Full wwPDB EM Validation Report ⓘ

Feb 5, 2024 – 05:04 PM JST

PDB ID	:	7XOE
EMDB ID	:	EMD-33346
Title	:	Cryo-EM structure of S glycoprotein encoded by the Covid-19 mRNA vaccine candidate RQ3013 (Prefusion state)
Authors	:	Wu, Z.; Yu, Z.; Tan, S.; Lu, J.; Lu, G.; Lin, J.
Deposited on	:	2022-05-01
Resolution	:	3.90 Å(reported)

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

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

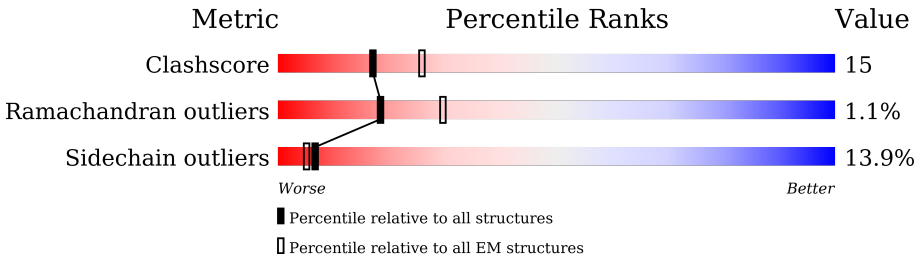
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
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	1293	51% 28% 19%
1	B	1293	52% 29% 17%
1	C	1293	52% 29% 17%
2	D	2	100%
2	E	2	50% 100%
2	F	2	50% 50%
2	G	2	50% 50%
2	H	2	50% 50%

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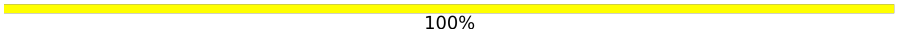
Mol	Chain	Length	Quality of chain
2	I	2	
2	J	2	
2	K	2	
2	L	2	
2	M	2	
2	N	2	
2	O	2	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	I	2	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 25587 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 Spike glycoprotein,peptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1053	Total	C	N	O	S	0	0
			8137	5193	1356	1553	35		
1	B	1079	Total	C	N	O	S	0	0
			8420	5380	1403	1599	38		
1	C	1078	Total	C	N	O	S	0	0
			8400	5365	1398	1599	38		

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	414	ASN	LYS	variant	UNP P0DTC2
A	481	LYS	GLU	variant	UNP P0DTC2
A	498	TYR	ASN	variant	UNP P0DTC2
A	567	ASP	ALA	variant	UNP P0DTC2
A	611	GLY	ASP	variant	UNP P0DTC2
A	678	HIS	PRO	variant	UNP P0DTC2
A	679	GLY	ARG	conflict	UNP P0DTC2
A	680	SER	ARG	conflict	UNP P0DTC2
A	682	SER	ARG	conflict	UNP P0DTC2
A	698	VAL	ALA	variant	UNP P0DTC2
A	713	ILE	THR	variant	UNP P0DTC2
A	979	ALA	SER	variant	UNP P0DTC2
A	1115	HIS	ASP	variant	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	414	ASN	LYS	variant	UNP P0DTC2
B	481	LYS	GLU	variant	UNP P0DTC2
B	498	TYR	ASN	variant	UNP P0DTC2
B	567	ASP	ALA	variant	UNP P0DTC2
B	611	GLY	ASP	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	678	HIS	PRO	variant	UNP P0DTC2
B	679	GLY	ARG	conflict	UNP P0DTC2
B	680	SER	ARG	conflict	UNP P0DTC2
B	682	SER	ARG	conflict	UNP P0DTC2
B	698	VAL	ALA	variant	UNP P0DTC2
B	713	ILE	THR	variant	UNP P0DTC2
B	979	ALA	SER	variant	UNP P0DTC2
B	1115	HIS	ASP	variant	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	414	ASN	LYS	variant	UNP P0DTC2
C	481	LYS	GLU	variant	UNP P0DTC2
C	498	TYR	ASN	variant	UNP P0DTC2
C	567	ASP	ALA	variant	UNP P0DTC2
C	611	GLY	ASP	variant	UNP P0DTC2
C	678	HIS	PRO	variant	UNP P0DTC2
C	679	GLY	ARG	conflict	UNP P0DTC2
C	680	SER	ARG	conflict	UNP P0DTC2
C	682	SER	ARG	conflict	UNP P0DTC2
C	698	VAL	ALA	variant	UNP P0DTC2
C	713	ILE	THR	variant	UNP P0DTC2
C	979	ALA	SER	variant	UNP P0DTC2
C	1115	HIS	ASP	variant	UNP P0DTC2

- Molecule 2 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
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	G	2	Total	C	N	O	0	0
			28	16	2	10		

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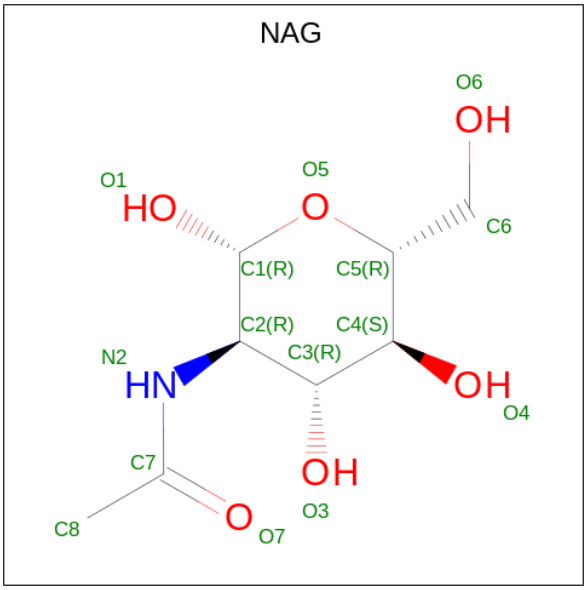
Mol	Chain	Residues	Atoms	AltConf	Trace
2	H	2	Total C N O 28 16 2 10	0	0
2	I	2	Total C N O 28 16 2 10	0	0
2	J	2	Total C N O 28 16 2 10	0	0
2	K	2	Total C N O 28 16 2 10	0	0
2	L	2	Total C N O 28 16 2 10	0	0
2	M	2	Total C N O 28 16 2 10	0	0
2	N	2	Total C N O 28 16 2 10	0	0
2	O	2	Total C N O 28 16 2 10	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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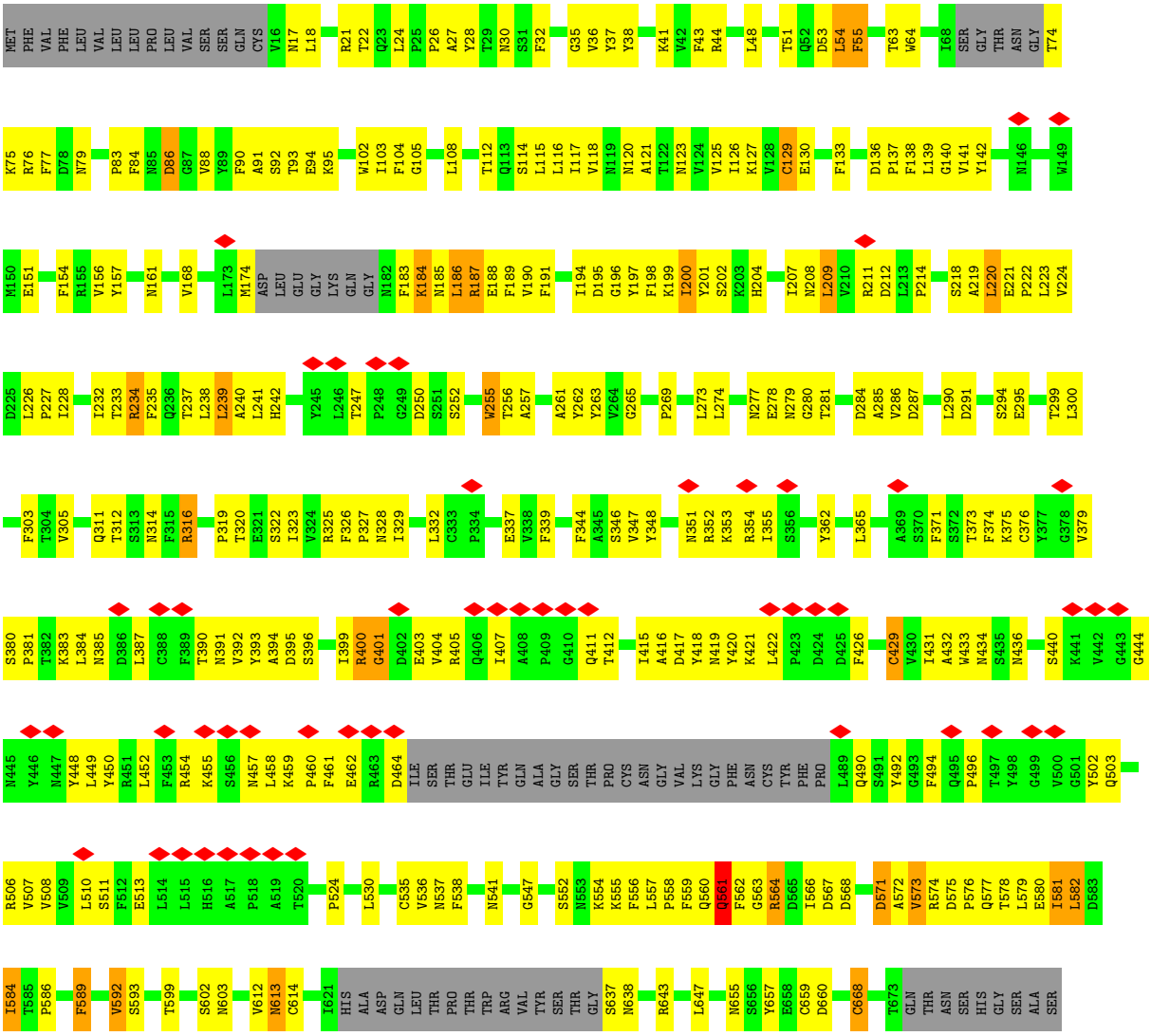
Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total C N O 14 8 1 5	0
3	A	1	Total C N O 14 8 1 5	0
3	A	1	Total C N O 14 8 1 5	0
3	A	1	Total C N O 14 8 1 5	0
3	A	1	Total C N O 14 8 1 5	0
3	B	1	Total C N O 14 8 1 5	0
3	B	1	Total C N O 14 8 1 5	0
3	B	1	Total C N O 14 8 1 5	0
3	B	1	Total C N O 14 8 1 5	0
3	B	1	Total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

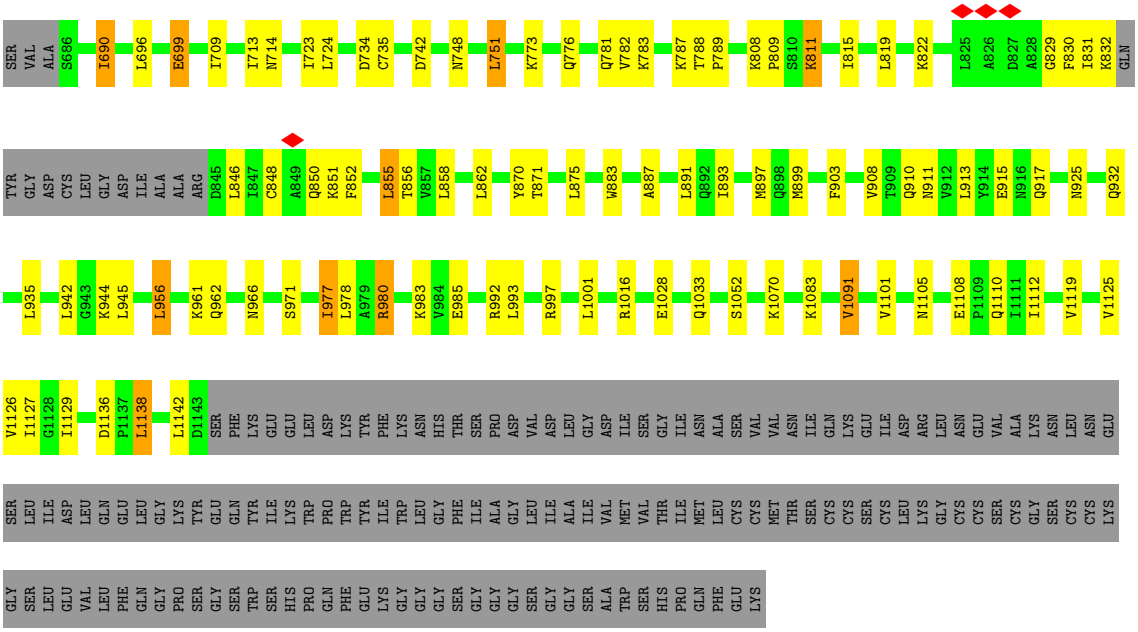
3 Residue-property plots (i)

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: Spike glycoprotein,peptide

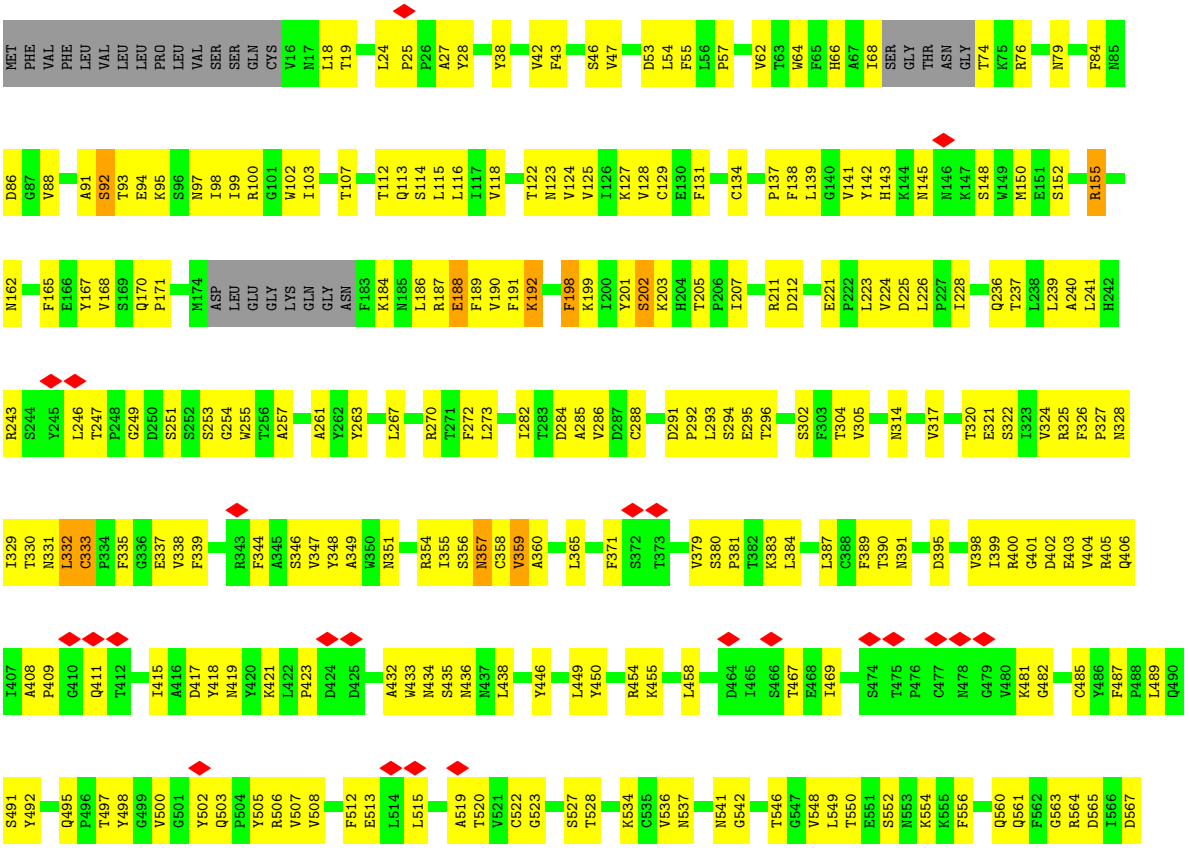
Chain A:

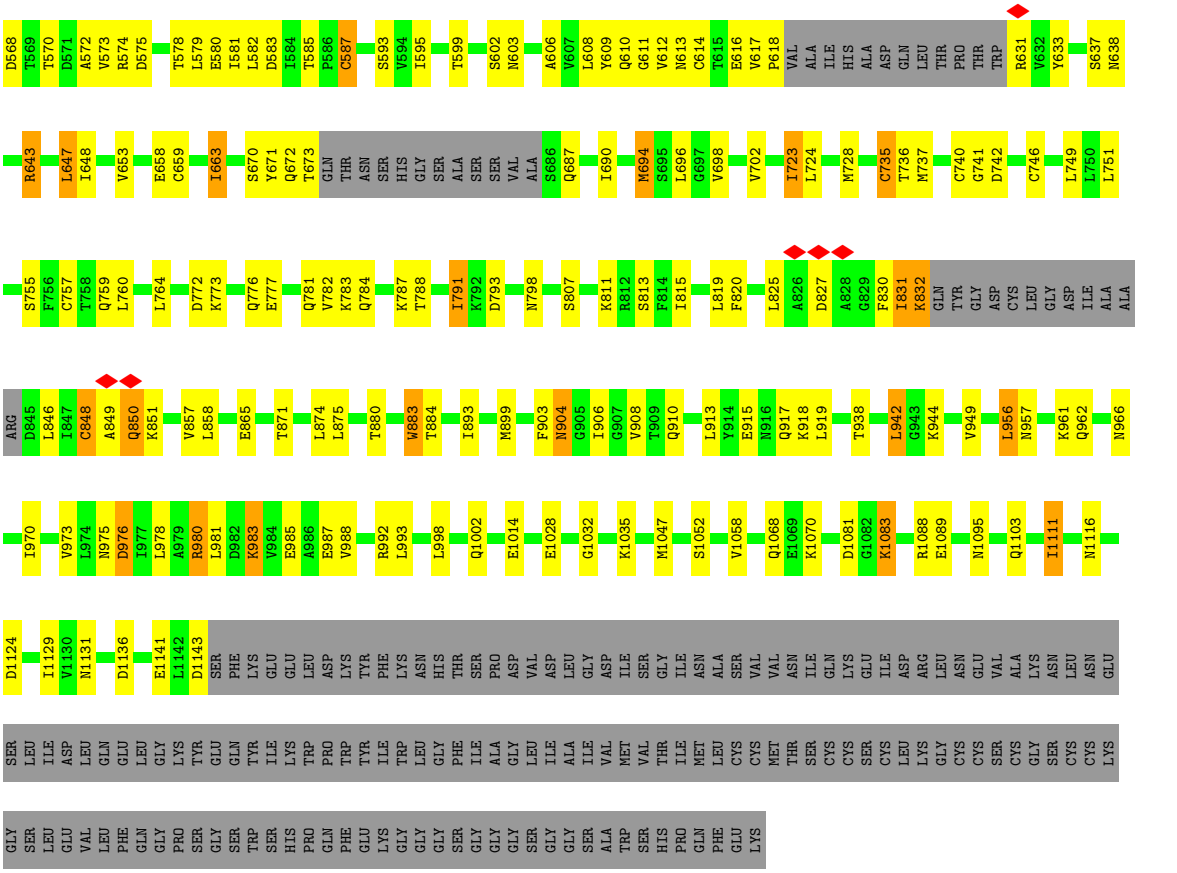




• Molecule 1: Spike glycoprotein,peptide

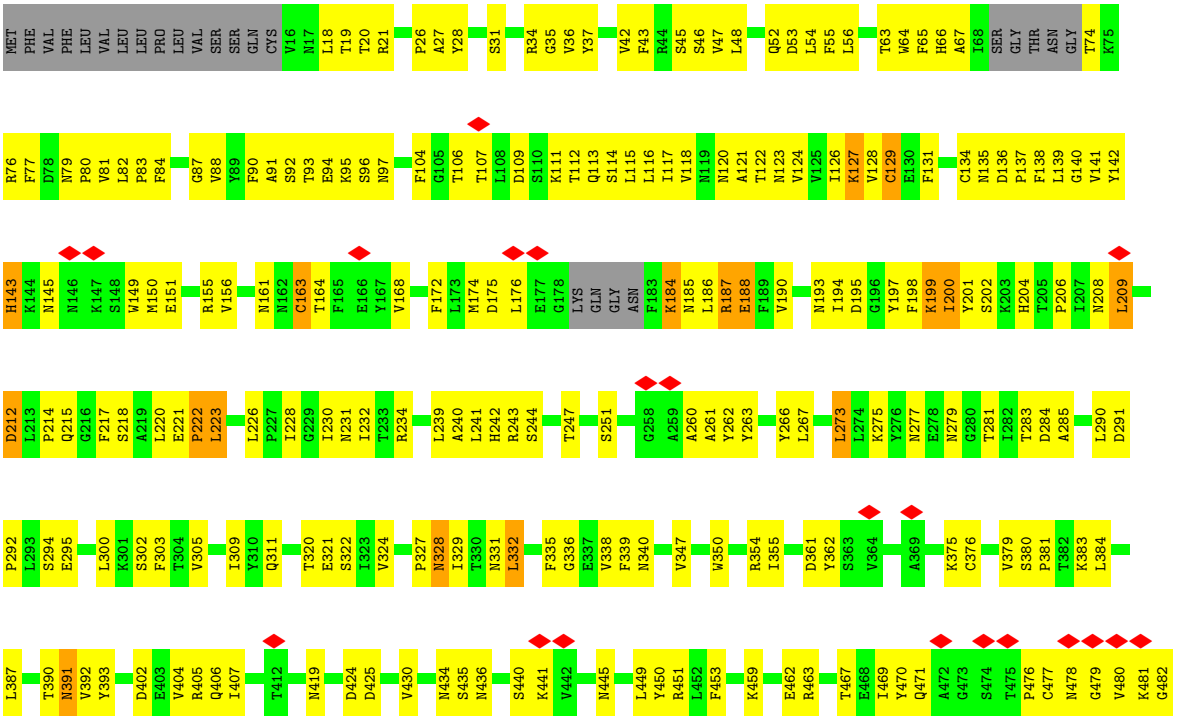
Chain B:

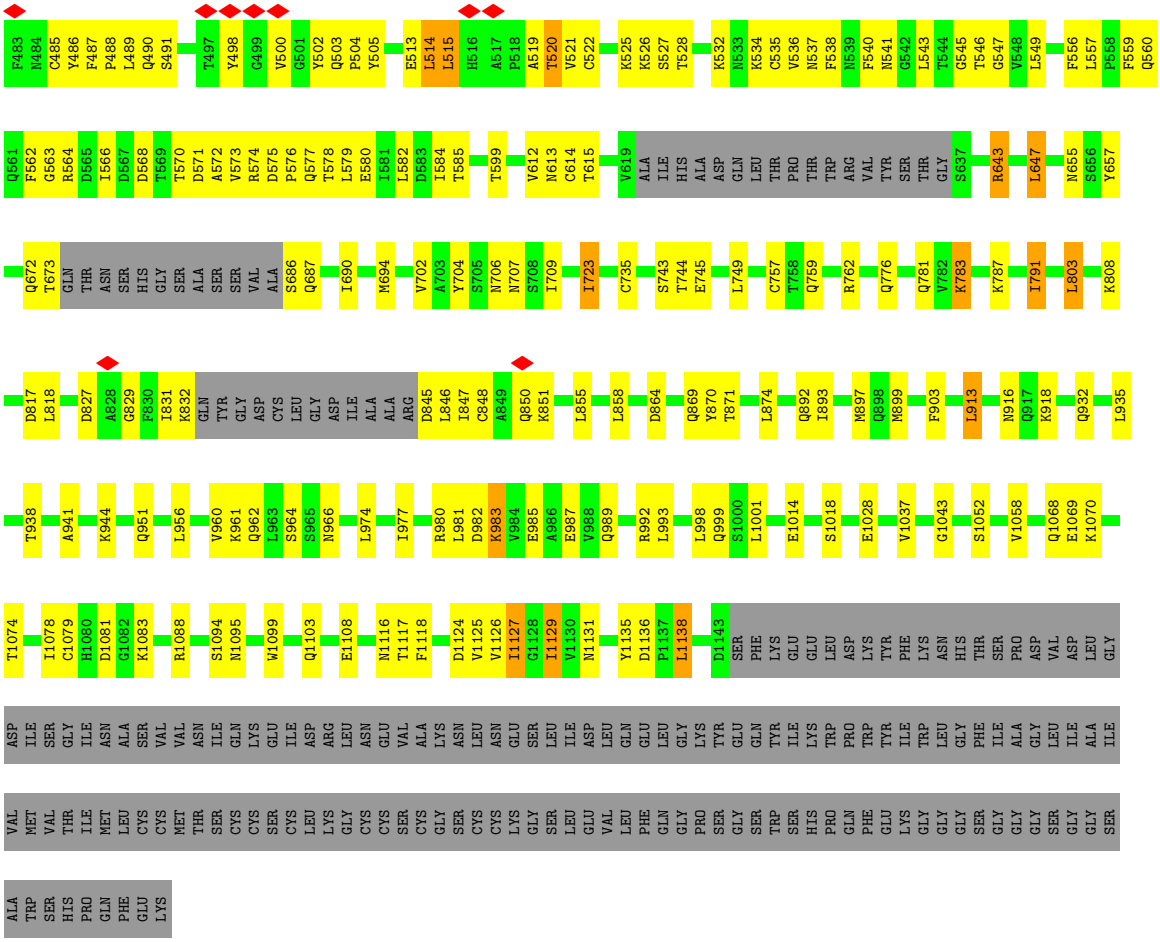




• Molecule 1: Spike glycoprotein,peptide

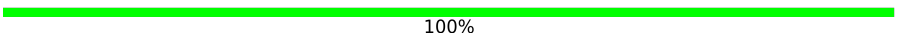
Chain C:





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

Chain D:



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

Chain E:

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

Chain F:

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

Chain G:

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

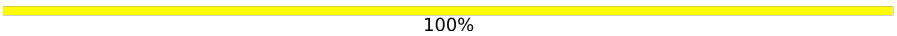
Chain H:

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

Chain I:

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

Chain J:



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

Chain K:

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

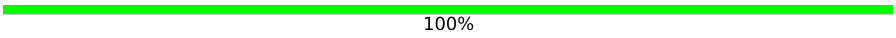
Chain L:

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

Chain M:

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

Chain N:



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

Chain O:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	14846	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.25	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.735	Depositor
Minimum map value	-0.661	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.039	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	563.2, 563.2, 563.2	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	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

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	0.58	0/8318	0.72	2/11329 (0.0%)
1	B	0.57	0/8615	0.67	0/11727
1	C	0.57	0/8592	0.69	1/11695 (0.0%)
All	All	0.57	0/25525	0.69	3/34751 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	129	CYS	CB-CA-C	-12.47	85.47	110.40
1	A	129	CYS	CB-CA-C	-8.55	93.30	110.40
1	A	429	CYS	CA-CB-SG	5.70	124.27	114.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8137	0	7889	261	0
1	B	8420	0	8210	261	0
1	C	8400	0	8193	273	0
2	D	28	0	25	0	0
2	E	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	28	0	25	1	0
2	G	28	0	25	0	0
2	H	28	0	25	1	0
2	I	28	0	25	7	0
2	J	28	0	25	0	0
2	K	28	0	25	0	0
2	L	28	0	25	1	0
2	M	28	0	25	1	0
2	N	28	0	25	0	0
2	O	28	0	25	1	0
3	A	112	0	104	0	0
3	B	98	0	91	2	0
3	C	84	0	78	6	0
All	All	25587	0	24865	777	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 15.

All (777) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:613:ASN:HD21	3:C:1301:NAG:C1	1.18	1.52
1:B:919:LEU:CD1	2:I:2:NAG:H62	1.60	1.31
1:B:919:LEU:HD13	2:I:2:NAG:C6	1.94	0.97
1:B:919:LEU:HD13	2:I:2:NAG:H62	0.97	0.95
1:A:137:PRO:HG3	1:A:156:VAL:HA	1.50	0.94
1:B:118:VAL:O	1:B:124:VAL:HA	1.67	0.94
1:A:104:PHE:HB2	1:A:115:LEU:HB3	1.51	0.91
1:B:919:LEU:CD1	2:I:2:NAG:C6	2.49	0.90
1:B:190:VAL:HG13	1:B:267:LEU:HD11	1.51	0.90
1:A:91:ALA:O	1:A:262:TYR:HA	1.71	0.89
1:A:563:GLY:HA3	1:A:571:ASP:H	1.37	0.87
1:C:118:VAL:O	1:C:124:VAL:HA	1.75	0.85
1:C:563:GLY:O	1:C:570:THR:HA	1.76	0.85
1:C:532:LYS:HA	1:C:549:LEU:HD21	1.60	0.84
1:C:390:THR:HB	1:C:519:ALA:HA	1.59	0.83
1:A:211:ARG:HE	1:A:214:PRO:HB3	1.46	0.81
1:B:391:ASN:O	1:B:512:PHE:HA	1.79	0.81
1:C:613:ASN:CG	3:C:1301:NAG:C1	2.49	0.81
1:A:552:SER:HB2	1:A:581:ILE:HB	1.63	0.79
1:B:18:LEU:HD11	1:B:255:TRP:HE1	1.44	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:ASP:OD1	1:B:263:TYR:OH	1.99	0.79
1:C:564:ARG:NE	1:C:568:ASP:OD2	2.17	0.77
1:A:390:THR:HG22	1:A:391:ASN:H	1.49	0.77
1:B:383:LYS:HD2	1:C:980:ARG:H	1.49	0.77
1:C:115:LEU:HG	1:C:230:ILE:HD11	1.64	0.77
1:C:354:ARG:NH1	1:C:393:TYR:OH	2.18	0.77
1:B:390:THR:O	1:B:513:GLU:O	2.03	0.77
1:A:337:GLU:O	1:A:353:LYS:NZ	2.18	0.76
1:B:305:VAL:HG22	1:B:599:THR:HG23	1.68	0.76
1:A:79:ASN:HD21	1:A:237:THR:HB	1.49	0.76
1:B:351:ASN:O	1:B:395:ASP:HA	1.86	0.76
1:A:355:ILE:HB	1:A:392:VAL:HB	1.69	0.75
1:C:571:ASP:HA	1:C:584:ILE:O	1.86	0.75
1:C:572:ALA:HA	1:C:582:LEU:O	1.85	0.75
1:A:137:PRO:HG2	1:A:238:LEU:HG	1.69	0.75
1:B:99:ILE:HA	1:B:239:LEU:HA	1.68	0.75
1:A:374:PHE:HE2	1:A:381:PRO:HB3	1.50	0.74
1:A:362:TYR:HD2	1:A:384:LEU:HD13	1.52	0.74
1:C:106:THR:HG23	1:C:107:THR:HG23	1.69	0.74
1:C:355:ILE:HB	1:C:392:VAL:HB	1.69	0.74
1:A:852:PHE:CZ	1:C:585:THR:HG23	2.22	0.74
1:C:139:LEU:HD12	1:C:240:ALA:HB2	1.70	0.74
1:A:352:ARG:HE	1:A:393:TYR:HB3	1.53	0.74
1:A:156:VAL:HB	1:A:157:TYR:HD1	1.53	0.73
1:B:57:PRO:HG3	1:B:270:ARG:HG3	1.71	0.73
1:C:21:ARG:NH2	1:C:74:THR:O	2.23	0.72
1:C:91:ALA:HB3	1:C:263:TYR:HD1	1.53	0.71
1:A:352:ARG:NE	1:A:393:TYR:HB3	2.05	0.71
1:A:18:LEU:HD22	1:A:255:TRP:HE1	1.55	0.71
1:B:398:VAL:HG12	1:B:506:ARG:HA	1.72	0.71
1:C:200:ILE:H	1:C:223:LEU:H	1.38	0.71
1:B:919:LEU:HD12	2:I:2:NAG:H62	1.67	0.71
1:C:284:ASP:OD1	1:C:285:ALA:N	2.22	0.71
1:C:291:ASP:O	1:C:294:SER:OG	2.07	0.71
1:C:127:LYS:HB3	1:C:131:PHE:HZ	1.56	0.71
1:B:400:ARG:HD3	1:B:502:TYR:HA	1.73	0.71
1:B:405:ARG:O	1:B:411:GLN:NE2	2.24	0.71
1:A:88:VAL:HA	1:A:265:GLY:O	1.91	0.70
1:C:143:HIS:HB3	1:C:244:SER:HA	1.73	0.70
1:A:284:ASP:OD1	1:A:285:ALA:N	2.24	0.70
1:B:18:LEU:HD12	1:B:19:THR:H	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:ILE:HD11	1:B:419:ASN:HD22	1.56	0.69
1:A:121:ALA:HA	1:A:174:MET:HG3	1.74	0.69
1:A:277:ASN:ND2	1:A:281:THR:OG1	2.25	0.69
1:A:554:LYS:HD3	1:A:555:LYS:H	1.57	0.69
1:B:27:ALA:HB3	1:B:64:TRP:HB3	1.74	0.69
1:A:118:VAL:HG22	1:A:125:VAL:HB	1.73	0.69
1:A:184:LYS:HA	1:A:207:ILE:HG23	1.75	0.69
1:A:138:PHE:HB2	1:A:241:LEU:HG	1.75	0.69
1:B:102:TRP:CD1	1:B:237:THR:HA	2.28	0.68
1:C:571:ASP:HB3	1:C:584:ILE:O	1.93	0.68
1:C:481:LYS:HE2	1:C:487:PHE:HB2	1.75	0.68
1:C:91:ALA:O	1:C:262:TYR:HA	1.93	0.68
1:B:383:LYS:HZ3	1:C:981:LEU:N	1.91	0.68
1:B:346:SER:HB3	1:B:349:ALA:HB3	1.76	0.68
1:C:686:SER:OG	1:C:687:GLN:N	2.26	0.68
1:A:83:PRO:HA	1:A:234:ARG:HG3	1.76	0.67
1:B:418:TYR:CD2	1:B:454:ARG:HB3	2.28	0.67
1:B:643:ARG:NH2	1:C:832:LYS:H	1.92	0.67
1:B:643:ARG:HH22	1:C:832:LYS:H	1.40	0.67
1:A:459:LYS:HB3	1:A:462:GLU:HG3	1.76	0.67
1:B:291:ASP:OD1	1:B:294:SER:OG	2.09	0.67
1:B:116:LEU:HB3	1:B:131:PHE:CZ	2.30	0.67
1:C:566:ILE:HD12	1:C:566:ILE:H	1.60	0.67
1:B:102:TRP:HD1	1:B:237:THR:HA	1.60	0.67
1:C:571:ASP:CB	1:C:584:ILE:O	2.43	0.67
1:A:327:PRO:HD3	1:A:541:ASN:OD1	1.94	0.66
1:B:125:VAL:HG12	1:B:127:LYS:HG3	1.76	0.66
1:A:137:PRO:HB3	1:A:156:VAL:HG22	1.76	0.66
1:A:198:PHE:HB3	1:A:226:LEU:HD13	1.76	0.66
1:B:243:ARG:HE	1:B:255:TRP:HB3	1.59	0.66
1:C:18:LEU:HD13	1:C:136:ASP:HB2	1.77	0.66
1:A:562:PHE:HD1	1:A:564:ARG:HH11	1.41	0.66
1:C:476:PRO:O	1:C:478:ASN:ND2	2.28	0.66
1:A:54:LEU:HA	1:A:269:PRO:HA	1.77	0.66
1:C:77:PHE:HZ	1:C:239:LEU:HD22	1.61	0.66
1:B:595:ILE:HD11	1:B:663:ILE:HD11	1.78	0.65
1:B:670:SER:OG	1:B:671:TYR:N	2.29	0.65
1:B:142:TYR:HD1	1:B:243:ARG:HB2	1.61	0.65
1:C:90:PHE:HA	1:C:263:TYR:O	1.97	0.65
1:A:228:ILE:HD11	1:A:232:ILE:HD11	1.79	0.65
1:C:27:ALA:HB3	1:C:64:TRP:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:381:PRO:HA	1:B:384:LEU:HD23	1.76	0.65
1:B:335:PHE:HA	1:B:338:VAL:HG12	1.78	0.65
1:B:481:LYS:HE3	1:B:487:PHE:HB2	1.79	0.65
1:C:324:VAL:H	1:C:528:THR:HB	1.60	0.65
1:C:613:ASN:OD1	1:C:615:THR:OG1	2.14	0.65
1:B:122:THR:HG1	1:B:123:ASN:H	1.45	0.64
1:B:127:LYS:HB3	1:B:129:CYS:SG	2.37	0.64
1:B:673:THR:HA	1:B:687:GLN:HG2	1.79	0.64
1:A:287:ASP:HB2	1:A:290:LEU:HD23	1.78	0.64
1:C:116:LEU:HD21	1:C:156:VAL:HG11	1.79	0.64
1:C:571:ASP:HA	1:C:584:ILE:HB	1.79	0.64
1:A:92:SER:HB3	1:A:185:ASN:O	1.97	0.64
1:A:376:CYS:HA	1:A:429:CYS:HB2	1.78	0.64
1:B:226:LEU:HB3	1:B:228:ILE:HG23	1.80	0.64
1:B:574:ARG:HG2	1:B:579:LEU:HA	1.78	0.64
1:B:498:TYR:HB2	1:B:502:TYR:HB2	1.79	0.64
1:C:199:LYS:HB3	1:C:222:PRO:HB3	1.79	0.64
1:B:243:ARG:HA	1:B:247:THR:HG21	1.80	0.63
1:C:470:TYR:N	1:C:486:TYR:O	2.28	0.63
1:A:75:LYS:HE2	1:A:257:ALA:HB2	1.81	0.63
1:B:432:ALA:HA	1:B:506:ARG:O	1.97	0.63
1:C:361:ASP:OD1	1:C:362:TYR:N	2.29	0.63
1:A:91:ALA:HB3	1:A:263:TYR:HD1	1.61	0.63
1:B:637:SER:OG	1:B:638:ASN:N	2.31	0.63
1:C:243:ARG:HA	1:C:247:THR:HG21	1.80	0.63
1:C:673:THR:HA	1:C:687:GLN:HA	1.79	0.63
1:C:390:THR:HA	1:C:520:THR:HG22	1.81	0.63
1:A:452:LEU:HD23	1:A:490:GLN:HB2	1.81	0.63
1:C:404:VAL:O	1:C:407:ILE:HG22	1.98	0.63
1:A:562:PHE:CD1	1:A:564:ARG:NH1	2.66	0.63
1:A:94:GLU:O	1:A:183:PHE:HA	1.98	0.62
1:B:500:VAL:HA	1:B:503:GLN:HG2	1.79	0.62
1:C:557:LEU:N	1:C:560:GLN:OE1	2.27	0.62
1:A:556:PHE:HZ	1:A:572:ALA:HB1	1.64	0.62
1:B:433:TRP:CZ2	1:B:506:ARG:HD2	2.34	0.62
1:B:284:ASP:OD1	1:B:285:ALA:N	2.29	0.62
1:C:21:ARG:NH1	1:C:77:PHE:O	2.32	0.62
1:C:563:GLY:N	1:C:572:ALA:HB3	2.14	0.62
1:C:305:VAL:HG22	1:C:599:THR:HG23	1.82	0.62
1:B:18:LEU:HD11	1:B:255:TRP:NE1	2.15	0.62
1:C:64:TRP:HE1	1:C:261:ALA:HB1	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:CYS:HB2	1:C:137:PRO:HB3	1.82	0.62
1:C:450:TYR:OH	1:C:490:GLN:OE1	2.15	0.62
1:C:571:ASP:CA	1:C:584:ILE:O	2.47	0.62
1:B:575:ASP:OD2	1:B:578:THR:N	2.33	0.61
1:C:477:CYS:HB2	1:C:480:VAL:HG22	1.80	0.61
1:B:919:LEU:HD12	2:I:2:NAG:C6	2.28	0.61
1:C:549:LEU:HD23	1:C:549:LEU:H	1.65	0.61
1:B:390:THR:C	1:B:513:GLU:O	2.38	0.61
1:C:117:ILE:HG22	1:C:126:ILE:HG23	1.82	0.61
1:A:535:CYS:HA	1:A:547:GLY:O	2.00	0.61
1:C:549:LEU:HD12	1:C:582:LEU:HD13	1.81	0.61
1:B:295:GLU:OE1	1:B:633:TYR:OH	2.18	0.61
1:B:360:ALA:H	1:B:523:GLY:HA2	1.66	0.61
1:C:104:PHE:HB2	1:C:115:LEU:HB2	1.82	0.60
1:C:441:LYS:HE3	1:C:445:ASN:HA	1.83	0.60
1:A:104:PHE:CB	1:A:115:LEU:HB3	2.29	0.60
1:C:850:GLN:HB3	1:C:855:LEU:HB2	1.81	0.60
1:B:139:LEU:HB2	1:B:241:LEU:HG	1.82	0.60
1:A:189:PHE:HD2	1:A:200:ILE:HG13	1.67	0.60
1:B:339:PHE:O	1:B:506:ARG:NH1	2.34	0.60
1:C:453:PHE:HD2	1:C:488:PRO:HA	1.67	0.60
1:B:602:SER:OG	1:B:603:ASN:N	2.35	0.60
1:A:348:TYR:HA	1:A:419:ASN:HB3	1.83	0.60
1:C:350:TRP:O	1:C:463:ARG:NH2	2.33	0.60
1:B:139:LEU:HB3	1:B:240:ALA:HA	1.84	0.59
1:A:323:ILE:CG2	1:A:325:ARG:HG2	2.33	0.59
1:C:114:SER:O	1:C:128:VAL:HA	2.03	0.59
1:A:207:ILE:HG13	1:A:211:ARG:NH1	2.17	0.59
1:A:362:TYR:CD2	1:A:384:LEU:HD13	2.36	0.59
1:C:375:LYS:HG2	1:C:430:VAL:HG22	1.85	0.59
1:B:91:ALA:HB3	1:B:263:TYR:HB2	1.83	0.59
1:B:139:LEU:HB2	1:B:241:LEU:H	1.67	0.59
1:C:390:THR:HG23	1:C:391:ASN:ND2	2.17	0.59
1:B:659:CYS:HB2	1:B:694:MET:HG3	1.84	0.58
1:C:141:VAL:HB	1:C:241:LEU:O	2.02	0.58
1:A:374:PHE:CE2	1:A:381:PRO:HB3	2.35	0.58
1:B:243:ARG:HH12	1:B:251:SER:HA	1.67	0.58
1:C:335:PHE:HA	1:C:338:VAL:HG22	1.84	0.58
1:C:488:PRO:HG2	1:C:489:LEU:HD12	1.83	0.58
1:C:575:ASP:OD2	1:C:578:THR:N	2.35	0.58
1:A:405:ARG:NH1	1:A:412:THR:O	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:2:NAG:H83	2:O:2:NAG:H3	1.84	0.58
1:B:24:LEU:HD12	1:B:25:PRO:HD2	1.86	0.58
1:C:190:VAL:HB	1:C:201:TYR:CD1	2.38	0.58
1:B:123:ASN:HB3	1:B:168:VAL:HG13	1.86	0.58
1:A:562:PHE:HD1	1:A:564:ARG:NH1	2.00	0.58
1:B:575:ASP:O	1:B:579:LEU:HD23	2.04	0.58
1:B:94:GLU:OE2	1:B:98:ILE:N	2.22	0.58
1:A:563:GLY:HA3	1:A:571:ASP:N	2.15	0.57
1:A:102:TRP:H	1:A:117:ILE:HG23	1.68	0.57
1:A:327:PRO:HA	1:A:576:PRO:HB2	1.85	0.57
1:B:609:TYR:O	1:B:611:GLY:N	2.37	0.57
1:B:436:ASN:ND2	1:B:503:GLN:OE1	2.38	0.57
1:A:371:PHE:HD2	1:A:374:PHE:HB2	1.69	0.57
1:C:87:GLY:HA3	1:C:190:VAL:HG13	1.87	0.57
1:B:68:ILE:H	1:B:76:ARG:HB3	1.69	0.57
1:B:554:LYS:HB3	1:B:556:PHE:HE1	1.69	0.57
1:A:574:ARG:HG2	1:A:579:LEU:HA	1.86	0.57
1:C:137:PRO:HB2	1:C:156:VAL:HA	1.87	0.57
1:C:449:LEU:HG	1:C:491:SER:HB2	1.86	0.57
1:B:418:TYR:HD2	1:B:454:ARG:HB3	1.70	0.57
1:C:574:ARG:HG2	1:C:579:LEU:HA	1.85	0.57
1:C:832:LYS:HZ1	1:C:847:ILE:HB	1.70	0.57
1:C:93:THR:HG23	1:C:261:ALA:HB3	1.85	0.56
1:A:79:ASN:ND2	1:A:237:THR:HB	2.19	0.56
1:B:973:VAL:HB	1:B:976:ASP:HB2	1.87	0.56
1:C:202:SER:H	1:C:221:GLU:H	1.51	0.56
1:C:469:ILE:HD13	1:C:479:GLY:HA2	1.87	0.56
1:B:38:TYR:CE2	1:B:282:ILE:HG13	2.40	0.56
1:C:88:VAL:H	1:C:190:VAL:HA	1.70	0.56
1:C:142:TYR:O	1:C:149:TRP:HA	2.04	0.56
1:A:454:ARG:NH1	1:A:464:ASP:OD2	2.38	0.56
1:A:26:PRO:HG2	1:A:28:TYR:HE1	1.71	0.56
1:B:293:LEU:O	1:B:296:THR:OG1	2.20	0.56
1:B:417:ASP:OD1	1:B:418:TYR:N	2.38	0.56
1:A:400:ARG:HB2	1:A:492:TYR:CE1	2.40	0.56
1:A:24:LEU:HD22	1:A:76:ARG:HH12	1.70	0.56
1:A:602:SER:OG	1:A:603:ASN:N	2.38	0.56
1:B:189:PHE:HB3	1:B:191:PHE:CZ	2.40	0.56
1:A:184:LYS:HA	1:A:207:ILE:CG2	2.36	0.56
1:B:170:GLN:NE2	1:B:171:PRO:O	2.39	0.56
1:B:565:ASP:OD2	1:B:567:ASP:HB3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:302:SER:OG	1:C:303:PHE:N	2.39	0.56
1:A:347:VAL:HG11	1:A:415:ILE:HD13	1.88	0.55
1:A:351:ASN:ND2	1:A:396:SER:HB2	2.20	0.55
1:A:789:PRO:HG3	1:C:704:TYR:HB3	1.88	0.55
1:C:391:ASN:HB2	1:C:513:GLU:HB3	1.87	0.55
1:C:831:ILE:C	1:C:832:LYS:HD2	2.27	0.55
1:B:142:TYR:HB3	1:B:152:SER:OG	2.07	0.55
1:C:450:TYR:CZ	1:C:490:GLN:HB2	2.41	0.55
2:H:2:NAG:H3	2:H:2:NAG:H83	1.87	0.55
1:C:201:TYR:CE2	1:C:222:PRO:HG3	2.41	0.55
1:A:431:ILE:HB	1:A:508:VAL:HG23	1.88	0.55
1:B:563:GLY:O	1:B:570:THR:HA	2.06	0.55
1:C:846:LEU:HB2	1:C:850:GLN:NE2	2.21	0.55
1:A:362:TYR:HB3	1:A:365:LEU:HB3	1.88	0.55
1:B:53:ASP:HB3	1:B:55:PHE:CE2	2.42	0.55
1:B:419:ASN:N	1:B:458:LEU:HD21	2.21	0.55
1:C:847:ILE:HA	1:C:850:GLN:OE1	2.07	0.55
1:A:436:ASN:HD21	1:A:496:PRO:HA	1.72	0.55
1:B:66:HIS:CE1	1:B:68:ILE:HG23	2.42	0.55
1:A:322:SER:HA	1:A:537:ASN:O	2.06	0.55
1:C:231:ASN:O	1:C:232:ILE:HD13	2.07	0.55
1:A:347:VAL:HG11	1:A:415:ILE:CD1	2.37	0.55
1:C:200:ILE:N	1:C:223:LEU:H	2.03	0.55
1:C:613:ASN:OD1	3:C:1301:NAG:C1	2.54	0.55
1:B:593:SER:OG	1:B:608:LEU:HB3	2.06	0.55
1:C:123:ASN:HB3	1:C:168:VAL:HG13	1.89	0.55
1:B:122:THR:HG1	1:B:123:ASN:N	2.05	0.54
1:B:408:ALA:HB3	1:B:411:GLN:HB2	1.88	0.54
1:A:556:PHE:CE2	1:A:561:GLN:HA	2.41	0.54
1:B:359:VAL:HA	1:B:522:CYS:O	2.07	0.54
1:C:141:VAL:HG21	1:C:242:HIS:CD2	2.41	0.54
1:C:562:PHE:C	1:C:572:ALA:HB3	2.27	0.54
1:A:277:ASN:OD1	1:A:280:GLY:N	2.40	0.54
1:A:846:LEU:HB2	1:A:850:GLN:NE2	2.22	0.54
1:A:18:LEU:HD23	1:A:252:SER:HA	1.88	0.54
1:B:549:LEU:HA	1:B:583:ASP:O	2.08	0.54
1:B:572:ALA:HA	1:B:582:LEU:O	2.07	0.54
1:A:323:ILE:HG22	1:A:325:ARG:HG2	1.90	0.54
1:C:90:PHE:CE1	1:C:262:TYR:HB2	2.43	0.54
1:A:433:TRP:HZ2	1:A:506:ARG:HH21	1.56	0.54
1:C:380:SER:OG	1:C:383:LYS:HG2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:871:THR:HG21	1:C:1052:SER:HB3	1.89	0.54
1:A:30:ASN:HB3	1:A:32:PHE:CZ	2.42	0.54
1:C:107:THR:HG21	1:C:112:THR:HG23	1.90	0.54
2:L:2:NAG:H83	2:L:2:NAG:H3	1.90	0.54
1:A:554:LYS:HD2	1:B:43:PHE:CZ	2.43	0.54
1:B:84:PHE:HZ	1:B:191:PHE:O	1.90	0.54
1:A:211:ARG:NE	1:A:214:PRO:HB3	2.19	0.53
1:A:436:ASN:OD1	1:A:440:SER:OG	2.26	0.53
1:B:27:ALA:CB	1:B:64:TRP:HB3	2.38	0.53
1:B:190:VAL:HG13	1:B:267:LEU:CD1	2.31	0.53
1:C:190:VAL:HB	1:C:201:TYR:HD1	1.72	0.53
1:A:37:TYR:HB2	1:A:201:TYR:CD2	2.43	0.53
1:A:455:LYS:H	1:A:455:LYS:HD2	1.72	0.53
1:C:140:GLY:O	1:C:151:GLU:HA	2.09	0.53
1:C:571:ASP:C	1:C:584:ILE:H	2.11	0.53
1:A:560:GLN:HB3	1:B:43:PHE:HB2	1.89	0.53
1:C:571:ASP:CA	1:C:584:ILE:H	2.21	0.53
1:A:383:LYS:HD3	1:A:387:LEU:HD21	1.89	0.53
1:B:127:LYS:HB2	1:B:131:PHE:HZ	1.73	0.53
1:C:65:PHE:HB2	1:C:262:TYR:CE1	2.43	0.53
1:B:387:LEU:HD13	1:B:389:PHE:HE1	1.74	0.53
1:A:133:PHE:HA	1:A:157:TYR:HA	1.91	0.53
1:C:832:LYS:HG2	1:C:851:LYS:HE2	1.91	0.53
1:B:141:VAL:HG21	1:B:240:ALA:HB1	1.91	0.53
1:B:383:LYS:HD2	1:C:980:ARG:N	2.23	0.53
1:C:26:PRO:HG2	1:C:28:TYR:CE1	2.44	0.53
1:A:637:SER:OG	1:A:638:ASN:N	2.39	0.53
1:B:390:THR:HB	1:B:519:ALA:HA	1.91	0.53
1:C:18:LEU:HD11	1:C:138:PHE:CE1	2.44	0.53
1:C:459:LYS:HB2	1:C:462:GLU:OE2	2.08	0.53
1:C:831:ILE:O	1:C:832:LYS:HD2	2.09	0.53
1:A:212:ASP:OD1	1:A:263:TYR:OH	2.27	0.53
1:B:292:PRO:O	1:B:296:THR:HG23	2.10	0.53
1:B:339:PHE:HE1	1:B:508:VAL:HG21	1.74	0.53
1:A:380:SER:OG	1:A:383:LYS:HG2	2.10	0.52
1:B:38:TYR:CZ	1:B:282:ILE:HG13	2.44	0.52
1:A:84:PHE:CE1	1:A:86:ASP:HA	2.44	0.52
1:B:189:PHE:HB3	1:B:191:PHE:CE1	2.45	0.52
1:A:142:TYR:H	1:A:151:GLU:HA	1.74	0.52
1:A:394:ALA:HA	1:A:510:LEU:HA	1.92	0.52
1:C:390:THR:HG23	1:C:391:ASN:HD22	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:436:ASN:OD1	1:C:504:PRO:HD2	2.10	0.52
1:C:91:ALA:HB3	1:C:263:TYR:CD1	2.39	0.52
1:C:92:SER:OG	1:C:94:GLU:HB2	2.09	0.52
1:B:129:CYS:SG	1:B:131:PHE:CZ	3.03	0.52
1:A:830:PHE:HA	1:A:832:LYS:HE2	1.91	0.51
1:B:66:HIS:HE1	1:B:68:ILE:HG23	1.75	0.51
1:B:141:VAL:HG12	1:B:143:HIS:CE1	2.45	0.51
1:B:326:PHE:HA	1:B:541:ASN:OD1	2.09	0.51
1:C:320:THR:HG21	1:C:534:LYS:NZ	2.25	0.51
1:A:114:SER:HB3	1:A:133:PHE:HE2	1.75	0.51
1:B:487:PHE:HE2	1:B:489:LEU:HD12	1.75	0.51
1:B:145:ASN:HD21	1:B:246:LEU:HD22	1.75	0.51
1:B:450:TYR:HB3	1:B:492:TYR:CE1	2.45	0.51
1:A:196:GLY:HA2	1:A:227:PRO:HA	1.91	0.51
1:A:320:THR:HB	1:A:536:VAL:HA	1.93	0.51
1:B:249:GLY:HA3	1:B:253:SER:OG	2.11	0.51
1:A:201:TYR:CE2	1:A:222:PRO:HB3	2.46	0.51
1:B:324:VAL:N	1:B:528:THR:OG1	2.30	0.51
1:B:333:CYS:HB3	1:B:335:PHE:CE2	2.46	0.51
1:C:424:ASP:OD1	1:C:425:ASP:N	2.44	0.51
1:A:384:LEU:HD12	1:A:385:ASN:N	2.25	0.51
1:B:243:ARG:HG2	1:B:255:TRP:HA	1.93	0.51
1:C:376:CYS:SG	1:C:381:PRO:HG3	2.51	0.51
1:B:270:ARG:HB2	1:B:272:PHE:HE1	1.76	0.51
1:C:322:SER:HA	1:C:537:ASN:O	2.10	0.51
1:A:400:ARG:O	1:A:401:GLY:C	2.48	0.51
1:B:534:LYS:C	1:B:548:VAL:HG12	2.31	0.51
1:B:537:ASN:HA	1:B:546:THR:HA	1.91	0.51
1:B:673:THR:HA	1:B:687:GLN:HA	1.93	0.51
1:C:120:ASN:OD1	1:C:121:ALA:N	2.42	0.51
1:C:419:ASN:HD21	1:C:451:ARG:H	1.58	0.51
1:A:94:GLU:HG2	1:A:185:ASN:HB2	1.93	0.51
1:B:142:TYR:CD1	1:B:243:ARG:HB2	2.43	0.51
1:B:574:ARG:HA	1:B:580:GLU:O	2.10	0.51
1:A:183:PHE:O	1:A:207:ILE:HG23	2.11	0.50
1:A:41:LYS:HB3	1:C:559:PHE:O	2.12	0.50
1:A:404:VAL:HA	1:A:407:ILE:HG13	1.93	0.50
1:B:405:ARG:HA	1:B:405:ARG:NE	2.26	0.50
1:C:129:CYS:HB3	1:C:161:ASN:O	2.11	0.50
1:A:852:PHE:HZ	1:C:585:THR:HG23	1.74	0.50
1:C:31:SER:HB2	1:C:56:LEU:HD21	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:827:ASP:C	1:C:845:ASP:HA	2.30	0.50
1:C:829:GLY:O	1:C:847:ILE:HG13	2.12	0.50
1:B:482:GLY:N	1:B:485:CYS:HB2	2.26	0.50
1:C:535:CYS:HA	1:C:547:GLY:O	2.12	0.50
1:C:67:ALA:HA	1:C:76:ARG:O	2.10	0.50
1:C:292:PRO:O	1:C:295:GLU:N	2.45	0.50
1:A:115:LEU:HD12	1:A:116:LEU:H	1.77	0.50
1:A:819:LEU:HD23	1:A:942:LEU:HD11	1.94	0.50
1:A:291:ASP:O	1:A:294:SER:OG	2.25	0.50
1:A:426:PHE:HZ	1:A:511:SER:HA	1.75	0.50
1:C:18:LEU:HD11	1:C:138:PHE:HE1	1.76	0.50
1:A:41:LYS:O	1:C:560:GLN:HA	2.11	0.50
1:A:104:PHE:CE2	1:A:235:PHE:HB3	2.47	0.50
1:B:469:ILE:H	1:B:469:ILE:HD12	1.76	0.50
1:B:573:VAL:O	1:B:582:LEU:HD12	2.11	0.50
1:C:121:ALA:HA	1:C:174:MET:HB2	1.94	0.50
1:C:212:ASP:HA	1:C:263:TYR:OH	2.12	0.50
1:A:137:PRO:CG	1:A:238:LEU:HG	2.38	0.50
1:A:613:ASN:OD1	1:A:613:ASN:N	2.45	0.50
1:A:344:PHE:CE1	1:A:506:ARG:HD3	2.47	0.49
1:B:273:LEU:HB3	1:B:286:VAL:CG1	2.42	0.49
1:C:122:THR:HA	1:C:172:PHE:O	2.11	0.49
1:C:471:GLN:HG3	1:C:485:CYS:SG	2.52	0.49
1:A:286:VAL:HG23	1:A:303:PHE:CE2	2.47	0.49
1:A:434:ASN:HD21	1:A:503:GLN:CB	2.25	0.49
1:B:549:LEU:HD13	1:B:583:ASP:O	2.12	0.49
1:B:205:THR:HG23	1:B:207:ILE:HG12	1.93	0.49
1:B:53:ASP:CG	1:B:54:LEU:H	2.16	0.49
1:B:255:TRP:CZ3	1:B:257:ALA:HB2	2.47	0.49
1:B:673:THR:CA	1:B:687:GLN:HG2	2.42	0.49
1:A:36:VAL:HA	1:A:55:PHE:HE1	1.77	0.49
1:A:91:ALA:O	1:A:262:TYR:CA	2.54	0.49
1:A:104:PHE:HB3	1:A:232:ILE:HG23	1.93	0.49
1:A:116:LEU:O	1:A:126:ILE:HA	2.11	0.49
1:B:347:VAL:HG22	1:B:398:VAL:O	2.12	0.49
1:C:117:ILE:HG13	1:C:117:ILE:O	2.12	0.49
1:A:139:LEU:HB2	1:A:240:ALA:HA	1.95	0.49
1:A:156:VAL:HB	1:A:157:TYR:CD1	2.42	0.49
1:A:185:ASN:HA	1:A:187:ARG:HH21	1.77	0.49
1:C:35:GLY:HA2	1:C:220:LEU:HD11	1.93	0.49
1:C:37:TYR:HB3	1:C:220:LEU:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:PHE:HB3	1:A:191:PHE:CZ	2.48	0.49
1:A:455:LYS:HD2	1:A:455:LYS:N	2.28	0.49
1:C:83:PRO:HA	1:C:234:ARG:HG3	1.93	0.49
1:A:27:ALA:O	1:A:64:TRP:N	2.46	0.49
1:B:391:ASN:HB3	1:B:513:GLU:H	1.77	0.49
1:B:564:ARG:HD2	1:B:568:ASP:OD2	2.13	0.49
1:C:155:ARG:HH12	1:C:251:SER:CB	2.25	0.49
1:A:557:LEU:HB3	1:A:558:PRO:HD2	1.95	0.49
1:A:709:ILE:HD12	1:A:1091:VAL:HG21	1.93	0.49
1:B:467:THR:HG22	1:B:489:LEU:HD11	1.95	0.49
1:C:290:LEU:HD23	1:C:291:ASP:HB3	1.95	0.49
1:A:405:ARG:NH2	1:A:411:GLN:OE1	2.46	0.48
1:C:141:VAL:HG23	1:C:240:ALA:HB3	1.95	0.48
1:A:233:THR:HG22	1:A:234:ARG:HD3	1.95	0.48
1:A:316:ARG:CB	1:A:589:PHE:H	2.27	0.48
1:B:317:VAL:HB	1:B:587:CYS:SG	2.53	0.48
1:B:552:SER:OG	1:B:581:ILE:HB	2.13	0.48
1:A:75:LYS:HG3	1:A:255:TRP:HZ3	1.77	0.48
1:A:90:PHE:HA	1:A:263:TYR:O	2.13	0.48
1:A:432:ALA:HA	1:A:506:ARG:O	2.13	0.48
1:B:92:SER:H	1:B:186:LEU:HD13	1.77	0.48
1:B:495:GLN:HB3	1:B:497:THR:HG23	1.94	0.48
1:C:174:MET:HB3	1:C:176:LEU:HD23	1.95	0.48
1:C:436:ASN:O	1:C:440:SER:OG	2.30	0.48
1:A:385:ASN:HB2	1:A:524:PRO:HD2	1.96	0.48
1:A:848:CYS:HA	1:A:851:LYS:HB2	1.95	0.48
1:B:125:VAL:HA	1:B:167:TYR:O	2.13	0.48
1:B:434:ASN:HB2	1:B:505:TYR:CZ	2.48	0.48
1:A:557:LEU:O	1:A:559:PHE:N	2.47	0.48
1:C:66:HIS:CD2	1:C:261:ALA:HB2	2.49	0.48
1:C:109:ASP:HB2	1:C:111:LYS:NZ	2.28	0.48
1:C:200:ILE:HB	1:C:223:LEU:HB2	1.93	0.48
1:C:612:VAL:HG12	1:C:614:CYS:HA	1.96	0.48
1:C:27:ALA:HB3	1:C:64:TRP:HB3	1.96	0.48
1:C:981:LEU:HD21	1:C:989:GLN:HG3	1.95	0.48
1:A:295:GLU:O	1:A:299:THR:HG23	2.14	0.48
1:A:980:ARG:HA	1:C:383:LYS:HD2	1.96	0.48
1:C:94:GLU:HG2	1:C:96:SER:H	1.78	0.48
1:A:138:PHE:HA	1:A:239:LEU:O	2.14	0.48
1:A:403:GLU:HG3	1:A:415:ILE:HD12	1.96	0.48
1:C:405:ARG:HD2	1:C:406:GLN:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:LEU:O	1:A:450:TYR:HB3	2.13	0.47
1:A:41:LYS:NZ	1:C:559:PHE:HB2	2.29	0.47
1:B:391:ASN:HB3	1:B:513:GLU:HB3	1.95	0.47
1:B:469:ILE:HG21	1:B:485:CYS:HB3	1.96	0.47
1:C:81:VAL:HG22	1:C:234:ARG:HG2	1.97	0.47
1:C:90:PHE:H	1:C:188:GLU:HA	1.78	0.47
1:C:574:ARG:HA	1:C:580:GLU:O	2.14	0.47
1:A:452:LEU:CD2	1:A:490:GLN:HB2	2.43	0.47
1:C:104:PHE:HD2	1:C:232:ILE:HG21	1.79	0.47
1:C:848:CYS:O	1:C:851:LYS:HB2	2.13	0.47
1:A:573:VAL:HG12	1:A:582:LEU:HB2	1.96	0.47
1:B:28:TYR:HB3	3:B:1301:NAG:O7	2.15	0.47
1:B:113:GLN:NE2	1:B:128:VAL:O	2.47	0.47
1:A:21:ARG:NH1	1:A:77:PHE:O	2.48	0.47
1:A:412:THR:OG1	1:A:417:ASP:OD2	2.25	0.47
1:C:449:LEU:HA	1:C:491:SER:HA	1.95	0.47
1:C:469:ILE:HD12	1:C:469:ILE:H	1.80	0.47
1:B:404:VAL:C	1:B:406:GLN:H	2.16	0.47
1:B:435:SER:HB3	1:B:438:LEU:HD21	1.96	0.47
1:B:143:HIS:HB2	1:B:148:SER:O	2.14	0.47
1:C:129:CYS:HA	1:C:163:CYS:HA	1.97	0.47
1:A:43:PHE:HB3	1:C:556:PHE:CZ	2.50	0.47
1:A:273:LEU:O	1:A:285:ALA:HA	2.15	0.47
1:A:351:ASN:HD21	1:A:396:SER:HB2	1.80	0.47
1:A:554:LYS:HD2	1:B:43:PHE:CE2	2.50	0.47
1:A:945:LEU:HD23	1:A:945:LEU:HA	1.77	0.47
1:B:292:PRO:HG3	1:B:633:TYR:CD2	2.50	0.46
1:B:321:GLU:O	1:B:536:VAL:HB	2.15	0.46
1:C:97:ASN:ND2	1:C:175:ASP:OD2	2.48	0.46
1:C:320:THR:HG23	1:C:321:GLU:HG2	1.97	0.46
1:C:471:GLN:HG2	1:C:476:PRO:HB3	1.97	0.46
1:C:540:PHE:CZ	1:C:573:VAL:HG11	2.50	0.46
1:A:380:SER:OG	1:A:383:LYS:NZ	2.36	0.46
1:B:322:SER:HA	1:B:537:ASN:O	2.16	0.46
1:B:325:ARG:HA	1:B:527:SER:OG	2.16	0.46
1:B:348:TYR:HB3	1:B:419:ASN:OD1	2.15	0.46
1:B:354:ARG:HD2	1:B:355:ILE:N	2.29	0.46
1:B:832:LYS:H	1:B:832:LYS:HG3	1.50	0.46
3:B:1306:NAG:H3	3:B:1306:NAG:H83	1.97	0.46
1:C:128:VAL:O	1:C:163:CYS:HA	2.15	0.46
1:A:422:LEU:HD23	1:A:426:PHE:CD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:ASN:O	1:B:100:ARG:HD3	2.15	0.46
1:B:438:LEU:HD23	1:B:438:LEU:H	1.80	0.46
1:C:983:LYS:HD2	1:C:983:LYS:HA	1.64	0.46
1:B:391:ASN:O	1:B:391:ASN:ND2	2.48	0.46
1:B:595:ILE:HB	1:B:606:ALA:HB3	1.98	0.46
1:B:658:GLU:HG2	1:B:659:CYS:N	2.31	0.46
1:A:187:ARG:HH12	1:A:204:HIS:HA	1.81	0.46
1:B:68:ILE:C	1:B:257:ALA:HB3	2.36	0.46
1:B:406:GLN:HB2	1:B:415:ILE:HG22	1.98	0.46
1:B:515:LEU:HD13	1:B:542:GLY:HA3	1.96	0.46
1:A:190:VAL:HB	1:A:201:TYR:HD1	1.81	0.46
1:B:79:ASN:ND2	1:B:236:GLN:HE21	2.13	0.46
1:B:295:GLU:OE2	1:B:631:ARG:NH1	2.48	0.46
1:B:383:LYS:CD	1:C:980:ARG:H	2.24	0.46
1:B:446:TYR:HB2	1:B:491:SER:OG	2.15	0.46
1:C:137:PRO:CB	1:C:156:VAL:HA	2.45	0.46
1:A:432:ALA:HB2	1:A:507:VAL:HG13	1.97	0.46
1:A:887:ALA:HB1	1:C:1043:GLY:HA2	1.97	0.46
1:C:300:LEU:HD23	1:C:300:LEU:O	2.15	0.46
1:B:791:ILE:H	1:B:791:ILE:HG13	1.47	0.46
1:C:94:GLU:HG2	1:C:95:LYS:N	2.30	0.46
1:C:94:GLU:HG3	1:C:260:ALA:CB	2.46	0.46
1:A:208:ASN:HB2	1:A:209:LEU:HD12	1.98	0.45
1:A:403:GLU:OE2	1:A:403:GLU:HA	2.15	0.45
1:A:575:ASP:O	1:A:579:LEU:HD23	2.16	0.45
1:B:983:LYS:HB2	1:B:983:LYS:HE2	1.50	0.45
1:C:848:CYS:HA	1:C:851:LYS:HG2	1.98	0.45
1:B:113:GLN:HG2	1:B:128:VAL:HG12	1.97	0.45
1:B:608:LEU:HG	1:B:609:TYR:N	2.29	0.45
1:B:942:LEU:HD13	1:B:942:LEU:HA	1.80	0.45
1:C:322:SER:CB	1:C:537:ASN:HB2	2.47	0.45
1:C:405:ARG:HD2	1:C:405:ARG:C	2.37	0.45
1:B:291:ASP:O	1:B:294:SER:OG	2.34	0.45
1:B:292:PRO:HG3	1:B:633:TYR:CE2	2.51	0.45
1:C:832:LYS:HE3	1:C:848:CYS:SG	2.57	0.45
3:C:1302:NAG:N2	3:C:1302:NAG:O4	2.50	0.45
1:A:24:LEU:HD22	1:A:76:ARG:NH1	2.31	0.45
1:A:564:ARG:HG3	1:A:568:ASP:HB3	1.98	0.45
1:A:811:LYS:HA	1:A:811:LYS:HD3	1.63	0.45
1:B:975:ASN:HA	1:B:978:LEU:HD12	1.99	0.45
1:C:266:TYR:HA	1:C:267:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:THR:HG23	1:A:261:ALA:HB3	1.98	0.45
1:A:354:ARG:NE	1:A:391:ASN:HD21	2.15	0.45
1:A:416:ALA:HA	1:A:420:TYR:O	2.17	0.45
1:B:1083:LYS:HE2	1:B:1083:LYS:HB2	1.52	0.45
1:C:93:THR:CG2	1:C:261:ALA:HB3	2.47	0.45
1:A:105:GLY:O	1:A:234:ARG:N	2.50	0.45
1:A:339:PHE:CD2	1:A:508:VAL:HG21	2.51	0.45
1:A:547:GLY:HA3	1:A:586:PRO:HA	1.99	0.45
1:A:556:PHE:HB2	1:A:574:ARG:HH21	1.81	0.45
1:B:357:ASN:H	1:B:520:THR:HB	1.81	0.45
1:B:848:CYS:HB2	1:B:849:ALA:H	1.64	0.45
1:C:113:GLN:HG3	1:C:129:CYS:C	2.37	0.45
1:C:336:GLY:O	1:C:340:ASN:HB2	2.16	0.45
1:C:540:PHE:CE2	1:C:573:VAL:HG11	2.52	0.45
1:B:138:PHE:HB2	1:B:155:ARG:HG3	1.98	0.45
1:B:291:ASP:OD1	1:B:291:ASP:N	2.49	0.45
1:B:573:VAL:HG13	1:B:582:LEU:HD13	1.99	0.45
1:B:740:CYS:HB3	1:B:746:CYS:HB3	1.91	0.45
1:C:291:ASP:OD1	1:C:294:SER:OG	2.33	0.45
1:A:354:ARG:HD2	1:A:393:TYR:CZ	2.51	0.45
1:B:134:CYS:O	1:B:137:PRO:HD3	2.17	0.45
1:B:365:LEU:HB2	1:B:371:PHE:HZ	1.81	0.45
1:B:672:GLN:HG2	1:B:673:THR:N	2.31	0.45
1:C:141:VAL:HG21	1:C:242:HIS:HD2	1.78	0.45
1:C:324:VAL:CG1	1:C:527:SER:HA	2.47	0.45
1:C:470:TYR:O	1:C:486:TYR:N	2.35	0.45
1:C:575:ASP:OD2	1:C:578:THR:HG23	2.17	0.45
1:C:791:ILE:H	1:C:791:ILE:HG13	1.45	0.45
1:A:209:LEU:HD12	1:A:209:LEU:H	1.82	0.45
1:A:326:PHE:O	1:A:577:GLN:NE2	2.44	0.45
1:A:457:ASN:ND2	1:A:458:LEU:H	2.14	0.45
1:A:855:LEU:HD13	1:A:855:LEU:HA	1.74	0.45
1:C:723:ILE:HG23	1:C:1058:VAL:HG22	1.99	0.45
1:A:91:ALA:HB3	1:A:263:TYR:CD1	2.48	0.44
1:A:190:VAL:O	1:A:200:ILE:HA	2.17	0.44
1:A:538:PHE:CE2	1:A:584:ILE:HD13	2.52	0.44
1:A:574:ARG:HA	1:A:580:GLU:O	2.17	0.44
1:B:93:THR:CG2	1:B:261:ALA:HB3	2.47	0.44
1:B:103:ILE:HG22	1:B:116:LEU:HD13	2.00	0.44
1:B:125:VAL:HG22	1:B:168:VAL:HG22	1.99	0.44
1:B:302:SER:HG	1:B:304:THR:H	1.63	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:LEU:HD13	1:B:332:LEU:HA	1.74	0.44
1:B:379:VAL:HA	1:C:980:ARG:HB3	1.99	0.44
1:C:434:ASN:HB2	1:C:505:TYR:CZ	2.52	0.44
1:A:74:THR:OG1	1:A:75:LYS:N	2.49	0.44
1:A:328:ASN:N	1:A:577:GLN:HG2	2.31	0.44
1:A:956:LEU:HD23	1:A:956:LEU:HA	1.72	0.44
1:C:514:LEU:H	1:C:514:LEU:HG	1.41	0.44
1:B:125:VAL:HG11	1:B:127:LYS:HE3	1.99	0.44
1:B:337:GLU:OE2	1:B:337:GLU:N	2.51	0.44
1:B:883:TRP:HD1	1:B:1032:GLY:HA2	1.81	0.44
1:C:228:ILE:HG22	1:C:230:ILE:HG23	2.00	0.44
1:B:421:LYS:HA	1:B:421:LYS:HD3	1.74	0.44
1:C:279:ASN:ND2	3:C:1304:NAG:O3	2.51	0.44
1:C:571:ASP:O	1:C:572:ALA:HB2	2.17	0.44
1:B:188:GLU:O	1:B:202:SER:HB3	2.18	0.44
1:C:332:LEU:HD22	1:C:332:LEU:HA	1.79	0.44
1:C:672:GLN:HG3	1:C:690:ILE:HG12	1.98	0.44
1:C:1079:CYS:HB2	1:C:1129:ILE:HG12	1.98	0.44
1:A:557:LEU:HD12	1:A:560:GLN:NE2	2.32	0.44
1:B:871:THR:HG21	1:B:1052:SER:HB2	1.99	0.44
1:C:48:LEU:HB3	1:C:273:LEU:HD11	1.98	0.44
1:C:536:VAL:O	1:C:546:THR:HA	2.16	0.44
1:A:314:ASN:HA	1:A:592:VAL:CG2	2.48	0.44
1:A:659:CYS:HB2	1:A:668:CYS:HB3	1.72	0.44
1:B:74:THR:C	1:B:76:ARG:H	2.21	0.44
1:B:211:ARG:HG2	1:B:212:ASP:H	1.83	0.44
1:B:399:ILE:HG22	1:B:507:VAL:HG21	1.98	0.44
1:C:126:ILE:HG13	1:C:226:LEU:HD23	2.00	0.44
1:B:383:LYS:NZ	1:C:981:LEU:N	2.65	0.44
1:B:1111:ILE:H	1:B:1111:ILE:HG12	1.63	0.44
1:C:115:LEU:HD21	1:C:228:ILE:HG21	1.99	0.44
1:C:459:LYS:HB2	1:C:462:GLU:CD	2.37	0.44
1:A:133:PHE:HD1	1:A:156:VAL:O	2.00	0.43
1:A:448:TYR:HB3	1:A:492:TYR:CD2	2.52	0.43
1:A:452:LEU:HB2	1:A:490:GLN:NE2	2.33	0.43
1:B:64:TRP:CD1	1:B:263:TYR:HE1	2.36	0.43
1:B:320:THR:OG1	1:B:321:GLU:HG2	2.18	0.43
1:B:360:ALA:H	1:B:523:GLY:CA	2.29	0.43
1:C:141:VAL:HG23	1:C:240:ALA:CB	2.48	0.43
1:C:338:VAL:HG23	1:C:339:PHE:CD2	2.53	0.43
1:C:563:GLY:HA3	1:C:571:ASP:OD1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:GLU:HG3	1:A:95:LYS:N	2.33	0.43
1:B:243:ARG:NH1	1:B:251:SER:HA	2.33	0.43
2:M:1:NAG:H61	2:M:2:NAG:H82	1.99	0.43
1:B:288:CYS:HA	1:B:294:SER:HB2	2.00	0.43
1:C:376:CYS:HB3	1:C:379:VAL:CG2	2.49	0.43
1:C:613:ASN:ND2	3:C:1301:NAG:C2	2.75	0.43
1:A:371:PHE:CD2	1:A:374:PHE:HB2	2.50	0.43
1:A:390:THR:HB	1:A:513:GLU:O	2.19	0.43
1:A:815:ILE:H	1:A:815:ILE:HG12	1.68	0.43
1:C:435:SER:O	1:C:504:PRO:HG2	2.18	0.43
1:C:541:ASN:HD21	1:C:576:PRO:HG3	1.83	0.43
1:C:575:ASP:C	1:C:577:GLN:H	2.22	0.43
1:A:140:GLY:HA2	1:A:241:LEU:O	2.17	0.43
1:A:452:LEU:HB2	1:A:490:GLN:HE21	1.82	0.43
1:A:773:LYS:HE3	1:A:773:LYS:HB3	1.70	0.43
1:B:192:LYS:HZ3	1:B:201:TYR:HE1	1.60	0.43
1:C:572:ALA:CA	1:C:582:LEU:O	2.61	0.43
1:C:938:THR:HG21	1:C:941:ALA:HB2	2.00	0.43
1:A:458:LEU:HD21	1:A:462:GLU:O	2.18	0.43
1:B:64:TRP:CG	1:B:263:TYR:CE1	3.07	0.43
1:C:90:PHE:HB3	1:C:187:ARG:O	2.18	0.43
1:C:141:VAL:HB	1:C:242:HIS:HA	2.00	0.43
1:A:247:THR:O	1:A:247:THR:OG1	2.34	0.43
1:A:829:GLY:HA2	1:C:643:ARG:HE	1.83	0.43
1:C:184:LYS:HB2	1:C:206:PRO:HA	2.00	0.43
1:A:305:VAL:H	1:A:599:THR:HG22	1.84	0.43
1:B:389:PHE:O	1:B:519:ALA:HB1	2.19	0.43
1:C:47:VAL:HG22	1:C:48:LEU:N	2.33	0.43
1:C:209:LEU:HD22	1:C:209:LEU:HA	1.82	0.43
1:C:320:THR:HG23	1:C:536:VAL:HG12	2.00	0.43
1:A:38:TYR:HE2	1:A:219:ALA:HB1	1.84	0.43
1:A:92:SER:H	1:A:186:LEU:HA	1.83	0.43
1:A:312:THR:O	1:A:592:VAL:HG11	2.18	0.43
1:A:327:PRO:HG3	1:A:541:ASN:HD21	1.83	0.43
1:A:351:ASN:O	1:A:395:ASP:HA	2.19	0.43
1:B:327:PRO:HD3	1:B:541:ASN:OD1	2.19	0.43
1:C:434:ASN:HD21	1:C:503:GLN:HG3	1.84	0.43
1:C:571:ASP:HA	1:C:584:ILE:CA	2.49	0.43
1:B:904:ASN:HD22	1:B:904:ASN:HA	1.71	0.43
1:C:80:PRO:HG2	1:C:82:LEU:HD21	2.00	0.43
1:C:281:THR:O	1:C:283:THR:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:515:LEU:HD22	1:C:515:LEU:HA	1.76	0.43
1:C:571:ASP:HA	1:C:584:ILE:CB	2.48	0.43
1:A:354:ARG:HD2	1:A:393:TYR:OH	2.19	0.42
1:C:185:ASN:HA	1:C:204:HIS:CE1	2.53	0.42
1:A:21:ARG:HD2	1:A:77:PHE:O	2.18	0.42
1:A:327:PRO:CA	1:A:576:PRO:HB2	2.48	0.42
1:B:94:GLU:HG2	1:B:95:LYS:N	2.34	0.42
1:B:773:LYS:HB3	1:B:773:LYS:HE3	1.82	0.42
1:A:115:LEU:HD12	1:A:116:LEU:N	2.34	0.42
1:A:373:THR:O	1:A:373:THR:OG1	2.32	0.42
1:A:562:PHE:HB2	1:B:42:VAL:HG13	2.02	0.42
1:B:114:SER:OG	1:B:131:PHE:HD2	2.01	0.42
1:B:198:PHE:HB2	1:B:226:LEU:HD12	2.01	0.42
1:C:19:THR:HG22	1:C:20:THR:N	2.35	0.42
1:C:347:VAL:O	1:C:350:TRP:HD1	2.02	0.42
1:C:538:PHE:CZ	1:C:545:GLY:HA3	2.53	0.42
1:C:993:LEU:HD23	1:C:993:LEU:HA	1.86	0.42
1:A:418:TYR:HA	1:A:454:ARG:HD3	2.02	0.42
1:A:202:SER:O	1:A:220:LEU:HA	2.19	0.42
1:B:450:TYR:HB3	1:B:492:TYR:CZ	2.55	0.42
1:B:846:LEU:HD12	1:B:846:LEU:HA	1.85	0.42
1:C:84:PHE:N	1:C:234:ARG:HA	2.34	0.42
1:A:226:LEU:HD12	1:A:226:LEU:N	2.34	0.42
1:A:339:PHE:CE2	1:A:508:VAL:HG21	2.55	0.42
1:A:421:LYS:HB3	1:A:460:PRO:HA	1.99	0.42
1:A:751:LEU:HD13	1:A:751:LEU:HA	1.81	0.42
1:B:107:THR:HG22	1:B:112:THR:OG1	2.19	0.42
1:B:850:GLN:H	1:B:850:GLN:HG3	1.68	0.42
1:C:79:ASN:OD1	1:C:79:ASN:N	2.51	0.42
1:C:480:VAL:HG23	1:C:482:GLY:H	1.84	0.42
1:C:647:LEU:HD12	1:C:647:LEU:HA	1.80	0.42
1:A:195:ASP:OD2	1:A:228:ILE:CG1	2.68	0.42
1:A:242:HIS:O	1:A:256:THR:N	2.52	0.42
1:B:548:VAL:HG22	1:B:585:THR:O	2.20	0.42
1:B:980:ARG:HE	1:B:980:ARG:HB2	1.62	0.42
1:A:394:ALA:HB2	1:A:510:LEU:HG	2.00	0.42
1:A:452:LEU:HD23	1:A:490:GLN:HE21	1.85	0.42
1:A:530:LEU:HD23	1:A:530:LEU:HA	1.70	0.42
1:A:862:LEU:HD23	1:A:862:LEU:HA	1.88	0.42
1:A:971:SER:HB2	1:A:977:ILE:HG12	2.01	0.42
1:B:575:ASP:O	1:B:579:LEU:N	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:981:LEU:HD12	1:B:981:LEU:HA	1.82	0.42
1:C:899:MET:HB3	1:C:913:LEU:HD11	2.02	0.42
1:A:27:ALA:HB3	1:A:64:TRP:O	2.20	0.42
1:A:136:ASP:HA	1:A:137:PRO:HD3	1.85	0.42
1:A:871:THR:HG21	1:A:1052:SER:HB3	2.01	0.42
1:B:983:LYS:H	1:B:983:LYS:HG3	1.71	0.42
1:B:993:LEU:HD23	1:B:993:LEU:HA	1.87	0.42
1:C:402:ASP:O	1:C:405:ARG:HG3	2.20	0.42
1:C:467:THR:HG23	1:C:489:LEU:HD13	2.01	0.42
1:C:1127:ILE:H	1:C:1127:ILE:HG12	1.65	0.42
1:A:278:GLU:HG2	1:A:279:ASN:N	2.33	0.42
1:A:401:GLY:O	1:A:404:VAL:HG22	2.19	0.42
1:A:444:GLY:HA2	1:A:494:PHE:O	2.20	0.42
1:A:911:ASN:HD22	1:C:1118:PHE:HE1	1.66	0.42
1:A:1138:LEU:HD23	1:A:1138:LEU:HA	1.75	0.42
1:B:380:SER:OG	1:B:383:LYS:HG3	2.20	0.42
1:C:469:ILE:O	1:C:471:GLN:NE2	2.53	0.42
1:C:574:ARG:HG3	1:C:574:ARG:HH11	1.85	0.42
1:C:1094:SER:HB3	1:C:1099:TRP:CD2	2.55	0.42
1:A:108:LEU:HD23	1:A:234:ARG:HH21	1.84	0.41
1:A:242:HIS:O	1:A:247:THR:HG21	2.19	0.41
1:A:831:ILE:HG13	1:A:831:ILE:O	2.20	0.41
1:A:925:ASN:O	2:F:1:NAG:H83	2.20	0.41
1:B:415:ILE:CD1	1:B:419:ASN:HD22	2.29	0.41
1:B:575:ASP:CG	1:B:578:THR:H	2.22	0.41
1:C:52:GLN:OE1	1:C:52:GLN:N	2.53	0.41
1:C:94:GLU:HG3	1:C:260:ALA:HB2	2.00	0.41
1:A:690:ILE:H	1:A:690:ILE:HG13	1.71	0.41
1:C:540:PHE:O	1:C:543:LEU:HB2	2.20	0.41
1:C:783:LYS:HD2	1:C:783:LYS:HA	1.80	0.41
1:A:400:ARG:NH2	1:A:502:TYR:HB3	2.35	0.41
1:A:993:LEU:HD23	1:A:993:LEU:HA	1.84	0.41
1:B:253:SER:OG	1:B:254:GLY:N	2.52	0.41
1:B:314:ASN:OD1	1:B:314:ASN:N	2.53	0.41
1:B:560:GLN:HB3	1:C:43:PHE:HB2	2.03	0.41
1:C:77:PHE:CZ	1:C:239:LEU:HD22	2.48	0.41
1:C:277:ASN:CG	1:C:279:ASN:H	2.23	0.41
1:A:379:VAL:HG13	1:A:387:LEU:HD12	2.02	0.41
1:A:434:ASN:HD21	1:A:503:GLN:HB3	1.84	0.41
1:A:554:LYS:HD3	1:A:555:LYS:N	2.31	0.41
1:C:277:ASN:HD21	1:C:279:ASN:HB2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:434:ASN:OD1	1:C:435:SER:N	2.54	0.41
1:C:436:ASN:OD1	1:C:503:GLN:HB3	2.20	0.41
1:A:573:VAL:O	1:A:581:ILE:HA	2.20	0.41
1:B:344:PHE:CD2	1:B:398:VAL:HG13	2.55	0.41
1:A:278:GLU:OE1	1:A:278:GLU:N	2.38	0.41
1:B:831:ILE:HD12	1:B:831:ILE:HA	1.82	0.41
1:A:112:THR:O	1:A:130:GLU:HA	2.21	0.41
1:A:123:ASN:HB3	1:A:168:VAL:HA	2.02	0.41
1:A:557:LEU:HB2	1:A:560:GLN:CD	2.40	0.41
1:B:401:GLY:O	1:B:404:VAL:HG12	2.21	0.41
1:C:64:TRP:CG	1:C:263:TYR:CE2	3.09	0.41
1:C:67:ALA:HB1	1:C:77:PHE:HD1	1.86	0.41
1:C:198:PHE:O	1:C:200:ILE:HG12	2.21	0.41
1:C:803:LEU:HD22	1:C:803:LEU:HA	1.82	0.41
1:A:22:THR:HG23	1:A:74:THR:HA	2.03	0.41
1:C:324:VAL:HG12	1:C:527:SER:HA	2.01	0.41
1:A:103:ILE:O	1:A:235:PHE:HA	2.21	0.41
1:A:127:LYS:HB3	1:A:129:CYS:SG	2.61	0.41
1:A:184:LYS:HB3	1:A:184:LYS:HE3	1.75	0.41
1:A:575:ASP:OD2	1:A:578:THR:HG23	2.20	0.41
1:B:150:MET:N	1:B:150:MET:SD	2.94	0.41
1:B:406:GLN:OE1	1:B:415:ILE:N	2.43	0.41
1:B:449:LEU:HG	1:B:491:SER:CB	2.50	0.41
1:B:647:LEU:HD13	1:B:647:LEU:HA	1.86	0.41
1:B:735:CYS:O	1:B:736:THR:C	2.58	0.41
1:C:64:TRP:CD1	1:C:65:PHE:N	2.89	0.41
1:C:498:TYR:HB3	1:C:502:TYR:HB2	2.01	0.41
1:A:300:LEU:HD23	1:A:300:LEU:HA	1.68	0.41
1:A:327:PRO:O	1:A:328:ASN:C	2.60	0.41
1:A:390:THR:HG22	1:A:391:ASN:N	2.26	0.41
1:A:422:LEU:HG	1:A:461:PHE:CZ	2.56	0.41
1:B:438:LEU:HD11	1:B:506:ARG:NH2	2.36	0.41
1:B:454:ARG:HH11	1:B:455:LYS:H	1.69	0.41
1:C:127:LYS:HB3	1:C:131:PHE:CZ	2.45	0.41
1:C:139:LEU:O	1:C:240:ALA:HB1	2.20	0.41
1:A:273:LEU:HD12	1:A:274:LEU:N	2.36	0.40
1:B:115:LEU:HD23	1:B:116:LEU:N	2.36	0.40
1:B:123:ASN:CB	1:B:168:VAL:HG13	2.51	0.40
1:B:409:PRO:HB3	1:B:423:PRO:O	2.21	0.40
1:B:554:LYS:HB3	1:B:556:PHE:CE1	2.54	0.40
1:C:34:ARG:HH21	1:C:214:PRO:HG2	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:107:THR:HB	1:C:111:LYS:HD3	2.02	0.40
1:B:211:ARG:HH12	1:B:212:ASP:HB3	1.86	0.40
1:B:273:LEU:HB3	1:B:286:VAL:HG12	2.04	0.40
1:B:819:LEU:HD23	1:B:942:LEU:HD21	2.03	0.40
1:C:94:GLU:OE1	1:C:97:ASN:N	2.54	0.40
1:B:246:LEU:HD23	1:B:246:LEU:H	1.86	0.40
1:B:402:ASP:OD1	1:B:403:GLU:HG3	2.21	0.40
1:B:481:LYS:HE3	1:B:487:PHE:CB	2.48	0.40
1:B:723:ILE:HG23	1:B:1058:VAL:HG22	2.02	0.40
1:B:956:LEU:HD22	1:B:956:LEU:HA	1.81	0.40
1:C:186:LEU:O	1:C:204:HIS:HA	2.22	0.40
1:C:1138:LEU:HD23	1:C:1138:LEU:HA	1.94	0.40
1:A:290:LEU:HD12	1:A:291:ASP:HB2	2.04	0.40
1:B:550:THR:CG2	1:B:583:ASP:HB2	2.51	0.40
1:B:815:ILE:H	1:B:815:ILE:HG12	1.78	0.40
1:C:500:VAL:HA	1:C:503:GLN:HG2	2.03	0.40
1:A:198:PHE:HB3	1:A:226:LEU:CD1	2.49	0.40
1:A:822:LYS:HE3	1:A:822:LYS:HB3	1.94	0.40
1:B:919:LEU:HD12	2:I:2:NAG:O6	2.22	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	1039/1293 (80%)	874 (84%)	151 (14%)	14 (1%)	12	48
1	B	1067/1293 (82%)	912 (86%)	142 (13%)	13 (1%)	13	49
1	C	1066/1293 (82%)	919 (86%)	139 (13%)	8 (1%)	19	57
All	All	3172/3879 (82%)	2705 (85%)	432 (14%)	35 (1%)	18	51

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	141	VAL
1	A	209	LEU
1	B	224	VAL
1	B	735	CYS
1	A	589	PHE
1	A	1127	ILE
1	B	610	GLN
1	B	616	GLU
1	B	1124	ASP
1	C	327	PRO
1	A	319	PRO
1	B	225	ASP
1	B	617	VAL
1	B	938	THR
1	C	208	ASN
1	A	86	ASP
1	A	316	ARG
1	A	401	GLY
1	B	357	ASN
1	C	328	ASN
1	C	1124	ASP
1	C	1136	ASP
1	A	561	GLN
1	A	699	GLU
1	A	1136	ASP
1	B	331	ASN
1	B	696	LEU
1	B	1136	ASP
1	C	197	TYR
1	A	35	GLY
1	A	120	ASN
1	C	391	ASN
1	B	741	GLY
1	A	809	PRO
1	C	1127	ILE

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	897/1120 (80%)	775 (86%)	122 (14%)	3 22
1	B	938/1120 (84%)	805 (86%)	133 (14%)	3 20
1	C	936/1120 (84%)	807 (86%)	129 (14%)	3 21
All	All	2771/3360 (82%)	2387 (86%)	384 (14%)	7 21

All (384) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	44	ARG
1	A	48	LEU
1	A	51	THR
1	A	53	ASP
1	A	54	LEU
1	A	55	PHE
1	A	63	THR
1	A	154	PHE
1	A	161	ASN
1	A	184	LYS
1	A	186	LEU
1	A	187	ARG
1	A	188	GLU
1	A	194	ILE
1	A	197	TYR
1	A	199	LYS
1	A	200	ILE
1	A	218	SER
1	A	220	LEU
1	A	221	GLU
1	A	223	LEU
1	A	224	VAL
1	A	234	ARG
1	A	239	LEU
1	A	250	ASP
1	A	255	TRP
1	A	311	GLN
1	A	329	ILE
1	A	332	LEU
1	A	346	SER
1	A	375	LYS
1	A	399	ILE
1	A	400	ARG

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Mol	Chain	Res	Type
1	A	561	GLN
1	A	564	ARG
1	A	566	ILE
1	A	567	ASP
1	A	571	ASP
1	A	573	VAL
1	A	581	ILE
1	A	582	LEU
1	A	584	ILE
1	A	592	VAL
1	A	593	SER
1	A	612	VAL
1	A	613	ASN
1	A	614	CYS
1	A	643	ARG
1	A	647	LEU
1	A	655	ASN
1	A	657	TYR
1	A	660	ASP
1	A	668	CYS
1	A	690	ILE
1	A	696	LEU
1	A	699	GLU
1	A	713	ILE
1	A	714	ASN
1	A	723	ILE
1	A	724	LEU
1	A	734	ASP
1	A	735	CYS
1	A	742	ASP
1	A	748	ASN
1	A	751	LEU
1	A	776	GLN
1	A	781	GLN
1	A	782	VAL
1	A	783	LYS
1	A	787	LYS
1	A	788	THR
1	A	808	LYS
1	A	811	LYS
1	A	855	LEU
1	A	856	THR

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Mol	Chain	Res	Type
1	A	858	LEU
1	A	870	TYR
1	A	875	LEU
1	A	883	TRP
1	A	891	LEU
1	A	893	ILE
1	A	897	MET
1	A	899	MET
1	A	903	PHE
1	A	908	VAL
1	A	910	GLN
1	A	913	LEU
1	A	915	GLU
1	A	917	GLN
1	A	932	GLN
1	A	935	LEU
1	A	944	LYS
1	A	956	LEU
1	A	961	LYS
1	A	962	GLN
1	A	966	ASN
1	A	977	ILE
1	A	978	LEU
1	A	980	ARG
1	A	983	LYS
1	A	985	GLU
1	A	992	ARG
1	A	997	ARG
1	A	1001	LEU
1	A	1016	ARG
1	A	1028	GLU
1	A	1033	GLN
1	A	1070	LYS
1	A	1083	LYS
1	A	1091	VAL
1	A	1101	VAL
1	A	1105	ASN
1	A	1108	GLU
1	A	1110	GLN
1	A	1112	ILE
1	A	1119	VAL
1	A	1125	VAL

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Mol	Chain	Res	Type
1	A	1126	VAL
1	A	1129	ILE
1	A	1138	LEU
1	A	1142	LEU
1	B	46	SER
1	B	47	VAL
1	B	62	VAL
1	B	86	ASP
1	B	88	VAL
1	B	92	SER
1	B	155	ARG
1	B	162	ASN
1	B	165	PHE
1	B	184	LYS
1	B	187	ARG
1	B	188	GLU
1	B	192	LYS
1	B	198	PHE
1	B	199	LYS
1	B	202	SER
1	B	203	LYS
1	B	221	GLU
1	B	223	LEU
1	B	328	ASN
1	B	329	ILE
1	B	330	THR
1	B	332	LEU
1	B	333	CYS
1	B	356	SER
1	B	358	CYS
1	B	359	VAL
1	B	561	GLN
1	B	587	CYS
1	B	612	VAL
1	B	613	ASN
1	B	614	CYS
1	B	618	PRO
1	B	643	ARG
1	B	647	LEU
1	B	648	ILE
1	B	653	VAL
1	B	663	ILE

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Mol	Chain	Res	Type
1	B	690	ILE
1	B	694	MET
1	B	698	VAL
1	B	702	VAL
1	B	723	ILE
1	B	724	LEU
1	B	728	MET
1	B	737	MET
1	B	742	ASP
1	B	749	LEU
1	B	751	LEU
1	B	755	SER
1	B	757	CYS
1	B	759	GLN
1	B	760	LEU
1	B	764	LEU
1	B	772	ASP
1	B	776	GLN
1	B	777	GLU
1	B	781	GLN
1	B	782	VAL
1	B	783	LYS
1	B	784	GLN
1	B	787	LYS
1	B	788	THR
1	B	791	ILE
1	B	793	ASP
1	B	798	ASN
1	B	807	SER
1	B	811	LYS
1	B	813	SER
1	B	820	PHE
1	B	825	LEU
1	B	827	ASP
1	B	830	PHE
1	B	831	ILE
1	B	832	LYS
1	B	848	CYS
1	B	850	GLN
1	B	851	LYS
1	B	857	VAL
1	B	858	LEU

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Mol	Chain	Res	Type
1	B	865	GLU
1	B	874	LEU
1	B	875	LEU
1	B	880	THR
1	B	883	TRP
1	B	884	THR
1	B	893	ILE
1	B	899	MET
1	B	903	PHE
1	B	904	ASN
1	B	906	ILE
1	B	908	VAL
1	B	910	GLN
1	B	913	LEU
1	B	915	GLU
1	B	917	GLN
1	B	918	LYS
1	B	942	LEU
1	B	944	LYS
1	B	949	VAL
1	B	956	LEU
1	B	957	ASN
1	B	961	LYS
1	B	962	GLN
1	B	966	ASN
1	B	970	ILE
1	B	976	ASP
1	B	980	ARG
1	B	983	LYS
1	B	985	GLU
1	B	987	GLU
1	B	988	VAL
1	B	992	ARG
1	B	998	LEU
1	B	1002	GLN
1	B	1014	GLU
1	B	1028	GLU
1	B	1035	LYS
1	B	1047	MET
1	B	1068	GLN
1	B	1070	LYS
1	B	1081	ASP

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Mol	Chain	Res	Type
1	B	1083	LYS
1	B	1088	ARG
1	B	1089	GLU
1	B	1095	ASN
1	B	1103	GLN
1	B	1111	ILE
1	B	1116	ASN
1	B	1129	ILE
1	B	1131	ASN
1	B	1141	GLU
1	B	1143	ASP
1	C	36	VAL
1	C	42	VAL
1	C	45	SER
1	C	46	SER
1	C	53	ASP
1	C	54	LEU
1	C	55	PHE
1	C	63	THR
1	C	127	LYS
1	C	135	ASN
1	C	143	HIS
1	C	145	ASN
1	C	150	MET
1	C	163	CYS
1	C	164	THR
1	C	184	LYS
1	C	187	ARG
1	C	188	GLU
1	C	193	ASN
1	C	194	ILE
1	C	195	ASP
1	C	199	LYS
1	C	200	ILE
1	C	209	LEU
1	C	212	ASP
1	C	215	GLN
1	C	217	PHE
1	C	218	SER
1	C	222	PRO
1	C	223	LEU
1	C	273	LEU

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Mol	Chain	Res	Type
1	C	275	LYS
1	C	309	ILE
1	C	311	GLN
1	C	328	ASN
1	C	329	ILE
1	C	331	ASN
1	C	332	LEU
1	C	384	LEU
1	C	387	LEU
1	C	514	LEU
1	C	515	LEU
1	C	520	THR
1	C	521	VAL
1	C	522	CYS
1	C	525	LYS
1	C	526	LYS
1	C	643	ARG
1	C	647	LEU
1	C	655	ASN
1	C	657	TYR
1	C	694	MET
1	C	702	VAL
1	C	706	ASN
1	C	707	ASN
1	C	709	ILE
1	C	723	ILE
1	C	735	CYS
1	C	743	SER
1	C	744	THR
1	C	745	GLU
1	C	749	LEU
1	C	757	CYS
1	C	759	GLN
1	C	762	ARG
1	C	776	GLN
1	C	781	GLN
1	C	783	LYS
1	C	787	LYS
1	C	791	ILE
1	C	803	LEU
1	C	808	LYS
1	C	817	ASP

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Mol	Chain	Res	Type
1	C	818	LEU
1	C	858	LEU
1	C	864	ASP
1	C	869	GLN
1	C	870	TYR
1	C	874	LEU
1	C	892	GLN
1	C	893	ILE
1	C	897	MET
1	C	903	PHE
1	C	913	LEU
1	C	916	ASN
1	C	918	LYS
1	C	932	GLN
1	C	935	LEU
1	C	944	LYS
1	C	951	GLN
1	C	956	LEU
1	C	960	VAL
1	C	961	LYS
1	C	962	GLN
1	C	964	SER
1	C	966	ASN
1	C	974	LEU
1	C	977	ILE
1	C	982	ASP
1	C	983	LYS
1	C	985	GLU
1	C	987	GLU
1	C	992	ARG
1	C	998	LEU
1	C	999	GLN
1	C	1001	LEU
1	C	1014	GLU
1	C	1018	SER
1	C	1028	GLU
1	C	1037	VAL
1	C	1068	GLN
1	C	1069	GLU
1	C	1070	LYS
1	C	1074	THR
1	C	1078	ILE

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Mol	Chain	Res	Type
1	C	1081	ASP
1	C	1083	LYS
1	C	1088	ARG
1	C	1095	ASN
1	C	1103	GLN
1	C	1108	GLU
1	C	1116	ASN
1	C	1117	THR
1	C	1125	VAL
1	C	1126	VAL
1	C	1129	ILE
1	C	1131	ASN
1	C	1135	TYR
1	C	1138	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	ASN
1	A	85	ASN
1	A	185	ASN
1	A	311	GLN
1	A	351	ASN
1	A	357	ASN
1	A	434	ASN
1	A	457	ASN
1	A	490	GLN
1	A	503	GLN
1	A	561	GLN
1	A	911	ASN
1	A	999	GLN
1	A	1105	ASN
1	B	97	ASN
1	B	113	GLN
1	B	162	ASN
1	B	236	GLN
1	B	391	ASN
1	B	414	ASN
1	B	478	ASN
1	B	495	GLN
1	B	533	ASN
1	B	850	GLN

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Mol	Chain	Res	Type
1	B	853	ASN
1	B	869	GLN
1	B	904	ASN
1	B	923	GLN
1	B	966	ASN
1	B	1002	GLN
1	B	1116	ASN
1	C	66	HIS
1	C	204	HIS
1	C	242	HIS
1	C	318	GLN
1	C	391	ASN
1	C	478	ASN
1	C	541	ASN
1	C	781	GLN
1	C	952	ASN
1	C	1008	GLN
1	C	1020	ASN
1	C	1080	HIS
1	C	1085	HIS

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

24 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	D	1	2	14,14,15	0.46	0	17,19,21	0.45	0
2	NAG	D	2	2	14,14,15	0.74	0	17,19,21	0.55	0
2	NAG	E	1	2	14,14,15	0.69	1 (7%)	17,19,21	0.91	1 (5%)
2	NAG	E	2	2	14,14,15	0.50	0	17,19,21	1.86	3 (17%)
2	NAG	F	1	2	14,14,15	1.46	2 (14%)	17,19,21	0.71	0
2	NAG	F	2	2	14,14,15	0.28	0	17,19,21	0.83	1 (5%)
2	NAG	G	1	2	14,14,15	0.69	1 (7%)	17,19,21	0.51	0
2	NAG	G	2	2	14,14,15	0.30	0	17,19,21	0.40	0
2	NAG	H	1	2	14,14,15	0.76	1 (7%)	17,19,21	0.47	0
2	NAG	H	2	2	14,14,15	0.44	0	17,19,21	1.23	1 (5%)
2	NAG	I	1	2	14,14,15	0.45	0	17,19,21	0.63	0
2	NAG	I	2	2	14,14,15	0.60	1 (7%)	17,19,21	1.14	2 (11%)
2	NAG	J	1	2	14,14,15	0.57	1 (7%)	17,19,21	0.43	0
2	NAG	J	2	2	14,14,15	0.47	0	17,19,21	1.29	2 (11%)
2	NAG	K	1	2	14,14,15	0.66	1 (7%)	17,19,21	0.53	0
2	NAG	K	2	2	14,14,15	0.32	0	17,19,21	0.41	0
2	NAG	L	1	2	14,14,15	0.44	0	17,19,21	0.70	0
2	NAG	L	2	2	14,14,15	0.39	0	17,19,21	1.37	2 (11%)
2	NAG	M	1	2	14,14,15	1.11	1 (7%)	17,19,21	0.60	0
2	NAG	M	2	2	14,14,15	0.36	0	17,19,21	0.50	0
2	NAG	N	1	2	14,14,15	0.50	0	17,19,21	0.54	0
2	NAG	N	2	2	14,14,15	0.29	0	17,19,21	0.40	0
2	NAG	O	1	2	14,14,15	0.55	0	17,19,21	0.49	0
2	NAG	O	2	2	14,14,15	1.25	1 (7%)	17,19,21	1.48	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	1	2	-	1/6/23/26	0/1/1/1
2	NAG	D	2	2	-	4/6/23/26	0/1/1/1
2	NAG	E	1	2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	2	-	3/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	NAG	G	1	2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	NAG	H	1	2	-	2/6/23/26	0/1/1/1
2	NAG	H	2	2	-	5/6/23/26	0/1/1/1
2	NAG	I	1	2	-	1/6/23/26	0/1/1/1
2	NAG	I	2	2	-	4/6/23/26	0/1/1/1
2	NAG	J	1	2	-	3/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
2	NAG	K	1	2	-	1/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
2	NAG	L	1	2	-	2/6/23/26	0/1/1/1
2	NAG	L	2	2	-	5/6/23/26	0/1/1/1
2	NAG	M	1	2	-	3/6/23/26	0/1/1/1
2	NAG	M	2	2	-	1/6/23/26	0/1/1/1
2	NAG	N	1	2	-	0/6/23/26	0/1/1/1
2	NAG	N	2	2	-	0/6/23/26	0/1/1/1
2	NAG	O	1	2	-	2/6/23/26	0/1/1/1
2	NAG	O	2	2	-	5/6/23/26	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1	NAG	O5-C1	-4.86	1.36	1.43
2	O	2	NAG	O5-C1	-4.33	1.36	1.43
2	M	1	NAG	O5-C1	-3.80	1.37	1.43
2	H	1	NAG	O5-C1	-2.67	1.39	1.43
2	K	1	NAG	O5-C1	-2.34	1.40	1.43
2	G	1	NAG	O5-C1	-2.34	1.40	1.43
2	F	1	NAG	C1-C2	-2.21	1.49	1.52
2	E	1	NAG	O5-C1	-2.08	1.40	1.43
2	J	1	NAG	O5-C1	-2.05	1.40	1.43
2	I	2	NAG	O5-C1	-2.03	1.40	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	2	NAG	C1-O5-C5	6.61	121.14	112.19
2	O	2	NAG	C2-N2-C7	4.47	129.26	122.90
2	L	2	NAG	C2-N2-C7	4.38	129.14	122.90
2	H	2	NAG	C2-N2-C7	4.23	128.92	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	2	NAG	C1-O5-C5	4.00	117.61	112.19
2	I	2	NAG	C1-O5-C5	3.47	116.90	112.19
2	F	2	NAG	C1-O5-C5	2.76	115.93	112.19
2	E	2	NAG	C3-C4-C5	2.74	115.13	110.24
2	J	2	NAG	C3-C4-C5	2.68	115.02	110.24
2	O	2	NAG	C1-O5-C5	2.45	115.52	112.19
2	L	2	NAG	C1-C2-N2	2.36	114.52	110.49
2	I	2	NAG	C3-C4-C5	2.33	114.40	110.24
2	E	2	NAG	O5-C5-C4	2.29	116.40	110.83
2	E	1	NAG	C1-O5-C5	2.15	115.11	112.19

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	O	2	NAG	O5-C5-C6-O6
2	I	2	NAG	C4-C5-C6-O6
2	M	1	NAG	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
2	O	2	NAG	C4-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
2	D	2	NAG	C8-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2
2	H	1	NAG	C8-C7-N2-C2
2	H	1	NAG	O7-C7-N2-C2
2	H	2	NAG	C8-C7-N2-C2
2	H	2	NAG	O7-C7-N2-C2
2	L	1	NAG	C8-C7-N2-C2
2	L	1	NAG	O7-C7-N2-C2
2	L	2	NAG	C8-C7-N2-C2
2	L	2	NAG	O7-C7-N2-C2
2	O	1	NAG	C8-C7-N2-C2
2	O	1	NAG	O7-C7-N2-C2
2	O	2	NAG	C8-C7-N2-C2
2	O	2	NAG	O7-C7-N2-C2
2	M	1	NAG	O5-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	D	2	NAG	C4-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
2	J	1	NAG	C4-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6
2	J	1	NAG	O5-C5-C6-O6
2	K	2	NAG	O5-C5-C6-O6
2	L	2	NAG	C4-C5-C6-O6
2	J	2	NAG	C4-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6
2	I	2	NAG	C1-C2-N2-C7
2	K	1	NAG	C4-C5-C6-O6
2	F	1	NAG	C3-C2-N2-C7
2	J	1	NAG	C3-C2-N2-C7
2	L	2	NAG	C3-C2-N2-C7
2	M	1	NAG	C3-C2-N2-C7
2	O	2	NAG	C3-C2-N2-C7
2	E	1	NAG	C4-C5-C6-O6
2	M	2	NAG	C4-C5-C6-O6
2	K	2	NAG	C1-C2-N2-C7
2	D	1	NAG	C1-C2-N2-C7
2	L	2	NAG	O5-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6
2	H	2	NAG	C3-C2-N2-C7
2	I	2	NAG	C3-C2-N2-C7

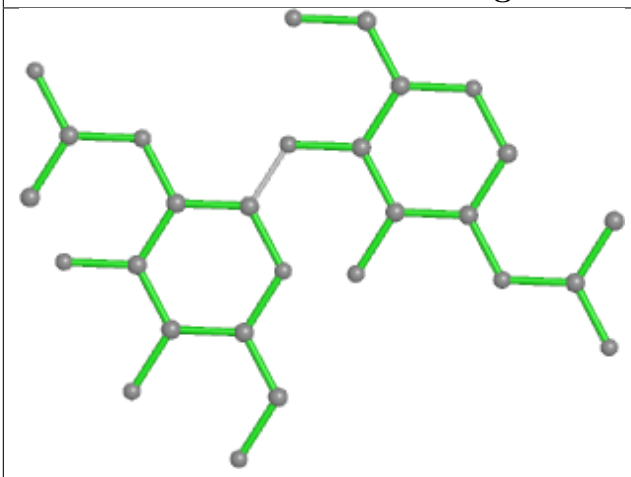
There are no ring outliers.

7 monomers are involved in 12 short contacts:

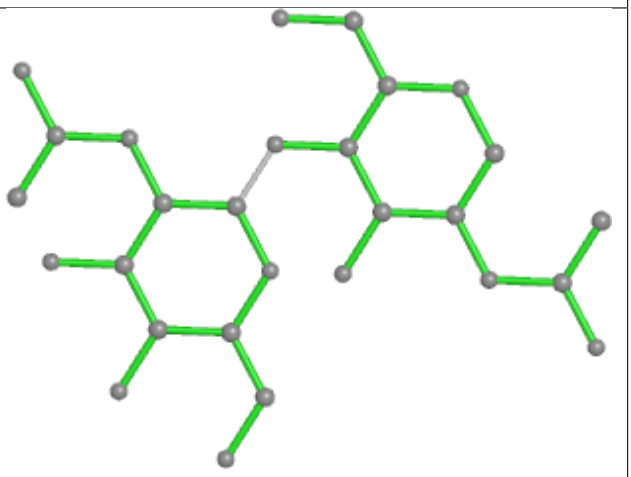
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	O	2	NAG	1	0
2	H	2	NAG	1	0
2	I	2	NAG	7	0
2	F	1	NAG	1	0
2	M	2	NAG	1	0
2	M	1	NAG	1	0
2	L	2	NAG	1	0

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

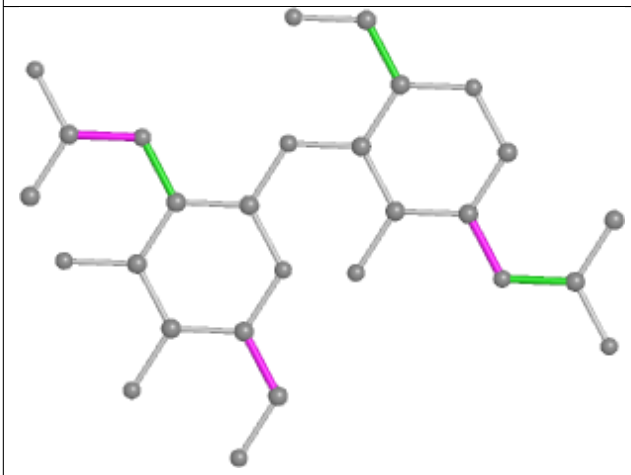
Oligosaccharide Chain D



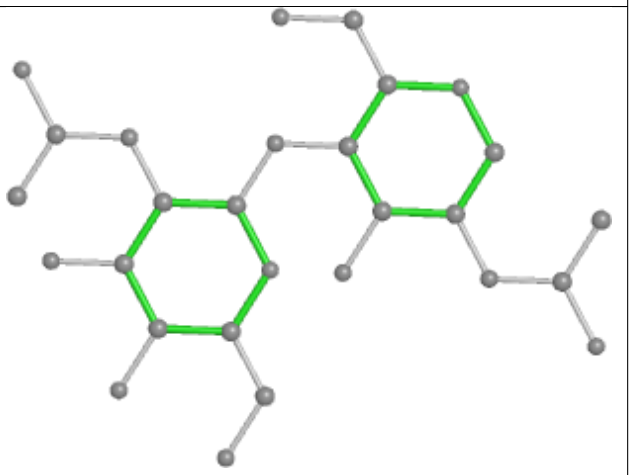
Bond lengths



Bond angles

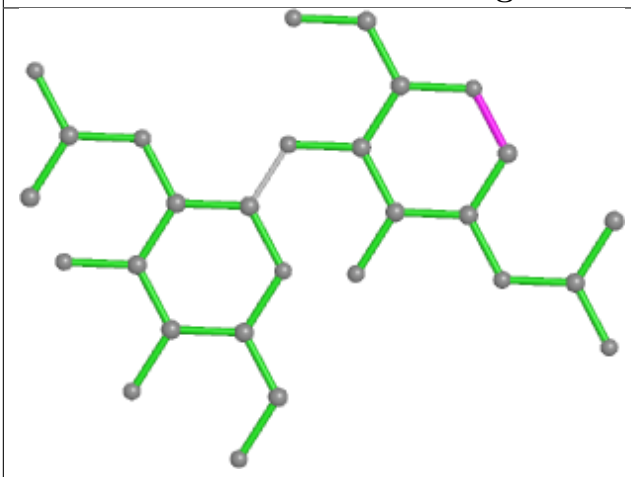


Torsions

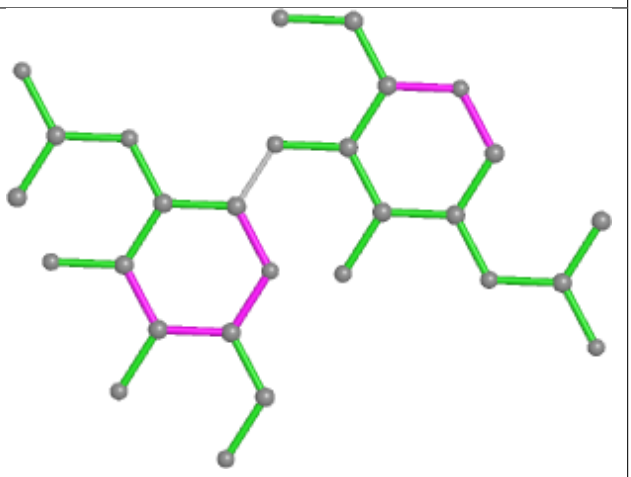


Rings

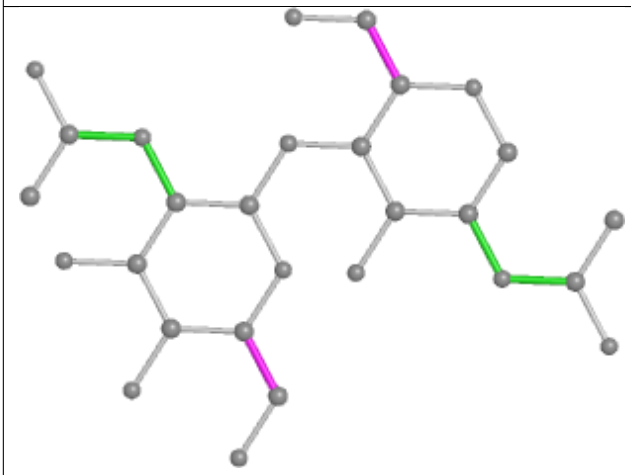
Oligosaccharide Chain E



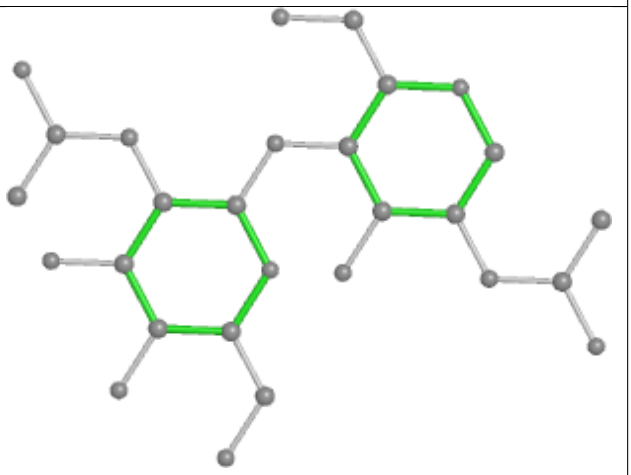
Bond lengths



Bond angles

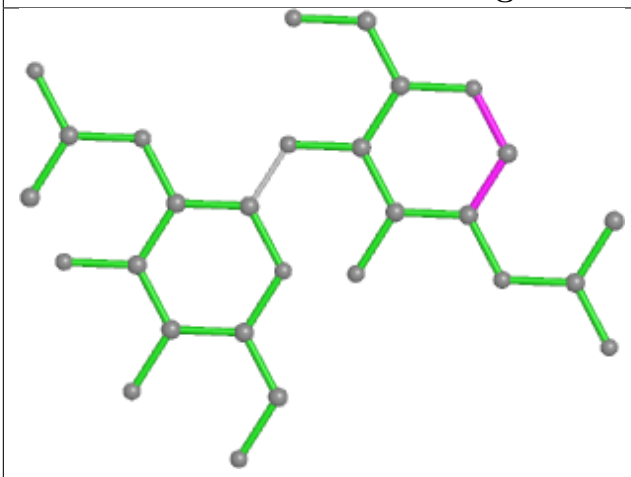


Torsions

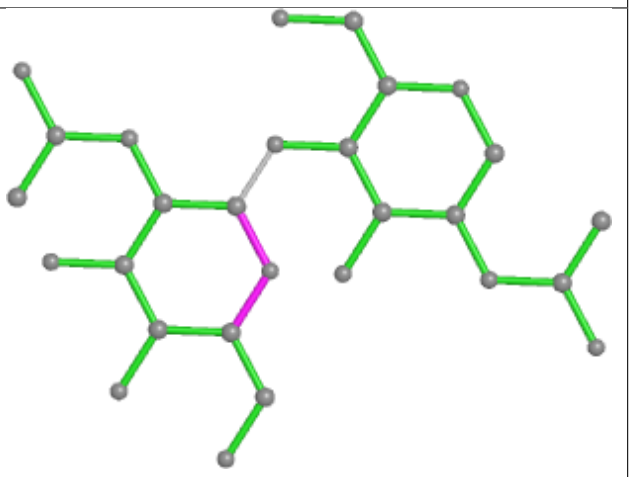


Rings

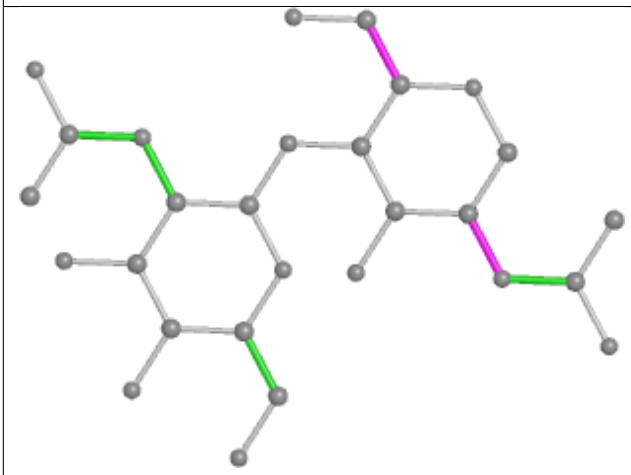
Oligosaccharide Chain F



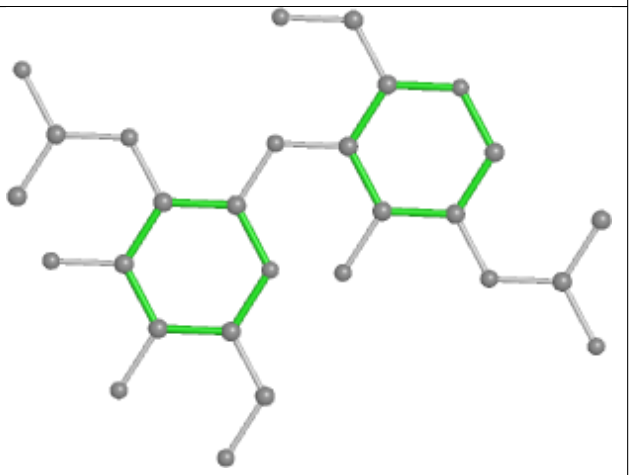
Bond lengths



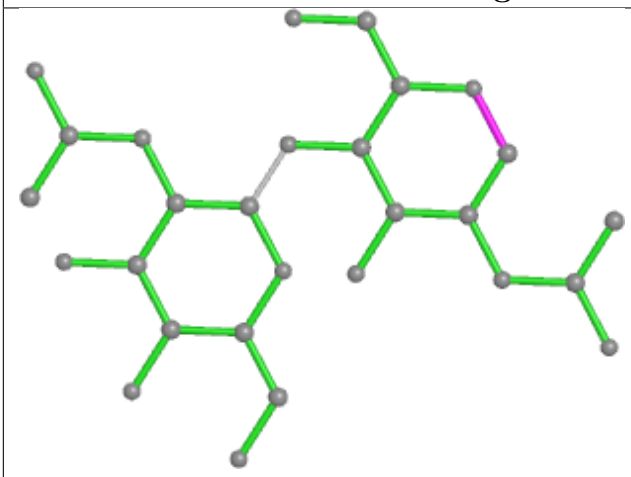
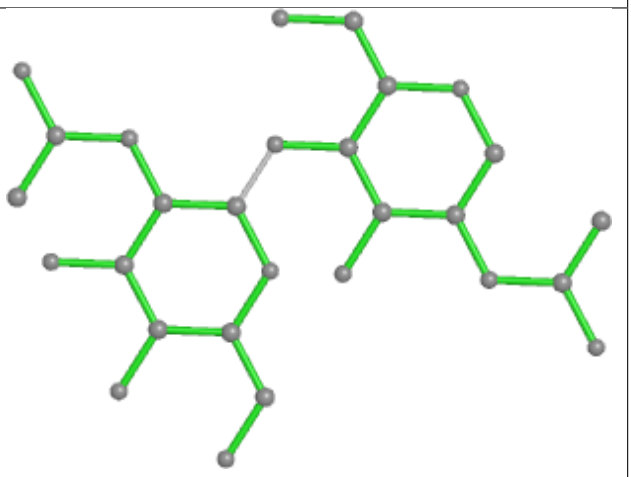
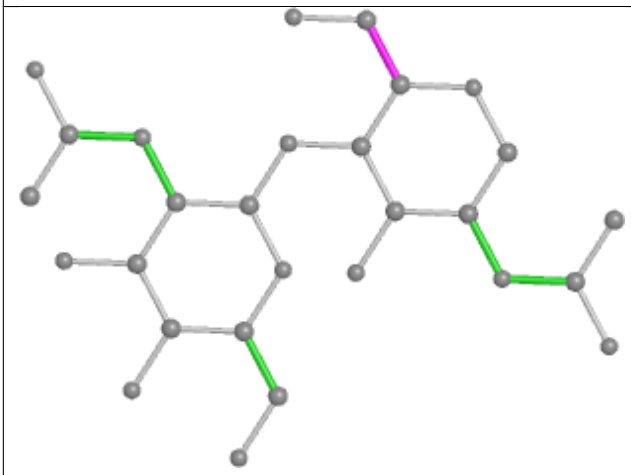
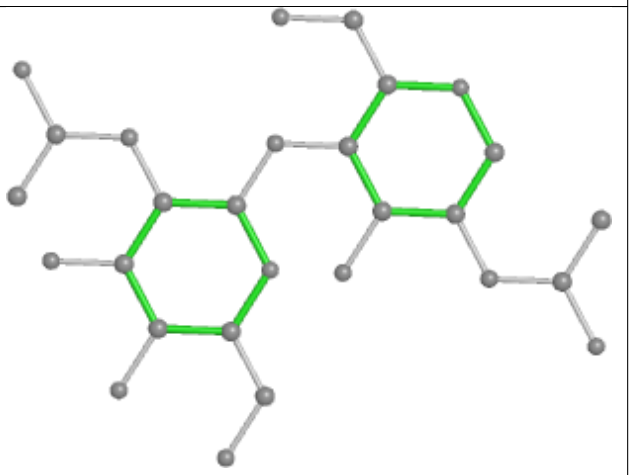
Bond angles



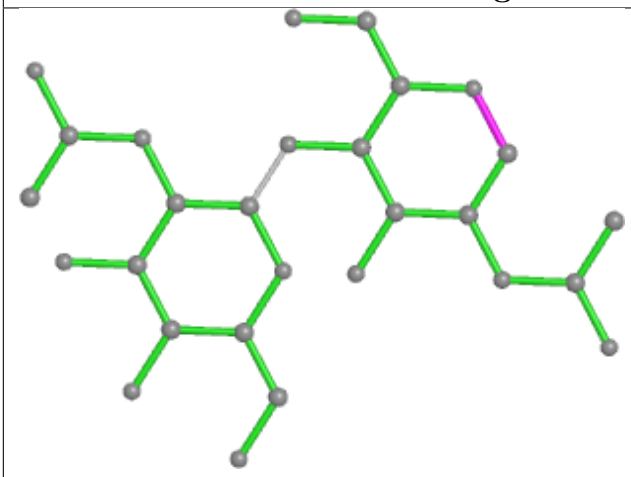
Torsions



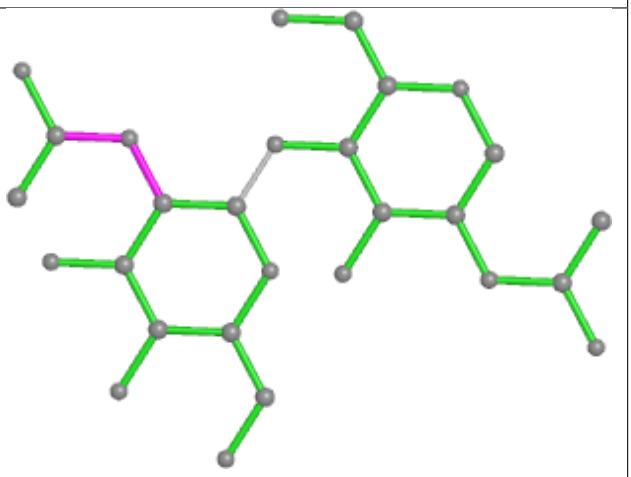
Rings

Oligosaccharide Chain G	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

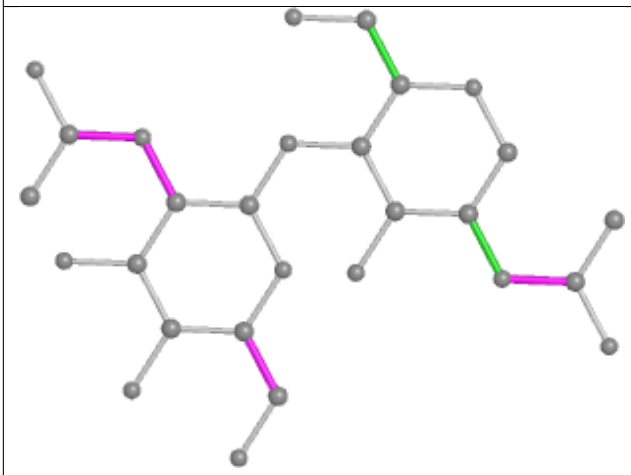
Oligosaccharide Chain H



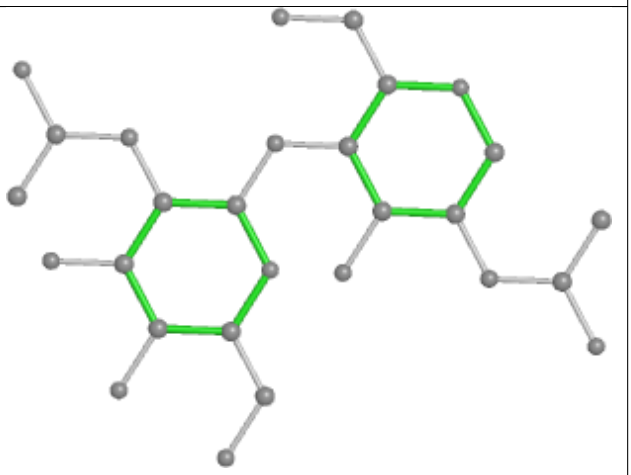
Bond lengths



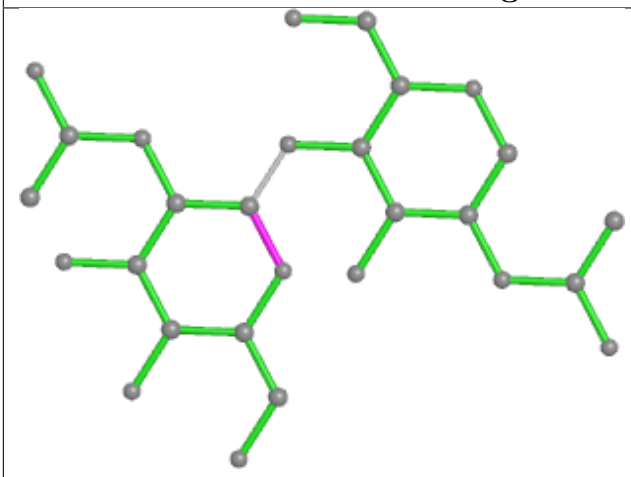
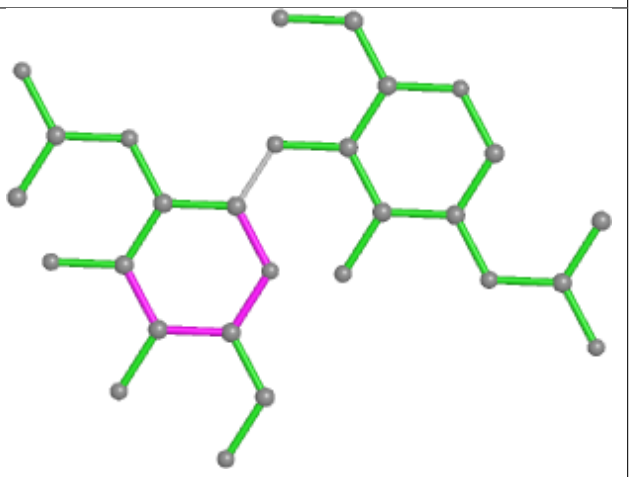
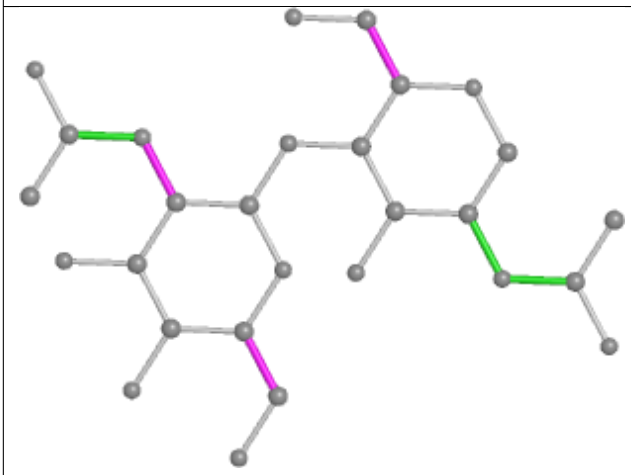
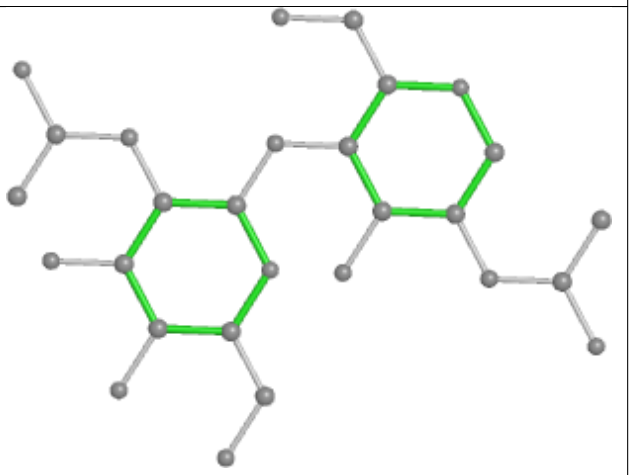
Bond angles



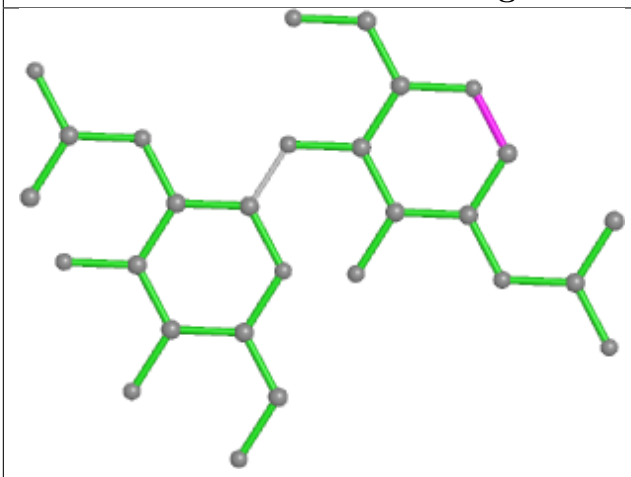
Torsions



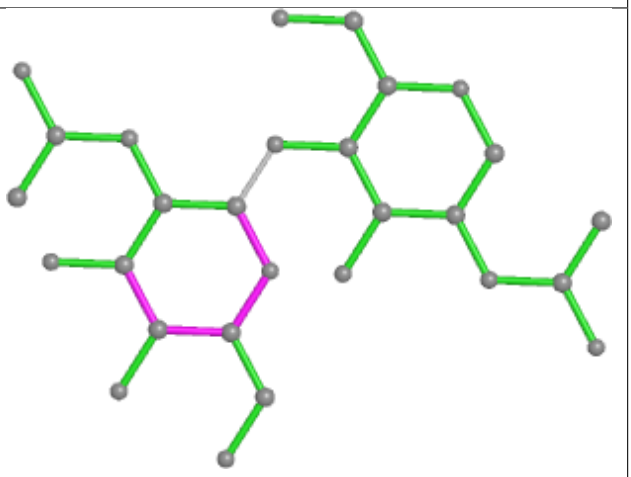
Rings

Oligosaccharide Chain I	
 Bond lengths	 Bond angles
 Torsions	 Rings

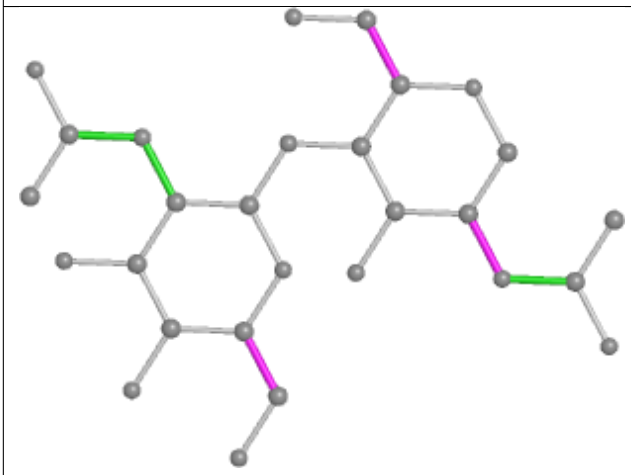
Oligosaccharide Chain J



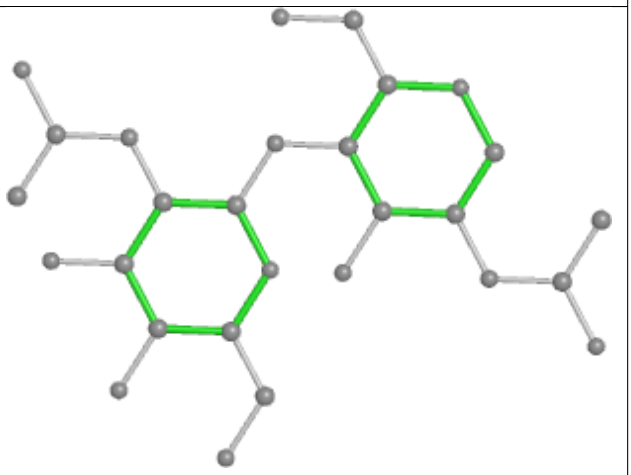
Bond lengths



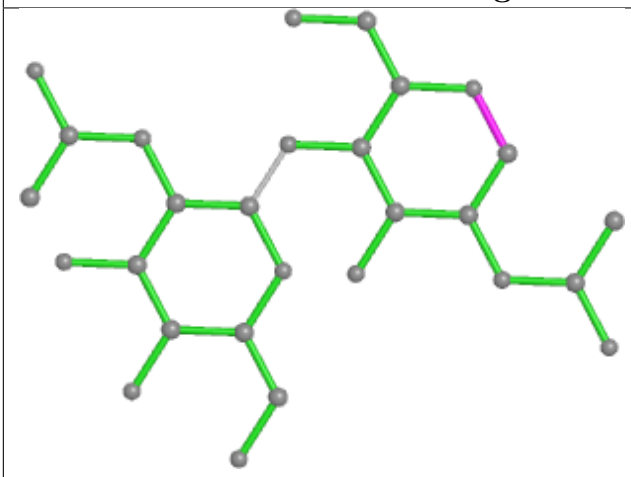
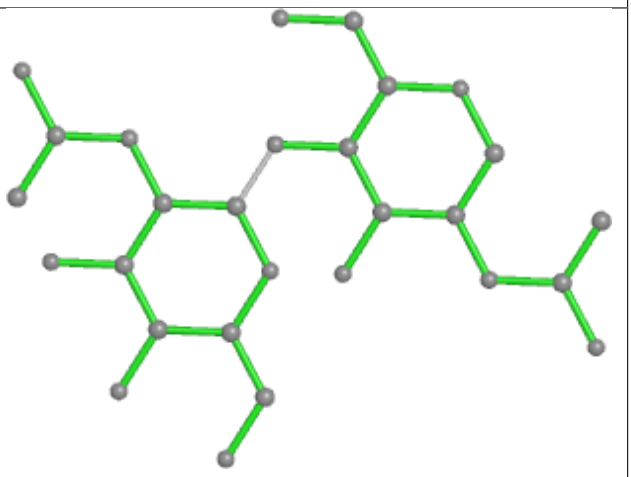
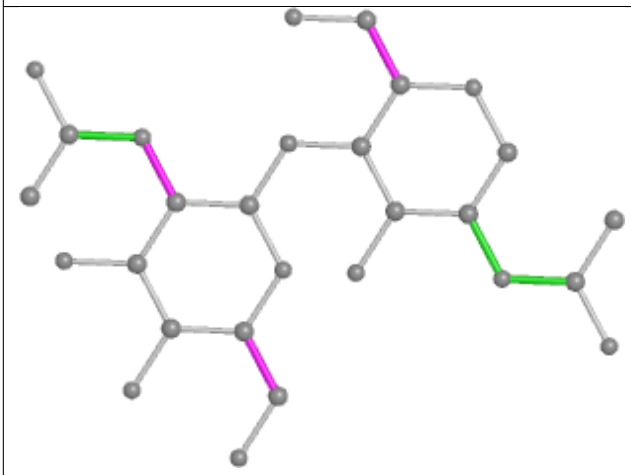
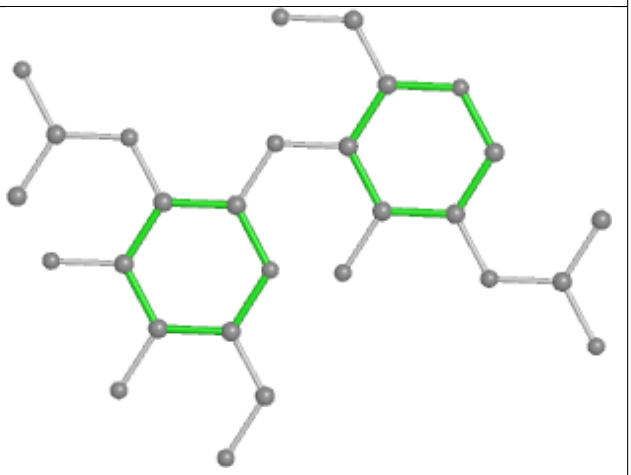
Bond angles



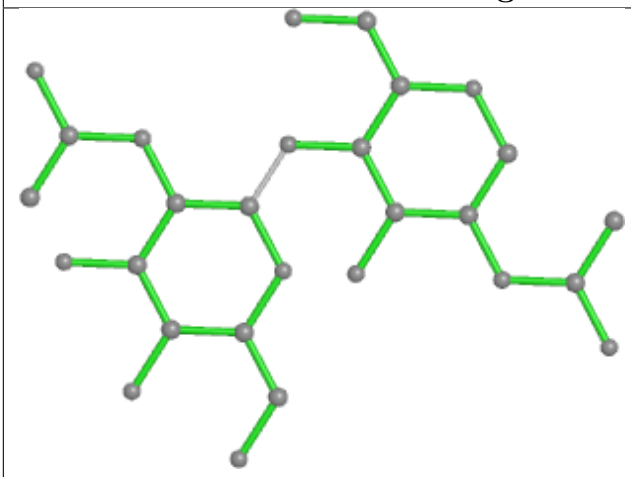
Torsions



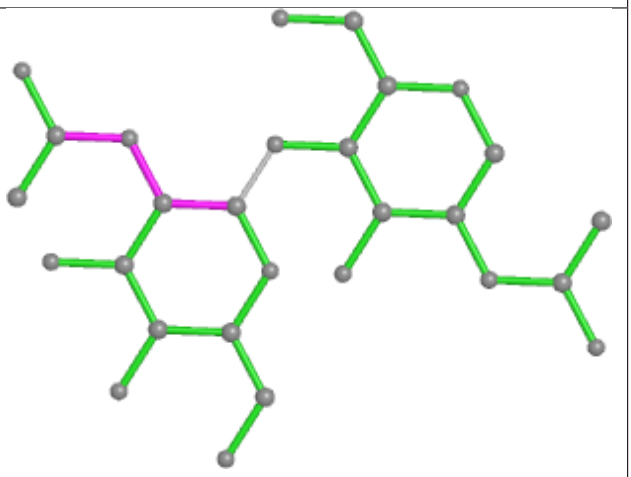
Rings

Oligosaccharide Chain K	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

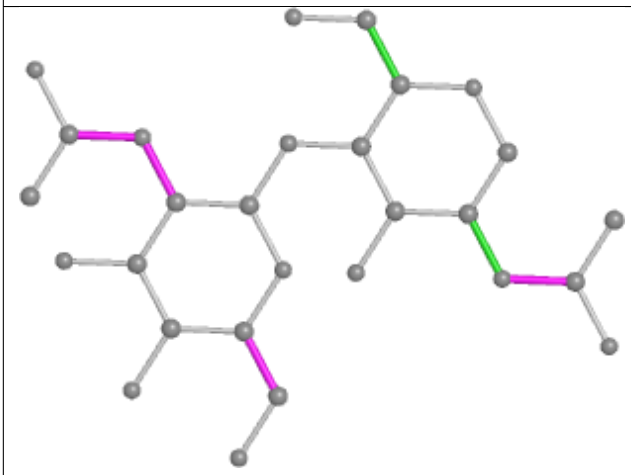
Oligosaccharide Chain L



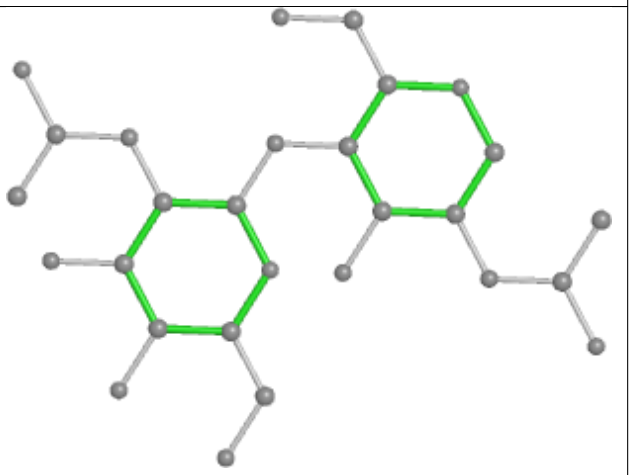
Bond lengths



Bond angles

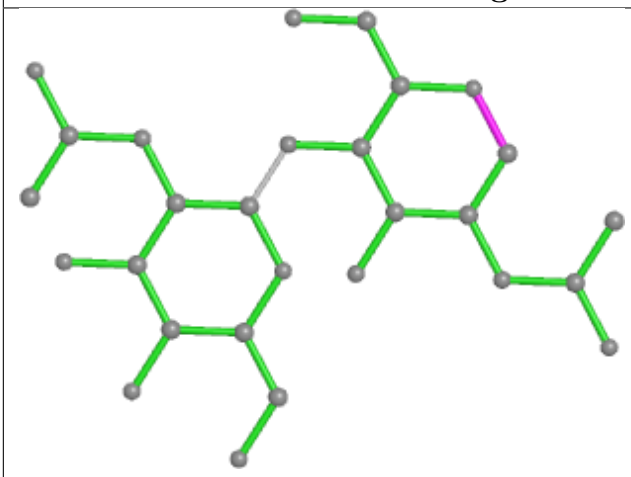


Torsions

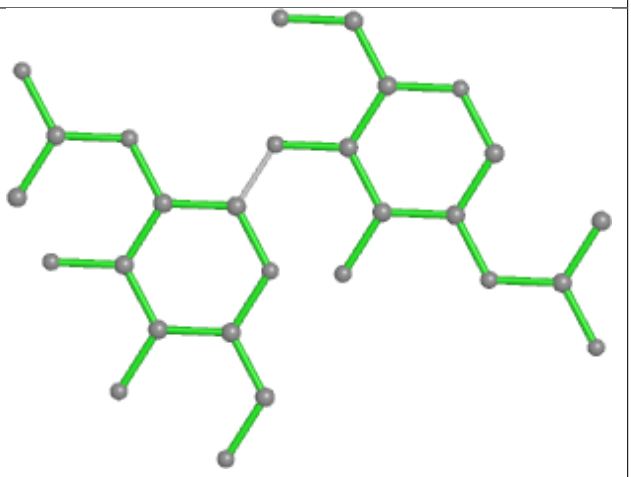


Rings

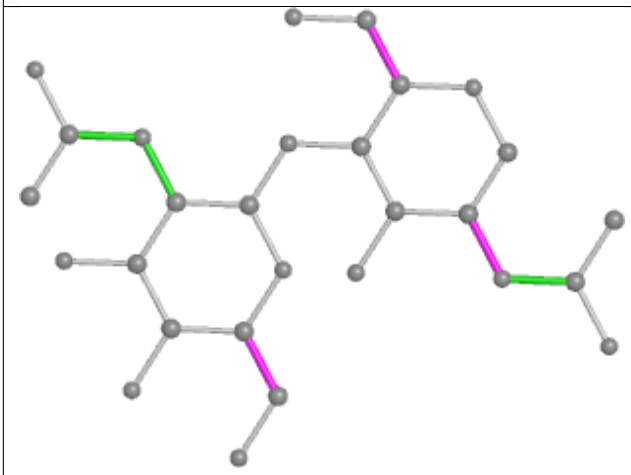
Oligosaccharide Chain M



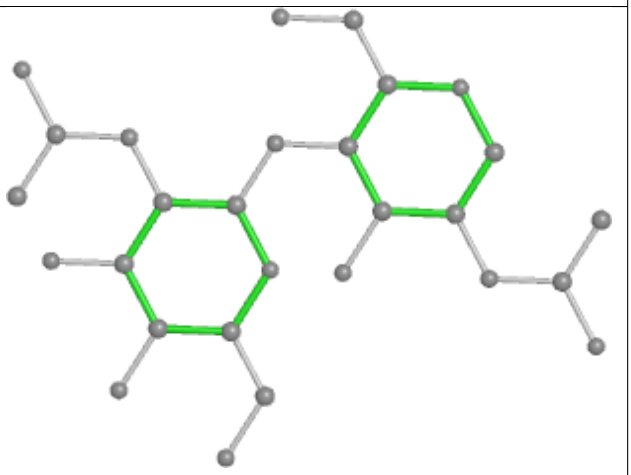
Bond lengths



Bond angles

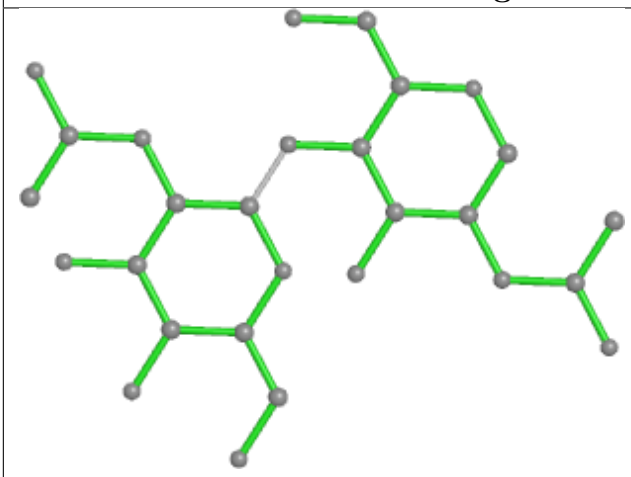


Torsions

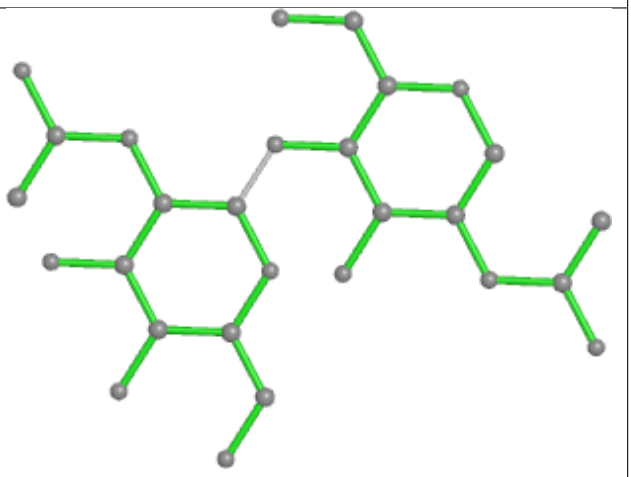


Rings

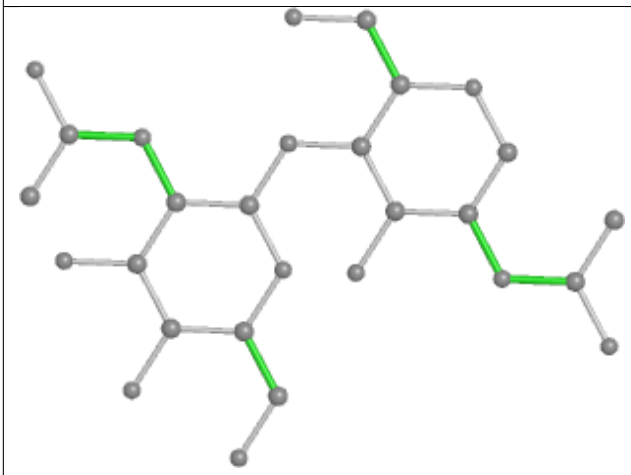
Oligosaccharide Chain N



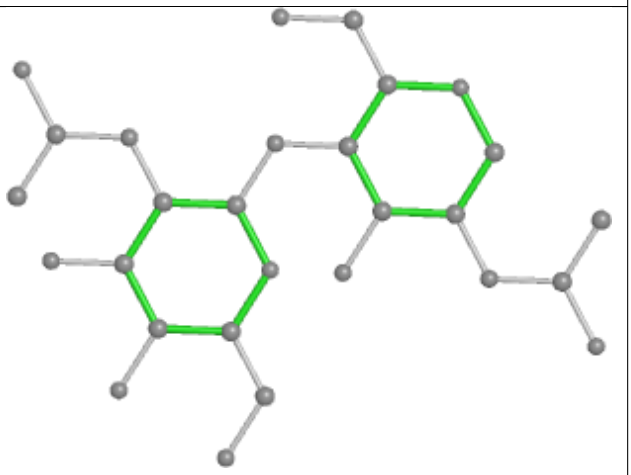
Bond lengths



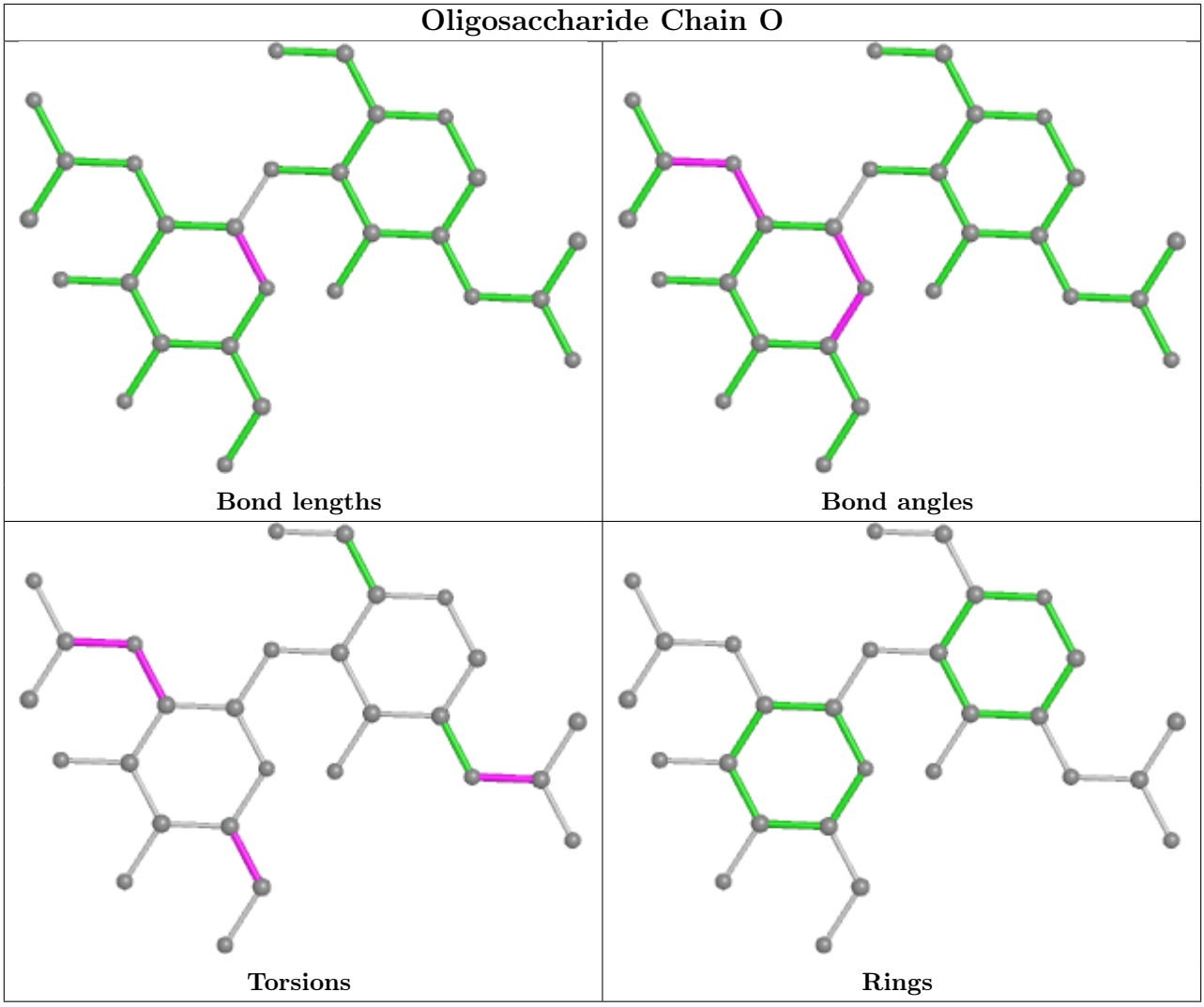
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

21 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	$\#\|Z\| > 2$
3	NAG	A	1308	1	14,14,15	0.37	0	17,19,21	0.99	1 (5%)
3	NAG	B	1301	1	14,14,15	0.28	0	17,19,21	0.54	0
3	NAG	B	1305	1	14,14,15	0.27	0	17,19,21	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	C	1301	1	14,14,15	0.24	0	17,19,21	0.42	0
3	NAG	C	1305	1	14,14,15	0.88	1 (7%)	17,19,21	1.20	2 (11%)
3	NAG	A	1307	1	14,14,15	0.41	0	17,19,21	0.50	0
3	NAG	A	1306	1	14,14,15	0.24	0	17,19,21	0.64	1 (5%)
3	NAG	C	1304	1	14,14,15	0.39	0	17,19,21	0.39	0
3	NAG	B	1306	1	14,14,15	1.32	1 (7%)	17,19,21	1.61	3 (17%)
3	NAG	A	1305	1	14,14,15	0.34	0	17,19,21	0.38	0
3	NAG	A	1304	1	14,14,15	0.31	0	17,19,21	0.44	0
3	NAG	C	1302	1	14,14,15	0.58	0	17,19,21	0.74	0
3	NAG	A	1302	1	14,14,15	0.23	0	17,19,21	0.46	0
3	NAG	A	1301	1	14,14,15	0.54	0	17,19,21	0.51	0
3	NAG	B	1303	1	14,14,15	0.31	0	17,19,21	0.62	0
3	NAG	B	1302	1	14,14,15	0.45	0	17,19,21	0.92	1 (5%)
3	NAG	C	1303	-	14,14,15	0.48	0	17,19,21	0.32	0
3	NAG	A	1303	1	14,14,15	0.16	0	17,19,21	0.39	0
3	NAG	B	1304	1	14,14,15	0.20	0	17,19,21	0.48	0
3	NAG	C	1306	1	14,14,15	0.27	0	17,19,21	0.68	1 (5%)
3	NAG	B	1307	1	14,14,15	0.23	0	17,19,21	0.42	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
3	NAG	A	1308	1	-	3/6/23/26	0/1/1/1
3	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1305	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1307	1	-	3/6/23/26	0/1/1/1
3	NAG	A	1306	1	-	1/6/23/26	0/1/1/1
3	NAG	C	1304	1	-	4/6/23/26	0/1/1/1
3	NAG	B	1306	1	-	3/6/23/26	0/1/1/1
3	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1304	1	-	1/6/23/26	0/1/1/1
3	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1302	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1301	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	1303	1	-	4/6/23/26	0/1/1/1
3	NAG	B	1302	1	-	6/6/23/26	0/1/1/1
3	NAG	C	1303	-	-	2/6/23/26	0/1/1/1
3	NAG	A	1303	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1304	1	-	3/6/23/26	0/1/1/1
3	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1307	1	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1306	NAG	O5-C1	-4.66	1.36	1.43
3	C	1305	NAG	O5-C1	-2.54	1.39	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1306	NAG	C2-N2-C7	4.48	129.28	122.90
3	C	1305	NAG	C1-O5-C5	3.56	117.02	112.19
3	B	1306	NAG	C3-C4-C5	3.20	115.95	110.24
3	C	1305	NAG	C3-C4-C5	2.74	115.12	110.24
3	A	1308	NAG	C2-N2-C7	2.54	126.53	122.90
3	B	1306	NAG	C1-C2-N2	2.40	114.58	110.49
3	C	1306	NAG	C1-O5-C5	2.38	115.42	112.19
3	A	1306	NAG	C1-O5-C5	2.15	115.10	112.19
3	B	1302	NAG	C1-O5-C5	2.03	114.94	112.19

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1308	NAG	C3-C2-N2-C7
3	A	1308	NAG	C8-C7-N2-C2
3	A	1308	NAG	O7-C7-N2-C2
3	B	1302	NAG	C8-C7-N2-C2
3	B	1302	NAG	O7-C7-N2-C2
3	C	1306	NAG	C4-C5-C6-O6
3	C	1302	NAG	C1-C2-N2-C7
3	C	1306	NAG	O5-C5-C6-O6
3	A	1307	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	B	1303	NAG	C8-C7-N2-C2
3	B	1302	NAG	O5-C5-C6-O6
3	B	1303	NAG	O5-C5-C6-O6
3	B	1304	NAG	O5-C5-C6-O6
3	B	1307	NAG	O5-C5-C6-O6
3	C	1305	NAG	O5-C5-C6-O6
3	C	1301	NAG	C4-C5-C6-O6
3	C	1301	NAG	O5-C5-C6-O6
3	C	1303	NAG	C4-C5-C6-O6
3	B	1303	NAG	O7-C7-N2-C2
3	C	1303	NAG	O5-C5-C6-O6
3	C	1304	NAG	C4-C5-C6-O6
3	B	1304	NAG	C4-C5-C6-O6
3	B	1306	NAG	C8-C7-N2-C2
3	B	1306	NAG	O7-C7-N2-C2
3	C	1304	NAG	C8-C7-N2-C2
3	C	1304	NAG	O7-C7-N2-C2
3	A	1307	NAG	C4-C5-C6-O6
3	C	1305	NAG	C4-C5-C6-O6
3	C	1304	NAG	O5-C5-C6-O6
3	A	1305	NAG	O5-C5-C6-O6
3	B	1302	NAG	C4-C5-C6-O6
3	B	1303	NAG	C4-C5-C6-O6
3	B	1301	NAG	O5-C5-C6-O6
3	A	1303	NAG	O5-C5-C6-O6
3	B	1307	NAG	C4-C5-C6-O6
3	B	1302	NAG	C1-C2-N2-C7
3	A	1305	NAG	C4-C5-C6-O6
3	A	1306	NAG	O5-C5-C6-O6
3	B	1305	NAG	C4-C5-C6-O6
3	B	1305	NAG	O5-C5-C6-O6
3	A	1307	NAG	C1-C2-N2-C7
3	A	1304	NAG	C3-C2-N2-C7
3	B	1301	NAG	C3-C2-N2-C7
3	B	1304	NAG	C3-C2-N2-C7
3	B	1306	NAG	C3-C2-N2-C7
3	C	1302	NAG	C3-C2-N2-C7
3	B	1302	NAG	C3-C2-N2-C7

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1301	NAG	1	0
3	C	1301	NAG	4	0
3	C	1304	NAG	1	0
3	B	1306	NAG	1	0
3	C	1302	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

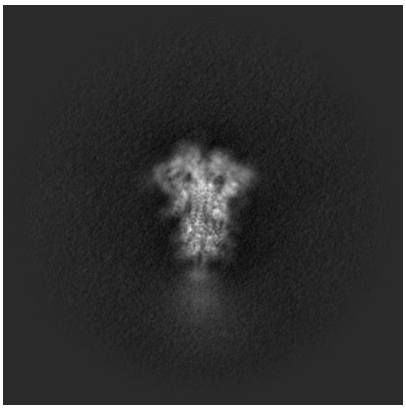
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-33346. These allow visual inspection of the internal detail of the map and identification of artifacts.

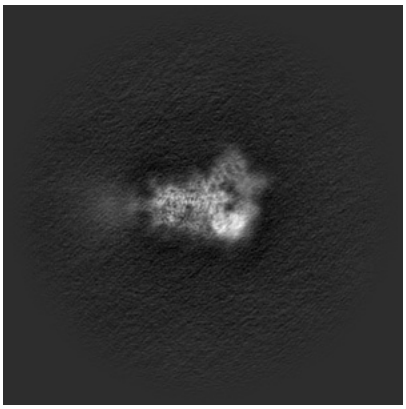
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

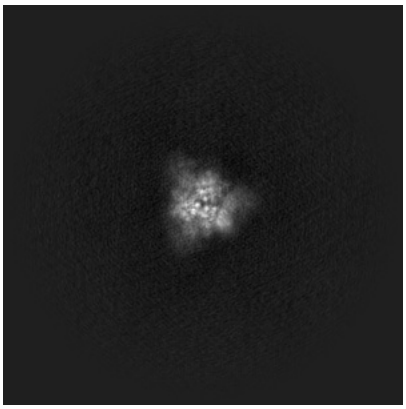
6.1.1 Primary map



X

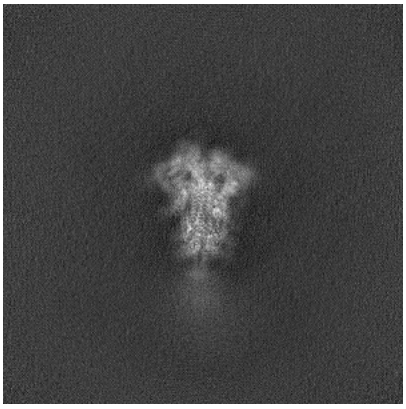


Y

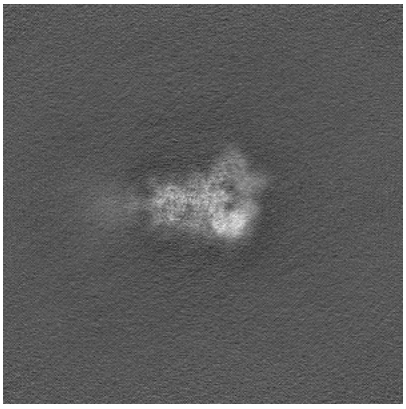


Z

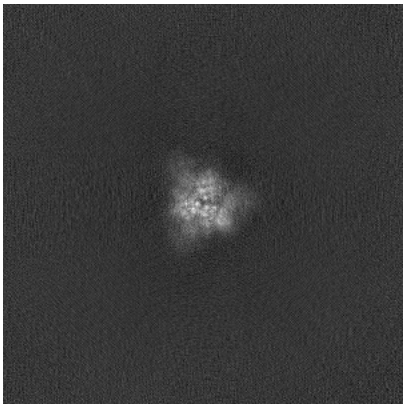
6.1.2 Raw map



X



Y

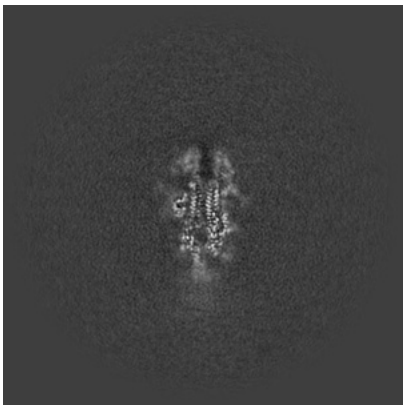


Z

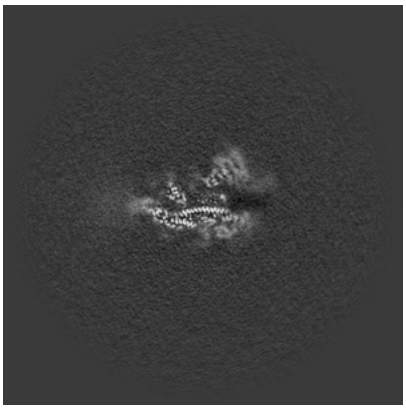
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

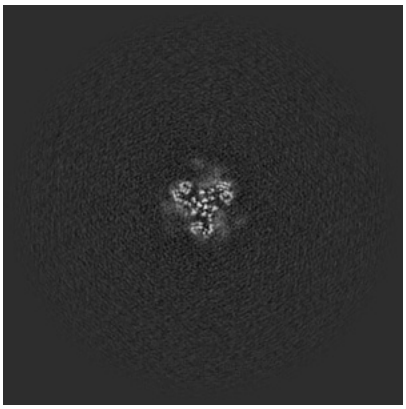
6.2.1 Primary map



X Index: 256

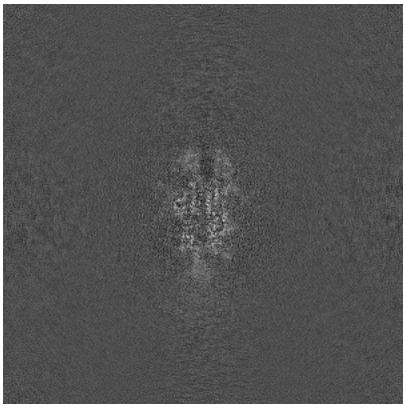


Y Index: 256

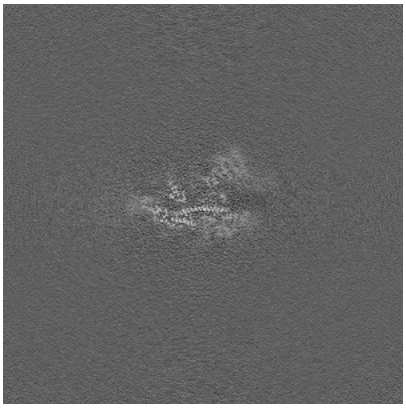


Z Index: 256

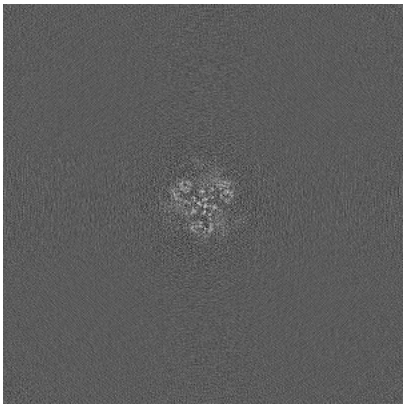
6.2.2 Raw map



X Index: 256



Y Index: 256

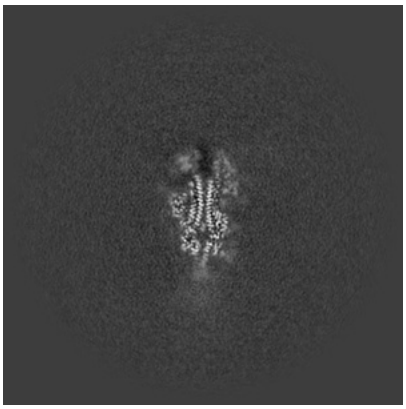


Z Index: 256

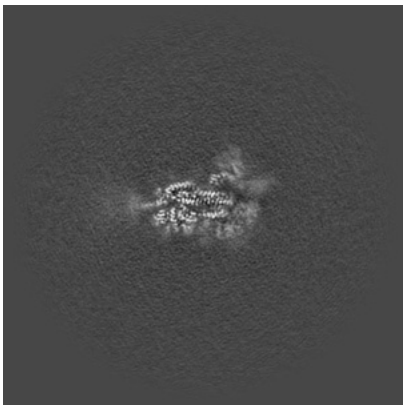
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

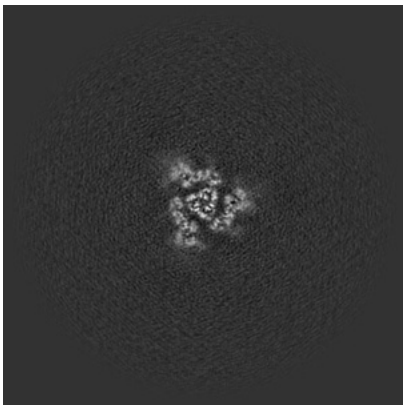
6.3.1 Primary map



X Index: 259

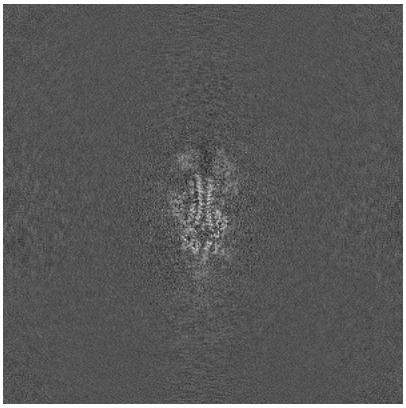


Y Index: 249

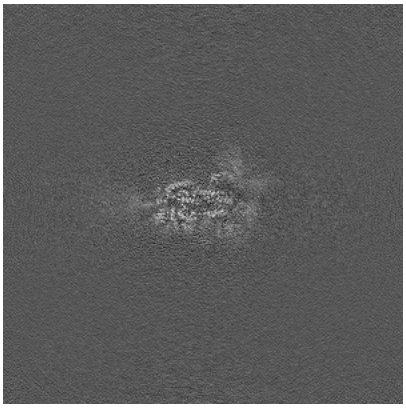


Z Index: 280

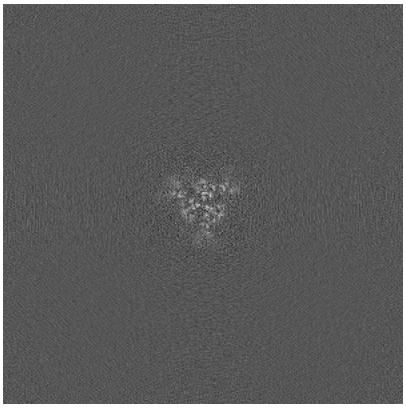
6.3.2 Raw map



X Index: 259



Y Index: 249

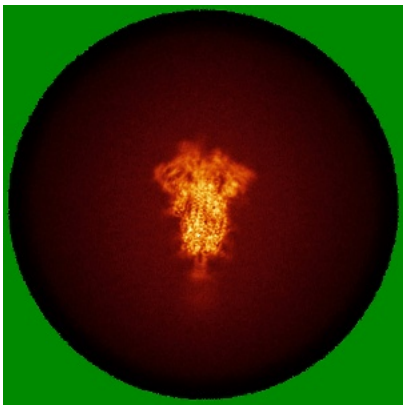


Z Index: 244

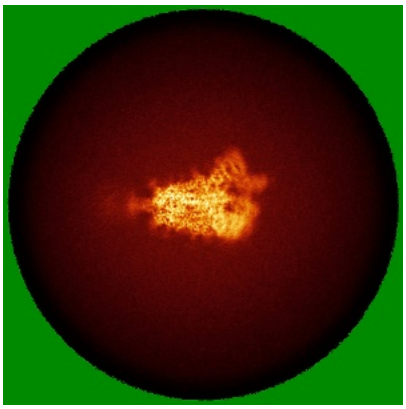
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

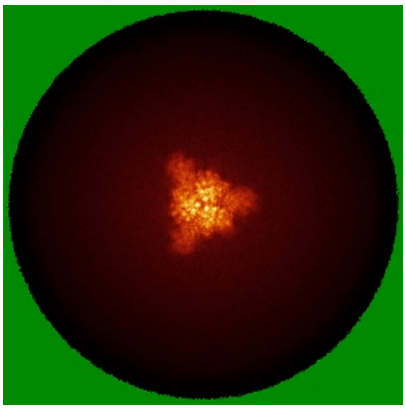
6.4.1 Primary map



X

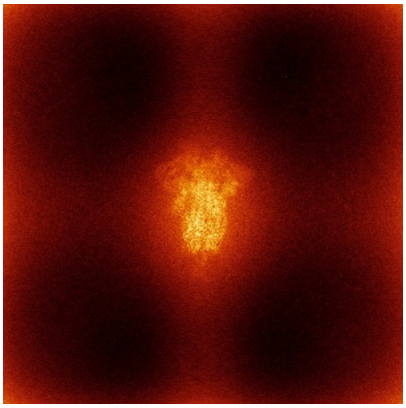


Y

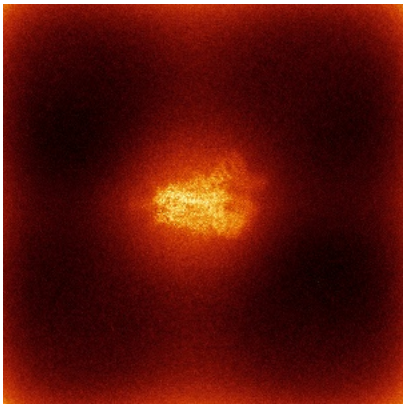


Z

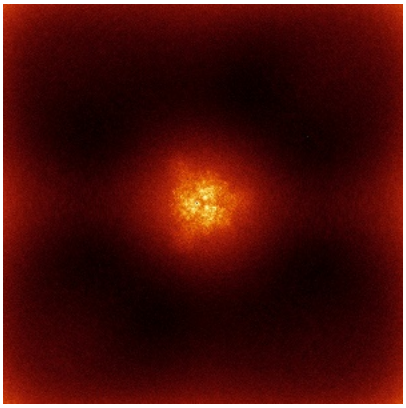
6.4.2 Raw map



X



Y



Z

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

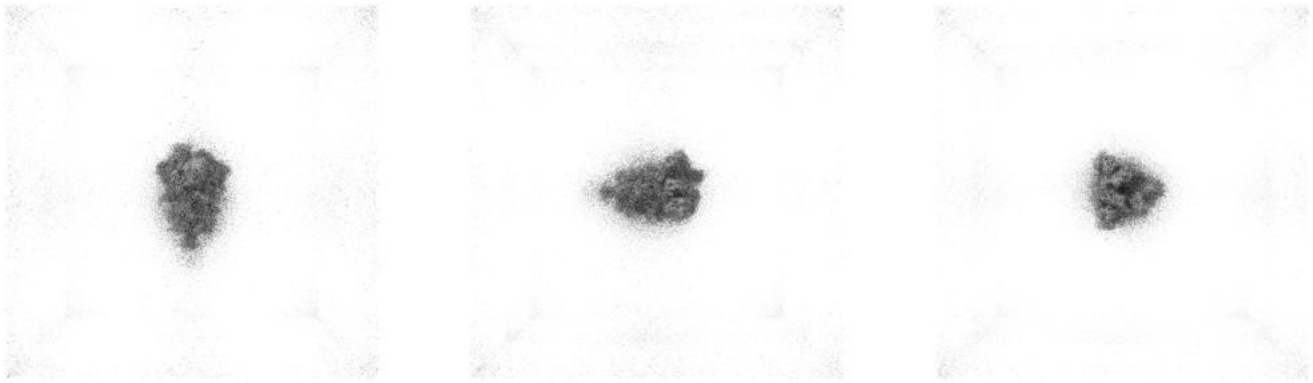
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

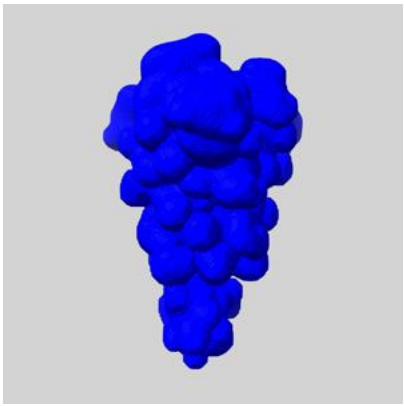
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

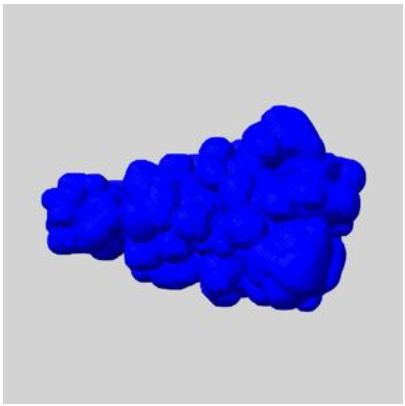
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

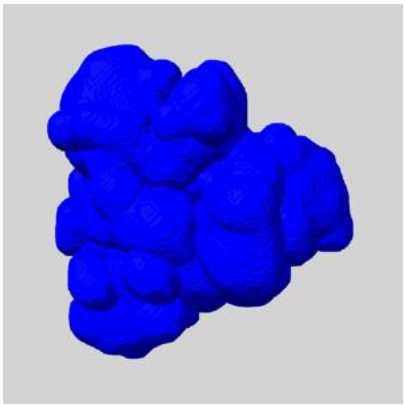
6.6.1 emd_33346_msk_1.map (i)



X



Y

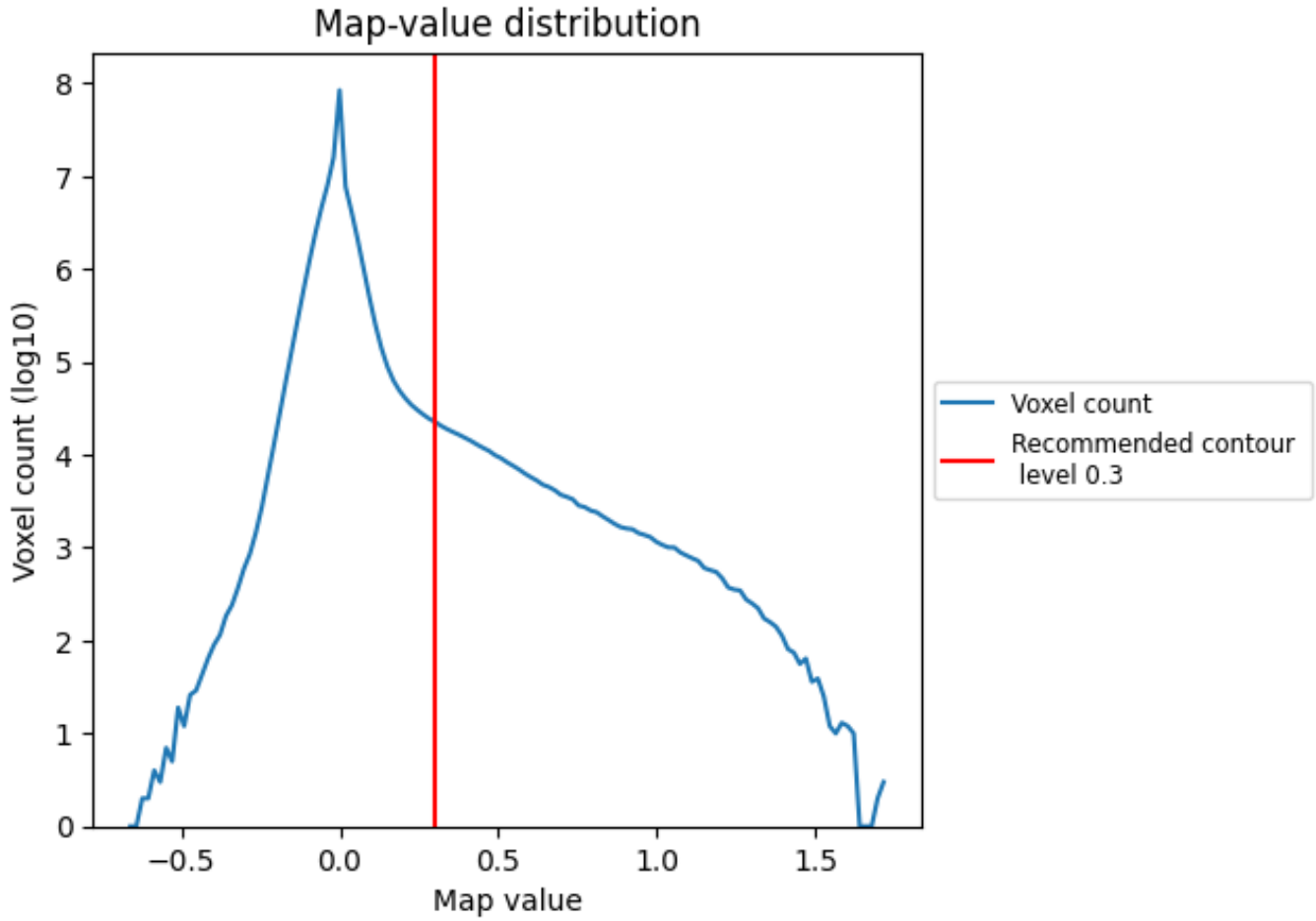


Z

7 Map analysis

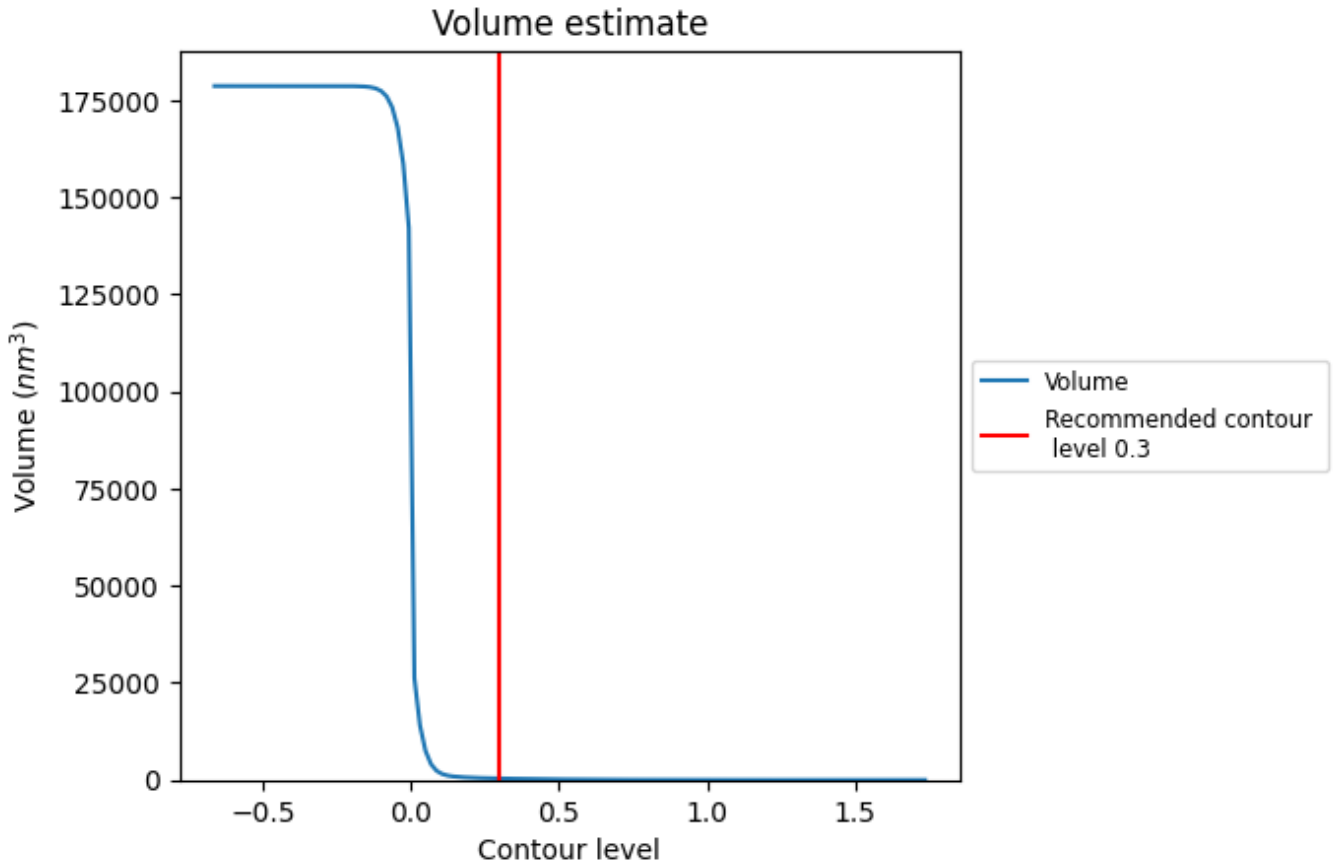
This section contains the results of statistical analysis of the map.

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.

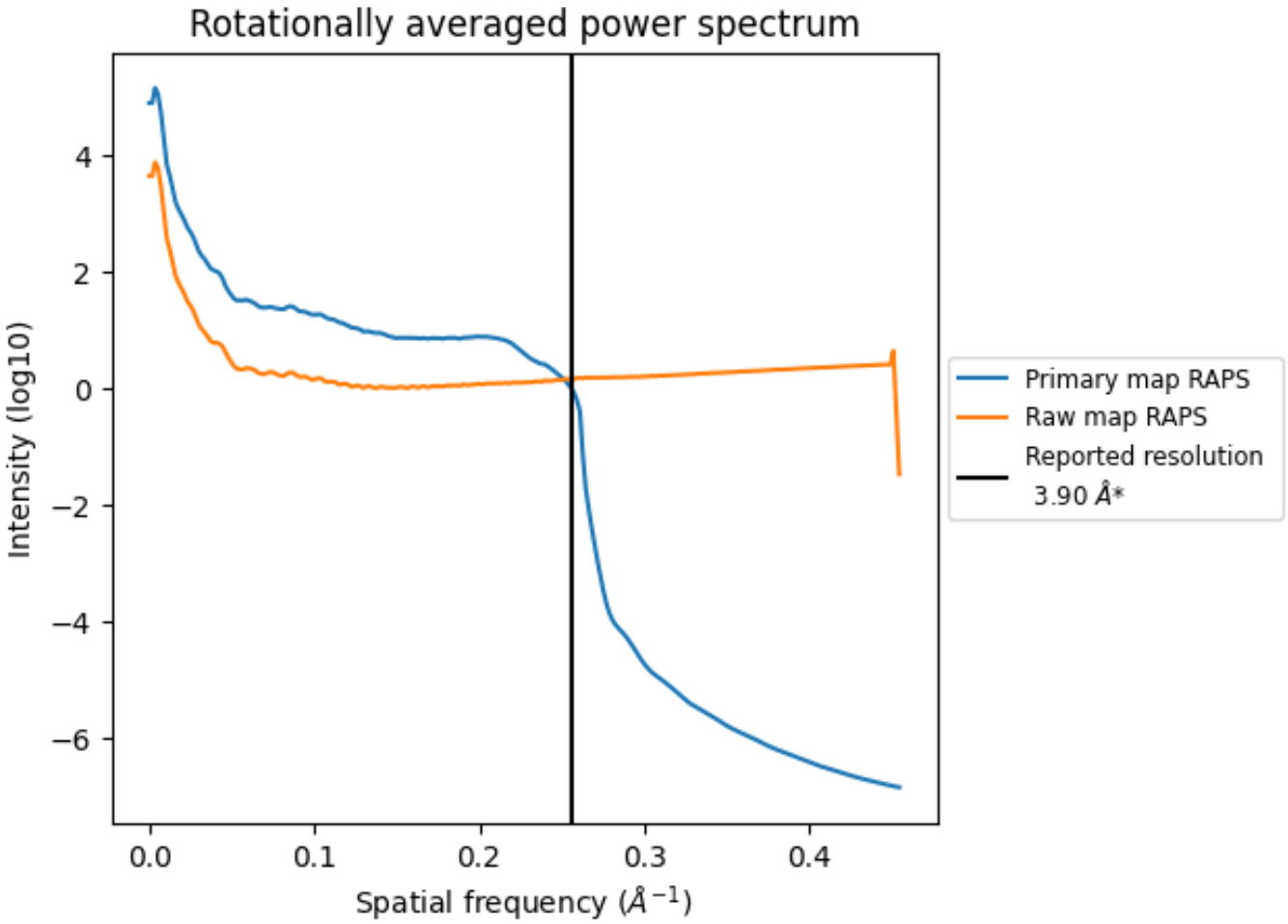
7.2 Volume estimate



The volume at the recommended contour level is 377 nm^3; this corresponds to an approximate mass of 341 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)

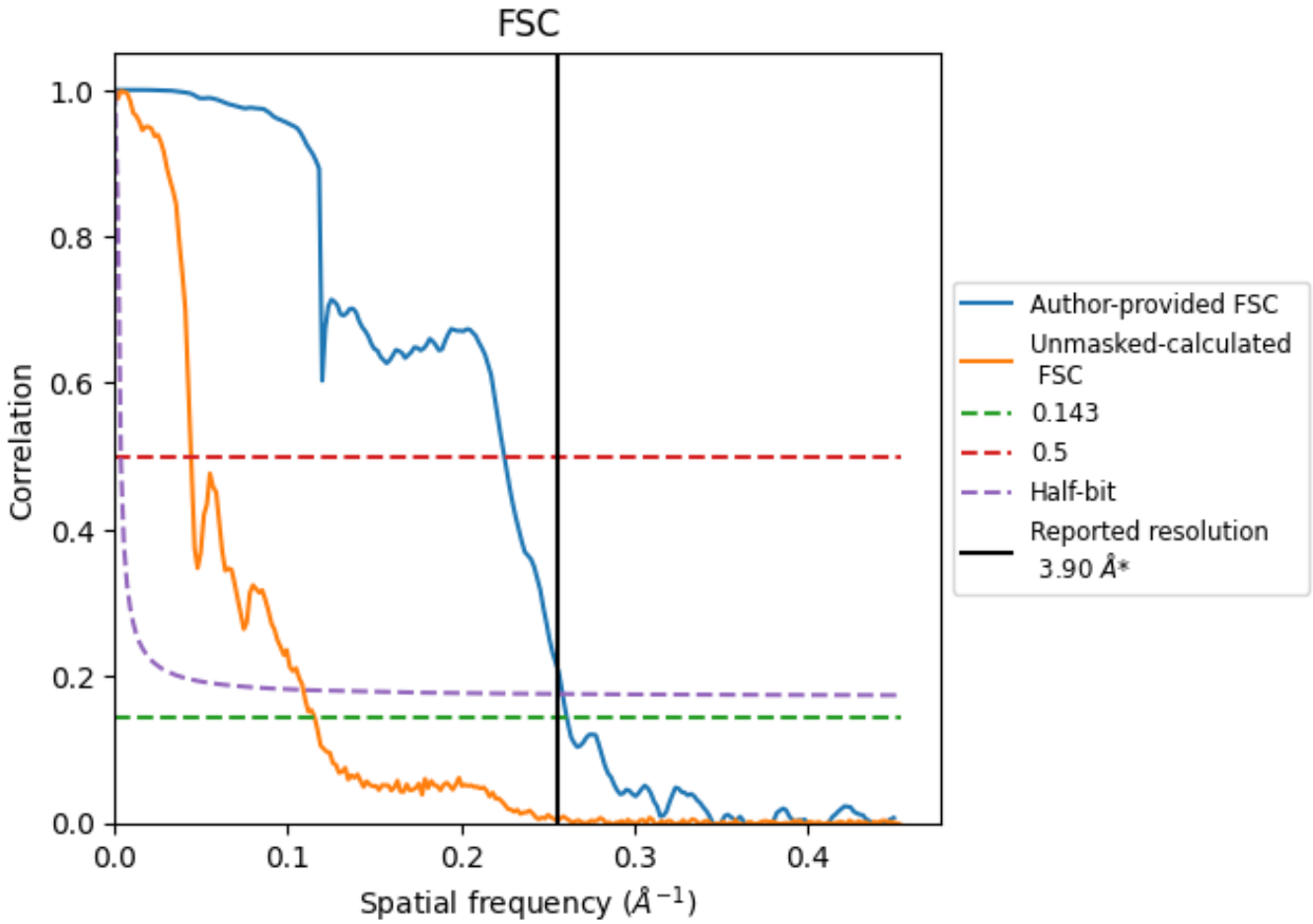


*Reported resolution corresponds to spatial frequency of 0.256 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.256 Å^{-1}

8.2 Resolution estimates (i)

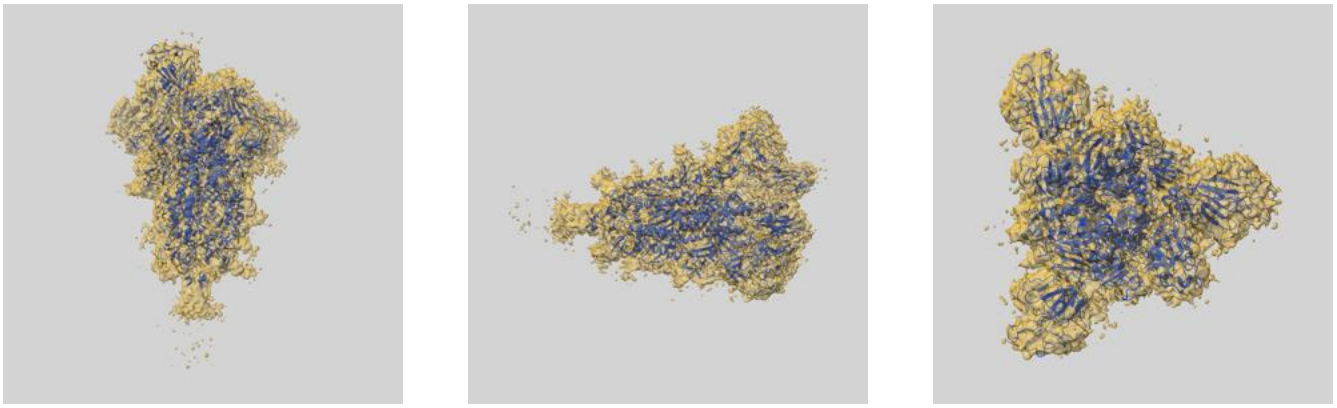
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.83	4.44	3.87
Unmasked-calculated*	8.65	22.73	9.18

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.65 differs from the reported value 3.9 by more than 10 %

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-33346 and PDB model 7XOE. Per-residue inclusion information can be found in section 3 on page 8.

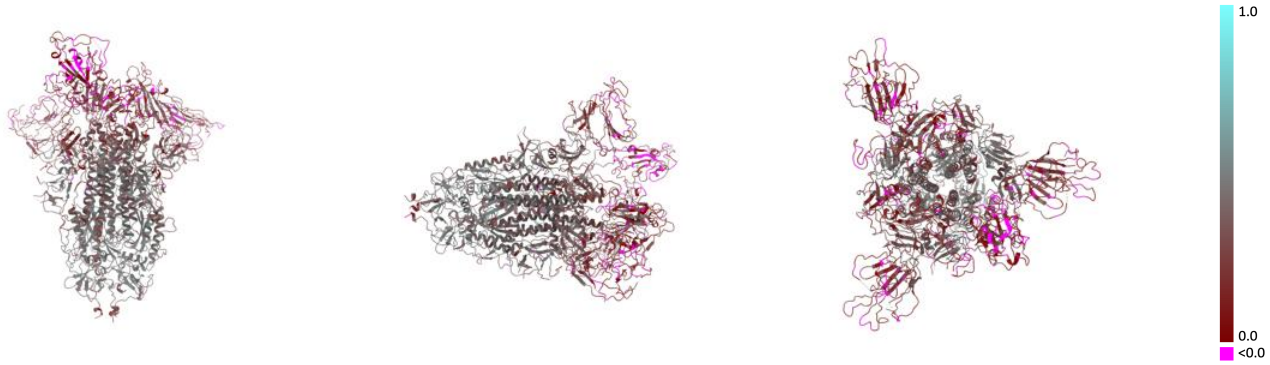
9.1 Map-model overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.3 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.

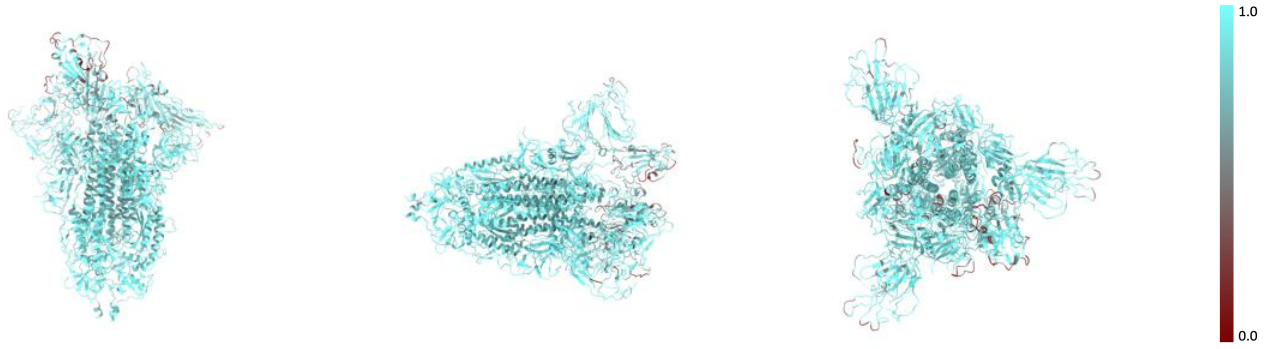
9.2 Q-score mapped to coordinate model (i)



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.

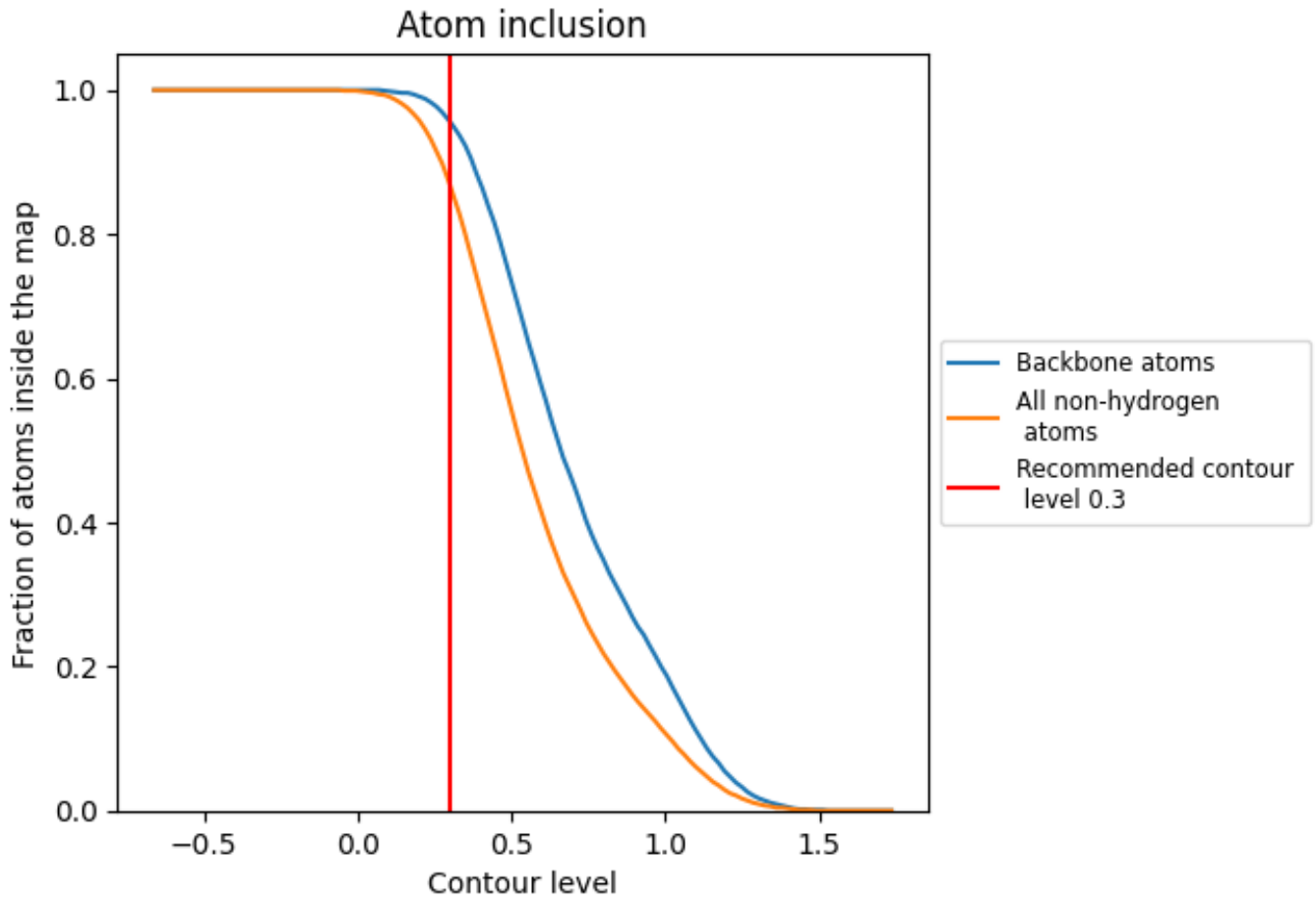
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.3).

9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8680	0.3010
A	0.8520	0.2910
B	0.8790	0.3090
C	0.8730	0.3060
D	0.7860	0.1180
E	0.4290	0.2730
F	0.6790	0.1170
G	0.8210	0.2630
H	0.9640	0.3490
I	0.7500	0.2270
J	0.8210	0.2860
K	0.7860	0.2290
L	0.9640	0.3780
M	0.8930	0.3590
N	0.8930	0.2410
O	0.8930	0.2390