



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 06:35 PM UTC

PDB ID : 6MF2 / pdb_00006mf2
Title : Improved Model of Human Coagulation Factor VIII
Authors : Smith, I.W.; Spiegel, P.C.
Deposited on : 2018-09-08
Resolution : 3.61 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

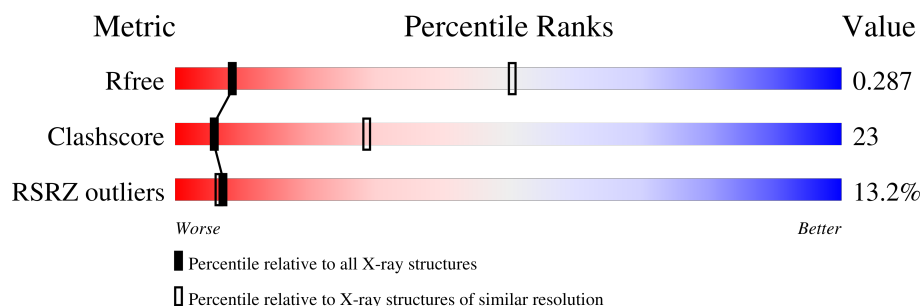
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.61 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	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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	1512	
2	B	3	
2	C	3	
2	D	3	

2 Entry composition [i](#)

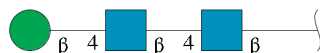
There are 6 unique types of molecules in this entry. The entry contains 10035 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1222	Total	C	N	O	S	0	0	0
			9914	6395	1675	1790	54			

- Molecule 2 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
2	B	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	C	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	D	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 5 is COPPER (I) ION (CCD ID: CU1) (formula: Cu).

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

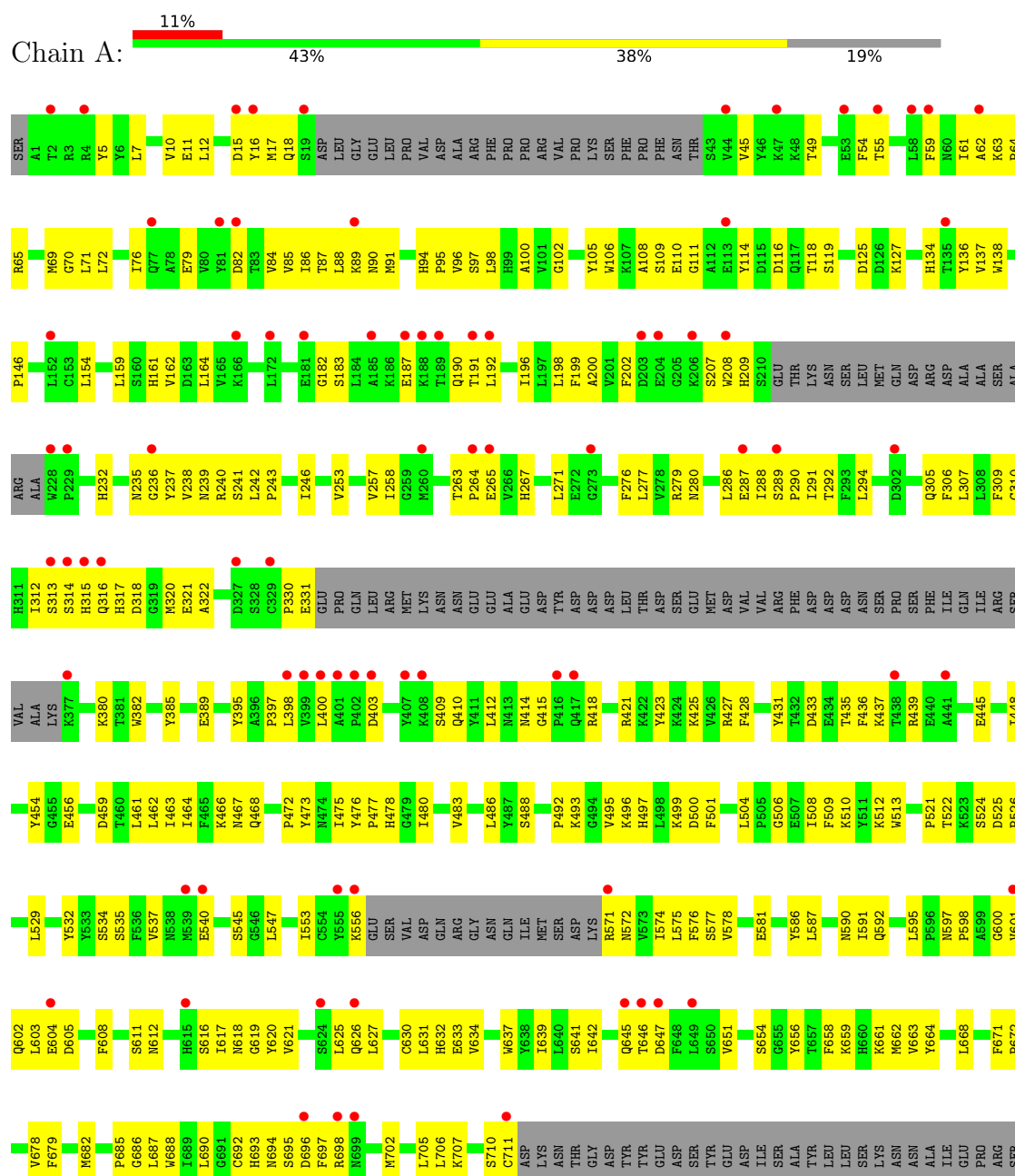
- Molecule 6 is water.

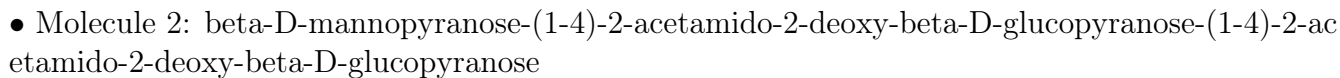
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	O	0	0
			1	1		

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





NAG1
NAG2
BMA3

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





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

Chain D:  67% 33%



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	134.57Å 134.57Å 359.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	57.36 – 3.61 57.36 – 3.61	Depositor EDS
% Data completeness (in resolution range)	81.7 (57.36-3.61) 80.4 (57.36-3.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	14.38 (at 3.57Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.252 , 0.284 0.254 , 0.287	Depositor DCC
R_{free} test set	1568 reflections (4.01%)	wwPDB-VP
Wilson B-factor (Å ²)	36.1	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 28.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.74	EDS
Total number of atoms	10035	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% 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: NAG, BMA, ZN, CU1, CA

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	0/10198	0.65	4/13824 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	305	GLN	CG-CD-NE2	-27.63	74.95	116.40
1	A	305	GLN	CG-CD-OE1	24.53	169.85	120.80
1	A	305	GLN	OE1-CD-NE2	-20.55	102.06	122.60
1	A	305	GLN	CA-CB-CG	5.67	125.44	114.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1864	ASN	Peptide
1	A	1915	ASN	Peptide
1	A	2141	ASN	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	9914	0	9682	455	1
2	B	39	0	34	4	0
2	C	39	0	34	0	0
2	D	39	0	34	0	0
3	A	1	0	0	0	0
4	A	1	0	0	0	0
5	A	1	0	0	0	0
6	A	1	0	0	0	0
All	All	10035	0	9784	456	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 23.

All (456) 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:496:LYS:H	1:A:496:LYS:HD3	1.33	0.92
1:A:2050:LEU:HD12	1:A:2055:TYR:HE2	1.37	0.89
1:A:1942:TRP:HE1	1:A:1988:MET:HE2	1.42	0.83
1:A:310:CYS:SG	1:A:317:HIS:ND1	2.45	0.83
1:A:312:ILE:HG21	1:A:317:HIS:CE1	2.14	0.82
1:A:2182:SER:O	1:A:2184:ALA:N	2.12	0.81
1:A:654:SER:O	1:A:656:TYR:N	2.17	0.78
1:A:307:LEU:HG	1:A:309:PHE:HB3	1.64	0.78
1:A:1747:LEU:HD23	1:A:1747:LEU:O	1.85	0.77
1:A:2081:ILE:HG21	1:A:2149:ILE:HD12	1.67	0.76
1:A:654:SER:HB2	1:A:688:TRP:HB3	1.66	0.76
1:A:2129:ASN:ND2	1:A:2134:GLY:O	2.19	0.76
1:A:1842:ASP:O	1:A:1844:GLU:N	2.19	0.75
1:A:2042:GLN:HG3	1:A:2047:ALA:HA	1.68	0.75
1:A:238:VAL:O	1:A:241:SER:OG	2.02	0.75
1:A:232:HIS:HB3	1:A:320:MET:HG2	1.69	0.75
1:A:1784:SER:OG	1:A:1805:ASN:OD1	2.06	0.74
1:A:289:SER:HG	1:A:292:THR:HG1	1.32	0.74
1:A:2105:TYR:HD2	1:A:2146:ALA:HB2	1.53	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2078:PRO:HB3	1:A:2107:LEU:HD11	1.69	0.73
1:A:289:SER:HB2	1:A:290:PRO:HD2	1.70	0.73
1:A:10:VAL:HG12	1:A:12:LEU:HD23	1.70	0.73
1:A:1709:TYR:OH	1:A:1732:LYS:NZ	2.17	0.73
1:A:71:LEU:HD13	1:A:236:GLY:HA3	1.71	0.73
1:A:2050:LEU:O	1:A:2052:ARG:N	2.20	0.72
1:A:159:LEU:HD13	1:A:164:LEU:HD11	1.71	0.72
1:A:1913:LYS:O	1:A:1916:TYR:N	2.21	0.72
1:A:694:ASN:O	1:A:696:ASP:N	2.22	0.72
1:A:2000:CYS:O	1:A:2002:ILE:N	2.20	0.72
1:A:1826:THR:HB	1:A:1829:GLU:HG3	1.71	0.71
1:A:2192:ALA:HB2	1:A:2230:LEU:HD12	1.73	0.70
1:A:1767:VAL:HG22	1:A:1768:GLU:HG3	1.73	0.70
1:A:90:ASN:ND2	1:A:94:HIS:O	2.24	0.70
1:A:2050:LEU:HD12	1:A:2055:TYR:CE2	2.24	0.69
1:A:2073:VAL:HG12	1:A:2074:ASP:H	1.57	0.68
1:A:2206:SER:O	1:A:2209:ARG:NH2	2.27	0.68
1:A:1709:TYR:HB3	1:A:1925:ILE:HG22	1.74	0.67
1:A:1919:HIS:CD2	1:A:2005:HIS:HD2	2.12	0.67
1:A:2241:THR:HG22	1:A:2325:GLY:HA2	1.76	0.67
1:A:1952:ASN:O	1:A:1954:HIS:N	2.27	0.67
1:A:2117:GLY:O	1:A:2119:SER:N	2.21	0.67
1:A:486:LEU:HD13	1:A:512:LYS:HB2	1.77	0.66
1:A:1865:PRO:HD2	1:A:1867:HIS:H	1.61	0.65
1:A:445:GLU:HA	1:A:625:LEU:HD11	1.77	0.65
1:A:2048:PRO:HA	1:A:2062:TRP:HB2	1.77	0.65
1:A:578:VAL:HG23	1:A:645:GLN:HG2	1.78	0.65
1:A:412:LEU:HA	1:A:421:ARG:HB3	1.76	0.65
1:A:1821:HIS:C	1:A:1823:MET:H	2.04	0.65
1:A:466:LYS:HB2	1:A:508:ILE:HG12	1.79	0.65
1:A:608:PHE:O	1:A:612:ASN:ND2	2.29	0.64
1:A:97:SER:OG	1:A:161:HIS:N	2.27	0.64
1:A:1881:THR:OG1	1:A:1882:ILE:N	2.31	0.64
1:A:389:GLU:OE2	1:A:431:TYR:OH	2.13	0.64
1:A:11:GLU:HG3	1:A:49:THR:HB	1.80	0.63
1:A:54:PHE:HD1	1:A:62:ALA:HA	1.62	0.63
1:A:522:THR:O	1:A:524:SER:N	2.31	0.63
1:A:2100:GLN:O	1:A:2154:THR:OG1	2.16	0.63
1:A:486:LEU:O	1:A:488:SER:N	2.32	0.63
1:A:1944:LEU:HB3	1:A:1978:LEU:HD11	1.80	0.63
1:A:641:SER:OG	1:A:645:GLN:OE1	2.16	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:ALA:HB2	1:A:138:TRP:CZ2	2.34	0.62
1:A:685:PRO:O	1:A:688:TRP:NE1	2.30	0.62
1:A:504:LEU:O	1:A:506:GLY:N	2.31	0.62
1:A:1826:THR:O	1:A:1828:ASP:N	2.32	0.62
1:A:89:LYS:HG2	1:A:91:MET:HG3	1.80	0.62
1:A:257:VAL:HB	1:A:294:LEU:HB2	1.80	0.62
1:A:2084:ILE:HD11	1:A:2164:MET:HE3	1.80	0.62
1:A:86:ILE:HG22	1:A:87:THR:H	1.63	0.62
1:A:1956:ILE:HD13	1:A:1978:LEU:HD12	1.81	0.62
1:A:314:SER:O	1:A:316:GLN:N	2.31	0.61
1:A:1911:THR:OG1	1:A:1914:GLU:OE2	2.18	0.61
1:A:591:ILE:HG23	1:A:595:LEU:HD22	1.83	0.61
1:A:310:CYS:HG	1:A:317:HIS:HD1	0.65	0.61
1:A:1967:LYS:C	1:A:1969:GLU:H	2.08	0.61
1:A:529:LEU:HD11	1:A:553:ILE:HB	1.82	0.60
1:A:1909:ASP:HA	1:A:1912:PHE:CE1	2.37	0.60
1:A:2028:ALA:N	1:A:2165:GLU:OE1	2.33	0.60
1:A:1880:PHE:CZ	1:A:1956:ILE:HG12	2.36	0.60
1:A:1927:ASP:HA	1:A:2012:THR:HA	1.84	0.60
1:A:1742:SER:O	1:A:1744:THR:N	2.35	0.59
1:A:276:PHE:CD2	1:A:286:LEU:HG	2.37	0.59
1:A:2162:LEU:HD11	1:A:2164:MET:HB3	1.84	0.59
1:A:1737:GLU:HG2	1:A:1747:LEU:HD22	1.84	0.59
1:A:105:TYR:HB2	1:A:109:SER:HB2	1.85	0.59
1:A:314:SER:HB2	1:A:646:THR:HB	1.84	0.59
1:A:581:GLU:HB2	1:A:612:ASN:HB3	1.84	0.59
1:A:496:LYS:HD3	1:A:496:LYS:N	2.14	0.59
1:A:65:ARG:NH2	1:A:70:GLY:O	2.36	0.58
1:A:627:LEU:HD11	1:A:637:TRP:HH2	1.68	0.58
1:A:2060:ASN:O	1:A:2163:ARG:HD3	2.03	0.58
1:A:1870:GLN:O	1:A:1872:THR:N	2.30	0.58
1:A:627:LEU:HD11	1:A:637:TRP:CH2	2.38	0.58
1:A:146:PRO:HB3	1:A:154:LEU:HG	1.86	0.58
1:A:586:TYR:O	1:A:590:ASN:ND2	2.37	0.58
1:A:2310:PRO:HG2	1:A:2317:ILE:HD13	1.85	0.58
1:A:1737:GLU:HB2	1:A:1761:PRO:HG3	1.86	0.57
1:A:1755:HIS:CE1	1:A:1876:PHE:HD1	2.22	0.57
1:A:454:TYR:HE2	1:A:456:GLU:HG3	1.68	0.57
1:A:69:MET:HG2	1:A:72:LEU:HB2	1.86	0.57
1:A:1780:SER:O	1:A:1809:PRO:HG3	2.03	0.57
1:A:2311:GLN:O	1:A:2313:TRP:HE3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1732:LYS:NZ	1:A:1885:GLU:OE2	2.37	0.57
1:A:2245:THR:HG23	1:A:2293:VAL:HG13	1.86	0.57
1:A:199:PHE:HB2	1:A:288:ILE:HD13	1.86	0.56
1:A:2186:SER:HB3	1:A:2189:GLN:HG3	1.88	0.56
1:A:2218:ALA:HB2	1:A:2248:VAL:HG11	1.86	0.56
1:A:1826:THR:O	1:A:1829:GLU:N	2.27	0.56
1:A:1877:ALA:O	1:A:1922:ASN:ND2	2.31	0.56
1:A:476:TYR:OH	1:A:483:VAL:HG11	2.05	0.56
1:A:397:PRO:HB2	1:A:398:LEU:HD22	1.88	0.56
1:A:94:HIS:HD1	1:A:208:TRP:CG	2.23	0.56
1:A:287:GLU:HB3	1:A:671:PHE:CE2	2.40	0.56
1:A:2096:LEU:HD21	1:A:2159:ARG:HH21	1.71	0.56
1:A:2229:TRP:HB3	1:A:2309:HIS:HD1	1.71	0.56
1:A:576:PHE:O	1:A:645:GLN:NE2	2.39	0.55
1:A:1954:HIS:ND1	1:A:2000:CYS:SG	2.71	0.55
1:A:1784:SER:N	1:A:1839:SER:OG	2.39	0.55
1:A:597:ASN:OD1	1:A:600:GLY:N	2.40	0.55
1:A:1996:TRP:HB2	1:A:2014:PHE:CE1	2.41	0.55
1:A:2219:TRP:HE3	1:A:2319:LEU:HB2	1.70	0.55
1:A:79:GLU:OE1	1:A:182:GLY:N	2.39	0.55
1:A:2084:ILE:HG13	1:A:2166:LEU:HD23	1.89	0.55
1:A:1864:ASN:HB3	1:A:1865:PRO:HD3	1.89	0.55
1:A:2276:GLN:HB2	1:A:2281:LYS:HB2	1.89	0.55
1:A:534:SER:OG	1:A:535:SER:N	2.39	0.55
1:A:467:ASN:OD1	1:A:468:GLN:N	2.40	0.54
1:A:525:ASP:HB2	1:A:526:PRO:HD2	1.89	0.54
1:A:1909:ASP:HA	1:A:1912:PHE:CD1	2.42	0.54
1:A:2212:LEU:O	1:A:2320:ARG:NH1	2.40	0.54
1:A:1750:GLY:O	1:A:1752:LEU:N	2.37	0.54
1:A:72:LEU:HD21	1:A:198:LEU:HD22	1.90	0.54
1:A:1954:HIS:CE1	1:A:2005:HIS:CE1	2.95	0.54
1:A:2057:GLY:C	1:A:2058:SER:HG	2.16	0.54
1:A:95:PRO:HB2	1:A:162:VAL:HG11	1.90	0.54
1:A:2141:ASN:HB3	2:B:1:NAG:HN2	1.72	0.54
1:A:1764:ARG:NE	1:A:1875:GLU:OE1	2.41	0.53
1:A:1865:PRO:HD2	1:A:1867:HIS:HB2	1.90	0.53
1:A:2193:SER:HB3	1:A:2229:TRP:CE2	2.42	0.53
1:A:1870:GLN:C	1:A:1872:THR:H	2.16	0.53
1:A:271:LEU:HD11	1:A:306:PHE:HB2	1.89	0.53
1:A:380:LYS:N	1:A:459:ASP:OD1	2.41	0.53
1:A:1759:LEU:HD22	1:A:1922:ASN:OD1	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2108:ASP:OD1	1:A:2109:GLY:N	2.41	0.53
1:A:86:ILE:HG21	1:A:98:LEU:HD21	1.91	0.53
1:A:127:LYS:HD2	1:A:162:VAL:HG12	1.89	0.53
1:A:1825:PRO:HG3	1:A:1833:LYS:HB3	1.91	0.53
1:A:1831:ASP:HB2	1:A:1941:ARG:NH1	2.24	0.53
1:A:626:GLN:HB3	1:A:707:LYS:HE2	1.91	0.53
1:A:2027:MET:HB3	1:A:2165:GLU:OE1	2.09	0.53
1:A:2088:GLY:O	1:A:2163:ARG:NH2	2.41	0.53
1:A:1953:ILE:HG22	1:A:1979:TYR:HD1	1.74	0.53
1:A:190:GLN:O	1:A:192:LEU:N	2.42	0.53
1:A:1976:TYR:CZ	1:A:1984:GLU:HG2	2.44	0.52
1:A:478:HIS:HD1	1:A:532:TYR:HE1	1.57	0.52
1:A:2195:TYR:HB3	1:A:2205:PRO:HD3	1.91	0.52
1:A:237:TYR:CD2	1:A:242:LEU:HA	2.45	0.52
1:A:425:LYS:HB3	1:A:545:SER:O	2.10	0.52
1:A:631:LEU:HB3	1:A:632:HIS:ND1	2.24	0.52
1:A:69:MET:O	1:A:235:ASN:HB3	2.09	0.52
1:A:418:ARG:NH1	1:A:608:PHE:HA	2.25	0.52
1:A:385:TYR:HE1	1:A:464:ILE:HD12	1.75	0.52
1:A:682:MET:HE1	1:A:706:LEU:HD21	1.91	0.52
1:A:587:LEU:O	1:A:591:ILE:HG13	2.09	0.52
1:A:5:TYR:HE2	1:A:76:ILE:HA	1.74	0.51
1:A:15:ASP:HB3	1:A:45:VAL:HG22	1.91	0.51
1:A:102:GLY:HA2	1:A:1962:VAL:HG12	1.92	0.51
1:A:410:GLN:O	1:A:611:SER:OG	2.27	0.51
1:A:2055:TYR:O	1:A:2060:ASN:ND2	2.40	0.51
1:A:2094:SER:HB3	1:A:2158:ILE:HD13	1.92	0.51
1:A:656:TYR:HE1	1:A:682:MET:HA	1.75	0.51
1:A:114:TYR:O	1:A:116:ASP:N	2.41	0.51
1:A:1913:LYS:O	1:A:1915:ASN:N	2.43	0.51
1:A:428:PHE:CE1	1:A:547:LEU:HD22	2.45	0.51
1:A:427:ARG:NE	1:A:448:ILE:HA	2.26	0.51
1:A:509:PHE:HD1	1:A:510:LYS:H	1.59	0.51
1:A:1920:ALA:HB1	1:A:1923:GLY:HA2	1.92	0.51
1:A:105:TYR:CZ	1:A:1960:GLY:HA2	2.46	0.51
1:A:1738:PHE:HD2	1:A:1743:PHE:HB3	1.75	0.51
1:A:433:ASP:OD1	1:A:435:THR:HG22	2.11	0.51
1:A:1908:GLU:HG2	1:A:1910:PRO:HD3	1.93	0.51
1:A:2244:THR:OG1	1:A:2322:GLU:O	2.28	0.51
1:A:59:PHE:HD2	1:A:89:LYS:HD3	1.75	0.51
1:A:85:VAL:HA	1:A:137:VAL:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1749:ARG:HB2	1:A:1753:ASN:HB2	1.92	0.51
1:A:286:LEU:HD22	1:A:294:LEU:HD22	1.92	0.50
1:A:710:SER:OG	1:A:711:CYS:N	2.43	0.50
1:A:1919:HIS:CD2	1:A:2008:ALA:HB3	2.45	0.50
1:A:1919:HIS:HD2	1:A:2005:HIS:O	1.93	0.50
1:A:425:LYS:NZ	1:A:581:GLU:OE2	2.35	0.50
1:A:1993:ALA:HA	1:A:2016:VAL:HG13	1.93	0.50
1:A:467:ASN:ND2	1:A:473:TYR:H	2.08	0.50
1:A:2223:VAL:O	1:A:2224:ASN:ND2	2.43	0.50
1:A:187:GLU:N	1:A:187:GLU:OE1	2.44	0.50
1:A:630:CYS:N	1:A:633:GLU:OE1	2.45	0.50
1:A:2141:ASN:CB	2:B:1:NAG:HN2	2.24	0.50
1:A:187:GLU:H	1:A:187:GLU:CD	2.19	0.50
1:A:592:GLN:HA	1:A:598:PRO:HG3	1.93	0.50
1:A:2223:VAL:HG11	1:A:2225:ASN:HD22	1.77	0.50
1:A:106:TRP:C	1:A:108:ALA:H	2.20	0.50
1:A:1787:SER:C	1:A:1789:LEU:H	2.20	0.50
1:A:1874:GLN:HG3	1:A:1938:GLN:HE21	1.77	0.50
1:A:1789:LEU:O	1:A:1791:SER:N	2.45	0.50
1:A:79:GLU:HB2	1:A:82:ASP:OD2	2.12	0.49
1:A:647:ASP:O	1:A:672:PRO:HD3	2.11	0.49
1:A:242:LEU:HB3	1:A:322:ALA:HB1	1.94	0.49
1:A:500:ASP:OD1	1:A:500:ASP:N	2.41	0.49
1:A:287:GLU:HB3	1:A:671:PHE:CD2	2.47	0.49
1:A:463:ILE:HG21	1:A:475:ILE:HD13	1.93	0.49
1:A:2086:THR:C	1:A:2129:ASN:HD21	2.19	0.49
1:A:695:SER:C	1:A:697:PHE:H	2.20	0.49
1:A:2038:THR:O	1:A:2071:ILE:HG13	2.12	0.49
1:A:435:THR:HG23	1:A:437:LYS:H	1.77	0.49
1:A:2057:GLY:O	1:A:2059:ILE:N	2.46	0.49
1:A:651:VAL:HG12	1:A:668:LEU:O	2.12	0.49
1:A:658:PHE:HB2	1:A:678:VAL:HB	1.93	0.49
1:A:106:TRP:O	1:A:108:ALA:N	2.42	0.49
1:A:1925:ILE:O	1:A:1928:THR:OG1	2.21	0.49
1:A:2220:ARG:HH21	1:A:2255:MET:HE1	1.77	0.49
1:A:1945:LEU:HD12	1:A:1946:SER:H	1.77	0.48
1:A:2244:THR:HG22	1:A:2294:VAL:HB	1.95	0.48
1:A:2245:THR:HG21	1:A:2260:PHE:CE1	2.48	0.48
1:A:456:GLU:O	1:A:459:ASP:HB2	2.13	0.48
1:A:1863:LEU:HD23	1:A:1869:ARG:O	2.13	0.48
1:A:316:GLN:HB3	1:A:317:HIS:H	1.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1695:THR:HG23	1:A:1770:ASN:HB2	1.96	0.48
1:A:2141:ASN:OD1	2:B:1:NAG:H3	2.12	0.48
1:A:617:ILE:HG22	1:A:625:LEU:HD23	1.95	0.48
1:A:1707:TRP:CD1	1:A:1708:ASP:H	2.31	0.48
1:A:1954:HIS:CE1	1:A:2010:MET:SD	3.07	0.48
1:A:2044:GLY:O	1:A:2046:TRP:N	2.35	0.48
1:A:183:SER:O	1:A:183:SER:OG	2.26	0.48
1:A:601:VAL:O	1:A:603:LEU:N	2.47	0.48
1:A:1772:MET:HB2	1:A:1816:PHE:HD1	1.77	0.48
1:A:1949:SER:O	1:A:1952:ASN:ND2	2.40	0.48
1:A:1997:ARG:NE	1:A:2011:SER:OG	2.44	0.48
1:A:2229:TRP:HB3	1:A:2309:HIS:ND1	2.29	0.48
1:A:316:GLN:OE1	1:A:318:ASP:N	2.43	0.48
1:A:198:LEU:O	1:A:200:ALA:N	2.47	0.48
1:A:414:ASN:OD1	1:A:415:GLY:N	2.46	0.48
1:A:2260:PHE:HZ	1:A:2295:ASN:HD22	1.61	0.48
1:A:7:LEU:HD23	1:A:88:LEU:HD13	1.96	0.47
1:A:16:TYR:O	1:A:18:GLN:N	2.45	0.47
1:A:54:PHE:CD1	1:A:62:ALA:HA	2.44	0.47
1:A:2194:SER:HB3	1:A:2222:GLN:HG2	1.95	0.47
1:A:118:THR:HG22	1:A:119:SER:H	1.78	0.47
1:A:257:VAL:HG21	1:A:286:LEU:HD13	1.95	0.47
1:A:1756:LEU:O	1:A:1758:LEU:N	2.47	0.47
1:A:1738:PHE:CD1	1:A:1746:PRO:HA	2.49	0.47
1:A:1755:HIS:CD2	1:A:1756:LEU:HD22	2.49	0.47
1:A:1805:ASN:ND2	1:A:1813:LYS:HE2	2.29	0.47
1:A:662:MET:HG3	1:A:1968:LYS:HG2	1.94	0.47
2:B:2:NAG:O3	2:B:3:BMA:O5	2.24	0.47
1:A:467:ASN:HD22	1:A:473:TYR:H	1.62	0.47
1:A:698:ARG:HB3	1:A:698:ARG:CZ	2.44	0.47
1:A:1763:ILE:HG23	1:A:1855:LEU:HG	1.96	0.47
1:A:237:TYR:CD2	1:A:242:LEU:HD13	2.50	0.47
1:A:425:LYS:HD3	1:A:448:ILE:HD11	1.97	0.47
1:A:2039:ALA:HB2	1:A:2048:PRO:HB3	1.96	0.47
1:A:277:LEU:HA	1:A:277:LEU:HD23	1.73	0.47
1:A:577:SER:HA	1:A:642:ILE:O	2.15	0.47
1:A:2086:THR:O	1:A:2129:ASN:ND2	2.39	0.47
1:A:5:TYR:CE2	1:A:76:ILE:HG23	2.50	0.47
1:A:664:TYR:CE2	1:A:1822:HIS:HA	2.49	0.47
1:A:1821:HIS:C	1:A:1823:MET:N	2.73	0.47
1:A:2081:ILE:HD13	1:A:2149:ILE:HB	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:VAL:CG2	1:A:645:GLN:HG2	2.45	0.46
1:A:65:ARG:NH1	1:A:72:LEU:O	2.39	0.46
1:A:263:THR:O	1:A:264:PRO:C	2.57	0.46
1:A:478:HIS:ND1	1:A:532:TYR:HE1	2.13	0.46
1:A:1782:PRO:HB3	1:A:1808:LYS:HA	1.96	0.46
1:A:571:ARG:HG2	1:A:572:ASN:H	1.81	0.46
1:A:1894:ASN:O	1:A:1895:MET:HE2	2.15	0.46
1:A:2001:LEU:HD23	1:A:2001:LEU:HA	1.72	0.46
1:A:279:ARG:HB2	1:A:280:ASN:H	1.55	0.46
1:A:433:ASP:OD1	1:A:433:ASP:N	2.48	0.46
1:A:461:LEU:HB2	1:A:513:TRP:HB2	1.96	0.46
1:A:645:GLN:C	1:A:647:ASP:H	2.22	0.46
1:A:1942:TRP:NE1	1:A:1988:MET:HE2	2.22	0.46
1:A:2180:MET:HB2	1:A:2322:GLU:HA	1.98	0.46
1:A:601:VAL:HG23	1:A:602:GLN:H	1.80	0.46
1:A:1910:PRO:HD2	1:A:1912:PHE:H	1.80	0.46
1:A:17:MET:HE2	1:A:239:ASN:HB2	1.97	0.46
1:A:525:ASP:N	1:A:525:ASP:OD1	2.48	0.46
1:A:2248:VAL:HG12	1:A:2320:ARG:CZ	2.46	0.46
1:A:586:TYR:N	1:A:586:TYR:CD1	2.84	0.46
1:A:1794:GLU:HB3	1:A:1795:ASP:H	1.44	0.46
1:A:2178:LEU:HD21	1:A:2325:GLY:C	2.41	0.46
1:A:1953:ILE:HG22	1:A:1979:TYR:CD1	2.51	0.46
1:A:207:SER:OG	1:A:208:TRP:N	2.48	0.45
1:A:476:TYR:CE1	1:A:483:VAL:HG11	2.52	0.45
1:A:1929:LEU:HB3	1:A:2012:THR:OG1	2.16	0.45
1:A:2086:THR:HG23	1:A:2162:LEU:HD13	1.97	0.45
1:A:687:LEU:HD11	1:A:705:LEU:HD23	1.99	0.45
1:A:540:GLU:OE1	1:A:540:GLU:N	2.49	0.45
1:A:1730:PHE:CD2	1:A:1885:GLU:HG3	2.50	0.45
1:A:1785:PHE:HB3	1:A:1815:TYR:CE2	2.51	0.45
1:A:1967:LYS:C	1:A:1969:GLU:N	2.74	0.45
1:A:1781:ARG:CZ	1:A:1781:ARG:HB3	2.45	0.45
1:A:1870:GLN:O	1:A:1871:VAL:HG22	2.17	0.45
1:A:2017:TYR:CZ	1:A:2143:PRO:HG3	2.51	0.45
1:A:2076:LEU:O	1:A:2147:ARG:NH1	2.50	0.45
1:A:1883:PHE:O	1:A:1917:ARG:HA	2.16	0.45
1:A:90:ASN:HD22	1:A:96:VAL:HG22	1.82	0.45
1:A:1994:GLY:H	1:A:2016:VAL:HG13	1.82	0.45
1:A:86:ILE:HG22	1:A:87:THR:N	2.29	0.45
1:A:313:SER:O	1:A:315:HIS:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:574:ILE:HG12	1:A:690:LEU:HD21	1.99	0.45
1:A:1805:ASN:HD21	1:A:1815:TYR:HE1	1.64	0.45
1:A:2082:HIS:HB2	1:A:2168:GLY:HA2	1.98	0.45
1:A:2178:LEU:HD21	1:A:2326:CYS:N	2.32	0.45
1:A:2098:ILE:HG21	1:A:2153:PRO:HB3	1.98	0.45
1:A:431:TYR:CE1	1:A:439:ARG:HG2	2.52	0.45
1:A:492:PRO:HB2	1:A:493:LYS:H	1.54	0.45
1:A:2072:LYS:HA	1:A:2150:ARG:HA	1.99	0.45
1:A:1856:LEU:HD11	1:A:1943:TYR:HE2	1.81	0.44
1:A:286:LEU:O	1:A:288:ILE:N	2.49	0.44
1:A:1733:VAL:HG22	1:A:1851:LEU:HD21	2.00	0.44
1:A:1942:TRP:HB2	1:A:1986:VAL:HG22	1.99	0.44
1:A:2298:ASP:O	1:A:2300:PRO:HD3	2.16	0.44
1:A:403:ASP:O	1:A:409:SER:HB2	2.17	0.44
1:A:661:LYS:O	1:A:662:MET:HB2	2.17	0.44
1:A:2047:ALA:HB3	1:A:2050:LEU:HD22	1.99	0.44
1:A:477:PRO:HG3	1:A:513:TRP:CE2	2.52	0.44
1:A:1784:SER:OG	1:A:1785:PHE:N	2.51	0.44
1:A:11:GLU:OE2	1:A:209:HIS:NE2	2.41	0.44
1:A:71:LEU:HD22	1:A:202:PHE:CZ	2.52	0.44
1:A:603:LEU:HB3	1:A:604:GLU:H	1.63	0.44
1:A:668:LEU:HD22	1:A:678:VAL:HG11	2.00	0.44
1:A:2105:TYR:CD2	1:A:2146:ALA:HB2	2.43	0.44
1:A:191:THR:HG23	1:A:192:LEU:H	1.82	0.44
1:A:1789:LEU:HD11	1:A:1835:TRP:CD1	2.53	0.44
1:A:1932:LEU:HB3	1:A:2014:PHE:HB3	1.99	0.44
1:A:1940:ILE:O	1:A:1987:GLU:HA	2.17	0.44
1:A:385:TYR:CE1	1:A:464:ILE:HD12	2.51	0.44
1:A:1924:TYR:HB3	1:A:1928:THR:HB	2.00	0.44
1:A:2038:THR:HG22	1:A:2039:ALA:H	1.82	0.44
1:A:55:THR:HG22	1:A:61:ILE:HB	1.99	0.43
1:A:575:LEU:O	1:A:618:ASN:N	2.38	0.43
1:A:267:HIS:ND1	1:A:320:MET:HE2	2.33	0.43
1:A:382:TRP:NE1	1:A:459:ASP:OD2	2.51	0.43
1:A:398:LEU:HD22	1:A:398:LEU:H	1.82	0.43
1:A:495:VAL:HG11	1:A:501:PHE:HB2	1.99	0.43
1:A:656:TYR:CE1	1:A:682:MET:HA	2.52	0.43
1:A:1869:ARG:HG2	1:A:1870:GLN:H	1.83	0.43
1:A:2043:TYR:HE2	1:A:2046:TRP:HD1	1.66	0.43
1:A:232:HIS:CD2	1:A:317:HIS:CD2	3.06	0.43
1:A:472:PRO:O	1:A:537:VAL:HG21	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2256:TYR:CE1	1:A:2314:VAL:HG11	2.53	0.43
1:A:240:ARG:HA	1:A:322:ALA:HA	1.99	0.43
1:A:617:ILE:O	1:A:619:GLY:N	2.51	0.43
1:A:17:MET:CE	1:A:239:ASN:HD22	2.31	0.43
1:A:84:VAL:HB	1:A:138:TRP:HB2	2.00	0.43
1:A:659:LYS:HE3	1:A:659:LYS:HB2	1.89	0.43
1:A:1826:THR:O	1:A:1827:LYS:C	2.61	0.43
1:A:1919:HIS:HB3	1:A:2010:MET:HB2	2.01	0.43
1:A:2264:SER:HB3	1:A:2301:LEU:HD21	2.00	0.43
1:A:1704:GLU:OE2	1:A:1780:SER:N	2.38	0.43
1:A:240:ARG:NE	1:A:321:GLU:OE1	2.46	0.43
1:A:289:SER:HB2	1:A:290:PRO:CD	2.45	0.43
1:A:2003:GLY:O	1:A:2007:HIS:N	2.48	0.43
1:A:2179:GLY:O	1:A:2185:ILE:HG13	2.19	0.43
1:A:98:LEU:HB3	1:A:136:TYR:CE2	2.54	0.43
1:A:483:VAL:HG23	1:A:513:TRP:CD1	2.54	0.43
1:A:687:LEU:HD12	1:A:707:LYS:HG2	2.00	0.43
1:A:63:LYS:HD2	1:A:64:PRO:HD2	2.00	0.43
1:A:125:ASP:HA	1:A:134:HIS:CD2	2.53	0.43
1:A:198:LEU:HD12	1:A:258:ILE:HB	2.00	0.43
1:A:428:PHE:CD1	1:A:547:LEU:HD22	2.54	0.43
1:A:395:TYR:O	1:A:620:TYR:HA	2.19	0.42
1:A:1870:GLN:C	1:A:1871:VAL:HG22	2.45	0.42
1:A:2097:TYR:CE1	1:A:2130:VAL:HA	2.54	0.42
1:A:2042:GLN:O	1:A:2043:TYR:HB3	2.19	0.42
1:A:2218:ALA:HB2	1:A:2248:VAL:CG1	2.49	0.42
1:A:2230:LEU:O	1:A:2307:ARG:HA	2.18	0.42
1:A:2286:ASN:N	1:A:2293:VAL:HG11	2.34	0.42
1:A:192:LEU:HD21	1:A:246:ILE:O	2.18	0.42
1:A:2265:SER:HB2	1:A:2271:TRP:CD2	2.55	0.42
1:A:2302:LEU:HB3	1:A:2303:THR:H	1.56	0.42
1:A:94:HIS:HD1	1:A:208:TRP:CD1	2.37	0.42
1:A:237:TYR:CE2	1:A:243:PRO:HD2	2.55	0.42
1:A:497:HIS:CD2	1:A:499:LYS:HB2	2.55	0.42
1:A:1707:TRP:CD1	1:A:1709:TYR:H	2.37	0.42
1:A:2258:LYS:HD2	1:A:2314:VAL:HG23	2.02	0.42
1:A:436:PHE:CE2	1:A:466:LYS:HB3	2.55	0.42
1:A:1755:HIS:ND1	1:A:1876:PHE:HD1	2.17	0.42
1:A:1804:LYS:HE2	1:A:1804:LYS:HB3	1.92	0.42
1:A:159:LEU:HD13	1:A:164:LEU:CD1	2.47	0.42
1:A:196:ILE:HD12	1:A:196:ILE:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:692:CYS:O	1:A:693:HIS:HB2	2.19	0.42
1:A:55:THR:CG2	1:A:61:ILE:HB	2.48	0.42
1:A:556:LYS:HD2	1:A:556:LYS:HA	1.70	0.42
1:A:2046:TRP:HZ3	1:A:2060:ASN:H	1.68	0.42
1:A:2136:LYS:HD3	1:A:2136:LYS:HA	1.83	0.42
1:A:2207:LYS:HD3	1:A:2216:SER:O	2.20	0.42
1:A:686:GLY:HA3	1:A:1803:ARG:HD2	2.01	0.41
1:A:1839:SER:HB3	1:A:1846:ASP:OD2	2.20	0.41
1:A:591:ILE:CG2	1:A:595:LEU:HD22	2.49	0.41
1:A:1738:PHE:CD2	1:A:1743:PHE:HB3	2.55	0.41
1:A:2023:THR:OG1	1:A:2024:PRO:HD2	2.20	0.41
1:A:2115:TYR:OH	1:A:2140:PHE:HB3	2.20	0.41
1:A:1926:MET:HG3	1:A:2009:GLY:CA	2.50	0.41
1:A:330:PRO:HB2	1:A:331:GLU:H	1.65	0.41
1:A:400:LEU:H	1:A:400:LEU:HD22	1.84	0.41
1:A:521:PRO:HA	1:A:525:ASP:OD2	2.20	0.41
1:A:663:VAL:HG21	1:A:1967:LYS:HA	2.02	0.41
1:A:702:MET:HE3	1:A:702:MET:HB2	1.93	0.41
1:A:1730:PHE:CZ	1:A:1918:PHE:HZ	2.39	0.41
1:A:1870:GLN:OE1	1:A:1941:ARG:NH1	2.53	0.41
1:A:2111:LYS:HB2	1:A:2111:LYS:HE3	1.91	0.41
1:A:192:LEU:HD11	1:A:253:VAL:HG23	2.03	0.41
1:A:2000:CYS:O	1:A:2002:ILE:HG12	2.21	0.41
1:A:2096:LEU:HD12	1:A:2158:ILE:HD12	2.02	0.41
1:A:2108:ASP:OD2	1:A:2111:LYS:HG2	2.20	0.41
1:A:2129:ASN:OD1	1:A:2129:ASN:N	2.53	0.41
1:A:59:PHE:CD2	1:A:89:LYS:HD3	2.55	0.41
1:A:110:GLU:HB3	1:A:111:GLY:H	1.68	0.41
1:A:264:PRO:HB3	1:A:1953:ILE:HD11	2.01	0.41
1:A:574:ILE:HB	1:A:639:ILE:HG12	2.02	0.41
1:A:616:SER:HA	1:A:621:VAL:HG12	2.01	0.41
1:A:1880:PHE:CD1	1:A:1880:PHE:N	2.89	0.41
1:A:1893:GLU:C	1:A:1895:MET:H	2.27	0.41
1:A:2266:GLN:NE2	1:A:2303:THR:HA	2.36	0.41
1:A:2274:PHE:CZ	1:A:2299:PRO:HG2	2.55	0.41
1:A:86:ILE:HD11	1:A:138:TRP:CZ3	2.56	0.41
1:A:1920:ALA:HB1	1:A:1923:GLY:CA	2.51	0.41
1:A:1989:LEU:HD12	1:A:1989:LEU:O	2.21	0.41
1:A:2087:GLN:HB3	1:A:2088:GLY:H	1.67	0.41
1:A:290:PRO:HB2	1:A:291:ILE:H	1.72	0.41
1:A:575:LEU:N	1:A:618:ASN:OD1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:631:LEU:C	1:A:633:GLU:H	2.28	0.41
1:A:634:VAL:HG12	1:A:679:PHE:CZ	2.55	0.41
1:A:1873:VAL:HG23	1:A:1939:ARG:C	2.46	0.41
1:A:1919:HIS:HB3	1:A:2010:MET:HE3	2.02	0.41
1:A:2246:GLN:OE1	1:A:2320:ARG:NE	2.53	0.41
1:A:164:LEU:HD12	1:A:164:LEU:HA	1.68	0.40
1:A:264:PRO:HB2	1:A:265:GLU:H	1.72	0.40
1:A:1878:LEU:HA	1:A:1922:ASN:ND2	2.37	0.40
1:A:1908:GLU:N	1:A:1908:GLU:OE1	2.54	0.40
1:A:2175:SER:O	1:A:2324:LEU:HD22	2.21	0.40
1:A:86:ILE:HG21	1:A:98:LEU:CD2	2.51	0.40
1:A:462:LEU:HA	1:A:462:LEU:HD12	1.86	0.40
1:A:476:TYR:CZ	1:A:483:VAL:HG11	2.56	0.40
1:A:603:LEU:O	1:A:605:ASP:N	2.54	0.40
1:A:2027:MET:HE1	1:A:2073:VAL:HG21	2.03	0.40
1:A:2105:TYR:HA	1:A:2148:TYR:O	2.21	0.40
1:A:317:HIS:CD2	1:A:317:HIS:N	2.89	0.40
1:A:423:TYR:CD2	1:A:581:GLU:HG3	2.56	0.40
1:A:1934:MET:CE	1:A:1990:PRO:HG3	2.52	0.40
1:A:2063:SER:HB2	1:A:2161:THR:HG23	2.03	0.40
1:A:480:ILE:H	1:A:480:ILE:HG13	1.72	0.40
1:A:2264:SER:OG	1:A:2301:LEU:HD11	2.22	0.40
1:A:662:MET:HE2	1:A:1968:LYS:HG2	2.02	0.40
1:A:1708:ASP:O	1:A:1710:GLY:N	2.54	0.40
1:A:1758:LEU:HD12	1:A:1758:LEU:HA	1.81	0.40
1:A:1876:PHE:CE2	1:A:1934:MET:HG2	2.56	0.40
1:A:2017:TYR:CE2	1:A:2143:PRO:HG3	2.56	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)
1:A:1821:HIS:NE2	1:A:2315:HIS:O[5_957]	2.17	0.03

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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](#)

9 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	B	1	2,1	14,14,15	0.67	1 (7%)	17,19,21	1.37	2 (11%)
2	NAG	B	2	2	14,14,15	0.22	0	17,19,21	0.75	0
2	BMA	B	3	2	11,11,12	0.60	0	15,15,17	1.20	2 (13%)
2	NAG	C	1	2,1	14,14,15	0.38	0	17,19,21	0.76	0
2	NAG	C	2	2	14,14,15	0.20	0	17,19,21	0.72	1 (5%)
2	BMA	C	3	2	11,11,12	0.67	0	15,15,17	0.80	0
2	NAG	D	1	2,1	14,14,15	0.33	0	17,19,21	0.40	0
2	NAG	D	2	2	14,14,15	0.33	0	17,19,21	0.52	0
2	BMA	D	3	2	11,11,12	1.16	2 (18%)	15,15,17	0.97	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	B	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	B	2	2	-	3/6/23/26	0/1/1/1
2	BMA	B	3	2	-	2/2/19/22	0/1/1/1
2	NAG	C	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	C	2	2	-	4/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	NAG	D	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	D	2	2	-	1/6/23/26	0/1/1/1
2	BMA	D	3	2	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3	BMA	C2-C3	2.62	1.56	1.52
2	D	3	BMA	C1-C2	2.59	1.58	1.52
2	B	1	NAG	O5-C1	2.18	1.47	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	NAG	C1-O5-C5	4.59	118.34	112.19
2	B	3	BMA	C1-O5-C5	3.43	116.78	112.19
2	C	2	NAG	C1-O5-C5	2.41	115.41	112.19
2	B	1	NAG	O3-C3-C2	-2.02	105.20	109.40
2	B	3	BMA	O2-C2-C3	-2.02	105.97	110.15

There are no chirality outliers.

All (16) torsion outliers are listed below:

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

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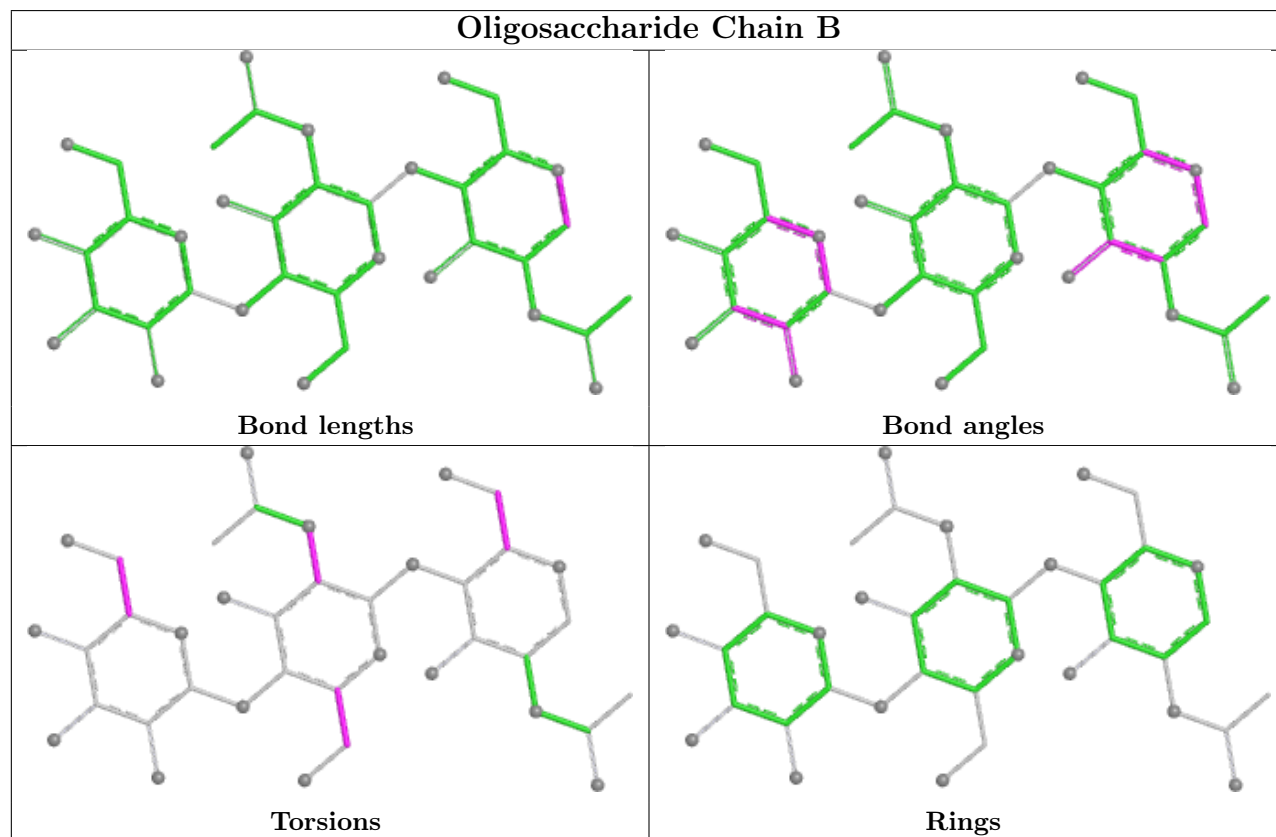
Mol	Chain	Res	Type	Atoms
2	B	3	BMA	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	B	2	NAG	C3-C2-N2-C7
2	C	1	NAG	C3-C2-N2-C7

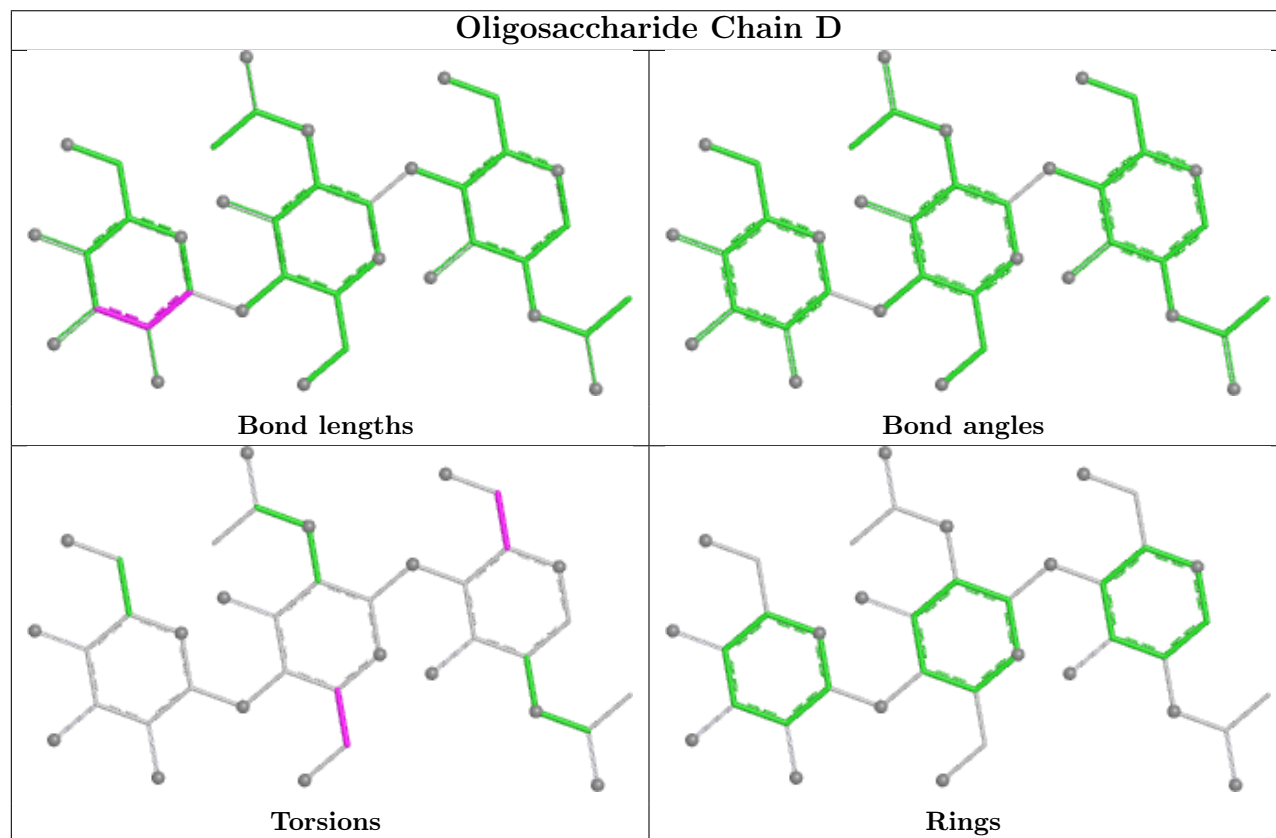
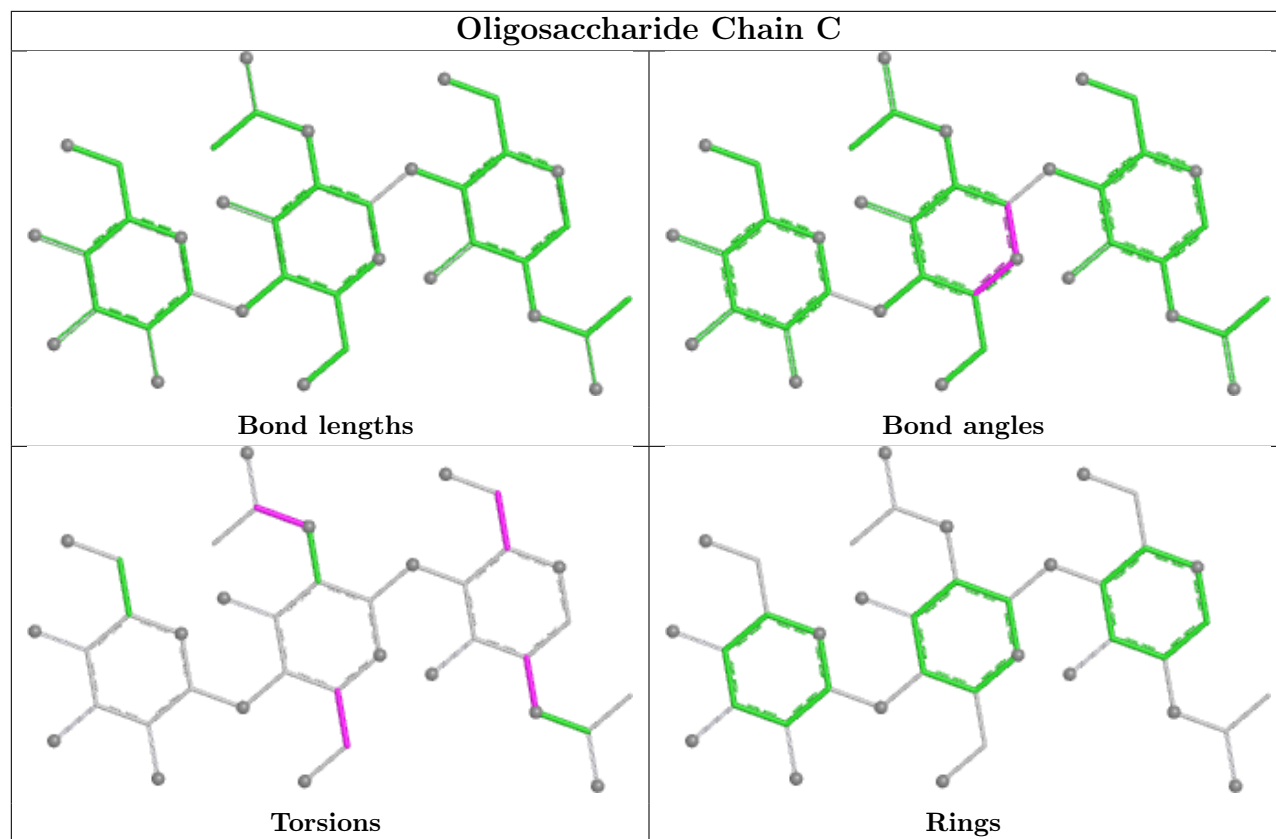
There are no ring outliers.

3 monomers are involved in 4 short contacts:

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

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





5.6 Ligand geometry

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

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, 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	1222/1512 (80%)	1.15	161 (13%) 7 6	18, 50, 86, 131	0

All (161) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	314	SER	6.1
1	A	191	THR	5.8
1	A	1795	ASP	5.5
1	A	1914	GLU	5.1
1	A	2332	TYR	5.0
1	A	189	THR	4.7
1	A	315	HIS	4.6
1	A	1748	TYR	4.5
1	A	2200	PHE	4.4
1	A	2141	ASN	4.3
1	A	1897	ARG	4.2
1	A	181	GLU	4.1
1	A	2004	GLU	4.1
1	A	1838	PHE	3.7
1	A	1739	THR	3.7
1	A	1745	GLN	3.6
1	A	329	CYS	3.4
1	A	2331	LEU	3.4
1	A	711	CYS	3.4
1	A	2330	ASP	3.4
1	A	403	ASP	3.4
1	A	1693	LYS	3.4
1	A	400	LEU	3.3
1	A	1844	GLU	3.3
1	A	260	MET	3.3
1	A	1802	PRO	3.3
1	A	228	TRP	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	398	LEU	3.2
1	A	696	ASP	3.2
1	A	47	LYS	3.2
1	A	1916	TYR	3.2
1	A	1727	VAL	3.1
1	A	1729	GLN	3.1
1	A	2275	PHE	3.1
1	A	646	THR	3.1
1	A	265	GLU	3.1
1	A	2252	LEU	3.1
1	A	1953	ILE	3.0
1	A	135	THR	3.0
1	A	2304	ARG	3.0
1	A	1910	PRO	2.9
1	A	19	SER	2.9
1	A	58	LEU	2.9
1	A	208	TRP	2.9
1	A	236	GLY	2.9
1	A	2030	GLY	2.9
1	A	698	ARG	2.9
1	A	377	LYS	2.9
1	A	4	ARG	2.8
1	A	1754	GLU	2.8
1	A	1909	ASP	2.8
1	A	2083	GLY	2.8
1	A	2231	GLN	2.8
1	A	185	ALA	2.8
1	A	2267	ASP	2.8
1	A	2059	ILE	2.8
1	A	287	GLU	2.8
1	A	539	MET	2.8
1	A	1757	GLY	2.8
1	A	2110	LYS	2.7
1	A	1915	ASN	2.7
1	A	2120	THR	2.7
1	A	571	ARG	2.7
1	A	203	ASP	2.7
1	A	1712	SER	2.7
1	A	53	GLU	2.7
1	A	2122	THR	2.7
1	A	313	SER	2.7
1	A	1908	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	417	GLN	2.6
1	A	273	GLY	2.6
1	A	555	TYR	2.6
1	A	647	ASP	2.6
1	A	1780	SER	2.6
1	A	264	PRO	2.6
1	A	699	ASN	2.6
1	A	1871	VAL	2.6
1	A	2202	THR	2.6
1	A	187	GLU	2.6
1	A	601	VAL	2.6
1	A	2116	ARG	2.5
1	A	1866	ALA	2.5
1	A	2113	GLN	2.5
1	A	407	TYR	2.5
1	A	2195	TYR	2.5
1	A	82	ASP	2.5
1	A	2280	VAL	2.5
1	A	2282	VAL	2.5
1	A	62	ALA	2.5
1	A	626	GLN	2.5
1	A	2270	GLN	2.5
1	A	188	LYS	2.5
1	A	399	VAL	2.5
1	A	624	SER	2.5
1	A	89	LYS	2.5
1	A	166	LYS	2.5
1	A	2043	TYR	2.5
1	A	1806	PHE	2.4
1	A	327	ASP	2.4
1	A	229	PRO	2.4
1	A	15	ASP	2.4
1	A	615	HIS	2.4
1	A	649	LEU	2.4
1	A	2305	TYR	2.4
1	A	2082	HIS	2.4
1	A	438	THR	2.4
1	A	401	ALA	2.4
1	A	152	LEU	2.4
1	A	2	THR	2.3
1	A	2191	THR	2.3
1	A	1740	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	1751	GLU	2.3
1	A	1841	VAL	2.3
1	A	2219	TRP	2.3
1	A	1939	ARG	2.3
1	A	1794	GLU	2.3
1	A	2081	ILE	2.3
1	A	172	LEU	2.3
1	A	16	TYR	2.3
1	A	113	GLU	2.3
1	A	204	GLU	2.3
1	A	540	GLU	2.3
1	A	289	SER	2.3
1	A	556	LYS	2.3
1	A	55	THR	2.3
1	A	44	VAL	2.3
1	A	441	ALA	2.2
1	A	77	GLN	2.2
1	A	2329	GLN	2.2
1	A	2134	GLY	2.2
1	A	2246	GLN	2.2
1	A	302	ASP	2.2
1	A	2174	CYS	2.2
1	A	192	LEU	2.2
1	A	604	GLU	2.2
1	A	1931	GLY	2.2
1	A	2091	GLN	2.1
1	A	2308	ILE	2.1
1	A	59	PHE	2.1
1	A	1728	PRO	2.1
1	A	1793	GLU	2.1
1	A	316	GLN	2.1
1	A	1821	HIS	2.1
1	A	2045	GLN	2.1
1	A	1924	TYR	2.1
1	A	1768	GLU	2.1
1	A	2238	MET	2.1
1	A	2260	PHE	2.1
1	A	645	GLN	2.1
1	A	81	TYR	2.1
1	A	2203	TRP	2.1
1	A	206	LYS	2.1
1	A	1894	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1843	LEU	2.1
1	A	2309	HIS	2.1
1	A	416	PRO	2.0
1	A	402	PRO	2.0
1	A	2201	ALA	2.0
1	A	2222	GLN	2.0
1	A	408	LYS	2.0
1	A	1803	ARG	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](#)

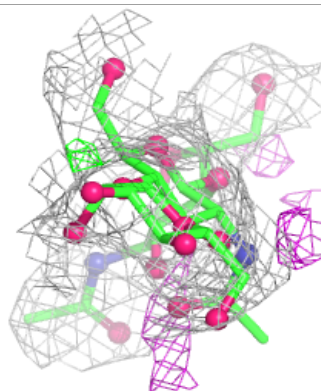
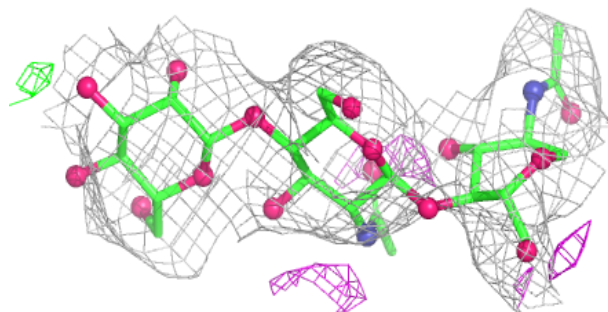
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	NAG	D	2	14/15	0.11	0.24	129,160,166,168	0
2	NAG	D	1	14/15	0.22	0.22	106,138,153,160	0
2	BMA	C	3	11/12	0.25	0.23	124,140,146,149	0
2	BMA	B	3	11/12	0.42	0.19	85,96,102,102	0
2	BMA	D	3	11/12	0.42	0.23	137,156,169,169	0
2	NAG	C	2	14/15	0.49	0.19	99,111,135,137	0
2	NAG	B	2	14/15	0.64	0.21	44,81,88,96	0
2	NAG	C	1	14/15	0.66	0.19	67,83,103,108	0
2	NAG	B	1	14/15	0.75	0.18	28,56,70,80	0

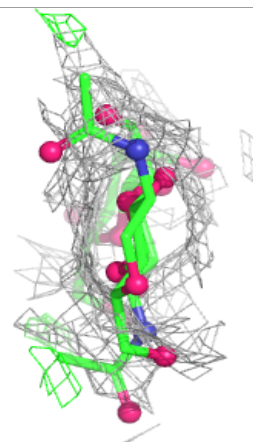
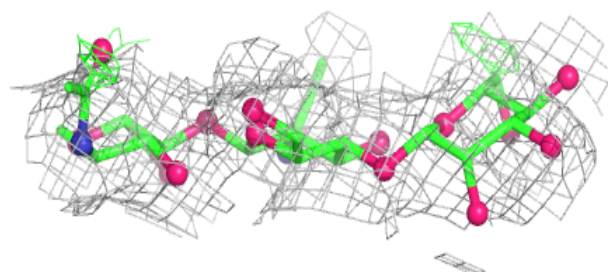
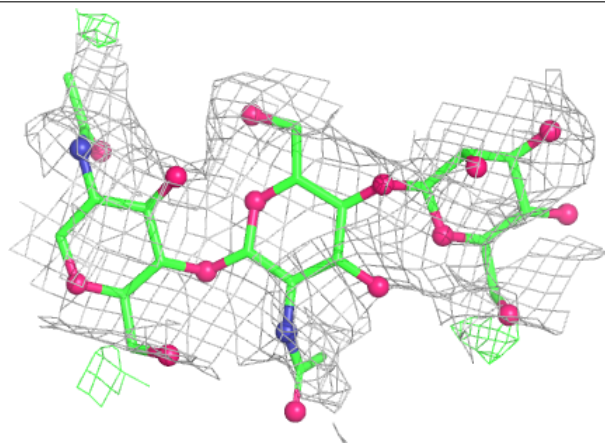
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

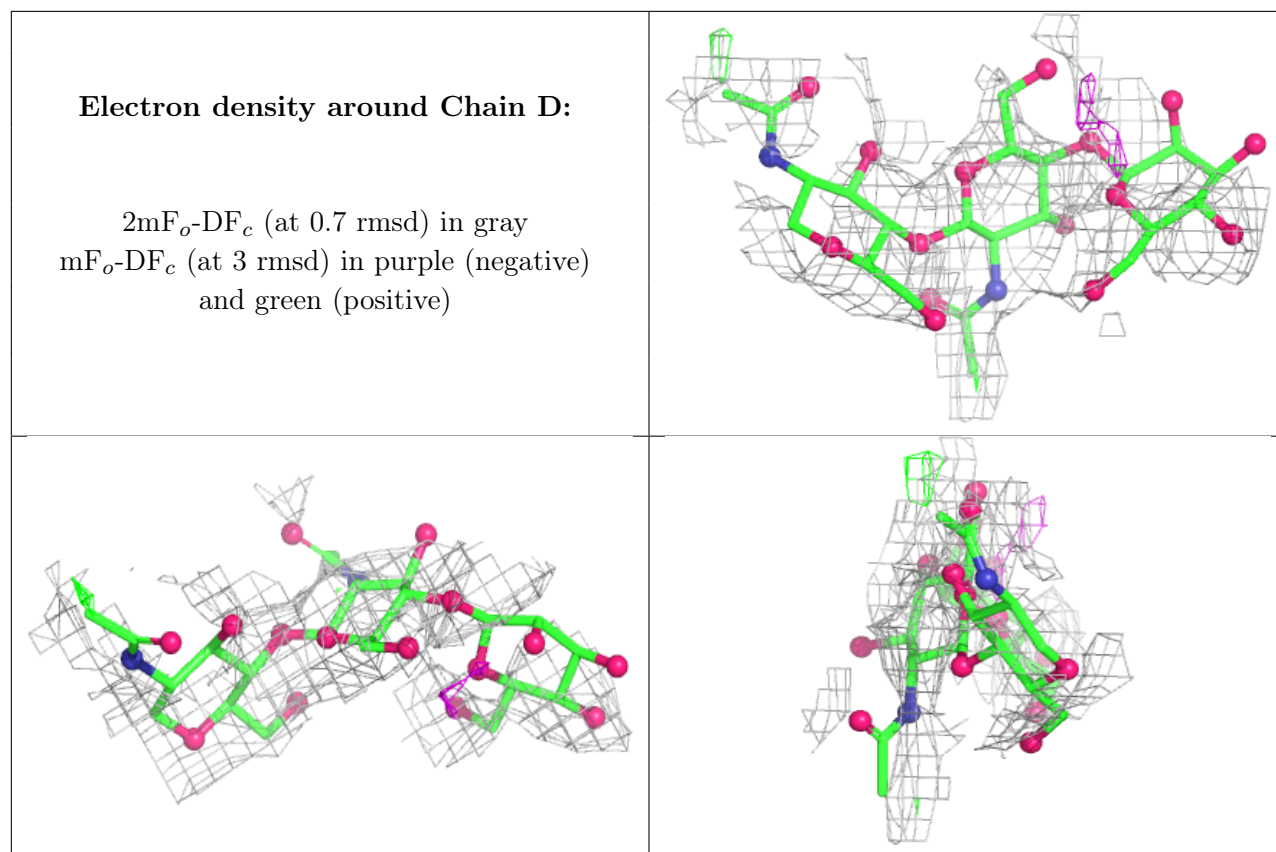
Electron density around Chain B:

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

**Electron density around Chain C:**

$2mF_o-DF_c$ (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
4	ZN	A	2411	1/1	0.98	0.04	55,55,55,55	0
5	CU1	A	2412	1/1	0.98	0.07	27,27,27,27	0
3	CA	A	2410	1/1	0.99	0.12	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.