



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:12 AM UTC

PDB ID : 6MF0 / pdb_00006mf0
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 types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

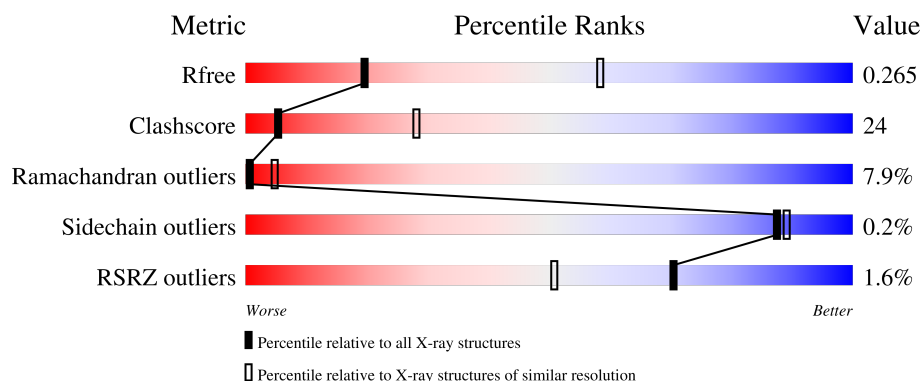
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	% 45% 36% • 14%
1	B	1467	% 42% 39% • 15%
2	C	5	80% 20%
2	E	5	20% 60% 20%
2	F	5	20% 60% 20%

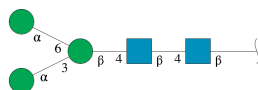
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Mol	Chain	Length	Quality of chain
3	D	3	 100%
4	G	7	 71% 29%
5	H	6	 50% 50%

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.

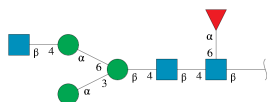


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	5	Total 61	C 34	N 2	O 25	0	0	0
2	E	5	Total 61	C 34	N 2	O 25	0	0	0
2	F	5	Total 61	C 34	N 2	O 25	0	0	0

-
- A diagram of a 1D chain with a green circle and two blue squares. The chain is represented by a horizontal line with a green circle at the left end, followed by a blue square, then another blue square, and finally a curly brace at the right end. The segments are labeled with β and 4 below the line.

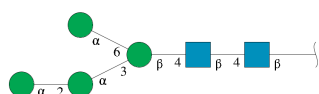
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	3	Total	C	N	O	0	0	0
			39	22	2	15			

- 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 (CCD ID: CA) (formula: Ca).

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

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

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

- Molecule 8 is COPPER (I) ION (CCD ID: CU1) (formula: Cu).

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

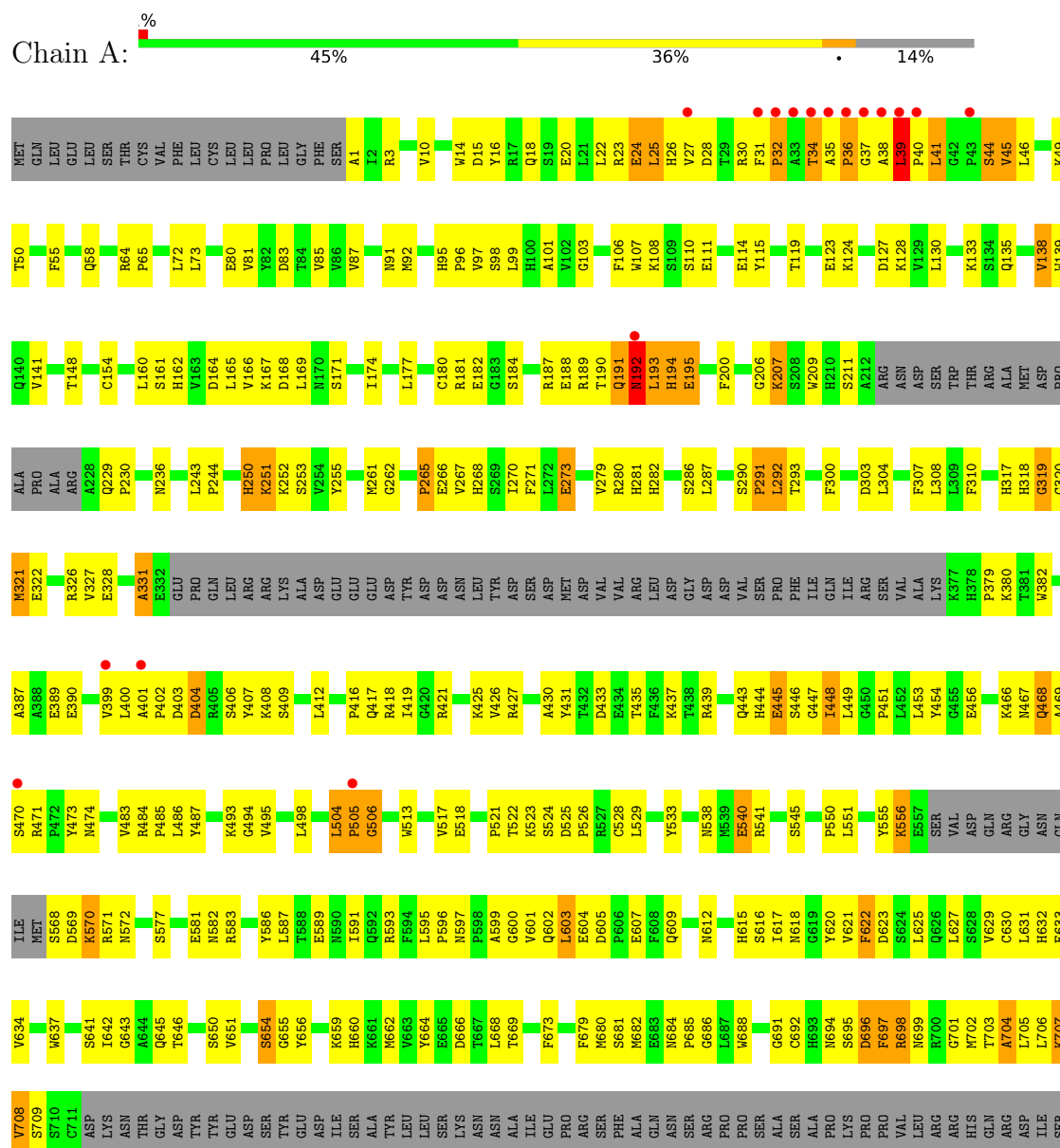
- Molecule 9 is water.

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

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 chimera



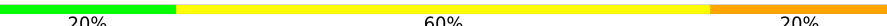
R2320	T2244	S2099	K2020	G1923	C1832	H1755	GLU	GLU	GLU	E589	T514	T435
M2321	T2245	Q2100	K2026	Y1924	K1833	L1756	ASP	ASP	PRO	F671	V515	F436
E2322	Q2246	F2101	G2026	Y1924	A1834	G1757	GLU	GLU	ARG	R593	E518	F437
G2325	G2247	I2102	M2027	M1925	V1835	L1758	ASN	ASN	SER	F594	E519	T438
C2326	V2248	M2103	A2028	D1927	A1836	G1759	GLN	GLN	PHE	M680	G520	R439
E2327	K2249	M2104	A2028	D1927	Y1837	G1760	ASP	ALA	ALA	A599	G520	E440
A2328	S2250	Y2105	S2029	L1928	Y1841	P1761	PRO	PRO	GLN	M682	P521	A441
Q2329	L2251	S2106	P1930	L1929	V1841	Y1762	ARG	ARG	ASN	E683	T522	I442
ASP	L2252	L2107	G1931	L1932	D1846	I1763	SER	SER	ASN	N684	S524	Q443
LEU	M2255	G2108	L1932	L1932	A1765	E1766	PHE	ARG	ARG	E607	P685	S446
TYR	V2257	Q2036	Q2036	Q1936	K1693	R1694	GLN	PRO	PRO	A610	P526	C447
	F2260	T2037	T2038	G1850	T1694	D1769	K1694	SER	SER	S611	R527	T448
	L2261	K2110	A2039	L1851	R1695	M1770	T1695	ALA	ALA	N612	E540	L449
	I2262	W2112		L1852	R1696	M1770	T1695	SER	SER	L613	P526	L449
	S2263	Q2114	Y2043	G1853	F1699	I1771	F1699	ALA	ALA	M614	R524	L452
	E2264	T2115	G2044	L1854	I1771	I1771	G691	PRO	PRO	H615	E540	L453
	S2265	R2116	Q2045	Y1942	L1855	V1773	C692	LYS	LYS	S534	E540	H378
	S2265	G2117	W2046	L1943	L1856	T1774	H693	PRO	PRO	S535	E540	H378
	W2271	N2118	A2047	L1944	L1857	F1775	N694	VAL	VAL	V537	E540	H378
	F2274	S2119	P2048	L1945	C1858	K1776	D1708	LEU	LEU	H618	E540	H378
	N2277	T2120	K2049	S1946	M1777	Q1777	Y1709	ARG	ARG	M539	E540	H378
	V2280	G2121	L2050	M1947	L1863	Q1778	E1713	ARG	ARG	P622	E540	H378
		L2123	A2051	L1953	E1875	R1781	S1714	HIS	HIS	D623	R541	L464
		N2124	L2053	F1876	F1876	P1782	P1715	GLN	GLN	T703	E540	L464
		V2125	H2054	V1965	F1879	Y1783	ARG	ARG	ARG	A704	E540	L466
		F2126	K1967	S1784	F1879	F1785	ALA	ASP	ASP	L705	E540	L466
		F2127	K1968	F1967	F1879	F1785	LEU	ILE	ILE	L706	E540	L466
			I2059	K1968	F1883	L1789	ARG	SER	SER	K707	E540	L466
			N2060	D1884	D1884	I1790	ASN	LEU	LEU	V708	E540	L466
			A2061	E1885	E1885	S1791	ALA	PRO	PRO	L631	E540	L466
			W2062	T1886	K1887	Y1792	ALA	THR	THR	H632	E540	L466
			S2063	K1887	K1887	Y1792	GLN	PHE	PHE	E633	E540	L466
			P2067	Y1890	Y1890	E1801	ASN	GLN	GLN	S710	E540	L466
			I2071	N1977	Y1890	P1802	LYS	PRO	PRO	K556	E540	L466
			K2072	L1978	E1893	R1803	GLY	GLU	GLU	S488	E540	L466
			L2076	Y1979	N1894	H1804	GLY	ASP	ASP	R489	E540	L466
			M2079	F1982	V1895	V1807	LYS	GLY	GLY	R490	E540	L466
			I2080	E1984	V1895	V1807	ASP	GLY	GLY	L491	E540	L466
			I2081	L1989	C1899	T1812	MET	GLY	GLY	P492	E540	L466
			I2084	P1990	GLN	R1812	ASP	GLY	GLY	S641	E540	L466
			K2085	V1993	ARG	T1812	TYR	ASP	ASP	G494	E540	L466
			T2086	G2003	ALA	R1813	GLY	TYR	TYR	V495	E540	L466
			Q2087	L2006	PRO	R1736	ASP	ASP	ASP	K496	E540	L466
			G2088	Q2007	CYS	E1737	ILE	ILE	ILE	H497	E540	L466
			A2089	A2008	HIS	F1738	PHE	PHE	PHE	L498	E540	L466
			K2092	G2009	LEU	G1741	GLY	GLY	GLY	D500	E540	L466
			F2093	A2008	GLN	S1742	THR	THR	THR	R570	E540	L466
			S2094	M2010	GLN	T1743	ILE	ILE	ILE	R571	E540	L466
			S2095	S2011	GLU	Q1820	GLU	GLU	GLU	N572	E540	L466
			L2096	T2012	GLU	H1821	THR	THR	THR	V573	E540	L466
			Y2097	Y1915	ASP	R1822	LYS	LYS	LYS	T574	E540	L466
			I2098	L2015	PRO	M1823	GLY	GLY	GLY	F668	E540	L466
					T1911	T1746	LEU	LEU	GLU	V659	E540	L466
					L1912	S1747	GLU	GLU	GLU	L575	E540	L466
					K1913	Y1748	ASP	ASP	ASP	H660	E540	L466
					E1827	L1748	PHE	PHE	PHE	F501	E540	L466
					N1915	R1749	LYS	LYS	LYS	N582	E540	L466
					N1915	L1752	ASN	ASN	ASN	V663	E540	L466
					N1915	D1828	ILE	ILE	ILE	Y511	E540	L466
					Y1916	F1830	TYR	TYR	TYR	L587	E540	L466
					F1917	K1754	ALA	ALA	ALA	K512	E540	L466
					L2015	T1821	TYR	TYR	TYR	T588	E540	L466

- 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%

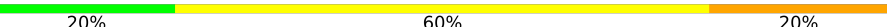


- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  20% 60% 20%

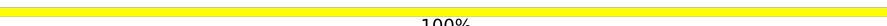


- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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

Chain H:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.00Å 135.86Å 196.11Å 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) 99.8 (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 3.19Å)	Xtriage
Refinement program	PHENIX 1.12_2829, PHENIX 1.12_2829	Depositor
R, R_{free}	0.206 , 0.287 (Not available) , 0.265	Depositor DCC
R_{free} test set	3077 reflections (4.93%)	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)	0.30 , 43.4	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	0.92	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: CA, FUC, MAN, ZN, BMA, CU1, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.48	4/10434 (0.0%)	0.85	8/14149 (0.1%)
1	B	0.44	2/10367 (0.0%)	0.74	8/14053 (0.1%)
All	All	0.46	6/20801 (0.0%)	0.80	16/28202 (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	A	191	GLN	CD-NE2	8.04	1.50	1.33
1	B	2104	MET	SD-CE	-7.84	1.59	1.79
1	B	2150	ARG	CZ-NH2	-7.36	1.23	1.33
1	A	191	GLN	CD-OE1	-7.34	1.09	1.23
1	A	192	ASN	N-CA	-5.68	1.38	1.46
1	A	191	GLN	CG-CD	-5.13	1.39	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	191	GLN	CG-CD-OE1	29.55	179.90	120.80
1	A	191	GLN	OE1-CD-NE2	-23.94	98.66	122.60
1	A	191	GLN	CG-CD-NE2	-23.31	81.43	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	191	GLN	CA-CB-CG	20.70	155.50	114.10
1	A	191	GLN	CB-CG-CD	-13.94	88.89	112.60
1	B	44	SER	N-CA-C	6.63	124.92	110.80
1	B	42	GLY	C-N-CD	-6.26	106.84	120.60
1	B	2150	ARG	NE-CZ-NH2	5.99	124.59	119.20
1	B	2150	ARG	NH1-CZ-NH2	-5.66	111.95	119.30
1	B	147	PRO	N-CA-C	5.65	124.11	112.47
1	B	2169	CYS	N-CA-C	5.62	122.78	110.80
1	B	631	LEU	CD1-CG-CD2	-5.38	98.97	110.80
1	A	191	GLN	N-CA-C	5.31	119.76	113.12
1	A	506	GLY	N-CA-C	-5.30	100.61	113.18
1	B	12	LEU	CD1-CG-CD2	-5.03	99.73	110.80
1	A	292	LEU	CA-CB-CG	-5.00	98.79	116.30

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	454	2
1	B	10084	0	9837	530	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	981	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 24.

All (981) 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:HE2	1:B:2150:ARG:HH21	1.08	1.17
1:B:2104:MET:CE	1:B:2150:ARG:HH21	1.60	1.12
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:2104:MET:HE2	1:B:2150:ARG:NH2	1.85	0.91
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:697:PHE:O	1:A:699:ASN:N	2.11	0.83
1:A:1993:VAL:HA	1:A:2016:VAL:HG23	1.59	0.83
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:A:2176:MET:HE3	1:A:2177:PRO:HD2	1.60	0.81
1:B:617:ILE:HG23	1:B:625:LEU:HD23	1.63	0.81
1:A:522:THR:O	1:A:524:SER:N	2.13	0.81
1:A:2100:GLN:HB3	1:A:2155:HIS:HB2	1.63	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:2180:MET:HE1	1:A:2232:VAL:HG21	1.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:1869:ARG:NH2	2:E:1:NAG:O7	2.25	0.70
1:B:1945:LEU:HG	1:B:1983:PHE:HD1	1.56	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:467:ASN:OD1	1:A:468:GLN:N	2.26	0.69
1:A:2162:LEU:HD11	1:A:2164:MET:HB3	1.75	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:80:GLU:HB2	1:B:181:ARG:O	1.93	0.69
1:B:625:LEU:HD12	1:B:626:GLN:H	1.58	0.69
1:B:1807:VAL:HG22	1:B:1813:ARG:NH1	2.07	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:317:HIS:CD2	2:C:2:NAG:H81	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:2250:SER:HB3	1:A:2255:MET:HE2	1.77	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:445:GLU:O	1:A:618:ASN:ND2	2.28	0.67
1:A:1742:SER:O	1:A:1744:THR:N	2.27	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:581:GLU:HB2	1:B:612:ASN:HB3	1.77	0.66
1:B:2087:GLN:HB3	1:B:2163:ARG:HB2	1.76	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:230:PRO:HB2	1:B:232:MET:HE3	1.76	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: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:66:ARG:NH1	1:B:73:LEU:O	2.29	0.65
1:B:2170:ASP:OD1	1:B:2175:SER:HB2	1.96	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:443:GLN:NE2	1:A:443:GLN:O	2.29	0.65
1:A:2261:LEU:HD12	1:A:2309:HIS:HB2	1.79	0.65
1:B:397:PRO:HD2	1:B:624:SER:HB3	1.77	0.65
1:B:2061:ALA:HB2	1:B:2163:ARG:HG3	1.79	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:208:SER:C	1:B:210:HIS:H	2.04	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
1:B:114:GLU:HB2	1:B:127:ASP:HB3	1.79	0.63
1:A:591:ILE:HG23	1:A:595:LEU:HD22	1.81	0.62
1:A:2246:GLN:HE21	1:A:2292:PRO:HD3	1.64	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:B:2183:LYS:HZ1	1:B:2212:LEU:HD11	1.64	0.62
1:A:453:LEU:HD22	1:A:533:TYR:CE2	2.34	0.62
1:A:2182:SER:C	1:A:2184:ALA:H	2.07	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:1934:MET:HE2	1:A:2016:VAL:HG12	1.80	0.62
1:A:2072:LYS:HB2	1:A:2150:ARG:HG3	1.80	0.62
1:B:68:PRO:HB2	1:B:244:PRO:HG2	1.82	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: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:A:182:GLU:H	1:A:182:GLU:CD	2.05	0.62
1:A:615:HIS:HB3	1:A:702:MET:HE3	1.81	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:315:SER:C	1:B:317:HIS:H	2.07	0.62
1:B:1927:ASP:HA	1:B:2012:THR:HA	1.79	0.61
1:B:27:VAL:HG11	1:B:62:VAL:CA	2.30	0.61
1:B:2147:ARG:HD3	1:B:2148:TYR:CE1	2.36	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:400:LEU:HD11	1:B:622:PHE:HB2	1.81	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:2162:LEU:HD21	1:B:2164:MET:HE2	1.83	0.61
1:B:261:MET:HE3	1:B:262:GLY:HA2	1.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:2026:GLY:HA3	1:A:2031:HIS:HB3	1.84	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:241:ARG:NH2	1:B:322:GLU:OE1	2.35	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:A:310:PHE:HB2	1:A:322:GLU:HG2	1.84	0.60
1:A:2174:CYS:O	1:A:2241:THR:HG21	2.02	0.60
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: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:A:1826:THR:HB	1:A:1829:GLU:HG3	1.84	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: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:2027:MET:HE1	1:A:2073:VAL:HG21	1.85	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1820:GLN:HG2	1:A:1823:MET:HE3	1.87	0.57
1:B:91:ASN:ND2	1:B:96:PRO:HA	2.20	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:A:1870:GLN:O	1:A:1871:VAL:HG22	2.04	0.57
1:A:268:HIS:CG	1:A:321:MET:HE2	2.38	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: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
4:G:2:NAG:H83	4:G:2:NAG:H3	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:617:ILE:HD12	1:A:703:THR:O	2.05	0.56
1:A:2196:PHE:HB2	1:A:2222:GLN:HA	1.87	0.56
1:B:2187:ASP:HB3	1:B:2206:SER:HB2	1.86	0.56
1:A:485:PRO:HD3	1:A:498:LEU:HD22	1.88	0.56
1:B:47:TYR:OH	1:B:230:PRO:HG3	2.05	0.56
1:B:238:TYR:HB3	1:B:242:SER:HB2	1.86	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:B:1883:PHE:O	1:B:1917:ARG:HA	2.04	0.56
1:B:2100:GLN:HB2	1:B:2154:THR:OG1	2.05	0.56
1:B:2223:VAL:HG12	1:B:2225:ASN:HD22	1.69	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:37:GLY:O	1:A:39:LEU:N	2.33	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: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:A:2074:ASP:CG	1:A:2147:ARG:HH21	2.14	0.56
1:B:2154:THR:O	1:B:2155:HIS:ND1	2.39	0.56
1:A:577:SER:HA	1:A:645:GLN:NE2	2.21	0.56
1:A:2096:LEU:HD23	1:A:2159:ARG:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:LEU:HD12	1:A:244:PRO:HD2	1.87	0.55
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: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:250:HIS:C	1:A:252:LYS:H	2.14	0.55
1:A:680:MET:SD	1:A:682:MET:HE1	2.47	0.55
1:A:1768:GLU:H	1:A:1819:VAL:HG13	1.72	0.55
1:B:589:GLU:OE1	1:B:593:ARG:NH1	2.40	0.55
1:B:1912:LEU:HD23	1:B:1912:LEU:H	1.70	0.55
1:A:380:LYS:HD3	1:A:382:TRP:CZ2	2.41	0.55
1:A:433:ASP:OD1	1:A:435:THR:HG22	2.06	0.55
1:B:60:PHE:CE2	1:B:90:LYS:HB2	2.42	0.55
1:B:267:VAL:HB	1:B:671:PHE:HE2	1.71	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:A:599:ALA:O	1:A:601:VAL:HG13	2.07	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: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:167:LYS:HD3	1:A:209:TRP:HA	1.87	0.55
1:A:1700:ILE:O	1:A:1775:PHE:HA	2.07	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:444:HIS:O	1:A:445:GLU:HB2	2.07	0.54
1:A:1934:MET:CE	1:A:2016:VAL:HG12	2.37	0.54
1:A:108:LYS:HG2	1:A:1996:TRP:CH2	2.42	0.54
1:A:193:LEU:HG	1:A:195:GLU:HG3	1.87	0.54
1:A:2042:GLN:HG3	1:A:2048:PRO:HD3	1.87	0.54
1:B:570:LYS:O	1:B:571:ARG:HB2	2.07	0.54
1:B:1743:PHE:CD2	1:B:1776:LYS:HD2	2.42	0.54
1:A:582:ASN:ND2	1:A:609:GLN:O	2.40	0.54
1:A:1993:VAL:HG11	1:A:2173:SER:HB2	1.89	0.54
1:B:1695:THR:HG23	1:B:1770:ASN:HB2	1.88	0.54
1:A:504:LEU:HB3	1:A:505:PRO:CD	2.37	0.54
1:A:1751:GLU:HG3	1:A:2117:GLY:HA2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:622:PHE:C	1:B:624:SER:H	2.13	0.54
1:B:1736:ARG:HE	1:B:1749:ARG:NH1	2.06	0.54
1:B:411:TYR:CE2	1:B:700:ARG:HB3	2.43	0.54
1:B:1707:TRP:CE2	1:B:1758:LEU:HD13	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:518:GLU:CD	1:B:518:GLU:H	2.15	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
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:B:615:HIS:HB3	1:B:702:MET:HE3	1.89	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:34:THR:C	1:A:36:PRO:HD3	2.33	0.53
1:A:654:SER:HB3	1:A:688:TRP:CE3	2.44	0.53
1:A:1834:ALA:HB2	1:A:1943:TYR:CD1	2.43	0.53
1:B:91:ASN:HD21	1:B:96:PRO:HA	1.72	0.53
1:A:44:SER:O	1:A:45:VAL:HG12	2.07	0.53
1:A:2116:ARG:HG3	1:A:2123:LEU:HA	1.89	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: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:A:2265:SER:O	1:A:2303:THR:HB	2.09	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:2180:MET:CE	1:A:2232:VAL:HG21	2.36	0.53
1:A:380:LYS:HD3	1:A:382:TRP:CH2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:ILE:HD12	1:A:419:ILE:H	1.74	0.53
1:A:2009:GLY:O	1:A:2011:SER:N	2.42	0.53
1:B:2261:LEU:HD12	1:B:2309:HIS:HB2	1.88	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:A:1846:ASP:HB3	1:A:1889:TRP:NE1	2.21	0.53
1:B:471:ARG:HH12	1:B:537:VAL:HG23	1.74	0.53
1:B:1749:ARG:HD2	1:B:1753:ASN:HB3	1.90	0.53
1:A:525:ASP:HB2	1:A:526:PRO:CD	2.38	0.52
1:A:2198:ASN:OD1	1:A:2199:MET:N	2.43	0.52
1:B:641:SER:C	1:B:642:ILE:HG13	2.34	0.52
1:A:692:CYS:C	1:A:694:ASN:H	2.16	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:654:SER:HB3	1:A:688:TRP:HE3	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
1:B:2085:LYS:HB2	1:B:2165:GLU:HB3	1.91	0.52
1:B:2115:TYR:C	1:B:2117:GLY:H	2.17	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:A:10:VAL:HG23	1:A:92:MET:HE3	1.92	0.52
1:B:394:ASP:HB3	1:B:422:LYS:HG3	1.92	0.52
1:B:2180:MET:HE2	1:B:2321:MET:HG2	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:A:680:MET:HG3	1:A:682:MET:HE1	1.91	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:518:GLU:H	1:A:518:GLU:CD	2.18	0.52
1:A:568:SER:HA	1:A:571:ARG:NH2	2.25	0.52
1:B:20:GLU:O	1:B:23:ARG:HG3	2.10	0.52
1:B:1945:LEU:HB2	1:B:1983:PHE:CE1	2.43	0.52
1:A:1:ALA:HB1	1:A:83:ASP:HA	1.91	0.52
1:A:1992:LYS:O	1:A:2016:VAL:HG21	2.10	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:497:HIS:HD2	1:B:498:LEU:N	2.08	0.51
1:B:2115:TYR:CE2	1:B:2117:GLY:HA2	2.45	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:315:SER:C	1:B:317:HIS:N	2.67	0.51
1:B:449:LEU:HD21	1:B:575:LEU:HD22	1.92	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:268:HIS:ND1	1:A:321:MET:HE2	2.26	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:A:2026:GLY:C	1:A:2032:ILE:HG13	2.35	0.51
1:B:497:HIS:CD2	1:B:498:LEU:N	2.78	0.51
1:B:2104:MET:HG3	1:B:2152:HIS:CD2	2.46	0.51
1:A:98:SER:O	1:A:161:SER:HA	2.10	0.51
1:A:589:GLU:O	1:A:593:ARG:HG3	2.11	0.51
1:B:29:THR:HG23	1:B:30:ARG:N	2.26	0.51
1:B:428:PHE:CZ	1:B:547:LEU:HD22	2.46	0.51
1:B:472:PRO:HG3	1:B:504:LEU:HD23	1.92	0.51
5:H:1:NAG:O3	5:H:2:NAG:O5	2.17	0.51
1:B:258:VAL:HB	1:B:295:LEU:HB2	1.93	0.51
1:B:2061:ALA:HB3	1:B:2089:ALA: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:B:522:THR:C	1:B:524:SER:H	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:684:ASN:O	1:A:708:VAL:HG21	2.11	0.50
1:A:1993:VAL:HA	1:A:2016:VAL:CG2	2.36	0.50
1:B:56:THR:OG1	1:B:62:VAL:HG21	2.12	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: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: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:B:2081:ILE:HG12	1:B:2149:ILE:HD11	1.93	0.50
1:A:14:TRP:NE1	1:A:16:TYR:HA	2.26	0.50
1:A:55:PHE:CZ	1:A:92:MET:HE1	2.47	0.50
1:A:2044:GLY:C	1:A:2046:TRP:H	2.19	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: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:A:2201:ALA:O	1:A:2202:THR:HG23	2.11	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:270:ILE:HD11	1:A:321:MET:HE3	1.93	0.49
1:A:1837:TYR:CZ	1:A:1853:GLY:HA3	2.47	0.49
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:OD1	1:B:126:ASP:N	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:290:SER:O	1:A:291:PRO:C	2.55	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:A:1757:GLY:C	1:A:1759:LEU:H	2.21	0.49
1:B:1924:TYR:HB2	1:B:1929:LEU:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:680:MET:CG	1:A:682:MET:HE1	2.42	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: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:A:1880:PHE:CE2	1:A:1921:ILE:HG12	2.47	0.49
1:A:2229:TRP:HB3	1:A:2309:HIS:ND1	2.28	0.49
1:B:603:LEU:HD23	1:B:603:LEU:O	2.13	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: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:540:GLU:HG2	1:B:541:ARG:HG3	1.93	0.48
1:B:2106:SER:O	1:B:2146:ALA:HB1	2.13	0.48
1:B:2180:MET:HB2	1:B:2322:GLU:CD	2.38	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:56:THR:H	1:B:62:VAL:HG23	1.77	0.48
1:B:453:LEU:HD13	1:B:533:TYR:HE2	1.78	0.48
1:B:27:VAL:HG22	1:B:28:ASP:H	1.78	0.48
1:B:1732:LYS:NZ	1:B:1885:GLU:OE2	2.38	0.48
1:B:2006:LEU:C	1:B:2008:ALA:H	2.21	0.48
1:B:2076:LEU:C	1:B:2147:ARG:HE	2.20	0.48
1:A:454:TYR:HE2	1:A:570:LYS:HE3	1.78	0.48
1:A:1963:PHE:CD2	1:A:1986:VAL:HB	2.49	0.48
1:B:2110:LYS:HD3	1:B:2112:TRP:NE1	2.23	0.48
1:A:192:ASN:O	1:A:194:HIS:N	2.45	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: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:2180:MET:HE1	1:A:2232:VAL:CG2	2.39	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:45:VAL:HG22	1:A:46:LEU:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:LYS:HB3	1:A:545:SER:O	2.13	0.48
1:A:685:PRO:HA	1:A:708:VAL:CG2	2.44	0.48
1:A:1694:ARG:O	1:A:1769:ASP:HB2	2.14	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:686:GLY:O	1:A:708:VAL:HG22	2.14	0.48
1:A:2044:GLY:O	1:A:2046:TRP:N	2.46	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:486:LEU:HD12	1:A:487:TYR:H	1.79	0.48
1:A:2053:LEU:HD13	1:A:2165:GLU:HB3	1.95	0.48
1:B:2179:GLY:HA3	1:B:2185:ILE:H	1.79	0.48
1:A:427:ARG:NE	1:A:448:ILE:HA	2.28	0.48
1:A:1936:GLN:O	1:A:1990:PRO:HG2	2.14	0.48
1:A:2048:PRO:C	1:A:2050:LEU:H	2.22	0.48
1:B:701:GLY:O	1:B:703:THR:N	2.47	0.48
1:B:2063:SER:HA	1:B:2160:SER:O	2.14	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:474:ASN:HB2	1:B:537:VAL:HG13	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:A:261:MET:HG2	1:A:262:GLY:H	1.79	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:B:1790:ILE:HD12	1:B:1790:ILE:O	2.13	0.47
1:B:2178:LEU:HD11	1:B:2325:GLY:HA3	1.96	0.47
1:B:60:PHE:HD2	1:B:90:LYS:HD3	1.80	0.47
1:B:1833:LYS:HG2	1:B:1834:ALA:H	1.80	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:1889:TRP:C	1:A:1891:PHE:H	2.22	0.47
1:A:58:GLN:OE1	1:A:58:GLN:N	2.42	0.47
1:A:602:GLN:HB3	1:A:605:ASP:CB	2.44	0.47
1:B:42:GLY:HA2	1:B:44:SER:H	1.79	0.47
1:B:174:ILE:HD13	1:B:199:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:2211:HIS:CE1	1:B:2292:PRO:HG3	2.49	0.47
1:A:292:LEU:HD13	1:A:2001:LEU:HB3	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:A:2196:PHE:HZ	1:A:2198:ASN:HD22	1.63	0.47
1:B:69:TRP:CH2	1:B:70:MET:HE2	2.50	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: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:251:LYS:HE3	1:B:496:LYS:O	2.13	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: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:26:HIS:CD2	1:B:65:PRO:HA	2.48	0.47
1:B:155:LEU:O	1:B:178:LEU:HA	2.15	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
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:A:20:GLU:HG3	1:A:23:ARG:NE	2.30	0.47
1:A:103:GLY:HA2	1:A:1962:VAL:HG12	1.97	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: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:387:ALA:HA	1:B:466:LYS:O	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:682:MET:N	1:B:682:MET:HE2	2.30	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:B:1707:TRP:CZ2	1:B:1758:LEU:HD13	2.50	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: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:2110:LYS:HA	1:B:2112:TRP:NE1	2.31	0.46
1:A:706:LEU:O	1:A:707:LYS:C	2.59	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
5:H:4:MAN:O3	5:H:5:MAN:H3	2.15	0.46
1:A:80:GLU:HA	1:A:180:CYS:O	2.16	0.46
1:A:2038:THR:O	1:A:2072:LYS:N	2.49	0.46
1:A:2182:SER:O	1:A:2182:SER:OG	2.28	0.46
1:B:12:LEU:C	1:B:12:LEU:HD12	2.40	0.46
1:B:574:ILE:O	1:B:639:ILE:HA	2.16	0.46
1:B:2107:LEU:CD2	1:B:2146:ALA:HA	2.44	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:128:LYS:HE3	1:A:128:LYS:HB3	1.70	0.45
1:A:200:PHE:HB3	1:A:321:MET:HE1	1.98	0.45
1:A:597:ASN:C	1:A:599:ALA:N	2.73	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:90:LYS:HG3	1:B:133:LYS:O	2.16	0.45
1:B:1831:ASP:HB2	1:B:1941:ARG:NH1	2.32	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:B:648:PHE:CE1	1:B:1953:ILE:HD11	2.51	0.45
1:B:1833:LYS:O	1:B:1834:ALA:HB2	2.16	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:70:MET:O	1:B:73:LEU:HB2	2.15	0.45
1:B:680:MET:SD	1:B:682:MET:HE1	2.57	0.45
1:B:1700:ILE:O	1:B:1775:PHE:HA	2.17	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:A:1708:ASP:C	1:A:1710:GLY:H	2.25	0.45
1:B:78:GLN:HG2	1:B:178:LEU:HD12	1.98	0.45
1:B:453:LEU:HD13	1:B:533:TYR:CE2	2.52	0.45
1:A:300:PHE:CE2	1:B:490:ARG:HG3	2.52	0.45
1:A:486:LEU:HG	1:A:487:TYR:CD2	2.51	0.45
1:A:629:VAL:HG23	1:A:708:VAL:HG12	1.99	0.45
1:A:642:ILE:HD13	1:A:673:PHE:HA	1.98	0.45
1:A:1888:SER:O	1:A:1889:TRP:C	2.60	0.45
1:B:69:TRP:CZ3	1:B:70:MET:HG2	2.50	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: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:A:49:LYS:HZ2	1:A:171:SER:HA	1.82	0.45
1:A:596:PRO:HG2	1:A:597:ASN:ND2	2.31	0.45
1:B:287:LEU:HD12	1:B:287:LEU:HA	1.67	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:HD23	1:A:1863:LEU:O	2.17	0.45
1:A:2250:SER:O	1:A:2251:LEU:C	2.59	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: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:16:TYR:CZ	1:B:232:MET:HG3	2.52	0.44
1:B:89:LEU:HD21	1:B:97:VAL:HG23	1.99	0.44
1:B:103:GLY:HA3	1:B:157:TYR:CD2	2.51	0.44
1:B:200:PHE:HE2	1:B:258:VAL:HG13	1.83	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:2203:TRP:CE3	1:B:2220:ARG:HG3	2.52	0.44
1:A:1764:ARG:HB3	1:A:1863:LEU:CD1	2.44	0.44
1:B:396:ALA:HB1	1:B:400:LEU:HD12	2.00	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: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:B:185:LEU:H	1:B:185:LEU:HG	1.59	0.44
1:B:2114:THR:HG21	1:B:2123:LEU:CD2	2.47	0.44
1:B:2170:ASP:OD1	1:B:2174:CYS:C	2.61	0.44
1:A:454:TYR:CE2	1:A:570:LYS:HE3	2.52	0.44
1:B:2186:SER:H	1:B:2189:GLN:CD	2.24	0.44
1:B:2217:ASN:OD1	1:B:2217:ASN:N	2.50	0.44
1:A:2248:VAL:C	1:A:2289:SER:HB2	2.43	0.44
1:B:69:TRP:CE3	1:B:70:MET:HG2	2.53	0.44
1:B:497:HIS:CE1	1:B:499:LYS:HG2	2.53	0.44
1:B:2262:ILE:HA	1:B:2307:ARG:O	2.16	0.44
1:A:191:GLN:HE22	1:A:331:ALA:H	1.65	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:230:PRO:HB2	1:B:232:MET:CE	2.44	0.44
1:B:485:PRO:HB3	1:B:509:PHE:CZ	2.53	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: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:1733:VAL:HB	1:B:1890:TYR:OH	2.17	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:1834:ALA:C	1:B:1983:PHE:HD2	2.26	0.44
1:B:2260:PHE:CE1	1:B:2308:ILE:HD12	2.53	0.44
1:A:24:GLU:O	1:A:25:LEU:HB2	2.18	0.43
1:A:165:LEU:HD12	1:A:165:LEU:HA	1.85	0.43
1:A:641:SER:O	1:A:642:ILE:HD13	2.17	0.43
1:A:669:THR:HG21	1:A:1979:TYR:HB3	2.00	0.43
1:A:697:PHE:C	1:A:699:ASN:N	2.76	0.43
1:B:12:LEU:HD12	1:B:13:SER:C	2.43	0.43
1:B:69:TRP:CZ2	1:B:70:MET:HE2	2.53	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:3:ARG:HB3	1:B:5:TYR:HE1	1.83	0.43
1:B:81:VAL:HA	1:B:141:VAL:CG1	2.47	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:A:15:ASP:O	1:A:16:TYR:HB2	2.18	0.43
1:A:433:ASP:OD1	1:A:433:ASP:N	2.52	0.43
1:A:87:VAL:HG11	1:A:99:LEU:HD21	2.01	0.43
1:A:1763:ILE:HG23	1:A:1855:LEU:HG	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1764:ARG:CZ	1:A:1869:ARG:HG3	2.48	0.43
1:B:81:VAL:HG12	1:B:82:TYR:CD2	2.53	0.43
1:B:2193:SER:HB3	1:B:2229:TRP:NE1	2.33	0.43
1:B:2225:ASN:HA	1:B:2313:TRP:HH2	1.84	0.43
1:A:1771:ILE:HD12	1:A:1817:TRP:NE1	2.33	0.43
1:A:1792:TYR:CD1	1:A:1792:TYR:N	2.86	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: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:A:50:THR:HG22	1:A:171:SER:HB2	2.00	0.43
1:A:484:ARG:HH21	1:B:514:THR:CG2	2.31	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: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:A:2074:ASP:OD1	1:A:2147:ARG:NH2	2.44	0.43
1:A:293:THR:HA	1:A:1977:ASN:HD21	1.82	0.43
1:A:627:LEU:HD11	1:A:637:TRP:HZ3	1.84	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: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:B:239:VAL:O	1:B:240:ASN:C	2.62	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:251:LYS:HD2	1:B:491:LEU:HD12	2.01	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:154:CYS:HA	1:A:180:CYS:HA	2.01	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:1709:TYR:CD2	1:B:1923:GLY:O	2.72	0.43
1:A:654:SER:C	1:A:656:TYR:N	2.77	0.42
1:B:114:GLU:HG3	1:B:124:LYS:HD3	2.00	0.42
1:B:452:LEU:HD23	1:B:550:PRO:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:493:LYS:O	1:A:495:VAL:N	2.48	0.42
1:A:1732:LYS:HB3	1:A:1849:SER:O	2.18	0.42
1:B:47:TYR:CG	1:B:205:GLU:HG3	2.54	0.42
1:B:89:LEU:HA	1:B:89:LEU:HD12	1.81	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:495:VAL:HG21	1:B:501:PHE:CD1	2.53	0.42
1:B:2255:MET:HE3	1:B:2255:MET:HB2	1.88	0.42
1:A:483:VAL:HG13	1:A:483:VAL:O	2.19	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:2251:LEU:C	1:A:2252:LEU:HG	2.44	0.42
1:B:169:LEU:HA	1:B:169:LEU:HD23	1.65	0.42
1:B:504:LEU:CD2	1:B:505:PRO:HD2	2.50	0.42
1:B:680:MET:HB3	1:B:682:MET:HE1	2.02	0.42
1:B:1876:PHE:CD2	1:B:1932:LEU:HD23	2.54	0.42
1:A:493:LYS:H	1:A:495:VAL:HG23	1.85	0.42
1:B:68:PRO:HB2	1:B:244:PRO:CG	2.47	0.42
1:B:685:PRO:HA	1:B:708:VAL:HG23	2.01	0.42
1:A:23:ARG:O	1:A:26:HIS:N	2.53	0.42
1:A:293:THR:HA	1:A:1977:ASN:ND2	2.34	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: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:1999:GLU:HB3	1:A:2006:LEU:HD13	2.01	0.42
1:B:193:LEU:CD1	1:B:252:LYS:HD3	2.49	0.42
1:B:395:TYR:CD2	1:B:614:MET:HE2	2.54	0.42
1:B:397:PRO:O	1:B:398:LEU:C	2.62	0.42
1:B:2171:LEU:HD23	1:B:2171:LEU:HA	1.78	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:A:1731:LYS:HB3	1:A:1890:TYR:HB3	2.02	0.42
1:A:1797:GLU:C	1:A:1799:GLY:H	2.27	0.42
1:A:1842:ASP:O	1:A:1843:LEU:C	2.62	0.42
1:A:1933:VAL:C	1:A:1934:MET:HG3	2.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:397:PRO:O	1:B:399:VAL:HG22	2.19	0.42
1:B:573:VAL:HG22	1:B:638:TYR:HB2	2.02	0.42
1:B:631:LEU:HB2	1:B:709:SER:C	2.45	0.42
1:B:654:SER:OG	1:B:689:ILE:HB	2.19	0.42
1:B:660:HIS:N	1:B:663:VAL:O	2.49	0.42
1:B:2127:PHE:O	1:B:2136:LYS:NZ	2.52	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:321:MET:HE2	1:B:321:MET:HB3	1.65	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:622:PHE:CD1	1:B:701:GLY:HA2	2.54	0.42
1:B:623:ASP:N	1:B:623:ASP:OD1	2.52	0.42
1:B:2117:GLY:CA	1:B:2124:MET:HB2	2.49	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:241:ARG:HD2	1:B:322:GLU:HB2	2.02	0.42
1:B:1745:GLN:HA	1:B:1746:PRO:HD3	1.82	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: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:HA	1:A:2020:LYS:HD3	1.84	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:OD1	1:A:127:ASP:N	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:58:GLN:CD	1:B:58:GLN:H	2.26	0.42
1:B:315:SER:HB2	1:B:318:HIS:H	1.85	0.42
1:B:1784:SER:HB3	1:B:1841:VAL:HG13	2.01	0.42
1:A:390:GLU:OE2	1:A:470:SER:N	2.53	0.41
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:B:621:VAL:C	1:B:622:PHE:O	2.63	0.41
1:B:1736:ARG:HE	1:B:1749:ARG:HH12	1.68	0.41
1:B:1978:LEU:HA	1:B:1978:LEU:HD23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:634:VAL:HG22	1:A:681:SER:HB2	2.03	0.41
1:B:527:ARG:HD3	1:B:527:ARG:HA	1.63	0.41
1:B:538:ASN:O	1:B:539:MET:C	2.62	0.41
1:B:2020:LYS:NZ	1:B:2327:GLU:OE1	2.47	0.41
1:B:2045:GLN:O	1:B:2059:ILE:HG21	2.20	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
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:B:2147:ARG:O	1:B:2147:ARG:HG2	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:A:540:GLU:HB3	1:A:583:ARG:HH21	1.85	0.41
1:A:1895:VAL:C	1:A:1897:ARG:N	2.78	0.41
1:B:2098:ILE:HD11	1:B:2153:PRO:HB3	2.02	0.41
1:A:55:PHE:HZ	1:A:92:MET:HE1	1.84	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:1953:ILE:HG22	1:A:1979:TYR:CD1	2.56	0.41
1:B:2189:GLN:HG2	1:B:2235:GLN:OE1	2.20	0.41
1:A:662:MET:HE2	1:A:662:MET:HB3	1.90	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:A:1895:VAL:C	1:A:1897:ARG:H	2.27	0.41
1:B:44:SER:O	1:B:46:LEU:N	2.52	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:2050:LEU:C	1:B:2052:ARG:H	2.28	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:7:LEU:HD23	1:B:52:PHE:CD1	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:A:95:HIS:HB2	1:A:96:PRO:HD2	2.02	0.41
1:A:418:ARG:NH2	1:A:607:GLU:HG2	2.35	0.41
1:A:696:ASP:C	1:A:697:PHE:O	2.63	0.41
1:A:2217:ASN:O	1:A:2218:ALA:HB2	2.20	0.41
1:B:1693:LYS:O	1:B:1769:ASP:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2043:TYR:HD1	1:B:2043:TYR:O	2.04	0.41
1:B:2247:GLY:N	1:B:2286:ASN:HD21	2.17	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
1:A:2115:TYR:CZ	1:A:2117:GLY:HA3	2.55	0.41
1:B:108:LYS:HE3	1:B:108:LYS:HB3	1.71	0.41
1:B:148:THR:CG2	1:B:1972:LYS: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:B:1766:GLU:HG2	1:B:1863:LEU:HD13	2.03	0.41
1:B:1789:LEU:HD12	1:B:1855:LEU:HD22	2.03	0.41
1:B:2084:ILE:CG2	1:B:2138:ASN: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:A:1870:GLN:CD	1:A:1941:ARG:HH12	2.29	0.41
1:B:15:ASP:HB2	1:B:45:VAL:CG2	2.51	0.41
1:B:130:LEU:HB2	1:B:133:LYS:CD	2.51	0.41
1:B:1879:PHE:HD1	1:B:1945:LEU:HB3	1.86	0.41
1:A:35:ALA:HB1	1:A:41:LEU:HD21	2.03	0.40
1:A:206:GLY:O	1:A:207:LYS:HB3	2.21	0.40
1:A:1870:GLN:C	1:A:1872:THR:H	2.29	0.40
1:A:2050:LEU:C	1:A:2052:ARG:H	2.30	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:B:2192:ALA:HB3	1:B:2205:PRO:HG3	2.03	0.40
1:A:685:PRO:HA	1:A:708:VAL:HG21	2.02	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:B:28:ASP:HB2	1:B:30:ARG:C	2.46	0.40
1:B:406:SER:O	1:B:407:TYR:C	2.64	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:2100:GLN:HB2	1:B:2154:THR:HG1	1.85	0.40
1:B:2302:LEU:HD13	1:B:2302:LEU:HA	1.97	0.40
1:A:389:GLU:C	1:A:426:VAL:HG23	2.46	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:A:1758:LEU:HD12	1:A:1758:LEU:HA	1.73	0.40
1:A:2080:ILE:HG12	1:A:2145:ILE:CD1	2.51	0.40
1:B:112:GLY:O	1:B:162:HIS:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:552:LEU:HD21	1:B:638:TYR:CE2	2.57	0.40
1:A:404:ASP:OD2	1:A:409:SER:HB3	2.20	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:2263:SER:OG	1:A:2307:ARG:HB2	2.21	0.40
1:B:135:GLN:HG3	1:B:136:THR:O	2.21	0.40
1:B:419:ILE:HG23	1:B:594:PHE:HB2	2.04	0.40
1:B:571:ARG:O	1:B:572:ASN:HB2	2.20	0.40
1:B:632:HIS:O	1:B:634:VAL:HG23	2.22	0.40
1:B:635:ALA:N	1:B:680:MET:O	2.53	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:A:271:PHE:CE1	1:A:286:SER:HB3	2.56	0.40
1:A:597:ASN:C	1:A:599:ALA:H	2.29	0.40
1:A:2195:TYR:CG	1:A:2195:TYR:O	2.74	0.40
1:B:59:LEU:H	1:B:59:LEU:HG	1.50	0.40
1:B:190:THR:C	1:B:192:ASN:H	2.29	0.40
1:B:702:MET:HE3	1:B:702:MET:HB2	1.95	0.40
1:B:1749:ARG:HH21	1:B:1749:ARG:HD3	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

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%)	0	4
1	B	1231/1467 (84%)	955 (78%)	182 (15%)	94 (8%)	1	5
All	All	2473/2934 (84%)	1921 (78%)	356 (14%)	196 (8%)	1	5

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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	65/1301 (5%)	65 (100%)	0	100	100
1	B	1088/1301 (84%)	1086 (100%)	2 (0%)	87	89
All	All	1153/2602 (44%)	1151 (100%)	2 (0%)	87	89

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	43	PRO
1	B	163	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	191	GLN
1	B	26	HIS
1	B	162	HIS
1	B	233	HIS
1	B	250	HIS
1	B	275	HIS
1	B	318	HIS
1	B	1796	GLN
1	B	1864	ASN
1	B	2007	GLN
1	B	2141	ASN
1	B	2172	ASN
1	B	2189	GLN
1	B	2225	ASN
1	B	2231	GLN

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	1.04	1 (7%)	17,19,21	2.12	3 (17%)
2	NAG	C	2	2	14,14,15	0.36	0	17,19,21	0.46	0
2	BMA	C	3	2	11,11,12	1.37	3 (27%)	15,15,17	1.11	0
2	MAN	C	4	2	11,11,12	0.79	0	15,15,17	0.94	1 (6%)
2	MAN	C	5	2	11,11,12	1.43	3 (27%)	15,15,17	1.99	3 (20%)
3	NAG	D	1	1,3	14,14,15	0.76	1 (7%)	17,19,21	1.44	3 (17%)
3	NAG	D	2	3	14,14,15	0.84	1 (7%)	17,19,21	1.29	2 (11%)
3	BMA	D	3	3	11,11,12	1.45	2 (18%)	15,15,17	0.81	0
2	NAG	E	1	1,2	14,14,15	0.54	0	17,19,21	0.69	0
2	NAG	E	2	2	14,14,15	0.66	0	17,19,21	1.91	5 (29%)
2	BMA	E	3	2	11,11,12	1.93	4 (36%)	15,15,17	1.09	0
2	MAN	E	4	2	11,11,12	1.60	2 (18%)	15,15,17	1.30	1 (6%)
2	MAN	E	5	2	11,11,12	0.85	0	15,15,17	0.97	0
2	NAG	F	1	1,2	14,14,15	0.27	0	17,19,21	0.46	0
2	NAG	F	2	2	14,14,15	0.71	1 (7%)	17,19,21	0.69	0
2	BMA	F	3	2	11,11,12	1.64	3 (27%)	15,15,17	2.29	6 (40%)
2	MAN	F	4	2	11,11,12	2.04	3 (27%)	15,15,17	2.85	5 (33%)
2	MAN	F	5	2	11,11,12	0.60	0	15,15,17	2.09	2 (13%)
4	NAG	G	1	1,4	14,14,15	0.59	0	17,19,21	1.12	1 (5%)
4	NAG	G	2	4	14,14,15	0.59	0	17,19,21	1.50	3 (17%)
4	BMA	G	3	4	11,11,12	1.16	2 (18%)	15,15,17	1.12	2 (13%)
4	MAN	G	4	4	11,11,12	1.05	1 (9%)	15,15,17	1.65	2 (13%)
4	NAG	G	5	4	14,14,15	0.41	0	17,19,21	1.56	3 (17%)
4	MAN	G	6	4	11,11,12	1.03	1 (9%)	15,15,17	1.70	3 (20%)
4	FUC	G	7	4	10,10,11	1.14	1 (10%)	14,14,16	1.09	0
5	NAG	H	1	1,5	14,14,15	0.66	1 (7%)	17,19,21	0.79	0
5	NAG	H	2	5	14,14,15	0.60	0	17,19,21	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	BMA	H	3	5	11,11,12	1.07	0	15,15,17	1.37	2 (13%)
5	MAN	H	4	5	11,11,12	0.98	0	15,15,17	1.15	1 (6%)
5	MAN	H	5	5	11,11,12	1.24	1 (9%)	15,15,17	1.10	1 (6%)
5	MAN	H	6	5	11,11,12	1.53	3 (27%)	15,15,17	0.99	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	-	5/6/23/26	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	-	6/6/23/26	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
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	-	3/6/23/26	0/1/1/1
5	NAG	H	2	5	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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 (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	4	MAN	C4-C5	-4.38	1.43	1.53
2	E	4	MAN	O5-C5	4.08	1.51	1.43
2	F	4	MAN	O5-C5	3.76	1.50	1.43
2	E	3	BMA	C1-C2	3.65	1.60	1.52
2	E	3	BMA	C2-C3	3.52	1.57	1.52
2	C	1	NAG	O5-C1	3.45	1.49	1.43
2	F	3	BMA	C2-C3	3.41	1.57	1.52
2	C	5	MAN	C1-C2	3.34	1.60	1.52
5	H	6	MAN	C4-C5	3.19	1.59	1.53
5	H	5	MAN	C1-C2	3.19	1.59	1.52
3	D	2	NAG	O5-C1	-2.81	1.39	1.43
4	G	3	BMA	C2-C3	2.63	1.56	1.52
3	D	3	BMA	C1-C2	2.60	1.58	1.52
3	D	1	NAG	O5-C1	-2.58	1.39	1.43
2	E	3	BMA	C4-C5	2.57	1.58	1.53
5	H	6	MAN	C1-C2	2.46	1.58	1.52
2	F	3	BMA	O3-C3	2.44	1.49	1.43
4	G	4	MAN	C4-C3	2.44	1.58	1.52
2	C	5	MAN	O5-C1	2.44	1.47	1.43
2	E	4	MAN	C1-C2	2.39	1.57	1.52
4	G	6	MAN	C1-C2	2.35	1.57	1.52
2	C	3	BMA	O5-C5	2.32	1.48	1.43
4	G	7	FUC	C2-C3	2.32	1.56	1.52
2	F	2	NAG	O5-C1	-2.24	1.39	1.43
2	F	4	MAN	C2-C3	2.22	1.55	1.52
5	H	1	NAG	O5-C1	-2.14	1.40	1.43
2	C	5	MAN	O5-C5	2.09	1.47	1.43
2	E	3	BMA	C4-C3	2.09	1.57	1.52
2	F	3	BMA	O5-C1	-2.07	1.40	1.43
2	C	3	BMA	C1-C2	2.07	1.57	1.52
4	G	3	BMA	C1-C2	2.02	1.57	1.52
3	D	3	BMA	C4-C3	2.01	1.57	1.52
2	C	3	BMA	C4-C3	2.00	1.57	1.52
5	H	6	MAN	O5-C1	-2.00	1.40	1.43

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	4	MAN	C1-O5-C5	7.26	121.92	112.19
2	F	5	MAN	C1-O5-C5	7.00	121.56	112.19
2	C	5	MAN	C1-O5-C5	6.27	120.59	112.19
2	C	1	NAG	C1-O5-C5	6.06	120.31	112.19
2	F	4	MAN	C2-C3-C4	5.99	121.39	110.86
4	G	6	MAN	C1-O5-C5	5.19	119.14	112.19
4	G	4	MAN	C1-O5-C5	5.09	119.01	112.19
2	F	3	BMA	C1-O5-C5	5.06	118.97	112.19
2	C	1	NAG	C2-N2-C7	4.87	129.43	122.90
2	E	2	NAG	C2-N2-C7	4.71	129.21	122.90
4	G	2	NAG	C2-N2-C7	4.61	129.07	122.90
2	F	3	BMA	O3-C3-C2	4.34	118.90	110.05
4	G	5	NAG	C2-N2-C7	3.87	128.08	122.90
2	E	2	NAG	C3-C4-C5	3.68	116.91	110.23
5	H	3	BMA	C1-O5-C5	3.34	116.66	112.19
2	E	4	MAN	C1-O5-C5	3.29	116.59	112.19
4	G	5	NAG	C1-C2-N2	-3.18	105.42	110.43
3	D	2	NAG	C3-C4-C5	3.14	115.92	110.23
4	G	3	BMA	C1-O5-C5	3.14	116.39	112.19
2	F	4	MAN	C1-C2-C3	3.13	114.20	109.64
3	D	2	NAG	C4-C3-C2	3.10	115.56	111.02
2	F	3	BMA	C3-C4-C5	3.04	115.75	110.23
3	D	1	NAG	C1-O5-C5	3.00	116.20	112.19
2	C	1	NAG	C1-C2-N2	2.94	115.06	110.43
3	D	1	NAG	C3-C4-C5	2.92	115.53	110.23
4	G	1	NAG	C2-N2-C7	2.90	126.78	122.90
2	F	4	MAN	O5-C5-C6	2.81	113.13	107.66
3	D	1	NAG	C2-N2-C7	2.68	126.49	122.90
4	G	2	NAG	C1-C2-N2	2.66	114.62	110.43
2	F	4	MAN	O3-C3-C4	-2.64	104.16	110.38
2	E	2	NAG	C1-O5-C5	2.63	115.72	112.19
2	C	5	MAN	C1-C2-C3	2.60	113.43	109.64
5	H	5	MAN	C1-O5-C5	2.51	115.55	112.19
5	H	4	MAN	O2-C2-C3	-2.48	105.01	110.15
4	G	6	MAN	O2-C2-C3	-2.45	105.08	110.15
4	G	5	NAG	C1-O5-C5	-2.41	108.95	112.19
4	G	6	MAN	C1-C2-C3	2.35	113.07	109.64
2	F	3	BMA	O5-C5-C4	2.34	116.51	110.83
2	C	5	MAN	O2-C2-C3	-2.22	105.56	110.15
2	E	2	NAG	C1-C2-N2	2.21	113.92	110.43
4	G	2	NAG	C1-O5-C5	2.18	115.11	112.19
2	F	5	MAN	O5-C1-C2	2.18	115.98	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2	NAG	O5-C5-C4	2.17	116.12	110.83
2	F	3	BMA	O5-C5-C6	-2.16	103.47	107.66
5	H	3	BMA	O2-C2-C3	-2.11	105.78	110.15
2	F	3	BMA	C2-C3-C4	2.07	114.50	110.86
2	C	4	MAN	O2-C2-C3	-2.07	105.87	110.15
4	G	4	MAN	O2-C2-C3	-2.05	105.91	110.15
4	G	3	BMA	O3-C3-C2	2.01	114.15	110.05

There are no chirality outliers.

All (55) torsion outliers are listed below:

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

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

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:

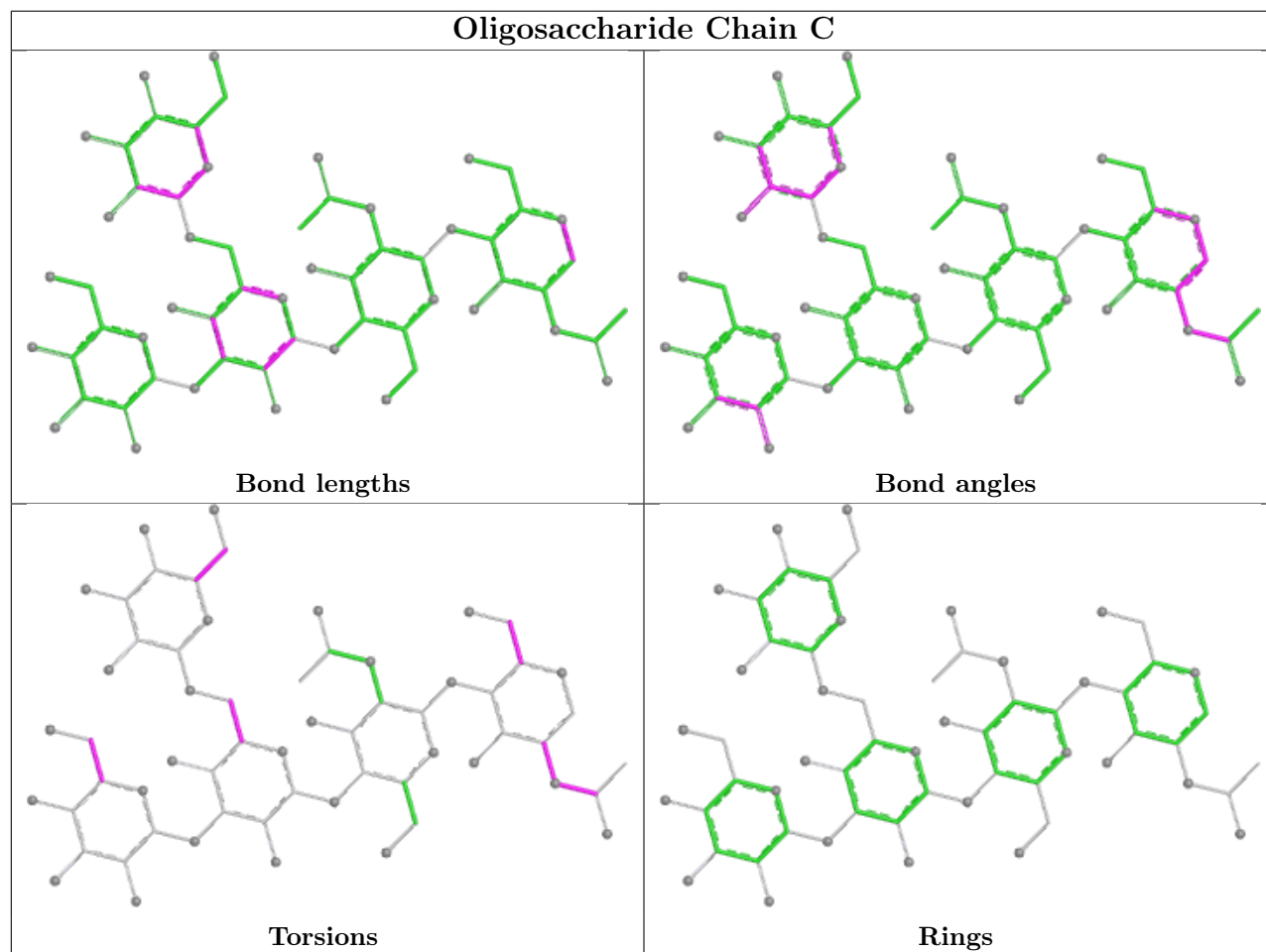
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	2	NAG	2	0
2	E	1	NAG	1	0
2	C	2	NAG	2	0
2	C	1	NAG	1	0
5	H	4	MAN	1	0
5	H	1	NAG	1	0
5	H	5	MAN	1	0

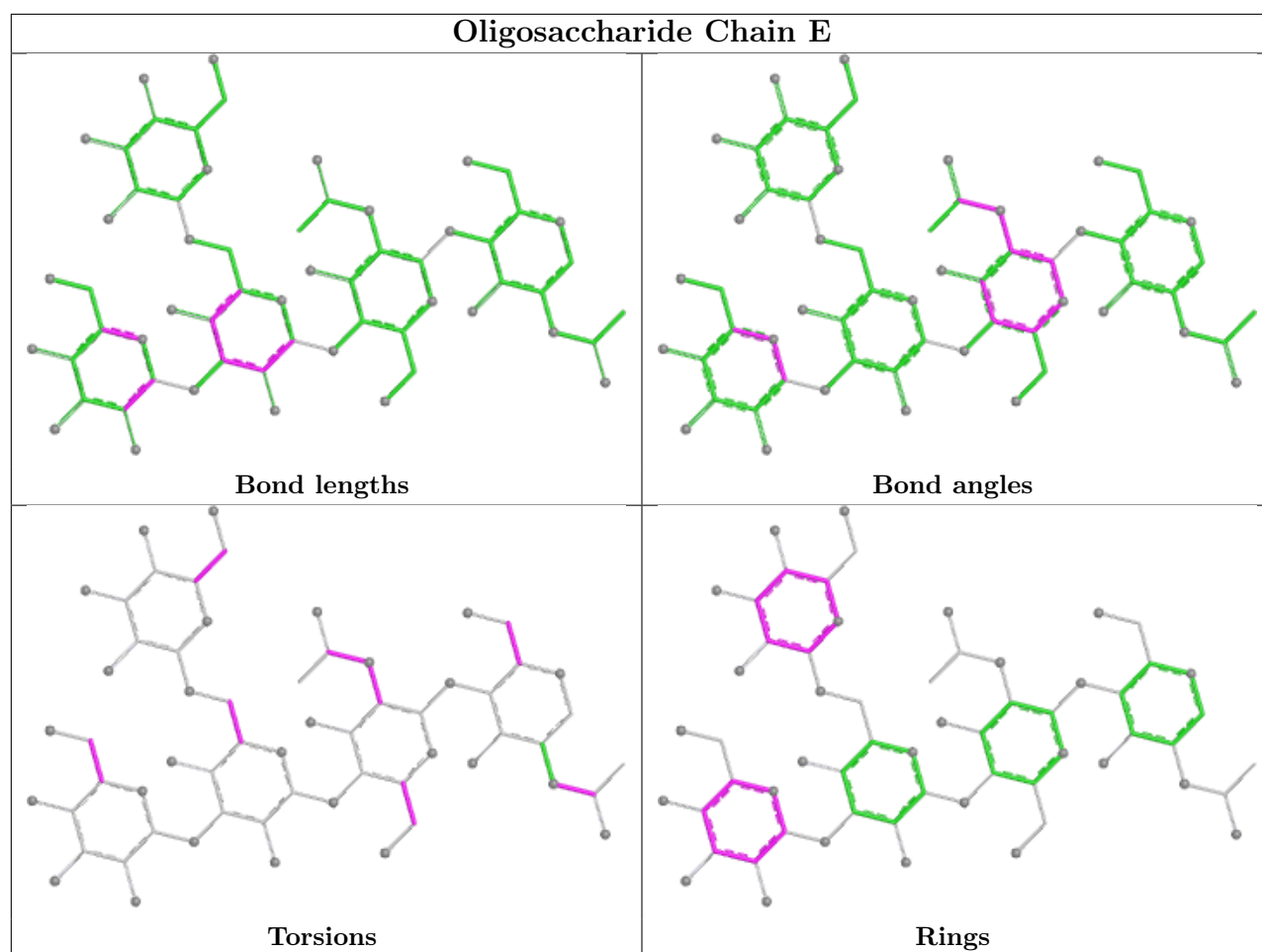
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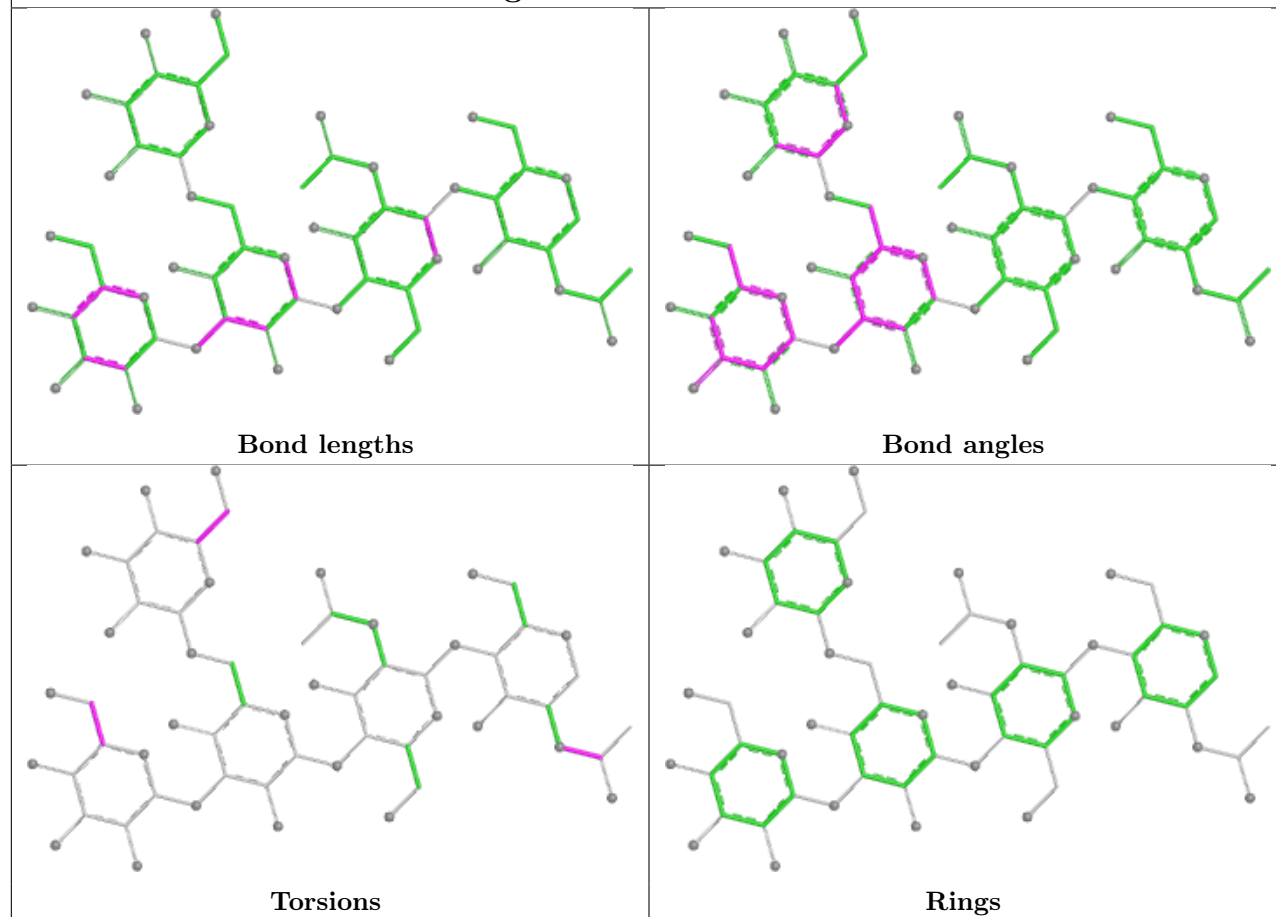
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2	NAG	1	0
4	G	1	NAG	1	0
2	F	4	MAN	0	2
5	H	2	NAG	1	0

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

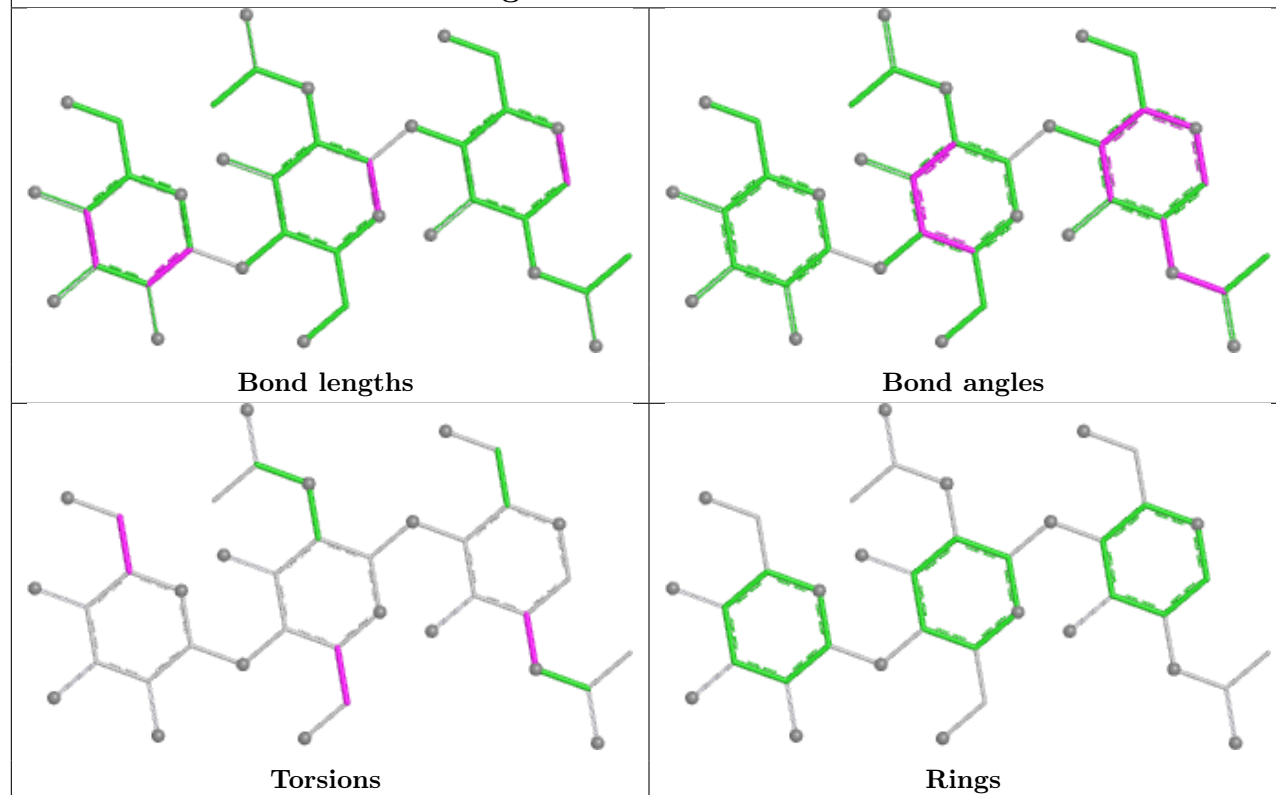


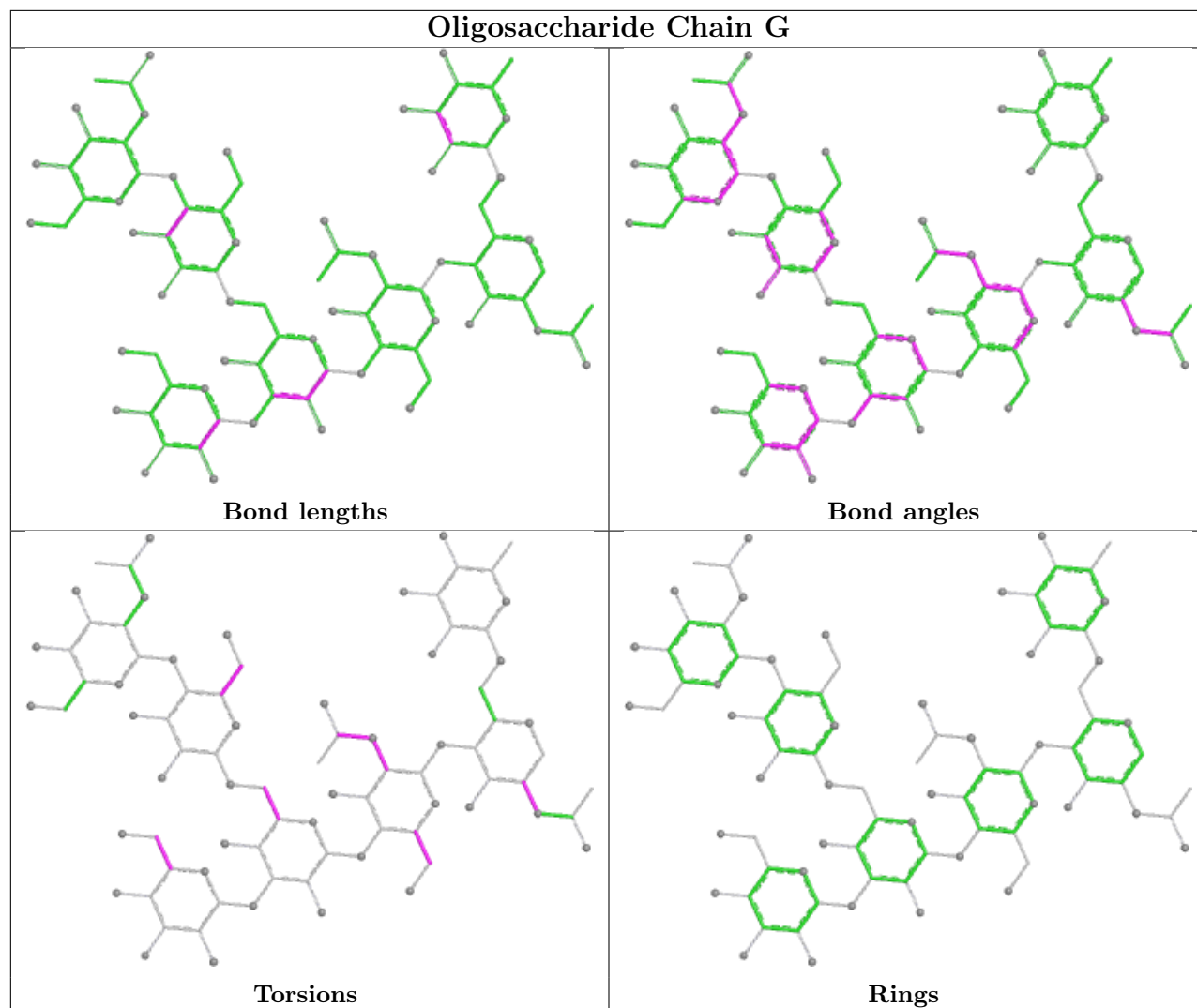


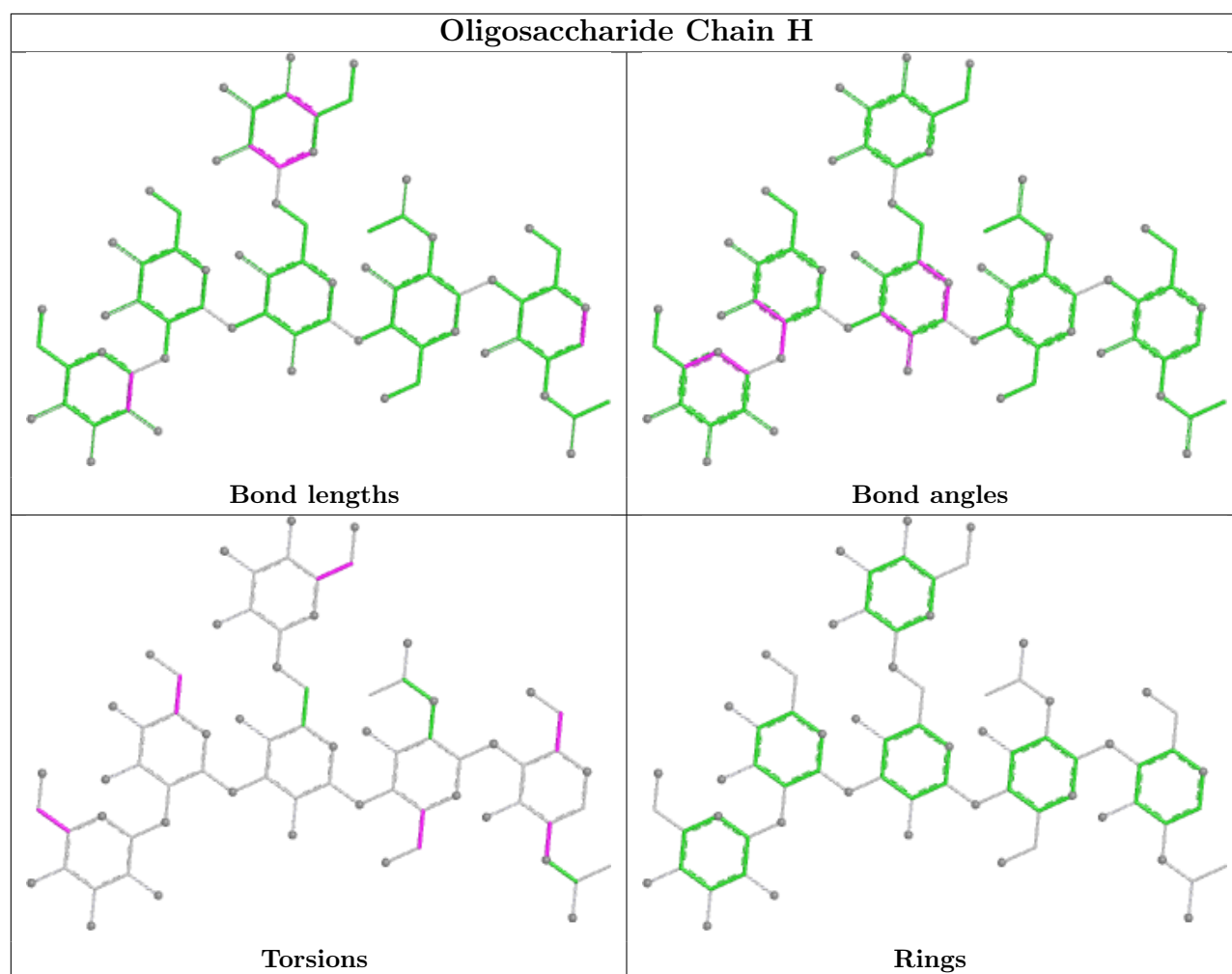
Oligosaccharide Chain F



Oligosaccharide Chain D







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%)	-0.19	18 (1%)	73 54	30, 48, 88, 273	0
1	B	1247/1467 (85%)	0.03	21 (1%)	69 49	30, 58, 130, 157	0
All	All	2503/2934 (85%)	-0.08	39 (1%)	70 51	30, 52, 119, 273	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2319	LEU	5.1
1	A	505	PRO	4.8
1	A	31	PHE	4.5
1	A	27	VAL	4.3
1	B	2122	THR	4.2
1	A	38	ALA	3.8
1	A	470	SER	3.5
1	A	34	THR	3.4
1	A	36	PRO	3.4
1	A	43	PRO	3.1
1	B	2329	GLN	3.0
1	B	2176	MET	3.0
1	B	2249	LYS	3.0
1	A	37	GLY	2.9
1	B	2293	VAL	2.8
1	A	39	LEU	2.8
1	B	2245	THR	2.8
1	A	33	ALA	2.8
1	A	399	VAL	2.7
1	B	2274	PHE	2.7
1	B	2244	THR	2.5
1	A	40	PRO	2.5
1	B	398	LEU	2.5
1	B	2257	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	32	PRO	2.4
1	B	107	TRP	2.4
1	A	192	ASN	2.4
1	A	35	ALA	2.4
1	B	2029	SER	2.4
1	B	1715	PRO	2.3
1	B	2252	LEU	2.3
1	B	2295	ASN	2.2
1	B	2328	ALA	2.2
1	B	2251	LEU	2.2
1	B	2317	ILE	2.1
1	A	1827	GLU	2.1
1	B	2120	THR	2.1
1	B	2277	ASN	2.0
1	A	401	ALA	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
3	NAG	D	2	14/15	0.17	0.16	114,145,152,154	0
2	MAN	F	5	11/12	0.18	0.16	149,151,160,160	0
4	MAN	G	6	11/12	0.26	0.14	128,135,144,145	0
4	FUC	G	7	10/11	0.26	0.12	124,134,139,144	0
2	MAN	E	4	11/12	0.30	0.14	117,124,129,131	0
2	BMA	F	3	11/12	0.32	0.17	131,138,150,151	0
2	NAG	F	2	14/15	0.33	0.17	130,144,153,154	0
4	NAG	G	1	14/15	0.33	0.18	99,116,124,128	0
2	BMA	C	3	11/12	0.36	0.14	144,158,163,164	0
2	MAN	C	4	11/12	0.36	0.12	148,158,161,163	0
5	MAN	H	5	11/12	0.45	0.13	125,134,142,149	0
3	NAG	D	1	14/15	0.48	0.13	95,131,141,144	0
2	MAN	C	5	11/12	0.48	0.11	138,145,151,156	0

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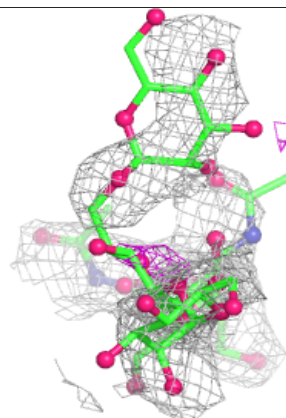
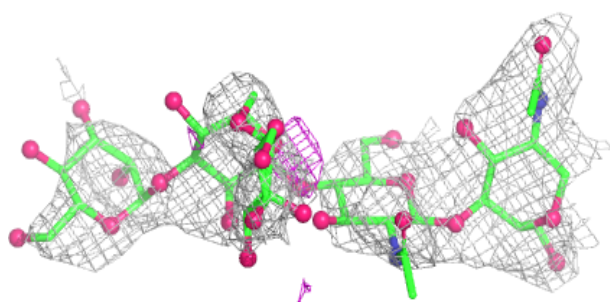
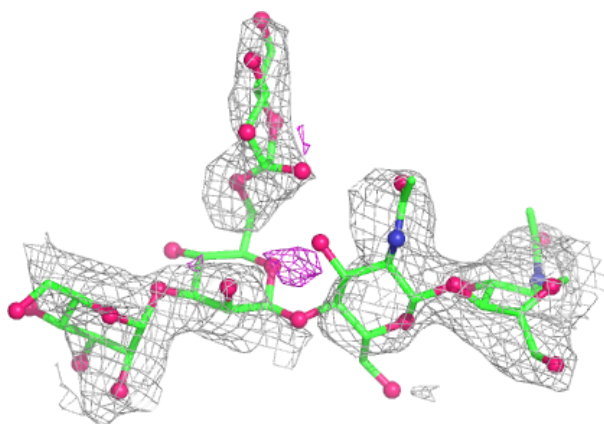
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	C	2	14/15	0.50	0.12	128,137,149,156	0
2	BMA	E	3	11/12	0.50	0.14	112,121,126,127	0
4	BMA	G	3	11/12	0.53	0.10	123,144,149,152	0
2	MAN	E	5	11/12	0.53	0.14	84,109,119,120	0
3	BMA	D	3	11/12	0.55	0.11	134,157,162,163	0
2	NAG	F	1	14/15	0.60	0.18	86,120,136,142	0
4	NAG	G	2	14/15	0.61	0.12	118,133,142,145	0
5	MAN	H	4	11/12	0.64	0.11	105,120,127,133	0
4	NAG	G	5	14/15	0.64	0.14	78,93,101,102	0
4	MAN	G	4	11/12	0.70	0.10	69,97,108,110	0
5	NAG	H	2	14/15	0.73	0.17	73,95,100,103	0
5	MAN	H	6	11/12	0.73	0.10	99,113,125,126	0
2	NAG	E	2	14/15	0.74	0.15	74,105,116,122	0
5	BMA	H	3	11/12	0.77	0.10	108,114,120,123	0
5	NAG	H	1	14/15	0.85	0.11	81,86,93,93	0
2	NAG	C	1	14/15	0.86	0.10	79,89,109,121	0
2	MAN	F	4	11/12	0.87	0.18	77,96,119,134	0
2	NAG	E	1	14/15	0.87	0.12	78,83,92,104	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.

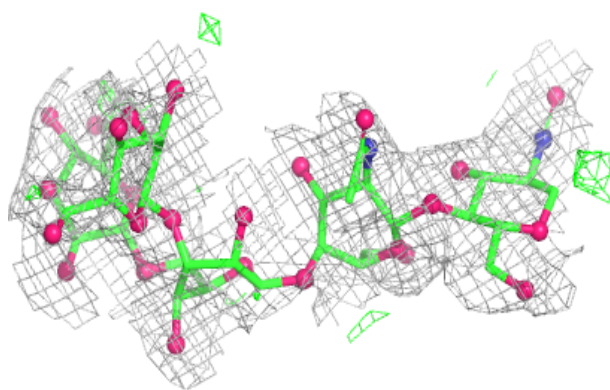
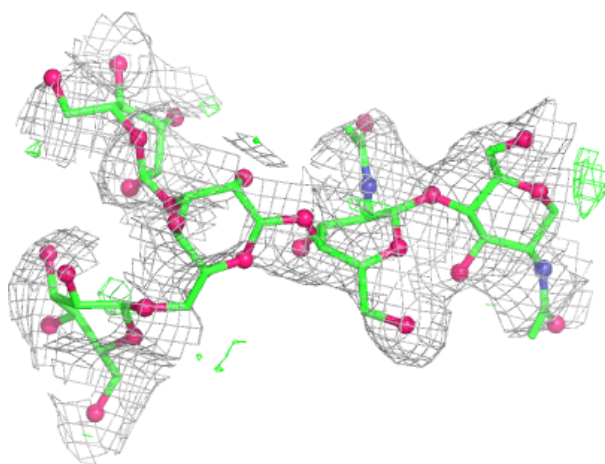
Electron density around Chain C:

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



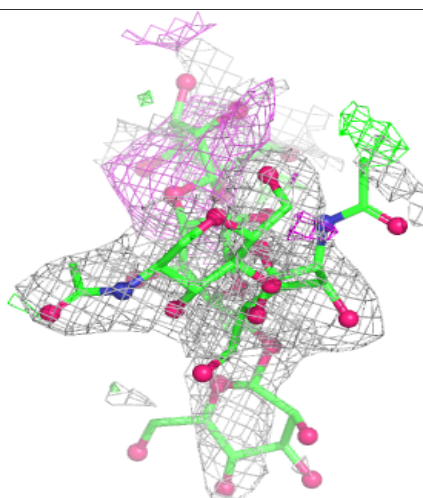
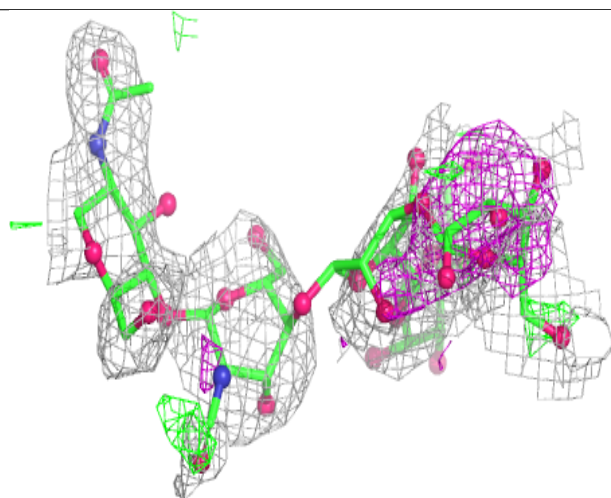
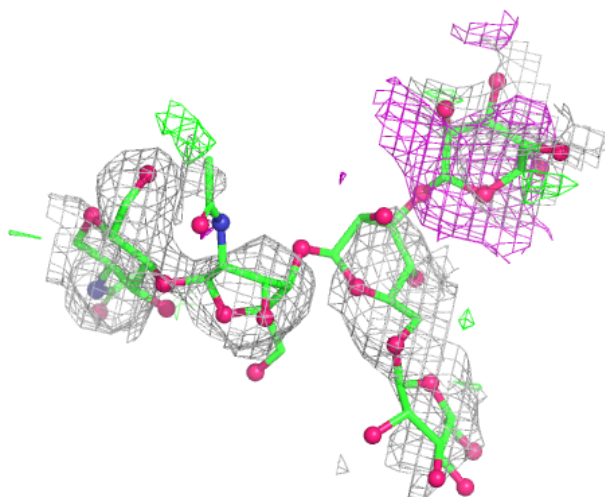
Electron density around Chain E:

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



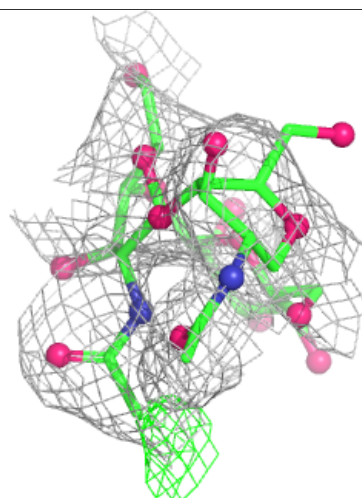
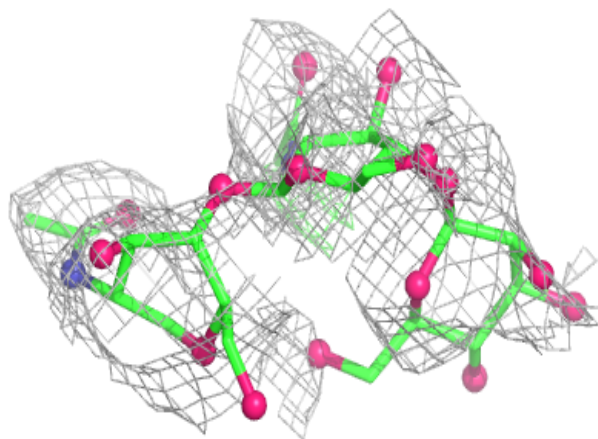
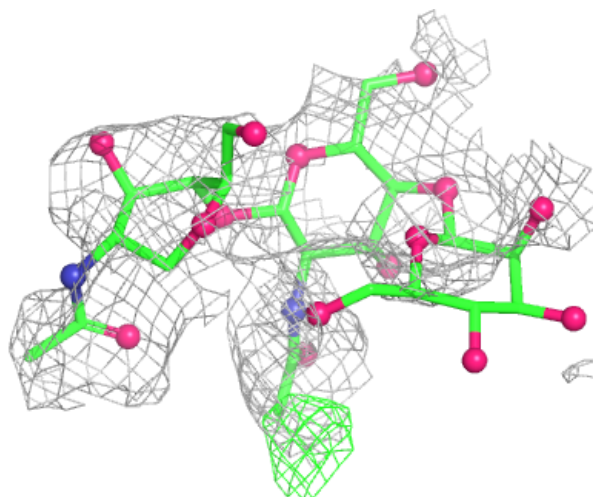
Electron density around Chain F:

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



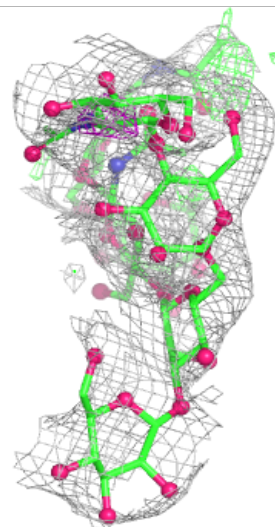
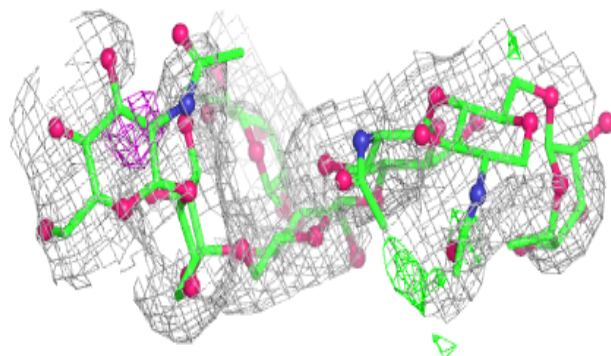
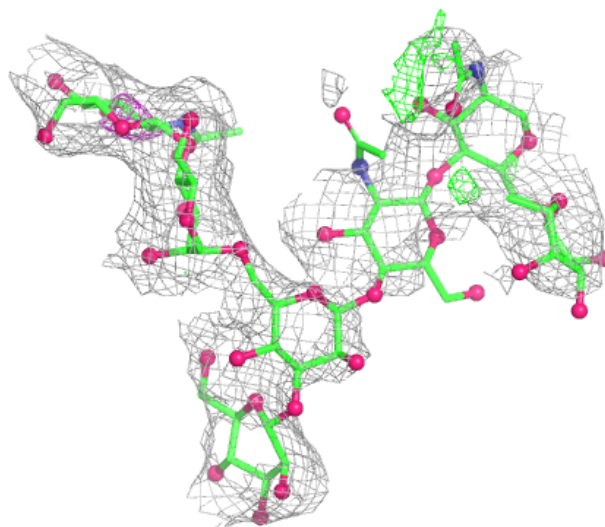
Electron density around Chain D:

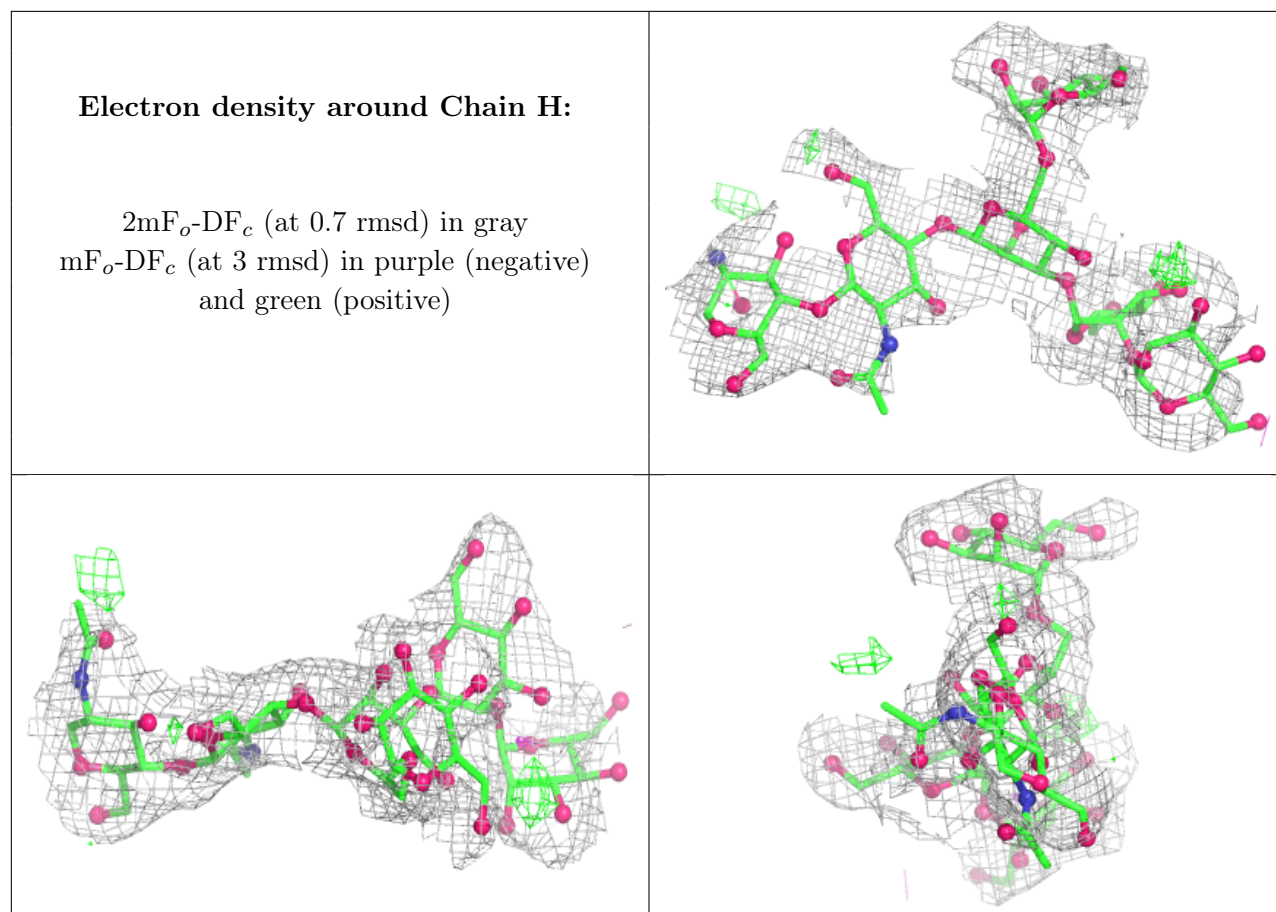
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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($\text{\AA}^2$)	Q<0.9
7	ZN	A	2415	1/1	0.97	0.04	46,46,46,46	0
6	CA	B	2419	1/1	0.99	0.06	59,59,59,59	0
6	CA	A	2414	1/1	0.99	0.06	40,40,40,40	0
7	ZN	B	2420	1/1	0.99	0.05	47,47,47,47	0
8	CU1	A	2416	1/1	0.99	0.07	40,40,40,40	0
8	CU1	B	2421	1/1	0.99	0.09	48,48,48,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.