



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 06:07 PM UTC

PDB ID : 9CWM / pdb_00009cwm
EMDB ID : EMD-45967
Title : Cryo-EM structure of human Low-density lipoprotein receptor-related protein 2
Authors : Zhang, Z.; Lyu, M.
Deposited on : 2024-07-29
Resolution : 3.30 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

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>.

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

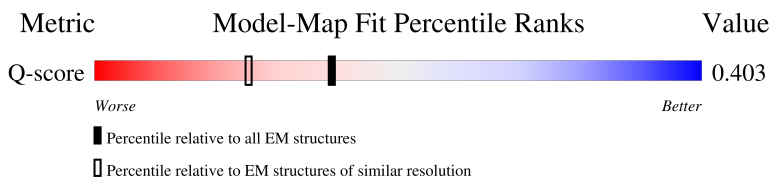
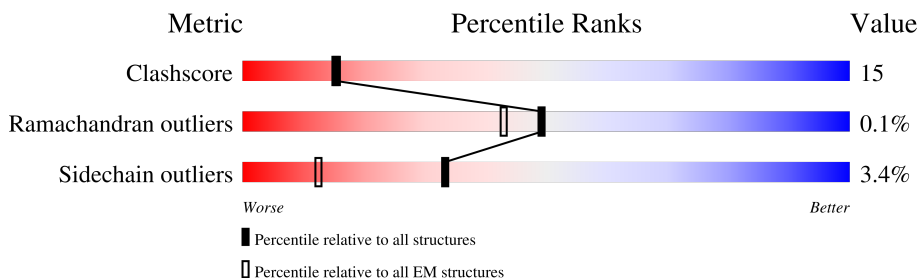
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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.




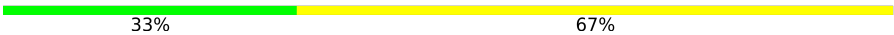


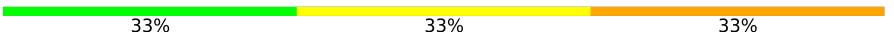



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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 ≥ 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	4655	
1	B	4655	
2	C	3	
2	D	3	

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Mol	Chain	Length	Quality of chain
2	E	3	 67%33%
2	F	3	 100%
2	I	3	 33%67%
2	J	3	 33%67%
2	K	3	 67%33%
2	L	3	 100%
2	N	3	 33%33%33%
3	G	2	 50%50%
3	H	2	 50%50%
3	M	2	 50%50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	G	1	-	-	X	-

2 Entry composition [i](#)

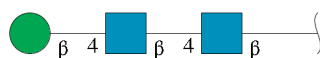
There are 4 unique types of molecules in this entry. The entry contains 58072 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Low-density lipoprotein receptor-related protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3695	Total	C	N	O	S	0	0
			28662	17831	4991	5563	277		
1	B	3692	Total	C	N	O	S	0	0
			28653	17828	4988	5560	277		

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



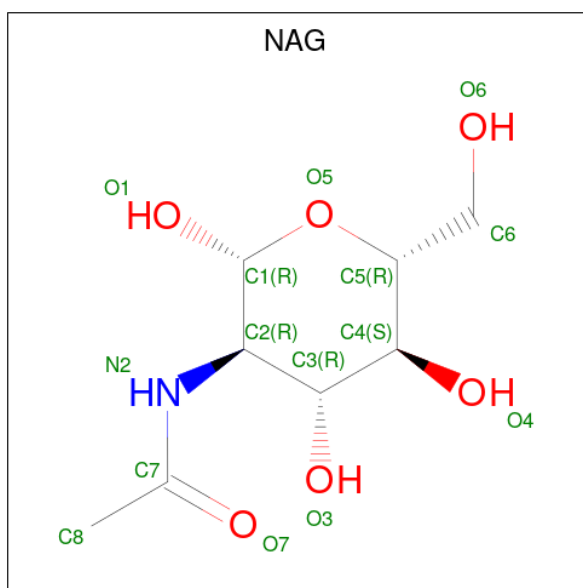
Mol	Chain	Residues	Atoms				AltConf	Trace
2	C	3	Total	C	N	O	0	0
			39	22	2	15		
2	D	3	Total	C	N	O	0	0
			39	22	2	15		
2	E	3	Total	C	N	O	0	0
			39	22	2	15		
2	F	3	Total	C	N	O	0	0
			39	22	2	15		
2	I	3	Total	C	N	O	0	0
			39	22	2	15		
2	J	3	Total	C	N	O	0	0
			39	22	2	15		
2	K	3	Total	C	N	O	0	0
			39	22	2	15		
2	L	3	Total	C	N	O	0	0
			39	22	2	15		
2	N	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 3 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
3	G	2	Total	C	N	O	0	0
			28	16	2	10		
3	H	2	Total	C	N	O	0	0
			28	16	2	10		
3	M	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	

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





D2242	S2106	S1961	M1834	S1677	H1566	V1451	G1350	CYS	G1209	D1129	T1023	H896	V673
Y2247	D2113	P1963	L1835	V1685	L1567	T1452	N1351	ASP	D1212	T1130	E1024	S897	S677
V2251	F2114	G1965	T1838	P1686	H1576	S1453	S1352	ARG	N1216	D1131	Q1025	D903	H678
S2254	S2115	I1966	R1841	L1687	R1578	Q1454	S1354	ASN	S1217	N1132	C1026	R904	L685
S2254	D2121	A1967	S1844	V1692	L1481	L1481	D1355	ASP	D1218	D1133	L1044	E910	G686
I2257	T2124	L1973	I1845	K1696	V1462	V1462	N1357	GLY	E1219	C1134	Q1045	E911	F687
I2258	R2125	Y1974	E1846	V1687	E1580	E1580	G1359	ASP	A1220	D1136	D1046	Q912	G686
R2262	R2126	T1976	L1848	R1581	R1581	G1465	G1360	ASP					F693
V2270	T2127	Q1979	D1853	M1584	M1584	G1466	G1362	SER	T1224	K1141	C1051	A935	G694
V2285	S2133	E1984	I1854	L1712	L1712	S1466	H1361	ASP	R1225	N1142	H1052	I936	F695
V2285	T2137	R1985	M1588	G1713	M1588	I1468	E1362	GLU	P1226			I937	T817
V2290	V2138	V1986	R1589	L1714	R1589	V1469	E1363	LYS	P1227	C1149	D1056	V939	R818
V2290	T2139	R1987	T1857	Q1718	T1590	I1480	C1364	ASP	G1228	Q1150	E1057	R688	R819
V2300	H2140	K1988	T1859	H1721	V1591	I1480	V1365	PRO	F1235	Q1153	L1059	R940	T820
I2300	G2141	G1991	D1864	H1722	V1592	S1483	Q1366	THR	Q1236	F1154	C1060	G944	I719
S2304	E2144	N2000	L1868	Y1723	V1593	D1484	E1367	GLN	C1237	N1155	G1061	R647	R720
K2305	G2146	G1991	D1864	Y1723	V1593	D1484	E1367	PRO	C1238	C1156	T1062	T948	V732
N2309	V2147	G1991	D1864	Y1723	V1593	D1484	E1367	ARG	E1239	P1157	N1065	V949	M733
P2312	A2151	G1991	D1864	Y1723	V1593	D1484	E1367	CYS	I1242	N1158	S1068	I957	F742
P2313	N2163	G1991	D1864	Y1723	V1593	D1484	E1367	PRO	I1243	R1160	A1071	I958	F743
D2318	A2164	G1991	D1864	Y1723	V1593	D1484	E1367	SER	I1244	C1161	F1072	H959	G745
N2319	T2165	G1991	D1864	Y1723	V1593	D1484	E1367	TRP		T1162	A1071	I960	V744
D2325	V2166	G1991	D1864	Y1723	V1593	D1484	E1367	GLN	E1249	F1166	F1072	K961	G746
V2326	E2168	G1991	D1864	Y1723	V1593	D1484	E1367	GLY	C1250	V1167	E1078	I961	D747
T2327	T2176	G1991	D1864	Y1723	V1593	D1484	E1367	ASN	D1251	G1177	E1079	I961	T843
D2330	N2177	G1991	D1864	Y1723	V1593	D1484	E1367	LEU	G1252	D1178	C1079	Q968	D748
K2331	R2181	G1991	D1864	Y1723	V1593	D1484	E1367	GLY	P1254	G1170	I1080	T969	
V2341	R2182	G1991	D1864	Y1723	V1593	D1484	E1367	HIS	D1255	K1172	W1084	N972	T754
P2345	P2192	G1991	D1864	Y1723	V1593	D1484	E1367	ILE	C1256	C1173	D1087	C974	I755
P2366	H2194	G1991	D1864	Y1723	V1593	D1484	E1367	CYS	L1257	I1175	K1088	M852	K762
T2374	V2197	G1991	D1864	Y1723	V1593	D1484	E1367	VAL	S1260	D1176	R1089	T978	I765
Q2376	D2198	G1991	D1864	Y1723	V1593	D1484	E1367	ASN	D1261	G1177	H1090	H979	F766
L2390	N2201	G1991	D1864	Y1723	V1593	D1484	E1367	LEU	E1262	S1178	D1091	P980	K767
A2393	W2206	G1991	D1864	Y1723	V1593	D1484	E1367	SER	H1263	D1179	C1092	N981	Q768
L2394	Y2209	G1991	D1864	Y1723	V1593	D1484	E1367	VAL	P1268	E1180	G1095	C988	K769
S2397	P2213	G1991	D1864	Y1723	V1593	D1484	E1367	CYS					G772
L2398	R2233	G1991	D1864	Y1723	V1593	D1484	E1367	ASP	S1273	V1184	S1096	T867	T773
S2400	P2236	G1991	D1864	Y1723	V1593	D1484	E1367	GLY	SER	L1185	D1097	V891	G774
L2401		G1991	D1864	Y1723	V1593	D1484	E1367	ILE	TYR	N1186	E1098	Q895	I777
		G1991	D1864	Y1723	V1593	D1484	E1367	PHE	PHE	C1187	H1099	R996	L778
		G1991	D1864	Y1723	V1593	D1484	E1367	ASP	HIS	Q1191	C1109	N873	L779
		G1991	D1864	Y1723	V1593	D1484	E1367	CYS	CYS	F1192	C1109	N873	A779
		G1991	D1864	Y1723	V1593	D1484	E1367	PRO	ASP	K1193	T1112	P1001	A780
		G1991	D1864	Y1723	V1593	D1484	E1367	ASN	ASN	D1198	Q1113	M1004	N761
		G1991	D1864	Y1723	V1593	D1484	E1367	GLY	GLY	T1201	Y1114	L884	
		G1991	D1864	Y1723	V1593	D1484	E1367	THR	ASN	G1202	M1118	N1009	N785
		G1991	D1864	Y1723	V1593	D1484	E1367	GLU	CYS	I1011	L1011	H010	W886
		G1991	D1864	Y1723	V1593	D1484	E1367	SER	ILE	V1203	C1121	L011	V786
		G1991	D1864	Y1723	V1593	D1484	E1367	PRO	HIS	T1204	I1122	G1015	A790
		G1991	D1864	Y1723	V1593	D1484	E1367	ALA	ARG	T1206	S1123	D1016	D882
		G1991	D1864	Y1723	V1593	D1484	E1367	TRP	ALA	N1205	W1124	D1016	R893
		G1991	D1864	Y1723	V1593	D1484	E1367	LEU	LEU	R1206	K1124	I894	I794
		G1991	D1864	Y1723	V1593	D1484	E1367				N1125	E1020	S795




F3847	LYS	L4179	E4293	VAL	LEU	GLU	GLN
E3848	PRO	T4180	Y4294	ALA	ASN	ASN	LYS
C3849	THR	S4181	W4295	VAL	MET	VAL	GLU
K3850	PRO	D4080	LEU	VAL	ASP	ASP	SER
N3851	LYS	Q4136	N4298	THR	ILE	ASN	VAL
V3852	PRO	T4190	Q4302	ILE	ASN	LYS	ALA
V3853	CYS	M4199	K4307	LEU	THR	ASN	THR
C3854	THR	T4202	T4308	LEU	SER	GLY	PRO
L3855	GLU	V4087	L4309	ILE	PHE	GLY	PRO
P3856	TYR	D4088	V4310	VAL	GLY	PRO	SER
P3857	GLU	Y4089	V4311	VAL	PRO	ILE	SER
Y3858	TYR	W4204	V4312	ILE	ASN	PRO	PRO
Y3859	LYS	G4205	M4312	GLY	THR	PRO	SER
D3862	CYS	P4208	W4313	ALA	ALA	SER	LEU
C3863	GLY	D4092	W4314	ALA	ILE	GLU	LEU
D3863	ASN	P4093	L4315	ALA	PRO	GLU	ALA
G3870	HIS	L4098	T4316	ILE	ASP	ILE	LYS
S3871	CYS	S4099	Q4317	ALA	ARG	PRO	PRO
D3872	ILE	V4100	I4320	PHE	GLY	GLU	LYS
E3873	PRO	V4101	F4321	ALA	THR	THR	PRO
E3874	HIS	Y4102	H4322	PHE	ALA	ASN	PRO
L3875	ASP	Y4103	Q4323	HIS	MET	PRO	SER
D3879	ASN	R4106	P4354	TYR	GLU	ARG	ARG
D3880	CYS	K4116	F4359	ARG	ASP	SER	ASP
F3889	ASP	L4223	C4367	THR	PHE	PRO	THR
ARG	ALA	L4228	F4369	THR	VAL	ALA	PRO
CYS	ASP	G4229	GLY	GLY	GLY	ALA	THR
ASN	ALA	I4120	SER	LEU	LEU	GLY	PRO
ASN	ASP	R4022	LEU	LEU	LYS	THR	THR
GLY	CYS	K4025	PRO	PRO	ILE	GLN	VAL
GLY	ASP	G4026	ALA	ALA	PRO	VAL	ALA
TRP	ASP	E4029	LEU	LEU	LYS	THR	THR
ILE	SER	C4030	PRO	PRO	ILE	ASP	GLU
TVR	ASP	V4031	LYS	LYS	PHE	ASN	THR
SER	GLU	D4034	LEU	PRO	GLU	LEU	PHE
HIS	LEU	G4035	SER	SER	ASN	PHE	LYS
GLU	GLY	F4036	LEU	LEU	PRO	LYS	ASP
VAL	CYS	T4037	THR	THR	MET	ARG	THR
CYS	ASN	Y4156	SER	SER	LYS	TYR	THR
LYS	LYS	S4038	LEU	LEU	SER	LYS	ALA
GLY	GLY	W4039	VAL	VAL	ALA	SER	ASN
LYS	VAL	S4040	LYS	LYS	GLN	GLN	VAL
GLU	ARG	D4041	C4410	PRO	THR	THR	LYS
ASP	ASP	R4042	E4411	GLU	ASP	ASP	GLU
THR	CYS	K4045	MET	ALA	ALA	ASN	ASP
GLY	CYS	R4046	ALA	ASN	VAL	PHE	GLY
ASP	GLY	C4047	SER	GLY	VAL	GLY	ASN
THR	GLY	L4057	LYS	VAL	VAL	VAL	PRO
ASN	ASN	Y4059	ILE	GLN	VAL	ILE	TYR
ILE	ILE	V4062	T4277	THR	THR	THR	ALA
CYS	CYS	R4063	D4278	ILE	PRO	PRO	ILE
THR	GLN	Y4067	L4284	PHE	ILE	ALA	GLN
ASN	ASN	Y4175	W4286	ARG	SER	GLN	GLN
CYS	CYS	W4178	ALA	THR	VAL	MET	VAL
GLN	GLN			ALA	THR	GLU	THR
ARG	ARG			ASP	VAL	ASN	VAL
					SER	GLU	SER

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

Chain C:  33% 67%

NAG1
NAG2
BNA3

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

Chain D:  33% 67%

NAG1
NAG2
BNA3

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

Chain E:  67% 33%



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

Chain F:



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

Chain I:



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

Chain J:



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

Chain K:



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

Chain L:



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

Chain N:



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

Chain G:  50% 50%

MAG1
MAG2

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

Chain H:  50% 50%

MAG1
MAG2

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

Chain M:  50% 50%

MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	111811	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.033	Depositor
Minimum map value	-0.060	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	547.84, 547.84, 547.84	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	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: BMA, 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	0.26	5/29362 (0.0%)	0.43	4/39957 (0.0%)
1	B	0.25	6/29354 (0.0%)	0.43	7/39946 (0.0%)
All	All	0.26	11/58716 (0.0%)	0.43	11/79903 (0.0%)

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

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

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	480	LYS	C-N	9.10	1.44	1.33
1	B	842	PHE	C-N	8.55	1.44	1.33
1	B	995	GLN	C-N	8.00	1.45	1.33
1	A	995	GLN	C-N	7.15	1.44	1.33
1	A	843	THR	C-N	6.31	1.41	1.33
1	B	841	PHE	C-N	-6.12	1.25	1.33
1	B	843	THR	C-N	6.04	1.42	1.33
1	A	481	ILE	C-N	5.63	1.41	1.33
1	B	367	GLY	C-N	5.59	1.41	1.33
1	B	996	ARG	C-N	5.46	1.40	1.33
1	A	996	ARG	C-N	5.04	1.39	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2726	GLY	N-CA-C	-9.85	102.41	115.32
1	A	2726	GLY	N-CA-C	-9.74	102.56	115.32
1	B	3819	GLY	N-CA-C	-6.17	107.74	115.08
1	B	842	PHE	O-C-N	5.58	129.92	123.17
1	A	480	LYS	O-C-N	5.54	130.43	123.23
1	B	995	GLN	O-C-N	5.45	130.23	123.15
1	B	1132	ASN	N-CA-C	-5.32	105.96	113.20
1	B	611	GLU	CB-CA-C	-5.17	110.59	116.54
1	A	995	GLN	O-C-N	5.16	129.46	122.96
1	B	3613	CYS	N-CA-C	-5.04	104.39	110.44
1	A	3881	VAL	CB-CA-C	-5.02	109.02	114.35

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	819	ARG	Sidechain

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	28662	0	26485	823	0
1	B	28653	0	26477	829	0
2	C	39	0	34	2	0
2	D	39	0	34	2	0
2	E	39	0	34	5	0
2	F	39	0	34	0	0
2	I	39	0	34	3	0
2	J	39	0	34	3	0
2	K	39	0	34	6	0
2	L	39	0	34	0	0
2	N	39	0	34	2	0
3	G	28	0	25	7	0
3	H	28	0	25	1	0
3	M	28	0	25	1	0
4	A	168	0	156	1	0
4	B	154	0	143	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	58072	0	53642	1640	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 15.

All (1640) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4329:SER:HB2	3:G:1:NAG:C1	1.75	1.16
1:A:4007:ASP:HA	1:A:4025:LYS:HA	1.10	1.09
1:B:1228:GLY:HA3	1:B:3195:SER:HA	1.51	0.91
1:A:4007:ASP:HA	1:A:4025:LYS:CA	2.00	0.90
1:B:3611:TRP:HA	1:B:3614:ASP:HB3	1.55	0.88
1:B:3239:LYS:HB2	2:K:1:NAG:H62	1.56	0.87
1:A:339:ASN:HB2	1:A:342:ASP:HB2	1.55	0.87
1:A:3239:LYS:HB2	2:E:1:NAG:H62	1.58	0.83
1:B:4208:PRO:HB2	1:B:4228:LEU:HB2	1.61	0.83
1:A:4007:ASP:CA	1:A:4025:LYS:HA	2.02	0.83
1:A:1228:GLY:HA3	1:A:3195:SER:HA	1.59	0.83
1:B:4293:GLU:HG2	1:B:4310:VAL:HG22	1.61	0.82
1:B:1352:SER:HA	1:B:1355:ASP:HB2	1.60	0.82
1:A:3255:PHE:HD2	2:E:1:NAG:H5	1.42	0.82
1:B:3998:ASN:HB2	1:B:4001:ASP:HB2	1.60	0.82
1:B:1159:HIS:HB2	1:B:1175:VAL:HG13	1.60	0.81
1:A:911:GLU:HG2	1:A:912:GLN:HG3	1.63	0.81
1:A:3255:PHE:CD2	2:E:1:NAG:H5	2.15	0.81
1:B:3255:PHE:HD2	2:K:1:NAG:H5	1.45	0.80
1:B:354:ILE:HG23	1:B:357:ILE:HB	1.62	0.80
1:B:3255:PHE:CD2	2:K:1:NAG:H5	2.17	0.80
1:B:2758:TYR:HB3	1:B:2763:TYR:HB2	1.66	0.78
1:B:4124:GLU:HG3	3:M:1:NAG:H83	1.66	0.78
1:B:1172:LYS:HE2	1:B:1177:GLY:HA3	1.64	0.78
1:B:3244:ILE:HG12	1:B:3251:ILE:HG12	1.67	0.77
1:B:3287:LEU:HD13	1:B:3323:PRO:HB2	1.65	0.77
1:A:1349:ASN:HB3	1:A:1370:GLY:HA3	1.67	0.76
1:A:4179:LEU:HD13	1:A:4199:MET:HE1	1.66	0.76
1:B:2398:LEU:HD22	1:B:2424:LEU:HD21	1.68	0.76
1:A:3063:GLU:HB2	1:A:3067:LEU:HB2	1.67	0.75
1:B:2489:MET:HA	1:B:2505:ARG:HA	1.67	0.75
1:B:2475:TRP:HZ2	1:B:2649:GLN:HB2	1.50	0.75
1:B:3063:GLU:HB2	1:B:3067:LEU:HB2	1.67	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3244:ILE:HG12	1:A:3251:ILE:HG12	1.68	0.74
1:B:3819:GLY:H	1:B:3835:ARG:HH21	1.32	0.74
1:A:3287:LEU:HD13	1:A:3323:PRO:HB2	1.69	0.74
1:A:3791:ARG:HH21	1:B:4142:MET:HG3	1.52	0.74
1:B:3326:LEU:HG	1:B:3335:LEU:HD11	1.69	0.73
1:A:2489:MET:HA	1:A:2505:ARG:HA	1.68	0.73
1:B:2686:ALA:HB2	1:B:2693:ILE:HD11	1.69	0.73
1:A:363:GLU:HB2	1:A:370:LEU:HB3	1.71	0.73
1:A:1461:LEU:HD23	1:A:1462:VAL:HG23	1.71	0.73
1:B:363:GLU:HB2	1:B:370:LEU:HB3	1.69	0.73
1:A:2707:CYS:HB3	1:A:2729:SER:HB3	1.71	0.73
1:A:4329:SER:CB	3:G:1:NAG:C1	2.62	0.73
1:A:1074:CYS:HB2	1:A:1078:GLU:HB2	1.71	0.72
1:B:4179:LEU:HD13	1:B:4199:MET:HE1	1.70	0.72
1:B:1461:LEU:HD23	1:B:1462:VAL:HG23	1.71	0.72
1:B:2759:ARG:NH1	1:B:2760:CYS:SG	2.63	0.72
1:A:3326:LEU:HG	1:A:3335:LEU:HD11	1.69	0.72
1:B:578:PHE:HB3	1:B:1175:VAL:HG12	1.71	0.72
1:A:1254:PRO:HG2	4:A:4702:NAG:H83	1.70	0.71
1:B:3104:SER:HA	1:B:3107:LYS:HB3	1.72	0.71
1:A:466:VAL:HB	1:A:469:PRO:HG3	1.73	0.71
1:B:1354:SER:H	1:B:1366:GLN:HE21	1.37	0.71
1:B:3836:PHE:HD2	1:B:3838:ASP:HB3	1.55	0.71
1:A:911:GLU:HB3	1:A:947:MET:HE2	1.72	0.71
1:B:817:THR:HG23	1:B:1001:PRO:HB3	1.71	0.71
1:A:4022:ARG:HB3	1:A:4029:GLU:HB3	1.73	0.71
1:A:3423:THR:HB	1:A:3451:PRO:HB2	1.73	0.71
1:A:1352:SER:HA	1:A:1355:ASP:HB2	1.73	0.71
1:A:481:ILE:HG13	1:A:496:LEU:HD23	1.73	0.70
1:B:1364:CYS:HA	1:B:1373:CYS:HA	1.73	0.70
1:B:3364:LEU:HD11	1:B:3367:PRO:HB3	1.71	0.70
1:A:2686:ALA:HB2	1:A:2693:ILE:HD11	1.71	0.70
1:A:883:ARG:HE	1:A:896:HIS:HD2	1.38	0.70
1:B:237:GLN:HB2	1:B:549:LYS:HD2	1.74	0.70
1:A:3364:LEU:HD11	1:A:3367:PRO:HB3	1.74	0.70
1:A:4208:PRO:HB2	1:A:4228:LEU:HB2	1.72	0.70
1:B:2707:CYS:HB3	1:B:2729:SER:HB3	1.72	0.70
1:B:1353:CYS:SG	1:B:1364:CYS:HB2	2.32	0.70
1:A:4142:MET:HG3	1:B:3791:ARG:HH21	1.57	0.70
1:A:991:VAL:HG23	1:A:995:GLN:HG3	1.73	0.69
1:B:1160:ARG:HE	1:B:1162:ILE:HG22	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2475:TRP:HZ2	1:A:2649:GLN:HB2	1.55	0.69
1:A:3796:ARG:NH2	1:A:3810:CYS:SG	2.65	0.69
1:B:1658:THR:HB	1:B:1686:PRO:HB2	1.73	0.69
1:A:744:VAL:HG22	1:A:958:LEU:HD13	1.74	0.69
1:B:3423:THR:HB	1:B:3451:PRO:HB2	1.73	0.69
1:B:3875:LEU:HB3	1:B:3879:LEU:HA	1.74	0.69
1:A:582:GLU:HG2	1:A:591:ARG:HE	1.58	0.69
1:B:4204:TRP:HA	1:B:4231:PRO:HD2	1.74	0.69
1:B:3796:ARG:NH2	1:B:3810:CYS:SG	2.66	0.69
1:B:395:SER:HB2	1:B:651:TYR:HB3	1.74	0.68
1:A:1826:LEU:HD22	1:A:1835:LEU:HD21	1.76	0.68
1:A:1658:THR:HB	1:A:1686:PRO:HB2	1.75	0.68
1:A:1435:SER:HB2	1:A:1452:THR:HB	1.75	0.68
1:B:911:GLU:HG2	1:B:912:GLN:HG3	1.76	0.68
1:A:829:ARG:NH1	1:A:873:ASN:OD1	2.27	0.67
1:A:1588:MET:SD	1:A:1718:GLN:NE2	2.66	0.67
1:B:1435:SER:HB2	1:B:1452:THR:HB	1.76	0.67
1:B:2608:THR:HG22	1:B:2615:ILE:HG12	1.75	0.67
1:A:3264:ILE:HG22	1:A:3265:ILE:HG13	1.77	0.67
1:B:847:ARG:NH2	1:B:1251:ASP:OD2	2.28	0.67
1:B:3578:CYS:HB3	1:B:3583:ASP:HB2	1.77	0.67
1:B:1114:TYR:N	1:B:1122:ILE:O	2.27	0.67
1:A:2608:THR:HG22	1:A:2615:ILE:HG12	1.75	0.67
1:A:3867:CYS:HB3	1:A:3870:GLY:HA3	1.77	0.66
1:B:1071:ALA:HB1	1:B:1079:CYS:HB3	1.77	0.66
1:B:1125:ASN:HA	1:B:1153:GLN:HE21	1.60	0.66
1:B:2474:ASP:HB2	1:B:2514:LEU:HD13	1.78	0.66
1:B:4022:ARG:HB3	1:B:4029:GLU:HB3	1.75	0.66
1:A:4062:VAL:HG23	1:A:4063:ARG:HG3	1.78	0.66
1:B:1256:CYS:SG	1:B:1260:SER:OG	2.53	0.66
1:A:4311:VAL:HG12	1:A:4312:ASN:H	1.61	0.66
1:B:1058:GLN:HG2	1:B:1059:LEU:HG	1.78	0.66
1:B:1365:VAL:H	1:B:1373:CYS:H	1.43	0.66
1:A:493:MET:HE1	1:A:673:VAL:HG11	1.78	0.66
1:A:3611:TRP:HA	1:A:3614:ASP:HB3	1.77	0.66
1:B:609:LEU:O	1:B:655:ARG:NH1	2.28	0.66
1:A:1256:CYS:SG	1:A:1260:SER:OG	2.54	0.66
1:A:4036:PHE:HB3	1:A:4047:CYS:HB3	1.77	0.66
1:B:1187:CYS:H	1:B:1193:LYS:HE3	1.61	0.66
1:A:229:CYS:HB2	1:A:233:ARG:HG2	1.76	0.66
1:A:2505:ARG:O	1:A:2542:ARG:NH1	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:991:VAL:HG23	1:B:995:GLN:HG3	1.77	0.65
1:B:3298:ASP:OD1	1:B:3298:ASP:N	2.29	0.65
1:B:4243:ARG:HH21	1:B:4256:THR:HG23	1.59	0.65
1:B:711:LEU:HD11	1:B:960:LEU:HG	1.78	0.65
1:B:2285:VAL:HG22	1:B:2290:ILE:HG22	1.79	0.65
1:A:1156:CYS:HB2	1:A:1160:ARG:H	1.60	0.65
1:A:765:ILE:HD11	1:A:786:VAL:HG21	1.77	0.65
1:B:582:GLU:HG2	1:B:591:ARG:HE	1.61	0.65
1:B:1588:MET:SD	1:B:1718:GLN:NE2	2.69	0.65
1:B:3204:SER:HB3	1:B:3232:LEU:HD23	1.79	0.65
1:B:3836:PHE:CZ	1:B:3840:ALA:HB3	2.32	0.65
1:A:1058:GLN:HG2	1:A:1059:LEU:HG	1.79	0.64
1:A:3578:CYS:HB3	1:A:3583:ASP:HB2	1.78	0.64
1:B:580:TYR:CE2	1:B:582:GLU:HB2	2.33	0.64
1:B:594:VAL:HG12	1:B:595:VAL:HG23	1.80	0.64
1:B:2531:LYS:HB3	1:B:2544:PRO:HB3	1.79	0.64
1:B:4062:VAL:HG23	1:B:4063:ARG:HG3	1.79	0.64
1:A:1367:GLU:HG3	1:A:1370:GLY:H	1.62	0.64
1:A:1187:CYS:H	1:A:1193:LYS:HE3	1.61	0.64
1:A:3142:LYS:N	1:A:3151:VAL:O	2.28	0.64
1:A:3362:THR:O	1:A:3399:ARG:NH1	2.28	0.64
1:B:3856:PRO:HG2	1:B:3859:TRP:HD1	1.62	0.64
1:A:1592:ILE:HG13	1:A:1593:VAL:HG23	1.80	0.64
1:A:3236:ARG:HD3	1:A:3459:PRO:HA	1.80	0.64
1:A:3846:MET:HG2	1:A:3857:PRO:HD3	1.79	0.64
1:B:3835:ARG:HD3	1:B:3841:TYR:HD2	1.61	0.64
1:B:3836:PHE:CD2	1:B:3838:ASP:HB3	2.32	0.64
1:A:1365:VAL:O	1:A:1372:LYS:HB3	1.98	0.64
1:B:3264:ILE:HG22	1:B:3265:ILE:HG13	1.80	0.64
1:A:2479:ARG:HH12	1:A:2499:ASN:HB2	1.63	0.63
1:A:3855:ILE:HD11	1:A:3867:CYS:HB2	1.80	0.63
1:B:1252:GLY:N	1:B:1262:GLU:OE1	2.29	0.63
1:A:1072:PHE:N	1:A:1080:ILE:O	2.31	0.63
1:A:570:ARG:HH11	1:A:583:THR:HG22	1.64	0.63
1:A:1159:HIS:HB2	1:A:1175:VAL:HG22	1.80	0.63
1:A:3298:ASP:N	1:A:3298:ASP:OD1	2.32	0.63
1:A:4204:TRP:HA	1:A:4231:PRO:HD2	1.80	0.63
1:A:602:PRO:HG3	1:A:621:LYS:HE2	1.81	0.63
1:A:620:THR:HA	1:A:1132:ASN:HB2	1.79	0.63
1:A:4279:ILE:HG12	1:A:4284:LEU:HG	1.81	0.63
1:B:366:PRO:HD2	1:B:368:ARG:HH22	1.61	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1237:CYS:SG	1:A:1260:SER:OG	2.57	0.63
1:A:1252:GLY:N	1:A:1262:GLU:OE1	2.30	0.63
1:B:3999:VAL:HG23	1:B:4000:PHE:HD1	1.62	0.63
1:A:2285:VAL:HG22	1:A:2290:ILE:HG22	1.80	0.63
1:B:3073:PRO:HA	1:B:3081:LYS:HD2	1.80	0.63
1:A:2398:LEU:HD22	1:A:2424:LEU:HD21	1.80	0.63
1:A:2759:ARG:NH2	1:A:2761:ASP:OD1	2.32	0.63
1:B:3720:HIS:ND1	1:B:3722:VAL:O	2.32	0.63
1:A:421:GLN:O	1:A:445:GLN:NE2	2.32	0.62
1:A:747:ASP:HA	1:A:961:LYS:HE3	1.81	0.62
1:A:3259:THR:HG21	2:E:1:NAG:C7	2.29	0.62
1:B:3362:THR:O	1:B:3399:ARG:NH1	2.28	0.62
1:B:4170:LYS:HG2	1:B:4174:ARG:HH21	1.63	0.62
1:A:1114:TYR:N	1:A:1122:ILE:O	2.31	0.62
1:B:1354:SER:HB3	1:B:1366:GLN:HG2	1.81	0.62
1:B:2683:TRP:HB3	1:B:2692:CYS:HB3	1.81	0.62
1:A:2683:TRP:HB3	1:A:2692:CYS:HB3	1.80	0.62
1:B:576:SER:HA	1:B:604:PRO:HD2	1.81	0.62
1:B:1826:LEU:HD22	1:B:1835:LEU:HD21	1.80	0.62
1:A:3720:HIS:ND1	1:A:3722:VAL:O	2.32	0.62
1:B:3834:THR:HB	1:B:3840:ALA:O	2.00	0.62
1:B:4279:ILE:HG12	1:B:4284:LEU:HG	1.82	0.62
1:B:2648:LYS:HB2	1:B:2650:GLN:HE22	1.65	0.61
1:A:423:ARG:HA	1:A:1089:ARG:HE	1.65	0.61
1:B:507:GLU:HB3	1:B:548:ARG:NH1	2.15	0.61
1:B:2182:ARG:NH1	1:B:2409:SER:OG	2.33	0.61
1:B:3259:THR:HG21	2:K:1:NAG:C7	2.30	0.61
1:A:1060:CYS:HA	1:A:1065:ASN:HD22	1.66	0.61
1:A:1381:LEU:HB3	1:A:1385:SER:HA	1.82	0.61
1:A:3872:ASP:HB3	1:A:3874:GLU:HG3	1.82	0.61
1:B:580:TYR:HE2	1:B:582:GLU:HB2	1.65	0.61
1:B:3496:ASP:OD2	1:B:3516:GLN:NE2	2.33	0.61
1:A:1160:ARG:HE	1:A:1162:ILE:HG22	1.66	0.61
1:A:3158:GLU:HG2	1:A:3159:MET:HG3	1.82	0.61
1:A:2756:TYR:HA	1:A:2759:ARG:HB3	1.81	0.61
1:B:365:ARG:HB3	1:B:368:ARG:NH2	2.15	0.61
1:A:609:LEU:O	1:A:655:ARG:NH1	2.34	0.61
1:A:2176:ILE:HB	2:C:1:NAG:H82	1.82	0.61
1:A:4020:HIS:NE2	1:A:4033:ALA:HB2	2.16	0.61
1:B:1405:TYR:HB2	1:B:1412:ARG:HB3	1.83	0.61
1:B:4311:VAL:HG12	1:B:4312:ASN:H	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:795:SER:OG	1:A:974:CYS:SG	2.59	0.60
1:B:883:ARG:NH2	1:B:903:ASP:O	2.33	0.60
1:B:4036:PHE:HB3	1:B:4047:CYS:HB3	1.84	0.60
1:A:2394:LEU:HD11	1:A:2633:LEU:HD13	1.83	0.60
1:A:3836:PHE:HD2	1:A:3838:ASP:HB3	1.66	0.60
1:B:421:GLN:O	1:B:445:GLN:NE2	2.33	0.60
1:A:2251:VAL:HG12	1:A:2258:ILE:HG12	1.83	0.60
1:B:1349:ASN:HB3	1:B:1370:GLY:HA3	1.81	0.60
1:B:2709:ASN:HB3	1:B:2727:ASP:CG	2.26	0.60
1:A:801:THR:HG22	1:A:808:ILE:HG12	1.83	0.60
1:B:2505:ARG:O	1:B:2542:ARG:NH1	2.34	0.60
1:A:523:TYR:CD2	1:A:540:ARG:HD2	2.36	0.60
1:A:2531:LYS:HB3	1:A:2544:PRO:HB3	1.83	0.60
1:A:3073:PRO:HA	1:A:3081:LYS:HD2	1.82	0.60
1:A:4067:TYR:CD2	1:A:4309:LEU:HD11	2.36	0.60
1:B:747:ASP:HA	1:B:961:LYS:HE3	1.83	0.60
1:A:352:CYS:HA	1:A:357:ILE:HD13	1.84	0.60
1:A:3094:CYS:H	1:A:3105:ASP:HB2	1.66	0.60
1:A:3204:SER:HB3	1:A:3232:LEU:HD23	1.84	0.60
1:B:1356:PHE:C	1:B:1358:GLY:H	2.08	0.60
1:A:527:SER:HB2	1:A:559:PRO:HB2	1.83	0.60
1:A:822:VAL:HG12	1:A:825:LEU:HD21	1.84	0.60
1:A:3496:ASP:OD2	1:A:3516:GLN:NE2	2.35	0.60
1:B:415:ARG:NH2	1:B:453:ILE:O	2.34	0.60
1:B:2251:VAL:HG12	1:B:2258:ILE:HG12	1.84	0.60
1:B:2390:LEU:HD13	1:B:2640:ILE:HD11	1.84	0.60
1:B:3025:ARG:NH1	1:B:3040:GLN:O	2.35	0.60
1:B:4178:TRP:HB3	1:B:4181:SER:HB3	1.82	0.60
1:A:3780:HIS:HE2	1:A:3824:LEU:HB2	1.66	0.60
1:B:1352:SER:HA	1:B:1355:ASP:CB	2.31	0.60
1:B:1510:LEU:HB3	1:B:1528:TYR:HB3	1.83	0.60
1:A:3454:ILE:O	1:A:3455:HIS:ND1	2.34	0.59
1:B:3176:CYS:O	1:B:3184:ARG:NH1	2.35	0.59
1:B:555:LYS:HE3	1:B:1175:VAL:HB	1.84	0.59
1:B:1358:GLY:O	1:B:1386:LYS:HD3	2.01	0.59
1:A:239:TRP:HA	1:A:242:ASP:HB3	1.84	0.59
1:A:1205:ASN:ND2	1:A:1212:ASP:OD2	2.36	0.59
1:A:2532:ILE:HG21	1:A:2565:LEU:HD21	1.85	0.59
1:B:1381:LEU:HB3	1:B:1385:SER:HA	1.84	0.59
1:A:1095:GLY:O	1:A:1099:HIS:N	2.34	0.59
1:A:1250:CYS:HB3	1:A:1268:PRO:HG3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4006:LEU:O	1:A:4008:ILE:HG13	2.01	0.59
1:B:3454:ILE:O	1:B:3455:HIS:ND1	2.35	0.59
1:A:347:VAL:HG22	1:A:349:PHE:H	1.66	0.59
1:A:847:ARG:NH2	1:A:1251:ASP:OD2	2.36	0.59
1:A:1060:CYS:SG	1:A:1061:GLY:N	2.73	0.59
1:A:1510:LEU:HB3	1:A:1528:TYR:HB3	1.85	0.59
1:B:661:ASN:HB3	1:B:664:LYS:HG3	1.84	0.59
1:B:2394:LEU:HD11	1:B:2633:LEU:HD13	1.84	0.59
1:A:3112:ASN:HB3	1:A:3115:HIS:HB2	1.84	0.59
1:B:423:ARG:NH1	1:B:1091:ASP:OD1	2.36	0.59
1:A:2474:ASP:HB2	1:A:2514:LEU:HD13	1.85	0.59
1:A:4280:PHE:HB2	1:A:4320:ILE:HD13	1.84	0.59
1:A:1871:GLY:N	1:A:1889:ASP:OD2	2.35	0.59
1:B:801:THR:HG22	1:B:808:ILE:HG12	1.85	0.59
1:B:558:TRP:HB2	1:B:577:ARG:HB2	1.83	0.59
1:B:602:PRO:HG3	1:B:621:LYS:HE2	1.83	0.59
1:B:1622:MET:HE3	1:B:1642:ILE:HD11	1.85	0.59
1:A:1356:PHE:C	1:A:1358:GLY:H	2.10	0.58
1:A:2648:LYS:HB2	1:A:2650:GLN:HE22	1.68	0.58
1:A:3200:TYR:CE1	2:D:1:NAG:H3	2.38	0.58
1:B:3226:LEU:HD13	1:B:3229:VAL:HG21	1.85	0.58
1:A:1062:THR:H	1:A:1065:ASN:HB2	1.68	0.58
1:A:1351:ASN:HA	1:A:1370:GLY:C	2.28	0.58
1:B:2739:HIS:O	1:B:2740:THR:C	2.46	0.58
1:B:3183:LEU:N	1:B:3192:ARG:O	2.35	0.58
3:G:1:NAG:H61	3:G:2:NAG:C7	2.33	0.58
1:A:817:THR:HG23	1:A:1001:PRO:HB3	1.85	0.58
1:A:1357:ASN:HA	1:A:1364:CYS:SG	2.43	0.58
1:A:2182:ARG:NH1	1:A:2409:SER:OG	2.36	0.58
1:A:2759:ARG:HD2	1:B:979:HIS:CG	2.38	0.58
1:B:887:VAL:HG22	1:B:894:ILE:HG12	1.85	0.58
1:B:2426:TYR:CD2	1:B:2643:VAL:HG13	2.39	0.58
1:B:2711:ARG:NH1	1:B:2724:ASP:O	2.36	0.58
1:A:1206:ARG:HA	1:A:1218:ASP:HB2	1.85	0.58
1:A:1351:ASN:HA	1:A:1370:GLY:CA	2.33	0.58
1:A:1358:GLY:O	1:A:1386:LYS:HD3	2.03	0.58
1:A:2533:GLU:HA	1:A:2544:PRO:HA	1.86	0.58
1:A:2686:ALA:N	1:A:2691:HIS:O	2.35	0.58
1:A:4313:PRO:HD3	1:B:4314:TRP:CE2	2.38	0.58
1:B:1871:GLY:N	1:B:1889:ASP:OD2	2.34	0.58
1:B:2739:HIS:CD2	1:B:2747:THR:HG21	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:574:VAL:HG12	1:A:581:ILE:HB	1.86	0.58
1:A:1405:TYR:HB2	1:A:1412:ARG:HB3	1.84	0.58
1:A:1658:THR:HG22	1:A:1665:VAL:HG22	1.86	0.58
1:B:1592:ILE:HG13	1:B:1593:VAL:HG23	1.84	0.58
1:B:2067:VAL:HG21	1:B:2300:ILE:HD13	1.86	0.58
1:B:2533:GLU:HA	1:B:2544:PRO:HA	1.85	0.58
1:B:3328:LEU:HG	1:B:3335:LEU:HD13	1.85	0.58
1:A:1046:ASP:HA	1:A:1068:SER:HB3	1.86	0.58
1:B:3200:TYR:CE1	2:J:1:NAG:H3	2.38	0.58
1:B:3599:TRP:N	1:B:3607:ILE:O	2.36	0.58
1:A:523:TYR:CE2	1:A:540:ARG:HD2	2.38	0.58
1:A:1945:ARG:NH2	1:A:1954:MET:SD	2.71	0.58
1:A:4293:GLU:HG2	1:A:4310:VAL:HG22	1.85	0.58
1:B:397:ILE:HG12	1:B:406:ILE:HG12	1.86	0.58
1:B:420:SER:O	1:B:1089:ARG:NH2	2.36	0.58
1:B:4101:VAL:HG21	1:B:4120:ILE:HD12	1.86	0.58
1:A:1617:SER:HA	1:A:1645:PRO:HD2	1.86	0.58
1:B:819:ARG:NH2	1:B:1001:PRO:O	2.37	0.58
1:B:1004:MET:HA	1:B:1015:GLY:HA2	1.86	0.58
1:B:3467:ASN:HD21	1:B:3469:CYS:HB2	1.68	0.58
1:A:1361:THR:HB	1:A:1388:CYS:H	1.69	0.58
1:A:3208:TYR:HH	1:A:3760:THR:HG1	1.50	0.57
1:B:402:ARG:HD3	1:B:1089:ARG:HH11	1.68	0.57
1:B:794:ILE:HG21	1:B:972:ASN:HB3	1.86	0.57
1:B:2598:LEU:HD11	1:B:2605:ILE:HD11	1.86	0.57
1:B:3142:LYS:N	1:B:3151:VAL:O	2.28	0.57
1:A:855:TRP:HB3	1:A:991:VAL:HG12	1.86	0.57
1:A:3423:THR:HG22	1:A:3430:VAL:HG22	1.86	0.57
1:A:3467:ASN:HD21	1:A:3469:CYS:HB2	1.69	0.57
1:A:4243:ARG:HH21	1:A:4256:THR:HG23	1.69	0.57
1:B:622:MET:HA	1:B:645:PRO:HD3	1.85	0.57
1:B:883:ARG:HH12	1:B:903:ASP:HB3	1.69	0.57
1:B:1172:LYS:HG2	1:B:1180:GLU:HB2	1.87	0.57
1:B:2704:SER:HA	1:B:2714:SER:HA	1.85	0.57
1:A:3176:CYS:O	1:A:3184:ARG:NH1	2.37	0.57
1:B:1617:SER:HA	1:B:1645:PRO:HD2	1.87	0.57
1:B:2491:ASN:HA	1:B:2502:VAL:HA	1.85	0.57
1:A:2683:TRP:HA	1:A:2693:ILE:O	2.05	0.57
1:A:3657:ASP:OD2	1:A:3706:ARG:NH2	2.35	0.57
1:B:746:ILE:HG13	1:B:961:LYS:HB3	1.86	0.57
1:A:1351:ASN:CG	1:A:1370:GLY:HA2	2.29	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3599:TRP:N	1:A:3607:ILE:O	2.36	0.57
1:B:4058:LEU:HD13	1:B:4311:VAL:HG21	1.86	0.57
1:B:754:THR:HA	1:B:769:LYS:HA	1.86	0.57
1:B:2399:ARG:HG2	1:B:2414:THR:HG23	1.87	0.57
1:B:3112:ASN:HB3	1:B:3115:HIS:HB2	1.86	0.57
1:B:3360:ILE:HD12	1:B:3399:ARG:HD2	1.86	0.57
1:B:3691:ARG:HG2	1:B:3693:ILE:HG23	1.85	0.57
1:A:4202:THR:HG22	1:A:4210:ILE:HG12	1.86	0.57
1:B:247:CYS:HB3	1:B:252:ASP:H	1.70	0.57
1:B:4007:ASP:HA	1:B:4025:LYS:HA	1.86	0.57
1:A:2711:ARG:HH11	1:A:2725:CYS:HA	1.69	0.57
1:B:1365:VAL:HG21	1:B:1374:LEU:HG	1.87	0.57
1:B:3657:ASP:OD2	1:B:3706:ARG:NH2	2.37	0.57
1:A:3203:PHE:HB3	1:A:3454:ILE:HG13	1.86	0.56
1:A:3691:ARG:HG2	1:A:3693:ILE:HG23	1.87	0.56
1:B:2510:ARG:NH2	1:B:2553:PRO:O	2.38	0.56
1:B:1254:PRO:HG2	4:B:4703:NAG:H83	1.87	0.56
1:A:402:ARG:HG2	1:A:425:VAL:HG12	1.87	0.56
1:A:1156:CYS:HB2	1:A:1159:HIS:HB3	1.87	0.56
1:A:1209:GLY:N	1:A:1219:GLU:OE1	2.37	0.56
1:A:1965:GLY:HA3	1:A:2006:GLY:HA2	1.86	0.56
1:A:3240:ARG:HD3	1:A:3253:ARG:HD2	1.87	0.56
1:A:3025:ARG:NH1	1:A:3040:GLN:O	2.38	0.56
1:B:2247:TYR:OH	1:B:2262:ARG:NH2	2.38	0.56
1:B:2683:TRP:HA	1:B:2693:ILE:O	2.04	0.56
1:B:4174:ARG:HD3	1:B:4374:PRO:HA	1.87	0.56
1:A:794:ILE:HG21	1:A:972:ASN:HB3	1.87	0.56
1:B:619:TRP:CD2	1:B:644:ARG:HD3	2.40	0.56
1:B:1362:HIS:HB3	1:B:1374:LEU:O	2.04	0.56
1:B:1965:GLY:HA3	1:B:2006:GLY:HA2	1.86	0.56
1:B:2432:ARG:HD2	1:B:2448:TYR:CD1	2.41	0.56
1:B:3575:HIS:O	1:B:3577:ASN:ND2	2.39	0.56
1:A:377:TYR:CE1	1:A:654:LEU:HD13	2.40	0.56
1:A:2711:ARG:NH1	1:A:2724:ASP:O	2.37	0.56
1:A:3312:VAL:HG11	1:A:3337:TRP:HZ2	1.70	0.56
1:A:706:ALA:O	1:A:708:GLN:NE2	2.38	0.56
1:A:3531:LYS:HA	1:A:3543:ASP:HB2	1.87	0.56
1:A:4101:VAL:HG21	1:A:4120:ILE:HD12	1.88	0.56
1:B:1846:GLU:HG3	1:B:1859:THR:HA	1.88	0.56
1:A:2426:TYR:CD2	1:A:2643:VAL:HG13	2.40	0.56
1:B:584:VAL:HB	1:B:588:GLY:HA2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1347:LEU:HB2	1:A:1369:PHE:HA	1.87	0.56
1:A:1622:MET:HE3	1:A:1642:ILE:HD11	1.86	0.56
1:A:3359:ILE:HG22	1:A:3360:ILE:HG12	1.88	0.56
1:B:1060:CYS:SG	1:B:1061:GLY:N	2.77	0.56
1:B:2545:ILE:HG22	1:B:2546:VAL:HG23	1.88	0.56
1:B:4202:THR:HG22	1:B:4210:ILE:HG12	1.88	0.56
1:A:2709:ASN:HB3	1:A:2727:ASP:CG	2.31	0.56
1:B:1439:LEU:HD21	1:B:1480:ILE:HD13	1.88	0.56
1:B:4359:PHE:HA	1:B:4367:CYS:HA	1.87	0.56
1:A:1113:GLN:HB3	1:A:1121:CYS:HB3	1.88	0.55
1:A:1136:ASP:OD1	1:A:1136:ASP:N	2.39	0.55
1:A:2510:ARG:NH2	1:A:2553:PRO:O	2.39	0.55
1:A:2644:VAL:HB	1:A:2648:LYS:HG2	1.88	0.55
1:B:1192:PHE:N	1:B:1201:ILE:O	2.38	0.55
1:B:2686:ALA:N	1:B:2691:HIS:O	2.36	0.55
1:B:574:VAL:HG12	1:B:581:ILE:HB	1.88	0.55
1:A:1555:ARG:NH1	1:A:1601:CYS:SG	2.80	0.55
1:A:4089:TYR:HB3	1:A:4101:VAL:HG22	1.89	0.55
1:B:1237:CYS:SG	1:B:1260:SER:OG	2.64	0.55
1:A:2067:VAL:HG21	1:A:2300:ILE:HD13	1.87	0.55
1:A:2432:ARG:HD2	1:A:2448:TYR:CD1	2.41	0.55
1:B:936:ILE:HG12	1:B:957:ILE:HD11	1.88	0.55
1:B:3842:CYS:SG	1:B:3848:GLU:HB3	2.46	0.55
1:B:1060:CYS:HA	1:B:1065:ASN:HD22	1.71	0.55
1:B:2644:VAL:HB	1:B:2648:LYS:HG2	1.88	0.55
1:B:3847:PHE:CE2	1:B:3855:ILE:HD13	2.42	0.55
1:B:1206:ARG:HA	1:B:1218:ASP:HB2	1.89	0.55
1:A:2168:GLU:OE2	1:A:2614:ARG:NH2	2.40	0.55
1:A:2704:SER:HA	1:A:2714:SER:HA	1.88	0.55
1:A:3415:ILE:O	1:A:3461:ARG:NH1	2.39	0.55
1:A:4170:LYS:HG2	1:A:4174:ARG:HH21	1.71	0.55
1:B:1354:SER:N	1:B:1366:GLN:HE21	2.03	0.55
1:A:1868:LEU:HD23	1:A:1910:VAL:HG23	1.89	0.55
1:A:2545:ILE:HG22	1:A:2546:VAL:HG23	1.88	0.55
1:A:4068:ASN:HB3	1:A:4071:SER:OG	2.06	0.55
1:B:366:PRO:HD2	1:B:368:ARG:NH2	2.22	0.55
1:B:1825:ASN:ND2	1:B:1875:GLY:HA2	2.22	0.55
1:B:3199:PRO:HB3	1:B:3458:HIS:HB2	1.89	0.55
1:B:4099:SER:O	1:B:4120:ILE:N	2.37	0.55
1:A:1354:SER:HB3	1:A:1366:GLN:HG2	1.89	0.55
1:B:1559:LEU:HD22	1:B:1584:MET:HE3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2144:GLU:HG3	1:B:2166:VAL:HG23	1.87	0.55
1:A:424:GLY:HA3	1:A:445:GLN:HE21	1.72	0.55
1:A:935:ALA:HB1	1:A:949:VAL:HG13	1.88	0.55
1:A:1191:GLN:HA	1:A:1202:GLY:HA2	1.88	0.55
1:A:1576:HIS:O	1:A:1578:ARG:NH1	2.40	0.55
1:A:1936:ALA:HB2	1:A:1966:ILE:HD11	1.87	0.55
1:A:2099:HIS:CE1	1:A:2194:HIS:HD2	2.25	0.55
1:A:2247:TYR:OH	1:A:2262:ARG:NH2	2.40	0.55
1:B:3311:CYS:HA	1:B:3319:CYS:HA	1.87	0.55
1:B:1354:SER:H	1:B:1366:GLN:NE2	2.03	0.54
1:B:3236:ARG:HD3	1:B:3459:PRO:HA	1.88	0.54
1:B:3284:LEU:N	1:B:3297:SER:O	2.37	0.54
1:B:3415:ILE:O	1:B:3461:ARG:NH1	2.41	0.54
1:A:3332:TYR:O	1:A:3485:GLY:N	2.40	0.54
1:B:2168:GLU:OE2	1:B:2614:ARG:NH2	2.40	0.54
1:B:527:SER:HB2	1:B:559:PRO:HB2	1.89	0.54
2:J:1:NAG:H61	2:J:2:NAG:H82	1.90	0.54
1:A:501:ARG:HG2	1:A:693:PHE:HE2	1.73	0.54
1:A:945:GLY:O	1:A:946:GLU:HG3	2.07	0.54
1:A:1846:GLU:HG3	1:A:1859:THR:HA	1.88	0.54
1:A:3328:LEU:HG	1:A:3335:LEU:HD13	1.90	0.54
1:B:2492:SER:HB3	1:B:2501:THR:HG23	1.89	0.54
1:B:2515:ASP:O	1:B:2519:GLY:N	2.40	0.54
1:B:3872:ASP:HB3	1:B:3874:GLU:HG2	1.89	0.54
1:A:1059:LEU:O	1:A:1065:ASN:ND2	2.40	0.54
1:A:1354:SER:H	1:A:1366:GLN:HE21	1.55	0.54
1:A:2141:GLY:H	1:A:2634:LEU:HD11	1.72	0.54
1:A:2556:LEU:HD23	1:A:2567:TRP:HB3	1.90	0.54
1:A:2709:ASN:HD21	1:A:2725:CYS:HB3	1.72	0.54
1:A:3039:CYS:HB2	1:A:3041:ASN:HD21	1.73	0.54
1:B:237:GLN:HE22	1:B:547:ASN:HB3	1.72	0.54
1:B:2425:ASP:O	1:B:2434:TYR:N	2.38	0.54
1:B:3211:ASN:HB3	1:B:3220:SER:HB3	1.90	0.54
1:B:3819:GLY:N	1:B:3835:ARG:HH21	2.05	0.54
1:A:3311:CYS:HA	1:A:3319:CYS:HA	1.89	0.54
1:A:3819:GLY:H	1:A:3835:ARG:HH21	1.54	0.54
1:B:239:TRP:HA	1:B:242:ASP:HB3	1.90	0.54
1:B:1347:LEU:HB2	1:B:1369:PHE:HA	1.90	0.54
1:B:2141:GLY:H	1:B:2634:LEU:HD11	1.72	0.54
1:B:3849:CYS:SG	1:B:3855:ILE:HD11	2.47	0.54
1:A:368:ARG:HG3	1:A:369:HIS:H	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:781:ASN:O	1:A:818:ARG:NH1	2.26	0.54
1:A:976:GLN:HB2	1:A:979:HIS:HB3	1.90	0.54
1:A:3861:CYS:SG	1:A:3874:GLU:HB2	2.48	0.54
1:A:4161:VAL:HA	1:A:4187:PRO:HD2	1.89	0.54
1:B:1072:PHE:N	1:B:1080:ILE:O	2.38	0.54
1:B:2711:ARG:HH11	1:B:2725:CYS:HA	1.72	0.54
1:B:3773:PRO:HD2	1:B:3776:TRP:CE3	2.43	0.54
1:B:3835:ARG:HD3	1:B:3841:TYR:CD2	2.43	0.54
1:A:420:SER:O	1:A:1089:ARG:NH2	2.41	0.54
1:A:2390:LEU:HD13	1:A:2640:ILE:HD11	1.88	0.54
1:B:473:ALA:HB3	1:B:482:TYR:HB2	1.89	0.54
1:B:570:ARG:HH11	1:B:583:THR:HG22	1.72	0.54
1:B:1159:HIS:O	1:B:1160:ARG:HB3	2.07	0.54
1:A:661:ASN:HB3	1:A:664:LYS:HG3	1.89	0.54
1:A:1437:LEU:HB2	1:A:1692:VAL:HB	1.90	0.54
1:B:790:ALA:HB3	1:B:799:TYR:HB2	1.89	0.54
1:B:1362:HIS:CG	1:B:1363:GLU:N	2.75	0.54
1:B:4160:ASP:HB3	1:B:4163:ASN:HB2	1.90	0.54
1:A:1559:LEU:HD22	1:A:1584:MET:HE3	1.89	0.54
1:A:3575:HIS:O	1:A:3577:ASN:ND2	2.40	0.54
1:B:365:ARG:HB2	1:B:368:ARG:C	2.33	0.54
1:B:381:ARG:HD3	1:B:384:TYR:HE1	1.73	0.54
1:B:1658:THR:HG22	1:B:1665:VAL:HG22	1.89	0.54
1:B:1906:ASP:HA	1:B:2034:LEU:HD13	1.90	0.54
1:B:3233:ASP:OD2	1:B:3277:VAL:N	2.33	0.54
1:B:4280:PHE:HB2	1:B:4320:ILE:HD13	1.90	0.54
1:B:2325:ASP:OD1	1:B:2326:VAL:N	2.41	0.53
1:A:1362:HIS:HB3	1:A:1374:LEU:O	2.09	0.53
1:A:1487:GLN:OE1	1:A:1491:TRP:NE1	2.36	0.53
1:A:2325:ASP:OD1	1:A:2326:VAL:N	2.40	0.53
1:B:582:GLU:HG3	1:B:583:THR:H	1.73	0.53
1:B:795:SER:OG	1:B:974:CYS:SG	2.65	0.53
1:A:2137:ILE:HG22	1:A:2138:VAL:HG23	1.90	0.53
1:A:4038:SER:OG	1:A:4040:SER:O	2.26	0.53
1:B:1235:PHE:N	1:B:1244:ILE:O	2.41	0.53
1:B:1349:ASN:OD1	1:B:1350:GLY:N	2.34	0.53
1:B:3039:CYS:HB2	1:B:3041:ASN:HD21	1.73	0.53
1:A:1091:ASP:N	1:A:1097:ASP:OD2	2.40	0.53
1:B:3359:ILE:HG22	1:B:3360:ILE:HG12	1.91	0.53
1:A:1235:PHE:N	1:A:1244:ILE:O	2.41	0.53
1:A:2693:ILE:HG22	1:A:2694:VAL:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3626:ASP:HB3	1:A:3629:HIS:HD2	1.74	0.53
1:A:4160:ASP:HB3	1:A:4163:ASN:HB2	1.90	0.53
1:A:4359:PHE:HA	1:A:4367:CYS:HA	1.91	0.53
1:B:1062:THR:H	1:B:1065:ASN:HB2	1.73	0.53
1:B:3823:CYS:HB3	1:B:3825:ASP:OD1	2.08	0.53
1:A:580:TYR:CE2	1:A:582:GLU:HB2	2.43	0.53
1:A:644:ARG:NH2	1:A:1132:ASN:O	2.42	0.53
1:A:2425:ASP:O	1:A:2434:TYR:N	2.39	0.53
1:B:1059:LEU:O	1:B:1065:ASN:ND2	2.42	0.53
1:B:1095:GLY:O	1:B:1099:HIS:N	2.41	0.53
1:B:2520:TYR:HA	1:B:2536:THR:HA	1.90	0.53
1:A:2318:ASP:OD1	1:A:2319:ASN:N	2.42	0.53
1:B:374:GLU:HG3	1:B:567:ILE:HD12	1.90	0.53
1:B:1405:TYR:N	1:B:1412:ARG:O	2.36	0.53
1:B:3094:CYS:H	1:B:3105:ASP:HB2	1.74	0.53
1:A:554:THR:O	1:A:591:ARG:NH1	2.36	0.53
1:A:639:TYR:HE2	1:A:641:ALA:HB2	1.73	0.53
1:A:1439:LEU:HD21	1:A:1480:ILE:HD13	1.89	0.53
1:A:2491:ASN:HA	1:A:2502:VAL:HA	1.91	0.53
1:B:1154:PHE:HE2	1:B:1174:CYS:SG	2.31	0.53
1:A:930:ASP:HB3	1:A:933:LEU:HB2	1.90	0.53
1:A:2775:CYS:HB2	1:B:978:THR:HG21	1.91	0.53
1:A:3509:MET:HB3	1:A:3511:MET:HG2	1.91	0.53
1:B:1156:CYS:HB2	1:B:1160:ARG:H	1.72	0.53
1:B:1825:ASN:HD22	1:B:1875:GLY:HA2	1.74	0.53
1:B:4208:PRO:HB2	1:B:4228:LEU:CB	2.35	0.53
1:A:580:TYR:HE2	1:A:582:GLU:HB2	1.74	0.53
1:A:1004:MET:HA	1:A:1015:GLY:HA2	1.91	0.53
1:A:1906:ASP:HA	1:A:2034:LEU:HD13	1.91	0.53
1:B:842:PHE:CE1	1:B:852:MET:HB2	2.44	0.53
1:A:594:VAL:HG12	1:A:595:VAL:HG23	1.90	0.52
1:A:1351:ASN:HA	1:A:1370:GLY:HA2	1.90	0.52
1:A:1825:ASN:ND2	1:A:1875:GLY:HA2	2.24	0.52
1:A:2598:LEU:HD11	1:A:2605:ILE:HD11	1.91	0.52
1:A:3773:PRO:HD2	1:A:3776:TRP:CE3	2.44	0.52
1:B:768:GLN:HE21	1:B:772:GLY:HA2	1.74	0.52
1:B:1945:ARG:NH2	1:B:1954:MET:SD	2.74	0.52
1:A:1356:PHE:C	1:A:1358:GLY:N	2.65	0.52
1:A:3798:CYS:SG	1:A:3799:HIS:N	2.82	0.52
1:B:460:GLU:CD	1:B:463:ASN:HD22	2.18	0.52
1:B:490:ARG:HA	1:B:506:THR:HG22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:834:HIS:CD2	1:B:837:ALA:H	2.27	0.52
1:B:1351:ASN:ND2	1:B:1370:GLY:HA2	2.25	0.52
1:B:2532:ILE:HG21	1:B:2565:LEU:HD21	1.91	0.52
1:B:2693:ILE:HG22	1:B:2694:VAL:H	1.73	0.52
1:B:4247:SER:HB3	1:B:4277:LEU:HD21	1.92	0.52
1:A:626:LYS:N	1:A:636:GLN:O	2.41	0.52
1:A:833:VAL:HG22	1:A:840:LEU:HD12	1.91	0.52
1:A:852:MET:HA	1:A:863:PRO:HA	1.92	0.52
1:A:2758:TYR:CD2	1:A:2765:ASP:HB2	2.44	0.52
1:B:1046:ASP:HA	1:B:1068:SER:HB3	1.91	0.52
1:A:3080:PHE:N	1:A:3088:ILE:O	2.37	0.52
1:A:3211:ASN:HB3	1:A:3220:SER:HB3	1.92	0.52
1:B:1225:ARG:O	1:B:1227:PRO:HD3	2.10	0.52
1:B:1484:ASP:HB3	1:B:1487:GLN:HB2	1.92	0.52
1:A:424:GLY:HA2	1:A:444:VAL:HB	1.90	0.52
1:A:576:SER:HA	1:A:604:PRO:HD2	1.91	0.52
1:A:2515:ASP:O	1:A:2519:GLY:N	2.43	0.52
1:A:3111:ILE:N	1:A:3113:GLU:OE2	2.40	0.52
1:B:1206:ARG:NH2	1:B:1217:SER:O	2.42	0.52
1:B:1250:CYS:HB3	1:B:1268:PRO:HG3	1.91	0.52
1:B:2556:LEU:HD23	1:B:2567:TRP:HB3	1.90	0.52
1:B:3047:LYS:HD3	1:B:3054:ASP:HB2	1.91	0.52
1:A:354:ILE:HD13	1:A:357:ILE:HD12	1.91	0.52
1:A:977:PRO:HD2	1:B:2776:LEU:HD22	1.91	0.52
1:B:3203:PHE:HB3	1:B:3454:ILE:HG13	1.92	0.52
1:B:3599:TRP:CE2	1:B:3612:GLN:HG3	2.45	0.52
1:B:3832:CYS:HB2	1:B:3833:PRO:HD2	1.91	0.52
1:A:713:PHE:HB3	1:A:960:LEU:HD12	1.90	0.52
1:A:1353:CYS:SG	1:A:1364:CYS:HB2	2.50	0.52
1:A:2688:ASN:HB2	1:A:2690:LYS:HE3	1.92	0.52
1:A:4060:ASP:HB3	1:A:4312:ASN:HD21	1.74	0.52
1:A:4174:ARG:HD3	1:A:4374:PRO:HA	1.92	0.52
1:A:4280:PHE:HB2	1:A:4320:ILE:HG21	1.92	0.52
1:B:578:PHE:CB	1:B:1175:VAL:HG12	2.39	0.52
1:B:1238:GLN:HE22	1:B:3178:CYS:H	1.57	0.52
1:B:1936:ALA:HB2	1:B:1966:ILE:HD11	1.90	0.52
1:A:1192:PHE:N	1:A:1201:ILE:O	2.43	0.52
1:A:1731:TRP:HB3	1:A:1740:CYS:SG	2.50	0.52
1:A:2432:ARG:NH2	1:A:2495:GLU:O	2.42	0.52
1:B:1205:ASN:ND2	1:B:1212:ASP:OD1	2.43	0.52
1:B:1731:TRP:HB3	1:B:1740:CYS:SG	2.50	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2318:ASP:OD1	1:B:2319:ASN:N	2.43	0.52
1:A:368:ARG:CG	1:A:369:HIS:H	2.23	0.51
1:A:1746:PRO:HB3	1:A:2011:HIS:HA	1.92	0.51
1:A:4020:HIS:CD2	1:A:4033:ALA:HB2	2.44	0.51
1:B:3332:TYR:O	1:B:3485:GLY:N	2.40	0.51
1:A:336:TYR:O	1:A:346:CYS:HB2	2.11	0.51
1:A:843:THR:CG2	1:A:872:PRO:HG2	2.39	0.51
1:B:1162:ILE:HG21	1:B:1173:ASP:HB3	1.93	0.51
1:B:1356:PHE:C	1:B:1358:GLY:N	2.65	0.51
1:B:3782:ASN:O	1:B:3782:ASN:ND2	2.43	0.51
1:A:946:GLU:O	1:A:947:MET:C	2.52	0.51
1:A:1073:THR:HA	1:A:1079:CYS:HA	1.92	0.51
1:B:1549:LYS:O	1:B:1589:ARG:NH1	2.34	0.51
1:B:1966:ILE:HG23	1:B:1973:LEU:HD11	1.92	0.51
1:A:2706:THR:HA	1:A:2712:CYS:HA	1.92	0.51
1:B:3245:ASP:O	1:B:3249:GLN:N	2.43	0.51
1:B:3509:MET:HB3	1:B:3511:MET:HG2	1.92	0.51
1:B:3688:THR:HB	1:B:3707:ASP:HB3	1.92	0.51
1:A:719:ILE:HD11	1:A:743:PHE:HB3	1.92	0.51
1:A:1685:TRP:HB3	1:A:1687:LEU:HD13	1.91	0.51
1:A:2523:TRP:NE1	1:A:2533:GLU:HB2	2.26	0.51
1:B:1113:GLN:HB3	1:B:1121:CYS:HB3	1.93	0.51
1:A:711:LEU:HD11	1:A:960:LEU:HG	1.92	0.51
1:A:862:LEU:HD12	1:A:863:PRO:HD2	1.92	0.51
1:A:907:LEU:HD22	1:A:943:ASP:HA	1.92	0.51
1:A:2569:ASP:HB3	1:A:2572:LEU:HB2	1.92	0.51
1:A:4091:TRP:CZ2	1:A:4323:GLN:HB2	2.46	0.51
1:B:441:THR:HG22	1:B:448:VAL:HG22	1.91	0.51
1:B:2242:ASP:OD2	1:B:2305:LYS:NZ	2.41	0.51
1:A:237:GLN:HE22	1:A:547:ASN:HB3	1.76	0.51
1:A:1484:ASP:HB3	1:A:1487:GLN:HB2	1.93	0.51
1:A:1650:LEU:O	1:A:1696:LYS:NZ	2.38	0.51
1:A:4224:VAL:HG23	1:A:4228:LEU:HD11	1.92	0.51
1:A:4232:THR:O	1:A:4247:SER:OG	2.29	0.51
1:B:465:SER:OG	1:B:501:ARG:NH1	2.43	0.51
1:B:1009:ASN:HD21	1:B:1011:LEU:HD12	1.75	0.51
1:B:1576:HIS:O	1:B:1578:ARG:NH1	2.41	0.51
1:B:1746:PRO:HB3	1:B:2011:HIS:HA	1.93	0.51
1:B:3862:ASP:O	1:B:3863:GLY:C	2.54	0.51
1:A:834:HIS:CD2	1:A:879:TRP:HZ3	2.28	0.51
1:A:2141:GLY:O	1:A:2163:ASN:ND2	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2534:ARG:HE	1:A:2545:ILE:HD11	1.75	0.51
1:A:3103:ASN:O	1:A:3107:LYS:HB3	2.11	0.51
1:B:1191:GLN:HA	1:B:1202:GLY:HA2	1.93	0.51
1:B:3798:CYS:SG	1:B:3799:HIS:N	2.84	0.51
1:A:1626:ASP:OD1	1:A:1626:ASP:N	2.41	0.51
1:A:4099:SER:O	1:A:4120:ILE:N	2.37	0.51
1:B:847:ARG:HD2	1:B:848:PRO:HA	1.92	0.51
1:B:1838:THR:HG23	1:B:1873:PRO:HG2	1.93	0.51
1:A:995:GLN:HA	1:B:2756:TYR:CE2	2.46	0.51
1:A:3329:HIS:HB2	1:A:3372:ILE:HD13	1.93	0.51
1:A:3479:LEU:HB2	1:A:3492:GLU:HB2	1.92	0.51
1:B:485:GLU:HG2	1:B:490:ARG:CZ	2.41	0.51
1:B:1187:CYS:SG	1:B:1193:LYS:HG2	2.51	0.51
1:B:1353:CYS:SG	1:B:1371:ALA:HA	2.51	0.51
1:B:1650:LEU:O	1:B:1696:LYS:NZ	2.35	0.51
1:B:3371:THR:HG23	1:B:3380:TYR:HB2	1.93	0.51
1:B:3398:HIS:HB2	1:B:3400:HIS:CE1	2.46	0.51
1:A:626:LYS:HB3	1:A:636:GLN:HB2	1.92	0.50
1:B:744:VAL:HG22	1:B:958:LEU:HD13	1.93	0.50
1:B:2523:TRP:NE1	1:B:2533:GLU:HB2	2.26	0.50
1:A:1198:ASP:N	1:A:1198:ASP:OD1	2.43	0.50
1:A:1378:GLY:HA3	1:A:1409:GLY:HA2	1.92	0.50
1:A:2176:ILE:HG22	1:A:2177:ASN:OD1	2.11	0.50
1:A:2653:ASN:HB3	1:A:2656:GLU:HG3	1.92	0.50
1:B:779:ALA:HB2	1:B:811:MET:HE1	1.93	0.50
1:B:1131:ASP:C	1:B:1133:ASP:H	2.19	0.50
1:B:1209:GLY:N	1:B:1219:GLU:OE1	2.41	0.50
1:B:3281:SER:O	1:B:3283:LYS:NZ	2.43	0.50
1:B:4091:TRP:CZ2	1:B:4323:GLN:HB2	2.47	0.50
1:A:3998:ASN:ND2	1:A:4000:PHE:H	2.09	0.50
1:B:3644:ASN:ND2	1:B:3662:ASP:OD2	2.45	0.50
1:B:4089:TYR:HB3	1:B:4101:VAL:HG22	1.92	0.50
1:A:1170:GLY:N	1:A:1180:GLU:OE2	2.45	0.50
1:A:3284:LEU:N	1:A:3297:SER:O	2.39	0.50
1:A:3782:ASN:O	1:A:3782:ASN:ND2	2.44	0.50
1:B:488:VAL:HG11	1:B:720:ARG:HD2	1.94	0.50
1:B:897:SER:HA	1:B:903:ASP:O	2.11	0.50
1:B:2603:GLN:HA	1:B:2620:LYS:HE3	1.93	0.50
1:B:2608:THR:HB	1:B:2637:PRO:HG2	1.93	0.50
1:B:2686:ALA:O	1:B:2690:LYS:N	2.34	0.50
1:A:3371:THR:HG23	1:A:3380:TYR:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:892:ASP:OD1	1:B:892:ASP:N	2.44	0.50
1:B:1198:ASP:OD1	1:B:1198:ASP:N	2.42	0.50
1:B:1967:ALA:HB1	1:B:2009:VAL:HG23	1.94	0.50
1:B:2137:ILE:HG22	1:B:2138:VAL:HG23	1.92	0.50
1:B:3208:TYR:HB3	1:B:3221:LEU:HD21	1.93	0.50
1:B:3799:HIS:HB2	1:B:3802:TYR:HD2	1.76	0.50
1:A:2492:SER:HB3	1:A:2501:THR:HG23	1.93	0.50
1:B:339:ASN:HB2	1:B:342:ASP:O	2.11	0.50
1:B:3531:LYS:HA	1:B:3543:ASP:HB2	1.93	0.50
1:A:1071:ALA:HB1	1:A:1079:CYS:HB3	1.93	0.50
1:A:3047:LYS:HD3	1:A:3054:ASP:HB2	1.93	0.50
1:A:3129:THR:OG1	1:A:3130:LEU:N	2.44	0.50
1:A:3183:LEU:N	1:A:3192:ARG:O	2.43	0.50
1:B:747:ASP:OD1	1:B:748:PHE:N	2.42	0.50
1:B:1367:GLU:HG3	1:B:1370:GLY:H	1.77	0.50
1:B:2476:ILE:HG13	1:B:2516:PRO:HB2	1.94	0.50
1:B:2758:TYR:HB2	1:B:2766:CYS:HB3	1.94	0.50
1:A:1518:TRP:HA	1:A:1521:ARG:HH21	1.77	0.50
1:A:4178:TRP:HB3	1:A:4181:SER:HB3	1.92	0.50
1:B:2257:ILE:HG13	1:B:2270:VAL:HG13	1.94	0.50
1:B:2432:ARG:NH2	1:B:2495:GLU:O	2.45	0.50
1:B:3626:ASP:HB3	1:B:3629:HIS:HD2	1.77	0.50
1:A:539:GLU:OE2	1:A:548:ARG:NE	2.45	0.50
1:A:892:ASP:OD1	1:A:892:ASP:N	2.44	0.50
1:B:336:TYR:O	1:B:346:CYS:HB2	2.11	0.50
1:B:556:LEU:HD11	1:B:559:PRO:HB3	1.93	0.50
1:B:940:ARG:NE	1:B:944:GLY:O	2.32	0.50
1:B:1685:TRP:HB3	1:B:1687:LEU:HD13	1.93	0.50
1:B:3608:PRO:HD2	1:B:3611:TRP:CE3	2.47	0.50
1:A:1549:LYS:O	1:A:1589:ARG:NH1	2.33	0.49
1:A:1822:PRO:HG3	1:A:1841:ARG:HH11	1.77	0.49
1:A:3599:TRP:CE2	1:A:3612:GLN:HG3	2.47	0.49
1:B:3111:ILE:N	1:B:3113:GLU:OE2	2.41	0.49
1:B:3855:ILE:HD12	1:B:3855:ILE:H	1.76	0.49
1:A:2167:SER:O	1:B:1618:TYR:OH	2.27	0.49
1:A:2449:ALA:HA	1:A:2456:HIS:CD2	2.47	0.49
1:B:1365:VAL:HG11	1:B:1372:LYS:HD3	1.94	0.49
1:B:2774:GLY:HA3	1:B:2777:PHE:HD2	1.77	0.49
1:B:3345:TYR:HD2	1:B:3347:GLY:H	1.60	0.49
1:B:3612:GLN:HG2	1:B:3629:HIS:HE1	1.75	0.49
1:B:3811:VAL:HG21	1:B:3822:ASP:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3829:GLU:HB3	1:B:3835:ARG:HH22	1.76	0.49
1:A:750:ALA:N	1:A:968:GLN:OE1	2.38	0.49
1:A:1225:ARG:O	1:A:1227:PRO:HD3	2.12	0.49
1:A:2426:TYR:CZ	1:A:2428:SER:HA	2.47	0.49
1:A:3398:HIS:HB2	1:A:3400:HIS:CE1	2.47	0.49
1:B:501:ARG:HG2	1:B:693:PHE:HE2	1.77	0.49
1:B:3312:VAL:HA	1:B:3356:LYS:HD3	1.94	0.49
1:B:3423:THR:HG22	1:B:3430:VAL:HG22	1.94	0.49
1:B:3804:GLN:HE21	1:B:3808:GLY:HA2	1.77	0.49
1:A:337:ILE:HA	1:A:346:CYS:HB2	1.94	0.49
1:A:3124:HIS:HE1	1:A:3141:TYR:CG	2.30	0.49
1:A:4008:ILE:N	1:A:4026:GLY:H	2.09	0.49
1:B:2345:PRO:HB2	1:B:2366:PRO:HB3	1.94	0.49
1:B:2548:SER:O	1:B:2585:ARG:NH1	2.38	0.49
1:B:4038:SER:OG	1:B:4040:SER:O	2.30	0.49
1:A:2393:ALA:HB2	1:A:2424:LEU:HG	1.93	0.49
1:A:2758:TYR:HB3	1:A:2763:TYR:HB2	1.94	0.49
1:A:2759:ARG:NE	1:A:2759:ARG:O	2.45	0.49
1:A:3199:PRO:HB3	1:A:3458:HIS:HB2	1.94	0.49
1:B:4116:LYS:HG2	1:B:4135:ASP:HA	1.94	0.49
1:A:768:GLN:HE21	1:A:772:GLY:HA2	1.77	0.49
1:A:1403:HIS:CD2	1:A:1403:HIS:H	2.29	0.49
1:A:1966:ILE:HG23	1:A:1973:LEU:HD11	1.94	0.49
1:A:1986:VAL:HB	1:A:1991:GLY:HA2	1.94	0.49
1:A:3513:SER:HB3	1:A:3593:HIS:CG	2.48	0.49
1:B:493:MET:HE1	1:B:673:VAL:HG11	1.94	0.49
1:B:744:VAL:HG13	1:B:959:HIS:HE1	1.78	0.49
1:B:3560:CYS:SG	1:B:3582:SER:HB3	2.53	0.49
1:A:754:THR:HG21	1:A:767:LYS:HE3	1.93	0.49
1:A:1416:ASP:OD1	1:A:1417:THR:N	2.45	0.49
1:A:1615:MET:HG3	1:A:1648:LEU:HD12	1.94	0.49
1:A:3268:ARG:HB2	1:A:3304:ARG:HH12	1.78	0.49
1:B:1822:PRO:HG3	1:B:1841:ARG:HH11	1.77	0.49
1:B:2706:THR:HA	1:B:2712:CYS:HA	1.94	0.49
1:B:3312:VAL:HG11	1:B:3337:TRP:HZ2	1.77	0.49
1:B:3821:ALA:HA	1:B:3829:GLU:HG2	1.94	0.49
1:A:359:ASP:O	1:A:629:LYS:NZ	2.40	0.49
1:A:894:ILE:HG13	1:A:913:MET:HE1	1.94	0.49
1:A:3081:LYS:HA	1:A:3087:CYS:HA	1.95	0.49
1:A:3360:ILE:HD12	1:A:3399:ARG:HD2	1.93	0.49
1:A:3608:PRO:HD2	1:A:3611:TRP:CE3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3644:ASN:ND2	1:A:3662:ASP:OD2	2.46	0.49
1:B:3780:HIS:N	1:B:3790:GLU:OE1	2.40	0.49
1:B:4230:TRP:CG	1:B:4250:LYS:HB2	2.48	0.49
1:A:338:ILE:HG23	1:A:347:VAL:HG12	1.95	0.49
1:A:1967:ALA:HB1	1:A:2009:VAL:HG23	1.95	0.49
1:A:2242:ASP:OD2	1:A:2305:LYS:NZ	2.42	0.49
1:A:2420:THR:O	1:A:2438:ASN:N	2.46	0.49
1:A:2557:THR:HG21	1:A:2599:THR:HA	1.94	0.49
1:A:3259:THR:HG21	2:E:1:NAG:N2	2.28	0.49
1:A:3835:ARG:HH11	1:A:3841:TYR:HD2	1.60	0.49
1:B:1437:LEU:HB2	1:B:1692:VAL:HB	1.93	0.49
1:B:2176:ILE:HG22	1:B:2177:ASN:OD1	2.13	0.49
1:B:3657:ASP:OD1	1:B:3706:ARG:NE	2.46	0.49
1:A:2513:VAL:HB	1:A:2522:TYR:HB2	1.94	0.49
1:A:3657:ASP:OD1	1:A:3706:ARG:NE	2.45	0.49
1:A:3688:THR:HB	1:A:3707:ASP:HB3	1.94	0.49
1:B:1986:VAL:HB	1:B:1991:GLY:HA2	1.94	0.49
1:B:2475:TRP:CZ2	1:B:2649:GLN:HB2	2.39	0.49
1:A:865:ILE:HG22	1:A:869:LEU:HD11	1.94	0.48
1:A:1357:ASN:O	1:A:1364:CYS:HB3	2.13	0.48
1:A:2144:GLU:HG3	1:A:2166:VAL:HG23	1.94	0.48
1:B:390:SER:HB2	4:B:4701:NAG:O5	2.13	0.48
1:B:1170:GLY:N	1:B:1180:GLU:OE2	2.44	0.48
1:B:1856:TYR:HB3	1:B:2046:ALA:HB2	1.94	0.48
1:B:2601:TYR:HB2	1:B:2642:THR:HG21	1.95	0.48
1:A:887:VAL:HG22	1:A:894:ILE:HG12	1.94	0.48
1:A:924:GLU:HA	1:A:941:LYS:HE3	1.94	0.48
1:A:1362:HIS:CG	1:A:1363:GLU:N	2.80	0.48
1:A:1519:VAL:HB	1:A:1561:PRO:HB2	1.95	0.48
1:A:2493:MET:HG2	1:A:2497:GLY:HA2	1.95	0.48
1:A:2550:LEU:HD11	1:A:2553:PRO:HB3	1.94	0.48
1:A:2603:GLN:HA	1:A:2620:LYS:HE3	1.94	0.48
1:A:3518:LEU:HD11	1:A:3522:ASN:HD22	1.78	0.48
1:B:2466:GLY:HA3	1:B:2486:LEU:HD22	1.94	0.48
1:B:3129:THR:OG1	1:B:3130:LEU:N	2.46	0.48
1:A:1848:LEU:HD11	1:A:1855:ARG:HB3	1.95	0.48
1:A:3245:ASP:O	1:A:3249:GLN:N	2.45	0.48
1:A:4102:TYR:OH	1:A:4171:LEU:HG	2.14	0.48
1:B:1378:GLY:HA3	1:B:1409:GLY:HA2	1.95	0.48
1:B:1518:TRP:HA	1:B:1521:ARG:HH21	1.78	0.48
1:B:2428:SER:O	1:B:2429:VAL:C	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2449:ALA:HA	1:B:2456:HIS:CD2	2.48	0.48
1:B:3081:LYS:HA	1:B:3087:CYS:HA	1.94	0.48
1:B:3259:THR:HG21	2:K:1:NAG:N2	2.28	0.48
1:B:3582:SER:HA	1:B:3585:ASP:HB2	1.95	0.48
1:B:3849:CYS:SG	1:B:3853:VAL:HB	2.53	0.48
1:A:582:GLU:HG3	1:A:583:THR:H	1.78	0.48
1:A:748:PHE:O	1:A:968:GLN:NE2	2.46	0.48
1:A:1844:SER:OG	1:A:1846:GLU:OE2	2.24	0.48
1:A:2475:TRP:CZ2	1:A:2649:GLN:HB2	2.44	0.48
1:A:3056:ASP:OD1	1:A:3056:ASP:N	2.44	0.48
1:B:639:TYR:HE1	1:B:641:ALA:HB2	1.79	0.48
1:B:2450:THR:H	1:B:2456:HIS:CE1	2.31	0.48
1:B:2569:ASP:HB3	1:B:2572:LEU:HB2	1.95	0.48
1:B:2654:PRO:HB2	1:B:2673:ALA:HB2	1.95	0.48
1:A:1551:LEU:HD11	1:A:1554:PRO:HB3	1.95	0.48
1:A:3103:ASN:HD21	1:A:3106:GLU:HG2	1.78	0.48
1:B:424:GLY:HA2	1:B:444:VAL:HB	1.95	0.48
1:B:494:VAL:HG12	1:B:501:ARG:HA	1.95	0.48
1:B:2393:ALA:HB2	1:B:2424:LEU:HG	1.93	0.48
1:B:2394:LEU:HD22	1:B:2399:ARG:CZ	2.43	0.48
1:A:484:VAL:HG22	1:A:491:ILE:HG12	1.95	0.48
1:A:940:ARG:HG3	1:A:946:GLU:HG3	1.95	0.48
1:A:945:GLY:C	1:A:946:GLU:HG3	2.39	0.48
1:B:1868:LEU:HD23	1:B:1910:VAL:HG23	1.94	0.48
1:B:3103:ASN:ND2	1:B:3105:ASP:OD1	2.47	0.48
1:A:563:THR:HG23	1:A:572:TYR:HB2	1.96	0.48
1:A:842:PHE:CE1	1:A:852:MET:HB2	2.49	0.48
1:A:974:CYS:HB3	1:A:981:ASN:HA	1.95	0.48
1:A:1903:ALA:HB2	1:A:1910:VAL:HG12	1.94	0.48
1:A:1927:ASP:OD2	1:A:1988:LYS:NZ	2.46	0.48
1:A:2036:VAL:HG12	1:A:2040:LEU:HB2	1.96	0.48
1:A:2686:ALA:HB3	1:A:2691:HIS:HB2	1.96	0.48
1:B:555:LYS:HB3	1:B:591:ARG:HH22	1.79	0.48
1:B:685:LEU:HB3	1:B:687:PHE:CE2	2.49	0.48
1:B:1580:GLU:HG2	1:B:1591:VAL:HG22	1.96	0.48
1:B:4208:PRO:O	1:B:4228:LEU:HD12	2.13	0.48
1:A:1074:CYS:N	1:A:1078:GLU:O	2.44	0.48
1:A:1154:PHE:CG	1:A:1155:ASN:N	2.82	0.48
1:A:1469:VAL:HG13	1:A:1687:LEU:HD23	1.96	0.48
1:A:3244:ILE:HD13	1:A:3272:ALA:HB1	1.96	0.48
1:B:1136:ASP:OD1	1:B:1136:ASP:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1156:CYS:CB	1:A:1159:HIS:HB3	2.43	0.48
1:A:2608:THR:HB	1:A:2637:PRO:HG2	1.95	0.48
1:B:1160:ARG:NE	1:B:1162:ILE:HG22	2.28	0.48
1:B:1362:HIS:O	1:B:1363:GLU:C	2.57	0.48
1:B:1755:ILE:HD12	1:B:1757:PHE:HE2	1.79	0.48
1:B:3329:HIS:HB2	1:B:3372:ILE:HD13	1.96	0.48
1:B:3859:TRP:HA	1:B:3862:ASP:HB3	1.96	0.48
1:A:788:SER:HB2	1:A:830:SER:HA	1.96	0.48
1:B:981:ASN:HA	1:B:988:CYS:HB2	1.96	0.48
1:B:1483:SER:HB2	1:B:1514:ILE:HD11	1.96	0.48
1:B:1487:GLN:OE1	1:B:1491:TRP:NE1	2.36	0.48
1:B:2502:VAL:H	1:B:2679:HIS:HB3	1.79	0.48
1:B:4000:PHE:HA	1:B:4004:SER:HB3	1.96	0.48
1:B:4175:TYR:HB3	1:B:4354:PRO:HB3	1.96	0.48
1:A:354:ILE:HB	1:A:357:ILE:HB	1.95	0.47
1:A:584:VAL:HB	1:A:588:GLY:HA2	1.96	0.47
1:A:883:ARG:HH12	1:A:903:ASP:HB3	1.79	0.47
1:A:2020:ASN:N	1:A:2023:SER:OG	2.38	0.47
1:A:3836:PHE:CD2	1:A:3838:ASP:HB3	2.47	0.47
1:B:3834:THR:HA	1:B:3841:TYR:CE2	2.49	0.47
1:A:867:THR:O	1:A:904:ARG:NH1	2.37	0.47
1:B:1465:GLY:HA3	1:B:1468:ILE:HD11	1.95	0.47
1:B:1510:LEU:HD23	1:B:1528:TYR:HB3	1.96	0.47
1:B:1903:ALA:HB2	1:B:1910:VAL:HG12	1.95	0.47
1:B:3220:SER:OG	1:B:3221:LEU:N	2.47	0.47
1:A:397:ILE:HG12	1:A:406:ILE:HG12	1.95	0.47
1:A:520:THR:HA	1:A:679:ARG:HH21	1.79	0.47
1:A:3103:ASN:ND2	1:A:3105:ASP:OD1	2.47	0.47
1:A:3801:GLU:N	1:A:3801:GLU:OE1	2.42	0.47
1:A:3819:GLY:N	1:A:3829:GLU:OE1	2.47	0.47
1:B:479:ASN:N	1:B:479:ASN:OD1	2.48	0.47
1:B:3244:ILE:HG21	1:B:3272:ALA:HB3	1.96	0.47
1:B:3294:LEU:HD21	1:B:3335:LEU:HD23	1.97	0.47
1:B:3533:ASP:HA	1:B:3551:ARG:NE	2.29	0.47
1:A:1175:VAL:HG23	1:A:1176:ASP:N	2.30	0.47
1:A:2548:SER:O	1:A:2585:ARG:NH1	2.39	0.47
1:A:3560:CYS:SG	1:A:3582:SER:HB3	2.54	0.47
1:A:4182:THR:O	1:A:4184:LEU:HG	2.14	0.47
1:A:4255:GLU:HG2	1:A:4266:VAL:HG22	1.96	0.47
1:B:972:ASN:OD1	1:B:973:ALA:N	2.43	0.47
1:B:1522:ASN:HD22	1:B:1537:LYS:HA	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1567:LEU:HD13	1:B:1581:ARG:HD2	1.96	0.47
2:I:1:NAG:H61	2:I:2:NAG:H82	1.95	0.47
1:A:395:SER:HB2	1:A:651:TYR:HB3	1.96	0.47
1:A:843:THR:HG21	1:A:872:PRO:O	2.15	0.47
1:A:883:ARG:HH21	1:A:896:HIS:CD2	2.32	0.47
1:A:2000:ASN:ND2	1:B:2254:SER:O	2.47	0.47
1:B:224:GLY:O	1:B:523:TYR:OH	2.32	0.47
1:B:781:ASN:O	1:B:818:ARG:NH1	2.25	0.47
1:B:1416:ASP:OD1	1:B:1417:THR:N	2.47	0.47
1:B:3513:SER:HB3	1:B:3593:HIS:CG	2.48	0.47
1:A:1354:SER:H	1:A:1366:GLN:NE2	2.13	0.47
1:A:1825:ASN:HD22	1:A:1875:GLY:HA2	1.80	0.47
1:A:1838:THR:HG23	1:A:1873:PRO:HG2	1.95	0.47
1:A:1937:VAL:HG12	1:A:1940:ARG:H	1.80	0.47
1:A:3110:GLY:C	1:A:3111:ILE:HD12	2.40	0.47
1:A:4247:SER:HB3	1:A:4277:LEU:HD21	1.96	0.47
1:B:2707:CYS:CB	1:B:2729:SER:HB3	2.42	0.47
1:A:446:ASN:HB3	1:A:467:GLU:HA	1.96	0.47
1:A:1154:PHE:N	1:A:1162:ILE:O	2.48	0.47
1:A:2345:PRO:HB2	1:A:2366:PRO:HB3	1.96	0.47
1:A:3078:HIS:C	1:A:3090:MET:HG2	2.40	0.47
1:A:3633:ARG:HB3	1:A:3641:ARG:HH12	1.79	0.47
1:B:347:VAL:HG22	1:B:349:PHE:H	1.80	0.47
1:B:351:ASP:OD1	1:B:351:ASP:N	2.47	0.47
1:B:467:GLU:N	1:B:485:GLU:OE2	2.46	0.47
1:B:513:ARG:HD2	1:B:605:PHE:HE1	1.79	0.47
1:B:1519:VAL:HB	1:B:1561:PRO:HB2	1.96	0.47
1:B:1937:VAL:HG12	1:B:1940:ARG:H	1.79	0.47
1:B:2568:VAL:HG12	1:B:2575:ILE:HG23	1.95	0.47
1:B:2653:ASN:HB3	1:B:2656:GLU:HG3	1.96	0.47
1:B:3390:GLU:HG2	1:B:3401:THR:HA	1.96	0.47
1:B:4312:ASN:N	1:B:4312:ASN:HD22	2.12	0.47
1:A:248:LYS:C	1:A:250:ASN:H	2.23	0.47
1:B:617:THR:HG22	1:B:624:VAL:HG22	1.97	0.47
1:B:852:MET:HE3	1:B:863:PRO:HB3	1.96	0.47
1:B:1141:LYS:O	1:B:1142:ASN:C	2.57	0.47
1:B:1551:LEU:HD11	1:B:1554:PRO:HB3	1.97	0.47
1:B:3599:TRP:HB2	1:B:3609:GLU:HA	1.96	0.47
1:B:4293:GLU:OE1	1:B:4307:LYS:HE2	2.15	0.47
1:A:1163:ASP:OD1	1:A:1164:LEU:N	2.47	0.47
1:A:2686:ALA:O	1:A:2690:LYS:N	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1615:MET:HG3	1:B:1648:LEU:HD12	1.97	0.47
1:B:1626:ASP:OD1	1:B:1626:ASP:N	2.45	0.47
1:B:1848:LEU:HD11	1:B:1855:ARG:HB3	1.97	0.47
1:B:1975:TYR:OH	1:B:1984:GLU:OE1	2.21	0.47
1:B:2490:ILE:N	1:B:2504:ALA:O	2.47	0.47
1:B:2599:THR:HG22	1:B:2606:TYR:HB2	1.97	0.47
1:B:3195:SER:HB2	1:B:3460:TYR:CZ	2.50	0.47
1:B:3633:ARG:HB3	1:B:3641:ARG:HH12	1.80	0.47
1:B:3875:LEU:HD22	1:B:3880:ASP:H	1.80	0.47
1:B:4067:TYR:CD2	1:B:4309:LEU:HD11	2.49	0.47
1:B:4255:GLU:HG2	1:B:4266:VAL:HG22	1.96	0.47
1:A:989:PHE:HB2	1:A:997:VAL:O	2.15	0.47
1:A:1031:PHE:N	1:A:1039:VAL:O	2.40	0.47
1:A:1405:TYR:N	1:A:1412:ARG:O	2.36	0.47
1:A:2124:ILE:HD11	1:A:2147:VAL:HG11	1.97	0.47
1:A:3312:VAL:HA	1:A:3356:LYS:HD3	1.96	0.47
1:B:2127:ILE:HA	1:B:2133:SER:O	2.14	0.47
1:B:2435:PHE:HZ	1:B:2458:PRO:HB3	1.80	0.47
1:B:3518:LEU:HD11	1:B:3522:ASN:HD22	1.80	0.47
1:A:539:GLU:CD	1:A:548:ARG:HE	2.23	0.46
1:A:1187:CYS:SG	1:A:1193:LYS:HG2	2.55	0.46
1:A:1618:TYR:OH	1:B:2167:SER:O	2.25	0.46
1:A:1667:ARG:NH2	1:A:1677:SER:OG	2.47	0.46
1:A:3533:ASP:HA	1:A:3551:ARG:NE	2.30	0.46
1:A:3775:ARG:HD2	1:A:3802:TYR:HE2	1.80	0.46
1:B:867:THR:O	1:B:904:ARG:NH1	2.34	0.46
1:A:465:SER:OG	1:A:501:ARG:NH1	2.48	0.46
1:A:490:ARG:HH21	1:A:501:ARG:NH2	2.13	0.46
1:A:829:ARG:HB2	1:A:845:TRP:CD1	2.50	0.46
1:A:1825:ASN:OD1	1:A:1826:LEU:N	2.48	0.46
1:A:2428:SER:O	1:A:2429:VAL:C	2.58	0.46
1:A:3047:LYS:HA	1:A:3052:ASP:HB2	1.98	0.46
1:A:3103:ASN:O	1:A:3107:LYS:N	2.41	0.46
1:A:3502:LEU:HD11	1:A:3507:TYR:HB2	1.96	0.46
1:B:400:ASN:OD1	1:B:401:GLY:N	2.47	0.46
1:B:490:ARG:HH21	1:B:501:ARG:NH2	2.12	0.46
1:B:518:ASP:OD1	1:B:520:THR:OG1	2.30	0.46
1:B:552:VAL:HG21	1:B:573:TRP:CH2	2.51	0.46
1:B:3376:ASN:ND2	1:B:3436:TYR:OH	2.48	0.46
1:A:910:ILE:HG21	1:A:913:MET:HB2	1.97	0.46
1:A:3640:PHE:HE2	1:A:3665:ASP:HA	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:513:ARG:HD2	1:B:605:PHE:CE1	2.51	0.46
1:B:677:SER:OG	1:B:678:HIS:N	2.48	0.46
1:B:2426:TYR:CZ	1:B:2428:SER:HA	2.51	0.46
1:A:1081:PRO:HD2	1:A:1084:TRP:CE3	2.50	0.46
1:A:2576:GLU:HG2	1:A:2587:VAL:HG22	1.98	0.46
1:A:4058:LEU:HD13	1:A:4311:VAL:HG21	1.97	0.46
1:B:1084:TRP:HB3	1:B:1091:ASP:OD2	2.16	0.46
1:B:1156:CYS:HB3	1:B:1159:HIS:HB3	1.98	0.46
1:B:1606:ASP:N	1:B:1606:ASP:OD1	2.48	0.46
1:B:4224:VAL:HG23	1:B:4228:LEU:HD11	1.97	0.46
1:B:4277:LEU:HB3	1:B:4284:LEU:HD21	1.96	0.46
1:A:949:VAL:HG11	1:A:952:SER:HB3	1.97	0.46
1:A:2192:PRO:HB3	1:A:2206:TRP:CD1	2.50	0.46
1:A:4312:ASN:ND2	1:A:4314:TRP:HB2	2.30	0.46
1:A:685:LEU:HB3	1:A:687:PHE:CE2	2.49	0.46
1:A:2254:SER:O	1:B:2000:ASN:ND2	2.48	0.46
1:A:3092:LYS:HB3	1:A:3099:ASP:OD2	2.15	0.46
1:A:3204:SER:O	1:A:3452:PHE:HB2	2.16	0.46
1:A:3220:SER:OG	1:A:3221:LEU:N	2.48	0.46
1:A:3458:HIS:CD2	1:A:3460:TYR:H	2.34	0.46
1:B:248:LYS:C	1:B:250:ASN:H	2.24	0.46
1:B:2523:TRP:NE1	1:B:2533:GLU:OE1	2.38	0.46
1:B:2550:LEU:HD11	1:B:2553:PRO:HB3	1.97	0.46
1:B:4057:LEU:HG	1:B:4321:PHE:HB2	1.98	0.46
1:B:4098:LEU:HD13	1:B:4380:PRO:HG2	1.97	0.46
1:A:847:ARG:HH11	1:A:848:PRO:HA	1.81	0.46
1:A:1097:ASP:OD1	1:A:1097:ASP:N	2.49	0.46
1:A:2568:VAL:HG13	1:A:2598:LEU:HD22	1.97	0.46
1:A:3270:PRO:HB2	1:A:3290:ARG:HB3	1.98	0.46
1:B:508:ASN:O	1:B:532:LEU:HG	2.16	0.46
1:B:862:LEU:HD12	1:B:863:PRO:HD2	1.98	0.46
1:B:2450:THR:O	1:B:2453:SER:OG	2.33	0.46
1:B:3103:ASN:O	1:B:3107:LYS:N	2.48	0.46
1:B:3573:ASN:OD1	1:B:3577:ASN:ND2	2.40	0.46
1:B:3626:ASP:HB3	1:B:3629:HIS:CD2	2.51	0.46
1:B:4186:GLN:HB3	1:B:4204:TRP:CZ3	2.51	0.46
1:B:4272:MET:HE1	1:B:4295:TRP:CE2	2.51	0.46
1:A:1422:GLU:HG2	1:A:1423:SER:H	1.80	0.46
1:A:4203:ASP:O	1:A:4208:PRO:HA	2.16	0.46
1:A:4329:SER:HB3	3:G:1:NAG:H5	1.97	0.46
1:B:1249:GLU:HA	1:B:1261:ASP:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1403:HIS:CD2	1:B:1403:HIS:H	2.31	0.46
1:B:2576:GLU:HG2	1:B:2587:VAL:HG22	1.97	0.46
1:B:3103:ASN:HD21	1:B:3106:GLU:HG2	1.81	0.46
1:B:4087:VAL:HG12	1:B:4103:TYR:HB3	1.97	0.46
1:A:406:ILE:HD11	1:A:417:LEU:HD22	1.98	0.46
1:A:1352:SER:HA	1:A:1355:ASP:CB	2.43	0.46
1:A:1856:TYR:HB3	1:A:2046:ALA:HB2	1.98	0.46
1:A:3238:GLU:HG3	1:A:3282:ARG:HH22	1.81	0.46
1:B:1825:ASN:OD1	1:B:1826:LEU:N	2.48	0.46
1:B:3273:GLU:OE2	1:B:3324:ARG:NH2	2.48	0.46
1:B:3458:HIS:CD2	1:B:3460:TYR:H	2.34	0.46
1:B:4092:ASP:OD1	1:B:4092:ASP:N	2.48	0.46
1:A:771:ASP:OD1	1:A:771:ASP:N	2.38	0.46
1:A:1580:GLU:HG2	1:A:1591:VAL:HG22	1.98	0.46
1:A:3345:TYR:HD2	1:A:3347:GLY:H	1.64	0.46
1:A:4068:ASN:ND2	3:H:1:NAG:O7	2.49	0.46
1:B:1154:PHE:CD1	1:B:1167:VAL:HG22	2.51	0.46
1:B:1828:LEU:HD12	1:B:1835:LEU:HD12	1.98	0.46
1:B:2725:CYS:HB2	1:B:2727:ASP:O	2.15	0.46
1:B:3729:ASN:N	1:B:3747:ASP:OD2	2.47	0.46
1:A:513:ARG:HD2	1:A:605:PHE:HE1	1.81	0.45
1:A:1606:ASP:OD1	1:A:1606:ASP:N	2.49	0.45
1:A:2572:LEU:HD13	1:A:2574:ARG:HH21	1.81	0.45
1:A:3294:LEU:HD21	1:A:3335:LEU:HD23	1.97	0.45
1:A:4252:ASP:OD1	1:A:4272:MET:N	2.49	0.45
1:B:1960:LEU:HD13	1:B:1963:PRO:HB3	1.98	0.45
1:B:3047:LYS:HA	1:B:3052:ASP:HB2	1.98	0.45
1:B:3453:ASP:OD1	1:B:3454:ILE:N	2.48	0.45
1:A:3233:ASP:OD2	1:A:3277:VAL:N	2.36	0.45
1:B:1251:ASP:N	1:B:1262:GLU:OE1	2.49	0.45
1:B:1365:VAL:H	1:B:1373:CYS:N	2.12	0.45
1:B:1956:LEU:HD23	1:B:1973:LEU:HD22	1.97	0.45
1:B:2557:THR:HG21	1:B:2599:THR:HA	1.99	0.45
1:A:518:ASP:OD1	1:A:521:VAL:HG22	2.17	0.45
1:A:1440:VAL:HG21	1:A:1665:VAL:HG21	1.97	0.45
1:A:2140:HIS:O	1:A:2181:ARG:NH1	2.35	0.45
1:A:2450:THR:H	1:A:2456:HIS:CE1	2.34	0.45
1:B:558:TRP:H	1:B:575:ASP:CG	2.24	0.45
1:B:1109:CYS:HB3	1:B:1113:GLN:HB2	1.99	0.45
1:B:2618:ALA:HB1	1:B:2623:GLY:HA2	1.98	0.45
1:B:3124:HIS:HE1	1:B:3141:TYR:CG	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4007:ASP:HA	1:B:4026:GLY:H	1.80	0.45
1:A:578:PHE:CG	1:A:1175:VAL:HG12	2.52	0.45
1:A:754:THR:HA	1:A:769:LYS:HA	1.97	0.45
1:A:1721:HIS:HB3	1:A:1723:TYR:CE2	2.52	0.45
1:A:2601:TYR:HB2	1:A:2642:THR:HG21	1.99	0.45
1:A:3226:LEU:HD13	1:A:3229:VAL:HG21	1.99	0.45
1:A:3533:ASP:HA	1:A:3551:ARG:HE	1.82	0.45
1:B:754:THR:HG21	1:B:767:LYS:HE3	1.97	0.45
1:B:1644:HIS:CE1	1:B:1660:ARG:HD3	2.52	0.45
1:A:978:THR:C	1:A:980:PRO:HD3	2.41	0.45
1:A:1158:ASN:HB3	1:A:1175:VAL:CG2	2.46	0.45
1:A:3517:PHE:N	1:A:3526:ILE:O	2.49	0.45
1:A:4312:ASN:HB3	1:B:4312:ASN:HB3	1.98	0.45
1:B:369:HIS:HE1	1:B:371:CYS:HB2	1.82	0.45
1:B:2124:ILE:HD11	1:B:2147:VAL:HG11	1.99	0.45
1:B:2572:LEU:HD13	1:B:2574:ARG:HE	1.81	0.45
1:B:3479:LEU:HB2	1:B:3492:GLU:HB2	1.99	0.45
1:A:381:ARG:HD3	1:A:384:TYR:HE1	1.81	0.45
1:A:2102:VAL:O	1:A:2334:GLN:NE2	2.40	0.45
1:A:4006:LEU:O	1:A:4007:ASP:C	2.59	0.45
1:B:622:MET:HE3	1:B:622:MET:HB2	1.63	0.45
1:B:1203:VAL:HA	1:B:1206:ARG:HB2	1.99	0.45
1:A:1203:VAL:HA	1:A:1206:ARG:HB2	1.99	0.45
1:A:1483:SER:HB2	1:A:1514:ILE:HD11	1.98	0.45
1:A:2127:ILE:HA	1:A:2133:SER:O	2.17	0.45
1:A:2155:VAL:HG21	1:A:2341:VAL:HG11	1.98	0.45
1:A:2450:THR:O	1:A:2453:SER:OG	2.29	0.45
1:A:3706:ARG:H	1:A:3706:ARG:HD2	1.81	0.45
1:A:4077:TYR:CE1	1:A:4120:ILE:HG12	2.51	0.45
1:A:4087:VAL:HG12	1:A:4103:TYR:HB3	1.98	0.45
1:B:597:GLY:N	1:B:1158:ASN:HD21	2.15	0.45
1:B:765:ILE:HD11	1:B:786:VAL:HG21	1.97	0.45
1:B:1949:ASP:OD1	1:B:1951:THR:OG1	2.28	0.45
1:B:3078:HIS:C	1:B:3090:MET:HG2	2.42	0.45
1:B:3801:GLU:OE1	1:B:3801:GLU:N	2.49	0.45
1:B:4280:PHE:HB2	1:B:4320:ILE:HG21	1.98	0.45
2:C:1:NAG:H61	2:C:2:NAG:H82	1.98	0.45
1:A:3660:CYS:HB3	1:A:3665:ASP:HB3	1.99	0.45
1:A:4285:TYR:HD2	1:A:4320:ILE:HD11	1.82	0.45
1:B:883:ARG:HH21	1:B:896:HIS:HD2	1.65	0.45
1:B:1747:PHE:HA	1:B:1761:LEU:HG	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2374:THR:HG23	1:B:2376:GLN:HE22	1.82	0.45
1:B:2426:TYR:HA	1:B:2433:ILE:HA	1.99	0.45
1:B:2738:LEU:HB3	1:B:2740:THR:HG23	1.99	0.45
1:B:2774:GLY:HA3	1:B:2777:PHE:CD2	2.51	0.45
1:B:3158:GLU:HG2	1:B:3159:MET:HG3	1.99	0.45
1:B:3533:ASP:HA	1:B:3551:ARG:HE	1.82	0.45
1:B:3775:ARG:HD2	1:B:3802:TYR:HE2	1.82	0.45
1:B:4006:LEU:O	1:B:4008:ILE:HG13	2.16	0.45
1:B:1087:ASP:OD1	1:B:1087:ASP:N	2.46	0.45
1:B:3204:SER:O	1:B:3452:PHE:HB2	2.17	0.45
1:A:558:TRP:HB2	1:A:577:ARG:HB2	1.99	0.45
1:A:1049:ASP:HB2	1:A:1054:ASN:HA	1.99	0.45
1:A:1494:PHE:HB2	1:A:1496:ASN:OD1	2.17	0.45
1:A:1567:LEU:HD13	1:A:1581:ARG:HD2	1.99	0.45
1:A:2520:TYR:HA	1:A:2536:THR:HA	1.98	0.45
1:A:3208:TYR:HB3	1:A:3221:LEU:HD21	1.98	0.45
1:B:910:ILE:HD12	1:B:939:VAL:HG11	1.99	0.45
1:B:1422:GLU:HG2	1:B:1423:SER:H	1.80	0.45
1:B:2709:ASN:HD21	1:B:2725:CYS:HB3	1.82	0.45
1:B:4059:PRO:HD2	1:B:4317:GLN:O	2.17	0.45
2:D:1:NAG:H61	2:D:2:NAG:H82	1.99	0.45
1:A:1109:CYS:HB3	1:A:1113:GLN:HB2	1.99	0.44
1:A:2725:CYS:HB2	1:A:2727:ASP:O	2.18	0.44
1:A:3236:ARG:NH2	1:A:3462:GLN:O	2.50	0.44
1:A:3567:SER:O	1:A:3570:THR:OG1	2.33	0.44
1:A:4008:ILE:H	1:A:4026:GLY:H	1.65	0.44
1:A:4171:LEU:HD12	1:A:4171:LEU:HA	1.77	0.44
1:B:695:PHE:HB3	1:B:704:CYS:HB3	1.99	0.44
1:B:830:SER:H	1:B:843:THR:HG23	1.81	0.44
1:B:3244:ILE:HD13	1:B:3272:ALA:HB1	1.99	0.44
1:B:4390:TYR:CD1	1:B:4400:LYS:HG2	2.52	0.44
1:A:1360:CYS:HB3	1:A:1373:CYS:HB3	1.74	0.44
1:A:1522:ASN:HD22	1:A:1537:LYS:HA	1.82	0.44
1:A:1883:GLY:C	1:A:1905:MET:HG3	2.42	0.44
1:A:4004:SER:O	1:A:4006:LEU:HG	2.18	0.44
1:A:4091:TRP:O	1:A:4093:PRO:HD3	2.17	0.44
1:B:1563:MET:HA	1:B:1566:HIS:CE1	2.51	0.44
1:B:1844:SER:OG	1:B:1846:GLU:OE2	2.25	0.44
1:B:3567:SER:O	1:B:3570:THR:OG1	2.33	0.44
1:A:2304:SER:HB3	1:A:2309:ASN:HD22	1.82	0.44
1:A:3799:HIS:HB2	1:A:3802:TYR:HD2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:626:LYS:N	1:B:636:GLN:O	2.47	0.44
1:B:2209:TYR:HB3	1:B:2236:PRO:HD2	2.00	0.44
1:B:2233:ILE:HD11	1:B:2236:PRO:HG3	1.98	0.44
1:B:2475:TRP:H	1:B:2475:TRP:HE3	1.64	0.44
1:B:4091:TRP:O	1:B:4093:PRO:HD3	2.17	0.44
1:A:584:VAL:HG12	1:A:591:ARG:HA	1.98	0.44
1:A:628:ASN:H	1:A:632:GLU:HB2	1.83	0.44
1:A:897:SER:HA	1:A:903:ASP:O	2.18	0.44
1:A:938:ARG:HB3	1:A:948:THR:HB	1.99	0.44
1:A:2653:ASN:HD21	1:A:2655:CYS:HB2	1.81	0.44
1:A:3110:GLY:N	1:A:3130:LEU:O	2.44	0.44
1:A:3110:GLY:H	1:A:3131:THR:HA	1.82	0.44
1:A:3615:THR:HA	1:A:3625:GLU:OE1	2.18	0.44
1:A:3682:THR:O	1:A:3695:LYS:N	2.51	0.44
1:A:3684:PHE:N	1:A:3693:ILE:O	2.41	0.44
1:A:3806:THR:OG1	1:A:3825:ASP:OD2	2.27	0.44
1:B:1044:LEU:HA	1:B:1056:ASP:HB2	2.00	0.44
1:B:1130:THR:HG1	1:B:1160:ARG:HH11	1.65	0.44
1:B:1154:PHE:CD2	1:B:1162:ILE:HD11	2.53	0.44
1:B:1830:TRP:HA	1:B:1833:ARG:HH21	1.83	0.44
1:B:1883:GLY:C	1:B:1905:MET:HG3	2.42	0.44
1:B:2140:HIS:O	1:B:2181:ARG:NH1	2.34	0.44
1:B:3298:ASP:OD1	1:B:3302:GLY:N	2.51	0.44
1:A:2490:ILE:N	1:A:2504:ALA:O	2.46	0.44
1:A:3278:ASP:OD2	1:A:3283:LYS:N	2.42	0.44
1:A:3599:TRP:HB2	1:A:3609:GLU:HA	2.00	0.44
1:B:350:ASP:HB3	1:B:353:GLN:HB2	1.99	0.44
1:B:865:ILE:HG22	1:B:869:LEU:HD11	1.98	0.44
1:B:935:ALA:HB1	1:B:949:VAL:HG13	1.99	0.44
1:B:1226:PRO:O	1:B:1228:GLY:N	2.44	0.44
1:B:1402:GLN:OE1	1:B:1416:ASP:N	2.50	0.44
1:B:1440:VAL:HG21	1:B:1665:VAL:HG21	1.99	0.44
1:B:1721:HIS:HB3	1:B:1723:TYR:CE2	2.52	0.44
1:B:2572:LEU:HD13	1:B:2574:ARG:HH21	1.81	0.44
1:B:3706:ARG:H	1:B:3706:ARG:HD2	1.81	0.44
1:B:3836:PHE:HD1	1:B:3843:GLN:HG3	1.83	0.44
1:B:4034:ASP:HB2	2:N:1:NAG:H5	1.98	0.44
1:A:3078:HIS:N	1:B:3078:HIS:HB3	2.33	0.44
1:A:3516:GLN:HA	1:A:3527:PRO:HA	1.99	0.44
1:A:4230:TRP:CG	1:A:4250:LYS:HB2	2.52	0.44
1:B:1347:LEU:N	1:B:1369:PHE:O	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2534:ARG:HE	1:B:2545:ILE:HD11	1.83	0.44
1:B:4212:SER:HB2	1:B:4223:LEU:HD11	2.00	0.44
1:A:612:GLY:HA2	1:A:629:LYS:HE2	1.98	0.44
1:A:683:ASP:OD1	1:A:683:ASP:N	2.50	0.44
1:A:714:SER:HA	1:A:719:ILE:HG12	1.98	0.44
1:A:1747:PHE:HA	1:A:1761:LEU:HG	1.99	0.44
1:A:2093:GLN:HE21	1:A:2093:GLN:HB3	1.63	0.44
1:A:3846:MET:HB3	1:A:3855:ILE:O	2.18	0.44
1:A:4098:LEU:HD13	1:A:4380:PRO:HG2	1.98	0.44
1:B:437:ARG:NH2	1:B:450:SER:OG	2.51	0.44
1:B:520:THR:HG22	1:B:659:ALA:HB2	2.00	0.44
1:B:2069:MET:HG2	1:B:2072:ALA:O	2.17	0.44
1:B:3789:ASP:OD1	1:B:3789:ASP:N	2.50	0.44
3:G:1:NAG:H61	3:G:2:NAG:N2	2.33	0.44
1:A:351:ASP:OD1	1:A:351:ASP:N	2.51	0.44
1:A:981:ASN:HA	1:A:988:CYS:HB2	2.00	0.44
1:A:1373:CYS:SG	1:A:1386:LYS:HG2	2.58	0.44
1:A:1834:ASN:ND2	1:A:2033:CYS:O	2.50	0.44
1:A:3612:GLN:HG2	1:A:3629:HIS:HE1	1.82	0.44
1:B:1751:VAL:HG21	1:B:1783:VAL:HB	2.00	0.44
1:B:2421:VAL:HG21	1:B:2435:PHE:HB2	2.00	0.44
1:B:4017:CYS:HB3	1:B:4021:CYS:HB2	1.99	0.44
1:B:4031:VAL:HA	1:B:4045:LYS:HD2	2.00	0.44
1:B:4083:TYR:HB3	1:B:4106:ARG:HG3	1.99	0.44
1:B:4396:LEU:HD12	1:B:4397:PRO:HD2	1.99	0.44
1:A:558:TRP:H	1:A:575:ASP:CG	2.26	0.44
1:A:847:ARG:HH21	1:A:1248:TRP:CD1	2.36	0.44
1:A:1206:ARG:NH1	1:A:1221:GLY:O	2.48	0.44
1:A:1675:ASN:N	1:A:1675:ASN:HD22	2.15	0.44
1:A:2209:TYR:HB3	1:A:2236:PRO:HD2	1.99	0.44
1:A:2466:GLY:HA3	1:A:2486:LEU:HD22	2.00	0.44
1:A:2502:VAL:HG23	1:A:2679:HIS:CD2	2.53	0.44
1:A:4273:ASN:OD1	1:A:4273:ASN:N	2.51	0.44
1:A:4327:ASN:ND2	3:G:1:NAG:O7	2.51	0.44
1:B:762:LYS:HA	1:B:1052:HIS:CE1	2.53	0.44
1:B:1467:TYR:H	1:B:1484:ASP:CG	2.26	0.44
1:B:1622:MET:HE1	1:B:1657:TRP:CE3	2.53	0.44
1:A:1173:ASP:N	1:A:1179:ASP:OD2	2.50	0.43
1:A:1266:CYS:HB3	1:A:1268:PRO:HD3	2.00	0.43
1:A:4000:PHE:HA	1:A:4004:SER:HB3	1.98	0.43
1:A:4390:TYR:CD1	1:A:4400:LYS:HG2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:TRP:CE2	1:B:630:PHE:HD1	2.36	0.43
1:B:480:LYS:NZ	1:B:495:ASN:OD1	2.31	0.43
1:B:875:LEU:HB3	1:B:884:LEU:HD11	2.00	0.43
1:B:3388:TYR:CD1	1:B:3390:GLU:HG3	2.53	0.43
1:B:3517:PHE:N	1:B:3526:ILE:O	2.51	0.43
1:A:473:ALA:HB1	1:A:517:VAL:HG22	1.99	0.43
1:A:661:ASN:HB3	1:A:664:LYS:HE3	2.00	0.43
1:A:1436:LEU:HD23	1:A:1436:LEU:H	1.82	0.43
1:A:1510:LEU:HD23	1:A:1528:TYR:HB3	1.99	0.43
1:A:2654:PRO:HB2	1:A:2673:ALA:HB2	1.99	0.43
1:B:1469:VAL:HG13	1:B:1687:LEU:HD23	1.99	0.43
1:B:2049:PHE:HA	1:B:2060:PRO:HA	2.01	0.43
1:B:2151:ALA:HB1	1:B:2197:VAL:HG12	2.00	0.43
1:B:3818:ASP:N	1:B:3829:GLU:OE1	2.52	0.43
1:B:3849:CYS:HB3	1:B:3870:GLY:CA	2.48	0.43
1:A:242:ASP:N	1:A:242:ASP:OD1	2.51	0.43
1:A:1216:ASN:O	1:A:1220:ALA:N	2.50	0.43
1:A:1960:LEU:HD13	1:A:1963:PRO:HB3	2.00	0.43
1:A:3434:ASN:HB3	1:A:3439:SER:H	1.84	0.43
1:A:4116:LYS:HG2	1:A:4135:ASP:HA	2.01	0.43
1:B:767:LYS:HB3	1:B:778:LEU:HD11	2.00	0.43
1:B:937:ILE:HG21	1:B:947:MET:HE2	2.00	0.43
1:B:1016:ASP:O	1:B:1020:GLU:N	2.46	0.43
1:B:1097:ASP:N	1:B:1097:ASP:OD1	2.52	0.43
1:B:1352:SER:CB	1:B:1358:GLY:HA2	2.48	0.43
1:B:4085:GLN:HG2	1:B:4145:ASP:HA	2.00	0.43
1:A:991:VAL:HB	1:A:992:PRO:HD2	2.00	0.43
1:A:1550:ASN:O	1:A:1589:ARG:NH2	2.52	0.43
1:A:2233:ILE:HD11	1:A:2236:PRO:HG3	1.99	0.43
1:A:2618:ALA:HB1	1:A:2623:GLY:HA2	2.01	0.43
1:A:3729:ASN:N	1:A:3747:ASP:OD2	2.48	0.43
1:A:3780:HIS:N	1:A:3790:GLU:OE1	2.43	0.43
1:A:4298:ASN:HB3	1:A:4302:GLN:O	2.18	0.43
1:B:402:ARG:CZ	1:B:1089:ARG:HD3	2.48	0.43
1:B:619:TRP:HB3	1:B:644:ARG:NH1	2.33	0.43
1:B:799:TYR:CD1	1:B:833:VAL:HG21	2.54	0.43
1:B:1555:ARG:NH1	1:B:1601:CYS:SG	2.90	0.43
1:B:1648:LEU:HD23	1:B:1649:THR:N	2.33	0.43
1:B:2401:LEU:HD21	1:B:2629:MET:HB3	2.00	0.43
1:B:3240:ARG:HD3	1:B:3253:ARG:HD2	1.99	0.43
1:B:3467:ASN:ND2	1:B:3469:CYS:HB2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3858:TYR:CE1	1:B:3859:TRP:CD1	3.06	0.43
1:A:493:MET:HE3	1:A:493:MET:HB3	1.87	0.43
1:A:524:LEU:N	1:A:541:ALA:O	2.51	0.43
1:A:543:MET:HB2	1:A:676:LEU:O	2.19	0.43
1:A:889:ALA:HA	1:A:916:PRO:HD2	1.99	0.43
1:A:3708:ASN:O	1:A:3712:GLN:HG3	2.19	0.43
1:B:1534:GLU:OE1	1:B:1543:ARG:NH2	2.49	0.43
1:B:1927:ASP:OD2	1:B:1988:LYS:NZ	2.41	0.43
1:B:2124:ILE:HB	1:B:2138:VAL:HB	2.00	0.43
1:B:4272:MET:HE2	1:B:4272:MET:HB2	1.86	0.43
1:A:682:ASN:ND2	1:A:687:PHE:O	2.43	0.43
1:A:2572:LEU:HD13	1:A:2574:ARG:HE	1.83	0.43
1:A:3275:LEU:HD21	1:A:3277:VAL:HG23	2.00	0.43
1:A:3365:GLU:HB2	1:A:3682:THR:HG21	2.00	0.43
1:A:4009:ASN:C	1:A:4011:CYS:N	2.77	0.43
1:B:643:LEU:H	1:B:643:LEU:HD12	1.83	0.43
1:B:2523:TRP:CE2	1:B:2533:GLU:HB2	2.54	0.43
1:B:2758:TYR:CD2	1:B:2765:ASP:HB2	2.53	0.43
1:B:3080:PHE:N	1:B:3088:ILE:O	2.43	0.43
1:B:3850:LYS:C	1:B:3852:HIS:H	2.25	0.43
1:A:1117:ASP:N	1:A:1136:ASP:OD2	2.52	0.43
1:A:1977:ASP:HB3	1:A:1980:TYR:HB2	2.00	0.43
1:A:2074:ARG:NH1	1:A:2085:GLU:OE2	2.51	0.43
1:A:2483:SER:HB2	1:A:2512:ILE:HD11	2.01	0.43
1:A:3458:HIS:HD2	1:A:3460:TYR:H	1.67	0.43
1:A:3873:GLU:H	1:A:3873:GLU:CD	2.27	0.43
1:A:4042:ARG:HA	1:A:4045:LYS:NZ	2.34	0.43
1:B:1357:ASN:HA	1:B:1364:CYS:SG	2.58	0.43
1:B:1820:VAL:HG13	1:B:1857:ARG:HD3	2.01	0.43
1:B:2141:GLY:O	1:B:2163:ASN:ND2	2.45	0.43
1:B:3846:MET:HB3	1:B:3857:PRO:HD3	2.01	0.43
1:A:368:ARG:NH1	1:A:369:HIS:CD2	2.87	0.43
1:A:1352:SER:HB2	1:A:1356:PHE:CZ	2.54	0.43
1:A:1622:MET:HE1	1:A:1657:TRP:CE3	2.53	0.43
1:A:1961:SER:OG	1:A:1979:GLN:HB2	2.18	0.43
1:A:4175:TYR:HB3	1:A:4354:PRO:HB3	2.01	0.43
1:B:488:VAL:CG1	1:B:720:ARG:HD2	2.49	0.43
1:B:3056:ASP:OD1	1:B:3056:ASP:N	2.51	0.43
1:B:3532:CYS:N	1:B:3543:ASP:O	2.52	0.43
1:B:3774:SER:O	1:B:3777:ILE:HG22	2.18	0.43
1:B:4158:TRP:CZ2	1:B:4167:GLU:HB2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:870:GLY:HA3	1:A:890:TYR:HB3	2.01	0.43
1:A:1402:GLN:OE1	1:A:1416:ASP:N	2.51	0.43
1:A:1648:LEU:HD23	1:A:1649:THR:N	2.34	0.43
1:A:1830:TRP:HA	1:A:1833:ARG:HH21	1.84	0.43
1:A:2619:ASN:OD1	1:A:2622:ASP:N	2.40	0.43
1:A:4103:TYR:CZ	1:A:4116:LYS:HB2	2.54	0.43
1:B:1129:ASP:O	1:B:1160:ARG:NH1	2.52	0.43
1:B:1149:CYS:O	1:B:1150:GLN:C	2.62	0.43
1:B:2397:SER:HA	1:B:2417:VAL:HG22	2.00	0.43
1:B:3834:THR:HB	1:B:3840:ALA:C	2.44	0.43
1:B:3835:ARG:HB2	1:B:3841:TYR:HA	2.00	0.43
1:B:4382:ARG:HB3	1:B:4409:TYR:CD1	2.54	0.43
1:A:446:ASN:N	1:A:446:ASN:OD1	2.51	0.43
1:A:1367:GLU:O	1:A:1368:PRO:C	2.60	0.43
1:A:2124:ILE:HB	1:A:2138:VAL:HB	1.99	0.43
1:A:2599:THR:HG22	1:A:2606:TYR:HB2	2.00	0.43
1:A:3089:GLU:HG2	1:A:3091:MET:H	1.83	0.43
1:A:3573:ASN:O	1:A:3605:ARG:NH2	2.50	0.43
1:B:1238:GLN:NE2	1:B:3178:CYS:H	2.17	0.43
1:B:1535:VAL:HG11	1:B:1714:LEU:HD11	2.01	0.43
1:B:2036:VAL:HG12	1:B:2040:LEU:HB2	1.99	0.43
1:B:3450:ARG:HB2	1:B:3452:PHE:CE2	2.53	0.43
1:A:521:VAL:HG23	1:A:523:TYR:CD1	2.54	0.42
1:A:937:ILE:HD12	1:A:937:ILE:N	2.34	0.42
1:A:977:PRO:HB2	1:B:2776:LEU:CB	2.48	0.42
1:A:2330:ASP:OD1	1:A:2331:LYS:N	2.51	0.42
1:A:3996:GLU:OE2	1:A:3998:ASN:HB3	2.19	0.42
1:A:4216:ASN:ND2	1:A:4345:ARG:HB3	2.34	0.42
1:A:4396:LEU:HD12	1:A:4397:PRO:HD2	2.01	0.42
1:B:452:ASP:OD2	1:B:457:ASN:ND2	2.51	0.42
1:B:539:GLU:CD	1:B:548:ARG:HE	2.27	0.42
1:B:579:ASP:HB3	1:B:601:ILE:O	2.19	0.42
1:B:1360:CYS:HB3	1:B:1373:CYS:HB3	1.65	0.42
1:B:1558:ALA:HB1	1:B:1605:ILE:HG13	2.00	0.42
1:B:2095:ARG:HD3	1:B:2095:ARG:HA	1.85	0.42
1:B:2550:LEU:HD21	1:B:2553:PRO:HB3	2.01	0.42
1:B:3135:CYS:SG	1:B:3136:SER:N	2.92	0.42
1:B:4311:VAL:HG12	1:B:4312:ASN:N	2.31	0.42
1:A:513:ARG:HD2	1:A:605:PHE:CE1	2.54	0.42
1:A:1084:TRP:HB3	1:A:1091:ASP:OD2	2.18	0.42
1:A:1578:ARG:NE	1:A:1580:GLU:OE2	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1644:HIS:CE1	1:A:1660:ARG:HD3	2.55	0.42
1:A:3298:ASP:OD1	1:A:3302:GLY:N	2.52	0.42
1:A:4059:PRO:HD2	1:A:4317:GLN:O	2.19	0.42
1:B:2106:SER:HA	2:I:2:NAG:O6	2.19	0.42
1:B:3093:LEU:HA	1:B:3105:ASP:HB2	2.02	0.42
1:B:4103:TYR:CZ	1:B:4116:LYS:HB2	2.54	0.42
1:B:4243:ARG:NE	1:B:4256:THR:OG1	2.52	0.42
1:A:1822:PRO:HG3	1:A:1841:ARG:NH1	2.34	0.42
1:A:2482:TYR:CZ	1:A:2491:ASN:HB2	2.55	0.42
1:A:3698:VAL:HA	1:A:3710:ASP:HB2	2.00	0.42
1:A:3819:GLY:N	1:A:3835:ARG:HH21	2.17	0.42
1:A:3843:GLN:HE21	1:A:3843:GLN:HB2	1.65	0.42
1:A:4031:VAL:HA	1:A:4045:LYS:HD2	2.00	0.42
1:B:733:MET:HE1	1:B:755:ILE:HD13	2.01	0.42
1:B:829:ARG:HD2	1:B:873:ASN:HA	2.01	0.42
1:B:830:SER:HB3	1:B:843:THR:HG22	2.01	0.42
1:B:1436:LEU:H	1:B:1436:LEU:HD23	1.85	0.42
1:B:3146:ASP:O	1:B:3148:ARG:NH1	2.52	0.42
1:B:3821:ALA:HA	1:B:3829:GLU:CG	2.49	0.42
1:B:4067:TYR:CZ	1:B:4072:GLU:HA	2.55	0.42
3:G:1:NAG:H61	3:G:2:NAG:H82	2.00	0.42
1:A:978:THR:OG1	1:B:2776:LEU:N	2.52	0.42
1:A:1175:VAL:HG23	1:A:1176:ASP:H	1.83	0.42
1:A:1558:ALA:HB1	1:A:1605:ILE:HG13	2.01	0.42
1:A:1878:VAL:HB	1:A:1905:MET:HE3	2.02	0.42
1:A:3774:SER:O	1:A:3777:ILE:HG22	2.19	0.42
1:A:4067:TYR:CG	1:A:4309:LEU:HD11	2.54	0.42
1:B:339:ASN:HD22	1:B:346:CYS:HA	1.84	0.42
1:B:1025:GLN:HG2	1:B:1026:CYS:SG	2.59	0.42
1:B:1263:HIS:CD2	1:B:1263:HIS:H	2.35	0.42
1:B:2653:ASN:HD21	1:B:2655:CYS:HB2	1.85	0.42
1:B:3270:PRO:HB2	1:B:3290:ARG:HB3	2.01	0.42
1:A:558:TRP:HB2	1:A:577:ARG:H	1.85	0.42
1:A:851:ILE:HB	1:A:865:ILE:HB	2.00	0.42
1:A:1571:SER:HB3	1:A:1600:PRO:HB2	2.01	0.42
1:A:1609:ASN:HB3	1:A:1611:LEU:HD23	2.01	0.42
1:A:2102:VAL:HG12	1:A:2109:ILE:HG12	2.01	0.42
1:A:2568:VAL:HG12	1:A:2575:ILE:HG23	2.00	0.42
1:A:2684:TYR:O	1:A:2693:ILE:HG13	2.20	0.42
1:A:3082:CYS:N	1:A:3086:ARG:O	2.37	0.42
1:A:3199:PRO:HG3	1:A:3416:PHE:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:431:PHE:O	1:B:656:GLN:NE2	2.47	0.42
1:B:1834:ASN:ND2	1:B:2033:CYS:O	2.51	0.42
1:B:2330:ASP:OD1	1:B:2331:LYS:N	2.53	0.42
1:B:3698:VAL:HA	1:B:3710:ASP:HB2	2.00	0.42
1:A:470:GLU:OE1	1:A:513:ARG:HD3	2.19	0.42
1:A:2568:VAL:HG12	1:A:2575:ILE:HG12	2.00	0.42
1:A:2739:HIS:CD2	1:A:2747:THR:HG21	2.54	0.42
1:A:3453:ASP:OD1	1:A:3454:ILE:N	2.52	0.42
1:A:3622:ASN:ND2	1:A:3625:GLU:HB2	2.35	0.42
1:A:3744:ASP:N	1:A:3750:ASP:OD2	2.52	0.42
1:B:885:TYR:CD2	1:B:896:HIS:HB3	2.54	0.42
1:B:1822:PRO:HG3	1:B:1841:ARG:NH1	2.34	0.42
1:B:2145:ASN:ND2	1:B:2165:PHE:O	2.53	0.42
1:B:3691:ARG:HD3	1:B:3705:CYS:HA	2.00	0.42
1:B:3848:GLU:HA	1:B:3853:VAL:O	2.20	0.42
1:A:964:ASP:HB3	1:A:967:ILE:HG13	2.02	0.42
1:A:3376:ASN:ND2	1:A:3436:TYR:OH	2.53	0.42
1:A:4311:VAL:HG12	1:A:4312:ASN:N	2.33	0.42
1:A:4329:SER:O	1:A:4330:VAL:C	2.63	0.42
1:B:356:GLY:O	1:B:383:GLN:NE2	2.52	0.42
1:B:1362:HIS:CG	1:B:1363:GLU:H	2.38	0.42
1:B:1365:VAL:CG1	1:B:1372:LYS:HD3	2.50	0.42
1:B:2198:ASP:OD2	1:B:2201:ASN:ND2	2.50	0.42
1:B:3517:PHE:HB2	1:B:3528:ILE:HD12	2.02	0.42
1:B:3819:GLY:N	1:B:3829:GLU:OE1	2.51	0.42
1:A:339:ASN:HD22	1:A:344:ARG:HA	1.85	0.42
1:A:441:THR:HG22	1:A:448:VAL:HG22	2.01	0.42
1:A:511:HIS:HB3	1:A:529:TRP:NE1	2.34	0.42
1:A:1205:ASN:HB3	1:A:1212:ASP:CG	2.45	0.42
1:A:1588:MET:SD	1:A:1717:SER:OG	2.77	0.42
1:A:1751:VAL:HG21	1:A:1783:VAL:HB	2.01	0.42
1:A:2469:ASP:N	1:A:2469:ASP:OD1	2.52	0.42
1:A:3135:CYS:SG	1:A:3136:SER:N	2.93	0.42
1:A:3209:LEU:O	1:A:3222:ILE:N	2.52	0.42
1:A:3706:ARG:HD2	1:A:3706:ARG:N	2.35	0.42
1:A:4067:TYR:CE2	1:A:4309:LEU:HD11	2.55	0.42
1:A:4154:ARG:C	1:A:4171:LEU:HD13	2.45	0.42
1:B:570:ARG:NH1	1:B:583:THR:HG22	2.35	0.42
1:B:3577:ASN:HD22	1:B:3583:ASP:CG	2.28	0.42
1:B:3682:THR:O	1:B:3695:LYS:N	2.53	0.42
1:A:698:ASP:OD1	1:A:699:THR:N	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1467:TYR:H	1:A:1484:ASP:CG	2.26	0.42
1:A:1784:GLU:OE1	1:A:1785:PHE:N	2.52	0.42
1:A:2644:VAL:HG12	1:A:2646:ASN:O	2.20	0.42
1:A:2758:TYR:HB2	1:A:2766:CYS:HB3	2.02	0.42
1:B:235:ILE:HG23	1:B:239:TRP:HE3	1.83	0.42
1:B:1205:ASN:HB3	1:B:1212:ASP:CG	2.45	0.42
1:B:2099:HIS:CE1	1:B:2194:HIS:HD2	2.38	0.42
1:B:3199:PRO:HG3	1:B:3416:PHE:CE2	2.55	0.42
1:B:3640:PHE:HE2	1:B:3665:ASP:HA	1.84	0.42
1:B:4242:ASP:OD1	1:B:4242:ASP:N	2.52	0.42
1:B:4314:TRP:O	1:B:4316:THR:HG23	2.19	0.42
1:A:507:GLU:HB3	1:A:548:ARG:NH1	2.35	0.42
1:A:558:TRP:CG	1:A:577:ARG:HB2	2.55	0.42
1:A:966:ASN:O	1:A:969:THR:OG1	2.38	0.42
1:A:1576:HIS:CE1	1:B:2213:PRO:HD2	2.55	0.42
1:A:1828:LEU:HD12	1:A:1835:LEU:HD12	2.02	0.42
1:A:4024:THR:HB	1:A:4027:SER:C	2.45	0.42
1:A:4158:TRP:CZ2	1:A:4167:GLU:HB2	2.55	0.42
1:B:441:THR:HB	1:B:469:PRO:HG2	2.01	0.42
1:B:628:ASN:H	1:B:632:GLU:HB2	1.85	0.42
1:B:785:ASN:HD22	1:B:804:HIS:HB2	1.85	0.42
1:B:1352:SER:O	1:B:1356:PHE:N	2.46	0.42
1:B:1514:ILE:HG23	1:B:1523:LEU:HD21	2.02	0.42
1:B:1550:ASN:O	1:B:1589:ARG:NH2	2.52	0.42
1:B:1667:ARG:NH2	1:B:1677:SER:OG	2.53	0.42
1:B:3516:GLN:HA	1:B:3527:PRO:HA	2.02	0.42
1:B:3708:ASN:O	1:B:3712:GLN:HG3	2.20	0.42
1:B:4298:ASN:HB3	1:B:4302:GLN:O	2.20	0.42
1:A:229:CYS:CB	1:A:233:ARG:HG2	2.48	0.41
1:A:490:ARG:HA	1:A:506:THR:HG22	2.01	0.41
1:A:1049:ASP:OD1	1:A:1049:ASP:N	2.50	0.41
1:A:2523:TRP:NE1	1:A:2533:GLU:OE1	2.43	0.41
1:A:3208:TYR:OH	1:A:3760:THR:OG1	2.23	0.41
1:A:3811:VAL:HG21	1:A:3822:ASP:HB3	2.02	0.41
1:A:4098:LEU:HA	1:A:4121:PRO:HA	2.02	0.41
1:A:4183:ASP:HB3	1:A:4220:ARG:HH12	1.85	0.41
1:B:563:THR:HG23	1:B:572:TYR:HB2	2.00	0.41
1:B:597:GLY:HA2	1:B:1158:ASN:OD1	2.20	0.41
1:B:777:ILE:O	1:B:816:LYS:NZ	2.40	0.41
1:B:1112:THR:HA	1:B:1124:LYS:HE3	2.02	0.41
1:B:2115:SER:HB2	1:B:2121:ASP:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3255:PHE:CE2	2:K:1:NAG:H5	2.55	0.41
1:B:4102:TYR:OH	1:B:4171:LEU:HG	2.20	0.41
1:A:365:ARG:HB2	1:A:368:ARG:C	2.44	0.41
1:A:1026:CYS:HB3	1:A:1030:SER:HB2	2.02	0.41
1:A:1060:CYS:SG	1:A:1065:ASN:HB3	2.60	0.41
1:A:2212:ARG:HH22	1:B:1597:ILE:H	1.68	0.41
1:A:2213:PRO:HD2	1:B:1576:HIS:CE1	2.55	0.41
1:A:2257:ILE:HG13	1:A:2270:VAL:HG13	2.02	0.41
1:A:3679:ASP:N	1:A:3683:GLU:HB2	2.35	0.41
1:A:3804:GLN:HE21	1:A:3808:GLY:HA2	1.84	0.41
1:A:4008:ILE:H	1:A:4026:GLY:N	2.18	0.41
1:A:4042:ARG:HA	1:A:4045:LYS:HZ1	1.85	0.41
1:B:793:TRP:CE2	1:B:968:GLN:HA	2.55	0.41
1:B:1786:ASP:HB3	1:B:1791:TYR:HB2	2.02	0.41
1:B:2192:PRO:HB3	1:B:2206:TRP:CD1	2.54	0.41
1:B:3192:ARG:HD3	1:B:3192:ARG:HA	1.95	0.41
1:B:4106:ARG:HA	1:B:4144:PRO:HD2	2.02	0.41
1:B:4154:ARG:C	1:B:4171:LEU:HD13	2.45	0.41
1:A:1112:THR:HA	1:A:1124:LYS:HE3	2.01	0.41
1:B:493:MET:HE3	1:B:493:MET:HB3	1.88	0.41
1:B:1216:ASN:O	1:B:1220:ALA:N	2.54	0.41
1:B:1635:VAL:HG12	1:B:1636:ILE:HG13	2.02	0.41
1:B:3082:CYS:N	1:B:3086:ARG:O	2.38	0.41
1:A:462:LEU:HD11	1:A:494:VAL:HG11	2.01	0.41
1:A:873:ASN:ND2	1:A:917:PHE:HD1	2.18	0.41
1:A:1365:VAL:HG21	1:A:1374:LEU:HD12	2.02	0.41
1:A:1446:ILE:HD11	1:A:1482:TRP:CG	2.55	0.41
1:A:2257:ILE:HD11	1:A:2270:VAL:HG22	2.02	0.41
1:A:2729:SER:O	1:A:2735:VAL:HG21	2.21	0.41
1:A:3844:ALA:HB3	1:A:3846:MET:HE3	2.01	0.41
1:A:4199:MET:HE3	1:A:4201:TRP:HZ3	1.85	0.41
1:B:522:GLY:C	1:B:543:MET:HG3	2.45	0.41
1:B:619:TRP:CD1	1:B:644:ARG:HG3	2.56	0.41
1:B:719:ILE:HD11	1:B:743:PHE:HB3	2.01	0.41
1:B:842:PHE:CZ	1:B:852:MET:HB2	2.56	0.41
1:B:1078:GLU:OE1	1:B:1092:CYS:HB2	2.20	0.41
1:B:1853:ASP:OD1	1:B:1853:ASP:N	2.48	0.41
1:B:1864:ASP:HB3	1:B:2083:HIS:CE1	2.55	0.41
1:B:2176:ILE:HB	2:I:1:NAG:H82	2.03	0.41
1:B:2531:LYS:HE2	1:B:2531:LYS:HB2	1.91	0.41
1:B:3093:LEU:HD22	1:B:3130:LEU:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3834:THR:HA	1:B:3841:TYR:CZ	2.56	0.41
1:A:2198:ASP:OD2	1:A:2201:ASN:ND2	2.49	0.41
1:A:2475:TRP:O	1:A:2476:ILE:C	2.64	0.41
1:A:2523:TRP:CE2	1:A:2533:GLU:HB2	2.55	0.41
1:A:4067:TYR:CZ	1:A:4072:GLU:HA	2.55	0.41
1:B:470:GLU:OE1	1:B:513:ARG:HD3	2.20	0.41
1:B:868:THR:HG21	1:B:1242:ILE:HG21	2.03	0.41
1:B:1236:GLN:NE2	1:B:3194:ASN:HD22	2.19	0.41
1:B:3502:LEU:HD11	1:B:3507:TYR:HB2	2.01	0.41
1:B:3706:ARG:HD2	1:B:3706:ARG:N	2.35	0.41
1:B:3744:ASP:N	1:B:3750:ASP:OD2	2.52	0.41
1:B:4285:TYR:HD1	1:B:4320:ILE:HD11	1.86	0.41
1:A:248:LYS:C	1:A:250:ASN:N	2.77	0.41
1:A:452:ASP:OD2	1:A:457:ASN:ND2	2.53	0.41
1:A:895:GLU:HG2	1:A:906:ARG:HB2	2.01	0.41
1:A:977:PRO:HB2	1:B:2776:LEU:HB3	2.02	0.41
1:A:1347:LEU:N	1:A:1369:PHE:O	2.53	0.41
1:A:1362:HIS:O	1:A:1363:GLU:C	2.61	0.41
1:A:2099:HIS:ND1	1:A:2194:HIS:HD2	2.19	0.41
1:A:3577:ASN:HD22	1:A:3583:ASP:CG	2.28	0.41
1:B:620:THR:HA	1:B:1132:ASN:HB2	2.01	0.41
1:B:1122:ILE:HD12	1:B:1133:ASP:OD2	2.21	0.41
1:B:1122:ILE:HG13	1:B:1134:CYS:HB3	2.02	0.41
1:B:1794:TRP:HZ3	1:B:1804:VAL:HG12	1.84	0.41
1:B:2096:ASN:O	1:B:2113:ASP:HA	2.20	0.41
1:B:2304:SER:HB3	1:B:2309:ASN:HD22	1.85	0.41
1:B:2513:VAL:HB	1:B:2522:TYR:HB2	2.02	0.41
1:B:2651:CYS:O	1:B:2652:ASN:C	2.61	0.41
1:A:793:TRP:CE2	1:A:968:GLN:HA	2.56	0.41
1:A:1037:ARG:NH1	1:A:1050:ASP:O	2.53	0.41
1:A:1239:GLU:HG3	1:A:1257:LEU:HB3	2.02	0.41
1:A:2707:CYS:CB	1:A:2729:SER:HB3	2.44	0.41
1:A:3640:PHE:N	1:A:3648:ILE:O	2.53	0.41
1:B:1872:PHE:H	1:B:1889:ASP:CG	2.28	0.41
1:B:1961:SER:OG	1:B:1979:GLN:HB2	2.20	0.41
1:B:2093:GLN:HE21	1:B:2093:GLN:HB3	1.65	0.41
1:B:2312:PRO:HA	1:B:2313:PRO:HD3	1.96	0.41
1:B:3243:TRP:HZ2	1:B:3261:LYS:HE3	1.85	0.41
1:B:3268:ARG:HB2	1:B:3304:ARG:HH12	1.86	0.41
1:B:3318:PHE:CZ	1:B:3361:SER:HB2	2.55	0.41
1:B:3614:ASP:OD1	1:B:3614:ASP:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3667:PRO:O	1:B:3670:GLU:N	2.54	0.41
1:B:4042:ARG:HA	1:B:4045:LYS:NZ	2.36	0.41
1:B:4246:TRP:CZ2	1:B:4255:GLU:HB2	2.55	0.41
1:A:350:ASP:HB3	1:A:353:GLN:HB2	2.01	0.41
1:A:925:HIS:CG	1:A:938:ARG:HD2	2.56	0.41
1:A:1076:HIS:N	1:A:1094:ASP:OD2	2.30	0.41
1:A:1965:GLY:H	1:A:1976:THR:HG23	1.86	0.41
1:A:4207:GLU:O	1:A:4208:PRO:C	2.62	0.41
1:B:462:LEU:HD11	1:B:494:VAL:HG11	2.03	0.41
1:B:523:TYR:HB3	1:B:525:PHE:CE1	2.56	0.41
1:B:1112:THR:O	1:B:1124:LYS:HG3	2.20	0.41
1:B:1162:ILE:HD12	1:B:1166:PHE:HB2	2.03	0.41
1:B:1373:CYS:SG	1:B:1386:LYS:HG2	2.60	0.41
1:B:3846:MET:CB	1:B:3857:PRO:HD3	2.50	0.41
1:A:535:GLU:HB2	1:A:537:LYS:HE3	2.03	0.41
1:A:556:LEU:HD11	1:A:559:PRO:HB3	2.03	0.41
1:A:681:ASP:OD1	1:A:682:ASN:N	2.53	0.41
1:A:834:HIS:NE2	1:A:836:PHE:HB2	2.36	0.41
1:A:917:PHE:HD2	1:A:958:LEU:HA	1.86	0.41
1:A:1112:THR:O	1:A:1124:LYS:HG3	2.20	0.41
1:A:1390:ASP:HB2	1:A:1408:ARG:NH1	2.35	0.41
1:A:1606:ASP:OD1	1:A:1650:LEU:HD13	2.21	0.41
1:A:1922:GLU:HG3	1:A:1963:PRO:O	2.20	0.41
1:A:2388:ASN:ND2	1:A:2601:TYR:OH	2.53	0.41
1:A:2501:THR:HB	1:A:2665:ILE:HD12	2.03	0.41
1:A:3281:SER:O	1:A:3283:LYS:NZ	2.52	0.41
1:A:3326:LEU:HD12	1:A:3326:LEU:HA	1.87	0.41
1:A:3655:ASP:HB2	1:A:3691:ARG:HH12	1.85	0.41
1:A:4121:PRO:C	1:A:4123:PHE:H	2.29	0.41
1:A:4165:ARG:NH2	1:A:4167:GLU:OE2	2.50	0.41
1:B:612:GLY:HA2	1:B:629:LYS:HE2	2.03	0.41
1:B:768:GLN:HA	1:B:774:GLY:O	2.21	0.41
1:B:1174:CYS:HB2	1:B:1178:SER:H	1.85	0.41
1:B:1352:SER:HB2	1:B:1358:GLY:HA2	2.03	0.41
1:B:1508:ILE:H	1:B:1508:ILE:HG13	1.49	0.41
1:B:1965:GLY:H	1:B:1976:THR:HG23	1.85	0.41
1:B:2438:ASN:O	1:B:2439:LEU:C	2.63	0.41
1:B:2684:TYR:O	1:B:2693:ILE:HG13	2.21	0.41
1:B:2685:LEU:HB3	1:B:2689:ARG:HA	2.03	0.41
1:B:2733:GLU:O	1:B:2737:ALA:N	2.54	0.41
1:B:3458:HIS:HD2	1:B:3460:TYR:H	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3633:ARG:NH2	1:B:3647:CYS:HB2	2.36	0.41
1:B:4411:GLU:OE1	1:B:4411:GLU:N	2.41	0.41
1:A:747:ASP:OD1	1:A:748:PHE:N	2.50	0.41
1:A:3020:ASP:OD1	1:A:3020:ASP:N	2.54	0.41
1:A:3025:ARG:HD3	1:A:3028:LEU:HD21	2.02	0.41
1:A:3090:MET:HE2	1:B:3091:MET:HG2	2.03	0.41
1:A:3551:ARG:HA	1:A:3559:GLN:NE2	2.36	0.41
1:A:3842:CYS:HB3	1:A:3846:MET:HB2	2.02	0.41
1:A:4170:LYS:HE2	1:A:4174:ARG:HH21	1.86	0.41
1:A:4246:TRP:CZ2	1:A:4255:GLU:HB2	2.56	0.41
1:B:742:PHE:O	1:B:744:VAL:HG23	2.21	0.41
1:B:845:TRP:CD1	1:B:845:TRP:H	2.39	0.41
1:B:1118:ASN:HD21	1:B:1136:ASP:H	1.69	0.41
1:B:1239:GLU:HG3	1:B:1257:LEU:HB3	2.03	0.41
1:B:2502:VAL:HG23	1:B:2679:HIS:CG	2.56	0.41
1:B:3092:LYS:HB3	1:B:3099:ASP:OD2	2.21	0.41
1:B:3312:VAL:HG11	1:B:3337:TRP:CZ2	2.55	0.41
1:B:3834:THR:O	1:B:3835:ARG:C	2.64	0.41
1:B:4257:ILE:HB	1:B:4261:GLY:HA2	2.03	0.41
1:A:1353:CYS:H	1:A:1371:ALA:HB2	1.86	0.40
1:A:1532:THR:HB	1:A:1545:VAL:HG13	2.03	0.40
1:A:1802:HIS:NE2	1:A:1813:VAL:HG22	2.37	0.40
1:A:1831:ILE:HD12	1:A:2018:SER:HA	2.03	0.40
1:A:2550:LEU:HD21	1:A:2553:PRO:HB3	2.03	0.40
1:A:2733:GLU:O	1:A:2734:SER:C	2.64	0.40
1:A:3201:LEU:N	1:A:3212:LEU:O	2.55	0.40
1:A:3391:TYR:CE1	1:A:3400:HIS:HB2	2.57	0.40
1:B:556:LEU:HG	1:B:559:PRO:HD3	2.02	0.40
1:B:1442:SER:OG	1:B:1443:GLN:N	2.54	0.40
1:B:1578:ARG:NE	1:B:1580:GLU:OE2	2.46	0.40
1:B:3110:GLY:C	1:B:3111:ILE:HD12	2.46	0.40
1:B:3200:TYR:CZ	2:J:1:NAG:H3	2.57	0.40
1:B:3858:TYR:O	1:B:3862:ASP:HB2	2.21	0.40
1:B:4203:ASP:C	1:B:4205:GLY:H	2.29	0.40
1:A:347:VAL:HG22	1:A:349:PHE:N	2.35	0.40
1:A:494:VAL:HG12	1:A:501:ARG:HA	2.03	0.40
1:A:932:ARG:HA	1:A:932:ARG:HD3	1.92	0.40
1:A:1163:ASP:HB3	1:A:1166:PHE:CD2	2.56	0.40
1:A:3307:LEU:HD23	1:A:3307:LEU:HA	1.88	0.40
1:A:3789:ASP:OD1	1:A:3789:ASP:N	2.54	0.40
1:A:4009:ASN:O	1:A:4010:GLU:C	2.65	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4092:ASP:OD1	1:A:4092:ASP:N	2.54	0.40
1:B:1060:CYS:SG	1:B:1065:ASN:HB3	2.61	0.40
1:B:2665:ILE:H	1:B:2665:ILE:HG13	1.64	0.40
1:A:423:ARG:NH2	1:A:1087:ASP:OD2	2.47	0.40
1:A:1375:CYS:SG	1:A:1381:LEU:HG	2.62	0.40
1:A:1872:PHE:H	1:A:1889:ASP:CG	2.28	0.40
1:A:3551:ARG:HA	1:A:3559:GLN:HE22	1.86	0.40
1:A:4175:TYR:OH	1:A:4372:GLU:N	2.53	0.40
1:A:4277:LEU:HB3	1:A:4284:LEU:HD21	2.03	0.40
1:B:535:GLU:O	1:B:537:LYS:HG3	2.21	0.40
1:B:746:ILE:CG1	1:B:961:LYS:HB3	2.51	0.40
1:B:1131:ASP:C	1:B:1133:ASP:N	2.77	0.40
1:B:1352:SER:HA	1:B:1355:ASP:CG	2.46	0.40
1:B:3278:ASP:OD2	1:B:3282:ARG:N	2.54	0.40
1:B:3875:LEU:HD22	1:B:3880:ASP:N	2.35	0.40
1:A:356:GLY:HA2	1:A:630:PHE:CG	2.56	0.40
1:A:1122:ILE:HD12	1:A:1133:ASP:OD2	2.21	0.40
1:A:1442:SER:OG	1:A:1443:GLN:N	2.55	0.40
1:A:1743:ASP:OD1	1:A:1744:ASP:N	2.53	0.40
1:A:3278:ASP:OD2	1:A:3282:ARG:N	2.53	0.40
1:A:3450:ARG:HB2	1:A:3452:PHE:CE2	2.56	0.40
1:A:4004:SER:O	1:A:4005:CYS:C	2.64	0.40
1:A:4106:ARG:HA	1:A:4144:PRO:HD2	2.03	0.40
1:A:4236:ILE:HB	1:A:4238:TYR:CZ	2.56	0.40
1:B:1132:ASN:O	1:B:1133:ASP:C	2.64	0.40
1:B:1365:VAL:HB	1:B:1372:LYS:HB3	2.04	0.40
1:B:2126:ARG:NE	1:B:2137:ILE:HD11	2.36	0.40
1:B:3513:SER:HB3	1:B:3593:HIS:ND1	2.36	0.40
1:B:4163:ASN:O	1:B:4165:ARG:HG3	2.22	0.40
1:B:4271:ALA:HB1	1:B:4286:TRP:NE1	2.37	0.40
1:A:603:HIS:CD2	1:A:619:TRP:HB2	2.56	0.40
1:A:632:GLU:HG3	1:A:634:ASN:H	1.85	0.40
1:A:749:ASP:HA	1:A:968:GLN:HE22	1.86	0.40
1:A:1462:VAL:HG13	1:A:1500:ARG:HH21	1.86	0.40
1:A:1508:ILE:H	1:A:1508:ILE:HG13	1.48	0.40
1:A:1975:TYR:OH	1:A:1984:GLU:OE1	2.21	0.40
1:A:3667:PRO:O	1:A:3670:GLU:N	2.54	0.40
1:A:3888:ARG:O	1:A:3889:PHE:C	2.65	0.40
1:A:4098:LEU:HD22	1:A:4380:PRO:HB2	2.04	0.40
1:A:4199:MET:HE3	1:A:4201:TRP:CZ3	2.57	0.40
1:B:379:LEU:HD12	1:B:384:TYR:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:793:TRP:CE3	1:B:968:GLN:HG2	2.56	0.40
1:B:1154:PHE:N	1:B:1162:ILE:O	2.55	0.40
1:B:1390:ASP:HB2	1:B:1408:ARG:NH1	2.35	0.40
1:B:1615:MET:HE3	1:B:1615:MET:HB2	1.90	0.40
1:B:2399:ARG:HG2	1:B:2414:THR:CG2	2.52	0.40
1:B:3331:GLN:O	1:B:3486:GLY:HA3	2.22	0.40
1:B:4314:TRP:O	1:B:4315:LEU:C	2.64	0.40
2:N:1:NAG:H82	2:N:1:NAG:H2	1.89	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	3683/4655 (79%)	3478 (94%)	203 (6%)	2 (0%)	48	75
1	B	3680/4655 (79%)	3478 (94%)	197 (5%)	5 (0%)	48	75
All	All	7363/9310 (79%)	6956 (94%)	400 (5%)	7 (0%)	49	75

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1160	ARG
1	A	821	VAL
1	A	960	LEU
1	B	821	VAL
1	B	646	TYR
1	B	1135	GLY
1	B	2417	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	3150/4105 (77%)	3047 (97%)	103 (3%)	33	59
1	B	3150/4105 (77%)	3038 (96%)	112 (4%)	31	58
All	All	6300/8210 (77%)	6085 (97%)	215 (3%)	33	59

All (215) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	374	GLU
1	A	446	ASN
1	A	453	ILE
1	A	464	VAL
1	A	466	VAL
1	A	488	VAL
1	A	581	ILE
1	A	683	ASP
1	A	746	ILE
1	A	810	VAL
1	A	821	VAL
1	A	887	VAL
1	A	892	ASP
1	A	969	THR
1	A	974	CYS
1	A	1023	THR
1	A	1051	CYS
1	A	1133	ASP
1	A	1184	VAL
1	A	1185	LEU
1	A	1187	CYS
1	A	1198	ASP
1	A	1224	THR
1	A	1238	GLN
1	A	1239	GLU
1	A	1363	GLU
1	A	1403	HIS

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Mol	Chain	Res	Type
1	A	1451	VAL
1	A	1454	GLN
1	A	1508	ILE
1	A	1648	LEU
1	A	1649	THR
1	A	1655	VAL
1	A	1712	LEU
1	A	1755	ILE
1	A	1784	GLU
1	A	1801	ILE
1	A	1820	VAL
1	A	1838	THR
1	A	1976	THR
1	A	2007	LEU
1	A	2036	VAL
1	A	2066	VAL
1	A	2093	GLN
1	A	2327	THR
1	A	2341	VAL
1	A	2421	VAL
1	A	2436	THR
1	A	2491	ASN
1	A	2493	MET
1	A	2501	THR
1	A	2513	VAL
1	A	2543	VAL
1	A	2593	VAL
1	A	2651	CYS
1	A	2705	PHE
1	A	2712	CYS
1	A	2747	THR
1	A	2759	ARG
1	A	2765	ASP
1	A	3035	ASN
1	A	3041	ASN
1	A	3045	ILE
1	A	3056	ASP
1	A	3067	LEU
1	A	3075	CYS
1	A	3078	HIS
1	A	3103	ASN
1	A	3129	THR

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Mol	Chain	Res	Type
1	A	3168	GLU
1	A	3278	ASP
1	A	3298	ASP
1	A	3346	ILE
1	A	3371	THR
1	A	3398	HIS
1	A	3413	ILE
1	A	3415	ILE
1	A	3420	ILE
1	A	3465	VAL
1	A	3552	PHE
1	A	3560	CYS
1	A	3578	CYS
1	A	3590	GLU
1	A	3619	CYS
1	A	3622	ASN
1	A	3629	HIS
1	A	3706	ARG
1	A	3744	ASP
1	A	3784	CYS
1	A	3843	GLN
1	A	3845	THR
1	A	3848	GLU
1	A	3859	TRP
1	A	4045	LYS
1	A	4120	ILE
1	A	4145	ASP
1	A	4156	ILE
1	A	4171	LEU
1	A	4179	LEU
1	A	4190	ILE
1	A	4219	ASP
1	A	4254	ILE
1	A	4273	ASN
1	B	339	ASN
1	B	354	ILE
1	B	452	ASP
1	B	464	VAL
1	B	466	VAL
1	B	479	ASN
1	B	481	ILE
1	B	488	VAL

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Mol	Chain	Res	Type
1	B	579	ASP
1	B	581	ILE
1	B	622	MET
1	B	642	SER
1	B	643	LEU
1	B	644	ARG
1	B	732	VAL
1	B	746	ILE
1	B	821	VAL
1	B	887	VAL
1	B	892	ASP
1	B	969	THR
1	B	974	CYS
1	B	978	THR
1	B	979	HIS
1	B	991	VAL
1	B	1023	THR
1	B	1051	CYS
1	B	1133	ASP
1	B	1184	VAL
1	B	1185	LEU
1	B	1187	CYS
1	B	1198	ASP
1	B	1224	THR
1	B	1262	GLU
1	B	1373	CYS
1	B	1403	HIS
1	B	1451	VAL
1	B	1454	GLN
1	B	1508	ILE
1	B	1612	LEU
1	B	1648	LEU
1	B	1649	THR
1	B	1655	VAL
1	B	1712	LEU
1	B	1755	ILE
1	B	1784	GLU
1	B	1801	ILE
1	B	1820	VAL
1	B	1838	THR
1	B	1976	THR
1	B	2007	LEU

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Mol	Chain	Res	Type
1	B	2036	VAL
1	B	2066	VAL
1	B	2327	THR
1	B	2341	VAL
1	B	2491	ASN
1	B	2493	MET
1	B	2513	VAL
1	B	2543	VAL
1	B	2593	VAL
1	B	2651	CYS
1	B	2705	PHE
1	B	2706	THR
1	B	2712	CYS
1	B	2739	HIS
1	B	2756	TYR
1	B	2776	LEU
1	B	3035	ASN
1	B	3041	ASN
1	B	3045	ILE
1	B	3056	ASP
1	B	3067	LEU
1	B	3075	CYS
1	B	3103	ASN
1	B	3129	THR
1	B	3168	GLU
1	B	3278	ASP
1	B	3298	ASP
1	B	3346	ILE
1	B	3371	THR
1	B	3398	HIS
1	B	3413	ILE
1	B	3415	ILE
1	B	3420	ILE
1	B	3446	ASN
1	B	3552	PHE
1	B	3560	CYS
1	B	3578	CYS
1	B	3590	GLU
1	B	3619	CYS
1	B	3622	ASN
1	B	3629	HIS
1	B	3706	ARG

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Mol	Chain	Res	Type
1	B	3744	ASP
1	B	3780	HIS
1	B	3784	CYS
1	B	3843	GLN
1	B	3858	TYR
1	B	4006	LEU
1	B	4041	ASP
1	B	4045	LYS
1	B	4080	ASP
1	B	4092	ASP
1	B	4120	ILE
1	B	4156	ILE
1	B	4171	LEU
1	B	4179	LEU
1	B	4190	ILE
1	B	4219	ASP
1	B	4254	ILE
1	B	4272	MET
1	B	4298	ASN
1	B	4312	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (132) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	353	GLN
1	A	369	HIS
1	A	410	HIS
1	A	445	GLN
1	A	489	ASN
1	A	547	ASN
1	A	596	HIS
1	A	661	ASN
1	A	696	GLN
1	A	716	GLN
1	A	768	GLN
1	A	785	ASN
1	A	896	HIS
1	A	976	GLN
1	A	986	HIS
1	A	1009	ASN
1	A	1064	ASN
1	A	1099	HIS

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Mol	Chain	Res	Type
1	A	1144	ASN
1	A	1153	GLN
1	A	1191	GLN
1	A	1231	HIS
1	A	1366	GLN
1	A	1454	GLN
1	A	1495	GLN
1	A	1522	ASN
1	A	1553	ASN
1	A	1575	HIS
1	A	1594	GLN
1	A	1754	HIS
1	A	1931	GLN
1	A	1969	HIS
1	A	2093	GLN
1	A	2194	HIS
1	A	2302	GLN
1	A	2376	GLN
1	A	2402	HIS
1	A	2529	HIS
1	A	2613	GLN
1	A	2636	GLN
1	A	2739	HIS
1	A	3041	ASN
1	A	3055	ASN
1	A	3103	ASN
1	A	3249	GLN
1	A	3303	HIS
1	A	3310	HIS
1	A	3376	ASN
1	A	3400	HIS
1	A	3458	HIS
1	A	3522	ASN
1	A	3600	GLN
1	A	3622	ASN
1	A	3787	ASN
1	A	3809	HIS
1	A	3843	GLN
1	A	3852	HIS
1	A	3998	ASN
1	A	4132	GLN
1	A	4163	ASN

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Mol	Chain	Res	Type
1	A	4240	ASN
1	B	237	GLN
1	B	339	ASN
1	B	353	GLN
1	B	369	HIS
1	B	410	HIS
1	B	445	GLN
1	B	596	HIS
1	B	603	HIS
1	B	661	ASN
1	B	696	GLN
1	B	708	GLN
1	B	729	GLN
1	B	768	GLN
1	B	785	ASN
1	B	834	HIS
1	B	896	HIS
1	B	976	GLN
1	B	1009	ASN
1	B	1099	HIS
1	B	1118	ASN
1	B	1142	ASN
1	B	1153	GLN
1	B	1158	ASN
1	B	1231	HIS
1	B	1236	GLN
1	B	1238	GLN
1	B	1351	ASN
1	B	1366	GLN
1	B	1454	GLN
1	B	1495	GLN
1	B	1522	ASN
1	B	1553	ASN
1	B	1575	HIS
1	B	1594	GLN
1	B	1754	HIS
1	B	1931	GLN
1	B	1969	HIS
1	B	2093	GLN
1	B	2145	ASN
1	B	2194	HIS
1	B	2302	GLN

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Mol	Chain	Res	Type
1	B	2376	GLN
1	B	2396	ASN
1	B	2402	HIS
1	B	2437	GLN
1	B	2529	HIS
1	B	2613	GLN
1	B	2636	GLN
1	B	3041	ASN
1	B	3055	ASN
1	B	3103	ASN
1	B	3115	HIS
1	B	3196	ASN
1	B	3249	GLN
1	B	3300	ASN
1	B	3303	HIS
1	B	3310	HIS
1	B	3376	ASN
1	B	3385	HIS
1	B	3400	HIS
1	B	3458	HIS
1	B	3522	ASN
1	B	3600	GLN
1	B	3622	ASN
1	B	3629	HIS
1	B	3787	ASN
1	B	3804	GLN
1	B	3843	GLN
1	B	4132	GLN
1	B	4163	ASN
1	B	4240	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

33 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	0.29	0	17,19,21	0.70	0
2	NAG	C	2	2	14,14,15	0.31	0	17,19,21	0.73	0
2	BMA	C	3	2	11,11,12	0.23	0	15,15,17	0.53	0
2	NAG	D	1	2,1	14,14,15	0.32	0	17,19,21	0.61	0
2	NAG	D	2	2	14,14,15	0.27	0	17,19,21	0.75	0
2	BMA	D	3	2	11,11,12	0.21	0	15,15,17	0.50	0
2	NAG	E	1	2,1	14,14,15	0.30	0	17,19,21	0.82	1 (5%)
2	NAG	E	2	2	14,14,15	0.26	0	17,19,21	0.68	0
2	BMA	E	3	2	11,11,12	0.21	0	15,15,17	0.55	0
2	NAG	F	1	2,1	14,14,15	0.25	0	17,19,21	0.50	0
2	NAG	F	2	2	14,14,15	0.29	0	17,19,21	0.61	0
2	BMA	F	3	2	11,11,12	0.21	0	15,15,17	0.56	0
3	NAG	G	1	3	14,14,15	0.40	0	17,19,21	0.76	0
3	NAG	G	2	3	14,14,15	0.40	0	17,19,21	2.00	4 (23%)
3	NAG	H	1	3,1	14,14,15	0.36	0	17,19,21	1.33	2 (11%)
3	NAG	H	2	3	14,14,15	0.39	0	17,19,21	2.00	4 (23%)
2	NAG	I	1	2,1	14,14,15	0.31	0	17,19,21	0.66	0
2	NAG	I	2	2	14,14,15	0.31	0	17,19,21	0.80	0
2	BMA	I	3	2	11,11,12	0.22	0	15,15,17	0.51	0
2	NAG	J	1	2,1	14,14,15	0.33	0	17,19,21	0.58	0
2	NAG	J	2	2	14,14,15	0.26	0	17,19,21	0.66	0
2	BMA	J	3	2	11,11,12	0.21	0	15,15,17	0.52	0
2	NAG	K	1	2,1	14,14,15	0.31	0	17,19,21	0.80	1 (5%)
2	NAG	K	2	2	14,14,15	0.25	0	17,19,21	0.68	0
2	BMA	K	3	2	11,11,12	0.22	0	15,15,17	0.56	0
2	NAG	L	1	2,1	14,14,15	0.25	0	17,19,21	0.49	0
2	NAG	L	2	2	14,14,15	0.27	0	17,19,21	0.63	0
2	BMA	L	3	2	11,11,12	0.21	0	15,15,17	0.55	0
3	NAG	M	1	3,1	14,14,15	0.42	0	17,19,21	1.05	1 (5%)
3	NAG	M	2	3	14,14,15	0.40	0	17,19,21	1.02	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	N	1	2,1	14,14,15	0.39	0	17,19,21	1.21	2 (11%)
2	NAG	N	2	2	14,14,15	0.41	0	17,19,21	1.10	1 (5%)
2	BMA	N	3	2	11,11,12	0.21	0	15,15,17	0.51	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	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	NAG	D	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	BMA	D	3	2	-	0/2/19/22	0/1/1/1
2	NAG	E	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	3/6/23/26	0/1/1/1
2	BMA	E	3	2	-	0/2/19/22	0/1/1/1
2	NAG	F	1	2,1	-	3/6/23/26	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
3	NAG	G	1	3	-	1/6/23/26	0/1/1/1
3	NAG	G	2	3	-	1/6/23/26	0/1/1/1
3	NAG	H	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	1/6/23/26	0/1/1/1
2	NAG	I	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
2	BMA	I	3	2	-	1/2/19/22	0/1/1/1
2	NAG	J	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
2	BMA	J	3	2	-	0/2/19/22	0/1/1/1
2	NAG	K	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	K	2	2	-	3/6/23/26	0/1/1/1
2	BMA	K	3	2	-	0/2/19/22	0/1/1/1
2	NAG	L	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	L	2	2	-	0/6/23/26	0/1/1/1
2	BMA	L	3	2	-	0/2/19/22	0/1/1/1
3	NAG	M	1	3,1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	M	2	3	-	2/6/23/26	0/1/1/1
2	NAG	N	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	N	2	2	-	2/6/23/26	0/1/1/1
2	BMA	N	3	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	2	NAG	O5-C5-C6	6.53	120.37	107.66
3	G	2	NAG	O5-C5-C6	6.52	120.35	107.66
2	N	2	NAG	O5-C1-C2	3.81	117.18	111.29
3	H	1	NAG	C1-C2-N2	3.69	116.25	110.43
3	H	1	NAG	C2-N2-C7	3.45	127.53	122.90
3	M	1	NAG	C2-N2-C7	3.12	127.08	122.90
3	M	2	NAG	C1-C2-N2	2.89	114.99	110.43
3	G	2	NAG	C4-C3-C2	2.74	115.03	111.02
2	N	1	NAG	C1-C2-N2	2.72	114.71	110.43
3	H	2	NAG	C4-C3-C2	2.71	114.99	111.02
3	M	2	NAG	C2-N2-C7	2.50	126.25	122.90
3	H	2	NAG	O3-C3-C4	2.46	116.18	110.38
3	G	2	NAG	O3-C3-C4	2.45	116.16	110.38
2	N	1	NAG	O5-C1-C2	2.40	115.00	111.29
2	E	1	NAG	C2-N2-C7	-2.17	119.99	122.90
2	K	1	NAG	C2-N2-C7	-2.07	120.12	122.90
3	G	2	NAG	O4-C4-C5	2.04	114.36	109.32
3	H	2	NAG	O4-C4-C5	2.04	114.35	109.32

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	E	2	NAG	C3-C2-N2-C7
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2
2	F	1	NAG	C1-C2-N2-C7
2	F	1	NAG	C8-C7-N2-C2
2	F	1	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
2	K	1	NAG	C8-C7-N2-C2
2	K	1	NAG	O7-C7-N2-C2
2	K	2	NAG	C3-C2-N2-C7
2	K	2	NAG	O7-C7-N2-C2
2	L	1	NAG	C1-C2-N2-C7
2	L	1	NAG	C8-C7-N2-C2
2	L	1	NAG	O7-C7-N2-C2
2	N	1	NAG	C8-C7-N2-C2
2	N	1	NAG	O7-C7-N2-C2
2	N	2	NAG	C8-C7-N2-C2
2	N	2	NAG	O7-C7-N2-C2
3	H	1	NAG	C1-C2-N2-C7
3	M	1	NAG	C8-C7-N2-C2
3	M	1	NAG	O7-C7-N2-C2
3	M	2	NAG	C1-C2-N2-C7
2	K	2	NAG	C8-C7-N2-C2
2	J	2	NAG	C8-C7-N2-C2
2	J	2	NAG	O7-C7-N2-C2
2	D	2	NAG	C8-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2
2	I	3	BMA	O5-C5-C6-O6
3	M	2	NAG	C3-C2-N2-C7
2	I	1	NAG	C8-C7-N2-C2
2	C	1	NAG	C8-C7-N2-C2
2	I	1	NAG	O7-C7-N2-C2
3	G	1	NAG	C1-C2-N2-C7
3	G	2	NAG	C1-C2-N2-C7
3	H	2	NAG	C1-C2-N2-C7
3	H	1	NAG	C3-C2-N2-C7
2	C	1	NAG	O7-C7-N2-C2

There are no ring outliers.

15 monomers are involved in 32 short contacts:

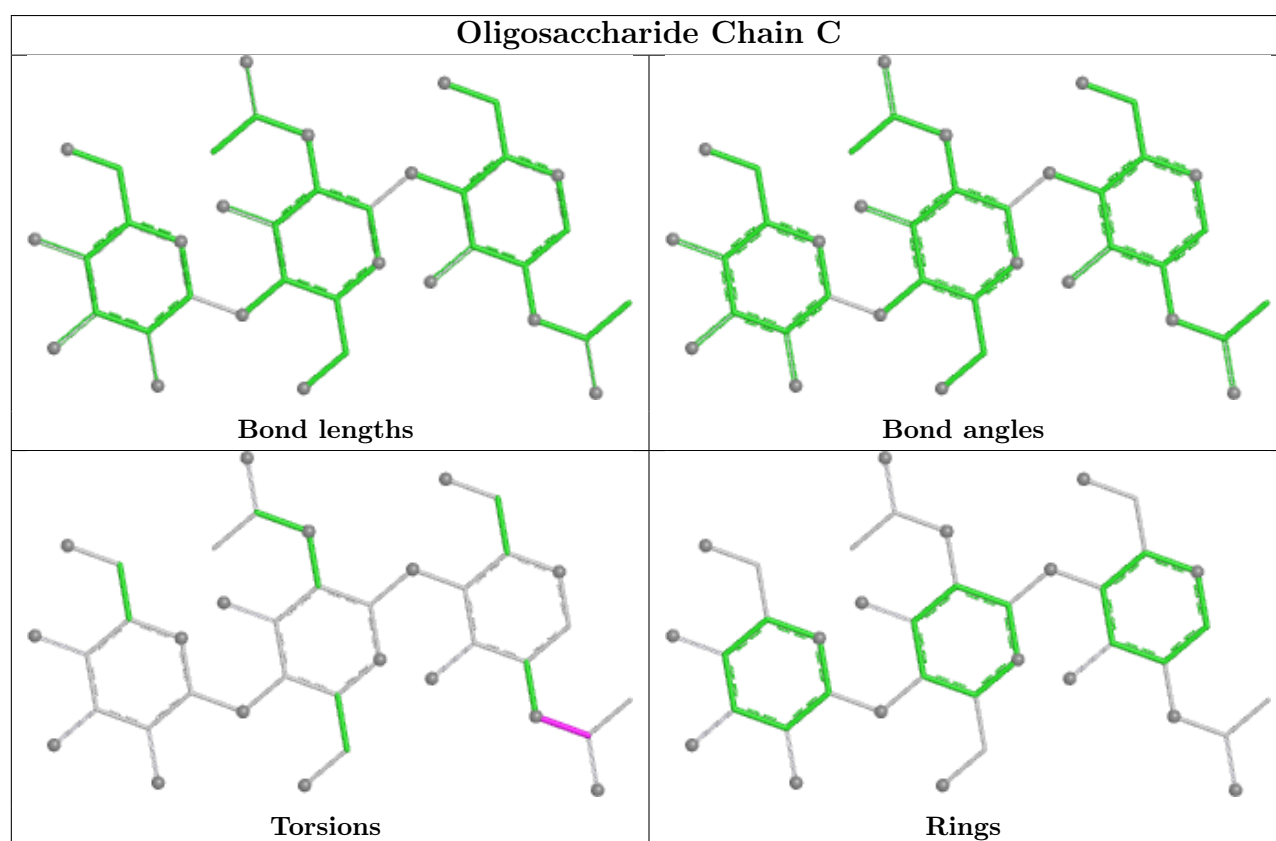
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	1	NAG	1	0
2	C	1	NAG	2	0
3	G	1	NAG	7	0
2	I	2	NAG	2	0
2	E	1	NAG	5	0
2	D	2	NAG	1	0
2	I	1	NAG	2	0

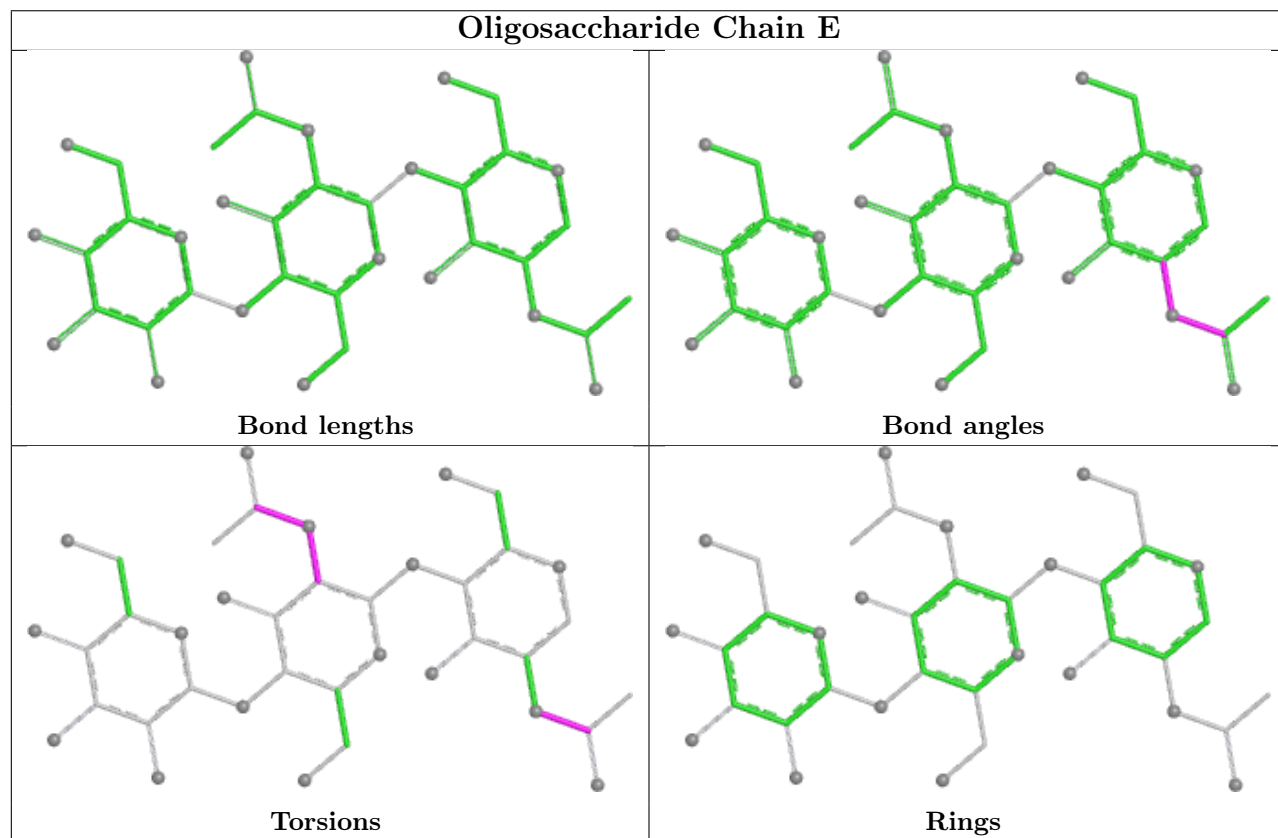
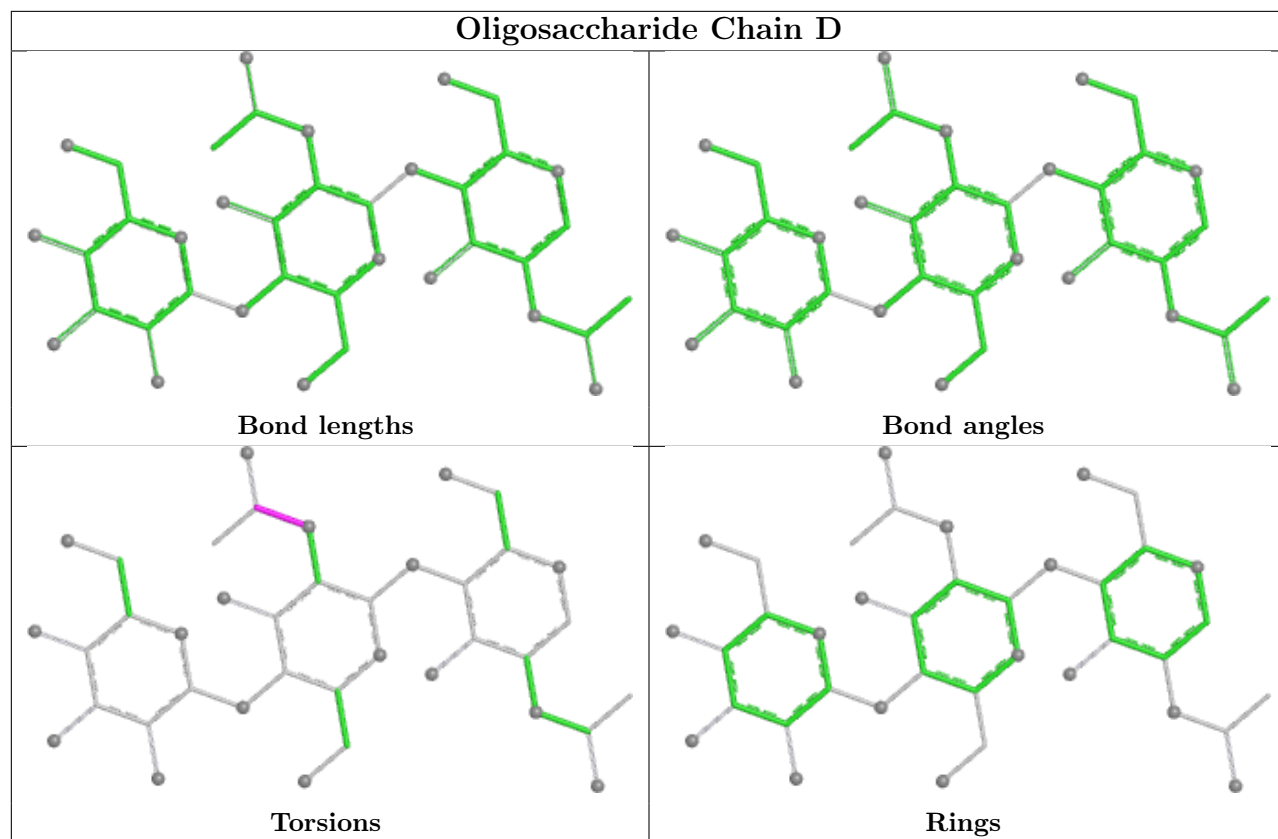
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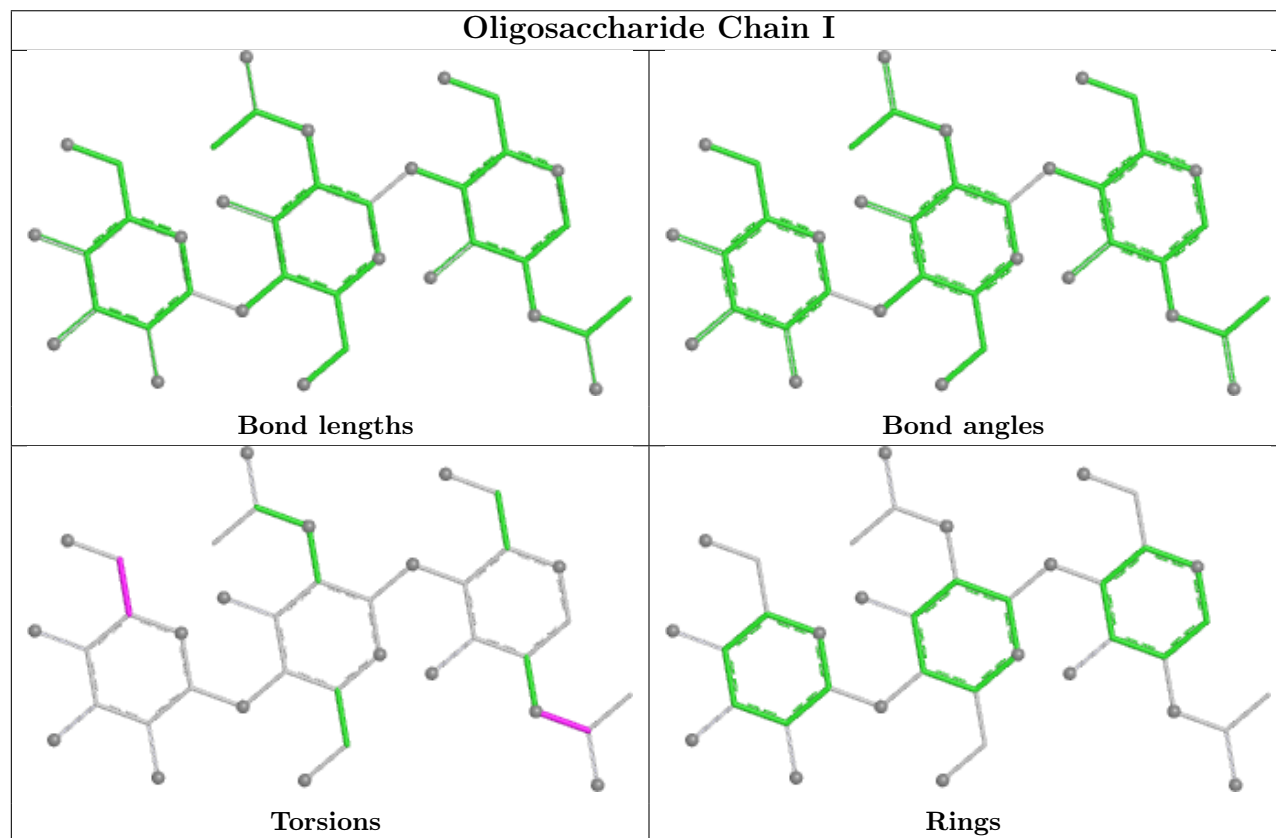
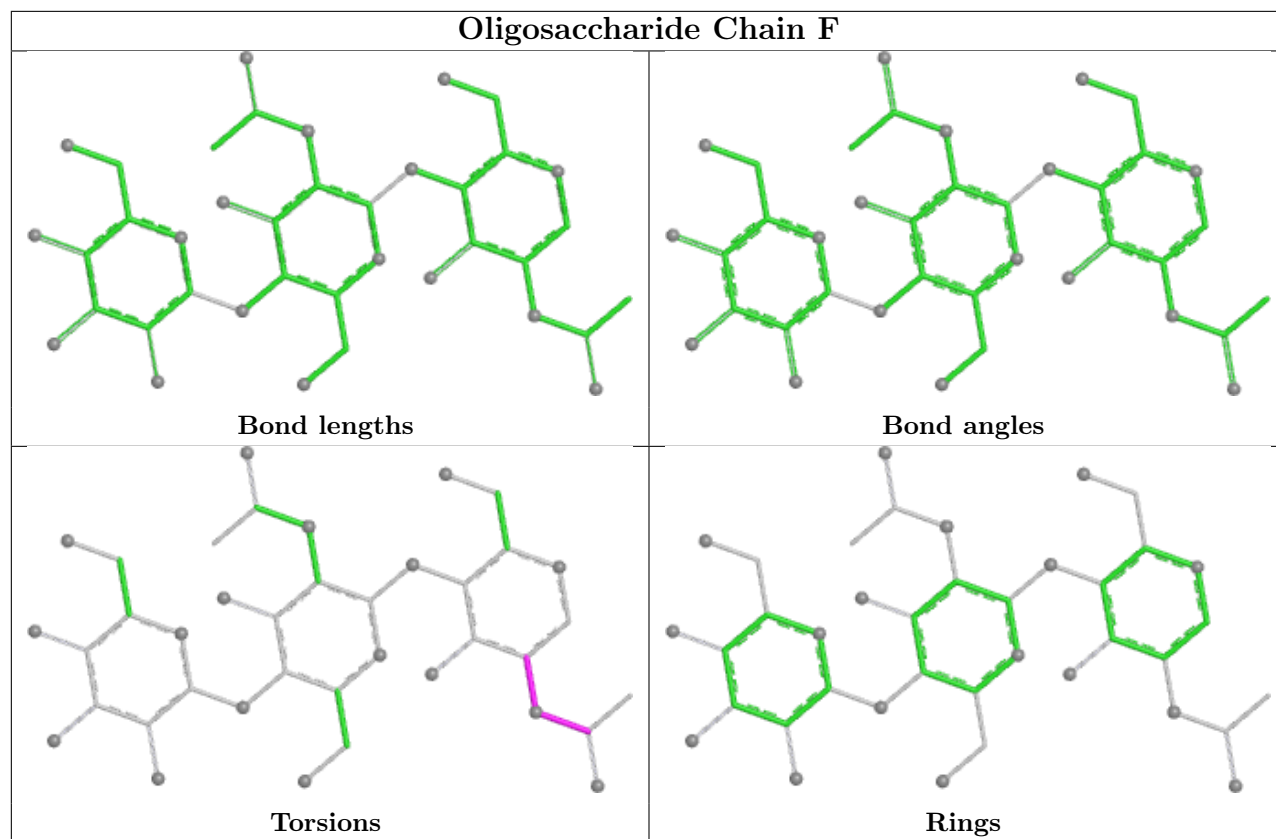
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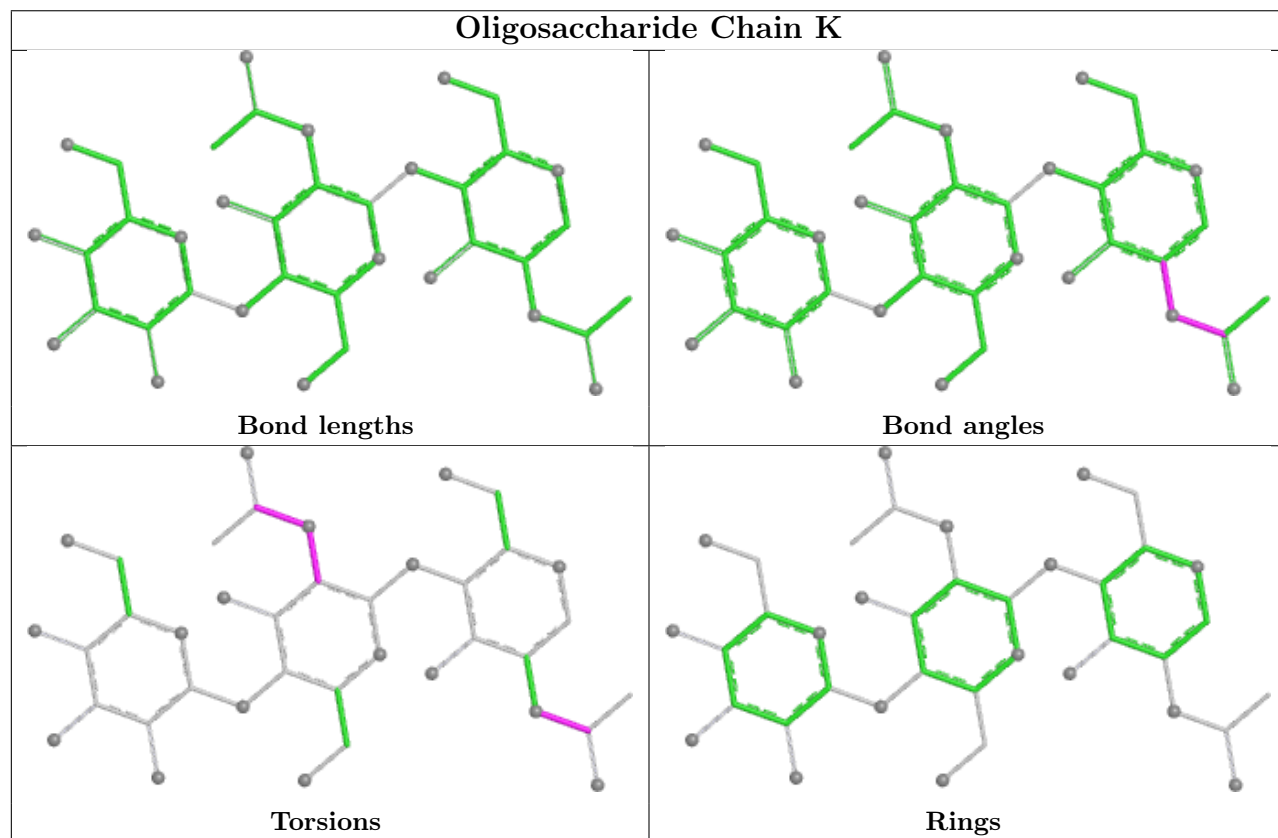
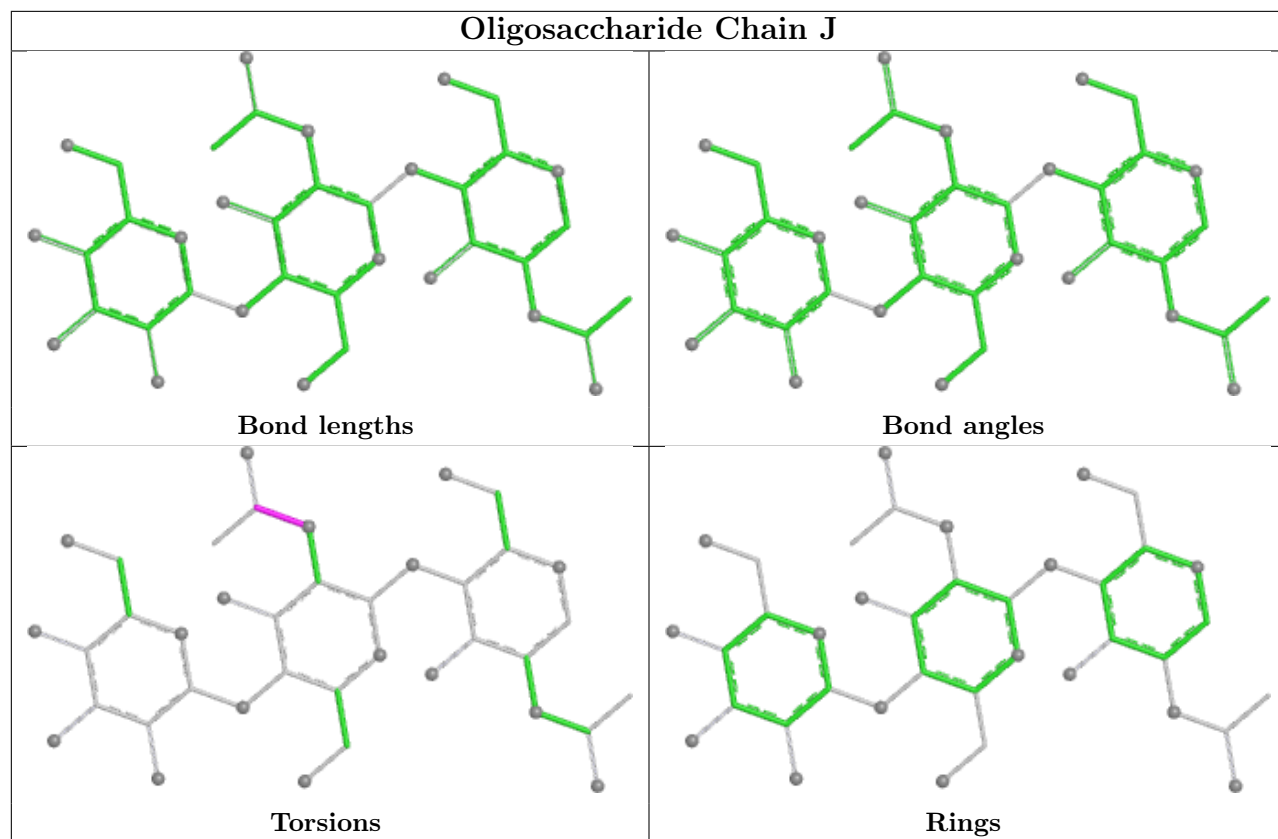
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	NAG	2	0
2	J	1	NAG	3	0
3	H	1	NAG	1	0
2	K	1	NAG	6	0
3	G	2	NAG	3	0
2	N	1	NAG	2	0
2	J	2	NAG	1	0
2	C	2	NAG	1	0

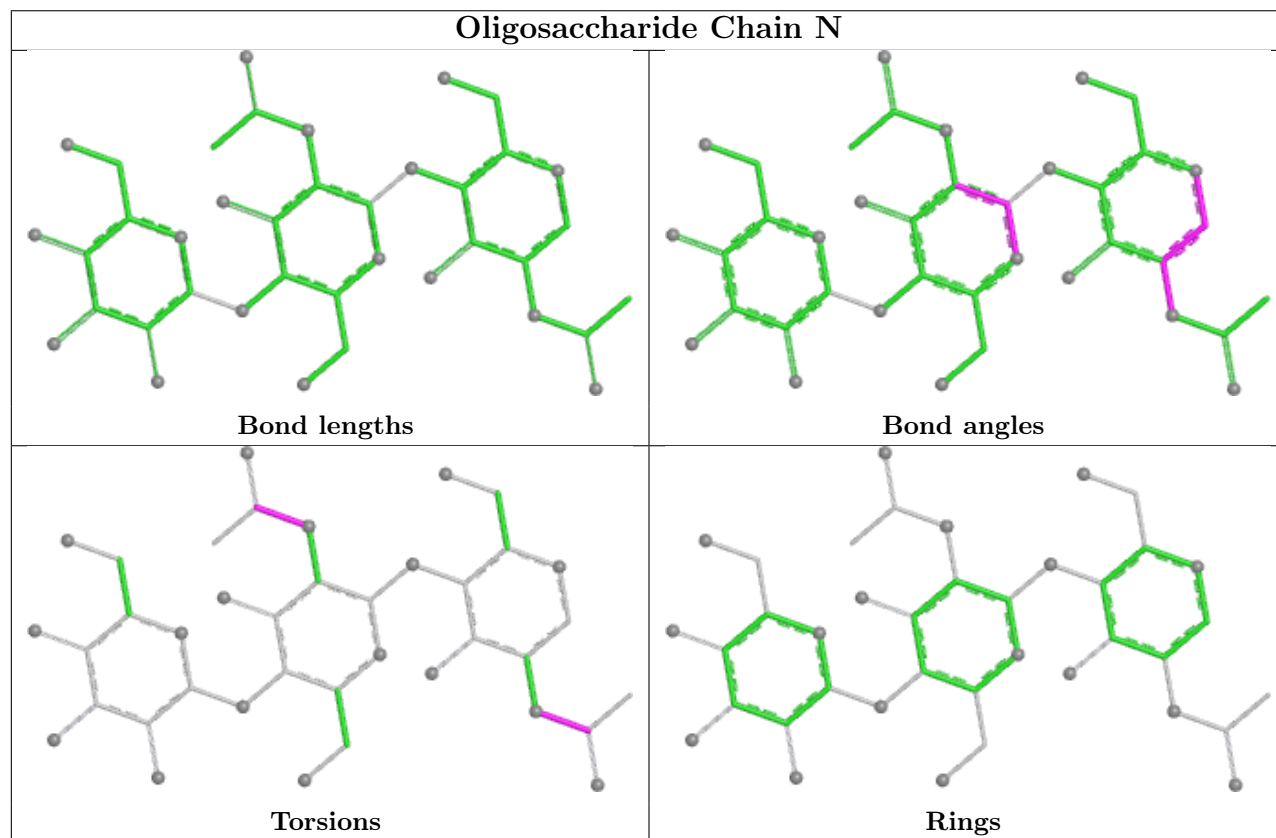
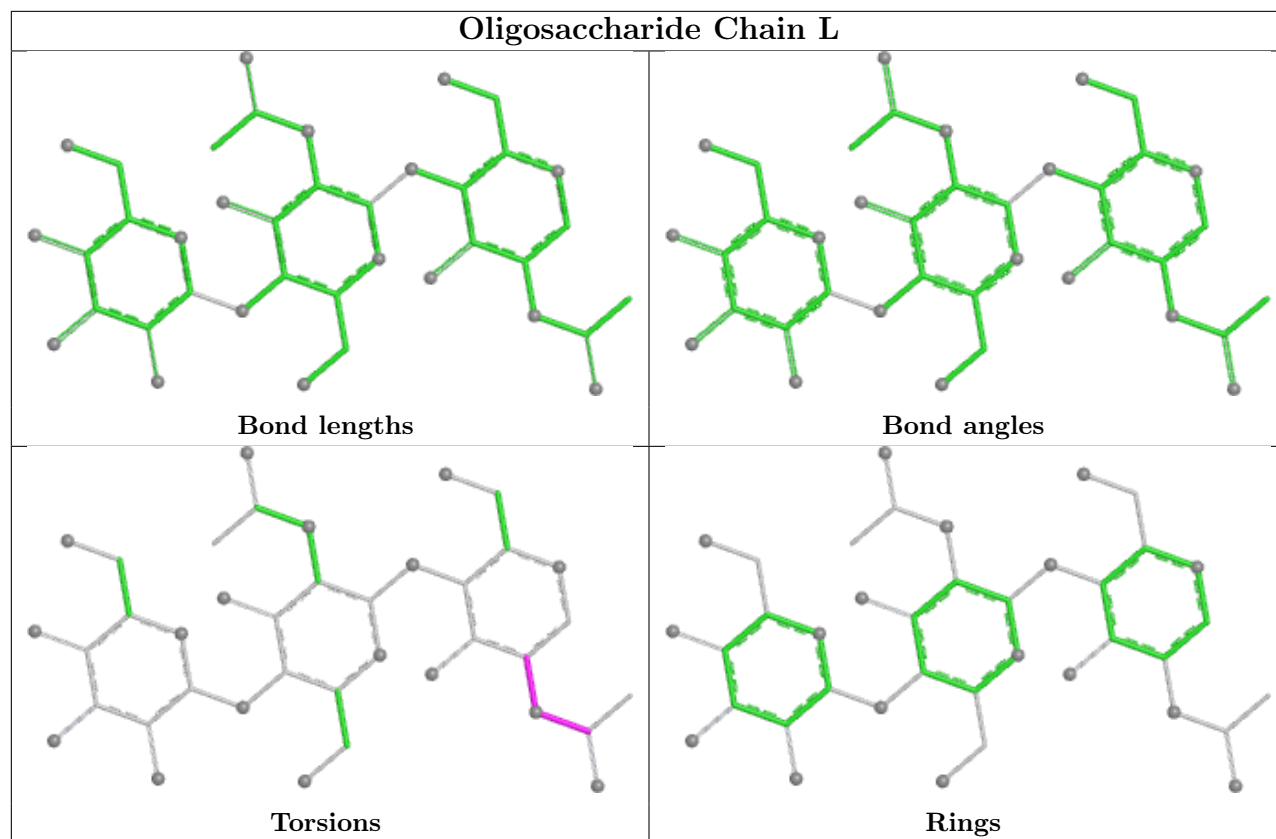
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

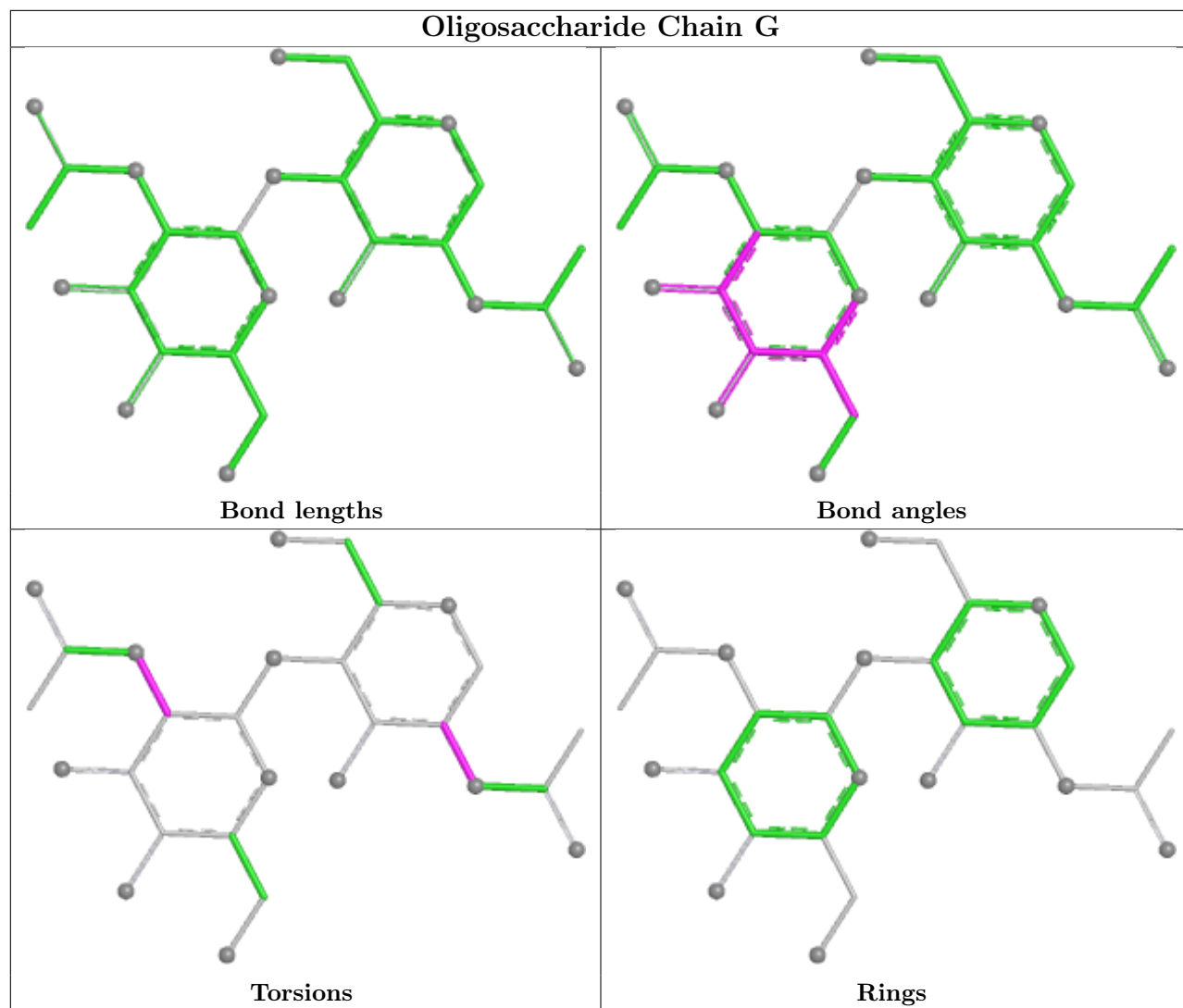


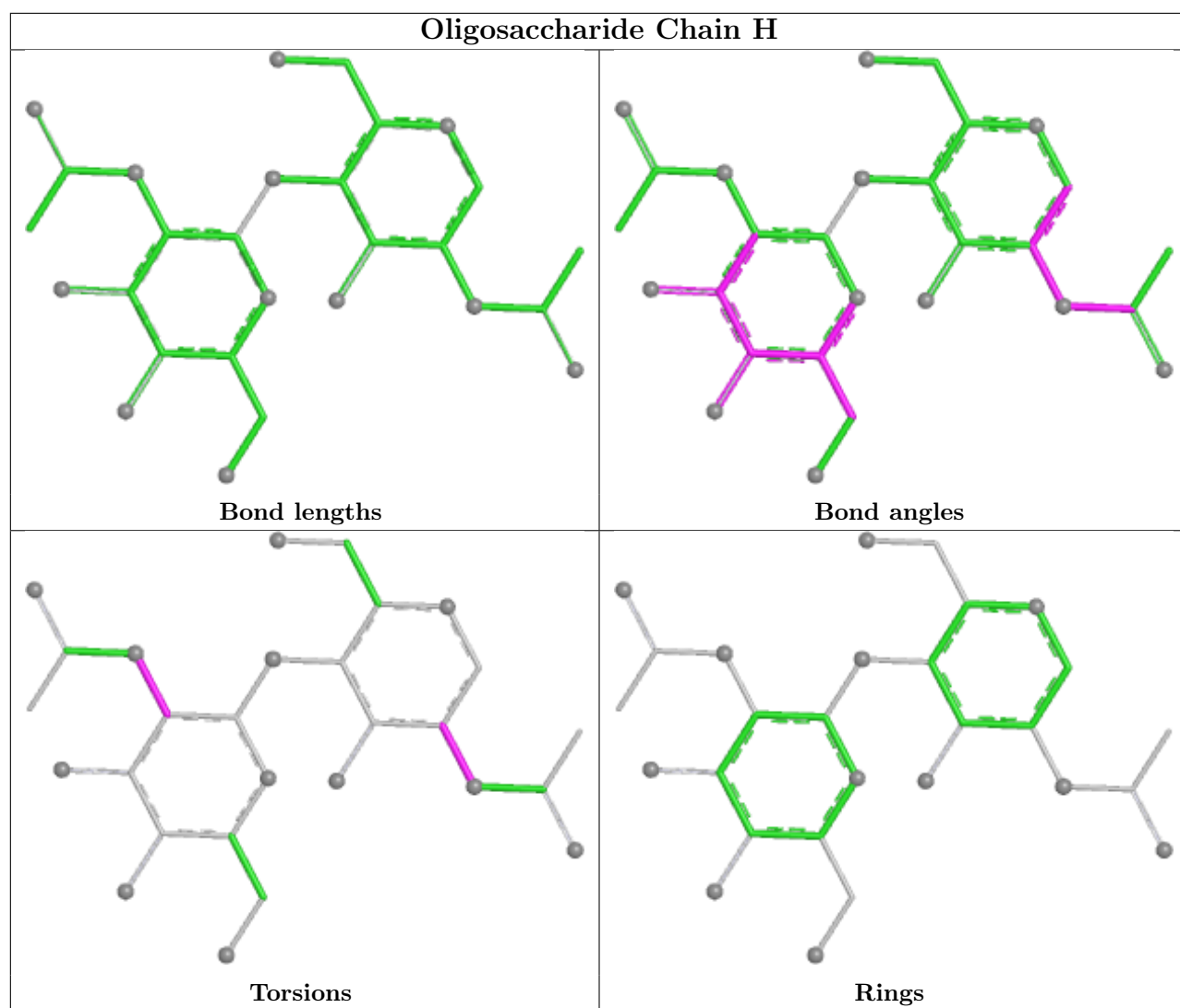


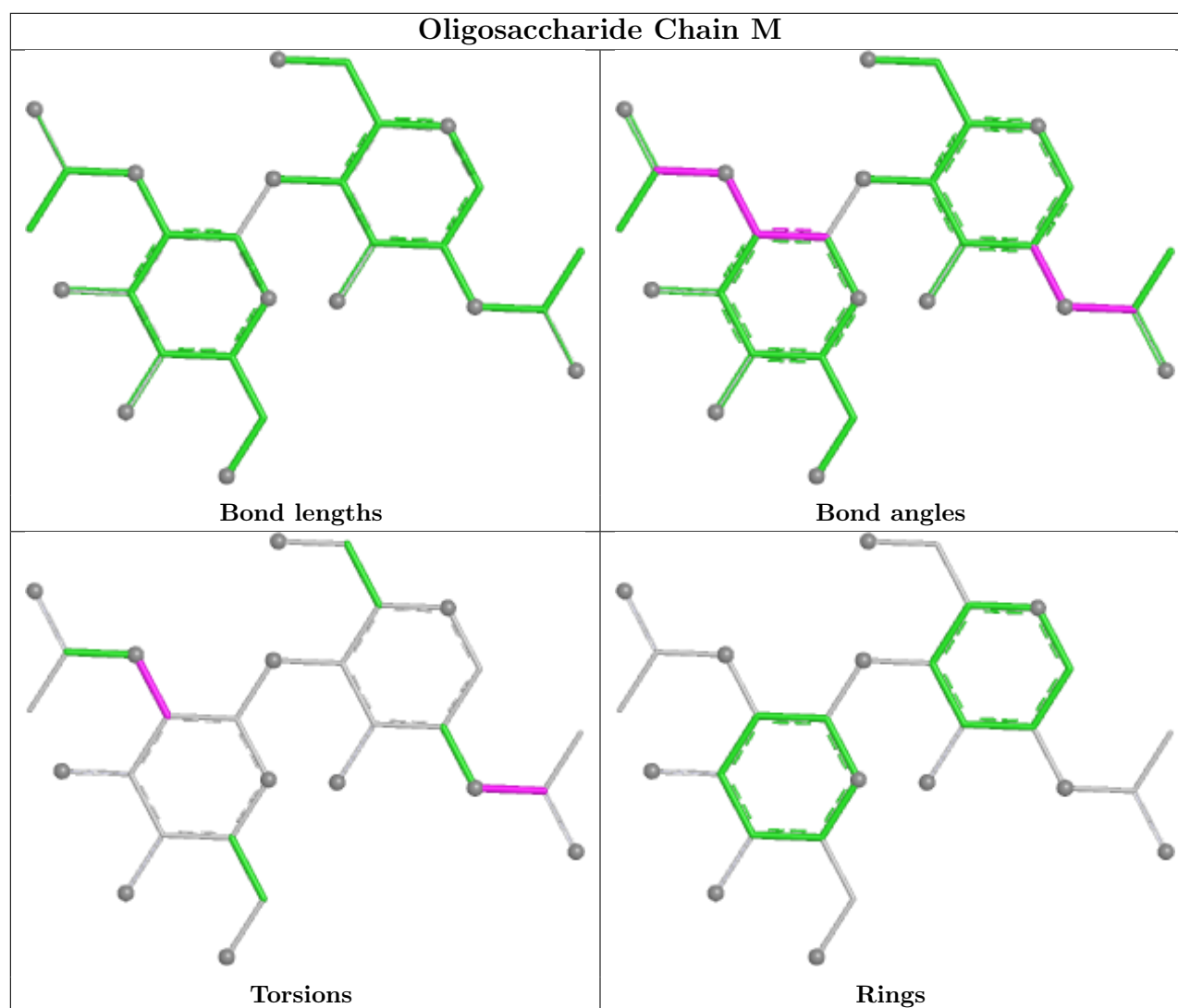












5.6 Ligand geometry [i](#)

23 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	$\# Z > 2$
4	NAG	A	4705	1	14,14,15	0.27	0	17,19,21	0.66	0
4	NAG	A	4709	1	14,14,15	0.27	0	17,19,21	0.69	0
4	NAG	B	4704	1	14,14,15	0.27	0	17,19,21	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	4703	1	14,14,15	0.28	0	17,19,21	0.66	0
4	NAG	A	4702	1	14,14,15	0.29	0	17,19,21	0.75	0
4	NAG	B	4709	1	14,14,15	0.28	0	17,19,21	0.64	0
4	NAG	A	4701	1	14,14,15	0.28	0	17,19,21	0.61	0
4	NAG	A	4711	1	14,14,15	0.38	0	17,19,21	0.50	0
4	NAG	B	4708	1	14,14,15	0.36	0	17,19,21	0.99	1 (5%)
4	NAG	B	4702	1	14,14,15	0.27	0	17,19,21	0.71	0
4	NAG	A	4704	1	14,14,15	0.28	0	17,19,21	0.60	0
4	NAG	B	4703	1	14,14,15	0.30	0	17,19,21	0.68	0
4	NAG	B	4705	1	14,14,15	0.28	0	17,19,21	0.61	0
4	NAG	B	4701	1	14,14,15	0.26	0	17,19,21	0.67	0
4	NAG	B	4710	1	14,14,15	0.28	0	17,19,21	0.64	0
4	NAG	A	4707	1	14,14,15	0.26	0	17,19,21	0.67	0
4	NAG	B	4711	1	14,14,15	0.38	0	17,19,21	0.48	0
4	NAG	A	4708	1	14,14,15	0.37	0	17,19,21	0.76	1 (5%)
4	NAG	B	4707	1	14,14,15	0.26	0	17,19,21	0.67	0
4	NAG	A	4710	1	14,14,15	0.26	0	17,19,21	0.52	0
4	NAG	A	4706	1	14,14,15	0.28	0	17,19,21	0.64	0
4	NAG	B	4706	1	14,14,15	0.27	0	17,19,21	0.67	0
4	NAG	A	4712	1	14,14,15	0.39	0	17,19,21	0.79	1 (5%)

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
4	NAG	A	4705	1	-	0/6/23/26	0/1/1/1
4	NAG	A	4709	1	-	2/6/23/26	0/1/1/1
4	NAG	B	4704	1	-	2/6/23/26	0/1/1/1
4	NAG	A	4703	1	-	3/6/23/26	0/1/1/1
4	NAG	A	4702	1	-	2/6/23/26	0/1/1/1
4	NAG	B	4709	1	-	0/6/23/26	0/1/1/1
4	NAG	A	4701	1	-	0/6/23/26	0/1/1/1
4	NAG	A	4711	1	-	0/6/23/26	0/1/1/1
4	NAG	B	4708	1	-	3/6/23/26	0/1/1/1
4	NAG	B	4702	1	-	2/6/23/26	0/1/1/1
4	NAG	A	4704	1	-	0/6/23/26	0/1/1/1
4	NAG	B	4703	1	-	2/6/23/26	0/1/1/1
4	NAG	B	4705	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	4701	1	-	0/6/23/26	0/1/1/1
4	NAG	B	4710	1	-	0/6/23/26	0/1/1/1
4	NAG	A	4707	1	-	3/6/23/26	0/1/1/1
4	NAG	B	4711	1	-	0/6/23/26	0/1/1/1
4	NAG	A	4708	1	-	1/6/23/26	0/1/1/1
4	NAG	B	4707	1	-	3/6/23/26	0/1/1/1
4	NAG	A	4710	1	-	3/6/23/26	0/1/1/1
4	NAG	A	4706	1	-	2/6/23/26	0/1/1/1
4	NAG	B	4706	1	-	0/6/23/26	0/1/1/1
4	NAG	A	4712	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	4708	NAG	C2-N2-C7	3.44	127.50	122.90
4	A	4712	NAG	C2-N2-C7	2.43	126.15	122.90
4	A	4708	NAG	C2-N2-C7	2.26	125.92	122.90

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	4707	NAG	C8-C7-N2-C2
4	A	4707	NAG	O7-C7-N2-C2
4	A	4710	NAG	C1-C2-N2-C7
4	A	4710	NAG	C8-C7-N2-C2
4	A	4710	NAG	O7-C7-N2-C2
4	B	4704	NAG	C8-C7-N2-C2
4	B	4704	NAG	O7-C7-N2-C2
4	B	4707	NAG	C3-C2-N2-C7
4	B	4707	NAG	C8-C7-N2-C2
4	B	4707	NAG	O7-C7-N2-C2
4	B	4708	NAG	C3-C2-N2-C7
4	B	4708	NAG	C8-C7-N2-C2
4	B	4708	NAG	O7-C7-N2-C2
4	A	4702	NAG	C8-C7-N2-C2
4	A	4702	NAG	O7-C7-N2-C2
4	B	4702	NAG	C8-C7-N2-C2
4	A	4706	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	B	4703	NAG	C8-C7-N2-C2
4	A	4703	NAG	C8-C7-N2-C2
4	A	4706	NAG	O7-C7-N2-C2
4	B	4702	NAG	O7-C7-N2-C2
4	B	4703	NAG	O7-C7-N2-C2
4	A	4703	NAG	O7-C7-N2-C2
4	A	4709	NAG	C8-C7-N2-C2
4	A	4707	NAG	C3-C2-N2-C7
4	A	4709	NAG	O7-C7-N2-C2
4	A	4708	NAG	C3-C2-N2-C7
4	A	4712	NAG	C3-C2-N2-C7
4	A	4703	NAG	C1-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	4702	NAG	1	0
4	B	4703	NAG	1	0
4	B	4701	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.

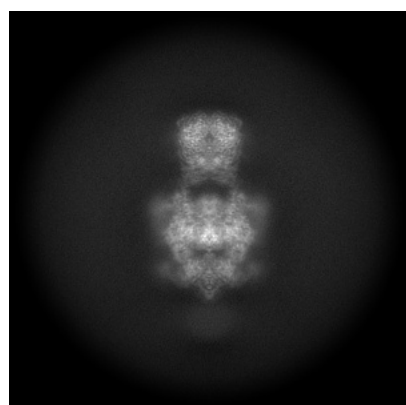
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45967. These allow visual inspection of the internal detail of the map and identification of artifacts.

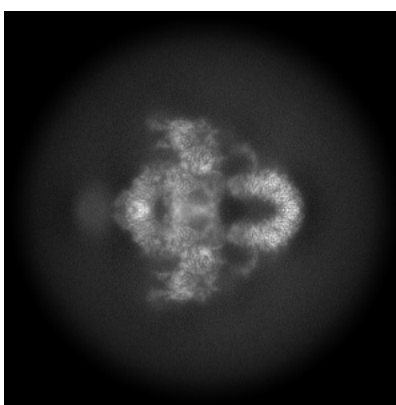
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

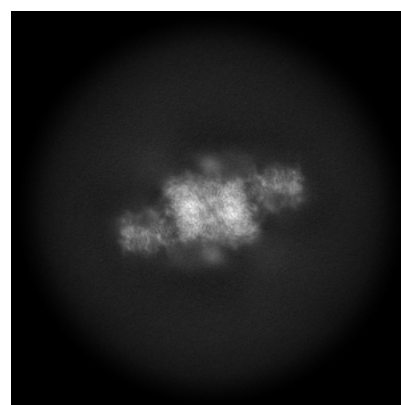
6.1.1 Primary map



X



Y

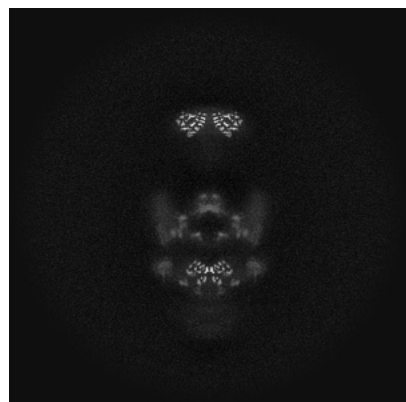


Z

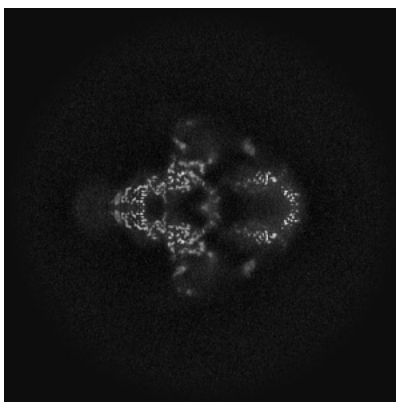
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

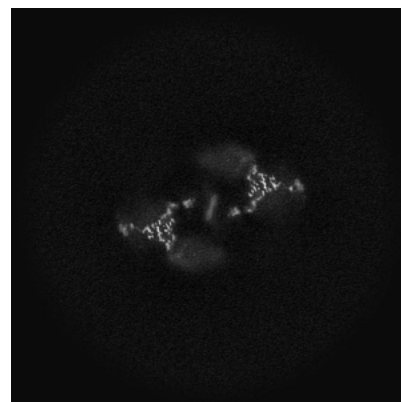
6.2.1 Primary map



X Index: 256



Y Index: 256

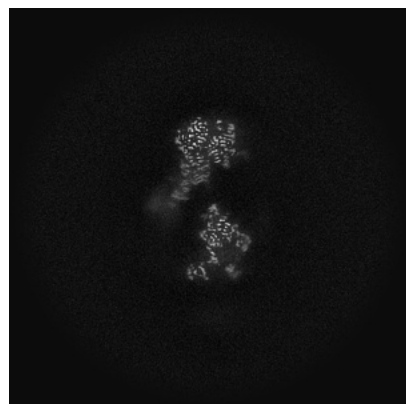


Z Index: 256

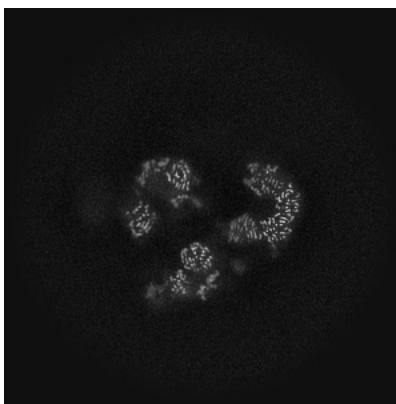
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

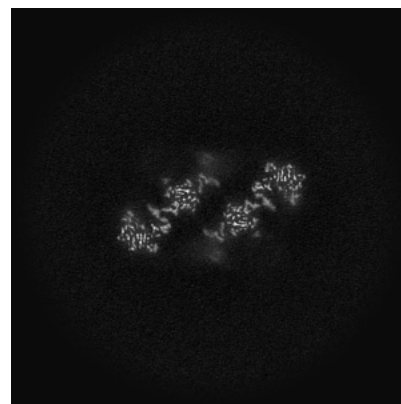
6.3.1 Primary map



X Index: 224



Y Index: 233

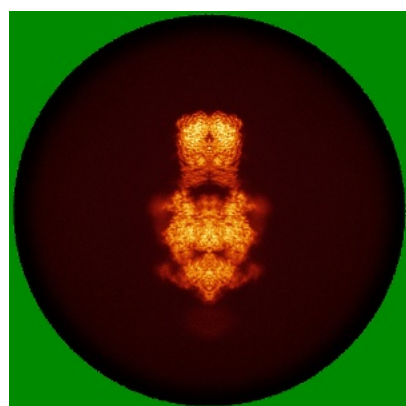


Z Index: 231

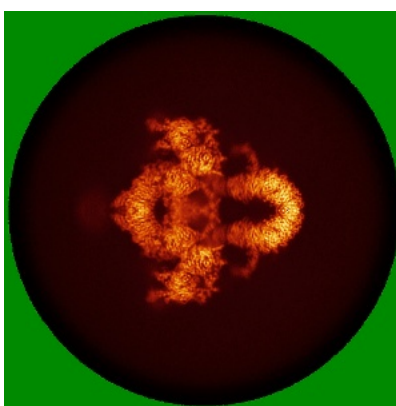
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

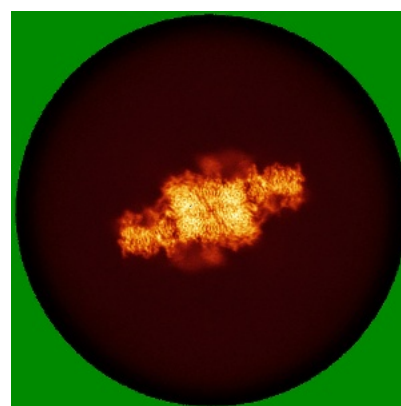
6.4.1 Primary map



X



Y

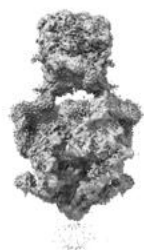


Z

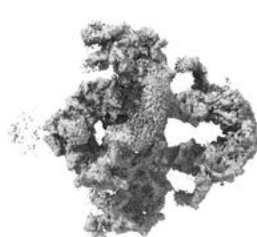
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

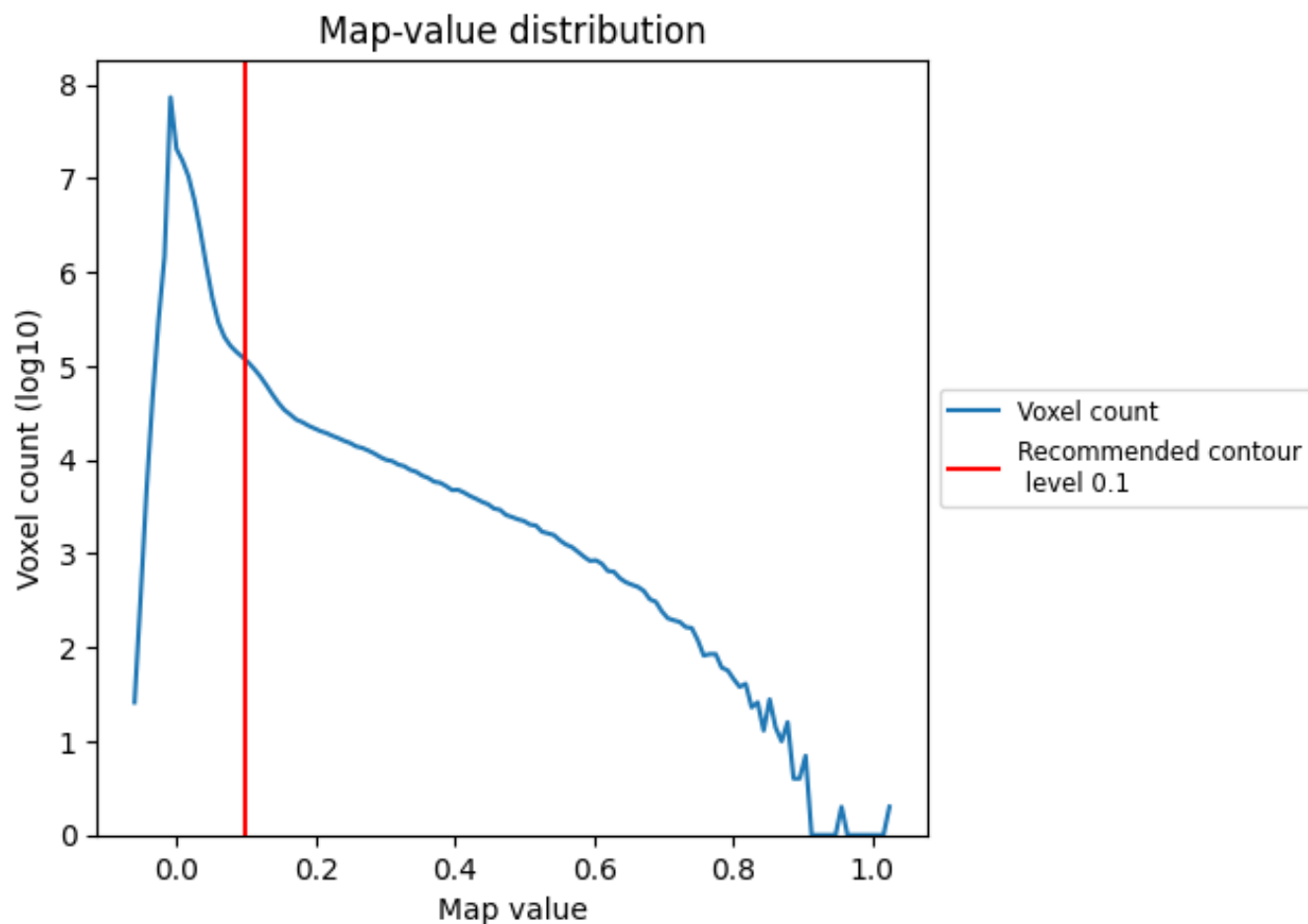
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

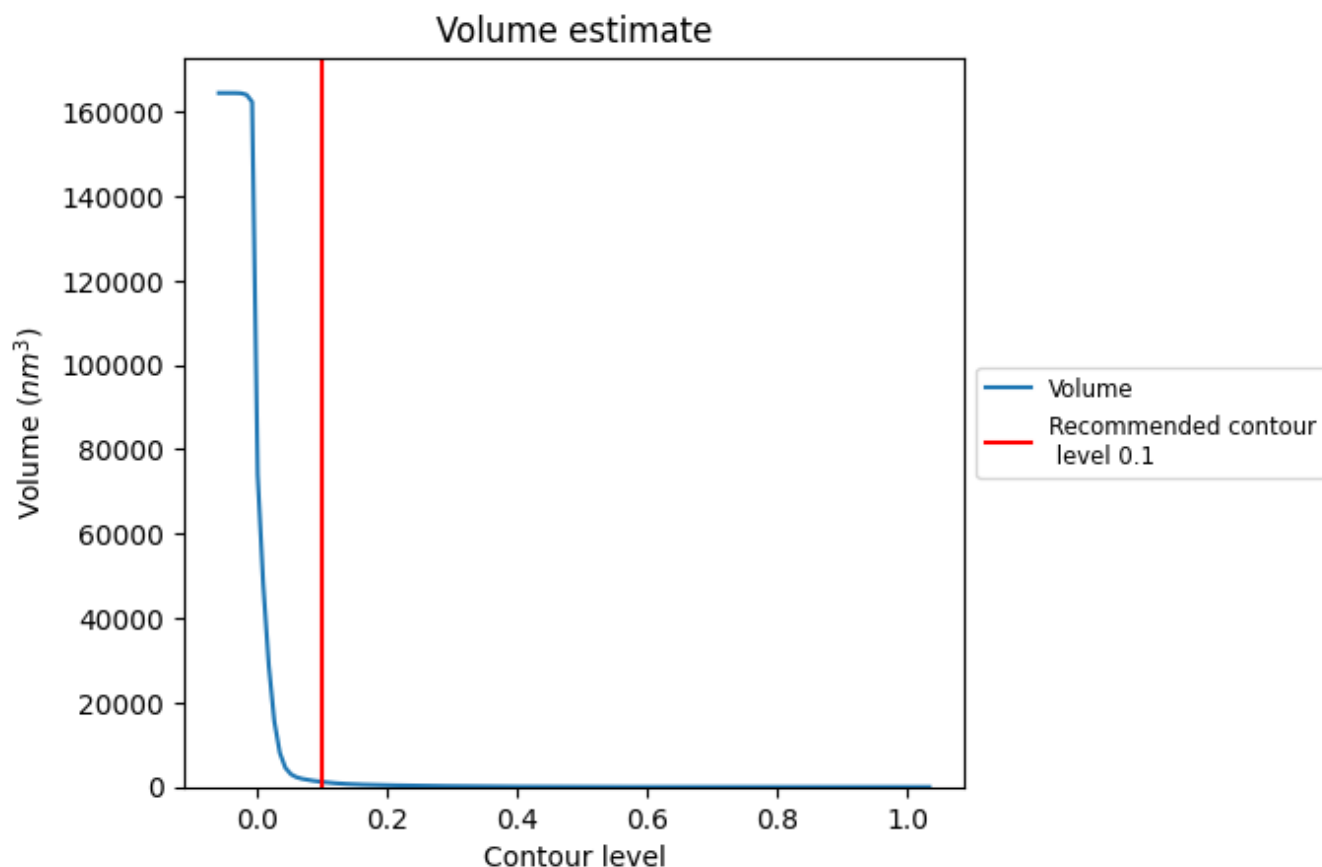
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

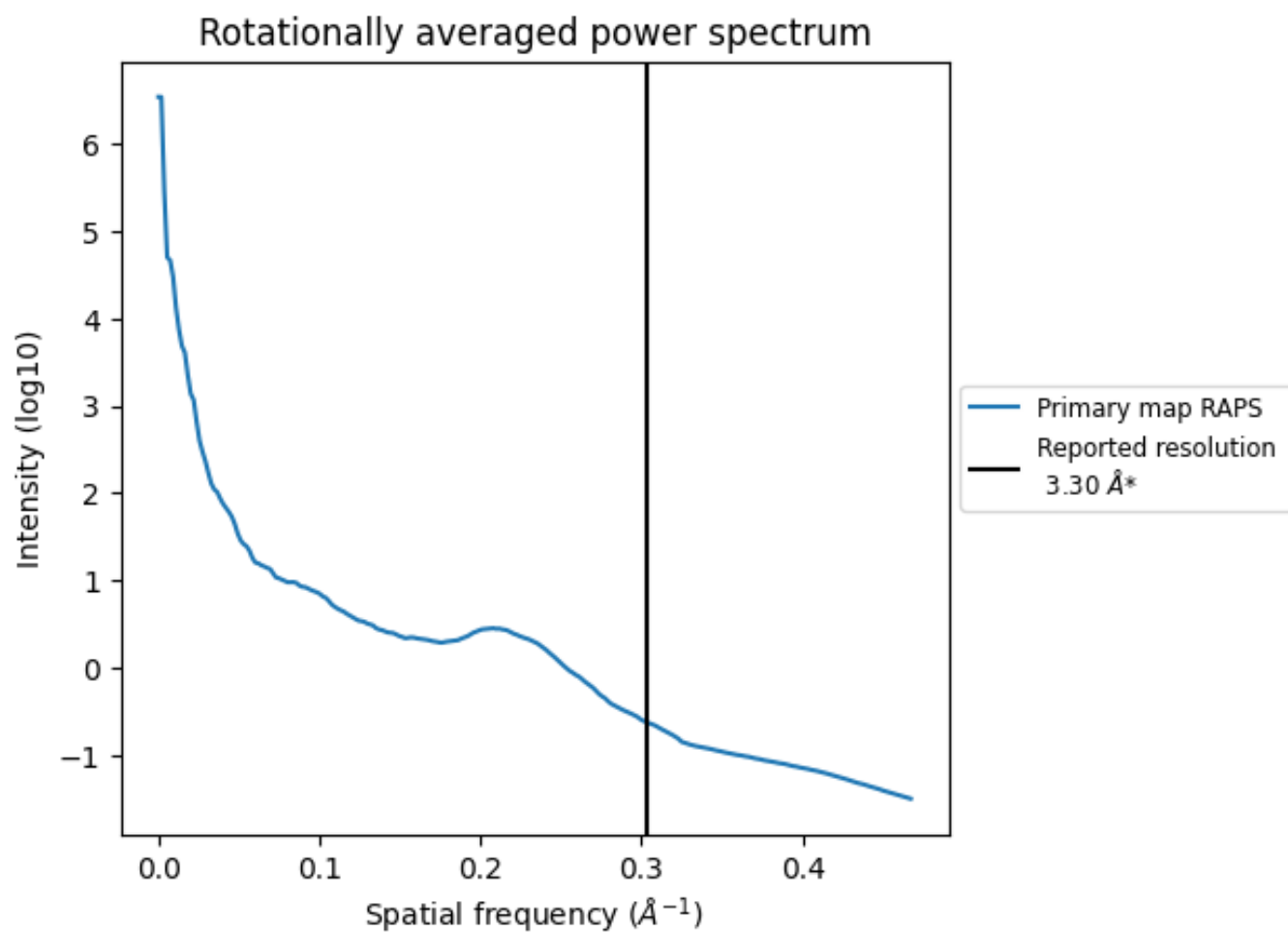
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1187 nm³; this corresponds to an approximate mass of 1072 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

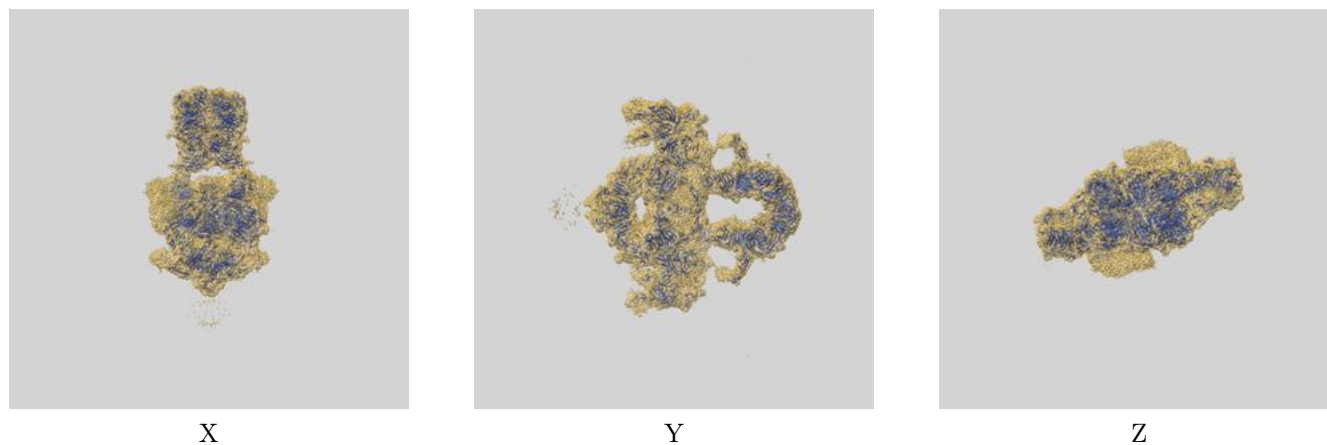
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

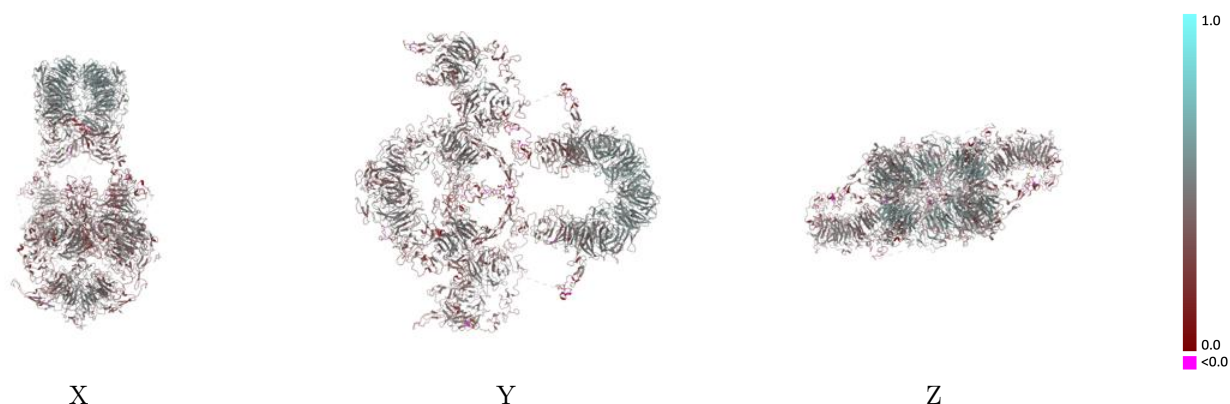
This section contains information regarding the fit between EMDB map EMD-45967 and PDB model 9CWM. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



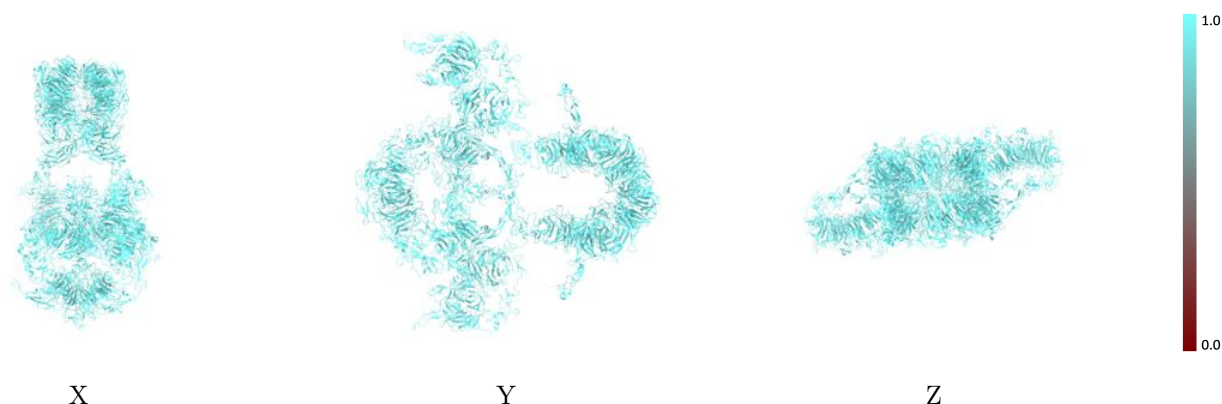
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



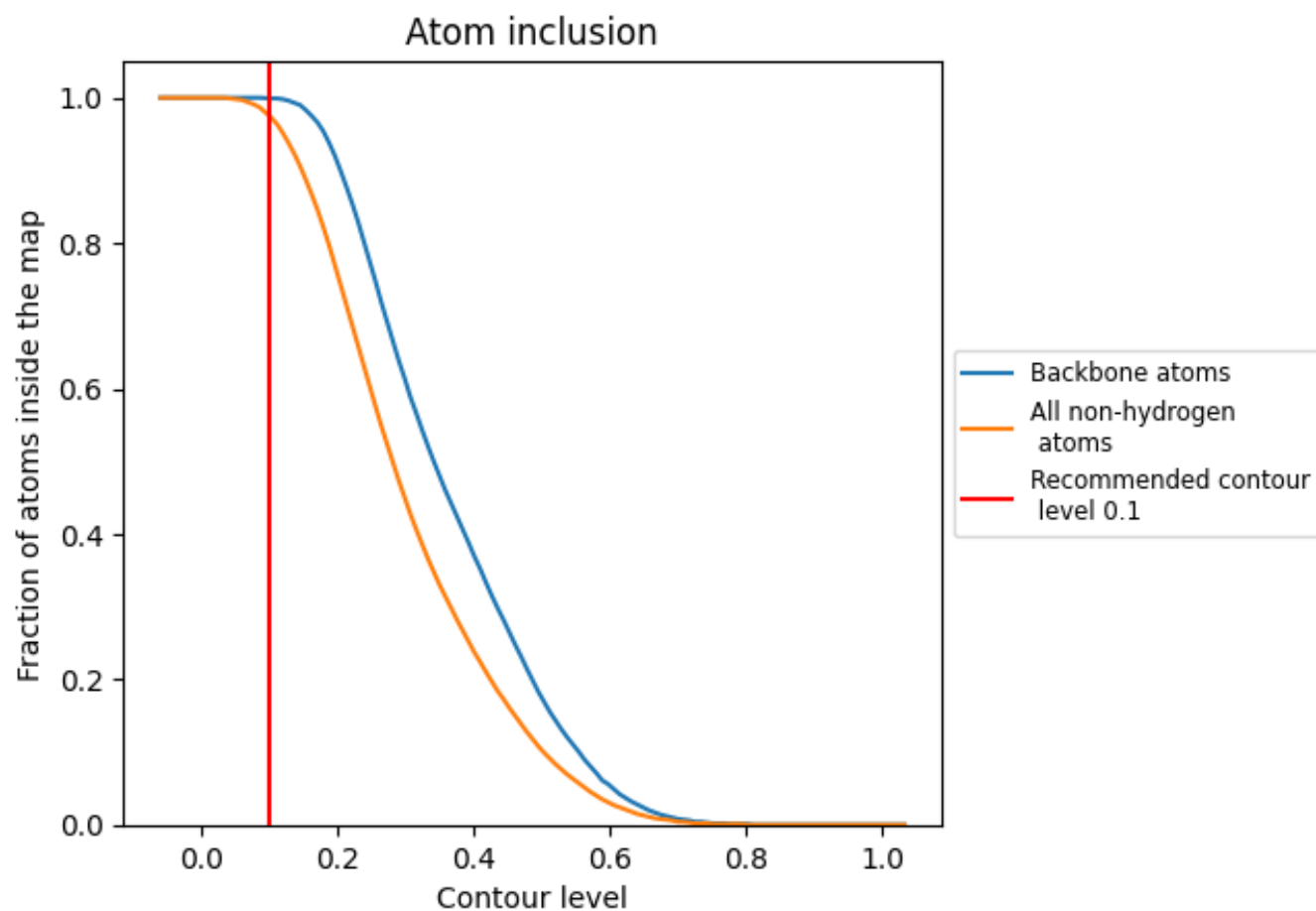
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).































9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 98% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9750	 0.4030
A	 0.9760	 0.4050
B	 0.9750	 0.4010
C	 0.9490	 0.4310
D	 0.9490	 0.3520
E	 1.0000	 0.4100
F	 0.8970	 0.1850
G	 0.8930	 0.3650
H	 1.0000	 0.4200
I	 0.9740	 0.4470
J	 0.9490	 0.3580
K	 1.0000	 0.4160
L	 0.8970	 0.2190
M	 0.9640	 0.3420
N	 0.8210	 0.1740

