



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 11:18 PM BST

PDB ID : 6MF0
Title : Crystal Structure Determination of Human/Porcine Chimera Coagulation Factor VIII
Authors : Smith, I.W.; Spiegel, P.C.
Deposited on : 2018-09-07
Resolution : 3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

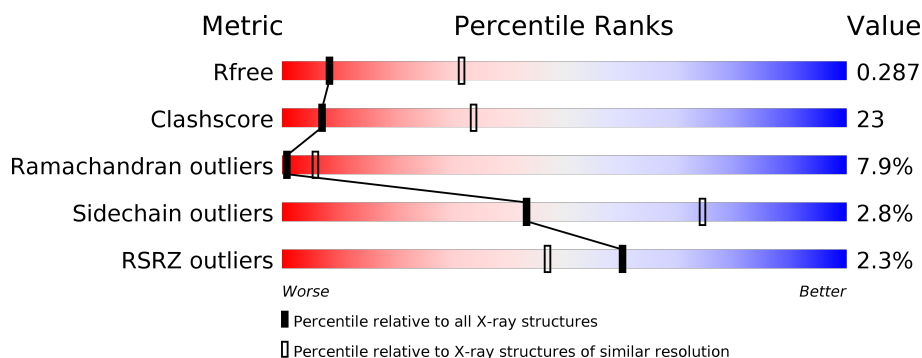
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	<div> <div>%</div> <div> <div></div> <div>46%</div> <div>35%</div> <div>5%</div> <div>14%</div> </div> </div>
1	B	1467	<div> <div>2%</div> <div> <div></div> <div>42%</div> <div>38%</div> <div>5%</div> <div>15%</div> </div> </div>
2	C	5	<div> <div></div> <div>80%</div> <div>20%</div> </div>
2	E	5	<div> <div></div> <div>20%</div> <div>60%</div> <div>20%</div> </div>
2	F	5	<div> <div></div> <div>20%</div> <div>60%</div> <div>20%</div> </div>
3	D	3	<div> <div></div> <div>100%</div> </div>

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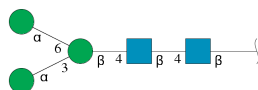
Mol	Chain	Length	Quality of chain
4	G	7	
5	H	6	

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
2	NAG	C	2	-	-	-	X
2	BMA	C	3	-	-	-	X
2	MAN	C	4	-	-	-	X
2	MAN	C	5	-	-	-	X
2	BMA	F	3	-	-	-	X
2	MAN	F	4	-	-	-	X
2	MAN	F	5	-	-	-	X
3	BMA	D	3	-	-	-	X
4	FUC	G	7	-	-	-	X
5	MAN	H	5	-	-	-	X

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 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

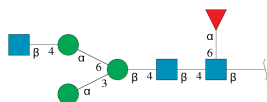


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	5	Total 61	C 34	N 2	O 25	0	0	0
2	E	5	Total 61	C 34	N 2	O 25	0	0	0
2	F	5	Total 61	C 34	N 2	O 25	0	0	0

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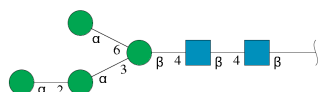
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	7	Total	C	N	O	0	0	0
			85	48	3	34			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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
5	H	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Ca	0	0
			1	1		
6	A	1	Total	Ca	0	0
			1	1		

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 8 is COPPER (I) ION (three-letter code: CU1) (formula: Cu).

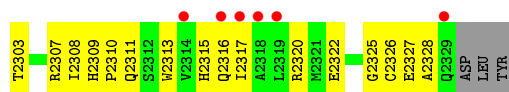
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total 1	Cu 1	0	0
8	A	1	Total 1	Cu 1	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	5	Total 5	O 5	0	0
9	B	1	Total 1	O 1	0	0

WORLDWIDE
PDB
PROTEIN DATA BANK

N2225	H2155	K2092	L2006	T1911	E1827	L1752	I1E	ASN	G668	E589	T514	T435	ASP
F2226	Y2156	F2093	Q2007	L1912	D1828	M1753	TTR	ALA	L668	R593	V515	F436	GLY
E2227	S2157	K1913	A2008	K1913	E1829	H1754	GLU	ILE	F671	R594	E518	K437	ASP
E2228	I2158	S2094	G2009	E1914	F1830	H1755	ASP	PRO	G675	R594	D519	T438	VAL
N2229	R2159	S2095	M2010	N1915	C1832	L1756	GLU	ARG	M680	A598	G520	R439	SER
L2230	S2160	L2096	S2011	Y1916	K1833	L1758	ASN	ASN	M680	L603	P521	P440	PRO
T2231	T2161	Y2097	T2012	R1917	K1833	L1759	GLN	PHE	M680	L603	T522	I442	PHE
D2233	L2162	I2098	L2015	F1918	W1835	G1760	ASP	ALA	S681	E507	K523	Q443	ILE
F2234	R2163	S2099	K2101	H1919	W1836	P1761	PRO	GLN	M682	E507	S524	S446	GLN
Q2235	M2164	Q2100	K2020	Y1837	Y1836	Y1762	ARG	ARG	M683	E507	D525	I447	ILE
K2239	E2165	I2102	K2020	G1923	Y1841	I1763	SER	ARG	N684	A610	P526	T448	ARG
T2244	C2169	I2103	G2026	Y1924	V1841	R1764	PHE	ARG	P685	S611	R527	L449	VAL
T2245	D2170	M2104	K2027	Y1925	D1846	A1765	GLN	PRO	G686	R612	G528	L453	ALA
Q2246	Y2105	S2106	A2028	D1927	D1946	E1766	K1693	PRO	R688	R613	L529	L452	LYS
G2247	T2107	L2107	K2032	T1928	D1946	E1766	R1694	SER	M688	R614	E534	L453	LYS
V2248	L2108	D2108	I2032	P1930	S1849	D1769	T1695	ALA	L690	R615	S534	R377	GLY
G2109	G2109	G1931	Q1936	G1931	G1850	M1770	T1695	SER	L690	R615	S534	R378	GLY
K2110	K2110	L1932	L1932	L1932	L1851	I1771	T1695	ALA	G691	R616	S535	R379	GLY
K2111	K2111	L1932	L1932	L1932	G1852	M1772	T1700	PRO	G692	R617	S535	R380	GLY
Q2112	Q2112	W112	A2039	Q1937	P1854	T1774	PRO	PRO	H693	R618	F536	R381	GLY
Q2113	Q2113	L1855	L1855	L1855	F1775	F1775	PRO	PRO	S695	R621	M538	L461	GLY
T2114	T2114	F1876	F1876	F1876	K1776	K1776	VAL	VAL	R699	R622	E540	L462	GLY
Y2115	Y2115	L1857	L1857	L1857	M1777	M1777	LEU	LEU	R700	R623	R541	L463	GLY
R2116	R2116	C1858	C1858	C1858	Q1778	Q1778	ARG	ARG	R700	R624	D542	L464	GLY
G2117	G2117	L1863	L1863	L1863	R1781	R1781	ARG	ARG	M702	R626	L547	L465	GLY
N2118	N2118	L1943	L1943	L1943	P1782	P1782	HIS	HIS	M702	R626	L547	L466	GLY
S2119	S2119	L1944	L1944	L1944	Y1783	Y1783	GLN	GLN	A704	R629	P550	R471	GLY
T2120	T2120	S1946	S1946	S1946	A1784	A1784	ASP	ASP	L705	R630	L551	P472	GLY
G2121	G2121	F1876	F1876	F1876	F1785	F1785	ILE	ILE	L706	R631	L552	Y473	GLY
T2122	T2122	F1879	F1879	F1879	R1789	R1789	SER	SER	K707	R632	L552	M474	GLY
L2123	L2123	F1883	F1883	F1883	L1790	L1790	ASN	ASN	R708	R633	K556	P485	GLY
M2124	M2124	D1884	D1884	D1884	S1791	S1791	LEU	LEU	S709	R634	GLU	L486	GLY
F2126	F2126	E1885	E1885	E1885	Y1792	Y1792	ALA	ALA	S710	R635	SER	L487	GLY
F2127	F2127	K1887	K1887	K1887	G1799	G1799	GLN	GLN	C711	R636	VAL	S488	GLY
S2133	S2133	Y1890	Y1890	Y1890	A1800	A1800	ASN	ASN	ASP	R637	ASP	R489	GLY
G2134	G2134	E1893	E1893	E1893	E1801	E1801	PRO	PRO	LYS	R638	GLN	R490	GLY
I2135	I2135	M1894	M1894	M1894	R1802	R1802	GLU	GLU	ASN	R639	ARG	L491	GLY
K2136	K2136	V1895	V1895	V1895	H1804	H1804	THR	THR	GLY	R640	GLY	P492	GLY
H2137	H2137	E1896	E1896	E1896	R1803	R1803	ASP	ASP	ASN	R641	ASN	K493	GLY
N2138	N2138	R1897	R1897	R1897	H1804	H1804	LYS	LYS	GLN	R642	GLN	G494	GLY
I2139	I2139	Y1897	Y1897	Y1897	Y1807	Y1807	MET	MET	TYR	R645	ILE	V495	GLY
F2140	F2140	L1977	L1977	L1977	T1812	T1812	ASP	ASP	GLU	R648	ASP	R497	GLY
N2141	N2141	Y1979	Y1979	Y1979	R1813	R1813	THR	THR	ASP	R651	R571	K498	GLY
P2142	P2142	Y1979	Y1979	Y1979	T1814	T1814	ILE	ILE	TYR	R651	R571	K499	GLY
G2143	G2143	Y1982	Y1982	Y1982	Y1815	Y1815	PHE	PHE	GLU	R654	R572	D500	GLY
I2144	I2144	F1983	F1983	F1983	F1816	F1816	SER	SER	ASP	R654	R572	F501	GLY
I2145	I2145	E1984	E1984	E1984	Y1819	Y1819	THR	THR	ILE	R655	R573	L504	GLY
A2146	A2146	Y1989	Y1989	Y1989	H1821	H1821	GLY	GLY	GLU	R656	R574	P505	GLY
R2147	R2147	Y1993	Y1993	Y1993	H1822	H1822	LYS	LYS	TYR	R657	R575	L504	GLY
Y2148	Y2148	G2003	G2003	G2003	M1823	M1823	GLU	GLU	LEU	R658	R575	L504	GLY
I2149	I2149	G2003	G2003	G2003	M1823	M1823	LEU	LEU	LEU	R659	R575	L504	GLY
R2150	R2150	G2003	G2003	G2003	M1823	M1823	ASP	ASP	LEU	R660	R575	L504	GLY
L2151	L2151	G2003	G2003	G2003	M1823	M1823	PHE	PHE	LEU	R661	R575	L504	GLY
H2152	H2152	G2003	G2003	G2003	M1823	M1823	ASP	ASP	LEU	R662	R575	L504	GLY
G2153	G2153	G2003	G2003	G2003	M1823	M1823	ASP	ASP	LEU	R663	R575	L504	GLY
T2154	T2154	G2003	G2003	G2003	M1823	M1823	ASP	ASP	LEU	R664	R575	L504	GLY



- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C: 80% 20%



- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 20% 60% 20%



- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 20% 60% 20%



- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 100%

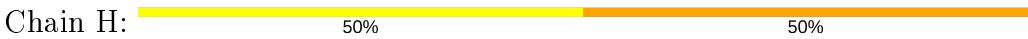


- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G: 71% 29%



- Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



HA01
HA02
HA03
HA04
HA05
HA06

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.00 Å 135.86 Å 196.11 Å 90.00° 90.15° 90.00°	Depositor
Resolution (Å)	49.03 – 3.20 49.03 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.03-3.20) 99.9 (49.03-3.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 3.19 Å)	Xtriage
Refinement program	PHENIX 1.12_2829, PHENIX 1.12_2829	Depositor
R, R_{free}	0.206 , 0.287 0.206 , 0.287	Depositor DCC
R_{free} test set	3077 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	62.6	Xtriage
Anisotropy	0.515	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 47.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.031 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	20622	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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: ZN, BMA, NAG, CU1, CA, FUC, MAN

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	0.54	5/10434 (0.0%)	0.78	8/14149 (0.1%)
1	B	0.49	1/10367 (0.0%)	0.72	7/14053 (0.0%)
All	All	0.51	6/20801 (0.0%)	0.75	15/28202 (0.1%)

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	11
1	B	0	6
All	All	0	17

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	2150	ARG	CZ-NH2	-7.05	1.23	1.33
1	A	191	GLN	CD-NE2	6.91	1.50	1.32
1	A	2174	CYS	CA-CB	-6.57	1.39	1.53
1	A	191	GLN	CD-OE1	-6.53	1.09	1.24
1	A	2016	VAL	CB-CG2	-5.65	1.41	1.52
1	A	191	GLN	CG-CD	-5.14	1.39	1.51

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	191	GLN	CG-CD-OE1	29.15	179.90	121.60
1	A	191	GLN	CA-CB-CG	19.14	155.50	113.40
1	A	191	GLN	CG-CD-NE2	-14.70	81.43	116.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	191	GLN	OE1-CD-NE2	-10.11	98.66	121.90
1	A	191	GLN	CB-CG-CD	-8.73	88.89	111.60
1	B	2150	ARG	NE-CZ-NH2	8.59	124.59	120.30
1	B	683	GLU	C-N-CA	-8.37	100.77	121.70
1	A	292	LEU	CA-CB-CG	-7.18	98.79	115.30
1	B	2150	ARG	NH1-CZ-NH2	-6.77	111.95	119.40
1	A	449	LEU	CA-CB-CG	6.76	130.86	115.30
1	B	42	GLY	C-N-CD	-6.26	106.84	120.60
1	B	2150	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	A	627	LEU	CA-CB-CG	5.56	128.08	115.30
1	B	199	LEU	CA-CB-CG	5.16	127.17	115.30
1	B	44	SER	N-CA-C	5.15	124.92	111.00

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2057	GLY	Peptide
1	A	2141	ASN	Peptide
1	A	2278	GLY	Peptide
1	A	2298	ASP	Peptide
1	A	24	GLU	Peptide
1	A	39	LEU	Peptide
1	A	404	ASP	Peptide
1	A	473	TYR	Peptide
1	A	570	LYS	Peptide
1	A	691	GLY	Peptide
1	A	696	ASP	Peptide
1	B	2119	SER	Peptide
1	B	2141	ASN	Peptide
1	B	2298	ASP	Peptide
1	B	244	PRO	Peptide
1	B	28	ASP	Peptide
1	B	684	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	10147	0	9905	424	2
1	B	10084	0	9837	506	1
2	C	61	0	52	3	0
2	E	61	0	52	2	0
2	F	61	0	52	0	2
3	D	39	0	34	0	0
4	G	85	0	73	2	0
5	H	72	0	61	2	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
9	A	5	0	0	0	0
9	B	1	0	0	0	0
All	All	20622	0	20066	927	3

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 (927) 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:B:2104:MET:CE	1:B:2150:ARG:HH21	1.60	1.12
1:B:2104:MET:HE2	1:B:2150:ARG:HH21	1.04	1.10
1:B:44:SER:O	1:B:46:LEU:HD12	1.66	0.95
1:A:1728:PRO:HG3	1:A:1897:ARG:HH21	1.29	0.94
1:B:1776:LYS:HG3	1:B:1812:THR:HG22	1.49	0.92
1:B:690:LEU:HB3	1:B:704:ALA:HB3	1.53	0.91
1:B:1752:LEU:HD13	1:B:2118:ASN:HB2	1.53	0.88
1:B:2212:LEU:O	1:B:2320:ARG:NH1	2.07	0.87
1:B:2185:ILE:O	1:B:2209:ARG:NH1	2.06	0.87
1:B:2104:MET:CE	1:B:2150:ARG:NH2	2.38	0.86
1:B:435:THR:HG23	1:B:437:LYS:H	1.41	0.85
1:B:2104:MET:HE2	1:B:2150:ARG:NH2	1.90	0.85
1:B:622:PHE:O	1:B:624:SER:N	2.09	0.85
1:B:82:TYR:HE1	1:B:143:LYS:HG2	1.42	0.84
1:B:2086:THR:HG22	1:B:2136:LYS:HB3	1.58	0.84
1:A:2182:SER:O	1:A:2184:ALA:N	2.11	0.83
1:A:1993:VAL:HA	1:A:2016:VAL:HG23	1.59	0.83
1:A:697:PHE:O	1:A:699:ASN:N	2.11	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:PRO:O	1:B:151:ASP:HB2	1.79	0.83
1:A:708:VAL:HG23	1:A:709:SER:H	1.42	0.83
1:B:27:VAL:HB	1:B:63:ALA:HB2	1.59	0.83
1:A:601:VAL:HG23	1:A:602:GLN:H	1.43	0.82
1:B:147:PRO:HG2	1:B:181:ARG:HG3	1.60	0.81
1:A:1846:ASP:HB3	1:A:1889:TRP:HE1	1.45	0.81
1:B:617:ILE:HG23	1:B:625:LEU:HD23	1.63	0.81
1:A:2100:GLN:HB3	1:A:2155:HIS:HB2	1.63	0.81
1:A:522:THR:O	1:A:524:SER:N	2.13	0.81
1:B:2096:LEU:HD23	1:B:2159:ARG:HB3	1.60	0.81
1:B:266:GLU:OE1	1:B:318:HIS:CE1	2.34	0.81
1:A:602:GLN:O	1:A:604:GLU:N	2.16	0.79
1:B:2110:LYS:HD3	1:B:2112:TRP:HE1	1.47	0.79
1:B:1696:ARG:HD2	1:B:1765:ALA:HA	1.64	0.79
1:A:435:THR:HG23	1:A:437:LYS:H	1.46	0.78
1:A:3:ARG:NH1	1:A:83:ASP:OD2	2.15	0.78
1:A:265:PRO:HG3	1:A:1951:GLU:HG2	1.65	0.78
1:A:50:THR:HG21	1:A:95:HIS:CE1	2.19	0.78
1:B:687:LEU:HD12	1:B:707:LYS:HB3	1.64	0.78
1:A:192:ASN:HB3	1:A:252:LYS:HG2	1.64	0.77
1:A:504:LEU:HB3	1:A:505:PRO:HD2	1.65	0.77
1:A:64:ARG:HD3	1:A:65:PRO:HD2	1.65	0.77
1:A:666:ASP:HB2	1:A:1835:TRP:HZ3	1.50	0.77
1:A:654:SER:O	1:A:656:TYR:N	2.18	0.76
1:A:1895:VAL:O	1:A:1897:ARG:N	2.20	0.75
1:B:2026:GLY:HA3	1:B:2032:ILE:HG13	1.69	0.75
1:A:326:ARG:NH1	1:A:328:GLU:OE2	2.19	0.75
1:B:1737:GLU:HB2	1:B:1761:PRO:HG3	1.68	0.75
1:B:1937:ASN:HA	1:B:1989:LEU:HD21	1.69	0.74
1:B:2100:GLN:HE22	1:B:2127:PHE:HE1	1.35	0.74
1:A:119:THR:HG23	1:A:123:GLU:HB2	1.70	0.74
1:B:651:VAL:HG12	1:B:668:LEU:O	1.89	0.73
1:A:114:GLU:HB2	1:A:127:ASP:HB3	1.71	0.73
1:B:382:TRP:HB2	1:B:461:LEU:HD23	1.71	0.73
1:A:1732:LYS:NZ	1:A:1885:GLU:OE2	2.21	0.72
1:B:2107:LEU:HD23	1:B:2146:ALA:HA	1.70	0.72
1:B:2244:THR:HB	1:B:2322:GLU:HB3	1.71	0.72
1:B:686:GLY:HA2	1:B:1801:GLU:HG3	1.70	0.72
1:A:188:GLU:HG3	1:A:193:LEU:HD13	1.72	0.72
1:B:306:GLN:HG2	1:B:326:ARG:HG2	1.71	0.72
1:A:443:GLN:HE22	1:A:446:SER:H	1.36	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:LEU:O	1:A:195:GLU:N	2.23	0.71
1:B:574:ILE:HD11	1:B:637:TRP:CE3	2.25	0.71
1:B:1777:ASN:OD1	1:B:1778:GLN:N	2.24	0.71
1:A:317:HIS:HD2	2:C:2:NAG:H81	1.56	0.70
1:A:504:LEU:O	1:A:506:GLY:N	2.24	0.70
1:B:1769:ASP:O	1:B:1819:VAL:HG12	1.91	0.70
1:A:2169:CYS:SG	1:A:2173:SER:HA	2.30	0.70
1:A:195:GLU:HG2	1:A:255:TYR:HB2	1.73	0.70
1:B:190:THR:O	1:B:192:ASN:N	2.24	0.70
1:B:574:ILE:HD11	1:B:637:TRP:HE3	1.56	0.70
1:B:82:TYR:CE1	1:B:143:LYS:HG2	2.26	0.70
1:B:396:ALA:HB3	1:B:421:ARG:HD3	1.73	0.70
1:B:485:PRO:HD3	1:B:498:LEU:HD11	1.74	0.70
1:A:443:GLN:NE2	1:A:446:SER:H	1.90	0.70
1:B:1945:LEU:HG	1:B:1983:PHE:HD1	1.56	0.70
1:A:1869:ARG:NH2	2:E:1:NAG:O7	2.25	0.70
1:B:266:GLU:OE1	1:B:318:HIS:HE1	1.71	0.70
1:A:483:VAL:HG23	1:A:513:TRP:CD1	2.26	0.70
1:B:525:ASP:HB2	1:B:526:PRO:HD2	1.74	0.70
1:B:6:TYR:HB3	1:B:60:PHE:CE1	2.27	0.70
1:B:27:VAL:HG11	1:B:62:VAL:HA	1.74	0.69
1:A:2162:LEU:HD11	1:A:2164:MET:HB3	1.75	0.69
1:A:467:ASN:OD1	1:A:468:GLN:N	2.26	0.69
1:A:1826:THR:HG22	1:A:1828:ASP:H	1.58	0.69
1:B:120:SER:HB2	1:B:123:GLU:HG3	1.74	0.69
1:A:2286:ASN:H	1:A:2293:VAL:HG11	1.56	0.69
1:B:1772:MET:HB2	1:B:1816:PHE:HD1	1.56	0.69
1:A:250:HIS:O	1:A:252:LYS:N	2.25	0.69
1:A:271:PHE:CZ	1:A:286:SER:HB3	2.28	0.69
1:B:1807:VAL:HG22	1:B:1813:ARG:NH1	2.07	0.69
1:B:625:LEU:HD12	1:B:626:GLN:H	1.58	0.69
1:B:80:GLU:HB2	1:B:181:ARG:O	1.93	0.69
1:A:616:SER:HA	1:A:621:VAL:HG12	1.75	0.68
1:B:189:ARG:HG3	1:B:193:LEU:HD22	1.75	0.68
1:A:1764:ARG:HB3	1:A:1863:LEU:HD11	1.73	0.68
1:A:1936:GLN:HB2	1:A:2018:SER:HA	1.76	0.68
1:A:317:HIS:CD2	2:C:2:NAG:H81	2.29	0.68
1:A:555:TYR:HD1	1:A:556:LYS:H	1.40	0.68
1:B:6:TYR:HB3	1:B:60:PHE:HE1	1.58	0.68
1:A:518:GLU:OE2	1:B:488:SER:OG	2.10	0.68
1:A:182:GLU:OE1	1:A:182:GLU:N	2.16	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:LEU:HD22	1:A:169:LEU:HD21	1.75	0.67
1:A:1756:LEU:HD21	1:A:1762:TYR:CE2	2.29	0.67
1:A:2055:TYR:HD1	1:A:2056:SER:H	1.41	0.67
1:B:2196:PHE:HB2	1:B:2222:GLN:HA	1.76	0.67
1:A:1742:SER:O	1:A:1744:THR:N	2.27	0.67
1:A:445:GLU:O	1:A:618:ASN:ND2	2.28	0.67
1:B:1945:LEU:HD22	1:B:1947:MET:HG2	1.76	0.67
1:A:107:TRP:O	1:A:108:LYS:HB2	1.95	0.67
1:B:2096:LEU:HD12	1:B:2096:LEU:H	1.59	0.67
1:B:2087:GLN:HB3	1:B:2163:ARG:HB2	1.76	0.66
1:B:581:GLU:HB2	1:B:612:ASN:HB3	1.77	0.66
1:A:1769:ASP:O	1:A:1819:VAL:HG12	1.94	0.66
1:B:1764:ARG:NH2	1:B:1875:GLU:OE1	2.27	0.66
1:B:2182:SER:O	1:B:2184:ALA:N	2.28	0.66
1:B:1976:TYR:CZ	1:B:1984:GLU:HG2	2.31	0.66
1:A:1927:ASP:HA	1:A:2012:THR:HA	1.77	0.66
1:A:2180:MET:HE1	1:A:2232:VAL:HG21	1.77	0.65
1:B:2246:GLN:HB3	1:B:2320:ARG:HB2	1.77	0.65
1:B:2224:ASN:ND2	1:B:2316:GLN:OE1	2.30	0.65
1:B:2170:ASP:OD1	1:B:2175:SER:HB2	1.96	0.65
1:B:66:ARG:NH1	1:B:73:LEU:O	2.29	0.65
1:B:208:SER:O	1:B:210:HIS:N	2.29	0.65
1:B:446:SER:HA	1:B:618:ASN:ND2	2.12	0.65
1:A:2261:LEU:HD12	1:A:2309:HIS:HB2	1.79	0.65
1:A:443:GLN:NE2	1:A:443:GLN:O	2.29	0.65
1:B:2061:ALA:HB2	1:B:2163:ARG:HG3	1.79	0.65
1:B:397:PRO:HD2	1:B:624:SER:HB3	1.77	0.65
1:A:2241:THR:HG22	1:A:2325:GLY:HA2	1.79	0.65
1:B:12:LEU:HD11	1:B:14:TRP:HB2	1.79	0.65
1:B:2015:LEU:HD11	1:B:2171:LEU:HD22	1.79	0.64
1:A:654:SER:HB2	1:A:688:TRP:HB3	1.78	0.64
1:A:1934:MET:HE2	1:A:2016:VAL:HG12	1.79	0.64
1:A:449:LEU:HD13	1:A:550:PRO:HD3	1.79	0.64
1:A:666:ASP:HB2	1:A:1835:TRP:CZ3	2.32	0.64
1:B:464:ILE:HG12	1:B:510:LYS:HE3	1.81	0.64
1:B:1884:ASP:OD1	1:B:1886:THR:OG1	2.15	0.63
1:B:2210:LEU:HA	1:B:2320:ARG:HB3	1.80	0.63
1:B:50:THR:HG21	1:B:95:HIS:NE2	2.13	0.63
1:A:2187:ASP:HB3	1:A:2206:SER:HB2	1.81	0.63
1:A:601:VAL:HG23	1:A:602:GLN:N	2.14	0.63
1:A:14:TRP:CE2	1:A:72:LEU:HD11	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:GLU:HB2	1:B:127:ASP:HB3	1.79	0.63
1:A:2246:GLN:HE21	1:A:2292:PRO:HD3	1.64	0.62
1:A:591:ILE:HG23	1:A:595:LEU:HD22	1.81	0.62
1:B:192:ASN:HB3	1:B:252:LYS:HD2	1.81	0.62
1:B:435:THR:HG23	1:B:437:LYS:N	2.13	0.62
1:A:453:LEU:HD22	1:A:533:TYR:CE2	2.34	0.62
1:B:2094:SER:HB3	1:B:2158:ILE:HD13	1.80	0.62
1:B:1893:GLU:O	1:B:1895:VAL:N	2.30	0.62
1:A:2072:LYS:HB2	1:A:2150:ARG:HG3	1.80	0.62
1:B:623:ASP:HB3	1:B:705:LEU:HG	1.81	0.62
1:B:654:SER:HB2	1:B:688:TRP:HB3	1.81	0.62
1:B:68:PRO:HB2	1:B:244:PRO:HG2	1.82	0.62
1:A:164:ASP:OD1	1:A:2007:GLN:NE2	2.32	0.62
1:A:1826:THR:O	1:A:1859:ARG:NH1	2.33	0.62
1:B:29:THR:HG23	1:B:30:ARG:H	1.64	0.62
1:B:631:LEU:HD22	1:B:632:HIS:CD2	2.34	0.62
1:B:1913:LYS:O	1:B:1915:ASN:N	2.32	0.62
1:B:147:PRO:HA	1:B:155:LEU:HD11	1.81	0.62
1:B:1927:ASP:HA	1:B:2012:THR:HA	1.79	0.61
1:B:2147:ARG:HD3	1:B:2148:TYR:CE1	2.36	0.61
1:B:27:VAL:HG11	1:B:62:VAL:CA	2.30	0.61
1:A:36:PRO:HB2	1:A:46:LEU:HD22	1.83	0.61
1:B:495:VAL:HG11	1:B:501:PHE:HB2	1.82	0.61
1:B:1732:LYS:HB3	1:B:1849:SER:O	2.01	0.61
1:B:1756:LEU:HD21	1:B:1762:TYR:CZ	2.36	0.61
1:B:400:LEU:HD11	1:B:622:PHE:HB2	1.81	0.61
1:B:2039:ALA:HA	1:B:2071:ILE:HA	1.83	0.61
1:A:91:ASN:ND2	1:A:97:VAL:HG22	2.16	0.60
1:B:1936:GLN:OE1	1:B:1993:VAL:HG23	2.01	0.60
1:B:250:HIS:CE1	1:B:304:LEU:HG	2.35	0.60
1:A:2026:GLY:HA3	1:A:2031:HIS:HB3	1.84	0.60
1:A:416:PRO:HA	1:A:596:PRO:HG3	1.83	0.60
1:A:651:VAL:HG12	1:A:668:LEU:O	2.00	0.60
1:A:80:GLU:HG2	1:A:184:SER:HB2	1.83	0.60
1:A:525:ASP:HB2	1:A:526:PRO:HD2	1.83	0.60
1:B:1733:VAL:HG13	1:B:1851:LEU:HG	1.82	0.60
1:B:2100:GLN:NE2	1:B:2127:PHE:CE1	2.70	0.60
1:B:2186:SER:HB3	1:B:2189:GLN:HG3	1.84	0.60
1:B:241:ARG:NH2	1:B:322:GLU:OE1	2.35	0.60
1:A:2174:CYS:O	1:A:2241:THR:HG21	2.02	0.60
1:A:310:PHE:HB2	1:A:322:GLU:HG2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:708:VAL:HG23	1:A:709:SER:N	2.16	0.60
1:B:113:ALA:HB2	1:B:162:HIS:CD2	2.37	0.60
1:A:1756:LEU:HD21	1:A:1762:TYR:HE2	1.67	0.59
1:B:1801:GLU:OE1	1:B:1803:ARG:NH2	2.34	0.59
1:A:1826:THR:HB	1:A:1829:GLU:HG3	1.84	0.59
1:A:50:THR:HG21	1:A:95:HIS:HE1	1.65	0.59
1:A:518:GLU:HG3	1:B:490:ARG:HH11	1.67	0.59
1:B:269:SER:O	1:B:311:CYS:HA	2.03	0.59
1:B:692:CYS:O	1:B:693:HIS:HB2	2.03	0.59
1:A:119:THR:CG2	1:A:123:GLU:HB2	2.33	0.58
1:A:504:LEU:CB	1:A:505:PRO:HD2	2.32	0.58
1:A:2246:GLN:HA	1:A:2286:ASN:HD21	1.69	0.58
1:A:1766:GLU:O	1:A:1819:VAL:HG11	2.03	0.58
1:B:208:SER:C	1:B:210:HIS:H	2.04	0.58
1:B:240:ASN:O	1:B:242:SER:N	2.37	0.58
1:B:315:SER:HB3	1:B:317:HIS:HB2	1.86	0.58
1:A:1925:VAL:HG22	1:A:1926:MET:HG2	1.86	0.58
1:A:2076:LEU:HA	1:A:2147:ARG:NH2	2.18	0.58
1:A:2281:LYS:HG2	1:A:2283:PHE:CE1	2.38	0.58
1:A:2182:SER:C	1:A:2184:ALA:H	2.07	0.58
1:A:601:VAL:CG2	1:A:602:GLN:H	2.16	0.58
1:B:1979:TYR:O	1:B:1982:VAL:HG22	2.03	0.58
1:A:692:CYS:SG	1:A:694:ASN:HB2	2.44	0.57
1:B:1945:LEU:HG	1:B:1983:PHE:CD1	2.38	0.57
1:A:1764:ARG:HG2	1:A:1856:LEU:HB2	1.86	0.57
1:B:2100:GLN:NE2	1:B:2127:PHE:HE1	2.01	0.57
1:B:1743:PHE:CE2	1:B:1776:LYS:HB2	2.39	0.57
1:A:2229:TRP:HB3	1:A:2309:HIS:HD1	1.70	0.57
1:B:2183:LYS:HZ1	1:B:2212:LEU:HD11	1.70	0.57
1:B:233:HIS:HB3	1:B:321:MET:HG3	1.86	0.57
1:A:620:TYR:HD2	1:A:625:LEU:HB2	1.70	0.57
1:B:631:LEU:HD22	1:B:632:HIS:NE2	2.20	0.57
1:B:656:TYR:CE2	1:B:682:MET:HA	2.39	0.57
1:B:91:ASN:ND2	1:B:96:PRO:HA	2.20	0.57
1:A:182:GLU:H	1:A:182:GLU:CD	2.05	0.57
1:A:1870:GLN:O	1:A:1871:VAL:HG22	2.04	0.57
1:A:631:LEU:HD11	1:A:685:PRO:HG3	1.87	0.57
1:B:29:THR:CG2	1:B:30:ARG:H	2.17	0.57
1:B:315:SER:C	1:B:317:HIS:H	2.07	0.57
1:A:2129:ASN:ND2	1:A:2134:GLY:O	2.36	0.57
1:B:497:HIS:HD2	1:B:498:LEU:H	1.53	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:2:NAG:H3	4:G:2:NAG:H83	1.87	0.57
1:A:627:LEU:HD23	1:A:705:LEU:O	2.04	0.57
1:B:12:LEU:HD23	1:B:25:LEU:HD21	1.86	0.57
1:A:166:VAL:HB	1:A:2007:GLN:HE22	1.69	0.56
1:A:401:ALA:HA	1:A:408:LYS:HE2	1.86	0.56
1:B:110:SER:CB	1:B:138:VAL:H	2.17	0.56
1:A:2196:PHE:HB2	1:A:2222:GLN:HA	1.87	0.56
1:A:617:ILE:HD12	1:A:703:THR:O	2.05	0.56
1:B:2187:ASP:HB3	1:B:2206:SER:HB2	1.86	0.56
1:B:1883:PHE:O	1:B:1917:ARG:HA	2.04	0.56
1:B:2223:VAL:HG12	1:B:2225:ASN:HD22	1.69	0.56
1:B:238:TYR:HB3	1:B:242:SER:HB2	1.86	0.56
1:A:485:PRO:HD3	1:A:498:LEU:HD22	1.88	0.56
1:B:2100:GLN:HB2	1:B:2154:THR:OG1	2.05	0.56
1:B:47:TYR:OH	1:B:230:PRO:HG3	2.05	0.56
1:B:449:LEU:HD22	1:B:550:PRO:HD3	1.87	0.56
1:B:656:TYR:HE2	1:B:682:MET:HA	1.71	0.56
1:A:1739:ALA:HB3	1:A:1745:GLN:HB3	1.87	0.56
1:B:396:ALA:HB2	1:B:412:LEU:HD22	1.86	0.56
1:A:2082:HIS:HD2	1:A:2143:PRO:HB3	1.70	0.56
1:B:98:SER:HB3	1:B:162:HIS:H	1.69	0.56
1:A:2080:ILE:HG12	1:A:2145:ILE:HD12	1.86	0.56
1:A:2100:GLN:HG2	1:A:2154:THR:OG1	2.05	0.56
1:A:37:GLY:O	1:A:39:LEU:N	2.33	0.56
1:B:120:SER:HB3	1:B:2298:ASP:O	2.06	0.56
1:A:443:GLN:NE2	1:A:446:SER:HB2	2.20	0.56
1:A:538:ASN:OD1	1:A:541:ARG:HB2	2.06	0.56
1:B:2154:THR:O	1:B:2155:HIS:ND1	2.39	0.56
1:A:2096:LEU:HD23	1:A:2159:ARG:HB2	1.88	0.56
1:A:577:SER:HA	1:A:645:GLN:NE2	2.21	0.56
1:A:1756:LEU:O	1:A:1759:LEU:HB2	2.05	0.55
1:A:2032:ILE:O	1:A:2052:ARG:NH2	2.30	0.55
1:A:2180:MET:CE	1:A:2232:VAL:HG21	2.36	0.55
1:A:243:LEU:HD12	1:A:244:PRO:HD2	1.87	0.55
1:A:1786:TYR:CE1	1:A:1790:ILE:HD11	2.41	0.55
1:B:267:VAL:HB	1:B:671:PHE:CE2	2.42	0.55
1:A:444:HIS:O	1:A:445:GLU:HB2	2.07	0.55
1:A:1768:GLU:H	1:A:1819:VAL:HG13	1.72	0.55
1:B:1912:LEU:H	1:B:1912:LEU:HD23	1.70	0.55
1:B:589:GLU:OE1	1:B:593:ARG:NH1	2.40	0.55
1:A:380:LYS:HD3	1:A:382:TRP:CZ2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:ASP:OD1	1:A:435:THR:HG22	2.06	0.55
1:B:2062:TRP:O	1:B:2161:THR:HA	2.06	0.55
1:B:2087:GLN:N	1:B:2163:ARG:O	2.39	0.55
1:B:267:VAL:HB	1:B:671:PHE:HE2	1.71	0.55
1:B:60:PHE:CE2	1:B:90:LYS:HB2	2.42	0.55
1:A:1697:HIS:CD2	1:A:1772:MET:HG2	2.42	0.55
1:A:1756:LEU:HD12	1:A:1759:LEU:HB3	1.88	0.55
1:A:1874:GLN:HE22	1:A:1934:MET:HA	1.71	0.55
1:A:2027:MET:HE3	1:A:2073:VAL:HG21	1.87	0.55
1:A:599:ALA:O	1:A:601:VAL:HG13	2.07	0.55
1:A:387:ALA:HA	1:A:466:LYS:O	2.07	0.55
1:B:410:GLN:OE1	1:B:418:ARG:NH2	2.38	0.55
1:B:685:PRO:HA	1:B:708:VAL:CG2	2.37	0.55
1:A:412:LEU:HD23	1:A:421:ARG:HB2	1.88	0.55
1:A:581:GLU:HB2	1:A:612:ASN:HB3	1.89	0.55
1:A:1700:ILE:O	1:A:1775:PHE:HA	2.07	0.55
1:A:167:LYS:HD3	1:A:209:TRP:HA	1.87	0.55
1:B:2230:LEU:O	1:B:2307:ARG:HA	2.07	0.55
2:E:2:NAG:H83	2:E:2:NAG:H3	1.89	0.55
1:A:1934:MET:CE	1:A:2016:VAL:HG12	2.37	0.54
1:A:193:LEU:HG	1:A:195:GLU:HG3	1.87	0.54
1:A:108:LYS:HG2	1:A:1996:TRP:CH2	2.42	0.54
1:A:2042:GLN:HG3	1:A:2048:PRO:HD3	1.87	0.54
1:B:1743:PHE:CD2	1:B:1776:LYS:HD2	2.42	0.54
1:B:570:LYS:O	1:B:571:ARG:HB2	2.07	0.54
1:A:1993:VAL:HG11	1:A:2173:SER:HB2	1.89	0.54
1:A:582:ASN:ND2	1:A:609:GLN:O	2.40	0.54
1:B:1695:THR:HG23	1:B:1770:ASN:HB2	1.88	0.54
1:A:1751:GLU:HG3	1:A:2117:GLY:HA2	1.88	0.54
1:A:504:LEU:HB3	1:A:505:PRO:CD	2.37	0.54
1:B:1736:ARG:HE	1:B:1749:ARG:NH1	2.06	0.54
1:B:1707:TRP:CE2	1:B:1758:LEU:HD13	2.43	0.54
1:B:411:TYR:CE2	1:B:700:ARG:HB3	2.43	0.54
1:A:1759:LEU:HD12	1:A:1852:ILE:HG23	1.88	0.54
1:A:1882:ILE:HG22	1:A:1952:ASN:OD1	2.07	0.54
1:A:2207:LYS:HD2	1:A:2216:SER:O	2.07	0.54
1:B:109:SER:O	1:B:126:ASP:HB3	2.08	0.54
1:B:440:GLU:HG2	1:B:441:ALA:H	1.72	0.54
1:B:1735:PHE:O	1:B:1760:GLY:HA2	2.06	0.54
1:A:1790:ILE:HD12	1:A:1790:ILE:O	2.07	0.54
1:B:110:SER:HB3	1:B:138:VAL:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:400:LEU:CD1	1:B:622:PHE:HB2	2.37	0.54
1:B:437:LYS:O	1:B:438:THR:HG23	2.08	0.54
1:A:2222:GLN:HG3	1:A:2223:VAL:HG23	1.90	0.54
1:B:1941:ARG:HD2	1:B:1943:TYR:OH	2.07	0.54
1:A:30:ARG:HG3	1:A:32:PRO:HD2	1.89	0.54
1:A:35:ALA:N	1:A:36:PRO:HD3	2.23	0.54
1:B:1784:SER:OG	1:B:1785:PHE:N	2.40	0.53
1:B:684:ASN:HB2	1:B:1792:TYR:H	1.72	0.53
1:B:389:GLU:OE1	1:B:431:TYR:OH	2.15	0.53
1:B:521:PRO:HG3	1:B:529:LEU:HD13	1.90	0.53
1:A:1834:ALA:HB2	1:A:1943:TYR:CD1	2.43	0.53
1:A:654:SER:HB3	1:A:688:TRP:CE3	2.44	0.53
1:B:91:ASN:HD21	1:B:96:PRO:HA	1.72	0.53
1:A:2116:ARG:HG3	1:A:2123:LEU:HA	1.89	0.53
1:A:44:SER:O	1:A:45:VAL:HG12	2.07	0.53
1:B:2239:LYS:HB3	1:B:2326:CYS:SG	2.49	0.53
1:A:1751:GLU:H	1:A:1754:LYS:HG3	1.73	0.53
1:A:1874:GLN:NE2	1:A:1934:MET:HA	2.23	0.53
1:A:2265:SER:O	1:A:2303:THR:HB	2.09	0.53
1:A:279:VAL:O	1:A:281:HIS:N	2.41	0.53
1:A:666:ASP:OD2	1:A:1788:SER:OG	2.24	0.53
1:B:166:VAL:HA	1:B:263:THR:HG21	1.89	0.53
1:B:457:VAL:HA	1:B:515:VAL:HG12	1.90	0.53
1:B:520:GLY:HA2	1:B:529:LEU:HD22	1.89	0.53
1:A:2009:GLY:O	1:A:2011:SER:N	2.42	0.53
1:A:380:LYS:HD3	1:A:382:TRP:CH2	2.43	0.53
1:A:419:ILE:HD12	1:A:419:ILE:H	1.74	0.53
1:B:2261:LEU:HD12	1:B:2309:HIS:HB2	1.88	0.53
1:A:1846:ASP:HB3	1:A:1889:TRP:NE1	2.21	0.53
1:A:630:CYS:O	1:A:633:GLU:HB2	2.09	0.53
1:A:650:SER:OG	1:A:669:THR:HG22	2.09	0.53
1:B:1749:ARG:HD2	1:B:1753:ASN:HB3	1.90	0.53
1:B:471:ARG:HH12	1:B:537:VAL:HG23	1.74	0.53
1:A:2198:ASN:OD1	1:A:2199:MET:N	2.43	0.52
1:A:525:ASP:HB2	1:A:526:PRO:CD	2.38	0.52
1:B:49:LYS:NZ	1:B:205:GLU:OE2	2.31	0.52
5:H:1:NAG:O3	5:H:2:NAG:O5	2.17	0.52
1:A:1738:PHE:CD2	1:A:1746:PRO:HA	2.44	0.52
1:B:495:VAL:HG21	1:B:501:PHE:HD1	1.74	0.52
1:A:1833:LYS:HD3	1:A:1835:TRP:CZ2	2.44	0.52
1:A:2036:GLN:NE2	1:A:2074:ASP:O	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:654:SER:HB3	1:A:688:TRP:HE3	1.74	0.52
1:B:2085:LYS:HB2	1:B:2165:GLU:HB3	1.91	0.52
1:A:417:GLN:NE2	1:A:605:ASP:OD2	2.39	0.52
1:B:152:PRO:HG2	1:B:154:CYS:O	2.10	0.52
1:B:394:ASP:HB3	1:B:422:LYS:HG3	1.92	0.52
1:A:1759:LEU:HD22	1:A:1922:ASN:OD1	2.09	0.52
1:A:1924:TYR:CD1	1:A:1928:THR:HG22	2.44	0.52
1:A:2308:ILE:HG21	1:A:2319:LEU:HD11	1.92	0.52
1:B:1776:LYS:HG3	1:B:1812:THR:CG2	2.31	0.52
1:B:238:TYR:CD2	1:B:243:LEU:HD12	2.44	0.52
1:B:575:LEU:HD12	1:B:640:LEU:HB2	1.90	0.52
1:A:568:SER:HA	1:A:571:ARG:NH2	2.25	0.52
1:B:1945:LEU:HB2	1:B:1983:PHE:CE1	2.43	0.52
1:B:20:GLU:O	1:B:23:ARG:HG3	2.10	0.52
1:A:1992:LYS:O	1:A:2016:VAL:HG21	2.10	0.52
1:A:1:ALA:HB1	1:A:83:ASP:HA	1.91	0.52
1:B:160:LEU:HD13	1:B:169:LEU:HD21	1.91	0.52
1:B:2026:GLY:O	1:B:2028:ALA:N	2.43	0.52
1:B:2187:ASP:OD1	1:B:2209:ARG:NH2	2.42	0.52
1:A:119:THR:HG22	1:A:124:LYS:HG3	1.91	0.51
1:B:535:SER:HB3	1:B:542:ASP:HB3	1.92	0.51
1:B:625:LEU:HD12	1:B:626:GLN:N	2.24	0.51
1:A:81:VAL:HG23	1:A:181:ARG:HA	1.92	0.51
1:A:470:SER:O	1:A:471:ARG:HG2	2.10	0.51
1:B:2115:TYR:CE2	1:B:2117:GLY:HA2	2.45	0.51
1:B:497:HIS:HD2	1:B:498:LEU:N	2.08	0.51
1:A:430:ALA:HB2	1:A:451:PRO:HG3	1.93	0.51
1:B:101:ALA:O	1:B:106:PHE:HZ	1.93	0.51
1:B:449:LEU:HD21	1:B:575:LEU:HD22	1.92	0.51
1:A:2074:ASP:CG	1:A:2147:ARG:HH21	2.14	0.51
1:A:692:CYS:HB3	1:A:698:ARG:HB2	1.93	0.51
1:B:2119:SER:HB2	1:B:2120:THR:HG23	1.93	0.51
1:B:395:TYR:CE2	1:B:614:MET:HG3	2.46	0.51
1:B:411:TYR:HE2	1:B:700:ARG:HB3	1.74	0.51
1:A:643:GLY:HA3	1:A:645:GLN:HE21	1.76	0.51
1:B:2009:GLY:O	1:B:2011:SER:N	2.43	0.51
1:A:34:THR:HB	1:A:36:PRO:HD3	1.93	0.51
1:B:2104:MET:HG3	1:B:2152:HIS:CD2	2.46	0.51
1:B:497:HIS:CD2	1:B:498:LEU:N	2.78	0.51
1:A:589:GLU:O	1:A:593:ARG:HG3	2.11	0.51
1:A:98:SER:O	1:A:161:SER:HA	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:THR:HG23	1:B:30:ARG:N	2.26	0.51
1:B:472:PRO:HG3	1:B:504:LEU:HD23	1.92	0.51
1:B:428:PHE:CZ	1:B:547:LEU:HD22	2.46	0.51
1:B:2061:ALA:HB3	1:B:2089:ALA:HB2	1.93	0.51
1:B:258:VAL:HB	1:B:295:LEU:HB2	1.93	0.51
1:A:1829:GLU:O	1:A:1859:ARG:NH2	2.44	0.50
1:B:1821:HIS:CG	1:B:1822:HIS:N	2.79	0.50
1:B:2086:THR:CG2	1:B:2136:LYS:HB3	2.33	0.50
1:A:15:ASP:OD2	1:A:18:GLN:HG2	2.11	0.50
1:A:2203:TRP:CD2	1:A:2220:ARG:HG3	2.46	0.50
1:B:71:GLY:HA3	1:B:236:ASN:O	2.11	0.50
1:B:396:ALA:HB1	1:B:400:LEU:HB2	1.93	0.50
1:B:456:GLU:OE1	1:B:556:LYS:HB2	2.11	0.50
1:A:634:VAL:HG13	1:A:679:PHE:CZ	2.46	0.50
1:B:117:ASP:OD1	1:B:117:ASP:N	2.37	0.50
1:B:1834:ALA:HB1	1:B:1983:PHE:HE2	1.76	0.50
1:B:1837:TYR:CZ	1:B:1853:GLY:HA3	2.46	0.50
1:B:2285:GLY:HA2	1:B:2293:VAL:HG11	1.93	0.50
1:A:1993:VAL:HA	1:A:2016:VAL:CG2	2.36	0.50
1:A:684:ASN:O	1:A:708:VAL:HG21	2.11	0.50
1:B:1926:MET:SD	1:B:2009:GLY:HA2	2.51	0.50
1:B:2225:ASN:HB2	1:B:2226:PRO:HD2	1.94	0.50
1:B:56:THR:OG1	1:B:62:VAL:HG21	2.12	0.50
1:A:2102:ILE:HG13	1:A:2152:HIS:HB2	1.92	0.50
1:A:2191:THR:O	1:A:2231:GLN:HB3	2.12	0.50
1:B:151:ASP:HB3	1:B:152:PRO:HD2	1.94	0.50
1:B:2081:ILE:HG12	1:B:2149:ILE:HD11	1.93	0.50
1:B:396:ALA:CB	1:B:400:LEU:HD12	2.41	0.50
1:B:629:VAL:CG2	1:B:708:VAL:HG12	2.42	0.50
1:A:14:TRP:NE1	1:A:16:TYR:HA	2.26	0.50
1:B:523:LYS:HA	1:B:527:ARG:HH12	1.76	0.50
1:B:640:LEU:HD22	1:B:642:ILE:HD11	1.93	0.50
1:A:517:VAL:HB	1:B:488:SER:HB2	1.93	0.50
1:A:1941:ARG:HD2	1:A:1943:TYR:OH	2.11	0.50
1:B:27:VAL:HG11	1:B:63:ALA:N	2.26	0.50
1:A:2201:ALA:O	1:A:2202:THR:HG23	2.11	0.50
1:A:192:ASN:HB3	1:A:252:LYS:CG	2.37	0.50
1:A:267:VAL:HG12	1:A:290:SER:HB3	1.93	0.50
1:B:1884:ASP:O	1:B:1887:LYS:N	2.45	0.50
1:B:2038:THR:O	1:B:2072:LYS:N	2.39	0.50
1:A:1837:TYR:CZ	1:A:1853:GLY:HA3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1924:TYR:HB2	1:A:1929:LEU:HB2	1.93	0.49
1:B:106:PHE:CD2	1:B:111:GLU:HG3	2.47	0.49
1:B:1772:MET:HB2	1:B:1816:PHE:CD1	2.43	0.49
1:B:2027:MET:HB2	1:B:2165:GLU:OE2	2.11	0.49
1:B:95:HIS:HB2	1:B:96:PRO:HD2	1.95	0.49
1:B:126:ASP:N	1:B:126:ASP:OD1	2.46	0.49
1:A:106:PHE:CE1	1:A:111:GLU:HG3	2.48	0.49
1:A:168:ASP:OD1	1:A:209:TRP:NE1	2.45	0.49
1:A:379:PRO:HG3	1:B:486:LEU:HD11	1.93	0.49
1:A:453:LEU:O	1:A:551:LEU:HD12	2.13	0.49
1:B:1924:TYR:HB2	1:B:1929:LEU:HB2	1.94	0.49
1:B:14:TRP:CE2	1:B:72:LEU:HD21	2.47	0.49
1:B:395:TYR:OH	1:B:425:LYS:NZ	2.23	0.49
1:B:518:GLU:H	1:B:518:GLU:CD	2.15	0.49
1:A:1886:THR:HA	1:A:1891:PHE:CD1	2.47	0.49
1:B:1789:LEU:HD22	1:B:1823:MET:HB3	1.94	0.49
1:A:406:SER:O	1:A:408:LYS:N	2.36	0.49
1:B:12:LEU:CD1	1:B:14:TRP:HB2	2.43	0.49
1:A:2055:TYR:HD1	1:A:2056:SER:N	2.08	0.49
1:B:2261:LEU:HA	1:B:2283:PHE:HD1	1.78	0.49
1:A:1880:PHE:CE2	1:A:1921:ILE:HG12	2.47	0.49
1:A:454:TYR:CE1	1:A:456:GLU:HG3	2.48	0.49
1:A:591:ILE:HA	1:A:595:LEU:HD13	1.95	0.49
1:B:1776:LYS:HG2	1:B:1777:ASN:O	2.13	0.49
1:B:1945:LEU:HB2	1:B:1983:PHE:HE1	1.78	0.49
1:B:603:LEU:HD23	1:B:603:LEU:O	2.13	0.49
1:A:34:THR:C	1:A:36:PRO:HD3	2.33	0.48
1:A:484:ARG:HH21	1:B:514:THR:HG21	1.77	0.48
1:A:660:HIS:O	1:A:662:MET:N	2.45	0.48
1:B:2106:SER:O	1:B:2146:ALA:HB1	2.13	0.48
1:B:540:GLU:HG2	1:B:541:ARG:HG3	1.93	0.48
1:A:1841:VAL:HG22	1:A:1846:ASP:OD2	2.12	0.48
1:B:42:GLY:HA2	1:B:44:SER:N	2.28	0.48
1:B:453:LEU:HD13	1:B:533:TYR:HE2	1.78	0.48
1:B:56:THR:H	1:B:62:VAL:HG23	1.77	0.48
1:A:250:HIS:C	1:A:252:LYS:H	2.14	0.48
1:B:27:VAL:HG22	1:B:28:ASP:H	1.78	0.48
1:A:1963:PHE:CD2	1:A:1986:VAL:HB	2.49	0.48
1:A:454:TYR:HE2	1:A:570:LYS:HE3	1.78	0.48
1:B:2110:LYS:HD3	1:B:2112:TRP:NE1	2.23	0.48
1:B:2104:MET:HE3	1:B:2112:TRP:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2115:TYR:C	1:B:2117:GLY:H	2.17	0.48
1:A:192:ASN:O	1:A:194:HIS:N	2.45	0.48
1:A:2034:ASP:OD2	1:A:2049:LYS:HB2	2.14	0.48
1:A:2052:ARG:O	1:A:2055:TYR:HB2	2.14	0.48
1:A:273:GLU:HG3	1:A:308:LEU:HB3	1.94	0.48
1:A:622:PHE:O	1:A:623:ASP:HB2	2.12	0.48
1:A:2043:TYR:HD2	1:A:2046:TRP:CD1	2.31	0.48
1:B:2096:LEU:HD21	1:B:2159:ARG:NH1	2.29	0.48
1:A:1694:ARG:O	1:A:1769:ASP:HB2	2.14	0.48
1:A:425:LYS:HB3	1:A:545:SER:O	2.13	0.48
1:A:45:VAL:HG22	1:A:46:LEU:H	1.78	0.48
1:A:685:PRO:HA	1:A:708:VAL:CG2	2.44	0.48
1:B:631:LEU:CD2	1:B:632:HIS:CD2	2.96	0.48
1:B:705:LEU:HD23	1:B:705:LEU:HA	1.53	0.48
1:A:2044:GLY:O	1:A:2046:TRP:N	2.46	0.48
1:A:686:GLY:O	1:A:708:VAL:HG22	2.14	0.48
1:B:200:PHE:HB3	1:B:321:MET:HE1	1.95	0.48
1:B:617:ILE:HG21	1:B:704:ALA:HB2	1.95	0.48
2:C:1:NAG:H83	2:C:1:NAG:H3	1.95	0.48
1:A:2053:LEU:HD13	1:A:2165:GLU:HB3	1.95	0.48
1:A:486:LEU:HD12	1:A:487:TYR:H	1.79	0.48
1:B:2179:GLY:HA3	1:B:2185:ILE:H	1.79	0.48
1:B:230:PRO:HB2	1:B:232:MET:CE	2.44	0.48
1:A:1936:GLN:O	1:A:1990:PRO:HG2	2.14	0.48
1:A:427:ARG:NE	1:A:448:ILE:HA	2.28	0.48
1:A:692:CYS:C	1:A:694:ASN:H	2.16	0.48
1:B:2063:SER:HA	1:B:2160:SER:O	2.14	0.48
1:B:701:GLY:O	1:B:703:THR:N	2.47	0.48
1:A:148:THR:O	1:A:181:ARG:NH2	2.36	0.47
1:B:640:LEU:HD23	1:B:675:GLY:HA3	1.94	0.47
1:A:304:LEU:HA	1:A:327:VAL:HG23	1.96	0.47
1:A:467:ASN:O	1:A:468:GLN:HG3	2.15	0.47
1:A:521:PRO:HG3	1:A:529:LEU:HD23	1.96	0.47
1:B:1834:ALA:HB1	1:B:1983:PHE:CE2	2.48	0.47
1:B:1929:LEU:HD23	1:B:1930:PRO:O	2.14	0.47
1:B:474:ASN:HB2	1:B:537:VAL:HG13	1.96	0.47
1:A:1819:VAL:HG21	1:A:1857:ILE:HD12	1.96	0.47
1:A:1913:LYS:O	1:A:1916:TYR:N	2.37	0.47
1:A:2185:ILE:O	1:A:2209:ARG:NH1	2.40	0.47
1:A:2187:ASP:OD1	1:A:2209:ARG:NH2	2.48	0.47
1:A:261:MET:HG2	1:A:262:GLY:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1790:ILE:O	1:B:1790:ILE:HD12	2.13	0.47
1:B:2178:LEU:HD11	1:B:2325:GLY:HA3	1.96	0.47
1:A:2229:TRP:HB3	1:A:2309:HIS:ND1	2.28	0.47
1:B:1833:LYS:HG2	1:B:1834:ALA:H	1.80	0.47
1:B:60:PHE:HD2	1:B:90:LYS:HD3	1.80	0.47
1:B:680:MET:HE3	1:B:680:MET:HB2	1.69	0.47
1:A:2026:GLY:C	1:A:2032:ILE:HG13	2.35	0.47
1:A:303:ASP:O	1:A:327:VAL:HG21	2.15	0.47
1:A:602:GLN:HB3	1:A:605:ASP:HB2	1.97	0.47
1:A:58:GLN:N	1:A:58:GLN:OE1	2.42	0.47
1:A:602:GLN:HB3	1:A:605:ASP:CB	2.44	0.47
1:B:174:ILE:HD13	1:B:199:LEU:HD21	1.96	0.47
1:B:2211:HIS:CE1	1:B:2292:PRO:HG3	2.49	0.47
1:B:42:GLY:HA2	1:B:44:SER:H	1.79	0.47
1:B:281:HIS:O	1:B:524:SER:HB2	2.15	0.47
1:B:607:GLU:HA	1:B:610:ALA:HB3	1.96	0.47
1:A:2196:PHE:HZ	1:A:2198:ASN:HD22	1.63	0.47
1:A:292:LEU:HD13	1:A:2001:LEU:HB3	1.96	0.47
1:A:518:GLU:H	1:A:518:GLU:CD	2.18	0.47
1:B:574:ILE:HD12	1:B:639:ILE:HG12	1.96	0.47
1:B:620:TYR:HB3	1:B:624:SER:HB2	1.96	0.47
1:A:1766:GLU:HG3	1:A:1863:LEU:HB3	1.96	0.47
1:A:1949:SER:O	1:A:1952:ASN:ND2	2.31	0.47
1:B:1735:PHE:CZ	1:B:1851:LEU:HD22	2.50	0.47
1:B:2049:LYS:O	1:B:2052:ARG:NH1	2.48	0.47
1:B:2086:THR:O	1:B:2135:ILE:HA	2.15	0.47
1:B:2100:GLN:H	1:B:2155:HIS:HB2	1.79	0.47
1:A:20:GLU:HG3	1:A:23:ARG:HG3	1.96	0.47
1:A:443:GLN:HE22	1:A:446:SER:N	2.09	0.47
1:A:568:SER:HA	1:A:571:ARG:HH21	1.80	0.47
1:A:645:GLN:O	1:A:646:THR:HB	2.13	0.47
1:A:251:LYS:HE3	1:B:496:LYS:O	2.13	0.47
1:B:641:SER:C	1:B:642:ILE:HG13	2.34	0.47
1:B:80:GLU:OE1	1:B:183:GLY:N	2.48	0.47
4:G:1:NAG:H3	4:G:2:NAG:H82	1.96	0.47
1:A:85:VAL:O	1:A:138:VAL:HA	2.13	0.47
1:B:155:LEU:O	1:B:178:LEU:HA	2.15	0.47
1:B:1789:LEU:HD11	1:B:1835:TRP:CD1	2.50	0.47
1:B:2274:PHE:HE2	1:B:2301:LEU:HD13	1.79	0.47
1:B:392:ASP:OD1	1:B:593:ARG:NH2	2.46	0.47
1:B:504:LEU:HD22	1:B:505:PRO:HD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:HIS:CD2	1:B:65:PRO:HA	2.48	0.47
1:A:103:GLY:HA2	1:A:1962:VAL:HG12	1.97	0.47
1:A:20:GLU:HG3	1:A:23:ARG:NE	2.30	0.47
1:A:2166:LEU:HD23	1:A:2166:LEU:HA	1.74	0.47
1:B:1781:ARG:HB2	1:B:1782:PRO:HD2	1.96	0.47
1:B:2228:GLU:O	1:B:2310:PRO:HD2	2.14	0.47
1:B:315:SER:C	1:B:317:HIS:N	2.67	0.47
1:A:49:LYS:HZ2	1:A:171:SER:HA	1.80	0.46
1:A:80:GLU:HG2	1:A:184:SER:CB	2.45	0.46
1:B:120:SER:O	1:B:123:GLU:N	2.48	0.46
1:B:1709:TYR:O	1:B:1928:THR:HG21	2.15	0.46
1:B:2247:GLY:H	1:B:2286:ASN:HD21	1.61	0.46
1:A:2046:TRP:CE2	1:A:2059:ILE:HG22	2.49	0.46
1:B:1738:PHE:HD2	1:B:1743:PHE:HA	1.81	0.46
1:B:2265:SER:O	1:B:2303:THR:HB	2.15	0.46
1:B:387:ALA:HA	1:B:466:LYS:O	2.15	0.46
1:A:417:GLN:OE1	1:A:602:GLN:HG3	2.15	0.46
1:A:526:PRO:HG2	1:A:528:CYS:O	2.16	0.46
1:A:582:ASN:HA	1:A:587:LEU:HD12	1.97	0.46
1:B:91:ASN:HB2	1:B:129:VAL:HG23	1.97	0.46
1:B:1707:TRP:CZ2	1:B:1758:LEU:HD13	2.50	0.46
1:B:17:ARG:HG3	1:B:242:SER:OG	2.15	0.46
1:B:400:LEU:HD23	1:B:400:LEU:HA	1.73	0.46
1:B:586:TYR:O	1:B:589:GLU:N	2.49	0.46
1:A:483:VAL:HG23	1:A:513:TRP:HD1	1.76	0.46
1:B:2092:LYS:HG2	1:B:2093:PHE:CD2	2.50	0.46
1:A:253:SER:HA	1:A:300:PHE:HA	1.98	0.46
1:B:2110:LYS:HA	1:B:2112:TRP:NE1	2.31	0.46
1:B:394:ASP:HB2	1:B:421:ARG:HG3	1.98	0.46
1:B:397:PRO:HD2	1:B:624:SER:CB	2.44	0.46
1:B:165:LEU:HD23	1:B:2003:GLY:HA2	1.97	0.46
1:A:1888:SER:O	1:A:1891:PHE:N	2.49	0.46
1:A:2021:CYS:O	1:A:2169:CYS:HB2	2.16	0.46
1:A:2263:SER:HB3	1:A:2273:LEU:HD23	1.98	0.46
1:B:119:THR:HB	1:B:123:GLU:HB2	1.97	0.46
1:B:1758:LEU:HD12	1:B:1758:LEU:HA	1.70	0.46
1:B:2060:ASN:O	1:B:2163:ARG:HD3	2.15	0.46
1:B:2088:GLY:O	1:B:2163:ARG:NH2	2.47	0.46
1:B:2265:SER:HB2	1:B:2271:TRP:CD2	2.51	0.46
1:B:2286:ASN:H	1:B:2293:VAL:HG11	1.80	0.46
1:B:522:THR:C	1:B:524:SER:H	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:4:MAN:O3	5:H:5:MAN:H3	2.15	0.46
1:A:2038:THR:O	1:A:2072:LYS:N	2.49	0.46
1:A:80:GLU:HA	1:A:180:CYS:O	2.16	0.46
1:B:2107:LEU:CD2	1:B:2146:ALA:HA	2.44	0.46
1:B:574:ILE:O	1:B:639:ILE:HA	2.16	0.46
1:A:454:TYR:HE1	1:A:456:GLU:HG3	1.81	0.46
1:B:397:PRO:O	1:B:399:VAL:N	2.49	0.46
1:B:657:THR:O	1:B:658:PHE:CG	2.69	0.46
1:A:1839:SER:HB2	1:A:1851:LEU:HD13	1.98	0.45
1:A:2233:ASP:HB2	1:A:2305:TYR:HE1	1.79	0.45
1:B:2048:PRO:HA	1:B:2062:TRP:CD1	2.50	0.45
1:B:2264:SER:HB2	1:B:2303:THR:OG1	2.17	0.45
1:B:255:TYR:HE1	1:B:298:GLN:HG3	1.82	0.45
1:B:407:TYR:CD2	1:B:408:LYS:HG2	2.51	0.45
1:B:498:LEU:HD22	1:B:511:TYR:HE1	1.82	0.45
1:B:521:PRO:HB3	1:B:526:PRO:O	2.16	0.45
1:B:582:ASN:HA	1:B:587:LEU:HD22	1.98	0.45
1:A:128:LYS:HB3	1:A:128:LYS:HE3	1.70	0.45
1:A:1788:SER:H	1:A:1790:ILE:HG13	1.80	0.45
1:A:1989:LEU:O	1:A:1989:LEU:HD12	2.16	0.45
1:A:2314:VAL:O	1:A:2316:GLN:N	2.49	0.45
1:B:1831:ASP:HB2	1:B:1941:ARG:NH1	2.32	0.45
1:B:90:LYS:HG3	1:B:133:LYS:O	2.16	0.45
1:A:2044:GLY:C	1:A:2046:TRP:H	2.19	0.45
1:B:1833:LYS:O	1:B:1834:ALA:HB2	2.16	0.45
1:B:648:PHE:CE1	1:B:1953:ILE:HD11	2.51	0.45
1:B:16:TYR:O	1:B:239:VAL:HG22	2.17	0.45
1:B:461:LEU:HB2	1:B:513:TRP:HB2	1.97	0.45
1:A:1774:THR:HG22	1:A:1814:THR:OG1	2.17	0.45
1:A:1789:LEU:HD11	1:A:1835:TRP:CD1	2.52	0.45
1:B:1700:ILE:O	1:B:1775:PHE:HA	2.17	0.45
1:B:70:MET:O	1:B:73:LEU:HB2	2.15	0.45
1:A:130:LEU:HB2	1:A:133:LYS:HD3	1.99	0.45
1:A:601:VAL:O	1:A:603:LEU:HD12	2.17	0.45
1:B:453:LEU:HD13	1:B:533:TYR:CE2	2.52	0.45
1:B:78:GLN:HG2	1:B:178:LEU:HD12	1.98	0.45
1:A:300:PHE:CE2	1:B:490:ARG:HG3	2.52	0.45
1:A:200:PHE:CD1	1:A:321:MET:HE3	2.50	0.45
1:A:486:LEU:HG	1:A:487:TYR:CD2	2.51	0.45
1:A:642:ILE:HD13	1:A:673:PHE:HA	1.98	0.45
1:A:629:VAL:HG23	1:A:708:VAL:HG12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1731:LYS:HB3	1:B:1894:ASN:HD21	1.82	0.45
1:B:1965:VAL:HG12	1:B:1971:TYR:O	2.17	0.45
1:B:2210:LEU:HD22	1:B:2322:GLU:HB2	1.99	0.45
1:B:2286:ASN:H	1:B:2293:VAL:CG1	2.29	0.45
1:B:269:SER:H	1:B:313:ILE:HD13	1.81	0.45
1:B:613:ILE:O	1:B:613:ILE:HG13	2.16	0.45
1:B:69:TRP:CZ3	1:B:70:MET:HG2	2.50	0.45
1:A:596:PRO:HG2	1:A:597:ASN:ND2	2.31	0.45
1:B:1789:LEU:HA	1:B:1789:LEU:HD23	1.62	0.45
1:B:2100:GLN:OE1	1:B:2125:VAL:HG12	2.17	0.45
1:B:287:LEU:HA	1:B:287:LEU:HD12	1.67	0.45
1:A:101:ALA:HB2	1:A:139:TRP:CZ2	2.51	0.45
1:B:457:VAL:HA	1:B:515:VAL:CG1	2.46	0.45
1:B:631:LEU:CD2	1:B:632:HIS:NE2	2.80	0.45
1:A:703:THR:O	1:A:704:ALA:HB3	2.17	0.45
1:B:1826:THR:HG23	1:B:1829:GLU:OE2	2.17	0.45
1:A:14:TRP:HZ3	1:A:22:LEU:HG	1.82	0.45
1:A:1863:LEU:O	1:A:1863:LEU:HD23	2.17	0.45
1:B:1819:VAL:HG21	1:B:1857:ILE:HD12	1.99	0.45
1:B:2102:ILE:HG22	1:B:2124:MET:O	2.17	0.45
1:A:1757:GLY:C	1:A:1759:LEU:H	2.21	0.44
1:A:290:SER:O	1:A:291:PRO:C	2.55	0.44
1:A:389:GLU:OE2	1:A:439:ARG:NH1	2.50	0.44
1:A:586:TYR:N	1:A:586:TYR:CD1	2.85	0.44
1:B:103:GLY:HA3	1:B:157:TYR:CD2	2.51	0.44
1:B:16:TYR:CZ	1:B:232:MET:HG3	2.52	0.44
1:B:200:PHE:HE2	1:B:258:VAL:HG13	1.83	0.44
1:B:2203:TRP:CE3	1:B:2220:ARG:HG3	2.52	0.44
1:B:310:PHE:HA	1:B:321:MET:O	2.18	0.44
1:B:664:TYR:CE2	1:B:1822:HIS:HB2	2.52	0.44
1:B:89:LEU:HD21	1:B:97:VAL:HG23	1.99	0.44
1:A:1764:ARG:HB3	1:A:1863:LEU:CD1	2.44	0.44
1:B:1699:PHE:CE1	1:B:1741:GLY:HA2	2.53	0.44
1:B:1790:ILE:HD13	1:B:1792:TYR:CE1	2.52	0.44
1:B:396:ALA:HB1	1:B:400:LEU:HD12	2.00	0.44
1:B:185:LEU:HG	1:B:185:LEU:H	1.59	0.44
1:B:2114:THR:HG21	1:B:2123:LEU:CD2	2.47	0.44
1:B:15:ASP:HB2	1:B:45:VAL:HG22	2.00	0.44
1:B:54:GLU:HG3	1:B:55:PHE:N	2.33	0.44
1:A:454:TYR:CE2	1:A:570:LYS:HE3	2.52	0.44
1:B:2217:ASN:N	1:B:2217:ASN:OD1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2262:ILE:HA	1:B:2307:ARG:O	2.16	0.44
1:B:497:HIS:CE1	1:B:499:LYS:HG2	2.53	0.44
1:B:69:TRP:CE3	1:B:70:MET:HG2	2.53	0.44
1:A:2047:ALA:O	1:A:2050:LEU:HD23	2.17	0.44
1:A:2236:LYS:HD3	1:A:2327:GLU:HG3	1.99	0.44
1:A:2255:MET:HB3	1:A:2316:GLN:HB2	1.98	0.44
1:A:191:GLN:HE22	1:A:331:ALA:H	1.65	0.44
1:B:12:LEU:CD2	1:B:25:LEU:HD11	2.48	0.44
1:B:238:TYR:CE2	1:B:243:LEU:HD12	2.52	0.44
1:B:2043:TYR:HB3	1:B:2046:TRP:HB2	1.99	0.44
1:B:2052:ARG:O	1:B:2163:ARG:HG2	2.18	0.44
1:B:2076:LEU:C	1:B:2147:ARG:HE	2.20	0.44
1:B:2180:MET:HB2	1:B:2322:GLU:CD	2.38	0.44
1:B:485:PRO:HB3	1:B:509:PHE:CZ	2.53	0.44
1:A:36:PRO:HB2	1:A:37:GLY:H	1.64	0.44
1:B:462:LEU:HD21	1:B:486:LEU:HD13	1.99	0.44
1:B:593:ARG:HD2	1:B:594:PHE:CE2	2.52	0.44
1:B:633:GLU:O	1:B:682:MET:HG2	2.17	0.44
1:A:165:LEU:HD23	1:A:2003:GLY:HA2	2.00	0.44
1:A:2267:ASP:OD1	1:A:2270:GLN:N	2.43	0.44
1:B:1755:HIS:HB3	1:B:1931:GLY:HA3	1.99	0.44
1:B:1828:ASP:O	1:B:1966:ARG:HG2	2.18	0.44
1:B:1733:VAL:HB	1:B:1890:TYR:OH	2.17	0.44
1:B:2006:LEU:C	1:B:2008:ALA:H	2.21	0.44
1:B:2260:PHE:CE1	1:B:2308:ILE:HD12	2.53	0.44
1:A:165:LEU:HA	1:A:165:LEU:HD12	1.85	0.43
1:A:669:THR:HG21	1:A:1979:TYR:HB3	2.00	0.43
1:A:24:GLU:O	1:A:25:LEU:HB2	2.18	0.43
1:A:641:SER:O	1:A:642:ILE:HD13	2.17	0.43
1:B:1875:GLU:HG2	1:B:1943:TYR:OH	2.18	0.43
1:B:2105:TYR:HB2	1:B:2146:ALA:CB	2.47	0.43
1:B:2140:PHE:CD2	1:B:2144:ILE:HG13	2.53	0.43
1:B:2244:THR:OG1	1:B:2294:VAL:HG22	2.18	0.43
1:A:73:LEU:HD12	1:A:236:ASN:ND2	2.33	0.43
1:A:400:LEU:O	1:A:408:LYS:HE2	2.18	0.43
1:B:124:LYS:HG2	1:B:127:ASP:OD2	2.18	0.43
1:B:1841:VAL:HG22	1:B:1846:ASP:OD2	2.18	0.43
1:B:1945:LEU:HD12	1:B:1983:PHE:CE1	2.52	0.43
1:B:2203:TRP:CD2	1:B:2216:SER:HB2	2.53	0.43
1:B:2224:ASN:HB3	1:B:2317:ILE:HG13	2.00	0.43
1:B:3:ARG:HB3	1:B:5:TYR:HE1	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:VAL:HA	1:B:141:VAL:CG1	2.47	0.43
1:A:15:ASP:O	1:A:16:TYR:HB2	2.18	0.43
1:A:433:ASP:N	1:A:433:ASP:OD1	2.52	0.43
1:B:208:SER:C	1:B:210:HIS:N	2.70	0.43
1:A:1763:ILE:HG23	1:A:1855:LEU:HG	1.99	0.43
1:A:1764:ARG:CZ	1:A:1869:ARG:HG3	2.48	0.43
1:A:87:VAL:HG11	1:A:99:LEU:HD21	2.01	0.43
1:B:2225:ASN:HA	1:B:2313:TRP:HH2	1.84	0.43
1:B:2193:SER:HB3	1:B:2229:TRP:NE1	2.33	0.43
1:B:81:VAL:HG12	1:B:82:TYR:CD2	2.53	0.43
1:A:1792:TYR:N	1:A:1792:TYR:CD1	2.86	0.43
1:A:1771:ILE:HD12	1:A:1817:TRP:NE1	2.33	0.43
1:B:1830:PHE:CE1	1:B:1966:ARG:HD2	2.53	0.43
1:B:1972:LYS:O	1:B:1973:MET:HG3	2.17	0.43
1:B:23:ARG:HH11	1:B:23:ARG:HG2	1.83	0.43
1:B:407:TYR:CE2	1:B:408:LYS:HG2	2.54	0.43
1:B:409:SER:HA	1:B:413:ASN:HB2	2.00	0.43
1:B:692:CYS:SG	1:B:693:HIS:N	2.90	0.43
1:A:2022:GLN:HG2	1:A:2082:HIS:HB2	2.01	0.43
1:A:2170:ASP:OD1	1:A:2175:SER:OG	2.35	0.43
1:A:50:THR:HG22	1:A:171:SER:HB2	2.00	0.43
1:B:133:LYS:HB3	1:B:134:SER:H	1.66	0.43
1:B:1755:HIS:NE2	1:B:1762:TYR:OH	2.32	0.43
1:B:2095:SER:O	1:B:2095:SER:OG	2.36	0.43
1:B:261:MET:HE3	1:B:262:GLY:HA2	1.99	0.43
1:A:484:ARG:HH21	1:B:514:THR:CG2	2.31	0.43
1:A:2048:PRO:C	1:A:2050:LEU:H	2.22	0.43
1:A:2074:ASP:OD1	1:A:2147:ARG:NH2	2.44	0.43
1:A:1732:LYS:HD3	1:A:1758:LEU:HD21	2.01	0.43
1:A:1883:PHE:O	1:A:1917:ARG:HA	2.19	0.43
1:A:293:THR:HA	1:A:1977:ASN:HD21	1.82	0.43
1:A:1945:LEU:HB2	1:A:1983:PHE:CE1	2.54	0.43
1:A:2273:LEU:O	1:A:2275:PHE:HD1	2.02	0.43
1:A:627:LEU:HD11	1:A:637:TRP:HZ3	1.84	0.43
1:B:1774:THR:HG22	1:B:1814:THR:HG23	2.01	0.43
1:B:2261:LEU:HA	1:B:2283:PHE:CD1	2.54	0.43
1:A:708:VAL:O	1:A:709:SER:HB3	2.19	0.43
1:B:1734:VAL:HG23	1:B:1736:ARG:HD3	2.01	0.43
1:B:1756:LEU:HD11	1:B:1762:TYR:CE2	2.54	0.43
1:B:2147:ARG:HD3	1:B:2148:TYR:CZ	2.53	0.43
1:A:251:LYS:HD2	1:B:491:LEU:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:CYS:HA	1:A:180:CYS:HA	2.01	0.43
1:A:1889:TRP:C	1:A:1891:PHE:H	2.22	0.43
1:B:1709:TYR:CD2	1:B:1923:GLY:O	2.72	0.43
1:B:312:HIS:O	1:B:312:HIS:ND1	2.51	0.43
1:B:397:PRO:HD3	1:B:620:TYR:HD2	1.84	0.43
1:B:114:GLU:HG3	1:B:124:LYS:HD3	2.00	0.42
1:B:2050:LEU:HD12	1:B:2055:TYR:CE2	2.53	0.42
1:B:2109:GLY:HA2	1:B:2148:TYR:CE1	2.53	0.42
1:B:2178:LEU:HD23	1:B:2178:LEU:HA	1.76	0.42
1:B:452:LEU:HD23	1:B:550:PRO:HG2	2.01	0.42
1:A:1732:LYS:HB3	1:A:1849:SER:O	2.18	0.42
1:A:493:LYS:O	1:A:495:VAL:N	2.48	0.42
1:B:229:GLN:HB3	1:B:230:PRO:CD	2.49	0.42
1:B:255:TYR:CE1	1:B:298:GLN:HG3	2.54	0.42
1:B:47:TYR:CG	1:B:205:GLU:HG3	2.54	0.42
1:B:495:VAL:HG21	1:B:501:PHE:CD1	2.53	0.42
1:B:89:LEU:HA	1:B:89:LEU:HD12	1.81	0.42
1:A:2045:GLN:O	1:A:2059:ILE:HD13	2.18	0.42
1:A:2104:MET:O	1:A:2150:ARG:N	2.51	0.42
1:A:483:VAL:O	1:A:483:VAL:HG13	2.19	0.42
1:B:169:LEU:HA	1:B:169:LEU:HD23	1.65	0.42
1:B:1876:PHE:CD2	1:B:1932:LEU:HD23	2.54	0.42
1:B:504:LEU:CD2	1:B:505:PRO:HD2	2.50	0.42
1:A:493:LYS:H	1:A:495:VAL:HG23	1.85	0.42
1:B:685:PRO:HA	1:B:708:VAL:HG23	2.01	0.42
1:B:68:PRO:HB2	1:B:244:PRO:CG	2.47	0.42
1:A:1693:LYS:HE2	1:A:1693:LYS:HB2	1.76	0.42
1:A:1924:TYR:HD1	1:A:1928:THR:HG22	1.84	0.42
1:A:293:THR:HA	1:A:1977:ASN:ND2	2.34	0.42
1:A:1999:GLU:HB3	1:A:2006:LEU:HD13	2.01	0.42
1:A:23:ARG:O	1:A:26:HIS:N	2.53	0.42
1:A:447:GLY:O	1:A:448:ILE:HG22	2.20	0.42
1:A:587:LEU:O	1:A:591:ILE:HG13	2.19	0.42
1:B:2171:LEU:HA	1:B:2171:LEU:HD23	1.78	0.42
1:B:193:LEU:CD1	1:B:252:LYS:HD3	2.49	0.42
1:A:1731:LYS:HB3	1:A:1890:TYR:HB3	2.02	0.42
1:A:270:ILE:HB	1:A:287:LEU:HB2	2.01	0.42
1:A:317:HIS:O	1:A:319:GLY:N	2.52	0.42
1:A:572:ASN:HB2	1:A:637:TRP:CE3	2.55	0.42
1:A:631:LEU:HD22	1:A:632:HIS:CD2	2.55	0.42
1:B:397:PRO:O	1:B:399:VAL:HG22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:573:VAL:HG22	1:B:638:TYR:HB2	2.02	0.42
1:B:660:HIS:N	1:B:663:VAL:O	2.49	0.42
1:B:654:SER:OG	1:B:689:ILE:HB	2.19	0.42
1:A:659:LYS:HE2	1:A:664:TYR:CZ	2.54	0.42
1:B:102:VAL:HG21	1:B:294:PHE:CE2	2.55	0.42
1:B:2117:GLY:CA	1:B:2124:MET:HB2	2.49	0.42
1:B:466:LYS:HD2	1:B:508:ILE:HD11	2.02	0.42
1:B:466:LYS:HD2	1:B:508:ILE:CD1	2.49	0.42
1:B:623:ASP:OD1	1:B:623:ASP:N	2.52	0.42
1:B:622:PHE:CD1	1:B:701:GLY:HA2	2.54	0.42
1:A:115:TYR:CZ	1:A:1997:ARG:HB2	2.55	0.42
1:A:1767:VAL:O	1:A:1768:GLU:HB2	2.19	0.42
1:A:1934:MET:O	1:A:2016:VAL:HA	2.20	0.42
1:A:2179:GLY:HA3	1:A:2184:ALA:HB3	2.02	0.42
1:B:1745:GLN:HA	1:B:1746:PRO:HD3	1.82	0.42
1:B:241:ARG:HD2	1:B:322:GLU:HB2	2.02	0.42
1:A:1838:PHE:HD2	1:A:1839:SER:O	2.03	0.42
1:A:1843:LEU:HD23	1:A:1843:LEU:HA	1.75	0.42
1:A:2020:LYS:HD3	1:A:2020:LYS:HA	1.84	0.42
1:A:282:HIS:CD2	1:A:525:ASP:HB3	2.54	0.42
1:A:522:THR:N	1:A:525:ASP:OD1	2.41	0.42
1:B:2157:SER:O	1:B:2158:ILE:HB	2.20	0.42
1:B:2257:VAL:HG22	1:B:2317:ILE:HG23	2.02	0.42
1:A:127:ASP:N	1:A:127:ASP:OD1	2.52	0.42
1:A:177:LEU:HD12	1:A:177:LEU:HA	1.82	0.42
1:A:320:GLY:O	1:A:322:GLU:N	2.53	0.42
1:B:1784:SER:HB3	1:B:1841:VAL:HG13	2.01	0.42
1:B:315:SER:HB2	1:B:318:HIS:H	1.85	0.42
1:A:1963:PHE:HD2	1:A:1986:VAL:HB	1.85	0.41
1:A:2286:ASN:N	1:A:2293:VAL:HG11	2.30	0.41
1:A:390:GLU:OE2	1:A:470:SER:N	2.53	0.41
1:B:1736:ARG:HE	1:B:1749:ARG:HH12	1.68	0.41
1:B:1978:LEU:HD23	1:B:1978:LEU:HA	1.77	0.41
1:B:2313:TRP:CE3	1:B:2317:ILE:HD11	2.54	0.41
1:A:631:LEU:HD22	1:A:632:HIS:NE2	2.35	0.41
1:A:634:VAL:HG22	1:A:681:SER:HB2	2.03	0.41
1:B:2045:GLN:O	1:B:2059:ILE:HG21	2.20	0.41
1:B:2020:LYS:NZ	1:B:2327:GLU:OE1	2.47	0.41
1:B:527:ARG:HA	1:B:527:ARG:HD3	1.63	0.41
1:A:106:PHE:HB2	1:A:110:SER:HB2	2.01	0.41
1:A:162:HIS:NE2	1:A:1999:GLU:OE2	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2147:ARG:HG2	1:B:2147:ARG:O	2.19	0.41
1:B:2189:GLN:HB3	1:B:2233:ASP:O	2.21	0.41
1:B:2192:ALA:HB1	1:B:2229:TRP:O	2.20	0.41
1:B:389:GLU:HG2	1:B:429:MET:SD	2.60	0.41
1:B:626:GLN:HA	1:B:705:LEU:HB2	2.03	0.41
1:A:540:GLU:HB3	1:A:583:ARG:HH21	1.85	0.41
1:B:2098:ILE:HD11	1:B:2153:PRO:HB3	2.02	0.41
1:A:1953:ILE:HG22	1:A:1979:TYR:CD1	2.56	0.41
1:A:417:GLN:O	1:A:418:ARG:NE	2.54	0.41
1:A:431:TYR:CE2	1:A:439:ARG:HG2	2.54	0.41
1:A:706:LEU:O	1:A:707:LYS:C	2.59	0.41
1:B:12:LEU:C	1:B:12:LEU:HD12	2.40	0.41
1:B:2189:GLN:HG2	1:B:2235:GLN:OE1	2.20	0.41
1:A:1781:ARG:O	1:A:1809:PRO:HG3	2.20	0.41
1:A:1807:VAL:HG22	1:A:1813:ARG:HB3	2.03	0.41
1:B:1832:CYS:HA	1:B:1858:CYS:HA	2.02	0.41
1:B:1940:ILE:HD12	1:B:1990:PRO:HG3	2.03	0.41
1:B:44:SER:O	1:B:46:LEU:N	2.52	0.41
1:A:188:GLU:O	1:A:190:THR:N	2.54	0.41
1:A:408:LYS:O	1:A:412:LEU:HD12	2.21	0.41
1:A:622:PHE:CD2	1:A:701:GLY:HA2	2.56	0.41
1:B:1967:LYS:O	1:B:1968:LYS:HB3	2.21	0.41
1:B:2053:LEU:HD23	1:B:2054:HIS:CG	2.56	0.41
1:B:2079:MET:HB3	1:B:2169:CYS:O	2.20	0.41
1:B:2274:PHE:CE2	1:B:2301:LEU:HD13	2.54	0.41
1:B:7:LEU:HD23	1:B:52:PHE:CD1	2.56	0.41
1:A:2217:ASN:O	1:A:2218:ALA:HB2	2.20	0.41
1:A:418:ARG:NH2	1:A:607:GLU:HG2	2.35	0.41
1:A:95:HIS:HB2	1:A:96:PRO:HD2	2.02	0.41
1:B:1693:LYS:O	1:B:1769:ASP:HB3	2.21	0.41
1:B:2043:TYR:O	1:B:2043:TYR:HD1	2.04	0.41
1:B:2247:GLY:N	1:B:2286:ASN:HD21	2.17	0.41
1:B:571:ARG:O	1:B:572:ASN:HB2	2.20	0.41
1:B:1789:LEU:HD12	1:B:1855:LEU:HD22	2.03	0.41
1:B:1766:GLU:HG2	1:B:1863:LEU:HD13	2.03	0.41
1:B:2084:ILE:CG2	1:B:2138:ASN:HB2	2.51	0.41
1:B:277:PHE:CD2	1:B:287:LEU:HB2	2.56	0.41
1:B:418:ARG:HD3	1:B:611:SER:CB	2.51	0.41
1:A:2115:TYR:CZ	1:A:2117:GLY:HA3	2.55	0.41
1:A:250:HIS:CE1	1:A:304:LEU:HG	2.56	0.41
1:A:273:GLU:HB2	1:A:307:PHE:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:597:ASN:C	1:A:599:ALA:N	2.73	0.41
1:B:108:LYS:HB3	1:B:108:LYS:HE3	1.71	0.41
1:B:148:THR:CG2	1:B:1972:LYS:HB2	2.51	0.41
1:A:26:HIS:O	1:A:28:ASP:N	2.54	0.41
1:A:498:LEU:HA	1:A:498:LEU:HD12	1.76	0.41
1:B:130:LEU:HB2	1:B:133:LYS:CD	2.51	0.41
1:B:15:ASP:HB2	1:B:45:VAL:CG2	2.51	0.41
1:B:1783:TYR:HH	1:B:1890:TYR:HH	1.68	0.41
1:B:1879:PHE:HD1	1:B:1945:LEU:HB3	1.86	0.41
1:B:29:THR:CG2	1:B:30:ARG:N	2.81	0.41
1:A:206:GLY:O	1:A:207:LYS:HB3	2.21	0.40
1:A:2080:ILE:HG13	1:A:2171:LEU:HD23	2.04	0.40
1:A:2115:TYR:CE2	1:A:2117:GLY:HA3	2.56	0.40
1:A:35:ALA:HB1	1:A:41:LEU:HD21	2.03	0.40
1:B:2192:ALA:HB3	1:B:2205:PRO:HG3	2.03	0.40
1:A:1708:ASP:C	1:A:1710:GLY:H	2.25	0.40
1:A:1778:GLN:HB3	1:A:1779:ALA:H	1.69	0.40
1:A:1940:ILE:HD12	1:A:1990:PRO:HD3	2.03	0.40
1:A:685:PRO:HA	1:A:708:VAL:HG21	2.02	0.40
1:B:1731:LYS:H	1:B:1894:ASN:HD21	1.68	0.40
1:B:2032:ILE:HG23	1:B:2036:GLN:NE2	2.36	0.40
1:B:2049:LYS:H	1:B:2049:LYS:HG3	1.57	0.40
1:B:2302:LEU:HD13	1:B:2302:LEU:HA	1.97	0.40
1:A:1758:LEU:HA	1:A:1758:LEU:HD12	1.73	0.40
1:A:1888:SER:O	1:A:1889:TRP:C	2.60	0.40
1:A:2080:ILE:HG12	1:A:2145:ILE:CD1	2.51	0.40
1:A:454:TYR:CE2	1:A:570:LYS:HG3	2.56	0.40
1:A:577:SER:O	1:A:616:SER:HB3	2.21	0.40
1:B:112:GLY:O	1:B:162:HIS:HB3	2.21	0.40
1:B:552:LEU:HD21	1:B:638:TYR:CE2	2.57	0.40
1:A:1753:ASN:HB3	1:A:1756:LEU:HD23	2.02	0.40
1:A:1781:ARG:CZ	1:A:1889:TRP:CZ2	3.05	0.40
1:A:1832:CYS:HA	1:A:1858:CYS:HA	2.03	0.40
1:A:2176:MET:HE3	1:A:2177:PRO:HD2	2.03	0.40
1:A:2263:SER:OG	1:A:2307:ARG:HB2	2.21	0.40
1:A:404:ASP:OD2	1:A:409:SER:HB3	2.20	0.40
1:B:135:GLN:HG3	1:B:136:THR:O	2.21	0.40
1:B:1936:GLN:HG3	1:B:1937:ASN:ND2	2.36	0.40
1:B:2193:SER:HB3	1:B:2229:TRP:CE2	2.57	0.40
1:B:419:ILE:HG23	1:B:594:PHE:HB2	2.04	0.40
1:B:632:HIS:O	1:B:634:VAL:HG23	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:635:ALA:N	1:B:680:MET:O	2.53	0.40
1:A:2195:TYR:O	1:A:2195:TYR:CG	2.74	0.40
1:A:271:PHE:CE1	1:A:286:SER:HB3	2.56	0.40
1:B:1749:ARG:HD3	1:B:1749:ARG:HH21	1.75	0.40
1:B:1756:LEU:HD21	1:B:1762:TYR:CE2	2.57	0.40
1:B:1792:TYR:HD2	1:B:1801:GLU:OE2	2.05	0.40
1:B:59:LEU:H	1:B:59:LEU:HG	1.50	0.40

All (3) 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:504:LEU:O	2:F:4:MAN:O6[1_455]	1.98	0.22
1:A:469:ALA:O	2:F:4:MAN:O2[1_455]	2.04	0.16
1:B:326:ARG:NH2	1:B:2094:SER:OG[2_457]	2.11	0.09

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	1242/1467 (85%)	966 (78%)	174 (14%)	102 (8%)	1	5
1	B	1231/1467 (84%)	955 (78%)	182 (15%)	94 (8%)	1	7
All	All	2473/2934 (84%)	1921 (78%)	356 (14%)	196 (8%)	1	6

All (196) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	32	PRO
1	A	36	PRO
1	A	39	LEU
1	A	40	PRO

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Mol	Chain	Res	Type
1	A	44	SER
1	A	45	VAL
1	A	207	LYS
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	407	TYR
1	A	505	PRO
1	A	556	LYS
1	A	603	LEU
1	A	655	GLY
1	A	695	SER
1	A	1796	GLN
1	A	1804	HIS
1	A	1871	VAL
1	A	1889	TRP
1	A	1896	GLU
1	A	1936	GLN
1	A	2010	MET
1	A	2120	THR
1	A	2183	LYS
1	A	2206	SER
1	A	2252	LEU
1	A	2284	GLN
1	B	29	THR
1	B	44	SER
1	B	46	LEU
1	B	181	ARG
1	B	191	GLN
1	B	209	TRP
1	B	250	HIS
1	B	265	PRO
1	B	331	ALA
1	B	398	LEU
1	B	571	ARG
1	B	622	PHE
1	B	685	PRO
1	B	695	SER
1	B	1694	ARG

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Mol	Chain	Res	Type
1	B	1695	THR
1	B	1709	TYR
1	B	1726	GLU
1	B	1765	ALA
1	B	1804	HIS
1	B	1894	ASN
1	B	1914	GLU
1	B	2142	PRO
1	B	2183	LYS
1	A	25	LEU
1	A	38	ALA
1	A	189	ARG
1	A	192	ASN
1	A	193	LEU
1	A	194	HIS
1	A	211	SER
1	A	280	ARG
1	A	399	VAL
1	A	403	ASP
1	A	445	GLU
1	A	523	LYS
1	A	600	GLY
1	A	707	LYS
1	A	1742	SER
1	A	1743	PHE
1	A	1938	GLN
1	A	2045	GLN
1	A	2092	LYS
1	A	2119	SER
1	A	2184	ALA
1	B	230	PRO
1	B	240	ASN
1	B	241	ARG
1	B	242	SER
1	B	397	PRO
1	B	407	TYR
1	B	409	SER
1	B	439	ARG
1	B	526	PRO
1	B	623	ASP
1	B	636	TYR
1	B	658	PHE

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Mol	Chain	Res	Type
1	B	693	HIS
1	B	702	MET
1	B	706	LEU
1	B	1713	GLU
1	B	1821	HIS
1	B	2010	MET
1	B	2027	MET
1	B	2044	GLY
1	B	2067	PRO
1	B	2180	MET
1	B	2280	VAL
1	B	2328	ALA
1	A	34	THR
1	A	195	GLU
1	A	230	PRO
1	A	251	LYS
1	A	266	GLU
1	A	319	GLY
1	A	468	GLN
1	A	654	SER
1	A	1751	GLU
1	A	1778	GLN
1	A	1897	ARG
1	A	2040	SER
1	A	2043	TYR
1	A	2067	PRO
1	A	2218	ALA
1	B	28	ASP
1	B	128	LYS
1	B	187	ARG
1	B	266	GLU
1	B	287	LEU
1	B	316	HIS
1	B	406	SER
1	B	414	ASN
1	B	493	LYS
1	B	539	MET
1	B	618	ASN
1	B	1747	SER
1	B	1752	LEU
1	B	1833	LYS
1	B	1913	LYS

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Mol	Chain	Res	Type
1	B	1930	PRO
1	B	2115	TYR
1	B	2135	ILE
1	B	2158	ILE
1	B	2286	ASN
1	B	2299	PRO
1	A	27	VAL
1	A	41	LEU
1	A	138	VAL
1	A	273	GLU
1	A	331	ALA
1	A	540	GLU
1	A	697	PHE
1	A	704	ALA
1	A	1890	TYR
1	A	2132	SER
1	A	2142	PRO
1	A	2286	ASN
1	A	2315	HIS
1	B	147	PRO
1	B	378	HIS
1	B	447	GLY
1	B	599	ALA
1	B	654	SER
1	B	1850	GLY
1	B	2092	LYS
1	B	2133	SER
1	B	2311	GLN
1	B	2315	HIS
1	A	135	GLN
1	A	187	ARG
1	A	569	ASP
1	A	622	PHE
1	A	698	ARG
1	A	1843	LEU
1	A	1860	ALA
1	A	2280	VAL
1	A	2303	THR
1	B	64	ARG
1	B	133	LYS
1	B	239	VAL
1	B	413	ASN

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Mol	Chain	Res	Type
1	B	443	GLN
1	B	2007	GLN
1	A	474	ASN
1	A	494	GLY
1	A	504	LEU
1	A	708	VAL
1	A	1713	GLU
1	A	1779	ALA
1	A	1797	GLU
1	A	2202	THR
1	B	2159	ARG
1	B	2175	SER
1	B	45	VAL
1	A	141	VAL
1	A	174	ILE
1	B	402	PRO
1	B	1741	GLY
1	A	31	PHE
1	A	402	PRO
1	A	448	ILE
1	B	229	GLN
1	B	1990	PRO
1	B	27	VAL
1	B	2098	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	1110/1301 (85%)	1074 (97%)	36 (3%)	39	71
1	B	1104/1301 (85%)	1079 (98%)	25 (2%)	50	78
All	All	2214/2602 (85%)	2153 (97%)	61 (3%)	43	74

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	GLU
1	A	39	LEU
1	A	66	ARG
1	A	106	PHE
1	A	133	LYS
1	A	153	PRO
1	A	185	LEU
1	A	193	LEU
1	A	208	SER
1	A	210	HIS
1	A	312	HIS
1	A	317	HIS
1	A	421	ARG
1	A	443	GLN
1	A	478	HIS
1	A	555	TYR
1	A	624	SER
1	A	647	ASP
1	A	654	SER
1	A	1801	GLU
1	A	1897	ARG
1	A	1949	SER
1	A	1983	PHE
1	A	1997	ARG
1	A	2000	CYS
1	A	2031	HIS
1	A	2034	ASP
1	A	2055	TYR
1	A	2110	LYS
1	A	2137	HIS
1	A	2157	SER
1	A	2206	SER
1	A	2220	ARG
1	A	2250	SER
1	A	2295	ASN
1	A	2319	LEU
1	B	43	PRO
1	B	94	SER
1	B	106	PHE
1	B	160	LEU
1	B	162	HIS
1	B	392	ASP
1	B	409	SER

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Mol	Chain	Res	Type
1	B	527	ARG
1	B	538	ASN
1	B	539	MET
1	B	616	SER
1	B	636	TYR
1	B	645	GLN
1	B	699	ASN
1	B	1709	TYR
1	B	1736	ARG
1	B	1784	SER
1	B	1899	CYS
1	B	1919	HIS
1	B	1946	SER
1	B	1983	PHE
1	B	2055	TYR
1	B	2104	MET
1	B	2206	SER
1	B	2286	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	191	GLN
1	A	317	HIS
1	A	443	GLN
1	A	2007	GLN
1	A	2082	HIS
1	A	2246	GLN
1	B	26	HIS
1	B	162	HIS
1	B	233	HIS
1	B	318	HIS
1	B	2189	GLN
1	B	2225	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 ⓘ

31 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	C	1	1,2	14,14,15	1.07	1 (7%)	17,19,21	2.05	3 (17%)
2	NAG	C	2	2	14,14,15	0.37	0	17,19,21	0.44	0
2	BMA	C	3	2	11,11,12	1.38	3 (27%)	15,15,17	1.21	0
2	MAN	C	4	2	11,11,12	0.81	0	15,15,17	1.00	1 (6%)
2	MAN	C	5	2	11,11,12	1.47	3 (27%)	15,15,17	2.08	4 (26%)
3	NAG	D	1	1,3	14,14,15	0.79	1 (7%)	17,19,21	1.41	3 (17%)
3	NAG	D	2	3	14,14,15	0.87	1 (7%)	17,19,21	1.29	2 (11%)
3	BMA	D	3	3	11,11,12	1.49	2 (18%)	15,15,17	0.91	0
2	NAG	E	1	1,2	14,14,15	0.54	0	17,19,21	0.67	0
2	NAG	E	2	2	14,14,15	0.68	0	17,19,21	1.85	5 (29%)
2	BMA	E	3	2	11,11,12	1.98	4 (36%)	15,15,17	1.27	1 (6%)
2	MAN	E	4	2	11,11,12	1.59	2 (18%)	15,15,17	1.36	2 (13%)
2	MAN	E	5	2	11,11,12	0.87	0	15,15,17	1.05	0
2	NAG	F	1	1,2	14,14,15	0.27	0	17,19,21	0.44	0
2	NAG	F	2	2	14,14,15	0.73	1 (7%)	17,19,21	0.68	0
2	BMA	F	3	2	11,11,12	1.69	3 (27%)	15,15,17	2.41	8 (53%)
2	MAN	F	4	2	11,11,12	2.04	4 (36%)	15,15,17	2.98	5 (33%)
2	MAN	F	5	2	11,11,12	0.62	0	15,15,17	2.20	3 (20%)
4	NAG	G	1	1,4	14,14,15	0.55	0	17,19,21	1.07	1 (5%)
4	NAG	G	2	4	14,14,15	0.55	0	17,19,21	1.42	3 (17%)
4	BMA	G	3	4	11,11,12	1.20	2 (18%)	15,15,17	1.17	2 (13%)
4	MAN	G	4	4	11,11,12	1.09	1 (9%)	15,15,17	1.65	2 (13%)
4	NAG	G	5	4	14,14,15	0.41	0	17,19,21	1.50	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MAN	G	6	4	11,11,12	1.04	1 (9%)	15,15,17	1.81	4 (26%)
4	FUC	G	7	4	10,10,11	1.17	1 (10%)	14,14,16	1.20	1 (7%)
5	NAG	H	1	1,5	14,14,15	0.68	1 (7%)	17,19,21	0.76	0
5	NAG	H	2	5	14,14,15	0.61	0	17,19,21	0.67	0
5	BMA	H	3	5	11,11,12	1.09	0	15,15,17	1.41	2 (13%)
5	MAN	H	4	5	11,11,12	0.99	0	15,15,17	1.26	1 (6%)
5	MAN	H	5	5	11,11,12	1.28	1 (9%)	15,15,17	1.17	1 (6%)
5	MAN	H	6	5	11,11,12	1.57	3 (27%)	15,15,17	1.04	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	1/2/19/22	0/1/1/1
2	MAN	C	4	2	-	2/2/19/22	0/1/1/1
2	MAN	C	5	2	-	1/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	BMA	D	3	3	-	2/2/19/22	0/1/1/1
2	NAG	E	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	E	2	2	-	6/6/23/26	0/1/1/1
2	BMA	E	3	2	-	2/2/19/22	0/1/1/1
2	MAN	E	4	2	-	2/2/19/22	1/1/1/1
2	MAN	E	5	2	-	2/2/19/22	1/1/1/1
2	NAG	F	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	BMA	F	3	2	-	0/2/19/22	0/1/1/1
2	MAN	F	4	2	-	2/2/19/22	0/1/1/1
2	MAN	F	5	2	-	1/2/19/22	0/1/1/1
4	NAG	G	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	G	2	4	-	5/6/23/26	0/1/1/1
4	BMA	G	3	4	-	2/2/19/22	0/1/1/1
4	MAN	G	4	4	-	1/2/19/22	0/1/1/1
4	NAG	G	5	4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	G	6	4	-	2/2/19/22	0/1/1/1
4	FUC	G	7	4	-	-	0/1/1/1
5	NAG	H	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	H	2	5	-	1/6/23/26	0/1/1/1
5	BMA	H	3	5	-	0/2/19/22	0/1/1/1
5	MAN	H	4	5	-	1/2/19/22	0/1/1/1
5	MAN	H	5	5	-	2/2/19/22	0/1/1/1
5	MAN	H	6	5	-	1/2/19/22	0/1/1/1

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	4	MAN	C4-C5	-4.45	1.43	1.53
2	E	4	MAN	O5-C5	3.91	1.51	1.43
2	E	3	BMA	C1-C2	3.83	1.60	1.52
2	E	3	BMA	C2-C3	3.64	1.57	1.52
2	C	1	NAG	O5-C1	3.62	1.49	1.43
2	F	4	MAN	O5-C5	3.61	1.50	1.43
2	F	3	BMA	C2-C3	3.53	1.57	1.52
2	C	5	MAN	C1-C2	3.50	1.60	1.52
5	H	5	MAN	C1-C2	3.34	1.59	1.52
5	H	6	MAN	C4-C5	3.23	1.59	1.53
3	D	2	NAG	O5-C1	-2.97	1.39	1.43
3	D	3	BMA	C1-C2	2.73	1.58	1.52
3	D	1	NAG	O5-C1	-2.72	1.39	1.43
4	G	3	BMA	C2-C3	2.71	1.56	1.52
2	E	3	BMA	C4-C5	2.60	1.58	1.53
5	H	6	MAN	C1-C2	2.58	1.58	1.52
2	F	3	BMA	O3-C3	2.55	1.49	1.43
2	C	5	MAN	O5-C1	2.55	1.47	1.43
2	E	4	MAN	C1-C2	2.51	1.57	1.52
4	G	4	MAN	C4-C3	2.49	1.58	1.52
4	G	6	MAN	C1-C2	2.46	1.57	1.52
4	G	7	FUC	C2-C3	2.40	1.56	1.52
2	F	2	NAG	O5-C1	-2.37	1.39	1.43
2	F	4	MAN	C2-C3	2.29	1.55	1.52
5	H	1	NAG	O5-C1	-2.26	1.40	1.43
2	C	3	BMA	O5-C5	2.23	1.48	1.43
2	F	3	BMA	O5-C1	-2.19	1.40	1.43
2	C	3	BMA	C1-C2	2.17	1.57	1.52
2	E	3	BMA	C4-C3	2.13	1.57	1.52
4	G	3	BMA	C1-C2	2.12	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	6	MAN	O5-C1	-2.12	1.40	1.43
2	F	4	MAN	O5-C1	2.06	1.47	1.43
3	D	3	BMA	C4-C3	2.06	1.57	1.52
2	C	3	BMA	C4-C3	2.05	1.57	1.52
2	C	5	MAN	O5-C5	2.01	1.47	1.43

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	4	MAN	C1-O5-C5	7.18	121.92	112.19
2	F	5	MAN	C1-O5-C5	6.92	121.56	112.19
2	C	5	MAN	C1-O5-C5	6.20	120.59	112.19
2	F	4	MAN	C2-C3-C4	6.07	121.39	110.89
2	C	1	NAG	C1-O5-C5	5.99	120.31	112.19
4	G	6	MAN	C1-O5-C5	5.13	119.14	112.19
4	G	4	MAN	C1-O5-C5	5.03	119.01	112.19
2	F	3	BMA	C1-O5-C5	5.01	118.97	112.19
2	F	3	BMA	O3-C3-C2	4.65	118.90	109.99
2	C	1	NAG	C2-N2-C7	4.58	129.43	122.90
2	E	2	NAG	C2-N2-C7	4.43	129.21	122.90
4	G	2	NAG	C2-N2-C7	4.33	129.07	122.90
2	F	4	MAN	O5-C5-C6	3.78	113.13	107.20
2	E	2	NAG	C3-C4-C5	3.74	116.91	110.24
2	F	4	MAN	C1-C2-C3	3.69	114.20	109.67
4	G	5	NAG	C2-N2-C7	3.64	128.08	122.90
2	F	5	MAN	O5-C1-C2	3.38	115.98	110.77
5	H	3	BMA	C1-O5-C5	3.29	116.66	112.19
2	E	4	MAN	C1-O5-C5	3.25	116.59	112.19
3	D	2	NAG	C3-C4-C5	3.19	115.92	110.24
3	D	2	NAG	C4-C3-C2	3.10	115.56	111.02
4	G	3	BMA	C1-O5-C5	3.10	116.39	112.19
2	F	3	BMA	C3-C4-C5	3.09	115.75	110.24
2	C	5	MAN	C1-C2-C3	3.06	113.43	109.67
4	G	5	NAG	C1-C2-N2	-2.97	105.42	110.49
3	D	1	NAG	C3-C4-C5	2.97	115.53	110.24
3	D	1	NAG	C1-O5-C5	2.96	116.20	112.19
4	G	6	MAN	C1-C2-C3	2.77	113.07	109.67
4	G	1	NAG	C2-N2-C7	2.72	126.78	122.90
2	C	1	NAG	C1-C2-N2	2.68	115.06	110.49
2	F	4	MAN	O3-C3-C4	-2.68	104.16	110.35
2	E	3	BMA	O5-C1-C2	-2.65	106.68	110.77
2	E	2	NAG	C1-O5-C5	2.60	115.72	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	4	MAN	O2-C2-C3	-2.56	105.01	110.14
4	G	6	MAN	O2-C2-C3	-2.52	105.08	110.14
3	D	1	NAG	C2-N2-C7	2.52	126.49	122.90
5	H	5	MAN	C1-O5-C5	2.48	115.55	112.19
4	G	2	NAG	C1-C2-N2	2.42	114.62	110.49
4	G	5	NAG	C1-O5-C5	-2.39	108.95	112.19
2	F	3	BMA	O5-C5-C6	-2.38	103.47	107.20
2	F	3	BMA	O5-C1-C2	-2.37	107.11	110.77
4	G	6	MAN	O5-C1-C2	2.34	114.38	110.77
2	F	3	BMA	O5-C5-C4	2.34	116.51	110.83
2	C	5	MAN	O2-C2-C3	-2.29	105.56	110.14
2	F	3	BMA	C1-C2-C3	-2.23	106.93	109.67
5	H	3	BMA	O2-C2-C3	-2.18	105.78	110.14
2	E	2	NAG	O5-C5-C4	2.17	116.12	110.83
4	G	3	BMA	O3-C3-C2	2.17	114.15	109.99
4	G	2	NAG	C1-O5-C5	2.15	115.11	112.19
2	C	5	MAN	O5-C1-C2	2.15	114.09	110.77
2	C	4	MAN	O2-C2-C3	-2.13	105.87	110.14
4	G	4	MAN	O2-C2-C3	-2.11	105.91	110.14
2	F	3	BMA	C2-C3-C4	2.09	114.50	110.89
2	F	5	MAN	O2-C2-C3	-2.03	106.08	110.14
2	E	2	NAG	C1-C2-N2	2.01	113.92	110.49
4	G	7	FUC	C1-C2-C3	2.01	112.13	109.67
2	E	4	MAN	O2-C2-C3	-2.00	106.13	110.14

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	1	NAG	C3-C2-N2-C7
2	E	4	MAN	O5-C5-C6-O6
2	C	4	MAN	C4-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
2	F	4	MAN	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	E	5	MAN	O5-C5-C6-O6
5	H	5	MAN	O5-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
3	D	3	BMA	C4-C5-C6-O6
2	E	4	MAN	C4-C5-C6-O6
5	H	5	MAN	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
4	G	2	NAG	C8-C7-N2-C2
4	G	2	NAG	O7-C7-N2-C2
2	F	1	NAG	C8-C7-N2-C2
2	F	1	NAG	O7-C7-N2-C2
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	E	1	NAG	C4-C5-C6-O6
2	E	5	MAN	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	E	3	BMA	O5-C5-C6-O6
2	F	4	MAN	C4-C5-C6-O6
2	C	4	MAN	O5-C5-C6-O6
3	D	3	BMA	O5-C5-C6-O6
4	G	6	MAN	O5-C5-C6-O6
3	D	1	NAG	C1-C2-N2-C7
4	G	4	MAN	O5-C5-C6-O6
4	G	3	BMA	C4-C5-C6-O6
2	F	5	MAN	O5-C5-C6-O6
2	C	5	MAN	O5-C5-C6-O6
5	H	4	MAN	O5-C5-C6-O6
5	H	6	MAN	O5-C5-C6-O6
2	E	3	BMA	C4-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
4	G	3	BMA	O5-C5-C6-O6
5	H	1	NAG	O5-C5-C6-O6
5	H	2	NAG	O5-C5-C6-O6
2	E	2	NAG	C3-C2-N2-C7
2	C	1	NAG	C3-C2-N2-C7
5	H	1	NAG	C3-C2-N2-C7
4	G	2	NAG	C3-C2-N2-C7
4	G	6	MAN	C4-C5-C6-O6
2	C	3	BMA	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	E	2	NAG	C1-C2-N2-C7

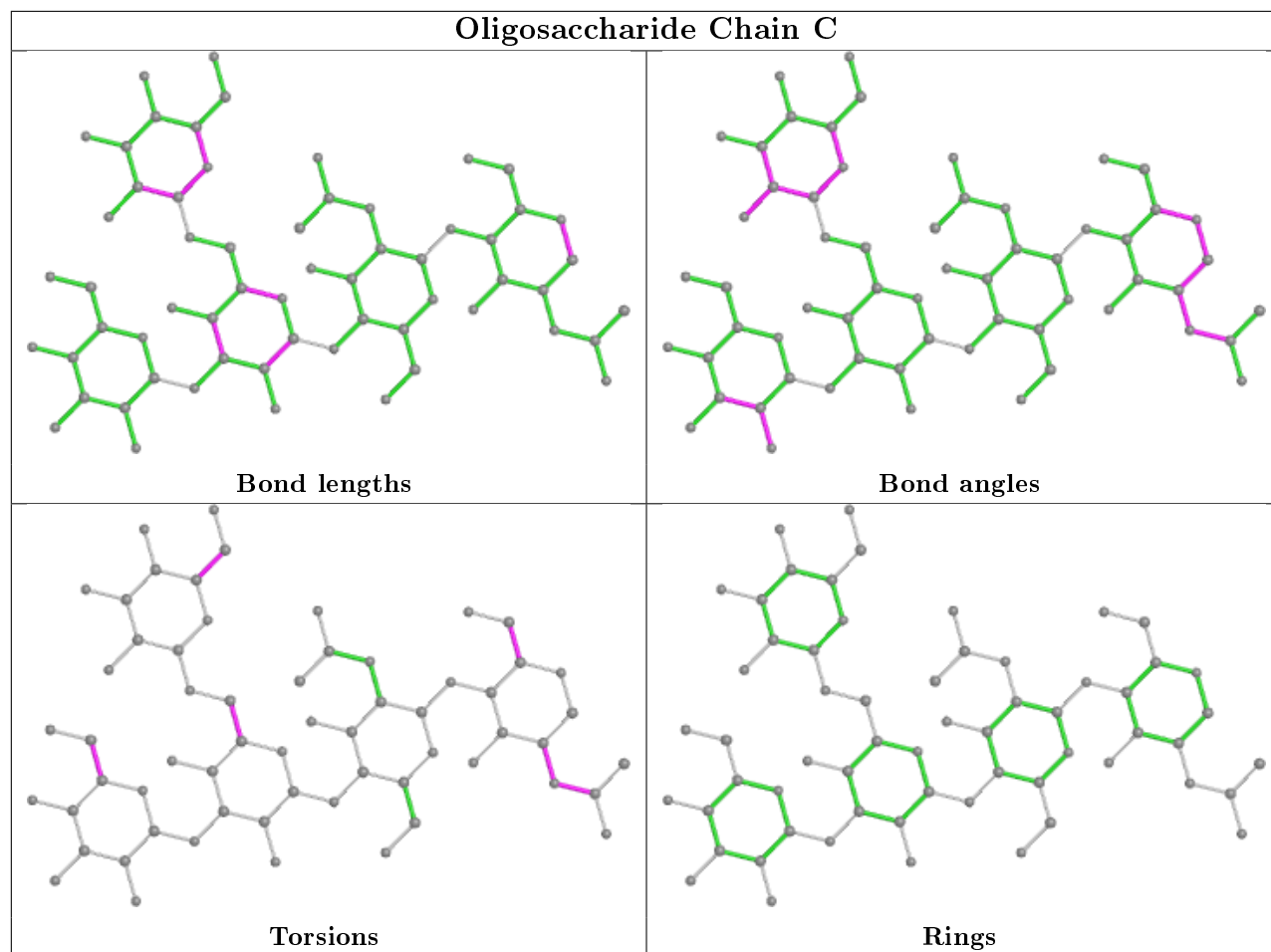
All (2) ring outliers are listed below:

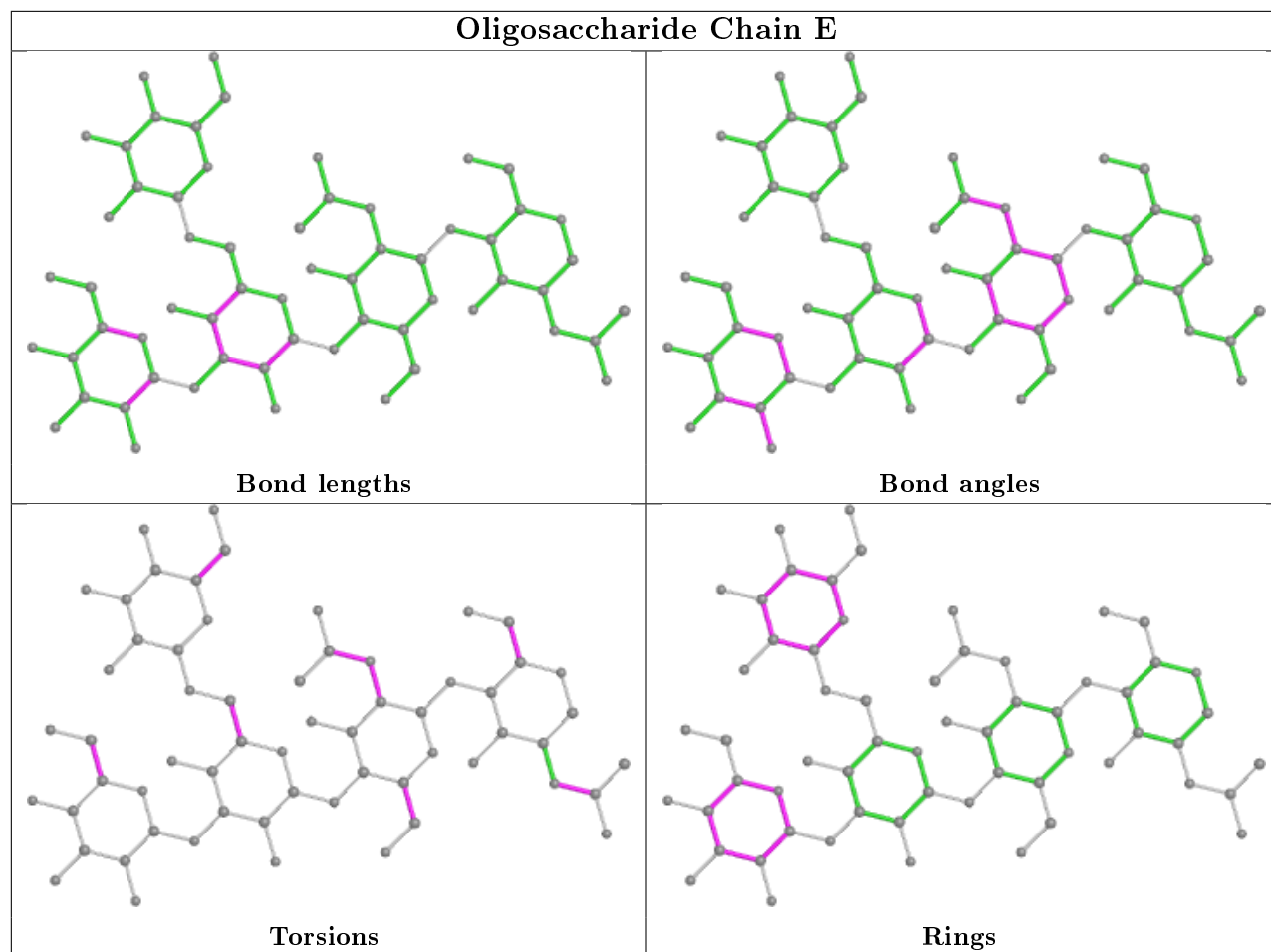
Mol	Chain	Res	Type	Atoms
2	E	5	MAN	C1-C2-C3-C4-C5-O5
2	E	4	MAN	C1-C2-C3-C4-C5-O5

11 monomers are involved in 11 short contacts:

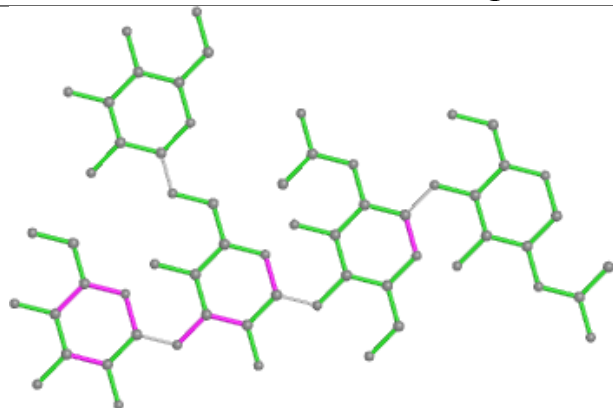
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2	NAG	1	0
2	C	1	NAG	1	0
5	H	1	NAG	1	0
4	G	2	NAG	2	0
2	F	4	MAN	0	2
5	H	4	MAN	1	0
2	E	1	NAG	1	0
2	C	2	NAG	2	0
5	H	5	MAN	1	0
4	G	1	NAG	1	0
5	H	2	NAG	1	0

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

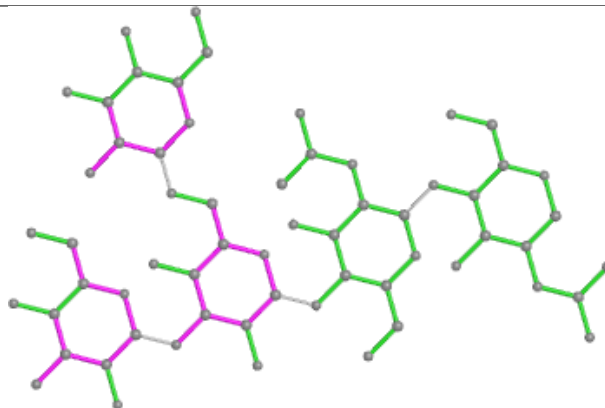




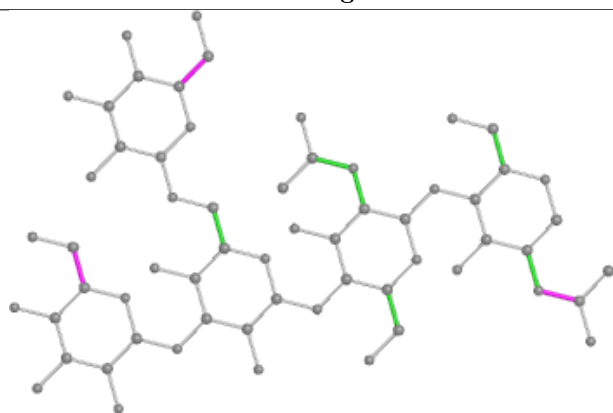
Oligosaccharide Chain F



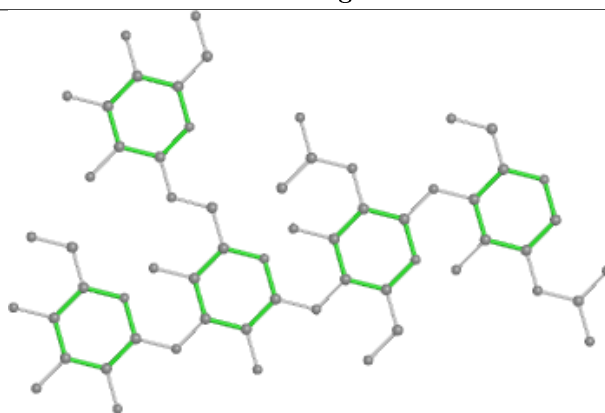
Bond lengths



Bond angles

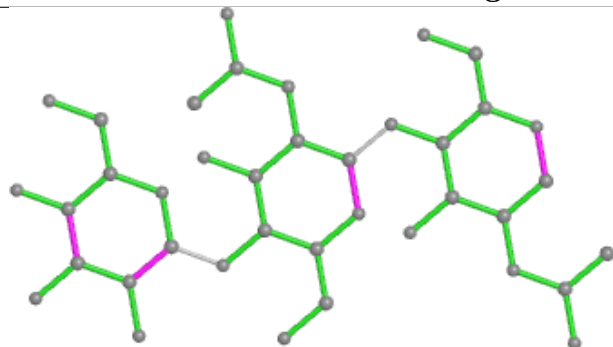


Torsions

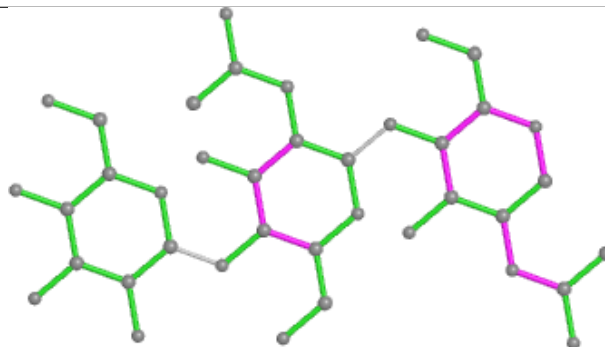


Rings

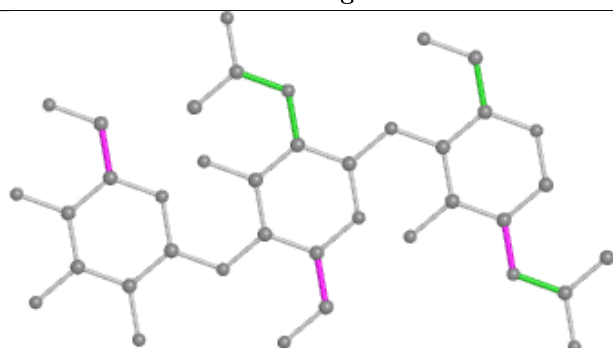
Oligosaccharide Chain D



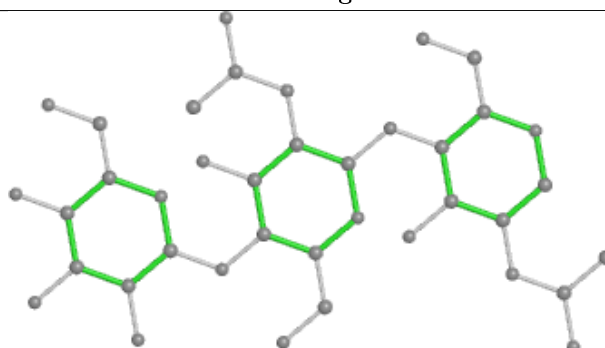
Bond lengths



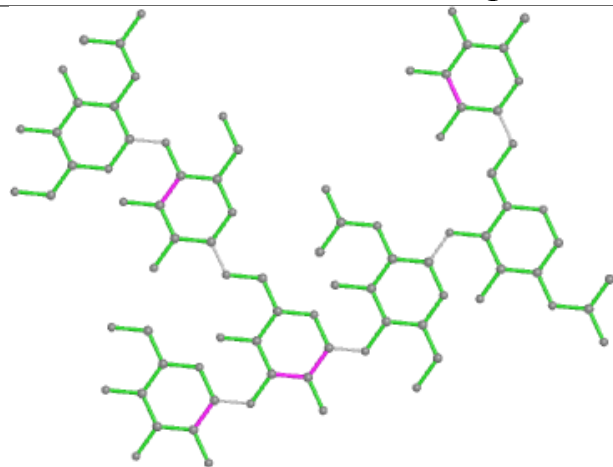
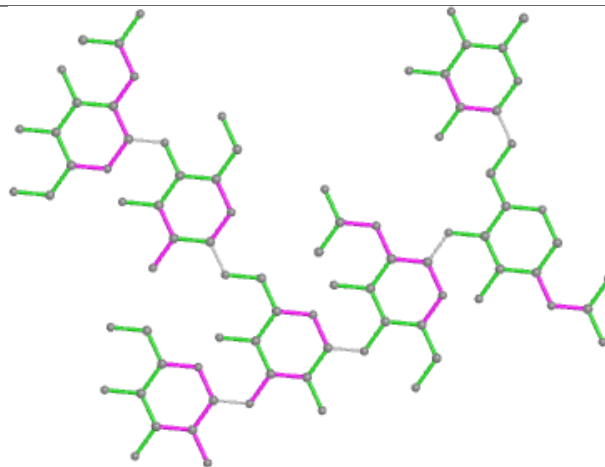
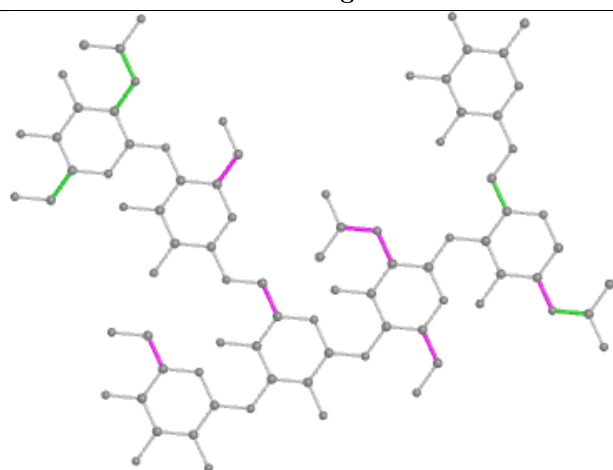
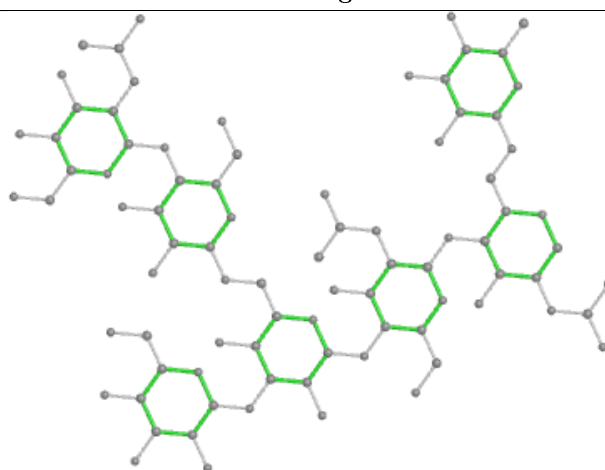
Bond angles

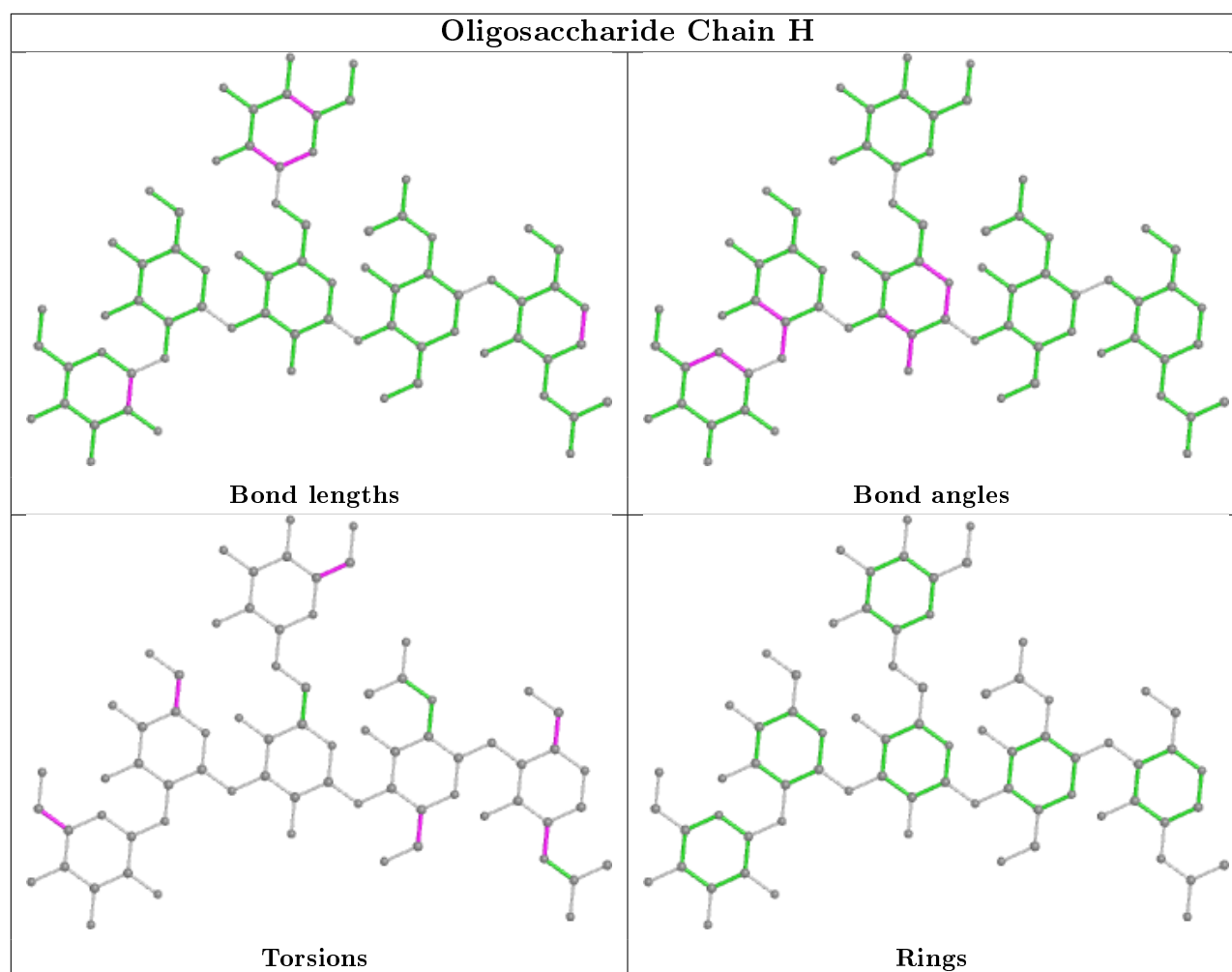


Torsions



Rings

Oligosaccharide Chain G**Bond lengths****Bond angles****Torsions****Rings**



5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 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 [i](#)

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	1256/1467 (85%)	-0.29	22 (1%) 68 55	30, 48, 88, 273	0
1	B	1247/1467 (85%)	-0.13	35 (2%) 53 37	30, 58, 130, 157	0
All	All	2503/2934 (85%)	-0.21	57 (2%) 60 47	30, 52, 119, 273	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	34	THR	9.4
1	A	37	GLY	9.1
1	A	40	PRO	8.6
1	A	33	ALA	7.9
1	B	2318	ALA	6.3
1	A	41	LEU	6.2
1	B	2319	LEU	6.1
1	B	2277	ASN	5.0
1	A	36	PRO	5.0
1	A	32	PRO	4.6
1	A	39	LEU	4.3
1	B	2245	THR	4.2
1	B	212	ALA	3.7
1	A	505	PRO	3.6
1	A	43	PRO	3.5
1	B	1899	CYS	3.4
1	B	2329	GLN	3.3
1	B	2217	ASN	3.3
1	A	399	VAL	3.2
1	B	1799	GLY	3.2
1	A	44	SER	3.2
1	B	2197	THR	3.2
1	A	42	GLY	3.1
1	A	38	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	569	ASP	3.0
1	B	1911	THR	3.0
1	B	2314	VAL	2.9
1	B	2199	MET	2.9
1	B	398	LEU	2.9
1	B	2316	GLN	2.9
1	B	2295	ASN	2.8
1	B	2279	LYS	2.8
1	A	190	THR	2.8
1	B	2122	THR	2.7
1	A	31	PHE	2.7
1	B	2317	ILE	2.6
1	B	2274	PHE	2.6
1	A	35	ALA	2.6
1	B	2258	LYS	2.6
1	B	2254	SER	2.6
1	B	2213	GLN	2.5
1	A	403	ASP	2.5
1	B	2202	THR	2.5
1	B	2250	SER	2.3
1	A	30	ARG	2.3
1	B	568	SER	2.3
1	B	1897	ARG	2.2
1	B	2198	ASN	2.2
1	B	2257	VAL	2.2
1	B	709	SER	2.2
1	A	317	HIS	2.2
1	B	2276	GLN	2.1
1	B	2214	GLY	2.1
1	A	400	LEU	2.1
1	B	2216	SER	2.1
1	B	2248	VAL	2.0
1	B	2269	HIS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

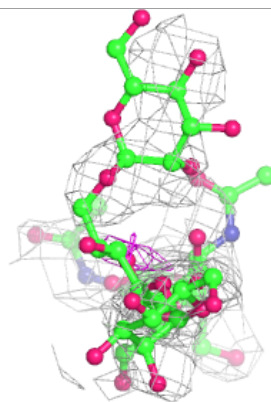
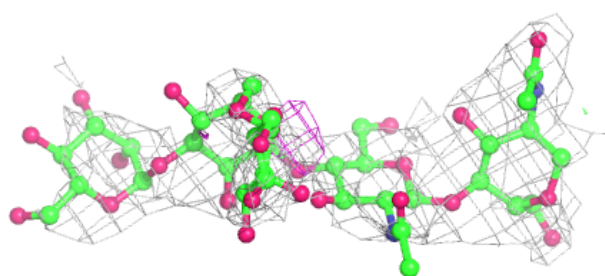
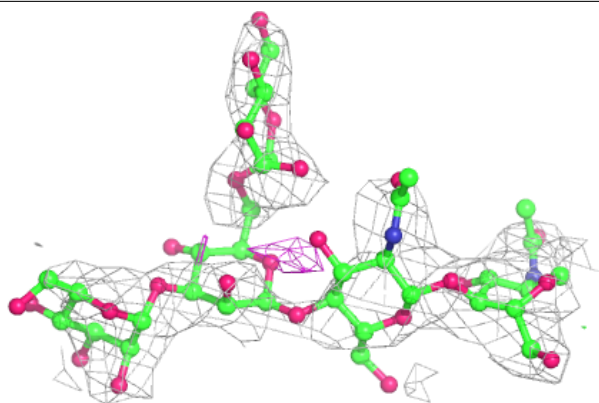
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	MAN	F	5	11/12	0.49	0.59	149,151,160,160	0
2	MAN	E	4	11/12	0.52	0.33	117,124,129,131	0
5	MAN	H	5	11/12	0.57	0.42	125,134,142,149	0
2	BMA	F	3	11/12	0.59	0.60	131,138,150,151	0
2	BMA	C	3	11/12	0.60	0.61	144,158,163,164	0
4	NAG	G	2	14/15	0.61	0.39	118,133,142,145	0
2	NAG	F	2	14/15	0.61	0.37	130,144,153,154	0
3	BMA	D	3	11/12	0.62	0.56	134,157,162,163	0
5	MAN	H	6	11/12	0.63	0.30	99,113,125,126	0
2	NAG	C	2	14/15	0.64	0.47	128,137,149,156	0
2	MAN	C	4	11/12	0.64	0.56	148,158,161,163	0
4	NAG	G	5	14/15	0.67	0.32	78,93,101,102	0
2	MAN	C	5	11/12	0.70	0.51	138,145,151,156	0
2	MAN	F	4	11/12	0.71	0.43	77,96,119,134	0
2	NAG	F	1	14/15	0.72	0.33	86,120,136,142	0
3	NAG	D	2	14/15	0.74	0.38	114,145,152,154	0
4	BMA	G	3	11/12	0.75	0.39	123,144,149,152	0
5	NAG	H	2	14/15	0.75	0.28	73,95,100,103	0
4	MAN	G	6	11/12	0.77	0.36	128,135,144,145	0
4	NAG	G	1	14/15	0.78	0.23	99,116,124,128	0
2	NAG	E	2	14/15	0.79	0.28	74,105,116,122	0
2	BMA	E	3	11/12	0.79	0.24	112,121,126,127	0
4	MAN	G	4	11/12	0.80	0.22	69,97,108,110	0
4	FUC	G	7	10/11	0.80	0.41	124,134,139,144	0
3	NAG	D	1	14/15	0.82	0.38	95,131,141,144	0
5	MAN	H	4	11/12	0.84	0.18	105,120,127,133	0
2	MAN	E	5	11/12	0.84	0.16	84,109,119,120	0
5	BMA	H	3	11/12	0.86	0.18	108,114,120,123	0
2	NAG	C	1	14/15	0.88	0.28	79,89,109,121	0
2	NAG	E	1	14/15	0.89	0.18	78,83,92,104	0
5	NAG	H	1	14/15	0.91	0.18	81,86,93,93	0

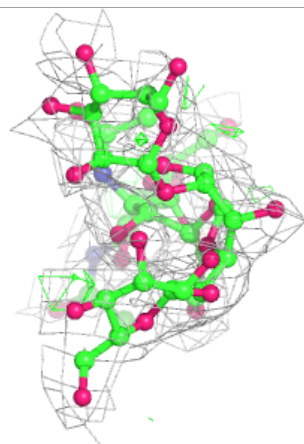
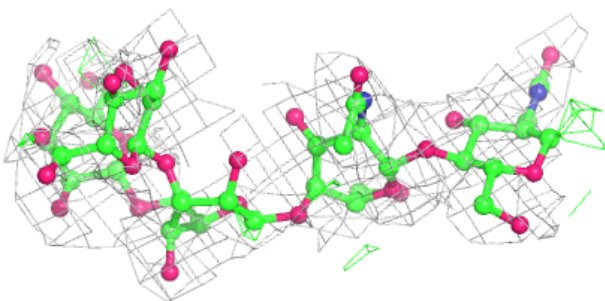
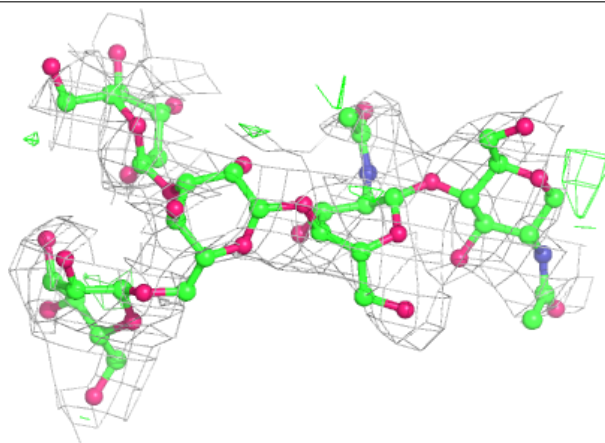
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

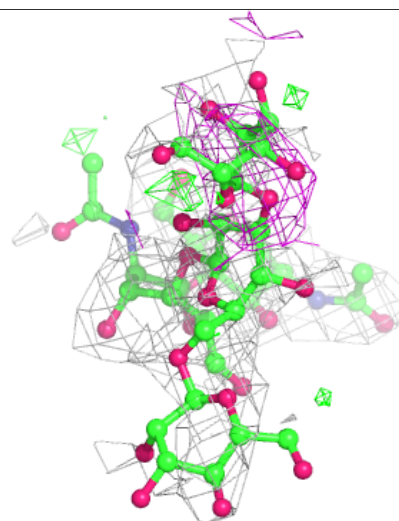
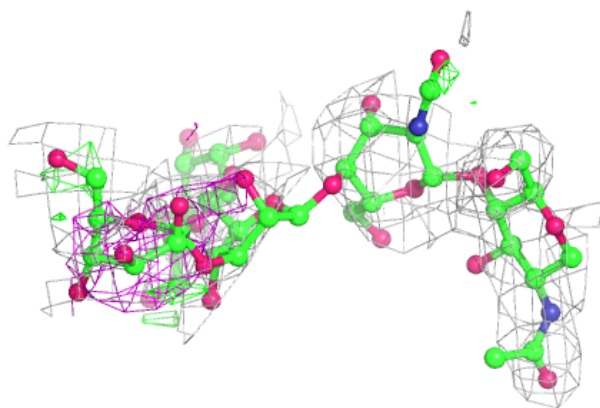
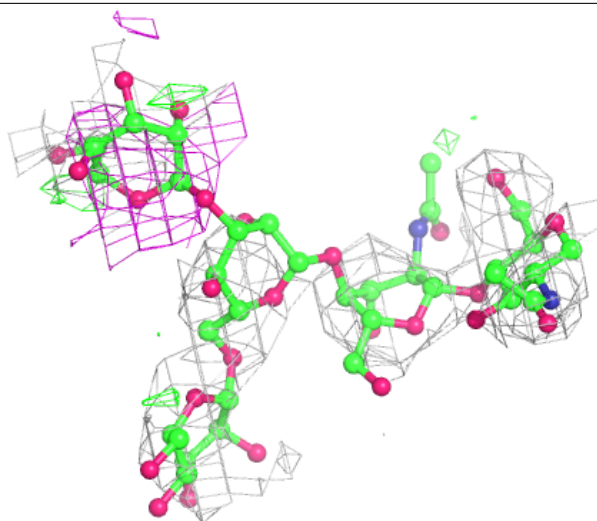
**Electron density around Chain E:**

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



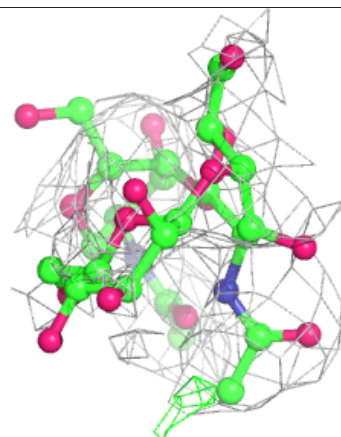
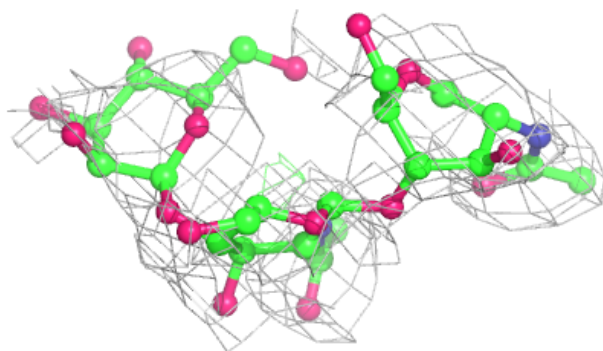
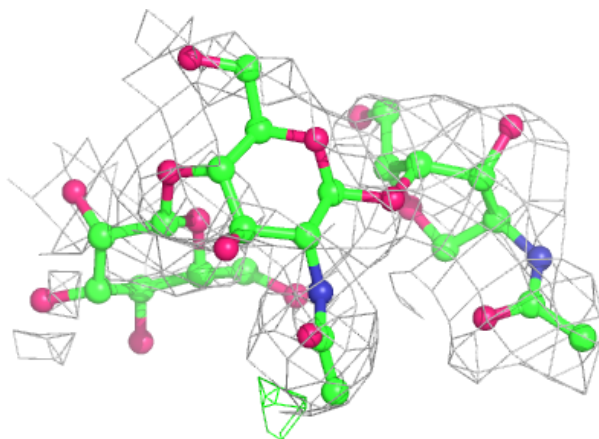
Electron density around Chain F:

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



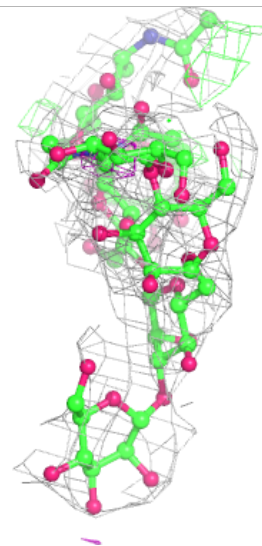
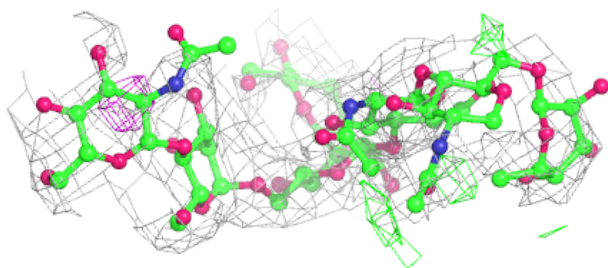
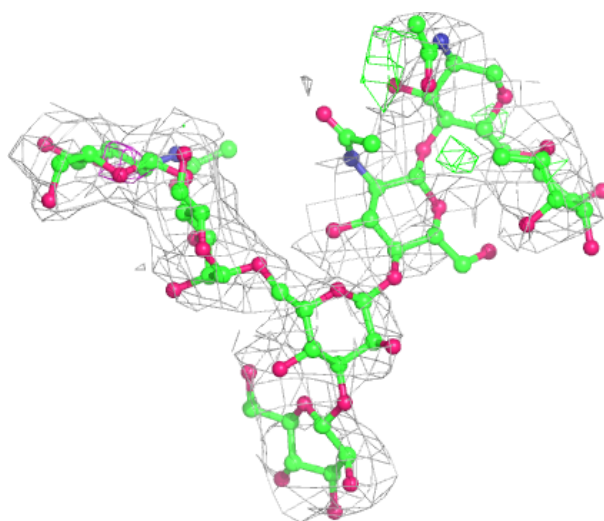
Electron density around Chain D:

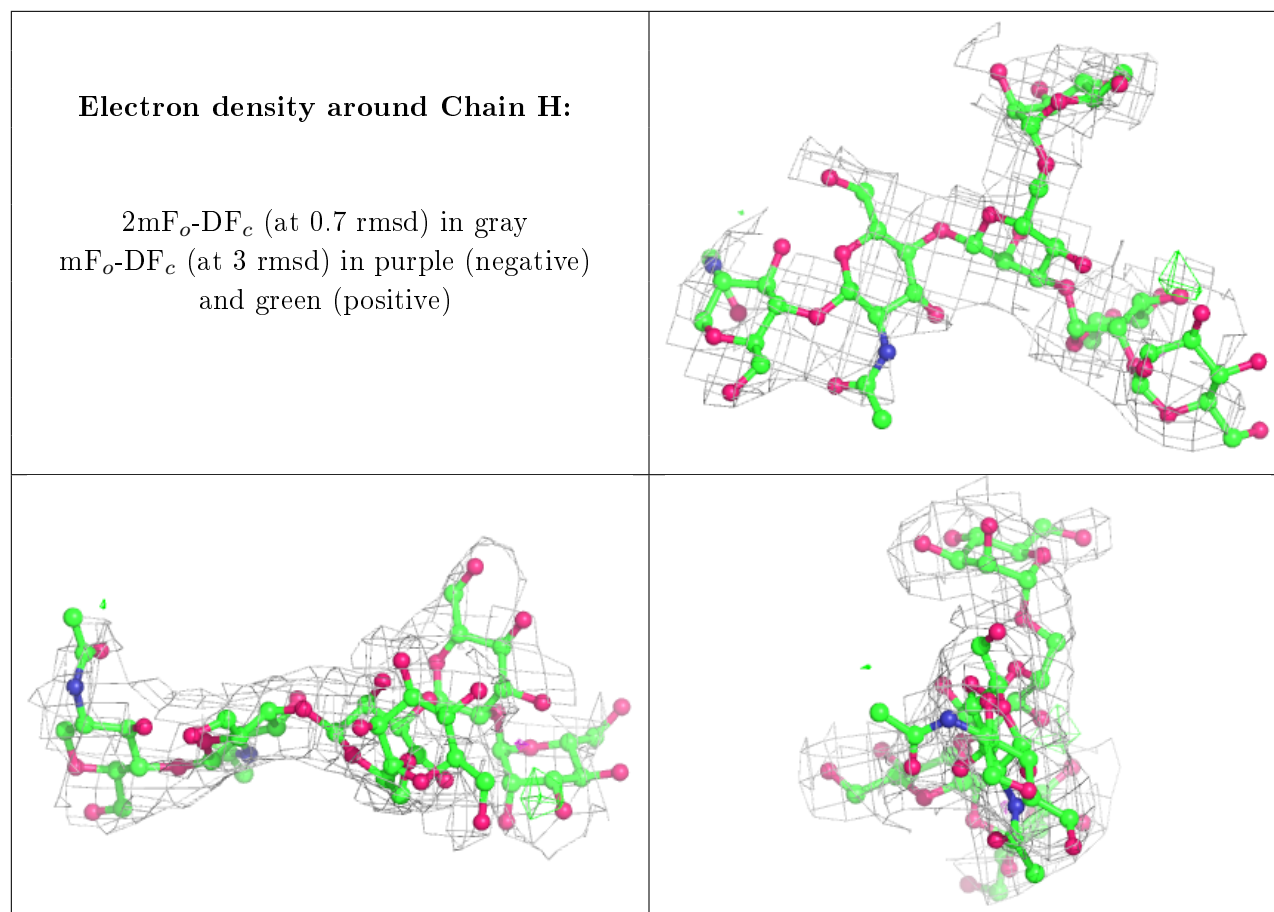
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain G:

$2mF_o-DF_c$ (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
7	ZN	A	2415	1/1	0.97	0.15	46,46,46,46	0
6	CA	B	2419	1/1	0.98	0.20	59,59,59,59	0
8	CU1	B	2421	1/1	0.99	0.22	48,48,48,48	0
8	CU1	A	2416	1/1	0.99	0.20	40,40,40,40	0
6	CA	A	2414	1/1	0.99	0.20	40,40,40,40	0
7	ZN	B	2420	1/1	1.00	0.19	47,47,47,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.