



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 09:23 AM BST

PDB ID : 1OAN  
Title : Crystal structure of the dengue 2 virus envelope protein  
Authors : Modis, Y.; Harrison, S.C.  
Deposited on : 2003-01-16  
Resolution : 2.75 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](mailto: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.

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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 : 2.13.1  
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) : 2.13.1

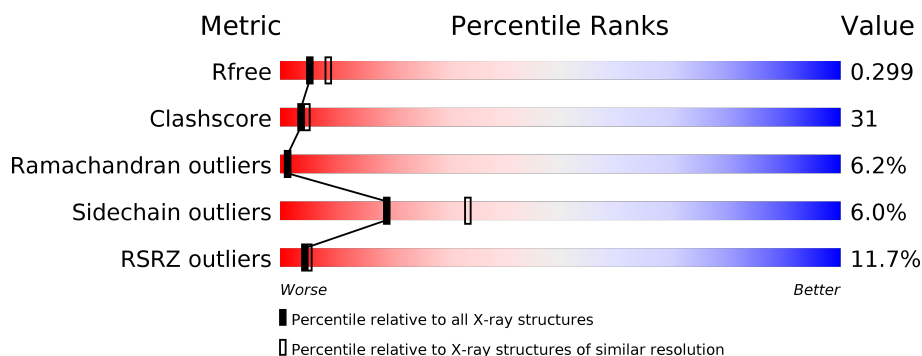
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	394	<div> <div>15%</div> <div>52%</div> <div>42%</div> <div>5%</div> </div>
1	B	394	<div> <div>8%</div> <div>47%</div> <div>47%</div> <div>5%</div> </div>
2	C	4	<div> <div>25%</div> <div>50%</div> <div>25%</div> </div>
2	D	4	<div> <div>25%</div> <div>50%</div> <div>25%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FUC	C	4	X	-	-	-
2	FUC	D	4	X	-	-	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6296 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.

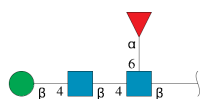
- Molecule 1 is a protein called ENVELOPE GLYCOPROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	394	Total	C	N	O	S	0	0	0
			3062	1931	526	579	26			
1	B	394	Total	C	N	O	S	0	0	0
			3062	1931	526	579	26			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	71	GLU	ASP	conflict	UNP P12823
A	390	ASN	ASP	conflict	UNP P12823
B	71	GLU	ASP	conflict	UNP P12823
B	390	ASN	ASP	conflict	UNP P12823

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	4	Total	C	N	O	0	0	0
			49	28	2	19			
2	D	4	Total	C	N	O	0	0	0
			49	28	2	19			

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

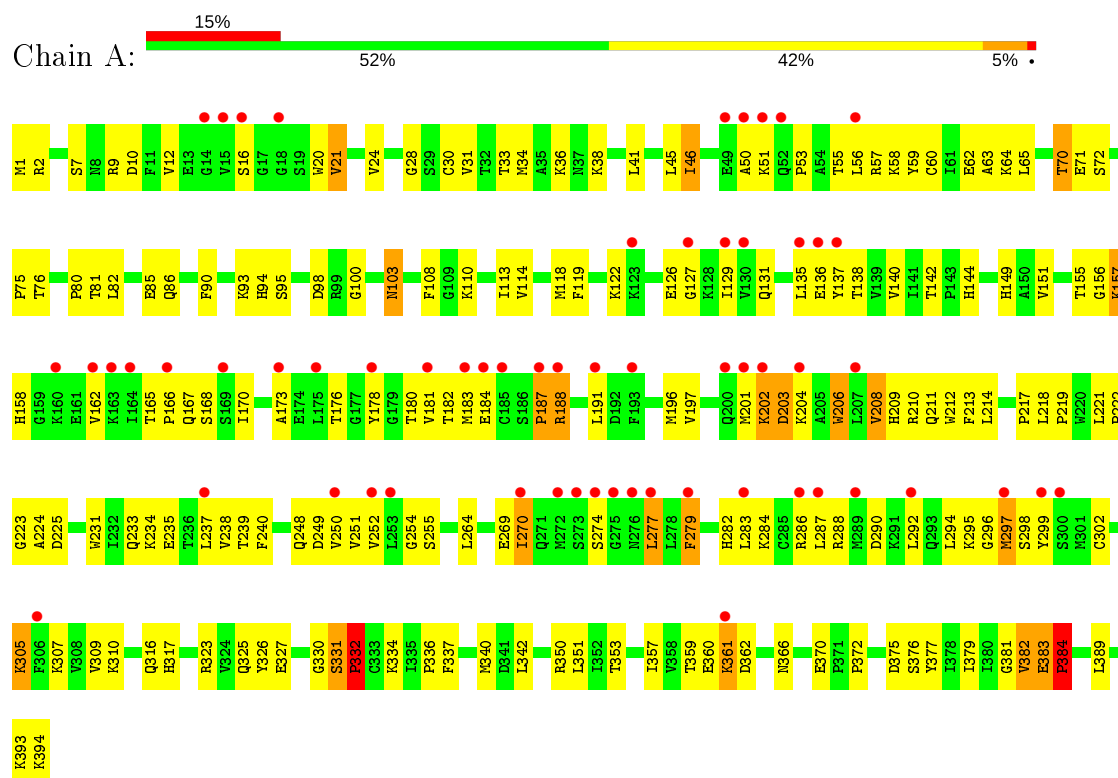
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	20	Total	O	0	0
			20	20		
5	B	25	Total	O	0	0
			25	25		

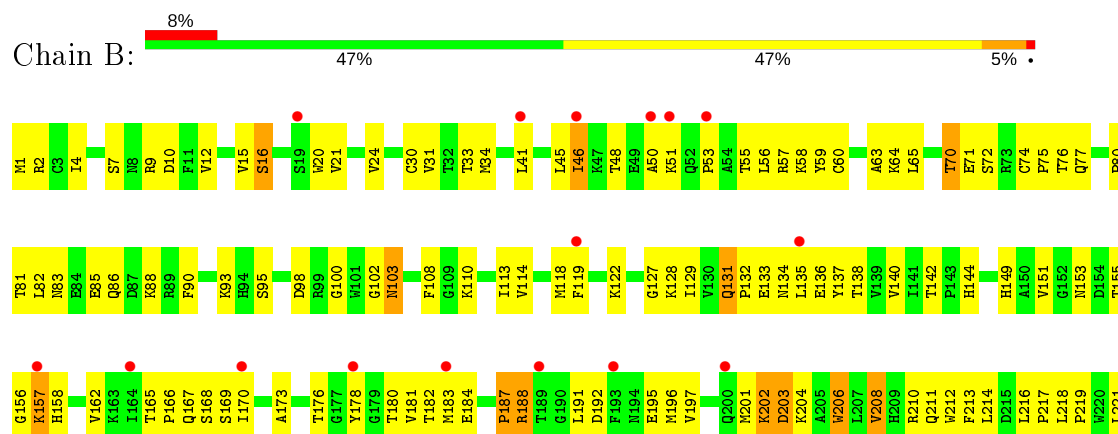
### 3 Residue-property plots

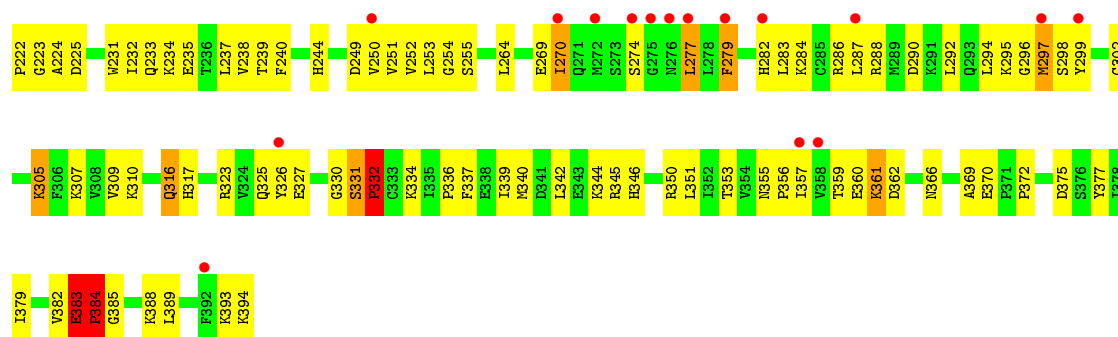
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: ENVELOPE GLYCOPROTEIN



#### • Molecule 1: ENVELOPE GLYCOPROTEIN





- Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C: 



- Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.54Å 81.54Å 288.62Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.10 – 2.75 48.10 – 2.75	Depositor EDS
% Data completeness (in resolution range)	83.2 (48.10-2.75) 83.2 (48.10-2.75)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.15 (at 2.77Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.261 , 0.296 0.265 , 0.299	Depositor DCC
$R_{free}$ test set	1539 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	59.7	Xtriage
Anisotropy	0.262	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 83.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.034 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	6296	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.62% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

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

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

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	0.44	0/3124	0.68	1/4219 (0.0%)
1	B	0.45	0/3124	0.68	1/4219 (0.0%)
All	All	0.44	0/6248	0.68	2/8438 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	384	PRO	CA-N-CD	-6.91	101.83	111.50
1	B	384	PRO	CA-N-CD	-5.65	103.59	111.50

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3062	0	3065	193	0
1	B	3062	0	3065	203	0
2	C	49	0	43	2	0
2	D	49	0	43	2	0
3	A	1	0	0	0	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	20	0	0	4	0
5	B	25	0	0	5	1
All	All	6296	0	6242	390	1

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 31.

All (390) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:GLU:HB3	1:A:384:PRO:HD2	1.43	1.01
1:B:323:ARG:HE	1:B:366:ASN:HD21	1.13	0.96
1:A:323:ARG:HE	1:A:366:ASN:HD21	1.09	0.95
1:B:182:THR:HG22	1:B:288:ARG:HB2	1.56	0.87
1:B:344:LYS:HG3	5:B:2017:HOH:O	1.77	0.85
1:A:182:THR:HG22	1:A:288:ARG:HB2	1.57	0.85
1:A:71:GLU:HG2	1:A:81:THR:H	1.40	0.84
1:B:71:GLU:HG2	1:B:81:THR:H	1.41	0.84
1:A:323:ARG:NE	1:A:366:ASN:HD21	1.75	0.83
1:B:345:ARG:HG2	1:B:346:HIS:CD2	2.17	0.79
1:B:323:ARG:NE	1:B:366:ASN:HD21	1.79	0.79
1:A:383:GLU:HB3	1:A:384:PRO:CD	2.13	0.79
1:A:342:LEU:HA	1:A:377:TYR:CE1	2.18	0.79
1:A:342:LEU:HD23	1:A:377:TYR:CE1	2.17	0.79
1:A:269:GLU:O	1:A:270:ILE:HG13	1.85	0.77
1:A:56:LEU:HD22	1:A:213:PHE:HE2	1.49	0.77
1:A:56:LEU:HD21	1:A:214:LEU:HD21	1.68	0.75
1:A:277:LEU:HB2	1:A:279:PHE:CE1	2.22	0.75
1:B:202:LYS:O	1:B:203:ASP:CG	2.25	0.75
1:A:394:LYS:OXT	1:A:394:LYS:HD3	1.86	0.74
1:B:394:LYS:HD3	1:B:394:LYS:OXT	1.87	0.74
1:B:277:LEU:HB2	1:B:279:PHE:CE1	2.23	0.74
1:B:383:GLU:HB3	1:B:384:PRO:HD2	1.67	0.74
1:B:269:GLU:O	1:B:270:ILE:HG13	1.88	0.74
1:B:56:LEU:HD21	1:B:214:LEU:HD21	1.70	0.73
1:B:56:LEU:HD22	1:B:213:PHE:HE2	1.53	0.73
1:A:305:LYS:H	1:A:305:LYS:NZ	1.86	0.72
1:B:383:GLU:OE1	5:B:2022:HOH:O	2.07	0.72
1:A:305:LYS:HZ2	1:A:305:LYS:H	1.36	0.72
1:A:165:THR:HB	1:A:168:SER:OG	1.89	0.72
1:B:217:PRO:O	1:B:218:LEU:HD23	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:ASP:OD2	1:B:195:GLU:HG2	1.90	0.71
1:B:336:PRO:HG2	1:B:382:VAL:HG23	1.70	0.71
1:B:305:LYS:CE	1:B:305:LYS:H	2.03	0.71
1:A:359:THR:O	1:A:360:GLU:HG3	1.91	0.71
1:B:100:GLY:H	1:B:103:ASN:HD21	1.37	0.71
1:B:296:GLY:C	1:B:298:SER:H	1.94	0.71
1:A:342:LEU:HD23	1:A:377:TYR:HE1	1.54	0.70
1:B:165:THR:HB	1:B:168:SER:OG	1.90	0.70
1:B:155:THR:HG22	1:B:157:LYS:H	1.57	0.70
1:A:20:TRP:HA	1:A:287:LEU:O	1.91	0.70
1:B:240:PHE:CE1	1:B:250:VAL:HG22	2.27	0.69
1:A:98:ASP:OD2	1:B:7:SER:HB2	1.93	0.69
1:B:240:PHE:HE1	1:B:250:VAL:HG22	1.57	0.69
1:B:305:LYS:H	1:B:305:LYS:NZ	1.90	0.69
1:A:305:LYS:H	1:A:305:LYS:CE	2.05	0.69
1:A:155:THR:HG22	1:A:157:LYS:H	1.58	0.69
1:B:20:TRP:HA	1:B:287:LEU:O	1.92	0.68
1:A:100:GLY:H	1:A:103:ASN:HD21	1.39	0.68
1:A:204:LYS:HB3	1:A:206:TRP:CH2	2.28	0.68
1:B:56:LEU:HD23	1:B:56:LEU:C	2.14	0.68
1:B:305:LYS:HE3	1:B:305:LYS:N	2.08	0.67
1:B:206:TRP:H	1:B:206:TRP:HE3	1.43	0.67
1:B:359:THR:O	1:B:360:GLU:HG3	1.94	0.67
1:A:173:ALA:HB3	1:A:181:VAL:HG13	1.77	0.67
1:A:71:GLU:HG3	1:A:80:PRO:HB3	1.75	0.67
1:B:20:TRP:CE3	1:B:286:ARG:HD2	2.30	0.67
1:A:20:TRP:CE3	1:A:286:ARG:HD2	2.31	0.66
1:B:344:LYS:NZ	1:B:344:LYS:HB3	2.10	0.66
1:B:206:TRP:CE3	1:B:206:TRP:N	2.64	0.66
1:B:337:PHE:CD2	1:B:351:LEU:HD21	2.31	0.66
1:B:344:LYS:HE3	1:B:388:LYS:HE3	1.77	0.66
1:B:71:GLU:HG3	1:B:80:PRO:HB3	1.76	0.66
1:B:170:ILE:HG13	1:B:184:GLU:HG3	1.77	0.66
1:A:305:LYS:HE3	1:A:305:LYS:N	2.11	0.65
1:B:305:LYS:H	1:B:305:LYS:HZ2	1.42	0.65
1:A:316:GLN:HE22	1:B:110:LYS:HE2	1.60	0.65
1:A:56:LEU:C	1:A:56:LEU:HD23	2.17	0.65
1:A:296:GLY:C	1:A:298:SER:H	1.99	0.65
1:B:170:ILE:CG1	1:B:184:GLU:HG3	2.27	0.65
1:A:382:VAL:HG22	5:A:2018:HOH:O	1.96	0.64
1:B:82:LEU:O	1:B:85:GLU:HB2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:383:GLU:HB3	1:B:384:PRO:CD	2.27	0.64
1:A:240:PHE:CE1	1:A:250:VAL:HG22	2.32	0.64
1:A:206:TRP:CE3	1:A:206:TRP:N	2.67	0.63
1:B:286:ARG:HE	1:B:288:ARG:HH21	1.44	0.63
1:A:162:VAL:HG11	1:A:183:MET:CE	2.28	0.63
1:B:173:ALA:HB3	1:B:181:VAL:HG13	1.80	0.63
1:B:202:LYS:O	1:B:203:ASP:OD2	2.17	0.63
1:B:162:VAL:HG11	1:B:183:MET:CE	2.29	0.63
1:A:217:PRO:O	1:A:218:LEU:HD23	1.99	0.63
1:B:240:PHE:CE1	1:B:250:VAL:HG13	2.34	0.63
1:B:137:TYR:CD2	1:B:283:LEU:HD22	2.34	0.63
1:A:206:TRP:H	1:A:206:TRP:HE3	1.47	0.63
1:A:286:ARG:HE	1:A:288:ARG:HH21	1.47	0.63
2:C:2:NAG:H4	2:C:3:BMA:O2	1.98	0.62
1:A:376:SER:C	1:A:377:TYR:CD1	2.73	0.62
1:A:383:GLU:CB	1:A:384:PRO:CD	2.77	0.62
1:B:296:GLY:HA3	1:B:299:TYR:CE2	2.34	0.62
1:B:100:GLY:H	1:B:103:ASN:ND2	1.96	0.62
1:B:166:PRO:CG	1:B:187:PRO:HG3	2.30	0.62
1:A:240:PHE:HE1	1:A:250:VAL:HG22	1.65	0.62
1:B:297:MET:HA	1:B:334:LYS:NZ	2.15	0.61
1:A:100:GLY:H	1:A:103:ASN:ND2	1.98	0.61
1:A:24:VAL:HG22	1:A:284:LYS:HG2	1.81	0.61
1:A:127:GLY:HA3	1:A:213:PHE:CZ	2.35	0.61
1:B:127:GLY:HA3	1:B:213:PHE:CZ	2.35	0.61
1:B:24:VAL:HG22	1:B:284:LYS:HG2	1.81	0.61
1:A:170:ILE:CG1	1:A:184:GLU:HG3	2.31	0.61
2:D:2:NAG:H4	2:D:3:BMA:O2	1.99	0.61
1:A:166:PRO:CG	1:A:187:PRO:HG3	2.31	0.61
1:A:221:LEU:HD13	1:A:225:ASP:OD2	2.01	0.60
1:A:137:TYR:CD2	1:A:283:LEU:HD22	2.36	0.60
1:A:270:ILE:HG22	1:A:270:ILE:O	2.02	0.60
1:B:206:TRP:HE3	1:B:206:TRP:N	1.97	0.60
1:A:206:TRP:N	1:A:206:TRP:HE3	1.98	0.60
1:A:340:MET:HG3	1:A:379:ILE:HG13	1.82	0.60
1:A:82:LEU:O	1:A:85:GLU:HB2	2.01	0.60
1:B:204:LYS:HB3	1:B:206:TRP:CH2	2.36	0.60
1:B:182:THR:CG2	1:B:288:ARG:HB2	2.31	0.60
1:B:340:MET:HG3	1:B:379:ILE:HG13	1.84	0.60
1:A:20:TRP:HE3	1:A:286:ARG:HD2	1.67	0.60
1:B:56:LEU:O	1:B:56:LEU:HD23	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:GLU:HG2	1:A:81:THR:N	2.16	0.59
1:B:270:ILE:HG22	1:B:270:ILE:O	2.02	0.59
1:B:191:LEU:HD13	1:B:196:MET:CE	2.33	0.58
1:A:383:GLU:HA	1:A:383:GLU:OE1	2.03	0.58
1:A:182:THR:CG2	1:A:288:ARG:HB2	2.30	0.58
1:A:323:ARG:HE	1:A:366:ASN:ND2	1.91	0.58
1:A:129:ILE:CD1	1:A:210:ARG:HH22	2.16	0.58
1:A:206:TRP:NE1	1:A:264:LEU:HB3	2.18	0.58
1:B:383:GLU:HA	1:B:383:GLU:OE1	2.03	0.57
1:B:221:LEU:HD13	1:B:225:ASP:OD2	2.04	0.57
1:B:20:TRP:HE3	1:B:286:ARG:HD2	1.67	0.57
1:A:55:THR:O	1:A:223:GLY:HA3	2.04	0.57
1:A:297:MET:HA	1:A:334:LYS:NZ	2.19	0.57
1:A:50:ALA:HA	1:A:135:LEU:HD23	1.87	0.57
1:A:34:MET:SD	1:A:350:ARG:NH2	2.78	0.57
1:B:296:GLY:HA3	1:B:299:TYR:CD2	2.40	0.57
1:B:50:ALA:HA	1:B:135:LEU:HD23	1.85	0.57
1:A:56:LEU:HD12	1:A:129:ILE:HD11	1.86	0.57
1:B:221:LEU:CD2	1:B:231:TRP:HA	2.35	0.57
1:A:53:PRO:HB3	1:A:129:ILE:O	2.04	0.56
1:A:65:LEU:HG	1:A:252:VAL:HG22	1.87	0.56
1:A:162:VAL:HG11	1:A:183:MET:HE1	1.87	0.56
1:A:350:ARG:HD3	1:A:370:GLU:OE1	2.05	0.56
1:A:251:VAL:HG21	1:B:204:LYS:HE3	1.86	0.56
1:A:7:SER:HB2	1:B:98:ASP:OD2	2.06	0.56
1:B:55:THR:O	1:B:223:GLY:HA3	2.05	0.56
1:B:162:VAL:HG11	1:B:183:MET:HE3	1.86	0.56
1:B:191:LEU:HD13	1:B:196:MET:HE3	1.88	0.56
1:B:202:LYS:HE2	1:B:202:LYS:HA	1.88	0.56
1:B:307:LYS:HB3	1:B:307:LYS:NZ	2.21	0.56
1:A:296:GLY:HA3	1:A:299:TYR:CE2	2.41	0.56
1:A:383:GLU:HG3	1:A:384:PRO:HD3	1.88	0.56
1:B:286:ARG:NE	1:B:288:ARG:HH21	2.04	0.56
1:B:350:ARG:HD3	1:B:370:GLU:OE1	2.06	0.56
1:B:305:LYS:CE	1:B:305:LYS:N	2.68	0.55
1:A:221:LEU:CD2	1:A:231:TRP:HA	2.37	0.55
1:B:129:ILE:CD1	1:B:210:ARG:HH22	2.18	0.55
1:B:9:ARG:HB3	1:B:317:HIS:CE1	2.41	0.55
1:A:151:VAL:HB	5:A:2009:HOH:O	2.07	0.55
1:B:206:TRP:NE1	1:B:264:LEU:HB3	2.22	0.55
1:B:342:LEU:HD21	1:B:375:ASP:CB	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:LYS:N	1:A:305:LYS:CE	2.68	0.55
1:A:337:PHE:CD2	1:A:351:LEU:HD21	2.41	0.55
1:A:197:VAL:HG23	1:A:210:ARG:HA	1.89	0.54
1:B:197:VAL:HG23	1:B:210:ARG:HA	1.88	0.54
1:A:307:LYS:NZ	1:A:307:LYS:HB3	2.22	0.54
1:A:234:LYS:O	1:A:238:VAL:HG23	2.07	0.54
1:A:240:PHE:CE1	1:A:250:VAL:HG13	2.43	0.54
1:A:165:THR:HB	1:A:168:SER:CB	2.38	0.54
1:A:70:THR:HA	1:A:82:LEU:HD11	1.90	0.54
1:B:53:PRO:HB3	1:B:129:ILE:O	2.07	0.54
1:B:344:LYS:HE3	1:B:388:LYS:CE	2.38	0.54
1:A:1:MET:HG3	1:A:144:HIS:HA	1.90	0.53
1:B:221:LEU:HD21	1:B:231:TRP:HA	1.90	0.53
1:A:286:ARG:NE	1:A:288:ARG:HH21	2.06	0.53
1:A:342:LEU:HD23	1:A:377:TYR:OH	2.09	0.53
1:B:235:GLU:CD	1:B:235:GLU:H	2.12	0.53
1:B:80:PRO:HG2	1:B:113:ILE:CA	2.39	0.53
1:B:65:LEU:HG	1:B:252:VAL:HG22	1.91	0.53
1:B:34:MET:SD	1:B:350:ARG:NH2	2.82	0.53
1:A:155:THR:CG2	1:A:157:LYS:HG3	2.39	0.53
1:B:1:MET:HG3	1:B:144:HIS:HA	1.90	0.53
1:A:235:GLU:H	1:A:235:GLU:CD	2.13	0.52
1:B:56:LEU:HD12	1:B:129:ILE:HD11	1.90	0.52
1:B:165:THR:HB	1:B:168:SER:CB	2.39	0.52
1:A:165:THR:HG22	1:A:167:GLN:H	1.75	0.52
1:B:336:PRO:HG2	1:B:382:VAL:CG2	2.37	0.52
1:A:204:LYS:HE3	1:B:251:VAL:HG21	1.92	0.52
1:B:64:LYS:HB2	1:B:122:LYS:HD2	1.91	0.52
1:A:202:LYS:O	1:A:203:ASP:OD2	2.27	0.52
1:A:75:PRO:O	1:A:76:THR:OG1	2.23	0.52
1:B:90:PHE:CZ	1:B:118:MET:HB2	2.44	0.52
1:B:114:VAL:O	1:B:114:VAL:HG13	2.10	0.52
1:A:64:LYS:HB2	1:A:122:LYS:HD2	1.92	0.51
1:B:155:THR:CG2	1:B:157:LYS:HG3	2.39	0.51
1:B:296:GLY:C	1:B:298:SER:N	2.63	0.51
1:A:80:PRO:HG2	1:A:113:ILE:CA	2.41	0.51
1:A:202:LYS:O	1:A:203:ASP:CG	2.48	0.51
1:A:296:GLY:HA3	1:A:299:TYR:CD2	2.46	0.51
1:B:165:THR:HG22	1:B:167:GLN:H	1.75	0.51
1:B:57:ARG:HG2	1:B:58:LYS:N	2.26	0.51
1:B:331:SER:CB	1:B:332:PRO:CD	2.88	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:LEU:HD21	1:A:231:TRP:HA	1.92	0.51
1:A:381:GLY:HA2	5:A:2018:HOH:O	2.10	0.51
1:B:45:LEU:HD12	1:B:138:THR:O	2.11	0.51
1:B:166:PRO:HG2	1:B:187:PRO:HG3	1.93	0.51
1:B:70:THR:HA	1:B:82:LEU:HD11	1.93	0.51
1:A:170:ILE:HG13	1:A:184:GLU:HG3	1.93	0.51
1:A:166:PRO:HB3	1:A:187:PRO:HD3	1.92	0.51
1:A:56:LEU:O	1:A:56:LEU:HD23	2.11	0.51
1:A:98:ASP:CG	1:B:7:SER:HB2	2.31	0.50
1:B:234:LYS:O	1:B:238:VAL:HG23	2.11	0.50
1:A:166:PRO:HG2	1:A:187:PRO:HG3	1.93	0.50
1:A:28:GLY:HA3	1:B:244:HIS:CD2	2.46	0.50
1:A:342:LEU:HD23	1:A:377:TYR:CZ	2.45	0.50
1:A:191:LEU:HD13	1:A:196:MET:CE	2.41	0.50
1:A:90:PHE:CZ	1:A:118:MET:HB2	2.47	0.50
1:A:239:THR:HB	1:A:251:VAL:CG1	2.42	0.50
1:A:342:LEU:HD21	1:A:375:ASP:CB	2.41	0.50
1:A:80:PRO:HB2	1:A:114:VAL:HG12	1.94	0.50
1:A:9:ARG:HB3	1:A:317:HIS:CE1	2.47	0.50
1:A:45:LEU:HD12	1:A:138:THR:O	2.11	0.50
1:B:71:GLU:HG2	1:B:81:THR:N	2.18	0.50
1:A:100:GLY:HA3	1:A:108:PHE:CD1	2.47	0.50
1:A:114:VAL:HG13	1:A:114:VAL:O	2.12	0.50
1:A:63:ALA:O	1:A:252:VAL:HG11	2.12	0.50
1:B:100:GLY:HA3	1:B:108:PHE:CD1	2.46	0.50
1:B:239:THR:HB	1:B:251:VAL:CG1	2.42	0.50
1:A:219:PRO:HG2	1:A:237:LEU:HD12	1.95	0.49
1:B:170:ILE:N	1:B:170:ILE:HD12	2.28	0.49
1:B:46:ILE:CG1	1:B:140:VAL:HG23	2.43	0.49
1:A:202:LYS:HA	1:A:202:LYS:HE2	1.95	0.48
1:B:166:PRO:HB3	1:B:187:PRO:HD3	1.94	0.48
1:B:173:ALA:O	1:B:180:THR:HG23	2.12	0.48
1:A:277:LEU:HD12	1:A:277:LEU:H	1.79	0.48
1:A:307:LYS:HZ3	1:A:307:LYS:HB3	1.77	0.48
1:A:46:ILE:CG1	1:A:140:VAL:HG23	2.44	0.48
1:B:95:SER:HB3	1:B:113:ILE:CG2	2.43	0.48
1:A:57:ARG:HG2	1:A:58:LYS:N	2.29	0.48
1:B:131:GLN:HG3	1:B:134:ASN:HD22	1.78	0.48
1:B:202:LYS:CA	1:B:202:LYS:HE2	2.44	0.48
1:B:197:VAL:CG2	1:B:210:ARG:HA	2.44	0.48
1:B:46:ILE:HG12	1:B:140:VAL:HG23	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:GLY:C	1:B:225:ASP:H	2.17	0.48
1:A:110:LYS:HE2	1:B:316:GLN:HE22	1.79	0.48
1:A:331:SER:CB	1:A:332:PRO:CD	2.92	0.48
1:B:131:GLN:HB2	1:B:133:GLU:OE1	2.14	0.47
1:B:277:LEU:H	1:B:277:LEU:HD12	1.79	0.47
1:A:173:ALA:HB3	1:A:181:VAL:CG1	2.43	0.47
1:A:309:VAL:CG2	1:A:325:GLN:HB2	2.44	0.47
1:B:233:GLN:HA	1:B:235:GLU:OE2	2.14	0.47
1:A:95:SER:HB3	1:A:113:ILE:CG2	2.44	0.47
1:A:197:VAL:CG2	1:A:210:ARG:HA	2.45	0.47
1:B:201:MET:O	1:B:203:ASP:N	2.47	0.47
1:B:342:LEU:HD21	1:B:375:ASP:HB2	1.95	0.47
1:B:345:ARG:HB2	1:B:345:ARG:NH1	2.29	0.47
1:B:251:VAL:HG22	1:B:252:VAL:N	2.30	0.47
1:A:56:LEU:HB2	1:A:129:ILE:HG13	1.97	0.47
1:A:223:GLY:C	1:A:225:ASP:H	2.17	0.47
1:B:309:VAL:CG2	1:B:325:GLN:HB2	2.44	0.47
1:B:383:GLU:O	1:B:385:GLY:N	2.48	0.47
1:A:51:LYS:HE3	1:A:136:GLU:HB2	1.96	0.47
1:A:204:LYS:HB3	1:A:206:TRP:CZ3	2.49	0.47
1:A:233:GLN:HA	1:A:235:GLU:OE2	2.14	0.47
1:B:51:LYS:HE3	1:B:136:GLU:HB2	1.96	0.47
1:A:309:VAL:HG21	1:A:325:GLN:HB2	1.97	0.47
1:A:208:VAL:HG21	1:A:212:TRP:CZ3	2.50	0.46
1:A:296:GLY:C	1:A:298:SER:N	2.68	0.46
1:A:342:LEU:HD21	1:A:375:ASP:HB2	1.97	0.46
1:A:377:TYR:CD1	1:A:377:TYR:N	2.83	0.46
1:B:72:SER:HB3	1:B:113:ILE:HG13	1.96	0.46
1:B:372:PRO:O	5:B:2020:HOH:O	2.21	0.46
1:B:56:LEU:CD2	1:B:56:LEU:C	2.82	0.46
1:A:155:THR:HG22	1:A:157:LYS:HG3	1.96	0.46
1:B:155:THR:HG22	1:B:157:LYS:HG3	1.98	0.46
1:A:119:PHE:CB	1:A:234:LYS:HD2	2.45	0.46
1:B:65:LEU:HD11	1:B:238:VAL:HG13	1.98	0.46
1:B:57:ARG:CG	1:B:58:LYS:N	2.79	0.46
1:B:83:ASN:ND2	5:B:2003:HOH:O	2.47	0.46
1:A:208:VAL:HG21	1:A:212:TRP:HZ3	1.81	0.46
1:B:309:VAL:HG21	1:B:325:GLN:HB2	1.98	0.46
1:A:239:THR:HB	1:A:251:VAL:HG12	1.98	0.46
1:A:360:GLU:O	1:A:362:ASP:N	2.49	0.46
1:B:60:CYS:HB2	1:B:231:TRP:CZ3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:CYS:HB2	1:A:231:TRP:CZ3	2.51	0.45
1:B:221:LEU:HG	1:B:231:TRP:CE3	2.51	0.45
1:A:170:ILE:HG12	1:A:184:GLU:HG3	1.98	0.45
1:B:119:PHE:CB	1:B:234:LYS:HD2	2.45	0.45
1:A:173:ALA:O	1:A:180:THR:HG23	2.15	0.45
1:A:206:TRP:CD1	1:A:264:LEU:HB3	2.50	0.45
1:A:296:GLY:O	1:A:299:TYR:HD2	2.00	0.45
1:B:173:ALA:HB3	1:B:181:VAL:CG1	2.46	0.45
1:A:310:LYS:HB3	1:A:323:ARG:HB3	1.97	0.45
1:B:63:ALA:O	1:B:252:VAL:HG11	2.17	0.45
1:A:201:MET:O	1:A:203:ASP:N	2.50	0.45
1:B:323:ARG:HE	1:B:366:ASN:ND2	1.96	0.45
1:B:339:ILE:HA	1:B:377:TYR:O	2.17	0.45
1:A:251:VAL:HG22	1:A:252:VAL:N	2.32	0.45
1:A:36:LYS:O	1:A:38:LYS:HG2	2.17	0.45
1:A:65:LEU:HD11	1:A:238:VAL:HG13	1.99	0.45
1:B:208:VAL:HG21	1:B:212:TRP:HZ3	1.82	0.45
1:A:302:CYS:HB3	1:A:326:TYR:CZ	2.52	0.44
1:A:95:SER:HB2	1:A:248:GLN:NE2	2.32	0.44
1:B:41:LEU:HD11	1:B:292:LEU:HD11	1.99	0.44
1:B:208:VAL:HG21	1:B:212:TRP:CZ3	2.52	0.44
1:A:296:GLY:O	1:A:299:TYR:CD2	2.70	0.44
1:A:336:PRO:HG2	5:A:2018:HOH:O	2.17	0.44
1:B:7:SER:O	1:B:317:HIS:CE1	2.71	0.44
1:B:372:PRO:O	1:B:393:LYS:HB3	2.18	0.44
1:B:219:PRO:HG2	1:B:237:LEU:HD12	2.00	0.44
1:B:240:PHE:HA	1:B:249:ASP:O	2.18	0.44
1:A:302:CYS:SG	1:A:334:LYS:O	2.75	0.44
1:B:178:TYR:CE1	1:B:295:LYS:HE3	2.52	0.44
1:B:239:THR:HB	1:B:251:VAL:HG12	1.99	0.43
1:B:377:TYR:HB3	1:B:379:ILE:HD11	2.00	0.43
1:A:56:LEU:C	1:A:56:LEU:CD2	2.85	0.43
1:A:62:GLU:HG2	1:A:122:LYS:HB2	2.01	0.43
1:A:334:LYS:HG2	1:A:357:ILE:HG22	2.00	0.43
1:A:46:ILE:HG12	1:A:140:VAL:HG23	2.01	0.43
1:A:210:ARG:O	1:A:213:PHE:HB3	2.19	0.43
1:A:353:THR:O	1:A:353:THR:HG22	2.19	0.43
1:A:72:SER:HB3	1:A:113:ILE:HG13	2.01	0.43
1:A:221:LEU:HG	1:A:231:TRP:CE3	2.54	0.43
1:A:12:VAL:O	1:A:33:THR:HA	2.18	0.43
1:B:12:VAL:O	1:B:33:THR:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:VAL:HB	5:B:2010:HOH:O	2.18	0.43
1:B:80:PRO:HB2	1:B:114:VAL:HG12	2.00	0.43
1:B:59:TYR:CD1	1:B:218:LEU:HB2	2.53	0.43
1:B:344:LYS:HB3	1:B:344:LYS:HZ3	1.83	0.42
1:A:41:LEU:HD11	1:A:292:LEU:HD11	2.00	0.42
1:A:10:ASP:O	1:A:31:VAL:HA	2.18	0.42
1:A:327:GLU:O	1:A:361:LYS:HE3	2.19	0.42
1:B:10:ASP:O	1:B:31:VAL:HA	2.19	0.42
1:B:383:GLU:CB	1:B:384:PRO:CD	2.96	0.42
1:B:302:CYS:HB3	1:B:326:TYR:CZ	2.54	0.42
1:B:310:LYS:HB3	1:B:323:ARG:HB3	2.00	0.42
1:B:331:SER:HB2	1:B:332:PRO:CD	2.49	0.42
1:B:360:GLU:O	1:B:362:ASP:N	2.52	0.42
1:B:74:CYS:HB2	1:B:77:GLN:HG3	2.01	0.42
1:A:222:PRO:O	1:A:225:ASP:HB2	2.20	0.42
1:B:355:ASN:N	1:B:356:PRO:HD3	2.34	0.42
1:B:75:PRO:O	1:B:76:THR:OG1	2.28	0.42
1:A:206:TRP:CD2	1:A:264:LEU:HD13	2.55	0.42
1:A:269:GLU:C	1:A:270:ILE:HG13	2.40	0.42
1:A:178:TYR:CE1	1:A:295:LYS:HE3	2.54	0.42
1:A:57:ARG:CG	1:A:58:LYS:N	2.83	0.42
1:A:85:GLU:OE1	1:A:94:HIS:NE2	2.31	0.42
1:A:188:ARG:CZ	1:A:284:LYS:HD2	2.50	0.42
1:B:296:GLY:O	1:B:299:TYR:HD2	2.03	0.42
1:B:339:ILE:HD11	1:B:369:ALA:HB1	2.02	0.42
1:B:56:LEU:HB2	1:B:129:ILE:HG13	2.02	0.42
1:B:57:ARG:CG	1:B:58:LYS:H	2.32	0.42
1:A:59:TYR:CD1	1:A:218:LEU:HB2	2.55	0.42
1:B:331:SER:CB	1:B:332:PRO:HD2	2.49	0.42
1:B:327:GLU:O	1:B:361:LYS:HE3	2.20	0.42
1:A:12:VAL:HG12	1:A:21:VAL:HG11	2.01	0.41
1:A:119:PHE:HB3	1:A:234:LYS:HD2	2.02	0.41
1:B:149:HIS:O	1:B:153:ASN:HB2	2.20	0.41
1:B:156:GLY:C	1:B:158:HIS:H	2.24	0.41
1:B:188:ARG:CZ	1:B:284:LYS:HD2	2.50	0.41
1:A:170:ILE:HD12	1:A:170:ILE:N	2.36	0.41
1:B:119:PHE:HB3	1:B:234:LYS:HD2	2.02	0.41
1:B:307:LYS:HB3	1:B:307:LYS:HZ3	1.84	0.41
1:B:334:LYS:HG2	1:B:357:ILE:HG22	2.03	0.41
1:B:149:HIS:HB3	2:D:1:NAG:H2	2.01	0.41
1:A:156:GLY:C	1:A:158:HIS:H	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:SER:C	1:B:170:ILE:HD12	2.41	0.41
1:B:206:TRP:CD1	1:B:264:LEU:HB3	2.56	0.41
1:B:232:ILE:HG22	1:B:233:GLN:HG3	2.02	0.41
1:B:48:THR:O	1:B:279:PHE:CE1	2.73	0.41
1:B:210:ARG:O	1:B:213:PHE:HB3	2.20	0.41
1:B:238:VAL:CG1	1:B:250:VAL:HG12	2.51	0.41
1:B:296:GLY:O	1:B:299:TYR:CD2	2.74	0.41
1:A:202:LYS:CA	1:A:202:LYS:HE2	2.51	0.41
1:A:240:PHE:HA	1:A:249:ASP:O	2.21	0.41
1:A:331:SER:CB	1:A:332:PRO:HD2	2.51	0.41
1:A:359:THR:O	1:A:360:GLU:CG	2.65	0.41
1:B:206:TRP:CD2	1:B:264:LEU:HD13	2.56	0.41
1:A:173:ALA:O	1:A:180:THR:HA	2.21	0.41
1:A:372:PRO:O	1:A:393:LYS:HB3	2.21	0.41
1:B:213:PHE:O	1:B:216:LEU:HG	2.20	0.41
1:B:253:LEU:HD12	1:B:253:LEU:HA	1.96	0.41
1:B:184:GLU:HB3	1:B:286:ARG:HB3	2.02	0.41
1:B:15:VAL:O	1:B:16:SER:C	2.59	0.40
1:A:191:LEU:HD13	1:A:196:MET:HE3	2.03	0.40
1:A:51:LYS:HE3	1:A:136:GLU:CB	2.51	0.40
1:B:131:GLN:O	1:B:132:PRO:C	2.60	0.40
1:B:191:LEU:HD22	1:B:196:MET:HE2	2.03	0.40
1:B:128:LYS:O	1:B:197:VAL:HG13	2.21	0.40
1:A:129:ILE:HD11	1:A:210:ARG:HH22	1.84	0.40
1:B:269:GLU:C	1:B:270:ILE:HG13	2.42	0.40
1:A:100:GLY:N	1:A:103:ASN:HD21	2.14	0.40
1:A:149:HIS:HB3	2:C:1:NAG:H2	2.03	0.40
1:A:188:ARG:HH11	1:A:188:ARG:HB2	1.86	0.40
1:A:221:LEU:HD23	1:A:231:TRP:HA	2.04	0.40
1:B:222:PRO:O	1:B:225:ASP:HB2	2.22	0.40
1:B:353:THR:O	1:B:353:THR:HG22	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:2003:HOH:O	5:B:2003:HOH:O[6_555]	1.99	0.21

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	A	392/394 (100%)	321 (82%)	48 (12%)	23 (6%)	<b>1</b>	<b>1</b>
1	B	392/394 (100%)	318 (81%)	48 (12%)	26 (7%)	<b>1</b>	<b>1</b>
All	All	784/788 (100%)	639 (82%)	96 (12%)	49 (6%)	<b>1</b>	<b>1</b>

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	176	THR
1	A	187	PRO
1	A	202	LYS
1	A	383	GLU
1	B	176	THR
1	B	187	PRO
1	B	202	LYS
1	B	383	GLU
1	A	16	SER
1	A	203	ASP
1	A	224	ALA
1	A	254	GLY
1	A	270	ILE
1	A	279	PHE
1	A	330	GLY
1	A	331	SER
1	A	361	LYS
1	B	16	SER
1	B	203	ASP
1	B	224	ALA
1	B	254	GLY
1	B	270	ILE
1	B	279	PHE
1	B	330	GLY
1	B	331	SER

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Mol	Chain	Res	Type
1	A	274	SER
1	A	282	HIS
1	A	332	PRO
1	A	384	PRO
1	B	274	SER
1	B	282	HIS
1	B	332	PRO
1	B	361	LYS
1	B	384	PRO
1	A	157	LYS
1	A	255	SER
1	A	294	LEU
1	B	46	ILE
1	B	157	LYS
1	B	294	LEU
1	B	297	MET
1	A	46	ILE
1	A	297	MET
1	B	88	LYS
1	A	126	GLU
1	B	255	SER
1	B	316	GLN
1	B	102	GLY
1	B	4	ILE

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	A	342/342 (100%)	321 (94%)	21 (6%)	18	33
1	B	342/342 (100%)	322 (94%)	20 (6%)	20	35
All	All	684/684 (100%)	643 (94%)	41 (6%)	19	33

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	21	VAL
1	A	30	CYS
1	A	70	THR
1	A	86	GLN
1	A	93	LYS
1	A	103	ASN
1	A	131	GLN
1	A	142	THR
1	A	188	ARG
1	A	206	TRP
1	A	208	VAL
1	A	209	HIS
1	A	211	GLN
1	A	277	LEU
1	A	290	ASP
1	A	305	LYS
1	A	332	PRO
1	A	382	VAL
1	A	384	PRO
1	A	389	LEU
1	B	2	ARG
1	B	21	VAL
1	B	30	CYS
1	B	70	THR
1	B	86	GLN
1	B	93	LYS
1	B	103	ASN
1	B	131	GLN
1	B	142	THR
1	B	188	ARG
1	B	206	TRP
1	B	208	VAL
1	B	211	GLN
1	B	277	LEU
1	B	290	ASP
1	B	305	LYS
1	B	332	PRO
1	B	383	GLU
1	B	384	PRO
1	B	389	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	GLN
1	A	86	GLN
1	A	103	ASN
1	A	131	GLN
1	A	149	HIS
1	A	200	GLN
1	A	244	HIS
1	A	248	GLN
1	A	256	GLN
1	A	316	GLN
1	A	366	ASN
1	B	77	GLN
1	B	83	ASN
1	B	86	GLN
1	B	103	ASN
1	B	131	GLN
1	B	134	ASN
1	B	149	HIS
1	B	200	GLN
1	B	244	HIS
1	B	248	GLN
1	B	316	GLN
1	B	317	HIS
1	B	366	ASN

### 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 ⓘ

8 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	C	1	1,2	14,14,15	0.68	0	17,19,21	0.67	0
2	NAG	C	2	2	14,14,15	0.74	0	17,19,21	1.00	1 (5%)
2	BMA	C	3	2	11,11,12	0.59	0	15,15,17	0.40	0
2	FUC	C	4	2	10,10,11	0.41	0	14,14,16	0.40	0
2	NAG	D	1	1,2	14,14,15	0.61	0	17,19,21	0.63	0
2	NAG	D	2	2	14,14,15	0.77	0	17,19,21	1.01	1 (5%)
2	BMA	D	3	2	11,11,12	0.64	0	15,15,17	0.39	0
2	FUC	D	4	2	10,10,11	0.47	0	14,14,16	0.44	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
2	NAG	C	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	BMA	C	3	2	-	2/2/19/22	0/1/1/1
2	FUC	C	4	2	1/1/4/5	-	0/1/1/1
2	NAG	D	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	BMA	D	3	2	-	2/2/19/22	0/1/1/1
2	FUC	D	4	2	1/1/4/5	-	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(°)	Ideal(°)
2	C	2	NAG	C4-C3-C2	2.54	114.73	111.02
2	D	2	NAG	C4-C3-C2	2.45	114.61	111.02

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	4	FUC	C1
2	D	4	FUC	C1



All (16) torsion outliers are listed below:

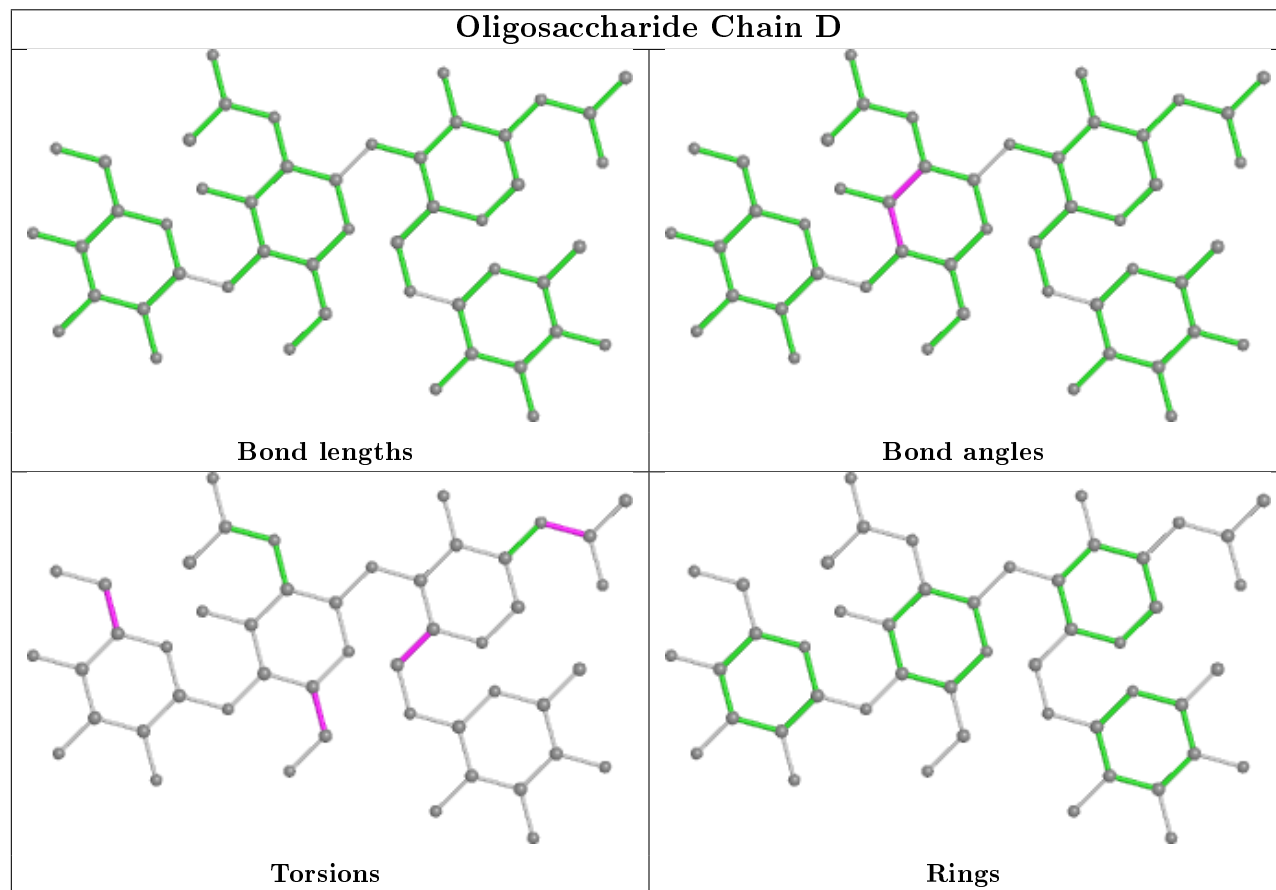
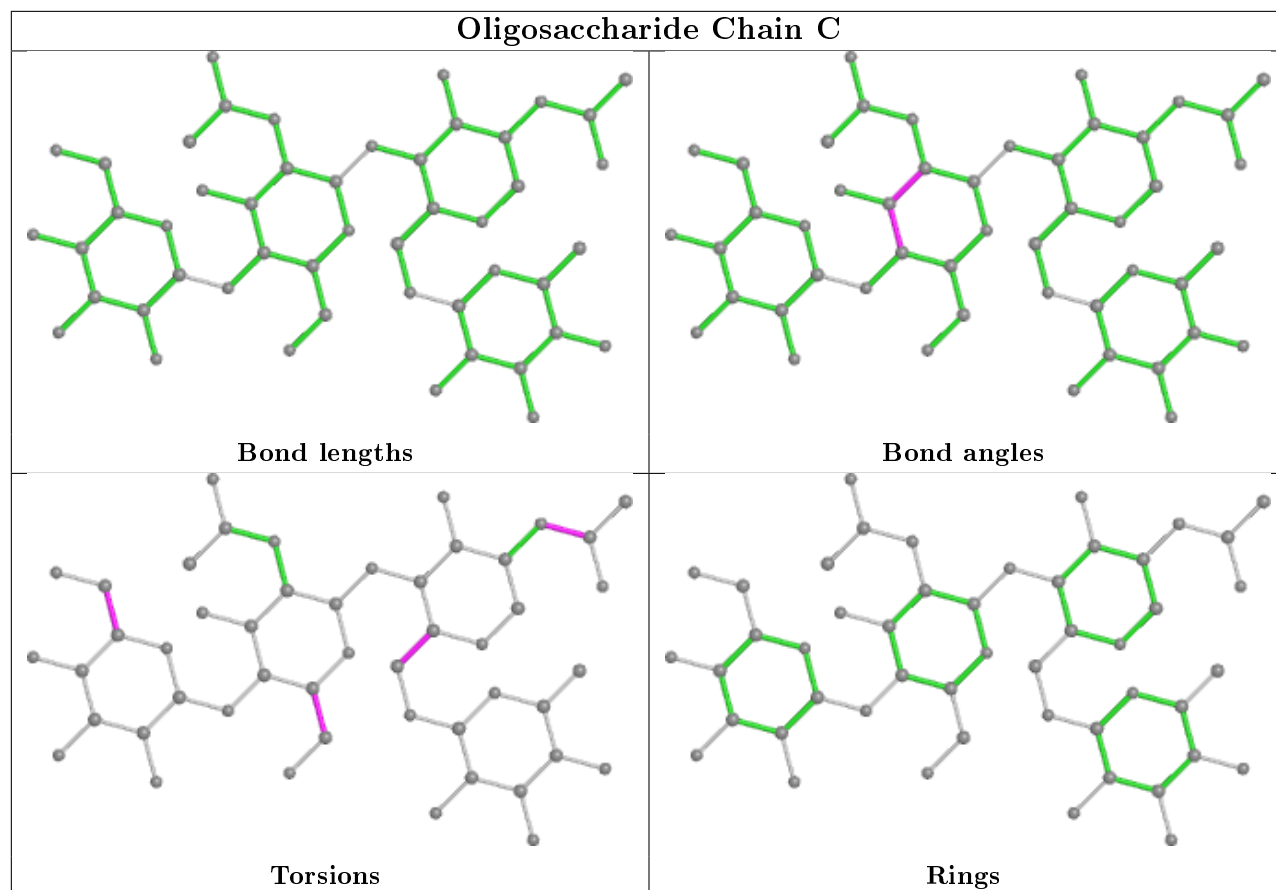
Mol	Chain	Res	Type	Atoms
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	C	2	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	C	3	BMA	O5-C5-C6-O6
2	D	3	BMA	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	D	3	BMA	C4-C5-C6-O6
2	C	3	BMA	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	NAG	1	0
2	C	3	BMA	1	0
2	D	1	NAG	1	0
2	C	1	NAG	1	0
2	D	2	NAG	1	0
2	D	3	BMA	1	0

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



## 5.6 Ligand geometry

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	A	1396	1	14,14,15	0.81	1 (7%)	17,19,21	0.60	0
4	NAG	B	1395	1	14,14,15	0.68	0	17,19,21	0.62	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
4	NAG	A	1396	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1395	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1396	NAG	C1-C2	2.00	1.55	1.52

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	394/394 (100%)	0.83	60 (15%) <b>2</b> <b>2</b>	29, 73, 131, 149	0
1	B	394/394 (100%)	0.65	32 (8%) <b>12</b> <b>14</b>	24, 69, 116, 149	0
All	All	788/788 (100%)	0.74	92 (11%) <b>4</b> <b>5</b>	24, 71, 126, 149	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	276	ASN	7.0
1	B	272	MET	6.8
1	B	50	ALA	5.7
1	A	14	GLY	5.6
1	B	276	ASN	5.5
1	A	162	VAL	5.1
1	B	275	GLY	5.1
1	A	51	LYS	5.0
1	A	164	ILE	4.8
1	A	200	GLN	4.7
1	A	275	GLY	4.5
1	A	297	MET	4.2
1	A	50	ALA	4.2
1	A	137	TYR	3.9
1	B	157	LYS	3.8
1	A	183	MET	3.7
1	B	297	MET	3.7
1	A	279	PHE	3.7
1	B	193	PHE	3.7
1	A	191	LEU	3.5
1	B	183	MET	3.5
1	A	16	SER	3.4
1	A	277	LEU	3.4
1	A	178	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	135	LEU	3.4
1	B	299	TYR	3.3
1	A	15	VAL	3.3
1	A	173	ALA	3.2
1	A	130	VAL	3.2
1	B	274	SER	3.2
1	B	282	HIS	3.1
1	B	119	PHE	3.1
1	A	163	LYS	3.0
1	A	289	MET	3.0
1	A	52	GLN	3.0
1	A	272	MET	2.9
1	A	274	SER	2.9
1	B	135	LEU	2.9
1	B	19	SER	2.9
1	B	164	ILE	2.9
1	B	326	TYR	2.9
1	A	286	ARG	2.8
1	B	200	GLN	2.8
1	A	202	LYS	2.8
1	A	270	ILE	2.8
1	A	253	LEU	2.8
1	A	185	CYS	2.8
1	B	392	PHE	2.7
1	A	127	GLY	2.7
1	A	18	GLY	2.6
1	A	193	PHE	2.6
1	A	181	VAL	2.6
1	B	189	THR	2.6
1	A	292	LEU	2.6
1	A	273	SER	2.5
1	A	166	PRO	2.5
1	B	170	ILE	2.5
1	B	279	PHE	2.5
1	A	123	LYS	2.4
1	A	188	ARG	2.4
1	A	204	LYS	2.4
1	A	136	GLU	2.4
1	A	207	LEU	2.4
1	A	56	LEU	2.4
1	A	237	LEU	2.4
1	A	299	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	129	ILE	2.3
1	A	175	LEU	2.3
1	B	250	VAL	2.3
1	A	187	PRO	2.3
1	A	306	PHE	2.3
1	B	53	PRO	2.2
1	A	250	VAL	2.2
1	A	283	LEU	2.2
1	B	51	LYS	2.2
1	B	358	VAL	2.2
1	B	287	LEU	2.2
1	B	178	TYR	2.2
1	A	160	LYS	2.1
1	B	357	ILE	2.1
1	B	41	LEU	2.1
1	A	49	GLU	2.1
1	A	361	LYS	2.1
1	B	46	ILE	2.1
1	A	184	GLU	2.1
1	B	270	ILE	2.1
1	A	169	SER	2.1
1	A	252	VAL	2.0
1	A	201	MET	2.0
1	A	300	SER	2.0
1	A	287	LEU	2.0
1	B	277	LEU	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<sup>th</sup> 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.

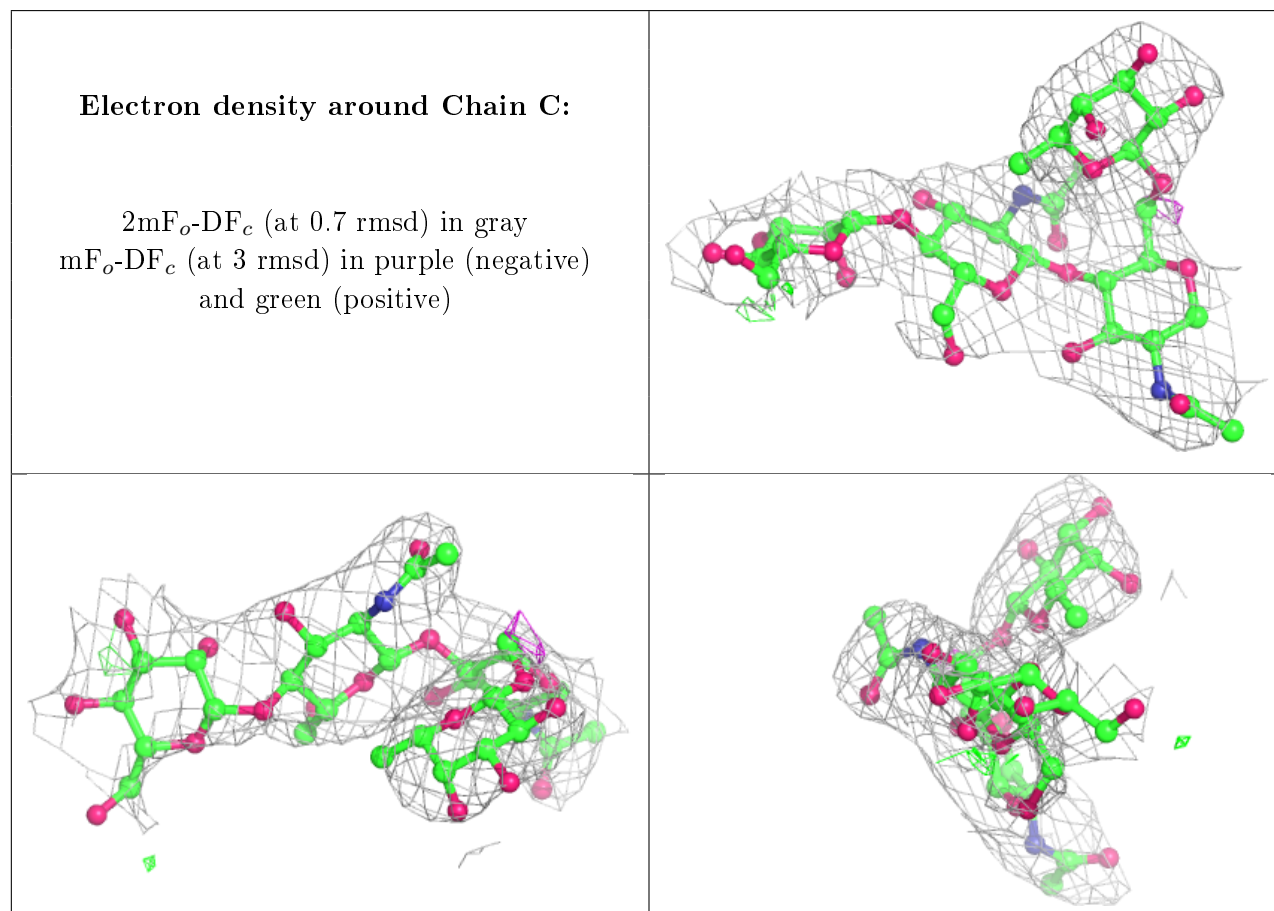
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	BMA	C	3	11/12	0.50	0.20	124,127,129,131	0
2	BMA	D	3	11/12	0.68	0.17	108,121,127,129	0

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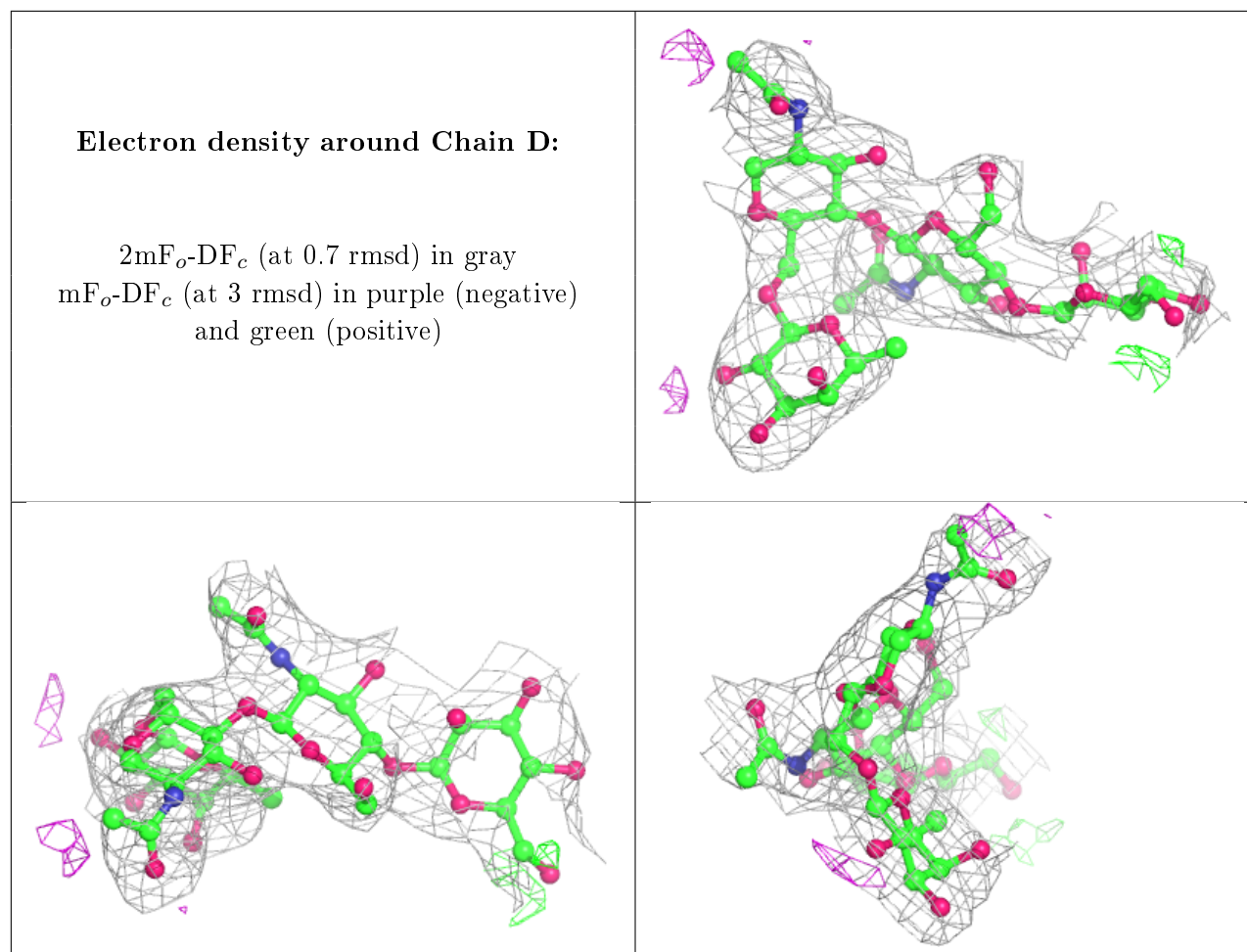
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	C	1	14/15	0.87	0.26	75,81,89,90	0
2	NAG	D	2	14/15	0.90	0.18	58,80,95,105	0
2	NAG	C	2	14/15	0.91	0.18	82,94,105,119	0
2	FUC	D	4	10/11	0.94	0.21	63,71,77,81	0
2	NAG	D	1	14/15	0.95	0.20	45,67,72,74	0
2	FUC	C	4	10/11	0.95	0.22	70,75,78,88	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.







## 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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
4	NAG	A	1396	14/15	0.82	0.16	88,98,103,104	0
4	NAG	B	1395	14/15	0.84	0.14	74,91,101,105	0
3	NA	A	1395	1/1	0.97	0.33	12,12,12,12	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.