Full wwPDB EM Validation Report

Nov 27, 2022 – 07:45 PM EST

PDB ID	:	7KO8
EMDB ID	:	EMD-22961
Title	:	Cryo-EM structure of the mature and infective Mayaro virus
Authors	:	Riberio-Filho, H.V.; Coimbra, L.D.; Cassago, A.; Rocha, R.P.F.; Padilha, A.C.M.; Schatz, M.; van Heel, M.G.; Portugal, R.V.; Trivella, D.B.B.; de Oliveira, P.S.L.; Marques, R.E.
Deposited on	:	2020-11-06
Resolution	:	4.40 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 (i) 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 (i)) were used in the production of this report:

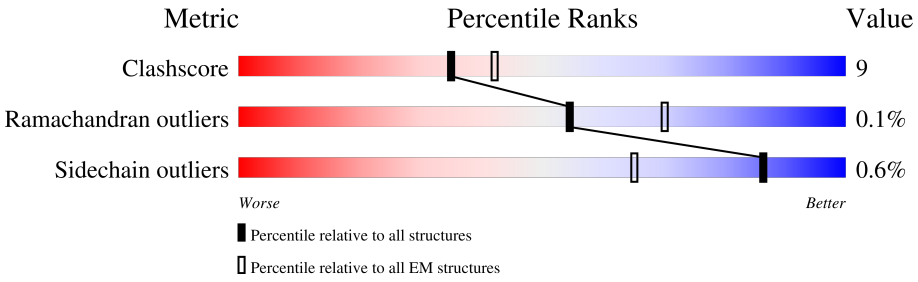
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.40 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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 <=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	258	26% 41% 17% 41%
1	D	258	19% 46% 13% 41%
1	G	258	26% 44% 15% 41%
1	J	258	19% 47% 11% · 41%
2	B	436	27% 80% 19% ·
2	E	436	15% 83% 16% ·
2	H	436	24% 81% 18% ·
2	L	436	20% 81% 18% ·

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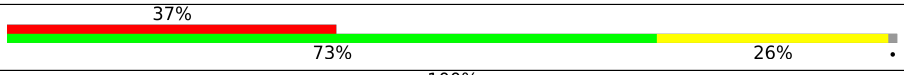
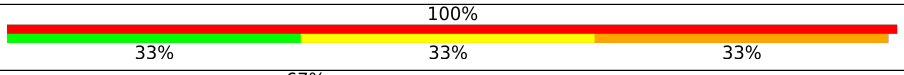
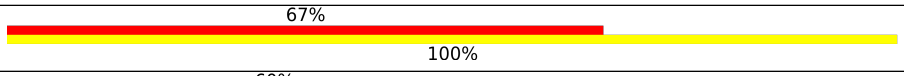
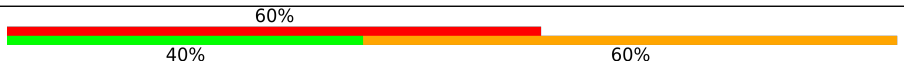
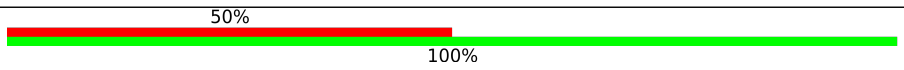
Mol	Chain	Length	Quality of chain
3	C	422	
3	F	422	
3	I	422	
3	M	422	
4	N	3	
4	P	3	
4	T	3	
5	O	5	
5	Q	5	
5	S	5	
5	U	5	
6	R	2	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 31153 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 Capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	152	Total	C	N	O	S	0	0
			1170	739	203	222	6		
1	D	152	Total	C	N	O	S	0	0
			1170	739	203	222	6		
1	G	152	Total	C	N	O	S	0	0
			1170	739	203	222	6		
1	J	152	Total	C	N	O	S	0	0
			1170	739	203	222	6		

- Molecule 2 is a protein called E1 glycoprotein.

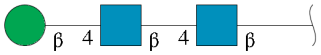
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	433	Total	C	N	O	S	0	0
			3290	2083	555	629	23		
2	E	433	Total	C	N	O	S	0	0
			3290	2083	555	629	23		
2	H	433	Total	C	N	O	S	0	0
			3290	2083	555	629	23		
2	L	433	Total	C	N	O	S	0	0
			3290	2083	555	629	23		

- Molecule 3 is a protein called E2 glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	416	Total	C	N	O	S	0	0
			3231	2032	574	603	22		
3	F	416	Total	C	N	O	S	0	0
			3231	2032	574	603	22		
3	I	416	Total	C	N	O	S	0	0
			3231	2032	574	603	22		
3	M	416	Total	C	N	O	S	0	0
			3231	2032	574	603	22		

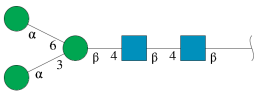
- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-b

eta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
5	O	5	Total	C	N	O	0	0
			61	34	2	25		
5	Q	5	Total	C	N	O	0	0
			61	34	2	25		
5	U	5	Total	C	N	O	0	0
			61	34	2	25		
5	S	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

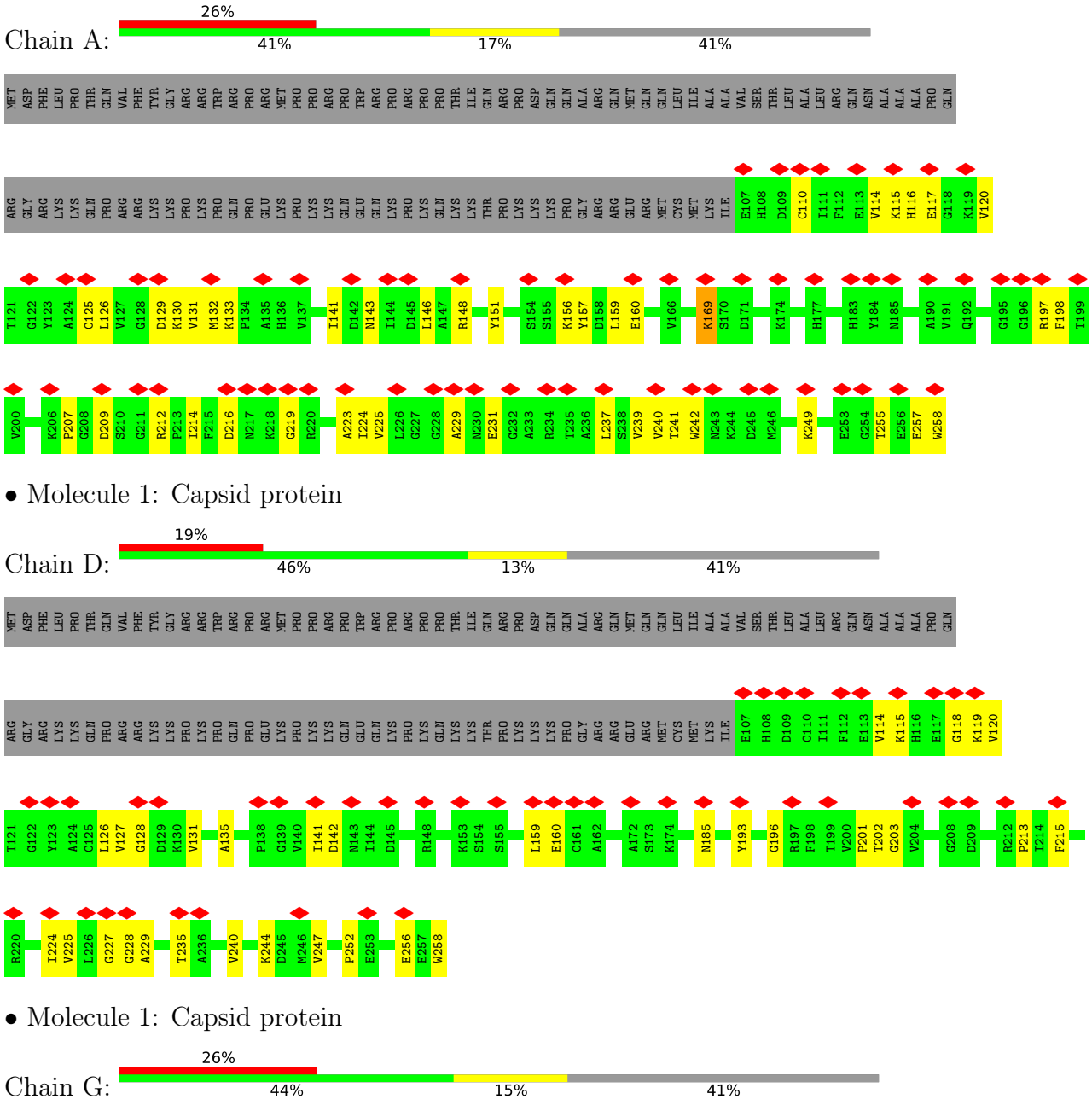
Mol	Chain	Residues	Atoms				AltConf	Trace
6	R	2	Total	C	N	O	0	0
			28	16	2	10		

3 Residue-property plots (i)

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

• Molecule 1: Capsid protein

Chain A:

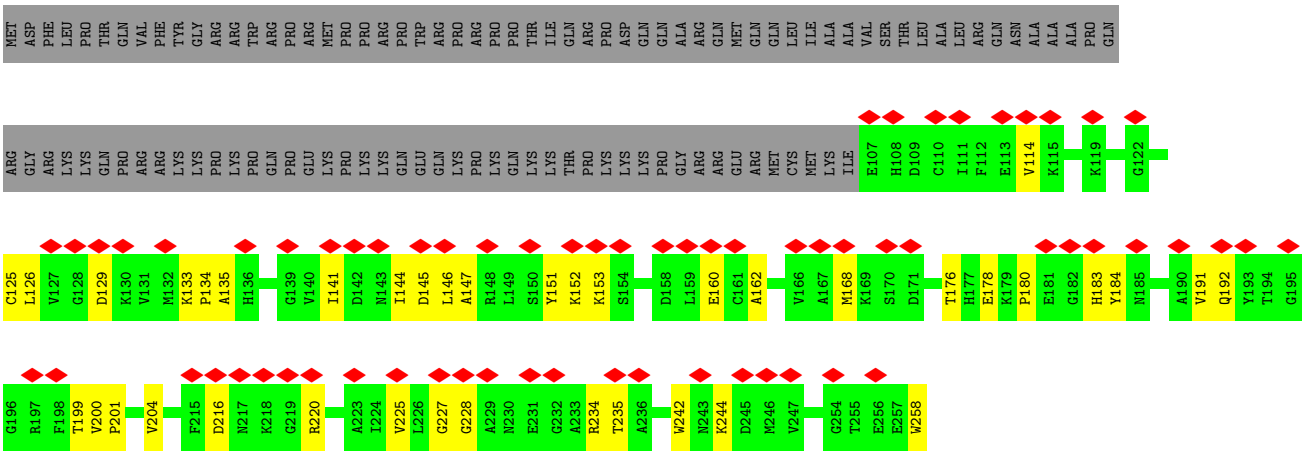


• Molecule 1: Capsid protein

Chain D:

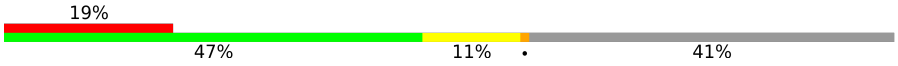
• Molecule 1: Capsid protein

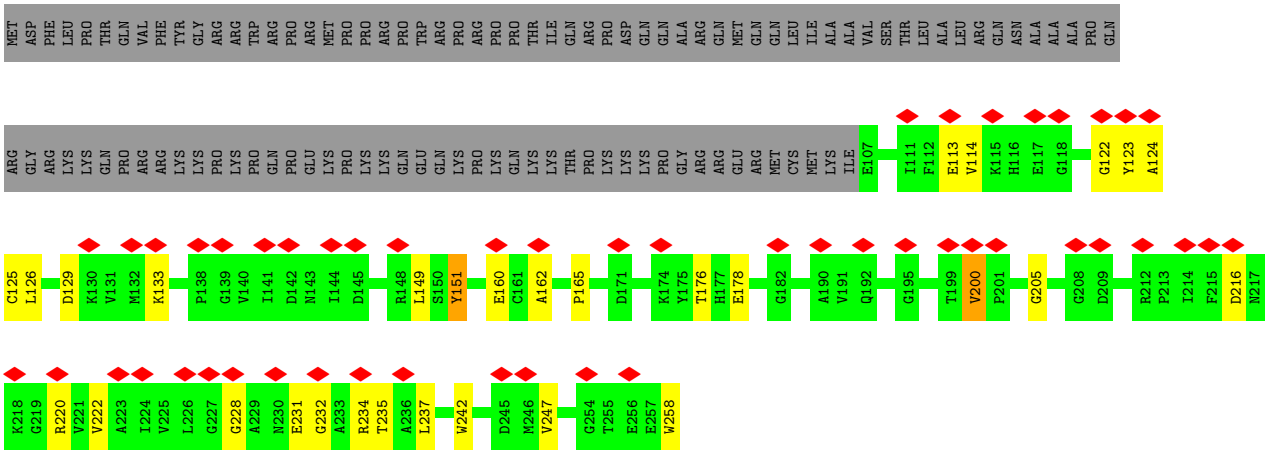
Chain G:



• Molecule 1: Capsid protein

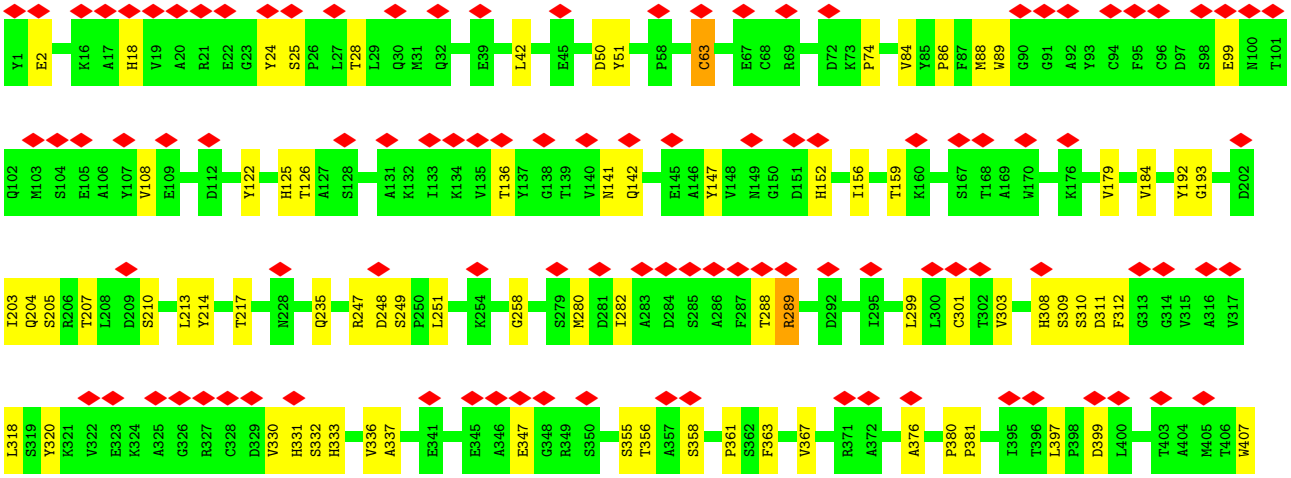
Chain J:

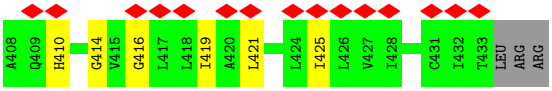




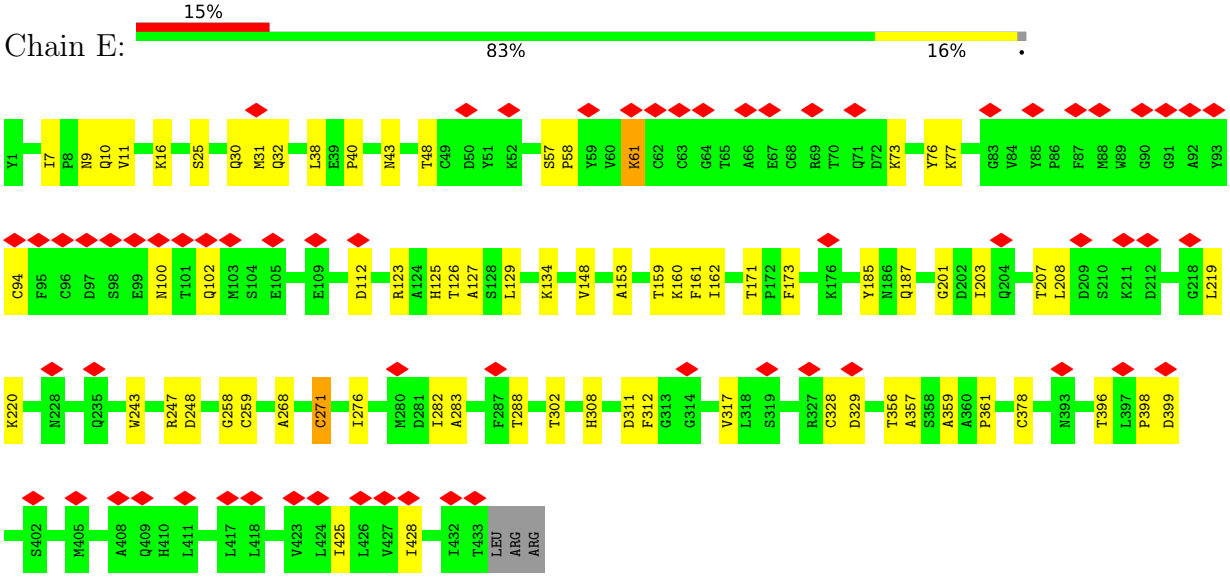
• Molecule 2: E1 glycoprotein

Chain B:

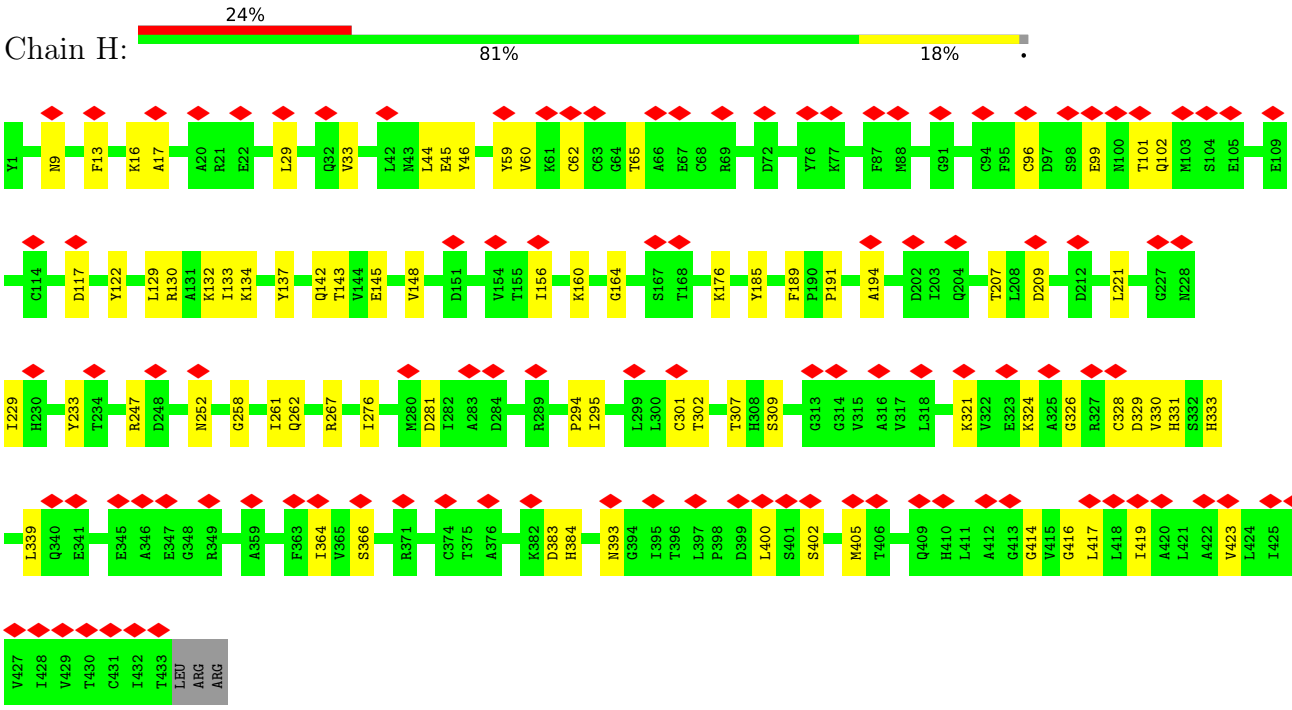




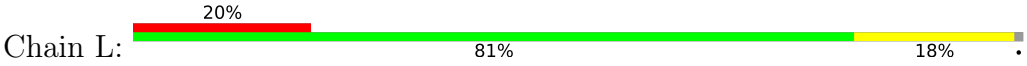
• Molecule 2: E1 glycoprotein

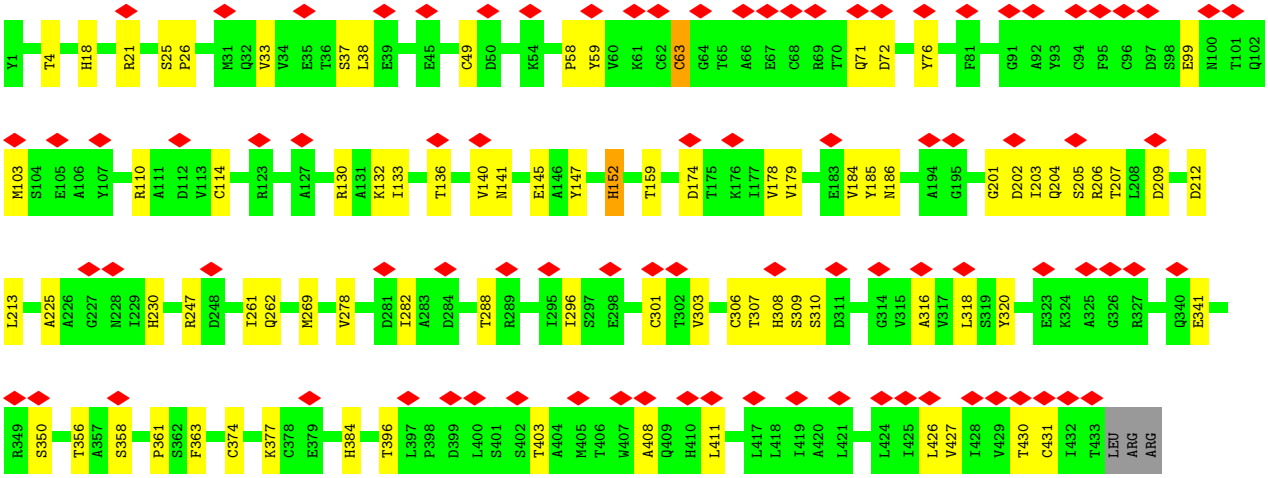


• Molecule 2: E1 glycoprotein



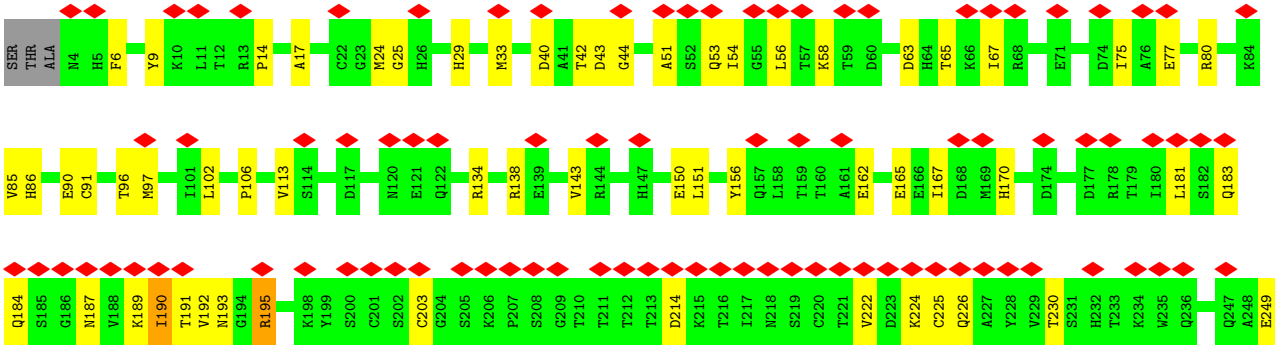
• Molecule 2: E1 glycoprotein





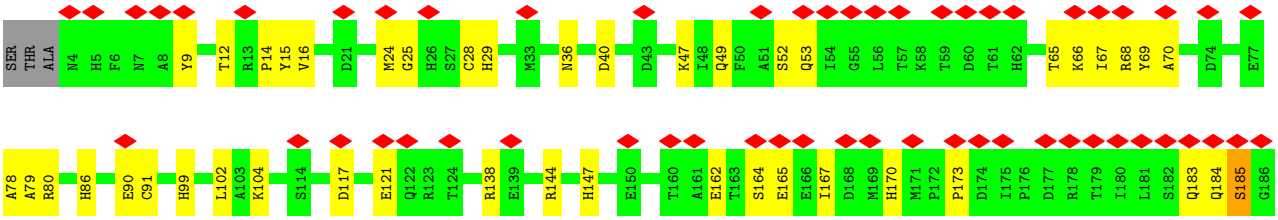
• Molecule 3: E2 glycoprotein

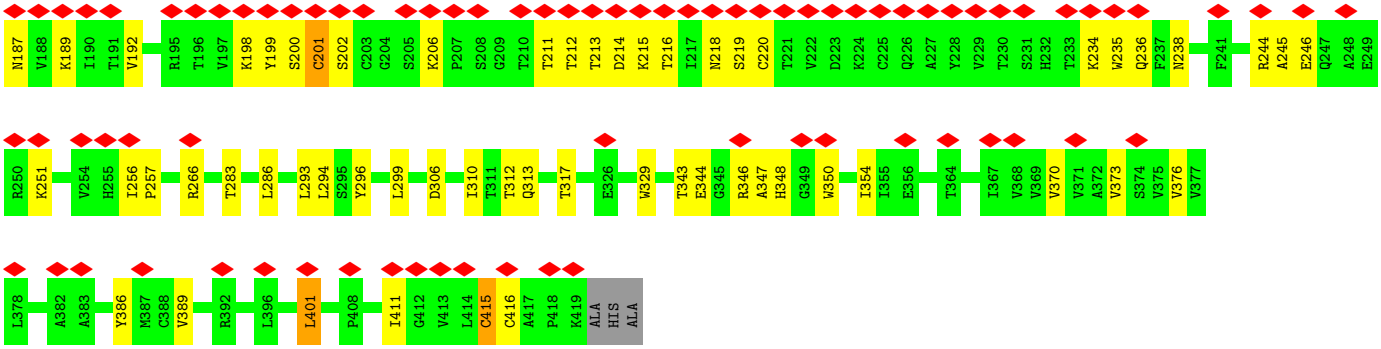
Chain C:



• Molecule 3: E2 glycoprotein

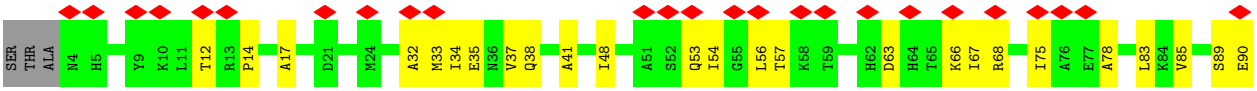
Chain F:

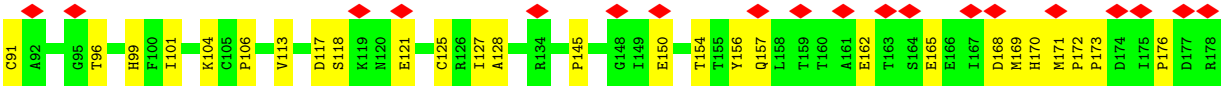


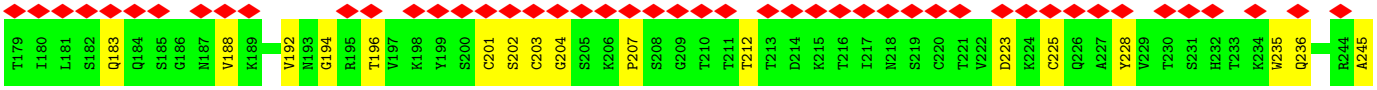


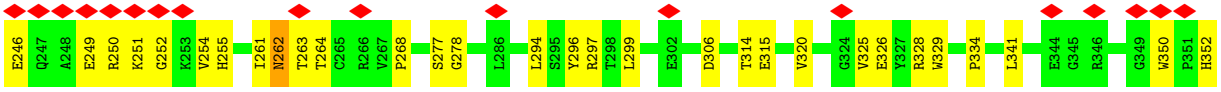
• Molecule 3: E2 glycoprotein

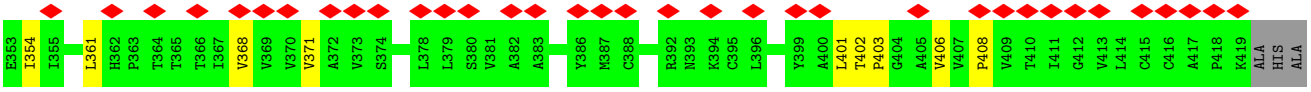
Chain I:





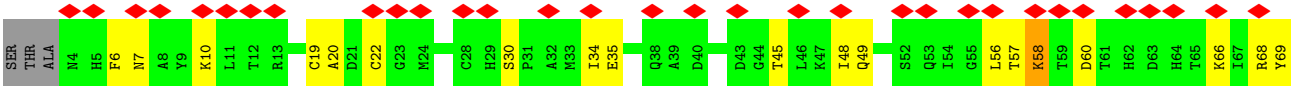


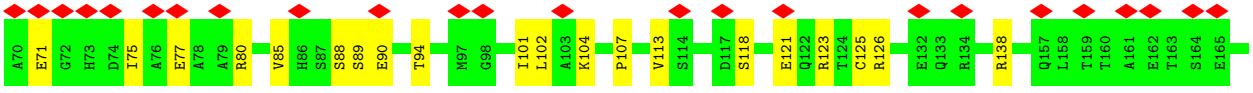


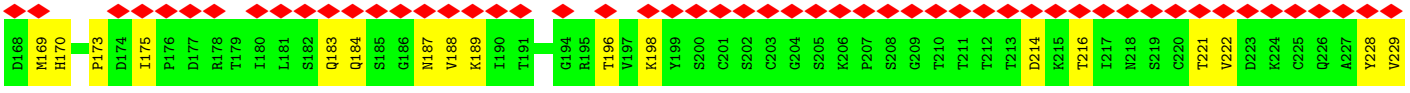


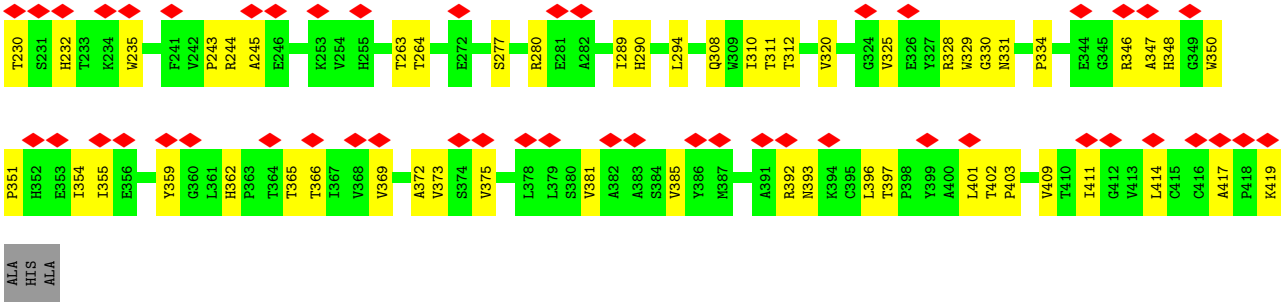
• Molecule 3: E2 glycoprotein

Chain M:







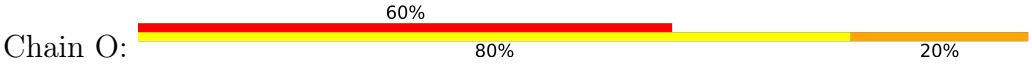


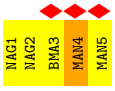
• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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

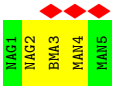
• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

• Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



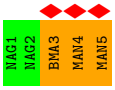


• Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



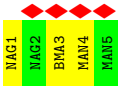
• Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:



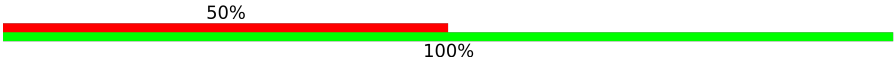
• Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:



• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	40179	Depositor
Resolution determination method	FSC 1/2 BIT CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	9.131	Depositor
Minimum map value	-7.538	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.553	Depositor
Recommended contour level	1.9	Depositor
Map size (Å)	885.9199, 885.9199, 885.9199	wwPDB
Map dimensions	800, 800, 800	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1074, 1.1074, 1.1074	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.34	0/1199	0.60	0/1623
1	D	0.32	0/1199	0.56	0/1623
1	G	0.32	0/1199	0.54	0/1623
1	J	0.35	0/1199	0.59	0/1623
2	B	0.36	0/3372	0.56	1/4606 (0.0%)
2	E	0.36	0/3372	0.56	0/4606
2	H	0.35	0/3372	0.57	0/4606
2	L	0.36	0/3372	0.58	1/4606 (0.0%)
3	C	0.33	0/3313	0.59	0/4522
3	F	0.34	0/3313	0.60	0/4522
3	I	0.32	0/3313	0.57	0/4522
3	M	0.32	0/3313	0.57	0/4522
All	All	0.34	0/31536	0.58	2/43004 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
1	J	0	1
2	B	0	1
2	H	0	2
2	L	0	1
3	C	0	6
3	F	0	5
3	I	0	4
All	All	0	22

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	299	LEU	CA-CB-CG	6.29	129.77	115.30
2	L	38	LEU	CA-CB-CG	5.17	127.20	115.30

There are no chirality outliers.

All (22) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	239	VAL	Peptide
2	B	414	GLY	Peptide
3	C	189	LYS	Peptide
3	C	190	ILE	Peptide
3	C	191	THR	Peptide
3	C	230	THR	Peptide
3	C	340	GLN	Peptide
3	C	6	PHE	Peptide
1	D	201	PRO	Peptide
3	F	185	SER	Peptide
3	F	200	SER	Peptide
3	F	201	CYS	Peptide
3	F	350	TRP	Peptide
3	F	415	CYS	Peptide
2	H	137	TYR	Peptide
2	H	364	ILE	Peptide
3	I	204	GLY	Peptide
3	I	249	GLU	Peptide
3	I	35	GLU	Peptide
3	I	350	TRP	Peptide
1	J	200	VAL	Peptide
2	L	152	HIS	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1170	0	1144	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1170	0	1146	21	0
1	G	1170	0	1146	27	0
1	J	1170	0	1146	24	0
2	B	3290	0	3210	51	0
2	E	3290	0	3209	43	0
2	H	3290	0	3211	45	0
2	L	3290	0	3213	51	0
3	C	3231	0	3198	58	0
3	F	3231	0	3198	65	0
3	I	3231	0	3194	67	0
3	M	3231	0	3192	74	0
4	N	39	0	33	1	0
4	P	39	0	34	1	0
4	T	39	0	34	0	0
5	O	61	0	52	2	0
5	Q	61	0	52	0	0
5	S	61	0	52	1	0
5	U	61	0	52	2	0
6	R	28	0	25	0	0
All	All	31153	0	30541	538	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 9.

All (538) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:LYS:HE3	1:J:232:GLY:HA3	1.35	1.08
1:A:169:LYS:HA	1:A:169:LYS:NZ	1.97	0.79
3:M:320:VAL:HG12	3:M:325:VAL:HG11	1.66	0.78
1:A:169:LYS:CE	1:J:232:GLY:HA3	2.14	0.77
1:A:169:LYS:HE2	1:J:231:GLU:O	1.86	0.75
3:I:56:LEU:HB2	3:I:68:ARG:HD3	1.68	0.74
2:B:108:VAL:HG21	2:B:217:THR:HG21	1.71	0.73
1:A:114:VAL:HA	1:A:141:ILE:HA	1.71	0.72
3:F:411:ILE:HA	3:F:415:CYS:HA	1.71	0.72
3:I:401:LEU:HD12	3:I:402:THR:HG23	1.71	0.71
3:C:193:ASN:ND2	3:C:195:ARG:O	2.23	0.71
2:H:416:GLY:HA2	2:H:419:ILE:HD12	1.72	0.71
3:M:396:LEU:HD11	3:M:414:LEU:HD22	1.71	0.71
2:E:171:THR:HG22	2:E:173:PHE:H	1.54	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:94:CYS:HB3	2:E:100:ASN:HD21	1.55	0.71
2:L:33:VAL:HG12	2:L:133:ILE:HG12	1.73	0.70
2:H:191:PRO:HD2	2:H:194:ALA:HB3	1.72	0.70
3:I:157:GLN:HB2	3:I:261:ILE:HG12	1.72	0.70
2:H:400:LEU:HG	2:H:405:MET:HG2	1.73	0.70
1:J:133:LYS:HB3	1:J:160:GLU:HB2	1.74	0.70
2:B:192:TYR:HA	2:B:204:GLN:HE22	1.55	0.69
4:P:3:BMA:O2	4:P:3:BMA:H62	1.93	0.69
2:B:258:GLY:HA3	3:C:299:LEU:HD13	1.76	0.68
3:I:250:ARG:HG3	3:I:252:GLY:H	1.59	0.68
2:H:142:GLN:HB3	2:H:156:ILE:HD11	1.75	0.67
2:L:207:THR:HG23	2:L:209:ASP:H	1.60	0.67
2:L:179:VAL:HG22	2:L:184:VAL:HG12	1.77	0.67
1:J:176:THR:HB	1:J:220:ARG:HD3	1.76	0.66
1:D:115:LYS:HG2	1:D:120:VAL:HG12	1.76	0.65
1:G:125:CYS:SG	1:G:126:LEU:N	2.69	0.65
3:M:57:THR:O	3:M:60:ASP:N	2.28	0.65
3:C:165:GLU:HB3	3:C:256:ILE:HB	1.79	0.65
3:F:206:LYS:NZ	3:F:220:CYS:SG	2.69	0.65
3:F:15:TYR:HB3	3:F:236:GLN:HE22	1.62	0.65
1:G:228:GLY:H	1:G:258:TRP:HB3	1.62	0.64
3:M:311:THR:HG23	3:M:312:THR:HG23	1.80	0.64
2:L:225:ALA:H	2:L:230:HIS:HE1	1.45	0.63
1:D:229:ALA:O	1:D:235:THR:OG1	2.15	0.63
1:G:151:TYR:HA	1:G:162:ALA:HB2	1.81	0.63
3:M:19:CYS:SG	3:M:20:ALA:N	2.72	0.62
1:A:110:CYS:SG	1:A:126:LEU:N	2.68	0.62
3:C:54:ILE:HG22	3:C:67:ILE:HB	1.81	0.62
2:E:187:GLN:HE22	2:E:243:TRP:HE1	1.48	0.62
3:C:85:VAL:HG22	3:C:113:VAL:HG12	1.82	0.62
2:H:132:LYS:HG2	2:H:145:GLU:HG2	1.80	0.62
3:M:77:GLU:O	3:M:118:SER:OG	2.17	0.62
2:B:179:VAL:HG22	2:B:184:VAL:HG12	1.82	0.61
2:E:48:THR:HG23	2:E:203:ILE:HB	1.82	0.61
3:F:347:ALA:O	3:F:348:HIS:ND1	2.33	0.61
3:F:66:LYS:HA	3:F:79:ALA:HA	1.83	0.61
3:M:48:ILE:HB	3:M:101:ILE:HG23	1.83	0.61
3:C:138:ARG:NH1	3:C:295:SER:OG	2.34	0.61
3:M:175:ILE:HB	3:M:229:VAL:HB	1.82	0.61
3:C:347:ALA:O	3:C:348:HIS:ND1	2.34	0.60
2:B:309:SER:OG	2:B:310:SER:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:16:LYS:NZ	2:H:339:LEU:O	2.34	0.60
3:I:168:ASP:OD1	3:I:250:ARG:NH1	2.34	0.60
1:A:114:VAL:HG22	1:A:141:ILE:HG22	1.82	0.60
2:B:88:MET:HG2	2:B:89:TRP:H	1.66	0.60
3:C:301:ARG:NH2	3:C:302:GLU:OE2	2.35	0.60
2:E:308:HIS:HB2	2:E:357:ALA:HA	1.83	0.60
2:L:174:ASP:OD2	2:L:186:ASN:ND2	2.34	0.60
3:M:6:PHE:O	3:M:10:LYS:NZ	2.35	0.60
1:G:225:VAL:HG22	1:G:227:GLY:H	1.66	0.59
3:M:184:GLN:O	3:M:187:ASN:ND2	2.34	0.59
3:I:17:ALA:HB3	3:I:33:MET:HG2	1.85	0.59
3:F:173:PRO:HA	3:F:245:ALA:HB2	1.85	0.59
1:D:247:VAL:HG11	3:F:401:LEU:HB3	1.84	0.59
2:B:217:THR:OG1	2:B:235:GLN:NE2	2.35	0.58
1:D:114:VAL:HG23	1:D:141:ILE:HA	1.85	0.58
2:E:359:ALA:HA	2:E:378:CYS:HB2	1.85	0.58
3:F:183:GLN:NE2	3:F:187:ASN:O	2.37	0.58
3:M:58:LYS:HB3	3:M:68:ARG:HH22	1.67	0.58
2:E:43:ASN:HB2	2:E:123:ARG:HB3	1.85	0.58
3:F:348:HIS:H	3:F:354:ILE:HG22	1.69	0.58
3:C:54:ILE:HD12	3:C:96:THR:HB	1.86	0.58
2:E:38:LEU:HB3	2:E:268:ALA:HB3	1.86	0.58
3:I:117:ASP:HB3	3:I:121:GLU:HB2	1.85	0.58
2:L:309:SER:OG	2:L:310:SER:N	2.36	0.58
2:B:247:ARG:NE	2:B:248:ASP:O	2.33	0.58
3:I:145:PRO:HG3	3:I:268:PRO:HB3	1.85	0.58
3:I:169:MET:O	3:I:170:HIS:ND1	2.37	0.58
2:L:37:SER:HA	2:L:269:MET:HA	1.85	0.58
1:D:142:ASP:OD1	1:D:142:ASP:N	2.35	0.58
2:B:184:VAL:HG23	2:B:251:LEU:HB3	1.85	0.57
3:F:65:THR:O	3:F:80:ARG:N	2.37	0.57
2:E:396:THR:HG22	2:E:398:PRO:HD2	1.86	0.57
3:M:85:VAL:HG22	3:M:113:VAL:HG12	1.85	0.57
3:C:25:GLY:O	3:F:144:ARG:NH2	2.37	0.57
1:D:126:LEU:HB3	1:D:131:VAL:HG12	1.85	0.57
2:L:185:TYR:OH	2:L:247:ARG:NE	2.35	0.57
3:C:58:LYS:HE3	3:C:75:ILE:HB	1.86	0.57
3:F:283:THR:HG22	3:F:317:THR:HG22	1.86	0.57
3:I:192:VAL:HG23	3:I:194:GLY:H	1.69	0.57
1:J:133:LYS:HE2	1:J:160:GLU:HG3	1.87	0.57
3:M:417:ALA:O	3:M:419:LYS:NZ	2.32	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:201:PRO:HA	1:G:234:ARG:HA	1.87	0.57
3:I:299:LEU:HD11	3:I:326:GLU:HG3	1.87	0.56
3:F:211:THR:HG21	3:F:215:LYS:HD2	1.86	0.56
2:H:221:LEU:HA	2:H:233:TYR:HA	1.87	0.56
1:A:169:LYS:HA	1:A:169:LYS:HZ3	1.68	0.56
2:B:24:TYR:HD1	2:B:289:ARG:HA	1.71	0.56
3:F:162:GLU:HG2	3:F:257:PRO:HA	1.86	0.56
2:H:301:CYS:SG	2:H:302:THR:N	2.78	0.56
3:M:355:ILE:O	3:M:359:TYR:HB3	2.05	0.56
3:C:33:MET:HB3	3:C:51:ALA:HB2	1.87	0.56
2:B:309:SER:OG	2:B:311:ASP:OD1	2.21	0.56
1:J:151:TYR:HB3	1:J:162:ALA:HB2	1.87	0.56
2:B:74:PRO:HG3	2:B:213:LEU:HD21	1.88	0.56
2:B:308:HIS:HB2	2:B:380:PRO:HA	1.87	0.56
2:H:60:VAL:HG12	2:H:102:GLN:HG3	1.87	0.56
2:E:311:ASP:OD1	2:E:312:PHE:N	2.39	0.56
1:G:133:LYS:NZ	1:G:134:PRO:O	2.30	0.56
3:I:196:THR:HG22	3:I:212:THR:HG22	1.88	0.56
1:D:119:LYS:HD2	1:G:145:ASP:OD2	2.05	0.55
2:E:25:SER:OG	2:E:288:THR:OG1	2.23	0.55
3:M:328:ARG:HD3	3:M:334:PRO:HG3	1.88	0.55
3:F:69:TYR:OH	3:F:117:ASP:OD1	2.25	0.55
1:G:199:THR:HG23	1:G:234:ARG:HE	1.71	0.55
1:J:242:TRP:CD1	3:M:402:THR:HG22	2.40	0.55
2:L:159:THR:HG23	2:L:282:ILE:HA	1.88	0.55
3:C:225:CYS:O	3:C:226:GLN:NE2	2.40	0.55
3:F:213:THR:OG1	3:F:214:ASP:N	2.39	0.55
1:J:228:GLY:HA2	1:J:237:LEU:HA	1.86	0.55
2:L:306:CYS:SG	2:L:307:THR:N	2.80	0.55
2:E:328:CYS:SG	2:E:329:ASP:N	2.80	0.55
3:I:262:ASN:OD1	5:S:1:NAG:N2	2.39	0.55
2:B:247:ARG:NH1	2:B:249:SER:OG	2.39	0.55
3:F:187:ASN:HA	3:F:218:ASN:HB3	1.87	0.55
2:L:110:ARG:HB2	2:L:213:LEU:HD13	1.87	0.55
2:L:261:ILE:O	2:L:262:GLN:NE2	2.40	0.55
3:C:143:VAL:HB	3:I:128:ALA:HB2	1.88	0.55
3:F:28:CYS:SG	3:F:29:HIS:N	2.80	0.55
3:M:169:MET:HB3	3:M:235:TRP:HB3	1.88	0.54
1:A:130:LYS:HZ1	3:C:404:GLY:H	1.55	0.54
2:B:303:VAL:HG11	2:B:376:ALA:HB2	1.89	0.54
1:J:149:LEU:HD11	1:J:165:PRO:HD3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:407:TRP:HA	2:B:410:HIS:HB2	1.89	0.54
3:I:57:THR:O	3:I:68:ARG:NH2	2.41	0.54
2:B:51:TYR:HB3	2:B:203:ILE:HG13	1.89	0.54
3:I:263:THR:O	3:I:264:THR:OG1	2.25	0.54
2:L:225:ALA:H	2:L:230:HIS:CE1	2.26	0.54
2:H:207:THR:HG23	2:H:209:ASP:H	1.72	0.54
2:L:427:VAL:O	2:L:431:CYS:N	2.41	0.54
3:M:392:ARG:HH11	3:M:414:LEU:H	1.56	0.54
3:M:58:LYS:HG2	3:M:68:ARG:HH12	1.73	0.54
3:M:401:LEU:HD23	3:M:401:LEU:H	1.71	0.54
2:E:207:THR:HG22	2:E:208:LEU:H	1.73	0.54
1:J:125:CYS:SG	1:J:126:LEU:N	2.80	0.54
1:J:216:ASP:OD1	1:J:220:ARG:N	2.42	0.53
3:I:254:VAL:HG12	3:I:255:HIS:H	1.74	0.53
2:L:59:TYR:HB3	2:L:103:MET:HB3	1.90	0.53
3:F:36:ASN:HB2	3:F:49:GLN:HE21	1.74	0.53
3:C:80:ARG:HE	3:C:96:THR:HG21	1.74	0.53
1:J:114:VAL:N	1:J:122:GLY:O	2.36	0.53
2:B:63:CYS:HA	2:B:99:GLU:HB2	1.91	0.53
3:F:235:TRP:CE2	3:F:251:LYS:HE3	2.44	0.53
2:H:307:THR:HG22	2:H:309:SER:HB3	1.91	0.53
3:F:170:HIS:HA	3:F:251:LYS:HB3	1.91	0.53
3:I:352:HIS:HB2	3:I:354:ILE:HG12	1.90	0.53
2:B:320:TYR:OH	2:B:347:GLU:N	2.41	0.53
3:C:167:ILE:HG23	3:C:256:ILE:HD11	1.91	0.52
1:D:135:ALA:HA	1:D:160:GLU:HG2	1.90	0.52
1:J:176:THR:OG1	1:J:178:GLU:OE1	2.26	0.52
3:M:173:PRO:HA	3:M:245:ALA:HB2	1.90	0.52
1:D:228:GLY:O	1:D:256:GLU:N	2.42	0.52
1:A:169:LYS:HA	1:A:169:LYS:CE	2.39	0.52
1:D:193:TYR:CZ	1:D:196:GLY:HA2	2.45	0.52
3:C:40:ASP:OD1	3:C:40:ASP:N	2.36	0.52
2:E:10:GLN:OE1	2:E:11:VAL:N	2.42	0.52
2:L:136:THR:HA	2:L:141:ASN:HB3	1.92	0.52
2:L:358:SER:OG	2:L:396:THR:O	2.27	0.52
3:M:94:THR:OG1	3:M:102:LEU:O	2.27	0.52
3:M:35:GLU:HB3	3:M:49:GLN:NE2	2.25	0.52
3:C:14:PRO:HD3	3:C:53:GLN:HE22	1.75	0.52
3:C:43:ASP:OD1	3:C:44:GLY:N	2.43	0.52
3:C:203:CYS:SG	3:C:224:LYS:HG2	2.50	0.52
2:L:384:HIS:HB2	3:M:277:SER:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:LYS:CE	1:J:231:GLU:O	2.57	0.52
3:F:147:HIS:HA	3:F:266:ARG:HH11	1.74	0.52
3:M:89:SER:OG	3:M:90:GLU:N	2.43	0.52
3:F:185:SER:CB	3:F:187:ASN:H	2.23	0.51
2:L:341:GLU:OE1	2:L:341:GLU:N	2.43	0.51
2:L:147:TYR:H	2:L:152:HIS:CE1	2.28	0.51
1:D:224:ILE:HG22	1:D:225:VAL:H	1.76	0.51
1:A:198:PHE:HZ	1:A:214:ILE:HD13	1.76	0.51
2:B:301:CYS:HB3	2:B:318:LEU:HB2	1.93	0.51
1:G:146:LEU:HD21	1:G:168:MET:HG3	1.92	0.51
1:A:229:ALA:HB2	1:A:255:THR:HA	1.92	0.51
2:E:258:GLY:HA3	3:F:299:LEU:HD13	1.91	0.51
2:L:4:THR:OG1	2:L:278:VAL:O	2.20	0.51
3:F:199:TYR:HE2	3:F:215:LYS:HD3	1.75	0.51
3:I:406:VAL:HG22	3:I:408:PRO:HD3	1.92	0.51
3:C:91:CYS:HB3	3:C:106:PRO:HD2	1.91	0.51
2:E:259:CYS:SG	2:E:268:ALA:HB1	2.51	0.51
2:H:65:THR:HG22	2:H:101:THR:HG21	1.93	0.51
1:J:129:ASP:H	3:M:403:PRO:HB3	1.76	0.51
3:I:34:ILE:HD11	3:I:48:ILE:HD12	1.92	0.51
2:B:397:LEU:HG	3:C:362:HIS:HE1	1.76	0.50
3:C:63:ASP:OD1	3:C:65:THR:N	2.43	0.50
2:E:159:THR:HG22	2:E:283:ALA:H	1.76	0.50
2:L:308:HIS:NE2	2:L:358:SER:O	2.44	0.50
2:B:159:THR:HG23	2:B:282:ILE:HA	1.93	0.50
3:M:45:THR:HG22	3:M:104:LYS:HD3	1.92	0.50
3:C:58:LYS:N	3:C:77:GLU:OE2	2.44	0.50
1:G:141:ILE:HB	1:G:147:ALA:HB2	1.94	0.50
2:B:358:SER:HB3	2:B:397:LEU:HA	1.92	0.50
3:C:181:LEU:HD22	3:C:192:VAL:HG21	1.92	0.50
1:J:200:VAL:HG23	1:J:235:THR:HB	1.93	0.50
1:A:115:LYS:HA	1:A:120:VAL:HA	1.93	0.50
1:A:129:ASP:H	1:A:130:LYS:HD2	1.75	0.50
3:F:244:ARG:HG3	3:F:246:GLU:H	1.77	0.50
2:L:132:LYS:HG3	2:L:145:GLU:HB3	1.93	0.50
3:C:181:LEU:HD13	3:C:192:VAL:HB	1.94	0.50
2:E:129:LEU:HB3	2:E:148:VAL:HG11	1.94	0.50
2:E:40:PRO:HA	2:E:127:ALA:HA	1.94	0.50
1:A:156:LYS:HE2	1:A:157:TYR:HE2	1.75	0.49
3:I:368:VAL:HA	3:I:371:VAL:HG22	1.93	0.49
3:F:343:THR:OG1	3:F:344:GLU:N	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:9:ASN:HD22	2:H:276:ILE:HD11	1.77	0.49
2:L:408:ALA:HA	2:L:411:LEU:HB3	1.94	0.49
3:C:150:GLU:OE1	3:C:150:GLU:N	2.45	0.49
3:F:165:GLU:HG3	3:F:256:ILE:HB	1.95	0.49
1:G:141:ILE:HD12	1:G:141:ILE:H	1.77	0.49
1:J:247:VAL:HG21	3:M:401:LEU:HD11	1.94	0.49
1:A:209:ASP:OD1	1:A:212:ARG:NH2	2.46	0.49
3:C:42:THR:HA	3:C:134:ARG:HH22	1.77	0.49
3:C:326:GLU:CD	3:C:336:ARG:HE	2.14	0.49
1:D:202:THR:OG1	1:D:203:GLY:N	2.44	0.49
1:D:213:PRO:HG2	1:D:215:PHE:HE1	1.78	0.49
3:M:393:ASN:OD1	3:M:397:THR:OG1	2.30	0.49
2:B:337:ALA:HA	2:B:356:THR:OG1	2.13	0.49
3:M:369:VAL:O	3:M:373:VAL:HG23	2.13	0.49
1:A:169:LYS:HZ3	1:A:169:LYS:CA	2.25	0.48
2:H:148:VAL:O	2:H:164:GLY:HA3	2.13	0.48
2:L:63:CYS:HB3	2:L:99:GLU:HB2	1.95	0.48
1:G:184:TYR:HB2	1:G:191:VAL:HG13	1.95	0.48
3:M:198:LYS:N	3:M:228:TYR:O	2.42	0.48
1:A:130:LYS:NZ	3:C:404:GLY:H	2.10	0.48
1:J:242:TRP:HE1	3:M:402:THR:HA	1.78	0.48
3:F:67:ILE:N	3:F:78:ALA:O	2.46	0.48
3:F:185:SER:HB2	3:F:187:ASN:H	1.77	0.48
3:F:47:LYS:HA	3:F:102:LEU:HA	1.96	0.48
1:G:114:VAL:HG22	1:G:141:ILE:HA	1.96	0.48
1:G:129:ASP:HB3	3:I:403:PRO:HB3	1.96	0.48
2:B:421:LEU:O	2:B:425:ILE:HG12	2.14	0.48
3:C:170:HIS:NE2	3:C:249:GLU:O	2.47	0.48
3:C:286:LEU:HD11	3:C:294:LEU:HD12	1.96	0.48
3:F:12:THR:HA	3:F:235:TRP:H	1.78	0.48
3:M:138:ARG:HH12	3:M:328:ARG:HE	1.60	0.48
3:M:308:GLN:HE22	3:M:310:ILE:HD11	1.77	0.48
1:A:231:GLU:OE1	1:A:231:GLU:N	2.46	0.48
2:L:363:PHE:HB2	2:L:374:CYS:HB3	1.96	0.48
3:M:71:GLU:OE2	3:M:123:ARG:NH1	2.47	0.48
2:H:134:LYS:HA	2:H:143:THR:HA	1.96	0.48
2:H:160:LYS:HB3	2:H:281:ASP:HB3	1.96	0.48
2:H:400:LEU:HD23	2:H:402:SER:H	1.79	0.48
3:C:373:VAL:HA	3:C:376:VAL:HG22	1.94	0.47
1:G:216:ASP:OD1	1:G:220:ARG:N	2.35	0.47
2:B:147:TYR:H	2:B:152:HIS:HD2	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:48:THR:HG21	2:E:201:GLY:HA2	1.97	0.47
2:H:252:ASN:O	3:I:297:ARG:NH2	2.47	0.47
2:B:136:THR:HG22	2:B:141:ASN:HB3	1.96	0.47
3:M:214:ASP:OD1	3:M:214:ASP:N	2.45	0.47
2:E:112:ASP:OD1	2:E:112:ASP:N	2.41	0.47
3:M:121:GLU:OE1	3:M:123:ARG:NH2	2.47	0.47
1:A:125:CYS:SG	1:A:126:LEU:N	2.87	0.47
1:A:198:PHE:CZ	1:A:214:ILE:HD13	2.50	0.47
3:C:86:HIS:HB3	3:C:90:GLU:HA	1.97	0.47
3:F:386:TYR:HA	3:F:389:VAL:HG22	1.96	0.47
2:L:130:ARG:HG2	2:L:147:TYR:CD1	2.48	0.47
1:G:183:HIS:CE1	1:G:192:GLN:HE22	2.32	0.47
3:M:196:THR:HG23	3:M:230:THR:HB	1.96	0.47
3:M:346:ARG:HG2	3:M:347:ALA:H	1.79	0.47
1:G:135:ALA:HB1	1:G:153:LYS:HE3	1.97	0.47
2:H:44:LEU:H	2:H:44:LEU:HD23	1.79	0.47
2:L:201:GLY:O	2:L:204:GLN:NE2	2.48	0.47
2:L:356:THR:HG21	2:L:361:PRO:HD3	1.97	0.47
2:E:187:GLN:NE2	2:E:243:TRP:HE1	2.13	0.46
3:F:40:ASP:OD1	3:F:40:ASP:N	2.43	0.46
5:O:4:MAN:O3	5:O:5:MAN:H61	2.15	0.46
3:F:24:MET:SD	3:F:24:MET:N	2.89	0.46
2:H:59:TYR:HE1	3:I:246:GLU:HG3	1.79	0.46
3:M:169:MET:O	3:M:170:HIS:ND1	2.48	0.46
3:M:221:THR:HG22	3:M:222:VAL:H	1.79	0.46
5:U:3:BMA:O2	5:U:5:MAN:O6	2.32	0.46
3:F:373:VAL:HA	3:F:376:VAL:HG12	1.97	0.46
1:G:200:VAL:O	1:G:235:THR:N	2.45	0.46
2:L:212:ASP:N	2:L:212:ASP:OD1	2.48	0.46
3:F:370:VAL:HA	3:F:373:VAL:HG12	1.97	0.46
2:H:328:CYS:SG	2:H:329:ASP:N	2.89	0.46
3:I:223:ASP:N	3:I:223:ASP:OD1	2.47	0.46
1:J:124:ALA:HB2	1:J:133:LYS:HG3	1.97	0.46
2:H:258:GLY:HA3	3:I:299:LEU:HD23	1.98	0.46
1:A:151:TYR:HB3	1:A:160:GLU:HG3	1.98	0.46
1:G:180:PRO:O	1:G:184:TYR:OH	2.28	0.46
2:H:117:ASP:N	2:H:117:ASP:OD1	2.48	0.46
1:J:231:GLU:OE2	1:J:234:ARG:N	2.49	0.46
5:U:3:BMA:H3	5:U:4:MAN:H2	1.53	0.46
2:L:58:PRO:HG2	3:M:243:PRO:HA	1.98	0.46
2:B:84:VAL:HG22	2:B:86:PRO:HD3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:125:HIS:ND1	2:B:126:THR:HG22	2.31	0.46
3:I:85:VAL:HG22	3:I:113:VAL:HA	1.98	0.46
2:B:416:GLY:O	2:B:419:ILE:HG22	2.16	0.45
3:M:66:LYS:HB3	3:M:66:LYS:HE2	1.84	0.45
3:M:125:CYS:SG	3:M:126:ARG:N	2.89	0.45
3:M:183:GLN:HE22	3:M:188:VAL:HG13	1.79	0.45
2:H:191:PRO:O	2:L:152:HIS:HA	2.17	0.45
4:N:1:NAG:H5	4:N:2:NAG:H83	1.99	0.45
2:B:89:TRP:HB2	3:C:29:HIS:CD2	2.51	0.45
1:D:118:GLY:HA3	1:G:144:ILE:HG12	1.98	0.45
2:L:147:TYR:H	2:L:152:HIS:HE1	1.62	0.45
3:M:34:ILE:HD11	3:M:113:VAL:HG22	1.97	0.45
3:M:409:VAL:C	3:M:411:ILE:H	2.20	0.45
1:A:214:ILE:HD11	1:A:223:ALA:HB3	1.98	0.45
3:C:319:PRO:O	3:C:325:VAL:HG21	2.17	0.45
3:F:189:LYS:HG2	3:F:216:THR:HB	1.98	0.45
2:H:62:CYS:HB2	2:H:96:CYS:HB2	1.99	0.45
2:L:403:THR:HG21	3:M:348:HIS:ND1	2.30	0.45
1:A:156:LYS:HE2	1:A:157:TYR:CE2	2.52	0.45
3:F:52:SER:OG	3:F:53:GLN:N	2.50	0.45
3:I:176:PRO:HA	3:I:228:TYR:HB3	1.98	0.45
3:M:56:LEU:HB3	3:M:68:ARG:HG2	1.98	0.45
3:I:277:SER:OG	3:I:278:GLY:N	2.50	0.45
2:B:25:SER:HG	2:B:288:THR:HG1	1.50	0.45
2:E:356:THR:OG1	2:E:357:ALA:N	2.50	0.45
3:F:86:HIS:HB3	3:F:90:GLU:HA	1.99	0.45
2:H:96:CYS:O	2:H:99:GLU:N	2.37	0.45
3:I:150:GLU:HB2	3:I:264:THR:HG21	1.99	0.45
1:J:205:GLY:HA3	1:J:258:TRP:CH2	2.51	0.45
3:M:289:ILE:O	3:M:290:HIS:ND1	2.50	0.45
2:B:336:VAL:HG12	2:B:356:THR:HG21	1.99	0.45
3:I:154:THR:HA	3:I:262:ASN:HB3	1.99	0.45
3:I:173:PRO:HB3	3:I:245:ALA:N	2.31	0.45
3:I:235:TRP:CD1	3:I:251:LYS:HD3	2.52	0.45
2:E:73:LYS:HB2	2:E:76:TYR:HB2	1.98	0.45
2:E:125:HIS:CD2	2:E:126:THR:HG22	2.52	0.45
3:I:12:THR:HG22	3:I:235:TRP:HB2	1.99	0.44
2:L:205:SER:OG	2:L:207:THR:O	2.33	0.44
3:I:14:PRO:HD2	3:I:75:ILE:HD12	1.99	0.44
3:I:67:ILE:HG23	3:I:78:ALA:HB3	1.98	0.44
2:L:18:HIS:CE1	2:L:26:PRO:HB2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:426:LEU:O	2:L:430:THR:OG1	2.35	0.44
3:M:7:ASN:HA	3:M:10:LYS:NZ	2.31	0.44
1:A:143:ASN:HD22	1:A:146:LEU:H	1.64	0.44
3:C:387:MET:HA	3:C:390:VAL:HG22	1.99	0.44
2:E:77:LYS:NZ	2:E:219:LEU:O	2.45	0.44
2:L:25:SER:OG	2:L:288:THR:OG1	2.35	0.44
2:L:49:CYS:HB2	2:L:114:CYS:HB2	1.85	0.44
3:M:263:THR:HG22	3:M:264:THR:H	1.81	0.44
1:D:127:VAL:HG12	1:D:128:GLY:H	1.81	0.44
3:F:25:GLY:HA3	3:I:104:LYS:NZ	2.33	0.44
3:I:63:ASP:OD2	3:I:66:LYS:N	2.51	0.44
3:C:183:GLN:HE22	3:C:222:VAL:HG11	1.83	0.44
3:C:348:HIS:HA	3:C:354:ILE:HG12	2.00	0.44
2:H:13:PHE:HD2	2:H:393:ASN:HD22	1.64	0.44
2:H:295:ILE:HG22	2:H:324:LYS:HB3	1.99	0.44
3:I:235:TRP:CG	3:I:251:LYS:HD3	2.52	0.44
3:M:244:ARG:HG2	3:M:245:ALA:O	2.18	0.44
3:C:162:GLU:O	3:C:255:HIS:ND1	2.41	0.44
2:H:129:LEU:HD12	2:H:130:ARG:H	1.82	0.44
3:F:138:ARG:HB3	3:F:293:LEU:HB2	1.99	0.44
3:I:171:MET:HB2	3:I:251:LYS:HE3	1.99	0.44
3:I:263:THR:HG23	3:I:264:THR:H	1.82	0.44
2:B:419:ILE:HD11	3:C:387:MET:HB3	2.00	0.44
2:E:58:PRO:HB3	2:E:102:GLN:HE21	1.82	0.44
2:E:61:LYS:HD2	2:E:61:LYS:HA	1.77	0.44
3:F:53:GLN:HE21	3:F:68:ARG:HD2	1.83	0.44
2:H:17:ALA:HB3	2:H:29:LEU:HG	1.99	0.44
3:I:165:GLU:N	3:I:165:GLU:OE1	2.51	0.44
2:L:18:HIS:HE1	2:L:26:PRO:HB2	1.82	0.44
1:A:207:PRO:HA	1:A:258:TRP:CD1	2.53	0.44
2:B:18:HIS:HA	2:B:28:THR:HG22	2.00	0.44
2:B:18:HIS:HB2	2:B:331:HIS:CD2	2.52	0.44
2:E:57:SER:N	3:F:238:ASN:OD1	2.50	0.44
2:E:185:TYR:OH	2:E:247:ARG:NE	2.50	0.44
3:F:286:LEU:HD22	3:F:329:TRP:CE2	2.53	0.44
3:I:83:LEU:HD21	3:I:101:ILE:HD12	1.99	0.44
3:M:396:LEU:HD21	3:M:414:LEU:HB2	1.99	0.44
3:F:16:VAL:HG23	3:F:70:ALA:HB3	2.00	0.43
2:L:178:VAL:HG13	2:L:185:TYR:HB2	1.99	0.43
2:B:399:ASP:N	2:B:399:ASP:OD1	2.49	0.43
2:E:153:ALA:HA	2:E:162:ILE:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:164:SER:O	3:F:164:SER:OG	2.30	0.43
3:F:234:LYS:HA	3:F:234:LYS:HD3	1.82	0.43
3:M:189:LYS:HG2	3:M:216:THR:HG22	1.99	0.43
1:A:132:MET:HB2	1:A:159:LEU:HD11	2.00	0.43
3:C:9:TYR:CD2	3:C:56:LEU:HD11	2.53	0.43
3:F:86:HIS:HA	3:F:91:CYS:H	1.83	0.43
3:F:167:ILE:HB	3:F:256:ILE:HD11	1.99	0.43
2:E:9:ASN:HB2	2:E:276:ILE:HG13	2.00	0.43
2:H:176:LYS:HB3	2:H:189:PHE:CE2	2.54	0.43
2:L:72:ASP:OD1	2:L:72:ASP:N	2.48	0.43
1:A:116:HIS:NE2	1:A:117:GLU:HG3	2.33	0.43
1:A:242:TRP:HB2	3:C:402:THR:HG23	1.99	0.43
3:I:294:LEU:HD13	3:I:329:TRP:HD1	1.84	0.43
3:M:372:ALA:HA	3:M:375:VAL:HG12	1.98	0.43
1:A:197:ARG:HA	1:A:197:ARG:HD3	1.78	0.43
3:C:24:MET:HG3	3:F:104:LYS:HG3	1.99	0.43
2:E:16:LYS:HD3	2:E:30:GLN:HB3	2.00	0.43
3:I:296:TYR:HE1	3:I:306:ASP:HB3	1.84	0.43
2:E:259:CYS:HB2	2:E:271:CYS:HB3	1.34	0.43
1:G:201:PRO:HG2	1:G:204:VAL:HG11	2.00	0.43
3:I:162:GLU:HB3	3:I:255:HIS:CD2	2.54	0.43
3:M:362:HIS:HB3	3:M:365:THR:OG1	2.19	0.43
1:A:216:ASP:OD1	1:A:219:GLY:N	2.30	0.43
2:B:24:TYR:CD1	2:B:289:ARG:HA	2.52	0.43
1:D:115:LYS:NZ	1:D:118:GLY:O	2.34	0.43
1:D:213:PRO:HA	1:D:224:ILE:HA	2.01	0.43
3:M:69:TYR:HE2	3:M:71:GLU:HB2	1.82	0.43
1:A:169:LYS:HZ3	1:A:169:LYS:CB	2.31	0.43
3:C:97:MET:HB3	3:C:258:PHE:HZ	1.84	0.43
3:M:58:LYS:CB	3:M:68:ARG:HH22	2.32	0.43
3:C:344:GLU:CD	3:C:345:GLY:H	2.22	0.43
2:E:248:ASP:OD1	2:E:248:ASP:N	2.44	0.43
3:I:172:PRO:HB3	3:I:236:GLN:HG3	2.01	0.43
3:C:289:ILE:HG23	3:C:290:HIS:CD2	2.54	0.42
2:H:262:GLN:OE1	2:H:267:ARG:NH1	2.51	0.42
2:E:7:ILE:HD11	2:E:31:MET:HG3	2.01	0.42
2:H:294:PRO:HG3	2:H:326:GLY:HA3	2.00	0.42
3:I:183:GLN:HA	3:I:188:VAL:HA	2.02	0.42
3:M:68:ARG:HD2	3:M:75:ILE:HG22	2.01	0.42
3:M:68:ARG:HH21	3:M:75:ILE:HG22	1.83	0.42
2:E:302:THR:OG1	2:E:317:VAL:O	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:414:GLY:O	2:H:417:LEU:HB3	2.20	0.42
3:I:341:LEU:HD22	3:I:361:LEU:HD11	2.01	0.42
2:L:303:VAL:HG23	2:L:316:ALA:HB2	2.02	0.42
2:L:318:LEU:HB2	2:L:350:SER:OG	2.18	0.42
3:M:351:PRO:HA	3:M:354:ILE:HG12	2.00	0.42
1:A:133:LYS:HB2	1:A:133:LYS:HE3	1.81	0.42
1:A:156:LYS:HG3	1:A:157:TYR:CD2	2.54	0.42
3:C:17:ALA:HB3	3:C:33:MET:HB2	2.01	0.42
3:C:184:GLN:HB2	3:C:187:ASN:HB2	2.01	0.42
1:G:176:THR:HG22	1:G:178:GLU:OE1	2.20	0.42
3:I:320:VAL:HG22	3:I:325:VAL:HG11	2.01	0.42
1:J:200:VAL:HG13	1:J:237:LEU:HD22	2.00	0.42
2:L:202:ASP:OD1	2:L:203:ILE:N	2.50	0.42
3:I:32:ALA:O	3:I:125:CYS:HB3	2.19	0.42
2:B:332:SER:OG	2:B:333:HIS:N	2.53	0.42
3:F:198:LYS:NZ	3:F:199:TYR:O	2.34	0.42
3:F:310:ILE:HD12	3:F:310:ILE:HA	1.93	0.42
1:G:199:THR:O	1:G:234:ARG:NH2	2.52	0.42
2:H:44:LEU:HB3	2:H:122:TYR:CE1	2.55	0.42
3:I:53:GLN:HG2	3:I:99:HIS:CD2	2.55	0.42
3:M:330:GLY:O	3:M:331:ASN:ND2	2.52	0.42
1:A:126:LEU:HD13	1:A:131:VAL:HG13	2.01	0.42
2:B:2:GLU:HA	2:B:280:MET:O	2.20	0.42
2:B:308:HIS:HB2	2:B:381:PRO:HD3	2.00	0.42
3:I:91:CYS:SG	3:I:106:PRO:HD2	2.60	0.42
2:H:261:ILE:HD13	2:H:261:ILE:HA	1.90	0.42
2:H:321:LYS:HA	2:H:321:LYS:HD2	1.85	0.42
3:I:294:LEU:HB2	3:I:329:TRP:HD1	1.84	0.42
3:I:294:LEU:HB2	3:I:329:TRP:CD1	2.55	0.42
3:M:230:THR:HG23	3:M:232:HIS:CD2	2.55	0.42
3:M:366:THR:HG22	3:M:369:VAL:HG11	2.02	0.42
3:C:288:PRO:HG3	3:C:310:ILE:HG22	2.02	0.42
3:F:184:GLN:O	3:F:184:GLN:HG2	2.20	0.42
2:H:330:VAL:HA	2:H:366:SER:O	2.20	0.42
2:H:331:HIS:HD2	2:H:333:HIS:HD2	1.66	0.42
1:A:240:VAL:HA	1:A:249:LYS:HA	2.01	0.41
3:C:151:LEU:HD23	3:C:151:LEU:HA	1.85	0.41
3:C:359:TYR:O	3:C:363:PRO:HB3	2.20	0.41
3:M:188:VAL:O	3:M:216:THR:HA	2.20	0.41
3:M:294:LEU:HB2	3:M:329:TRP:HD1	1.85	0.41
3:M:350:TRP:CD2	3:M:351:PRO:HD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:205:SER:OG	2:B:207:THR:O	2.36	0.41
3:C:358:TYR:O	3:C:366:THR:HG21	2.20	0.41
1:D:159:LEU:HD21	1:D:240:VAL:HG21	2.03	0.41
2:E:399:ASP:OD1	2:E:399:ASP:N	2.53	0.41
2:E:425:ILE:HA	2:E:428:ILE:HG22	2.01	0.41
3:F:9:TYR:HE2	3:F:99:HIS:HB2	1.85	0.41
3:F:192:VAL:HG12	3:F:214:ASP:HB2	2.03	0.41
3:I:314:THR:HG22	3:I:315:GLU:H	1.86	0.41
3:I:41:ALA:HB2	3:I:156:TYR:CE1	2.55	0.41
2:L:301:CYS:SG	2:L:374:CYS:HB2	2.60	0.41
1:D:244:LYS:HB2	1:D:244:LYS:HE3	1.84	0.41
3:I:89:SER:OG	3:I:90:GLU:N	2.53	0.41
3:I:127:ILE:HD12	3:I:127:ILE:HA	1.91	0.41
1:J:113:GLU:HA	1:J:123:TYR:HD1	1.84	0.41
3:M:22:CYS:SG	3:M:30:SER:HB2	2.61	0.41
2:E:220:LYS:HE3	2:E:220:LYS:HB2	1.83	0.41
3:F:296:TYR:CE1	3:F:306:ASP:HB3	2.55	0.41
1:G:135:ALA:HB2	1:G:160:GLU:HG3	2.02	0.41
2:H:383:ASP:OD1	2:H:384:HIS:N	2.52	0.41
3:I:117:ASP:OD1	3:I:118:SER:N	2.53	0.41
3:M:381:VAL:O	3:M:385:VAL:HG23	2.20	0.41
3:F:312:THR:HG22	3:F:313:GLN:H	1.85	0.41
3:F:346:ARG:HD2	3:F:346:ARG:HA	1.84	0.41
1:G:242:TRP:HD1	3:I:402:THR:HG22	1.85	0.41
2:H:185:TYR:CE2	2:H:247:ARG:HB3	2.55	0.41
3:I:328:ARG:HH21	3:I:334:PRO:HG3	1.85	0.41
5:O:1:NAG:H62	5:O:2:NAG:HN2	1.86	0.41
2:B:361:PRO:HB2	2:B:363:PHE:HD1	1.86	0.41
3:F:121:GLU:N	3:F:121:GLU:OE1	2.53	0.41
2:L:377:LYS:HB2	3:M:348:HIS:CE1	2.56	0.41
3:C:306:ASP:OD1	3:C:307:GLU:N	2.53	0.41
1:D:227:GLY:HA2	1:D:258:TRP:HB2	2.03	0.41
2:H:229:ILE:HD13	2:H:229:ILE:HA	1.95	0.41
2:H:419:ILE:O	2:H:423:VAL:HG23	2.20	0.41
3:I:202:SER:HA	3:I:207:PRO:HA	2.03	0.41
2:B:42:LEU:HD23	2:B:122:TYR:CG	2.56	0.41
2:B:193:GLY:O	2:B:214:TYR:OH	2.30	0.41
2:B:311:ASP:OD1	2:B:311:ASP:N	2.54	0.41
3:C:279:LYS:HG2	3:C:280:ARG:HG2	2.02	0.41
2:E:356:THR:HG21	2:E:361:PRO:HG3	2.02	0.41
3:F:14:PRO:HG3	3:F:53:GLN:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:33:VAL:HA	2:H:133:ILE:HG22	2.03	0.41
2:H:45:GLU:HG2	2:H:46:TYR:H	1.84	0.41
3:I:201:CYS:O	3:I:203:CYS:N	2.54	0.41
1:A:237:LEU:HD12	1:A:237:LEU:HA	1.89	0.41
2:B:207:THR:HG22	2:B:210:SER:HB2	2.02	0.41
3:C:190:ILE:N	3:C:214:ASP:OD1	2.54	0.41
3:M:88:SER:OG	3:M:107:PRO:O	2.31	0.41
2:B:312:PHE:HA	2:B:355:SER:OG	2.21	0.40
3:F:201:CYS:HB3	3:F:202:SER:H	1.79	0.40
3:F:206:LYS:HE2	3:F:219:SER:HB3	2.02	0.40
2:L:71:GLN:HB3	2:L:76:TYR:CZ	2.56	0.40
1:A:224:ILE:HG13	1:A:225:VAL:H	1.85	0.40
2:B:330:VAL:HG12	2:B:367:VAL:HB	2.03	0.40
1:G:244:LYS:HD2	1:G:244:LYS:HA	1.90	0.40
3:I:37:VAL:HG23	3:I:38:GLN:H	1.86	0.40
3:M:58:LYS:HB2	3:M:58:LYS:HE3	1.91	0.40
2:B:142:GLN:HG3	2:B:156:ILE:HG21	2.02	0.40
3:C:102:LEU:HD11	3:C:156:TYR:HD2	1.85	0.40
3:F:184:GLN:OE1	3:F:184:GLN:N	2.55	0.40
2:L:141:ASN:OD1	2:L:141:ASN:N	2.54	0.40
2:L:206:ARG:HD3	2:L:206:ARG:HA	1.93	0.40
2:B:50:ASP:OD1	2:B:51:TYR:N	2.55	0.40
3:F:294:LEU:HB2	3:F:329:TRP:HD1	1.85	0.40
1:G:152:LYS:HD3	1:G:153:LYS:H	1.86	0.40
1:A:257:GLU:H	1:A:257:GLU:HG3	1.73	0.40
1:D:185:ASN:N	1:D:185:ASN:OD1	2.53	0.40
2:E:32:GLN:HE21	2:E:134:LYS:HE3	1.86	0.40
2:E:159:THR:HG22	2:E:282:ILE:HA	2.02	0.40
3:I:54:ILE:HG22	3:I:67:ILE:HG13	2.03	0.40
3:I:54:ILE:HD12	3:I:96:THR:HB	2.03	0.40
2:L:296:ILE:HG21	2:L:320:TYR:CD1	2.57	0.40
3:M:294:LEU:HD13	3:M:329:TRP:HB2	2.03	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	150/258 (58%)	137 (91%)	13 (9%)	0	100	100
1	D	150/258 (58%)	137 (91%)	12 (8%)	1 (1%)	22	62
1	G	150/258 (58%)	139 (93%)	11 (7%)	0	100	100
1	J	150/258 (58%)	133 (89%)	17 (11%)	0	100	100
2	B	431/436 (99%)	389 (90%)	42 (10%)	0	100	100
2	E	431/436 (99%)	394 (91%)	37 (9%)	0	100	100
2	H	431/436 (99%)	378 (88%)	53 (12%)	0	100	100
2	L	431/436 (99%)	379 (88%)	51 (12%)	1 (0%)	47	81
3	C	414/422 (98%)	353 (85%)	61 (15%)	0	100	100
3	F	414/422 (98%)	359 (87%)	54 (13%)	1 (0%)	47	81
3	I	414/422 (98%)	366 (88%)	48 (12%)	0	100	100
3	M	414/422 (98%)	354 (86%)	59 (14%)	1 (0%)	47	81
All	All	3980/4464 (89%)	3518 (88%)	458 (12%)	4 (0%)	54	85

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	140	VAL
3	F	212	THR
3	M	58	LYS
1	D	252	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	124/220 (56%)	121 (98%)	3 (2%)	49	69
1	D	124/220 (56%)	124 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	124/220 (56%)	124 (100%)	0	100	100
1	J	124/220 (56%)	122 (98%)	2 (2%)	62	79
2	B	360/363 (99%)	358 (99%)	2 (1%)	86	92
2	E	360/363 (99%)	356 (99%)	4 (1%)	73	85
2	H	360/363 (99%)	360 (100%)	0	100	100
2	L	360/363 (99%)	358 (99%)	2 (1%)	86	92
3	C	363/366 (99%)	361 (99%)	2 (1%)	86	92
3	F	363/366 (99%)	361 (99%)	2 (1%)	86	92
3	I	363/366 (99%)	361 (99%)	2 (1%)	86	92
3	M	363/366 (99%)	361 (99%)	2 (1%)	86	92
All	All	3388/3796 (89%)	3367 (99%)	21 (1%)	86	92

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	148	ARG
1	A	169	LYS
1	A	241	THR
2	B	63	CYS
2	B	289	ARG
3	C	195	ARG
3	C	253	LYS
2	E	61	LYS
2	E	160	LYS
2	E	161	PHE
2	E	271	CYS
3	F	401	LEU
3	F	416	CYS
3	I	225	CYS
3	I	262	ASN
1	J	151	TYR
1	J	222	VAL
2	L	21	ARG
2	L	63	CYS
3	M	80	ARG
3	M	280	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	143	ASN
1	A	187	HIS
2	B	10	GLN
2	B	152	HIS
2	B	196	GLN
2	B	204	GLN
2	B	235	GLN
2	B	391	ASN
3	C	157	GLN
3	C	183	GLN
3	C	218	ASN
3	C	290	HIS
3	C	308	GLN
3	C	362	HIS
2	E	43	ASN
2	E	100	ASN
2	E	125	HIS
2	E	187	GLN
2	E	204	GLN
2	E	270	ASN
2	E	340	GLN
3	F	49	GLN
3	F	53	GLN
3	F	236	GLN
3	F	287	HIS
3	F	308	GLN
3	F	331	ASN
3	F	332	HIS
3	F	340	GLN
1	G	192	GLN
2	H	9	ASN
2	H	125	HIS
2	H	152	HIS
2	H	331	HIS
3	I	49	GLN
3	I	99	HIS
3	I	131	HIS
1	J	192	GLN
2	L	9	ASN
2	L	18	HIS
2	L	152	HIS
2	L	230	HIS
2	L	244	GLN

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Mol	Chain	Res	Type
2	L	262	GLN
3	M	247	GLN
3	M	331	ASN
3	M	362	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

31 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	$\#\|Z\| > 2$
4	NAG	N	1	4,2	14,14,15	0.79	1 (7%)	17,19,21	1.08	1 (5%)
4	NAG	N	2	4	14,14,15	0.19	0	17,19,21	0.40	0
4	BMA	N	3	4	11,11,12	0.74	0	15,15,17	0.83	0
5	NAG	O	1	3,5	14,14,15	0.30	0	17,19,21	0.60	0
5	NAG	O	2	5	14,14,15	0.29	0	17,19,21	0.59	0
5	BMA	O	3	5	11,11,12	0.69	0	15,15,17	1.06	1 (6%)
5	MAN	O	4	5	11,11,12	0.83	0	15,15,17	1.18	2 (13%)
5	MAN	O	5	5	11,11,12	0.25	0	15,15,17	0.67	0
4	NAG	P	1	4,2	14,14,15	0.32	0	17,19,21	0.76	1 (5%)
4	NAG	P	2	4	14,14,15	1.29	1 (7%)	17,19,21	1.24	1 (5%)
4	BMA	P	3	4	11,11,12	0.40	0	15,15,17	1.17	2 (13%)
5	NAG	Q	1	3,5	14,14,15	0.56	0	17,19,21	0.66	0
5	NAG	Q	2	5	14,14,15	0.55	0	17,19,21	1.74	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	BMA	Q	3	5	11,11,12	0.82	0	15,15,17	1.54	3 (20%)
5	MAN	Q	4	5	11,11,12	0.36	0	15,15,17	0.96	1 (6%)
5	MAN	Q	5	5	11,11,12	0.26	0	15,15,17	0.84	0
6	NAG	R	1	6,2	14,14,15	0.27	0	17,19,21	0.47	0
6	NAG	R	2	6	14,14,15	0.33	0	17,19,21	0.40	0
5	NAG	S	1	3,5	14,14,15	0.33	0	17,19,21	0.43	0
5	NAG	S	2	5	14,14,15	0.26	0	17,19,21	0.37	0
5	BMA	S	3	5	11,11,12	0.46	0	15,15,17	2.06	3 (20%)
5	MAN	S	4	5	11,11,12	0.23	0	15,15,17	0.91	1 (6%)
5	MAN	S	5	5	11,11,12	0.19	0	15,15,17	0.86	0
4	NAG	T	1	4,2	14,14,15	0.33	0	17,19,21	0.83	1 (5%)
4	NAG	T	2	4	14,14,15	0.47	0	17,19,21	0.94	2 (11%)
4	BMA	T	3	4	11,11,12	0.45	0	15,15,17	1.00	1 (6%)
5	NAG	U	1	3,5	14,14,15	0.24	0	17,19,21	0.57	0
5	NAG	U	2	5	14,14,15	0.19	0	17,19,21	0.48	0
5	BMA	U	3	5	11,11,12	0.54	0	15,15,17	1.60	2 (13%)
5	MAN	U	4	5	11,11,12	0.28	0	15,15,17	0.90	1 (6%)
5	MAN	U	5	5	11,11,12	0.27	0	15,15,17	0.91	1 (6%)

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
4	NAG	N	1	4,2	-	3/6/23/26	0/1/1/1
4	NAG	N	2	4	-	4/6/23/26	0/1/1/1
4	BMA	N	3	4	-	1/2/19/22	0/1/1/1
5	NAG	O	1	3,5	-	2/6/23/26	0/1/1/1
5	NAG	O	2	5	-	2/6/23/26	0/1/1/1
5	BMA	O	3	5	-	0/2/19/22	0/1/1/1
5	MAN	O	4	5	-	0/2/19/22	0/1/1/1
5	MAN	O	5	5	-	2/2/19/22	0/1/1/1
4	NAG	P	1	4,2	-	4/6/23/26	0/1/1/1
4	NAG	P	2	4	-	3/6/23/26	0/1/1/1
4	BMA	P	3	4	-	1/2/19/22	1/1/1/1
5	NAG	Q	1	3,5	-	3/6/23/26	0/1/1/1
5	NAG	Q	2	5	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BMA	Q	3	5	-	0/2/19/22	0/1/1/1
5	MAN	Q	4	5	-	2/2/19/22	0/1/1/1
5	MAN	Q	5	5	-	0/2/19/22	0/1/1/1
6	NAG	R	1	6,2	-	4/6/23/26	0/1/1/1
6	NAG	R	2	6	-	1/6/23/26	0/1/1/1
5	NAG	S	1	3,5	-	2/6/23/26	0/1/1/1
5	NAG	S	2	5	-	3/6/23/26	0/1/1/1
5	BMA	S	3	5	-	2/2/19/22	0/1/1/1
5	MAN	S	4	5	-	0/2/19/22	0/1/1/1
5	MAN	S	5	5	-	0/2/19/22	0/1/1/1
4	NAG	T	1	4,2	-	3/6/23/26	0/1/1/1
4	NAG	T	2	4	-	2/6/23/26	0/1/1/1
4	BMA	T	3	4	-	0/2/19/22	0/1/1/1
5	NAG	U	1	3,5	-	0/6/23/26	0/1/1/1
5	NAG	U	2	5	-	3/6/23/26	0/1/1/1
5	BMA	U	3	5	-	2/2/19/22	0/1/1/1
5	MAN	U	4	5	-	0/2/19/22	0/1/1/1
5	MAN	U	5	5	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	P	2	NAG	O5-C1	-4.03	1.37	1.43
4	N	1	NAG	C1-C2	2.45	1.56	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	Q	2	NAG	C2-N2-C7	6.06	131.53	122.90
5	S	3	BMA	O5-C5-C6	5.88	116.43	107.20
5	U	3	BMA	O5-C5-C6	4.81	114.74	107.20
5	Q	3	BMA	O3-C3-C2	4.07	117.79	109.99
5	S	3	BMA	O3-C3-C4	-3.57	102.09	110.35
4	P	2	NAG	C4-C3-C2	3.47	116.11	111.02
4	N	1	NAG	C1-O5-C5	3.38	116.77	112.19
4	P	3	BMA	C1-O5-C5	3.11	116.41	112.19
5	O	4	MAN	C1-O5-C5	3.10	116.39	112.19
5	O	3	BMA	C1-O5-C5	2.96	116.20	112.19
5	U	3	BMA	O3-C3-C2	-2.88	104.49	109.99
5	Q	2	NAG	C1-C2-N2	2.75	115.18	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	Q	4	MAN	C1-O5-C5	2.70	115.85	112.19
4	P	1	NAG	C1-O5-C5	2.63	115.76	112.19
4	P	3	BMA	O5-C5-C6	2.53	111.17	107.20
4	T	2	NAG	C1-O5-C5	2.43	115.48	112.19
5	O	4	MAN	O2-C2-C3	-2.32	105.49	110.14
5	S	3	BMA	C6-C5-C4	-2.22	107.80	113.00
5	Q	3	BMA	C3-C4-C5	-2.21	106.30	110.24
4	T	1	NAG	C1-O5-C5	2.18	115.14	112.19
5	Q	3	BMA	O5-C1-C2	-2.16	107.44	110.77
4	T	2	NAG	C2-N2-C7	2.15	125.97	122.90
5	U	4	MAN	O5-C1-C2	-2.14	107.46	110.77
5	U	5	MAN	O5-C1-C2	-2.14	107.47	110.77
4	T	3	BMA	O5-C5-C6	2.10	110.50	107.20
5	S	4	MAN	O5-C1-C2	-2.04	107.62	110.77

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	O	1	NAG	O5-C5-C6-O6
4	N	1	NAG	O5-C5-C6-O6
5	U	3	BMA	O5-C5-C6-O6
5	O	5	MAN	O5-C5-C6-O6
5	S	1	NAG	O5-C5-C6-O6
4	N	1	NAG	C4-C5-C6-O6
4	P	2	NAG	C4-C5-C6-O6
5	O	1	NAG	C4-C5-C6-O6
4	N	2	NAG	C4-C5-C6-O6
6	R	1	NAG	O5-C5-C6-O6
5	Q	4	MAN	O5-C5-C6-O6
5	U	3	BMA	C4-C5-C6-O6
4	P	1	NAG	O5-C5-C6-O6
4	N	2	NAG	C8-C7-N2-C2
4	N	2	NAG	O7-C7-N2-C2
4	P	1	NAG	C8-C7-N2-C2
4	P	1	NAG	O7-C7-N2-C2
5	Q	2	NAG	C8-C7-N2-C2
5	Q	2	NAG	O7-C7-N2-C2
5	U	2	NAG	C8-C7-N2-C2
5	U	2	NAG	O7-C7-N2-C2
5	S	2	NAG	C8-C7-N2-C2
5	S	2	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
6	R	1	NAG	C8-C7-N2-C2
6	R	1	NAG	O7-C7-N2-C2
4	T	1	NAG	C4-C5-C6-O6
6	R	1	NAG	C4-C5-C6-O6
5	O	5	MAN	C4-C5-C6-O6
4	P	1	NAG	C4-C5-C6-O6
5	O	2	NAG	C4-C5-C6-O6
4	N	2	NAG	O5-C5-C6-O6
5	S	1	NAG	C4-C5-C6-O6
4	P	3	BMA	O5-C5-C6-O6
4	P	2	NAG	O5-C5-C6-O6
4	T	1	NAG	O5-C5-C6-O6
5	S	2	NAG	O5-C5-C6-O6
4	N	3	BMA	O5-C5-C6-O6
5	O	2	NAG	O5-C5-C6-O6
6	R	2	NAG	O5-C5-C6-O6
5	Q	1	NAG	C4-C5-C6-O6
4	T	2	NAG	O5-C5-C6-O6
5	S	3	BMA	C4-C5-C6-O6
5	Q	4	MAN	C4-C5-C6-O6
5	S	3	BMA	O5-C5-C6-O6
4	N	1	NAG	C3-C2-N2-C7
4	P	2	NAG	C3-C2-N2-C7
4	T	1	NAG	C3-C2-N2-C7
4	T	2	NAG	C3-C2-N2-C7
5	Q	1	NAG	C3-C2-N2-C7
5	Q	2	NAG	C3-C2-N2-C7
5	Q	1	NAG	O5-C5-C6-O6
5	U	2	NAG	C4-C5-C6-O6

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	P	3	BMA	C1-C2-C3-C4-C5-O5

11 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	O	5	MAN	1	0
5	U	4	MAN	1	0
4	N	1	NAG	1	0
5	O	4	MAN	1	0

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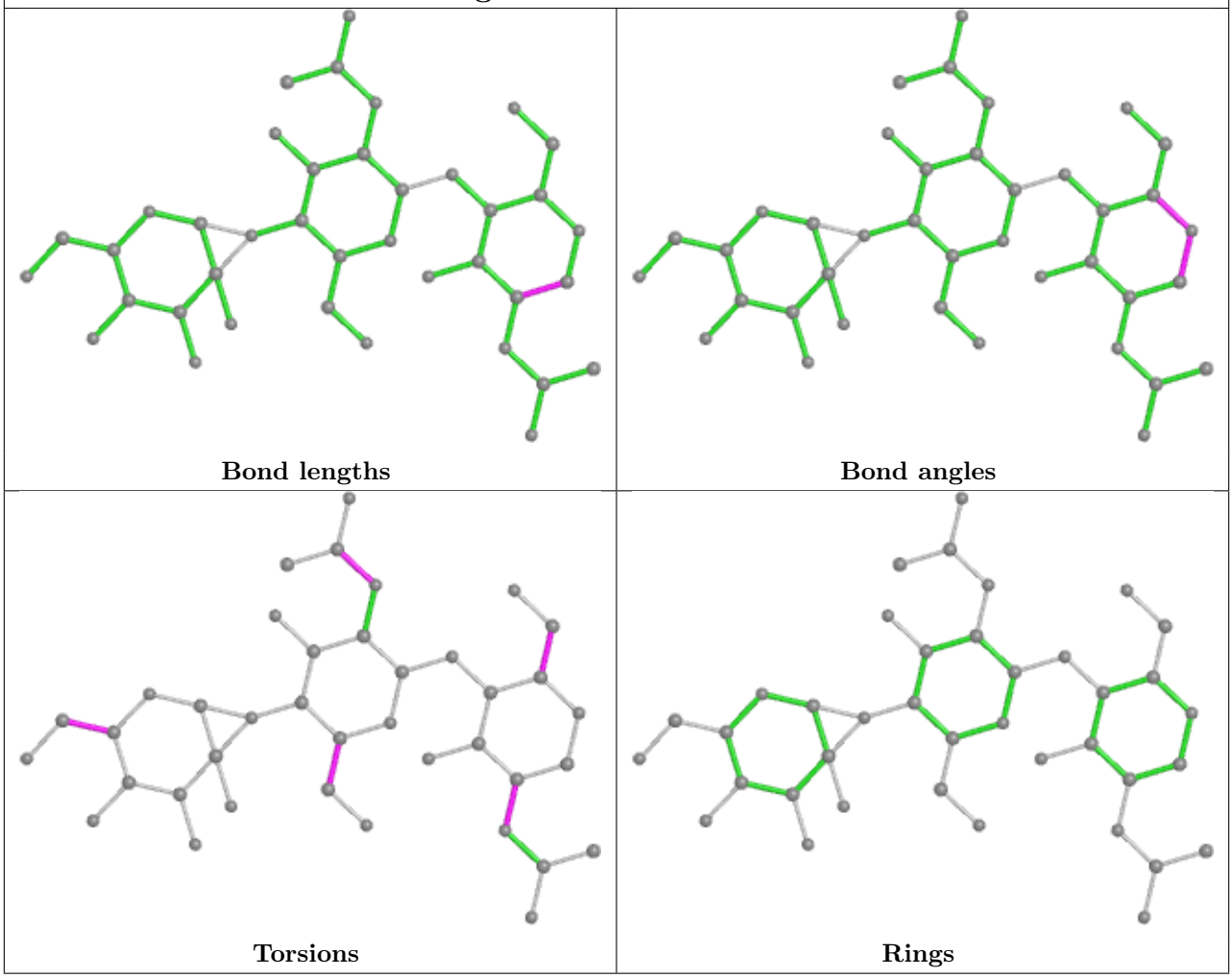
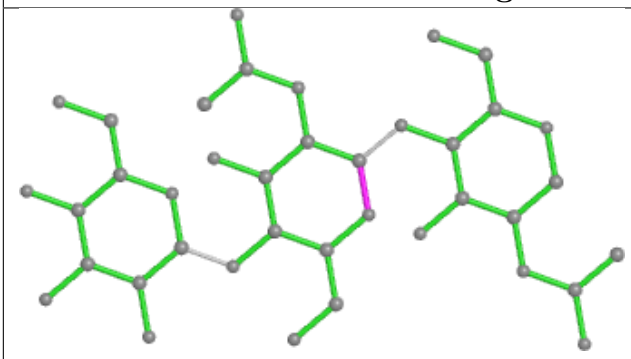
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	S	1	NAG	1	0
5	O	1	NAG	1	0
5	O	2	NAG	1	0
5	U	5	MAN	1	0
5	U	3	BMA	2	0
4	P	3	BMA	1	0
4	N	2	NAG	1	0

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

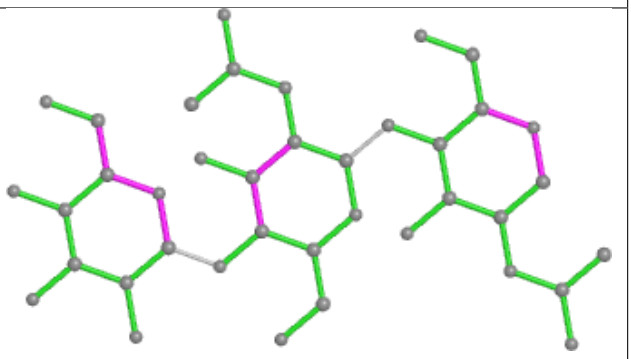
Oligosaccharide Chain N



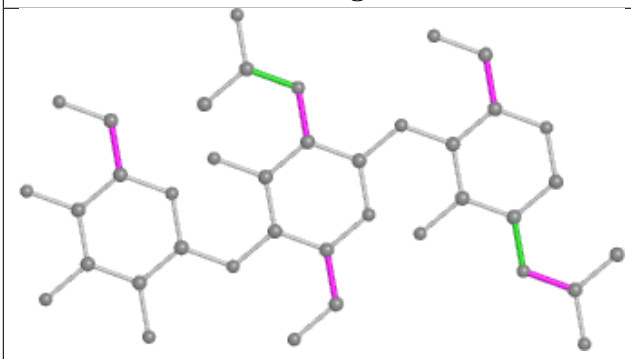
Oligosaccharide Chain P



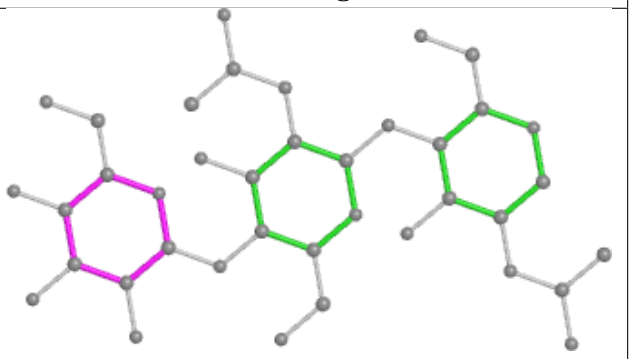
Bond lengths



Bond angles

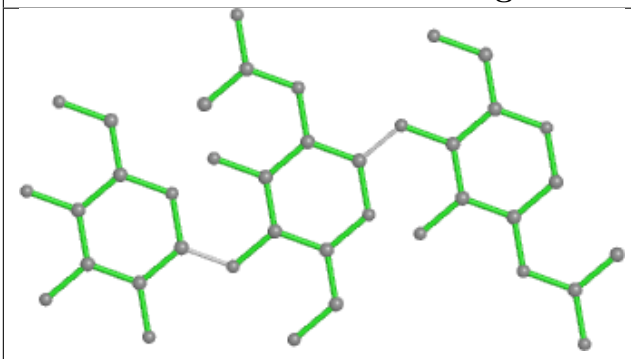


Torsions

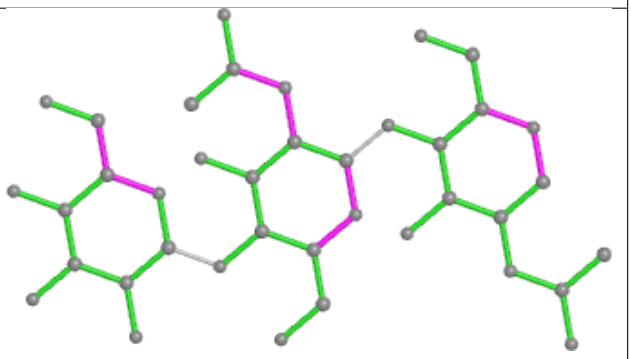


Rings

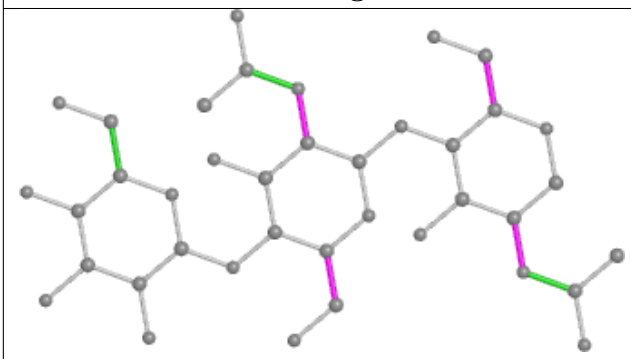
Oligosaccharide Chain T



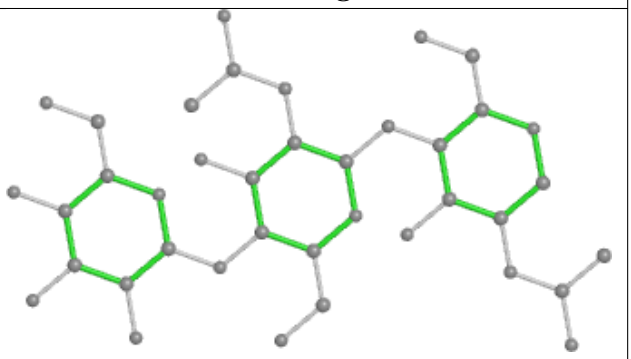
Bond lengths



Bond angles

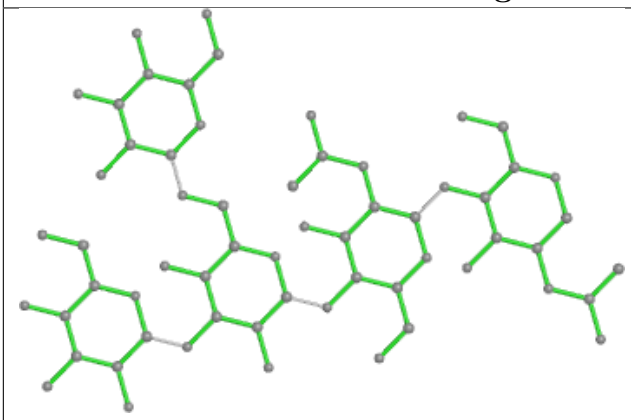


Torsions

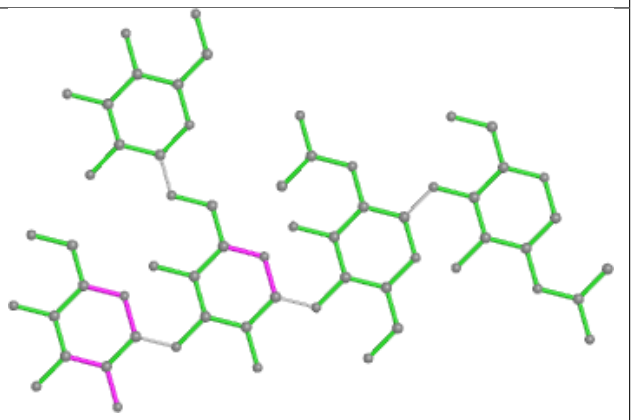


Rings

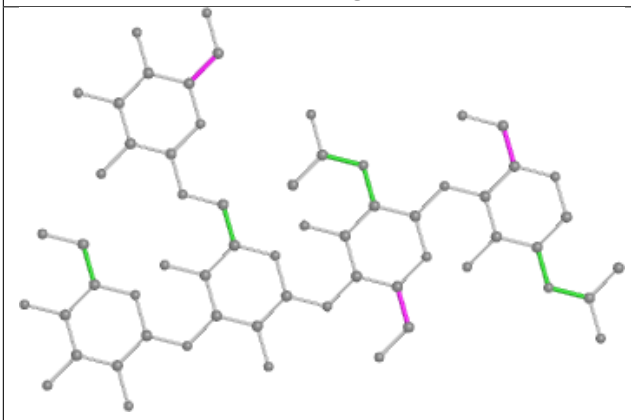
Oligosaccharide Chain O



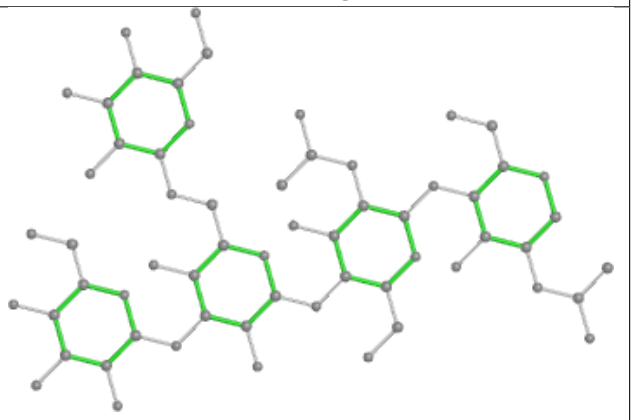
Bond lengths



Bond angles

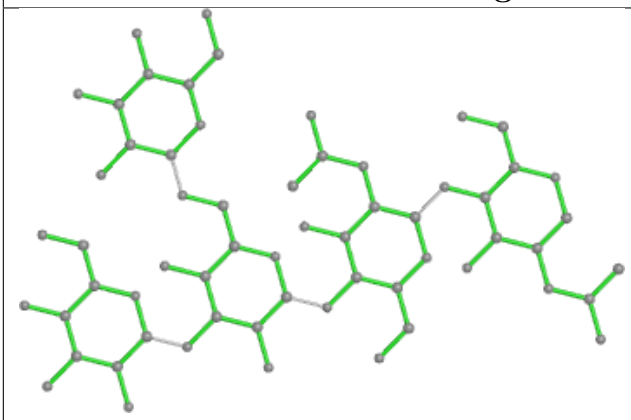


Torsions

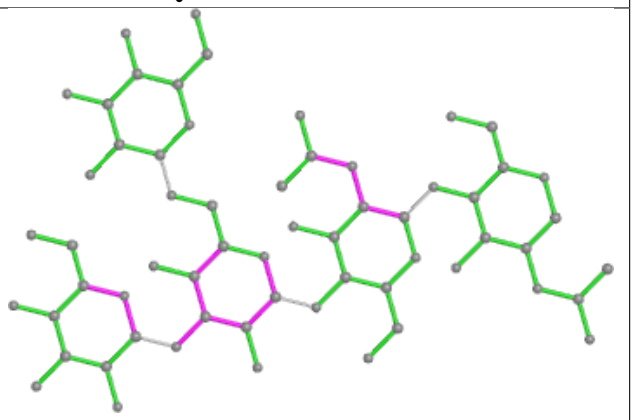


Rings

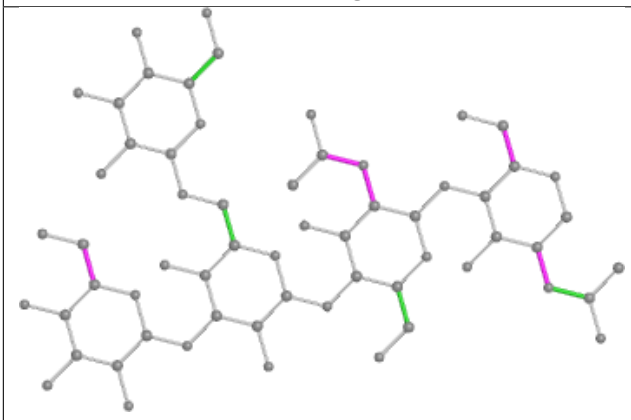
Oligosaccharide Chain Q



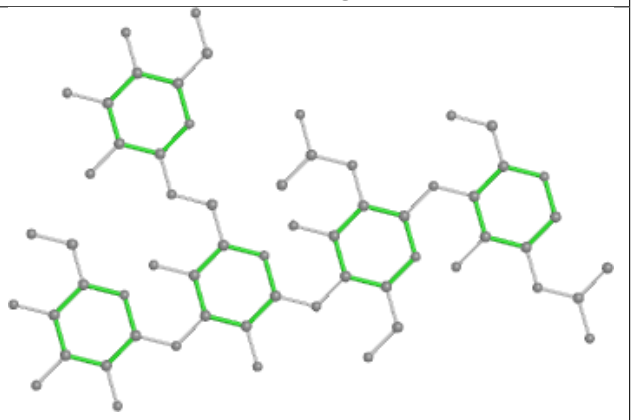
Bond lengths



Bond angles

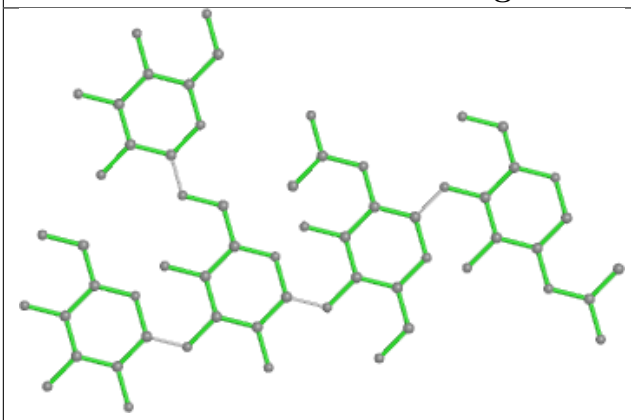


Torsions

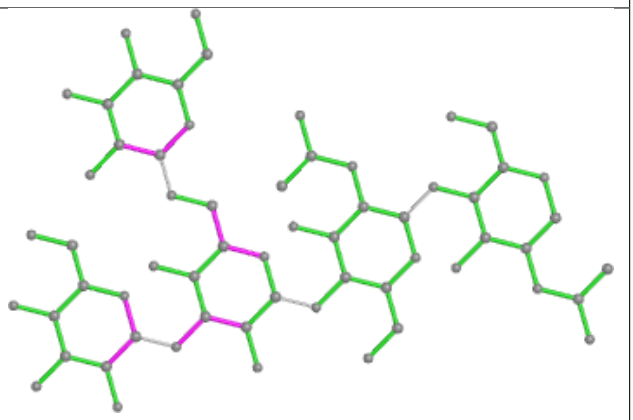


Rings

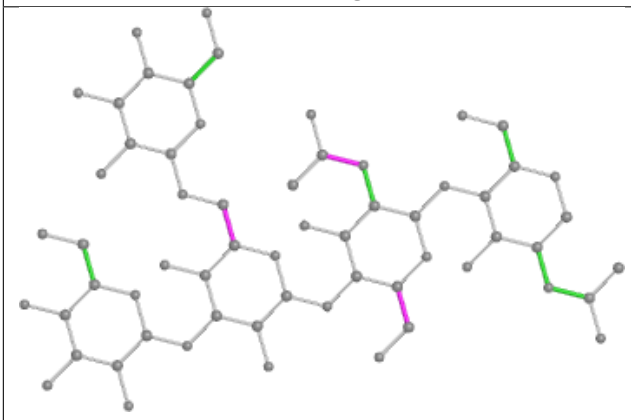
Oligosaccharide Chain U



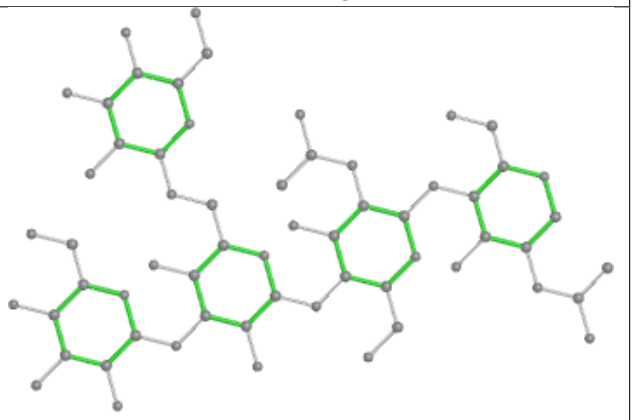
Bond lengths



Bond angles

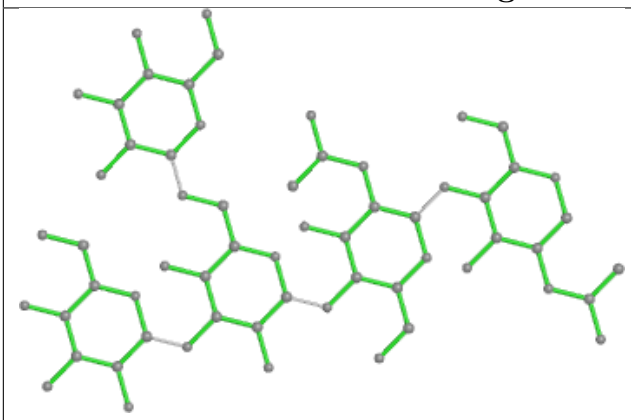


Torsions

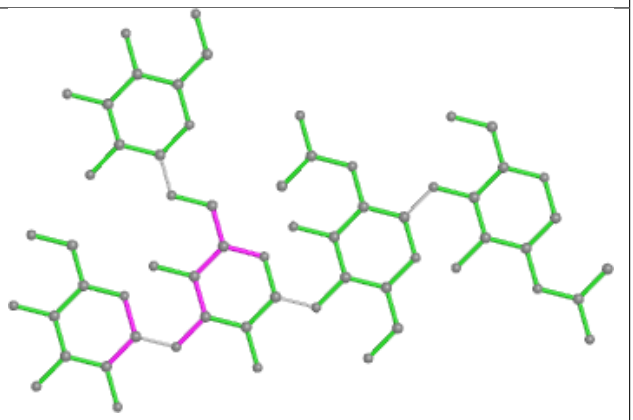


Rings

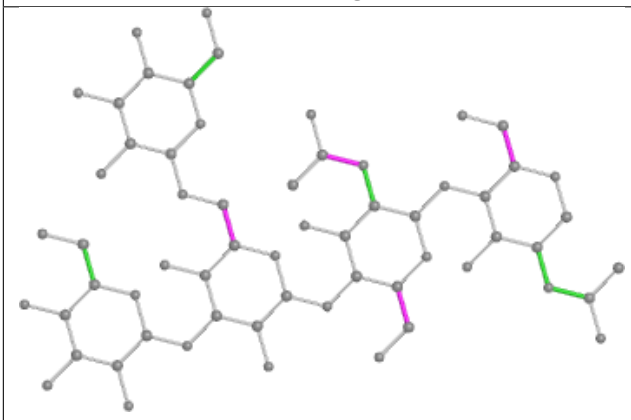
Oligosaccharide Chain S



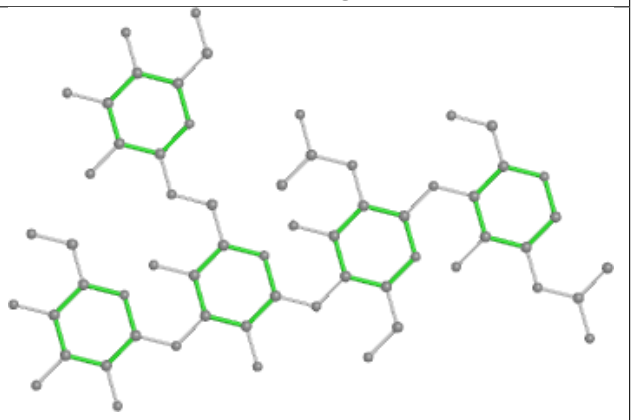
Bond lengths



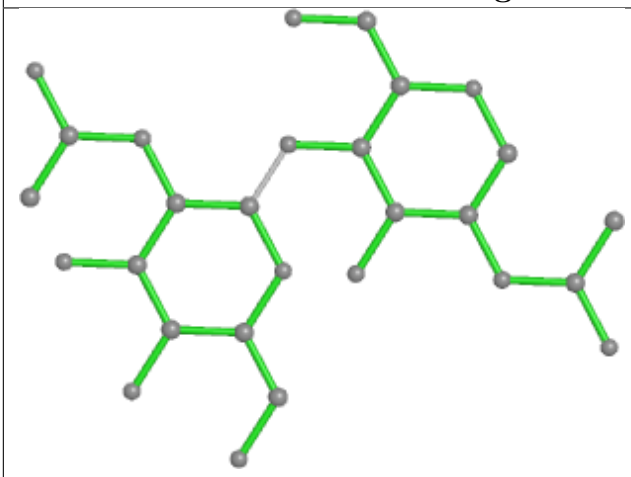
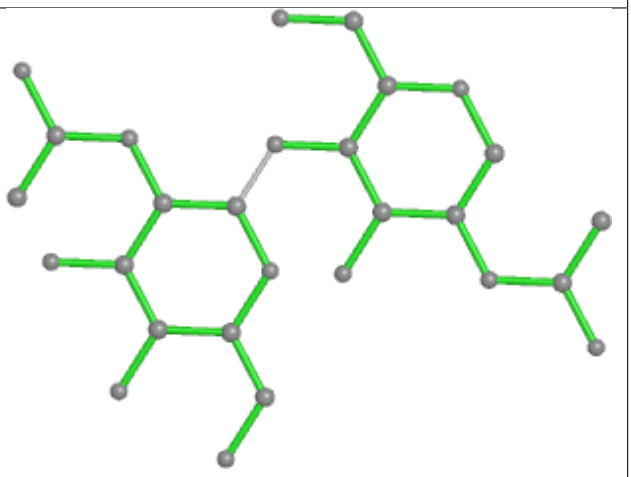
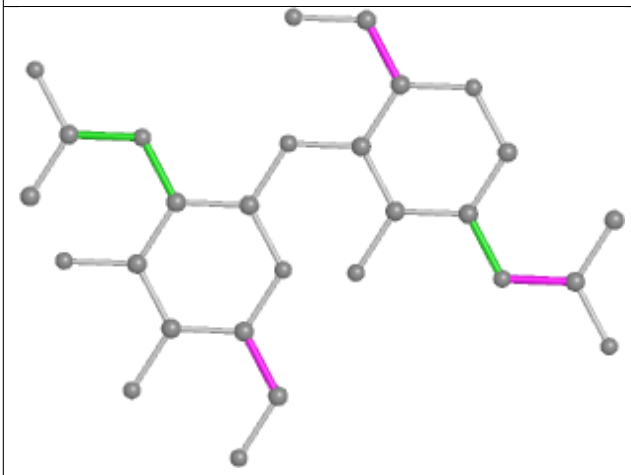
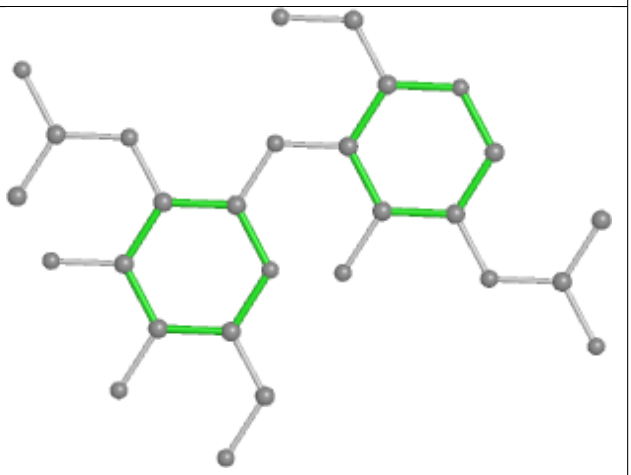
Bond angles



Torsions



Rings

Oligosaccharide Chain R	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

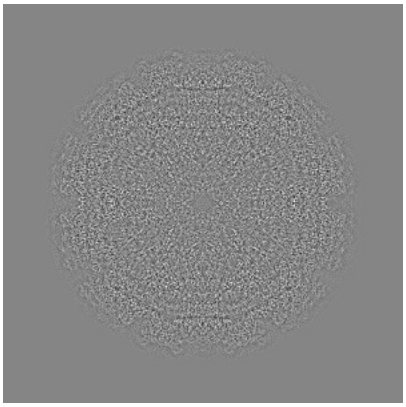
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-22961. These allow visual inspection of the internal detail of the map and identification of artifacts.

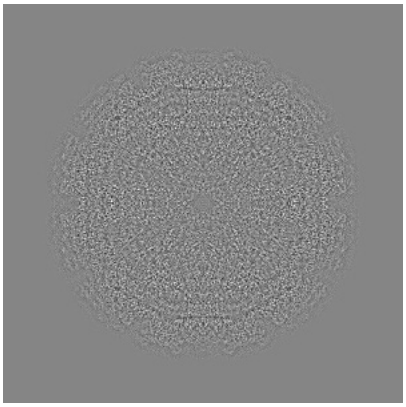
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

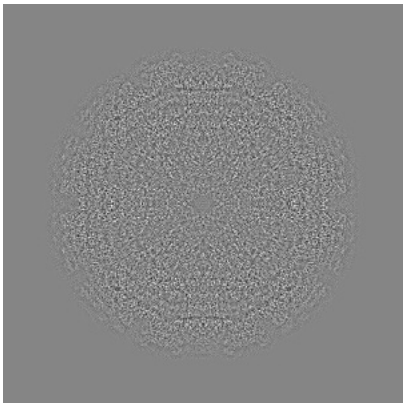
6.1.1 Primary map



X



Y

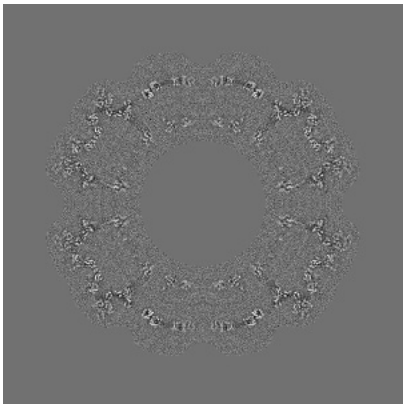


Z

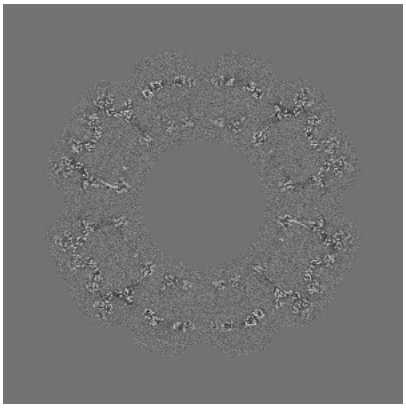
The images above show the map projected in three orthogonal directions.

6.2 Central slices

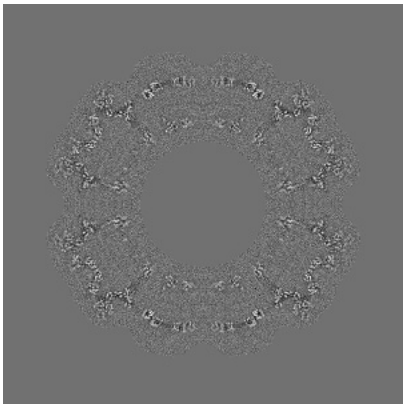
6.2.1 Primary map



X Index: 400



Y Index: 400

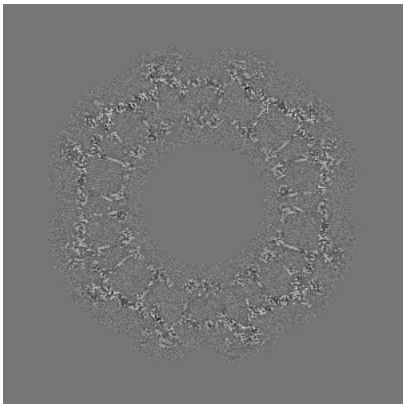


Z Index: 400

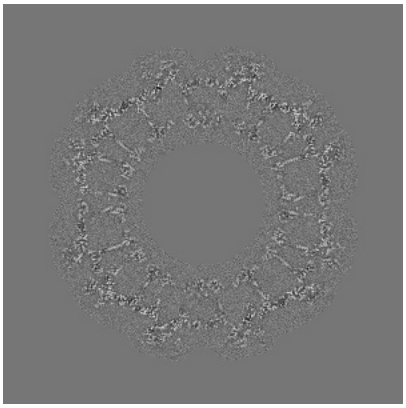
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

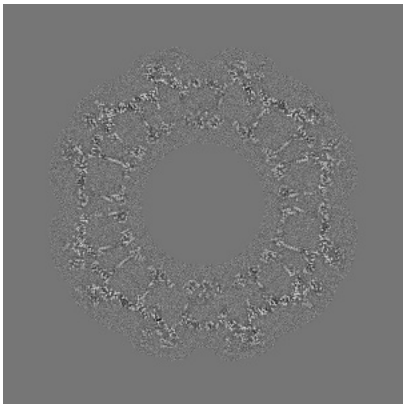
6.3.1 Primary map



X Index: 426



Y Index: 373

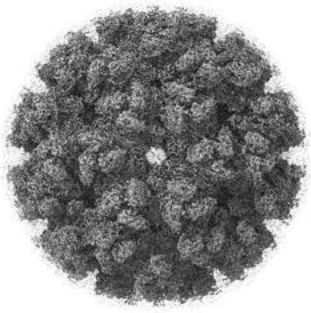


Z Index: 426

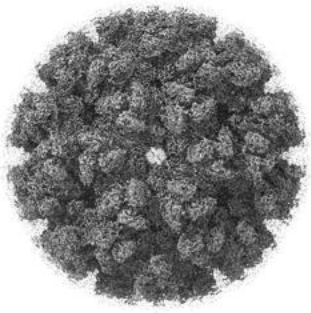
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

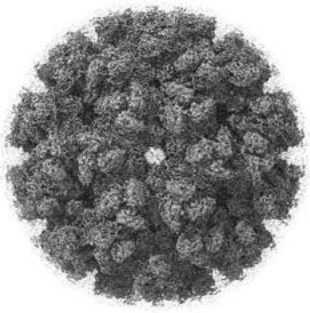
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.9. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

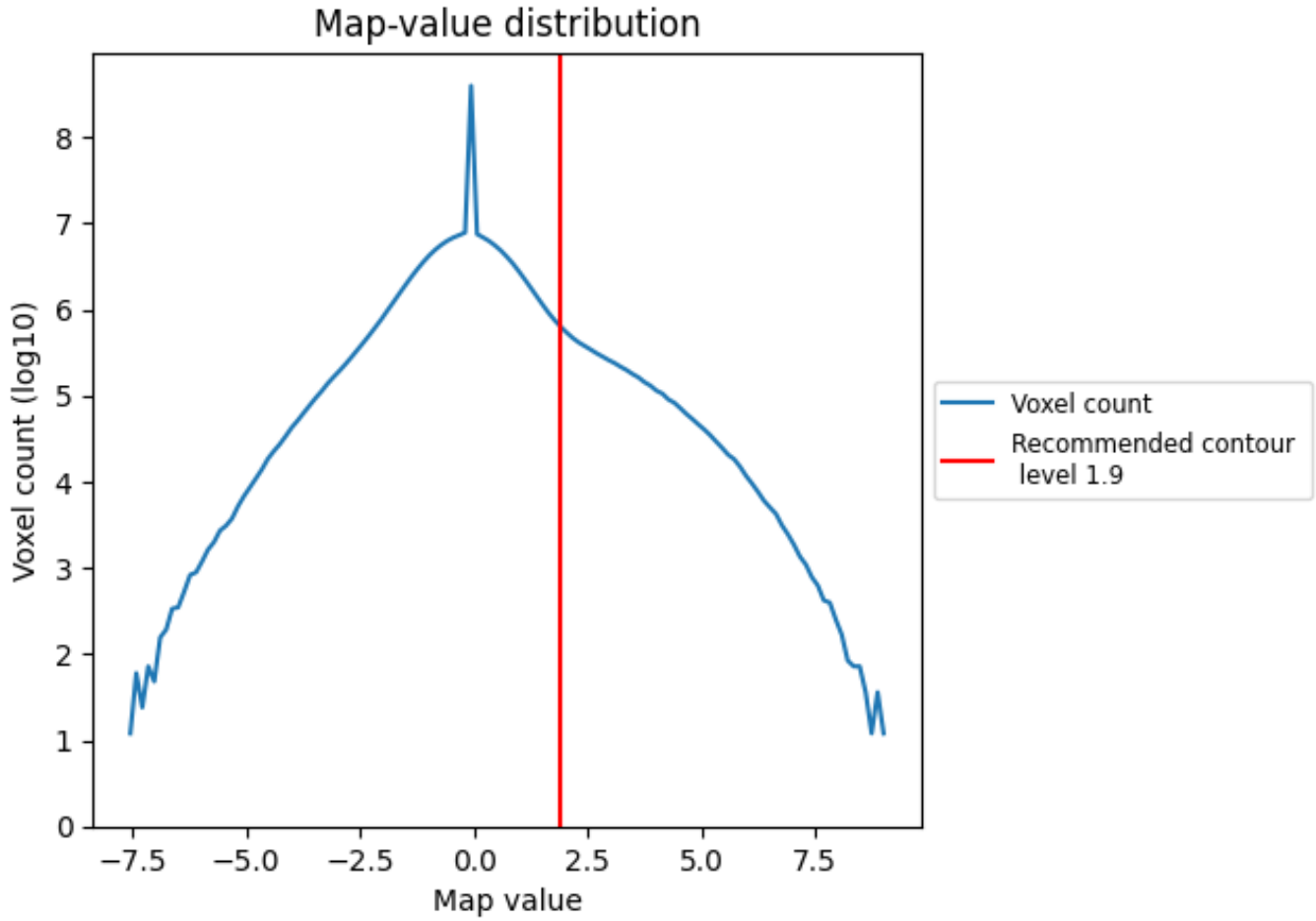
6.5 Mask visualisation (i)

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

7 Map analysis

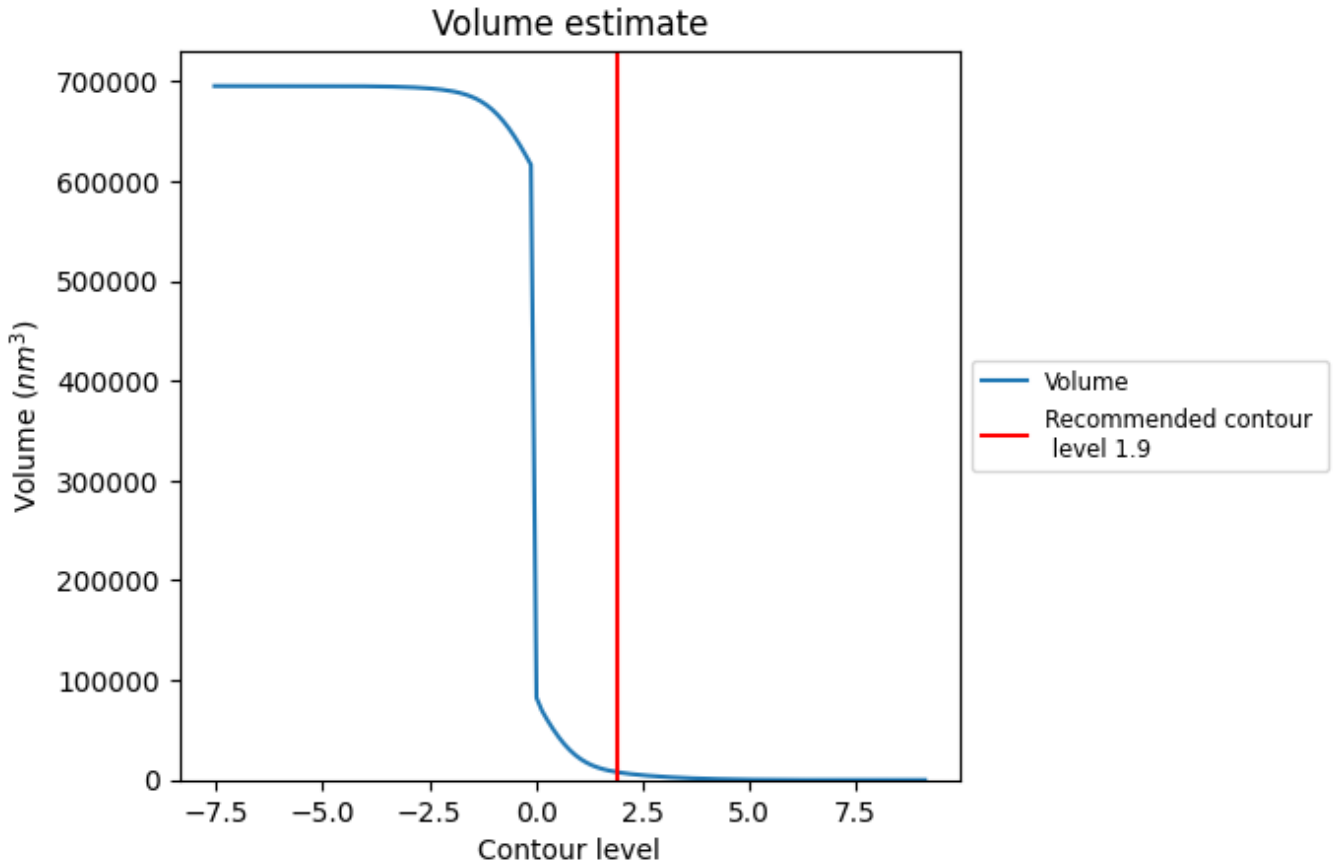
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

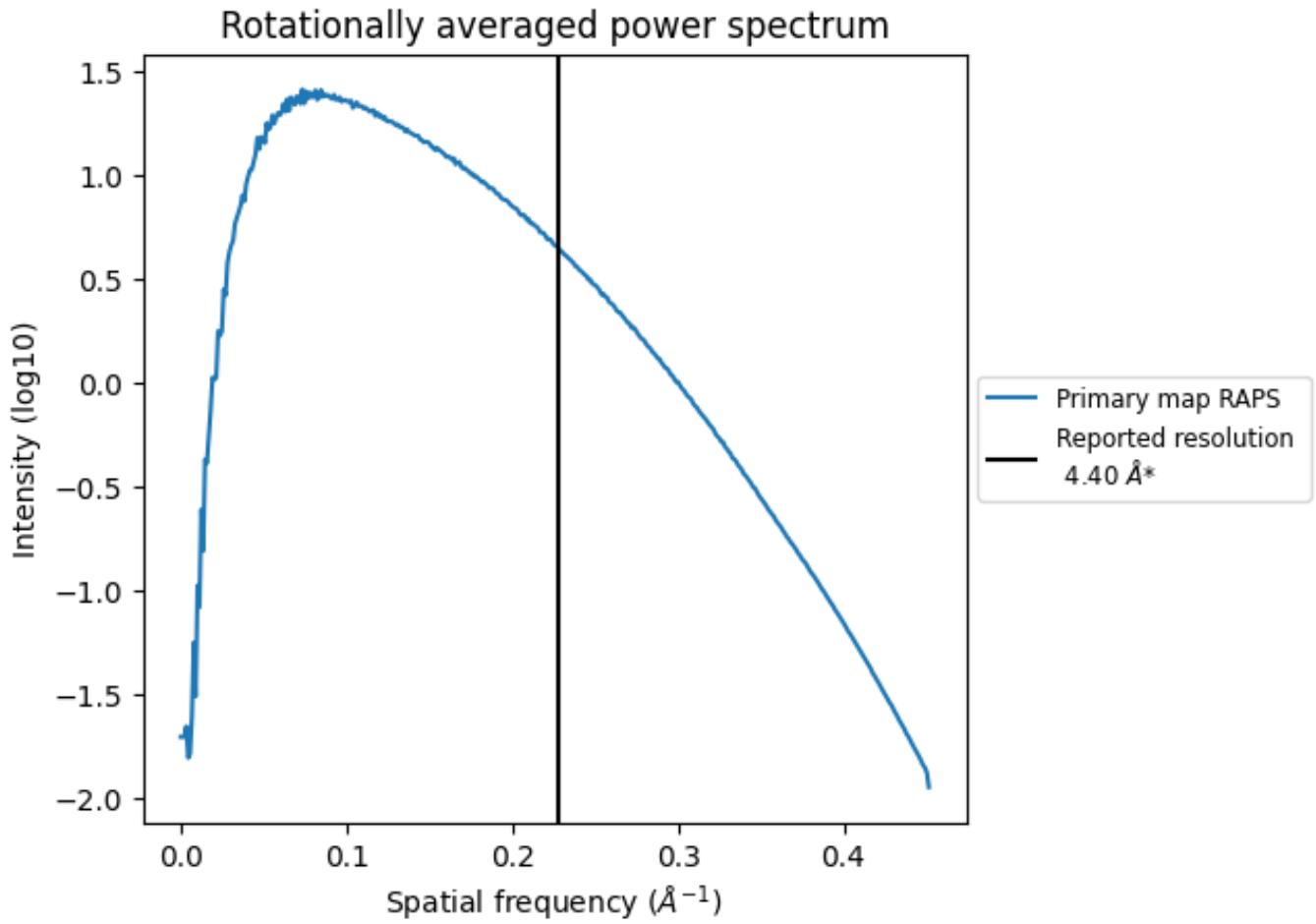
7.2 Volume estimate



The volume at the recommended contour level is 7919 nm^3; this corresponds to an approximate mass of 7154 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.227 Å^{-1}

8 Fourier-Shell correlation

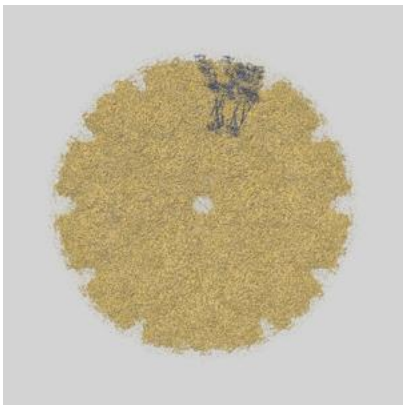
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

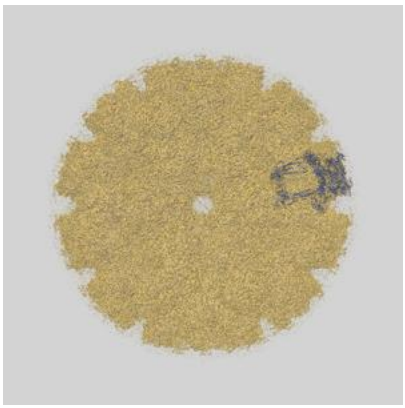
This section contains information regarding the fit between EMDB map EMD-22961 and PDB model 7KO8. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlays

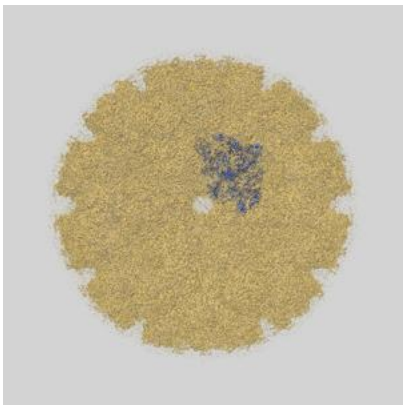
9.1.1 Map-model overlay



X

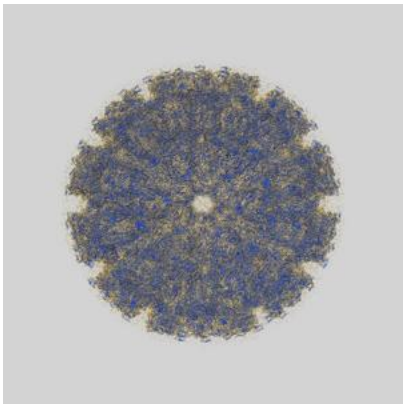


Y

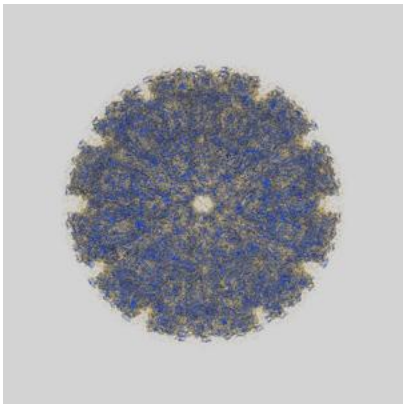


Z

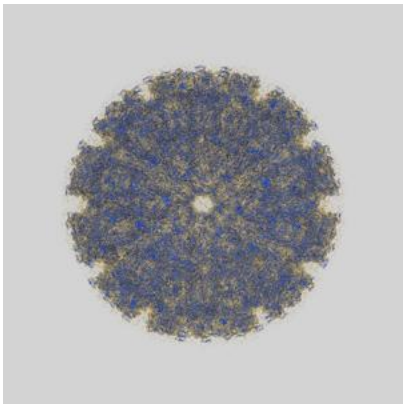
9.1.2 Map-model assembly overlay



X



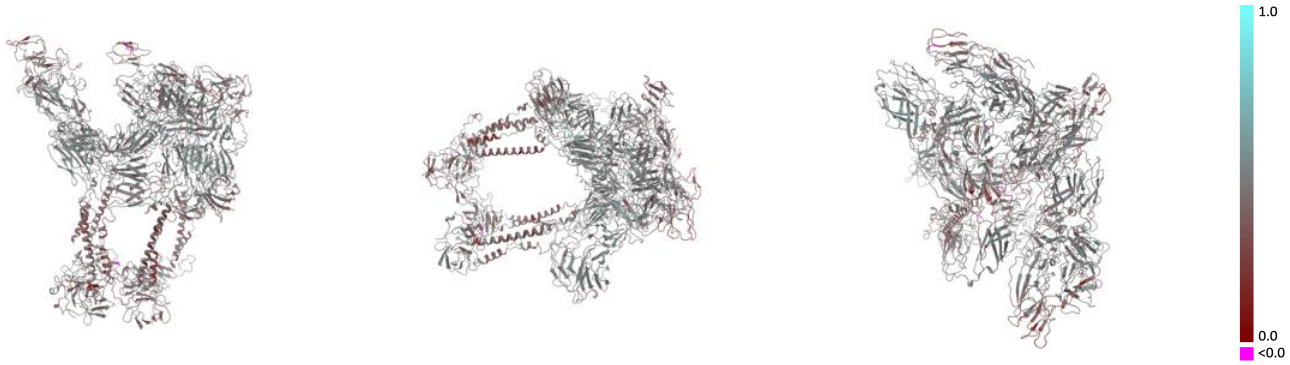
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.9 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.

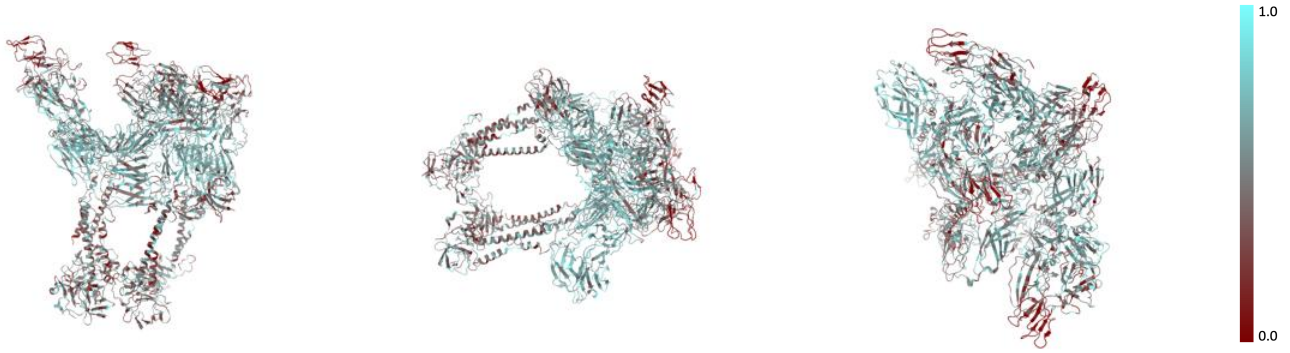
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

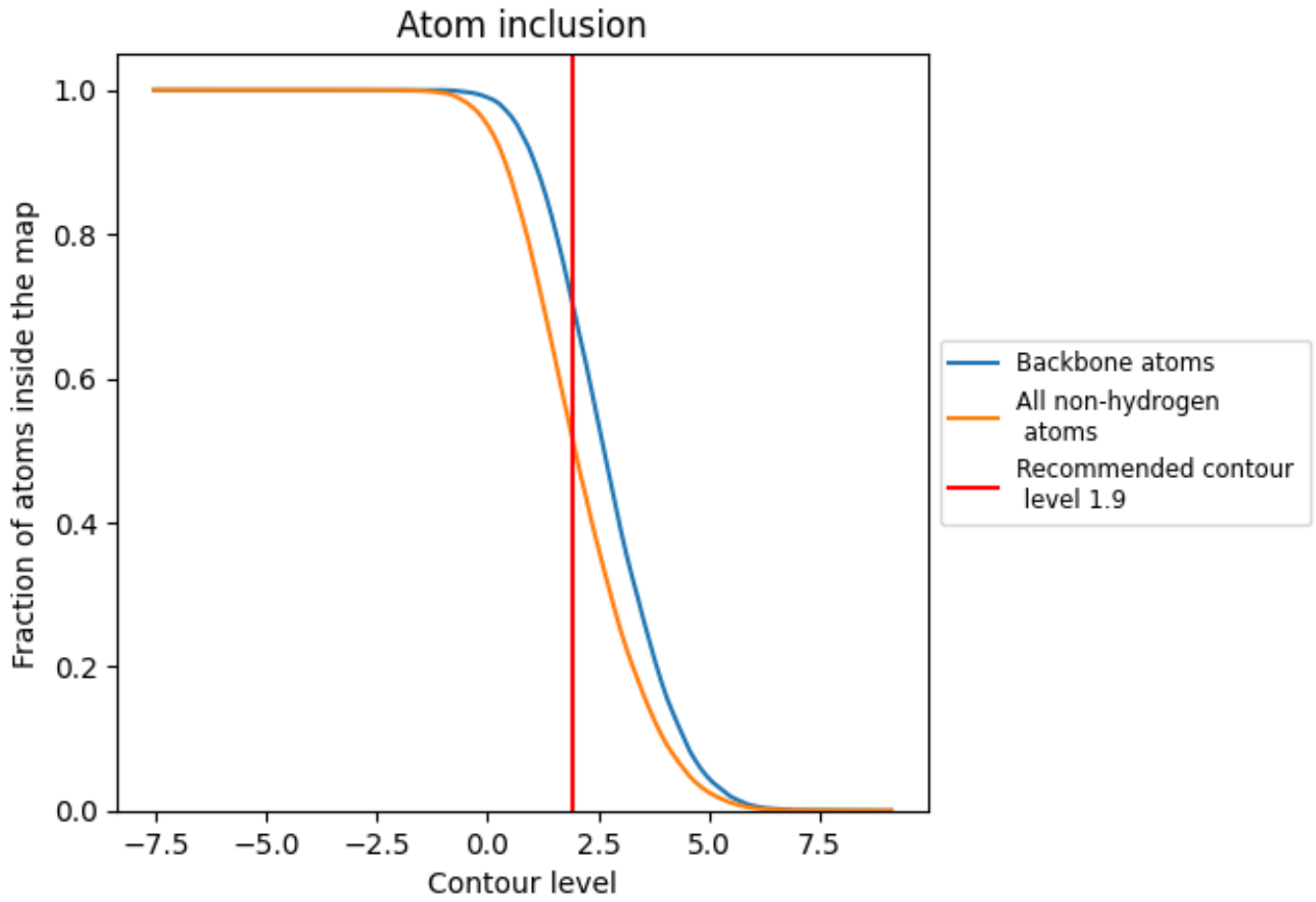
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (1.9).

9.4 Atom inclusion (i)



At the recommended contour level, 71% of all backbone atoms, 52% 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 (1.9) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5205	0.4460
A	0.4400	0.4130
B	0.5465	0.4560
C	0.5039	0.4410
D	0.4983	0.4510
E	0.6151	0.4730
F	0.5043	0.4420
G	0.4461	0.4270
H	0.5582	0.4540
I	0.4812	0.4420
J	0.4983	0.4210
L	0.5687	0.4560
M	0.4872	0.4370
N	0.1538	0.3160
O	0.2787	0.4100
P	0.2564	0.3550
Q	0.2951	0.3070
R	0.2500	0.4210
S	0.2295	0.3330
T	0.2308	0.3300
U	0.2623	0.4120