Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2023 – 06:34 AM EDT

PDB ID	:	7MWX
Title	:	Structure of the core ectodomain of the hepatitis C virus envelope glycoprotein 2 with tamarin CD81
Authors	:	Kumar, A.; Hossain, R.A.; Yost, S.A.; Bu, W.; Wang, Y.; Dearborn, A.D.; Grakoui, A.; Cohen, J.I.; Marcotrigiano, J.
Deposited on	:	2021-05-17
Resolution	:	3.32 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp
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:

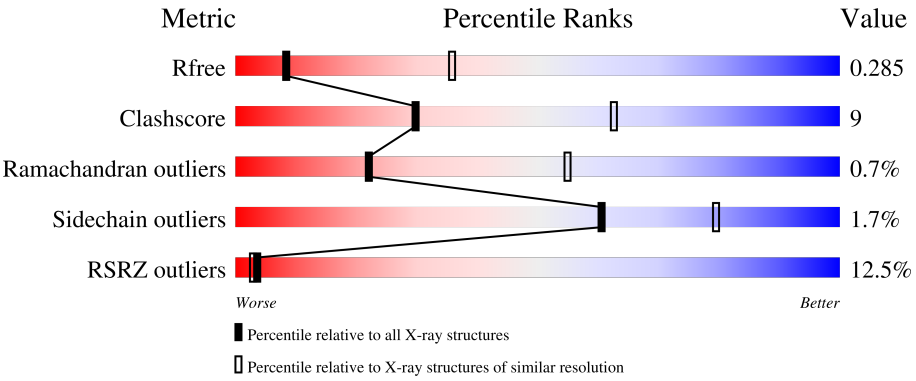
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.32 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1089 (3.36-3.28)
Clashscore	141614	1137 (3.36-3.28)
Ramachandran outliers	138981	1115 (3.36-3.28)
Sidechain outliers	138945	1114 (3.36-3.28)
RSRZ outliers	127900	1059 (3.36-3.28)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	C	259	20% 46% 19% · 34%
1	G	259	18% 46% 22% · 31%
2	A	218	7% 90% 9% ·
2	E	218	6% 81% 17% ·
3	B	218	7% 89% 11%

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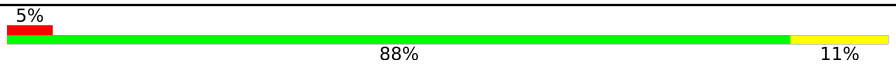
Mol	Chain	Length	Quality of chain
3	F	218	
4	D	93	
4	H	93	
5	I	3	
6	J	2	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 10459 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Core protein precursor eE2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	172	Total	C	N	O	S	0	0	0
			1289	828	214	233	14			
1	G	180	Total	C	N	O	S	0	0	0
			1328	845	222	247	14			

- Molecule 2 is a protein called 2A12 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	218	Total	C	N	O	S	0	0	0
			1607	1009	264	329	5			
2	E	218	Total	C	N	O	S	0	0	0
			1628	1020	266	337	5			

- Molecule 3 is a protein called 2A12 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	218	Total	C	N	O	S	0	0	0
			1659	1030	277	344	8			
3	F	218	Total	C	N	O	S	0	0	0
			1676	1040	282	346	8			

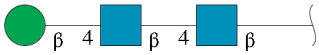
- Molecule 4 is a protein called CD81 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	81	Total	C	N	O	S	0	0	0
			555	338	94	118	5			
4	H	84	Total	C	N	O	S	0	0	0
			608	374	102	127	5			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	7	THR	-	cloning artifact	UNP Q9N0J9
D	8	GLY	-	cloning artifact	UNP Q9N0J9
D	9	SER	-	cloning artifact	UNP Q9N0J9
H	7	THR	-	cloning artifact	UNP Q9N0J9
H	8	GLY	-	cloning artifact	UNP Q9N0J9
H	9	SER	-	cloning artifact	UNP Q9N0J9

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

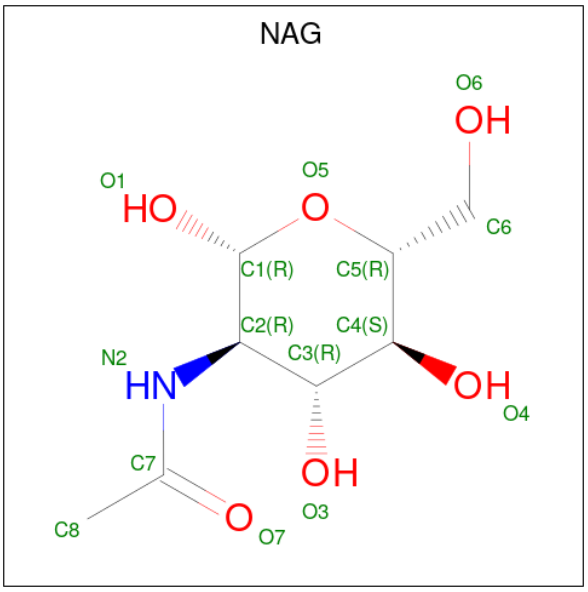


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	3	Total	C	N	O	0	0	0
			39	22	2	15			

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

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

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



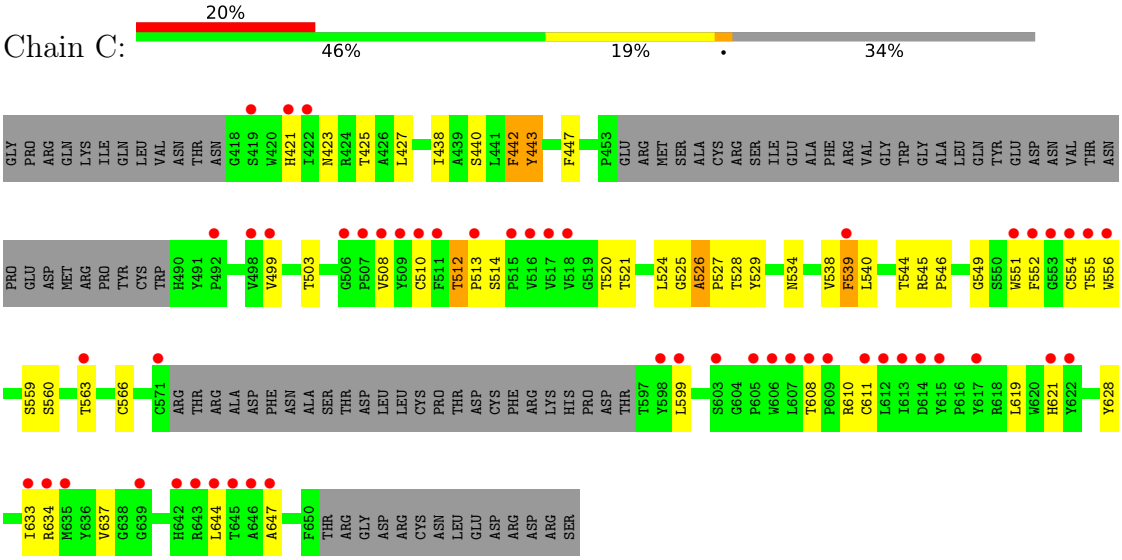
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total C N O 14 8 1 5	0	0
7	C	1	Total C N O 14 8 1 5	0	0
7	G	1	Total C N O 14 8 1 5	0	0

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 electron 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 dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

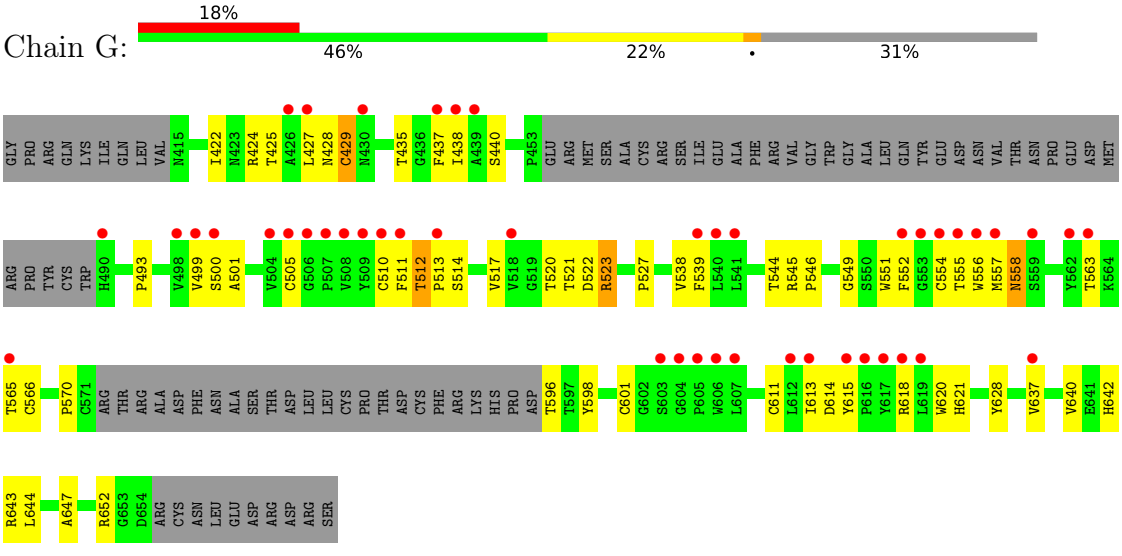
• Molecule 1: Core protein precursor eE2

Chain C:



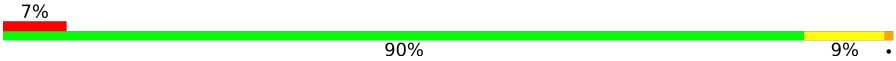
• Molecule 1: Core protein precursor eE2

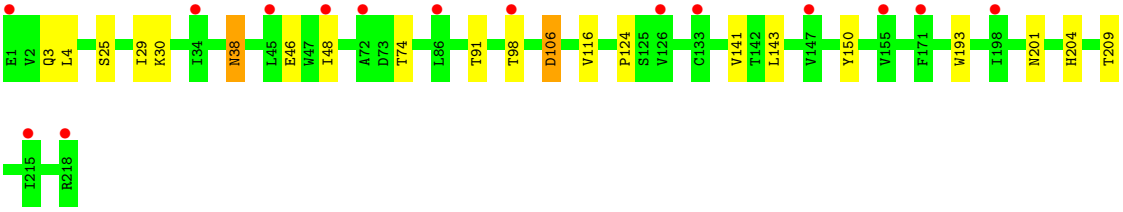
Chain G:



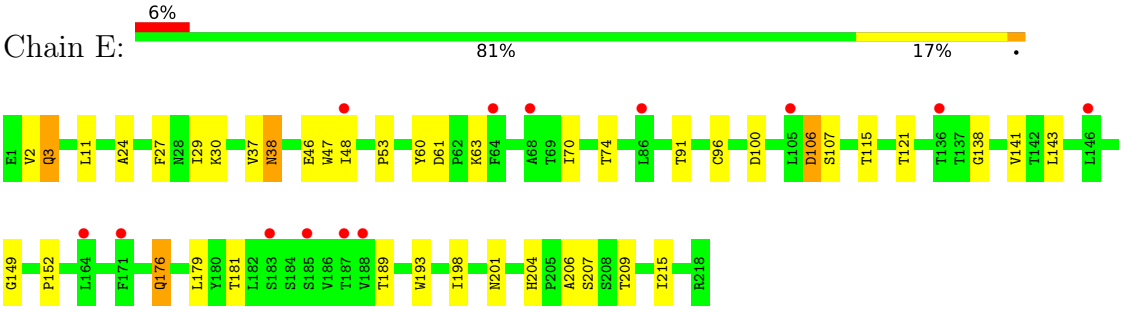
• Molecule 2: 2A12 Fab Heavy Chain

Chain A:

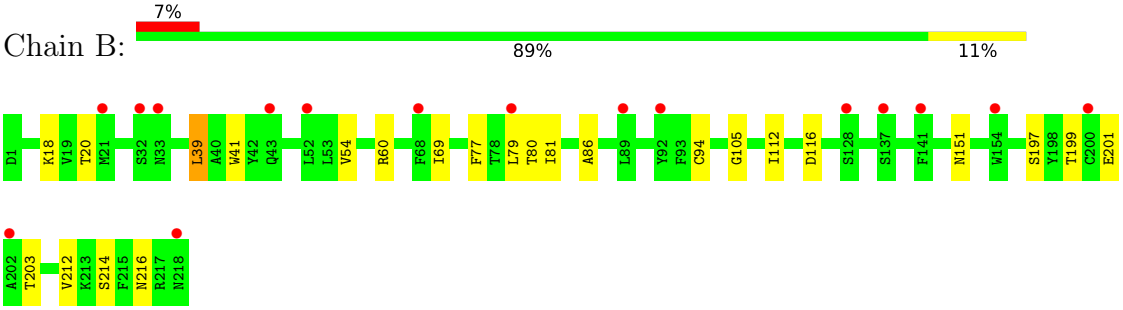




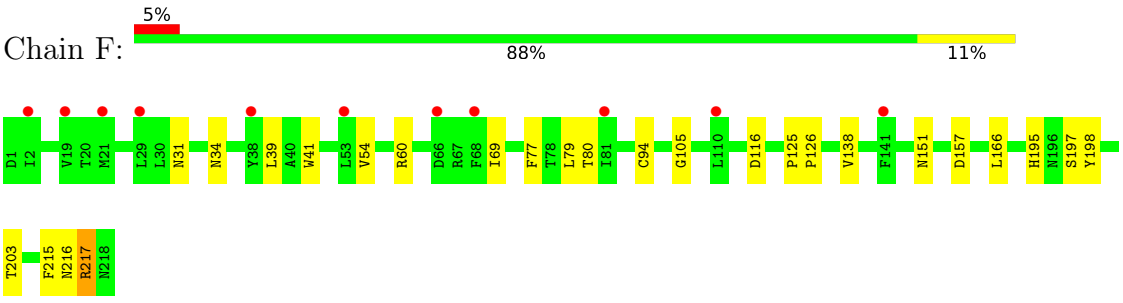
• Molecule 2: 2A12 Fab Heavy Chain



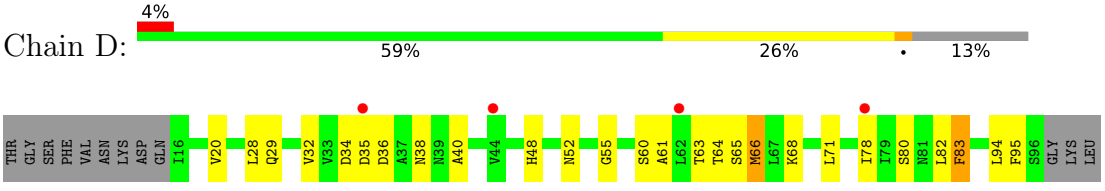
• Molecule 3: 2A12 Fab Light Chain



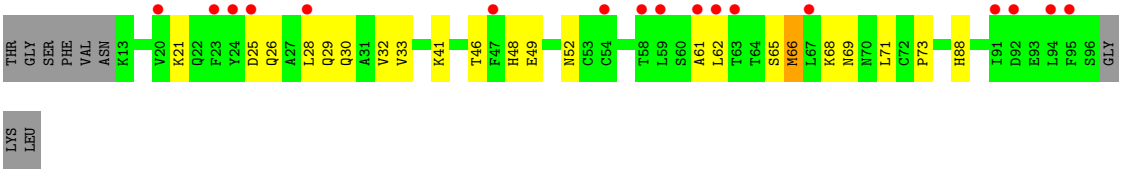
• Molecule 3: 2A12 Fab Light Chain



• Molecule 4: CD81 protein



• Molecule 4: CD81 protein

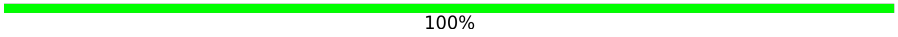


• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

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

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	76.95Å 127.77Å 212.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	53.09 – 3.32 54.74 – 3.32	Depositor EDS
% Data completeness (in resolution range)	99.4 (53.09-3.32) 99.5 (54.74-3.32)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.82 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.239 , 0.283 0.242 , 0.285	Depositor DCC
R_{free} test set	1593 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	124.4	Xtriage
Anisotropy	0.499	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 103.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	10459	wwPDB-VP
Average B, all atoms (Å^2)	168.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	C	0.26	0/1335	0.54	0/1837
1	G	0.27	0/1372	0.56	0/1889
2	A	0.25	0/1647	0.46	0/2263
2	E	0.25	0/1668	0.50	1/2288 (0.0%)
3	B	0.24	0/1696	0.42	0/2310
3	F	0.25	0/1713	0.42	0/2329
4	D	0.26	0/559	0.47	0/764
4	H	0.25	0/614	0.45	0/834
All	All	0.25	0/10604	0.48	1/14514 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	100	ASP	CB-CG-OD2	5.19	122.97	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	558	ASN	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1289	0	1167	42	0
1	G	1328	0	1189	51	0
2	A	1607	0	1532	12	0
2	E	1628	0	1564	31	0
3	B	1659	0	1543	12	0
3	F	1676	0	1578	15	0
4	D	555	0	495	21	0
4	H	608	0	561	18	0
5	I	39	0	34	2	0
6	J	28	0	25	0	0
7	C	28	0	26	0	0
7	G	14	0	13	0	0
All	All	10459	0	9727	189	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (189) 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)
2:E:29:ILE:HD13	2:E:53:PRO:CB	1.93	0.98
1:C:421:HIS:HB3	4:D:80:SER:H	1.31	0.95
1:G:501:ALA:H	1:G:538:VAL:HG22	1.34	0.92
2:A:91:THR:HG22	2:A:116:VAL:H	1.38	0.89
1:G:538:VAL:HG12	1:G:539:PHE:H	1.37	0.88
2:E:29:ILE:HD13	2:E:53:PRO:HB2	1.56	0.84
4:D:29:GLN:HA	4:D:32:VAL:HG22	1.62	0.81
1:C:513:PRO:HG3	1:C:637:VAL:HG21	1.64	0.79
2:E:29:ILE:HD13	2:E:53:PRO:HB3	1.67	0.76
1:G:427:LEU:HD23	1:G:428:ASN:H	1.52	0.75
2:E:11:LEU:HD13	2:E:152:PRO:HG3	1.70	0.74
1:G:521:THR:HG22	1:G:539:PHE:HD2	1.54	0.73
1:C:521:THR:H	1:C:539:PHE:HA	1.52	0.73
1:G:513:PRO:HG2	1:G:637:VAL:HG21	1.73	0.71
1:C:544:THR:HG23	1:C:549:GLY:HA3	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:538:VAL:HG12	1:G:539:PHE:N	2.06	0.70
1:C:634:ARG:NH1	2:A:106:ASP:OD2	2.25	0.69
3:F:217:ARG:HH11	3:F:217:ARG:HA	1.57	0.69
1:G:544:THR:HG23	1:G:549:GLY:HA3	1.75	0.69
2:E:91:THR:HG23	2:E:115:THR:HA	1.75	0.69
1:C:438:ILE:HD13	4:D:60:SER:HB2	1.75	0.68
1:G:521:THR:OG1	1:G:522:ASP:N	2.27	0.68
2:E:29:ILE:HD12	2:E:30:LYS:N	2.09	0.68
1:G:440:SER:HB2	1:G:620:TRP:HZ3	1.59	0.67
1:G:501:ALA:HB2	1:G:538:VAL:HA	1.79	0.65
2:A:38:ASN:HB3	2:A:48:ILE:HD11	1.78	0.64
1:G:538:VAL:CG1	1:G:539:PHE:H	2.11	0.64
3:B:201:GLU:HG2	3:B:212:VAL:HG12	1.80	0.63
1:G:521:THR:HA	1:G:539:PHE:HB3	1.78	0.63
2:E:149:GLY:HA2	2:E:179:LEU:HG	1.82	0.62
1:C:512:THR:OG1	1:C:513:PRO:HD2	2.00	0.61
1:C:526:ALA:H	1:C:527:PRO:CD	2.13	0.61
1:G:501:ALA:N	1:G:538:VAL:HG22	2.12	0.61
1:C:520:THR:HA	1:C:539:PHE:HB3	1.83	0.59
1:C:442:PHE:H	4:D:83:PHE:HB2	1.66	0.59
2:E:29:ILE:HD11	2:E:74:THR:HG22	1.85	0.58
1:C:628:TYR:HB3	1:C:647:ALA:HB1	1.87	0.57
1:G:551:TRP:NE1	1:G:554:CYS:SG	2.77	0.57
1:C:423:ASN:HB3	4:D:78:ILE:O	2.05	0.57
1:C:608:THR:HG23	1:C:610:ARG:H	1.67	0.57
1:G:555:THR:HG22	1:G:621:HIS:HD2	1.68	0.57
4:D:35:ASP:HB3	4:D:65:SER:OG	2.04	0.57
1:G:425:THR:HG21	1:G:520:THR:HA	1.87	0.57
1:G:521:THR:HG22	1:G:539:PHE:CD2	2.38	0.57
4:H:28:LEU:HD12	4:H:62:LEU:HD13	1.87	0.56
1:G:422:ILE:HB	1:G:517:VAL:HG11	1.86	0.56
1:C:510:CYS:HA	1:C:554:CYS:HA	1.87	0.56
4:H:49:GLU:HG2	4:H:73:PRO:HB3	1.88	0.56
2:E:38:ASN:HB3	2:E:48:ILE:HD11	1.88	0.55
1:C:556:TRP:HZ3	1:C:566:CYS:HB2	1.71	0.55
4:D:63:THR:HA	4:D:66:MET:SD	2.46	0.55
1:G:493:PRO:HB3	1:G:565:THR:HG23	1.89	0.55
2:A:143:LEU:HD11	2:A:193:TRP:CD1	2.42	0.55
1:C:514:SER:HA	1:C:644:LEU:HD21	1.89	0.54
2:A:4:LEU:HD11	2:A:98:THR:HG23	1.87	0.54
1:G:546:PRO:HG3	1:G:551:TRP:HA	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:126:PRO:HD3	3:F:138:VAL:HG22	1.88	0.54
1:G:500:SER:HA	1:G:538:VAL:HG21	1.90	0.54
4:D:66:MET:SD	4:D:66:MET:N	2.64	0.54
5:I:1:NAG:H3	5:I:1:NAG:H83	1.89	0.53
2:A:29:ILE:HD11	2:A:74:THR:HA	1.90	0.53
2:E:29:ILE:CD1	2:E:53:PRO:HB2	2.34	0.52
3:F:116:ASP:OD1	3:F:116:ASP:N	2.43	0.52
1:C:546:PRO:HG3	1:C:551:TRP:HA	1.91	0.52
2:E:24:ALA:HB1	2:E:27:PHE:CE1	2.45	0.52
1:G:628:TYR:HB3	1:G:647:ALA:HB1	1.92	0.52
1:G:499:VAL:O	1:G:538:VAL:HG11	2.11	0.51
3:B:54:VAL:HG22	3:B:60:ARG:HA	1.92	0.51
1:G:422:ILE:HD13	1:G:517:VAL:HG11	1.93	0.51
1:G:614:ASP:HA	1:G:618:ARG:HD3	1.92	0.51
1:G:523:ARG:HH22	4:H:68:LYS:NZ	2.10	0.50
1:G:563:THR:HG21	1:G:621:HIS:O	2.11	0.50
4:D:28:LEU:O	4:D:32:VAL:HG13	2.12	0.50
1:C:545:ARG:O	1:C:549:GLY:N	2.44	0.50
1:C:633:ILE:HG22	1:C:634:ARG:H	1.76	0.50
1:G:555:THR:HG22	1:G:621:HIS:CD2	2.46	0.50
1:G:556:TRP:CH2	1:G:566:CYS:HB2	2.47	0.50
3:B:20:THR:HG22	3:B:80:THR:HB	1.94	0.50
1:C:421:HIS:HB3	4:D:80:SER:N	2.13	0.50
4:D:94:LEU:HD12	4:H:46:THR:HG22	1.94	0.50
4:H:32:VAL:HA	4:H:41:LYS:HD2	1.94	0.49
1:C:554:CYS:H	1:C:566:CYS:HB3	1.78	0.49
3:F:151:ASN:HB3	3:F:203:THR:HB	1.94	0.49
1:C:508:VAL:HG13	1:C:556:TRP:HB3	1.94	0.49
1:C:521:THR:N	1:C:538:VAL:O	2.45	0.49
1:C:503:THR:O	1:C:559:SER:HB2	2.12	0.49
3:B:151:ASN:HB3	3:B:203:THR:HB	1.95	0.49
3:F:54:VAL:HG22	3:F:60:ARG:HA	1.95	0.48
1:G:513:PRO:HB2	1:G:642:HIS:CG	2.49	0.48
4:H:33:VAL:HG22	4:H:41:LYS:HD3	1.95	0.48
2:E:204:HIS:HB3	2:E:209:THR:HB	1.95	0.48
2:A:204:HIS:HB3	2:A:209:THR:HB	1.95	0.48
4:H:26:GLN:O	4:H:30:GLN:HG2	2.14	0.48
1:G:499:VAL:HG12	1:G:500:SER:H	1.79	0.48
3:F:198:TYR:HB2	3:F:215:PHE:CE1	2.49	0.48
3:B:41:TRP:CE2	3:B:79:LEU:HB2	2.50	0.47
4:H:25:ASP:O	4:H:29:GLN:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:124:PRO:HB3	2:A:150:TYR:HB3	1.97	0.47
1:G:510:CYS:HA	1:G:554:CYS:HA	1.96	0.47
2:E:141:VAL:O	2:E:189:THR:OG1	2.24	0.47
2:E:143:LEU:HG	2:E:198:ILE:HD11	1.97	0.47
4:D:48:HIS:O	4:D:52:ASN:N	2.47	0.47
2:E:176:GLN:OE1	2:E:181:THR:OG1	2.30	0.47
1:G:513:PRO:CG	1:G:637:VAL:HG21	2.44	0.46
1:G:596:THR:HG22	1:G:598:TYR:H	1.80	0.46
3:B:69:ILE:HB	3:B:80:THR:HG23	1.98	0.46
2:A:141:VAL:HG21	2:A:193:TRP:CE3	2.51	0.46
3:F:94:CYS:O	3:F:105:GLY:N	2.49	0.46
1:G:546:PRO:HG2	1:G:552:PHE:CE2	2.51	0.46
1:C:427:LEU:HD11	4:D:64:THR:HB	1.98	0.45
1:G:643:ARG:NH2	2:E:106:ASP:OD1	2.48	0.45
4:H:33:VAL:HG13	4:H:41:LYS:HD3	1.98	0.45
4:H:65:SER:O	4:H:69:ASN:ND2	2.46	0.45
2:A:38:ASN:OD1	2:A:46:GLU:HB3	2.16	0.45
2:E:38:ASN:OD1	2:E:46:GLU:HB3	2.17	0.45
1:C:440:SER:HA	1:C:443:TYR:HB3	1.98	0.45
1:C:524:LEU:HD12	1:C:525:GLY:H	1.81	0.45
4:H:21:LYS:HG3	4:H:88:HIS:NE2	2.32	0.45
4:H:68:LYS:HA	4:H:68:LYS:HD2	1.74	0.45
1:C:528:THR:OG1	1:C:529:TYR:N	2.50	0.45
1:G:438:ILE:HD11	4:H:61:ALA:HA	1.98	0.45
3:B:199:THR:HG23	3:B:214:SER:HB3	1.99	0.45
2:A:3:GLN:HB3	2:A:25:SER:HB2	1.97	0.45
1:G:523:ARG:HH22	4:H:68:LYS:HZ1	1.65	0.45
3:B:86:ALA:HA	3:B:112:ILE:HD13	1.99	0.45
1:G:557:MET:HG3	1:G:558:ASN:N	2.32	0.44
2:E:29:ILE:HD12	2:E:29:ILE:C	2.36	0.44
2:E:143:LEU:HD23	2:E:189:THR:HG21	1.98	0.44
2:E:60:TYR:HE1	2:E:70:ILE:HG13	1.81	0.44
3:F:41:TRP:CE2	3:F:79:LEU:HB2	2.52	0.44
4:H:66:MET:HA	4:H:69:ASN:HD21	1.83	0.44
1:C:608:THR:HG22	1:C:611:CYS:HB2	1.99	0.44
4:D:34:ASP:CG	4:D:35:ASP:H	2.21	0.44
1:C:447:PHE:CZ	1:C:619:LEU:HB3	2.54	0.43
1:G:545:ARG:O	1:G:549:GLY:N	2.52	0.43
1:G:437:PHE:CD2	1:G:438:ILE:HG23	2.53	0.43
3:B:18:LYS:HA	3:B:81:ILE:O	2.19	0.43
3:F:197:SER:HB2	3:F:216:ASN:OD1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:560:SER:HB3	5:I:1:NAG:H82	2.01	0.43
1:G:611:CYS:HA	1:G:647:ALA:O	2.19	0.43
2:E:37:VAL:HG22	2:E:47:TRP:HA	2.01	0.43
1:C:545:ARG:HD3	1:C:599:LEU:O	2.19	0.42
1:G:557:MET:SD	1:G:563:THR:HG22	2.59	0.42
2:E:193:TRP:CH2	2:E:215:ILE:HB	2.54	0.42
3:F:125:PRO:HB3	3:F:215:PHE:CE2	2.54	0.42
1:G:613:ILE:HG12	1:G:644:LEU:HD23	2.01	0.42
1:G:429:CYS:HB3	1:G:505:CYS:HB2	1.74	0.42
3:B:94:CYS:O	3:B:105:GLY:N	2.52	0.42
4:D:36:ASP:HB3	4:D:71:LEU:HD13	2.02	0.42
4:D:20:VAL:HG11	4:D:95:PHE:CZ	2.55	0.42
3:F:39:LEU:HD13	3:F:77:PHE:CD1	2.54	0.42
4:D:38:ASN:C	4:D:40:ALA:H	2.23	0.42
2:E:176:GLN:HB3	3:F:166:LEU:HD11	2.02	0.42
2:E:179:LEU:HD12	2:E:179:LEU:HA	1.85	0.42
2:E:215:ILE:H	2:E:215:ILE:HG12	1.68	0.42
3:B:197:SER:OG	3:B:216:ASN:OD1	2.35	0.42
1:G:637:VAL:HG23	1:G:640:VAL:HG13	2.01	0.42
4:H:28:LEU:HD21	4:H:66:MET:HE1	2.02	0.42
1:C:512:THR:HG23	1:C:514:SER:H	1.84	0.42
1:C:563:THR:HG21	1:C:621:HIS:O	2.19	0.42
3:B:39:LEU:HD13	3:B:77:PHE:CD1	2.54	0.42
2:E:2:VAL:O	2:E:3:GLN:HB3	2.20	0.42
1:G:512:THR:HG22	1:G:514:SER:O	2.20	0.42
1:C:425:THR:HB	1:C:520:THR:HG23	2.02	0.42
2:E:2:VAL:HG12	2:E:107:SER:CB	2.50	0.42
1:C:540:LEU:H	1:C:540:LEU:HD23	1.85	0.41
1:C:556:TRP:CZ3	1:C:566:CYS:HB2	2.53	0.41
2:E:61:ASP:OD1	2:E:63:LYS:HG2	2.20	0.41
4:H:66:MET:O	4:H:71:LEU:N	2.52	0.41
1:C:552:PHE:HE2	1:C:599:LEU:HA	1.86	0.41
3:F:31:ASN:ND2	3:F:34:ASN:OD1	2.53	0.41
1:C:438:ILE:HG21	4:D:61:ALA:HA	2.03	0.41
3:F:157:ASP:OD2	3:F:195:HIS:ND1	2.54	0.41
1:G:435:THR:HG23	1:G:437:PHE:HB2	2.03	0.41
2:E:204:HIS:CE1	2:E:206:ALA:HB3	2.55	0.41
2:E:121:THR:HG22	2:E:207:SER:HB3	2.02	0.41
1:G:424:ARG:NE	1:G:424:ARG:HA	2.36	0.41
1:G:511:PHE:HZ	1:G:615:TYR:CD1	2.39	0.41
3:F:69:ILE:HB	3:F:80:THR:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:499:VAL:HG11	1:C:539:PHE:HE1	1.86	0.40
2:A:30:LYS:HE3	2:A:30:LYS:HB3	1.88	0.40
4:D:82:LEU:HD12	4:D:82:LEU:HA	1.86	0.40
4:H:48:HIS:O	4:H:52:ASN:N	2.54	0.40
1:C:555:THR:HG22	1:C:621:HIS:HD2	1.87	0.40
4:D:71:LEU:H	4:D:71:LEU:HG	1.66	0.40
1:G:511:PHE:C	1:G:551:TRP:HB2	2.41	0.40
4:D:55:GLY:HA3	4:D:63:THR:CG2	2.51	0.40
2:E:193:TRP:HH2	2:E:215:ILE:O	2.05	0.40
1:C:520:THR:OG1	1:C:524:LEU:HB2	2.20	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 X-ray entries followed by that with respect to entries of similar resolution.

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	C	166/259 (64%)	142 (86%)	20 (12%)	4 (2%)	6 29
1	G	174/259 (67%)	146 (84%)	24 (14%)	4 (2%)	6 30
2	A	216/218 (99%)	207 (96%)	9 (4%)	0	100 100
2	E	216/218 (99%)	201 (93%)	13 (6%)	2 (1%)	17 49
3	B	216/218 (99%)	207 (96%)	9 (4%)	0	100 100
3	F	216/218 (99%)	207 (96%)	9 (4%)	0	100 100
4	D	79/93 (85%)	69 (87%)	10 (13%)	0	100 100
4	H	82/93 (88%)	75 (92%)	7 (8%)	0	100 100
All	All	1365/1576 (87%)	1254 (92%)	101 (7%)	10 (1%)	22 55

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	512	THR
1	C	526	ALA
1	G	512	THR
1	G	570	PRO
2	E	138	GLY
1	C	442	PHE
1	G	429	CYS
1	G	527	PRO
1	C	534	ASN
2	E	3	GLN

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 X-ray entries followed by that with respect to entries of similar resolution.

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	C	137/227 (60%)	135 (98%)	2 (2%)	65	81
1	G	140/227 (62%)	137 (98%)	3 (2%)	53	76
2	A	180/187 (96%)	177 (98%)	3 (2%)	60	79
2	E	186/187 (100%)	181 (97%)	5 (3%)	44	72
3	B	187/195 (96%)	185 (99%)	2 (1%)	73	85
3	F	191/195 (98%)	190 (100%)	1 (0%)	88	93
4	D	58/82 (71%)	55 (95%)	3 (5%)	23	55
4	H	66/82 (80%)	65 (98%)	1 (2%)	65	81
All	All	1145/1382 (83%)	1125 (98%)	20 (2%)	60	79

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	443	TYR
1	C	539	PHE
1	G	523	ARG
1	G	601	CYS
1	G	652	ARG
2	A	38	ASN

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Mol	Chain	Res	Type
2	A	106	ASP
2	A	201	ASN
3	B	39	LEU
3	B	116	ASP
4	D	66	MET
4	D	68	LYS
4	D	83	PHE
2	E	38	ASN
2	E	96	CYS
2	E	106	ASP
2	E	176	GLN
2	E	201	ASN
3	F	217	ARG
4	H	66	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

5 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	$\#\|Z\| > 2$
5	NAG	I	1	5,1	14,14,15	0.51	0	17,19,21	1.30	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	I	2	5	14,14,15	0.30	0	17,19,21	0.43	0
5	BMA	I	3	5	11,11,12	0.62	0	15,15,17	0.77	0
6	NAG	J	1	6,1	14,14,15	0.25	0	17,19,21	0.43	0
6	NAG	J	2	6	14,14,15	0.26	0	17,19,21	0.55	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
5	NAG	I	1	5,1	-	5/6/23/26	0/1/1/1
5	NAG	I	2	5	-	4/6/23/26	0/1/1/1
5	BMA	I	3	5	-	0/2/19/22	0/1/1/1
6	NAG	J	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	J	2	6	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	I	1	NAG	C2-N2-C7	4.33	129.07	122.90
5	I	1	NAG	C1-C2-N2	2.03	113.96	110.49

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	I	2	NAG	O5-C5-C6-O6
5	I	1	NAG	C8-C7-N2-C2
5	I	1	NAG	O7-C7-N2-C2
5	I	2	NAG	C8-C7-N2-C2
5	I	2	NAG	O7-C7-N2-C2
6	J	1	NAG	C4-C5-C6-O6
5	I	2	NAG	C4-C5-C6-O6
6	J	1	NAG	O5-C5-C6-O6
5	I	1	NAG	C4-C5-C6-O6
5	I	1	NAG	O5-C5-C6-O6
6	J	2	NAG	O5-C5-C6-O6
6	J	2	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
5	I	1	NAG	C3-C2-N2-C7

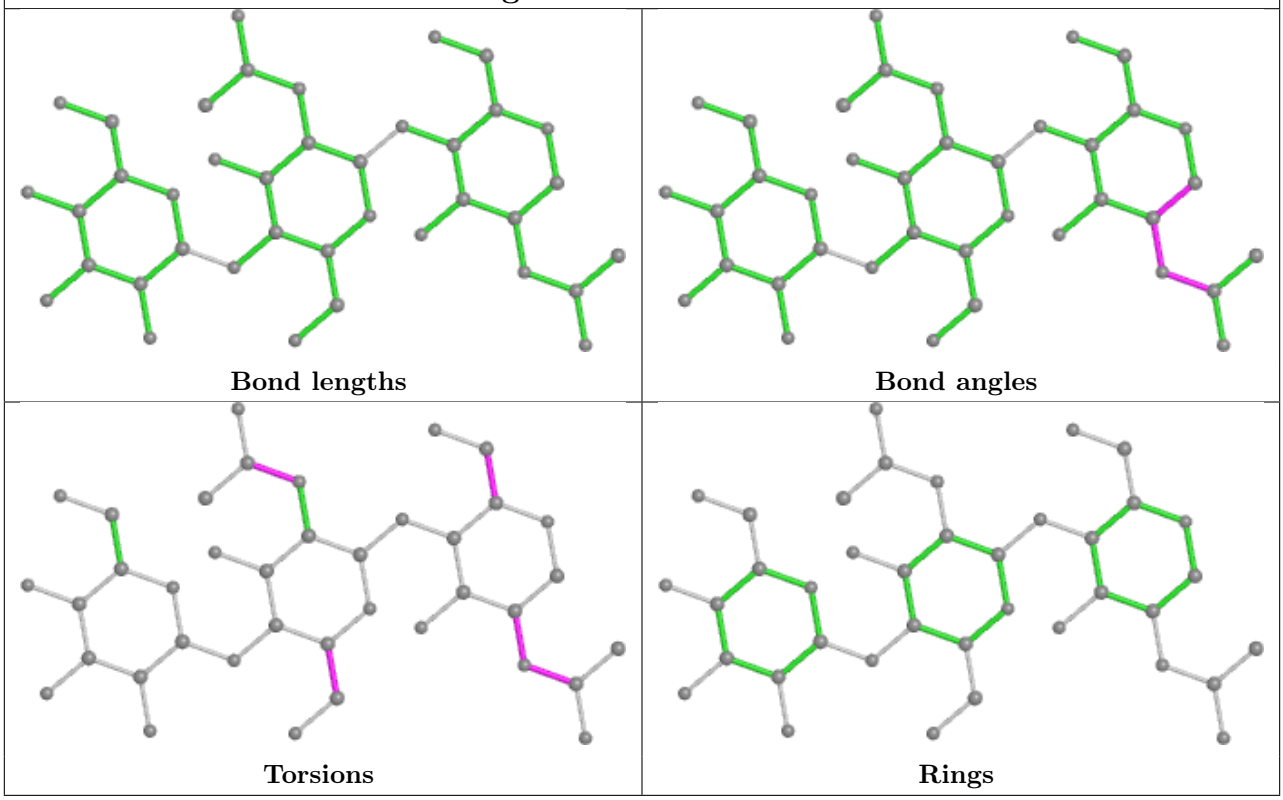
There are no ring outliers.

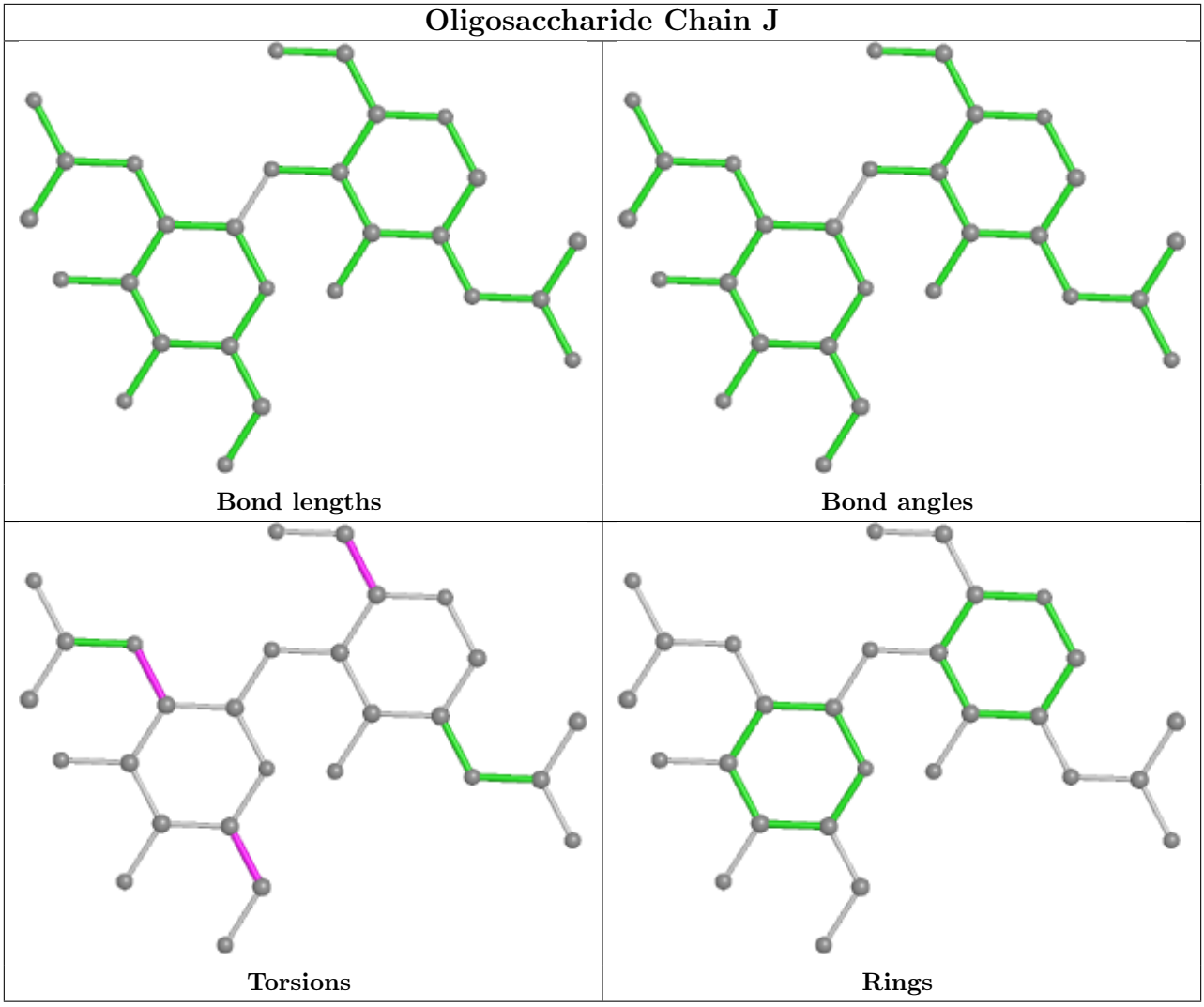
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	I	1	NAG	2	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 I





5.6 Ligand geometry (i)

3 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	$\#\|Z\| > 2$
7	NAG	C	701	1	14,14,15	0.40	0	17,19,21	0.52	0
7	NAG	G	701	1	14,14,15	0.24	0	17,19,21	0.43	0
7	NAG	C	702	1	14,14,15	0.27	0	17,19,21	0.50	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
7	NAG	C	701	1	-	3/6/23/26	0/1/1/1
7	NAG	G	701	1	-	2/6/23/26	0/1/1/1
7	NAG	C	702	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	702	NAG	O5-C5-C6-O6
7	C	702	NAG	C4-C5-C6-O6
7	G	701	NAG	C4-C5-C6-O6
7	C	701	NAG	C4-C5-C6-O6
7	C	701	NAG	O5-C5-C6-O6
7	G	701	NAG	O5-C5-C6-O6
7	C	701	NAG	C1-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

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 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	C	172/259 (66%)	1.33	52 (30%) 0 0	121, 209, 273, 347	0
1	G	180/259 (69%)	1.01	46 (25%) 0 0	119, 214, 290, 351	0
2	A	218/218 (100%)	0.44	15 (6%) 16 17	90, 121, 164, 222	0
2	E	218/218 (100%)	0.31	13 (5%) 21 22	80, 136, 205, 257	0
3	B	218/218 (100%)	0.36	16 (7%) 15 15	94, 139, 204, 301	0
3	F	218/218 (100%)	0.24	11 (5%) 28 28	108, 143, 202, 226	0
4	D	81/93 (87%)	-0.01	4 (4%) 29 29	163, 228, 294, 355	0
4	H	84/93 (90%)	0.76	17 (20%) 1 0	169, 219, 288, 328	0
All	All	1389/1576 (88%)	0.55	174 (12%) 3 3	80, 155, 264, 355	0

All (174) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	509	TYR	10.5
1	C	613	ILE	9.1
1	C	511	PHE	7.6
1	C	518	VAL	7.1
1	G	506	GLY	6.7
1	C	507	PRO	6.6
1	G	426	ALA	6.6
1	C	607	LEU	6.6
1	C	612	LEU	6.4
1	C	513	PRO	6.3
1	C	515	PRO	6.1
1	C	644	LEU	6.0
1	C	646	ALA	6.0
4	H	62	LEU	5.9
1	C	508	VAL	5.8
1	C	555	THR	5.8

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Mol	Chain	Res	Type	RSRZ
1	G	563	THR	5.6
1	G	499	VAL	5.5
1	G	556	TRP	5.5
1	C	552	PHE	5.4
1	G	505	CYS	5.3
1	C	539	PHE	5.2
1	C	609	PRO	5.2
1	C	517	VAL	5.2
4	H	92	ASP	5.1
1	C	499	VAL	4.9
1	G	557	MET	4.8
1	G	427	LEU	4.8
1	C	635	MET	4.7
1	C	647	ALA	4.7
1	G	607	LEU	4.7
1	C	598	TYR	4.6
4	H	95	PHE	4.4
1	C	492	PRO	4.4
1	G	539	PHE	4.3
1	G	430	ASN	4.2
1	C	603	SER	4.1
1	G	619	LEU	4.1
1	C	510	CYS	4.1
4	H	63	THR	4.1
1	C	516	VAL	4.1
1	G	554	CYS	4.0
1	G	559	SER	4.0
1	C	599	LEU	4.0
1	G	518	VAL	4.0
1	G	438	ILE	4.0
1	G	513	PRO	4.0
1	G	510	CYS	3.9
1	C	642	HIS	3.9
1	G	507	PRO	3.8
1	G	508	VAL	3.8
1	G	565	THR	3.8
1	G	498	VAL	3.8
1	C	606	TRP	3.8
1	G	437	PHE	3.8
4	D	35	ASP	3.8
1	G	605	PRO	3.8
1	G	540	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	645	THR	3.6
1	G	555	THR	3.6
2	E	188	VAL	3.6
4	H	61	ALA	3.6
1	C	614	ASP	3.6
1	G	606	TRP	3.6
1	G	612	LEU	3.6
1	C	506	GLY	3.5
2	A	45	LEU	3.5
1	C	556	TRP	3.4
2	A	171	PHE	3.4
4	H	24	TYR	3.4
3	F	68	PHE	3.4
1	G	552	PHE	3.4
1	C	419	SER	3.3
4	H	54	CYS	3.3
1	C	554	CYS	3.2
1	C	498	VAL	3.2
1	G	604	GLY	3.2
2	E	171	PHE	3.2
4	H	58	THR	3.2
1	C	615	TYR	3.1
1	C	633	ILE	3.1
2	A	133	CYS	3.1
1	G	613	ILE	3.1
1	C	563	THR	3.1
4	H	28	LEU	3.0
4	H	67	LEU	3.0
4	H	47	PHE	2.8
3	F	53	LEU	2.8
1	G	618	ARG	2.8
4	H	20	VAL	2.8
3	B	89	LEU	2.8
3	B	33	ASN	2.8
1	G	541	LEU	2.7
1	G	603	SER	2.7
3	B	68	PHE	2.7
2	A	72	ALA	2.7
1	G	509	TYR	2.7
2	E	136	THR	2.7
1	G	615	TYR	2.7
1	C	639	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	608	THR	2.6
1	G	504	VAL	2.6
1	C	643	ARG	2.6
2	E	48	ILE	2.6
1	C	622	TYR	2.5
1	C	553	GLY	2.5
2	E	183	SER	2.5
4	H	91	ILE	2.5
3	B	92	TYR	2.5
3	B	141	PHE	2.5
3	F	21	MET	2.5
4	H	25	ASP	2.5
3	B	137	SER	2.5
1	G	553	GLY	2.5
3	B	43	GLN	2.5
3	F	19	VAL	2.4
1	C	605	PRO	2.4
3	B	21	MET	2.4
2	E	187	THR	2.4
1	C	551	TRP	2.4
3	F	110	LEU	2.4
3	B	218	ASN	2.4
1	C	571	CYS	2.3
3	F	66	ASP	2.3
3	B	202	ALA	2.3
2	A	126	VAL	2.3
1	G	511	PHE	2.3
3	B	154	TRP	2.3
1	G	500	SER	2.3
4	D	78	ILE	2.3
1	C	621	HIS	2.3
2	A	147	VAL	2.3
1	C	634	ARG	2.3
2	A	155	VAL	2.3
2	A	218	ARG	2.3
3	F	38	TYR	2.3
3	B	200	CYS	2.2
2	E	146	LEU	2.2
4	D	62	LEU	2.2
1	C	611	CYS	2.2
2	E	64	PHE	2.2
4	D	44	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	637	VAL	2.2
2	E	164	LEU	2.2
2	A	34	ILE	2.2
1	G	617	TYR	2.2
2	A	86	LEU	2.2
2	E	68	ALA	2.2
2	E	105	LEU	2.1
4	H	94	LEU	2.1
1	G	439	ALA	2.1
1	C	422	ILE	2.1
3	F	81	ILE	2.1
2	A	98	THR	2.1
3	F	141	PHE	2.1
4	H	23	PHE	2.1
2	E	185	SER	2.1
3	B	128	SER	2.1
3	B	52	LEU	2.1
1	G	490	HIS	2.1
1	G	616	PRO	2.1
1	G	562	TYR	2.1
2	A	215	ILE	2.1
3	F	2	ILE	2.1
3	F	29	LEU	2.1
2	A	48	ILE	2.1
4	H	59	LEU	2.1
2	A	1	GLU	2.1
2	A	198	ILE	2.0
2	E	86	LEU	2.0
3	B	32	SER	2.0
3	B	79	LEU	2.0
1	C	421	HIS	2.0
1	C	617	TYR	2.0

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

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

6.3 Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

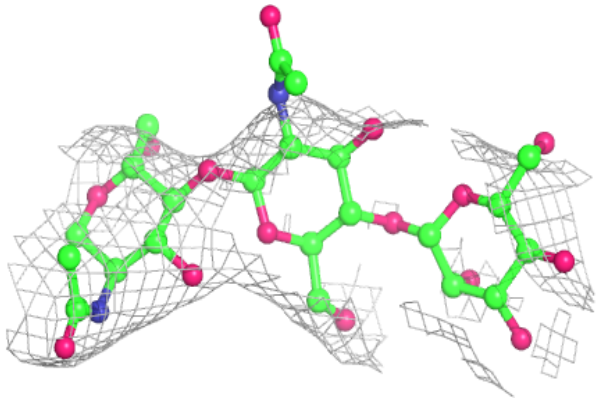
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

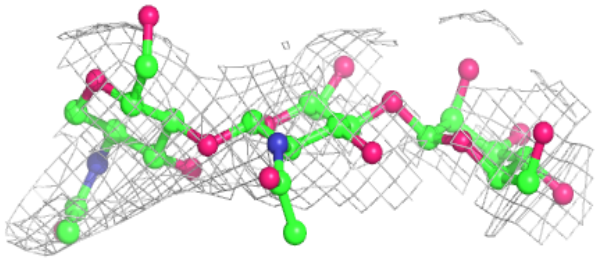
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NAG	J	2	14/15	0.72	0.24	272,316,333,333	0
5	BMA	I	3	11/12	0.76	0.18	207,250,262,265	0
5	NAG	I	2	14/15	0.80	0.24	232,276,302,307	0
6	NAG	J	1	14/15	0.89	0.20	246,278,321,325	0
5	NAG	I	1	14/15	0.90	0.25	190,227,241,265	0

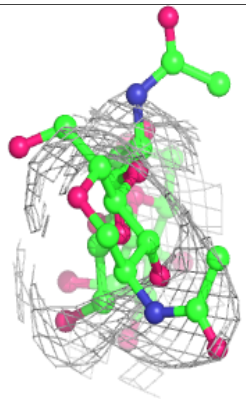
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain I:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

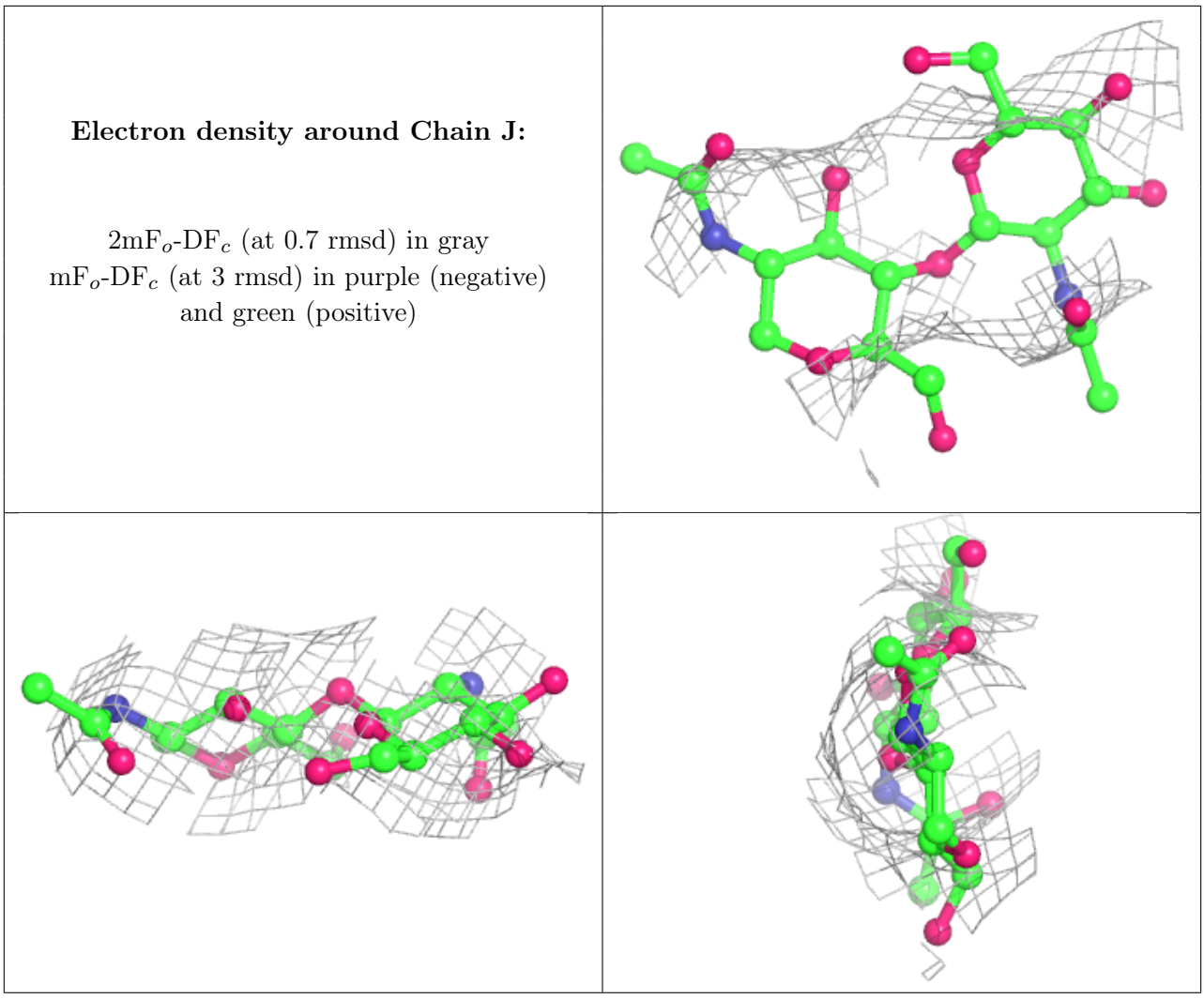






Electron density around Chain J:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	NAG	C	702	14/15	0.51	0.29	156,207,230,240	0
7	NAG	C	701	14/15	0.59	0.24	218,249,259,260	0
7	NAG	G	701	14/15	0.67	0.20	150,226,238,249	0

6.5 Other polymers

There are no such residues in this entry.