	0.51
9:K:1626:LEU:O	9:K:1630:ASN:HB3	2.10	0.51
7:H:124:LEU:HB3	7:H:144:TYR:HB2	1.92	0.51
9:K:1208:GLN:O	9:K:1212:TYR:HB2	2.11	0.51
2:B:283:LYS:HE3	7:H:81:TRP:HA	1.92	0.51
8:I:140:SER:OG	8:I:143:SER:OG	2.27	0.51
9:K:362:MET:HG3	9:K:389:ILE:HD11	1.93	0.51
10:J:120:SER:N	10:J:123:ARG:HB3	2.25	0.50
9:K:369:LEU:HD13	9:K:385:PHE:HD2	1.75	0.50
9:K:1161:GLU:HA	9:K:1164:ILE:HG23	1.94	0.50
1:A:69:ARG:HH12	1:A:420:ARG:HH12	1.59	0.50
11:D:164:TRP:HA	11:D:167:PHE:HD2	1.76	0.50
9:K:432:GLU:O	9:K:435:LYS:HG2	2.12	0.50
1:A:124:ASP:O	1:A:147:LYS:NZ	2.44	0.50
1:A:705:GLN:HE21	1:A:756:PHE:HE1	1.59	0.50
9:K:1060:GLN:HB3	9:K:1125:MET:HG3	1.93	0.50
9:K:1573:GLN:HG2	9:K:1575:PRO:HD2	1.93	0.50
7:H:163:ASP:N	7:H:163:ASP:OD1	2.45	0.50
9:K:1162:ILE:HA	9:K:1165:PHE:HB3	1.94	0.50
11:D:50:LYS:HG3	11:D:51:GLN:HG3	1.94	0.50
1:A:182:GLY:N	1:A:284:VAL:O	2.43	0.50
1:A:219:TRP:CZ2	1:A:246:GLN:HG3	2.47	0.50
9:K:299:TYR:HA	9:K:305:ALA:HA	1.93	0.49
10:J:65:ARG:NH2	10:J:67:ASN:OD1	2.42	0.49
10:J:229:LEU:HD23	10:J:229:LEU:H	1.75	0.49
3:C:9:ASP:O	3:C:12:ILE:HG22	2.12	0.49
9:K:679:PHE:CZ	9:K:714:ASP:HB3	2.48	0.49
1:A:175:TYR:HA	1:A:190:GLY:HA2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:647:TYR:O	1:A:692:THR:OG1	2.30	0.49
9:K:171:THR:HA	9:K:198:LEU:HD11	1.94	0.49
1:A:31:ASP:HA	1:A:944:GLN:O	2.12	0.49
9:K:1586:VAL:HG23	9:K:1590:ARG:HG3	1.95	0.49
9:K:639:ASN:OD1	9:K:640:LEU:N	2.46	0.49
9:K:1217:ARG:HH12	9:K:1649:LEU:HD21	1.78	0.49
9:K:1250:LEU:O	9:K:1253:THR:OG1	2.25	0.49
6:G:57:LYS:NZ	6:G:59:GLN:OE1	2.45	0.48
9:K:241:VAL:O	9:K:244:PRO:HD2	2.13	0.48
9:K:1179:ASN:O	9:K:1183:GLY:N	2.34	0.48
1:A:212:GLN:OE1	1:A:214:ARG:NH2	2.46	0.48
1:A:687:ARG:HG2	1:A:688:LYS:H	1.78	0.48
6:G:70:ASP:HB3	6:G:73:GLU:HB2	1.94	0.48
9:K:298:CYS:HB2	9:K:313:PRO:HB3	1.94	0.48
2:B:209:GLU:OE2	2:B:212:ARG:NH2	2.46	0.48
1:A:485:LEU:HD23	1:A:488:LEU:HD21	1.96	0.48
9:K:748:PHE:O	9:K:752:ALA:N	2.36	0.48
10:J:276:HIS:CE1	10:J:328:CYS:HG	2.32	0.48
1:A:26:GLN:HA	1:A:29:LYS:HD2	1.96	0.48
9:K:1647:LYS:HG3	9:K:1650:ASP:HB2	1.96	0.48
9:K:753:VAL:HA	9:K:756:LEU:HB3	1.95	0.48
1:A:547:GLY:HA3	1:A:557:TRP:NE1	2.29	0.48
9:K:648:VAL:HA	9:K:651:ILE:HG22	1.96	0.48
5:F:55:TYR:HB2	5:F:96:TYR:CZ	2.49	0.48
9:K:147:PHE:CG	9:K:151:ASP:HB2	2.49	0.48
1:A:683:GLY:HA3	1:A:696:TRP:NE1	2.29	0.47
1:A:331:THR:HG22	1:A:380:VAL:HG21	1.95	0.47
7:H:17:HIS:CE1	7:H:26:VAL:HB	2.49	0.47
10:J:276:HIS:O	10:J:279:GLN:HG2	2.13	0.47
9:K:744:LEU:O	9:K:748:PHE:N	2.39	0.47
1:A:39:LYS:HD2	1:A:428:HIS:CE1	2.50	0.47
9:K:366:THR:HG21	9:K:1459:ARG:HE	1.78	0.47
9:K:1621:LYS:O	9:K:1625:ASN:ND2	2.46	0.47
3:C:118:VAL:HG13	3:C:119:LEU:HD22	1.95	0.47
9:K:1340:VAL:HA	9:K:1343:ILE:HG12	1.95	0.47
9:K:1345:ASP:HB2	9:K:1376:PHE:CB	2.45	0.47
9:K:1378:LEU:O	9:K:1382:MET:N	2.41	0.47
9:K:1642:LYS:H	9:K:1642:LYS:HD2	1.78	0.47
1:A:243:ARG:HH21	1:A:267:GLU:HG2	1.79	0.47
9:K:1294:LYS:O	9:K:1325:HIS:N	2.36	0.47
2:B:9:ASP:N	2:B:9:ASP:OD1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:70:LYS:HE2	3:C:74:LEU:HD11	1.96	0.47
9:K:1244:LEU:HA	9:K:1247:VAL:HG22	1.97	0.47
9:K:1605:MET:HG2	9:K:1652:VAL:HG11	1.95	0.47
10:J:108:LEU:HG	10:J:110:LYS:H	1.80	0.47
10:J:120:SER:H	10:J:123:ARG:HB3	1.80	0.47
10:J:133:GLN:O	10:J:136:ARG:NH2	2.48	0.47
8:I:91:SER:O	8:I:95:ARG:HG3	2.15	0.47
10:J:294:VAL:O	10:J:322:TYR:OH	2.32	0.47
9:K:201:ILE:HG21	9:K:243:ARG:HH21	1.80	0.46
9:K:1436:ASN:HB3	9:K:1439:THR:HG21	1.97	0.46
1:A:188:ALA:HB3	1:A:200:VAL:HG23	1.96	0.46
9:K:1337:LEU:O	9:K:1340:VAL:HG12	2.15	0.46
10:J:246:SER:N	10:J:249:GLU:OE2	2.42	0.46
10:J:360:THR:HG23	10:J:361:HIS:ND1	2.30	0.46
9:K:1565:VAL:HA	9:K:1569:LEU:HD13	1.96	0.46
1:A:420:ARG:HG2	1:A:434:GLN:HA	1.96	0.46
9:K:707:ASP:OD2	9:K:710:SER:OG	2.31	0.46
5:F:49:LEU:O	5:F:52:PHE:HB2	2.15	0.46
9:K:144:TYR:HD1	9:K:159:LEU:HD23	1.81	0.46
1:A:812:GLU:OE2	1:A:827:ARG:NH1	2.49	0.46
9:K:111:ASN:HB2	9:K:115:ARG:HD2	1.98	0.46
9:K:1434:ALA:HB2	9:K:1480:ALA:H	1.80	0.46
1:A:469:LEU:HA	1:A:472:GLU:HG2	1.98	0.46
1:A:549:GLU:OE1	1:A:552:SER:OG	2.29	0.45
1:A:565:LYS:HA	1:A:565:LYS:HD3	1.67	0.45
3:C:32:HIS:NE2	3:C:187:LEU:HD21	2.32	0.45
5:F:72:ARG:HG3	5:F:73:ARG:HD3	1.99	0.45
8:I:151:ASP:OD1	8:I:152:VAL:N	2.47	0.45
9:K:1532:ARG:HH12	9:K:1540:HIS:HB2	1.81	0.45
10:J:360:THR:HG23	10:J:361:HIS:HD1	1.81	0.45
9:K:280:ILE:O	9:K:284:ILE:HG12	2.17	0.45
9:K:440:TRP:CD1	10:J:342:LEU:HD12	2.51	0.45
10:J:65:ARG:HH12	10:J:67:ASN:HB3	1.81	0.45
7:H:29:LEU:HG	7:H:60:LEU:HD11	1.97	0.45
7:H:29:LEU:HD11	7:H:75:LEU:HD23	1.97	0.45
7:H:148:GLU:HB2	7:H:149:ASN:H	1.62	0.45
8:I:69:ARG:HH22	8:I:97:ARG:HH12	1.64	0.45
9:K:1413:LEU:HA	9:K:1416:VAL:HG22	1.97	0.45
9:K:1552:TYR:O	9:K:1554:PRO:HD3	2.15	0.45
2:B:20:ARG:O	2:B:24:GLU:HG2	2.17	0.45
10:J:250:VAL:O	10:J:254:ILE:HG12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:VAL:HG13	1:A:912:TYR:CZ	2.51	0.45
1:A:921:GLY:HA3	1:A:938:TYR:CZ	2.51	0.45
6:G:45:PHE:CD1	6:G:112:ILE:HD11	2.52	0.45
9:K:325:GLN:HG3	9:K:330:THR:HG21	1.98	0.45
9:K:606:VAL:HG11	9:K:615:GLY:HA3	1.98	0.45
9:K:276:LEU:O	9:K:279:ILE:HG22	2.17	0.45
1:A:153:LEU:HD22	1:A:163:TRP:CZ2	2.52	0.45
1:A:440:VAL:HG13	1:A:441:VAL:HG23	1.98	0.45
1:A:466:GLN:HA	1:A:469:LEU:HB3	1.97	0.45
3:C:32:HIS:CD2	3:C:191:ASN:HB3	2.49	0.45
10:J:45:GLU:HG3	10:J:80:VAL:HA	1.99	0.45
7:H:125:ILE:HG23	7:H:141:ILE:HG23	1.99	0.45
9:K:1181:PHE:HA	9:K:1184:PHE:HB2	1.98	0.45
9:K:1434:ALA:HB2	9:K:1479:CYS:HA	1.99	0.45
1:A:775:GLN:HE21	1:A:775:GLN:HB2	1.61	0.45
7:H:154:ARG:O	7:H:160:TYR:OH	2.29	0.45
9:K:1435:LEU:HD13	9:K:1446:ASN:HD22	1.82	0.45
9:K:1326:TYR:O	9:K:1332:ASN:ND2	2.50	0.45
10:J:124:LEU:HD13	10:J:170:PRO:HD2	1.99	0.45
10:J:96:LYS:HZ3	10:J:115:ILE:HG12	1.81	0.44
1:A:761:LEU:HB2	1:A:771:HIS:HB3	1.98	0.44
9:K:748:PHE:HA	9:K:751:ILE:HB	1.99	0.44
9:K:1654:PRO:HA	9:K:1658:ASP:HB2	1.99	0.44
9:K:1207:ARG:HG3	9:K:1208:GLN:N	2.31	0.44
10:J:55:ALA:HB1	10:J:58:LYS:HD2	1.99	0.44
11:D:15:PHE:HD1	11:D:15:PHE:HA	1.69	0.44
9:K:405:SER:HA	9:K:1531:THR:HG22	1.99	0.44
9:K:624:LEU:HD12	9:K:627:ILE:HD12	1.98	0.44
10:J:95:ILE:HD13	10:J:104:TRP:HE3	1.83	0.44
10:J:307:ARG:O	10:J:307:ARG:NH1	2.50	0.44
1:A:25:ASP:O	1:A:29:LYS:NZ	2.39	0.44
9:K:109:LEU:HA	9:K:115:ARG:HH12	1.82	0.44
9:K:358:GLN:NE2	9:K:363:GLU:O	2.51	0.44
10:J:296:SER:HB3	10:J:299:VAL:HG23	1.99	0.44
1:A:52:LYS:HE2	1:A:69:ARG:NH1	2.33	0.44
9:K:1598:LEU:HD23	9:K:1602:GLY:HA2	1.99	0.44
3:C:153:GLN:NE2	3:C:162:ASP:O	2.50	0.44
7:H:148:GLU:OE1	7:H:149:ASN:N	2.50	0.44
9:K:1250:LEU:O	9:K:1254:ILE:HG12	2.17	0.44
10:J:179:PRO:O	10:J:288:ILE:N	2.36	0.44
10:J:343:GLU:O	10:J:347:GLU:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:PRO:HA	1:A:245:LEU:HD13	2.00	0.44
9:K:1215:LYS:HD3	9:K:1641:TRP:HZ2	1.83	0.44
9:K:1425:ILE:O	9:K:1428:GLN:NE2	2.51	0.44
10:J:66:THR:O	10:J:90:LYS:N	2.51	0.44
9:K:1408:LEU:N	9:K:1409:PRO:HD2	2.33	0.43
10:J:99:TYR:HB2	10:J:105:ILE:HD11	2.00	0.43
10:J:355:VAL:HG22	10:J:358:ARG:HH21	1.83	0.43
1:A:208:GLU:OE1	1:A:208:GLU:N	2.48	0.43
9:K:185:PHE:HE2	9:K:195:TRP:HB2	1.83	0.43
1:A:206:ASP:HB3	1:A:208:GLU:OE1	2.18	0.43
1:A:686:LEU:HD11	1:A:690:LEU:HA	1.99	0.43
9:K:533:LEU:HD21	9:K:566:LEU:HD22	2.00	0.43
9:K:622:VAL:HA	9:K:625:LEU:HG	2.00	0.43
9:K:685:ARG:H	9:K:685:ARG:HD2	1.82	0.43
9:K:1612:ALA:O	9:K:1616:THR:HG23	2.18	0.43
9:K:1632:GLU:O	9:K:1636:ILE:HG12	2.18	0.43
1:A:472:GLU:HG3	1:A:473:PHE:HD1	1.84	0.43
4:E:46:VAL:HG13	5:F:44:LEU:HD21	2.00	0.43
9:K:1246:PHE:HE1	9:K:1383:ARG:HH12	1.66	0.43
3:C:139:LYS:HG3	3:C:164:SER:HB3	2.00	0.43
10:J:191:GLU:O	10:J:195:MET:HG2	2.19	0.43
9:K:620:ARG:HH22	9:K:1062:MET:HA	1.83	0.43
1:A:577:THR:OG1	1:A:578:THR:N	2.51	0.43
7:H:165:PRO:O	7:H:168:GLN:HG3	2.19	0.43
1:A:941:ASP:OD1	1:A:941:ASP:N	2.51	0.43
9:K:241:VAL:HG13	9:K:667:LEU:HB3	2.01	0.43
9:K:537:ASN:HB2	9:K:623:ARG:HH22	1.82	0.43
9:K:1432:LYS:O	9:K:1479:CYS:HB3	2.19	0.43
1:A:162:LYS:HG2	1:A:163:TRP:HD1	1.84	0.43
1:A:932:THR:HG22	1:A:948:TYR:HD1	1.84	0.43
9:K:1375:PHE:O	9:K:1379:PHE:N	2.50	0.43
10:J:52:LEU:O	10:J:56:LYS:N	2.52	0.43
10:J:188:LYS:NZ	10:J:197:GLN:OE1	2.46	0.43
8:I:101:VAL:HG13	8:I:106:GLY:HA3	2.01	0.43
9:K:126:PHE:O	9:K:130:ILE:HG12	2.19	0.43
9:K:158:ASN:O	9:K:162:VAL:HG23	2.19	0.43
9:K:397:LEU:HD13	9:K:1519:PHE:CD1	2.53	0.43
9:K:1398:LEU:O	9:K:1402:ILE:HG12	2.18	0.43
9:K:1560:ILE:H	9:K:1560:ILE:HG12	1.50	0.43
7:H:93:TYR:HA	7:H:125:ILE:O	2.19	0.42
9:K:257:VAL:O	9:K:261:ILE:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:279:ILE:HD12	9:K:279:ILE:HA	1.91	0.42
9:K:1189:PHE:O	9:K:1194:GLU:HG2	2.18	0.42
1:A:187:TRP:CD1	1:A:201:LYS:HG2	2.54	0.42
4:E:58:TYR:O	4:E:61:VAL:HG12	2.18	0.42
9:K:237:ARG:HH11	9:K:240:ARG:HH22	1.67	0.42
9:K:1546:LYS:HE2	9:K:1610:LEU:HD11	2.01	0.42
10:J:52:LEU:O	10:J:56:LYS:HG2	2.18	0.42
9:K:1370:ARG:HG3	9:K:1373:ILE:HB	2.00	0.42
1:A:186:VAL:HG23	1:A:204:VAL:HG22	2.01	0.42
1:A:257:ARG:HH11	1:A:308:GLY:HA3	1.84	0.42
5:F:11:PRO:HA	5:F:12:PRO:HD3	1.96	0.42
9:K:750:ALA:HA	9:K:753:VAL:HB	2.00	0.42
9:K:1184:PHE:HA	9:K:1187:VAL:HB	2.00	0.42
1:A:146:LEU:HD22	1:A:178:VAL:HG23	2.01	0.42
1:A:243:ARG:HH12	1:A:261:LEU:HB2	1.84	0.42
1:A:412:LYS:HD3	1:A:416:SER:HB2	2.01	0.42
9:K:378:ARG:NH2	9:K:1452:GLN:OE1	2.42	0.42
9:K:1182:VAL:HA	9:K:1185:VAL:HB	2.00	0.42
10:J:339:GLU:OE1	10:J:339:GLU:N	2.52	0.42
1:A:889:GLN:NE2	1:A:892:GLU:OE2	2.52	0.42
9:K:745:LEU:O	9:K:748:PHE:HB2	2.20	0.42
9:K:1345:ASP:HB2	9:K:1376:PHE:HB2	2.01	0.42
10:J:95:ILE:HD13	10:J:104:TRP:CE3	2.53	0.42
9:K:197:LEU:O	9:K:201:ILE:HG12	2.19	0.42
9:K:729:VAL:O	9:K:732:TYR:HB3	2.19	0.42
9:K:1381:VAL:O	9:K:1384:LEU:HB2	2.18	0.42
10:J:179:PRO:HG2	10:J:287:PRO:HB3	2.01	0.42
10:J:277:PRO:HB3	10:J:289:ILE:HD13	2.01	0.42
1:A:243:ARG:NH1	1:A:261:LEU:HB2	2.34	0.42
1:A:722:GLN:HE21	11:D:170:PRO:HB3	1.84	0.42
5:F:103:LEU:HA	5:F:103:LEU:HD12	1.73	0.42
9:K:383:ILE:H	9:K:383:ILE:HD12	1.85	0.42
9:K:753:VAL:O	9:K:756:LEU:HB3	2.20	0.42
9:K:1345:ASP:HB2	9:K:1376:PHE:CG	2.55	0.42
9:K:749:LEU:O	9:K:752:ALA:HB3	2.19	0.42
10:J:212:ILE:HD13	10:J:266:LEU:HB3	2.01	0.42
10:J:203:PHE:CZ	10:J:346:CYS:HB3	2.55	0.42
2:B:70:ASP:OD1	2:B:71:LEU:N	2.52	0.41
10:J:58:LYS:HE2	10:J:58:LYS:HB2	1.91	0.41
10:J:347:GLU:O	10:J:351:GLU:HG2	2.20	0.41
11:D:16:LYS:HB3	11:D:17:TRP:H	1.70	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:573:MET:SD	1:A:573:MET:N	2.92	0.41
3:C:12:ILE:HD11	3:C:135:PHE:CD1	2.55	0.41
8:I:71:ARG:NH1	8:I:108:TYR:OH	2.53	0.41
8:I:114:ARG:CZ	8:I:126:GLY:HA3	2.50	0.41
9:K:172:VAL:O	9:K:176:LEU:HG	2.20	0.41
9:K:627:ILE:HG23	9:K:630:ILE:HD12	2.01	0.41
10:J:307:ARG:HA	10:J:307:ARG:HD2	1.92	0.41
1:A:587:CYS:SG	1:A:606:PRO:HG3	2.60	0.41
1:A:619:LEU:HD13	1:A:623:ILE:HG13	2.02	0.41
9:K:1377:ARG:O	9:K:1380:ARG:HB2	2.19	0.41
9:K:1437:ASP:HA	9:K:1442:ASN:ND2	2.34	0.41
9:K:1621:LYS:HZ3	9:K:1625:ASN:HA	1.85	0.41
10:J:111:GLU:HA	10:J:359:ALA:HA	2.03	0.41
9:K:1201:GLU:CD	9:K:1207:ARG:HE	2.24	0.41
9:K:1332:ASN:HA	9:K:1335:ASP:OD2	2.20	0.41
10:J:211:ARG:NH2	10:J:354:GLU:OE1	2.50	0.41
2:B:283:LYS:NZ	7:H:84:ASP:HB2	2.35	0.41
3:C:144:LEU:HB3	3:C:148:PHE:CD1	2.56	0.41
9:K:261:ILE:HG23	9:K:746:ASN:ND2	2.36	0.41
9:K:357:PHE:O	9:K:360:ILE:HG22	2.20	0.41
9:K:747:VAL:O	9:K:750:ALA:HB3	2.20	0.41
9:K:1295:PRO:HA	9:K:1326:TYR:HB2	2.02	0.41
9:K:1477:LYS:HE3	9:K:1477:LYS:HB3	1.87	0.41
1:A:956:LEU:HD21	1:A:960:TYR:CD2	2.56	0.41
2:B:64:LEU:HD23	2:B:64:LEU:HA	1.92	0.41
8:I:166:GLY:O	8:I:169:ARG:NH1	2.49	0.41
9:K:339:PRO:HB2	9:K:343:ILE:H	1.85	0.41
9:K:372:VAL:O	9:K:376:VAL:HG12	2.21	0.41
9:K:1120:ASN:OD1	9:K:1121:VAL:N	2.53	0.41
9:K:1597:PRO:HB2	9:K:1603:THR:O	2.21	0.41
1:A:154:HIS:CE1	1:A:161:LEU:HD13	2.56	0.41
1:A:889:GLN:O	1:A:892:GLU:HG3	2.20	0.41
2:B:199:LYS:HD3	2:B:199:LYS:HA	1.92	0.41
9:K:408:PHE:CD2	9:K:1531:THR:HB	2.56	0.41
9:K:518:ARG:HA	9:K:577:SER:HB2	2.03	0.41
9:K:1330:ALA:O	9:K:1333:THR:OG1	2.30	0.41
10:J:73:VAL:N	10:J:86:ASN:OD1	2.53	0.41
10:J:337:LEU:HD23	10:J:345:ALA:HB1	2.02	0.41
7:H:135:ASP:OD1	7:H:135:ASP:N	2.54	0.41
8:I:143:SER:HA	8:I:182:ASN:O	2.21	0.41
9:K:285:ILE:HD13	9:K:1378:LEU:HD22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:619:LEU:O	9:K:623:ARG:HG2	2.20	0.41
9:K:1022:VAL:O	9:K:1025:PRO:HD2	2.21	0.41
9:K:1408:LEU:HD11	9:K:1522:VAL:HG12	2.03	0.41
9:K:1446:ASN:HD21	9:K:1448:GLN:NE2	2.19	0.41
9:K:1549:TRP:CZ3	9:K:1569:LEU:HD23	2.56	0.41
1:A:439:LYS:HA	1:A:439:LYS:HD2	1.92	0.40
3:C:115:VAL:O	3:C:119:LEU:HB2	2.20	0.40
6:G:69:VAL:HG22	6:G:96:VAL:HG22	2.03	0.40
9:K:167:LEU:HD11	9:K:202:ILE:HA	2.02	0.40
9:K:274:LEU:HA	9:K:277:PHE:HD2	1.87	0.40
9:K:295:HIS:O	9:K:335:GLY:N	2.44	0.40
1:A:573:MET:HB2	1:A:628:LEU:HD22	2.02	0.40
2:B:105:ASP:N	2:B:105:ASP:OD1	2.55	0.40
2:B:136:LYS:HB3	2:B:139:GLU:OE1	2.21	0.40
9:K:1140:LEU:HD22	9:K:1143:ARG:HH22	1.85	0.40
7:H:77:LEU:HD23	7:H:77:LEU:HA	1.91	0.40
9:K:550:ASN:ND2	9:K:554:GLU:OE2	2.55	0.40
9:K:1391:GLY:O	9:K:1394:ILE:HG12	2.22	0.40
9:K:1653:VAL:HG12	9:K:1658:ASP:H	1.87	0.40
10:J:79:PRO:HD3	10:J:103:TRP:CD1	2.57	0.40
2:B:188:ASN:HB3	2:B:191:TYR:HD2	1.86	0.40
9:K:533:LEU:HD11	9:K:566:LEU:HD13	2.02	0.40
10:J:203:PHE:HD2	10:J:204:LEU:HD22	1.87	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	930/973 (96%)	886 (95%)	44 (5%)	0	100	100
2	B	289/291 (99%)	282 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	212/258 (82%)	199 (94%)	13 (6%)	0	100	100
4	E	99/101 (98%)	98 (99%)	1 (1%)	0	100	100
5	F	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
6	G	114/116 (98%)	108 (95%)	6 (5%)	0	100	100
7	H	189/208 (91%)	177 (94%)	12 (6%)	0	100	100
8	I	146/157 (93%)	145 (99%)	1 (1%)	0	100	100
9	K	1102/1550 (71%)	1014 (92%)	88 (8%)	0	100	100
10	J	292/324 (90%)	287 (98%)	5 (2%)	0	100	100
11	D	39/170 (23%)	31 (80%)	7 (18%)	1 (3%)	4	22
All	All	3510/4248 (83%)	3321 (95%)	188 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	D	45	VAL

### 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	824/858 (96%)	806 (98%)	18 (2%)	47	68
2	B	250/250 (100%)	246 (98%)	4 (2%)	58	75
3	C	198/234 (85%)	195 (98%)	3 (2%)	60	76
4	E	85/85 (100%)	84 (99%)	1 (1%)	67	80
5	F	79/79 (100%)	77 (98%)	2 (2%)	42	65
6	G	102/102 (100%)	98 (96%)	4 (4%)	27	53
7	H	169/180 (94%)	164 (97%)	5 (3%)	36	61
8	I	127/131 (97%)	123 (97%)	4 (3%)	35	60
9	K	983/1367 (72%)	955 (97%)	28 (3%)	38	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	J	262/287 (91%)	261 (100%)	1 (0%)	89	93
11	D	37/141 (26%)	33 (89%)	4 (11%)	5	20
All	All	3116/3714 (84%)	3042 (98%)	74 (2%)	45	66

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	THR
1	A	62	VAL
1	A	197	VAL
1	A	211	GLN
1	A	327	THR
1	A	407	ILE
1	A	442	LEU
1	A	463	THR
1	A	483	MET
1	A	504	LYS
1	A	573	MET
1	A	775	GLN
1	A	794	GLN
1	A	814	THR
1	A	852	THR
1	A	892	GLU
1	A	912	TYR
1	A	948	TYR
2	B	238	HIS
2	B	270	PHE
2	B	280	TYR
2	B	291	THR
3	C	38	LEU
3	C	60	VAL
3	C	135	PHE
4	E	32	ARG
5	F	73	ARG
5	F	103	LEU
6	G	60	ASP
6	G	67	VAL
6	G	72	GLU
6	G	112	ILE
7	H	133	THR
7	H	148	GLU

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Mol	Chain	Res	Type
7	H	158	HIS
7	H	184	VAL
7	H	187	ASP
8	I	58	HIS
8	I	115	ARG
8	I	135	CYS
8	I	176	VAL
9	K	127	GLU
9	K	137	ASN
9	K	143	ILE
9	K	248	VAL
9	K	332	CYS
9	K	346	PHE
9	K	354	LEU
9	K	404	LEU
9	K	418	ARG
9	K	518	ARG
9	K	535	PHE
9	K	597	CYS
9	K	664	ILE
9	K	665	PHE
9	K	685	ARG
9	K	755	ASN
9	K	1164	ILE
9	K	1242	GLU
9	K	1245	MET
9	K	1340	VAL
9	K	1381	VAL
9	K	1435	LEU
9	K	1503	TYR
9	K	1518	LEU
9	K	1527	PHE
9	K	1560	ILE
9	K	1585	ARG
9	K	1609	THR
10	J	223	LEU
11	D	15	PHE
11	D	43	TYR
11	D	45	VAL
11	D	50	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	222	HIS
1	A	262	GLN
1	A	273	GLN
1	A	280	GLN
1	A	705	GLN
1	A	952	GLN
3	C	195	GLN
4	E	19	HIS
4	E	48	GLN
7	H	199	ASN
8	I	188	GLN
9	K	158	ASN
9	K	325	GLN
9	K	358	GLN
9	K	429	GLN
9	K	443	GLN
9	K	581	GLN
9	K	671	GLN
9	K	701	GLN
9	K	1199	ASN
9	K	1206	GLN
9	K	1259	GLN
9	K	1445	ASN
9	K	1446	ASN
9	K	1517	ASN
9	K	1599	ASN
10	J	47	GLN
10	J	50	GLN
10	J	251	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 ⓘ

6 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	$\# Z  > 2$
12	NAG	L	1	1,12	14,14,15	0.24	0	17,19,21	0.41	0
12	NAG	L	2	12	14,14,15	0.24	0	17,19,21	0.45	0
12	NAG	M	1	1,12	14,14,15	0.23	0	17,19,21	0.43	0
12	NAG	M	2	12	14,14,15	0.25	0	17,19,21	0.43	0
12	NAG	N	1	8,12	14,14,15	0.80	1 (7%)	17,19,21	1.43	3 (17%)
12	NAG	N	2	12	14,14,15	0.22	0	17,19,21	0.51	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	NAG	L	1	1,12	-	0/6/23/26	0/1/1/1
12	NAG	L	2	12	-	2/6/23/26	0/1/1/1
12	NAG	M	1	1,12	-	2/6/23/26	0/1/1/1
12	NAG	M	2	12	-	0/6/23/26	0/1/1/1
12	NAG	N	1	8,12	-	6/6/23/26	0/1/1/1
12	NAG	N	2	12	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	N	1	NAG	C1-C2	2.66	1.56	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	N	1	NAG	C2-N2-C7	4.39	128.78	122.90
12	N	1	NAG	C1-O5-C5	2.22	115.16	112.19
12	N	1	NAG	C1-C2-N2	2.15	113.82	110.43

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	N	1	NAG	C4-C5-C6-O6
12	L	2	NAG	O5-C5-C6-O6
12	N	1	NAG	O5-C5-C6-O6
12	N	1	NAG	C8-C7-N2-C2
12	N	1	NAG	O7-C7-N2-C2
12	L	2	NAG	C4-C5-C6-O6
12	M	1	NAG	O5-C5-C6-O6
12	N	2	NAG	C4-C5-C6-O6
12	M	1	NAG	C4-C5-C6-O6
12	N	1	NAG	C1-C2-N2-C7
12	N	1	NAG	C3-C2-N2-C7
12	N	2	NAG	O5-C5-C6-O6

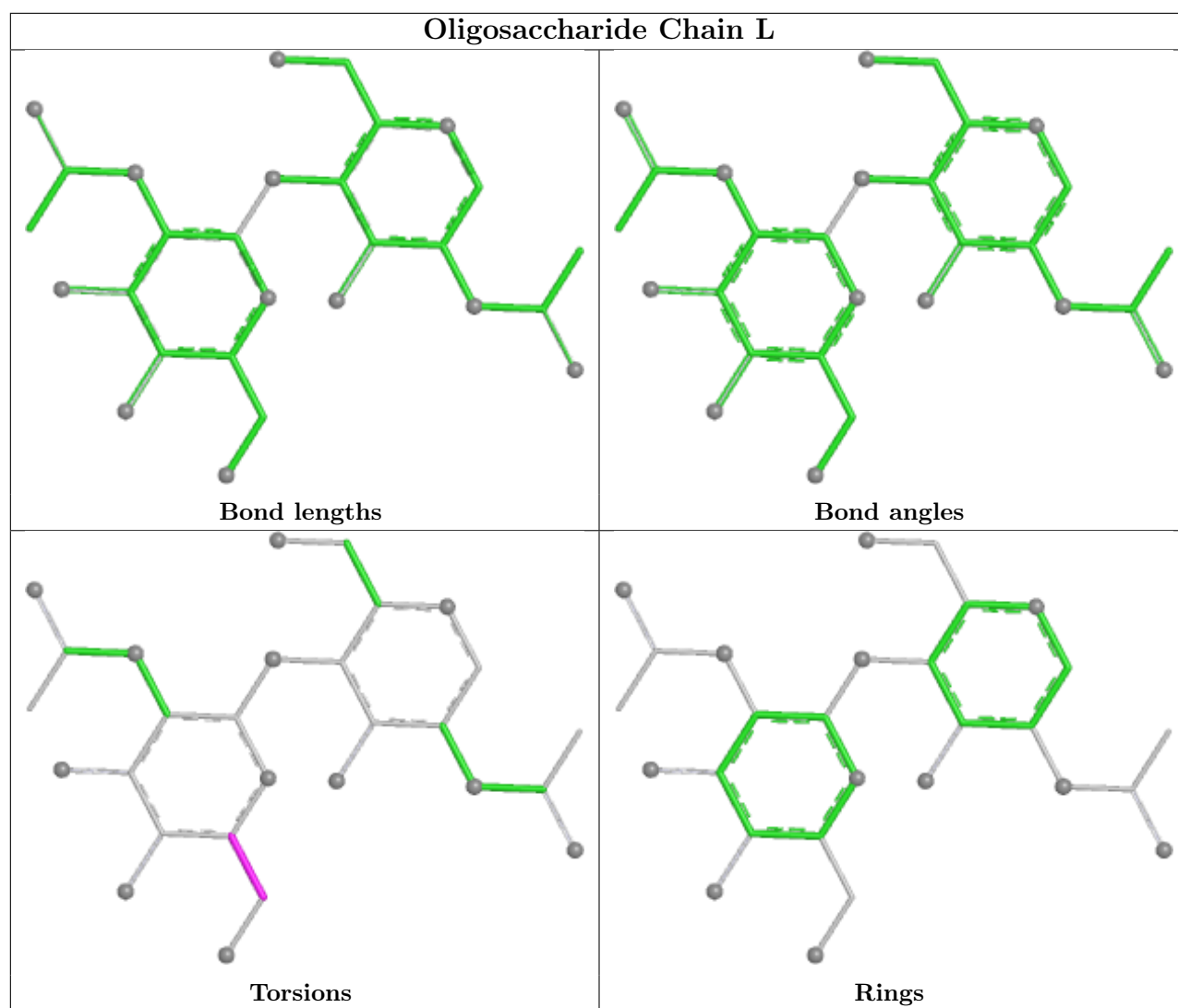
There are no ring outliers.

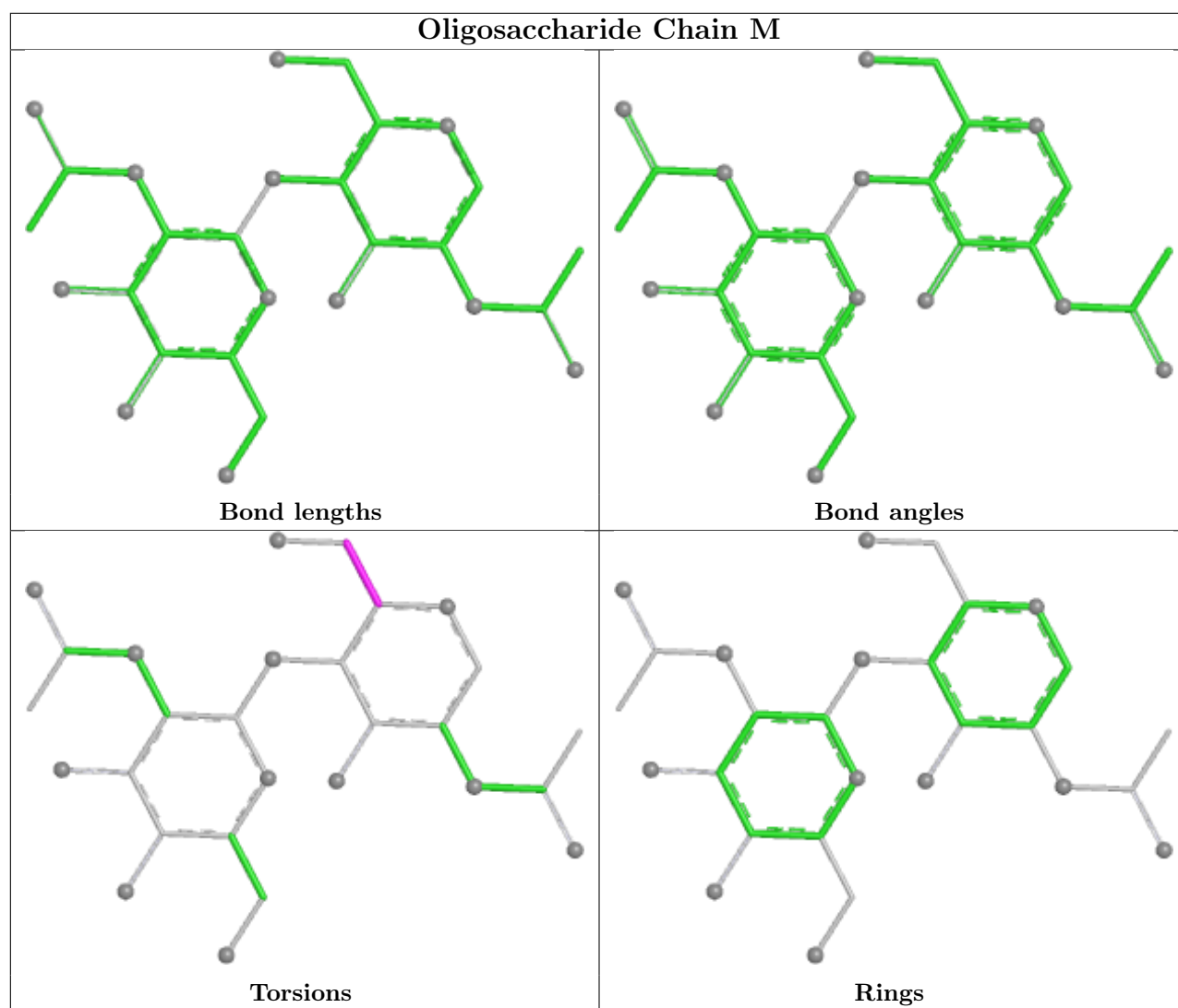
1 monomer is involved in 1 short contact:

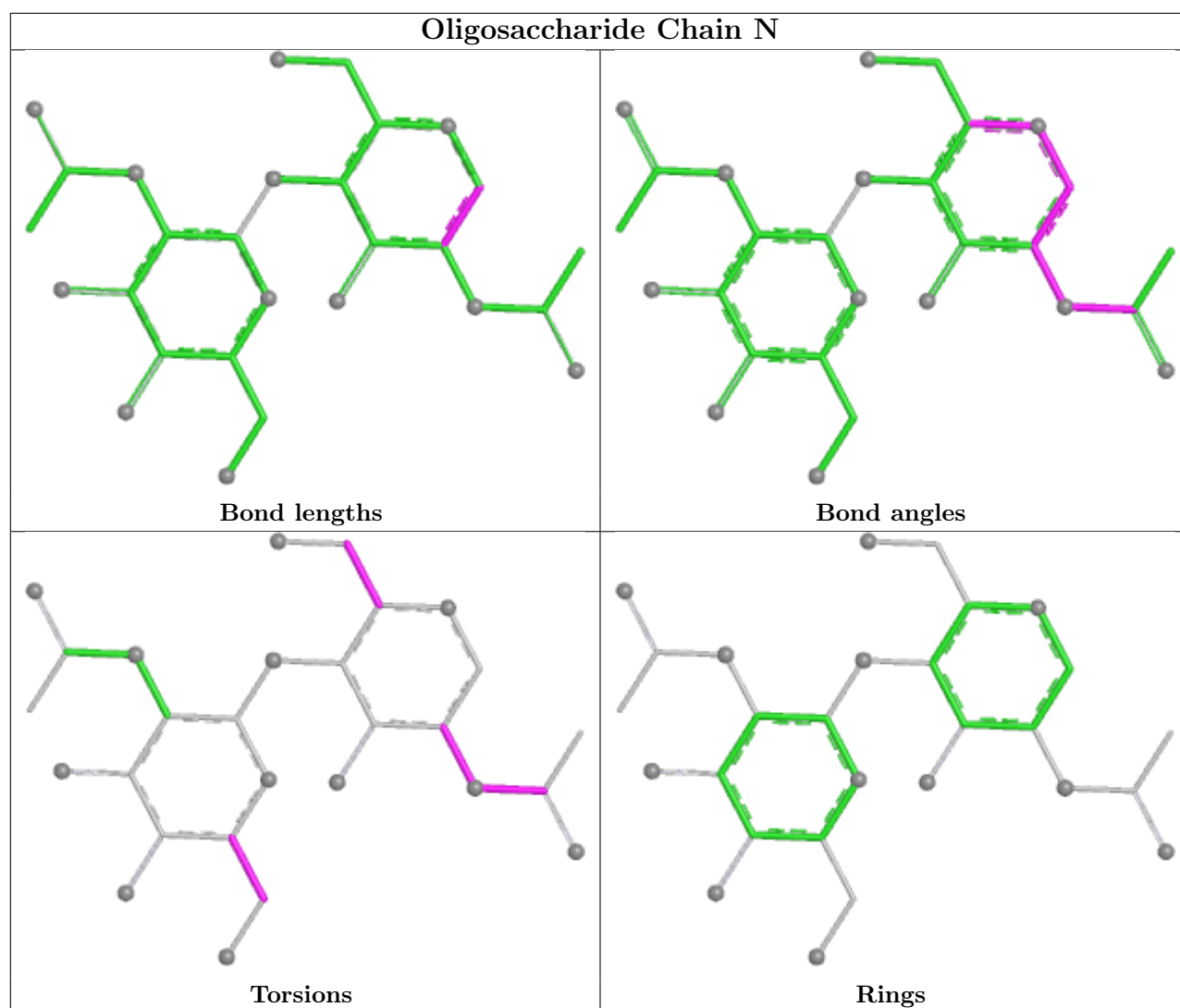
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	N	1	NAG	1	0

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](#)

2 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	$\# Z  > 2$
14	9Z9	K	1701	-	44,44,44	1.19	4 (9%)	64,68,68	1.05	5 (7%)
13	NAG	A	1001	1	14,14,15	0.27	0	17,19,21	0.40	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	9Z9	K	1701	-	-	4/12/100/100	0/6/6/6
13	NAG	A	1001	1	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	K	1701	9Z9	C76-C73	2.81	1.56	1.51
14	K	1701	9Z9	C79-C78	2.19	1.55	1.51
14	K	1701	9Z9	O80-C73	2.16	1.45	1.42
14	K	1701	9Z9	C09-C08	2.11	1.57	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	K	1701	9Z9	C77-C78-C79	2.85	112.05	108.59
14	K	1701	9Z9	O80-C79-C78	-2.78	108.60	112.17
14	K	1701	9Z9	C17-C16-C13	2.61	115.30	111.45
14	K	1701	9Z9	C19-C18-C17	2.39	114.23	110.33
14	K	1701	9Z9	C18-C17-C16	2.26	114.11	110.97

There are no chirality outliers.

All (4) torsion outliers are listed below:

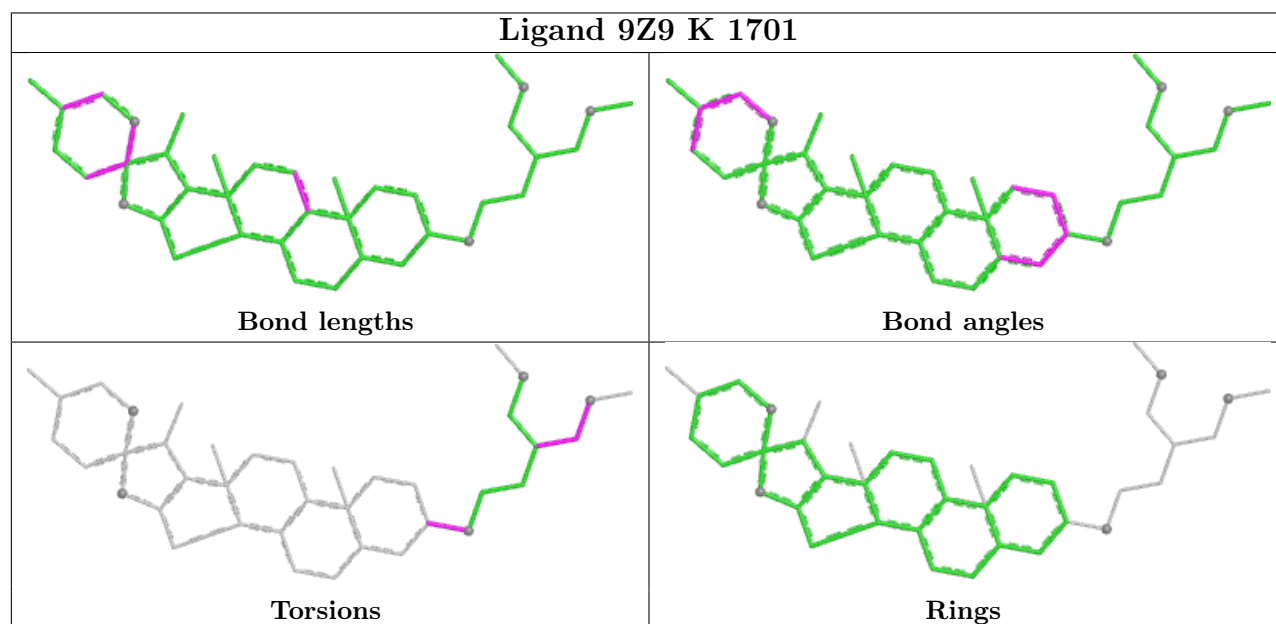
Mol	Chain	Res	Type	Atoms
14	K	1701	9Z9	C16-C17-O20-C21
14	K	1701	9Z9	C18-C17-O20-C21
14	K	1701	9Z9	C23-C24-O25-C26
14	K	1701	9Z9	C22-C23-C24-O25

There are no ring outliers.

No monomer is involved in short contacts.

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.

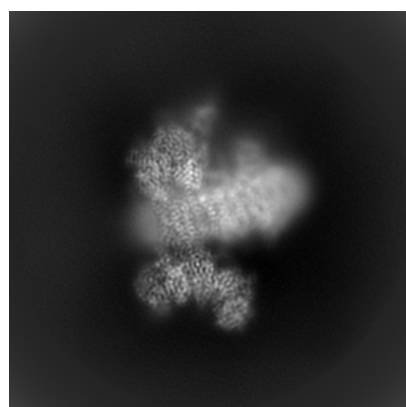
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-28376. These allow visual inspection of the internal detail of the map and identification of artifacts.

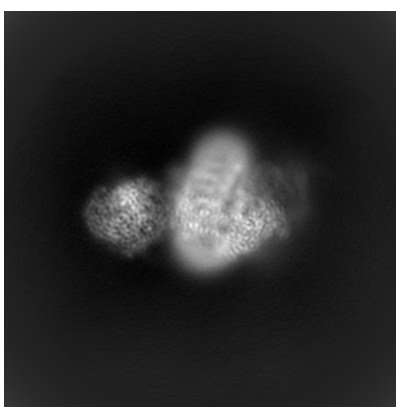
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

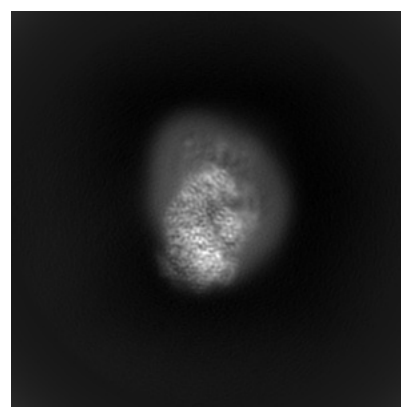
#### 6.1.1 Primary map



X



Y

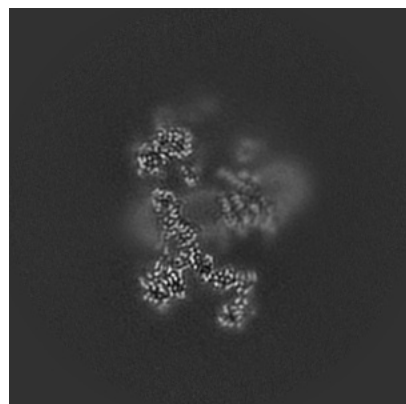


Z

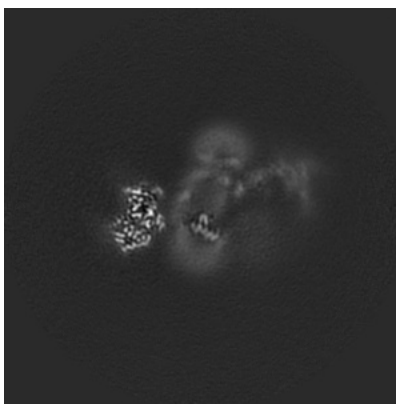
The images above show the map projected in three orthogonal directions.

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

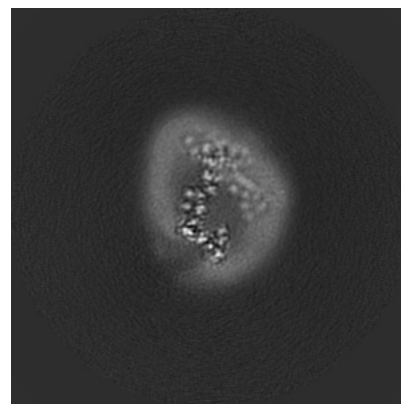
#### 6.2.1 Primary map



X Index: 220



Y Index: 220

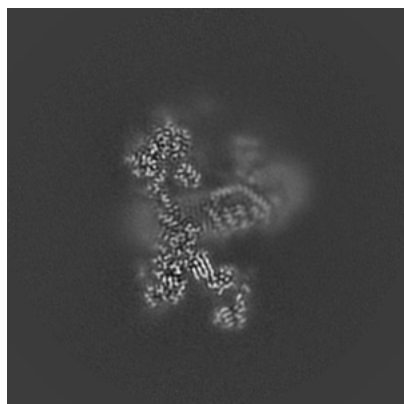


Z Index: 220

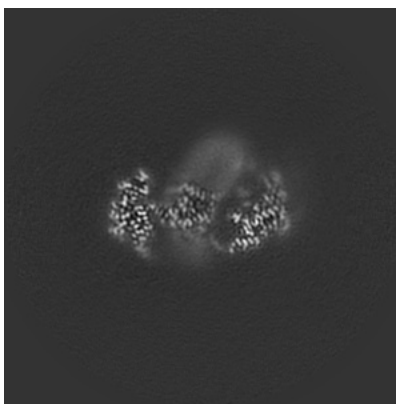
The images above show central slices of the map in three orthogonal directions.

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

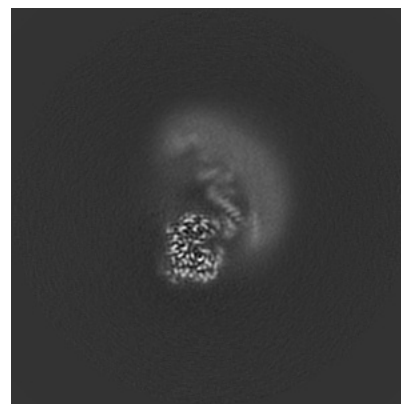
### 6.3.1 Primary map



X Index: 213



Y Index: 187

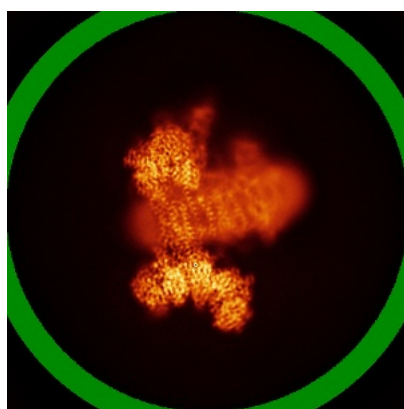


Z Index: 259

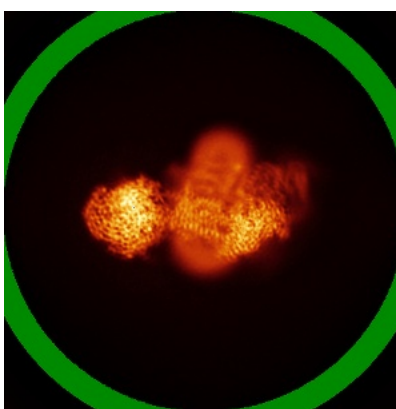
The images above show the largest variance slices of the map in three orthogonal directions.

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

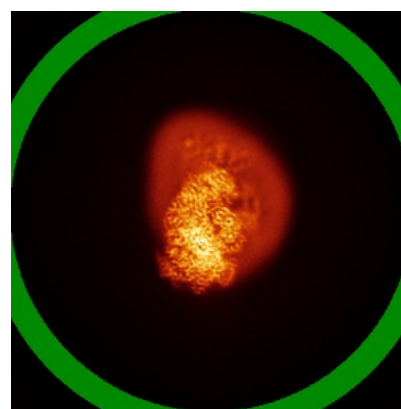
### 6.4.1 Primary map



X



Y

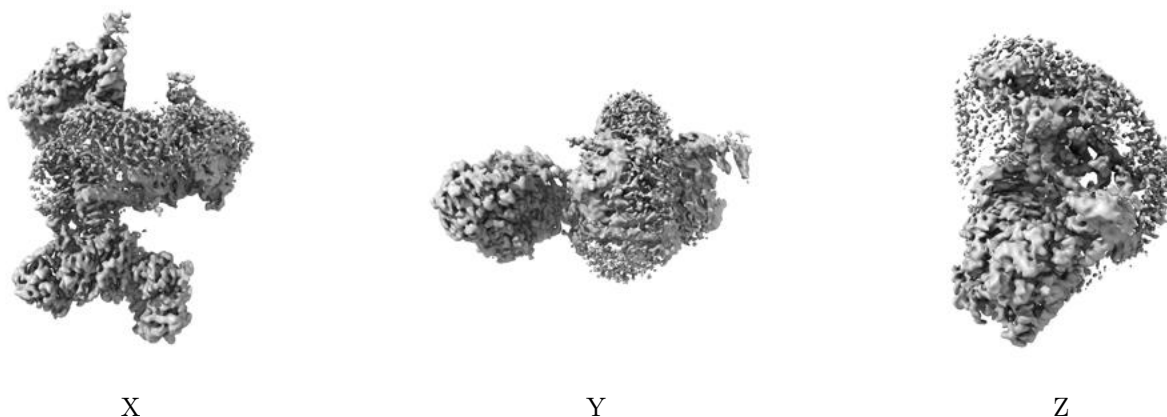


Z

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 5.93. 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](#)

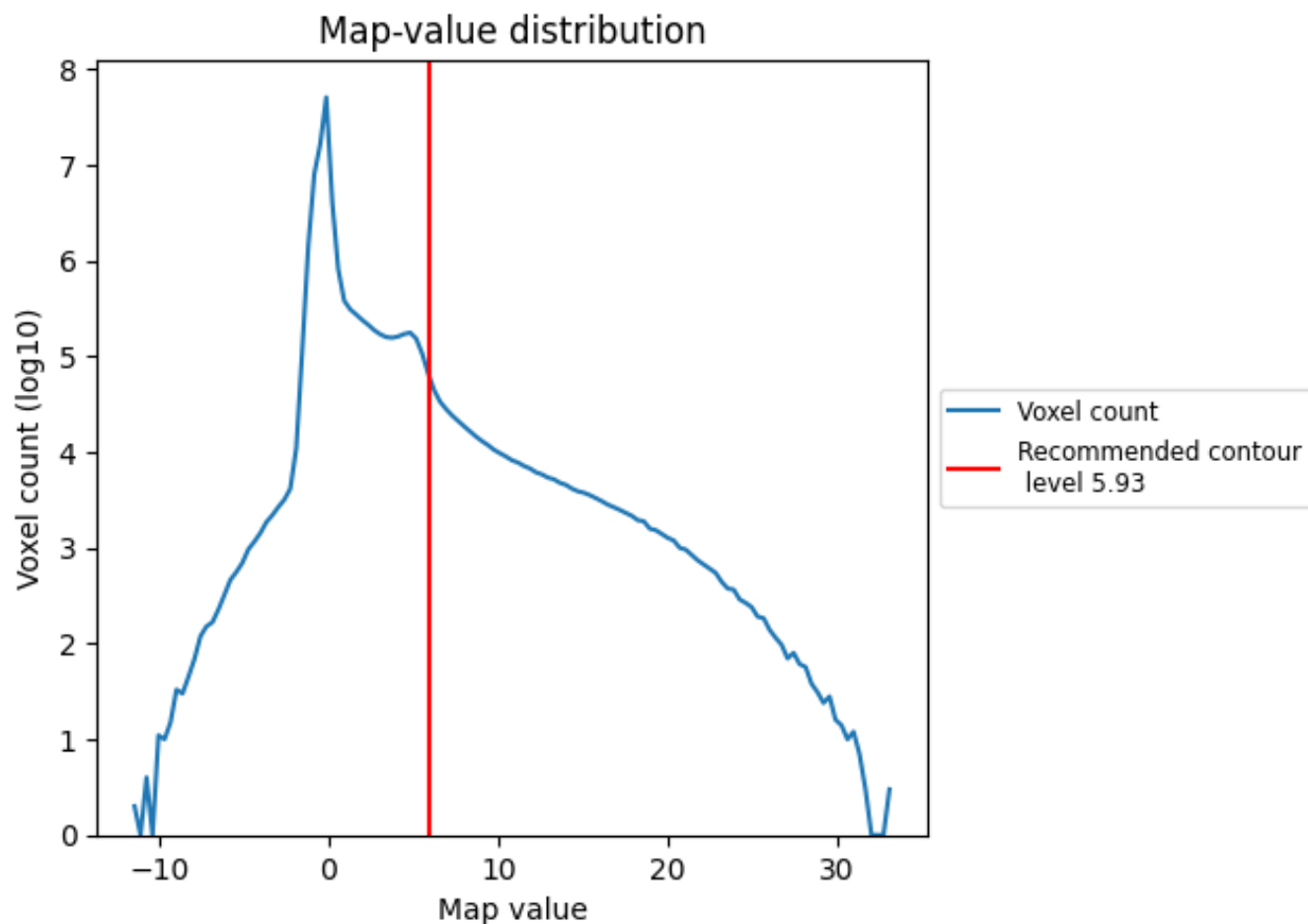
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

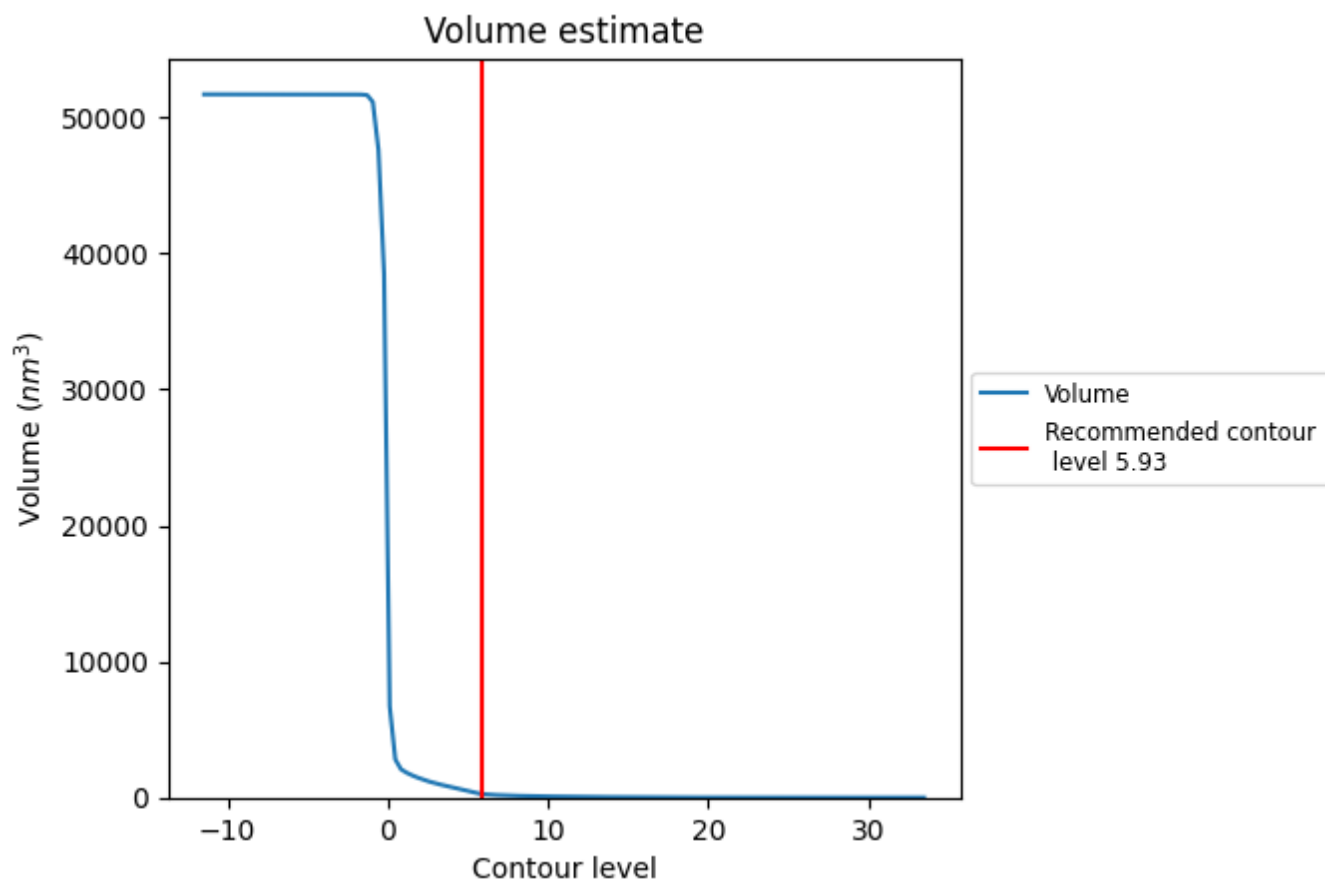
This section contains the results of statistical analysis of the map.

### 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.

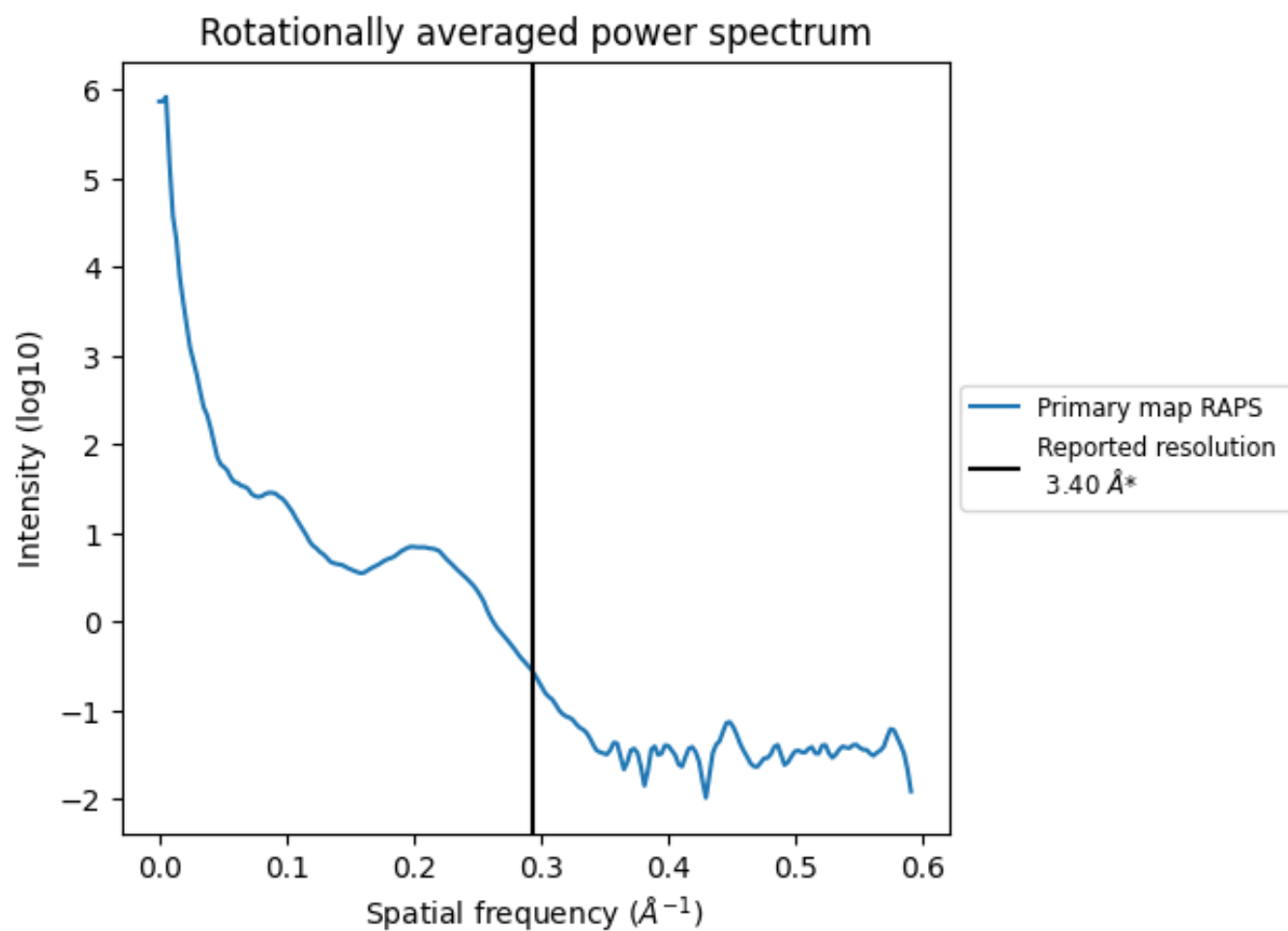
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 260 nm<sup>3</sup>; this corresponds to an approximate mass of 235 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 0.294 Å<sup>-1</sup>

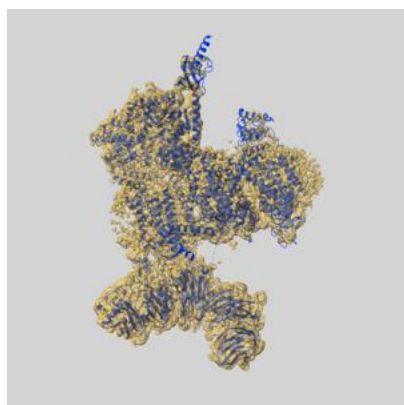
## 8 Fourier-Shell correlation ⓘ

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

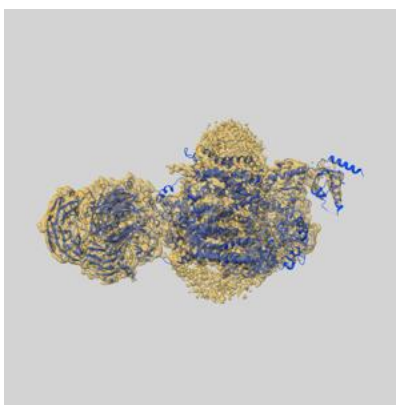
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-28376 and PDB model 8EOI. Per-residue inclusion information can be found in section [3](#) on page [8](#).

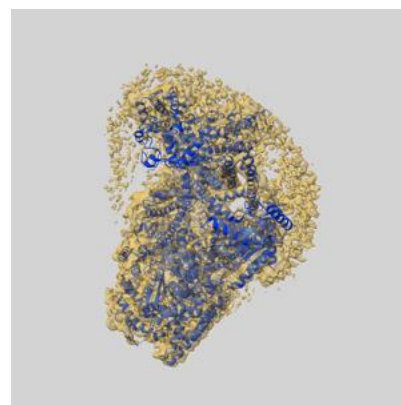
### 9.1 Map-model overlay [i](#)



X



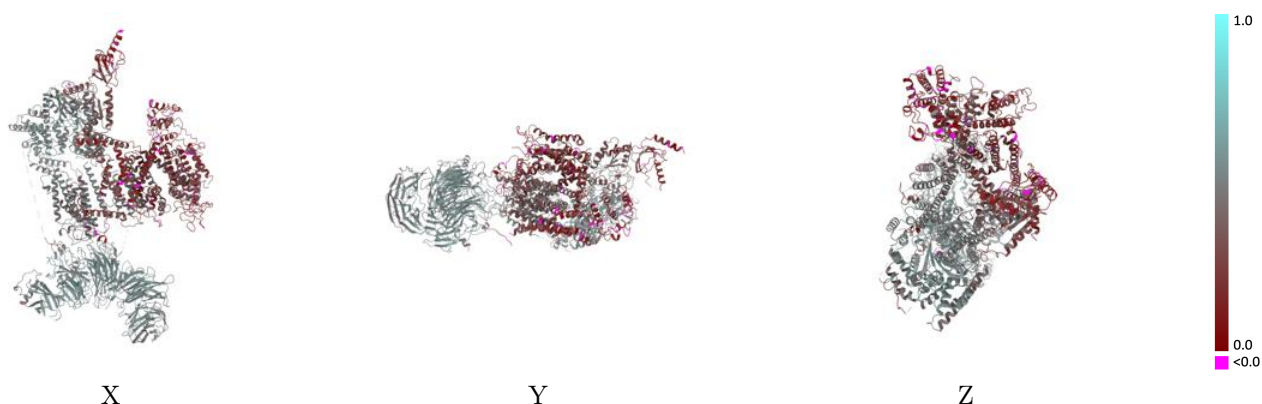
Y



Z

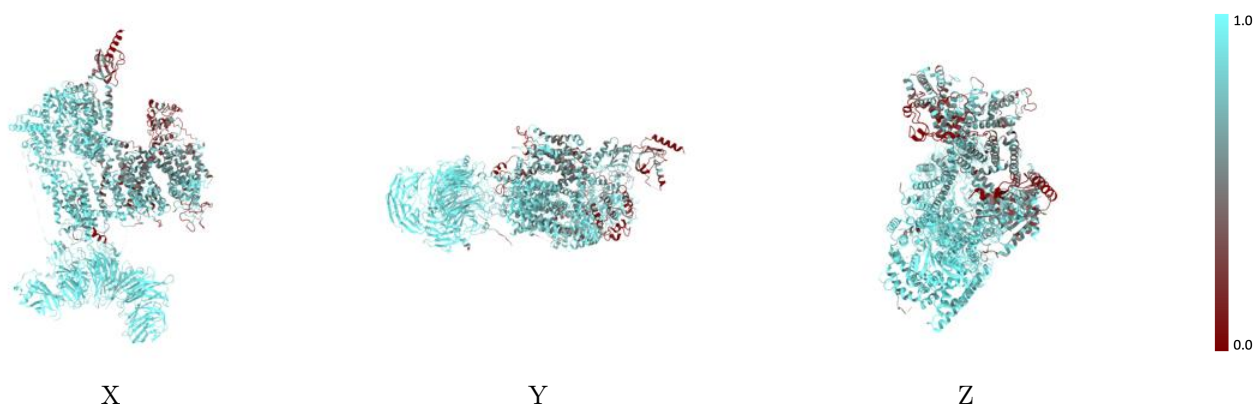
The images above show the 3D surface view of the map at the recommended contour level 5.93 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



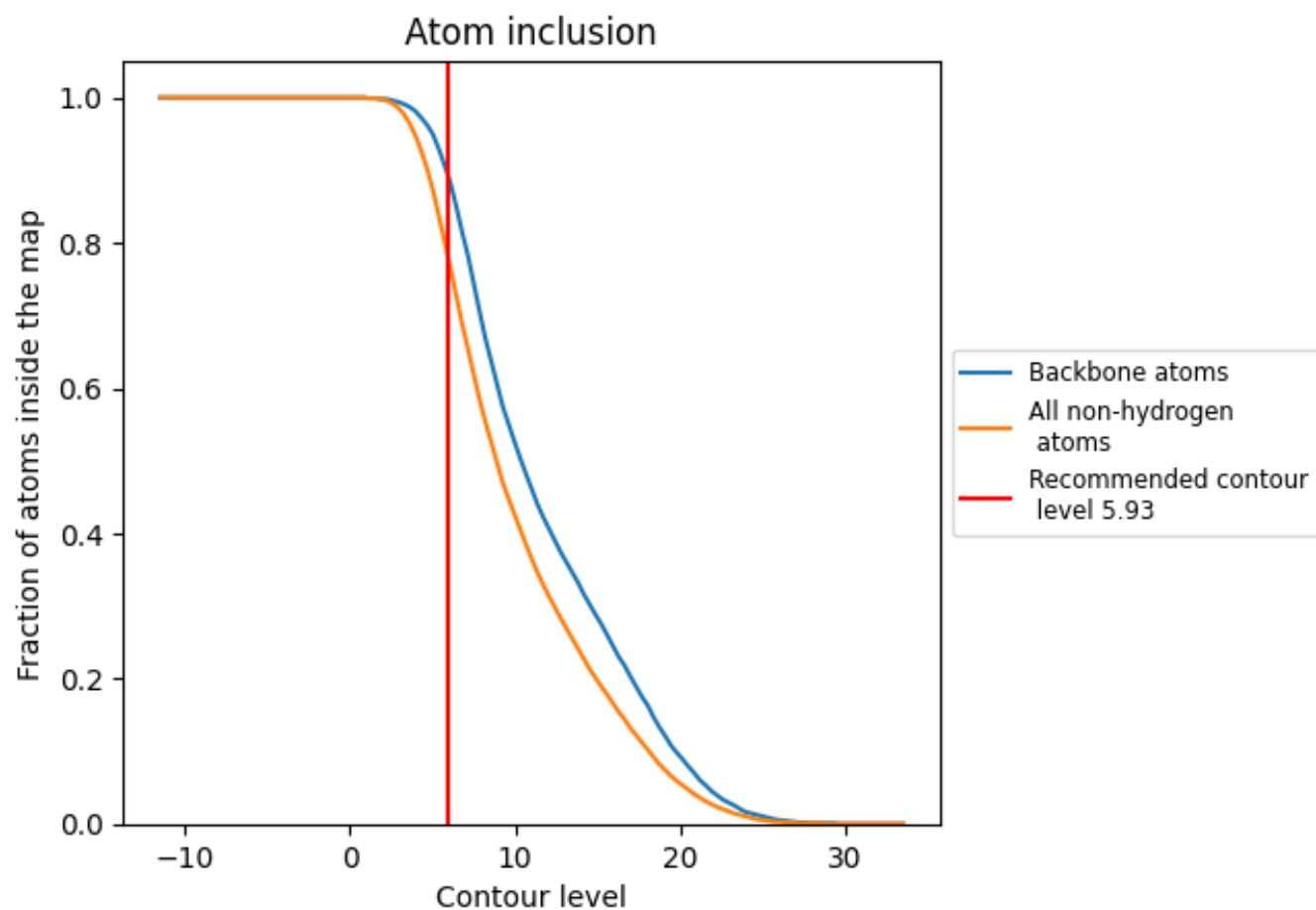
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (5.93).

## 9.4 Atom inclusion ⓘ



At the recommended contour level, 89% of all backbone atoms, 78% 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 (5.93) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7820	<div></div> 0.4110
A	<div></div> 0.9350	<div></div> 0.5170
B	<div></div> 0.9220	<div></div> 0.5170
C	<div></div> 0.8700	<div></div> 0.4660
D	<div></div> 0.8590	<div></div> 0.4460
E	<div></div> 0.8650	<div></div> 0.4790
F	<div></div> 0.9170	<div></div> 0.4890
G	<div></div> 0.9190	<div></div> 0.5110
H	<div></div> 0.9400	<div></div> 0.5150
I	<div></div> 0.9550	<div></div> 0.5060
J	<div></div> 0.5200	<div></div> 0.3060
K	<div></div> 0.5840	<div></div> 0.2580
L	<div></div> 0.9290	<div></div> 0.5140
M	<div></div> 0.8210	<div></div> 0.4770
N	<div></div> 0.7500	<div></div> 0.4250

1.0

0.0

<0.0