



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 26, 2024 – 01:26 PM EDT

PDB ID : 6MF2
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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

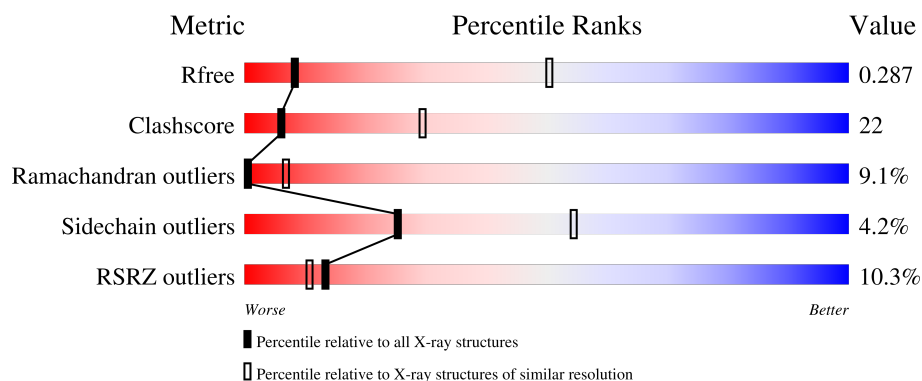
1 Overall quality at a glance

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}	164625	1563 (3.70-3.50)
Clashscore	180529	1665 (3.70-3.50)
Ramachandran outliers	177936	1641 (3.70-3.50)
Sidechain outliers	177891	1640 (3.70-3.50)
RSRZ outliers	164620	1562 (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	<div> <div>8%</div> <div>40%</div> <div>35%</div> <div>6%</div> <div>19%</div> </div>
2	B	3	<div> <div>33%</div> <div>67%</div> </div>
2	C	3	<div> <div>67%</div> <div>33%</div> </div>
2	D	3	<div> <div>67%</div> <div>33%</div> </div>

2 Entry composition [i](#)

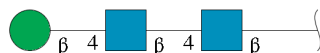
There are 6 unique types of molecules in this entry. The entry contains 10035 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (three-letter code: CA) (formula: Ca).

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

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 5 is COPPER (I) ION (three-letter code: CU1) (formula: Cu).

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

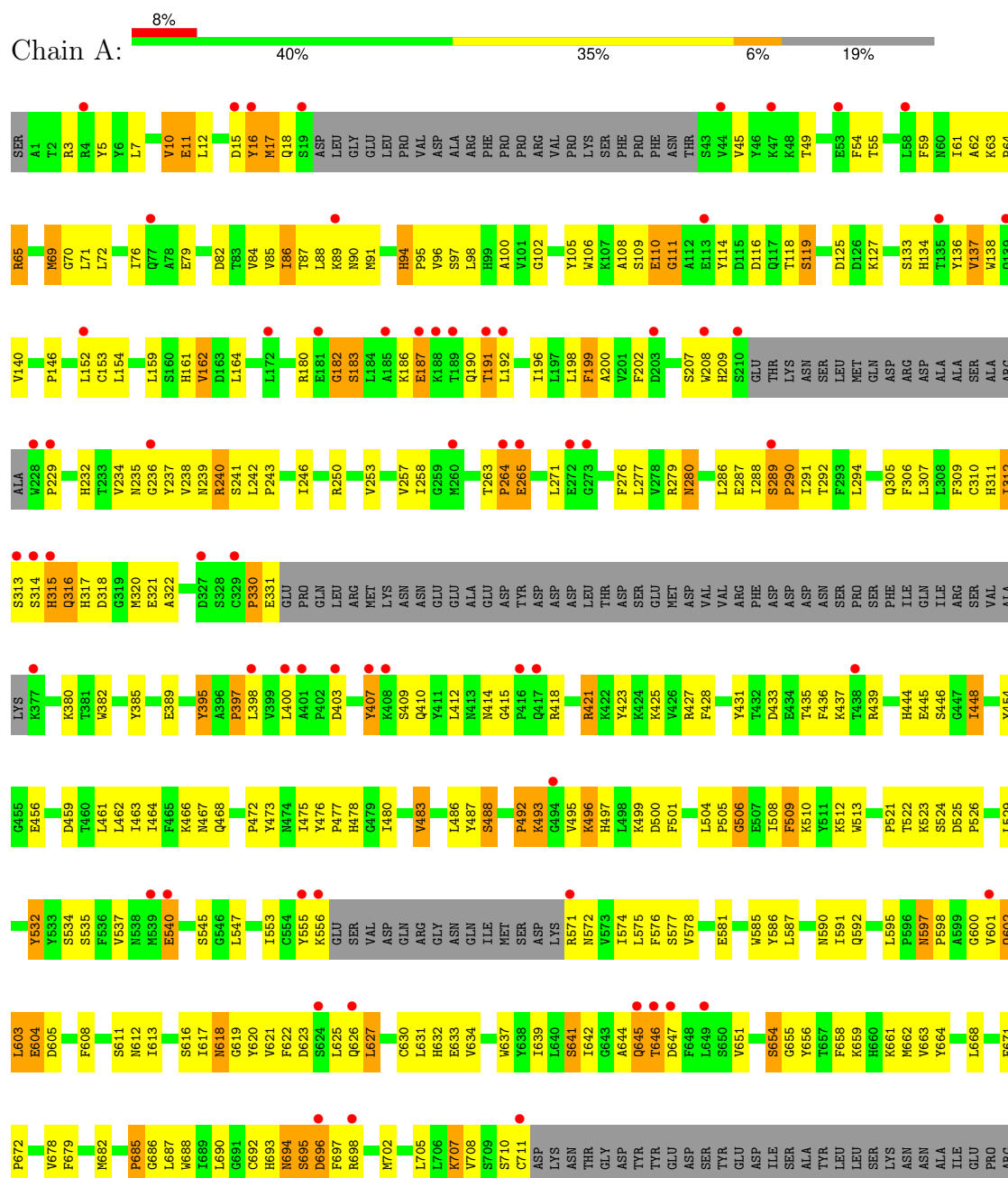
- Molecule 6 is water.

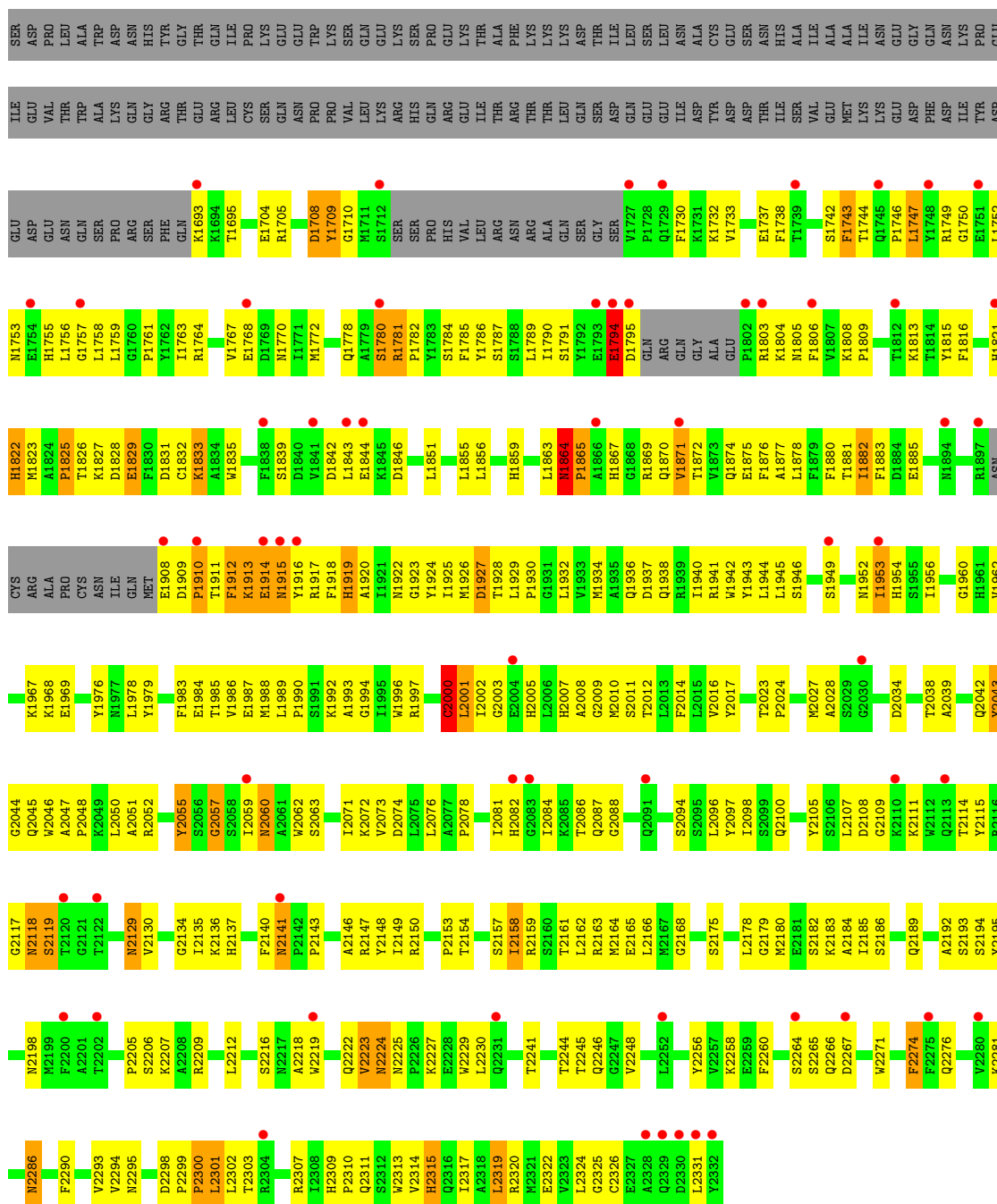
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	O	0	0
			1	1		

3 Residue-property plots [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: Coagulation factor VIII





- 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





- 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) 81.8 (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	2191 reflections (4.92%)	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 , 27.4	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	0.75	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: CA, CU1, BMA, NAG, 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	0.31	0/10198	0.62	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-OE1	24.13	169.85	121.60
1	A	305	GLN	CG-CD-NE2	-17.39	74.95	116.70
1	A	305	GLN	OE1-CD-NE2	-8.63	102.06	121.90
1	A	305	GLN	CA-CB-CG	5.47	125.44	113.40

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	438	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	439	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 22.

All (439) 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: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:1709:TYR:OH	1:A:1732:LYS:NZ	2.17	0.76
1:A:2129:ASN:ND2	1:A:2134:GLY:O	2.19	0.76
1:A:310:CYS:SG	1:A:317:HIS:ND1	2.45	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:2105:TYR:HD2	1:A:2146:ALA:HB2	1.53	0.74
1:A:2078:PRO:HB3	1:A:2107:LEU:HD11	1.69	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:289:SER:HG	1:A:292:THR:HG1	1.33	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: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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:529:LEU:HD11	1:A:553:ILE:HB	1.82	0.60
1:A:1821:HIS:C	1:A:1823:MET:H	2.04	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:310:CYS:HG	1:A:317:HIS:HD1	0.64	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
1:A:2245:THR:HG23	1:A:2293:VAL:HG13	1.86	0.57
1:A:1732:LYS:NZ	1:A:1885:GLU:OE2	2.37	0.57
1:A:199:PHE:HB2	1:A:288:ILE:HD13	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1967:LYS:C	1:A:1969:GLU:H	2.08	0.56
1:A:397:PRO:HB2	1:A:398:LEU:HD22	1.88	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: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: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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:710:SER:OG	1:A:711:CYS:N	2.43	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
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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: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
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1934:MET:HE3	1:A:1990:PRO:HG3	1.95	0.47
1:A:1805:ASN:ND2	1:A:1813:LYS:HE2	2.29	0.47
1:A:1942:TRP:HE1	1:A:1988:MET:CE	2.28	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:2081:ILE:HD13	1:A:2149:ILE:HB	1.95	0.47
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: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: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:2180:MET:HB2	1:A:2322:GLU:HA	1.98	0.46
1:A:1925:ILE:O	1:A:1928:THR:OG1	2.21	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:187:GLU:H	1:A:187:GLU:CD	2.19	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:1781:ARG:CZ	1:A:1781:ARG:HB3	2.45	0.45
1:A:1787:SER:C	1:A:1789:LEU:H	2.20	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
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:695:SER:C	1:A:697:PHE:H	2.20	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:2086:THR:C	1:A:2129:ASN:HD21	2.19	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:473:TYR:HH	1:A:585:TRP:HD1	1.63	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: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
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: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:1870:GLN:C	1:A:1872:THR:H	2.16	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:106:TRP:C	1:A:108:ALA:H	2.20	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: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
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:263:THR:O	1:A:264:PRO:C	2.57	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:645:GLN:C	1:A:647:ASP:H	2.22	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:17:MET:HE2	1:A:239:ASN:HB2	2.03	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:1821:HIS:C	1:A:1823:MET:N	2.73	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: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:2178:LEU:HD21	1:A:2325:GLY:C	2.41	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
1:A:634:VAL:HG12	1:A:679:PHE:CZ	2.55	0.41
1:A:1927:ASP:N	1:A:1927:ASP:OD1	2.54	0.41
1:A:2246:GLN:OE1	1:A:2320:ARG:NE	2.53	0.41
1:A:1967:LYS:C	1:A:1969:GLU:N	2.74	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:2105:TYR:HA	1:A:2148:TYR:O	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:1934:MET:CE	1:A:1990:PRO:HG3	2.52	0.40
1:A:2264:SER:OG	1:A:2301:LEU:HD11	2.22	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

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	1204/1512 (80%)	841 (70%)	254 (21%)	109 (9%)	0 7

All (109) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	ILE
1	A	110	GLU
1	A	133	SER
1	A	191	THR
1	A	264	PRO
1	A	290	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	311	HIS
1	A	312	ILE
1	A	315	HIS
1	A	316	GLN
1	A	483	VAL
1	A	492	PRO
1	A	655	GLY
1	A	708	VAL
1	A	1743	PHE
1	A	1790	ILE
1	A	1794	GLU
1	A	1827	LYS
1	A	1864	ASN
1	A	1871	VAL
1	A	1910	PRO
1	A	1914	GLU
1	A	1953	ILE
1	A	2001	LEU
1	A	2051	ALA
1	A	2118	ASN
1	A	2183	LYS
1	A	2223	VAL
1	A	2224	ASN
1	A	140	VAL
1	A	199	PHE
1	A	330	PRO
1	A	397	PRO
1	A	523	LYS
1	A	602	GLN
1	A	618	ASN
1	A	644	ALA
1	A	654	SER
1	A	695	SER
1	A	702	MET
1	A	1708	ASP
1	A	1709	TYR
1	A	1757	GLY
1	A	1780	SER
1	A	1859	HIS
1	A	1865	PRO
1	A	1882	ILE
1	A	1913	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1937	ASP
1	A	1985	THR
1	A	2000	CYS
1	A	2060	ASN
1	A	2114	THR
1	A	2274	PHE
1	A	2331	LEU
1	A	3	ARG
1	A	16	TYR
1	A	119	SER
1	A	137	VAL
1	A	182	GLY
1	A	265	GLU
1	A	407	TYR
1	A	444	HIS
1	A	446	SER
1	A	493	LYS
1	A	603	LEU
1	A	645	GLN
1	A	1936	GLN
1	A	2045	GLN
1	A	2057	GLY
1	A	2198	ASN
1	A	2227	LYS
1	A	2315	HIS
1	A	10	VAL
1	A	17	MET
1	A	186	LYS
1	A	448	ILE
1	A	540	GLU
1	A	604	GLU
1	A	613	ILE
1	A	646	THR
1	A	1747	LEU
1	A	1778	GLN
1	A	1781	ARG
1	A	1822	HIS
1	A	1825	PRO
1	A	1829	GLU
1	A	1843	LEU
1	A	2158	ILE
1	A	2286	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2290	PHE
1	A	2301	LEU
1	A	69	MET
1	A	229	PRO
1	A	289	SER
1	A	487	TYR
1	A	694	ASN
1	A	696	ASP
1	A	505	PRO
1	A	622	PHE
1	A	707	LYS
1	A	2135	ILE
1	A	162	VAL
1	A	506	GLY
1	A	111	GLY
1	A	1930	PRO
1	A	2300	PRO
1	A	685	PRO
1	A	234	VAL

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	1087/1350 (80%)	1041 (96%)	46 (4%)	25 54

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLU
1	A	65	ARG
1	A	94	HIS
1	A	152	LEU
1	A	153	CYS
1	A	180	ARG
1	A	183	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	187	GLU
1	A	240	ARG
1	A	250	ARG
1	A	280	ASN
1	A	395	TYR
1	A	407	TYR
1	A	421	ARG
1	A	488	SER
1	A	496	LYS
1	A	509	PHE
1	A	532	TYR
1	A	555	TYR
1	A	597	ASN
1	A	623	ASP
1	A	627	LEU
1	A	641	SER
1	A	1693	LYS
1	A	1705	ARG
1	A	1786	TYR
1	A	1794	GLU
1	A	1806	PHE
1	A	1832	CYS
1	A	1833	LYS
1	A	1912	PHE
1	A	1919	HIS
1	A	1927	ASP
1	A	1983	PHE
1	A	1992	LYS
1	A	2000	CYS
1	A	2034	ASP
1	A	2043	TYR
1	A	2055	TYR
1	A	2118	ASN
1	A	2119	SER
1	A	2129	ASN
1	A	2137	HIS
1	A	2157	SER
1	A	2267	ASP
1	A	2319	LEU

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

Mol	Chain	Res	Type
1	A	77	GLN
1	A	305	GLN
1	A	497	HIS
1	A	1919	HIS
1	A	2005	HIS

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 ⓘ

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	1,2	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	1,2	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	1,2	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	1,2	-	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	1,2	-	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	1,2	-	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

Continued on next page...

Continued from previous page...

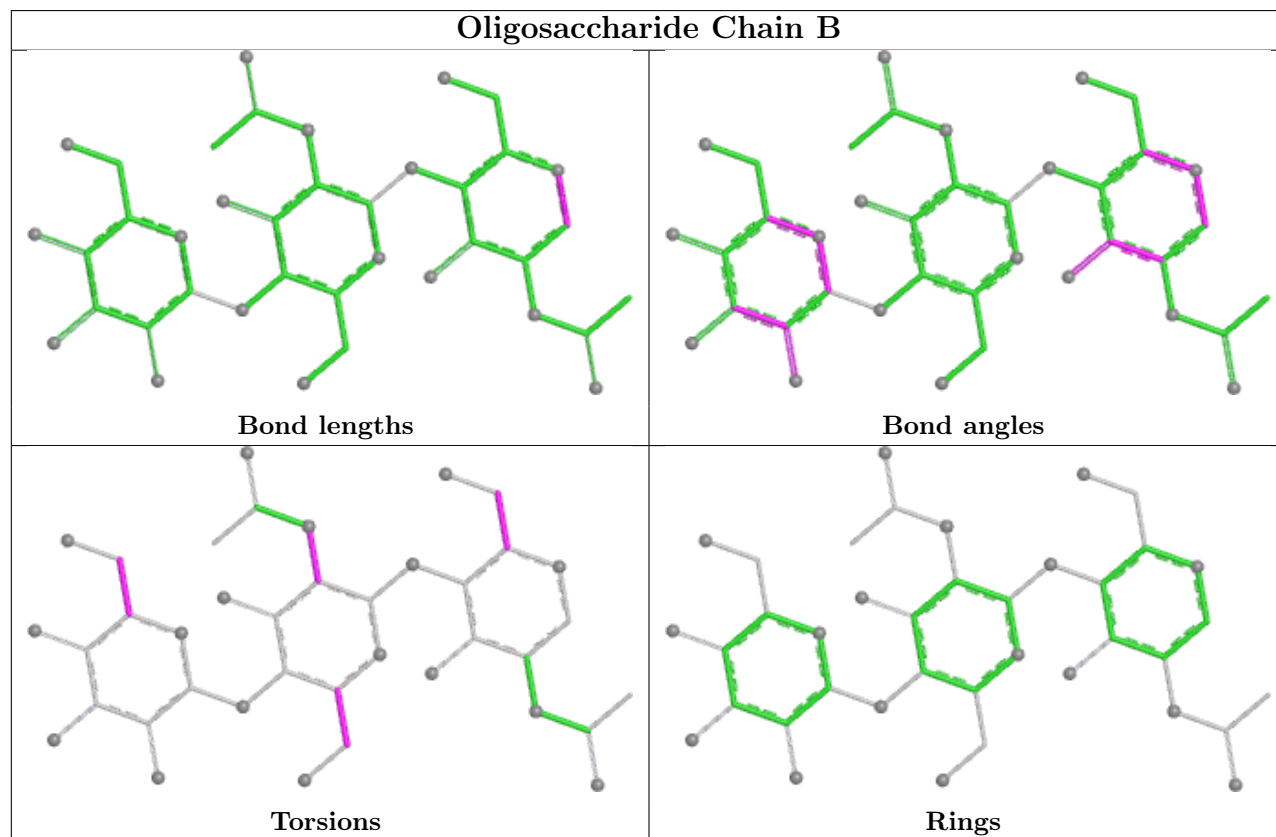
Mol	Chain	Res	Type	Atoms
2	B	3	BMA	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	B	2	NAG	C3-C2-N2-C7
2	C	1	NAG	C3-C2-N2-C7

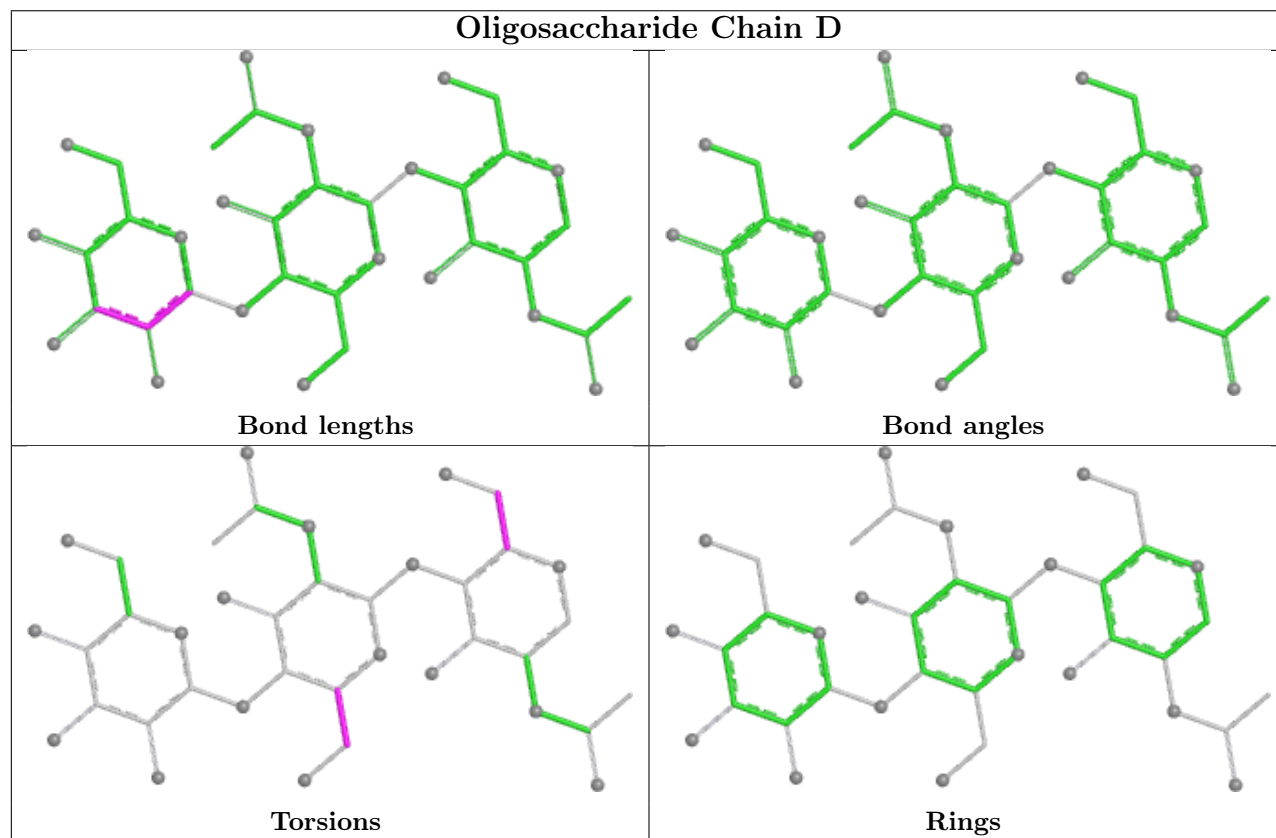
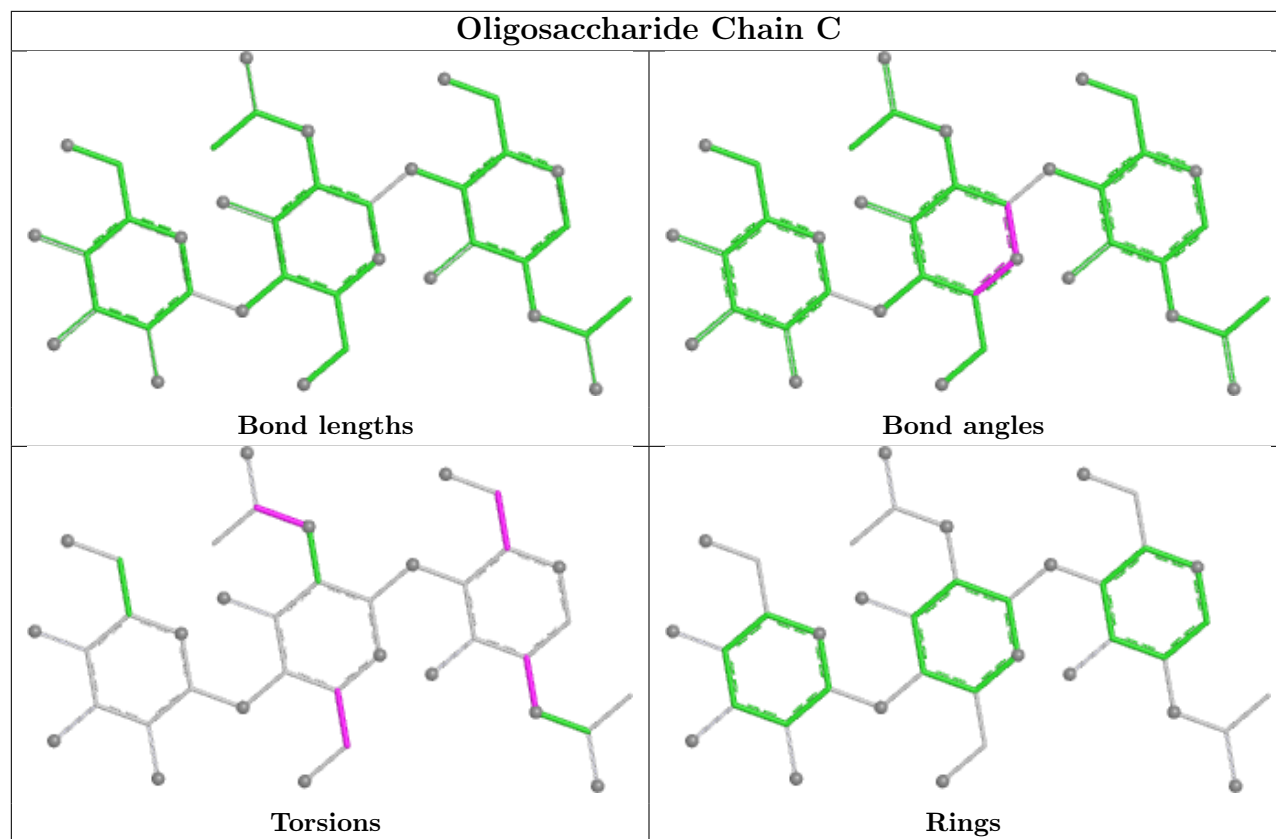
There are no ring outliers.

3 monomers are involved in 4 short contacts:

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

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





5.6 Ligand geometry

Of 3 ligands modelled in this entry, 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%)	0.96	126 (10%)	13 11	18, 50, 86, 131	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	314	SER	6.0
1	A	191	THR	4.8
1	A	315	HIS	4.4
1	A	1795	ASP	4.4
1	A	1748	TYR	4.3
1	A	2332	TYR	4.1
1	A	189	THR	4.0
1	A	2331	LEU	4.0
1	A	2200	PHE	4.0
1	A	1914	GLU	4.0
1	A	1897	ARG	3.9
1	A	2141	ASN	3.8
1	A	2004	GLU	3.6
1	A	400	LEU	3.6
1	A	260	MET	3.5
1	A	646	THR	3.4
1	A	1739	THR	3.3
1	A	1838	PHE	3.3
1	A	181	GLU	3.3
1	A	1693	LYS	3.2
1	A	1844	GLU	3.2
1	A	47	LYS	3.1
1	A	2252	LEU	3.0
1	A	2330	ASP	3.0
1	A	1712	SER	3.0
1	A	711	CYS	3.0
1	A	236	GLY	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	188	LYS	2.9
1	A	1871	VAL	2.9
1	A	403	ASP	2.9
1	A	696	ASP	2.9
1	A	313	SER	2.9
1	A	1953	ILE	2.9
1	A	417	GLN	2.9
1	A	1915	ASN	2.9
1	A	1802	PRO	2.8
1	A	2275	PHE	2.8
1	A	265	GLU	2.8
1	A	228	TRP	2.8
1	A	1727	VAL	2.8
1	A	15	ASP	2.8
1	A	152	LEU	2.7
1	A	1745	GLN	2.7
1	A	1916	TYR	2.7
1	A	601	VAL	2.7
1	A	647	ASP	2.7
1	A	4	ARG	2.6
1	A	19	SER	2.6
1	A	539	MET	2.6
1	A	135	THR	2.6
1	A	377	LYS	2.6
1	A	2091	GLN	2.6
1	A	1780	SER	2.6
1	A	264	PRO	2.5
1	A	2231	GLN	2.5
1	A	58	LEU	2.5
1	A	172	LEU	2.5
1	A	2120	THR	2.5
1	A	626	GLN	2.5
1	A	2059	ILE	2.5
1	A	203	ASP	2.5
1	A	556	LYS	2.5
1	A	1894	ASN	2.4
1	A	2280	VAL	2.4
1	A	624	SER	2.4
1	A	2030	GLY	2.4
1	A	2329	GLN	2.4
1	A	698	ARG	2.4
1	A	229	PRO	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	289	SER	2.4
1	A	645	GLN	2.4
1	A	273	GLY	2.4
1	A	1757	GLY	2.4
1	A	187	GLU	2.4
1	A	398	LEU	2.4
1	A	1866	ALA	2.3
1	A	407	TYR	2.3
1	A	329	CYS	2.3
1	A	2113	GLN	2.3
1	A	438	THR	2.3
1	A	555	TYR	2.3
1	A	571	ARG	2.3
1	A	185	ALA	2.3
1	A	2267	ASP	2.3
1	A	1910	PRO	2.3
1	A	139	GLN	2.3
1	A	2122	THR	2.2
1	A	208	TRP	2.2
1	A	1754	GLU	2.2
1	A	1908	GLU	2.2
1	A	2110	LYS	2.2
1	A	2202	THR	2.2
1	A	2304	ARG	2.2
1	A	494	GLY	2.2
1	A	1812	THR	2.2
1	A	89	LYS	2.2
1	A	2082	HIS	2.2
1	A	1729	GLN	2.2
1	A	192	LEU	2.2
1	A	1751	GLU	2.2
1	A	53	GLU	2.1
1	A	113	GLU	2.1
1	A	2219	TRP	2.1
1	A	2264	SER	2.1
1	A	540	GLU	2.1
1	A	2083	GLY	2.1
1	A	1841	VAL	2.1
1	A	1794	GLU	2.1
1	A	401	ALA	2.1
1	A	44	VAL	2.1
1	A	77	GLN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	649	LEU	2.1
1	A	16	TYR	2.1
1	A	1843	LEU	2.1
1	A	408	LYS	2.1
1	A	1821	HIS	2.1
1	A	416	PRO	2.1
1	A	1806	PHE	2.1
1	A	2328	ALA	2.1
1	A	1949	SER	2.1
1	A	1803	ARG	2.0
1	A	272	GLU	2.0
1	A	327	ASP	2.0
1	A	1768	GLU	2.0
1	A	1793	GLU	2.0
1	A	210	SER	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](#)

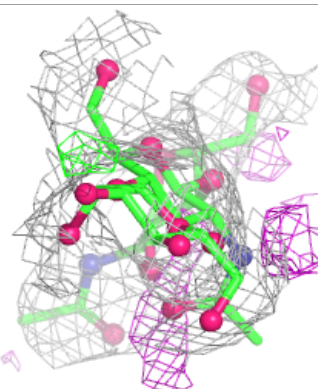
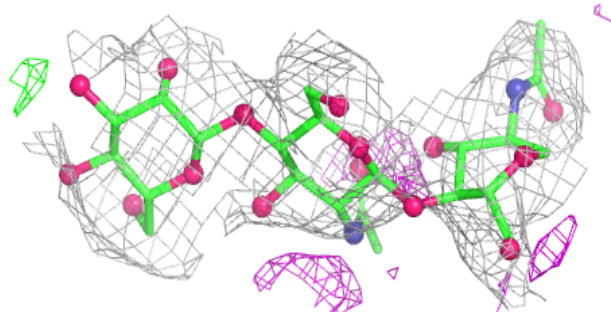
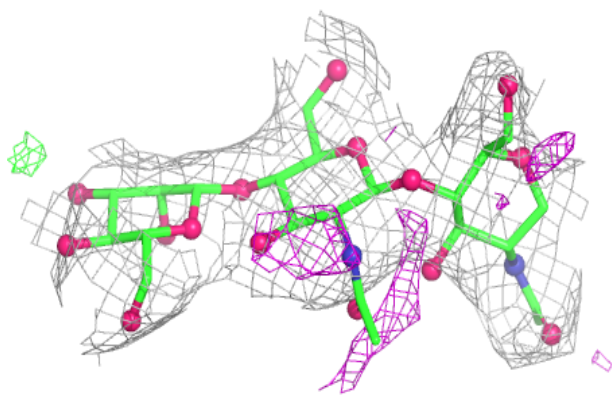
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	D	1	14/15	0.07	0.24	106,138,153,160	0
2	NAG	D	2	14/15	0.12	0.24	129,160,166,168	0
2	BMA	C	3	11/12	0.31	0.21	124,140,146,149	0
2	BMA	D	3	11/12	0.42	0.25	137,156,169,169	0
2	BMA	B	3	11/12	0.43	0.17	85,96,102,102	0
2	NAG	C	2	14/15	0.54	0.18	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	0.70	0.18	67,83,103,108	0
2	NAG	B	1	14/15	0.76	0.17	28,56,70,80	0

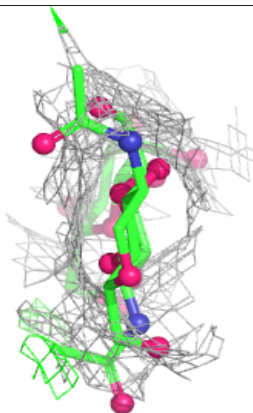
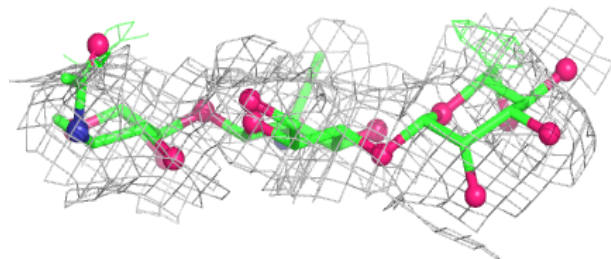
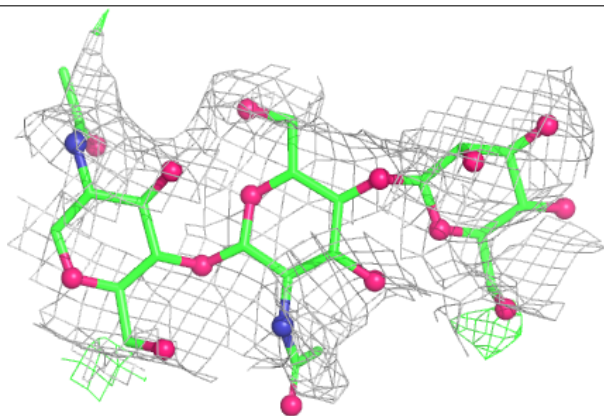
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

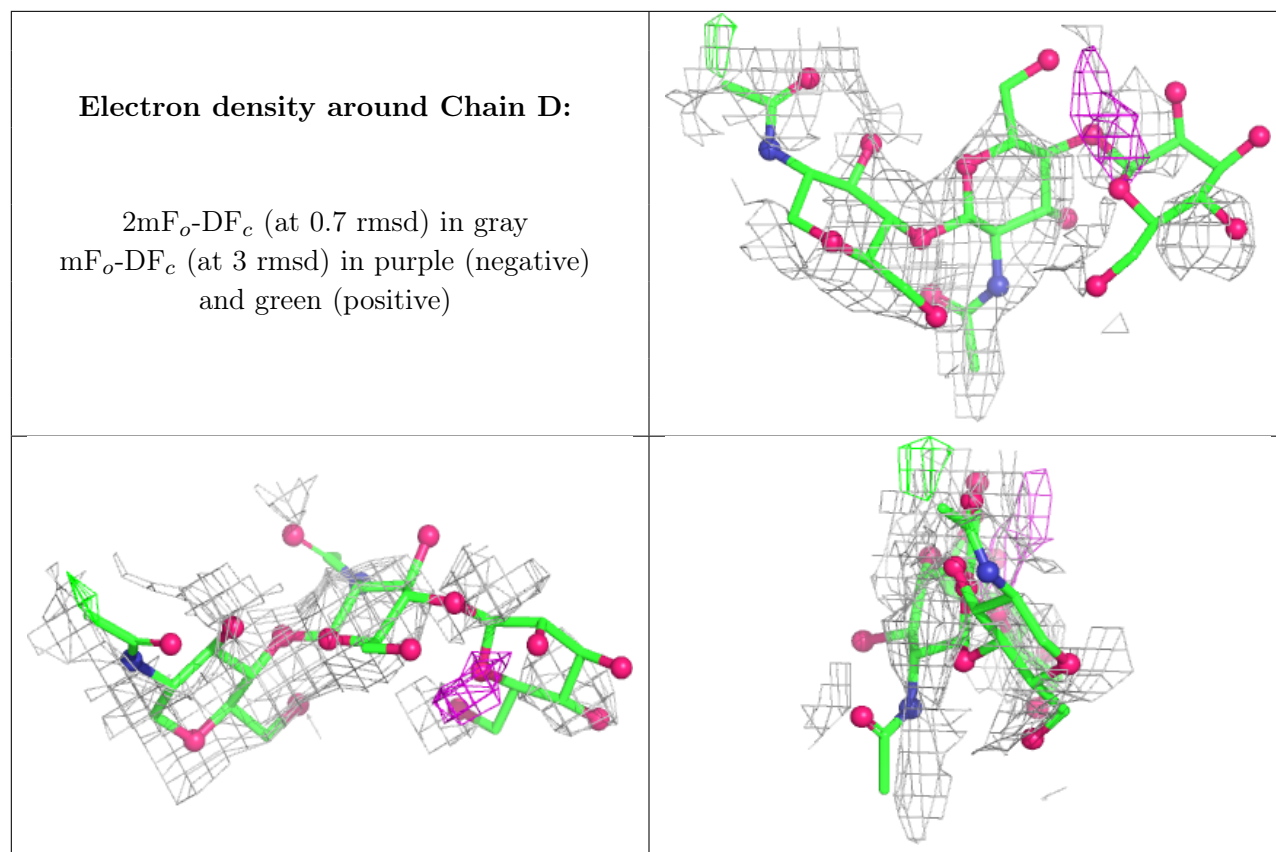
Electron density around Chain B:

$2mF_o-DF_c$ (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(\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	0.13	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.