



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:47 PM UTC

PDB ID : 7KBT / pdb_00007kbt
Title : Factor VIII in complex with the anti-C2 domain antibody, G99
Authors : Ronayne, E.K.; Gish, J.; Wilson, C.; Peters, S.; Spencer, H.T.; Spiegel, P.C.; Childers, K.C.
Deposited on : 2020-10-02
Resolution : 4.15 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

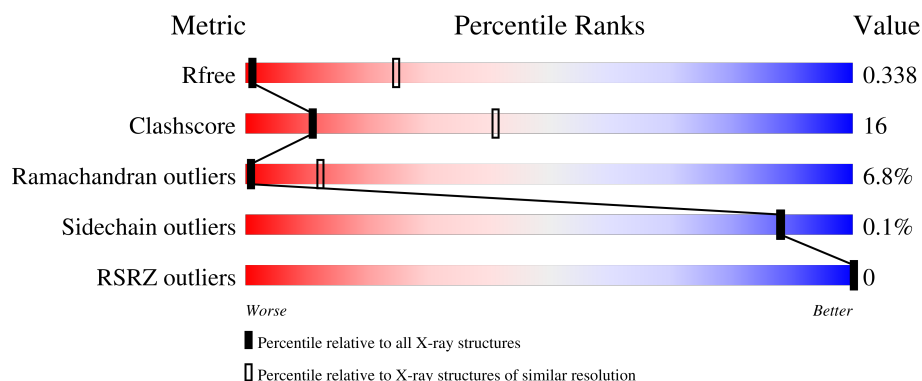
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.15 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}	180053	1077 (4.50-3.82)
Clashscore	190562	1019 (4.48-3.84)
Ramachandran outliers	187476	1035 (4.50-3.82)
Sidechain outliers	187428	1022 (4.50-3.82)
RSRZ outliers	180081	1074 (4.50-3.82)

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 $\leq 5\%$. 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	1467	
2	E	224	
3	F	214	
4	B	2	
4	G	2	

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

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

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 11366 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 Coagulation factor VIII,Coagulation factor VIII,Coagulation factor VIII,Coagulation factor VIII,Coagulation factor VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1233	Total	C	N	O	S	0	0	0
			9809	6272	1700	1785	52			

- Molecule 2 is a protein called G99 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	115	Total	C	N	O	S	0	0	0
			818	503	139	173	3			

- Molecule 3 is a protein called G99 light chain.

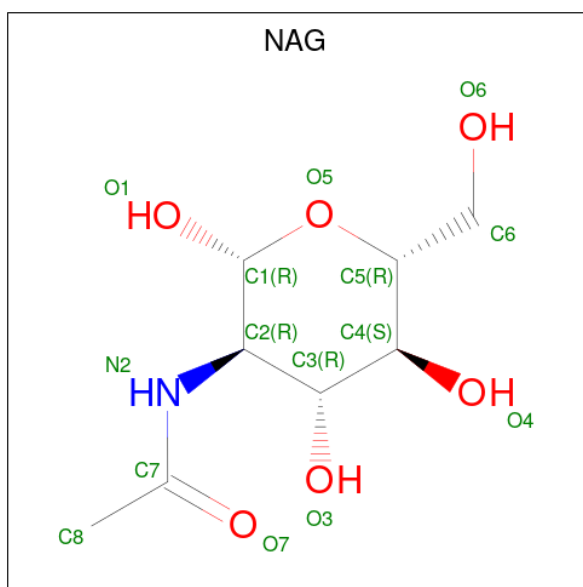
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	96	Total	C	N	O	S	0	0	0
			666	403	120	140	3			

- Molecule 4 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
4	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	B	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 6 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Cu	0	0
			1	1		

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Zn	0	0
			1	1		

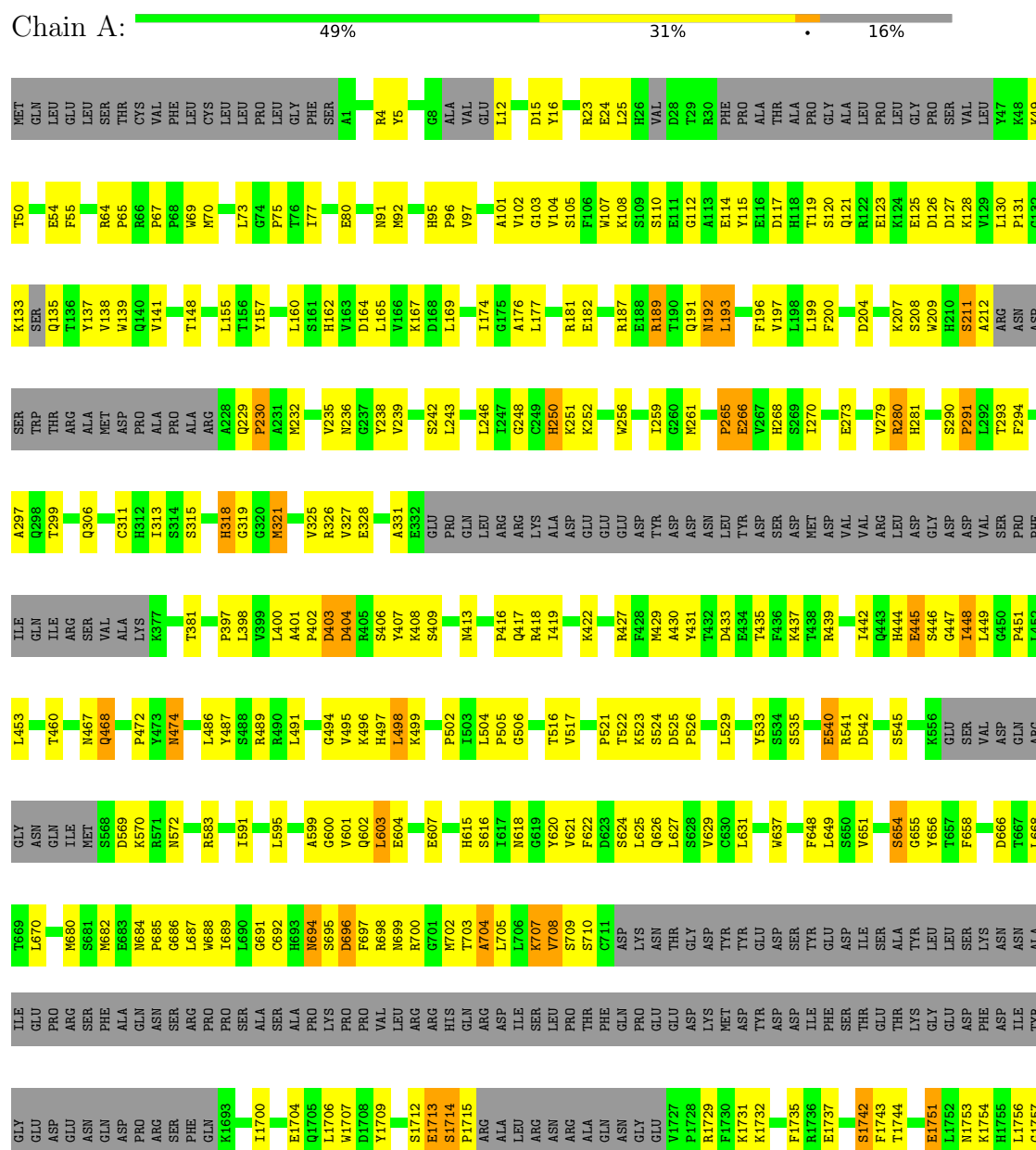
- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca).

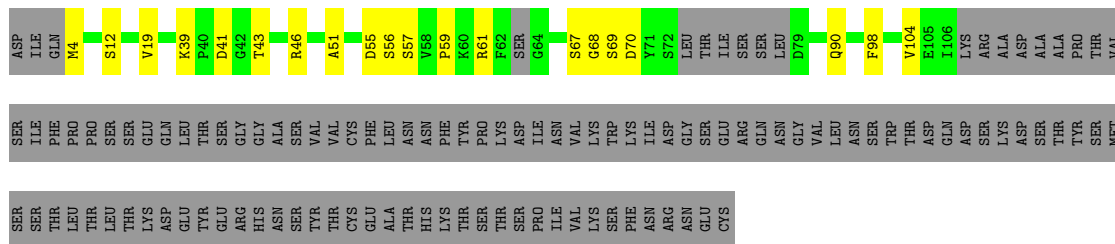
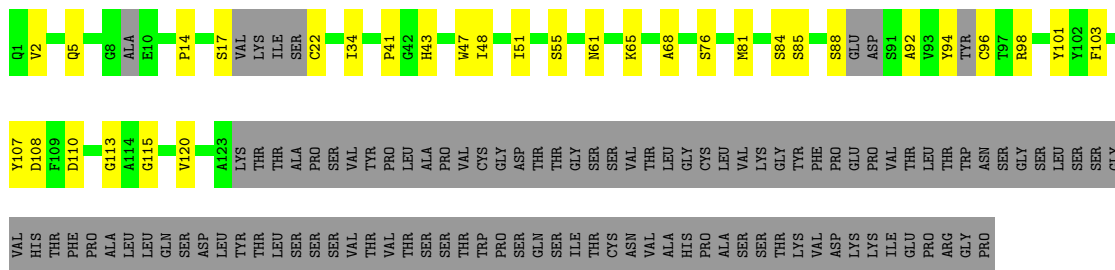
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Ca	0	0
			1	1		

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: Coagulation factor VIII,Coagulation factor VIII,Coagulation factor VIII,Coagulation factor VIII,Coagulation factor VIII





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

Chain G:  50% 50%

MAG1
MAG2

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

Chain B:  100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	132.24Å 132.24Å 380.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.48 – 4.15 25.48 – 4.15	Depositor EDS
% Data completeness (in resolution range)	99.1 (25.48-4.15) 99.1 (25.48-4.15)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 4.10Å)	Xtriage
Refinement program	PHENIX (1.16_3549: ???)	Depositor
R, R_{free}	0.300 , 0.338 0.303 , 0.338	Depositor DCC
R_{free} test set	2000 reflections (7.56%)	wwPDB-VP
Wilson B-factor (Å ²)	195.9	Xtriage
Anisotropy	0.363	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 202.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11366	wwPDB-VP
Average B, all atoms (Å ²)	253.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.13% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

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

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	0.22	0/10070	0.66	0/13647
2	E	0.20	0/833	0.33	0/1129
3	F	0.14	0/673	0.43	0/906
All	All	0.21	0/11576	0.63	0/15682

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2057	GLY	Peptide
1	A	2141	ASN	Peptide
1	A	2178	LEU	Mainchain
1	A	2278	GLY	Peptide
1	A	404	ASP	Peptide
1	A	570	LYS	Peptide
1	A	691	GLY	Peptide
1	A	696	ASP	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9809	0	9455	339	0
2	E	818	0	700	18	0
3	F	666	0	587	11	0
4	B	28	0	25	0	0
4	G	28	0	25	1	0
5	A	14	0	13	0	0
6	A	1	0	0	0	0
7	A	1	0	0	0	0
8	A	1	0	0	0	0
All	All	11366	0	10805	363	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 16.

All (363) 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:1781:ARG:HG2	1:A:1782:PRO:HD2	1.49	0.93
1:A:540:GLU:HG2	1:A:583:ARG:HH21	1.39	0.85
1:A:64:ARG:HH21	1:A:65:PRO:HD2	1.41	0.85
1:A:1927:ASP:HA	1:A:2012:THR:HA	1.58	0.84
1:A:54:GLU:HG2	1:A:75:PRO:HG3	1.58	0.83
1:A:1846:ASP:HB3	1:A:1889:TRP:HE1	1.46	0.81
1:A:708:VAL:HG23	1:A:709:SER:H	1.45	0.81
1:A:12:LEU:N	1:A:49:LYS:O	2.17	0.77
3:F:4:MET:HE2	3:F:90:GLN:HB2	1.67	0.77
1:A:2246:GLN:HB3	1:A:2320:ARG:HB2	1.66	0.76
1:A:401:ALA:O	1:A:403:ASP:N	2.19	0.75
1:A:266:GLU:OE1	1:A:318:HIS:NE2	2.19	0.75
1:A:1874:GLN:HE22	1:A:1934:MET:HA	1.51	0.75
1:A:406:SER:O	1:A:408:LYS:N	2.15	0.75
1:A:2261:LEU:HD11	1:A:2282:VAL:HG12	1.69	0.75
1:A:2179:GLY:HA3	1:A:2184:ALA:HB3	1.69	0.73
1:A:2100:GLN:HB2	1:A:2155:HIS:HB2	1.70	0.73
1:A:243:LEU:HD12	1:A:246:LEU:HD23	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:THR:HG23	1:A:437:LYS:H	1.53	0.73
1:A:256:TRP:HE1	1:A:299:THR:HG22	1.54	0.72
1:A:293:THR:HA	1:A:1977:ASN:HD21	1.54	0.72
1:A:2274:PHE:HB3	1:A:2281:LYS:HE2	1.71	0.72
1:A:2265:SER:O	1:A:2303:THR:OG1	2.09	0.71
1:A:80:GLU:HG2	1:A:182:GLU:HA	1.73	0.71
1:A:120:SER:OG	1:A:123:GLU:OE1	2.08	0.70
1:A:2187:ASP:OD1	1:A:2209:ARG:NH2	2.25	0.69
1:A:1709:TYR:O	1:A:1925:VAL:HG12	1.93	0.68
1:A:467:ASN:OD1	1:A:468:GLN:N	2.27	0.68
1:A:130:LEU:HG	1:A:131:PRO:HD2	1.75	0.67
2:E:34:ILE:HD11	2:E:51:ILE:HD12	1.77	0.67
1:A:620:TYR:HB3	1:A:624:SER:HB2	1.77	0.66
1:A:615:HIS:HB3	1:A:702:MET:HE3	1.78	0.66
1:A:2236:LYS:NZ	1:A:2237:THR:OG1	2.29	0.66
1:A:238:TYR:HD2	1:A:243:LEU:HA	1.60	0.66
1:A:2142:PRO:HG3	4:G:1:NAG:H81	1.78	0.65
1:A:1993:VAL:HA	1:A:2016:VAL:HG23	1.78	0.65
1:A:280:ARG:O	1:A:281:HIS:ND1	2.30	0.65
1:A:1782:PRO:HB3	1:A:1809:PRO:HD3	1.78	0.65
3:F:56:SER:OG	3:F:57:SER:N	2.30	0.64
1:A:1776:LYS:HD2	1:A:1812:THR:HB	1.78	0.64
1:A:1756:LEU:HD21	1:A:1762:TYR:CE2	2.32	0.64
1:A:121:GLN:OE1	1:A:121:GLN:N	2.31	0.64
1:A:114:GLU:HB2	1:A:127:ASP:HB3	1.80	0.64
1:A:1946:SER:HB3	1:A:1978:LEU:HD22	1.80	0.64
1:A:160:LEU:HD22	1:A:169:LEU:HD21	1.79	0.63
1:A:1805:ASN:O	1:A:1813:ARG:NH1	2.32	0.63
1:A:80:GLU:CG	1:A:182:GLU:HA	2.28	0.63
1:A:2198:ASN:OD1	1:A:2199:MET:N	2.32	0.63
1:A:504:LEU:O	1:A:506:GLY:N	2.32	0.63
1:A:666:ASP:HB2	1:A:1835:TRP:HZ3	1.64	0.62
1:A:2169:CYS:SG	1:A:2173:SER:HA	2.39	0.62
1:A:2260:PHE:HE1	1:A:2262:ILE:HD11	1.63	0.62
1:A:235:VAL:HG23	1:A:321:MET:HA	1.81	0.62
1:A:326:ARG:NH1	1:A:328:GLU:OE2	2.33	0.62
1:A:73:LEU:HD21	1:A:199:LEU:HB2	1.81	0.62
1:A:2027:MET:HE1	1:A:2073:VAL:HG21	1.81	0.62
1:A:427:ARG:HE	1:A:448:ILE:HA	1.65	0.61
2:E:47:TRP:HE3	2:E:61:ASN:HD22	1.49	0.61
1:A:522:THR:O	1:A:524:SER:N	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2044:GLY:C	1:A:2046:TRP:H	2.08	0.61
1:A:110:SER:OG	1:A:137:TYR:O	2.09	0.60
1:A:2274:PHE:HD2	1:A:2281:LYS:HD3	1.66	0.60
1:A:73:LEU:HD12	1:A:236:ASN:ND2	2.16	0.60
1:A:239:VAL:O	1:A:242:SER:OG	2.18	0.60
1:A:649:LEU:HA	1:A:694:ASN:ND2	2.18	0.58
1:A:2021:CYS:SG	1:A:2175:SER:OG	2.61	0.58
1:A:696:ASP:HA	1:A:699:ASN:OD1	2.03	0.58
1:A:2106:SER:N	1:A:2148:TYR:O	2.36	0.58
1:A:54:GLU:HG2	1:A:75:PRO:CG	2.33	0.58
1:A:2194:SER:OG	1:A:2228:GLU:OE2	2.21	0.58
1:A:654:SER:O	1:A:656:TYR:N	2.36	0.57
1:A:293:THR:HA	1:A:1977:ASN:ND2	2.18	0.57
1:A:496:LYS:H	1:A:496:LYS:HD3	1.68	0.57
1:A:2246:GLN:HE22	1:A:2292:PRO:HD3	1.70	0.57
1:A:189:ARG:HB3	1:A:192:ASN:OD1	2.05	0.57
1:A:591:ILE:HG23	1:A:595:LEU:HD22	1.87	0.57
1:A:680:MET:HE2	1:A:682:MET:SD	2.45	0.57
1:A:2254:SER:O	1:A:2315:HIS:ND1	2.37	0.57
1:A:2281:LYS:HZ2	1:A:2283:PHE:HE2	1.53	0.57
2:E:108:ASP:O	3:F:46:ARG:NH1	2.34	0.57
1:A:444:HIS:O	1:A:445:GLU:HB2	2.04	0.57
1:A:2235:GLN:O	1:A:2304:ARG:NH1	2.37	0.57
1:A:497:HIS:C	1:A:499:LYS:H	2.13	0.56
1:A:601:VAL:HG23	1:A:602:GLN:H	1.70	0.56
1:A:73:LEU:HD12	1:A:236:ASN:HD22	1.69	0.56
1:A:525:ASP:HB2	1:A:526:PRO:HD2	1.87	0.56
1:A:1870:GLN:O	1:A:1871:VAL:HG22	2.05	0.56
1:A:1706:LEU:HD21	1:A:1729:ARG:HD3	1.87	0.56
1:A:686:GLY:O	1:A:708:VAL:HG22	2.06	0.56
1:A:649:LEU:HA	1:A:694:ASN:HD21	1.70	0.56
1:A:107:TRP:O	1:A:108:LYS:HB2	2.04	0.55
1:A:1786:TYR:CD1	1:A:1790:ILE:HD11	2.42	0.55
1:A:311:CYS:SG	1:A:313:ILE:HG22	2.48	0.54
1:A:541:ARG:HG2	1:A:583:ARG:HB3	1.89	0.54
1:A:629:VAL:HG23	1:A:708:VAL:HG12	1.88	0.54
1:A:104:VAL:HG12	1:A:105:SER:H	1.73	0.54
1:A:694:ASN:O	1:A:696:ASP:N	2.41	0.54
1:A:5:TYR:CE2	1:A:77:ILE:HG23	2.43	0.54
1:A:491:LEU:HD23	1:A:495:VAL:HB	1.89	0.54
1:A:601:VAL:O	1:A:603:LEU:N	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1951:GLU:OE2	1:A:1952:ASN:ND2	2.40	0.54
1:A:2115:TYR:OH	1:A:2142:PRO:HD2	2.08	0.54
1:A:2104:MET:O	1:A:2150:ARG:N	2.36	0.54
1:A:2119:SER:O	1:A:2121:GLY:N	2.40	0.54
1:A:1826:THR:HG22	1:A:1828:ASP:H	1.73	0.54
1:A:162:HIS:NE2	1:A:1999:GLU:OE2	2.33	0.53
1:A:204:ASP:OD2	1:A:207:LYS:NZ	2.38	0.53
1:A:2201:ALA:HB1	1:A:2203:TRP:NE1	2.23	0.53
1:A:246:LEU:HD12	1:A:325:VAL:HG13	1.89	0.53
1:A:692:CYS:HB3	1:A:698:ARG:HB2	1.90	0.53
1:A:631:LEU:HD11	1:A:685:PRO:HB3	1.91	0.53
1:A:1781:ARG:C	1:A:1809:PRO:HG3	2.33	0.53
1:A:176:ALA:HB2	1:A:197:VAL:HG11	1.92	0.52
1:A:2100:GLN:O	1:A:2154:THR:HG22	2.09	0.52
1:A:2091:GLN:O	1:A:2093:PHE:N	2.42	0.52
1:A:1764:ARG:HG2	1:A:1856:LEU:HB2	1.91	0.52
1:A:2193:SER:HB3	2:E:103:PHE:CD2	2.44	0.52
1:A:2273:LEU:HD21	2:E:101:TYR:CE1	2.45	0.52
1:A:1894:ASN:HA	1:A:1896:GLU:HG3	1.92	0.52
2:E:14:PRO:HG3	2:E:120:VAL:HG12	1.92	0.51
1:A:687:LEU:HD21	1:A:705:LEU:HD23	1.92	0.51
1:A:248:GLY:O	1:A:327:VAL:HA	2.10	0.51
1:A:429:MET:HE2	1:A:439:ARG:HD3	1.92	0.51
1:A:148:THR:O	1:A:181:ARG:NH2	2.35	0.51
1:A:200:PHE:HE2	1:A:270:ILE:HG21	1.76	0.51
1:A:447:GLY:O	1:A:448:ILE:HG22	2.09	0.51
1:A:1832:CYS:HA	1:A:1858:CYS:HA	1.93	0.51
1:A:1834:ALA:HB2	1:A:1943:TYR:CD1	2.46	0.51
1:A:2103:ILE:HD13	1:A:2140:PHE:CE1	2.46	0.51
3:F:39:LYS:HB2	3:F:43:THR:HB	1.92	0.51
1:A:1870:GLN:C	1:A:1872:THR:H	2.19	0.51
1:A:4:ARG:O	1:A:5:TYR:HD1	1.93	0.51
1:A:2080:ILE:HG12	1:A:2145:ILE:HD12	1.91	0.51
1:A:2246:GLN:HE22	1:A:2292:PRO:CD	2.23	0.51
1:A:1829:GLU:O	1:A:1859:ARG:NH2	2.44	0.50
1:A:708:VAL:HG23	1:A:709:SER:N	2.22	0.50
2:E:88:SER:HA	2:E:120:VAL:HB	1.93	0.50
1:A:1732:LYS:NZ	1:A:1885:GLU:OE2	2.28	0.50
1:A:409:SER:HB2	1:A:413:ASN:HD22	1.77	0.50
1:A:2250:SER:O	1:A:2252:LEU:N	2.45	0.50
2:E:110:ASP:HA	3:F:46:ARG:HD3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:MET:O	1:A:236:ASN:ND2	2.42	0.50
1:A:1808:GLN:HB2	1:A:1811:GLU:HG2	1.92	0.50
1:A:2101:PHE:HE2	1:A:2103:ILE:HD11	1.76	0.50
1:A:50:THR:HG21	1:A:95:HIS:NE2	2.27	0.50
3:F:12:SER:HA	3:F:104:VAL:HG12	1.92	0.50
1:A:290:SER:O	1:A:291:PRO:C	2.55	0.50
1:A:1742:SER:O	1:A:1744:THR:N	2.44	0.50
1:A:2009:GLY:O	1:A:2011:SER:N	2.45	0.50
1:A:429:MET:HE1	1:A:442:ILE:HG22	1.95	0.49
1:A:2262:ILE:HD13	1:A:2281:LYS:HZ1	1.77	0.49
1:A:1756:LEU:HD21	1:A:1762:TYR:HE2	1.76	0.49
1:A:2036:GLN:NE2	1:A:2074:ASP:O	2.44	0.49
1:A:2207:LYS:HE2	1:A:2216:SER:O	2.12	0.49
1:A:684:ASN:O	1:A:708:VAL:HG21	2.12	0.49
1:A:1712:SER:OG	1:A:1713:GLU:OE1	2.21	0.49
1:A:2049:LYS:HG3	1:A:2050:LEU:HD22	1.93	0.49
1:A:119:THR:HG23	1:A:123:GLU:HB2	1.95	0.49
1:A:1764:ARG:HB3	1:A:1863:LEU:HD11	1.94	0.49
1:A:91:ASN:ND2	1:A:97:VAL:HG22	2.27	0.49
1:A:2027:MET:HA	1:A:2032:ILE:CG2	2.43	0.49
1:A:2313:TRP:HB3	1:A:2317:ILE:HD13	1.94	0.49
1:A:1737:GLU:HB2	1:A:1761:PRO:HG3	1.94	0.48
1:A:2098:ILE:HD13	1:A:2162:LEU:HD13	1.95	0.48
1:A:2112:TRP:CZ3	1:A:2150:ARG:HB2	2.48	0.48
1:A:182:GLU:H	1:A:182:GLU:CD	2.19	0.48
1:A:1808:GLN:O	1:A:1810:ASN:N	2.46	0.48
1:A:2042:GLN:O	1:A:2044:GLY:N	2.47	0.48
1:A:495:VAL:HG12	1:A:498:LEU:H	1.78	0.48
1:A:1934:MET:SD	1:A:1940:ILE:HD13	2.54	0.48
1:A:2228:GLU:HG3	1:A:2229:TRP:N	2.29	0.48
1:A:77:ILE:HD12	1:A:177:LEU:HD13	1.95	0.48
1:A:666:ASP:HB2	1:A:1835:TRP:CZ3	2.48	0.48
1:A:1707:TRP:HB3	1:A:1732:LYS:HG3	1.95	0.48
1:A:1756:LEU:O	1:A:1759:LEU:HB2	2.14	0.48
1:A:2241:THR:HA	1:A:2300:PRO:HB3	1.95	0.48
1:A:486:LEU:HG	1:A:487:TYR:CD2	2.49	0.47
1:A:2058:SER:OG	1:A:2059:ILE:N	2.45	0.47
1:A:2241:THR:HG22	1:A:2325:GLY:HA2	1.96	0.47
1:A:616:SER:HA	1:A:621:VAL:HG12	1.96	0.47
1:A:2164:MET:HE3	1:A:2164:MET:HB2	1.76	0.47
1:A:489:ARG:HE	1:A:489:ARG:HB2	1.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:ASP:OD1	1:A:404:ASP:N	2.47	0.47
1:A:658:PHE:HA	1:A:680:MET:HB3	1.95	0.47
1:A:697:PHE:O	1:A:700:ARG:N	2.43	0.47
2:E:110:ASP:OD1	2:E:110:ASP:N	2.47	0.47
1:A:2053:LEU:HG	1:A:2087:GLN:OE1	2.15	0.47
1:A:268:HIS:ND1	1:A:321:MET:HE2	2.30	0.47
1:A:631:LEU:HD12	1:A:710:SER:HB3	1.97	0.47
1:A:2103:ILE:HD13	1:A:2140:PHE:HE1	1.79	0.47
1:A:2116:ARG:HG3	1:A:2123:LEU:HA	1.97	0.47
1:A:1936:GLN:O	1:A:1990:PRO:HG2	2.15	0.47
1:A:540:GLU:HG2	1:A:583:ARG:NH2	2.18	0.47
3:F:41:ASP:OD1	3:F:41:ASP:N	2.44	0.47
1:A:602:GLN:O	1:A:604:GLU:N	2.46	0.47
1:A:648:PHE:CZ	1:A:1953:ILE:HD11	2.50	0.47
1:A:2046:TRP:CZ2	1:A:2059:ILE:HG22	2.50	0.47
1:A:155:LEU:HD11	1:A:1972:LYS:O	2.15	0.46
1:A:1751:GLU:H	1:A:1754:LYS:HG3	1.80	0.46
1:A:2038:THR:O	1:A:2072:LYS:N	2.48	0.46
1:A:703:THR:O	1:A:704:ALA:HB3	2.15	0.46
1:A:1846:ASP:HB3	1:A:1889:TRP:NE1	2.24	0.46
3:F:67:SER:O	3:F:70:ASP:N	2.40	0.46
1:A:1759:LEU:HD22	1:A:1922:ASN:ND2	2.29	0.46
1:A:2080:ILE:HG13	1:A:2171:LEU:HD23	1.97	0.46
1:A:164:ASP:HB3	1:A:167:LYS:HB2	1.96	0.46
1:A:266:GLU:CD	1:A:318:HIS:HE2	2.23	0.46
1:A:525:ASP:HB2	1:A:526:PRO:CD	2.44	0.46
1:A:1735:PHE:O	1:A:1760:GLY:HA2	2.16	0.46
1:A:102:VAL:HG13	1:A:1957:HIS:CE1	2.50	0.46
1:A:472:PRO:HB2	1:A:502:PRO:HB2	1.98	0.46
1:A:2093:PHE:HD1	1:A:2093:PHE:H	1.64	0.46
1:A:67:PRO:HD2	1:A:70:MET:HE3	1.98	0.46
1:A:497:HIS:O	1:A:499:LYS:N	2.48	0.46
1:A:2096:LEU:HD23	1:A:2159:ARG:HB2	1.97	0.46
2:E:96:CYS:O	2:E:113:GLY:N	2.48	0.46
1:A:279:VAL:O	1:A:281:HIS:N	2.49	0.46
1:A:599:ALA:O	1:A:601:VAL:HG13	2.16	0.46
1:A:230:PRO:HB2	1:A:232:MET:HE3	1.97	0.45
1:A:703:THR:OG1	1:A:704:ALA:N	2.48	0.45
1:A:2228:GLU:HG3	1:A:2229:TRP:H	1.81	0.45
1:A:1762:TYR:OH	1:A:1877:ALA:N	2.49	0.45
1:A:637:TRP:HE1	1:A:682:MET:HE1	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1731:LYS:HD3	1:A:1890:TYR:HB3	1.98	0.45
1:A:2274:PHE:HD1	1:A:2301:LEU:HD12	1.81	0.45
1:A:1753:ASN:HB3	1:A:1756:LEU:HD23	1.98	0.45
1:A:591:ILE:O	1:A:595:LEU:HB2	2.17	0.45
1:A:651:VAL:HG12	1:A:668:LEU:O	2.16	0.45
1:A:2230:LEU:HB3	1:A:2308:ILE:HG22	1.99	0.45
1:A:279:VAL:HG12	1:A:297:ALA:HB2	1.99	0.45
1:A:542:ASP:O	1:A:545:SER:OG	2.31	0.45
1:A:1781:ARG:HH21	1:A:1783:TYR:HE1	1.64	0.45
1:A:1996:TRP:HB2	1:A:2014:PHE:CZ	2.52	0.45
1:A:445:GLU:O	1:A:618:ASN:ND2	2.50	0.45
1:A:1714:SER:HA	1:A:1715:PRO:HD2	1.88	0.45
1:A:1732:LYS:HD3	1:A:1758:LEU:HD21	1.99	0.45
1:A:1783:TYR:O	1:A:1807:VAL:HB	2.17	0.45
1:A:2026:GLY:O	1:A:2032:ILE:HG22	2.16	0.45
1:A:2107:LEU:HD13	1:A:2146:ALA:HA	1.98	0.45
1:A:130:LEU:H	1:A:133:LYS:NZ	2.15	0.44
1:A:2070:TRP:HB3	1:A:2152:HIS:CE1	2.52	0.44
1:A:2112:TRP:CH2	1:A:2148:TYR:HB3	2.51	0.44
1:A:1826:THR:HB	1:A:1829:GLU:HG3	2.00	0.44
1:A:1732:LYS:HD3	1:A:1758:LEU:HD11	1.99	0.44
1:A:2178:LEU:HD13	1:A:2323:VAL:HB	1.99	0.44
1:A:64:ARG:HD2	1:A:65:PRO:HD2	1.99	0.44
2:E:98:ARG:NH2	2:E:107:TYR:HB3	2.33	0.44
1:A:692:CYS:C	1:A:694:ASN:H	2.26	0.44
1:A:2187:ASP:HB3	1:A:2206:SER:HB2	1.99	0.44
2:E:68:ALA:HA	2:E:81:MET:HE3	2.00	0.44
1:A:23:ARG:C	1:A:25:LEU:N	2.76	0.44
1:A:91:ASN:HD21	1:A:96:PRO:HA	1.82	0.44
1:A:165:LEU:HD23	1:A:2003:GLY:HA2	2.00	0.44
1:A:250:HIS:O	1:A:252:LYS:N	2.44	0.44
1:A:259:ILE:HG23	1:A:294:PHE:CE1	2.52	0.44
1:A:430:ALA:HB2	1:A:451:PRO:HG3	1.99	0.43
1:A:1757:GLY:C	1:A:1759:LEU:H	2.26	0.43
1:A:1820:GLN:HG2	1:A:1823:MET:HE3	1.99	0.43
2:E:41:PRO:HD3	2:E:92:ALA:HA	2.00	0.43
1:A:69:TRP:CE2	1:A:196:PHE:HD1	2.35	0.43
1:A:467:ASN:O	1:A:468:GLN:HG3	2.17	0.43
1:A:497:HIS:C	1:A:499:LYS:N	2.76	0.43
1:A:1924:TYR:CD1	1:A:1928:THR:HG22	2.54	0.43
1:A:1781:ARG:O	1:A:1809:PRO:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2174:CYS:HG	1:A:2326:CYS:HG	1.59	0.43
1:A:103:GLY:HA2	1:A:1962:VAL:HG12	2.00	0.43
1:A:1894:ASN:C	1:A:1896:GLU:H	2.27	0.43
1:A:516:THR:OG1	1:A:517:VAL:N	2.51	0.43
1:A:692:CYS:SG	1:A:694:ASN:HB2	2.59	0.43
1:A:1758:LEU:HD23	1:A:1883:PHE:CZ	2.53	0.43
1:A:1769:ASP:O	1:A:1819:VAL:HG12	2.19	0.43
1:A:2193:SER:HB2	1:A:2228:GLU:CD	2.44	0.43
1:A:101:ALA:HB2	1:A:139:TRP:CZ2	2.53	0.43
1:A:486:LEU:HD12	1:A:487:TYR:H	1.83	0.43
1:A:1768:GLU:H	1:A:1819:VAL:HG13	1.82	0.43
1:A:306:GLN:HA	1:A:325:VAL:O	2.19	0.43
1:A:422:LYS:HB2	1:A:422:LYS:HE3	1.82	0.43
1:A:125:GLU:HB2	1:A:135:GLN:HE22	1.83	0.43
1:A:1778:GLN:HB3	1:A:1779:ALA:H	1.59	0.43
1:A:1784:SER:OG	1:A:1805:ASN:OD1	2.37	0.43
1:A:2098:ILE:HG21	1:A:2101:PHE:HB3	2.01	0.43
1:A:2192:ALA:HB2	1:A:2230:LEU:HD12	2.01	0.43
1:A:431:TYR:CE2	1:A:439:ARG:HG2	2.53	0.43
1:A:15:ASP:O	1:A:16:TYR:HB2	2.19	0.42
1:A:55:PHE:CZ	1:A:92:MET:HE1	2.54	0.42
1:A:2258:LYS:HB2	1:A:2258:LYS:HE3	1.84	0.42
1:A:397:PRO:HD2	1:A:624:SER:HB3	2.01	0.42
1:A:2027:MET:O	1:A:2052:ARG:NH1	2.52	0.42
1:A:2044:GLY:O	1:A:2046:TRP:N	2.50	0.42
1:A:2207:LYS:HB3	1:A:2207:LYS:HE3	1.78	0.42
1:A:2236:LYS:HG3	1:A:2237:THR:N	2.34	0.42
1:A:115:TYR:CE2	1:A:117:ASP:HB3	2.54	0.42
1:A:626:GLN:HB3	1:A:707:LYS:HE2	2.01	0.42
1:A:101:ALA:HB2	1:A:139:TRP:CH2	2.54	0.42
1:A:265:PRO:HB2	1:A:266:GLU:H	1.55	0.42
1:A:398:LEU:HD22	1:A:398:LEU:HA	1.86	0.42
1:A:2088:GLY:C	1:A:2163:ARG:HH21	2.26	0.42
1:A:1929:LEU:HD23	1:A:2012:THR:HG21	2.02	0.42
1:A:418:ARG:CZ	1:A:607:GLU:HG2	2.50	0.42
1:A:680:MET:HE3	1:A:680:MET:HB2	1.76	0.42
1:A:1704:GLU:OE2	1:A:1780:SER:N	2.49	0.42
1:A:2080:ILE:HG22	1:A:2082:HIS:CE1	2.55	0.42
1:A:182:GLU:OE1	1:A:182:GLU:N	2.25	0.42
1:A:381:THR:HG22	1:A:460:THR:OG1	2.19	0.42
1:A:2044:GLY:C	1:A:2046:TRP:N	2.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2194:SER:HB2	1:A:2222:GLN:HB2	2.02	0.42
1:A:2313:TRP:CE3	1:A:2317:ILE:HD11	2.55	0.42
1:A:119:THR:CG2	1:A:123:GLU:HB2	2.50	0.42
1:A:192:ASN:HB2	1:A:193:LEU:H	1.64	0.42
1:A:246:LEU:HD11	1:A:325:VAL:HG22	2.01	0.42
1:A:315:SER:O	1:A:318:HIS:HB2	2.20	0.42
1:A:446:SER:O	1:A:449:LEU:HG	2.19	0.42
1:A:453:LEU:HD22	1:A:533:TYR:CE2	2.55	0.42
1:A:1874:GLN:NE2	1:A:1934:MET:HA	2.25	0.42
1:A:2116:ARG:CG	1:A:2123:LEU:HA	2.50	0.42
1:A:167:LYS:HB3	1:A:209:TRP:CD1	2.55	0.41
1:A:417:GLN:O	1:A:418:ARG:NE	2.52	0.41
1:A:1700:ILE:O	1:A:1775:PHE:HA	2.20	0.41
1:A:2105:TYR:HA	1:A:2149:ILE:HA	2.02	0.41
3:F:68:GLY:HA2	3:F:69:SER:HA	1.51	0.41
1:A:211:SER:HB2	1:A:212:ALA:H	1.62	0.41
1:A:2128:GLY:O	1:A:2136:LYS:HG2	2.20	0.41
2:E:94:TYR:C	2:E:115:GLY:HA2	2.45	0.41
3:F:55:ASP:OD1	3:F:56:SER:N	2.37	0.41
1:A:2204:SER:O	1:A:2207:LYS:HG2	2.20	0.41
1:A:2230:LEU:O	1:A:2307:ARG:HA	2.20	0.41
1:A:2258:LYS:HE2	1:A:2314:VAL:HG23	2.02	0.41
1:A:2182:SER:C	1:A:2184:ALA:H	2.28	0.41
2:E:5:GLN:O	2:E:22:CYS:HA	2.20	0.41
3:F:59:PRO:HG2	3:F:61:ARG:NH2	2.35	0.41
1:A:670:LEU:HD23	1:A:670:LEU:HA	1.79	0.41
1:A:69:TRP:CE2	1:A:196:PHE:CD1	3.09	0.41
1:A:165:LEU:HA	1:A:165:LEU:HD12	1.81	0.41
1:A:2260:PHE:CE1	1:A:2262:ILE:HD11	2.49	0.41
1:A:2280:VAL:HB	2:E:55:SER:HB3	2.01	0.41
1:A:208:SER:OG	1:A:209:TRP:N	2.53	0.41
1:A:433:ASP:OD1	1:A:435:THR:HG22	2.20	0.41
1:A:474:ASN:O	1:A:535:SER:HB2	2.21	0.41
1:A:684:ASN:HD21	1:A:1791:SER:HA	1.86	0.41
1:A:1998:ILE:HG13	1:A:2014:PHE:CE1	2.56	0.41
1:A:157:TYR:HB2	1:A:177:LEU:HB3	2.03	0.41
1:A:627:LEU:HD23	1:A:705:LEU:O	2.20	0.41
1:A:654:SER:HB2	1:A:688:TRP:HB3	2.02	0.41
1:A:689:ILE:O	1:A:689:ILE:HG13	2.21	0.41
1:A:708:VAL:O	1:A:709:SER:HB3	2.20	0.41
1:A:1760:GLY:N	1:A:1852:ILE:O	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:GLY:HA2	1:A:126:ASP:O	2.21	0.41
1:A:1889:TRP:C	1:A:1891:PHE:H	2.28	0.41
1:A:2248:VAL:O	1:A:2289:SER:HB2	2.21	0.41
1:A:620:TYR:CD1	1:A:625:LEU:HB2	2.56	0.40
1:A:2033:ARG:HB2	1:A:2035:PHE:CE1	2.56	0.40
1:A:2260:PHE:C	1:A:2261:LEU:HD12	2.46	0.40
1:A:169:LEU:HB3	1:A:261:MET:HE3	2.04	0.40
1:A:55:PHE:HZ	1:A:92:MET:HE1	1.85	0.40
1:A:128:LYS:HB3	1:A:128:LYS:HE3	1.78	0.40
1:A:521:PRO:HG3	1:A:529:LEU:HD23	2.03	0.40
1:A:1803:ARG:O	1:A:1804:HIS:C	2.64	0.40
2:E:61:ASN:O	2:E:65:LYS:HG2	2.20	0.40
1:A:189:ARG:O	1:A:191:GLN:N	2.54	0.40
1:A:2176:MET:HE3	1:A:2176:MET:HB2	1.90	0.40
1:A:2027:MET:HA	1:A:2032:ILE:HG22	2.04	0.40
1:A:2281:LYS:NZ	1:A:2297:LEU:HD21	2.37	0.40
2:E:17:SER:HA	2:E:84:SER:HA	2.03	0.40

There are no symmetry-related clashes.

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	1211/1467 (82%)	952 (79%)	170 (14%)	89 (7%)	1	11
2	E	105/224 (47%)	82 (78%)	19 (18%)	4 (4%)	2	20
3	F	90/214 (42%)	63 (70%)	24 (27%)	3 (3%)	3	21
All	All	1406/1905 (74%)	1097 (78%)	213 (15%)	96 (7%)	1	12

All (96) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	192	ASN
1	A	229	GLN
1	A	250	HIS
1	A	265	PRO
1	A	291	PRO
1	A	318	HIS
1	A	321	MET
1	A	402	PRO
1	A	407	TYR
1	A	416	PRO
1	A	505	PRO
1	A	572	ASN
1	A	603	LEU
1	A	655	GLY
1	A	1713	GLU
1	A	1796	GLN
1	A	1804	HIS
1	A	1871	VAL
1	A	1889	TRP
1	A	1936	GLN
1	A	2010	MET
1	A	2120	THR
1	A	2183	LYS
1	A	2206	SER
1	A	24	GLU
1	A	189	ARG
1	A	280	ARG
1	A	400	LEU
1	A	403	ASP
1	A	419	ILE
1	A	445	GLU
1	A	468	GLN
1	A	523	LYS
1	A	600	GLY
1	A	707	LYS
1	A	1743	PHE
1	A	1809	PRO
1	A	2092	LYS
1	A	2119	SER
1	A	2184	ALA
1	A	2199	MET
1	A	2251	LEU
2	E	43	HIS

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Mol	Chain	Res	Type
3	F	19	VAL
1	A	193	LEU
1	A	211	SER
1	A	230	PRO
1	A	251	LYS
1	A	266	GLU
1	A	319	GLY
1	A	1742	SER
1	A	1751	GLU
1	A	1778	GLN
1	A	1897	ARG
1	A	1938	GLN
1	A	2040	SER
1	A	2043	TYR
1	A	2045	GLN
1	A	2067	PRO
1	A	2218	ALA
1	A	2252	LEU
2	E	85	SER
3	F	98	PHE
1	A	138	VAL
1	A	273	GLU
1	A	331	ALA
1	A	498	LEU
1	A	654	SER
1	A	694	ASN
1	A	695	SER
1	A	704	ALA
1	A	1714	SER
1	A	1798	GLN
1	A	2132	SER
1	A	2315	HIS
2	E	76	SER
3	F	51	ALA
1	A	187	ARG
1	A	540	GLU
1	A	569	ASP
1	A	622	PHE
1	A	1810	ASN
1	A	1843	LEU
1	A	1860	ALA
1	A	1890	TYR

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Mol	Chain	Res	Type
1	A	2142	PRO
1	A	474	ASN
1	A	708	VAL
1	A	1779	ALA
1	A	2058	SER
1	A	2116	ARG
1	A	141	VAL
1	A	174	ILE
1	A	448	ILE
1	A	494	GLY
2	E	48	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	1052/1301 (81%)	1052 (100%)	0	100	100
2	E	80/191 (42%)	79 (99%)	1 (1%)	61	71
3	F	64/191 (34%)	64 (100%)	0	100	100
All	All	1196/1683 (71%)	1195 (100%)	1 (0%)	88	88

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	2	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	268	HIS
1	A	684	ASN
1	A	694	ASN
1	A	1745	GLN
1	A	1770	ASN

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Mol	Chain	Res	Type
1	A	1864	ASN
1	A	1894	ASN
1	A	1938	GLN
1	A	2100	GLN
1	A	2129	ASN
1	A	2172	ASN
1	A	2189	GLN
1	A	2286	ASN
2	E	59	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 ⓘ

4 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	B	1	4,1	14,14,15	0.43	0	17,19,21	0.52	0
4	NAG	B	2	4	14,14,15	0.28	0	17,19,21	0.65	0
4	NAG	G	1	4,1	14,14,15	0.69	1 (7%)	17,19,21	0.67	1 (5%)
4	NAG	G	2	4	14,14,15	0.91	1 (7%)	17,19,21	1.26	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	B	2	4	1/1/5/7	4/6/23/26	0/1/1/1
4	NAG	G	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	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)
4	G	2	NAG	O5-C1	-2.39	1.39	1.43
4	G	1	NAG	O5-C1	2.18	1.47	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	2	NAG	C4-C3-C2	2.72	115.00	111.02
4	G	2	NAG	C2-N2-C7	2.62	126.41	122.90
4	G	1	NAG	C1-O5-C5	2.07	114.97	112.19

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	2	NAG	C1

All (9) torsion outliers are listed below:

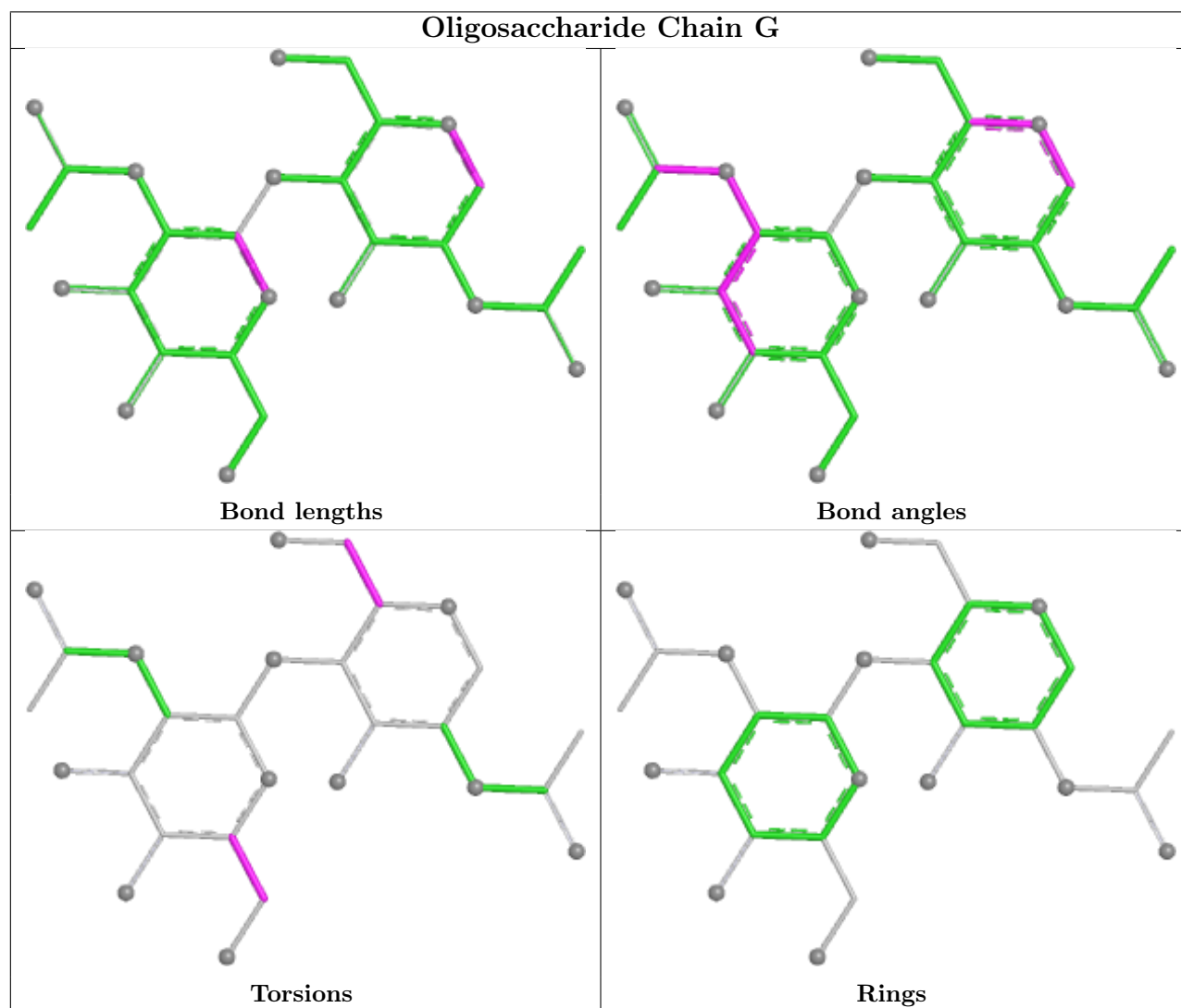
Mol	Chain	Res	Type	Atoms
4	B	1	NAG	O5-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
4	B	1	NAG	C4-C5-C6-O6
4	B	2	NAG	C8-C7-N2-C2
4	B	2	NAG	O7-C7-N2-C2
4	G	1	NAG	O5-C5-C6-O6
4	B	2	NAG	C4-C5-C6-O6
4	B	2	NAG	O5-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6

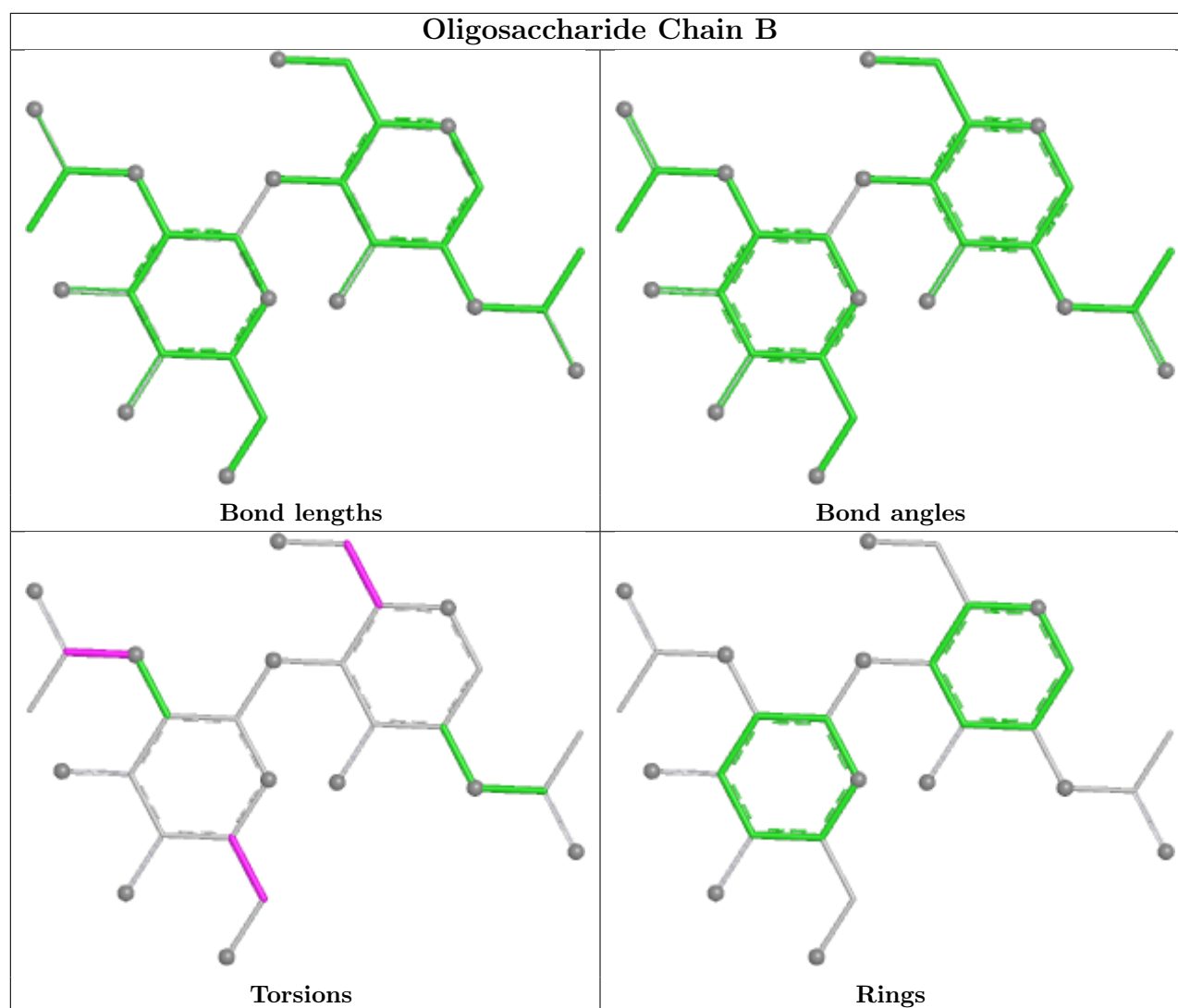
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	1	NAG	1	0

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





5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 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	$\# Z > 2$
5	NAG	A	2401	1	14,14,15	0.31	0	17,19,21	0.53	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	A	2401	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2401	NAG	C4-C5-C6-O6
5	A	2401	NAG	O5-C5-C6-O6
5	A	2401	NAG	C1-C2-N2-C7
5	A	2401	NAG	C3-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 [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, 95th 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	A	1233/1467 (84%)	-0.54	0 100 100	194, 241, 289, 329	0
2	E	115/224 (51%)	-0.59	0 100 100	265, 306, 326, 335	0
3	F	96/214 (44%)	-0.50	0 100 100	277, 329, 358, 365	0
All	All	1444/1905 (75%)	-0.54	0 100 100	194, 247, 324, 365	0

There are no RSRZ outliers to report.

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](#)

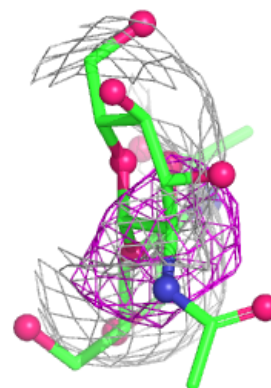
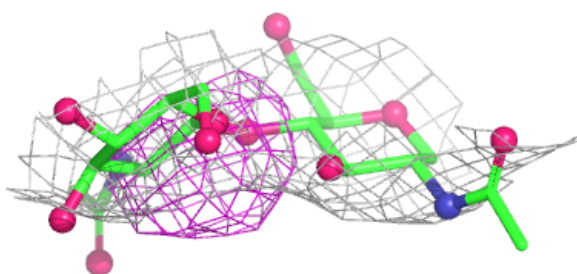
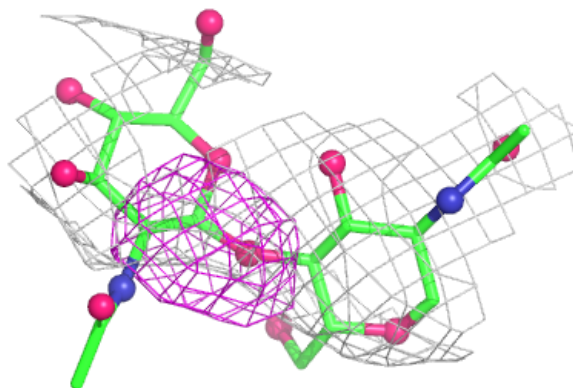
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q < 0.9
4	NAG	G	1	14/15	-	-	243,253,266,267	0
4	NAG	G	2	14/15	-	-	224,248,256,258	0
4	NAG	B	1	14/15	-	-	261,277,285,288	0
4	NAG	B	2	14/15	-	-	301,312,318,318	0

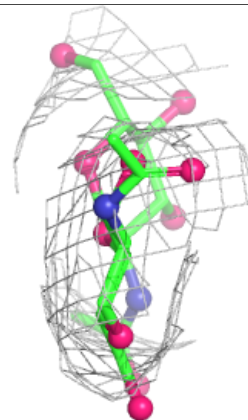
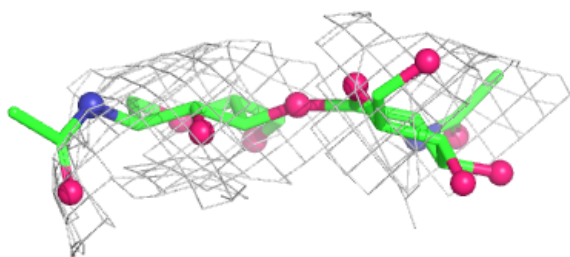
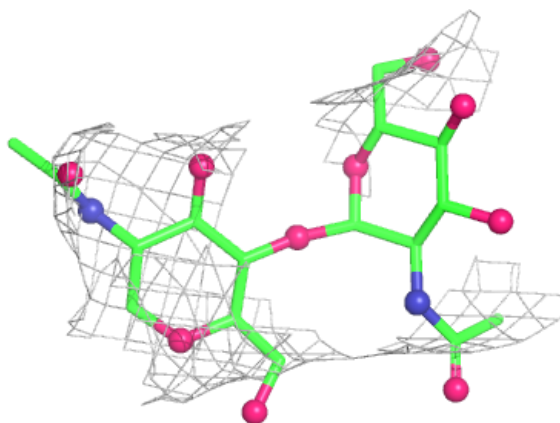
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain G:

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

**Electron density around Chain B:**

$2mF_o-DF_c$ (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, 95th 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
5	NAG	A	2401	14/15	0.50	0.07	273,291,300,302	0
7	ZN	A	2403	1/1	0.97	0.07	213,213,213,213	0
6	CU	A	2402	1/1	0.98	0.03	229,229,229,229	0
8	CA	A	2404	1/1	0.98	0.06	210,210,210,210	0

6.5 Other polymers [i](#)

There are no such residues in this entry.