



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2023 – 01:32 PM EDT

PDB ID : 7RKU  
Title : Structure of the SARS-CoV-2 receptor binding domain in complex with the human neutralizing antibody Fab fragment, C022  
Authors : Jette, C.A.; Bjorkman, P.J.; Barnes, C.O.  
Deposited on : 2021-07-22  
Resolution : 3.20 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.

The types of validation reports are described at

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

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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 : 2.35.1  
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

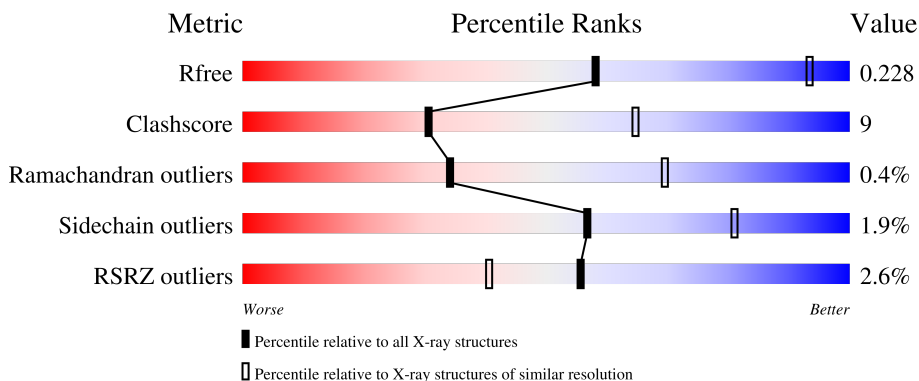
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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  $\geq 3$ , 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	212	75% 17% • 8%
1	B	212	73% 19% 8%
1	C	212	2% 74% 17% • 8%
1	D	212	72% 18% • 8%
2	E	240	72% 24% •

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Mol	Chain	Length	Quality of chain
2	G	240	<p>6% 64% 29% 7%</p>
2	H	240	<p>73% 22%</p>
2	J	240	<p>5% 68% 26% 6%</p>
3	F	215	<p>78% 20%</p>
3	I	215	<p>7% 78% 21%</p>
3	K	215	<p>7% 75% 23%</p>
3	L	215	<p>82% 16%</p>
4	M	3	<p>67% 33%</p>
4	N	3	<p>33% 67%</p>

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 19802 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 Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	196	1552	995	259	290	8	0	0	0
1	B	196	1552	995	259	290	8	0	0	0
1	C	195	1541	988	257	288	8	0	0	0
1	D	194	1536	985	256	287	8	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	534	HIS	-	expression tag	UNP P0DTC2
A	535	HIS	-	expression tag	UNP P0DTC2
A	536	HIS	-	expression tag	UNP P0DTC2
A	537	HIS	-	expression tag	UNP P0DTC2
A	538	HIS	-	expression tag	UNP P0DTC2
A	539	HIS	-	expression tag	UNP P0DTC2
B	534	HIS	-	expression tag	UNP P0DTC2
B	535	HIS	-	expression tag	UNP P0DTC2
B	536	HIS	-	expression tag	UNP P0DTC2
B	537	HIS	-	expression tag	UNP P0DTC2
B	538	HIS	-	expression tag	UNP P0DTC2
B	539	HIS	-	expression tag	UNP P0DTC2
C	534	HIS	-	expression tag	UNP P0DTC2
C	535	HIS	-	expression tag	UNP P0DTC2
C	536	HIS	-	expression tag	UNP P0DTC2
C	537	HIS	-	expression tag	UNP P0DTC2
C	538	HIS	-	expression tag	UNP P0DTC2
C	539	HIS	-	expression tag	UNP P0DTC2
D	534	HIS	-	expression tag	UNP P0DTC2
D	535	HIS	-	expression tag	UNP P0DTC2
D	536	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	537	HIS	-	expression tag	UNP P0DTC2
D	538	HIS	-	expression tag	UNP P0DTC2
D	539	HIS	-	expression tag	UNP P0DTC2

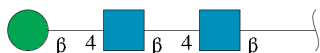
- Molecule 2 is a protein called C022 Antibody Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	E	231	Total	C	N	O	S	0	0	0
			1747	1112	288	343	4			
2	G	223	Total	C	N	O	S	0	0	0
			1692	1081	278	329	4			
2	H	231	Total	C	N	O	S	0	0	0
			1746	1111	288	343	4			
2	J	225	Total	C	N	O	S	0	0	0
			1703	1087	280	332	4			

- Molecule 3 is a protein called C022 Antibody Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	F	213	Total	C	N	O	S	0	2	0
			1654	1038	274	336	6			
3	I	214	Total	C	N	O	S	0	2	0
			1660	1041	275	337	7			
3	K	214	Total	C	N	O	S	0	2	0
			1659	1040	275	337	7			
3	L	213	Total	C	N	O	S	0	2	0
			1654	1038	274	336	6			

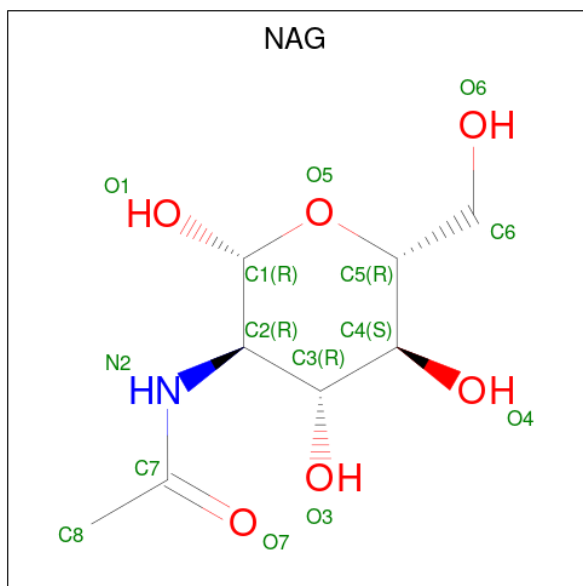
- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:

C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



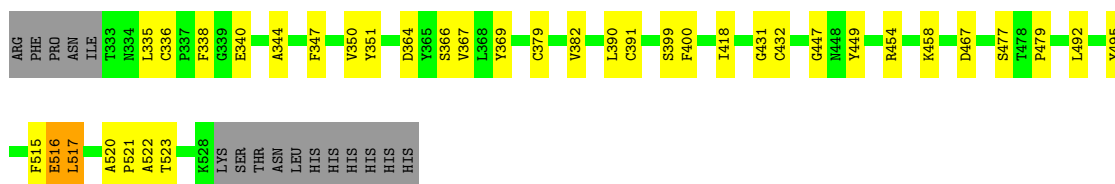
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	C	1	14	8	1	5	0	0
5	D	1	14	8	1	5	0	0

### 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.

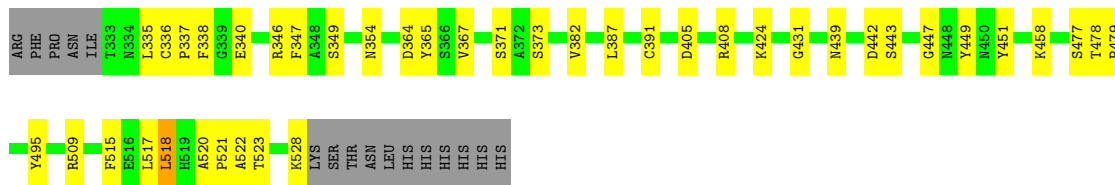
- Molecule 1: Spike protein S1

Chain A: 




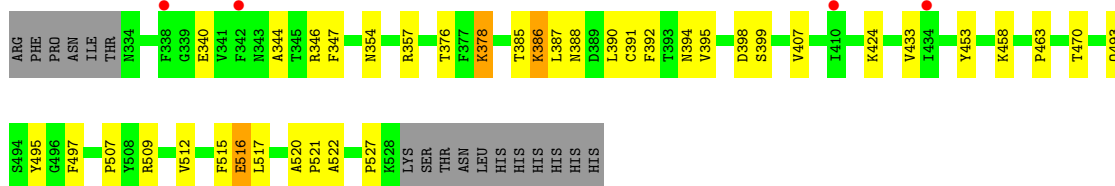
- Molecule 1: Spike protein S1

Chain B: 



- Molecule 1: Spike protein S1

Chain C: 



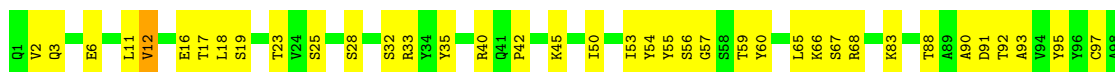
- Molecule 1: Spike protein S1

Chain D: 

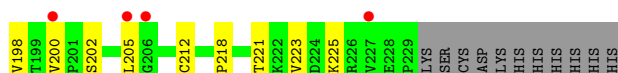
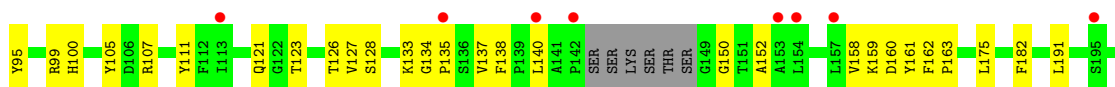




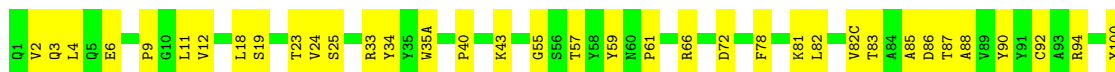
• Molecule 2: C022 Antibody Fab Heavy Chain



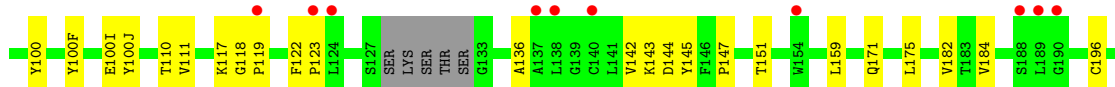
• Molecule 2: C022 Antibody Fab Heavy Chain



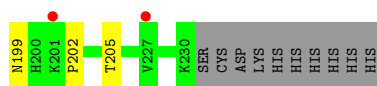
• Molecule 2: C022 Antibody Fab Heavy Chain



• Molecule 2: C022 Antibody Fab Heavy Chain







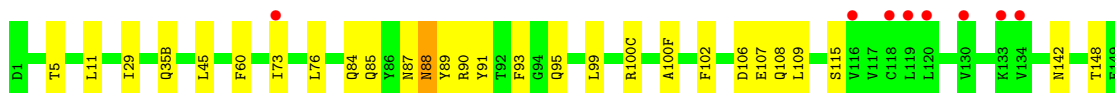
- Molecule 3: C022 Antibody Fab Light Chain

Chain F: 78% 20% ..



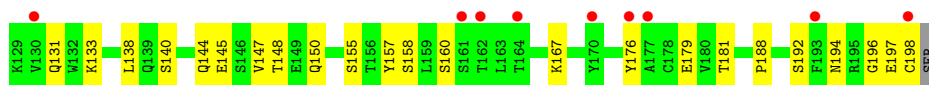
- Molecule 3: C022 Antibody Fab Light Chain

Chain I: 7% 78% 21%



- Molecule 3: C022 Antibody Fab Light Chain

Chain K: 7% 75% 23%



- Molecule 3: C022 Antibody Fab Light Chain

Chain L: % 82% 16% ..




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

Chain M:  67% 33%

MAG1  
MAG2  
BMA3

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

Chain N:  33% 67%

MAG1  
MAG2  
BMA3

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	178.38Å 178.38Å 247.32Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.60 – 3.20 44.60 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.6 (44.60-3.20) 99.6 (44.60-3.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.06 (at 3.19Å)	Xtrriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, $R_{free}$	0.188 , 0.231 0.187 , 0.228	Depositor DCC
$R_{free}$ test set	3595 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	125.1	Xtrriage
Anisotropy	0.000	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 95.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.449 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	19802	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	124.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% 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: BMA, 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	0.62	2/1596 (0.1%)	0.74	1/2172 (0.0%)
1	B	0.57	0/1596	0.77	4/2172 (0.2%)
1	C	0.60	0/1585	0.71	1/2158 (0.0%)
1	D	0.60	0/1580	0.72	1/2151 (0.0%)
2	E	0.54	0/1796	0.75	0/2453
2	G	0.54	0/1740	0.74	1/2378 (0.0%)
2	H	0.53	0/1795	0.76	1/2451 (0.0%)
2	J	0.51	0/1751	0.74	0/2393
3	F	0.54	0/1696	0.71	0/2302
3	I	0.55	0/1702	0.74	0/2310
3	K	0.56	0/1701	0.73	0/2308
3	L	0.54	0/1696	0.74	1/2302 (0.0%)
All	All	0.56	2/20234 (0.0%)	0.74	10/27550 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	516	GLU	CG-CD	7.83	1.63	1.51
1	A	516	GLU	CB-CG	6.91	1.65	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	12	VAL	C-N-CA	-7.71	102.42	121.70
1	B	517	LEU	CA-CB-CG	6.97	131.33	115.30
1	B	518	LEU	CA-CB-CG	-6.04	101.40	115.30
1	A	517	LEU	CA-CB-CG	5.81	128.66	115.30
1	B	335	LEU	C-N-CA	-5.58	107.74	121.70
1	B	424	LYS	C-N-CA	-5.54	107.85	121.70
3	L	181	LEU	CA-CB-CG	5.51	127.97	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	4	LEU	CA-CB-CG	5.46	127.86	115.30
1	D	378	LYS	CD-CE-NZ	5.36	124.02	111.70
1	C	378	LYS	CD-CE-NZ	5.04	123.29	111.70

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	1552	0	1472	22	0
1	B	1552	0	1472	20	0
1	C	1541	0	1454	26	0
1	D	1536	0	1452	29	0
2	E	1747	0	1702	36	0
2	G	1692	0	1643	44	0
2	H	1746	0	1698	32	0
2	J	1703	0	1650	39	0
3	F	1654	0	1610	34	0
3	I	1660	0	1615	30	0
3	K	1659	0	1611	37	0
3	L	1654	0	1610	28	0
4	M	39	0	34	0	0
4	N	39	0	34	0	0
5	C	14	0	13	0	0
5	D	14	0	11	0	0
All	All	19802	0	19081	357	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 (357) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:126:ARG:HH12	3:K:147[B]:VAL:HG21	1.24	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:142:ARG:HH12	3:F:163[B]:VAL:HG21	1.44	0.82
2:G:92:THR:HG23	2:G:126:THR:HA	1.67	0.77
3:L:142:ARG:HH12	3:L:163[B]:VAL:HG21	1.51	0.76
2:G:23:THR:HG22	2:G:79:GLN:HG2	1.66	0.75
2:E:42:PRO:HG2	2:E:45:LYS:HB2	1.69	0.75
2:J:87:THR:HG23	2:J:110:THR:HA	1.67	0.75
3:K:181:THR:HG22	3:K:188:PRO:HB3	1.69	0.74
3:F:6:GLN:HE22	3:F:87:TYR:HA	1.52	0.74
2:G:16:GLU:HG2	2:G:17:THR:H	1.53	0.74
3:L:29:ILE:HA	3:L:92:ASN:HD22	1.51	0.72
2:G:89:ALA:HA	2:G:127:VAL:HG11	1.71	0.72
2:H:40:PRO:HG2	2:H:43:LYS:HB2	1.71	0.70
3:K:24:ARG:HG3	3:K:24:ARG:HH11	1.58	0.69
2:J:84:ALA:HA	2:J:111:VAL:HG11	1.75	0.69
3:I:35(B):GLN:HB2	3:I:45:LEU:HD11	1.73	0.69
3:K:35(B):GLN:HB2	3:K:45:LEU:HD11	1.75	0.68
2:G:175:LEU:HD21	2:G:198:VAL:HG21	1.75	0.68
3:L:89:GLN:NE2	3:L:96:TYR:HD2	1.92	0.68
3:K:126:ARG:NH1	3:K:147[B]:VAL:HG21	2.04	0.67
2:E:35:TYR:CE1	2:E:54:TYR:HD2	2.12	0.67
2:G:42:PRO:HG2	2:G:45:LYS:HB2	1.76	0.66
2:H:3:GLN:HG3	2:H:25:SER:HB2	1.76	0.66
2:G:53:ILE:HD13	2:G:73:VAL:HG13	1.78	0.65
2:H:200:HIS:CD2	2:H:202:PRO:HD2	2.31	0.65
2:J:16:GLU:HG2	2:J:17:THR:H	1.62	0.65
1:D:360:ASN:HB3	2:E:146:SER:HB3	1.80	0.64
2:E:216:HIS:CD2	2:E:218:PRO:HD2	2.33	0.63
3:K:6:GLN:HE22	3:K:82(C):TYR:HA	1.64	0.63
2:H:2:VAL:HG21	2:H:94:ARG:HH21	1.63	0.63
2:J:119:PRO:HB3	2:J:145:TYR:HB3	1.80	0.62
2:G:21:THR:HG22	2:G:81:SER:HB3	1.81	0.62
2:G:133:LYS:NZ	2:G:160:ASP:O	2.31	0.62
1:C:391:CYS:HB3	1:C:522:ALA:HB1	1.81	0.62
3:I:181:THR:HG22	3:I:188:PRO:HB3	1.81	0.62
2:J:40:PRO:HG2	2:J:43:LYS:HB2	1.81	0.61
2:E:135:PRO:HB3	2:E:161:TYR:HB3	1.82	0.61
2:J:51:ILE:HD13	2:J:71:VAL:HG13	1.81	0.61
2:G:93:ALA:HB3	2:G:95:TYR:CE1	2.36	0.61
2:G:99:ARG:HD2	2:G:100:HIS:O	2.01	0.60
3:I:5:THR:HA	3:I:95:GLN:HE22	1.66	0.60
3:F:89:GLN:NE2	3:F:96:TYR:HD2	2.00	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:109:LEU:HD22	3:I:167:LYS:HG3	1.83	0.59
1:C:520:ALA:HB1	1:C:521:PRO:HD2	1.84	0.59
2:G:3:GLN:HG3	2:G:25:SER:HB2	1.85	0.59
2:H:87:THR:HG23	2:H:110:THR:HA	1.85	0.59
1:C:388:ASN:HB3	1:C:527:PRO:HD2	1.83	0.59
2:E:54:TYR:HE1	2:E:55:TYR:CE2	2.20	0.59
1:D:357:ARG:NH1	1:D:394:ASN:OD1	2.35	0.59
3:F:76:SER:OG	3:F:77:SER:N	2.34	0.59
2:G:13:LYS:HA	2:G:128:SER:O	2.02	0.59
1:C:395:VAL:HG22	1:C:515:PHE:HD1	1.68	0.59
2:G:34:TYR:CG	2:G:99:ARG:HD3	2.38	0.59
2:J:66:ARG:NH1	2:J:86:ASP:OD2	2.25	0.59
3:I:85:GLN:NE2	3:I:90:ARG:O	2.36	0.59
2:G:135:PRO:HD2	2:G:221:THR:HG21	1.84	0.58
2:G:135:PRO:HB3	2:G:161:TYR:HB3	1.84	0.58
1:A:364:ASP:O	1:A:367:VAL:HG12	2.03	0.58
2:E:2:VAL:HG21	2:E:99:ARG:NH1	2.18	0.58
3:K:133:LYS:HG2	3:K:138:LEU:HD23	1.86	0.58
2:E:6:GLU:OE2	2:E:97:CYS:SG	2.63	0.57
1:C:386:LYS:O	1:C:390:LEU:HD13	2.04	0.57
2:J:159:LEU:HD21	2:J:182:VAL:HG21	1.86	0.57
1:C:385:THR:HG22	1:C:386:LYS:HG3	1.87	0.57
2:E:57:GLY:O	2:E:59:THR:HG23	2.05	0.57
2:J:117:LYS:NZ	2:J:118:GLY:O	2.38	0.57
1:D:376:THR:HG23	1:D:378:LYS:HE3	1.88	0.56
2:E:19:SER:HB3	2:E:83:LYS:HG2	1.88	0.56
1:C:517:LEU:HD12	1:C:517:LEU:O	2.05	0.56
1:D:366:SER:HA	1:D:369:TYR:HB3	1.87	0.56
2:J:21:THR:HG22	2:J:79:SER:HB3	1.87	0.56
1:B:364:ASP:O	1:B:367:VAL:HG12	2.06	0.55
2:H:11:LEU:HD21	2:H:146:PHE:CE1	2.41	0.55
3:K:87:ASN:OD1	3:K:88:ASN:N	2.39	0.55
2:H:11:LEU:HD21	2:H:146:PHE:HE1	1.71	0.55
1:B:439:ASN:O	1:B:443:SER:OG	2.24	0.55
3:F:6:GLN:NE2	3:F:88:CYS:H	2.04	0.55
1:A:391:CYS:HB3	1:A:522:ALA:HB1	1.89	0.55
2:E:3:GLN:HB2	2:E:25:SER:HB2	1.89	0.55
2:E:11:LEU:HD21	2:E:162:PHE:CE1	2.41	0.55
2:J:94:ARG:HD2	2:J:95:HIS:O	2.07	0.55
1:B:391:CYS:HB3	1:B:522:ALA:HB1	1.88	0.54
2:G:160:ASP:HB3	2:G:191:LEU:HD12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:354:ASN:O	1:C:398:ASP:HA	2.08	0.54
2:J:143:LYS:HE3	3:K:115:SER:OG	2.08	0.54
1:D:388:ASN:HB3	1:D:527:PRO:HD2	1.89	0.54
3:F:108:ARG:NH1	3:F:109:THR:HG23	2.22	0.54
2:J:88:ALA:HB3	2:J:90:TYR:CE1	2.43	0.54
3:L:166:GLN:HE21	3:L:171:SER:HB3	1.73	0.54
3:L:37:GLN:HB2	3:L:47:LEU:HD11	1.90	0.54
1:D:455:LEU:HD22	1:D:456:PHE:CE2	2.43	0.54
3:K:24:ARG:NH1	3:K:68:GLU:OE2	2.34	0.54
1:B:382:VAL:HG12	1:C:470:THR:OG1	2.08	0.53
1:D:395:VAL:HG22	1:D:515:PHE:HD1	1.73	0.53
3:F:37:GLN:HB2	3:F:47:LEU:HD11	1.89	0.53
3:L:89:GLN:NE2	3:L:96:TYR:CD2	2.76	0.53
1:D:517:LEU:HD12	1:D:517:LEU:O	2.07	0.53
3:F:108:ARG:HG2	3:F:109:THR:H	1.73	0.53
2:J:100:TYR:CE1	2:J:100(F):TYR:HD1	2.26	0.53
3:K:29:ILE:HA	3:K:87:ASN:HD22	1.74	0.53
3:I:194:ASN:HB2	3:I:198:CYS:C	2.29	0.53
3:I:176:TYR:O	3:I:192:SER:HB2	2.09	0.53
2:H:55:GLY:O	2:H:57:THR:HG23	2.09	0.53
1:D:520:ALA:HB1	1:D:521:PRO:HD2	1.91	0.52
1:A:369:TYR:O	2:G:107:ARG:HD2	2.09	0.52
2:H:88:ALA:HB3	2:H:90:TYR:CE2	2.44	0.52
1:D:392:PHE:HD1	1:D:517:LEU:HD23	1.74	0.52
2:H:66:ARG:NH1	2:H:82:LEU:HD21	2.23	0.52
2:J:24:VAL:HG23	2:J:76:ASN:ND2	2.25	0.52
3:F:166:GLN:HE21	3:F:171:SER:HB3	1.74	0.52
1:B:447:GLY:HA3	1:B:449:TYR:CE1	2.44	0.52
3:K:89:TYR:HA	3:K:91:TYR:HE1	1.74	0.52
1:B:405:ASP:OD1	1:B:408:ARG:NH1	2.42	0.52
1:D:386:LYS:O	1:D:390:LEU:HD13	2.10	0.52
2:E:6:GLU:OE2	2:E:120:GLY:HA3	2.09	0.52
2:J:34:TYR:CG	2:J:94:ARG:HD3	2.45	0.52
1:B:371:SER:OG	1:B:373:SER:HB3	2.09	0.51
1:C:453:TYR:CE1	1:C:493:GLN:HB3	2.45	0.51
1:C:347:PHE:CD1	1:C:509:ARG:NH1	2.78	0.51
2:H:6:GLU:OE2	2:H:92:CYS:SG	2.68	0.51
3:I:148:THR:HG23	3:I:158:SER:O	2.09	0.51
2:J:12:VAL:HG21	2:J:18:LEU:HB3	1.92	0.51
3:K:24:ARG:HG3	3:K:24:ARG:NH1	2.25	0.51
1:A:521:PRO:O	1:A:523:THR:HG23	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:176:TYR:O	3:K:192:SER:HB2	2.11	0.51
3:I:150:GLN:HG3	3:I:157:TYR:CE1	2.45	0.51
1:A:382:VAL:HG12	1:D:470:THR:OG1	2.11	0.51
2:J:100:TYR:CE1	2:J:100(F):TYR:CD1	2.99	0.51
3:K:76:LEU:HD11	3:K:99:LEU:HD21	1.93	0.51
3:L:75:ILE:HG21	3:L:78:LEU:HD12	1.93	0.51
1:C:376:THR:HG23	1:C:378:LYS:HE3	1.93	0.50
3:I:87:ASN:O	3:I:88:ASN:HB2	2.11	0.50
3:F:89:GLN:NE2	3:F:96:TYR:CD2	2.78	0.50
2:H:4:LEU:HD21	2:H:35(A):TRP:HZ3	1.76	0.50
2:E:66:LYS:O	2:E:67:SER:OG	2.17	0.50
2:E:12:VAL:HG12	2:E:16:GLU:HB2	1.94	0.50
3:K:148:THR:HG23	3:K:158:SER:O	2.11	0.50
3:K:150:GLN:HG3	3:K:157:TYR:CE1	2.46	0.50
2:J:117:LYS:NZ	2:J:144:ASP:O	2.40	0.50
1:C:385:THR:O	1:C:386:LYS:HB2	2.12	0.50
3:F:142:ARG:NH1	3:F:163[B]:VAL:HG21	2.21	0.50
2:E:54:TYR:HD1	2:E:56:SER:H	1.58	0.49
2:G:89:ALA:HA	2:G:127:VAL:CG1	2.42	0.49
2:G:105:TYR:CE1	2:G:111:TYR:HD1	2.30	0.49
2:H:40:PRO:HA	2:H:88:ALA:HA	1.94	0.49
3:L:166:GLN:NE2	3:L:171:SER:HB3	2.27	0.49
2:H:18:LEU:HB2	2:H:82(C):VAL:HG11	1.93	0.49
3:F:75:ILE:HG21	3:F:78:LEU:HD12	1.93	0.49
1:C:433:VAL:HG22	1:C:512:VAL:HG22	1.94	0.49
2:J:24:VAL:HG21	2:J:29:ILE:HG13	1.95	0.49
3:L:106:ILE:HB	3:L:166:GLN:HE22	1.77	0.49
3:K:150:GLN:HG3	3:K:157:TYR:CZ	2.48	0.49
3:L:193:ALA:HB2	3:L:208:SER:HB2	1.95	0.49
2:H:61:PRO:HG2	3:L:1:ASP:OD1	2.13	0.49
3:I:170:TYR:O	3:I:176:TYR:OH	2.30	0.49
1:C:347:PHE:CE2	1:C:399:SER:HB2	2.48	0.49
2:J:30:SER:HB2	2:J:73:THR:HG23	1.95	0.49
2:E:60:TYR:CE2	3:F:94:TYR:CD2	3.01	0.48
3:K:125:PRO:HB2	3:K:127:GLU:OE1	2.13	0.48
1:D:406:GLU:OE1	1:D:495:TYR:OH	2.25	0.48
3:K:6:GLN:NE2	3:K:83:CYS:H	2.12	0.48
3:F:193:ALA:HB2	3:F:208:SER:HB2	1.95	0.48
2:G:225:LYS:HE3	3:I:107:GLU:OE1	2.13	0.48
3:L:83:PHE:CE2	3:L:106:ILE:HG12	2.49	0.48
1:A:477:SER:O	1:A:479:PRO:HD3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:PHE:CE2	1:B:509:ARG:HB3	2.49	0.48
2:J:144:ASP:HB3	2:J:175:LEU:HD12	1.96	0.48
3:L:89:GLN:HE22	3:L:96:TYR:HD2	1.60	0.48
2:H:119:PRO:HB3	2:H:145:TYR:HB3	1.96	0.48
2:E:105:TYR:CE1	2:E:111:TYR:CD1	3.02	0.48
3:F:166:GLN:NE2	3:F:171:SER:HB3	2.28	0.48
2:E:11:LEU:HD21	2:E:162:PHE:HE1	1.78	0.47
3:F:6:GLN:HE21	3:F:88:CYS:H	1.62	0.47
2:H:100:TYR:CE1	2:H:100(F):TYR:CD1	3.02	0.47
2:J:136:ALA:HB3	2:J:184:VAL:HG23	1.96	0.47
3:L:29:ILE:HA	3:L:92:ASN:ND2	2.25	0.47
1:C:392:PHE:HB3	1:C:516:GLU:O	2.14	0.47
2:E:170:TRP:CZ3	2:E:212:CYS:HB3	2.49	0.47
1:B:521:PRO:O	1:B:523:THR:HG23	2.13	0.47
2:G:105:TYR:CE1	2:G:111:TYR:CD1	3.01	0.47
2:E:6:GLU:OE1	2:E:122:GLY:N	2.44	0.47
3:K:194:ASN:HB2	3:K:198:CYS:C	2.34	0.47
3:F:29:ILE:HA	3:F:92:ASN:HD22	1.79	0.47
2:G:152:ALA:HB1	2:G:205:LEU:HD21	1.96	0.47
1:C:395:VAL:HG22	1:C:515:PHE:CD1	2.49	0.47
3:F:197:THR:HG22	3:F:204:PRO:HB3	1.97	0.47
1:B:520:ALA:HB1	1:B:521:PRO:HD2	1.96	0.47
2:G:21:THR:HG22	2:G:81:SER:CB	2.45	0.47
3:I:84:GLN:HB2	3:I:93:PHE:CD2	2.49	0.47
2:J:67:VAL:HG12	2:J:82:LEU:HG	1.95	0.47
1:B:336:CYS:O	1:B:338:PHE:N	2.44	0.47
1:D:338:PHE:CE2	1:D:363:ALA:HB1	2.49	0.47
2:H:83:THR:HB	2:H:85:ALA:H	1.80	0.47
1:C:392:PHE:HD1	1:C:517:LEU:HD23	1.79	0.47
1:D:364:ASP:O	1:D:367:VAL:HG12	2.14	0.47
1:A:351:TYR:CE2	1:A:492:LEU:HD21	2.50	0.47
2:E:124:LEU:HG	2:E:125:VAL:N	2.30	0.47
3:I:89:TYR:HA	3:I:91:TYR:HE1	1.80	0.47
2:J:119:PRO:HD2	2:J:205:THR:HG21	1.96	0.47
2:H:18:LEU:HD11	2:H:109:VAL:HG11	1.97	0.46
3:I:76:LEU:HD12	3:I:76:LEU:HA	1.72	0.46
1:A:336:CYS:O	1:A:338:PHE:N	2.41	0.46
1:B:431:GLY:HA2	1:B:515:PHE:CD2	2.51	0.46
3:I:142:ASN:HB2	3:I:163:LEU:HD11	1.97	0.46
3:L:28:SER:HA	3:L:68:GLY:O	2.14	0.46
3:K:60:PHE:CE1	3:K:73:ILE:HG12	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:SER:HA	1:A:369:TYR:CE1	2.50	0.46
3:F:2:ILE:HD13	3:F:29:ILE:HG22	1.97	0.46
2:G:11:LEU:HD22	2:G:162:PHE:HE1	1.80	0.46
2:E:42:PRO:HA	2:E:93:ALA:HA	1.98	0.46
2:G:135:PRO:HB2	2:G:158:VAL:HG13	1.96	0.46
2:H:154:TRP:CZ3	2:H:196:CYS:HB3	2.51	0.46
1:C:497:PHE:CD2	1:C:507:PRO:HB3	2.50	0.46
3:L:76:SER:OG	3:L:77:SER:N	2.48	0.46
1:A:520:ALA:HB1	1:A:521:PRO:HD2	1.97	0.46
2:H:2:VAL:HG21	2:H:94:ARG:NH2	2.29	0.46
3:I:29:ILE:HA	3:I:87:ASN:HD22	1.81	0.46
3:K:131:GLN:HB3	3:K:179:GLU:HB3	1.99	0.45
3:L:105:GLU:HB3	3:L:166:GLN:OE1	2.16	0.45
2:E:68:ARG:NH2	2:E:91:ASP:OD1	2.48	0.45
2:E:140:LEU:HB3	3:F:118:PHE:CD1	2.52	0.45
2:G:133:LYS:NZ	2:G:134:GLY:O	2.46	0.45
3:I:91:TYR:HD1	3:I:91:TYR:N	2.15	0.45
3:K:89:TYR:CD1	3:K:89:TYR:N	2.83	0.45
3:I:76:LEU:HD11	3:I:99:LEU:HD21	1.98	0.45
2:J:151:THR:OG1	2:J:199:ASN:HB3	2.17	0.45
3:I:60:PHE:CE1	3:I:73:ILE:HG12	2.51	0.45
3:I:169:ASP:HA	3:I:172:LYS:HD3	1.97	0.45
1:A:379:CYS:HA	1:A:432:CYS:HA	1.99	0.45
1:A:447:GLY:HA3	1:A:449:TYR:CE1	2.52	0.45
3:L:120:PRO:HD3	3:L:132:VAL:HG22	1.99	0.45
2:E:92:THR:HG23	2:E:126:THR:HA	1.99	0.45
2:E:105:TYR:CE1	2:E:111:TYR:HD1	2.35	0.45
2:H:131:THR:HG22	2:H:133:GLY:H	1.81	0.45
1:B:442:ASP:HB3	1:B:451:TYR:HE2	1.81	0.44
2:E:40:ARG:HB3	2:E:50:ILE:HD11	1.99	0.44
2:E:53:ILE:HG13	2:E:59:THR:HG22	1.98	0.44
2:G:140:LEU:HB3	3:I:102:PHE:CD2	2.52	0.44
1:D:347:PHE:CD2	1:D:509:ARG:NH1	2.85	0.44
1:D:381:GLY:HA3	1:D:430:THR:HG22	1.98	0.44
2:G:16:GLU:HG2	2:G:17:THR:N	2.29	0.44
2:G:182:PHE:CE2	3:I:160:SER:HB3	2.51	0.44
2:G:225:LYS:HD2	2:G:225:LYS:HA	1.71	0.44
3:K:20:THR:HG22	3:K:72:THR:OG1	2.17	0.44
2:H:4:LEU:HD22	2:H:24:VAL:HG22	1.99	0.44
1:A:335:LEU:HD23	1:A:336:CYS:N	2.32	0.44
1:A:458:LYS:HA	1:A:458:LYS:HD2	1.59	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:424:LYS:HB3	1:C:463:PRO:HA	1.98	0.44
3:F:83:PHE:CE2	3:F:106:ILE:HG12	2.52	0.44
3:F:90:GLN:HG2	3:F:91:TYR:N	2.32	0.44
2:H:35(A):TRP:HB3	2:H:78:PHE:CZ	2.53	0.44
1:A:350:VAL:HA	1:A:400:PHE:HB2	1.99	0.44
1:B:346:ARG:HH12	1:B:354:ASN:ND2	2.16	0.44
3:F:125:LEU:HD22	3:F:183:LYS:HG3	1.99	0.44
2:E:28:SER:O	2:E:32:SER:OG	2.35	0.44
3:F:108:ARG:HG2	3:F:109:THR:N	2.31	0.44
2:G:18:LEU:HD23	2:G:19:SER:N	2.32	0.44
3:L:166:GLN:HG3	3:L:173:TYR:CZ	2.53	0.44
3:L:197:THR:HG22	3:L:204:PRO:HB3	1.99	0.44
1:B:458:LYS:HA	1:B:458:LYS:HD2	1.69	0.44
2:G:152:ALA:HB3	2:G:200:VAL:HG23	1.99	0.44
3:I:91:TYR:N	3:I:91:TYR:CD1	2.85	0.44
3:F:201:LEU:HD13	3:F:205:VAL:HG23	2.00	0.43
1:B:408:ARG:NH2	3:K:52:LEU:O	2.51	0.43
3:I:150:GLN:HG3	3:I:157:TYR:CZ	2.53	0.43
2:J:122:PHE:CG	3:K:108:GLN:HB2	2.53	0.43
3:F:105:GLU:HB3	3:F:166:GLN:OE1	2.18	0.43
3:K:109:LEU:HD22	3:K:167:LYS:HG3	2.00	0.43
3:L:201:LEU:HD13	3:L:205:VAL:HG23	2.00	0.43
1:C:340:GLU:O	1:C:344:ALA:HB2	2.18	0.43
2:G:163:PRO:HD2	2:G:218:PRO:CB	2.49	0.43
1:A:390:LEU:HD21	1:D:470:THR:HG21	2.00	0.43
2:H:34:TYR:CG	2:H:94:ARG:HD3	2.54	0.43
2:J:87:THR:OG1	2:J:111:VAL:HG12	2.18	0.43
2:G:138:PHE:CG	3:I:108:GLN:HB2	2.54	0.43
2:H:108:LEU:HG	2:H:109:VAL:N	2.33	0.43
1:D:354:ASN:O	1:D:398:ASP:HA	2.18	0.43
2:G:14:PRO:HD3	2:G:128:SER:O	2.19	0.43
3:L:108:ARG:NH2	3:L:109:THR:HG23	2.34	0.43
1:C:357:ARG:NH1	1:C:394:ASN:OD1	2.52	0.43
2:E:65:LEU:HD23	2:E:65:LEU:HA	1.81	0.43
1:A:347:PHE:CE2	1:A:399:SER:HB2	2.54	0.43
2:G:150:GLY:HA2	2:G:202:SER:OG	2.19	0.43
3:I:11:LEU:HD23	3:I:99:LEU:HD13	2.00	0.43
3:K:91:TYR:HD1	3:K:91:TYR:N	2.17	0.43
3:K:126:ARG:HB3	3:K:157:TYR:CD2	2.54	0.43
1:A:431:GLY:HA2	1:A:515:PHE:CD2	2.54	0.42
3:F:141:PRO:HB2	3:F:143:GLU:OE1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:108:ARG:HH21	3:L:109:THR:HG23	1.84	0.42
1:D:392:PHE:HB3	1:D:516:GLU:O	2.18	0.42
2:J:11:LEU:HA	2:J:110:THR:O	2.18	0.42
2:E:18:LEU:HD11	2:E:125:VAL:HG11	2.00	0.42
3:K:196:GLY:O	3:K:197:GLU:HB3	2.19	0.42
1:D:455:LEU:O	1:D:455:LEU:HD23	2.18	0.42
2:E:138:PHE:HB3	3:F:121:SER:OG	2.20	0.42
3:F:166:GLN:HG3	3:F:173:TYR:CZ	2.54	0.42
2:J:119:PRO:HB2	2:J:142:VAL:HG13	2.01	0.42
2:G:71:ILE:HD13	2:G:71:ILE:HG21	1.78	0.42
2:J:123:PRO:O	3:K:105:SER:HB3	2.19	0.42
3:L:2:ILE:H	3:L:2:ILE:HG13	1.63	0.42
1:B:337:PRO:O	1:B:340:GLU:HB2	2.19	0.42
2:E:54:TYR:CE1	2:E:55:TYR:CD2	3.07	0.42
3:F:106:ILE:HB	3:F:166:GLN:HE22	1.85	0.42
2:G:159:LYS:HE3	3:I:115:SER:OG	2.20	0.42
1:B:365:TYR:CD2	1:B:387:LEU:HB3	2.55	0.42
3:F:94:TYR:CD1	3:F:94:TYR:N	2.87	0.42
3:F:165:GLU:HA	3:F:165:GLU:OE1	2.20	0.42
2:J:3:GLN:C	2:J:4:LEU:HD12	2.39	0.42
2:J:171:GLN:HA	3:K:144:GLN:HE22	1.83	0.42
1:A:418:ILE:HD13	1:A:418:ILE:HA	1.87	0.42
1:C:347:PHE:HD1	1:C:509:ARG:NH1	2.17	0.42
1:D:357:ARG:HH12	1:D:394:ASN:CG	2.22	0.42
1:D:361:CYS:O	1:D:524:VAL:HA	2.20	0.42
1:D:385:THR:O	1:D:386:LYS:HB2	2.19	0.42
3:F:124:GLN:HG2	3:F:129:THR:O	2.20	0.42
3:L:12:SER:HB3	3:L:107:LYS:HB2	2.01	0.42
2:J:8:GLY:HA3	2:J:20:VAL:HG12	2.02	0.42
1:D:388:ASN:O	1:D:526:GLY:HA3	2.20	0.41
2:G:8:GLY:HA3	2:G:20:VAL:HG12	2.01	0.41
2:H:19:SER:HB3	2:H:81:LYS:HD3	2.02	0.41
1:C:387:LEU:HD23	1:C:387:LEU:HA	1.81	0.41
1:D:369:TYR:CE1	1:D:385:THR:HG22	2.55	0.41
1:D:458:LYS:HD2	1:D:458:LYS:HA	1.82	0.41
2:E:93:ALA:HB3	2:E:95:TYR:CE1	2.55	0.41
3:L:165:GLU:OE1	3:L:165:GLU:HA	2.19	0.41
1:B:518:LEU:HD23	1:B:518:LEU:HA	1.78	0.41
2:E:88:THR:HB	2:E:90:ALA:H	1.85	0.41
2:G:137:VAL:HG21	2:G:223:VAL:HB	2.03	0.41
2:J:12:VAL:HG21	2:J:18:LEU:CB	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:91:TYR:N	3:K:91:TYR:CD1	2.88	0.41
3:L:193:ALA:HB2	3:L:208:SER:CB	2.49	0.41
2:H:66:ARG:HH11	2:H:82:LEU:HD21	1.85	0.41
1:B:477:SER:O	1:B:479:PRO:HD3	2.20	0.41
3:K:78:PRO:HB3	3:K:155:SER:OG	2.20	0.41
1:C:458:LYS:HD2	1:C:458:LYS:HA	1.89	0.41
1:A:517:LEU:HD12	1:A:517:LEU:O	2.21	0.41
1:D:497:PHE:CD2	1:D:507:PRO:HB3	2.56	0.41
3:F:21:ILE:HG12	3:F:102:THR:HG21	2.03	0.41
2:G:163:PRO:HD2	2:G:218:PRO:HB2	2.02	0.41
2:H:124:LEU:HB3	3:L:118:PHE:CD1	2.55	0.41
2:J:55:GLY:O	2:J:57:THR:HG23	2.21	0.41
2:J:31:SER:HA	2:J:53:TYR:CE2	2.56	0.41
1:A:454:ARG:NH2	1:A:467:ASP:O	2.51	0.40
2:G:40:ARG:HB3	2:G:50:ILE:HD11	2.02	0.40
3:I:100(C):ARG:NH2	3:I:100(F):ALA:HB2	2.36	0.40
2:J:147:PRO:HD2	2:J:202:PRO:CB	2.52	0.40
1:C:385:THR:O	1:C:386:LYS:CB	2.69	0.40
2:G:57:GLY:O	2:G:59:THR:HG23	2.21	0.40
1:D:347:PHE:CE1	1:D:399:SER:HB2	2.56	0.40
2:H:9:PRO:HD3	2:H:19:SER:O	2.21	0.40
3:I:196:GLY:O	3:I:197:GLU:HB3	2.21	0.40
2:J:100(I):GLU:HB3	2:J:100(J):TYR:H	1.69	0.40
3:K:145:GLU:HA	3:K:160:SER:O	2.21	0.40
1:A:340:GLU:O	1:A:344:ALA:HB2	2.21	0.40
2:H:57:THR:HG1	2:H:59:TYR:HE2	1.70	0.40
2:H:66:ARG:NH1	2:H:86:ASP:OD2	2.49	0.40
3:K:87:ASN:CG	3:K:88:ASN:H	2.25	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	A	194/212 (92%)	183 (94%)	11 (6%)	0	100	100
1	B	194/212 (92%)	184 (95%)	10 (5%)	0	100	100
1	C	193/212 (91%)	181 (94%)	11 (6%)	1 (0%)	29	67
1	D	192/212 (91%)	183 (95%)	9 (5%)	0	100	100
2	E	229/240 (95%)	217 (95%)	11 (5%)	1 (0%)	34	69
2	G	219/240 (91%)	203 (93%)	15 (7%)	1 (0%)	29	67
2	H	229/240 (95%)	215 (94%)	11 (5%)	3 (1%)	12	47
2	J	221/240 (92%)	210 (95%)	11 (5%)	0	100	100
3	F	213/215 (99%)	199 (93%)	14 (7%)	0	100	100
3	I	214/215 (100%)	202 (94%)	11 (5%)	1 (0%)	29	67
3	K	214/215 (100%)	202 (94%)	10 (5%)	2 (1%)	17	56
3	L	213/215 (99%)	199 (93%)	14 (7%)	0	100	100
All	All	2525/2668 (95%)	2378 (94%)	138 (6%)	9 (0%)	34	69

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	K	89	TYR
2	H	129	LYS
2	H	131	THR
3	I	88	ASN
2	E	148	SER
2	H	134	GLY
3	K	87	ASN
1	C	386	LYS
2	G	31	SER

### 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	A	169/185 (91%)	167 (99%)	2 (1%)	71	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	169/185 (91%)	165 (98%)	4 (2%)	49	77
1	C	167/185 (90%)	163 (98%)	4 (2%)	49	77
1	D	167/185 (90%)	163 (98%)	4 (2%)	49	77
2	E	197/207 (95%)	192 (98%)	5 (2%)	47	77
2	G	189/207 (91%)	184 (97%)	5 (3%)	46	76
2	H	197/207 (95%)	191 (97%)	6 (3%)	41	73
2	J	190/207 (92%)	189 (100%)	1 (0%)	88	95
3	F	190/190 (100%)	186 (98%)	4 (2%)	53	79
3	I	191/190 (100%)	189 (99%)	2 (1%)	76	90
3	K	191/190 (100%)	188 (98%)	3 (2%)	62	84
3	L	190/190 (100%)	188 (99%)	2 (1%)	73	88
All	All	2207/2328 (95%)	2165 (98%)	42 (2%)	57	81

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	495	TYR
1	A	516	GLU
1	B	349	SER
1	B	478	THR
1	B	495	TYR
1	B	528	LYS
1	C	346	ARG
1	C	407	VAL
1	C	495	TYR
1	C	516	GLU
1	D	345	THR
1	D	430	THR
1	D	495	TYR
1	D	516	GLU
2	E	12	VAL
2	E	17	THR
2	E	23	THR
2	E	33	ARG
2	E	199	THR
3	F	6	GLN
3	F	31	SER
3	F	94	TYR

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Mol	Chain	Res	Type
3	F	122	ASP
2	G	54	TYR
2	G	75	THR
2	G	121	GLN
2	G	123	THR
2	G	212	CYS
2	H	23	THR
2	H	33	ARG
2	H	72	ASP
2	H	130	SER
2	H	160	THR
2	H	183	THR
3	I	106	ASP
3	I	186	SER
2	J	196	CYS
3	K	5	THR
3	K	106	ASP
3	K	140	SER
3	L	109	THR
3	L	142	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
3	F	6	GLN
2	G	118	HIS
3	I	150	GLN
3	K	6	GLN
3	L	198	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates i

6 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	M	1	4,1	14,14,15	0.37	0	17,19,21	0.82	0
4	NAG	M	2	4	14,14,15	0.24	0	17,19,21	0.60	0
4	BMA	M	3	4	11,11,12	2.42	3 (27%)	15,15,17	1.93	5 (33%)
4	NAG	N	1	4,1	14,14,15	0.72	1 (7%)	17,19,21	0.89	1 (5%)
4	NAG	N	2	4	14,14,15	0.29	0	17,19,21	0.47	0
4	BMA	N	3	4	11,11,12	1.50	2 (18%)	15,15,17	1.12	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	M	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	M	2	4	-	2/6/23/26	0/1/1/1
4	BMA	M	3	4	-	2/2/19/22	0/1/1/1
4	NAG	N	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	N	2	4	-	2/6/23/26	0/1/1/1
4	BMA	N	3	4	-	2/2/19/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	3	BMA	C4-C3	4.73	1.64	1.52
4	M	3	BMA	C4-C5	4.49	1.62	1.53
4	M	3	BMA	C1-C2	3.78	1.60	1.52
4	N	1	NAG	O5-C1	2.55	1.47	1.43
4	N	3	BMA	O5-C1	2.45	1.47	1.43
4	N	3	BMA	C2-C3	2.24	1.55	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	3	BMA	C3-C4-C5	4.54	118.33	110.24
4	M	3	BMA	O2-C2-C1	3.48	116.27	109.15
4	N	3	BMA	C1-O5-C5	2.95	116.19	112.19
4	M	3	BMA	C2-C3-C4	2.91	115.94	110.89
4	M	3	BMA	C1-C2-C3	-2.60	106.48	109.67
4	N	1	NAG	C1-O5-C5	2.32	115.34	112.19
4	M	3	BMA	C1-O5-C5	-2.30	109.08	112.19

There are no chirality outliers.

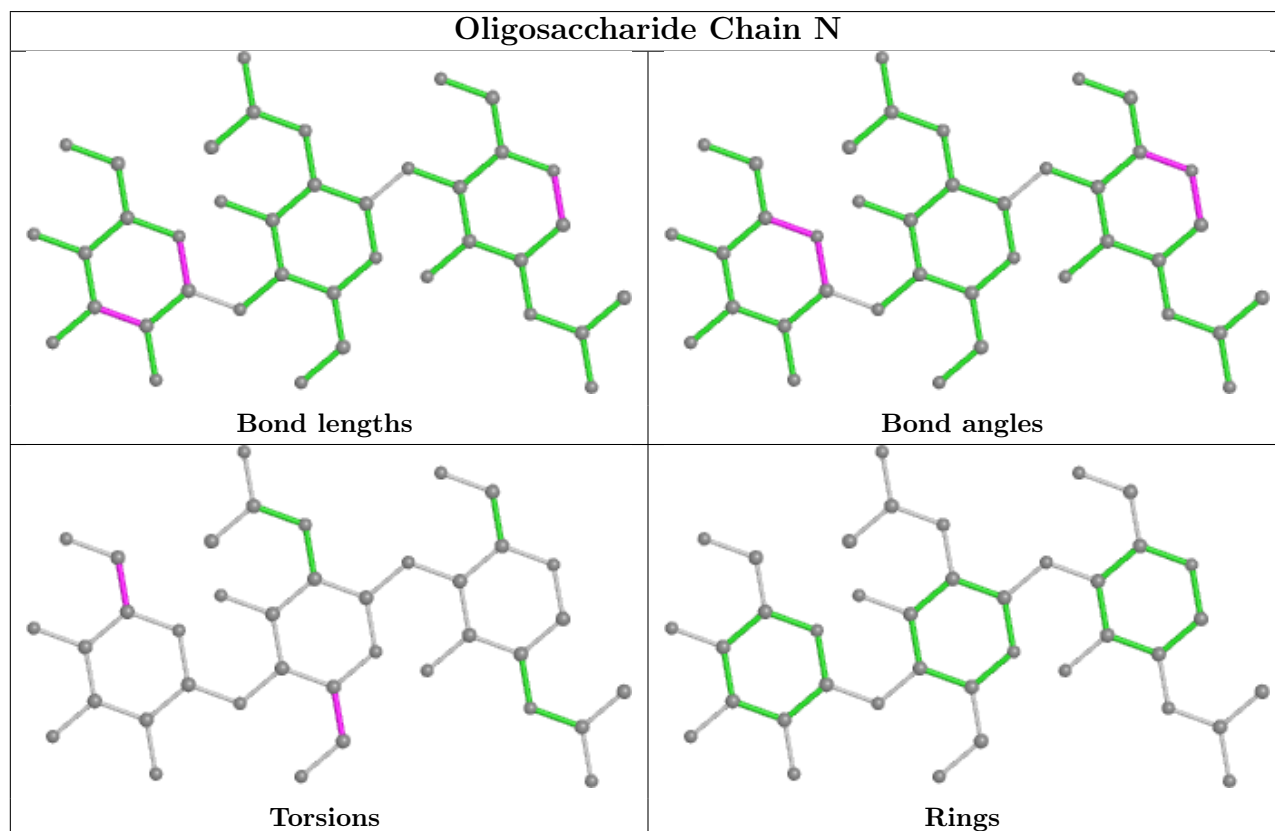
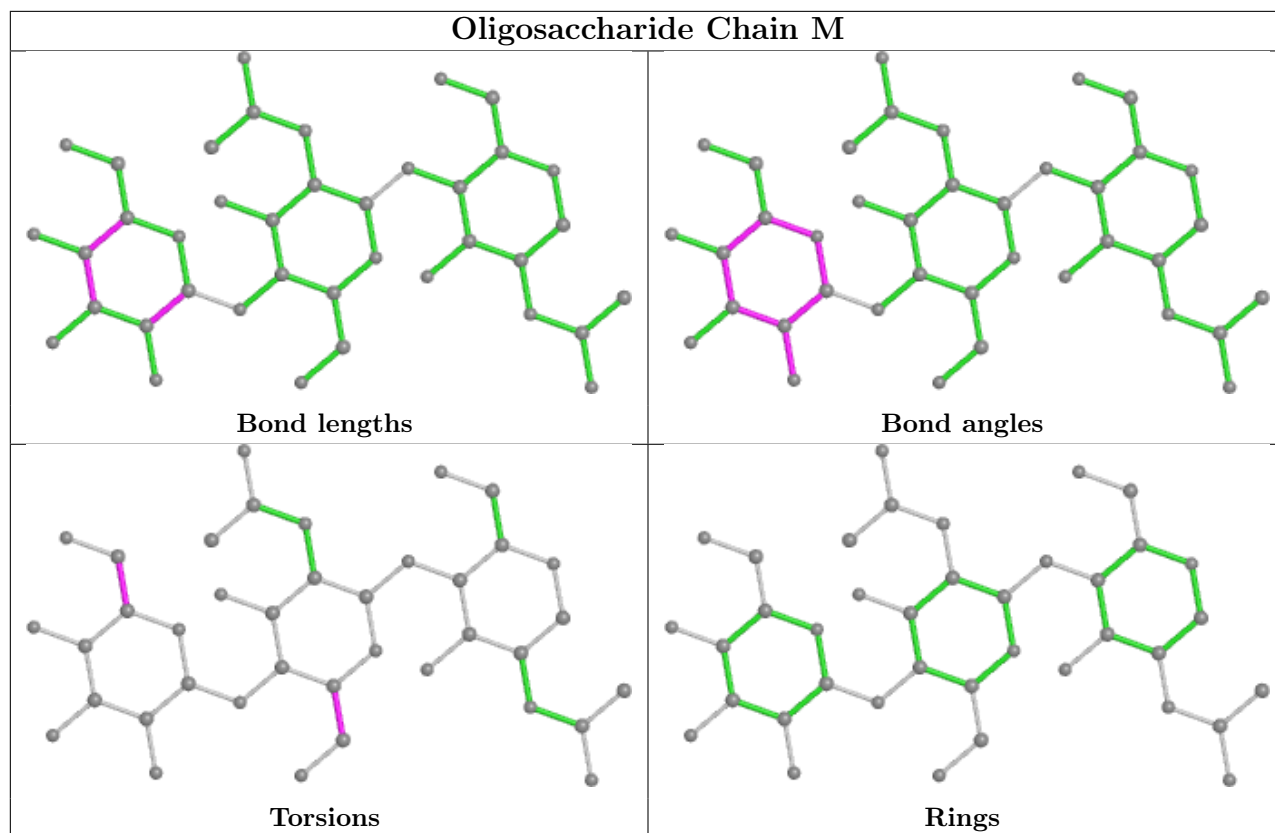
All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	M	3	BMA	C4-C5-C6-O6
4	M	3	BMA	O5-C5-C6-O6
4	N	2	NAG	O5-C5-C6-O6
4	N	3	BMA	O5-C5-C6-O6
4	N	2	NAG	C4-C5-C6-O6
4	M	2	NAG	C4-C5-C6-O6
4	M	2	NAG	O5-C5-C6-O6
4	N	3	BMA	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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



## 5.6 Ligand geometry

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	C	601	1	14,14,15	1.10	1 (7%)	17,19,21	0.67	1 (5%)
5	NAG	D	601	1	14,14,15	1.49	1 (7%)	17,19,21	0.96	1 (5%)

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	C	601	1	-	1/6/23/26	0/1/1/1
5	NAG	D	601	1	-	1/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	601	NAG	O5-C1	5.42	1.52	1.43
5	C	601	NAG	O5-C1	3.87	1.49	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	601	NAG	C4-C3-C2	-2.44	107.45	111.02
5	C	601	NAG	C1-O5-C5	2.05	114.97	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	601	NAG	O5-C5-C6-O6
5	D	601	NAG	O5-C5-C6-O6

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	196/212 (92%)	0.21	0 <b>100</b> <b>100</b>	82, 112, 158, 176	0
1	B	196/212 (92%)	0.26	0 <b>100</b> <b>100</b>	79, 113, 157, 169	0
1	C	195/212 (91%)	0.15	4 (2%) 63 49	90, 121, 157, 173	0
1	D	194/212 (91%)	0.15	2 (1%) 82 72	93, 121, 159, 177	0
2	E	231/240 (96%)	0.12	0 <b>100</b> <b>100</b>	85, 110, 150, 187	0
2	G	223/240 (92%)	0.44	15 (6%) 17 10	79, 141, 196, 215	0
2	H	231/240 (96%)	0.20	1 (0%) 92 89	87, 109, 148, 178	0
2	J	225/240 (93%)	0.42	12 (5%) 26 14	79, 141, 201, 222	0
3	F	213/215 (99%)	0.19	0 <b>100</b> <b>100</b>	92, 114, 143, 156	0
3	I	214/215 (99%)	0.42	14 (6%) 18 11	77, 131, 205, 216	0
3	K	214/215 (99%)	0.38	16 (7%) 14 8	77, 129, 206, 216	0
3	L	213/215 (99%)	0.18	2 (0%) 84 75	91, 114, 140, 156	0
All	All	2545/2668 (95%)	0.26	66 (2%) 56 40	77, 117, 192, 222	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	124	LEU	6.4
2	G	206	GLY	5.5
2	G	205	LEU	5.5
3	I	198	CYS	5.4
2	J	189	LEU	4.9
3	I	119	LEU	4.9
3	K	119	LEU	4.2
3	I	130	VAL	4.2
3	K	176	TYR	4.0
3	K	198	CYS	4.0
3	K	130	VAL	3.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	I	170	TYR	3.7
2	G	154	LEU	3.7
2	G	227	VAL	3.5
2	J	138	LEU	3.4
3	K	170	TYR	3.3
3	I	176	TYR	2.9
1	C	338	PHE	2.8
3	K	162	THR	2.8
3	K	177	ALA	2.8
2	J	190	GLY	2.7
3	K	117	VAL	2.7
2	G	142	PRO	2.7
2	J	227	VAL	2.7
3	K	120	LEU	2.6
2	J	140	CYS	2.6
2	J	119	PRO	2.6
3	I	133	LYS	2.6
2	J	123	PRO	2.6
2	G	140	LEU	2.6
2	H	121	VAL	2.5
2	J	201	LYS	2.5
3	I	116	VAL	2.4
3	I	134	VAL	2.4
2	J	188	SER	2.4
3	I	120	LEU	2.4
3	K	111	SER	2.4
3	L	73	LEU	2.3
3	K	116	VAL	2.3
2	G	135	PRO	2.3
1	C	434	ILE	2.3
3	L	19	VAL	2.3
2	G	157	LEU	2.2
1	C	342	PHE	2.2
3	I	162	THR	2.2
3	K	128	ALA	2.2
3	K	161	SER	2.2
2	G	195	SER	2.2
3	I	118	CYS	2.2
2	G	153	ALA	2.2
3	K	164	THR	2.2
2	J	137	ALA	2.2
3	I	165	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	G	10	GLY	2.1
2	J	154	TRP	2.1
1	D	434	ILE	2.1
2	G	113	ILE	2.1
1	D	342	PHE	2.1
2	G	47	LEU	2.1
3	I	194	ASN	2.1
2	G	200	VAL	2.1
3	I	73	ILE	2.1
2	G	80	PHE	2.0
3	K	193	PHE	2.0
1	C	410	ILE	2.0
3	K	101	ILE	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](#)

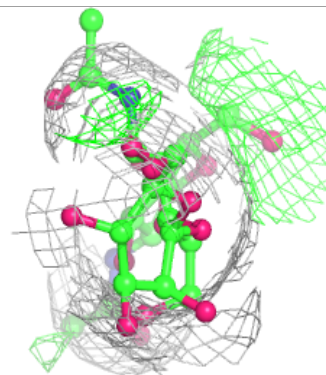
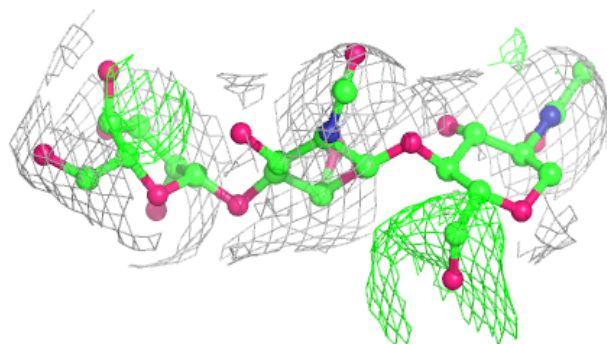
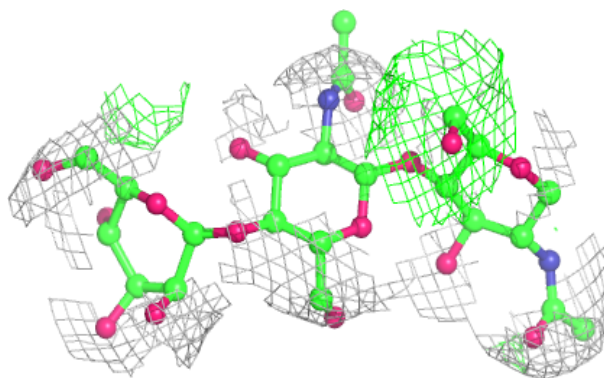
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
4	NAG	M	1	14/15	0.84	0.21	113,137,151,154	0
4	NAG	N	1	14/15	0.86	0.21	114,136,149,157	0
4	BMA	M	3	11/12	0.91	0.14	157,172,174,175	0
4	BMA	N	3	11/12	0.93	0.08	152,176,185,189	0
4	NAG	N	2	14/15	0.96	0.10	149,165,179,185	0
4	NAG	M	2	14/15	0.96	0.12	145,161,169,172	0

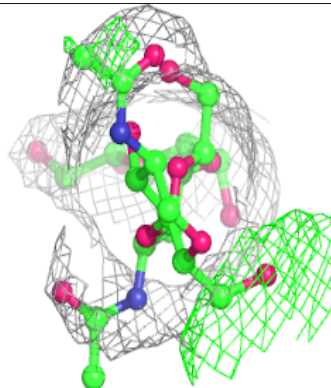
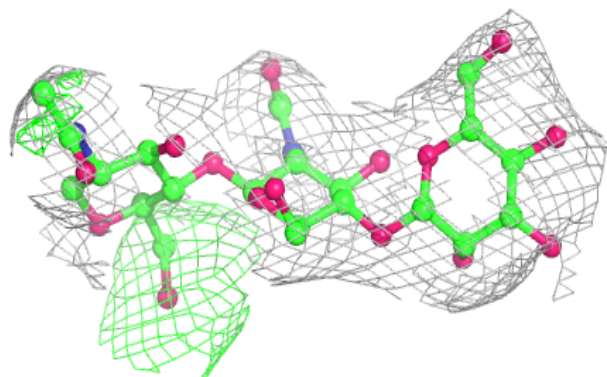
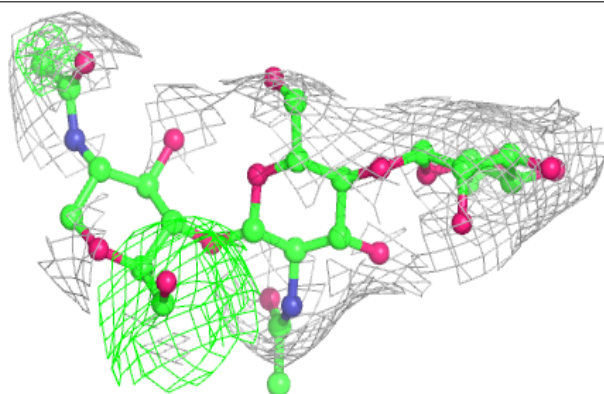
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around Chain M:**

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

**Electron density around Chain N:**

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



## 6.4 Ligands [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
5	NAG	D	601	14/15	0.70	0.18	133,148,154,155	0
5	NAG	C	601	14/15	0.77	0.25	138,148,164,166	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.