



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 03:14 AM UTC

PDB ID : 8EOI / pdb_00008eoi
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

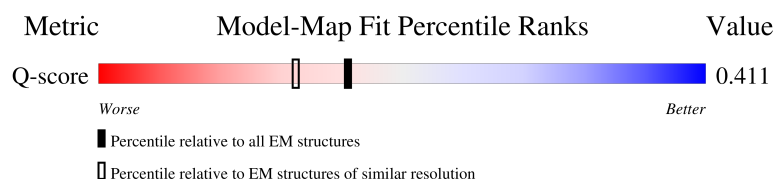
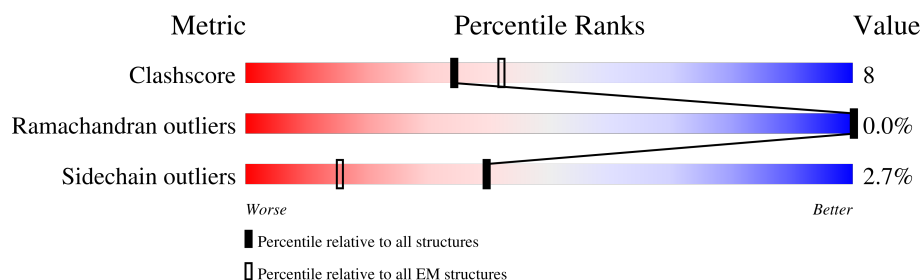
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMD 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 3.40 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

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

Mol	Chain	Length	Quality of chain
1	A	973	
2	B	291	
3	C	258	
4	E	101	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	F	100	85% 14%
6	G	116	82% 16%
7	H	208	75% 16% 7%
8	I	157	80% 16%
9	K	1550	17% 50% 21% 28%
10	J	324	29% 63% 28% 9%
11	D	170	19% 6% 74%
12	L	2	100%
12	M	2	100%
12	N	2	50% 50%

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.



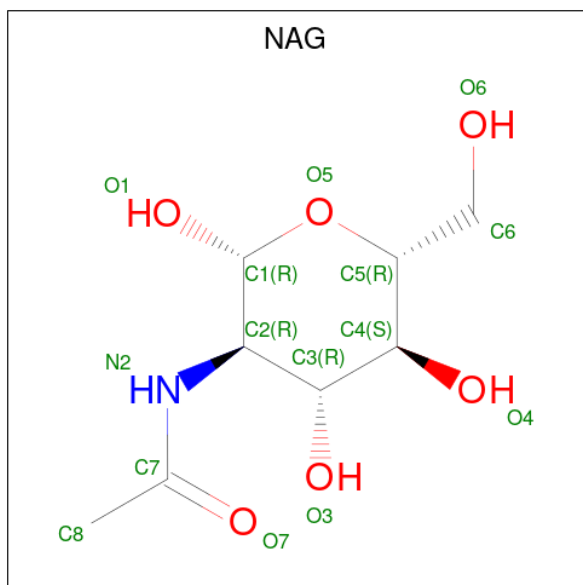
Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	2	Total	C	N	O		0	0
			28	16	2	10			
12	M	2	Total	C	N	O		0	0
			28	16	2	10			

Continued on next page...

Continued from previous page...

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

- Molecule 13 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

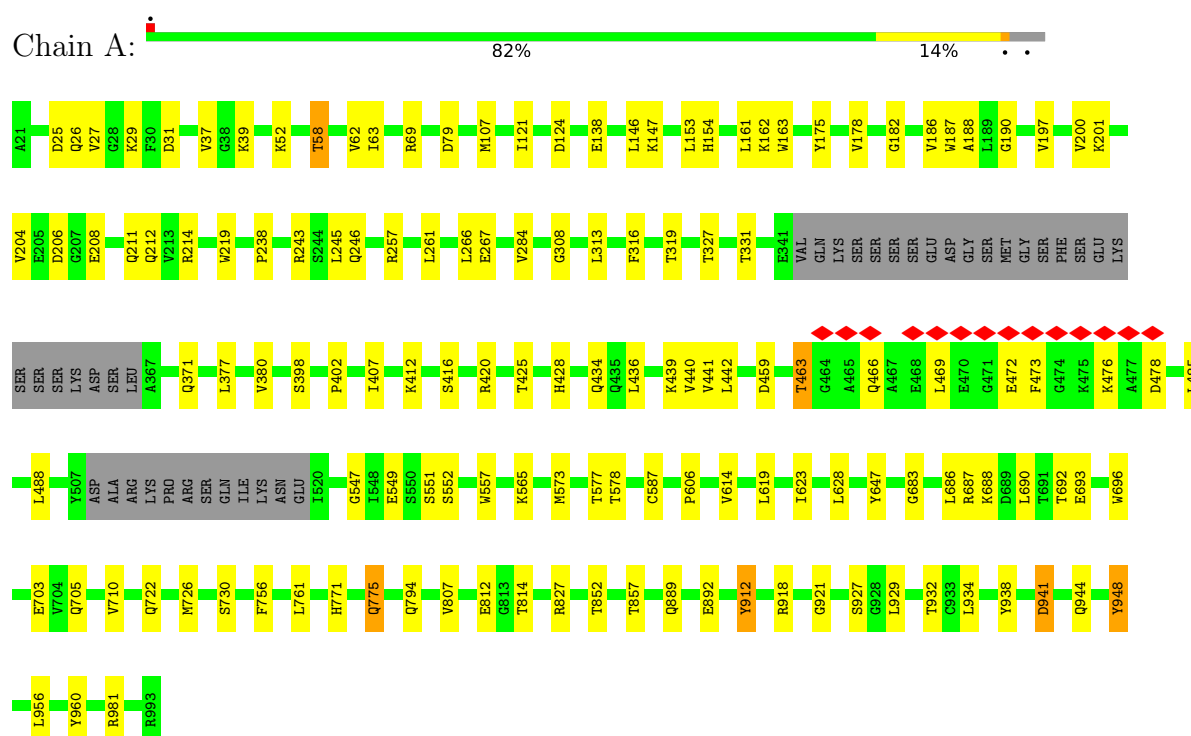
- Molecule 14 is (3beta,14beta,17beta,25R)-3-[4-methoxy-3-(methoxymethyl)butoxy]spirost-5-en (CCD ID: 9Z9) (formula: $C_{34}H_{56}O_5$).



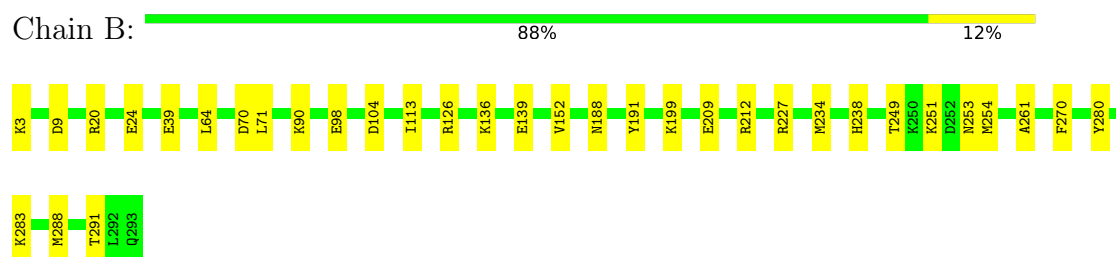
3 Residue-property plots

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

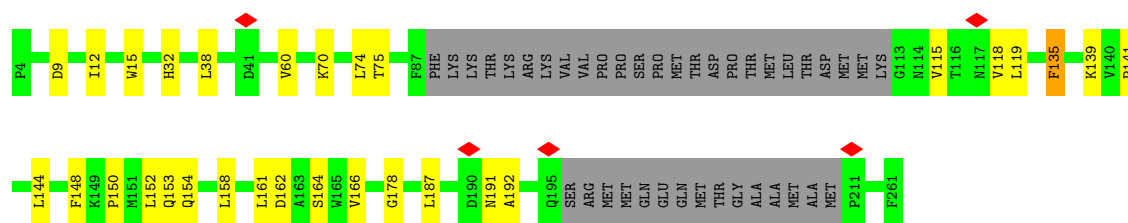


• Molecule 2: ER membrane protein complex subunit 2



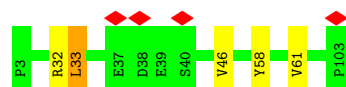
• Molecule 3: ER membrane protein complex subunit 3





- Molecule 4: ER membrane protein complex subunit 5

Chain E: 95%



- Molecule 5: ER membrane protein complex subunit 6

Chain F: 85%



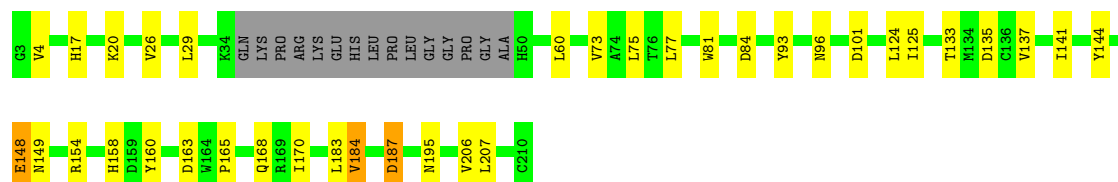
- Molecule 6: ER membrane protein complex subunit 7

Chain G: 82%



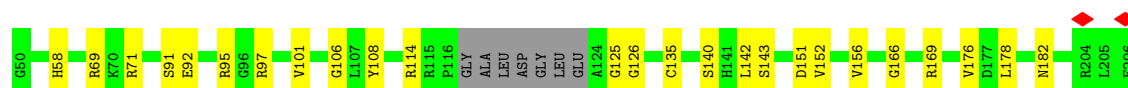
- Molecule 7: ER membrane protein complex subunit 8

Chain H: 75%



- Molecule 8: ER membrane protein complex subunit 10

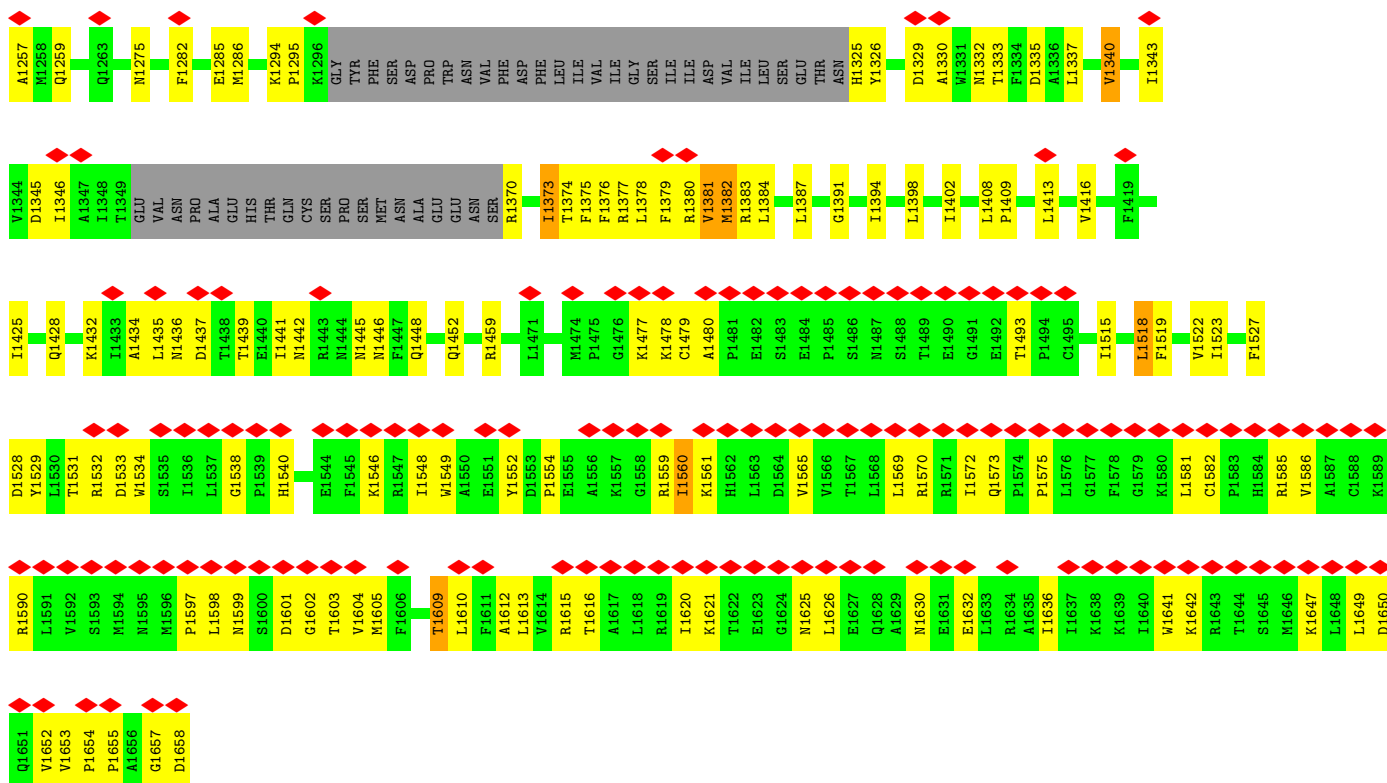
Chain I: 80%



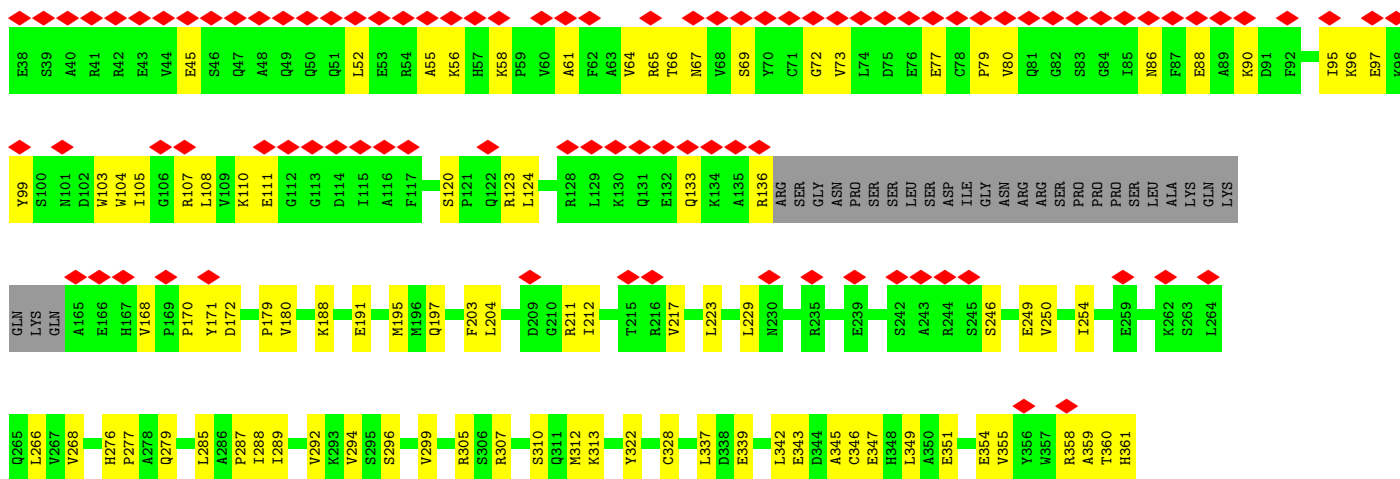
- Molecule 9: Voltage-dependent L-type calcium channel subunit alpha-1C

Chain K: 17% 50% 21% 28%

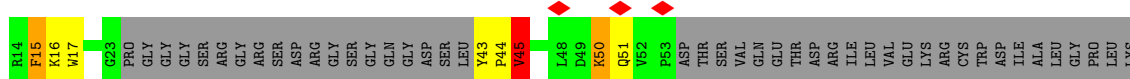




• Molecule 10: Voltage-dependent L-type calcium channel subunit beta-3



• Molecule 11: ER membrane protein complex subunit 4



GLN
ILE
PRO
MET
ASN
LEU
PHE
ILE
MET
TYR
MET
ALA
GLY
ASN
THR
ILE
SER
ILE
PHE
PRO
THR
MET
MET
VAL
CYS
MET
MET
ALA
TRP
ARG
PRO
ILE
GLN
ALA
LEU
MET
MET
ALA
ILE
SER
ALA
THR
PHE
LYS
MET
LEU
GLU
SER
SER
SER
GLN
LYS
PHE
LEU
GLN
GLY
LEU
VAL
TYR
LEU
ILE

GLY
ASN
LEU
MET
GLY
LEU
ALA
LEU
ALA
VAL
TYR
MET
LYS
CYS
GLN
SER
MET
GLY
LEU
LEU
PRO
THR
H160
M164
F167
P170
R173
F176
L183

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

Chain L: 100%

MAG1
MAG2

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

Chain M: 100%

MAG1
MAG2

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

Chain N: 50% 50%

MAG1
MAG2

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 (Å)	372.504, 372.504, 372.504	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: 9Z9, 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	0.10	0/7615	0.28	0/10346
2	B	0.09	0/2447	0.22	0/3288
3	C	0.11	0/1819	0.29	0/2464
4	E	0.08	0/827	0.21	0/1118
5	F	0.11	0/803	0.29	0/1089
6	G	0.09	0/956	0.28	0/1298
7	H	0.11	0/1583	0.32	1/2156 (0.0%)
8	I	0.09	0/1170	0.24	0/1589
9	K	0.10	0/9237	0.29	1/12522 (0.0%)
10	J	0.08	0/2408	0.24	0/3252
11	D	0.13	0/374	0.48	0/504
All	All	0.10	0/29239	0.28	2/39626 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
7	H	137	VAL	N-CA-C	-5.83	108.17	113.71
9	K	1373	ILE	N-CA-C	-5.39	108.02	113.20

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	79	0
2	B	2403	0	2355	18	0
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	21	0
8	I	1150	0	1124	12	0
9	K	9024	0	9261	238	0
10	J	2364	0	2400	61	0
11	D	363	0	349	7	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	465	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 (465) 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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:1199:ASN:HD21	9:K:1204:LYS:HA	1.61	0.65
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
10:J:305:ARG:HG2	10:J:312:MET:HE1	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
2:B:261:ALA:HB1	2:B:288:MET:HE3	1.81	0.61
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:1127:ALA:O	9:K:1130:THR:OG1	2.17	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:726:MET:SD	1:A:730:SER:OG	2.58	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:25:ASP:O	1:A:29:LYS:NZ	2.39	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
1:A:107:MET:HE2	1:A:121:ILE:HD11	1.92	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:B:234:MET:HE3	7:H:73:VAL:HG22	1.96	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
9:K:1613:LEU:O	9:K:1616:THR:OG1	2.22	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
9:K:1201:GLU:CD	9:K:1207:ARG:HE	2.24	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
2:B:251:LYS:HA	2:B:254:MET:HE3	1.97	0.45
7:H:29:LEU:HG	7:H:60:LEU:HD11	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
9:K:571:MET:HE3	9:K:596:VAL:HG21	1.98	0.45
9:K:1621:LYS:HZ3	9:K:1625:ASN:HA	1.82	0.45
10:J:250:VAL:O	10:J:254:ILE:HG12	2.16	0.45
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:184:LEU:C	9:K:187:PRO:HD2	2.42	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
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:624:LEU:HB2	9:K:1062:MET:HE3	1.99	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
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
9:K:1286:MET:HE2	9:K:1286:MET:HB3	1.77	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
9:K:1652:VAL:C	9:K:1655:PRO:HD2	2.43	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:1216:ALA:C	9:K:1217:ARG:HE	2.27	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
10:J:111:GLU:HA	10:J:359:ALA:HA	2.03	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
9:K:1062:MET:HE2	9:K:1062:MET:HB2	1.85	0.40
11:D:44:PRO:O	11:D:45:VAL:C	2.64	0.40
1:A:573:MET:HB2	1:A:628:LEU:HD22	2.02	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
9:K:758:ASP:CG	9:K:1182:VAL:HG11	2.47	0.40
9:K:1177:MET:HE3	9:K:1177:MET:HB3	2.00	0.40
10:J:203:PHE:HD2	10:J:204:LEU:HD22	1.87	0.40
10:J:246:SER:H	10:J:249:GLU:CD	2.27	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	930/973 (96%)	886 (95%)	44 (5%)	0	100	100
2	B	289/291 (99%)	282 (98%)	7 (2%)	0	100	100
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	21
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%)	799 (97%)	25 (3%)	36	59

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	250/250 (100%)	244 (98%)	6 (2%)	43	62
3	C	198/234 (85%)	194 (98%)	4 (2%)	48	65
4	E	85/85 (100%)	83 (98%)	2 (2%)	43	62
5	F	79/79 (100%)	78 (99%)	1 (1%)	61	71
6	G	102/102 (100%)	96 (94%)	6 (6%)	18	44
7	H	169/180 (94%)	162 (96%)	7 (4%)	27	52
8	I	127/131 (97%)	123 (97%)	4 (3%)	35	59
9	K	983/1367 (72%)	961 (98%)	22 (2%)	45	63
10	J	262/287 (91%)	258 (98%)	4 (2%)	57	69
11	D	37/141 (26%)	33 (89%)	4 (11%)	6	22
All	All	3116/3714 (84%)	3031 (97%)	85 (3%)	40	60

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	THR
1	A	62	VAL
1	A	63	ILE
1	A	197	VAL
1	A	211	GLN
1	A	313	LEU
1	A	327	THR
1	A	377	LEU
1	A	407	ILE
1	A	436	LEU
1	A	442	LEU
1	A	463	THR
1	A	614	VAL
1	A	703	GLU
1	A	710	VAL
1	A	775	GLN
1	A	794	GLN
1	A	807	VAL
1	A	814	THR
1	A	852	THR
1	A	857	THR
1	A	912	TYR
1	A	929	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	941	ASP
1	A	948	TYR
2	B	104	ASP
2	B	152	VAL
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	75	THR
3	C	135	PHE
4	E	32	ARG
4	E	33	LEU
5	F	103	LEU
6	G	52	VAL
6	G	67	VAL
6	G	72	GLU
6	G	112	ILE
6	G	123	VAL
6	G	150	ILE
7	H	4	VAL
7	H	133	THR
7	H	148	GLU
7	H	158	HIS
7	H	184	VAL
7	H	187	ASP
7	H	207	LEU
8	I	58	HIS
8	I	135	CYS
8	I	156	VAL
8	I	176	VAL
9	K	127	GLU
9	K	129	ILE
9	K	137	ASN
9	K	143	ILE
9	K	248	VAL
9	K	275	VAL
9	K	346	PHE
9	K	354	LEU
9	K	400	VAL
9	K	404	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	K	518	ARG
9	K	664	ILE
9	K	665	PHE
9	K	755	ASN
9	K	1164	ILE
9	K	1340	VAL
9	K	1381	VAL
9	K	1382	MET
9	K	1518	LEU
9	K	1527	PHE
9	K	1560	ILE
9	K	1609	THR
10	J	168	VAL
10	J	217	VAL
10	J	223	LEU
10	J	292	VAL
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 (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	HIS
1	A	95	GLN
1	A	154	HIS
1	A	222	HIS
1	A	262	GLN
1	A	273	GLN
1	A	397	GLN
1	A	428	HIS
1	A	435	GLN
1	A	496	GLN
1	A	705	GLN
1	A	718	HIS
1	A	722	GLN
1	A	914	GLN
1	A	952	GLN
2	B	169	HIS
2	B	185	ASN
2	B	194	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	11	ASN
3	C	195	GLN
4	E	19	HIS
4	E	27	HIS
4	E	48	GLN
6	G	74	HIS
6	G	124	ASN
7	H	146	HIS
7	H	199	ASN
8	I	155	ASN
8	I	188	GLN
9	K	158	ASN
9	K	300	ASN
9	K	325	GLN
9	K	358	GLN
9	K	429	GLN
9	K	443	GLN
9	K	537	ASN
9	K	560	ASN
9	K	671	GLN
9	K	701	GLN
9	K	1190	GLN
9	K	1199	ASN
9	K	1206	GLN
9	K	1259	GLN
9	K	1272	ASN
9	K	1325	HIS
9	K	1332	ASN
9	K	1445	ASN
9	K	1446	ASN
9	K	1526	ASN
9	K	1540	HIS
9	K	1541	HIS
9	K	1599	ASN
10	J	47	GLN
10	J	50	GLN
10	J	206	HIS
10	J	251	GLN
10	J	341	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	12,8	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	12,8	-	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:

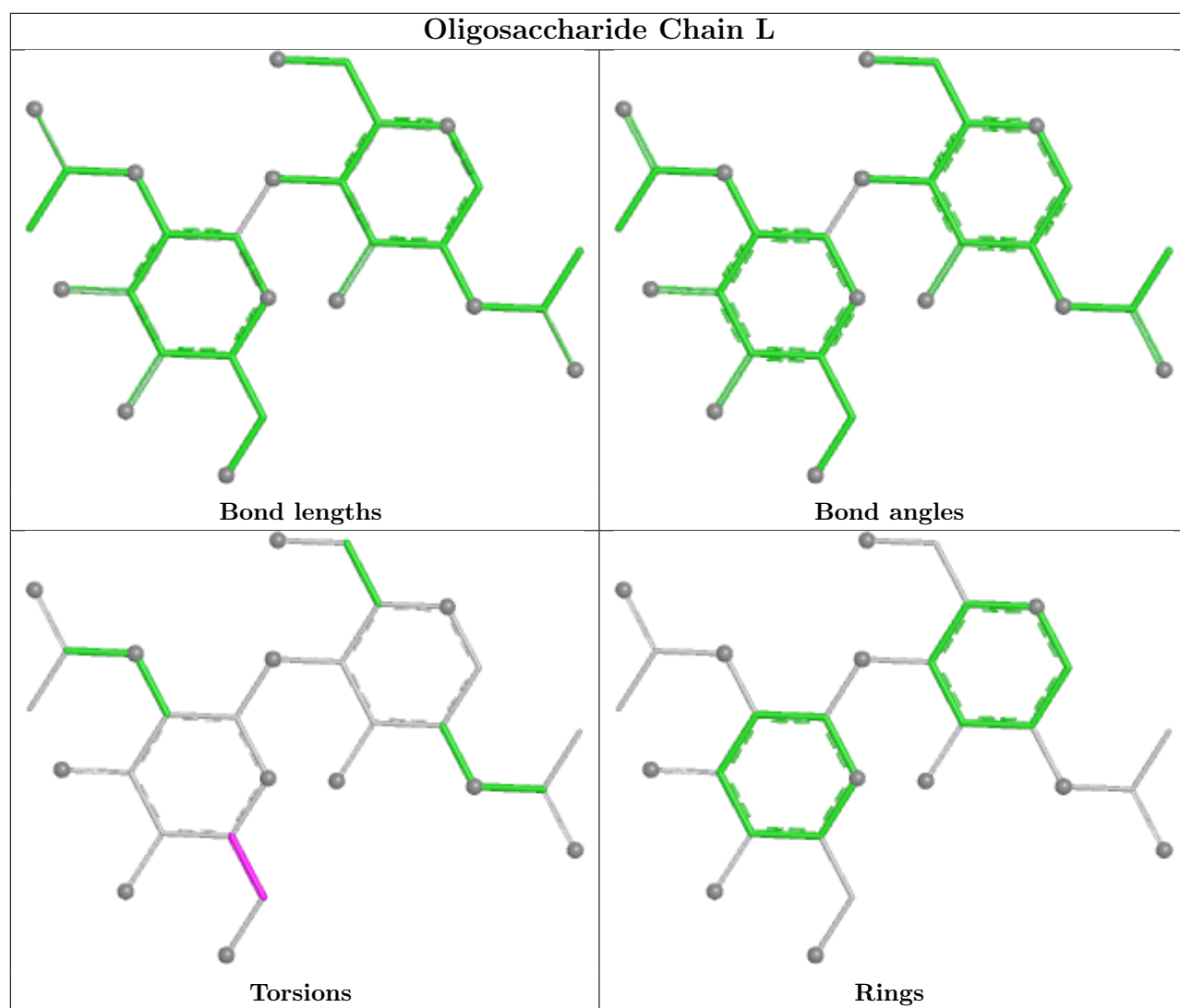
Mol	Chain	Res	Type	Atoms
12	N	1	NAG	C4-C5-C6-O6
12	L	2	NAG	O5-C5-C6-O6
12	N	1	NAG	O5-C5-C6-O6
12	N	1	NAG	C8-C7-N2-C2
12	N	1	NAG	O7-C7-N2-C2
12	L	2	NAG	C4-C5-C6-O6
12	M	1	NAG	O5-C5-C6-O6
12	N	2	NAG	C4-C5-C6-O6
12	M	1	NAG	C4-C5-C6-O6
12	N	1	NAG	C1-C2-N2-C7
12	N	1	NAG	C3-C2-N2-C7
12	N	2	NAG	O5-C5-C6-O6

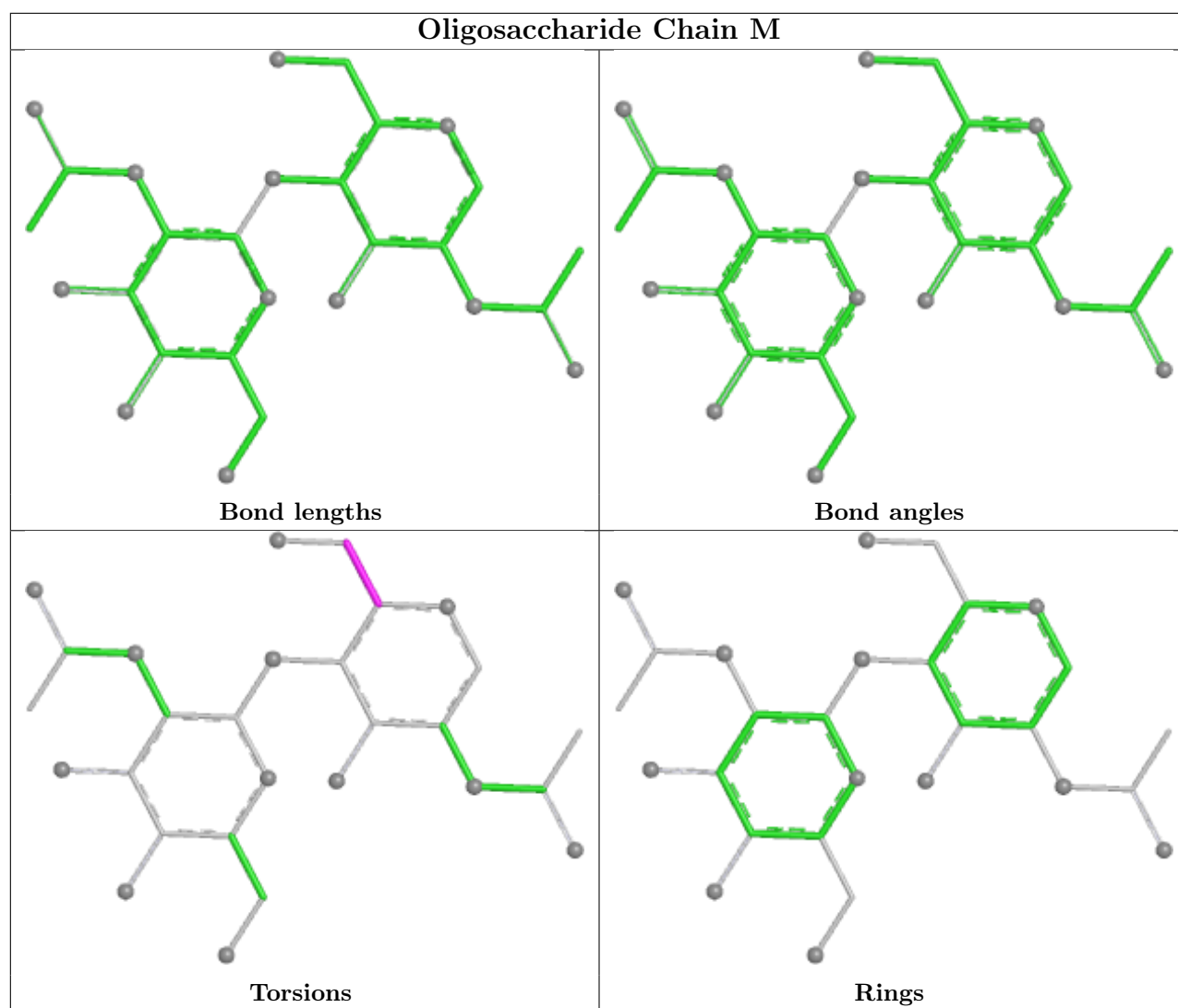
There are no ring outliers.

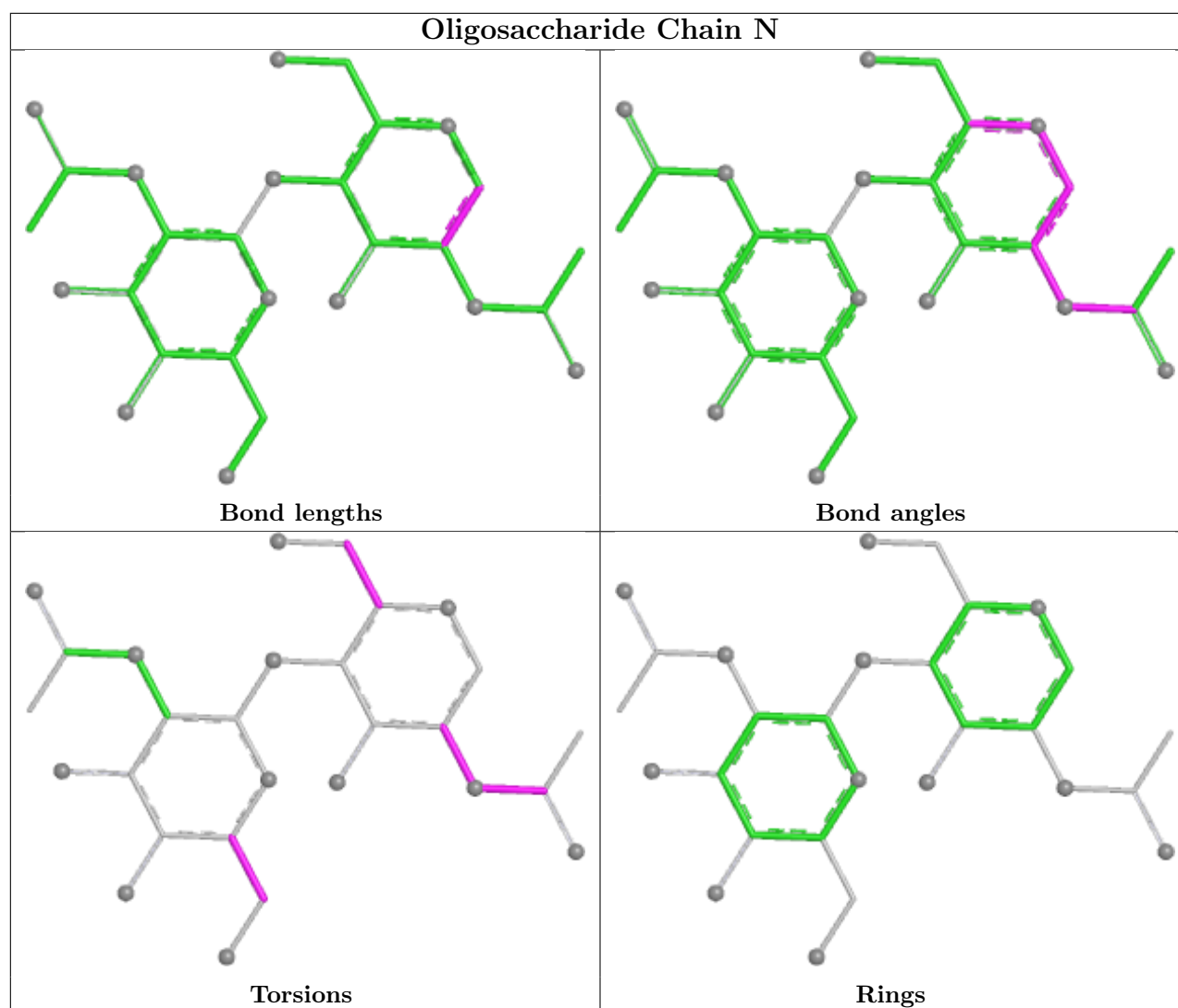
1 monomer is involved in 1 short contact:

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

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
13	NAG	A	1001	1	-	0/6/23/26	0/1/1/1
14	9Z9	K	1701	-	-	4/12/100/100	0/6/6/6

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:

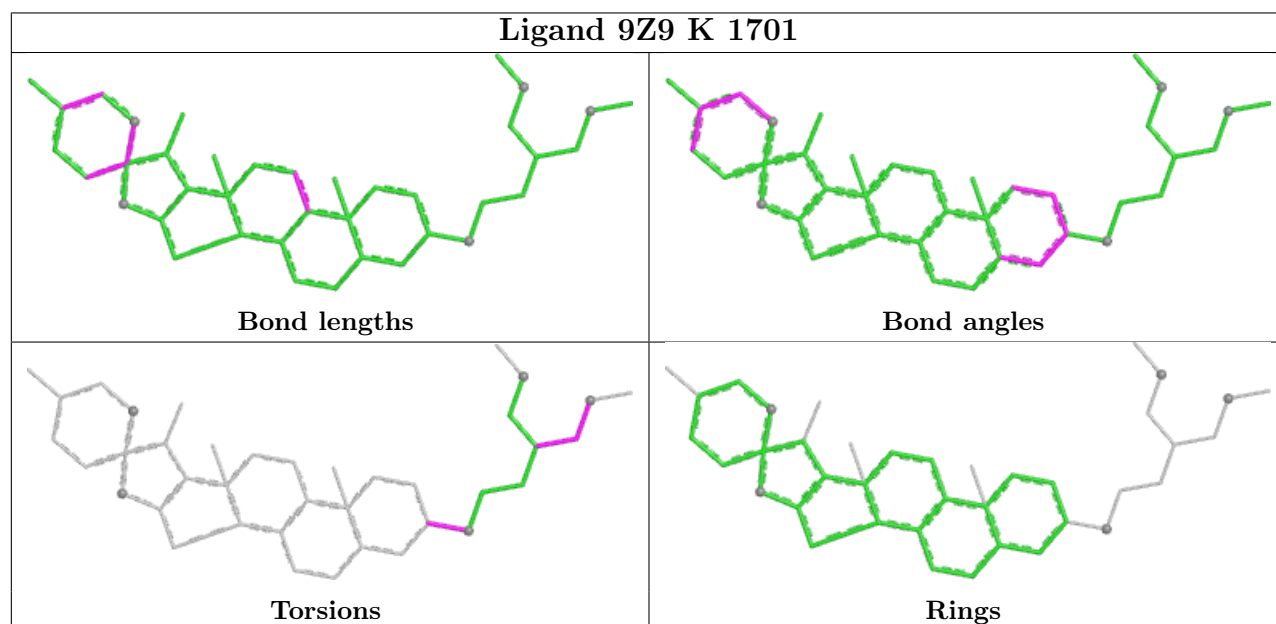
Mol	Chain	Res	Type	Atoms
14	K	1701	9Z9	C16-C17-O20-C21
14	K	1701	9Z9	C18-C17-O20-C21
14	K	1701	9Z9	C23-C24-O25-C26
14	K	1701	9Z9	C22-C23-C24-O25

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.

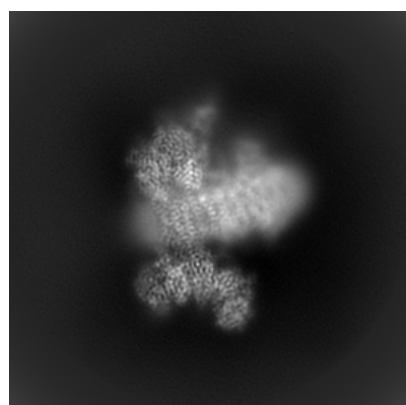
6 Map visualisation [i](#)

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.

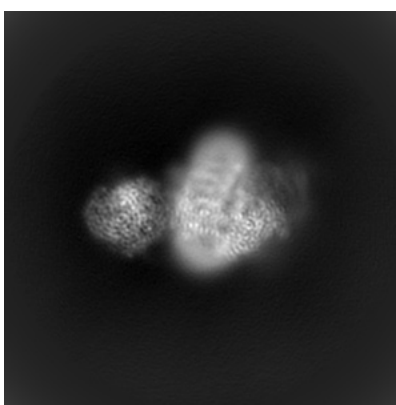
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

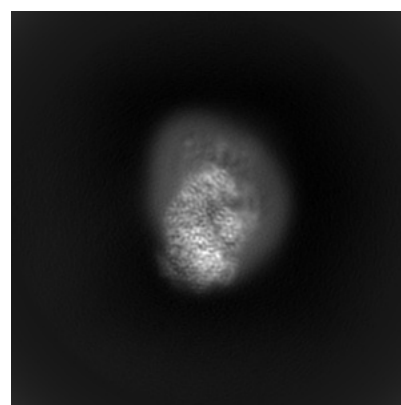
6.1.1 Primary map



X



Y

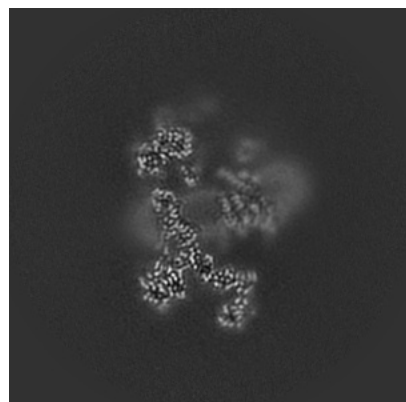


Z

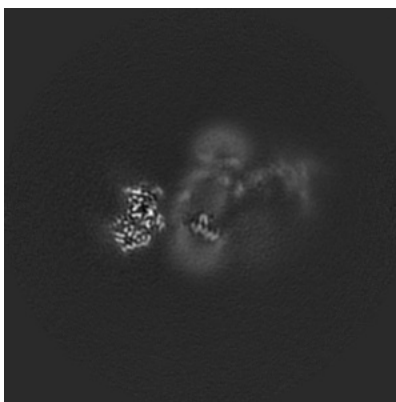
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

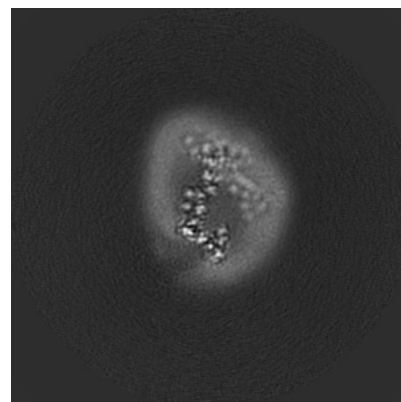
6.2.1 Primary map



X Index: 220



Y Index: 220

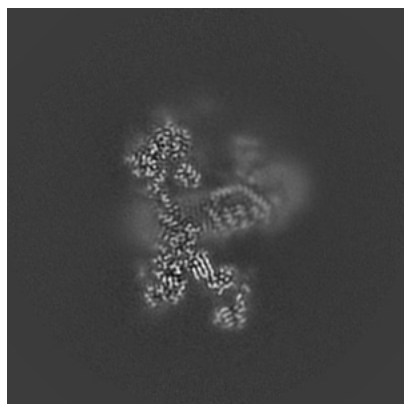


Z Index: 220

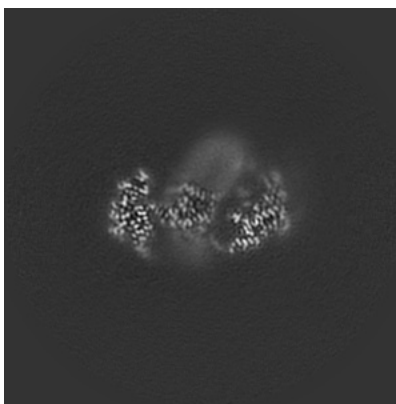
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

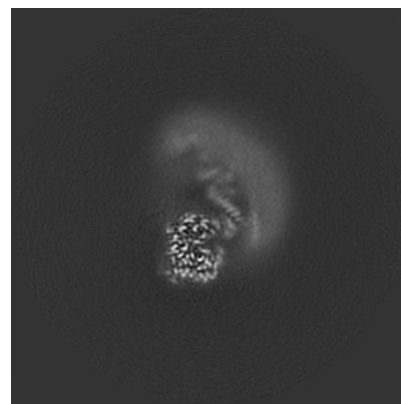
6.3.1 Primary map



X Index: 213



Y Index: 187

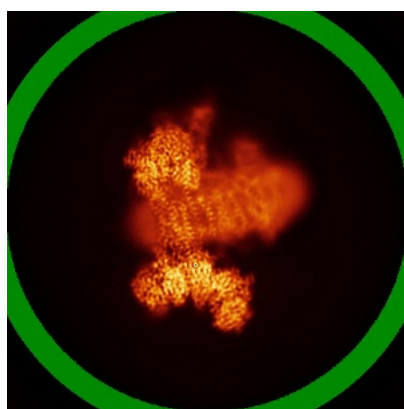


Z Index: 259

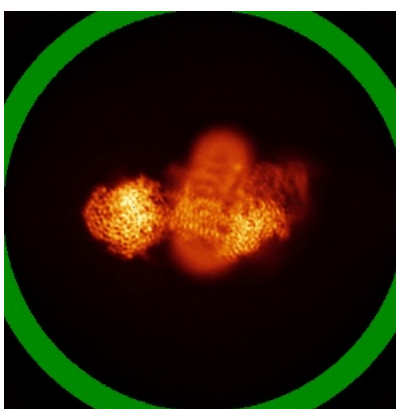
The images above show the largest variance slices of the map in three orthogonal directions.

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

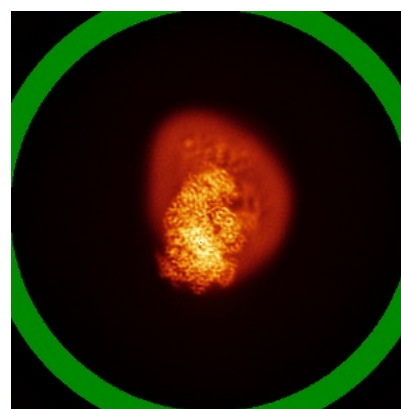
6.4.1 Primary map



X



Y

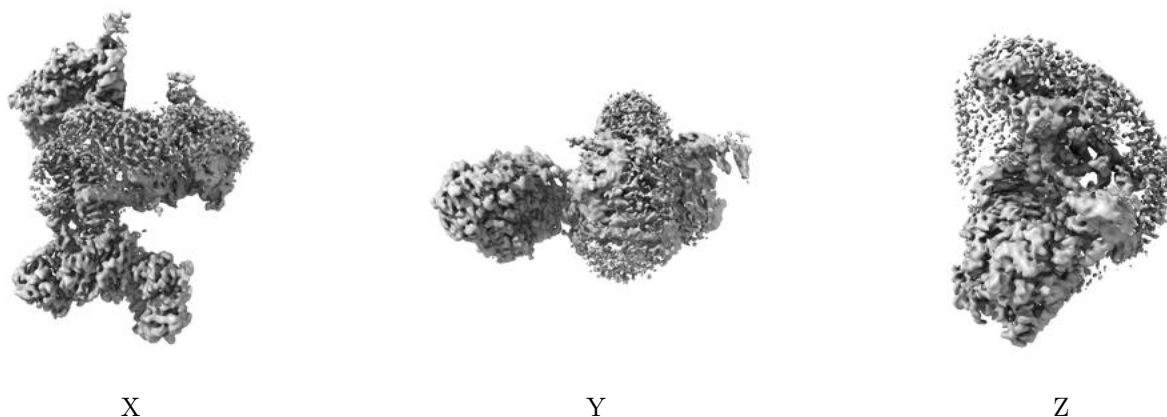


Z

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.

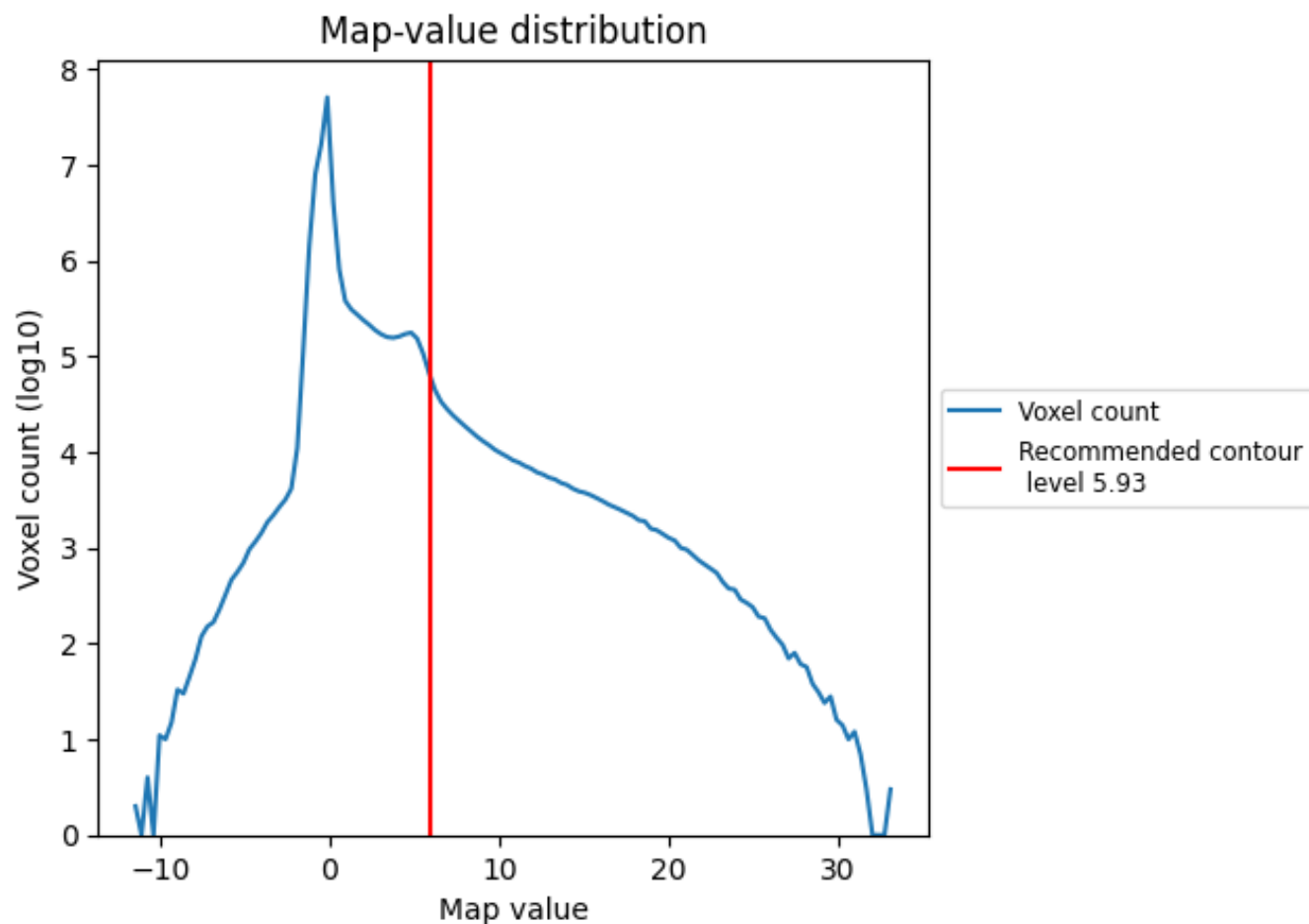
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

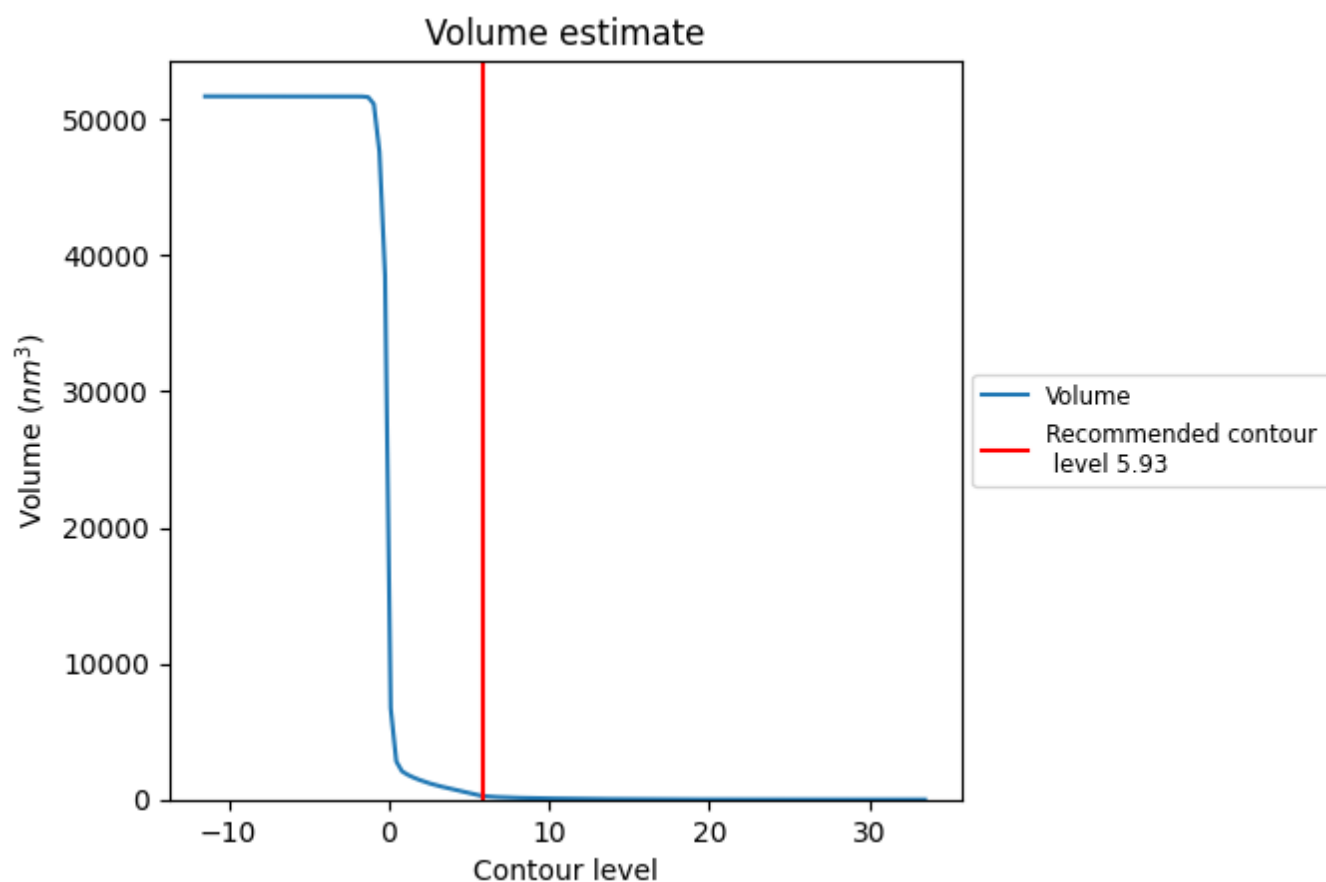
This section contains the results of statistical analysis of the map.

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.

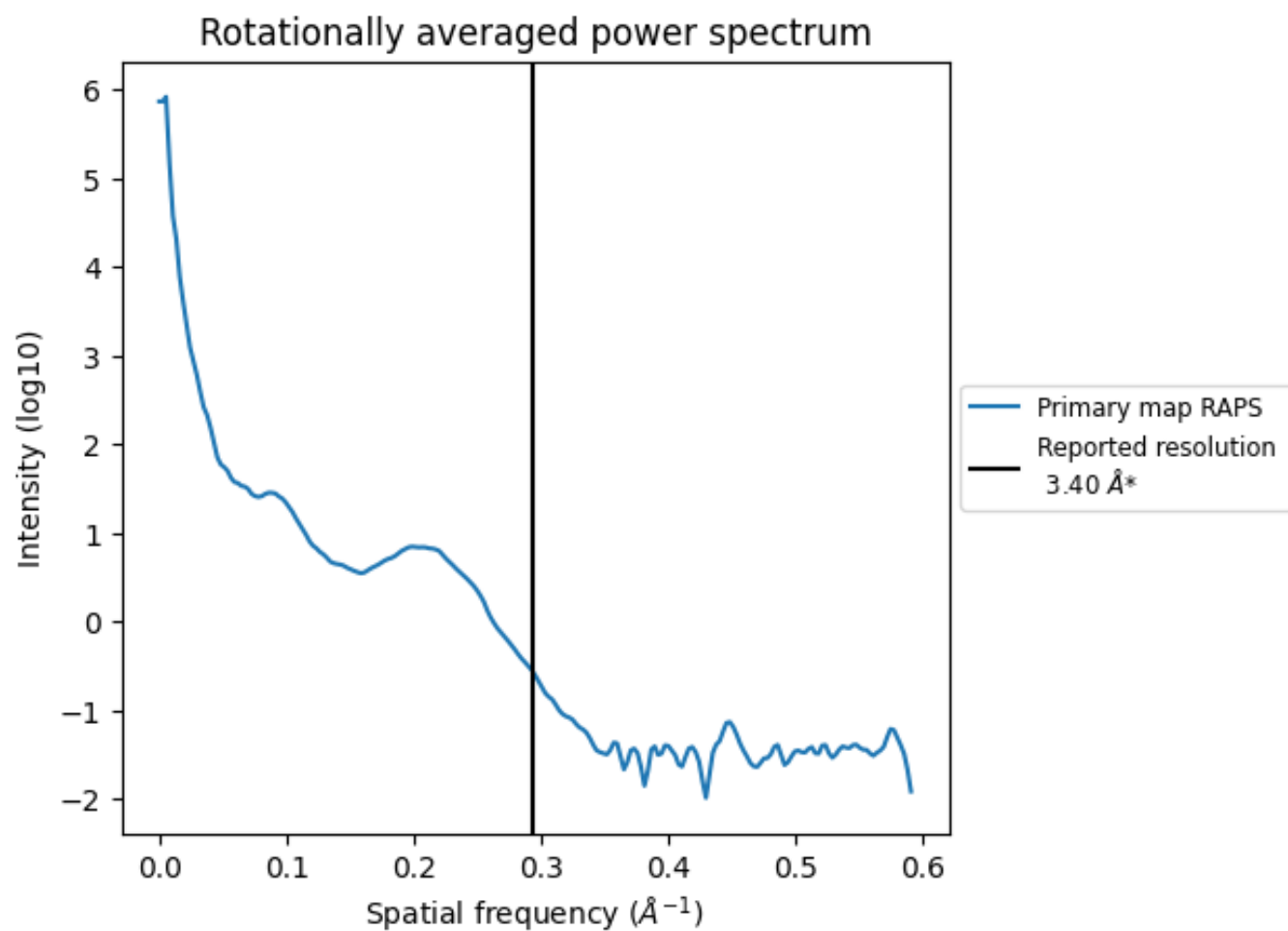
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 260 nm³; 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⁻¹

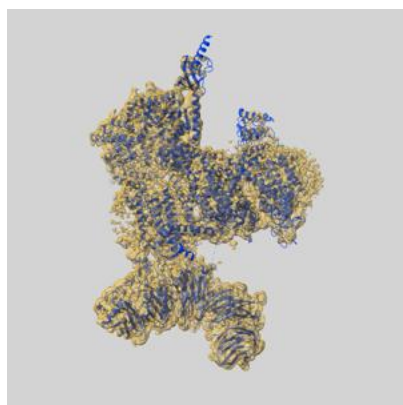
8 Fourier-Shell correlation ⓘ

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

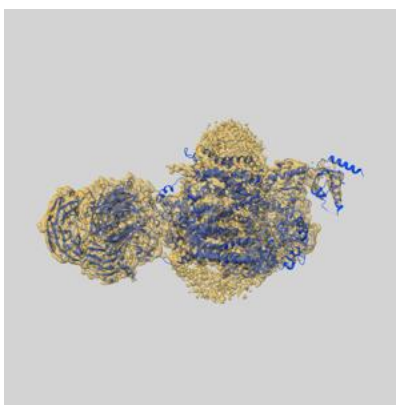
9 Map-model fit [i](#)

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](#).

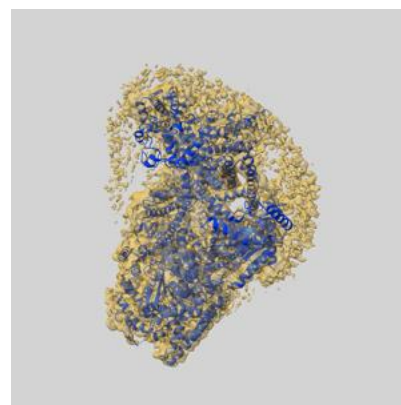
9.1 Map-model overlay [i](#)



X



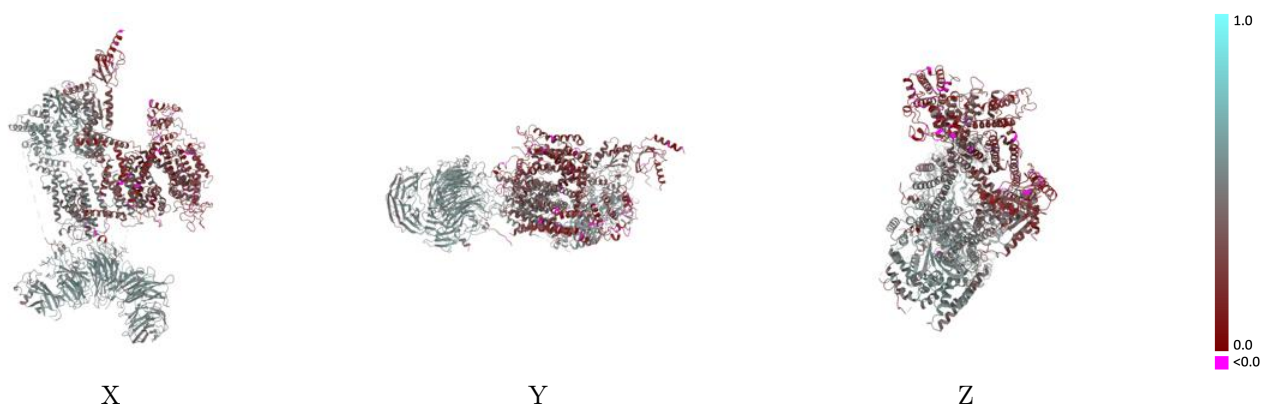
Y



Z

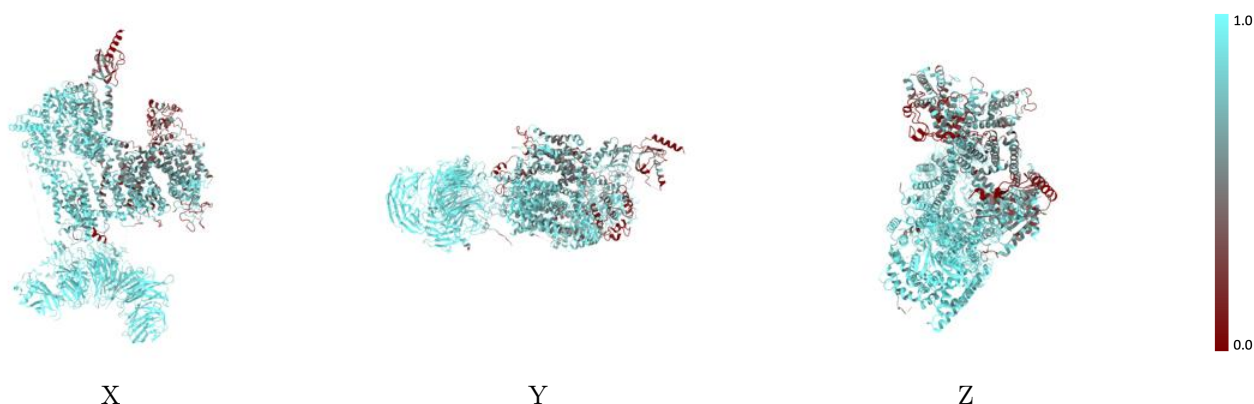
The images above show the 3D surface view of the map at the recommended contour level 5.93 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



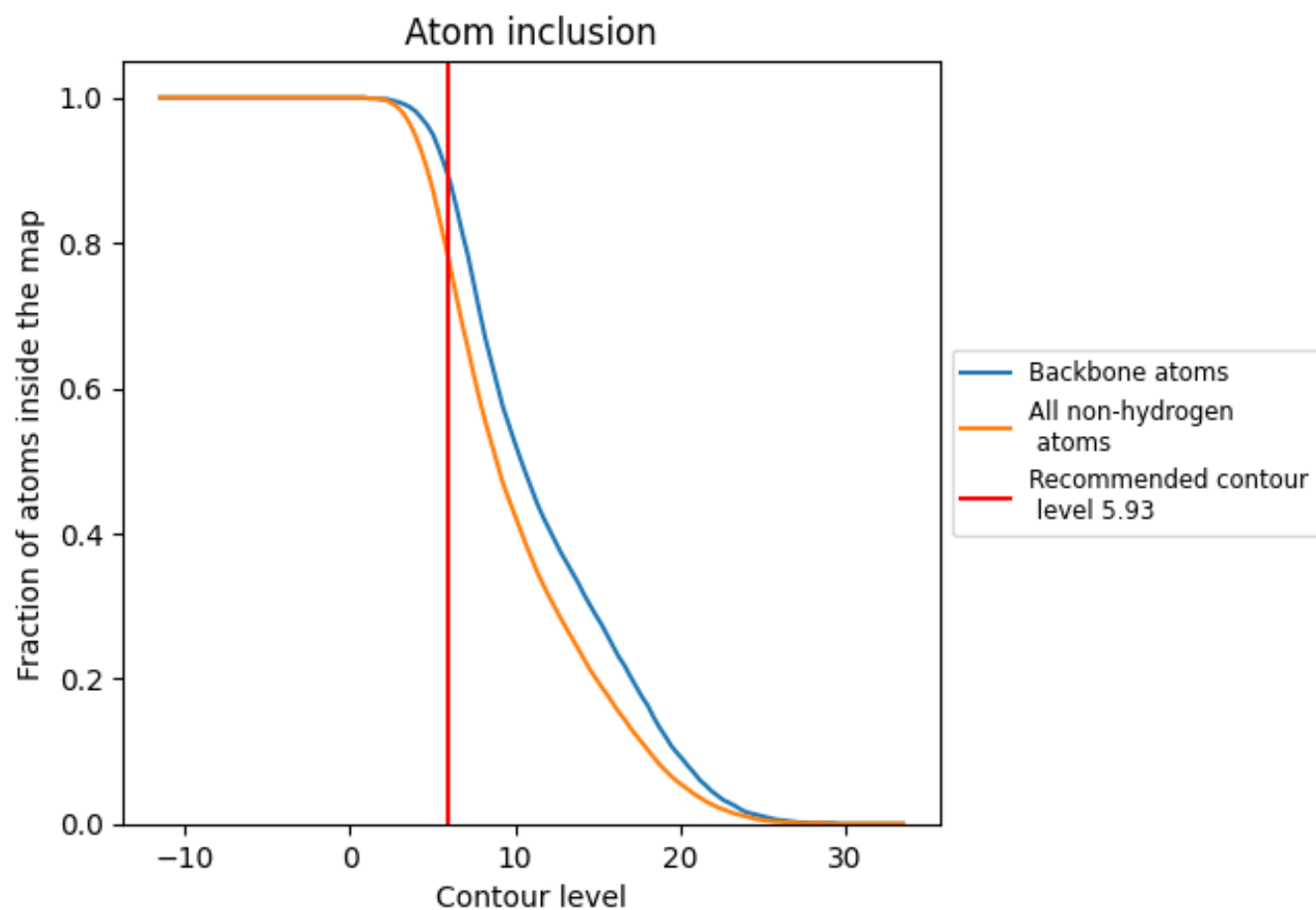
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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	 0.7820	 0.4110
A	 0.9350	 0.5170
B	 0.9220	 0.5170
C	 0.8700	 0.4660
D	 0.8590	 0.4460
E	 0.8650	 0.4790
F	 0.9170	 0.4890
G	 0.9190	 0.5110
H	 0.9400	 0.5150
I	 0.9550	 0.5060
J	 0.5200	 0.3060
K	 0.5840	 0.2580
L	 0.9290	 0.5140
M	 0.8210	 0.4770
N	 0.7500	 0.4250

