



## Full wwPDB EM Validation Report ⓘ

May 14, 2024 – 10:16 am BST

PDB ID : 8R50  
EMDB ID : EMD-18889  
Title : Mouse teneurin-3 compact dimer - A1B1 isoform  
Authors : Gogou, C.; Meijer, D.H.  
Deposited on : 2023-11-15  
Resolution : 3.10 Å (reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

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>.

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

EMDB validation analysis : 0.0.1.dev92  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

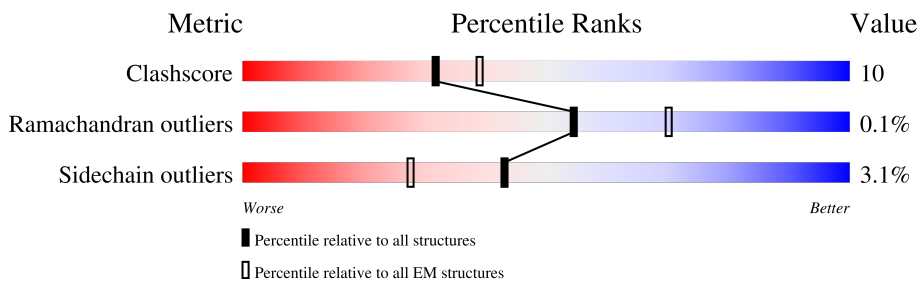
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.10 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	2407	
1	B	2407	
2	C	2	
2	D	2	
2	E	2	
2	F	2	
2	G	2	
2	H	2	
2	I	2	

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Mol	Chain	Length	Quality of chain
2	J	2	 100%

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 29752 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Teneurin-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	1889	14651	9292	2523	2773	63	0	0
1	A	1889	14651	9292	2523	2773	63	0	0

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	312	MET	-	initiating methionine	UNP Q9WTS6
B	313	ALA	-	expression tag	UNP Q9WTS6
B	314	ARG	-	expression tag	UNP Q9WTS6
B	315	PRO	-	expression tag	UNP Q9WTS6
B	316	LEU	-	expression tag	UNP Q9WTS6
B	317	CYS	-	expression tag	UNP Q9WTS6
B	318	THR	-	expression tag	UNP Q9WTS6
B	319	LEU	-	expression tag	UNP Q9WTS6
B	320	LEU	-	expression tag	UNP Q9WTS6
B	321	LEU	-	expression tag	UNP Q9WTS6
B	322	LEU	-	expression tag	UNP Q9WTS6
B	323	MET	-	expression tag	UNP Q9WTS6
B	324	ALA	-	expression tag	UNP Q9WTS6
B	325	THR	-	expression tag	UNP Q9WTS6
B	326	LEU	-	expression tag	UNP Q9WTS6
B	327	ALA	-	expression tag	UNP Q9WTS6
B	328	GLY	-	expression tag	UNP Q9WTS6
B	329	ALA	-	expression tag	UNP Q9WTS6
B	330	LEU	-	expression tag	UNP Q9WTS6
B	331	ALA	-	expression tag	UNP Q9WTS6
B	332	GLY	-	expression tag	UNP Q9WTS6
B	333	SER	-	expression tag	UNP Q9WTS6
B	334	HIS	-	expression tag	UNP Q9WTS6
B	335	HIS	-	expression tag	UNP Q9WTS6
B	336	HIS	-	expression tag	UNP Q9WTS6
B	337	HIS	-	expression tag	UNP Q9WTS6

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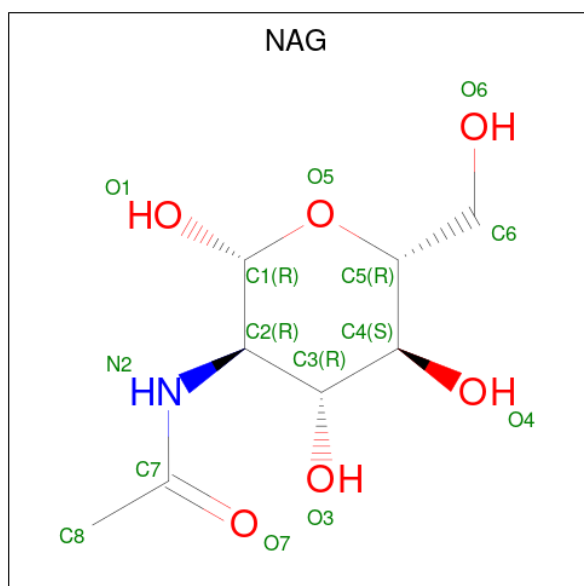
Chain	Residue	Modelled	Actual	Comment	Reference
B	338	HIS	-	expression tag	UNP Q9WTS6
B	339	HIS	-	expression tag	UNP Q9WTS6
B	340	GLY	-	expression tag	UNP Q9WTS6
B	341	SER	-	expression tag	UNP Q9WTS6
B	2332	ILE	THR	conflict	UNP Q9WTS6
B	2716	ALA	-	expression tag	UNP Q9WTS6
B	2717	ALA	-	expression tag	UNP Q9WTS6
B	2718	ALA	-	expression tag	UNP Q9WTS6
A	312	MET	-	initiating methionine	UNP Q9WTS6
A	313	ALA	-	expression tag	UNP Q9WTS6
A	314	ARG	-	expression tag	UNP Q9WTS6
A	315	PRO	-	expression tag	UNP Q9WTS6
A	316	LEU	-	expression tag	UNP Q9WTS6
A	317	CYS	-	expression tag	UNP Q9WTS6
A	318	THR	-	expression tag	UNP Q9WTS6
A	319	LEU	-	expression tag	UNP Q9WTS6
A	320	LEU	-	expression tag	UNP Q9WTS6
A	321	LEU	-	expression tag	UNP Q9WTS6
A	322	LEU	-	expression tag	UNP Q9WTS6
A	323	MET	-	expression tag	UNP Q9WTS6
A	324	ALA	-	expression tag	UNP Q9WTS6
A	325	THR	-	expression tag	UNP Q9WTS6
A	326	LEU	-	expression tag	UNP Q9WTS6
A	327	ALA	-	expression tag	UNP Q9WTS6
A	328	GLY	-	expression tag	UNP Q9WTS6
A	329	ALA	-	expression tag	UNP Q9WTS6
A	330	LEU	-	expression tag	UNP Q9WTS6
A	331	ALA	-	expression tag	UNP Q9WTS6
A	332	GLY	-	expression tag	UNP Q9WTS6
A	333	SER	-	expression tag	UNP Q9WTS6
A	334	HIS	-	expression tag	UNP Q9WTS6
A	335	HIS	-	expression tag	UNP Q9WTS6
A	336	HIS	-	expression tag	UNP Q9WTS6
A	337	HIS	-	expression tag	UNP Q9WTS6
A	338	HIS	-	expression tag	UNP Q9WTS6
A	339	HIS	-	expression tag	UNP Q9WTS6
A	340	GLY	-	expression tag	UNP Q9WTS6
A	341	SER	-	expression tag	UNP Q9WTS6
A	2332	ILE	THR	conflict	UNP Q9WTS6
A	2716	ALA	-	expression tag	UNP Q9WTS6
A	2717	ALA	-	expression tag	UNP Q9WTS6
A	2718	ALA	-	expression tag	UNP Q9WTS6

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	C	2	Total	C	N	O	0	0
			28	16	2	10		
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	G	2	Total	C	N	O	0	0
			28	16	2	10		
2	H	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		
2	J	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



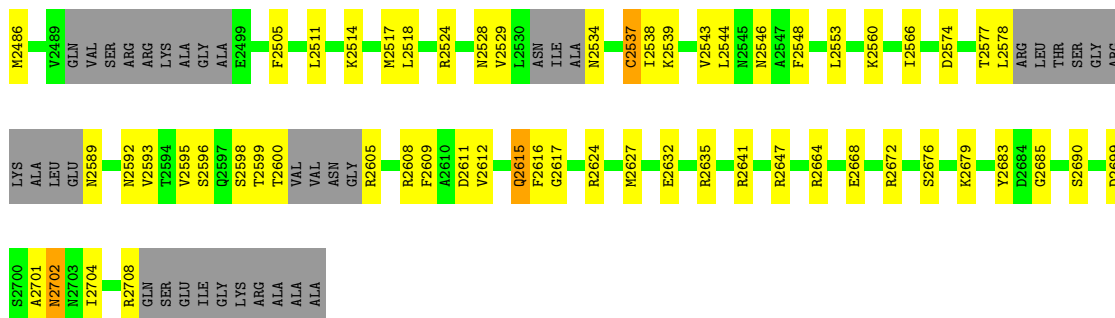
Mol	Chain	Residues	Atoms				AltConf
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			15	8	1	6	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			15	8	1	6	
3	A	1	Total	C	N	O	0
			14	8	1	5	







A2320	L2189	S2045	M1910	M1751	V1593	G1469	ASP THR	S1289	H1129	P992	L853	GLY TRP
S2324	D2195	N2051	S1912	M1752	V1594	G1470	S1350	L1260	V1130	E996	S858	ASN
L2327	R2196	D2064	V1913	L1753	S1595	ASN	M1351	T1261	Y1139	H1001	T859	GLY
M2328	L2200	V2077	R1914	L1754	Q1599	C1472	H1352	ALA	K1140	E1002	L862	HIS
K2330	L2207	D2081	H1916	V1763	I1605	S1477	I1353	LYS	P1152	E1003	S866	ASN
Q2333	L2207	D2081	H1916	E1764	I1606	G1478	D1363	D1285	P1153	T1004	P1153	GLY
F2342	Q2215	D2082	I1921	R1768	G1606	G1478	L1364	N1269	V1154	L1011	T875	ILE
N2345	R2216	N2083	S1922	K1483	T1607	K1483	P1368	M1159	M1159	K1012	A1876	ALA
F2348	G2217	Q2084	R1923	Q1771	A1616	S1496	F1368	M1371	C1169	R1019	T877	VAL
G2353	T2218	I2085	I1924	V1776	L1621	P1497	S1372	S1372	G1169	ASP	G878	ASP
H2355	E2219	T2092	R1928	V1785	F1624	D1498	I1373	CYS	C1172	S1025	Q879	CYS
Y2359	S2223	Y2093	M1929	V1785	A1504	A1504	V1374	LEU	C1172	V1026	A883	LYS
D2360	T2224	T2094	I1930	D1794	K1636	A1505	V1375	PRO	D1177	L1027	D894	ILE
T2363	S2225	Y2106	Y1931	F1795	S1637	L1506	I1384	PHE	G1178	K1028	K749	HIS
Y2369	S2234	Q2107	M1932	D1796	D1638	V1514	I1385	ASP	M1179	M1031	L785	VAL
D2360	V2241	Y2108	I1941	R1797	E1639	S1515	E1396	GLU	K1180	M892	C786	CYS
T2363	L2248	E2109	T1942	H1808	T1640	S1523	ASN	ALA	L1181	K1042	N757	MET
R2371	V2252	Y2116	R1960	ARG	G1641	M1524	R1388	ARG	P1184	H1044	S758	GLY
R2379	V2252	I2118	R1971	K1810	D1647	P1524	Q1389	GLY	V1185	L1045	R761	TRP
D2384	H2261	M2125	R1974	L1813	M1656	P1522	R1396	GLY	A1186	M1046	C782	GLY
I2391	L2262	G2126	E1974	R1814	P1660	Q1535	P1397	GLY	L1187	V1049	T763	GLY
D2394	Q2263	R2127	Y1977	R1826	Q1535	Q1535	H1399	GLY	I1191	V1050	Q774	GLY
F2398	F2264	R2131	Y1978	V1832	Y1538	I1539	CYS	GLN	G1198	Q1055	R778	TRP
M2399	F2265	I2135	S1979	M1833	H1546	I1539	VAL	VAL	D1199	K1056	R781	ILE
V2415	F2266	V1982	T1980	T1838	Q1547	H1548	PRO	PRO	W1057	W1057	G781	LEU
Y2418	F2266	S1983	R1981	T1838	Q1547	Y1548	GLY	VAL	F1200	F1058	C782	LYS
L2419	A2267	P2137	S1983	Q1844	T1549	T1549	VAL	VAL	L1064	L1064	D783	ALA
W2425	D2268	N2140	K1994	S1847	Y1553	V1553	PRO	PRO	T1067	T1067	M786	CYS
I2437	H2277	K2143	M1997	I1848	R1721	Y1559	VAL	VAL	F1068	F1068	L801	ALA
F2440	Y2290	A2144	L1998	Q1849	I1722	Y1559	GLY	GLY	D1071	D1071	F802	ALA
W2425	L2293	A2145	S2000	R1850	N1560	N1560	LYS	LYS	P941	P941	Y820	CYS
I2437	L2297	Y2158	C2005	K1856	S1564	R1565	H1412	H1412	D1222	T1073	P825	HIS
F2440	E2301	M2164	T2006	G1863	R1566	D1566	Y1428	Y1428	F1223	D1074	P825	ARG
P2441	D2306	L2171	T2006	R1864	V1569	T1570	L1432	L1432	S1226	A1075	T830	ALA
L2454	E2307	N2172	T2006	G1864	T1570	T1570	L1442	L1442	P1229	E1093	Q833	ALA
V2469	F2308	G2173	T2010	R1864	Y1732	Y1732	SER	SER	Y1094	Y1094	SER	THR
R2475	S2312	N2174	R2010	Y1880	Q1733	Q1733	R1443	R1443	L1102	L1102	L835	GLN
K2478	D2313	N2179	P2035	V1886	T1734	T1734	R1444	R1444	W1193	W1193	Q840	THR
	T2315	P2180	R1749	I1886	G1741	T1573	V1448	V1448	F1234	F1234	D964	CYS
	T2317	S2183	R1750	I1896	A1743	I1582	T1449	T1449	L1235	L1235	L965	ASP
			R2042	F1897	M1744	I1582	T1450	T1450	P1239	P1239	A842	CYS
				E1898	N1744	R1583	ASP	ASP	V1240	V1240	A843	LYS
				L1905	P1745	R1584	G1452	G1452	T1241	T1241	K844	THR
				I1908	T1746	D1585	ARG	ARG	Q1111	Q1111	R970	CYS
				I1908	R1749	M1589	PRO	PRO	L1244	L1244	Y847	GLY
				T1909	R1750	M1589	L1345	L1345	E1114	E1114	S985	ASP
							C1347	C1347	L1115	L1115	S986	ASN
									S1247	S1247	F852	TRP



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

Chain C:  100%



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

Chain D:  100%



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

Chain E:  50%



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

Chain F:  100%



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

Chain G:  100%




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

Chain H:  100%

MAG1  
MAG2

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

Chain I:  50% 50%

MAG1  
MAG2

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

Chain J:  100%

MAG1  
MAG2

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	57545	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50.0	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.25	0/14968	0.50	0/20337
1	B	0.25	0/14968	0.50	0/20337
All	All	0.25	0/29936	0.50	0/40674

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	14651	0	14020	277	0
1	B	14651	0	14020	273	0
2	C	28	0	25	0	0
2	D	28	0	25	0	0
2	E	28	0	25	4	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
2	H	28	0	25	0	0
2	I	28	0	25	4	0
2	J	28	0	25	0	0
3	A	113	0	106	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	113	0	106	4	0
All	All	29752	0	28452	553	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (553) 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:1913:VAL:HG12	1:B:1913:VAL:O	1.68	0.92
1:A:1913:VAL:HG12	1:A:1913:VAL:O	1.68	0.89
1:A:1312:LEU:HD21	1:A:1323:LYS:HG3	1.66	0.77
1:B:1312:LEU:HD21	1:B:1323:LYS:HG3	1.66	0.77
1:A:1074:ASP:OD1	1:A:1075:ALA:N	2.19	0.76
1:B:1074:ASP:OD1	1:B:1075:ALA:N	2.19	0.74
1:A:2145:ALA:HB3	1:A:2158:TYR:HB2	1.70	0.74
1:B:2145:ALA:HB3	1:B:2158:TYR:HB2	1.70	0.74
1:A:928:ARG:HG3	1:A:930:PRO:HD2	1.70	0.73
1:B:928:ARG:HG3	1:B:930:PRO:HD2	1.70	0.73
1:A:1240:VAL:HG23	1:A:1241:THR:HG23	1.73	0.71
1:B:1240:VAL:HG23	1:B:1241:THR:HG23	1.73	0.71
1:B:1913:VAL:O	1:B:1913:VAL:CG1	2.39	0.71
1:A:1913:VAL:O	1:A:1913:VAL:CG1	2.39	0.70
1:A:2418:TYR:O	1:A:2425:TRP:NE1	2.26	0.69
1:B:2164:MET:SD	1:B:2164:MET:N	2.66	0.69
1:A:2164:MET:SD	1:A:2164:MET:N	2.66	0.68
1:B:2418:TYR:O	1:B:2425:TRP:NE1	2.26	0.68
1:B:2543:VAL:HG12	1:B:2574:ASP:HB2	1.77	0.67
1:B:1247:SER:HB3	1:B:1305:MET:HE1	1.77	0.67
1:B:1569:VAL:O	1:B:1584:ARG:NH2	2.25	0.67
1:A:1569:VAL:O	1:A:1584:ARG:NH2	2.25	0.66
1:A:1247:SER:HB3	1:A:1305:MET:HE1	1.75	0.66
1:B:1140:LYS:NZ	1:B:1538:TYR:OH	2.29	0.66
1:A:2543:VAL:HG12	1:A:2574:ASP:HB2	1.77	0.65
1:A:1140:LYS:NZ	1:A:1538:TYR:OH	2.29	0.64
1:B:2511:LEU:HG	1:B:2616:PHE:HB3	1.79	0.64
1:B:1616:ALA:HB2	1:B:1621:LEU:HD11	1.79	0.64
1:A:2511:LEU:HG	1:A:2616:PHE:HB3	1.79	0.64
1:A:1616:ALA:HB2	1:A:1621:LEU:HD11	1.79	0.64
1:A:2330:LYS:NZ	1:A:2345:ASN:O	2.29	0.63
1:B:892:ASN:HB3	1:B:927:GLU:HB2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1977:TYR:HB2	1:A:2225:SER:HB2	1.80	0.63
1:B:1977:TYR:HB2	1:B:2225:SER:HB2	1.79	0.63
1:A:2029:VAL:H	1:A:2263:GLN:HE22	1.46	0.62
1:A:892:ASN:HB3	1:A:927:GLU:HB2	1.81	0.62
1:B:2029:VAL:H	1:B:2263:GLN:HE22	1.46	0.62
1:B:1368:PRO:HG2	1:B:1428:TYR:HA	1.81	0.62
1:A:2668:GLU:O	1:A:2672:ARG:NH1	2.32	0.61
1:B:2668:GLU:O	1:B:2672:ARG:NH1	2.32	0.61
1:B:963:CYS:SG	1:B:964:ASP:N	2.73	0.61
1:B:1351:MET:SD	1:B:1351:MET:N	2.74	0.61
1:B:2330:LYS:NZ	1:B:2345:ASN:O	2.29	0.61
1:A:963:CYS:SG	1:A:964:ASP:N	2.73	0.61
1:A:1368:PRO:HG2	1:A:1428:TYR:HA	1.81	0.61
1:A:2600:THR:HG22	1:A:2605:ARG:HH12	1.66	0.61
1:B:1259:SER:O	1:B:1269:ASN:ND2	2.33	0.61
1:A:889:ILE:O	1:A:928:ARG:NH1	2.34	0.61
1:A:1259:SER:O	1:A:1269:ASN:ND2	2.33	0.61
1:A:2196:ARG:HB3	1:A:2207:LEU:HD22	1.82	0.61
1:B:889:ILE:O	1:B:928:ARG:NH1	2.34	0.61
1:A:2164:MET:O	1:A:2179:ASN:ND2	2.35	0.60
1:B:2196:ARG:HB3	1:B:2207:LEU:HD22	1.82	0.60
1:B:2600:THR:HG22	1:B:2605:ARG:HH12	1.66	0.60
1:A:2174:ASN:OD1	1:A:2399:ASN:ND2	2.32	0.60
1:B:892:ASN:ND2	1:B:927:GLU:OE1	2.34	0.60
1:B:1639:GLU:HG2	1:B:1640:THR:HG23	1.84	0.60
1:B:2174:ASN:OD1	1:B:2399:ASN:ND2	2.32	0.60
1:A:1111:GLN:NE2	1:A:1114:GLU:OE2	2.35	0.60
1:A:1639:GLU:HG2	1:A:1640:THR:HG23	1.84	0.60
1:B:1111:GLN:NE2	1:B:1114:GLU:OE2	2.35	0.59
1:A:1351:MET:N	1:A:1351:MET:SD	2.74	0.59
1:B:1768:ARG:NH2	1:B:1794:ASP:OD2	2.34	0.59
1:A:1768:ARG:NH2	1:A:1794:ASP:OD2	2.34	0.59
1:A:892:ASN:ND2	1:A:927:GLU:OE1	2.34	0.59
1:A:1363:ASP:OD1	1:A:1364:LEU:N	2.36	0.59
1:B:840:GLN:HA	1:B:844:LYS:HE2	1.84	0.59
1:B:2164:MET:O	1:B:2179:ASN:ND2	2.35	0.59
1:A:840:GLN:HA	1:A:844:LYS:HE2	1.84	0.59
1:A:965:LEU:O	1:A:1389:GLN:NE2	2.37	0.58
1:A:2215:GLN:NE2	1:A:2217:GLY:O	2.36	0.58
1:B:1910:MET:HB2	1:B:1914:ALA:HB3	1.86	0.58
1:B:1184:PRO:HB2	1:B:1504:ALA:HB1	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2215:GLN:NE2	1:B:2217:GLY:O	2.36	0.58
1:A:1184:PRO:HB2	1:A:1504:ALA:HB1	1.84	0.58
1:B:965:LEU:O	1:B:1389:GLN:NE2	2.37	0.58
1:B:1363:ASP:OD1	1:B:1364:LEU:N	2.36	0.57
1:B:2548:PHE:HB2	1:B:2566:ILE:HG12	1.85	0.57
1:A:1910:MET:HB2	1:A:1914:ALA:HB3	1.85	0.57
1:A:941:PRO:HG2	1:A:944:VAL:HG11	1.86	0.57
1:A:1981:ARG:NH1	1:A:1983:SER:OG	2.38	0.57
1:A:2548:PHE:HB2	1:A:2566:ILE:HG12	1.85	0.57
1:A:2641:ARG:NH2	1:A:2685:GLY:O	2.37	0.57
1:A:859:THR:HG21	1:A:913:ASP:HB2	1.87	0.57
1:A:1532:PRO:O	1:A:1535:GLN:NE2	2.36	0.57
1:A:2134:LYS:NZ	1:A:2137:PRO:O	2.34	0.57
1:A:2333:GLN:HG3	1:A:2342:PHE:HD2	1.69	0.57
1:B:1373:ILE:HB	1:B:1384:ILE:HB	1.86	0.57
1:A:862:LEU:HD21	1:A:866:SER:HA	1.86	0.57
1:B:2333:GLN:HG3	1:B:2342:PHE:HD2	1.69	0.57
1:B:1031:MET:HB2	1:B:1064:LEU:HB3	1.87	0.56
1:B:1981:ARG:NH1	1:B:1983:SER:OG	2.38	0.56
2:I:2:NAG:H3	2:I:2:NAG:H3	1.87	0.56
1:B:941:PRO:HG2	1:B:944:VAL:HG11	1.86	0.56
1:B:2189:LEU:HD22	1:B:2200:LEU:HA	1.87	0.56
1:B:2632:GLU:OE1	1:B:2635:ARG:NH1	2.39	0.56
1:B:859:THR:HG21	1:B:913:ASP:HB2	1.87	0.56
1:B:862:LEU:HD21	1:B:866:SER:HA	1.86	0.56
2:E:2:NAG:H3	2:E:2:NAG:H3	1.87	0.56
3:B:2805:NAG:H3	3:B:2805:NAG:H3	1.88	0.56
1:A:1373:ILE:HB	1:A:1384:ILE:HB	1.86	0.56
1:A:2189:LEU:HD22	1:A:2200:LEU:HA	1.87	0.56
3:A:2805:NAG:H3	3:A:2805:NAG:H3	1.88	0.56
1:B:1886:VAL:HG12	1:B:1896:ILE:HG23	1.88	0.55
1:A:1477:SER:OG	1:A:1478:GLY:N	2.40	0.55
1:A:1589:MET:HG3	1:A:1605:ILE:HG21	1.88	0.55
1:A:1031:MET:HB2	1:A:1064:LEU:HB3	1.87	0.55
1:B:1589:MET:HG3	1:B:1605:ILE:HG21	1.88	0.55
1:A:2632:GLU:OE1	1:A:2635:ARG:NH1	2.38	0.55
1:B:1027:LEU:O	1:B:1068:PHE:N	2.40	0.55
1:A:1886:VAL:HG12	1:A:1896:ILE:HG23	1.88	0.55
1:B:1808:HIS:O	1:B:1810:LYS:N	2.40	0.55
1:B:1532:PRO:O	1:B:1535:GLN:NE2	2.36	0.55
1:A:2029:VAL:H	1:A:2263:GLN:NE2	2.04	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1028:LYS:HD2	1:A:1067:THR:HG22	1.89	0.54
1:A:1740:ALA:HB1	1:A:1744:ASN:HD21	1.71	0.54
1:B:1477:SER:OG	1:B:1478:GLY:N	2.40	0.54
1:B:1740:ALA:HB1	1:B:1744:ASN:HD21	1.71	0.54
1:A:1808:HIS:O	1:A:1810:LYS:N	2.40	0.54
1:B:1917:THR:HB	1:B:1932:ASN:HB2	1.89	0.54
1:B:2029:VAL:H	1:B:2263:GLN:NE2	2.04	0.54
1:B:2134:LYS:NZ	1:B:2137:PRO:O	2.34	0.54
1:B:2641:ARG:NH2	1:B:2685:GLY:O	2.37	0.54
1:A:1019:ARG:NH2	1:A:1140:LYS:O	2.40	0.54
1:A:1235:LEU:HD23	1:A:1244:LEU:HD11	1.90	0.54
1:B:1235:LEU:HD23	1:B:1244:LEU:HD11	1.90	0.54
1:B:2290:TYR:HE2	1:B:2301:GLU:HG3	1.72	0.54
1:B:842:ALA:HB3	1:B:1115:LEU:HD11	1.90	0.53
1:B:1104:GLU:OE1	1:B:1106:ARG:NH1	2.41	0.53
1:B:1749:LYS:HG3	1:B:1764:GLU:HB2	1.89	0.53
1:A:2290:TYR:HE2	1:A:2301:GLU:HG3	1.72	0.53
1:B:1589:MET:HB3	1:B:1605:ILE:HG13	1.89	0.53
1:A:842:ALA:HB3	1:A:1115:LEU:HD11	1.90	0.53
1:B:1019:ARG:NH2	1:B:1140:LYS:O	2.40	0.53
1:B:1187:LEU:HD11	1:B:1504:ALA:HB2	1.91	0.53
1:B:2672:ARG:O	1:B:2676:SER:OG	2.26	0.53
1:B:1364:LEU:HB3	1:B:1375:VAL:HG23	1.90	0.53
1:B:2035:TYR:OH	1:B:2267:ALA:O	2.27	0.53
1:A:1813:LEU:HD21	1:A:1826:TRP:HD1	1.73	0.53
1:A:1960:ARG:NH1	1:A:2223:TYR:O	2.40	0.53
1:A:1104:GLU:OE1	1:A:1106:ARG:NH1	2.41	0.53
1:A:1589:MET:HB3	1:A:1605:ILE:HG13	1.89	0.53
1:A:1917:THR:HB	1:A:1932:ASN:HB2	1.89	0.53
1:B:1028:LYS:HD2	1:B:1067:THR:HG22	1.89	0.53
1:B:1186:ALA:HB3	1:B:1198:GLY:HA3	1.90	0.53
1:A:1749:LYS:HG3	1:A:1764:GLU:HB2	1.89	0.53
1:A:2035:TYR:OH	1:A:2267:ALA:O	2.27	0.53
1:B:1960:ARG:NH1	1:B:2223:TYR:O	2.40	0.53
1:A:1186:ALA:HB3	1:A:1198:GLY:HA3	1.90	0.53
1:B:1226:SER:HB2	1:B:1229:PRO:HA	1.91	0.52
1:A:1364:LEU:HB3	1:A:1375:VAL:HG23	1.90	0.52
1:A:2672:ARG:O	1:A:2676:SER:OG	2.26	0.52
1:B:2092:THR:HB	1:B:2109:GLU:HB3	1.92	0.52
1:A:1027:LEU:O	1:A:1068:PHE:N	2.40	0.52
1:A:2092:THR:HB	1:A:2109:GLU:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1187:LEU:HD11	1:A:1504:ALA:HB2	1.91	0.52
1:A:2595:VAL:HG23	1:A:2612:VAL:HG22	1.92	0.52
1:B:1353:ILE:HD13	1:B:1388:ARG:HD3	1.92	0.52
1:A:1523:SER:OG	1:A:1524:MET:SD	2.67	0.52
1:A:1978:ASP:HB3	1:A:2702:ASN:HB2	1.91	0.52
2:I:1:NAG:O3	2:I:2:NAG:N2	2.43	0.52
1:B:1813:LEU:HD21	1:B:1826:TRP:HD1	1.74	0.52
1:B:1641:GLY:HA2	1:B:2514:LYS:HE2	1.92	0.51
1:B:1928:ARG:HD3	1:B:1941:ILE:HD13	1.92	0.51
1:A:1722:ILE:HB	1:A:1730:SER:HB3	1.92	0.51
2:E:1:NAG:O3	2:E:2:NAG:N2	2.43	0.51
1:B:1044:HIS:NE2	1:B:1093:GLU:OE1	2.36	0.51
1:B:2598:SER:N	1:B:2609:PHE:O	2.42	0.51
1:B:926:PHE:HD2	1:B:934:GLN:HB2	1.76	0.51
1:A:926:PHE:HD2	1:A:934:GLN:HB2	1.76	0.51
1:B:1444:ARG:HB2	1:B:1456:LEU:HD11	1.92	0.51
1:B:2595:VAL:HG23	1:B:2612:VAL:HG22	1.92	0.51
1:B:2578:LEU:HD22	1:B:2593:VAL:HG21	1.93	0.51
1:B:1182:LEU:HD23	1:B:1200:PHE:HB3	1.92	0.51
1:B:1978:ASP:HB3	1:B:2702:ASN:HB2	1.91	0.51
1:A:1226:SER:HB2	1:A:1229:PRO:HA	1.91	0.51
1:A:1432:LEU:O	1:A:1448:VAL:N	2.41	0.51
2:E:1:NAG:H61	2:E:2:NAG:O5	2.11	0.51
2:I:1:NAG:H61	2:I:2:NAG:O5	2.11	0.51
1:A:883:ALA:HB2	1:A:954:LYS:HE3	1.93	0.51
1:A:996:GLU:OE2	1:A:2469:VAL:N	2.41	0.51
1:B:1722:ILE:HB	1:B:1730:SER:HB3	1.92	0.51
1:B:892:ASN:ND2	3:B:2807:NAG:O5	2.44	0.51
1:B:1323:LYS:N	1:B:1331:SER:O	2.44	0.51
1:A:1524:MET:SD	1:A:1524:MET:N	2.84	0.51
1:A:1698:ASP:OD2	1:A:1713:GLN:NE2	2.44	0.50
1:A:892:ASN:ND2	3:A:2807:NAG:O5	2.44	0.50
1:A:2125:MET:HB3	1:A:2127:ARG:HG3	1.93	0.50
1:A:2598:SER:N	1:A:2609:PHE:O	2.42	0.50
1:A:1004:THR:O	1:A:1012:LYS:HB2	2.12	0.50
1:A:1182:LEU:HD23	1:A:1200:PHE:HB3	1.92	0.50
1:A:1928:ARG:HD3	1:A:1941:ILE:HD13	1.92	0.50
1:B:986:SER:HB3	1:B:2475:ARG:HH11	1.76	0.50
1:B:1523:SER:OG	1:B:1524:MET:SD	2.67	0.50
1:B:2560:LYS:NZ	1:B:2617:GLY:O	2.44	0.50
1:A:1353:ILE:HD13	1:A:1388:ARG:HD3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1728:LEU:HB2	1:A:2014:PRO:HD3	1.94	0.50
1:B:883:ALA:HB2	1:B:954:LYS:HE3	1.93	0.50
1:A:2317:THR:HB	1:A:2355:HIS:H	1.77	0.50
1:B:1728:LEU:HB2	1:B:2014:PRO:HD3	1.94	0.50
1:A:1444:ARG:HB2	1:A:1456:LEU:HD11	1.92	0.50
1:B:1003:GLU:HG2	1:B:1012:LYS:HD3	1.93	0.50
1:A:1641:GLY:HA2	1:A:2514:LYS:HE2	1.92	0.50
1:B:1524:MET:SD	1:B:1524:MET:N	2.84	0.50
1:B:1918:MET:HB3	1:B:2505:PHE:CG	2.47	0.50
1:A:1442:ILE:HD11	1:A:1444:ARG:HD3	1.94	0.50
1:A:1560:ASN:HB2	1:A:1573:THR:HB	1.94	0.50
1:A:2252:VAL:O	1:A:2264:PHE:N	2.40	0.50
1:B:1004:THR:O	1:B:1012:LYS:HB2	2.12	0.50
1:B:2317:THR:HB	1:B:2355:HIS:H	1.77	0.50
1:B:2241:VAL:HG13	1:B:2256:THR:HG22	1.94	0.49
1:A:1323:LYS:N	1:A:1331:SER:O	2.44	0.49
1:A:1647:ASP:HB2	1:A:1656:ASN:OD1	2.12	0.49
1:A:1918:MET:HB3	1:A:2505:PHE:CG	2.47	0.49
1:A:2578:LEU:HD22	1:A:2593:VAL:HG21	1.93	0.49
1:B:1698:ASP:OD2	1:B:1713:GLN:NE2	2.44	0.49
1:B:1832:LEU:HD21	1:B:2082:ILE:HD12	1.94	0.49
1:A:986:SER:HB3	1:A:2475:ARG:HH11	1.77	0.49
1:A:1031:MET:HE1	1:A:1045:LEU:HD22	1.93	0.49
1:B:858:SER:OG	1:B:859:THR:N	2.46	0.49
1:B:1974:GLU:OE2	1:B:1981:ARG:NH2	2.46	0.49
1:B:2313:ASP:OD1	1:B:2315:THR:OG1	2.30	0.49
1:B:2330:LYS:NZ	1:B:2348:PHE:O	2.37	0.49
1:A:2180:PRO:HG2	1:A:2183:SER:HB3	1.94	0.49
1:B:1442:ILE:HD11	1:B:1444:ARG:HD3	1.94	0.49
1:B:1129:HIS:O	1:B:1546:HIS:HB2	2.13	0.49
1:B:1982:VAL:HG22	1:B:1998:LEU:HD12	1.95	0.49
1:A:1974:GLU:OE2	1:A:1981:ARG:NH2	2.46	0.49
1:B:985:ARG:NH2	1:B:1001:HIS:O	2.45	0.49
1:B:1031:MET:HE1	1:B:1045:LEU:HD22	1.95	0.49
1:B:1560:ASN:HB2	1:B:1573:THR:HB	1.94	0.49
1:A:778:ARG:HG2	1:A:786:MET:SD	2.53	0.49
1:A:1044:HIS:NE2	1:A:1093:GLU:OE1	2.36	0.49
1:B:1647:ASP:HB2	1:B:1656:ASN:OD1	2.12	0.49
1:B:2252:VAL:O	1:B:2264:PHE:N	2.41	0.49
1:A:1003:GLU:HG2	1:A:1012:LYS:HD3	1.93	0.49
1:A:2313:ASP:OD1	1:A:2315:THR:OG1	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2529:VAL:HG21	1:A:2538:ILE:HD13	1.95	0.49
1:A:2560:LYS:NZ	1:A:2617:GLY:O	2.44	0.49
1:B:2125:MET:HB3	1:B:2127:ARG:HG3	1.93	0.48
1:A:1566:ASP:OD1	1:A:1588:ARG:NH2	2.46	0.48
1:A:2241:VAL:HG13	1:A:2256:THR:HG22	1.94	0.48
1:B:2180:PRO:HG2	1:B:2183:SER:HB3	1.94	0.48
1:B:2529:VAL:HG21	1:B:2538:ILE:HD13	1.95	0.48
1:A:985:ARG:NH2	1:A:1001:HIS:O	2.45	0.48
1:A:1980:THR:HG23	1:A:2000:SER:HB3	1.95	0.48
1:B:761:ARG:NH1	1:A:2611:ASP:OD2	2.46	0.48
1:B:1566:ASP:OD1	1:B:1588:ARG:NH2	2.46	0.48
1:B:2589:ASN:ND2	1:A:1607:THR:OG1	2.46	0.48
1:B:778:ARG:HG2	1:B:786:MET:SD	2.53	0.48
1:B:1733:GLN:HB2	1:B:1749:LYS:HB3	1.96	0.48
1:A:1832:LEU:HD21	1:A:2082:ILE:HD12	1.94	0.48
1:A:858:SER:OG	1:A:859:THR:N	2.46	0.48
1:A:1129:HIS:O	1:A:1546:HIS:HB2	2.13	0.48
1:A:1191:ILE:HD11	1:A:1239:PRO:HA	1.95	0.48
1:A:1046:MET:HG2	1:A:1055:GLN:HG2	1.96	0.48
1:B:2010:ARG:NH2	1:B:2017:ASP:OD2	2.47	0.48
1:A:918:GLY:HA2	1:A:940:ILE:HG13	1.96	0.48
1:B:1769:LYS:HE2	1:B:1771:GLN:HB2	1.96	0.47
1:A:1713:GLN:HB3	1:A:1721:ARG:HB2	1.96	0.47
1:B:918:GLY:HA2	1:B:940:ILE:HG13	1.96	0.47
1:B:1046:MET:HG2	1:B:1055:GLN:HG2	1.96	0.47
1:B:1845:ILE:O	1:B:1859:TYR:OH	2.29	0.47
1:A:844:LYS:HE3	1:A:844:LYS:HB2	1.68	0.47
1:B:970:ARG:HH21	1:B:1385:THR:HG21	1.79	0.47
1:B:2248:LEU:HD13	1:B:2454:LEU:HD13	1.95	0.47
1:A:2135:ILE:HD11	1:A:2320:ALA:HB2	1.95	0.47
1:A:2624:ARG:HD3	1:A:2627:MET:SD	2.54	0.47
1:B:2106:ILE:O	1:B:2117:TRP:HA	2.14	0.47
1:B:2172:ASN:ND2	1:B:2195:ASP:OD2	2.43	0.47
1:B:2440:PHE:HD1	1:B:2441:PRO:HD2	1.79	0.47
1:B:2135:ILE:HD11	1:B:2320:ALA:HB2	1.96	0.47
1:A:1982:VAL:HG22	1:A:1998:LEU:HD12	1.95	0.47
1:B:1320:MET:HB2	1:B:1334:LEU:HD13	1.96	0.47
1:B:1997:ASN:HB3	1:B:2006:THR:HG23	1.97	0.47
1:A:758:SER:O	1:A:758:SER:OG	2.32	0.47
1:A:985:ARG:HH22	1:A:992:PRO:HB3	1.80	0.47
1:A:1320:MET:HB2	1:A:1334:LEU:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2248:LEU:HD13	1:A:2454:LEU:HD13	1.95	0.47
1:B:1980:THR:HG23	1:B:2000:SER:HB3	1.95	0.47
1:B:2595:VAL:HB	1:B:2612:VAL:HG13	1.97	0.47
1:A:1444:ARG:HA	1:A:1459:GLY:HA3	1.97	0.47
1:A:1448:VAL:HG22	1:A:1454:ILE:HG12	1.97	0.47
1:B:2624:ARG:HD3	1:B:2627:MET:SD	2.54	0.47
1:B:1191:ILE:HD11	1:B:1239:PRO:HA	1.95	0.47
1:B:1444:ARG:HA	1:B:1459:GLY:HA3	1.97	0.47
1:B:1448:VAL:HG22	1:B:1454:ILE:HG12	1.97	0.47
1:A:2010:ARG:NH2	1:A:2017:ASP:OD2	2.47	0.47
1:A:2553:LEU:HD23	1:A:2553:LEU:HA	1.75	0.47
1:B:1713:GLN:HB3	1:B:1721:ARG:HB2	1.96	0.46
1:A:970:ARG:HH21	1:A:1385:THR:HG21	1.79	0.46
1:A:1042:LYS:HG2	1:A:1057:TRP:HE1	1.80	0.46
1:A:2440:PHE:HD1	1:A:2441:PRO:HD2	1.79	0.46
1:A:921:SER:N	1:A:1239:PRO:O	2.46	0.46
1:A:1721:ARG:NH2	1:A:1729:ASP:OD1	2.45	0.46
1:B:1584:ARG:O	1:B:1585:ASP:HB3	2.14	0.46
1:B:2596:SER:HB2	1:A:763:THR:HA	1.98	0.46
1:A:1584:ARG:O	1:A:1585:ASP:HB3	2.15	0.46
1:A:1733:GLN:HB2	1:A:1749:LYS:HB3	1.96	0.46
1:A:1769:LYS:HE2	1:A:1771:GLN:HB2	1.96	0.46
1:A:2106:ILE:O	1:A:2117:TRP:HA	2.14	0.46
1:A:2297:LEU:O	1:A:2312:SER:OG	2.30	0.46
1:B:985:ARG:HH22	1:B:992:PRO:HB3	1.80	0.46
1:B:1750:ARG:HB3	1:B:1763:VAL:HG13	1.97	0.46
1:B:758:SER:O	1:B:758:SER:OG	2.32	0.46
1:B:1607:THR:OG1	1:A:2589:ASN:ND2	2.46	0.46
1:A:1049:VAL:HG13	1:A:1050:VAL:HG22	1.98	0.46
1:B:763:THR:HA	1:A:2596:SER:HB2	1.97	0.46
1:B:996:GLU:OE2	1:B:2469:VAL:N	2.41	0.46
1:A:2595:VAL:HB	1:A:2612:VAL:HG13	1.97	0.46
1:B:1595:SER:HB2	1:B:1599:GLN:HB3	1.98	0.46
1:A:1206:ILE:HG13	1:A:1212:VAL:HG22	1.97	0.46
1:A:1731:HIS:NE2	1:A:1733:GLN:OE1	2.42	0.46
1:A:2539:LYS:HG2	1:A:2577:THR:HB	1.98	0.46
1:B:1042:LYS:HG2	1:B:1057:TRP:HE1	1.80	0.46
1:B:2353:GLY:HA3	1:B:2359:TYR:HB2	1.98	0.46
1:B:2683:TYR:OH	1:B:2708:ARG:NH2	2.49	0.46
1:A:757:ASN:ND2	1:A:781:GLY:O	2.48	0.46
1:A:1595:SER:HB2	1:A:1599:GLN:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1997:ASN:HB3	1:A:2006:THR:HG23	1.97	0.46
1:B:853:LEU:HD22	1:B:859:THR:HB	1.98	0.46
1:B:1660:PRO:O	1:B:1922:ARG:NE	2.49	0.46
1:B:2534:ASN:N	1:B:2537:CYS:SG	2.89	0.46
1:A:1203:VAL:N	1:A:1216:LEU:O	2.48	0.46
1:A:1921:ILE:HG12	1:A:1930:ILE:HD11	1.98	0.46
1:B:2414:ASP:OD1	1:B:2414:ASP:N	2.49	0.45
1:A:1582:ILE:HD11	1:A:1584:ARG:NH2	2.32	0.45
1:B:1539:ILE:HD12	1:B:1548:TYR:HE1	1.82	0.45
1:A:2574:ASP:O	1:A:2577:THR:OG1	2.35	0.45
1:A:2683:TYR:OH	1:A:2708:ARG:NH2	2.49	0.45
1:B:919:GLY:N	1:B:940:ILE:O	2.43	0.45
1:B:921:SER:N	1:B:1239:PRO:O	2.46	0.45
1:B:1750:ARG:HD3	1:B:1752:MET:SD	2.56	0.45
1:B:2611:ASP:OD2	1:A:761:ARG:NH1	2.44	0.45
1:A:2534:ASN:N	1:A:2537:CYS:SG	2.89	0.45
1:B:1308:ASP:HB2	1:B:1371:ASN:HD21	1.82	0.45
1:B:1582:ILE:HD11	1:B:1584:ARG:NH2	2.31	0.45
1:A:1750:ARG:HB3	1:A:1763:VAL:HG13	1.97	0.45
1:B:969:VAL:N	1:B:1094:TYR:OH	2.50	0.45
1:B:1058:PHE:HB3	1:B:1064:LEU:HD21	1.99	0.45
1:B:1923:SER:OG	1:B:1924:ILE:N	2.49	0.45
1:A:1847:SER:HB2	1:A:1856:LYS:HG3	1.98	0.45
1:B:1206:ILE:HG13	1:B:1212:VAL:HG22	1.97	0.45
1:B:1721:ARG:NH2	1:B:1729:ASP:OD1	2.45	0.45
1:B:1921:ILE:HG12	1:B:1930:ILE:HD11	1.98	0.45
1:B:2574:ASP:O	1:B:2577:THR:OG1	2.35	0.45
1:A:1130:VAL:HG13	1:A:1139:TYR:HB2	1.98	0.45
1:B:1734:THR:CG2	1:B:1745:PRO:HB2	2.47	0.45
1:B:1838:THR:OG1	1:B:1847:SER:OG	2.28	0.45
1:A:1305:MET:HE2	1:A:1305:MET:HB3	1.92	0.45
1:A:1734:THR:CG2	1:A:1745:PRO:HB2	2.47	0.45
1:B:1532:PRO:HB3	1:B:1746:THR:HG22	1.98	0.45
1:B:1731:HIS:NE2	1:B:1733:GLN:OE1	2.42	0.45
1:B:1754:LEU:HD21	1:B:2015:LEU:HD13	1.99	0.45
1:B:1838:THR:HG21	3:B:2803:NAG:H62	1.99	0.45
1:B:2605:ARG:HD2	1:B:2605:ARG:O	2.17	0.45
1:A:1660:PRO:O	1:A:1922:ARG:NE	2.49	0.45
1:B:1071:ASP:HB3	1:B:1073:THR:HG22	1.98	0.45
1:B:1847:SER:HB2	1:B:1856:LYS:HG3	1.98	0.45
1:A:1850:ARG:HD2	1:A:2415:VAL:HG12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1049:VAL:HG13	1:B:1050:VAL:HG22	1.98	0.45
1:B:2539:LYS:HG2	1:B:2577:THR:HB	1.98	0.45
1:A:969:VAL:N	1:A:1094:TYR:OH	2.50	0.45
1:A:1923:SER:OG	1:A:1924:ILE:N	2.49	0.45
1:A:853:LEU:HD22	1:A:859:THR:HB	1.98	0.44
1:A:1582:ILE:HG22	1:A:1593:VAL:HG13	1.99	0.44
1:A:1750:ARG:HD3	1:A:1752:MET:SD	2.56	0.44
1:A:2327:LEU:HD23	1:A:2327:LEU:HA	1.82	0.44
1:B:1582:ILE:HG22	1:B:1593:VAL:HG13	1.99	0.44
1:B:1916:HIS:HB3	1:B:1931:TYR:HE1	1.82	0.44
1:A:1905:LEU:HD21	1:A:1908:ILE:HD11	1.99	0.44
1:A:2353:GLY:HA3	1:A:2359:TYR:HB2	1.98	0.44
1:A:954:LYS:HB3	1:A:954:LYS:HE2	1.78	0.44
1:A:1532:PRO:HB3	1:A:1746:THR:HG22	1.98	0.44
1:B:1130:VAL:HG13	1:B:1139:TYR:HB2	1.98	0.44
1:A:783:ASP:OD1	1:A:783:ASP:N	2.51	0.44
1:A:1754:LEU:HD21	1:A:2015:LEU:HD13	1.99	0.44
1:B:1911:PRO:HB2	1:B:2171:LEU:HB3	1.99	0.44
1:A:919:GLY:N	1:A:940:ILE:O	2.43	0.44
1:A:1071:ASP:HB3	1:A:1073:THR:HG22	1.98	0.44
1:B:1004:THR:HG22	1:B:1636:LYS:HE2	1.99	0.44
1:A:801:LEU:HD12	1:A:801:LEU:HA	1.85	0.44
1:A:884:ASP:OD1	1:A:884:ASP:N	2.40	0.44
1:A:2255:LYS:HB2	1:A:2261:HIS:CD2	2.52	0.44
1:B:986:SER:HB3	1:B:2475:ARG:HD3	2.00	0.44
1:B:2297:LEU:O	1:B:2312:SER:OG	2.30	0.44
1:A:1004:THR:HG22	1:A:1636:LYS:HE2	1.99	0.44
1:A:1058:PHE:HB3	1:A:1064:LEU:HD21	1.99	0.44
1:A:1308:ASP:HB2	1:A:1371:ASN:HD21	1.82	0.44
1:A:1838:THR:OG1	1:A:1847:SER:OG	2.28	0.44
2:I:1:NAG:H4	2:I:2:NAG:H2	1.77	0.44
1:B:1432:LEU:O	1:B:1448:VAL:N	2.41	0.44
1:B:1850:ARG:HD2	1:B:2415:VAL:HG12	1.99	0.44
1:B:2265:PHE:HB2	1:B:2277:HIS:HB2	1.99	0.44
1:A:2605:ARG:HD2	1:A:2605:ARG:O	2.17	0.44
1:B:1378:ASN:HB3	1:B:1379:ASN:H	1.57	0.43
1:B:2449:GLU:H	1:B:2449:GLU:HG2	1.61	0.43
1:B:920:ALA:HB2	1:B:1191:ILE:HG23	2.00	0.43
1:B:1102:LEU:HD12	1:B:1102:LEU:H	1.83	0.43
1:B:1905:LEU:HD21	1:B:1908:ILE:HD11	1.99	0.43
1:A:1004:THR:HG21	1:A:1624:PHE:HZ	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1838:THR:HG21	3:A:2803:NAG:H62	1.99	0.43
1:B:801:LEU:HD12	1:B:801:LEU:HA	1.85	0.43
1:B:2189:LEU:HD21	1:B:2200:LEU:HD12	2.01	0.43
1:B:2478:LYS:HE3	1:B:2478:LYS:HB3	1.86	0.43
1:B:2599:THR:HA	1:B:2608:ARG:HA	1.99	0.43
1:A:1102:LEU:HD12	1:A:1102:LEU:H	1.84	0.43
1:A:1539:ILE:HD12	1:A:1548:TYR:HE1	1.81	0.43
1:B:1307:ILE:HG12	1:B:1313:ILE:HG12	2.00	0.43
1:B:1855:GLU:OE2	1:B:1868:ARG:NH1	2.46	0.43
1:A:2140:ASN:H	3:A:2805:NAG:H2	1.84	0.43
1:A:2524:ARG:HH22	1:A:2546:ASN:HB3	1.83	0.43
1:B:2074:LYS:HE3	1:B:2074:LYS:HB3	1.80	0.43
1:A:749:LYS:HB2	1:A:749:LYS:HE2	1.83	0.43
1:A:1396:ARG:HA	1:A:1396:ARG:HD3	1.79	0.43
1:A:1911:PRO:HB2	1:A:2171:LEU:HB3	1.99	0.43
1:A:2371:ARG:CZ	1:A:2384:ASP:HB2	2.49	0.43
1:A:2647:ARG:HB3	1:A:2701:ALA:HB2	2.01	0.43
1:B:2255:LYS:HB2	1:B:2261:HIS:CD2	2.53	0.43
1:B:2647:ARG:HB3	1:B:2701:ALA:HB2	2.01	0.43
1:A:1916:HIS:HB3	1:A:1931:TYR:HE1	1.83	0.43
1:B:1004:THR:HG21	1:B:1624:PHE:HZ	1.82	0.43
1:B:1763:VAL:HG23	1:B:1785:VAL:HG22	2.01	0.43
1:A:802:ILE:HD12	1:A:802:ILE:HA	1.82	0.43
1:A:820:TYR:CE2	1:A:928:ARG:HD2	2.54	0.43
1:A:1307:ILE:HG12	1:A:1313:ILE:HG12	2.00	0.43
1:A:2265:PHE:HB2	1:A:2277:HIS:HB2	1.99	0.43
1:B:1153:PRO:HB2	1:B:1514:VAL:HG13	2.00	0.43
1:B:2555:PHE:O	1:B:2562:THR:OG1	2.30	0.43
1:A:2599:THR:HA	1:A:2608:ARG:HA	1.99	0.43
1:A:920:ALA:HB2	1:A:1191:ILE:HG23	2.00	0.43
1:A:1153:PRO:HB2	1:A:1514:VAL:HG13	2.00	0.43
1:A:2116:TYR:OH	1:A:2118:ILE:HD11	2.19	0.43
1:B:875:VAL:HG12	1:B:877:ARG:HG3	2.01	0.43
1:A:2307:GLU:HG3	1:A:2324:SER:HB3	2.00	0.43
1:B:1169:CYS:HB2	1:B:1172:CYS:HB3	1.44	0.42
1:B:2371:ARG:CZ	1:B:2384:ASP:HB2	2.49	0.42
1:B:2518:LEU:HD11	1:B:2544:LEU:HD13	2.02	0.42
1:A:1844:GLN:NE2	1:A:1863:GLY:O	2.51	0.42
1:A:2330:LYS:NZ	1:A:2348:PHE:O	2.37	0.42
1:B:1847:SER:HB2	1:B:1856:LYS:HE2	2.01	0.42
1:B:2131:ARG:O	1:B:2144:TYR:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2140:ASN:H	3:B:2805:NAG:H2	1.84	0.42
1:B:2524:ARG:HH22	1:B:2546:ASN:HB3	1.83	0.42
1:A:986:SER:HB3	1:A:2475:ARG:HD3	2.00	0.42
1:A:2518:LEU:HD11	1:A:2544:LEU:HD13	2.02	0.42
1:B:757:ASN:ND2	1:B:781:GLY:O	2.48	0.42
1:B:1203:VAL:N	1:B:1216:LEU:O	2.49	0.42
1:B:2306:ASP:HB3	1:B:2308:PHE:HE1	1.85	0.42
1:A:875:VAL:HG12	1:A:877:ARG:HG3	2.01	0.42
1:A:1496:SER:OG	1:A:1498:ASP:OD2	2.27	0.42
1:A:2704:ILE:HD13	1:A:2704:ILE:HA	1.87	0.42
1:B:749:LYS:HB2	1:B:749:LYS:HE2	1.83	0.42
1:B:955:LYS:HA	1:B:955:LYS:HD2	1.88	0.42
1:B:1505:ASP:N	1:B:1505:ASP:OD1	2.53	0.42
1:B:2116:TYR:OH	1:B:2118:ILE:HD11	2.19	0.42
1:B:2307:GLU:HG3	1:B:2324:SER:HB3	2.00	0.42
1:A:1154:VAL:HG11	1:A:1742:THR:HG21	2.01	0.42
1:A:1505:ASP:OD1	1:A:1505:ASP:N	2.53	0.42
1:A:825:PRO:HB2	1:A:830:ILE:HD11	2.02	0.42
1:A:1169:CYS:HB2	1:A:1172:CYS:HB3	1.44	0.42
1:B:820:TYR:CE2	1:B:928:ARG:HD2	2.54	0.42
1:B:2166:ARG:HH21	1:B:2179:ASN:HD21	1.67	0.42
1:B:2350:LEU:HD23	1:B:2350:LEU:HA	1.81	0.42
1:B:2511:LEU:HD12	1:B:2511:LEU:H	1.85	0.42
1:A:2189:LEU:HD21	1:A:2200:LEU:HD12	2.00	0.42
1:B:2219:GLU:HA	1:B:2234:SER:HA	2.01	0.42
1:A:1564:SER:OG	1:A:1570:THR:OG1	2.37	0.42
1:A:1763:VAL:HG23	1:A:1785:VAL:HG22	2.01	0.42
1:B:1771:GLN:HA	1:B:1776:VAL:HA	2.02	0.42
1:A:2517:MET:CG	1:A:2528:ASN:H	2.33	0.42
1:B:1152:PRO:HA	1:B:1153:PRO:HD3	1.93	0.42
1:B:1154:VAL:HG11	1:B:1742:THR:HG21	2.01	0.42
1:B:1396:ARG:HD3	1:B:1396:ARG:HA	1.79	0.42
1:A:1105:LYS:HB3	1:A:1105:LYS:HE3	1.68	0.42
1:B:783:ASP:OD1	1:B:783:ASP:N	2.51	0.42
1:B:2517:MET:CG	1:B:2528:ASN:H	2.32	0.42
1:B:2589:ASN:HD22	1:A:1607:THR:HG1	1.66	0.42
1:A:1025:SER:OG	1:A:1111:GLN:O	2.38	0.42
1:B:1549:THR:HG22	1:B:1559:TYR:HB2	2.02	0.41
1:A:774:GLN:H	1:A:774:GLN:HG2	1.60	0.41
1:A:2306:ASP:HB3	1:A:2308:PHE:HE1	1.85	0.41
1:B:1011:LEU:HD11	1:B:1572:VAL:HG11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1152:PRO:HA	1:A:1153:PRO:HD3	1.93	0.41
1:A:1549:THR:HG22	1:A:1559:TYR:HB2	2.02	0.41
1:A:1886:VAL:HA	1:A:1896:ILE:HA	2.03	0.41
1:B:941:PRO:HD2	1:B:944:VAL:HG21	2.02	0.41
1:A:2131:ARG:O	1:A:2144:TYR:HB2	2.19	0.41
1:A:2172:ASN:ND2	1:A:2195:ASP:OD2	2.43	0.41
1:B:1025:SER:OG	1:B:1111:GLN:O	2.38	0.41
1:B:1553:VAL:O	1:B:1797:ARG:NH2	2.53	0.41
1:B:1844:GLN:NE2	1:B:1863:GLY:O	2.51	0.41
1:A:1771:GLN:HA	1:A:1776:VAL:HA	2.02	0.41
1:A:1942:THR:O	1:A:1942:THR:OG1	2.37	0.41
1:B:1274:ALA:HA	1:B:1296:GLU:HG2	2.03	0.41
1:B:1305:MET:HE2	1:B:1305:MET:HB3	1.89	0.41
1:B:1785:VAL:HG21	1:B:2437:ILE:HG12	2.02	0.41
1:B:1886:VAL:HG12	1:B:1896:ILE:HG12	2.02	0.41
1:B:1886:VAL:HA	1:B:1896:ILE:HA	2.03	0.41
1:A:1847:SER:HB2	1:A:1856:LYS:HE2	2.01	0.41
2:E:1:NAG:H4	2:E:2:NAG:H2	1.77	0.41
1:A:1833:MET:HB3	1:A:1850:ARG:NH1	2.35	0.41
1:A:1848:ILE:HD12	1:A:2419:ILE:HD13	2.02	0.41
1:A:2116:TYR:OH	1:A:2312:SER:O	2.24	0.41
1:B:825:PRO:HB2	1:B:830:ILE:HD11	2.02	0.41
1:B:1749:LYS:NZ	1:B:1764:GLU:OE1	2.49	0.41
1:B:1926:TYR:HB3	1:B:1951:LEU:HD12	2.02	0.41
1:B:2358:LEU:HD12	1:B:2358:LEU:HA	1.82	0.41
1:A:755:LEU:HD23	1:A:755:LEU:HA	1.93	0.41
1:A:879:GLN:HA	1:A:910:GLY:O	2.21	0.41
1:A:1011:LEU:HD11	1:A:1572:VAL:HG11	2.02	0.41
1:A:1553:VAL:O	1:A:1797:ARG:NH2	2.53	0.41
1:A:1864:ARG:HB3	1:A:1880:TYR:CZ	2.56	0.41
1:A:2219:GLU:HA	1:A:2234:SER:HA	2.01	0.41
1:A:1159:MET:HG2	1:A:1181:LEU:HD11	2.03	0.41
1:A:2077:VAL:HG11	1:A:2293:LEU:HD11	2.03	0.41
1:B:879:GLN:HA	1:B:910:GLY:O	2.21	0.41
1:B:1116:ASP:OD1	1:B:1116:ASP:N	2.52	0.41
1:B:1945:ASN:OD1	1:B:1946:GLU:N	2.53	0.41
1:A:820:TYR:HE2	1:A:929:SER:H	1.69	0.41
1:A:1274:ALA:HA	1:A:1296:GLU:HG2	2.02	0.41
1:A:1749:LYS:NZ	1:A:1764:GLU:OE1	2.50	0.41
1:A:1994:LYS:HA	1:A:1994:LYS:HD3	1.84	0.41
1:A:2166:ARG:HH21	1:A:2179:ASN:HD21	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2216:ARG:NH2	1:A:2363:THR:O	2.36	0.41
1:B:1714:ILE:HD11	1:B:2469:VAL:HG23	2.03	0.41
1:B:2327:LEU:HD23	1:B:2327:LEU:HA	1.82	0.41
1:A:1582:ILE:HB	1:A:1593:VAL:HG22	2.03	0.41
1:A:1886:VAL:HG12	1:A:1896:ILE:HG12	2.03	0.41
1:A:1898:GLU:H	1:A:1898:GLU:HG2	1.70	0.41
1:B:1040:LEU:HD23	1:B:1040:LEU:HA	1.91	0.40
1:B:1299:LEU:HD23	1:B:1317:ASP:OD2	2.21	0.40
1:B:1833:MET:HB3	1:B:1850:ARG:NH1	2.35	0.40
1:B:2391:ILE:HG13	1:B:2398:PHE:CG	2.57	0.40
1:A:1714:ILE:HD11	1:A:2469:VAL:HG23	2.03	0.40
1:B:752:CYS:HB2	1:B:755:LEU:HA	2.04	0.40
1:B:802:ILE:HD12	1:B:802:ILE:HA	1.82	0.40
1:B:2274:ARG:HD3	1:B:2291:TYR:CD1	2.57	0.40
1:A:941:PRO:HD2	1:A:944:VAL:HG21	2.02	0.40
1:A:2391:ILE:HG13	1:A:2398:PHE:CG	2.57	0.40
1:B:1159:MET:HG2	1:B:1181:LEU:HD11	2.03	0.40
1:B:1864:ARG:HB3	1:B:1880:TYR:CZ	2.56	0.40
1:B:2562:THR:HG22	1:B:2620:ALA:HB3	2.03	0.40
1:A:2511:LEU:HD12	1:A:2511:LEU:H	1.85	0.40
1:B:844:LYS:HE3	1:B:844:LYS:HB2	1.68	0.40
1:B:1582:ILE:HB	1:B:1593:VAL:HG22	2.03	0.40
1:A:1200:PHE:HA	1:A:1233:TYR:OH	2.21	0.40
1:A:2085:ILE:HG23	1:A:2094:THR:HG22	2.04	0.40
1:A:877:ARG:HA	1:A:912:PHE:O	2.22	0.40
1:A:1785:VAL:HG21	1:A:2437:ILE:HG12	2.02	0.40
1:A:1971:ARG:HA	1:A:1971:ARG:HD2	1.96	0.40
1:A:2478:LYS:HE3	1:A:2478:LYS:HB3	1.86	0.40
1:A:2592:ASN:HD22	1:A:2615:GLN:HE22	1.69	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	1858/2407 (77%)	1709 (92%)	148 (8%)	1 (0%)	51	83
1	B	1858/2407 (77%)	1708 (92%)	149 (8%)	1 (0%)	51	83
All	All	3716/4814 (77%)	3417 (92%)	297 (8%)	2 (0%)	54	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1229	PRO
1	A	1229	PRO

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	1544/2075 (74%)	1496 (97%)	48 (3%)	40	70
1	B	1544/2075 (74%)	1497 (97%)	47 (3%)	41	71
All	All	3088/4150 (74%)	2993 (97%)	95 (3%)	43	70

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	820	TYR
1	B	847	TYR
1	B	852	PHE
1	B	945	PHE
1	B	951	LEU
1	B	1177	ASP
1	B	1179	ASN
1	B	1200	PHE
1	B	1222	ASP
1	B	1223	PHE
1	B	1320	MET
1	B	1333	LEU
1	B	1351	MET
1	B	1483	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	1505	ASP
1	B	1506	LEU
1	B	1515	SER
1	B	1638	ASP
1	B	1671	MET
1	B	1716	TYR
1	B	1796	ASP
1	B	1814	ARG
1	B	1856	LYS
1	B	2005	CYS
1	B	2042	ARG
1	B	2045	SER
1	B	2051	ASN
1	B	2064	ASP
1	B	2081	ASP
1	B	2084	GLN
1	B	2108	TYR
1	B	2125	MET
1	B	2164	MET
1	B	2262	LEU
1	B	2268	ASP
1	B	2328	MET
1	B	2360	ASP
1	B	2379	ARG
1	B	2394	ASP
1	B	2486	MET
1	B	2537	CYS
1	B	2615	GLN
1	B	2664	ARG
1	B	2679	LYS
1	B	2690	SER
1	B	2699	ASP
1	B	2702	ASN
1	A	820	TYR
1	A	847	TYR
1	A	852	PHE
1	A	945	PHE
1	A	951	LEU
1	A	1177	ASP
1	A	1179	ASN
1	A	1200	PHE
1	A	1222	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	1223	PHE
1	A	1320	MET
1	A	1333	LEU
1	A	1351	MET
1	A	1483	LYS
1	A	1505	ASP
1	A	1506	LEU
1	A	1515	SER
1	A	1638	ASP
1	A	1671	MET
1	A	1716	TYR
1	A	1796	ASP
1	A	1814	ARG
1	A	1856	LYS
1	A	2005	CYS
1	A	2042	ARG
1	A	2045	SER
1	A	2051	ASN
1	A	2064	ASP
1	A	2081	ASP
1	A	2084	GLN
1	A	2108	TYR
1	A	2125	MET
1	A	2143	LYS
1	A	2164	MET
1	A	2262	LEU
1	A	2268	ASP
1	A	2328	MET
1	A	2360	ASP
1	A	2379	ARG
1	A	2394	ASP
1	A	2486	MET
1	A	2537	CYS
1	A	2615	GLN
1	A	2664	ARG
1	A	2679	LYS
1	A	2690	SER
1	A	2699	ASP
1	A	2702	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1969	GLN
1	B	2263	GLN
1	B	2534	ASN
1	A	1969	GLN
1	A	2263	GLN
1	A	2534	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

16 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	2,1	14,14,15	0.19	0	17,19,21	0.41	0
2	NAG	C	2	2	14,14,15	0.20	0	17,19,21	0.42	0
2	NAG	D	1	2,1	14,14,15	0.32	0	17,19,21	0.39	0
2	NAG	D	2	2	14,14,15	0.24	0	17,19,21	0.42	0
2	NAG	E	1	2,1	14,14,15	0.24	0	17,19,21	0.49	0
2	NAG	E	2	2	14,14,15	0.62	1 (7%)	17,19,21	1.27	1 (5%)
2	NAG	F	1	2,1	14,14,15	0.25	0	17,19,21	0.57	0
2	NAG	F	2	2	14,14,15	0.22	0	17,19,21	0.40	0
2	NAG	G	1	2,1	14,14,15	0.20	0	17,19,21	0.40	0
2	NAG	G	2	2	14,14,15	0.21	0	17,19,21	0.42	0
2	NAG	H	1	2,1	14,14,15	0.32	0	17,19,21	0.39	0
2	NAG	H	2	2	14,14,15	0.25	0	17,19,21	0.42	0
2	NAG	I	1	2,1	14,14,15	0.24	0	17,19,21	0.49	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	I	2	2	14,14,15	0.62	0	17,19,21	1.26	1 (5%)
2	NAG	J	1	2,1	14,14,15	0.24	0	17,19,21	0.57	0
2	NAG	J	2	2	14,14,15	0.23	0	17,19,21	0.40	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	2,1	-	4/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	NAG	D	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	D	2	2	-	1/6/23/26	0/1/1/1
2	NAG	E	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	E	2	2	-	5/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	H	2	2	-	1/6/23/26	0/1/1/1
2	NAG	I	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	I	2	2	-	5/6/23/26	0/1/1/1
2	NAG	J	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2	NAG	C1-C2	2.02	1.55	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	2	NAG	C2-N2-C7	4.30	129.03	122.90
2	E	2	NAG	C2-N2-C7	4.30	129.03	122.90

There are no chirality outliers.

All (42) torsion outliers are listed below:

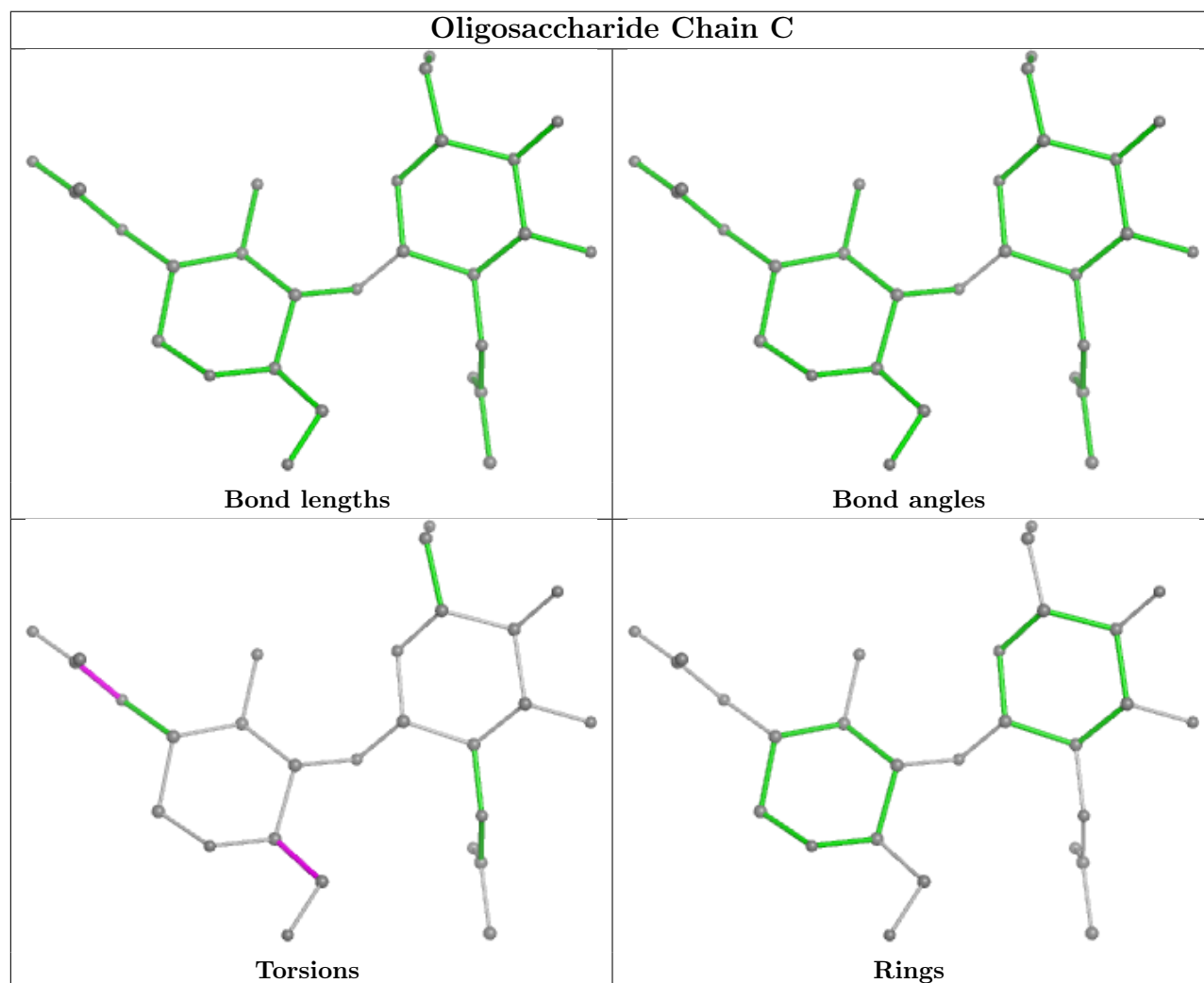
Mol	Chain	Res	Type	Atoms
2	E	1	NAG	O5-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6
2	I	1	NAG	C4-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2
2	F	2	NAG	C8-C7-N2-C2
2	F	2	NAG	O7-C7-N2-C2
2	G	1	NAG	C8-C7-N2-C2
2	G	1	NAG	O7-C7-N2-C2
2	H	1	NAG	C8-C7-N2-C2
2	H	1	NAG	O7-C7-N2-C2
2	I	1	NAG	C8-C7-N2-C2
2	I	1	NAG	O7-C7-N2-C2
2	I	2	NAG	C8-C7-N2-C2
2	I	2	NAG	O7-C7-N2-C2
2	J	2	NAG	C8-C7-N2-C2
2	J	2	NAG	O7-C7-N2-C2
2	C	1	NAG	O5-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	I	2	NAG	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
2	J	1	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
2	E	2	NAG	C3-C2-N2-C7
2	F	1	NAG	C3-C2-N2-C7
2	I	2	NAG	C3-C2-N2-C7
2	J	1	NAG	C3-C2-N2-C7

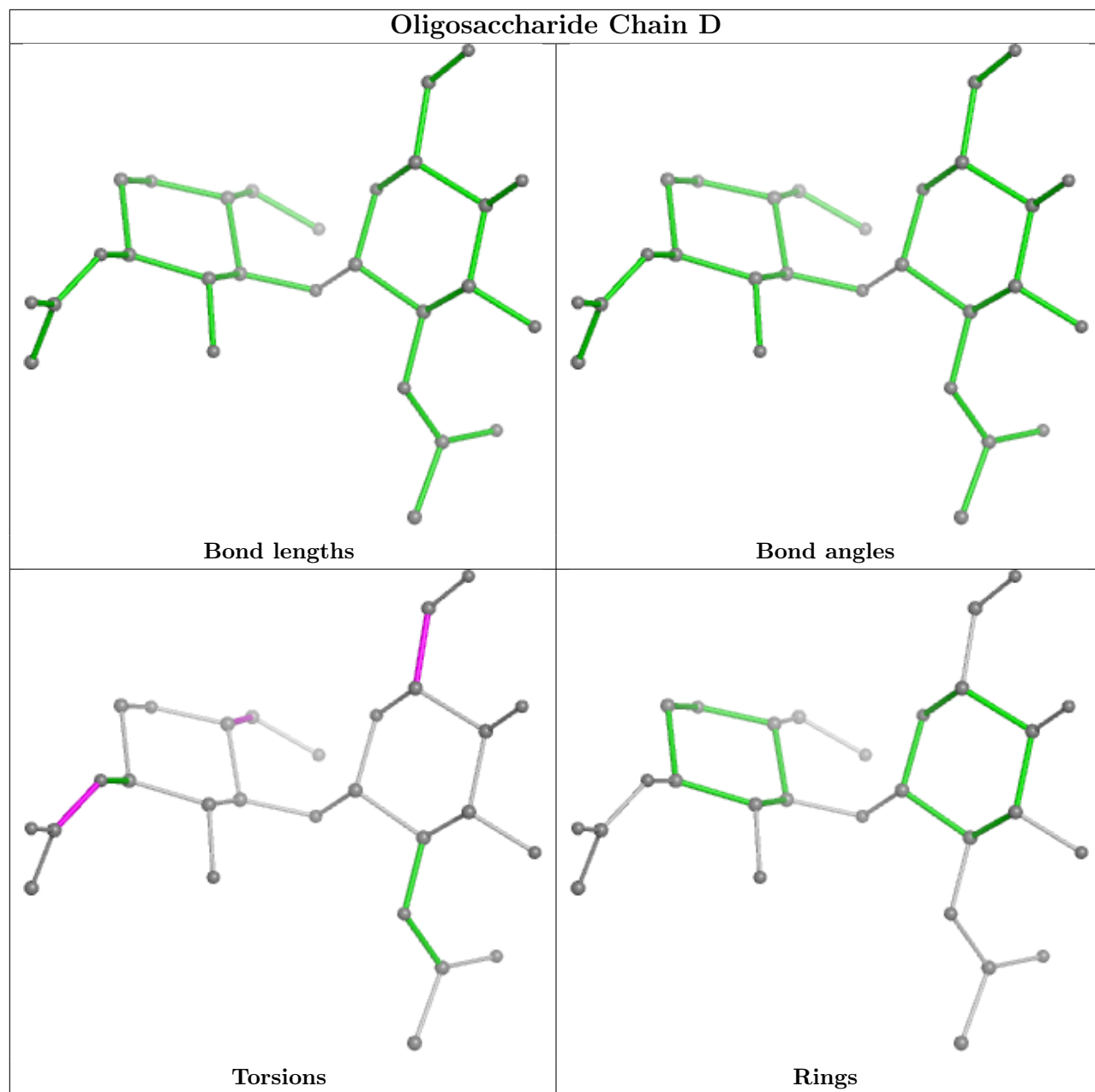
There are no ring outliers.

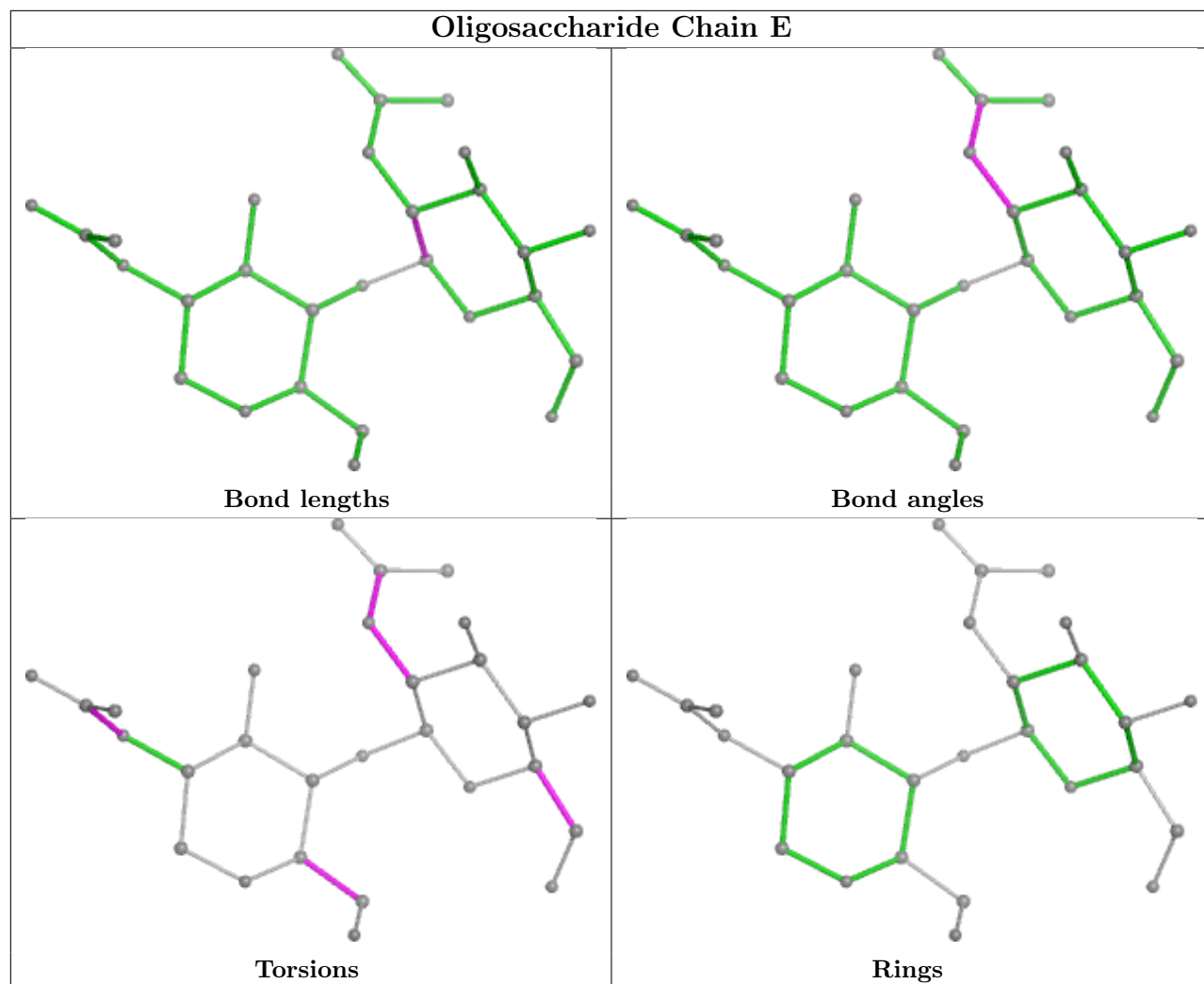
4 monomers are involved in 8 short contacts:

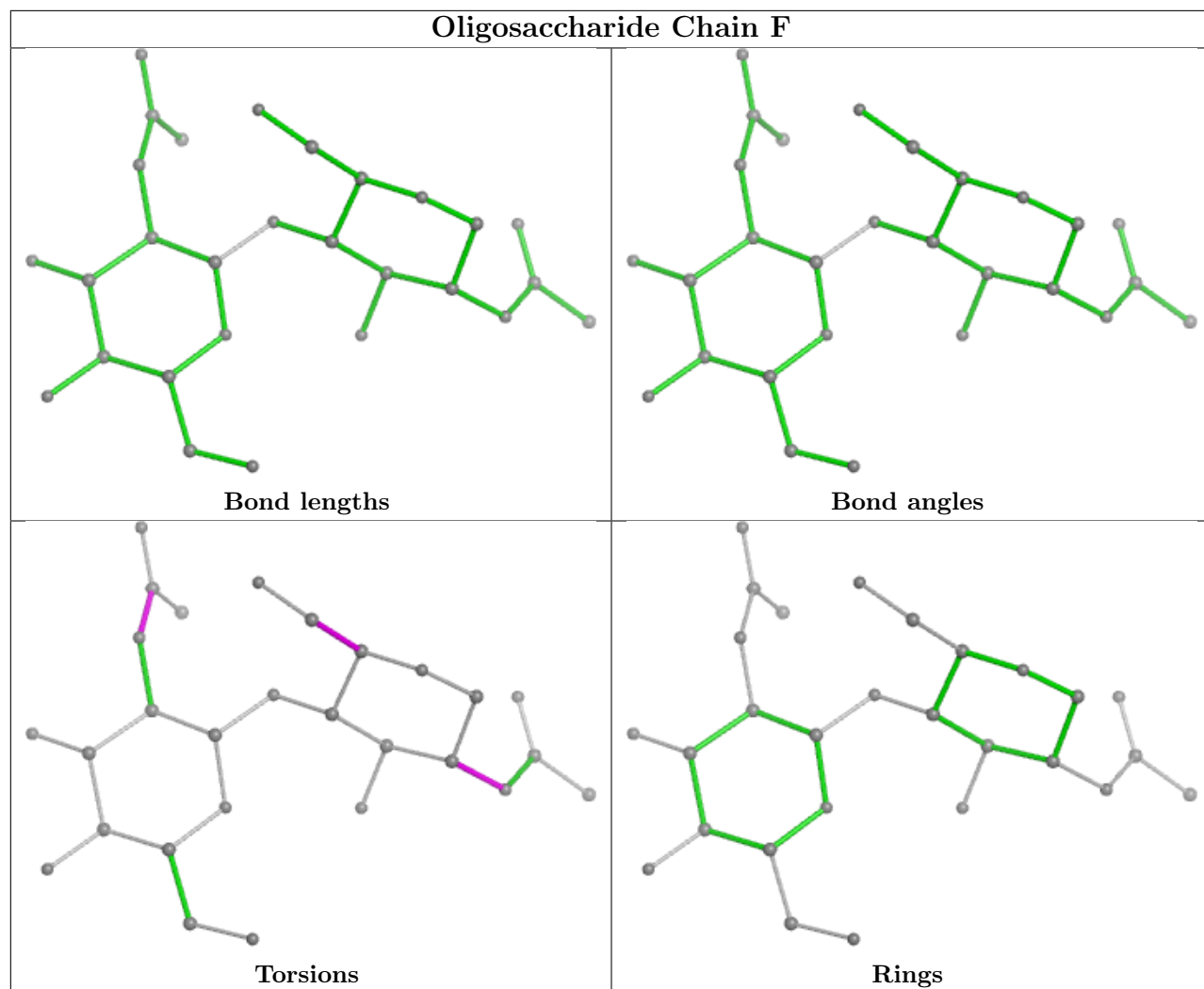
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	2	NAG	4	0
2	I	1	NAG	3	0
2	E	2	NAG	4	0
2	E	1	NAG	3	0

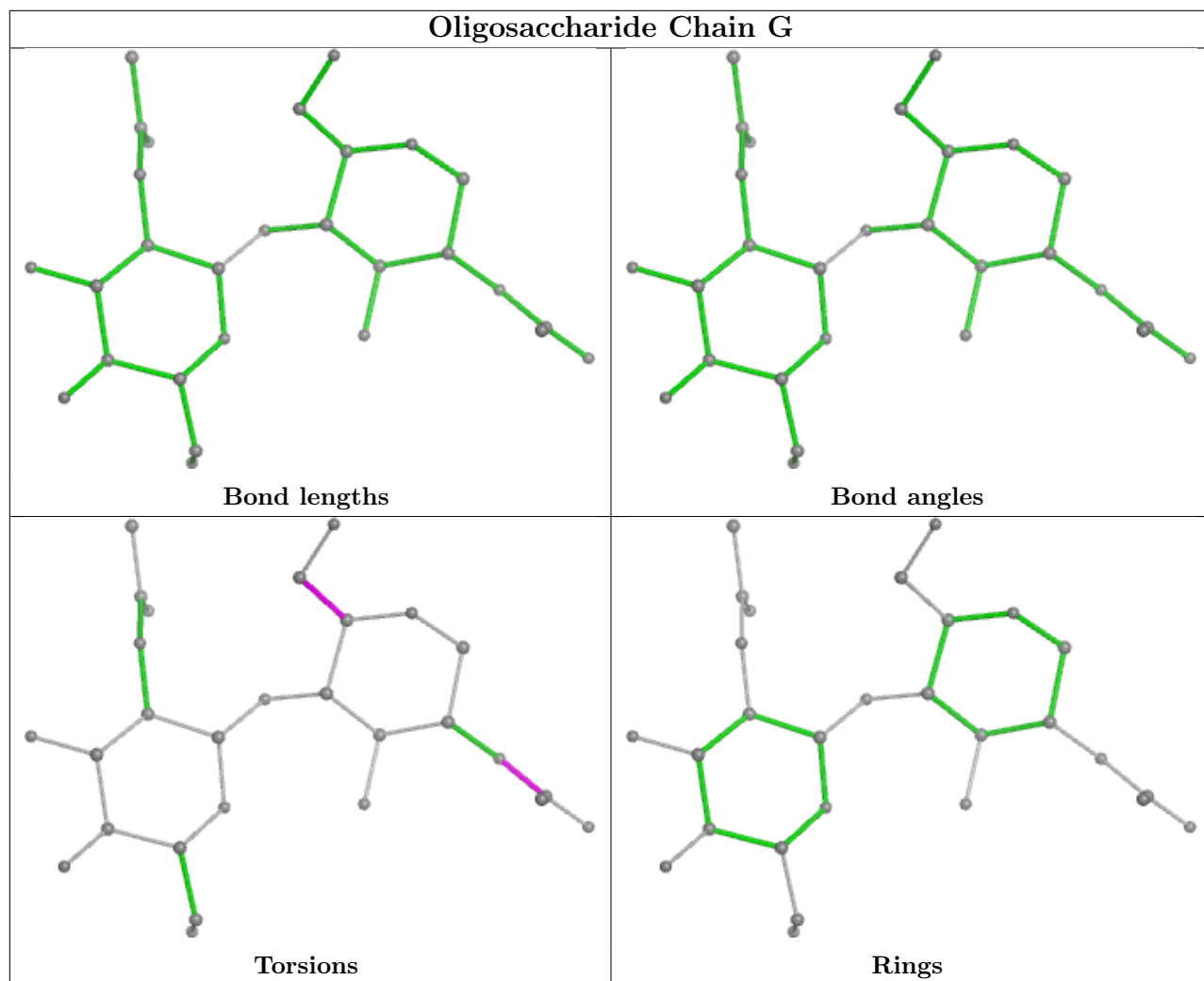
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

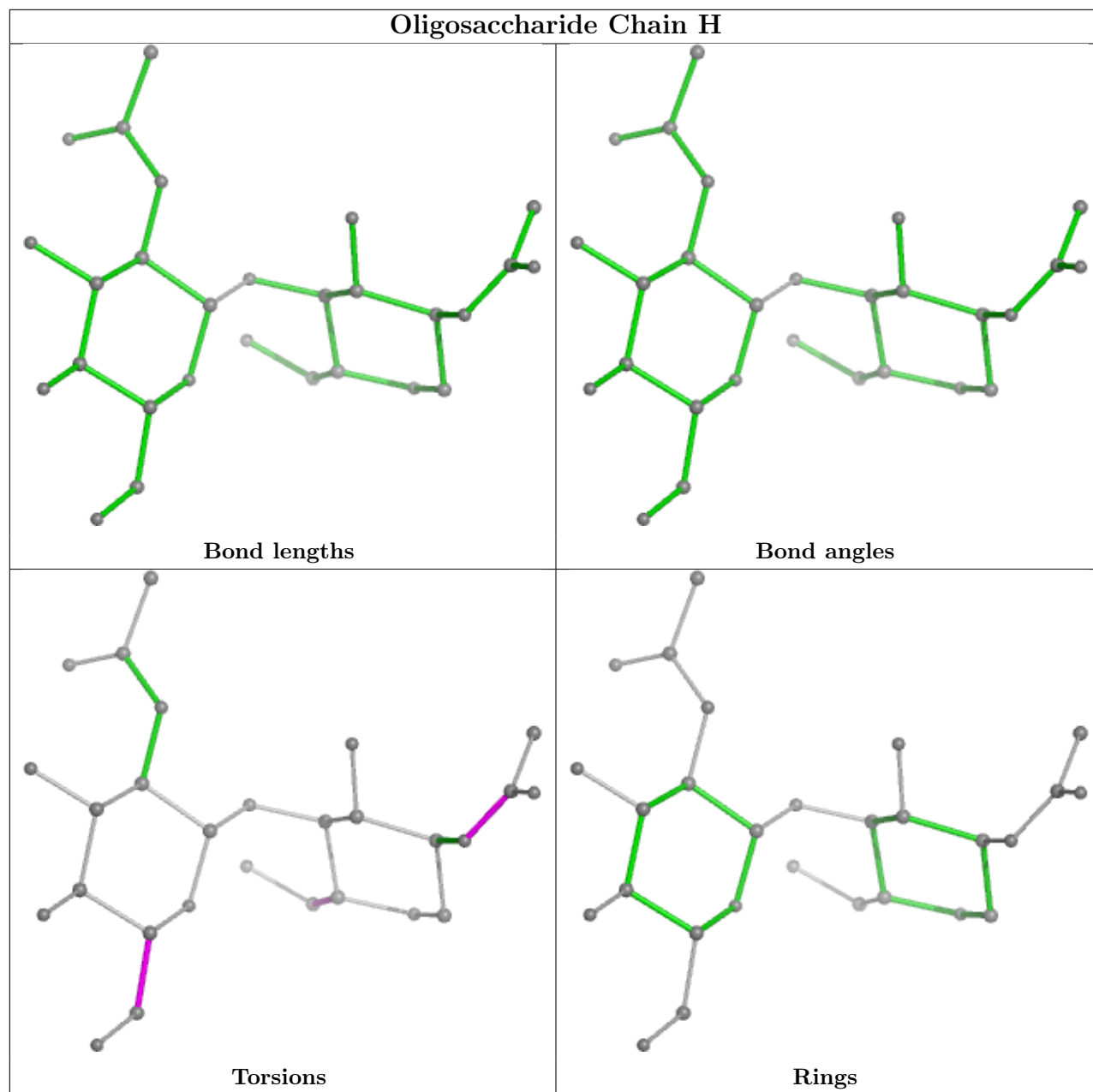




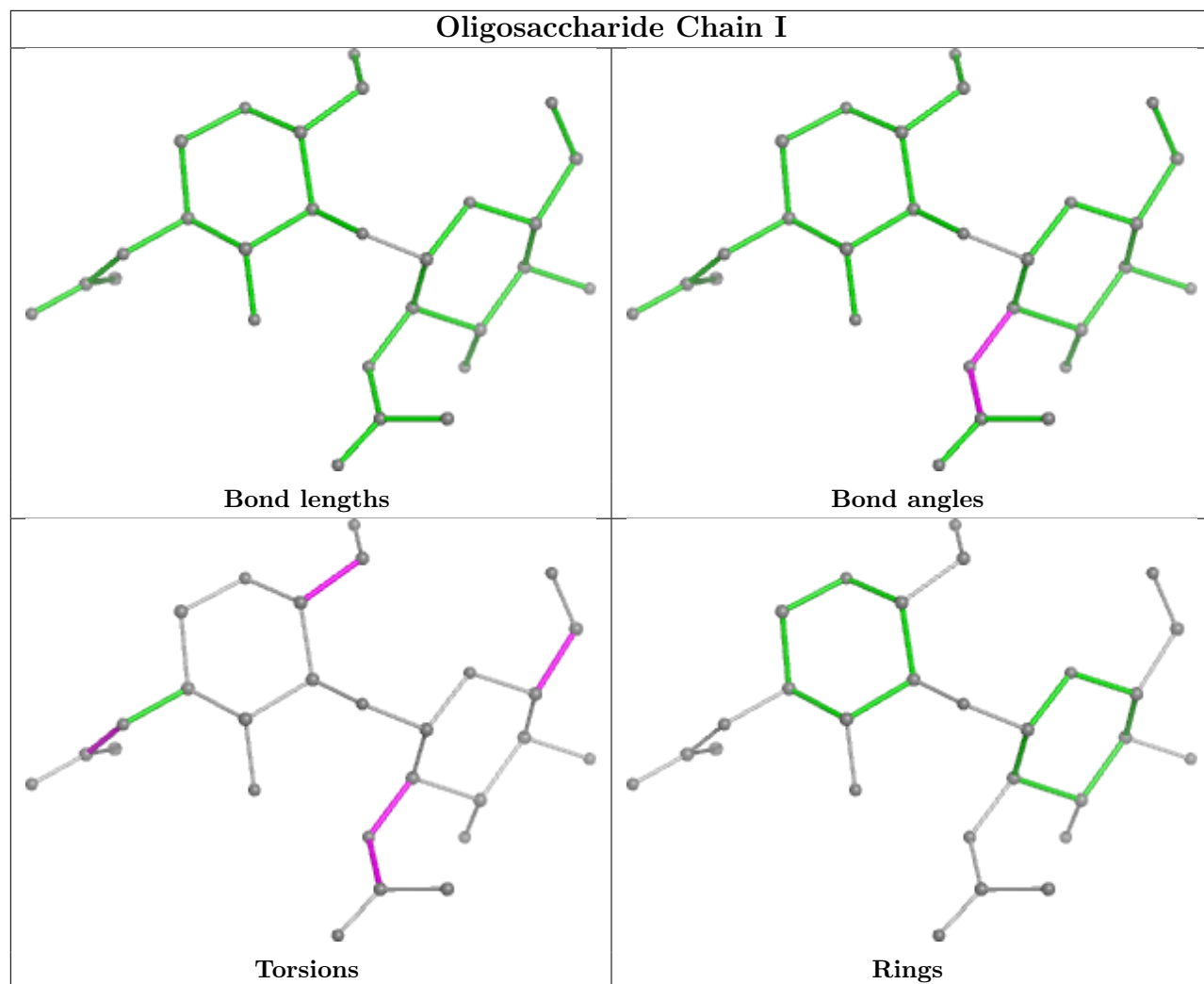


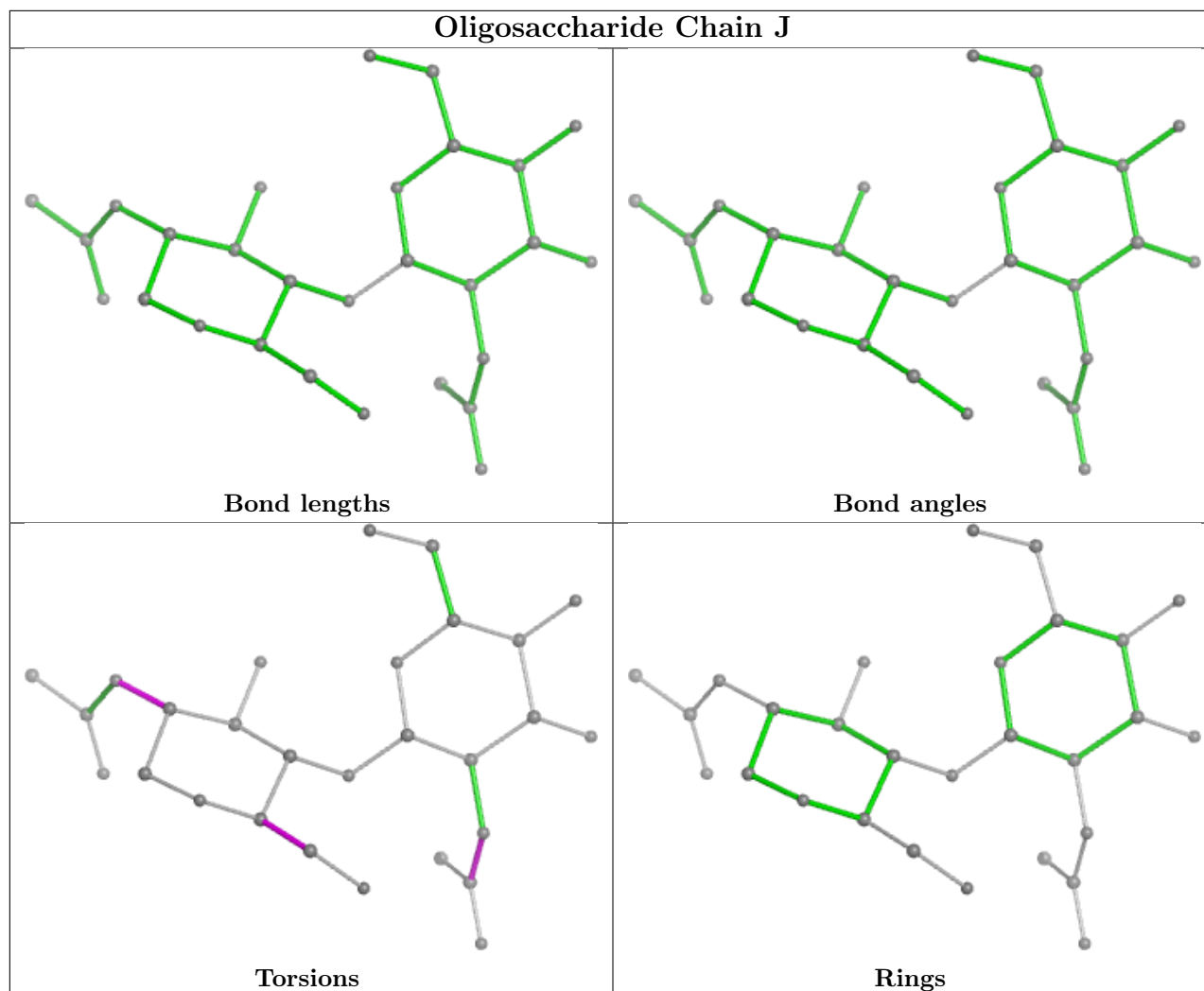












## 5.6 Ligand geometry [i](#)

16 ligands 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	$\# Z  > 2$
3	NAG	A	2805	1	14,14,15	0.56	0	17,19,21	1.25	1 (5%)
3	NAG	B	2806	1	14,14,15	0.24	0	17,19,21	0.44	0
3	NAG	B	2802	1	14,14,15	0.21	0	17,19,21	0.42	0
3	NAG	B	2804	1	14,14,15	0.23	0	17,19,21	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	A	2808	1	14,14,15	0.22	0	17,19,21	0.41	0
3	NAG	A	2804	1	14,14,15	0.23	0	17,19,21	0.40	0
3	NAG	B	2807	-	15,15,15	0.20	0	21,21,21	0.28	0
3	NAG	A	2806	1	14,14,15	0.22	0	17,19,21	0.43	0
3	NAG	A	2803	1	14,14,15	0.21	0	17,19,21	0.46	0
3	NAG	A	2802	1	14,14,15	0.20	0	17,19,21	0.43	0
3	NAG	B	2801	1	14,14,15	0.19	0	17,19,21	0.42	0
3	NAG	A	2807	-	15,15,15	0.20	0	21,21,21	0.28	0
3	NAG	A	2801	1	14,14,15	0.20	0	17,19,21	0.42	0
3	NAG	B	2805	1	14,14,15	0.56	0	17,19,21	1.26	1 (5%)
3	NAG	B	2803	1	14,14,15	0.21	0	17,19,21	0.46	0
3	NAG	B	2808	1	14,14,15	0.21	0	17,19,21	0.42	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
3	NAG	A	2805	1	-	5/6/23/26	0/1/1/1
3	NAG	B	2806	1	-	2/6/23/26	0/1/1/1
3	NAG	B	2802	1	-	4/6/23/26	0/1/1/1
3	NAG	B	2804	1	-	2/6/23/26	0/1/1/1
3	NAG	A	2808	1	-	2/6/23/26	0/1/1/1
3	NAG	A	2804	1	-	2/6/23/26	0/1/1/1
3	NAG	B	2807	-	-	4/6/26/26	0/1/1/1
3	NAG	A	2806	1	-	2/6/23/26	0/1/1/1
3	NAG	A	2803	1	-	4/6/23/26	0/1/1/1
3	NAG	A	2802	1	-	4/6/23/26	0/1/1/1
3	NAG	B	2801	1	-	1/6/23/26	0/1/1/1
3	NAG	A	2807	-	-	4/6/26/26	0/1/1/1
3	NAG	A	2801	1	-	1/6/23/26	0/1/1/1
3	NAG	B	2805	1	-	5/6/23/26	0/1/1/1
3	NAG	B	2803	1	-	4/6/23/26	0/1/1/1
3	NAG	B	2808	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2805	NAG	C2-N2-C7	4.29	129.01	122.90
3	A	2805	NAG	C2-N2-C7	4.26	128.97	122.90

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2804	NAG	O5-C5-C6-O6
3	B	2805	NAG	O5-C5-C6-O6
3	A	2804	NAG	O5-C5-C6-O6
3	A	2805	NAG	O5-C5-C6-O6
3	B	2804	NAG	C4-C5-C6-O6
3	A	2804	NAG	C4-C5-C6-O6
3	B	2802	NAG	O5-C5-C6-O6
3	B	2807	NAG	O5-C5-C6-O6
3	A	2802	NAG	O5-C5-C6-O6
3	A	2807	NAG	O5-C5-C6-O6
3	B	2805	NAG	C4-C5-C6-O6
3	A	2805	NAG	C4-C5-C6-O6
3	B	2806	NAG	O5-C5-C6-O6
3	A	2806	NAG	O5-C5-C6-O6
3	B	2807	NAG	C4-C5-C6-O6
3	A	2807	NAG	C4-C5-C6-O6
3	B	2802	NAG	C8-C7-N2-C2
3	B	2802	NAG	O7-C7-N2-C2
3	B	2803	NAG	C8-C7-N2-C2
3	B	2803	NAG	O7-C7-N2-C2
3	B	2805	NAG	C8-C7-N2-C2
3	B	2805	NAG	O7-C7-N2-C2
3	B	2807	NAG	C8-C7-N2-C2
3	B	2807	NAG	O7-C7-N2-C2
3	A	2802	NAG	C8-C7-N2-C2
3	A	2802	NAG	O7-C7-N2-C2
3	A	2803	NAG	C8-C7-N2-C2
3	A	2803	NAG	O7-C7-N2-C2
3	A	2805	NAG	C8-C7-N2-C2
3	A	2805	NAG	O7-C7-N2-C2
3	A	2807	NAG	C8-C7-N2-C2
3	A	2807	NAG	O7-C7-N2-C2
3	B	2806	NAG	C4-C5-C6-O6
3	A	2806	NAG	C4-C5-C6-O6
3	B	2808	NAG	O5-C5-C6-O6
3	A	2808	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	B	2808	NAG	C4-C5-C6-O6
3	A	2808	NAG	C4-C5-C6-O6
3	B	2802	NAG	C4-C5-C6-O6
3	A	2802	NAG	C4-C5-C6-O6
3	A	2803	NAG	C4-C5-C6-O6
3	B	2803	NAG	C4-C5-C6-O6
3	B	2803	NAG	O5-C5-C6-O6
3	A	2803	NAG	O5-C5-C6-O6
3	B	2805	NAG	C3-C2-N2-C7
3	A	2805	NAG	C3-C2-N2-C7
3	B	2801	NAG	C4-C5-C6-O6
3	A	2801	NAG	C4-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2805	NAG	2	0
3	B	2807	NAG	1	0
3	A	2803	NAG	1	0
3	A	2807	NAG	1	0
3	B	2805	NAG	2	0
3	B	2803	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-18889. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections

This section was not generated.

### 6.2 Central slices

This section was not generated.

### 6.3 Largest variance slices

This section was not generated.

### 6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

### 6.5 Orthogonal surface views

This section was not generated.

### 6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis

This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution

This section was not generated.

### 7.2 Volume estimate versus contour level

This section was not generated.

### 7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.



## 9 Map-model fit

This section was not generated.