



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 01:35 AM UTC

PDB ID : 7CAK / pdb_00007cak
EMDB ID : EMD-30333
Title : SARS-CoV-2 S trimer with three RBD in the open state and complexed with three H014 Fab
Authors : Zhe, L.; Cao, L.; Deng, Y.; Sun, Y.; Wang, N.; Xie, L.; Wang, Y.; Rao, Z.; Qin, C.; Wang, X.
Deposited on : 2020-06-08
Resolution : 3.58 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:

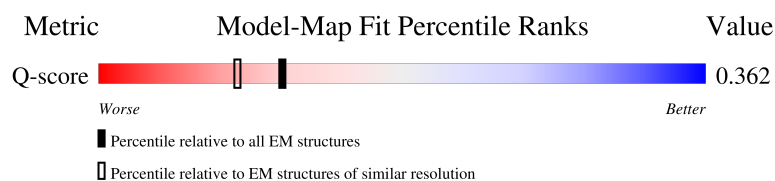
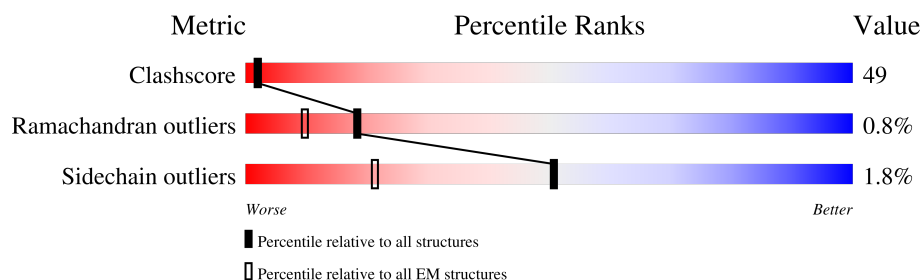
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.58 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	12629 (3.08 - 4.08)

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	1208	
1	B	1208	
1	C	1208	
2	D	210	

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Mol	Chain	Length	Quality of chain
2	F	210	
2	H	210	
3	E	223	
3	G	223	
3	I	223	
4	J	2	
4	K	2	
4	L	2	
4	M	2	
4	N	2	
4	O	2	
4	P	2	
4	Q	2	
4	R	2	
4	S	2	
4	T	2	
4	U	2	
4	V	2	
4	W	2	
4	X	2	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 30263 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1028	Total	C	N	O	S	0	0
			8029	5128	1336	1528	37		
1	B	1028	Total	C	N	O	S	0	0
			8033	5130	1337	1529	37		
1	C	1028	Total	C	N	O	S	0	0
			8033	5130	1337	1529	37		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	682	GLY	ARG	engineered mutation	UNP P0DTC2
A	683	SER	ARG	engineered mutation	UNP P0DTC2
A	685	SER	ARG	engineered mutation	UNP P0DTC2
A	835	MET	LYS	engineered mutation	UNP P0DTC2
A	844	MET	ILE	engineered mutation	UNP P0DTC2
A	846	TYR	ALA	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	682	GLY	ARG	engineered mutation	UNP P0DTC2
B	683	SER	ARG	engineered mutation	UNP P0DTC2
B	685	SER	ARG	engineered mutation	UNP P0DTC2
B	835	MET	LYS	engineered mutation	UNP P0DTC2
B	844	MET	ILE	engineered mutation	UNP P0DTC2
B	846	TYR	ALA	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	682	GLY	ARG	engineered mutation	UNP P0DTC2
C	683	SER	ARG	engineered mutation	UNP P0DTC2
C	685	SER	ARG	engineered mutation	UNP P0DTC2
C	835	MET	LYS	engineered mutation	UNP P0DTC2
C	844	MET	ILE	engineered mutation	UNP P0DTC2
C	846	TYR	ALA	engineered mutation	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2

- Molecule 2 is a protein called Light chain of H014 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	107	Total	C	N	O	S	0	0
			837	534	140	161	2		
2	F	107	Total	C	N	O	S	0	0
			837	534	140	161	2		
2	H	107	Total	C	N	O	S	0	0
			837	534	140	161	2		

- Molecule 3 is a protein called Heavy chain of H014 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	122	Total	C	N	O	S	0	0
			939	598	148	189	4		
3	G	122	Total	C	N	O	S	0	0
			939	598	148	189	4		
3	I	122	Total	C	N	O	S	0	0
			939	598	148	189	4		

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



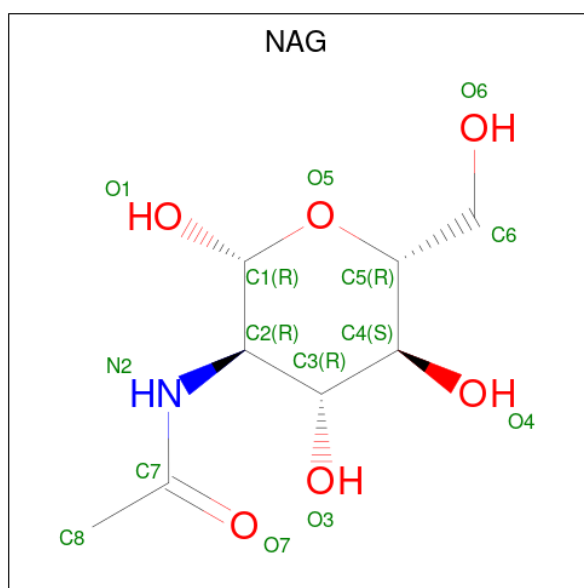
Mol	Chain	Residues	Atoms				AltConf	Trace
4	J	2	Total	C	N	O	0	0
			28	16	2	10		
4	K	2	Total	C	N	O	0	0
			28	16	2	10		
4	L	2	Total	C	N	O	0	0
			28	16	2	10		
4	M	2	Total	C	N	O	0	0
			28	16	2	10		
4	N	2	Total	C	N	O	0	0
			28	16	2	10		
4	O	2	Total	C	N	O	0	0
			28	16	2	10		
4	P	2	Total	C	N	O	0	0
			28	16	2	10		
4	Q	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				AltConf	Trace
4	R	2	Total	C	N	O	0	0
			28	16	2	10		
4	S	2	Total	C	N	O	0	0
			28	16	2	10		
4	T	2	Total	C	N	O	0	0
			28	16	2	10		
4	U	2	Total	C	N	O	0	0
			28	16	2	10		
4	V	2	Total	C	N	O	0	0
			28	16	2	10		
4	W	2	Total	C	N	O	0	0
			28	16	2	10		
4	X	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



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

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

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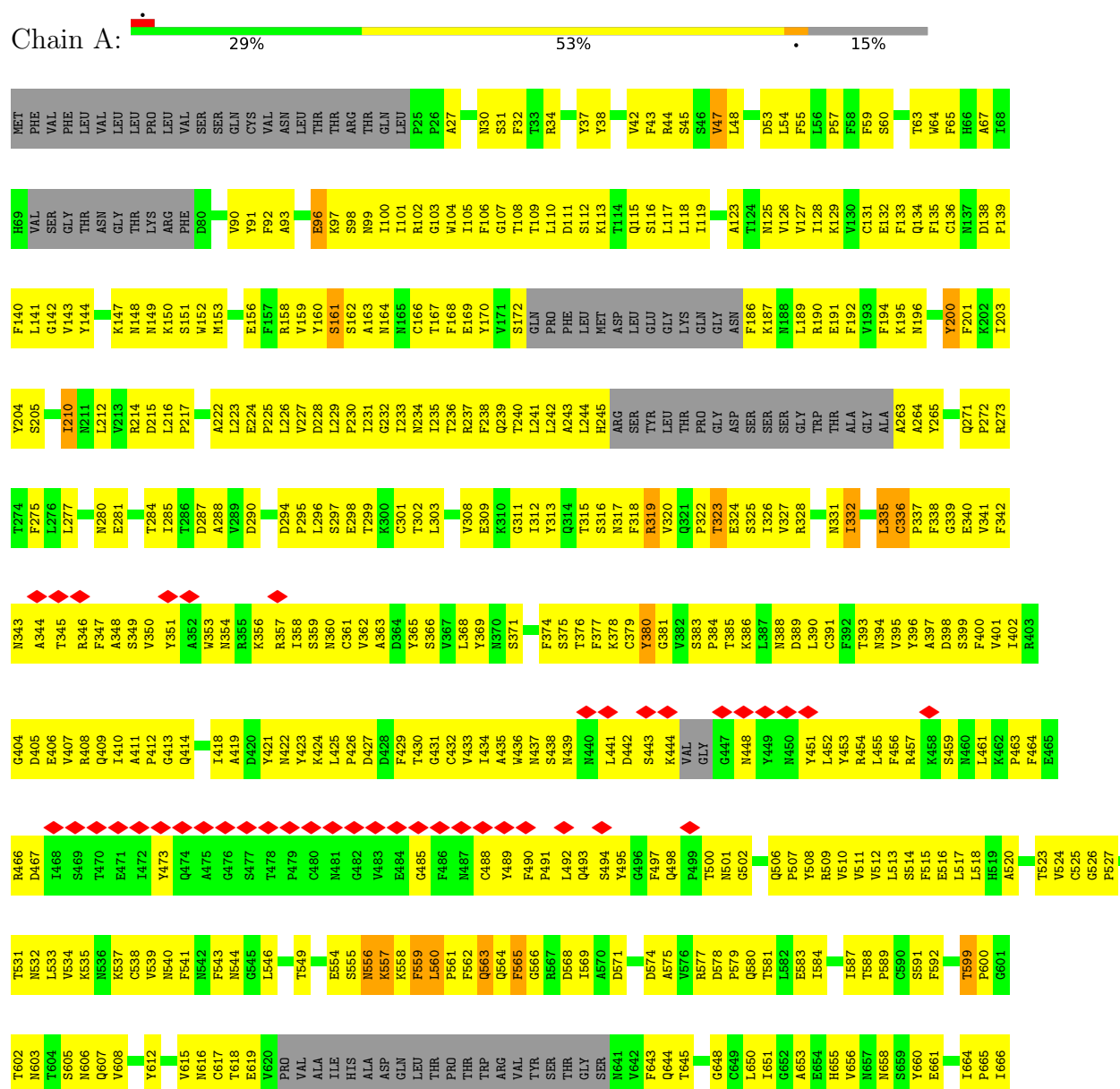
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Mol	Chain	Residues	Atoms				AltConf
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Spike glycoprotein



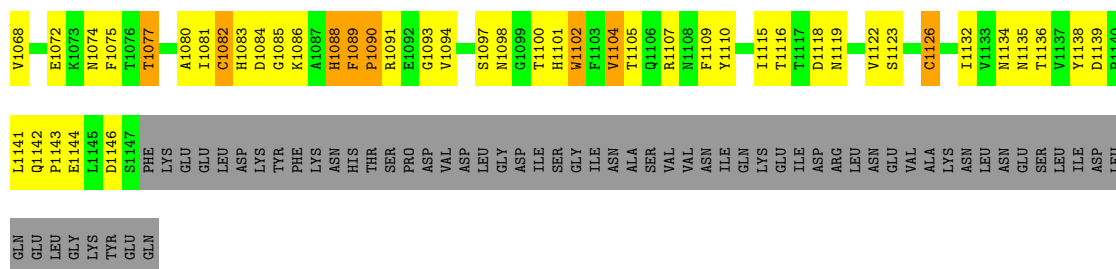
ASP	D1084	I1013	L945	L878	K814	M740	A868	T602	P527	F464	I402	F342
LYS	G1085	R1014	G946	A879	R815	T741	G669	S605	P531	E465	R403	N343
PHE	A1087	E1017	X947	G880	S816	I742	I670	S606	T531	R466	G404	A344
LYS	H1088	I1018	L948	T881	I818	C743	C671	N606	N532	D405	D405	T345
ASN	F1089	R1019	D950	T882	E819	G744	A672	Q607	L533	E406	V407	R346
HIS	P1090	A1020	V951	S884	D820	S746	Y674	Y612	V534	X408	Q409	F347
THR	R1091	S1021	Y952	G885	L821	T747	T675	Y615	K537	T470	I410	A348
SER	E1092	N1022	N953	W886	L822	E748	T676	N616	C538	E471	A411	S349
PRO	G1093	N1023	Q954	T887	F823	C749	THR	Y539	V539	I472	P412	V350
ASP	V1094	L1024	N955	F888	N824	S750	N617	N540	N540	Y473	G413	Y351
VAL	F1095	A1025	A956	G887	K825	N751	ASN	F541	F541	Q474	Q414	A352
ASP	V1096	A1026	Q957	G891	V826	L754	SER	T618	N642	A475	W353	W353
LEU	S1097	T1027	A958	A892	T827	L754	GLY	E619	F543	G476	K354	K354
GLN	K1098	M1028	L959	A893	LEU	S758	ALA	V620	N544	G476	K355	K355
CYS	G1099	M1029	N960	L894	ASP	F759	SER	VAL	L546	T478	D420	R357
ASP	T961	S1030	T961	P897	ALA	C760	SER	ALA	T549	P479	Y421	I358
ILE	H1101	V1033	L962	P898	GLY	T761	SER	ILE	S555	C480	N422	S359
GLY	W1102	L1034	V963	A899	PHE	Q762	VAL	HIS	K557	N481	Y423	N360
ILE	F1103	L1034	X964	M900	ILE	L763	ALA	ALA	N556	L425	K424	C361
ASN	V1104	K1038	Q965	Q901	GLN	N764	S889	ASP	K557	G482	P426	V362
ALA	T1105	K1038	L966	M902	GLN	R765	Q690	LEU	K558	V483	D427	A363
SER	Q1106	K1038	L966	Y904	TYR	A766	Y695	THR	L560	E484	D428	D364
VAL	R1107	G1043	F970	Y904	GLY	L767	T866	PRO	P561	G485	F429	Y365
VAL	N1108	G1044	L977	R905	ASP	T768	M697	THR	F562	G485	T430	S366
ASN	F1109	K1045	N978	R906	CYS	I770	T697	THR	Q563	V367	G431	L368
ILE	Y1047	G1046	N978	N907	LEU	I770	T697	THR	Q563	Y369	C432	Y369
LYS	T1115	H1048	L981	G908	GLY	A771	E702	ARG	Q564	N487	V433	C370
GLU	T1116	L1049	S982	I909	ASP	V772	N703	VAL	Q564	C488	I434	S371
ILE	T1117	M1050	R983	G910	MET	E773	S704	TYR	F565	C488	A435	A372
ASP	D1118	S1051	L984	Y911	ALA	Q774	Y707	SER	G566	Y489	W436	S373
ARG	N1119	Q1055	D985	T912	TYR	D775	THR	THR	R567	F490	M437	F374
LEU	Q1056	S1055	P987	Q913	ARG	K776	S708	GLY	I569	P491	S438	S375
ASN	A1056	P1057	E988	N914	ASP	N777	N709	SER	A570	L492	M439	F377
GLU	S1123	P1057	L989	V915	L849	T778	I712	N641	D571	Q493	M440	T376
VAL	G1126	V1060	E990	L916	I850	K786	I712	V642	D574	S494	L441	K378
ALA	L1132	V1061	Y991	Y917	K854	Q787	I714	F643	A575	S494	D442	C379
LYS	I1132	V1061	Q992	N919	P855	T791	N717	Q644	D575	G496	L441	Y380
ASN	V1133	L1064	D994	Q920	N856	T792	T719	T645	V576	F497	S443	G381
ASN	N1134	H1065	D994	I923	G857	T792	T719	G648	D578	Q498	K444	V382
GLU	N1135	V1065	D994	A924	L858	D796	I720	C649	P579	P499	VAL	S383
SER	T1136	T1066	R995	N925	T859	F797	S721	L850	Q580	T500	GLY	T385
SER	V1137	Y1067	L997	Q926	V860	F797	S721	I851	T581	N501	G447	K386
ILE	Y1138	V1068	T998	F927	V860	F797	S721	G852	L582	G502	M448	L387
ASP	D1139	P1069	G999	Q926	L864	F800	N801	E854	T581	G502	Y449	N388
LEU	P1140	A1070	R1000	F927	L865	N801	N801	E854	L584	Q506	M450	D389
LEU	L1141	Q1071	L1001	Q926	T866	F802	N801	E854	I584	P507	N451	L390
GLN	Q1142	E1072	Q1002	G932	D867	S803	N801	E854	I584	Q506	N451	C391
LEU	P1143	K1073	S1003	G932	E868	Q804	N801	E854	I584	Q506	N451	C391
GLY	E1144	N1074	L1004	Q935	M869	L805	N801	E854	I584	Q506	N451	C391
LYS	F1075	F1075	Q1005	D936	I870	L806	N801	E854	I584	Q506	N451	C391
TYR	T1076	T1076	Q1005	D936	A871	P807	N801	E854	I584	Q506	N451	C391
GLU	T1077	T1077	Y1007	L938	Q872	D808	N801	E854	I584	Q506	N451	C391
GLN	PHE	A1080	T1008	T941	T874	S810	N801	E854	I584	Q506	N451	C391
	LYS	L1081	T1009	A942	S875	K811	N801	E854	I584	Q506	N451	C391
	GLU	C1082	Q1010	S943	A875	P812	N801	E854	I584	Q506	N451	C391
	LEU	H1083	L1012	A944	L877	S813	N801	E854	I584	Q506	N451	C391

• Molecule 1: Spike glycoprotein

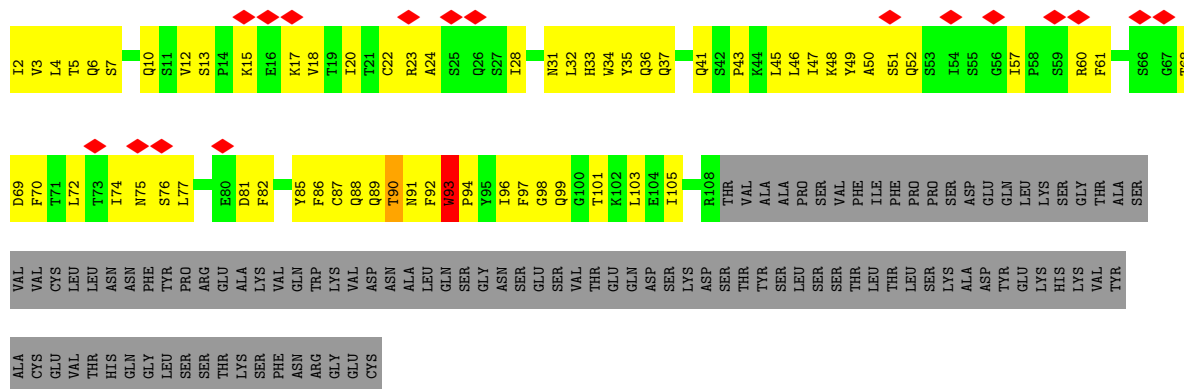
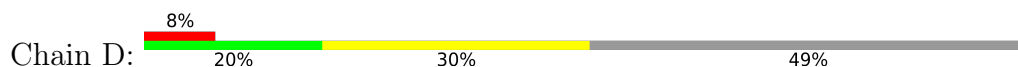
Chain C:  29% 53% 15%

MET	P25	P26	A27	N30	S31	F32	F33	R34	Y37	Y38	K41	F43	R44	S45	S46	V47	L48	D53	L54	F55	F56	F57	F58	F59	S60	T63	M64	F65	H66	A67
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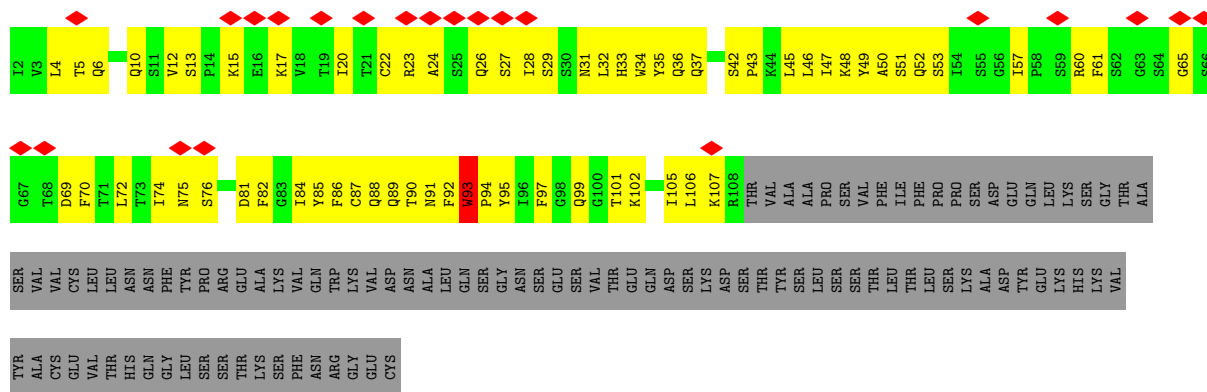
L986	L997	T998	G999	L1000	L1001	K1002	S1003	L1004	T1005	T1006	L1007	L1008	T1009	L1010	L1011	L1012	L1013	L1014	L1015	L1016	L1017	L1018	L1019	L1020	S1021	L1022	L1023	L1024	L1025	L1026	L1027	L1028	L1029	S1030	L1033	L1034	K1038	C1043	L1044	L1045	G1046	L1047	H1048	L1049	M1050	S1051	Q1054	L1060	V1061	H1064	V1065	L1066	Y1067							
N928	S929	A930	D931	G932	K933	L934	Q935	D936	L937	L938	T941	A942	S943	A944	L945	G946	K947	L948	L949	Q949	D950	L951	V952	N953	Q954	N955	A956	Q957	L958	A959	L959	N960	T961	L962	K963	K964	Q965	L966	F970	L977	N978	D979	L980	L981	S982	R983	L984	D985	P986	E987	E988	E989	E990	V991	I992	Q993	N994	Q995	D996	R995
L865	T866	D867	E868	M869	L870	A871	Q872	L873	T874	S875	A876	L877	L878	A879	G880	L881	T882	T883	S884	G885	W886	T887	F888	G891	A892	A893	L894	P897	F898	A899	M900	Q901	M902	A903	Y904	R905	P906	N907	G908	L909	V911	T912	Q913	N914	V915	L916	Y917	F918	N919	Q920	I923	A924	N925	F926	F927					
Q804	I805	L806	P807	D808	P809	S810	K811	P812	T813	S814	R815	S816	F817	I818	E819	D820	L821	L822	F823	M824	K825	W826	T827	LEU	ALA	ASP	ALA	GLY	PHE	ILE	MET	GLN	TYR	GLY	ASP	CYS	LEU	GLY	ASP	MET	ALA	TYR	ARG	ASP	L849	I850	C851	A852	Q853	K854	F855	N856	G857	L858	T859	V860	L861	L864		
L726	V729	S730	M731	T732	K733	P734	D735	T736	L737	T738	T739	M740	L741	L742	G743	G744	S745	L746	T747	E748	C749	N750	N751	L754	S758	F759	C760	T761	L762	L763	N764	R765	A766	L767	T768	G769	I770	A771	E772	E773	L774	D775	K776	N777	T778	K779	Q780	T781	P782	D796	F800	N801	F802	S803						
Q804	I805	L806	P807	D808	P809	S810	K811	P812	T813	S814	R815	S816	F817	I818	E819	D820	L821	L822	F823	M824	K825	W826	T827	LEU	ALA	ASP	ALA	GLY	PHE	ILE	MET	GLN	TYR	GLY	ASP	CYS	LEU	GLY	ASP	MET	ALA	TYR	ARG	ASP	L849	I850	C851	A852	Q853	K854	F855	N856	G857	L858	T859	V860	L861	L864		
L865	T866	D867	E868	M869	L870	A871	Q872	L873	T874	S875	A876	L877	L878	A879	G880	L881	T882	T883	S884	G885	W886	T887	F888	G891	A892	A893	L894	P897	F898	A899	M900	Q901	M902	A903	Y904	R905	P906	N907	G908	L909	V911	T912	Q913	N914	V915	L916	Y917	F918	N919	Q920	I923	A924	N925	F926	F927					
N928	S929	A930	D931	G932	K933	L934	Q935	D936	L937	L938	T941	A942	S943	A944	L945	G946	K947	L948	L949	Q949	D950	L951	V952	N953	Q954	N955	A956	Q957	L958	A959	L959	N960	T961	L962	K963	K964	Q965	L966	F970	L977	N978	D979	L980	L981	S982	R983	L984	D985	P986	E987	E988	E989	E990	V991	I992	Q993	N994	Q995	D996	R995
I68	H69	VAL	SER	GLY	THR	ASN	GLY	THR	LYS	ARG	PHE	D80	V90	Y91	F92	A93	E96	K97	S98	N99	I100	I101	R102	G103	W104	E105	F106	Y107	G108	T109	GLN	PRO	PHE	LEU	MET	ASP	LEU	GLU	GLY	LYS	GLN	GLY	ASN	F186	K187	N188	L189	R190	E191	F192	V193	E194	K195	Q196	F197	N198	Y200	F201	K202	
P139	F140	L141	G142	F143	Y144	K147	N148	L149	K150	ARG	S151	P152	M153	E156	F157	R158	V159	Y160	S161	A162	G163	N164	M165	C166	T167	F168	E169	Y170	V171	GLN	PRO	PHE	LEU	MET	ASP	LEU	GLU	GLY	LYS	GLN	GLY	ASN	F186	K187	N188	L189	R190	E191	F192	V193	E194	K195	Q196	F197	N198	Y200	F201	K202		
I203	Y204	S205	K206	I210	K211	L212	V213	R214	D215	L216	P217	A222	L223	E224	P225	L226	V227	D228	L229	P230	G231	G232	C233	I234	N235	L236	T237	F238	Q239	T240	L241	L242	A243	L244	H245	ARG	SER	TYR	LEU	THR	PRO	GLY	ASP	SER	SER	SER	GLY	THR	ALA	ALA	A263	A264	Y265	Q271						
P272	R273	T274	G275	L276	F277	K278	Y279	N280	E281	T284	L285	F286	D287	A288	V289	D290	D294	P295	L296	S297	E298	S299	N300	C301	T302	L303	K304	S305	F306	T307	V308	E309	K310	G311	L312	Y313	T315	S316	N317	F318	R319	V320	P322	T323	E324	S325	L326	D327	R328	N331	I332	L335	C336	D398						
P337	F338	G339	E340	F341	F342	N343	A344	T345	R346	F347	A348	S349	V350	Y351	A352	W353	N354	R355	K356	L358	S359	N360	C361	V362	A363	D364	S365	V367	L368	Y369	K370	S371	F374	S375	T376	F377	K378	C379	Y380	G381	V382	S383	L387	N388	D389	L390	C391	F392	T393	N394	V395	Y396	A397	D398						
S399	F400	V401	I402	R403	E405	D406	A406	V407	R408	Q409	I410	A411	P412	G413	Q414	I418	A419	D420	Y421	N422	Y423	K424	L425	P426	D427	D428	F429	T430	G431	C432	V433	I434	A435	W436	N437	S438	N439	N440	L441	D442	S443	K444	VAL	GLY	G447	N448	N450	Y451	Y453	R454	L455	F456	R457	K458	S459	N460				
L461	K462	P463	F464	E465	R466	D467	I468	S469	T470	E471	I472	A473	Q474	A475	G476	T477	S478	P479	C480	M481	G482	V483	E484	G485	F486	M487	C488	Y489	F490	P491	L492	Q493	S494	Y495	G496	F497	Q498	P499	T500	N501	G502	V503	Q506	P507	Y508	V510	R511	V512	L513	S514	F515	L517	H519	A520						
T523	V524	C525	G526	P527	K528	T531	N532	L533	V534	K535	M536	K537	C538	V539	F541	N542	F543	N544	G545	L546	T549	E554	S555	N556	K557	K558	F559	L560	P561	Q562	Q563	Q564	F565	G566	D567	D568	I569	A570	D571	D574	A575	V576	R577	D578	P579	Q580	L582	E583	I584	I587	T588	P589								
C590	S591	F592	G593	G594	V595	T599	P600	G601	T602	S605	N606	Q607	V608	Y612	V615	N616	C617	T618	E619	PRO	VAL	ALA	ILE	HIS	ALA	ASP	GLN	LEU	THR	PRO	THR	TRP	ARG	VAL	TYR	SER	THR	GLY	SER	N641	V642	F643	Q644	T645	G648	C649	L650	I651	G652	A653	E654	V656								
M657	M658	S659	V660	E661	I664	P665	L666	G667	A668	G669	I670	C671	A672	Y674	Q675	T676	GLN	THR	ASN	SER	PRO	GLY	SER	ALA	SER	VAL	ALA	ASP	GLN	LEU	THR	THR	ARG	VAL	TYR	SER	THR	GLY	SER	N641	V642	F643	Q644	T645	G648	C649	L650	I651	G652	A653	E654	V656								
L726	V729	S730	M731	T732	K733	P734	D735	T736	L737	T738	T739	M740	L741	L742	G743	G744	S745	L746	T747	E748	C749	N750	N751	L754	S758	F759	C760	T761	L762	L763	N764	R765	A766	L767	T768	G769	I770	A771	E772	E773	L774	D775	K776	N777	T778	K779	Q780	T781	P782	D796	F800	N801	F802	S803						
Q804	I805	L806	P807	D808	P809	S810	K811	P812	T813	S814	R815	S816	F817	I818	E819	D820	L821	L822	F823	M824	K825	W826	T827	LEU	ALA	ASP	ALA	GLY	PHE	ILE	MET	GLN	TYR	GLY	ASP	CYS	LEU	GLY	ASP	MET	ALA	TYR	ARG	ASP	L849	I850	C851	A852	Q853	K854	F855	N856	G857	L858	T859	V860	L861	L864		
L865	T866	D867	E868	M869	L870	A871	Q872	L873	T874	S875	A876	L877	L878	A879	G880	L881	T882	T883	S884	G885	W886	T887	F888	G891	A892	A893	L894	P897	F898	A899	M900	Q901	M902	A903	Y904	R905	P906	N907	G908	L909	V911	T912	Q913	N914	V915	L916	Y917	F918	N919	Q920	I923	A924	N925	F926	F927					
N928	S929	A930	D931	G932	K933	L934	Q935	D936	L937	L938	T941	A942	S943	A944	L945	G946	K947	L948	L949	Q949	D950	L951	V952	N953	Q954	N955	A956	Q957	L958	A959	L959	N960	T961	L962	K963	K964	Q965	L966	F970	L977	N978	D979	L980	L981	S982	R983	L984	D985	P986	E987	E988	E989	E990	V991	I992	Q993	N994	Q995	D996	R995



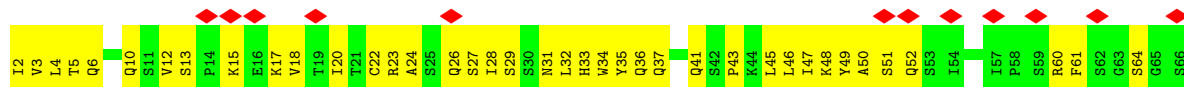
• Molecule 2: Light chain of H014 Fab



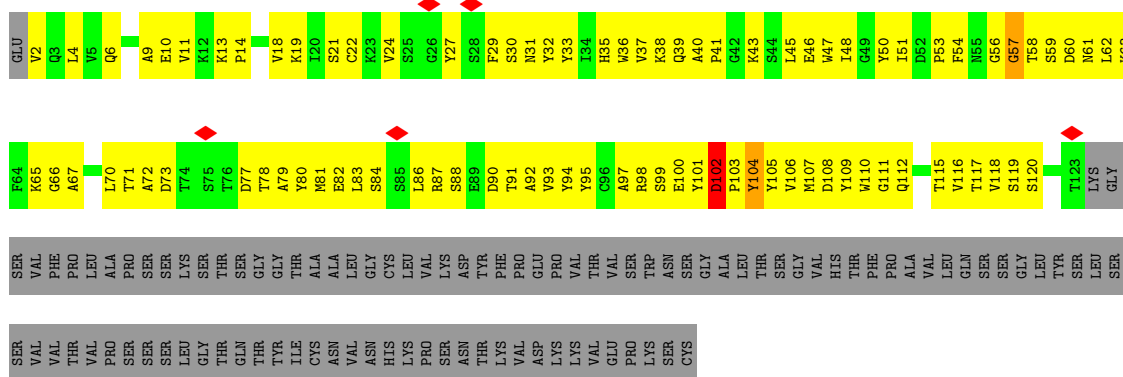
• Molecule 2: Light chain of H014 Fab



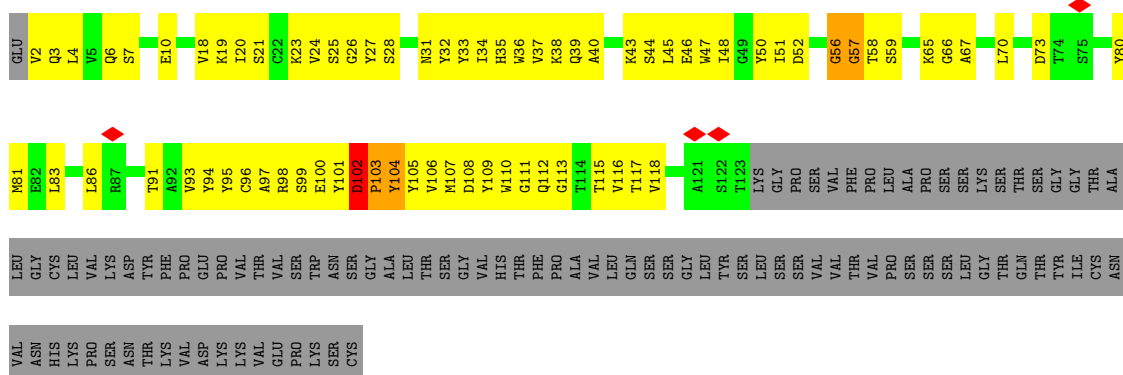
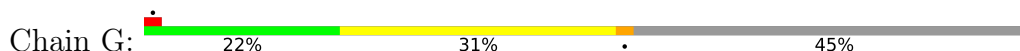
• Molecule 2: Light chain of H014 Fab



- Molecule 3: Heavy chain of H014 Fab

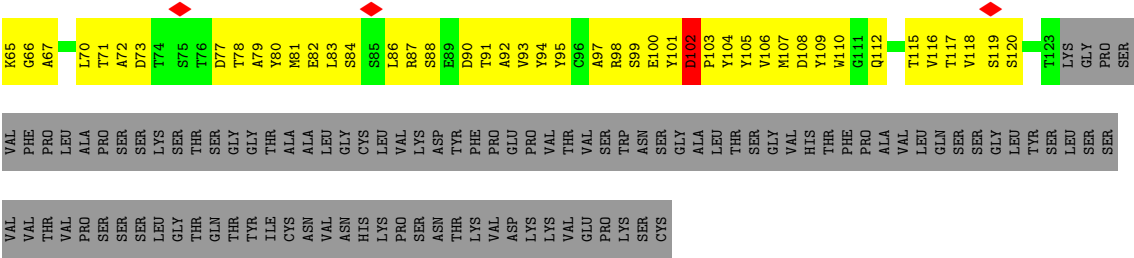


- Molecule 3: Heavy chain of H014 Fab



- Molecule 3: Heavy chain of H014 Fab





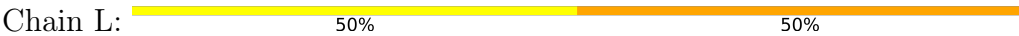
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



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



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



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



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



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



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



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



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



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



MAG1
MAG2

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

Chain V:  50% 50%

MAG1
MAG2

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

Chain W:  50% 50%

MAG1
MAG2

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

Chain X:  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	110970	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.084	Depositor
Minimum map value	-0.035	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0045	Depositor
Map size ($\text{\AA}$)	416.0, 416.0, 416.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.04, 1.04, 1.04	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.36	8/8214 (0.1%)	1.02	20/11179 (0.2%)
1	B	1.36	9/8218 (0.1%)	1.02	20/11184 (0.2%)
1	C	1.36	9/8218 (0.1%)	1.02	20/11184 (0.2%)
2	D	0.32	0/857	0.73	2/1160 (0.2%)
2	F	0.35	0/857	0.79	0/1160
2	H	0.32	0/857	0.73	2/1160 (0.2%)
3	E	0.37	0/963	0.67	0/1311
3	G	0.38	0/963	0.65	0/1311
3	I	0.36	0/963	0.67	0/1311
All	All	1.24	26/30110 (0.1%)	0.97	64/40960 (0.2%)

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	7
1	B	0	6
1	C	0	7
2	D	0	1
2	F	0	1
2	H	0	1
3	G	0	2
3	I	0	1
All	All	0	26

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	335	LEU	C-N	10.12	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	335	LEU	C-N	10.05	1.46	1.33
1	B	335	LEU	C-N	10.02	1.46	1.33
1	C	336	CYS	C-N	7.22	1.50	1.33
1	A	336	CYS	C-N	7.20	1.50	1.33
1	B	336	CYS	C-N	7.20	1.50	1.33
1	B	901	GLN	CB-CG	-6.08	1.34	1.52
1	A	901	GLN	CB-CG	-6.06	1.34	1.52
1	C	901	GLN	CB-CG	-6.06	1.34	1.52
1	A	1060	VAL	CB-CG1	-5.81	1.33	1.52
1	C	1060	VAL	CB-CG1	-5.79	1.33	1.52
1	B	1060	VAL	CB-CG1	-5.77	1.33	1.52
1	C	729	VAL	CB-CG1	-5.39	1.34	1.52
1	A	729	VAL	CB-CG1	-5.37	1.34	1.52
1	B	729	VAL	CB-CG1	-5.36	1.34	1.52
1	C	866	THR	CA-CB	-5.35	1.45	1.53
1	B	907	ASN	CB-CG	-5.32	1.38	1.52
1	A	907	ASN	CB-CG	-5.31	1.38	1.52
1	C	907	ASN	CB-CG	-5.29	1.38	1.52
1	C	898	PHE	CB-CG	-5.26	1.38	1.50
1	B	898	PHE	CB-CG	-5.25	1.38	1.50
1	A	898	PHE	CB-CG	-5.23	1.38	1.50
1	B	1102	TRP	CB-CG	-5.13	1.34	1.50
1	A	1102	TRP	CB-CG	-5.12	1.34	1.50
1	C	1102	TRP	CB-CG	-5.10	1.34	1.50
1	B	948	LEU	CG-CD1	-5.00	1.36	1.52

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	733	LYS	CA-C-N	-7.29	108.74	122.73
1	A	733	LYS	C-N-CA	-7.29	108.74	122.73
1	C	733	LYS	CA-C-N	-7.26	108.79	122.73
1	C	733	LYS	C-N-CA	-7.26	108.79	122.73
1	B	733	LYS	CA-C-N	-7.25	108.80	122.73
1	B	733	LYS	C-N-CA	-7.25	108.80	122.73
1	A	1088	HIS	CA-C-N	-6.83	110.05	123.56
1	A	1088	HIS	C-N-CA	-6.83	110.05	123.56
1	B	1088	HIS	CA-C-N	-6.82	110.06	123.56
1	B	1088	HIS	C-N-CA	-6.82	110.06	123.56
1	C	1088	HIS	CA-C-N	-6.80	110.09	123.56
1	C	1088	HIS	C-N-CA	-6.80	110.09	123.56
1	B	720	ILE	CA-C-N	-6.52	110.64	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	720	ILE	C-N-CA	-6.52	110.64	122.12
1	A	720	ILE	CA-C-N	-6.50	110.69	122.12
1	A	720	ILE	C-N-CA	-6.50	110.69	122.12
1	C	720	ILE	CA-C-N	-6.46	110.75	122.12
1	C	720	ILE	C-N-CA	-6.46	110.75	122.12
1	A	887	THR	CA-C-N	-5.76	110.42	121.94
1	A	887	THR	C-N-CA	-5.76	110.42	121.94
1	B	887	THR	CA-C-N	-5.74	110.45	121.94
1	B	887	THR	C-N-CA	-5.74	110.45	121.94
1	C	887	THR	CA-C-N	-5.74	110.46	121.94
1	C	887	THR	C-N-CA	-5.74	110.46	121.94
1	A	335	LEU	CA-C-N	5.68	132.08	122.65
1	A	335	LEU	C-N-CA	5.68	132.08	122.65
1	C	1082	CYS	CA-C-N	-5.67	110.70	121.54
1	C	1082	CYS	C-N-CA	-5.67	110.70	121.54
1	C	335	LEU	CA-C-N	5.67	132.06	122.65
1	C	335	LEU	C-N-CA	5.67	132.06	122.65
1	B	335	LEU	CA-C-N	5.67	132.05	122.65
1	B	335	LEU	C-N-CA	5.67	132.05	122.65
1	B	1082	CYS	CA-C-N	-5.66	110.73	121.54
1	B	1082	CYS	C-N-CA	-5.66	110.73	121.54
1	A	1082	CYS	CA-C-N	-5.65	110.74	121.54
1	A	1082	CYS	C-N-CA	-5.65	110.74	121.54
2	D	90	THR	CA-C-N	5.52	132.09	121.54
2	D	90	THR	C-N-CA	5.52	132.09	121.54
2	H	90	THR	CA-C-N	5.51	132.06	121.54
2	H	90	THR	C-N-CA	5.51	132.06	121.54
1	C	1090	PRO	CA-C-N	-5.38	112.66	120.29
1	C	1090	PRO	C-N-CA	-5.38	112.66	120.29
1	A	1090	PRO	CA-C-N	-5.36	112.68	120.29
1	A	1090	PRO	C-N-CA	-5.36	112.68	120.29
1	B	1090	PRO	CA-C-N	-5.34	112.71	120.29
1	B	1090	PRO	C-N-CA	-5.34	112.71	120.29
1	C	800	PHE	N-CA-C	-5.29	102.65	110.48
1	A	800	PHE	N-CA-C	-5.27	102.68	110.48
1	B	800	PHE	N-CA-C	-5.26	102.69	110.48
1	C	1050	MET	CA-C-N	-5.12	112.25	121.62
1	C	1050	MET	C-N-CA	-5.12	112.25	121.62
1	B	1050	MET	CA-C-N	-5.11	112.26	121.62
1	B	1050	MET	C-N-CA	-5.11	112.26	121.62
1	A	1050	MET	CA-C-N	-5.11	112.27	121.62
1	A	1050	MET	C-N-CA	-5.11	112.27	121.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	813	SER	CA-C-N	-5.04	115.00	122.41
1	A	813	SER	C-N-CA	-5.04	115.00	122.41
1	B	813	SER	CA-C-N	-5.04	115.00	122.41
1	B	813	SER	C-N-CA	-5.04	115.00	122.41
1	C	813	SER	CA-C-N	-5.03	115.02	122.41
1	C	813	SER	C-N-CA	-5.03	115.02	122.41
1	A	878	LEU	CB-CG-CD2	-5.01	95.66	110.70
1	C	878	LEU	CB-CG-CD2	-5.01	95.67	110.70
1	B	878	LEU	CB-CG-CD2	-5.01	95.67	110.70

There are no chirality outliers.

All (26) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1126	CYS	Peptide
1	A	200	TYR	Peptide
1	A	210	ILE	Peptide
1	A	380	TYR	Peptide
1	A	516	GLU	Peptide
1	A	565	PHE	Peptide
1	A	96	GLU	Peptide
1	B	1126	CYS	Peptide
1	B	200	TYR	Peptide
1	B	210	ILE	Peptide
1	B	380	TYR	Peptide
1	B	516	GLU	Peptide
1	B	96	GLU	Peptide
1	C	1126	CYS	Peptide
1	C	200	TYR	Peptide
1	C	210	ILE	Peptide
1	C	380	TYR	Peptide
1	C	516	GLU	Peptide
1	C	565	PHE	Peptide
1	C	96	GLU	Peptide
2	D	93	TRP	Peptide
2	F	93	TRP	Peptide
3	G	102	ASP	Peptide
3	G	56	GLY	Peptide
2	H	93	TRP	Peptide
3	I	102	ASP	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8029	0	7803	863	0
1	B	8033	0	7807	818	0
1	C	8033	0	7806	809	0
2	D	837	0	820	94	0
2	F	837	0	820	84	0
2	H	837	0	820	86	0
3	E	939	0	891	123	0
3	G	939	0	891	107	0
3	I	939	0	891	112	0
4	J	28	0	25	1	0
4	K	28	0	25	0	0
4	L	28	0	25	2	0
4	M	28	0	25	0	0
4	N	28	0	25	0	0
4	O	28	0	25	1	0
4	P	28	0	25	0	0
4	Q	28	0	25	2	0
4	R	28	0	25	0	0
4	S	28	0	25	1	0
4	T	28	0	25	1	0
4	U	28	0	25	0	0
4	V	28	0	25	2	0
4	W	28	0	25	0	0
4	X	28	0	25	1	0
5	A	140	0	130	14	0
5	B	140	0	130	13	0
5	C	140	0	130	13	0
All	All	30263	0	29314	2923	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 49.

All (2923) 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:43:PHE:CD2	1:B:559:PHE:HE1	1.02	1.63
1:A:43:PHE:CD2	1:B:559:PHE:CE1	1.93	1.56
1:B:324:GLU:CD	1:B:325:SER:H	1.07	1.51
1:C:318:PHE:CZ	1:C:615:VAL:HG11	1.62	1.33
1:A:43:PHE:CG	1:B:559:PHE:CE1	2.18	1.31
1:A:323:THR:HG22	1:A:324:GLU:OE1	1.34	1.26
2:H:95:TYR:OH	3:I:105:TYR:CD2	1.86	1.26
1:B:324:GLU:CD	1:B:325:SER:N	1.92	1.22
2:H:95:TYR:OH	3:I:105:TYR:CE2	1.81	1.22
1:C:559:PHE:CZ	1:C:565:PHE:O	1.93	1.22
1:B:318:PHE:CZ	1:B:615:VAL:HG11	1.78	1.19
1:A:559:PHE:HE2	1:A:564:GLN:O	1.26	1.17
1:A:319:ARG:NH1	1:C:740:MET:SD	2.18	1.16
1:C:320:VAL:HG23	1:C:591:SER:HB2	1.30	1.13
1:C:408:ARG:HD3	3:I:102:ASP:CG	1.74	1.12
1:A:318:PHE:CZ	1:A:615:VAL:HG11	1.84	1.11
1:A:740:MET:SD	1:B:319:ARG:NH1	2.25	1.09
3:G:102:ASP:HB3	3:G:103:PRO:CD	1.84	1.06
1:A:318:PHE:HZ	1:A:615:VAL:HG11	0.93	1.06
1:B:850:ILE:H	1:B:850:ILE:HD12	1.19	1.06
1:C:559:PHE:CE2	1:C:565:PHE:O	2.08	1.06
1:C:318:PHE:HZ	1:C:615:VAL:CG1	1.70	1.05
1:C:408:ARG:HD3	3:I:102:ASP:OD2	1.54	1.05
1:A:559:PHE:CE2	1:A:564:GLN:O	2.09	1.04
3:E:102:ASP:HB3	3:E:103:PRO:HD2	1.34	1.04
1:B:318:PHE:HZ	1:B:615:VAL:CG1	1.71	1.03
3:G:99:SER:OG	3:G:105:TYR:HD1	1.40	1.03
1:B:324:GLU:CG	1:B:325:SER:H	1.72	1.02
1:B:43:PHE:HB2	1:C:563:GLN:HG2	1.42	0.99
1:B:318:PHE:HZ	1:B:615:VAL:HG11	0.85	0.99
1:B:324:GLU:CG	1:B:325:SER:N	2.27	0.98
1:B:320:VAL:HG23	1:B:591:SER:HB2	1.46	0.98
1:A:323:THR:CG2	1:A:324:GLU:OE1	2.13	0.97
1:A:559:PHE:HE2	1:A:564:GLN:C	1.73	0.96
1:C:865:LEU:HD23	1:C:870:ILE:HD13	1.45	0.95
3:I:102:ASP:HB3	3:I:103:PRO:CD	1.97	0.95
1:A:43:PHE:HD2	1:B:559:PHE:HE1	1.11	0.94
2:F:35:TYR:HB2	2:F:86:PHE:HB2	1.49	0.94
1:C:559:PHE:HZ	1:C:565:PHE:C	1.76	0.94
1:A:375:SER:HA	2:D:92:PHE:H	1.30	0.94
3:E:102:ASP:HB3	3:E:103:PRO:CD	1.98	0.94
2:H:95:TYR:CZ	3:I:105:TYR:CD2	2.54	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:850:ILE:H	1:C:850:ILE:HD12	1.29	0.94
1:A:1135:ASN:OD1	1:A:1136:THR:N	2.01	0.94
1:C:320:VAL:HG23	1:C:591:SER:CB	1.98	0.93
2:F:10:GLN:HG3	2:F:20:ILE:HG12	1.47	0.93
1:C:1135:ASN:OD1	1:C:1136:THR:N	2.01	0.93
1:A:328:ARG:HH22	1:A:533:LEU:HB2	1.34	0.92
1:A:559:PHE:HB2	1:A:584:ILE:HD11	1.52	0.92
1:C:559:PHE:CZ	1:C:565:PHE:C	2.47	0.92
1:B:1135:ASN:OD1	1:B:1136:THR:N	2.02	0.91
1:C:328:ARG:HH22	1:C:533:LEU:HB2	1.34	0.91
3:G:35:HIS:HB2	3:G:97:ALA:HB3	1.53	0.91
1:A:557:LYS:O	1:A:584:ILE:HG21	1.69	0.90
1:B:328:ARG:HH22	1:B:533:LEU:HB2	1.34	0.90
1:A:375:SER:HA	2:D:92:PHE:N	1.86	0.90
1:A:320:VAL:HG23	1:A:591:SER:HB2	1.53	0.89
3:G:102:ASP:HB3	3:G:103:PRO:HD2	1.52	0.89
1:A:43:PHE:HA	1:B:563:GLN:NE2	1.85	0.89
3:G:10:GLU:HB2	3:G:116:VAL:HG22	1.51	0.89
1:A:318:PHE:HZ	1:A:615:VAL:CG1	1.85	0.88
3:G:102:ASP:OD2	3:G:103:PRO:HD3	1.74	0.88
1:A:353:TRP:O	1:A:466:ARG:NH2	2.07	0.88
3:E:103:PRO:O	3:E:105:TYR:CD2	2.27	0.88
1:A:43:PHE:CB	1:B:559:PHE:CE1	2.56	0.88
1:C:359:SER:HA	1:C:523:THR:HB	1.56	0.88
1:B:1019:ARG:NH2	1:B:1023:ASN:OD1	2.07	0.88
1:B:133:PHE:HB3	1:B:163:ALA:HA	1.55	0.87
1:A:323:THR:HG21	1:A:537:LYS:NZ	1.89	0.87
1:C:353:TRP:O	1:C:466:ARG:NH2	2.07	0.87
1:B:353:TRP:O	1:B:466:ARG:NH2	2.07	0.87
1:C:318:PHE:HZ	1:C:615:VAL:HG11	0.77	0.87
1:C:1019:ARG:NH2	1:C:1023:ASN:OD1	2.07	0.87
1:B:359:SER:HA	1:B:523:THR:HB	1.56	0.87
1:C:133:PHE:HB3	1:C:163:ALA:HA	1.55	0.87
1:C:786:LYS:NZ	1:C:891:GLY:O	2.08	0.87
1:A:133:PHE:HB3	1:A:163:ALA:HA	1.55	0.87
1:A:1019:ARG:NH2	1:A:1023:ASN:OD1	2.07	0.86
1:B:786:LYS:NZ	1:B:891:GLY:O	2.08	0.86
1:B:811:LYS:NZ	1:B:820:ASP:OD2	2.09	0.86
1:A:786:LYS:NZ	1:A:891:GLY:O	2.08	0.86
3:G:99:SER:HG	3:G:105:TYR:HD1	1.20	0.86
1:A:898:PHE:O	1:A:901:GLN:N	2.08	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:898:PHE:O	1:B:901:GLN:N	2.09	0.85
1:C:101:ILE:HG12	1:C:242:LEU:HD21	1.57	0.85
1:C:309:GLU:OE1	1:C:309:GLU:N	2.09	0.85
1:A:309:GLU:OE1	1:A:309:GLU:N	2.09	0.85
3:G:93:VAL:HG22	3:G:115:THR:HG22	1.58	0.85
1:A:359:SER:HA	1:A:523:THR:HB	1.56	0.85
1:B:1043:CYS:HB3	1:B:1048:HIS:CD2	2.12	0.85
1:B:37:TYR:OH	1:B:195:LYS:NZ	2.10	0.85
2:D:24:ALA:HB3	2:D:28:ILE:HG22	1.59	0.85
1:A:101:ILE:HG12	1:A:242:LEU:HD21	1.57	0.85
1:C:811:LYS:NZ	1:C:820:ASP:OD2	2.09	0.85
1:B:703:ASN:OD1	1:B:704:SER:N	2.10	0.84
1:A:1043:CYS:HB3	1:A:1048:HIS:CD2	2.12	0.84
1:B:309:GLU:N	1:B:309:GLU:OE1	2.09	0.84
1:C:898:PHE:O	1:C:901:GLN:N	2.08	0.84
1:A:703:ASN:OD1	1:A:704:SER:N	2.10	0.84
1:C:37:TYR:OH	1:C:195:LYS:NZ	2.10	0.84
1:C:316:SER:O	1:C:595:VAL:N	2.11	0.84
1:C:1043:CYS:HB3	1:C:1048:HIS:CD2	2.12	0.84
3:I:35:HIS:HB2	3:I:97:ALA:HB3	1.60	0.84
1:A:405:ASP:HA	3:E:103:PRO:HG3	1.58	0.83
1:A:811:LYS:NZ	1:A:820:ASP:OD2	2.09	0.83
1:A:544:ASN:HD21	1:A:579:PRO:HB3	1.43	0.83
3:G:102:ASP:CB	3:G:103:PRO:CD	2.56	0.83
1:B:101:ILE:HG12	1:B:242:LEU:HD21	1.57	0.83
1:C:703:ASN:OD1	1:C:704:SER:N	2.10	0.83
1:A:850:ILE:HD12	1:A:850:ILE:H	1.42	0.83
1:B:864:LEU:HD12	1:B:864:LEU:O	1.78	0.83
1:C:287:ASP:OD1	1:C:288:ALA:N	2.12	0.83
1:C:318:PHE:CZ	1:C:615:VAL:CG1	2.52	0.83
1:A:37:TYR:OH	1:A:195:LYS:NZ	2.10	0.83
1:A:559:PHE:HB2	1:A:584:ILE:CD1	2.09	0.82
1:A:112:SER:OG	1:A:164:ASN:ND2	2.12	0.82
1:A:773:GLU:O	1:A:776:LYS:N	2.13	0.82
3:E:35:HIS:HB2	3:E:97:ALA:HB3	1.60	0.82
1:C:112:SER:OG	1:C:164:ASN:ND2	2.12	0.82
2:H:24:ALA:HB3	2:H:28:ILE:HG22	1.59	0.82
1:B:287:ASP:OD1	1:B:288:ALA:N	2.12	0.82
1:B:773:GLU:O	1:B:776:LYS:N	2.13	0.82
1:C:544:ASN:HD21	1:C:579:PRO:HB3	1.43	0.82
1:B:379:CYS:HA	1:B:432:CYS:HA	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:PHE:CG	1:B:559:PHE:CD1	2.68	0.81
1:A:225:PRO:HD2	1:B:562:PHE:CD2	2.14	0.81
1:B:112:SER:OG	1:B:164:ASN:ND2	2.12	0.81
1:B:115:GLN:HA	1:B:132:GLU:HG2	1.61	0.81
1:B:544:ASN:HD21	1:B:579:PRO:HB3	1.43	0.81
1:C:773:GLU:O	1:C:776:LYS:N	2.13	0.81
1:C:317:ASN:HB3	1:C:593:GLY:O	1.81	0.81
3:G:99:SER:OG	3:G:105:TYR:CD1	2.30	0.81
1:B:858:LEU:H	1:B:858:LEU:HD12	1.44	0.81
1:A:287:ASP:OD1	1:A:288:ALA:N	2.12	0.81
3:I:102:ASP:OD2	3:I:103:PRO:HD3	1.81	0.81
1:A:115:GLN:HA	1:A:132:GLU:HG2	1.61	0.81
1:B:99:ASN:O	1:B:102:ARG:NE	2.15	0.80
1:C:115:GLN:HA	1:C:132:GLU:HG2	1.61	0.80
1:B:559:PHE:HZ	1:B:566:GLY:CA	1.95	0.80
1:A:280:ASN:OD1	1:A:284:THR:N	2.15	0.80
1:B:436:TRP:HE1	1:B:509:ARG:HD2	1.46	0.80
1:A:559:PHE:CE1	1:C:43:PHE:HB3	2.17	0.80
1:B:90:VAL:HG12	1:B:91:TYR:O	1.82	0.80
1:C:280:ASN:OD1	1:C:284:THR:N	2.15	0.80
1:A:379:CYS:HA	1:A:432:CYS:HA	1.62	0.80
1:A:299:THR:O	1:A:302:THR:N	2.14	0.80
1:A:436:TRP:HE1	1:A:509:ARG:HD2	1.46	0.79
1:A:99:ASN:O	1:A:102:ARG:NE	2.15	0.79
1:C:99:ASN:O	1:C:102:ARG:NE	2.15	0.79
1:A:375:SER:HB3	2:D:91:ASN:HB2	1.63	0.79
1:A:43:PHE:HD1	1:B:563:GLN:OE1	1.64	0.79
1:A:90:VAL:HG12	1:A:91:TYR:O	1.82	0.79
1:C:901:GLN:O	1:C:904:TYR:N	2.15	0.79
1:C:804:GLN:OE1	1:C:935:GLN:NE2	2.16	0.79
1:B:804:GLN:OE1	1:B:935:GLN:NE2	2.16	0.79
1:C:379:CYS:HA	1:C:432:CYS:HA	1.62	0.79
1:C:438:SER:HB3	1:C:509:ARG:HG3	1.64	0.79
1:A:804:GLN:OE1	1:A:935:GLN:NE2	2.16	0.79
1:B:280:ASN:OD1	1:B:284:THR:N	2.15	0.79
1:C:90:VAL:HG12	1:C:91:TYR:O	1.82	0.79
1:C:299:THR:O	1:C:302:THR:N	2.14	0.79
1:B:901:GLN:O	1:B:904:TYR:N	2.15	0.79
1:C:869:MET:O	1:C:872:GLN:N	2.16	0.78
1:A:408:ARG:HD3	3:E:102:ASP:CG	2.07	0.78
1:B:320:VAL:HG23	1:B:591:SER:CB	2.14	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:438:SER:HB3	1:B:509:ARG:HG3	1.64	0.78
1:B:869:MET:O	1:B:872:GLN:N	2.16	0.78
2:D:4:LEU:HA	2:D:24:ALA:HA	1.66	0.78
1:C:436:TRP:HE1	1:C:509:ARG:HD2	1.46	0.78
1:A:901:GLN:O	1:A:904:TYR:N	2.15	0.78
2:F:6:GLN:O	2:F:99:GLN:NE2	2.16	0.78
1:A:438:SER:HB3	1:A:509:ARG:HG3	1.64	0.78
3:I:93:VAL:HG22	3:I:115:THR:HG22	1.65	0.78
1:A:737:ASP:OD1	1:A:739:THR:N	2.17	0.78
1:A:557:LYS:O	1:A:584:ILE:HG13	1.85	0.77
1:B:299:THR:O	1:B:302:THR:N	2.15	0.77
1:B:737:ASP:OD1	1:B:739:THR:N	2.17	0.77
1:B:796:ASP:OD1	1:B:796:ASP:N	2.15	0.77
1:C:737:ASP:OD1	1:C:739:THR:N	2.17	0.77
1:B:461:LEU:HD21	1:B:467:ASP:HB2	1.67	0.77
1:C:796:ASP:OD1	1:C:796:ASP:N	2.15	0.77
1:B:134:GLN:O	1:B:161:SER:N	2.17	0.77
1:C:1072:GLU:OE1	1:C:1072:GLU:N	2.17	0.77
2:F:6:GLN:NE2	2:F:87:CYS:SG	2.58	0.77
1:C:461:LEU:HD21	1:C:467:ASP:HB2	1.67	0.77
2:F:22:CYS:N	2:F:70:PHE:O	2.18	0.77
2:D:93:TRP:CD2	2:D:94:PRO:HD3	2.19	0.77
3:E:93:VAL:HG22	3:E:115:THR:HG22	1.65	0.77
3:G:100:GLU:HB2	3:G:104:TYR:O	1.85	0.77
1:A:461:LEU:HD21	1:A:467:ASP:HB2	1.67	0.76
1:A:863:PRO:O	1:A:865:LEU:O	2.02	0.76
2:F:93:TRP:CD2	2:F:94:PRO:HD3	2.19	0.76
1:A:1072:GLU:N	1:A:1072:GLU:OE1	2.17	0.76
2:H:4:LEU:HA	2:H:24:ALA:HA	1.66	0.76
1:A:424:LYS:HB3	1:A:461:LEU:HB2	1.67	0.76
1:C:317:ASN:CB	1:C:593:GLY:O	2.34	0.76
1:C:320:VAL:HG21	1:C:591:SER:OG	1.84	0.76
2:F:48:LYS:N	2:F:52:GLN:O	2.14	0.76
1:B:454:ARG:HD3	1:B:457:ARG:HB2	1.68	0.76
2:F:97:PHE:HD2	3:G:45:LEU:HB3	1.50	0.76
2:H:93:TRP:CD2	2:H:94:PRO:HD3	2.19	0.76
1:A:375:SER:CB	2:D:91:ASN:HB2	2.15	0.76
1:C:559:PHE:HZ	1:C:566:GLY:N	1.83	0.76
3:E:102:ASP:CB	3:E:103:PRO:CD	2.63	0.76
1:A:869:MET:O	1:A:872:GLN:N	2.16	0.76
1:B:1072:GLU:OE1	1:B:1072:GLU:N	2.17	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:331:ASN:OD1	1:B:332:ILE:N	2.19	0.76
1:C:331:ASN:HB3	5:C:1304:NAG:C7	2.16	0.76
2:F:24:ALA:HB3	2:F:28:ILE:HG22	1.68	0.76
1:B:560:LEU:HB2	1:B:563:GLN:HB2	1.65	0.75
1:C:134:GLN:O	1:C:161:SER:N	2.17	0.75
1:C:850:ILE:HD12	1:C:850:ILE:N	2.02	0.75
1:A:796:ASP:OD1	1:A:796:ASP:N	2.15	0.75
1:A:320:VAL:HG23	1:A:591:SER:CB	2.15	0.75
1:A:331:ASN:OD1	1:A:332:ILE:N	2.19	0.75
1:A:454:ARG:HD3	1:A:457:ARG:HB2	1.68	0.75
1:B:43:PHE:HB2	1:C:563:GLN:CG	2.16	0.75
1:B:331:ASN:HB3	5:B:1304:NAG:C7	2.16	0.75
1:C:424:LYS:HB3	1:C:461:LEU:HB2	1.67	0.75
1:A:873:TYR:O	1:A:876:ALA:N	2.20	0.75
1:A:134:GLN:O	1:A:161:SER:N	2.17	0.75
1:C:873:TYR:O	1:C:876:ALA:N	2.20	0.75
3:I:102:ASP:CB	3:I:103:PRO:CD	2.65	0.75
1:A:281:GLU:HB2	5:A:1303:NAG:H82	1.69	0.75
1:A:331:ASN:HB3	5:A:1304:NAG:C7	2.16	0.75
1:A:405:ASP:OD2	3:E:104:TYR:OH	2.04	0.75
1:C:331:ASN:OD1	1:C:332:ILE:N	2.19	0.75
3:G:102:ASP:HB3	3:G:103:PRO:HD3	1.67	0.75
1:B:564:GLN:OE1	1:B:564:GLN:HA	1.87	0.74
2:D:12:VAL:HG21	2:D:18:VAL:HB	1.68	0.74
1:A:861:LEU:N	1:A:861:LEU:HD23	2.02	0.74
3:I:102:ASP:HB3	3:I:103:PRO:HD3	1.70	0.74
1:C:311:GLY:HA2	1:C:664:ILE:HG23	1.70	0.74
1:B:424:LYS:HB3	1:B:461:LEU:HB2	1.67	0.74
1:B:873:TYR:O	1:B:876:ALA:N	2.20	0.74
1:C:568:ASP:OD1	1:C:569:ILE:N	2.20	0.74
1:C:880:GLY:O	1:C:884:SER:OG	2.05	0.74
1:A:196:ASN:HD21	1:A:235:ILE:HD12	1.53	0.74
1:A:854:LYS:HZ3	1:A:854:LYS:HB3	1.52	0.74
1:B:196:ASN:HD21	1:B:235:ILE:HD12	1.53	0.74
1:B:880:GLY:O	1:B:884:SER:OG	2.05	0.74
1:A:540:ASN:OD1	1:A:541:PHE:N	2.21	0.74
1:C:196:ASN:HD21	1:C:235:ILE:HD12	1.53	0.74
1:C:454:ARG:HD3	1:C:457:ARG:HB2	1.68	0.73
2:H:12:VAL:HG21	2:H:18:VAL:HB	1.68	0.73
1:B:123:ALA:HB3	5:B:1302:NAG:H83	1.71	0.73
1:B:540:ASN:OD1	1:B:541:PHE:N	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:568:ASP:OD1	1:B:569:ILE:N	2.20	0.73
1:A:311:GLY:HA2	1:A:664:ILE:HG23	1.70	0.73
1:A:850:ILE:HD12	1:A:850:ILE:N	2.03	0.73
1:B:850:ILE:HD12	1:B:850:ILE:N	2.01	0.73
1:C:123:ALA:HB3	5:C:1302:NAG:H83	1.71	0.73
1:B:273:ARG:NH1	1:B:290:ASP:OD2	2.22	0.73
1:B:323:THR:HG21	1:B:537:LYS:NZ	2.04	0.73
1:C:375:SER:N	1:C:435:ALA:O	2.22	0.73
1:B:281:GLU:HB2	5:B:1303:NAG:H82	1.69	0.73
1:B:375:SER:N	1:B:435:ALA:O	2.22	0.73
1:C:273:ARG:NH1	1:C:290:ASP:OD2	2.22	0.73
1:C:540:ASN:OD1	1:C:541:PHE:N	2.21	0.73
1:A:401:VAL:HG22	1:A:509:ARG:HG2	1.71	0.73
1:B:311:GLY:HA2	1:B:664:ILE:HG23	1.70	0.73
1:B:876:ALA:O	1:B:879:ALA:N	2.22	0.73
1:A:906:PHE:O	1:A:909:ILE:N	2.21	0.73
1:B:747:THR:O	1:B:751:ASN:N	2.19	0.73
1:C:865:LEU:HD23	1:C:870:ILE:CD1	2.19	0.73
1:C:906:PHE:O	1:C:909:ILE:N	2.21	0.73
1:A:123:ALA:HB3	5:A:1302:NAG:H83	1.71	0.72
1:A:880:GLY:O	1:A:884:SER:OG	2.05	0.72
1:B:864:LEU:HD12	1:B:864:LEU:C	2.13	0.72
1:A:357:ARG:HH12	1:C:167:THR:HA	1.53	0.72
1:A:375:SER:N	1:A:435:ALA:O	2.22	0.72
1:A:717:ASN:OD1	1:A:718:PHE:N	2.23	0.72
1:A:876:ALA:O	1:A:879:ALA:N	2.22	0.72
1:C:281:GLU:HB2	5:C:1303:NAG:H82	1.69	0.72
1:A:568:ASP:OD1	1:A:569:ILE:N	2.21	0.72
1:C:560:LEU:HB2	1:C:563:GLN:HB2	1.70	0.72
1:B:108:THR:O	1:B:237:ARG:NH2	2.23	0.72
1:B:717:ASN:OD1	1:B:718:PHE:N	2.23	0.72
1:A:339:GLY:O	1:A:343:ASN:N	2.23	0.72
1:A:273:ARG:NH1	1:A:290:ASP:OD2	2.22	0.72
1:C:402:ILE:O	1:C:508:TYR:N	2.23	0.72
1:C:350:VAL:HG21	1:C:418:ILE:HD12	1.72	0.72
1:C:876:ALA:O	1:C:879:ALA:N	2.22	0.72
1:C:717:ASN:OD1	1:C:718:PHE:N	2.23	0.72
3:I:102:ASP:CB	3:I:103:PRO:HD3	2.20	0.72
1:B:339:GLY:O	1:B:343:ASN:N	2.23	0.71
2:D:5:THR:HB	2:D:23:ARG:HB3	1.72	0.71
1:A:1139:ASP:OD1	1:A:1141:LEU:N	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:ARG:HB3	1:B:192:PHE:CZ	2.25	0.71
1:C:1100:THR:HG1	1:C:1101:HIS:HD1	1.37	0.71
1:A:108:THR:O	1:A:237:ARG:NH2	2.23	0.71
1:C:108:THR:O	1:C:237:ARG:NH2	2.23	0.71
1:C:190:ARG:HB3	1:C:192:PHE:CZ	2.25	0.71
1:A:562:PHE:CE2	1:C:225:PRO:HD2	2.26	0.71
1:B:401:VAL:HG22	1:B:509:ARG:HG2	1.71	0.71
3:G:65:LYS:HE3	3:G:67:ALA:HA	1.72	0.71
1:A:856:ASN:O	1:A:858:LEU:N	2.24	0.71
1:B:1139:ASP:OD1	1:B:1141:LEU:N	2.23	0.71
1:C:401:VAL:HG22	1:C:509:ARG:HG2	1.71	0.71
1:A:350:VAL:HG21	1:A:418:ILE:HD12	1.72	0.70
1:A:402:ILE:O	1:A:508:TYR:N	2.23	0.70
1:A:1100:THR:HG1	1:A:1101:HIS:HD1	1.38	0.70
1:A:380:TYR:N	1:A:431:GLY:O	2.18	0.70
1:A:599:THR:OG1	1:A:600:PRO:O	2.09	0.70
1:B:906:PHE:O	1:B:909:ILE:N	2.21	0.70
1:C:320:VAL:CG2	1:C:591:SER:CB	2.70	0.70
1:C:1139:ASP:OD1	1:C:1141:LEU:N	2.23	0.70
1:A:190:ARG:HB3	1:A:192:PHE:CZ	2.25	0.70
1:C:599:THR:OG1	1:C:600:PRO:O	2.09	0.70
3:E:29:PHE:HZ	3:E:72:ALA:HB1	1.57	0.70
3:I:102:ASP:CG	3:I:103:PRO:HD3	2.17	0.70
1:A:414:GLN:NE2	3:E:101:TYR:OH	2.22	0.70
1:B:339:GLY:HA2	5:B:1305:NAG:H81	1.74	0.70
1:B:856:ASN:C	1:B:858:LEU:HD12	2.16	0.70
1:C:104:TRP:HB3	1:C:106:PHE:CE1	2.26	0.70
2:H:5:THR:HB	2:H:23:ARG:HB3	1.72	0.70
1:A:281:GLU:OE1	1:A:281:GLU:N	2.20	0.70
1:B:380:TYR:N	1:B:431:GLY:O	2.18	0.70
1:B:599:THR:OG1	1:B:600:PRO:O	2.09	0.70
1:C:351:TYR:HA	1:C:422:ASN:HB2	1.73	0.70
1:A:104:TRP:HB3	1:A:106:PHE:CE1	2.26	0.70
1:B:104:TRP:HB3	1:B:106:PHE:CE1	2.26	0.70
1:B:350:VAL:HG21	1:B:418:ILE:HD12	1.72	0.70
1:C:850:ILE:H	1:C:850:ILE:CD1	2.03	0.70
1:C:851:CYS:HA	1:C:854:LYS:HE2	1.72	0.70
2:H:64:SER:HG	2:H:71:THR:HG1	1.35	0.70
3:I:29:PHE:HZ	3:I:72:ALA:HB1	1.57	0.70
1:A:361:CYS:N	1:A:523:THR:O	2.17	0.69
1:B:351:TYR:HA	1:B:422:ASN:HB2	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:SER:OG	1:A:317:ASN:N	2.24	0.69
1:B:709:ASN:ND2	5:B:1309:NAG:O7	2.25	0.69
1:B:1100:THR:HG1	1:B:1101:HIS:HD1	1.38	0.69
2:D:6:GLN:NE2	2:D:87:CYS:SG	2.66	0.69
1:A:357:ARG:NH1	1:C:167:THR:HA	2.08	0.69
1:C:339:GLY:O	1:C:343:ASN:N	2.23	0.69
1:A:532:ASN:OD1	1:A:533:LEU:N	2.23	0.69
1:A:854:LYS:HZ3	1:A:854:LYS:CB	2.05	0.69
1:C:339:GLY:HA2	5:C:1305:NAG:H81	1.74	0.69
1:C:747:THR:O	1:C:751:ASN:N	2.19	0.69
1:A:709:ASN:ND2	5:A:1309:NAG:O7	2.25	0.69
1:A:858:LEU:N	1:A:858:LEU:HD12	2.07	0.69
1:C:709:ASN:ND2	5:C:1309:NAG:O7	2.25	0.69
1:B:676:THR:H	1:B:690:GLN:HG2	1.58	0.69
1:C:126:VAL:HB	1:C:172:SER:HB2	1.75	0.69
1:C:422:ASN:HB3	1:C:454:ARG:H	1.57	0.69
1:A:128:ILE:HD12	1:A:170:TYR:HD2	1.58	0.69
1:A:187:LYS:O	1:A:210:ILE:N	2.21	0.69
1:A:422:ASN:HB3	1:A:454:ARG:H	1.57	0.69
1:A:763:LEU:O	1:A:766:ALA:N	2.25	0.69
1:B:763:LEU:O	1:B:766:ALA:N	2.25	0.69
1:B:850:ILE:H	1:B:850:ILE:CD1	1.98	0.69
1:C:532:ASN:OD1	1:C:533:LEU:N	2.23	0.69
3:G:102:ASP:CB	3:G:103:PRO:HD3	2.22	0.69
2:H:6:GLN:NE2	2:H:87:CYS:SG	2.65	0.69
1:C:763:LEU:O	1:C:766:ALA:N	2.25	0.69
2:F:22:CYS:HB3	2:F:70:PHE:HB2	1.74	0.69
1:A:339:GLY:HA2	5:A:1305:NAG:H81	1.74	0.69
1:B:128:ILE:HD12	1:B:170:TYR:HD2	1.58	0.69
3:E:65:LYS:HE3	3:E:67:ALA:HA	1.75	0.69
1:B:402:ILE:O	1:B:508:TYR:N	2.23	0.68
1:B:532:ASN:OD1	1:B:533:LEU:N	2.23	0.68
3:G:38:LYS:O	3:G:46:GLU:N	2.26	0.68
1:B:422:ASN:HB3	1:B:454:ARG:H	1.57	0.68
1:B:858:LEU:HD12	1:B:858:LEU:N	2.08	0.68
1:C:143:VAL:N	1:C:244:LEU:O	2.27	0.68
1:A:143:VAL:N	1:A:244:LEU:O	2.27	0.68
1:A:351:TYR:HA	1:A:422:ASN:HB2	1.73	0.68
1:A:866:THR:O	1:A:869:MET:N	2.26	0.68
1:C:726:ILE:HG12	1:C:1061:VAL:HG22	1.75	0.68
1:A:143:VAL:HB	1:A:245:HIS:HA	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:ILE:C	1:B:106:PHE:HD1	2.01	0.68
1:B:134:GLN:HE21	1:B:135:PHE:H	1.41	0.68
1:B:866:THR:O	1:B:869:MET:N	2.26	0.68
1:B:1093:GLY:HA2	1:B:1107:ARG:HH11	1.57	0.68
1:C:1093:GLY:HA2	1:C:1107:ARG:HH11	1.57	0.68
1:A:43:PHE:CE2	1:B:559:PHE:CE1	2.75	0.68
1:A:676:THR:H	1:A:690:GLN:HG2	1.58	0.68
1:B:143:VAL:HB	1:B:245:HIS:HA	1.76	0.68
1:B:348:ALA:O	1:B:400:PHE:HA	1.94	0.68
1:C:406:GLU:HB3	1:C:418:ILE:HG13	1.76	0.68
3:G:35:HIS:O	3:G:97:ALA:N	2.25	0.68
1:A:126:VAL:HB	1:A:172:SER:HB2	1.75	0.68
1:A:733:LYS:NZ	1:A:775:ASP:OD2	2.21	0.68
1:C:320:VAL:CG2	1:C:591:SER:OG	2.41	0.68
1:C:676:THR:H	1:C:690:GLN:HG2	1.58	0.68
1:B:143:VAL:N	1:B:244:LEU:O	2.27	0.68
1:B:406:GLU:HB3	1:B:418:ILE:HG13	1.76	0.68
1:C:380:TYR:N	1:C:431:GLY:O	2.18	0.68
1:C:341:VAL:HG21	1:C:397:ALA:HB3	1.75	0.68
1:A:1093:GLY:HA2	1:A:1107:ARG:HH11	1.57	0.68
1:B:281:GLU:OE1	1:B:281:GLU:N	2.20	0.68
1:C:348:ALA:O	1:C:400:PHE:HA	1.94	0.68
2:D:6:GLN:O	2:D:99:GLN:NE2	2.27	0.68
3:E:40:ALA:HB3	3:E:43:LYS:HB2	1.75	0.68
1:A:726:ILE:HG12	1:A:1061:VAL:HG22	1.75	0.68
2:H:5:THR:N	2:H:23:ARG:O	2.26	0.68
1:C:864:LEU:O	1:C:864:LEU:HD12	1.94	0.67
1:A:348:ALA:O	1:A:400:PHE:HA	1.94	0.67
1:B:126:VAL:HB	1:B:172:SER:HB2	1.75	0.67
1:B:224:GLU:H	1:B:224:GLU:CD	2.02	0.67
1:C:105:ILE:C	1:C:106:PHE:HD1	2.01	0.67
1:C:224:GLU:H	1:C:224:GLU:CD	2.02	0.67
1:A:43:PHE:HB3	1:B:559:PHE:CE1	2.28	0.67
1:B:200:TYR:HE1	1:B:230:PRO:HB3	1.60	0.67
1:C:128:ILE:HD12	1:C:170:TYR:HD2	1.58	0.67
1:C:866:THR:O	1:C:869:MET:N	2.26	0.67
2:D:5:THR:N	2:D:23:ARG:O	2.26	0.67
1:A:200:TYR:HE1	1:A:230:PRO:HB3	1.60	0.67
1:A:224:GLU:H	1:A:224:GLU:CD	2.02	0.67
1:A:452:LEU:HD21	1:A:492:LEU:HB3	1.77	0.67
1:C:200:TYR:HE1	1:C:230:PRO:HB3	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:361:CYS:N	1:C:523:THR:O	2.17	0.67
1:A:747:THR:O	1:A:751:ASN:N	2.19	0.67
1:A:105:ILE:C	1:A:106:PHE:HD1	2.01	0.67
1:A:324:GLU:HG2	1:A:325:SER:H	1.60	0.67
2:H:6:GLN:O	2:H:99:GLN:NE2	2.27	0.67
3:I:65:LYS:HE3	3:I:67:ALA:HA	1.75	0.67
1:A:341:VAL:HG21	1:A:397:ALA:HB3	1.75	0.67
1:A:560:LEU:HD13	1:A:561:PRO:HD2	1.76	0.67
1:B:324:GLU:HG2	1:B:325:SER:N	2.08	0.67
1:B:341:VAL:HG21	1:B:397:ALA:HB3	1.75	0.67
1:A:406:GLU:HB3	1:A:418:ILE:HG13	1.76	0.67
1:B:906:PHE:O	1:B:907:ASN:C	2.38	0.66
1:C:143:VAL:HB	1:C:245:HIS:HA	1.76	0.66
1:A:323:THR:CB	1:A:537:LYS:HE3	2.25	0.66
3:I:40:ALA:HB3	3:I:43:LYS:HB2	1.75	0.66
1:B:1022:ALA:O	1:B:1025:ALA:N	2.28	0.66
1:A:378:LYS:HE2	3:E:57:GLY:HA2	1.76	0.66
1:A:1022:ALA:O	1:A:1025:ALA:N	2.28	0.66
1:B:361:CYS:N	1:B:523:THR:O	2.17	0.66
1:B:452:LEU:HD21	1:B:492:LEU:HB3	1.77	0.66
1:B:560:LEU:HD12	1:B:562:PHE:HE1	1.60	0.66
3:I:102:ASP:HB3	3:I:103:PRO:HD2	1.75	0.66
1:A:323:THR:HB	1:A:539:VAL:HG12	1.77	0.66
1:A:43:PHE:CD1	1:B:563:GLN:OE1	2.48	0.66
1:A:134:GLN:HE21	1:A:135:PHE:H	1.41	0.66
1:A:323:THR:OG1	1:A:537:LYS:HE3	1.96	0.66
1:B:800:PHE:CD1	1:B:800:PHE:N	2.63	0.66
1:C:134:GLN:HE21	1:C:135:PHE:H	1.41	0.66
1:A:323:THR:HG21	1:A:537:LYS:HZ2	1.60	0.66
1:B:726:ILE:HG12	1:B:1061:VAL:HG22	1.75	0.66
1:C:187:LYS:O	1:C:210:ILE:N	2.21	0.66
1:C:800:PHE:HD1	1:C:800:PHE:H	1.43	0.66
3:G:6:GLN:NE2	3:G:96:CYS:H	1.94	0.66
1:C:281:GLU:OE1	1:C:281:GLU:N	2.20	0.66
1:C:906:PHE:O	1:C:907:ASN:C	2.38	0.66
1:C:452:LEU:HD21	1:C:492:LEU:HB3	1.77	0.65
2:D:93:TRP:CE3	2:D:94:PRO:HD3	2.31	0.65
1:A:559:PHE:CE2	1:A:564:GLN:C	2.65	0.65
2:H:93:TRP:CE3	2:H:94:PRO:HD3	2.31	0.65
1:B:800:PHE:H	1:B:800:PHE:HD1	1.44	0.65
1:C:103:GLY:HA3	1:C:241:LEU:HB2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:97:ALA:HB1	3:G:107:MET:HB3	1.78	0.65
1:C:748:GLU:CD	1:C:748:GLU:H	2.04	0.65
2:F:37:GLN:HB2	2:F:43:PRO:HG3	1.77	0.65
1:B:800:PHE:HD2	1:B:927:PHE:HD2	1.45	0.65
1:C:800:PHE:HD2	1:C:927:PHE:HD2	1.45	0.65
1:C:1022:ALA:O	1:C:1025:ALA:N	2.28	0.65
2:F:32:LEU:HD21	2:F:87:CYS:HB2	1.77	0.65
1:A:800:PHE:HD1	1:A:800:PHE:H	1.44	0.65
2:H:95:TYR:CE2	3:I:105:TYR:CG	2.85	0.65
1:A:43:PHE:HD2	1:B:559:PHE:CE1	1.92	0.65
1:A:418:ILE:HA	1:A:422:ASN:OD1	1.97	0.65
3:G:102:ASP:CG	3:G:103:PRO:HD3	2.21	0.65
1:C:578:ASP:HB3	1:C:581:THR:O	1.97	0.65
1:A:901:GLN:O	1:A:903:ALA:N	2.30	0.65
1:C:978:ASN:HA	1:C:981:LEU:HD12	1.79	0.65
2:H:33:HIS:CE1	3:I:106:VAL:HG12	2.32	0.65
1:A:43:PHE:CD2	1:B:559:PHE:CD1	2.80	0.64
1:A:318:PHE:CZ	1:A:615:VAL:CG1	2.70	0.64
1:B:143:VAL:HG22	1:B:151:SER:HB2	1.79	0.64
1:A:748:GLU:CD	1:A:748:GLU:H	2.04	0.64
1:B:802:PHE:HD1	1:B:805:ILE:HD11	1.61	0.64
1:C:800:PHE:HD1	1:C:800:PHE:N	1.95	0.64
1:C:802:PHE:HD1	1:C:805:ILE:HD11	1.61	0.64
1:C:905:ARG:NH1	1:C:1049:LEU:O	2.28	0.64
2:F:48:LYS:HG3	3:G:106:VAL:HG11	1.79	0.64
1:A:578:ASP:HB3	1:A:581:THR:O	1.97	0.64
1:A:906:PHE:O	1:A:907:ASN:C	2.38	0.64
1:B:800:PHE:N	1:B:800:PHE:HD1	1.95	0.64
1:B:978:ASN:HA	1:B:981:LEU:HD12	1.79	0.64
1:C:351:TYR:CE2	1:C:452:LEU:HB3	2.33	0.64
2:D:22:CYS:N	2:D:70:PHE:O	2.31	0.64
2:D:33:HIS:CE1	3:E:106:VAL:HG12	2.32	0.64
3:G:2:VAL:HB	3:G:26:GLY:HA3	1.79	0.64
1:B:103:GLY:HA3	1:B:241:LEU:HB2	1.79	0.64
1:C:452:LEU:HA	1:C:494:SER:HA	1.80	0.64
1:A:43:PHE:HB2	1:B:563:GLN:HG2	1.79	0.64
1:A:143:VAL:HG22	1:A:151:SER:HB2	1.80	0.64
1:A:605:SER:OG	1:A:606:ASN:N	2.31	0.64
1:A:800:PHE:HD2	1:A:927:PHE:HD2	1.45	0.64
1:A:1100:THR:OG1	1:A:1101:HIS:ND1	2.30	0.64
1:B:376:THR:OG1	3:G:50:TYR:OH	2.14	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:418:ILE:HA	1:C:422:ASN:OD1	1.97	0.64
1:B:418:ILE:HA	1:B:422:ASN:OD1	1.97	0.64
1:A:159:VAL:HB	1:A:160:TYR:HD1	1.62	0.64
1:A:374:PHE:O	2:D:93:TRP:N	2.30	0.64
1:A:905:ARG:NH1	1:A:1049:LEU:O	2.28	0.64
1:B:144:TYR:N	1:B:151:SER:O	2.30	0.64
1:B:309:GLU:H	1:B:309:GLU:CD	2.05	0.64
1:B:901:GLN:O	1:B:903:ALA:N	2.30	0.64
3:E:24:VAL:HG21	3:E:29:PHE:HD1	1.63	0.64
1:A:103:GLY:HA3	1:A:241:LEU:HB2	1.79	0.64
1:B:578:ASP:HB3	1:B:581:THR:O	1.97	0.64
1:C:159:VAL:HB	1:C:160:TYR:HD1	1.62	0.64
1:A:401:VAL:HA	1:A:509:ARG:HA	1.80	0.64
1:A:978:ASN:HA	1:A:981:LEU:HD12	1.79	0.64
1:C:559:PHE:HZ	1:C:565:PHE:O	1.57	0.64
1:C:901:GLN:O	1:C:903:ALA:N	2.30	0.64
1:A:589:PRO:HD3	1:C:855:PHE:CE1	2.32	0.63
1:B:328:ARG:HG3	1:B:579:PRO:HG2	1.80	0.63
1:B:351:TYR:CE2	1:B:452:LEU:HB3	2.33	0.63
1:B:381:GLY:HA3	1:B:430:THR:HG23	1.80	0.63
1:B:733:LYS:NZ	1:B:775:ASP:OD2	2.21	0.63
1:C:143:VAL:HG22	1:C:151:SER:HB2	1.79	0.63
1:A:802:PHE:HD1	1:A:805:ILE:HD11	1.62	0.63
1:B:855:PHE:CE1	1:C:589:PRO:HD3	2.32	0.63
1:C:361:CYS:O	1:C:525:CYS:N	2.29	0.63
1:B:904:TYR:OH	1:C:1094:VAL:HG12	1.98	0.63
1:C:864:LEU:HD12	1:C:864:LEU:C	2.24	0.63
1:C:1100:THR:OG1	1:C:1101:HIS:ND1	2.30	0.63
1:A:324:GLU:OE1	1:A:324:GLU:N	2.32	0.63
1:A:328:ARG:HG3	1:A:579:PRO:HG2	1.80	0.63
1:A:351:TYR:CE2	1:A:452:LEU:HB3	2.33	0.63
1:B:452:LEU:HA	1:B:494:SER:HA	1.80	0.63
1:C:328:ARG:HG3	1:C:579:PRO:HG2	1.80	0.63
1:A:144:TYR:N	1:A:151:SER:O	2.30	0.63
1:A:309:GLU:H	1:A:309:GLU:CD	2.06	0.63
1:C:309:GLU:H	1:C:309:GLU:CD	2.05	0.63
2:F:69:ASP:OD1	2:F:70:PHE:N	2.32	0.63
1:A:324:GLU:HG2	1:A:325:SER:N	2.14	0.63
1:B:748:GLU:H	1:B:748:GLU:CD	2.04	0.63
1:A:719:THR:HG22	1:A:1068:VAL:O	1.99	0.63
1:A:800:PHE:HD1	1:A:800:PHE:N	1.95	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1102:TRP:HB2	1:A:1135:ASN:HD22	1.64	0.63
1:B:377:PHE:O	3:G:59:SER:HB3	1.99	0.63
1:C:725:GLU:OE1	1:C:1064:HIS:NE2	2.30	0.63
3:I:72:ALA:HA	3:I:79:ALA:HA	1.81	0.63
1:A:452:LEU:HA	1:A:494:SER:HA	1.80	0.63
1:B:426:PRO:HD2	1:B:429:PHE:HB2	1.81	0.63
1:C:317:ASN:HB3	1:C:594:GLY:HA2	1.81	0.63
1:A:43:PHE:HB3	1:B:559:PHE:CZ	2.34	0.63
1:A:378:LYS:NZ	3:E:58:THR:O	2.20	0.63
1:A:856:ASN:C	1:A:858:LEU:H	2.07	0.63
1:C:401:VAL:HA	1:C:509:ARG:HA	1.80	0.63
1:A:408:ARG:CD	3:E:102:ASP:CG	2.71	0.62
1:C:139:PRO:HB3	1:C:159:VAL:O	1.99	0.62
1:C:719:THR:HG22	1:C:1068:VAL:O	1.99	0.62
3:E:97:ALA:HB1	3:E:107:MET:HB2	1.80	0.62
3:E:102:ASP:CB	3:E:103:PRO:HD2	2.21	0.62
2:F:4:LEU:HA	2:F:24:ALA:HA	1.81	0.62
1:B:159:VAL:HB	1:B:160:TYR:HD1	1.62	0.62
1:B:905:ARG:NH1	1:B:1049:LEU:O	2.28	0.62
1:C:800:PHE:N	1:C:800:PHE:CD1	2.63	0.62
1:C:801:ASN:ND2	4:V:1:NAG:O7	2.32	0.62
1:A:167:THR:HA	1:B:357:ARG:HH12	1.64	0.62
1:B:187:LYS:O	1:B:210:ILE:N	2.21	0.62
1:C:408:ARG:HD3	3:I:102:ASP:OD1	1.98	0.62
3:E:72:ALA:HA	3:E:79:ALA:HA	1.81	0.62
1:A:141:LEU:O	1:A:244:LEU:N	2.30	0.62
1:A:324:GLU:CG	1:A:325:SER:H	2.12	0.62
1:B:801:ASN:ND2	4:Q:1:NAG:O7	2.33	0.62
1:C:381:GLY:HA3	1:C:430:THR:HG23	1.81	0.62
1:A:361:CYS:O	1:A:525:CYS:N	2.29	0.62
3:I:35:HIS:N	3:I:97:ALA:O	2.32	0.62
1:A:1077:THR:OG1	1:C:900:MET:SD	2.58	0.62
1:B:318:PHE:CZ	1:B:615:VAL:CG1	2.61	0.62
1:C:224:GLU:OE1	1:C:224:GLU:N	2.27	0.62
1:B:316:SER:OG	1:B:317:ASN:N	2.24	0.62
1:C:1018:ILE:O	1:C:1021:SER:N	2.33	0.62
3:I:24:VAL:HG21	3:I:29:PHE:HD1	1.63	0.62
1:A:303:LEU:HD12	1:A:308:VAL:HG22	1.82	0.62
1:A:901:GLN:HE21	1:A:905:ARG:HE	1.47	0.62
1:B:401:VAL:HA	1:B:509:ARG:HA	1.80	0.62
1:A:139:PRO:HB3	1:A:159:VAL:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:800:PHE:N	1:A:800:PHE:CD1	2.63	0.62
1:B:1100:THR:OG1	1:B:1101:HIS:ND1	2.30	0.62
1:C:577:ARG:HA	1:C:583:GLU:O	2.00	0.62
1:C:865:LEU:HB3	1:C:870:ILE:HD11	1.82	0.62
2:F:88:GLN:HG2	2:F:97:PHE:CD1	2.34	0.62
1:B:719:THR:HG22	1:B:1068:VAL:O	1.98	0.62
3:G:6:GLN:NE2	3:G:96:CYS:SG	2.59	0.62
1:A:577:ARG:HA	1:A:583:GLU:O	2.00	0.61
1:A:605:SER:OG	1:A:607:GLN:N	2.27	0.61
1:B:93:ALA:O	1:B:265:TYR:HB2	2.00	0.61
1:B:139:PRO:HB3	1:B:159:VAL:O	1.99	0.61
1:B:295:PRO:HB2	1:B:608:VAL:HG21	1.81	0.61
1:B:378:LYS:NZ	3:G:56:GLY:O	2.25	0.61
1:C:557:LYS:CB	1:C:584:ILE:HG21	2.29	0.61
1:C:733:LYS:NZ	1:C:775:ASP:OD2	2.21	0.61
1:C:992:GLN:O	1:C:995:ARG:N	2.33	0.61
3:I:97:ALA:HB1	3:I:107:MET:HB2	1.80	0.61
1:A:992:GLN:O	1:A:995:ARG:N	2.33	0.61
1:A:1018:ILE:O	1:A:1021:SER:N	2.33	0.61
1:B:577:ARG:HA	1:B:583:GLU:O	2.00	0.61
1:C:295:PRO:HB2	1:C:608:VAL:HG21	1.81	0.61
1:C:605:SER:OG	1:C:606:ASN:N	2.31	0.61
1:C:1102:TRP:HB2	1:C:1135:ASN:HD22	1.64	0.61
1:A:559:PHE:CE1	1:C:43:PHE:CB	2.83	0.61
1:A:801:ASN:ND2	4:L:1:NAG:O7	2.33	0.61
1:B:1102:TRP:HB2	1:B:1135:ASN:HD22	1.64	0.61
2:H:22:CYS:N	2:H:70:PHE:O	2.31	0.61
1:A:381:GLY:HA3	1:A:430:THR:HG23	1.81	0.61
1:B:901:GLN:HE21	1:B:905:ARG:HE	1.47	0.61
1:B:992:GLN:O	1:B:995:ARG:N	2.33	0.61
1:C:323:THR:HG22	1:C:324:GLU:HG3	1.81	0.61
2:F:20:ILE:HD12	2:F:85:TYR:HD2	1.65	0.61
1:A:224:GLU:OE1	1:A:224:GLU:N	2.27	0.61
1:A:557:LYS:HB2	1:A:584:ILE:HG21	1.82	0.61
1:B:34:ARG:NH1	1:B:217:PRO:O	2.34	0.61
1:C:901:GLN:HE21	1:C:905:ARG:HE	1.47	0.61
1:B:303:LEU:HD12	1:B:308:VAL:HG22	1.82	0.61
3:E:35:HIS:N	3:E:97:ALA:O	2.32	0.61
3:I:29:PHE:CZ	3:I:72:ALA:HB1	2.35	0.61
1:A:619:GLU:OE1	1:A:619:GLU:N	2.26	0.61
1:A:1094:VAL:HG12	1:C:904:TYR:OH	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1102:TRP:HB2	1:A:1135:ASN:ND2	2.16	0.61
1:B:605:SER:OG	1:B:607:GLN:N	2.27	0.61
1:B:1018:ILE:O	1:B:1021:SER:N	2.33	0.61
1:C:93:ALA:O	1:C:265:TYR:HB2	2.00	0.61
1:A:34:ARG:NH1	1:A:217:PRO:O	2.34	0.61
1:A:1072:GLU:HG2	1:C:894:LEU:HD21	1.82	0.61
1:A:426:PRO:HD2	1:A:429:PHE:HB2	1.81	0.61
1:C:316:SER:O	1:C:595:VAL:HB	2.00	0.61
1:C:326:ILE:O	1:C:326:ILE:HG22	2.01	0.61
1:C:426:PRO:HD2	1:C:429:PHE:HB2	1.81	0.61
1:A:295:PRO:HB2	1:A:608:VAL:HG21	1.81	0.61
1:B:900:MET:SD	1:C:1077:THR:OG1	2.55	0.61
1:C:605:SER:OG	1:C:607:GLN:N	2.27	0.61
2:F:35:TYR:CZ	2:F:45:LEU:HD13	2.36	0.61
1:B:1089:PHE:N	1:B:1089:PHE:HD1	1.98	0.60
1:C:303:LEU:HD12	1:C:308:VAL:HG22	1.82	0.60
1:C:321:GLN:OE1	1:C:321:GLN:HA	1.99	0.60
2:F:34:TRP:HD1	2:F:47:ILE:HB	1.65	0.60
1:A:356:LYS:O	1:A:396:TYR:HA	2.01	0.60
1:A:725:GLU:OE1	1:A:1064:HIS:NE2	2.30	0.60
1:B:1102:TRP:HB2	1:B:1135:ASN:ND2	2.16	0.60
1:C:34:ARG:NH1	1:C:217:PRO:O	2.34	0.60
1:A:1089:PHE:N	1:A:1089:PHE:HD1	1.98	0.60
1:B:323:THR:HG21	1:B:537:LYS:CE	2.32	0.60
3:E:29:PHE:CZ	3:E:72:ALA:HB1	2.35	0.60
1:A:42:VAL:HG22	1:B:565:PHE:HE2	1.67	0.60
1:A:385:THR:CG2	3:E:65:LYS:HE2	2.32	0.60
1:B:894:LEU:HD21	1:C:1072:GLU:HG2	1.82	0.60
1:C:515:PHE:HD2	1:C:517:LEU:H	1.49	0.60
2:H:37:GLN:HB2	2:H:43:PRO:HG3	1.82	0.60
1:C:67:ALA:HB3	1:C:263:ALA:HB3	1.84	0.60
3:G:91:THR:HG23	3:G:117:THR:HA	1.83	0.60
1:A:93:ALA:O	1:A:265:TYR:HB2	2.00	0.60
1:A:904:TYR:OH	1:B:1094:VAL:HG12	2.01	0.60
1:B:444:LYS:HD2	1:B:448:ASN:HB2	1.83	0.60
1:C:970:PHE:CD2	1:C:999:GLY:HA3	2.36	0.60
1:C:1080:ALA:O	1:C:1081:ILE:HG13	2.02	0.60
1:A:970:PHE:CD2	1:A:999:GLY:HA3	2.36	0.60
1:B:1088:HIS:ND1	1:B:1122:VAL:HG22	2.17	0.60
1:A:190:ARG:HB3	1:A:192:PHE:CE1	2.37	0.60
1:A:856:ASN:C	1:A:858:LEU:N	2.57	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:970:PHE:CD2	1:B:999:GLY:HA3	2.36	0.60
1:C:860:VAL:O	1:C:860:VAL:HG12	2.01	0.60
1:A:57:PRO:HG2	1:A:271:GLN:OE1	2.02	0.60
1:A:515:PHE:HD2	1:A:517:LEU:H	1.49	0.60
1:B:190:ARG:HB3	1:B:192:PHE:CE1	2.37	0.60
1:B:356:LYS:O	1:B:396:TYR:HA	2.01	0.60
1:C:356:LYS:O	1:C:396:TYR:HA	2.01	0.60
1:C:430:THR:HG21	1:C:517:LEU:HG	1.84	0.60
2:D:37:GLN:HB2	2:D:43:PRO:HG3	1.82	0.60
3:E:18:VAL:HG12	3:E:86:LEU:HD21	1.84	0.60
1:B:361:CYS:O	1:B:525:CYS:N	2.29	0.60
1:B:854:LYS:HA	1:B:858:LEU:O	2.02	0.60
1:B:1080:ALA:O	1:B:1081:ILE:HG13	2.02	0.60
1:C:444:LYS:HD2	1:C:448:ASN:HB2	1.83	0.60
1:C:600:PRO:HB3	1:C:674:TYR:HB2	1.84	0.60
1:C:1102:TRP:HB2	1:C:1135:ASN:ND2	2.16	0.60
2:H:32:LEU:HD21	2:H:87:CYS:HB2	1.84	0.60
1:A:134:GLN:NE2	1:A:135:PHE:H	2.00	0.59
1:B:134:GLN:NE2	1:B:135:PHE:H	2.00	0.59
1:C:1089:PHE:N	1:C:1089:PHE:CD1	2.70	0.59
2:D:33:HIS:NE2	3:E:105:TYR:O	2.35	0.59
3:E:13:LYS:NZ	3:E:120:SER:O	2.33	0.59
1:A:1080:ALA:O	1:A:1081:ILE:HG13	2.02	0.59
1:B:434:ILE:O	1:B:510:VAL:HA	2.02	0.59
2:D:35:TYR:HB2	2:D:86:PHE:HB2	1.84	0.59
1:A:434:ILE:O	1:A:510:VAL:HA	2.03	0.59
1:A:860:VAL:O	1:A:860:VAL:HG12	2.01	0.59
1:C:434:ILE:O	1:C:510:VAL:HA	2.03	0.59
1:C:559:PHE:HB2	1:C:584:ILE:HD11	1.83	0.59
1:A:430:THR:HG21	1:A:517:LEU:HG	1.84	0.59
1:B:385:THR:HG21	3:G:65:LYS:HE2	1.83	0.59
1:B:430:THR:HG21	1:B:517:LEU:HG	1.84	0.59
1:C:1088:HIS:ND1	1:C:1122:VAL:HG22	2.17	0.59
1:C:1089:PHE:N	1:C:1089:PHE:HD1	1.98	0.59
1:A:327:VAL:O	1:A:531:THR:N	2.35	0.59
1:A:363:ALA:N	1:A:525:CYS:O	2.34	0.59
1:A:1089:PHE:N	1:A:1089:PHE:CD1	2.70	0.59
1:B:860:VAL:O	1:B:860:VAL:HG12	2.01	0.59
1:C:57:PRO:HG2	1:C:271:GLN:OE1	2.02	0.59
2:D:88:GLN:HG2	2:D:97:PHE:CD1	2.37	0.59
1:B:525:CYS:SG	1:B:526:GLY:N	2.76	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:190:ARG:HB3	1:C:192:PHE:CE1	2.37	0.59
1:C:525:CYS:SG	1:C:526:GLY:N	2.76	0.59
2:D:32:LEU:HD21	2:D:87:CYS:HB2	1.84	0.59
1:A:398:ASP:O	1:A:511:VAL:HA	2.02	0.59
1:C:323:THR:OG1	1:C:537:LYS:HE3	2.03	0.59
1:A:43:PHE:HD1	1:B:563:GLN:CD	2.10	0.59
1:B:141:LEU:O	1:B:244:LEU:N	2.30	0.59
1:B:363:ALA:N	1:B:525:CYS:O	2.34	0.59
1:C:107:GLY:H	1:C:235:ILE:HG23	1.68	0.59
1:C:239:GLN:HG2	1:C:240:THR:O	2.03	0.59
2:F:95:TYR:HB2	2:F:97:PHE:HE1	1.68	0.59
2:H:88:GLN:HG2	2:H:97:PHE:CD1	2.37	0.59
1:A:107:GLY:H	1:A:235:ILE:HG23	1.68	0.59
1:A:650:LEU:HD21	1:A:653:ALA:HB3	1.85	0.59
1:A:1088:HIS:ND1	1:A:1122:VAL:HG22	2.17	0.59
1:B:515:PHE:HD2	1:B:517:LEU:H	1.49	0.59
1:B:132:GLU:O	1:B:164:ASN:N	2.36	0.58
1:A:132:GLU:O	1:A:164:ASN:N	2.36	0.58
1:A:395:VAL:HA	1:A:514:SER:O	2.03	0.58
1:A:444:LYS:HD2	1:A:448:ASN:HB2	1.83	0.58
1:A:849:LEU:HD23	1:A:849:LEU:O	2.03	0.58
1:A:855:PHE:CE1	1:B:589:PRO:HD3	2.38	0.58
1:B:396:TYR:HB2	1:B:514:SER:HB2	1.85	0.58
1:B:490:PHE:CE2	1:B:492:LEU:HB2	2.38	0.58
1:B:498:GLN:O	1:B:501:ASN:N	2.36	0.58
1:C:134:GLN:NE2	1:C:135:PHE:H	2.00	0.58
1:C:395:VAL:HA	1:C:514:SER:O	2.03	0.58
1:C:587:ILE:HG22	1:C:588:THR:H	1.68	0.58
1:A:67:ALA:HB3	1:A:263:ALA:HB3	1.84	0.58
1:A:97:LYS:HE2	1:A:186:PHE:HE1	1.68	0.58
1:A:365:TYR:HD1	1:A:368:LEU:HD12	1.69	0.58
1:A:377:PHE:HB3	2:D:93:TRP:CD1	2.39	0.58
1:A:587:ILE:HG22	1:A:588:THR:H	1.68	0.58
1:B:587:ILE:HG22	1:B:588:THR:H	1.68	0.58
1:B:605:SER:OG	1:B:606:ASN:N	2.31	0.58
1:B:856:ASN:O	1:B:858:LEU:HD12	2.03	0.58
1:C:97:LYS:HE2	1:C:186:PHE:HE1	1.68	0.58
1:A:239:GLN:HG2	1:A:240:THR:O	2.03	0.58
1:A:986:PRO:O	1:A:990:GLU:HG2	2.03	0.58
1:A:1050:MET:O	1:A:1051:SER:OG	2.21	0.58
1:B:107:GLY:H	1:B:235:ILE:HG23	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:365:TYR:HD1	1:C:368:LEU:HD12	1.69	0.58
1:C:396:TYR:HB2	1:C:514:SER:HB2	1.85	0.58
3:E:58:THR:HG22	3:E:70:LEU:HB2	1.85	0.58
1:A:676:THR:HG23	1:A:690:GLN:HA	1.86	0.58
1:B:67:ALA:HB3	1:B:263:ALA:HB3	1.84	0.58
1:B:398:ASP:O	1:B:511:VAL:HA	2.02	0.58
1:B:725:GLU:OE1	1:B:1064:HIS:NE2	2.30	0.58
1:C:398:ASP:O	1:C:511:VAL:HA	2.02	0.58
1:C:650:LEU:HD21	1:C:653:ALA:HB3	1.85	0.58
1:B:57:PRO:HG2	1:B:271:GLN:OE1	2.02	0.58
1:B:97:LYS:HE2	1:B:186:PHE:HE1	1.68	0.58
3:E:100:GLU:HG2	3:E:106:VAL:HG22	1.85	0.58
3:I:35:HIS:CD2	3:I:99:SER:HB2	2.39	0.58
1:A:396:TYR:HB2	1:A:514:SER:HB2	1.85	0.58
1:A:600:PRO:HB3	1:A:674:TYR:HB2	1.84	0.58
1:B:1089:PHE:N	1:B:1089:PHE:CD1	2.70	0.58
1:C:170:TYR:OH	1:C:172:SER:OG	2.20	0.58
2:H:35:TYR:HB2	2:H:86:PHE:HB2	1.84	0.58
3:I:18:VAL:HG12	3:I:86:LEU:HD21	1.84	0.58
1:A:854:LYS:O	1:A:854:LYS:HG2	2.02	0.58
1:A:894:LEU:HD21	1:B:1072:GLU:HG2	1.85	0.58
1:B:800:PHE:HD2	1:B:927:PHE:CD2	2.21	0.58
1:C:363:ALA:N	1:C:525:CYS:O	2.34	0.58
1:C:800:PHE:HD2	1:C:927:PHE:CD2	2.21	0.58
3:I:47:TRP:HZ2	3:I:50:TYR:HB3	1.69	0.58
3:I:100:GLU:HG2	3:I:106:VAL:HG22	1.85	0.58
1:A:393:THR:HB	1:A:520:ALA:HB3	1.86	0.58
1:A:525:CYS:SG	1:A:526:GLY:N	2.76	0.58
1:B:986:PRO:O	1:B:990:GLU:HG2	2.03	0.58
2:D:35:TYR:CZ	2:D:45:LEU:HD13	2.38	0.58
3:E:47:TRP:HZ2	3:E:50:TYR:HB3	1.69	0.58
2:F:5:THR:N	2:F:23:ARG:O	2.36	0.58
1:A:490:PHE:CE2	1:A:492:LEU:HB2	2.38	0.58
1:A:616:ASN:ND2	5:A:1307:NAG:O7	2.37	0.58
1:A:955:ASN:O	1:A:958:ALA:N	2.37	0.58
1:A:1088:HIS:HD1	1:A:1122:VAL:HG22	1.69	0.58
1:A:1089:PHE:HB3	1:A:1090:PRO:HD2	1.86	0.58
1:B:616:ASN:ND2	5:B:1307:NAG:O7	2.37	0.58
1:B:650:LEU:HD21	1:B:653:ALA:HB3	1.85	0.58
1:C:132:GLU:O	1:C:164:ASN:N	2.36	0.58
1:C:676:THR:HG23	1:C:690:GLN:HA	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:807:PRO:HA	1:C:816:SER:HB3	1.86	0.58
3:I:13:LYS:NZ	3:I:120:SER:O	2.33	0.58
1:A:957:GLN:O	1:A:957:GLN:NE2	2.37	0.57
1:B:239:GLN:HG2	1:B:240:THR:O	2.03	0.57
1:B:320:VAL:HG21	1:B:591:SER:OG	2.03	0.57
1:C:616:ASN:ND2	5:C:1307:NAG:O7	2.37	0.57
2:H:31:ASN:CG	2:H:90:THR:HG21	2.29	0.57
2:H:35:TYR:CZ	2:H:45:LEU:HD13	2.38	0.57
1:A:807:PRO:HA	1:A:816:SER:HB3	1.86	0.57
1:B:27:ALA:O	1:B:64:TRP:HB3	2.05	0.57
1:B:125:ASN:HB2	5:B:1302:NAG:H81	1.86	0.57
1:B:395:VAL:HA	1:B:514:SER:O	2.03	0.57
3:G:73:ASP:HB2	3:G:80:TYR:HE2	1.70	0.57
1:B:327:VAL:O	1:B:531:THR:N	2.35	0.57
1:B:600:PRO:HB3	1:B:674:TYR:HB2	1.85	0.57
1:B:800:PHE:CD2	1:B:927:PHE:HD2	2.22	0.57
1:C:393:THR:HB	1:C:520:ALA:HB3	1.86	0.57
2:D:31:ASN:CG	2:D:90:THR:HG21	2.29	0.57
1:C:490:PHE:CE2	1:C:492:LEU:HB2	2.38	0.57
1:C:574:ASP:OD2	1:C:575:ALA:N	2.38	0.57
1:C:645:THR:OG1	1:C:648:GLY:N	2.29	0.57
2:F:34:TRP:O	2:F:46:LEU:N	2.36	0.57
1:A:404:GLY:HA2	1:A:508:TYR:CD2	2.40	0.57
1:A:555:SER:OG	1:A:584:ILE:O	2.22	0.57
1:A:786:LYS:HG3	1:A:787:GLN:H	1.70	0.57
1:A:800:PHE:HD2	1:A:927:PHE:CD2	2.22	0.57
1:C:1089:PHE:HB3	1:C:1090:PRO:HD2	1.86	0.57
1:A:485:GLY:H	1:A:488:CYS:HB2	1.69	0.57
1:B:343:ASN:ND2	5:B:1305:NAG:O7	2.38	0.57
1:B:955:ASN:O	1:B:958:ALA:N	2.37	0.57
1:B:1089:PHE:HB3	1:B:1090:PRO:HD2	1.86	0.57
1:C:404:GLY:HA2	1:C:508:TYR:CD2	2.40	0.57
1:C:559:PHE:CE2	1:C:565:PHE:C	2.80	0.57
1:C:986:PRO:O	1:C:990:GLU:HG2	2.03	0.57
2:F:12:VAL:O	2:F:105:ILE:HA	2.03	0.57
1:A:125:ASN:HB2	5:A:1302:NAG:H81	1.86	0.57
1:A:1043:CYS:HB3	1:A:1048:HIS:HD2	1.68	0.57
1:B:224:GLU:OE1	1:B:224:GLU:N	2.27	0.57
1:B:393:THR:HB	1:B:520:ALA:HB3	1.86	0.57
1:B:574:ASP:OD2	1:B:575:ALA:N	2.38	0.57
1:B:807:PRO:HA	1:B:816:SER:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:LEU:O	1:C:244:LEU:N	2.30	0.57
2:F:22:CYS:SG	2:F:32:LEU:HD11	2.45	0.57
2:F:43:PRO:HD2	3:G:110:TRP:HZ3	1.68	0.57
2:F:93:TRP:CE3	2:F:94:PRO:HD3	2.39	0.57
1:A:800:PHE:CD2	1:A:927:PHE:HD2	2.22	0.57
1:B:365:TYR:HD1	1:B:368:LEU:HD12	1.68	0.57
1:B:438:SER:O	1:B:442:ASP:N	2.38	0.57
1:C:619:GLU:OE1	1:C:619:GLU:N	2.26	0.57
3:E:35:HIS:CD2	3:E:99:SER:HB2	2.39	0.57
3:G:4:LEU:HD23	3:G:24:VAL:HG22	1.86	0.57
1:A:666:ILE:HD11	1:A:672:ALA:HB2	1.87	0.57
1:B:676:THR:HG23	1:B:690:GLN:HA	1.86	0.57
1:B:786:LYS:HG3	1:B:787:GLN:H	1.70	0.57
3:E:73:ASP:O	3:E:77:ASP:N	2.38	0.57
3:G:6:GLN:OE1	3:G:113:GLY:N	2.31	0.57
3:I:58:THR:HG22	3:I:70:LEU:HB2	1.85	0.57
3:I:73:ASP:O	3:I:77:ASP:N	2.38	0.57
1:A:390:LEU:HD11	1:A:518:LEU:HD11	1.87	0.57
1:A:574:ASP:OD2	1:A:575:ALA:N	2.38	0.57
1:B:390:LEU:HD11	1:B:518:LEU:HD11	1.87	0.57
1:B:559:PHE:CZ	1:B:566:GLY:CA	2.83	0.57
1:C:485:GLY:H	1:C:488:CYS:HB2	1.69	0.57
1:C:766:ALA:O	1:C:769:GLY:N	2.38	0.57
1:B:1088:HIS:HD1	1:B:1122:VAL:HG22	1.69	0.56
1:C:144:TYR:N	1:C:151:SER:O	2.30	0.56
1:C:502:GLY:O	1:C:506:GLN:HG3	2.05	0.56
1:C:858:LEU:HD12	1:C:858:LEU:N	2.20	0.56
3:G:33:TYR:CE1	3:G:101:TYR:CD1	2.92	0.56
1:B:485:GLY:H	1:B:488:CYS:HB2	1.69	0.56
1:C:27:ALA:O	1:C:64:TRP:HB3	2.05	0.56
2:F:34:TRP:CD1	2:F:47:ILE:HB	2.39	0.56
1:A:498:GLN:O	1:A:501:ASN:N	2.36	0.56
1:A:766:ALA:O	1:A:769:GLY:N	2.38	0.56
1:B:347:PHE:CE2	1:B:509:ARG:HB3	2.40	0.56
1:B:957:GLN:NE2	1:B:957:GLN:O	2.37	0.56
1:C:327:VAL:O	1:C:531:THR:N	2.37	0.56
1:C:666:ILE:HD11	1:C:672:ALA:HB2	1.87	0.56
1:C:800:PHE:CD2	1:C:927:PHE:HD2	2.22	0.56
1:A:27:ALA:O	1:A:64:TRP:HB3	2.04	0.56
1:A:343:ASN:ND2	5:A:1305:NAG:O7	2.38	0.56
1:A:347:PHE:CE2	1:A:509:ARG:HB3	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:766:ALA:O	1:B:769:GLY:N	2.38	0.56
1:C:125:ASN:HB2	5:C:1302:NAG:H81	1.86	0.56
1:B:502:GLY:O	1:B:506:GLN:HG3	2.05	0.56
1:B:645:THR:OG1	1:B:648:GLY:N	2.29	0.56
1:B:914:ASN:HD22	1:C:1123:SER:HB2	1.69	0.56
1:C:347:PHE:CE2	1:C:509:ARG:HB3	2.40	0.56
1:C:557:LYS:O	1:C:584:ILE:HG13	2.05	0.56
1:C:955:ASN:O	1:C:958:ALA:N	2.37	0.56
3:I:37:VAL:O	3:I:95:TYR:N	2.36	0.56
1:A:336:CYS:SG	1:A:524:VAL:HG22	2.46	0.56
1:C:655:HIS:CD2	1:C:656:VAL:H	2.24	0.56
1:C:901:GLN:C	1:C:903:ALA:N	2.63	0.56
1:A:655:HIS:CD2	1:A:656:VAL:H	2.24	0.56
1:B:404:GLY:HA2	1:B:508:TYR:CD2	2.40	0.56
1:C:336:CYS:SG	1:C:524:VAL:HG22	2.46	0.56
1:C:901:GLN:HE21	1:C:905:ARG:NE	2.04	0.56
2:D:36:GLN:NE2	2:D:81:ASP:O	2.38	0.56
2:F:33:HIS:HA	2:F:47:ILE:O	2.05	0.56
1:B:37:TYR:HA	1:B:223:LEU:H	1.71	0.56
1:C:438:SER:O	1:C:442:ASP:N	2.38	0.56
1:C:786:LYS:HG3	1:C:787:GLN:H	1.70	0.56
1:C:957:GLN:O	1:C:957:GLN:NE2	2.38	0.56
2:F:17:LYS:HG2	2:F:75:ASN:HA	1.88	0.56
1:A:228:ASP:OD1	1:A:229:LEU:N	2.39	0.56
1:C:343:ASN:ND2	5:C:1305:NAG:O7	2.38	0.56
1:C:390:LEU:HD11	1:C:518:LEU:HD11	1.87	0.56
1:A:37:TYR:HA	1:A:223:LEU:H	1.71	0.56
1:A:438:SER:O	1:A:442:ASP:N	2.38	0.56
1:A:901:GLN:HE21	1:A:905:ARG:NE	2.04	0.56
1:B:323:THR:HG21	1:B:537:LYS:HE3	1.87	0.56
1:B:336:CYS:SG	1:B:524:VAL:HG22	2.46	0.56
1:B:655:HIS:CD2	1:B:656:VAL:H	2.24	0.56
1:B:655:HIS:CD2	1:B:656:VAL:N	2.74	0.56
1:B:901:GLN:C	1:B:903:ALA:N	2.63	0.56
1:C:498:GLN:O	1:C:501:ASN:N	2.36	0.56
3:E:56:GLY:O	3:E:58:THR:N	2.38	0.56
1:A:354:ASN:HD22	1:A:399:SER:HB3	1.71	0.55
1:A:365:TYR:CD1	1:A:368:LEU:HD12	2.41	0.55
1:A:560:LEU:HD12	1:A:562:PHE:HE1	1.70	0.55
1:B:147:LYS:CB	1:B:152:TRP:HE1	2.19	0.55
1:B:324:GLU:OE1	1:B:325:SER:N	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1067:TYR:CD2	1:B:1067:TYR:O	2.60	0.55
1:C:37:TYR:HA	1:C:223:LEU:H	1.71	0.55
1:C:1050:MET:O	1:C:1051:SER:OG	2.21	0.55
3:E:35:HIS:O	3:E:97:ALA:N	2.30	0.55
2:H:36:GLN:NE2	2:H:81:ASP:O	2.38	0.55
3:I:90:ASP:O	3:I:94:TYR:OH	2.19	0.55
1:A:655:HIS:CD2	1:A:656:VAL:N	2.74	0.55
1:A:900:MET:SD	1:B:1077:THR:OG1	2.61	0.55
1:B:645:THR:OG1	1:B:648:GLY:O	2.15	0.55
1:C:1088:HIS:HD1	1:C:1122:VAL:HG22	1.69	0.55
2:F:34:TRP:O	2:F:45:LEU:HD12	2.06	0.55
2:H:15:LYS:HA	2:H:76:SER:HA	1.88	0.55
3:I:56:GLY:O	3:I:58:THR:N	2.38	0.55
1:A:557:LYS:O	1:A:584:ILE:CG2	2.49	0.55
1:A:731:MET:HG2	1:A:774:GLN:OE1	2.07	0.55
1:A:901:GLN:C	1:A:903:ALA:N	2.63	0.55
1:B:365:TYR:CD1	1:B:368:LEU:HD12	2.41	0.55
1:B:375:SER:CB	1:B:436:TRP:HA	2.36	0.55
1:B:914:ASN:HD22	1:C:1123:SER:CB	2.19	0.55
1:C:802:PHE:CD1	1:C:805:ILE:HD11	2.41	0.55
3:G:40:ALA:HB3	3:G:43:LYS:HB2	1.88	0.55
1:B:409:GLN:HB3	1:B:418:ILE:HB	1.89	0.55
2:D:15:LYS:HA	2:D:76:SER:HA	1.89	0.55
1:A:502:GLY:O	1:A:506:GLN:HG3	2.05	0.55
1:B:1141:LEU:O	1:B:1144:GLU:N	2.39	0.55
3:G:58:THR:HG22	3:G:70:LEU:HB2	1.89	0.55
1:A:1067:TYR:CD2	1:A:1067:TYR:O	2.60	0.55
1:B:148:ASN:OD1	1:B:149:ASN:N	2.40	0.55
1:B:378:LYS:O	1:B:433:VAL:N	2.34	0.55
1:B:1027:THR:O	1:B:1030:SER:N	2.40	0.55
1:C:375:SER:CB	1:C:436:TRP:HA	2.37	0.55
1:C:409:GLN:HB3	1:C:418:ILE:HB	1.89	0.55
1:C:1067:TYR:CD2	1:C:1067:TYR:O	2.60	0.55
1:B:320:VAL:CG2	1:B:591:SER:OG	2.54	0.55
1:B:901:GLN:HE21	1:B:905:ARG:NE	2.04	0.55
1:C:147:LYS:CB	1:C:152:TRP:HE1	2.19	0.55
1:C:861:LEU:N	1:C:861:LEU:HD23	2.21	0.55
1:A:295:PRO:O	1:A:298:GLU:N	2.39	0.55
1:A:544:ASN:ND2	1:A:579:PRO:HB3	2.19	0.55
1:B:167:THR:HA	1:C:357:ARG:HH12	1.72	0.55
1:C:1116:THR:H	1:C:1119:ASN:ND2	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:6:GLN:HA	3:I:21:SER:O	2.07	0.55
1:A:147:LYS:CB	1:A:152:TRP:HE1	2.19	0.55
1:A:375:SER:CB	1:A:436:TRP:HA	2.36	0.55
1:A:409:GLN:HB3	1:A:418:ILE:HB	1.89	0.55
1:B:354:ASN:HD22	1:B:399:SER:HB3	1.71	0.55
1:C:228:ASP:OD1	1:C:229:LEU:N	2.39	0.55
1:C:1043:CYS:HB3	1:C:1048:HIS:HD2	1.68	0.55
3:E:38:LYS:O	3:E:46:GLU:N	2.40	0.55
3:G:112:GLN:OE1	3:G:112:GLN:N	2.36	0.55
1:A:201:PHE:CE2	1:A:203:ILE:HG13	2.42	0.55
1:B:802:PHE:CD1	1:B:805:ILE:HD11	2.41	0.55
1:C:655:HIS:CD2	1:C:656:VAL:N	2.74	0.55
1:C:1000:ARG:O	1:C:1003:SER:N	2.40	0.55
3:E:6:GLN:HA	3:E:21:SER:O	2.07	0.55
1:A:136:CYS:H	1:A:139:PRO:HG3	1.72	0.54
1:A:1027:THR:O	1:A:1030:SER:N	2.40	0.54
1:B:201:PHE:CE2	1:B:203:ILE:HG13	2.42	0.54
1:B:228:ASP:OD1	1:B:229:LEU:N	2.39	0.54
1:B:666:ILE:HD11	1:B:672:ALA:HB2	1.87	0.54
1:B:731:MET:HG2	1:B:774:GLN:OE1	2.07	0.54
1:A:323:THR:HG21	1:A:537:LYS:HZ1	1.70	0.54
1:A:1000:ARG:O	1:A:1003:SER:N	2.40	0.54
1:C:365:TYR:CD1	1:C:368:LEU:HD12	2.41	0.54
1:C:544:ASN:ND2	1:C:579:PRO:HB3	2.19	0.54
1:C:1004:LEU:O	1:C:1007:TYR:N	2.41	0.54
3:G:4:LEU:N	3:G:109:TYR:HE2	2.05	0.54
1:A:1084:ASP:HB2	1:A:1086:LYS:NZ	2.22	0.54
1:B:118:LEU:HD23	1:B:129:LYS:HE2	1.89	0.54
1:B:1000:ARG:O	1:B:1003:SER:N	2.40	0.54
1:A:90:VAL:HG21	1:A:238:PHE:CE1	2.42	0.54
1:A:144:TYR:HD2	1:A:152:TRP:CD1	2.25	0.54
1:A:746:SER:OG	1:A:748:GLU:OE1	2.15	0.54
1:B:1084:ASP:HB2	1:B:1086:LYS:NZ	2.22	0.54
1:B:1143:PRO:HA	1:B:1146:ASP:HB2	1.90	0.54
1:A:412:PRO:HB3	1:A:426:PRO:O	2.08	0.54
1:A:1116:THR:H	1:A:1119:ASN:ND2	2.05	0.54
1:B:100:ILE:HG22	1:B:242:LEU:HD22	1.89	0.54
1:B:1085:GLY:HA2	1:B:1126:CYS:SG	2.48	0.54
1:C:90:VAL:HG21	1:C:238:PHE:CE1	2.42	0.54
1:C:201:PHE:CE2	1:C:203:ILE:HG13	2.42	0.54
1:C:214:ARG:HB3	1:C:214:ARG:CZ	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:365:TYR:CE2	1:C:369:TYR:CE1	2.96	0.54
1:A:118:LEU:HD23	1:A:129:LYS:HE2	1.89	0.54
1:A:557:LYS:HB2	1:A:584:ILE:CG2	2.38	0.54
1:B:214:ARG:HB3	1:B:214:ARG:CZ	2.38	0.54
1:B:650:LEU:HD23	1:B:650:LEU:C	2.33	0.54
1:C:1027:THR:O	1:C:1030:SER:N	2.40	0.54
1:C:1085:GLY:HA2	1:C:1126:CYS:SG	2.48	0.54
2:D:28:ILE:HG21	2:D:68:THR:HA	1.90	0.54
3:G:6:GLN:HE22	3:G:96:CYS:H	1.55	0.54
3:G:33:TYR:CZ	3:G:101:TYR:CD1	2.95	0.54
1:B:90:VAL:HG21	1:B:238:PHE:CE1	2.42	0.54
1:B:144:TYR:HD2	1:B:152:TRP:CD1	2.25	0.54
1:B:763:LEU:HD22	1:B:1008:VAL:HG21	1.90	0.54
1:C:731:MET:HG2	1:C:774:GLN:OE1	2.06	0.54
3:G:28:SER:OG	3:G:31:ASN:ND2	2.41	0.54
1:A:42:VAL:HG22	1:B:565:PHE:CE2	2.43	0.54
1:A:320:VAL:CG2	1:A:591:SER:OG	2.56	0.54
1:A:557:LYS:CB	1:A:584:ILE:HG21	2.38	0.54
1:A:1008:VAL:O	1:A:1011:GLN:N	2.41	0.54
1:B:136:CYS:H	1:B:139:PRO:HG3	1.72	0.54
1:B:323:THR:HG21	1:B:537:LYS:HZ2	1.72	0.54
1:C:354:ASN:HD22	1:C:399:SER:HB3	1.71	0.54
1:C:897:PRO:HD2	1:C:900:MET:HB2	1.90	0.54
2:F:34:TRP:CE3	2:F:72:LEU:HB2	2.43	0.54
1:B:110:LEU:HD13	1:B:237:ARG:NH2	2.23	0.54
1:B:619:GLU:OE1	1:B:619:GLU:N	2.26	0.54
1:C:148:ASN:OD1	1:C:149:ASN:N	2.40	0.54
1:C:350:VAL:HB	1:C:402:ILE:HG22	1.90	0.54
1:C:1141:LEU:O	1:C:1144:GLU:N	2.39	0.54
2:D:33:HIS:HA	2:D:47:ILE:O	2.08	0.54
3:I:91:THR:HA	3:I:116:VAL:O	2.08	0.54
1:A:214:ARG:HB3	1:A:214:ARG:CZ	2.38	0.54
1:A:562:PHE:CD2	1:C:225:PRO:HD2	2.43	0.54
1:C:53:ASP:OD1	1:C:54:LEU:N	2.41	0.54
1:C:100:ILE:HG22	1:C:242:LEU:HD22	1.89	0.54
1:C:959:LEU:O	1:C:962:LEU:N	2.41	0.54
3:E:37:VAL:O	3:E:95:TYR:N	2.36	0.54
3:I:18:VAL:O	3:I:83:LEU:N	2.34	0.54
3:I:66:GLY:O	3:I:84:SER:OG	2.21	0.54
1:A:53:ASP:OD1	1:A:54:LEU:N	2.41	0.53
1:A:148:ASN:OD1	1:A:149:ASN:N	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:THR:HG22	1:A:435:ALA:H	1.73	0.53
1:A:650:LEU:C	1:A:650:LEU:HD23	2.33	0.53
1:A:1004:LEU:O	1:A:1007:TYR:N	2.41	0.53
1:B:318:PHE:CE1	1:B:592:PHE:O	2.61	0.53
1:B:365:TYR:CE2	1:B:369:TYR:CE1	2.96	0.53
1:C:136:CYS:H	1:C:139:PRO:HG3	1.72	0.53
1:C:406:GLU:OE2	1:C:495:TYR:OH	2.19	0.53
1:A:110:LEU:HD13	1:A:237:ARG:NH2	2.23	0.53
1:A:320:VAL:HG21	1:A:591:SER:OG	2.08	0.53
1:A:802:PHE:CD1	1:A:805:ILE:HD11	2.41	0.53
1:A:1085:GLY:HA2	1:A:1126:CYS:SG	2.48	0.53
1:B:559:PHE:HZ	1:B:566:GLY:HA3	1.72	0.53
1:B:891:GLY:HA2	1:C:1045:LYS:HZ1	1.73	0.53
1:C:360:ASN:H	1:C:523:THR:HA	1.74	0.53
1:C:1084:ASP:HB2	1:C:1086:LYS:NZ	2.22	0.53
2:H:33:HIS:HA	2:H:47:ILE:O	2.08	0.53
3:I:51:ILE:HD12	3:I:70:LEU:HB3	1.90	0.53
1:A:187:LYS:HD2	1:A:210:ILE:O	2.08	0.53
1:A:360:ASN:H	1:A:523:THR:HA	1.74	0.53
1:A:437:ASN:HA	1:A:508:TYR:HD1	1.74	0.53
1:B:140:PHE:HD2	1:B:141:LEU:O	1.91	0.53
1:C:187:LYS:HD2	1:C:210:ILE:O	2.09	0.53
1:C:412:PRO:HB3	1:C:426:PRO:O	2.08	0.53
3:G:27:TYR:CE2	3:G:98:ARG:HD3	2.43	0.53
1:A:91:TYR:CG	1:A:92:PHE:N	2.76	0.53
1:A:108:THR:OG1	1:A:109:THR:N	2.42	0.53
1:A:959:LEU:O	1:A:962:LEU:N	2.41	0.53
1:B:1004:LEU:O	1:B:1007:TYR:N	2.41	0.53
1:C:110:LEU:HD13	1:C:237:ARG:NH2	2.23	0.53
1:C:144:TYR:HD2	1:C:152:TRP:CD1	2.25	0.53
1:C:1008:VAL:O	1:C:1011:GLN:N	2.41	0.53
1:A:350:VAL:HB	1:A:402:ILE:HG22	1.90	0.53
1:B:350:VAL:HB	1:B:402:ILE:HG22	1.90	0.53
1:B:959:LEU:O	1:B:962:LEU:N	2.41	0.53
1:B:1116:THR:H	1:B:1119:ASN:ND2	2.05	0.53
1:C:376:THR:HG22	1:C:435:ALA:H	1.73	0.53
2:D:93:TRP:CG	2:D:94:PRO:HD3	2.43	0.53
3:E:60:ASP:OD2	3:E:65:LYS:NZ	2.42	0.53
1:A:93:ALA:HB1	1:A:189:LEU:HD11	1.91	0.53
1:A:100:ILE:HG22	1:A:242:LEU:HD22	1.89	0.53
1:A:365:TYR:CE2	1:A:369:TYR:CE1	2.96	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:568:ASP:O	1:A:571:ASP:N	2.34	0.53
1:B:360:ASN:H	1:B:523:THR:HA	1.74	0.53
1:B:412:PRO:HB3	1:B:426:PRO:O	2.08	0.53
1:B:453:TYR:N	1:B:493:GLN:O	2.39	0.53
1:C:140:PHE:HD2	1:C:141:LEU:O	1.91	0.53
3:E:51:ILE:HD12	3:E:70:LEU:HB3	1.90	0.53
2:F:91:ASN:N	2:F:95:TYR:HE1	2.07	0.53
3:G:4:LEU:HD12	3:G:110:TRP:HA	1.91	0.53
1:B:53:ASP:OD1	1:B:54:LEU:N	2.41	0.53
1:B:93:ALA:HB1	1:B:189:LEU:HD11	1.91	0.53
1:B:375:SER:OG	1:B:436:TRP:HA	2.09	0.53
1:C:91:TYR:CG	1:C:92:PHE:N	2.76	0.53
1:C:378:LYS:O	1:C:433:VAL:N	2.34	0.53
1:C:722:VAL:HG22	1:C:1065:VAL:HG22	1.91	0.53
3:G:109:TYR:C	3:G:110:TRP:HD1	2.16	0.53
2:H:34:TRP:CZ3	2:H:87:CYS:HB3	2.44	0.53
1:A:105:ILE:HG13	1:A:241:LEU:HD11	1.91	0.53
1:A:914:ASN:HD22	1:B:1123:SER:CB	2.22	0.53
1:B:320:VAL:CG2	1:B:591:SER:CB	2.86	0.53
1:C:128:ILE:HD12	1:C:170:TYR:CD2	2.43	0.53
1:C:555:SER:OG	1:C:584:ILE:O	2.22	0.53
1:C:1143:PRO:HA	1:C:1146:ASP:HB2	1.90	0.53
2:D:23:ARG:HE	2:D:69:ASP:HB2	1.74	0.53
2:D:34:TRP:CZ3	2:D:87:CYS:HB3	2.44	0.53
3:E:4:LEU:HD21	3:E:27:TYR:OH	2.09	0.53
3:E:91:THR:HA	3:E:116:VAL:O	2.08	0.53
1:A:763:LEU:HD22	1:A:1008:VAL:HG21	1.90	0.53
1:B:897:PRO:HD2	1:B:900:MET:HB2	1.90	0.53
1:C:375:SER:OG	1:C:436:TRP:HA	2.09	0.53
1:C:437:ASN:HA	1:C:508:TYR:HD1	1.74	0.53
1:C:886:TRP:O	1:C:888:PHE:N	2.42	0.53
2:D:43:PRO:HD2	3:E:110:TRP:HZ3	1.74	0.53
3:E:19:LYS:HA	3:E:82:GLU:HA	1.91	0.53
3:E:30:SER:HA	3:E:53:PRO:HB2	1.91	0.53
2:H:28:ILE:HG21	2:H:68:THR:HA	1.90	0.53
2:H:36:GLN:HB2	2:H:46:LEU:HD11	1.91	0.53
3:I:4:LEU:HD21	3:I:27:TYR:OH	2.09	0.53
1:C:295:PRO:O	1:C:298:GLU:N	2.39	0.53
2:F:97:PHE:CZ	3:G:47:TRP:HB2	2.44	0.53
1:A:106:PHE:CD1	1:A:238:PHE:HB2	2.44	0.52
1:B:106:PHE:CD1	1:B:238:PHE:HB2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:376:THR:HG22	1:B:435:ALA:H	1.73	0.52
1:B:1043:CYS:HB3	1:B:1048:HIS:HD2	1.68	0.52
1:C:108:THR:HG21	4:T:1:NAG:O5	2.10	0.52
1:C:650:LEU:HD23	1:C:650:LEU:C	2.33	0.52
1:C:959:LEU:O	1:C:960:ASN:C	2.52	0.52
1:C:1139:ASP:CG	1:C:1142:GLN:H	2.17	0.52
2:F:22:CYS:O	2:F:70:PHE:N	2.41	0.52
3:G:37:VAL:O	3:G:95:TYR:N	2.38	0.52
3:I:35:HIS:O	3:I:97:ALA:N	2.30	0.52
1:A:886:TRP:O	1:A:888:PHE:N	2.42	0.52
1:A:1084:ASP:HB2	1:A:1086:LYS:HZ3	1.74	0.52
1:A:1139:ASP:CG	1:A:1142:GLN:H	2.17	0.52
1:B:340:GLU:O	1:B:344:ALA:HB2	2.09	0.52
1:B:437:ASN:HA	1:B:508:TYR:HD1	1.74	0.52
1:B:886:TRP:O	1:B:888:PHE:N	2.42	0.52
1:B:1084:ASP:HB2	1:B:1086:LYS:HZ3	1.74	0.52
1:C:93:ALA:HB1	1:C:189:LEU:HD11	1.91	0.52
1:C:118:LEU:HD23	1:C:129:LYS:HE2	1.89	0.52
1:C:877:LEU:O	1:C:881:THR:OG1	2.22	0.52
3:I:19:LYS:HA	3:I:82:GLU:HA	1.91	0.52
1:A:108:THR:HG21	4:J:1:NAG:O5	2.10	0.52
1:B:91:TYR:CG	1:B:92:PHE:N	2.76	0.52
1:B:347:PHE:HB2	1:B:401:VAL:HG23	1.91	0.52
1:B:534:VAL:HG11	1:B:537:LYS:HE2	1.92	0.52
1:B:722:VAL:HG22	1:B:1065:VAL:HG22	1.91	0.52
1:B:959:LEU:O	1:B:960:ASN:C	2.52	0.52
1:C:240:THR:OG1	1:C:241:LEU:N	2.42	0.52
2:F:97:PHE:HD2	3:G:45:LEU:CB	2.21	0.52
3:G:33:TYR:CE1	3:G:101:TYR:HD1	2.27	0.52
1:A:140:PHE:HD2	1:A:141:LEU:O	1.91	0.52
1:A:290:ASP:O	1:A:297:SER:HB3	2.10	0.52
1:A:340:GLU:O	1:A:344:ALA:HB2	2.09	0.52
1:A:603:ASN:OD1	5:A:1306:NAG:O5	2.23	0.52
1:A:914:ASN:HD22	1:B:1123:SER:HB2	1.74	0.52
1:A:1143:PRO:HA	1:A:1146:ASP:HB2	1.90	0.52
1:B:295:PRO:O	1:B:298:GLU:N	2.39	0.52
1:B:748:GLU:OE1	1:B:748:GLU:N	2.39	0.52
1:C:105:ILE:HG13	1:C:241:LEU:HD11	1.91	0.52
1:C:763:LEU:HD22	1:C:1008:VAL:HG21	1.90	0.52
1:C:1091:ARG:N	1:C:1119:ASN:O	2.31	0.52
3:E:10:GLU:HG3	3:E:18:VAL:HG23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:21:SER:HA	3:I:80:TYR:HD1	1.74	0.52
3:I:30:SER:HA	3:I:53:PRO:HB2	1.91	0.52
1:A:534:VAL:HG11	1:A:537:LYS:HE2	1.92	0.52
1:A:897:PRO:HD2	1:A:900:MET:HB2	1.90	0.52
1:B:191:GLU:O	1:B:205:SER:HA	2.10	0.52
1:C:340:GLU:O	1:C:344:ALA:HB2	2.09	0.52
1:C:866:THR:O	1:C:868:GLU:N	2.43	0.52
2:D:34:TRP:O	2:D:46:LEU:N	2.38	0.52
3:G:50:TYR:O	3:G:58:THR:HA	2.09	0.52
2:H:77:LEU:HD22	2:H:105:ILE:HD11	1.91	0.52
1:A:65:PHE:HD2	1:A:265:TYR:HH	1.56	0.52
1:A:748:GLU:OE1	1:A:748:GLU:N	2.39	0.52
1:B:105:ILE:HG13	1:B:241:LEU:HD11	1.91	0.52
1:B:127:VAL:HG11	5:B:1302:NAG:H5	1.91	0.52
1:B:187:LYS:HD2	1:B:210:ILE:O	2.08	0.52
1:C:645:THR:OG1	1:C:648:GLY:O	2.15	0.52
3:G:3:GLN:HA	3:G:109:TYR:OH	2.09	0.52
3:G:38:LYS:N	3:G:46:GLU:O	2.31	0.52
1:A:191:GLU:O	1:A:205:SER:HA	2.10	0.52
1:A:377:PHE:HA	1:A:434:ILE:HG12	1.92	0.52
1:A:866:THR:O	1:A:868:GLU:N	2.43	0.52
1:B:342:PHE:HE1	1:B:511:VAL:HG11	1.75	0.52
2:D:97:PHE:HD2	3:E:45:LEU:HB3	1.75	0.52
3:E:27:TYR:CD1	3:E:32:TYR:HD2	2.27	0.52
2:F:93:TRP:CG	2:F:94:PRO:HD3	2.45	0.52
1:A:1082:CYS:N	1:A:1132:ILE:HD11	2.25	0.52
1:A:1100:THR:OG1	1:A:1101:HIS:N	2.42	0.52
1:A:1123:SER:HB2	1:C:914:ASN:HD22	1.75	0.52
1:B:103:GLY:HA2	1:B:119:ILE:O	2.10	0.52
1:B:290:ASP:O	1:B:297:SER:HB3	2.10	0.52
1:B:406:GLU:OE2	1:B:495:TYR:OH	2.19	0.52
1:B:866:THR:O	1:B:868:GLU:N	2.43	0.52
1:B:1139:ASP:CG	1:B:1142:GLN:H	2.17	0.52
1:C:149:ASN:CG	1:C:152:TRP:HA	2.35	0.52
1:C:1082:CYS:N	1:C:1132:ILE:HD11	2.25	0.52
2:D:34:TRP:O	2:D:45:LEU:HD12	2.10	0.52
3:E:38:LYS:N	3:E:46:GLU:O	2.23	0.52
2:H:93:TRP:CG	2:H:94:PRO:HD3	2.43	0.52
1:A:127:VAL:HG11	5:A:1302:NAG:H5	1.91	0.52
1:A:347:PHE:HB2	1:A:401:VAL:HG23	1.91	0.52
1:C:342:PHE:HE1	1:C:511:VAL:HG11	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:378:LYS:HE3	1:C:380:TYR:HA	1.92	0.52
1:C:994:ASP:O	1:C:998:THR:N	2.42	0.52
1:A:587:ILE:HG22	1:A:588:THR:N	2.25	0.52
1:A:722:VAL:HG22	1:A:1065:VAL:HG22	1.91	0.52
1:B:191:GLU:C	1:B:192:PHE:CD1	2.88	0.52
1:B:225:PRO:HD2	1:C:562:PHE:CD2	2.45	0.52
1:C:150:LYS:O	1:C:151:SER:OG	2.23	0.52
1:C:294:ASP:N	1:C:294:ASP:OD1	2.42	0.52
1:C:323:THR:HG21	1:C:537:LYS:NZ	2.25	0.52
3:I:60:ASP:OD2	3:I:65:LYS:NZ	2.42	0.52
1:A:103:GLY:HA2	1:A:119:ILE:O	2.10	0.51
1:A:240:THR:OG1	1:A:241:LEU:N	2.42	0.51
1:B:995:ARG:O	1:B:999:GLY:N	2.36	0.51
1:C:365:TYR:HE2	1:C:369:TYR:CE1	2.28	0.51
1:C:560:LEU:HD12	1:C:562:PHE:HE1	1.74	0.51
2:F:6:GLN:HE22	2:F:87:CYS:N	2.08	0.51
2:H:23:ARG:HE	2:H:69:ASP:HB2	1.74	0.51
1:A:375:SER:OG	1:A:436:TRP:HA	2.09	0.51
1:A:861:LEU:HD23	1:A:861:LEU:H	1.72	0.51
1:A:1141:LEU:O	1:A:1144:GLU:N	2.39	0.51
1:B:128:ILE:HD12	1:B:170:TYR:CD2	2.42	0.51
1:B:1083:HIS:HB2	1:B:1088:HIS:CD2	2.45	0.51
1:C:453:TYR:N	1:C:493:GLN:O	2.39	0.51
1:C:559:PHE:HZ	1:C:566:GLY:CA	2.24	0.51
1:C:658:ASN:ND2	1:C:660:TYR:OH	2.43	0.51
1:C:748:GLU:N	1:C:748:GLU:OE1	2.39	0.51
2:D:22:CYS:HB3	2:D:70:PHE:HB2	1.92	0.51
1:A:658:ASN:ND2	1:A:660:TYR:OH	2.42	0.51
1:A:904:TYR:C	1:A:906:PHE:N	2.68	0.51
1:B:141:LEU:O	1:B:243:ALA:HA	2.10	0.51
1:B:376:THR:HG1	3:G:50:TYR:HH	1.45	0.51
1:B:435:ALA:HA	1:B:510:VAL:HG22	1.93	0.51
1:C:127:VAL:HG11	5:C:1302:NAG:H5	1.91	0.51
1:C:290:ASP:O	1:C:297:SER:HB3	2.10	0.51
1:C:421:TYR:HD1	1:C:457:ARG:HB3	1.75	0.51
1:C:435:ALA:HA	1:C:510:VAL:HG22	1.93	0.51
1:C:534:VAL:HG11	1:C:537:LYS:HE2	1.92	0.51
2:D:3:VAL:HG22	2:D:96:ILE:HD13	1.92	0.51
3:G:35:HIS:CD2	3:G:99:SER:HB2	2.45	0.51
2:H:95:TYR:CE2	3:I:105:TYR:CD2	2.97	0.51
1:A:54:LEU:HD23	1:A:272:PRO:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:LEU:O	1:A:243:ALA:HA	2.10	0.51
1:A:302:THR:HG22	1:A:303:LEU:HD23	1.93	0.51
1:A:365:TYR:HE2	1:A:369:TYR:CE1	2.28	0.51
1:A:429:PHE:HE1	1:A:514:SER:HA	1.76	0.51
1:B:1082:CYS:N	1:B:1132:ILE:HD11	2.25	0.51
1:C:106:PHE:CD1	1:C:238:PHE:HB2	2.44	0.51
1:C:191:GLU:C	1:C:192:PHE:CD1	2.88	0.51
1:C:398:ASP:HB2	1:C:512:VAL:HB	1.92	0.51
1:C:429:PHE:HE1	1:C:514:SER:HA	1.76	0.51
1:C:540:ASN:HA	1:C:549:THR:HG23	1.93	0.51
1:C:723:THR:OG1	1:C:724:THR:N	2.41	0.51
2:D:77:LEU:HD22	2:D:105:ILE:HD11	1.91	0.51
2:H:97:PHE:HD2	3:I:45:LEU:HB3	1.75	0.51
1:A:135:PHE:HA	1:A:160:TYR:HA	1.93	0.51
1:A:149:ASN:CG	1:A:152:TRP:HA	2.35	0.51
1:A:191:GLU:C	1:A:192:PHE:CD1	2.88	0.51
1:A:559:PHE:CZ	1:A:566:GLY:CA	2.90	0.51
1:B:108:THR:HG21	4:O:1:NAG:O5	2.10	0.51
1:B:302:THR:HG22	1:B:303:LEU:HD23	1.93	0.51
1:B:323:THR:HB	1:B:539:VAL:HG12	1.93	0.51
1:B:1027:THR:O	1:B:1028:LYS:C	2.53	0.51
1:C:103:GLY:HA2	1:C:119:ILE:O	2.10	0.51
1:C:191:GLU:O	1:C:205:SER:HA	2.10	0.51
3:E:24:VAL:HB	3:E:77:ASP:HB3	1.93	0.51
3:E:103:PRO:O	3:E:105:TYR:CE2	2.62	0.51
2:H:34:TRP:O	2:H:45:LEU:HD12	2.10	0.51
3:I:61:ASN:OD1	3:I:63:LYS:HD3	2.10	0.51
1:A:393:THR:O	1:A:523:THR:OG1	2.23	0.51
1:A:419:ALA:O	1:A:424:LYS:HD3	2.11	0.51
1:B:419:ALA:O	1:B:424:LYS:HD3	2.11	0.51
1:B:453:TYR:CE2	1:B:455:LEU:HB2	2.46	0.51
1:B:1006:THR:O	1:B:1010:GLN:HG2	2.11	0.51
1:C:347:PHE:HB2	1:C:401:VAL:HG23	1.91	0.51
1:C:1083:HIS:HB2	1:C:1088:HIS:CD2	2.45	0.51
3:E:21:SER:HA	3:E:80:TYR:HD1	1.74	0.51
3:I:38:LYS:O	3:I:46:GLU:N	2.40	0.51
1:A:342:PHE:HE1	1:A:511:VAL:HG11	1.75	0.51
1:A:563:GLN:HG2	1:C:41:LYS:O	2.11	0.51
1:A:858:LEU:N	1:A:858:LEU:CD1	2.73	0.51
1:A:1006:THR:O	1:A:1010:GLN:HG2	2.11	0.51
1:A:1123:SER:CB	1:C:914:ASN:HD22	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:THR:OG1	1:B:241:LEU:N	2.42	0.51
1:C:65:PHE:HD2	1:C:265:TYR:CZ	2.29	0.51
1:C:141:LEU:O	1:C:243:ALA:HA	2.10	0.51
1:C:302:THR:HG22	1:C:303:LEU:HD23	1.93	0.51
3:I:24:VAL:HB	3:I:77:ASP:HB3	1.93	0.51
3:I:27:TYR:CD1	3:I:32:TYR:HD2	2.27	0.51
1:A:65:PHE:HD2	1:A:265:TYR:CZ	2.29	0.51
1:A:150:LYS:O	1:A:151:SER:OG	2.22	0.51
1:A:886:TRP:HB2	1:A:1034:LEU:O	2.11	0.51
1:B:135:PHE:HA	1:B:160:TYR:HA	1.93	0.51
1:B:294:ASP:OD1	1:B:294:ASP:N	2.42	0.51
1:B:429:PHE:HE1	1:B:514:SER:HA	1.76	0.51
1:B:994:ASP:O	1:B:998:THR:N	2.42	0.51
1:B:1043:CYS:CB	1:B:1048:HIS:CD2	2.92	0.51
1:C:453:TYR:CE2	1:C:455:LEU:HB2	2.46	0.51
1:C:656:VAL:HG12	1:C:658:ASN:H	1.76	0.51
1:C:1100:THR:OG1	1:C:1101:HIS:N	2.42	0.51
2:D:36:GLN:HB2	2:D:46:LEU:HD11	1.91	0.51
3:I:10:GLU:HG3	3:I:18:VAL:HG23	1.91	0.51
1:A:324:GLU:CG	1:A:325:SER:N	2.73	0.51
1:A:435:ALA:HA	1:A:510:VAL:HG22	1.93	0.51
1:A:1045:LYS:HZ1	1:C:891:GLY:HA2	1.76	0.51
1:B:618:THR:OG1	1:B:619:GLU:N	2.43	0.51
1:B:1008:VAL:O	1:B:1011:GLN:N	2.41	0.51
1:C:675:GLN:HG3	1:C:676:THR:O	2.11	0.51
1:C:904:TYR:O	1:C:906:PHE:N	2.44	0.51
3:E:61:ASN:OD1	3:E:63:LYS:HD3	2.10	0.51
1:A:43:PHE:CD1	1:B:559:PHE:CD1	2.99	0.51
1:A:328:ARG:NH1	1:A:578:ASP:OD2	2.44	0.51
1:B:111:ASP:C	1:B:113:LYS:H	2.18	0.51
1:B:328:ARG:NH1	1:B:578:ASP:OD2	2.44	0.51
1:B:398:ASP:HB2	1:B:512:VAL:HB	1.92	0.51
1:B:587:ILE:HG22	1:B:588:THR:N	2.25	0.51
1:B:886:TRP:HB2	1:B:1034:LEU:O	2.11	0.51
1:C:112:SER:O	1:C:132:GLU:HB3	2.11	0.51
1:C:316:SER:O	1:C:595:VAL:CB	2.58	0.51
2:F:48:LYS:O	2:F:52:GLN:HB2	2.11	0.51
3:G:35:HIS:N	3:G:97:ALA:O	2.34	0.51
1:A:112:SER:O	1:A:132:GLU:HB3	2.11	0.50
1:A:453:TYR:N	1:A:493:GLN:O	2.39	0.50
1:A:540:ASN:HA	1:A:549:THR:HG23	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:SER:O	1:B:132:GLU:HB3	2.11	0.50
1:B:544:ASN:ND2	1:B:579:PRO:HB3	2.19	0.50
1:B:740:MET:HA	1:B:743:CYS:O	2.11	0.50
1:C:719:THR:HG23	1:C:720:ILE:N	2.26	0.50
2:H:22:CYS:HB3	2:H:70:PHE:HB2	1.92	0.50
3:I:4:LEU:N	3:I:109:TYR:HE2	2.09	0.50
1:A:91:TYR:O	1:A:92:PHE:HB2	2.11	0.50
1:A:315:THR:OG1	1:A:316:SER:N	2.44	0.50
1:A:378:LYS:HE3	1:A:380:TYR:HA	1.92	0.50
1:A:398:ASP:HB2	1:A:512:VAL:HB	1.92	0.50
1:A:402:ILE:HG12	1:A:508:TYR:O	2.12	0.50
1:A:645:THR:OG1	1:A:648:GLY:N	2.29	0.50
1:A:1083:HIS:HB2	1:A:1088:HIS:CD2	2.45	0.50
1:B:402:ILE:HG12	1:B:508:TYR:O	2.12	0.50
1:B:421:TYR:HD1	1:B:457:ARG:HB3	1.75	0.50
1:C:97:LYS:HE2	1:C:186:PHE:CE1	2.46	0.50
1:C:335:LEU:C	1:C:361:CYS:HB2	2.37	0.50
1:A:204:TYR:HB3	1:A:223:LEU:HB3	1.94	0.50
1:A:453:TYR:CE2	1:A:455:LEU:HB2	2.46	0.50
1:B:65:PHE:HD2	1:B:265:TYR:CZ	2.29	0.50
1:B:149:ASN:CG	1:B:152:TRP:HA	2.35	0.50
1:B:192:PHE:HB3	1:B:194:PHE:CE1	2.47	0.50
1:B:204:TYR:HB3	1:B:223:LEU:HB3	1.94	0.50
1:B:374:PHE:HA	1:B:436:TRP:HB3	1.93	0.50
1:B:904:TYR:O	1:B:906:PHE:N	2.44	0.50
1:C:135:PHE:HA	1:C:160:TYR:HA	1.93	0.50
1:C:1006:THR:O	1:C:1010:GLN:HG2	2.11	0.50
3:G:51:ILE:HG12	3:G:52:ASP:N	2.26	0.50
3:I:38:LYS:N	3:I:46:GLU:O	2.23	0.50
1:A:335:LEU:C	1:A:361:CYS:HB2	2.37	0.50
1:A:421:TYR:HD1	1:A:457:ARG:HB3	1.75	0.50
1:A:656:VAL:HG12	1:A:658:ASN:N	2.27	0.50
1:A:904:TYR:O	1:A:906:PHE:N	2.44	0.50
1:B:376:THR:O	1:B:434:ILE:HG23	2.12	0.50
1:C:707:TYR:C	1:C:707:TYR:CD1	2.90	0.50
2:D:47:ILE:HA	2:D:52:GLN:O	2.12	0.50
2:F:26:GLN:HG3	2:F:27:SER:H	1.76	0.50
2:F:42:SER:HB2	3:G:110:TRP:CE3	2.46	0.50
3:G:20:ILE:HD12	3:G:94:TYR:HD2	1.76	0.50
2:H:17:LYS:HG2	2:H:75:ASN:HA	1.93	0.50
1:A:64:TRP:CD1	1:A:65:PHE:N	2.80	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:LEU:HD21	1:B:119:ILE:HD11	1.93	0.50
1:B:656:VAL:HG12	1:B:658:ASN:H	1.76	0.50
1:C:111:ASP:C	1:C:113:LYS:H	2.18	0.50
1:C:377:PHE:HA	1:C:434:ILE:HG12	1.92	0.50
1:C:564:GLN:OE1	1:C:564:GLN:HA	2.06	0.50
1:C:587:ILE:HG22	1:C:588:THR:N	2.25	0.50
1:C:656:VAL:HG12	1:C:658:ASN:N	2.27	0.50
1:C:904:TYR:C	1:C:906:PHE:N	2.68	0.50
2:D:17:LYS:HG2	2:D:75:ASN:HA	1.94	0.50
2:H:3:VAL:HG22	2:H:96:ILE:HD13	1.92	0.50
1:A:877:LEU:O	1:A:881:THR:OG1	2.22	0.50
1:A:1027:THR:O	1:A:1028:LYS:C	2.53	0.50
1:B:97:LYS:HE2	1:B:186:PHE:CE1	2.46	0.50
1:B:378:LYS:HE3	1:B:380:TYR:HA	1.92	0.50
1:B:904:TYR:C	1:B:906:PHE:N	2.68	0.50
1:C:64:TRP:CD1	1:C:65:PHE:N	2.80	0.50
1:C:192:PHE:HB3	1:C:194:PHE:CE1	2.47	0.50
2:D:12:VAL:HG12	2:D:13:SER:N	2.27	0.50
2:F:84:ILE:HG12	2:F:102:LYS:HA	1.93	0.50
3:G:33:TYR:HD2	3:G:105:TYR:HE1	1.60	0.50
1:A:388:ASN:HA	1:A:527:PRO:HD2	1.94	0.50
1:A:560:LEU:HB2	1:A:563:GLN:HB2	1.94	0.50
1:A:959:LEU:O	1:A:960:ASN:C	2.52	0.50
1:B:64:TRP:CD1	1:B:65:PHE:N	2.80	0.50
1:B:407:VAL:HG21	1:B:435:ALA:HB2	1.94	0.50
1:B:733:LYS:HE3	1:B:771:ALA:O	2.12	0.50
1:C:328:ARG:NH1	1:C:578:ASP:OD2	2.44	0.50
1:C:376:THR:O	1:C:434:ILE:HG23	2.12	0.50
3:E:11:VAL:HG22	3:E:117:THR:HB	1.94	0.50
2:H:12:VAL:HG12	2:H:13:SER:N	2.27	0.50
3:I:11:VAL:HG22	3:I:117:THR:HB	1.94	0.50
1:A:111:ASP:C	1:A:113:LYS:H	2.18	0.50
1:A:430:THR:HG22	1:A:515:PHE:CE2	2.47	0.50
1:A:560:LEU:HD12	1:A:562:PHE:CE1	2.47	0.50
1:A:891:GLY:HA2	1:B:1045:LYS:HZ1	1.76	0.50
1:B:377:PHE:HA	1:B:434:ILE:HG12	1.92	0.50
1:B:1100:THR:OG1	1:B:1101:HIS:N	2.42	0.50
1:C:108:THR:HG23	1:C:234:ASN:O	2.12	0.50
1:C:441:LEU:HD22	1:C:509:ARG:HH21	1.77	0.50
3:G:6:GLN:H	3:G:112:GLN:HE22	1.59	0.50
2:H:5:THR:O	2:H:23:ARG:N	2.35	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:GLN:OE1	1:A:115:GLN:N	2.45	0.50
1:A:740:MET:HA	1:A:743:CYS:O	2.11	0.50
1:B:143:VAL:HG13	1:B:151:SER:HA	1.94	0.50
1:B:540:ASN:HA	1:B:549:THR:HG23	1.93	0.50
1:B:707:TYR:CD1	1:B:707:TYR:C	2.90	0.50
1:B:936:ASP:N	1:B:936:ASP:OD1	2.44	0.50
1:C:204:TYR:HB3	1:C:223:LEU:HB3	1.94	0.50
1:C:1142:GLN:O	1:C:1146:ASP:N	2.45	0.50
2:D:34:TRP:CE3	2:D:72:LEU:HB2	2.47	0.50
2:D:82:PHE:HD2	2:D:105:ILE:HD12	1.77	0.50
3:E:4:LEU:N	3:E:109:TYR:HE2	2.09	0.50
2:H:43:PRO:HD2	3:I:110:TRP:HZ3	1.75	0.50
1:A:143:VAL:HG13	1:A:151:SER:HA	1.94	0.49
1:A:656:VAL:HG12	1:A:658:ASN:H	1.76	0.49
1:A:709:ASN:OD1	1:A:709:ASN:N	2.43	0.49
1:B:65:PHE:HD2	1:B:265:TYR:HH	1.57	0.49
1:B:656:VAL:HG12	1:B:658:ASN:N	2.27	0.49
1:B:1088:HIS:C	1:B:1089:PHE:HD1	2.20	0.49
1:C:54:LEU:HD23	1:C:272:PRO:HA	1.93	0.49
1:C:233:ILE:HG22	1:C:234:ASN:O	2.12	0.49
1:C:374:PHE:HA	1:C:436:TRP:HB3	1.93	0.49
1:C:419:ALA:O	1:C:424:LYS:HD3	2.11	0.49
1:C:618:THR:OG1	1:C:619:GLU:N	2.43	0.49
1:C:661:GLU:O	1:C:695:TYR:OH	2.30	0.49
1:C:733:LYS:HE3	1:C:771:ALA:O	2.12	0.49
1:C:886:TRP:HB2	1:C:1034:LEU:O	2.11	0.49
1:A:225:PRO:HD2	1:B:562:PHE:CE2	2.47	0.49
1:A:233:ILE:HG22	1:A:234:ASN:O	2.12	0.49
1:A:349:SER:HB2	1:A:351:TYR:CE2	2.47	0.49
1:B:54:LEU:HD23	1:B:272:PRO:HA	1.93	0.49
1:B:115:GLN:OE1	1:B:115:GLN:N	2.45	0.49
1:B:233:ILE:HG22	1:B:234:ASN:O	2.12	0.49
1:B:335:LEU:C	1:B:361:CYS:HB2	2.37	0.49
1:A:170:TYR:OH	1:A:172:SER:OG	2.20	0.49
1:A:441:LEU:HD22	1:A:509:ARG:HH21	1.77	0.49
1:A:618:THR:OG1	1:A:619:GLU:N	2.43	0.49
1:A:1088:HIS:CE1	1:A:1122:VAL:HG22	2.48	0.49
1:B:759:PHE:O	1:B:760:CYS:C	2.54	0.49
1:B:902:MET:HE1	1:B:1049:LEU:HD13	1.95	0.49
1:C:407:VAL:HG21	1:C:435:ALA:HB2	1.94	0.49
3:G:35:HIS:ND1	3:G:50:TYR:HB3	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:GLY:N	1:A:235:ILE:HG23	2.27	0.49
1:A:192:PHE:HB3	1:A:194:PHE:CE1	2.47	0.49
1:A:294:ASP:OD1	1:A:294:ASP:N	2.42	0.49
1:A:436:TRP:NE1	1:A:509:ARG:HB2	2.27	0.49
1:B:91:TYR:O	1:B:92:PHE:HB2	2.11	0.49
1:B:365:TYR:HE2	1:B:369:TYR:CE1	2.28	0.49
1:B:709:ASN:N	1:B:709:ASN:OD1	2.43	0.49
1:C:91:TYR:O	1:C:92:PHE:HB2	2.11	0.49
1:C:1021:SER:O	1:C:1021:SER:OG	2.30	0.49
2:H:34:TRP:CE3	2:H:72:LEU:HB2	2.47	0.49
3:I:71:THR:O	3:I:80:TYR:N	2.28	0.49
1:A:376:THR:O	1:A:434:ILE:HG23	2.12	0.49
1:B:107:GLY:N	1:B:235:ILE:HG23	2.27	0.49
1:B:349:SER:HB2	1:B:351:TYR:CE2	2.47	0.49
1:B:431:GLY:HA3	1:B:513:LEU:O	2.13	0.49
1:B:568:ASP:O	1:B:571:ASP:N	2.34	0.49
1:B:858:LEU:H	1:B:858:LEU:CD1	2.18	0.49
1:C:402:ILE:HG12	1:C:508:TYR:O	2.12	0.49
1:C:740:MET:HA	1:C:743:CYS:O	2.11	0.49
1:C:883:THR:OG1	1:C:884:SER:N	2.45	0.49
1:C:1088:HIS:C	1:C:1089:PHE:HD1	2.20	0.49
3:G:10:GLU:HG3	3:G:18:VAL:HG23	1.95	0.49
3:G:91:THR:HA	3:G:116:VAL:O	2.12	0.49
2:H:47:ILE:HA	2:H:52:GLN:O	2.12	0.49
1:A:97:LYS:HE2	1:A:186:PHE:CE1	2.46	0.49
1:A:562:PHE:CE2	1:C:225:PRO:CD	2.95	0.49
1:A:675:GLN:HG3	1:A:676:THR:O	2.11	0.49
1:A:733:LYS:HE3	1:A:771:ALA:O	2.12	0.49
1:A:759:PHE:CD2	1:A:1001:LEU:HD21	2.48	0.49
1:A:1088:HIS:C	1:A:1089:PHE:HD1	2.20	0.49
1:B:441:LEU:HD22	1:B:509:ARG:HH21	1.77	0.49
1:B:806:LEU:HD23	1:B:806:LEU:HA	1.54	0.49
1:C:65:PHE:HD2	1:C:265:TYR:HH	1.58	0.49
1:C:324:GLU:O	1:C:540:ASN:HB3	2.12	0.49
1:C:430:THR:HG22	1:C:515:PHE:CE2	2.47	0.49
1:C:709:ASN:N	1:C:709:ASN:OD1	2.43	0.49
2:F:82:PHE:HB3	2:F:105:ILE:HD12	1.93	0.49
3:G:47:TRP:HZ2	3:G:50:TYR:CD2	2.29	0.49
3:G:73:ASP:HB2	3:G:80:TYR:CE2	2.46	0.49
1:A:128:ILE:HD12	1:A:170:TYR:CD2	2.43	0.49
1:A:407:VAL:HG21	1:A:435:ALA:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:869:MET:O	1:A:870:ILE:C	2.56	0.49
1:A:883:THR:OG1	1:A:884:SER:N	2.45	0.49
1:A:902:MET:HE1	1:A:1049:LEU:HD13	1.95	0.49
1:A:1091:ARG:N	1:A:1119:ASN:O	2.31	0.49
1:A:1142:GLN:O	1:A:1146:ASP:N	2.45	0.49
1:B:127:VAL:HG21	5:B:1302:NAG:H5	1.95	0.49
1:B:159:VAL:HB	1:B:160:TYR:CD1	2.46	0.49
1:B:906:PHE:O	1:B:908:GLY:N	2.46	0.49
1:C:349:SER:HB2	1:C:351:TYR:CE2	2.47	0.49
1:C:759:PHE:CD2	1:C:1001:LEU:HD21	2.48	0.49
3:E:6:GLN:H	3:E:112:GLN:HE22	1.61	0.49
3:I:67:ALA:HB3	3:I:84:SER:OG	2.13	0.49
1:A:374:PHE:HA	1:A:436:TRP:HB3	1.93	0.49
1:B:315:THR:OG1	1:B:316:SER:N	2.44	0.49
1:C:107:GLY:N	1:C:235:ILE:HG23	2.27	0.49
1:C:419:ALA:O	1:C:424:LYS:HB2	2.13	0.49
1:C:436:TRP:NE1	1:C:509:ARG:HB2	2.27	0.49
1:C:995:ARG:O	1:C:999:GLY:N	2.36	0.49
1:C:997:ILE:O	1:C:998:THR:C	2.56	0.49
1:A:108:THR:HG23	1:A:234:ASN:O	2.12	0.49
1:A:167:THR:HA	1:B:357:ARG:NH1	2.28	0.49
1:A:759:PHE:O	1:A:760:CYS:C	2.54	0.49
1:A:1091:ARG:NH1	1:A:1118:ASP:O	2.46	0.49
1:B:191:GLU:C	1:B:192:PHE:HD1	2.21	0.49
1:B:378:LYS:HD3	3:G:57:GLY:HA2	1.94	0.49
1:B:658:ASN:ND2	1:B:660:TYR:OH	2.43	0.49
1:B:1088:HIS:CE1	1:B:1122:VAL:HG22	2.47	0.49
3:G:19:LYS:HA	3:G:81:MET:O	2.12	0.49
2:H:82:PHE:HD2	2:H:105:ILE:HD12	1.77	0.49
1:B:92:PHE:CD1	1:B:93:ALA:N	2.81	0.49
1:B:746:SER:OG	1:B:748:GLU:OE1	2.15	0.49
1:B:759:PHE:CD2	1:B:1001:LEU:HD21	2.48	0.49
1:B:821:LEU:O	1:B:825:LYS:HG2	2.13	0.49
1:B:1142:GLN:O	1:B:1146:ASP:N	2.45	0.49
1:C:115:GLN:N	1:C:115:GLN:OE1	2.45	0.49
1:C:117:LEU:HD21	1:C:119:ILE:HD11	1.93	0.49
1:C:503:VAL:HG21	2:H:29:SER:HA	1.94	0.49
1:C:759:PHE:O	1:C:760:CYS:C	2.54	0.49
1:C:869:MET:O	1:C:870:ILE:C	2.56	0.49
1:A:227:VAL:HG12	1:A:228:ASP:N	2.28	0.48
1:A:375:SER:O	2:D:91:ASN:HA	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:707:TYR:CD1	1:A:707:TYR:C	2.90	0.48
1:A:821:LEU:O	1:A:825:LYS:HG2	2.13	0.48
1:B:430:THR:HG22	1:B:515:PHE:CE2	2.47	0.48
1:B:675:GLN:HG3	1:B:676:THR:O	2.11	0.48
1:C:105:ILE:HD12	1:C:241:LEU:HD21	1.95	0.48
1:C:191:GLU:C	1:C:192:PHE:HD1	2.21	0.48
1:C:402:ILE:HD13	1:C:410:ILE:HD12	1.95	0.48
3:E:87:ARG:HG3	3:E:90:ASP:H	1.78	0.48
3:G:112:GLN:H	3:G:112:GLN:CD	2.21	0.48
2:H:43:PRO:HB2	3:I:110:TRP:CH2	2.48	0.48
1:A:127:VAL:HG21	5:A:1302:NAG:H5	1.94	0.48
1:A:402:ILE:HD13	1:A:410:ILE:HD12	1.95	0.48
1:A:619:GLU:H	1:A:619:GLU:CD	2.14	0.48
1:A:984:LEU:HB3	1:A:988:GLU:OE1	2.13	0.48
1:B:1091:ARG:N	1:B:1119:ASN:O	2.31	0.48
1:C:315:THR:OG1	1:C:316:SER:N	2.44	0.48
1:C:388:ASN:HA	1:C:527:PRO:HD2	1.94	0.48
1:C:431:GLY:HA3	1:C:513:LEU:O	2.13	0.48
1:C:856:ASN:HB2	1:C:858:LEU:HD13	1.95	0.48
1:C:936:ASP:OD1	1:C:936:ASP:N	2.44	0.48
2:F:65:GLY:HA2	2:F:70:PHE:HA	1.95	0.48
2:H:34:TRP:HD1	2:H:47:ILE:HB	1.79	0.48
2:H:37:GLN:HG3	2:H:41:GLN:O	2.13	0.48
3:I:13:LYS:HD2	3:I:120:SER:HA	1.96	0.48
1:A:419:ALA:O	1:A:424:LYS:HB2	2.13	0.48
1:A:431:GLY:HA3	1:A:513:LEU:O	2.13	0.48
1:B:436:TRP:NE1	1:B:509:ARG:HB2	2.27	0.48
1:B:984:LEU:HB3	1:B:988:GLU:OE1	2.13	0.48
1:C:92:PHE:CD1	1:C:93:ALA:N	2.81	0.48
1:C:341:VAL:HG11	1:C:397:ALA:HB1	1.96	0.48
1:C:878:LEU:HD12	1:C:878:LEU:O	2.13	0.48
1:C:902:MET:HE1	1:C:1049:LEU:HD13	1.95	0.48
1:C:916:LEU:O	1:C:919:ASN:N	2.45	0.48
1:C:996:LEU:HA	1:C:996:LEU:HD23	1.46	0.48
2:D:34:TRP:HD1	2:D:47:ILE:HB	1.79	0.48
3:E:67:ALA:HB3	3:E:84:SER:OG	2.13	0.48
2:F:32:LEU:HD13	2:F:70:PHE:CG	2.48	0.48
3:G:4:LEU:CD2	3:G:24:VAL:HG22	2.43	0.48
1:A:328:ARG:HB3	1:A:543:PHE:CD1	2.48	0.48
1:B:106:PHE:CD1	1:B:106:PHE:N	2.81	0.48
1:B:108:THR:HG22	1:B:236:THR:H	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:TYR:OH	1:B:172:SER:OG	2.20	0.48
1:B:436:TRP:O	1:B:508:TYR:HA	2.13	0.48
1:B:612:TYR:CE1	1:B:651:ILE:HD12	2.49	0.48
1:C:187:LYS:HA	1:C:210:ILE:O	2.14	0.48
1:C:323:THR:HG21	1:C:537:LYS:HZ2	1.78	0.48
1:C:821:LEU:O	1:C:825:LYS:HG2	2.13	0.48
1:C:914:ASN:OD1	1:C:915:VAL:N	2.47	0.48
1:C:919:ASN:O	1:C:920:GLN:C	2.57	0.48
1:C:1018:ILE:O	1:C:1022:ALA:N	2.43	0.48
1:B:419:ALA:O	1:B:424:LYS:HB2	2.13	0.48
1:C:143:VAL:HG13	1:C:151:SER:HA	1.94	0.48
1:C:328:ARG:HB3	1:C:543:PHE:CD1	2.48	0.48
1:C:984:LEU:HB3	1:C:988:GLU:OE1	2.13	0.48
2:D:43:PRO:HB2	3:E:110:TRP:CH2	2.48	0.48
3:E:65:LYS:HE3	3:E:67:ALA:CA	2.43	0.48
1:A:108:THR:HG22	1:A:236:THR:H	1.79	0.48
1:A:378:LYS:NZ	3:E:56:GLY:O	2.37	0.48
1:A:426:PRO:HG3	1:A:463:PRO:HB3	1.96	0.48
1:A:773:GLU:O	1:A:775:ASP:N	2.47	0.48
1:B:108:THR:HG23	1:B:234:ASN:O	2.12	0.48
1:B:328:ARG:HB3	1:B:543:PHE:CD1	2.48	0.48
1:B:619:GLU:H	1:B:619:GLU:CD	2.14	0.48
1:B:869:MET:O	1:B:870:ILE:C	2.56	0.48
1:B:873:TYR:C	1:B:875:SER:N	2.71	0.48
1:B:878:LEU:HD12	1:B:878:LEU:O	2.13	0.48
1:B:883:THR:OG1	1:B:884:SER:N	2.45	0.48
1:B:1021:SER:O	1:B:1021:SER:OG	2.30	0.48
1:B:1115:ILE:HA	1:B:1119:ASN:HD22	1.78	0.48
1:C:422:ASN:HB3	1:C:454:ARG:HB3	1.96	0.48
1:C:1084:ASP:HB2	1:C:1086:LYS:HZ3	1.77	0.48
1:C:1091:ARG:NH1	1:C:1118:ASP:O	2.46	0.48
3:E:13:LYS:HD2	3:E:120:SER:HA	1.96	0.48
2:H:34:TRP:O	2:H:46:LEU:N	2.38	0.48
1:A:804:GLN:CD	1:A:935:GLN:NE2	2.72	0.48
1:B:150:LYS:O	1:B:151:SER:OG	2.22	0.48
1:B:555:SER:OG	1:B:584:ILE:O	2.22	0.48
1:B:726:ILE:HG22	1:B:948:LEU:HD13	1.95	0.48
1:B:773:GLU:O	1:B:775:ASP:N	2.47	0.48
1:C:159:VAL:HB	1:C:160:TYR:CD1	2.46	0.48
1:C:280:ASN:HD21	1:C:284:THR:HB	1.78	0.48
1:C:391:CYS:CB	1:C:525:CYS:HA	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:906:PHE:O	1:C:908:GLY:N	2.46	0.48
2:F:15:LYS:HA	2:F:76:SER:HA	1.95	0.48
1:A:280:ASN:HD21	1:A:284:THR:HB	1.78	0.48
1:A:436:TRP:O	1:A:508:TYR:HA	2.13	0.48
1:A:612:TYR:CE1	1:A:651:ILE:HD12	2.49	0.48
1:A:854:LYS:CB	1:A:854:LYS:NZ	2.73	0.48
1:A:906:PHE:O	1:A:908:GLY:N	2.46	0.48
1:A:997:ILE:O	1:A:998:THR:C	2.56	0.48
1:B:105:ILE:HD12	1:B:241:LEU:HD21	1.95	0.48
1:B:661:GLU:O	1:B:695:TYR:OH	2.30	0.48
1:B:1008:VAL:O	1:B:1009:THR:C	2.57	0.48
1:B:1091:ARG:NH1	1:B:1118:ASP:O	2.46	0.48
1:C:106:PHE:CD1	1:C:106:PHE:N	2.81	0.48
1:C:436:TRP:O	1:C:508:TYR:HA	2.13	0.48
1:C:497:PHE:CE1	1:C:507:PRO:HB3	2.49	0.48
1:C:767:LEU:HD23	1:C:770:ILE:HD12	1.95	0.48
1:C:773:GLU:O	1:C:775:ASP:N	2.47	0.48
1:C:1004:LEU:O	1:C:1005:GLN:C	2.56	0.48
3:G:109:TYR:C	3:G:110:TRP:CD1	2.92	0.48
3:I:6:GLN:H	3:I:112:GLN:HE22	1.61	0.48
3:I:87:ARG:HG3	3:I:90:ASP:H	1.78	0.48
1:A:92:PHE:CD1	1:A:93:ALA:N	2.81	0.48
1:A:117:LEU:HD21	1:A:119:ILE:HD11	1.93	0.48
1:A:191:GLU:C	1:A:192:PHE:HD1	2.21	0.48
1:A:341:VAL:HG11	1:A:397:ALA:HB1	1.96	0.48
1:A:869:MET:HE1	1:B:669:GLY:HA3	1.95	0.48
1:A:936:ASP:N	1:A:936:ASP:OD1	2.44	0.48
1:B:719:THR:HG23	1:B:720:ILE:N	2.26	0.48
1:C:108:THR:HG22	1:C:236:THR:H	1.79	0.48
1:C:347:PHE:HE2	1:C:509:ARG:HB3	1.79	0.48
1:C:619:GLU:H	1:C:619:GLU:CD	2.14	0.48
1:C:726:ILE:HG22	1:C:948:LEU:HD13	1.95	0.48
2:F:20:ILE:HD12	2:F:85:TYR:CD2	2.47	0.48
1:A:105:ILE:HD12	1:A:241:LEU:HD21	1.95	0.48
1:A:497:PHE:CE1	1:A:507:PRO:HB3	2.49	0.48
1:A:559:PHE:CZ	1:C:43:PHE:HB3	2.48	0.48
1:A:702:GLU:CD	1:A:703:ASN:N	2.72	0.48
1:B:347:PHE:HE2	1:B:509:ARG:HB3	1.79	0.48
1:B:702:GLU:CD	1:B:703:ASN:N	2.72	0.48
1:B:901:GLN:NE2	1:B:905:ARG:HE	2.11	0.48
1:C:737:ASP:OD1	1:C:737:ASP:C	2.57	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:109:TYR:O	3:G:110:TRP:HD1	1.97	0.48
1:A:347:PHE:HE2	1:A:509:ARG:HB3	1.79	0.47
1:A:914:ASN:OD1	1:A:915:VAL:N	2.47	0.47
1:A:1049:LEU:HA	1:A:1049:LEU:HD23	1.39	0.47
1:A:1115:ILE:HA	1:A:1119:ASN:HD22	1.78	0.47
1:B:331:ASN:H	1:B:580:GLN:HA	1.79	0.47
1:B:388:ASN:HA	1:B:527:PRO:HD2	1.94	0.47
1:B:391:CYS:CB	1:B:525:CYS:HA	2.44	0.47
1:B:767:LEU:HD23	1:B:770:ILE:HD12	1.95	0.47
1:B:914:ASN:OD1	1:B:915:VAL:N	2.47	0.47
1:B:966:LEU:HA	1:B:966:LEU:HD23	1.58	0.47
1:C:227:VAL:HG12	1:C:228:ASP:N	2.28	0.47
1:C:393:THR:O	1:C:523:THR:OG1	2.23	0.47
1:C:804:GLN:CD	1:C:935:GLN:NE2	2.72	0.47
1:C:1088:HIS:CE1	1:C:1122:VAL:HG22	2.48	0.47
1:C:1115:ILE:HA	1:C:1119:ASN:HD22	1.78	0.47
1:A:43:PHE:HB2	1:B:563:GLN:CG	2.44	0.47
1:A:129:LYS:HG2	1:A:169:GLU:OE1	2.14	0.47
1:A:187:LYS:HA	1:A:210:ILE:O	2.14	0.47
1:A:277:LEU:HD23	1:A:277:LEU:HA	1.48	0.47
1:A:405:ASP:CG	3:E:104:TYR:OH	2.57	0.47
1:A:878:LEU:HD12	1:A:878:LEU:O	2.13	0.47
1:A:894:LEU:HA	1:A:894:LEU:HD23	1.52	0.47
1:A:950:ASP:O	1:A:951:VAL:C	2.56	0.47
1:B:723:THR:OG1	1:B:724:THR:N	2.41	0.47
1:B:791:THR:HB	1:B:792:PRO:HD2	1.96	0.47
1:B:864:LEU:C	1:B:864:LEU:CD1	2.86	0.47
1:B:876:ALA:O	1:B:877:LEU:C	2.57	0.47
1:C:950:ASP:O	1:C:951:VAL:C	2.56	0.47
2:D:60:ARG:HB2	2:D:75:ASN:O	2.14	0.47
3:G:47:TRP:CZ2	3:G:50:TYR:HD2	2.32	0.47
1:A:320:VAL:CG2	1:A:591:SER:CB	2.91	0.47
1:A:560:LEU:CB	1:A:563:GLN:HB2	2.44	0.47
1:A:719:THR:HG23	1:A:720:ILE:N	2.26	0.47
1:A:919:ASN:O	1:A:920:GLN:C	2.57	0.47
1:A:946:GLY:O	1:A:950:ASP:N	2.47	0.47
1:A:1018:ILE:O	1:A:1022:ALA:N	2.43	0.47
1:B:227:VAL:HG12	1:B:228:ASP:N	2.28	0.47
1:B:240:THR:O	1:B:241:LEU:HD23	2.15	0.47
1:C:66:HIS:N	1:C:80:ASP:OD2	2.43	0.47
1:C:331:ASN:H	1:C:580:GLN:HA	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:946:GLY:O	1:C:950:ASP:N	2.47	0.47
3:G:3:GLN:HB2	3:G:25:SER:OG	2.14	0.47
3:G:47:TRP:HZ2	3:G:50:TYR:HD2	1.61	0.47
1:A:107:GLY:HA2	1:A:235:ILE:HG12	1.96	0.47
1:A:117:LEU:HD12	1:A:118:LEU:H	1.80	0.47
1:A:159:VAL:HB	1:A:160:TYR:CD1	2.46	0.47
1:A:901:GLN:NE2	1:A:905:ARG:HE	2.11	0.47
1:B:66:HIS:N	1:B:80:ASP:OD2	2.43	0.47
1:B:117:LEU:HD12	1:B:118:LEU:H	1.80	0.47
1:B:129:LYS:HG2	1:B:169:GLU:OE1	2.14	0.47
1:B:167:THR:HA	1:C:357:ARG:NH1	2.30	0.47
1:B:341:VAL:HG11	1:B:397:ALA:HB1	1.96	0.47
1:B:402:ILE:HD13	1:B:410:ILE:HD12	1.94	0.47
1:B:422:ASN:HB3	1:B:454:ARG:HB3	1.96	0.47
1:B:426:PRO:HG3	1:B:463:PRO:HB3	1.96	0.47
1:C:568:ASP:O	1:C:571:ASP:N	2.34	0.47
1:C:599:THR:HG1	1:C:600:PRO:N	2.08	0.47
1:C:702:GLU:CD	1:C:703:ASN:N	2.72	0.47
1:C:853:GLN:O	1:C:858:LEU:HB2	2.15	0.47
1:A:405:ASP:CG	3:E:104:TYR:HH	2.23	0.47
1:A:429:PHE:CZ	1:A:512:VAL:HG13	2.50	0.47
1:A:994:ASP:O	1:A:998:THR:N	2.42	0.47
1:B:187:LYS:HA	1:B:210:ILE:O	2.14	0.47
1:B:497:PHE:CE1	1:B:507:PRO:HB3	2.49	0.47
1:B:950:ASP:O	1:B:951:VAL:C	2.56	0.47
1:C:117:LEU:HD12	1:C:118:LEU:H	1.80	0.47
1:C:473:TYR:N	1:C:489:TYR:O	2.46	0.47
1:C:612:TYR:CE1	1:C:651:ILE:HD12	2.49	0.47
1:C:900:MET:HE2	1:C:900:MET:HB3	1.46	0.47
3:E:10:GLU:O	3:E:116:VAL:HG13	2.15	0.47
2:H:4:LEU:HD22	2:H:22:CYS:SG	2.54	0.47
2:H:89:GLN:HB3	2:H:96:ILE:H	1.80	0.47
1:A:391:CYS:CB	1:A:525:CYS:HA	2.44	0.47
1:A:439:ASN:HB2	1:A:507:PRO:HD2	1.97	0.47
1:A:873:TYR:O	1:A:875:SER:N	2.48	0.47
1:B:338:PHE:HB3	1:B:342:PHE:CE2	2.50	0.47
1:B:804:GLN:CD	1:B:935:GLN:NE2	2.72	0.47
1:C:127:VAL:HG21	5:C:1302:NAG:H5	1.94	0.47
1:C:876:ALA:O	1:C:877:LEU:C	2.57	0.47
1:C:901:GLN:NE2	1:C:905:ARG:HE	2.11	0.47
2:D:37:GLN:HG3	2:D:41:GLN:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:48:ILE:HG21	3:E:81:MET:SD	2.55	0.47
2:F:32:LEU:HD21	2:F:87:CYS:CB	2.43	0.47
3:I:48:ILE:HG21	3:I:81:MET:SD	2.55	0.47
1:A:59:PHE:N	1:A:59:PHE:CD1	2.82	0.47
1:A:328:ARG:HG3	1:A:579:PRO:CG	2.45	0.47
1:A:375:SER:OG	2:D:91:ASN:ND2	2.48	0.47
1:A:425:LEU:HD11	1:A:512:VAL:HG21	1.97	0.47
1:A:712:ILE:HB	1:A:1077:THR:HG21	1.97	0.47
1:A:767:LEU:HD23	1:A:770:ILE:HD12	1.95	0.47
1:A:876:ALA:O	1:A:877:LEU:C	2.57	0.47
1:A:1008:VAL:O	1:A:1009:THR:C	2.57	0.47
1:B:600:PRO:HG3	1:B:674:TYR:CD1	2.50	0.47
1:B:816:SER:O	1:B:817:PHE:C	2.57	0.47
1:B:914:ASN:HA	1:C:1089:PHE:CE2	2.50	0.47
1:B:1018:ILE:O	1:B:1022:ALA:N	2.43	0.47
1:C:107:GLY:HA2	1:C:235:ILE:HG12	1.96	0.47
1:C:196:ASN:ND2	1:C:235:ILE:HD12	2.27	0.47
1:C:305:SER:OG	1:C:307:THR:O	2.20	0.47
1:C:350:VAL:HA	1:C:400:PHE:HB2	1.97	0.47
1:C:408:ARG:CD	3:I:102:ASP:CG	2.68	0.47
1:C:429:PHE:HD1	1:C:464:PHE:HZ	1.61	0.47
1:C:429:PHE:CZ	1:C:512:VAL:HG13	2.50	0.47
1:C:557:LYS:HB2	1:C:584:ILE:HG21	1.95	0.47
1:C:617:CYS:N	1:C:644:GLN:OE1	2.48	0.47
1:C:712:ILE:HB	1:C:1077:THR:HG21	1.97	0.47
1:C:791:THR:HB	1:C:792:PRO:HD2	1.97	0.47
1:C:873:TYR:O	1:C:875:SER:N	2.48	0.47
1:C:897:PRO:O	1:C:898:PHE:C	2.58	0.47
1:C:1083:HIS:CD2	1:C:1084:ASP:OD1	2.68	0.47
3:E:18:VAL:O	3:E:83:LEU:N	2.34	0.47
2:F:48:LYS:HG3	3:G:106:VAL:CG1	2.43	0.47
2:F:94:PRO:HB3	3:G:47:TRP:CZ3	2.50	0.47
1:A:63:THR:HG22	1:A:65:PHE:CE1	2.50	0.47
1:A:378:LYS:O	1:A:433:VAL:N	2.34	0.47
1:A:429:PHE:HD1	1:A:464:PHE:HZ	1.61	0.47
1:A:726:ILE:HG22	1:A:948:LEU:HD13	1.95	0.47
1:B:425:LEU:HD11	1:B:512:VAL:HG21	1.97	0.47
1:B:455:LEU:HG	1:B:456:PHE:CE2	2.50	0.47
1:C:59:PHE:N	1:C:59:PHE:CD1	2.82	0.47
1:C:959:LEU:HA	1:C:959:LEU:HD23	1.58	0.47
3:E:107:MET:HB2	3:E:110:TRP:HE1	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:802:PHE:O	1:A:803:SER:C	2.56	0.47
1:B:107:GLY:HA2	1:B:235:ILE:HG12	1.96	0.47
1:B:231:ILE:HG13	1:B:232:GLY:N	2.30	0.47
1:B:393:THR:OG1	1:B:394:ASN:N	2.47	0.47
1:B:737:ASP:OD1	1:B:737:ASP:C	2.57	0.47
1:B:919:ASN:O	1:B:920:GLN:C	2.56	0.47
1:C:439:ASN:HB2	1:C:507:PRO:HD2	1.97	0.47
1:C:763:LEU:O	1:C:764:ASN:C	2.58	0.47
2:D:22:CYS:HB2	2:D:34:TRP:CH2	2.50	0.47
2:D:61:PHE:HZ	2:D:81:ASP:OD1	1.98	0.47
2:H:22:CYS:HB2	2:H:34:TRP:CH2	2.50	0.47
1:A:43:PHE:HA	1:B:563:GLN:HE21	1.73	0.47
1:A:140:PHE:CZ	1:A:158:ARG:HD2	2.50	0.47
1:A:617:CYS:N	1:A:644:GLN:OE1	2.48	0.47
1:A:1083:HIS:CD2	1:A:1084:ASP:OD1	2.68	0.47
1:B:133:PHE:CD2	1:B:135:PHE:HE1	2.33	0.47
1:B:429:PHE:HD1	1:B:464:PHE:HZ	1.62	0.47
1:C:240:THR:O	1:C:241:LEU:HD23	2.15	0.47
1:C:426:PRO:HG3	1:C:463:PRO:HB3	1.96	0.47
1:C:600:PRO:HG3	1:C:674:TYR:CD1	2.50	0.47
1:C:822:LEU:HA	1:C:822:LEU:HD23	1.68	0.47
1:C:1012:LEU:HD23	1:C:1012:LEU:HA	1.60	0.47
2:D:4:LEU:HD22	2:D:22:CYS:SG	2.54	0.47
1:A:231:ILE:HG13	1:A:232:GLY:N	2.30	0.46
1:A:323:THR:HG21	1:A:537:LYS:CE	2.44	0.46
1:A:455:LEU:HG	1:A:456:PHE:CE2	2.50	0.46
1:A:566:GLY:HA2	1:C:43:PHE:HB3	1.97	0.46
1:A:661:GLU:O	1:A:695:TYR:OH	2.30	0.46
1:A:676:THR:HG23	1:A:690:GLN:HG2	1.97	0.46
1:A:723:THR:OG1	1:A:724:THR:N	2.41	0.46
1:A:773:GLU:C	1:A:775:ASP:N	2.72	0.46
1:A:855:PHE:CD1	1:B:589:PRO:HG3	2.50	0.46
1:B:280:ASN:HD21	1:B:284:THR:HB	1.78	0.46
1:C:338:PHE:HB3	1:C:342:PHE:CE2	2.50	0.46
2:D:48:LYS:N	2:D:52:GLN:O	2.40	0.46
3:I:14:PRO:HD3	3:I:119:SER:C	2.40	0.46
1:A:240:THR:O	1:A:241:LEU:HD23	2.15	0.46
1:A:331:ASN:H	1:A:580:GLN:HA	1.79	0.46
1:A:453:TYR:HB3	1:A:495:TYR:CE2	2.51	0.46
1:B:328:ARG:HG3	1:B:579:PRO:CG	2.45	0.46
1:B:429:PHE:CZ	1:B:512:VAL:HG13	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1083:HIS:CD2	1:B:1084:ASP:OD1	2.68	0.46
1:C:224:GLU:CD	1:C:224:GLU:N	2.72	0.46
1:C:425:LEU:HD11	1:C:512:VAL:HG21	1.97	0.46
1:C:451:TYR:O	1:C:494:SER:OG	2.33	0.46
1:C:773:GLU:C	1:C:775:ASP:N	2.72	0.46
1:C:873:TYR:C	1:C:875:SER:N	2.71	0.46
1:A:422:ASN:HB3	1:A:454:ARG:HB3	1.96	0.46
1:A:556:ASN:OD1	1:A:556:ASN:N	2.38	0.46
1:A:737:ASP:OD1	1:A:737:ASP:C	2.57	0.46
1:A:816:SER:O	1:A:817:PHE:C	2.57	0.46
1:B:63:THR:HG22	1:B:65:PHE:CE1	2.50	0.46
1:B:366:SER:HA	1:B:369:TYR:CD2	2.51	0.46
1:B:873:TYR:O	1:B:875:SER:N	2.48	0.46
1:B:897:PRO:O	1:B:898:PHE:C	2.58	0.46
1:B:997:ILE:O	1:B:998:THR:C	2.56	0.46
1:C:366:SER:HA	1:C:369:TYR:CD2	2.51	0.46
1:C:455:LEU:HG	1:C:456:PHE:CE2	2.50	0.46
1:C:816:SER:O	1:C:817:PHE:C	2.57	0.46
1:C:915:VAL:O	1:C:916:LEU:C	2.59	0.46
1:C:1027:THR:O	1:C:1028:LYS:C	2.53	0.46
2:D:5:THR:O	2:D:23:ARG:N	2.35	0.46
2:H:2:ILE:O	2:H:96:ILE:HD12	2.15	0.46
2:H:61:PHE:HZ	2:H:81:ASP:OD1	1.98	0.46
1:A:106:PHE:CD1	1:A:106:PHE:N	2.81	0.46
1:A:133:PHE:CD2	1:A:135:PHE:HE1	2.33	0.46
1:A:225:PRO:CD	1:B:562:PHE:CD2	2.95	0.46
1:A:802:PHE:O	1:A:805:ILE:N	2.49	0.46
1:A:961:THR:O	1:A:965:GLN:HG2	2.16	0.46
1:C:327:VAL:HB	1:C:531:THR:HG23	1.95	0.46
1:C:802:PHE:O	1:C:803:SER:C	2.56	0.46
2:D:46:LEU:HD22	2:D:61:PHE:CD2	2.50	0.46
3:G:86:LEU:HB3	3:G:118:VAL:HG21	1.97	0.46
2:H:10:GLN:O	2:H:103:LEU:HD12	2.15	0.46
3:I:107:MET:HB2	3:I:110:TRP:HE1	1.80	0.46
1:A:299:THR:O	1:A:301:CYS:N	2.49	0.46
1:A:350:VAL:HA	1:A:400:PHE:HB2	1.97	0.46
1:A:377:PHE:CB	2:D:93:TRP:CD1	2.98	0.46
1:A:385:THR:HG21	3:E:65:LYS:HE2	1.95	0.46
1:A:600:PRO:HG3	1:A:674:TYR:CD1	2.50	0.46
1:A:873:TYR:C	1:A:875:SER:N	2.71	0.46
1:A:913:GLN:O	1:A:916:LEU:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1043:CYS:CB	1:A:1048:HIS:CD2	2.92	0.46
1:B:43:PHE:CD2	1:C:559:PHE:CE1	3.03	0.46
1:B:215:ASP:OD1	1:B:216:LEU:N	2.42	0.46
1:B:299:THR:O	1:B:301:CYS:N	2.49	0.46
1:B:439:ASN:HB2	1:B:507:PRO:HD2	1.97	0.46
1:B:451:TYR:O	1:B:494:SER:OG	2.33	0.46
1:B:911:VAL:HG12	1:B:912:THR:O	2.16	0.46
1:B:916:LEU:O	1:B:919:ASN:N	2.45	0.46
1:B:946:GLY:O	1:B:950:ASP:N	2.47	0.46
1:B:961:THR:O	1:B:965:GLN:HG2	2.16	0.46
1:C:129:LYS:HG2	1:C:169:GLU:OE1	2.14	0.46
1:C:191:GLU:O	1:C:192:PHE:HD1	1.98	0.46
1:C:371:SER:HB3	5:C:1305:NAG:H3	1.97	0.46
3:E:38:LYS:NZ	3:E:46:GLU:OE1	2.24	0.46
2:F:28:ILE:HD13	2:F:70:PHE:CZ	2.50	0.46
1:A:806:LEU:HA	1:A:806:LEU:HD23	1.54	0.46
1:A:911:VAL:HG12	1:A:912:THR:O	2.16	0.46
1:B:676:THR:HG23	1:B:690:GLN:HG2	1.97	0.46
1:C:63:THR:HG22	1:C:65:PHE:CE1	2.50	0.46
1:C:231:ILE:HG13	1:C:232:GLY:N	2.30	0.46
1:C:328:ARG:HG3	1:C:579:PRO:CG	2.45	0.46
1:C:363:ALA:HB3	1:C:388:ASN:HA	1.98	0.46
1:C:559:PHE:HE2	1:C:565:PHE:O	1.87	0.46
3:E:41:PRO:HD3	3:E:92:ALA:HA	1.97	0.46
2:F:12:VAL:HG12	2:F:13:SER:H	1.81	0.46
2:F:35:TYR:CE1	2:F:88:GLN:HG3	2.50	0.46
1:A:115:GLN:HB2	1:A:233:ILE:HG12	1.98	0.46
1:A:363:ALA:HB3	1:A:388:ASN:HA	1.98	0.46
1:A:366:SER:HA	1:A:369:TYR:CD2	2.51	0.46
1:A:453:TYR:HE2	1:A:455:LEU:HD13	1.81	0.46
1:A:791:THR:HB	1:A:792:PRO:HD2	1.96	0.46
1:B:44:ARG:HB3	1:B:47:VAL:CG1	2.46	0.46
1:B:161:SER:OG	1:B:162:SER:N	2.48	0.46
1:B:913:GLN:O	1:B:916:LEU:N	2.49	0.46
1:C:136:CYS:N	1:C:139:PRO:HG3	2.31	0.46
1:C:161:SER:OG	1:C:162:SER:N	2.48	0.46
1:C:299:THR:O	1:C:301:CYS:N	2.49	0.46
1:C:374:PHE:O	2:H:93:TRP:HB2	2.15	0.46
3:E:10:GLU:HB2	3:E:116:VAL:HG22	1.98	0.46
3:E:33:TYR:CE1	3:E:101:TYR:CD1	3.02	0.46
2:F:13:SER:OG	2:F:106:LEU:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:31:ASN:OD1	2:F:32:LEU:N	2.49	0.46
2:H:46:LEU:HD22	2:H:61:PHE:CD2	2.50	0.46
2:H:60:ARG:HB2	2:H:75:ASN:O	2.14	0.46
1:A:136:CYS:O	1:A:139:PRO:HD3	2.16	0.46
1:A:215:ASP:OD1	1:A:216:LEU:N	2.42	0.46
1:A:429:PHE:HD1	1:A:464:PHE:CZ	2.33	0.46
1:B:41:LYS:HD3	1:C:562:PHE:O	2.16	0.46
1:B:371:SER:HB3	5:B:1305:NAG:H3	1.97	0.46
1:B:453:TYR:HB3	1:B:495:TYR:CE2	2.50	0.46
1:B:1049:LEU:HA	1:B:1049:LEU:HD23	1.39	0.46
1:C:38:TYR:CE2	1:C:285:ILE:HG13	2.51	0.46
1:C:140:PHE:CZ	1:C:158:ARG:HD2	2.51	0.46
1:C:215:ASP:OD1	1:C:216:LEU:N	2.42	0.46
1:C:453:TYR:HE2	1:C:455:LEU:HD13	1.81	0.46
3:G:20:ILE:HD11	3:G:116:VAL:CG2	2.46	0.46
3:I:10:GLU:O	3:I:116:VAL:HG13	2.15	0.46
1:A:338:PHE:HB3	1:A:342:PHE:CE2	2.50	0.46
1:A:371:SER:HB3	5:A:1305:NAG:H3	1.97	0.46
1:B:38:TYR:CE2	1:B:285:ILE:HG13	2.51	0.46
1:B:140:PHE:CZ	1:B:158:ARG:HD2	2.51	0.46
1:B:432:CYS:HB2	1:B:513:LEU:H	1.81	0.46
1:B:671:CYS:O	1:B:695:TYR:CE1	2.69	0.46
1:C:64:TRP:HE1	1:C:264:ALA:HB1	1.81	0.46
1:C:336:CYS:SG	1:C:362:VAL:N	2.89	0.46
1:C:671:CYS:O	1:C:695:TYR:CE1	2.69	0.46
1:C:911:VAL:HG12	1:C:912:THR:O	2.16	0.46
1:C:961:THR:O	1:C:965:GLN:HG2	2.16	0.46
2:F:31:ASN:CG	2:F:49:TYR:HA	2.41	0.46
1:A:192:PHE:HB3	1:A:194:PHE:HE1	1.81	0.46
1:A:323:THR:OG1	1:A:537:LYS:CE	2.64	0.46
1:B:136:CYS:O	1:B:139:PRO:HD3	2.16	0.46
1:B:191:GLU:O	1:B:192:PHE:HD1	1.98	0.46
1:B:429:PHE:HD1	1:B:464:PHE:CZ	2.34	0.46
1:B:555:SER:OG	1:B:584:ILE:HG22	2.16	0.46
1:B:712:ILE:HB	1:B:1077:THR:HG21	1.97	0.46
1:B:773:GLU:C	1:B:775:ASP:N	2.72	0.46
1:B:900:MET:HB3	1:B:900:MET:HE2	1.46	0.46
1:B:1004:LEU:O	1:B:1005:GLN:C	2.56	0.46
1:C:115:GLN:HB2	1:C:233:ILE:HG12	1.98	0.46
1:C:136:CYS:O	1:C:139:PRO:HD3	2.16	0.46
1:C:802:PHE:O	1:C:805:ILE:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:913:GLN:O	1:C:916:LEU:N	2.49	0.46
1:C:1100:THR:HG1	1:C:1101:HIS:CE1	2.31	0.46
2:F:45:LEU:HD23	3:G:108:ASP:OD1	2.15	0.46
2:F:91:ASN:N	2:F:95:TYR:CE1	2.84	0.46
3:I:37:VAL:HB	3:I:95:TYR:HB2	1.98	0.46
1:A:196:ASN:ND2	1:A:235:ILE:HD12	2.27	0.45
1:A:645:THR:OG1	1:A:648:GLY:O	2.15	0.45
1:A:856:ASN:CB	1:A:858:LEU:HD13	2.46	0.45
1:B:136:CYS:N	1:B:139:PRO:HG3	2.31	0.45
1:B:398:ASP:N	1:B:512:VAL:O	2.49	0.45
1:B:453:TYR:HE2	1:B:455:LEU:HD13	1.81	0.45
1:B:557:LYS:O	1:B:584:ILE:HG21	2.16	0.45
1:B:560:LEU:HD22	1:B:560:LEU:HA	1.82	0.45
1:B:770:ILE:O	1:B:773:GLU:N	2.49	0.45
1:B:904:TYR:O	1:B:905:ARG:C	2.57	0.45
2:D:89:GLN:HB3	2:D:96:ILE:H	1.80	0.45
2:F:33:HIS:ND1	3:G:106:VAL:HG12	2.31	0.45
3:G:4:LEU:O	3:G:111:GLY:HA2	2.16	0.45
3:G:27:TYR:CD1	3:G:32:TYR:HD2	2.34	0.45
3:G:97:ALA:HB1	3:G:107:MET:CB	2.44	0.45
1:A:669:GLY:HA3	1:C:869:MET:HE1	1.99	0.45
1:B:242:LEU:HA	1:B:242:LEU:HD23	1.73	0.45
1:B:336:CYS:SG	1:B:362:VAL:N	2.89	0.45
1:B:617:CYS:N	1:B:644:GLN:OE1	2.48	0.45
1:B:1064:HIS:O	1:B:1066:THR:HG23	2.17	0.45
1:C:152:TRP:HB3	1:C:153:MET:H	1.57	0.45
1:C:313:TYR:CD1	1:C:313:TYR:N	2.85	0.45
1:C:408:ARG:CD	3:I:102:ASP:OD2	2.45	0.45
1:C:767:LEU:HD23	1:C:767:LEU:HA	1.60	0.45
1:C:1043:CYS:CB	1:C:1048:HIS:CD2	2.92	0.45
2:D:69:ASP:OD1	2:D:70:PHE:N	2.50	0.45
2:F:12:VAL:HG12	2:F:13:SER:N	2.32	0.45
1:A:64:TRP:HE1	1:A:264:ALA:HB1	1.81	0.45
1:A:191:GLU:O	1:A:192:PHE:HD1	1.98	0.45
1:A:313:TYR:N	1:A:313:TYR:CD1	2.85	0.45
1:A:555:SER:OG	1:A:584:ILE:HG22	2.16	0.45
1:A:877:LEU:HA	1:A:877:LEU:HD23	1.79	0.45
1:A:904:TYR:O	1:A:905:ARG:C	2.57	0.45
1:A:959:LEU:HD23	1:A:959:LEU:HA	1.58	0.45
1:B:350:VAL:HA	1:B:400:PHE:HB2	1.97	0.45
1:B:363:ALA:HB3	1:B:388:ASN:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:557:LYS:O	1:B:584:ILE:HG13	2.16	0.45
1:B:802:PHE:O	1:B:805:ILE:N	2.49	0.45
1:C:44:ARG:HB3	1:C:47:VAL:CG1	2.46	0.45
1:C:133:PHE:CD2	1:C:135:PHE:HE1	2.33	0.45
1:C:429:PHE:HD1	1:C:464:PHE:CZ	2.33	0.45
1:C:676:THR:HG23	1:C:690:GLN:HG2	1.97	0.45
2:D:48:LYS:HD2	3:E:106:VAL:HG11	1.97	0.45
3:G:4:LEU:N	3:G:109:TYR:CE2	2.84	0.45
3:G:86:LEU:HB3	3:G:118:VAL:CG2	2.46	0.45
3:I:4:LEU:HD21	3:I:24:VAL:HG22	1.98	0.45
3:I:41:PRO:HD3	3:I:92:ALA:HA	1.97	0.45
3:I:65:LYS:HE3	3:I:67:ALA:CA	2.43	0.45
1:A:395:VAL:HG11	1:A:524:VAL:HG21	1.98	0.45
1:A:418:ILE:HG23	1:A:423:TYR:HB3	1.98	0.45
1:A:667:GLY:O	1:A:668:ALA:C	2.59	0.45
1:A:770:ILE:O	1:A:773:GLU:N	2.49	0.45
1:A:915:VAL:O	1:A:916:LEU:C	2.59	0.45
1:A:945:LEU:O	1:A:946:GLY:C	2.59	0.45
1:B:667:GLY:O	1:B:668:ALA:C	2.59	0.45
1:B:773:GLU:O	1:B:774:GLN:C	2.57	0.45
1:B:805:ILE:HB	1:B:1054:GLN:HE22	1.82	0.45
1:C:1064:HIS:O	1:C:1066:THR:HG23	2.17	0.45
3:E:14:PRO:HD3	3:E:119:SER:C	2.40	0.45
3:E:50:TYR:O	3:E:58:THR:HA	2.17	0.45
2:F:32:LEU:HB3	2:F:50:ALA:HB2	1.99	0.45
3:G:6:GLN:CD	3:G:111:GLY:HA3	2.41	0.45
1:A:38:TYR:CE2	1:A:285:ILE:HG13	2.51	0.45
1:A:38:TYR:CG	1:B:562:PHE:HZ	2.35	0.45
1:A:136:CYS:N	1:A:139:PRO:HG3	2.31	0.45
1:A:378:LYS:HE2	3:E:57:GLY:CA	2.45	0.45
1:A:419:ALA:C	1:A:424:LYS:HD3	2.42	0.45
1:A:485:GLY:N	1:A:488:CYS:HB2	2.32	0.45
1:B:222:ALA:C	1:B:223:LEU:HD12	2.42	0.45
1:B:485:GLY:N	1:B:488:CYS:HB2	2.32	0.45
1:B:763:LEU:O	1:B:764:ASN:C	2.58	0.45
1:B:767:LEU:HD23	1:B:767:LEU:HA	1.60	0.45
1:C:143:VAL:HG13	1:C:151:SER:CB	2.47	0.45
1:C:432:CYS:HB2	1:C:513:LEU:H	1.81	0.45
1:C:457:ARG:NH2	1:C:461:LEU:HD23	2.32	0.45
1:C:555:SER:OG	1:C:584:ILE:HG22	2.16	0.45
1:C:587:ILE:CG2	1:C:588:THR:H	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1097:SER:OG	1:C:1098:ASN:N	2.50	0.45
3:E:37:VAL:HB	3:E:95:TYR:HB2	1.98	0.45
2:H:48:LYS:HD2	3:I:106:VAL:HG11	1.97	0.45
2:H:69:ASP:OD1	2:H:70:PHE:N	2.50	0.45
1:A:322:PRO:HA	1:A:538:CYS:SG	2.56	0.45
1:A:473:TYR:HB2	1:A:491:PRO:HB3	1.98	0.45
1:A:671:CYS:O	1:A:695:TYR:CE1	2.69	0.45
1:A:1021:SER:O	1:A:1021:SER:OG	2.30	0.45
1:B:353:TRP:H	1:B:466:ARG:HE	1.65	0.45
1:B:739:THR:O	1:B:742:ILE:N	2.49	0.45
1:B:894:LEU:HD13	1:C:715:PRO:HD3	1.99	0.45
1:C:453:TYR:HB3	1:C:495:TYR:CE2	2.51	0.45
1:C:739:THR:O	1:C:742:ILE:N	2.49	0.45
1:C:902:MET:HB3	1:C:902:MET:HE3	1.62	0.45
2:D:10:GLN:O	2:D:103:LEU:HD12	2.15	0.45
2:F:49:TYR:C	2:F:51:SER:H	2.24	0.45
3:G:100:GLU:CB	3:G:104:TYR:O	2.60	0.45
2:H:12:VAL:HG12	2:H:13:SER:H	1.81	0.45
1:A:44:ARG:HB3	1:A:47:VAL:CG1	2.46	0.45
1:A:55:PHE:CD2	1:A:275:PHE:CD2	3.05	0.45
1:A:144:TYR:HB3	1:A:152:TRP:HB2	1.99	0.45
1:A:323:THR:HG22	1:A:324:GLU:N	2.32	0.45
1:A:384:PRO:HG3	3:E:60:ASP:HB3	1.99	0.45
1:A:436:TRP:CE2	1:A:509:ARG:HB2	2.52	0.45
1:A:1064:HIS:O	1:A:1066:THR:HG23	2.17	0.45
1:B:59:PHE:N	1:B:59:PHE:CD1	2.82	0.45
1:B:802:PHE:O	1:B:803:SER:C	2.56	0.45
1:B:877:LEU:O	1:B:881:THR:OG1	2.22	0.45
1:C:398:ASP:N	1:C:512:VAL:O	2.49	0.45
1:C:419:ALA:C	1:C:424:LYS:HD3	2.42	0.45
3:G:33:TYR:CE1	3:G:101:TYR:CE1	3.05	0.45
2:H:32:LEU:HD13	2:H:70:PHE:CB	2.47	0.45
3:I:50:TYR:O	3:I:58:THR:HA	2.17	0.45
1:A:133:PHE:CE2	1:A:135:PHE:HE1	2.35	0.45
1:A:336:CYS:SG	1:A:362:VAL:N	2.89	0.45
1:A:473:TYR:N	1:A:489:TYR:O	2.46	0.45
1:A:587:ILE:CG2	1:A:588:THR:H	2.29	0.45
1:A:715:PRO:HD3	1:C:894:LEU:HD13	1.99	0.45
1:A:739:THR:O	1:A:742:ILE:N	2.49	0.45
1:A:763:LEU:O	1:A:764:ASN:C	2.58	0.45
1:B:418:ILE:HG23	1:B:423:TYR:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:894:LEU:HA	1:B:894:LEU:HD23	1.52	0.45
1:C:108:THR:OG1	1:C:109:THR:N	2.42	0.45
1:C:322:PRO:HA	1:C:538:CYS:SG	2.56	0.45
1:C:353:TRP:H	1:C:466:ARG:HE	1.65	0.45
1:C:560:LEU:HD12	1:C:562:PHE:CE1	2.51	0.45
1:C:916:LEU:HA	1:C:916:LEU:HD12	1.54	0.45
3:E:2:VAL:N	3:E:27:TYR:HD2	2.15	0.45
3:E:56:GLY:C	3:E:58:THR:H	2.25	0.45
3:I:2:VAL:N	3:I:27:TYR:HD2	2.15	0.45
3:I:10:GLU:HB2	3:I:116:VAL:HG22	1.98	0.45
1:A:105:ILE:C	1:A:106:PHE:CD1	2.90	0.45
1:A:916:LEU:O	1:A:919:ASN:N	2.45	0.45
1:B:200:TYR:CD1	1:B:230:PRO:HA	2.52	0.45
1:B:225:PRO:HD2	1:C:562:PHE:CE2	2.52	0.45
1:B:419:ALA:C	1:B:424:LYS:HD3	2.42	0.45
1:B:457:ARG:NH2	1:B:461:LEU:HD23	2.32	0.45
1:C:133:PHE:CE2	1:C:135:PHE:HE1	2.35	0.45
1:C:222:ALA:C	1:C:223:LEU:HD12	2.42	0.45
1:C:395:VAL:HG11	1:C:524:VAL:HG21	1.98	0.45
1:C:770:ILE:O	1:C:773:GLU:N	2.49	0.45
1:C:934:ILE:HD12	1:C:934:ILE:HG23	1.67	0.45
1:A:133:PHE:HD2	1:A:160:TYR:HB2	1.82	0.45
1:A:966:LEU:HA	1:A:966:LEU:HD23	1.58	0.45
1:A:1000:ARG:O	1:A:1001:LEU:C	2.60	0.45
1:A:1003:SER:O	1:A:1003:SER:OG	2.35	0.45
1:A:1011:GLN:O	1:A:1012:LEU:C	2.60	0.45
1:B:395:VAL:HG11	1:B:524:VAL:HG21	1.98	0.45
1:B:587:ILE:CG2	1:B:588:THR:H	2.29	0.45
1:B:866:THR:C	1:B:868:GLU:N	2.74	0.45
1:C:354:ASN:HB2	1:C:399:SER:HB3	1.99	0.45
1:C:725:GLU:C	1:C:726:ILE:HG13	2.42	0.45
1:C:1003:SER:O	1:C:1003:SER:OG	2.35	0.45
2:D:2:ILE:O	2:D:96:ILE:HD12	2.15	0.45
2:D:32:LEU:HD13	2:D:70:PHE:CB	2.47	0.45
2:D:43:PRO:HG2	3:E:45:LEU:HD21	1.99	0.45
2:D:49:TYR:C	2:D:51:SER:H	2.25	0.45
3:E:4:LEU:HD21	3:E:24:VAL:HG22	1.98	0.45
3:E:102:ASP:CG	3:E:103:PRO:HD3	2.42	0.45
3:I:35:HIS:CD2	3:I:107:MET:HE2	2.52	0.45
1:A:200:TYR:CD1	1:A:230:PRO:HA	2.52	0.44
1:A:451:TYR:O	1:A:494:SER:OG	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:GLN:HB2	1:B:233:ILE:HG12	1.98	0.44
1:B:801:ASN:C	1:B:801:ASN:OD1	2.60	0.44
1:B:994:ASP:O	1:B:995:ARG:C	2.59	0.44
1:C:342:PHE:CE1	1:C:511:VAL:HG11	2.53	0.44
1:C:418:ILE:HG23	1:C:423:TYR:HB3	1.99	0.44
1:C:436:TRP:CE2	1:C:509:ARG:HB2	2.52	0.44
1:C:746:SER:OG	1:C:748:GLU:OE1	2.15	0.44
1:C:892:ALA:O	1:C:894:LEU:HG	2.18	0.44
1:C:994:ASP:O	1:C:995:ARG:C	2.59	0.44
2:D:7:SER:O	2:D:101:THR:OG1	2.27	0.44
1:A:318:PHE:O	1:A:318:PHE:CG	2.70	0.44
1:A:535:LYS:NZ	1:A:554:GLU:OE2	2.37	0.44
1:B:55:PHE:CD2	1:B:275:PHE:CD2	3.05	0.44
1:B:108:THR:OG1	1:B:109:THR:N	2.42	0.44
1:B:192:PHE:HB3	1:B:194:PHE:HE1	1.81	0.44
1:C:144:TYR:HB3	1:C:152:TRP:HB2	1.99	0.44
1:C:410:ILE:HG13	1:C:418:ILE:HG21	2.00	0.44
1:C:439:ASN:HA	1:C:443:SER:OG	2.18	0.44
1:C:809:PRO:O	1:C:814:LYS:HE2	2.18	0.44
1:C:877:LEU:HA	1:C:877:LEU:HD23	1.79	0.44
1:C:1008:VAL:O	1:C:1009:THR:C	2.57	0.44
3:G:31:ASN:O	3:G:101:TYR:HB2	2.17	0.44
3:G:39:GLN:HG3	3:G:44:SER:O	2.18	0.44
2:H:49:TYR:C	2:H:51:SER:H	2.25	0.44
1:A:353:TRP:H	1:A:466:ARG:HE	1.65	0.44
1:A:386:LYS:O	1:A:390:LEU:HB3	2.17	0.44
1:A:439:ASN:HA	1:A:443:SER:OG	2.18	0.44
1:A:581:THR:HG23	1:A:583:GLU:OE2	2.18	0.44
1:A:897:PRO:O	1:A:898:PHE:C	2.58	0.44
1:A:901:GLN:C	1:A:903:ALA:H	2.25	0.44
1:A:916:LEU:O	1:A:917:TYR:C	2.60	0.44
1:B:105:ILE:C	1:B:106:PHE:CD1	2.90	0.44
1:B:168:PHE:CG	1:B:169:GLU:N	2.86	0.44
1:B:473:TYR:N	1:B:489:TYR:O	2.46	0.44
1:B:869:MET:HE1	1:C:669:GLY:HA3	1.98	0.44
1:B:915:VAL:O	1:B:916:LEU:C	2.59	0.44
1:B:945:LEU:O	1:B:946:GLY:C	2.59	0.44
1:C:141:LEU:HB3	1:C:243:ALA:HA	1.99	0.44
1:C:192:PHE:HB3	1:C:194:PHE:HE1	1.81	0.44
1:C:328:ARG:HH22	1:C:533:LEU:CB	2.17	0.44
1:C:473:TYR:HB2	1:C:491:PRO:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:97:PHE:CZ	3:E:47:TRP:HB2	2.52	0.44
3:G:4:LEU:HG	3:G:109:TYR:CE2	2.52	0.44
1:A:43:PHE:CD1	1:B:563:GLN:CD	2.93	0.44
1:A:386:LYS:HD3	1:A:389:ASP:HB3	2.00	0.44
1:B:41:LYS:O	1:C:563:GLN:HA	2.16	0.44
1:B:152:TRP:HB3	1:B:153:MET:H	1.57	0.44
1:B:313:TYR:N	1:B:313:TYR:CD1	2.85	0.44
1:B:386:LYS:O	1:B:390:LEU:HB3	2.17	0.44
1:B:822:LEU:HA	1:B:822:LEU:HD23	1.68	0.44
1:B:1097:SER:OG	1:B:1098:ASN:N	2.50	0.44
1:C:133:PHE:HD2	1:C:160:TYR:HB2	1.82	0.44
1:C:901:GLN:C	1:C:903:ALA:H	2.25	0.44
1:C:1011:GLN:O	1:C:1012:LEU:C	2.60	0.44
2:D:31:ASN:OD1	2:D:32:LEU:N	2.51	0.44
3:I:56:GLY:C	3:I:58:THR:H	2.25	0.44
1:A:222:ALA:C	1:A:223:LEU:HD12	2.42	0.44
1:A:559:PHE:CE1	1:C:43:PHE:CD2	3.05	0.44
1:A:801:ASN:C	1:A:801:ASN:OD1	2.60	0.44
1:A:805:ILE:HB	1:A:1054:GLN:HE22	1.82	0.44
1:A:809:PRO:O	1:A:814:LYS:HE2	2.18	0.44
1:A:892:ALA:O	1:A:894:LEU:HG	2.18	0.44
1:B:143:VAL:HG13	1:B:151:SER:CB	2.47	0.44
1:B:351:TYR:HB3	1:B:453:TYR:HA	2.00	0.44
1:B:436:TRP:NE1	1:B:509:ARG:HD2	2.24	0.44
1:B:912:THR:HG22	1:B:914:ASN:H	1.83	0.44
1:B:1038:LYS:HE3	1:B:1038:LYS:HB3	1.66	0.44
1:C:55:PHE:CD2	1:C:275:PHE:CD2	3.05	0.44
1:C:386:LYS:O	1:C:390:LEU:HB3	2.17	0.44
1:C:667:GLY:O	1:C:668:ALA:C	2.59	0.44
1:C:866:THR:C	1:C:868:GLU:N	2.74	0.44
1:C:1081:ILE:HD13	1:C:1135:ASN:HB3	2.00	0.44
3:G:4:LEU:HA	3:G:23:LYS:O	2.18	0.44
1:A:54:LEU:O	1:A:55:PHE:HD1	2.00	0.44
1:A:224:GLU:CD	1:A:224:GLU:N	2.72	0.44
1:A:410:ILE:HG13	1:A:418:ILE:HG21	2.00	0.44
1:A:422:ASN:HB3	1:A:454:ARG:CB	2.48	0.44
1:A:802:PHE:O	1:A:804:GLN:N	2.50	0.44
1:A:1014:ARG:O	1:A:1017:GLU:N	2.47	0.44
1:A:1097:SER:OG	1:A:1098:ASN:N	2.50	0.44
1:A:1142:GLN:N	1:A:1143:PRO:HD2	2.33	0.44
1:B:64:TRP:HE1	1:B:264:ALA:HB1	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:TYR:HB3	1:B:152:TRP:HB2	1.99	0.44
1:B:326:ILE:HD12	1:B:532:ASN:O	2.18	0.44
1:B:410:ILE:HG13	1:B:418:ILE:HG21	2.00	0.44
1:B:802:PHE:O	1:B:804:GLN:N	2.50	0.44
1:C:200:TYR:CD1	1:C:230:PRO:HA	2.52	0.44
1:C:351:TYR:HB3	1:C:453:TYR:HA	2.00	0.44
1:C:386:LYS:HD3	1:C:389:ASP:HB3	2.00	0.44
1:C:805:ILE:HB	1:C:1054:GLN:HE22	1.82	0.44
1:C:901:GLN:O	1:C:902:MET:C	2.58	0.44
2:D:12:VAL:HG12	2:D:13:SER:H	1.81	0.44
3:E:35:HIS:CD2	3:E:107:MET:HE2	2.52	0.44
2:H:32:LEU:HD13	2:H:70:PHE:CG	2.53	0.44
1:A:168:PHE:CG	1:A:169:GLU:N	2.86	0.44
1:A:863:PRO:O	1:A:864:LEU:C	2.60	0.44
1:A:912:THR:HG22	1:A:914:ASN:H	1.83	0.44
1:B:809:PRO:O	1:B:814:LYS:HE2	2.18	0.44
1:B:892:ALA:O	1:B:894:LEU:HG	2.18	0.44
1:C:90:VAL:HG11	1:C:238:PHE:CZ	2.53	0.44
1:C:138:ASP:O	1:C:140:PHE:HD1	2.01	0.44
1:C:802:PHE:O	1:C:804:GLN:N	2.50	0.44
2:F:34:TRP:CD2	2:F:72:LEU:HB2	2.52	0.44
3:G:10:GLU:HG3	3:G:18:VAL:CG2	2.48	0.44
2:H:60:ARG:O	2:H:74:ILE:HA	2.18	0.44
1:A:326:ILE:HD12	1:A:532:ASN:O	2.18	0.44
1:A:432:CYS:HB2	1:A:513:LEU:H	1.81	0.44
1:A:725:GLU:C	1:A:726:ILE:HG13	2.42	0.44
1:A:995:ARG:O	1:A:999:GLY:N	2.36	0.44
1:B:90:VAL:HG11	1:B:238:PHE:CZ	2.53	0.44
1:B:473:TYR:HB2	1:B:491:PRO:HB3	1.98	0.44
1:B:543:PHE:O	1:B:546:LEU:N	2.51	0.44
1:B:901:GLN:O	1:B:902:MET:C	2.59	0.44
1:B:1134:ASN:O	1:B:1135:ASN:HB2	2.18	0.44
1:C:1000:ARG:O	1:C:1001:LEU:C	2.60	0.44
2:F:33:HIS:CE1	3:G:106:VAL:HG12	2.52	0.44
2:F:43:PRO:HD2	3:G:110:TRP:CZ3	2.51	0.44
3:G:7:SER:HB3	3:G:21:SER:OG	2.18	0.44
2:H:43:PRO:HG2	3:I:45:LEU:HD21	1.99	0.44
3:I:65:LYS:HA	3:I:65:LYS:HD2	1.71	0.44
1:A:141:LEU:HB3	1:A:243:ALA:HA	1.99	0.44
1:A:143:VAL:HG13	1:A:151:SER:CB	2.47	0.44
1:A:376:THR:HG22	1:A:435:ALA:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:ARG:NH2	1:A:461:LEU:HD23	2.32	0.44
1:B:141:LEU:HB3	1:B:243:ALA:HA	1.99	0.44
1:B:898:PHE:O	1:B:900:MET:N	2.50	0.44
1:B:1081:ILE:HD13	1:B:1135:ASN:HB3	2.00	0.44
1:C:773:GLU:O	1:C:774:GLN:C	2.57	0.44
1:C:806:LEU:HD23	1:C:806:LEU:HA	1.54	0.44
1:C:1038:LYS:HB3	1:C:1038:LYS:HE3	1.66	0.44
2:D:12:VAL:O	2:D:105:ILE:HA	2.18	0.44
2:D:74:ILE:HG21	2:D:77:LEU:HD23	2.00	0.44
3:E:31:ASN:C	3:E:101:TYR:HB2	2.43	0.44
3:E:41:PRO:HD3	3:E:91:THR:O	2.18	0.44
2:F:82:PHE:HB3	2:F:105:ILE:CD1	2.48	0.44
3:I:9:ALA:HA	3:I:115:THR:O	2.18	0.44
1:A:543:PHE:O	1:A:546:LEU:N	2.51	0.43
1:A:898:PHE:O	1:A:900:MET:N	2.50	0.43
1:B:436:TRP:CE2	1:B:509:ARG:HB2	2.52	0.43
1:B:1000:ARG:O	1:B:1001:LEU:C	2.60	0.43
1:C:295:PRO:O	1:C:296:LEU:C	2.61	0.43
1:C:408:ARG:CD	3:I:102:ASP:OD1	2.65	0.43
1:C:897:PRO:O	1:C:900:MET:N	2.49	0.43
1:C:898:PHE:O	1:C:900:MET:N	2.51	0.43
2:F:31:ASN:OD1	2:F:49:TYR:HA	2.18	0.43
3:G:32:TYR:CD2	3:G:98:ARG:HD2	2.53	0.43
2:H:6:GLN:HE22	2:H:87:CYS:N	2.16	0.43
1:A:904:TYR:N	1:A:904:TYR:CD1	2.83	0.43
1:A:1012:LEU:HD23	1:A:1012:LEU:HA	1.60	0.43
1:A:1134:ASN:O	1:A:1135:ASN:HB2	2.18	0.43
1:B:439:ASN:HA	1:B:443:SER:OG	2.18	0.43
1:C:168:PHE:CG	1:C:169:GLU:N	2.86	0.43
1:C:1142:GLN:N	1:C:1143:PRO:HD2	2.33	0.43
3:G:39:GLN:HG3	3:G:44:SER:C	2.43	0.43
2:H:12:VAL:O	2:H:105:ILE:HA	2.18	0.43
3:I:88:SER:HA	3:I:118:VAL:O	2.18	0.43
3:I:98:ARG:NH2	3:I:108:ASP:HB2	2.33	0.43
1:A:64:TRP:CD1	1:A:65:PHE:H	2.37	0.43
1:A:138:ASP:O	1:A:140:PHE:HD1	2.01	0.43
1:A:866:THR:C	1:A:868:GLU:N	2.74	0.43
1:A:916:LEU:HA	1:A:916:LEU:HD12	1.54	0.43
1:B:125:ASN:OD1	5:B:1302:NAG:H81	2.19	0.43
1:B:328:ARG:HH22	1:B:533:LEU:CB	2.17	0.43
1:B:342:PHE:CE1	1:B:511:VAL:HG11	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:725:GLU:C	1:B:726:ILE:HG13	2.42	0.43
1:B:1003:SER:O	1:B:1003:SER:OG	2.35	0.43
1:B:1018:ILE:HD12	1:B:1018:ILE:HG23	1.56	0.43
1:B:1142:GLN:N	1:B:1143:PRO:HD2	2.33	0.43
1:C:54:LEU:O	1:C:55:PHE:HD1	2.00	0.43
1:C:318:PHE:O	1:C:318:PHE:CG	2.70	0.43
1:C:759:PHE:HD1	1:C:762:GLN:HE21	1.66	0.43
1:C:825:LYS:HE2	1:C:938:LEU:O	2.19	0.43
1:C:966:LEU:HA	1:C:966:LEU:HD23	1.58	0.43
2:D:6:GLN:HE22	2:D:87:CYS:N	2.16	0.43
3:E:36:TRP:CD1	3:E:70:LEU:HD22	2.52	0.43
3:I:35:HIS:CG	3:I:47:TRP:HE1	2.36	0.43
1:A:354:ASN:HB2	1:A:399:SER:HB3	1.99	0.43
1:A:773:GLU:O	1:A:774:GLN:C	2.57	0.43
1:A:825:LYS:HE2	1:A:938:LEU:O	2.19	0.43
1:A:901:GLN:O	1:A:902:MET:C	2.59	0.43
1:A:1004:LEU:O	1:A:1005:GLN:C	2.56	0.43
1:B:64:TRP:CD1	1:B:65:PHE:H	2.37	0.43
1:B:123:ALA:O	1:B:124:THR:OG1	2.35	0.43
1:B:133:PHE:CE2	1:B:135:PHE:HE1	2.35	0.43
1:B:133:PHE:HD2	1:B:160:TYR:HB2	1.82	0.43
1:B:378:LYS:HA	1:B:378:LYS:HD2	1.74	0.43
1:B:1011:GLN:O	1:B:1012:LEU:C	2.60	0.43
1:B:1139:ASP:OD2	1:B:1142:GLN:N	2.50	0.43
1:C:96:GLU:HB3	1:C:99:ASN:H	1.83	0.43
1:C:141:LEU:HD23	1:C:243:ALA:HB2	1.99	0.43
1:C:559:PHE:CD2	1:C:563:GLN:HB3	2.53	0.43
1:C:584:ILE:HA	1:C:584:ILE:HD13	1.77	0.43
1:C:801:ASN:OD1	1:C:801:ASN:C	2.60	0.43
3:E:33:TYR:HB2	3:E:99:SER:HB3	2.01	0.43
2:H:48:LYS:N	2:H:52:GLN:O	2.39	0.43
2:H:85:TYR:HE2	2:H:103:LEU:HD22	1.84	0.43
3:I:36:TRP:CD1	3:I:70:LEU:HD22	2.52	0.43
1:A:430:THR:HG21	1:A:517:LEU:CD2	2.49	0.43
1:A:884:SER:HA	1:A:894:LEU:O	2.19	0.43
1:B:318:PHE:CG	1:B:318:PHE:O	2.70	0.43
1:B:437:ASN:HA	1:B:508:TYR:CD1	2.53	0.43
1:B:559:PHE:CZ	1:B:566:GLY:HA2	2.51	0.43
1:B:559:PHE:HD1	1:B:559:PHE:HA	1.72	0.43
1:B:953:ASN:O	1:B:954:GLN:C	2.61	0.43
1:C:136:CYS:HB2	1:C:139:PRO:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:376:THR:HG22	1:C:435:ALA:N	2.33	0.43
1:C:402:ILE:HG21	1:C:410:ILE:HD11	2.01	0.43
2:D:85:TYR:HE2	2:D:103:LEU:HD22	1.84	0.43
2:F:20:ILE:CD1	2:F:85:TYR:HD2	2.31	0.43
2:H:97:PHE:CZ	3:I:47:TRP:HB2	2.52	0.43
1:A:136:CYS:HB2	1:A:139:PRO:N	2.34	0.43
1:A:161:SER:OG	1:A:162:SER:N	2.48	0.43
1:A:294:ASP:O	1:A:295:PRO:C	2.61	0.43
1:A:295:PRO:O	1:A:296:LEU:C	2.61	0.43
1:A:351:TYR:HB3	1:A:453:TYR:HA	2.00	0.43
1:A:437:ASN:HA	1:A:508:TYR:CD1	2.53	0.43
1:A:994:ASP:O	1:A:995:ARG:C	2.59	0.43
1:A:996:LEU:HD23	1:A:996:LEU:HA	1.46	0.43
1:B:54:LEU:HD23	1:B:272:PRO:CA	2.49	0.43
1:B:141:LEU:HD23	1:B:243:ALA:HB2	1.99	0.43
1:B:422:ASN:HB3	1:B:454:ARG:CB	2.48	0.43
1:B:805:ILE:O	1:B:816:SER:OG	2.30	0.43
1:B:916:LEU:O	1:B:917:TYR:C	2.60	0.43
1:C:212:LEU:HD23	1:C:215:ASP:O	2.19	0.43
1:C:422:ASN:HB3	1:C:454:ARG:CB	2.48	0.43
1:C:963:VAL:O	1:C:964:LYS:C	2.60	0.43
3:E:33:TYR:CE1	3:E:101:TYR:HD1	2.37	0.43
3:E:66:GLY:O	3:E:84:SER:OG	2.21	0.43
3:E:71:THR:O	3:E:80:TYR:N	2.28	0.43
2:H:34:TRP:CD2	2:H:72:LEU:HB2	2.54	0.43
3:I:31:ASN:O	3:I:101:TYR:HB2	2.19	0.43
1:A:96:GLU:HB3	1:A:99:ASN:H	1.83	0.43
1:A:141:LEU:HD23	1:A:243:ALA:HB2	1.99	0.43
1:A:402:ILE:HG21	1:A:410:ILE:HD11	2.01	0.43
1:A:778:THR:O	1:A:778:THR:HG22	2.19	0.43
1:A:1081:ILE:HD13	1:A:1135:ASN:HB3	2.00	0.43
1:B:402:ILE:HG21	1:B:410:ILE:HD11	2.01	0.43
1:B:825:LYS:HE2	1:B:938:LEU:O	2.19	0.43
1:B:884:SER:HA	1:B:894:LEU:O	2.19	0.43
1:B:1009:THR:O	1:B:1010:GLN:C	2.59	0.43
1:B:1029:MET:HE2	1:B:1029:MET:HB2	1.91	0.43
1:B:1104:VAL:O	1:B:1104:VAL:HG13	2.19	0.43
1:C:106:PHE:O	1:C:116:SER:OG	2.30	0.43
1:C:884:SER:HA	1:C:894:LEU:O	2.19	0.43
1:C:1109:PHE:O	1:C:1110:TYR:C	2.61	0.43
2:D:23:ARG:HH11	2:D:69:ASP:HB2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:9:ALA:HA	3:E:115:THR:O	2.18	0.43
2:F:36:GLN:OE1	2:F:46:LEU:HD21	2.18	0.43
2:H:23:ARG:HH11	2:H:69:ASP:HB2	1.83	0.43
1:A:90:VAL:HG11	1:A:238:PHE:CZ	2.53	0.43
1:A:342:PHE:CE1	1:A:511:VAL:HG11	2.53	0.43
1:B:386:LYS:HD3	1:B:389:ASP:HB3	2.00	0.43
1:B:581:THR:HG23	1:B:583:GLU:OE2	2.18	0.43
1:C:394:ASN:O	1:C:515:PHE:HA	2.19	0.43
1:C:581:THR:HG23	1:C:583:GLU:OE2	2.18	0.43
1:C:759:PHE:O	1:C:762:GLN:N	2.51	0.43
2:D:85:TYR:N	2:D:101:THR:O	2.47	0.43
3:E:4:LEU:HD23	3:E:24:VAL:HA	2.00	0.43
3:E:35:HIS:CG	3:E:47:TRP:HE1	2.36	0.43
3:E:98:ARG:NH2	3:E:108:ASP:HB2	2.34	0.43
2:F:31:ASN:CG	2:F:90:THR:HG21	2.44	0.43
3:G:10:GLU:O	3:G:116:VAL:HA	2.18	0.43
1:A:308:VAL:HB	1:A:602:THR:HG23	2.00	0.43
1:A:359:SER:CA	1:A:523:THR:HB	2.40	0.43
1:A:393:THR:OG1	1:A:394:ASN:N	2.48	0.43
1:A:713:ALA:O	1:C:894:LEU:HD22	2.19	0.43
1:B:54:LEU:O	1:B:55:PHE:HD1	2.00	0.43
1:B:136:CYS:HB2	1:B:139:PRO:N	2.33	0.43
1:B:273:ARG:HA	1:B:273:ARG:HD3	1.68	0.43
1:B:308:VAL:HB	1:B:602:THR:HG23	2.00	0.43
1:C:54:LEU:HD23	1:C:272:PRO:CA	2.49	0.43
1:C:123:ALA:O	1:C:124:THR:OG1	2.35	0.43
1:C:318:PHE:CE1	1:C:592:PHE:O	2.72	0.43
1:C:341:VAL:CG2	1:C:356:LYS:HD3	2.49	0.43
1:C:412:PRO:HB3	1:C:427:ASP:HA	2.01	0.43
1:C:437:ASN:HA	1:C:508:TYR:CD1	2.53	0.43
1:C:805:ILE:HG21	1:C:805:ILE:HD13	1.73	0.43
1:C:945:LEU:O	1:C:946:GLY:C	2.59	0.43
3:E:88:SER:HA	3:E:118:VAL:O	2.18	0.43
2:H:31:ASN:OD1	2:H:32:LEU:N	2.51	0.43
3:I:41:PRO:HD3	3:I:91:THR:O	2.18	0.43
1:A:341:VAL:CG2	1:A:356:LYS:HD3	2.49	0.43
1:A:378:LYS:HZ3	3:E:58:THR:N	2.17	0.43
1:A:914:ASN:HA	1:B:1089:PHE:CE2	2.54	0.43
1:A:1136:THR:O	1:A:1136:THR:OG1	2.37	0.43
1:B:295:PRO:O	1:B:296:LEU:C	2.61	0.43
1:B:354:ASN:HB2	1:B:399:SER:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:430:THR:HG21	1:B:517:LEU:CD2	2.49	0.43
1:B:1004:LEU:HA	1:B:1004:LEU:HD23	1.71	0.43
1:C:125:ASN:OD1	5:C:1302:NAG:H81	2.19	0.43
1:C:537:LYS:O	1:C:539:VAL:HG13	2.19	0.43
1:C:543:PHE:O	1:C:546:LEU:N	2.51	0.43
1:C:714:ILE:HD13	1:C:1105:THR:HG21	2.01	0.43
1:C:763:LEU:HA	1:C:763:LEU:HD23	1.62	0.43
1:C:1049:LEU:HA	1:C:1049:LEU:HD23	1.39	0.43
2:D:32:LEU:HD13	2:D:70:PHE:CG	2.53	0.43
2:D:60:ARG:O	2:D:74:ILE:HA	2.18	0.43
2:F:37:GLN:HB2	2:F:86:PHE:HE2	1.84	0.43
1:A:212:LEU:HD23	1:A:215:ASP:O	2.19	0.42
1:A:375:SER:HB2	1:A:436:TRP:HA	2.00	0.42
1:A:398:ASP:N	1:A:512:VAL:O	2.49	0.42
1:A:963:VAL:O	1:A:964:LYS:C	2.60	0.42
1:B:138:ASP:O	1:B:140:PHE:HD1	2.01	0.42
1:B:158:ARG:HG3	1:B:158:ARG:O	2.19	0.42
1:B:341:VAL:CG2	1:B:356:LYS:HD3	2.49	0.42
1:C:485:GLY:N	1:C:488:CYS:HB2	2.31	0.42
1:C:671:CYS:SG	1:C:697:MET:HB3	2.59	0.42
1:C:768:THR:O	1:C:769:GLY:C	2.61	0.42
1:C:912:THR:HG22	1:C:914:ASN:H	1.83	0.42
2:F:57:ILE:CG2	2:F:61:PHE:HD2	2.32	0.42
2:H:94:PRO:O	2:H:96:ILE:HG13	2.19	0.42
1:A:158:ARG:O	1:A:158:ARG:HG3	2.19	0.42
1:A:383:SER:HB2	1:A:386:LYS:HG2	2.01	0.42
1:A:412:PRO:CB	1:A:427:ASP:HA	2.49	0.42
1:A:671:CYS:SG	1:A:697:MET:HB3	2.59	0.42
1:B:381:GLY:CA	1:B:430:THR:HG23	2.49	0.42
1:C:92:PHE:CE1	1:C:93:ALA:O	2.72	0.42
1:C:381:GLY:CA	1:C:430:THR:HG23	2.49	0.42
1:C:778:THR:O	1:C:778:THR:HG22	2.19	0.42
1:C:858:LEU:HD12	1:C:858:LEU:H	1.84	0.42
1:C:1014:ARG:O	1:C:1017:GLU:N	2.47	0.42
2:D:4:LEU:HD23	2:D:89:GLN:HB2	2.01	0.42
2:D:94:PRO:O	2:D:96:ILE:HG13	2.19	0.42
2:H:74:ILE:HG21	2:H:77:LEU:HD23	2.00	0.42
3:I:4:LEU:HD23	3:I:24:VAL:HA	2.00	0.42
1:A:98:SER:OG	1:A:100:ILE:HG12	2.19	0.42
1:A:101:ILE:HA	1:A:242:LEU:CD2	2.49	0.42
1:A:108:THR:HG22	1:A:236:THR:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:897:PRO:O	1:A:900:MET:N	2.49	0.42
1:A:1004:LEU:HA	1:A:1004:LEU:HD23	1.71	0.42
1:B:96:GLU:HB3	1:B:99:ASN:H	1.83	0.42
1:B:388:ASN:CA	1:B:527:PRO:HD2	2.50	0.42
1:B:394:ASN:O	1:B:515:PHE:HA	2.19	0.42
1:B:671:CYS:SG	1:B:697:MET:HB3	2.59	0.42
1:B:1143:PRO:O	1:B:1146:ASP:HB3	2.19	0.42
1:C:324:GLU:HB2	1:C:325:SER:H	1.56	0.42
1:C:1134:ASN:O	1:C:1135:ASN:HB2	2.18	0.42
1:C:1138:TYR:OH	1:C:1143:PRO:HG3	2.20	0.42
3:I:18:VAL:HG13	3:I:83:LEU:HB3	2.02	0.42
1:A:48:LEU:H	1:A:48:LEU:HG	1.60	0.42
1:A:125:ASN:OD1	5:A:1302:NAG:H81	2.19	0.42
1:A:375:SER:CA	2:D:91:ASN:HB2	2.50	0.42
1:A:430:THR:HG21	1:A:517:LEU:CG	2.50	0.42
1:A:563:GLN:HA	1:C:41:LYS:O	2.19	0.42
1:A:1109:PHE:O	1:A:1110:TYR:C	2.61	0.42
1:B:101:ILE:HA	1:B:242:LEU:CD2	2.49	0.42
1:B:108:THR:HG22	1:B:236:THR:N	2.35	0.42
1:B:299:THR:O	1:B:300:LYS:C	2.63	0.42
1:B:431:GLY:HA2	1:B:515:PHE:CE1	2.55	0.42
1:B:901:GLN:C	1:B:903:ALA:H	2.25	0.42
1:B:925:ASN:O	1:B:926:GLN:C	2.62	0.42
1:C:431:GLY:HA2	1:C:515:PHE:CE1	2.55	0.42
1:C:916:LEU:O	1:C:917:TYR:C	2.60	0.42
1:C:1104:VAL:HG13	1:C:1104:VAL:O	2.19	0.42
2:D:34:TRP:CD2	2:D:72:LEU:HB2	2.54	0.42
2:D:35:TYR:O	2:D:85:TYR:HA	2.20	0.42
3:E:109:TYR:C	3:E:110:TRP:HD1	2.27	0.42
2:H:35:TYR:O	2:H:85:TYR:HA	2.20	0.42
2:H:35:TYR:OH	3:I:107:MET:HG2	2.19	0.42
1:A:345:THR:HG22	1:A:346:ARG:NH1	2.35	0.42
1:A:412:PRO:HB3	1:A:427:ASP:HA	2.01	0.42
1:A:804:GLN:HE21	4:L:1:NAG:H62	1.85	0.42
1:A:900:MET:HB3	1:A:900:MET:HE2	1.46	0.42
1:B:411:ALA:HB3	1:B:414:GLN:CG	2.50	0.42
1:B:498:GLN:O	1:B:500:THR:N	2.52	0.42
1:B:560:LEU:HD12	1:B:562:PHE:CE1	2.48	0.42
1:B:797:PHE:HD1	1:B:797:PHE:HA	1.65	0.42
1:C:44:ARG:HB3	1:C:47:VAL:HG11	2.02	0.42
1:C:319:ARG:H	1:C:319:ARG:HG2	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:375:SER:HB2	1:C:436:TRP:HA	2.00	0.42
1:C:535:LYS:NZ	1:C:554:GLU:OE2	2.37	0.42
1:C:712:ILE:HG21	1:C:712:ILE:HD13	1.82	0.42
1:C:1009:THR:O	1:C:1010:GLN:C	2.59	0.42
3:G:81:MET:HE1	3:G:94:TYR:CG	2.54	0.42
3:I:109:TYR:C	3:I:110:TRP:HD1	2.27	0.42
1:A:44:ARG:HB3	1:A:47:VAL:HG11	2.02	0.42
1:A:378:LYS:NZ	3:E:58:THR:OG1	2.53	0.42
1:A:402:ILE:HD12	1:A:406:GLU:HB2	2.02	0.42
1:A:591:SER:O	1:A:592:PHE:HB2	2.19	0.42
1:A:819:GLU:O	1:A:823:PHE:HD2	2.03	0.42
1:A:894:LEU:HD22	1:B:713:ALA:O	2.19	0.42
1:A:1009:THR:O	1:A:1010:GLN:C	2.59	0.42
1:B:229:LEU:HA	1:B:229:LEU:HD23	1.78	0.42
1:B:341:VAL:HG22	1:B:356:LYS:HD3	2.01	0.42
1:B:412:PRO:CB	1:B:427:ASP:HA	2.50	0.42
1:B:421:TYR:HB3	1:B:454:ARG:HG2	2.01	0.42
1:B:712:ILE:HD13	1:B:712:ILE:HG21	1.82	0.42
1:B:759:PHE:HD1	1:B:762:GLN:HE21	1.66	0.42
1:B:950:ASP:O	1:B:953:ASN:N	2.53	0.42
1:B:1014:ARG:O	1:B:1017:GLU:N	2.47	0.42
1:C:98:SER:OG	1:C:100:ILE:HG12	2.19	0.42
1:C:383:SER:HB2	1:C:386:LYS:HG2	2.01	0.42
1:C:411:ALA:HB3	1:C:414:GLN:CG	2.50	0.42
1:C:498:GLN:O	1:C:500:THR:N	2.52	0.42
1:C:1011:GLN:O	1:C:1015:ALA:N	2.33	0.42
2:D:31:ASN:O	2:D:90:THR:OG1	2.32	0.42
3:I:27:TYR:CE2	3:I:98:ARG:HD3	2.55	0.42
1:A:54:LEU:HD23	1:A:272:PRO:CA	2.49	0.42
1:A:92:PHE:CE1	1:A:93:ALA:O	2.72	0.42
1:A:140:PHE:HB2	1:A:242:LEU:O	2.20	0.42
1:A:421:TYR:HB3	1:A:454:ARG:HG2	2.01	0.42
1:A:537:LYS:O	1:A:539:VAL:HG13	2.19	0.42
1:B:43:PHE:HB3	1:C:559:PHE:CZ	2.55	0.42
1:B:457:ARG:NH1	1:B:459:SER:O	2.51	0.42
1:B:759:PHE:O	1:B:762:GLN:N	2.51	0.42
1:B:763:LEU:HA	1:B:763:LEU:HD23	1.62	0.42
1:B:778:THR:O	1:B:778:THR:HG22	2.19	0.42
1:B:931:ILE:O	1:B:932:GLY:C	2.62	0.42
1:C:345:THR:HG22	1:C:346:ARG:NH1	2.35	0.42
1:C:421:TYR:HB3	1:C:454:ARG:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:10:GLN:HG2	2:F:101:THR:HG21	2.00	0.42
2:F:29:SER:HB2	2:F:90:THR:OG1	2.20	0.42
2:F:60:ARG:HH21	2:F:81:ASP:CG	2.28	0.42
3:G:36:TRP:O	3:G:48:ILE:HG22	2.20	0.42
3:I:33:TYR:HB2	3:I:99:SER:HB3	2.01	0.42
3:I:116:VAL:HG12	3:I:118:VAL:HG23	2.01	0.42
1:A:106:PHE:O	1:A:116:SER:OG	2.30	0.42
1:A:231:ILE:HG13	1:A:232:GLY:H	1.85	0.42
1:A:341:VAL:HG22	1:A:356:LYS:HD3	2.01	0.42
1:A:759:PHE:O	1:A:762:GLN:N	2.51	0.42
1:A:915:VAL:HG12	1:A:916:LEU:N	2.35	0.42
1:A:1104:VAL:HG13	1:A:1104:VAL:O	2.19	0.42
1:A:1138:TYR:OH	1:A:1143:PRO:HG3	2.20	0.42
1:B:325:SER:O	1:B:326:ILE:HD13	2.20	0.42
1:B:664:ILE:O	1:B:665:PRO:C	2.61	0.42
1:B:709:ASN:ND2	5:B:1309:NAG:C7	2.83	0.42
1:B:804:GLN:HE21	4:Q:1:NAG:H62	1.85	0.42
1:B:963:VAL:O	1:B:964:LYS:C	2.60	0.42
1:C:108:THR:HG22	1:C:236:THR:N	2.35	0.42
1:C:299:THR:O	1:C:300:LYS:C	2.63	0.42
1:C:341:VAL:HG22	1:C:356:LYS:HD3	2.01	0.42
1:C:430:THR:HG21	1:C:517:LEU:CD2	2.49	0.42
1:C:750:SER:O	1:C:754:LEU:HG	2.20	0.42
1:C:904:TYR:O	1:C:905:ARG:C	2.57	0.42
1:A:43:PHE:HB2	1:B:563:GLN:CD	2.45	0.42
1:A:101:ILE:HA	1:A:242:LEU:HD23	2.02	0.42
1:A:325:SER:O	1:A:326:ILE:HD13	2.20	0.42
1:A:411:ALA:HB3	1:A:414:GLN:CG	2.50	0.42
1:A:431:GLY:HA2	1:A:515:PHE:CE1	2.55	0.42
1:A:805:ILE:HD13	1:A:805:ILE:HG21	1.73	0.42
1:A:817:PHE:O	1:A:818:ILE:C	2.63	0.42
1:B:30:ASN:HD22	1:B:32:PHE:HE1	1.67	0.42
1:B:98:SER:OG	1:B:100:ILE:HG12	2.19	0.42
1:B:212:LEU:HD23	1:B:215:ASP:O	2.19	0.42
1:B:402:ILE:HD12	1:B:406:GLU:C	2.45	0.42
1:B:719:THR:CG2	1:B:1068:VAL:HB	2.50	0.42
1:B:737:ASP:OD2	1:B:740:MET:N	2.48	0.42
1:B:747:THR:HG22	1:B:751:ASN:ND2	2.35	0.42
1:B:750:SER:O	1:B:754:LEU:HG	2.20	0.42
1:C:30:ASN:HD22	1:C:32:PHE:HE1	1.67	0.42
1:C:93:ALA:HA	1:C:190:ARG:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:294:ASP:O	1:C:295:PRO:C	2.61	0.42
1:C:308:VAL:HB	1:C:602:THR:HG23	2.00	0.42
1:C:402:ILE:HD12	1:C:406:GLU:HB2	2.02	0.42
1:C:412:PRO:CB	1:C:427:ASP:HA	2.50	0.42
1:C:567:ARG:HB3	1:C:568:ASP:H	1.71	0.42
1:C:588:THR:HG23	1:C:589:PRO:HD2	2.01	0.42
1:C:591:SER:O	1:C:592:PHE:HB2	2.19	0.42
1:C:737:ASP:OD2	1:C:740:MET:N	2.48	0.42
1:C:804:GLN:HE21	4:V:1:NAG:H62	1.85	0.42
1:C:931:ILE:O	1:C:932:GLY:C	2.62	0.42
1:C:1005:GLN:O	1:C:1006:THR:C	2.62	0.42
3:E:18:VAL:HG13	3:E:83:LEU:HB3	2.02	0.42
3:E:87:ARG:HG2	3:E:90:ASP:CG	2.45	0.42
2:H:4:LEU:HD23	2:H:89:GLN:HB2	2.01	0.42
1:A:108:THR:HG22	1:A:236:THR:HG23	2.02	0.42
1:A:242:LEU:HD23	1:A:242:LEU:HA	1.73	0.42
1:A:559:PHE:CE1	1:A:566:GLY:CA	3.03	0.42
1:A:560:LEU:HD22	1:A:560:LEU:HA	1.73	0.42
1:A:759:PHE:HD1	1:A:762:GLN:HE21	1.66	0.42
1:A:850:ILE:N	1:A:850:ILE:CD1	2.73	0.42
1:A:1005:GLN:O	1:A:1006:THR:C	2.62	0.42
1:A:1089:PHE:CE2	1:C:914:ASN:HA	2.54	0.42
1:B:894:LEU:HD22	1:C:713:ALA:O	2.20	0.42
1:C:99:ASN:O	1:C:102:ARG:NH2	2.53	0.42
1:C:233:ILE:HD13	1:C:233:ILE:HG21	1.87	0.42
1:C:402:ILE:HD12	1:C:406:GLU:C	2.45	0.42
1:C:819:GLU:O	1:C:823:PHE:HD2	2.03	0.42
1:C:953:ASN:O	1:C:954:GLN:C	2.61	0.42
1:C:1018:ILE:HD12	1:C:1018:ILE:HG23	1.56	0.42
2:D:35:TYR:OH	3:E:107:MET:HG2	2.19	0.42
3:E:6:GLN:H	3:E:112:GLN:NE2	2.17	0.42
3:E:98:ARG:O	3:E:107:MET:HA	2.20	0.42
3:E:116:VAL:HG12	3:E:118:VAL:HG23	2.01	0.42
2:F:84:ILE:HA	2:F:102:LYS:HA	2.02	0.42
1:A:30:ASN:HD22	1:A:32:PHE:HE1	1.67	0.41
1:A:397:ALA:HB2	1:A:513:LEU:HD23	2.02	0.41
1:A:410:ILE:HG12	1:A:423:TYR:HD2	1.85	0.41
1:A:498:GLN:O	1:A:500:THR:N	2.52	0.41
1:A:664:ILE:O	1:A:665:PRO:C	2.61	0.41
1:A:768:THR:O	1:A:769:GLY:C	2.61	0.41
1:A:931:ILE:O	1:A:932:GLY:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1029:MET:HE2	1:A:1029:MET:HB2	1.91	0.41
1:B:376:THR:HG22	1:B:435:ALA:N	2.33	0.41
1:B:584:ILE:HD13	1:B:584:ILE:HA	1.77	0.41
1:B:669:GLY:O	1:B:697:MET:HG2	2.20	0.41
1:B:1005:GLN:O	1:B:1006:THR:C	2.62	0.41
1:B:1109:PHE:O	1:B:1110:TYR:C	2.61	0.41
2:F:4:LEU:HD23	2:F:89:GLN:HB2	2.01	0.41
2:F:60:ARG:HG3	2:F:61:PHE:CD1	2.55	0.41
3:I:87:ARG:HG2	3:I:90:ASP:CG	2.45	0.41
1:A:394:ASN:O	1:A:515:PHE:HA	2.19	0.41
1:A:588:THR:HG23	1:A:589:PRO:HD2	2.01	0.41
1:A:750:SER:O	1:A:754:LEU:HG	2.20	0.41
1:A:767:LEU:HD23	1:A:767:LEU:HA	1.60	0.41
1:A:1116:THR:H	1:A:1119:ASN:HD22	1.68	0.41
1:A:1143:PRO:O	1:A:1146:ASP:HB3	2.19	0.41
1:B:92:PHE:CE1	1:B:93:ALA:O	2.72	0.41
1:B:375:SER:HB2	1:B:436:TRP:HA	2.00	0.41
1:B:397:ALA:HB2	1:B:513:LEU:HD23	2.02	0.41
1:B:402:ILE:HD12	1:B:406:GLU:HB2	2.02	0.41
1:B:588:THR:HG23	1:B:589:PRO:HD2	2.01	0.41
1:B:591:SER:O	1:B:592:PHE:HB2	2.19	0.41
1:B:643:PHE:CD1	1:B:655:HIS:HB2	2.55	0.41
1:B:714:ILE:HD13	1:B:1105:THR:HG21	2.01	0.41
1:B:1056:ALA:HB1	1:B:1057:PRO:HD2	2.02	0.41
1:B:1138:TYR:OH	1:B:1143:PRO:HG3	2.20	0.41
1:C:64:TRP:CD1	1:C:65:PHE:H	2.37	0.41
1:C:140:PHE:HB2	1:C:242:LEU:O	2.20	0.41
1:C:354:ASN:HB2	1:C:399:SER:H	1.85	0.41
1:C:664:ILE:O	1:C:665:PRO:C	2.61	0.41
1:C:709:ASN:ND2	5:C:1309:NAG:C7	2.83	0.41
1:C:759:PHE:HD1	1:C:762:GLN:NE2	2.18	0.41
1:C:806:LEU:O	1:C:807:PRO:C	2.63	0.41
3:E:38:LYS:HG3	3:E:94:TYR:CE1	2.56	0.41
1:A:43:PHE:HB3	1:B:566:GLY:HA2	2.03	0.41
1:A:152:TRP:HB3	1:A:153:MET:H	1.57	0.41
1:A:357:ARG:NH1	1:C:166:CYS:O	2.53	0.41
1:A:457:ARG:NH1	1:A:459:SER:O	2.51	0.41
1:A:669:GLY:O	1:A:697:MET:HG2	2.20	0.41
1:A:744:GLY:O	1:A:746:SER:N	2.53	0.41
1:A:759:PHE:HD1	1:A:762:GLN:NE2	2.18	0.41
1:B:537:LYS:O	1:B:539:VAL:HG13	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:695:TYR:CD1	1:B:695:TYR:N	2.88	0.41
1:B:768:THR:O	1:B:769:GLY:C	2.61	0.41
1:B:953:ASN:O	1:B:957:GLN:N	2.39	0.41
1:B:1024:LEU:HD12	1:B:1024:LEU:HA	1.72	0.41
1:C:101:ILE:HA	1:C:242:LEU:CD2	2.50	0.41
1:C:108:THR:HG22	1:C:236:THR:HG23	2.02	0.41
1:C:158:ARG:HG3	1:C:158:ARG:O	2.19	0.41
1:C:950:ASP:O	1:C:953:ASN:N	2.53	0.41
1:C:977:LEU:HA	1:C:977:LEU:HD12	1.75	0.41
1:C:1094:VAL:H	1:C:1094:VAL:HG22	1.67	0.41
1:C:1143:PRO:O	1:C:1146:ASP:HB3	2.19	0.41
3:E:35:HIS:HB3	3:E:47:TRP:HE1	1.85	0.41
2:F:46:LEU:O	2:F:53:SER:HA	2.19	0.41
3:G:47:TRP:CZ2	3:G:50:TYR:CD2	3.07	0.41
3:G:100:GLU:CG	3:G:104:TYR:O	2.68	0.41
3:I:35:HIS:HE1	3:I:105:TYR:CD1	2.38	0.41
1:A:309:GLU:O	1:A:313:TYR:OH	2.34	0.41
1:A:385:THR:OG1	3:E:65:LYS:HE2	2.20	0.41
1:A:719:THR:CG2	1:A:1068:VAL:HB	2.50	0.41
1:B:64:TRP:NE1	1:B:65:PHE:O	2.53	0.41
1:B:915:VAL:HG12	1:B:916:LEU:N	2.35	0.41
1:B:917:TYR:HD2	1:C:1089:PHE:CE2	2.38	0.41
1:B:982:SER:OG	1:B:983:ARG:N	2.54	0.41
1:C:64:TRP:NE1	1:C:65:PHE:O	2.53	0.41
1:C:397:ALA:HB2	1:C:513:LEU:HD23	2.02	0.41
1:C:528:LYS:HE2	1:C:528:LYS:HB2	1.85	0.41
1:C:543:PHE:O	1:C:546:LEU:HB3	2.20	0.41
2:H:10:GLN:HG3	2:H:20:ILE:HG12	2.02	0.41
3:I:38:LYS:HG3	3:I:94:TYR:CE1	2.55	0.41
3:I:109:TYR:C	3:I:110:TRP:CD1	2.98	0.41
1:A:99:ASN:O	1:A:102:ARG:NH2	2.53	0.41
1:A:106:PHE:HD1	1:A:106:PHE:N	2.18	0.41
1:A:386:LYS:HA	1:A:389:ASP:HB3	2.02	0.41
1:A:709:ASN:ND2	5:A:1309:NAG:C7	2.83	0.41
1:A:1047:TYR:O	1:A:1066:THR:HB	2.20	0.41
1:B:44:ARG:HB3	1:B:47:VAL:HG11	2.02	0.41
1:B:337:PRO:HD2	1:B:358:ILE:HG23	2.03	0.41
1:B:717:ASN:O	1:B:1070:ALA:N	2.51	0.41
1:B:897:PRO:O	1:B:900:MET:N	2.49	0.41
1:C:118:LEU:N	1:C:129:LYS:O	2.53	0.41
1:C:337:PRO:HD2	1:C:358:ILE:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:791:THR:HG21	1:C:806:LEU:HD13	2.02	0.41
2:D:23:ARG:NE	2:D:69:ASP:HB2	2.36	0.41
3:E:6:GLN:N	3:E:112:GLN:HE22	2.19	0.41
3:E:27:TYR:CE2	3:E:98:ARG:HD3	2.55	0.41
2:F:106:LEU:O	2:F:107:LYS:HB3	2.21	0.41
3:G:27:TYR:CE1	3:G:32:TYR:HD2	2.38	0.41
3:G:66:GLY:HA3	3:G:83:LEU:HD12	2.02	0.41
3:I:6:GLN:H	3:I:112:GLN:NE2	2.17	0.41
1:A:402:ILE:HD12	1:A:406:GLU:C	2.45	0.41
1:A:560:LEU:HB2	1:A:563:GLN:NE2	2.36	0.41
1:A:741:TYR:CD2	1:A:741:TYR:C	2.98	0.41
1:A:850:ILE:H	1:A:850:ILE:CD1	2.23	0.41
1:A:1011:GLN:O	1:A:1015:ALA:N	2.33	0.41
1:B:65:PHE:HD2	1:B:265:TYR:OH	2.04	0.41
1:B:345:THR:HG22	1:B:346:ARG:NH1	2.35	0.41
1:B:383:SER:HB2	1:B:386:LYS:HG2	2.01	0.41
1:B:412:PRO:HB3	1:B:427:ASP:HA	2.01	0.41
1:B:819:GLU:O	1:B:823:PHE:HD2	2.03	0.41
1:B:1095:PHE:HD1	1:B:1095:PHE:HA	1.70	0.41
1:C:150:LYS:C	1:C:152:TRP:H	2.29	0.41
1:C:353:TRP:CG	1:C:423:TYR:CE1	3.09	0.41
1:C:786:LYS:H	1:C:786:LYS:HG2	1.54	0.41
1:C:870:ILE:O	1:C:874:THR:HG23	2.21	0.41
1:C:887:THR:H	1:C:887:THR:HG23	1.64	0.41
3:E:4:LEU:CD2	3:E:24:VAL:HG22	2.50	0.41
2:F:33:HIS:O	2:F:88:GLN:N	2.52	0.41
2:F:60:ARG:O	2:F:74:ILE:HA	2.21	0.41
2:H:23:ARG:NE	2:H:69:ASP:HB2	2.36	0.41
1:A:150:LYS:C	1:A:152:TRP:H	2.29	0.41
1:A:229:LEU:HD23	1:A:229:LEU:HA	1.78	0.41
1:A:353:TRP:CG	1:A:423:TYR:CE1	3.09	0.41
1:A:354:ASN:HB2	1:A:399:SER:H	1.85	0.41
1:A:643:PHE:CD1	1:A:655:HIS:HB2	2.56	0.41
1:A:797:PHE:HD1	1:A:797:PHE:HA	1.65	0.41
1:A:874:THR:H	1:A:874:THR:HG23	1.60	0.41
1:A:907:ASN:O	1:A:908:GLY:C	2.63	0.41
1:A:980:ILE:H	1:A:980:ILE:HG13	1.63	0.41
1:A:1038:LYS:HE3	1:A:1038:LYS:HB3	1.66	0.41
1:A:1056:ALA:HB1	1:A:1057:PRO:HD2	2.02	0.41
1:A:1139:ASP:OD2	1:A:1142:GLN:N	2.50	0.41
1:B:140:PHE:HB2	1:B:242:LEU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:666:ILE:HB	1:B:670:ILE:O	2.21	0.41
1:B:726:ILE:CG2	1:B:948:LEU:HD13	2.51	0.41
1:B:758:SER:O	1:B:759:PHE:C	2.64	0.41
1:B:791:THR:HG21	1:B:806:LEU:HD13	2.02	0.41
1:B:817:PHE:O	1:B:818:ILE:C	2.63	0.41
1:B:907:ASN:O	1:B:908:GLY:C	2.63	0.41
1:B:1074:ASN:O	1:B:1075:PHE:CG	2.74	0.41
1:C:101:ILE:HA	1:C:242:LEU:HD23	2.02	0.41
1:C:226:LEU:HD23	1:C:226:LEU:HA	1.85	0.41
1:C:226:LEU:HB2	1:C:227:VAL:HG23	2.02	0.41
1:C:409:GLN:CB	1:C:418:ILE:HB	2.51	0.41
1:C:719:THR:CG2	1:C:1068:VAL:HB	2.50	0.41
1:C:805:ILE:H	1:C:805:ILE:HG12	1.68	0.41
1:C:941:THR:HG22	1:C:943:SER:H	1.86	0.41
1:C:1047:TYR:O	1:C:1066:THR:HB	2.20	0.41
3:E:109:TYR:C	3:E:110:TRP:CD1	2.98	0.41
3:G:56:GLY:O	3:G:58:THR:N	2.53	0.41
1:A:226:LEU:HB2	1:A:227:VAL:HG23	2.02	0.41
1:A:273:ARG:HA	1:A:273:ARG:HD3	1.68	0.41
1:A:377:PHE:O	3:E:59:SER:HB3	2.21	0.41
1:A:378:LYS:HA	1:A:378:LYS:HD2	1.74	0.41
1:A:913:GLN:O	1:A:914:ASN:C	2.62	0.41
1:A:953:ASN:O	1:A:954:GLN:C	2.61	0.41
1:A:1100:THR:HG1	1:A:1101:HIS:N	2.17	0.41
1:B:226:LEU:CB	1:B:227:VAL:HG23	2.51	0.41
1:B:312:ILE:O	1:B:312:ILE:HG23	2.21	0.41
1:B:587:ILE:HG21	1:B:587:ILE:HD13	1.80	0.41
1:B:759:PHE:HD1	1:B:762:GLN:NE2	2.18	0.41
1:B:916:LEU:HD12	1:B:916:LEU:HA	1.53	0.41
1:C:317:ASN:OD1	1:C:317:ASN:N	2.53	0.41
1:C:386:LYS:HA	1:C:389:ASP:HB3	2.02	0.41
1:C:758:SER:O	1:C:759:PHE:C	2.64	0.41
1:C:980:ILE:H	1:C:980:ILE:HG13	1.63	0.41
1:C:982:SER:OG	1:C:983:ARG:N	2.54	0.41
1:C:1074:ASN:O	1:C:1075:PHE:CG	2.74	0.41
2:F:43:PRO:HB2	3:G:110:TRP:CH2	2.56	0.41
1:A:93:ALA:HA	1:A:190:ARG:O	2.20	0.41
1:A:226:LEU:HD23	1:A:226:LEU:HA	1.85	0.41
1:A:328:ARG:HH22	1:A:533:LEU:CB	2.17	0.41
1:A:354:ASN:O	1:A:398:ASP:HA	2.21	0.41
1:A:584:ILE:HA	1:A:584:ILE:HD13	1.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:726:ILE:CG2	1:A:948:LEU:HD13	2.51	0.41
1:A:807:PRO:O	1:A:809:PRO:HD3	2.21	0.41
1:A:883:THR:H	1:A:883:THR:HG23	1.72	0.41
1:A:923:ILE:O	1:A:924:ALA:C	2.63	0.41
1:A:950:ASP:O	1:A:953:ASN:N	2.53	0.41
1:A:1074:ASN:O	1:A:1075:PHE:CG	2.74	0.41
1:B:97:LYS:H	1:B:97:LYS:HG2	1.64	0.41
1:B:101:ILE:HA	1:B:242:LEU:HD23	2.02	0.41
1:B:111:ASP:O	1:B:112:SER:HB3	2.21	0.41
1:B:150:LYS:C	1:B:152:TRP:H	2.29	0.41
1:B:203:ILE:CG2	1:B:204:TYR:N	2.84	0.41
1:B:206:LYS:HA	1:B:206:LYS:HD2	1.92	0.41
1:B:216:LEU:HA	1:B:216:LEU:HD23	1.84	0.41
1:B:331:ASN:N	1:B:580:GLN:HG2	2.36	0.41
1:B:354:ASN:O	1:B:398:ASP:HA	2.21	0.41
1:B:393:THR:O	1:B:523:THR:OG1	2.23	0.41
1:B:560:LEU:CB	1:B:563:GLN:HB2	2.44	0.41
1:B:864:LEU:HG	1:B:865:LEU:HD12	2.02	0.41
1:B:870:ILE:HG23	1:B:870:ILE:HD12	1.85	0.41
1:B:887:THR:H	1:B:887:THR:HG23	1.64	0.41
1:B:1047:TYR:O	1:B:1066:THR:HB	2.20	0.41
1:C:206:LYS:HA	1:C:206:LYS:HD2	1.92	0.41
1:C:214:ARG:HG2	1:C:215:ASP:HB2	2.03	0.41
1:C:229:LEU:HA	1:C:229:LEU:HD23	1.78	0.41
1:C:279:TYR:CD1	1:C:279:TYR:N	2.89	0.41
1:C:388:ASN:CA	1:C:527:PRO:HD2	2.50	0.41
1:C:457:ARG:NH1	1:C:459:SER:O	2.51	0.41
1:C:541:PHE:CD1	1:C:541:PHE:C	2.99	0.41
1:C:560:LEU:CB	1:C:563:GLN:HB2	2.45	0.41
1:C:741:TYR:CD2	1:C:741:TYR:C	2.98	0.41
1:C:744:GLY:O	1:C:746:SER:N	2.53	0.41
1:C:925:ASN:O	1:C:926:GLN:C	2.62	0.41
1:C:929:SER:O	1:C:932:GLY:N	2.54	0.41
2:D:37:GLN:NE2	3:E:39:GLN:OE1	2.52	0.41
3:G:86:LEU:HD23	3:G:86:LEU:HA	1.92	0.41
2:H:26:GLN:HG3	2:H:27:SER:H	1.86	0.41
2:H:45:LEU:HD23	3:I:108:ASP:OD1	2.21	0.41
2:H:85:TYR:N	2:H:101:THR:O	2.47	0.41
3:I:30:SER:HA	3:I:53:PRO:CB	2.51	0.41
3:I:62:LEU:O	3:I:63:LYS:C	2.64	0.41
1:A:226:LEU:CB	1:A:227:VAL:HG23	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:PRO:HD2	1:A:358:ILE:HG12	2.03	0.41
1:A:388:ASN:CA	1:A:527:PRO:HD2	2.50	0.41
1:A:543:PHE:O	1:A:546:LEU:HB3	2.20	0.41
1:A:714:ILE:HD13	1:A:1105:THR:HG21	2.01	0.41
1:A:758:SER:O	1:A:759:PHE:C	2.64	0.41
1:A:822:LEU:HA	1:A:822:LEU:HD23	1.68	0.41
1:A:1093:GLY:HA2	1:A:1107:ARG:NH1	2.31	0.41
1:B:372:ALA:O	2:F:92:PHE:HA	2.20	0.41
1:B:744:GLY:O	1:B:746:SER:N	2.53	0.41
1:B:902:MET:HE3	1:B:902:MET:HB3	1.62	0.41
1:B:960:ASN:O	1:B:961:THR:C	2.63	0.41
1:C:669:GLY:O	1:C:697:MET:HG2	2.20	0.41
1:C:740:MET:O	1:C:741:TYR:C	2.64	0.41
1:C:786:LYS:HG3	1:C:787:GLN:N	2.35	0.41
1:C:818:ILE:O	1:C:819:GLU:C	2.63	0.41
1:C:854:LYS:HA	1:C:858:LEU:O	2.21	0.41
1:C:1004:LEU:HA	1:C:1004:LEU:HD23	1.71	0.41
3:E:92:ALA:O	3:E:115:THR:HA	2.21	0.41
2:H:32:LEU:HB3	2:H:50:ALA:HB2	2.03	0.41
1:A:45:SER:O	1:A:47:VAL:HG12	2.21	0.40
1:A:64:TRP:NE1	1:A:65:PHE:O	2.53	0.40
1:A:65:PHE:HD2	1:A:265:TYR:OH	2.04	0.40
1:A:111:ASP:C	1:A:134:GLN:OE1	2.65	0.40
1:A:216:LEU:HA	1:A:216:LEU:HD23	1.83	0.40
1:A:541:PHE:CD1	1:A:541:PHE:C	2.99	0.40
1:A:546:LEU:HD22	1:A:565:PHE:CE1	2.56	0.40
1:A:666:ILE:HB	1:A:670:ILE:O	2.21	0.40
1:A:715:PRO:HD3	1:C:894:LEU:CD1	2.51	0.40
1:A:756:TYR:HD1	1:B:970:PHE:HD1	1.69	0.40
1:A:941:THR:HG22	1:A:943:SER:H	1.86	0.40
1:B:170:TYR:CG	1:B:171:VAL:N	2.90	0.40
1:B:280:ASN:O	1:B:283:GLY:N	2.49	0.40
1:B:337:PRO:HD2	1:B:358:ILE:HG12	2.03	0.40
1:B:870:ILE:O	1:B:874:THR:HG23	2.21	0.40
1:B:1100:THR:HG1	1:B:1101:HIS:N	2.19	0.40
1:C:48:LEU:HA	1:C:48:LEU:HD23	1.90	0.40
1:C:410:ILE:HG12	1:C:423:TYR:HD2	1.85	0.40
1:C:1139:ASP:OD2	1:C:1142:GLN:N	2.50	0.40
2:D:22:CYS:SG	2:D:32:LEU:HD11	2.62	0.40
2:D:45:LEU:HD23	3:E:108:ASP:OD1	2.21	0.40
3:E:31:ASN:O	3:E:101:TYR:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:62:LEU:O	3:E:63:LYS:C	2.64	0.40
2:H:82:PHE:CD2	2:H:105:ILE:HB	2.56	0.40
3:I:4:LEU:CD2	3:I:24:VAL:HG22	2.50	0.40
3:I:28:SER:OG	3:I:31:ASN:HB2	2.22	0.40
3:I:98:ARG:O	3:I:107:MET:HA	2.20	0.40
1:A:413:GLY:HA3	3:E:54:PHE:CE2	2.56	0.40
1:A:670:ILE:HA	1:A:670:ILE:HD13	1.83	0.40
1:A:925:ASN:O	1:A:926:GLN:C	2.62	0.40
1:B:99:ASN:O	1:B:102:ARG:NH2	2.53	0.40
1:B:111:ASP:C	1:B:134:GLN:OE1	2.65	0.40
1:B:353:TRP:CG	1:B:423:TYR:CE1	3.09	0.40
1:B:354:ASN:HB2	1:B:399:SER:H	1.85	0.40
1:B:726:ILE:HD13	1:B:945:LEU:CD2	2.51	0.40
1:B:894:LEU:CD1	1:C:715:PRO:HD3	2.51	0.40
1:B:923:ILE:O	1:B:924:ALA:C	2.63	0.40
1:B:941:THR:HG22	1:B:943:SER:H	1.86	0.40
1:B:1116:THR:H	1:B:1119:ASN:HD22	1.68	0.40
1:C:131:CYS:HA	1:C:166:CYS:HA	2.03	0.40
1:C:170:TYR:CG	1:C:171:VAL:N	2.90	0.40
1:C:277:LEU:HA	1:C:277:LEU:HD23	1.48	0.40
1:C:695:TYR:CD1	1:C:695:TYR:N	2.88	0.40
1:C:737:ASP:OD2	1:C:740:MET:HB3	2.22	0.40
1:C:1050:MET:C	1:C:1051:SER:HG	2.22	0.40
2:D:10:GLN:HG3	2:D:20:ILE:HG12	2.02	0.40
2:D:32:LEU:HB3	2:D:50:ALA:HB2	2.03	0.40
1:A:32:PHE:HA	1:A:59:PHE:CD1	2.56	0.40
1:A:131:CYS:HA	1:A:166:CYS:HA	2.03	0.40
1:A:142:GLY:H	1:A:156:GLU:CB	2.34	0.40
1:A:212:LEU:HD11	1:A:214:ARG:NH1	2.37	0.40
1:A:312:ILE:O	1:A:312:ILE:HG23	2.21	0.40
1:A:327:VAL:HB	1:A:531:THR:HG23	2.04	0.40
1:A:331:ASN:N	1:A:580:GLN:HG2	2.36	0.40
1:A:455:LEU:HG	1:A:456:PHE:CD2	2.57	0.40
1:B:108:THR:HG22	1:B:236:THR:HG23	2.02	0.40
1:B:142:GLY:H	1:B:156:GLU:CB	2.34	0.40
1:B:294:ASP:O	1:B:295:PRO:C	2.61	0.40
1:B:543:PHE:O	1:B:546:LEU:HB3	2.20	0.40
1:B:786:LYS:HG3	1:B:787:GLN:N	2.35	0.40
1:B:1050:MET:C	1:B:1051:SER:HG	2.12	0.40
1:C:37:TYR:HB2	1:C:223:LEU:O	2.22	0.40
1:C:111:ASP:C	1:C:134:GLN:OE1	2.65	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:643:PHE:CD1	1:C:655:HIS:HB2	2.55	0.40
1:C:666:ILE:HB	1:C:670:ILE:O	2.21	0.40
1:C:923:ILE:O	1:C:924:ALA:C	2.63	0.40
2:D:34:TRP:CD1	2:D:47:ILE:HB	2.55	0.40
3:E:4:LEU:O	3:E:111:GLY:HA2	2.22	0.40
2:F:29:SER:OG	2:F:91:ASN:OD1	2.26	0.40
3:G:34:ILE:HB	3:G:51:ILE:HG22	2.03	0.40
2:H:34:TRP:CD1	2:H:47:ILE:HB	2.55	0.40
3:I:92:ALA:O	3:I:115:THR:HA	2.21	0.40
4:X:1:NAG:H62	4:X:2:NAG:H82	2.04	0.40
1:A:31:SER:OG	1:A:60:SER:N	2.55	0.40
1:A:37:TYR:HB2	1:A:223:LEU:O	2.21	0.40
1:A:907:ASN:N	1:A:907:ASN:OD1	2.52	0.40
1:A:917:TYR:HD2	1:B:1089:PHE:CE2	2.40	0.40
1:A:934:ILE:HD12	1:A:934:ILE:HG23	1.67	0.40
1:B:31:SER:OG	1:B:60:SER:N	2.55	0.40
1:B:45:SER:O	1:B:47:VAL:HG12	2.21	0.40
1:B:131:CYS:HA	1:B:166:CYS:HA	2.03	0.40
1:B:214:ARG:HG2	1:B:215:ASP:HB2	2.03	0.40
1:B:453:TYR:CD1	1:B:495:TYR:CE2	3.10	0.40
1:B:541:PHE:CD1	1:B:541:PHE:C	2.99	0.40
1:B:1100:THR:HG1	1:B:1101:HIS:CE1	2.33	0.40
1:C:31:SER:OG	1:C:60:SER:N	2.55	0.40
1:C:142:GLY:H	1:C:156:GLU:CB	2.34	0.40
1:C:212:LEU:HD11	1:C:214:ARG:NH1	2.37	0.40
1:C:226:LEU:CB	1:C:227:VAL:HG23	2.51	0.40
3:E:22:CYS:O	3:E:78:THR:HA	2.21	0.40
3:E:97:ALA:HB1	3:E:107:MET:CB	2.50	0.40
3:I:6:GLN:N	3:I:112:GLN:HE22	2.19	0.40
3:I:22:CYS:O	3:I:78:THR:HA	2.21	0.40
1:A:106:PHE:HB3	1:A:235:ILE:HD13	2.04	0.40
1:A:737:ASP:OD2	1:A:740:MET:HB3	2.22	0.40
1:A:786:LYS:HG3	1:A:787:GLN:N	2.35	0.40
1:A:870:ILE:O	1:A:874:THR:HG23	2.21	0.40
1:A:1024:LEU:HA	1:A:1024:LEU:HD12	1.72	0.40
1:B:32:PHE:HA	1:B:59:PHE:CD1	2.57	0.40
1:B:81:ASN:ND2	1:B:239:GLN:HE21	2.19	0.40
1:B:231:ILE:HG13	1:B:232:GLY:H	1.85	0.40
1:B:347:PHE:CE2	1:B:509:ARG:HD3	2.57	0.40
1:B:430:THR:HG21	1:B:517:LEU:CG	2.50	0.40
1:B:737:ASP:OD2	1:B:740:MET:HB3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:977:LEU:HA	1:B:977:LEU:HD12	1.75	0.40
1:B:1050:MET:O	1:B:1051:SER:OG	2.21	0.40
1:B:1086:LYS:HE2	1:B:1086:LYS:HB2	1.89	0.40
1:C:45:SER:O	1:C:47:VAL:HG12	2.21	0.40
1:C:317:ASN:HB2	1:C:593:GLY:O	2.17	0.40
1:C:985:ASP:N	1:C:988:GLU:OE1	2.52	0.40
2:D:35:TYR:CE2	2:D:45:LEU:HB2	2.57	0.40
2:D:57:ILE:CG2	2:D:61:PHE:HD2	2.34	0.40
2:D:87:CYS:O	2:D:98:GLY:N	2.46	0.40
3:I:35:HIS:HB3	3:I:47:TRP:HE1	1.85	0.40
4:S:1:NAG:H62	4:S:2:NAG:H82	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	1012/1208 (84%)	899 (89%)	106 (10%)	7 (1%)	18	51
1	B	1012/1208 (84%)	906 (90%)	101 (10%)	5 (0%)	24	57
1	C	1012/1208 (84%)	900 (89%)	106 (10%)	6 (1%)	21	54
2	D	105/210 (50%)	96 (91%)	8 (8%)	1 (1%)	12	44
2	F	105/210 (50%)	98 (93%)	6 (6%)	1 (1%)	12	44
2	H	105/210 (50%)	96 (91%)	8 (8%)	1 (1%)	12	44
3	E	120/223 (54%)	113 (94%)	4 (3%)	3 (2%)	4	28
3	G	120/223 (54%)	112 (93%)	5 (4%)	3 (2%)	4	28
3	I	120/223 (54%)	112 (93%)	5 (4%)	3 (2%)	4	28
All	All	3711/4923 (75%)	3332 (90%)	349 (9%)	30 (1%)	18	49

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	856	ASN
3	G	102	ASP
3	I	102	ASP
1	A	332	ILE
1	A	557	LYS
1	A	857	GLY
1	B	332	ILE
1	C	332	ILE
3	E	104	TYR
1	A	161	SER
1	B	161	SER
1	C	161	SER
1	A	902	MET
1	B	902	MET
1	C	902	MET
3	E	57	GLY
3	E	102	ASP
3	I	57	GLY
3	I	104	TYR
2	F	93	TRP
3	G	103	PRO
1	A	1033	VAL
1	B	1033	VAL
1	C	1033	VAL
2	D	93	TRP
2	H	93	TRP
3	G	57	GLY
1	A	770	ILE
1	B	770	ILE
1	C	770	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	896/1054 (85%)	879 (98%)	17 (2%)	50	67
1	B	897/1054 (85%)	879 (98%)	18 (2%)	48	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	897/1054 (85%)	875 (98%)	22 (2%)	42	63
2	D	95/189 (50%)	95 (100%)	0	100	100
2	F	95/189 (50%)	95 (100%)	0	100	100
2	H	95/189 (50%)	95 (100%)	0	100	100
3	E	101/190 (53%)	100 (99%)	1 (1%)	68	75
3	G	101/190 (53%)	100 (99%)	1 (1%)	68	75
3	I	101/190 (53%)	101 (100%)	0	100	100
All	All	3278/4299 (76%)	3219 (98%)	59 (2%)	51	68

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	VAL
1	A	319	ARG
1	A	323	THR
1	A	556	ASN
1	A	558	LYS
1	A	559	PHE
1	A	560	LEU
1	A	563	GLN
1	A	599	THR
1	A	800	PHE
1	A	850	ILE
1	A	853	GLN
1	A	854	LYS
1	A	861	LEU
1	A	1077	THR
1	A	1089	PHE
1	A	1104	VAL
1	B	47	VAL
1	B	319	ARG
1	B	321	GLN
1	B	558	LYS
1	B	559	PHE
1	B	560	LEU
1	B	564	GLN
1	B	599	THR
1	B	800	PHE
1	B	849	LEU
1	B	850	ILE

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Mol	Chain	Res	Type
1	B	854	LYS
1	B	858	LEU
1	B	859	THR
1	B	864	LEU
1	B	1077	THR
1	B	1089	PHE
1	B	1104	VAL
1	C	47	VAL
1	C	317	ASN
1	C	319	ARG
1	C	324	GLU
1	C	325	SER
1	C	558	LYS
1	C	559	PHE
1	C	560	LEU
1	C	563	GLN
1	C	564	GLN
1	C	599	THR
1	C	800	PHE
1	C	849	LEU
1	C	850	ILE
1	C	853	GLN
1	C	854	LYS
1	C	861	LEU
1	C	864	LEU
1	C	865	LEU
1	C	1077	THR
1	C	1089	PHE
1	C	1104	VAL
3	E	102	ASP
3	G	104	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	66	HIS
1	A	69	HIS
1	A	164	ASN
1	A	196	ASN
1	A	207	HIS
1	A	239	GLN

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Mol	Chain	Res	Type
1	A	354	ASN
1	A	414	GLN
1	A	437	ASN
1	A	506	GLN
1	A	779	GLN
1	A	935	GLN
1	A	1108	ASN
1	A	1119	ASN
1	B	30	ASN
1	B	66	HIS
1	B	69	HIS
1	B	164	ASN
1	B	196	ASN
1	B	207	HIS
1	B	239	GLN
1	B	354	ASN
1	B	437	ASN
1	B	655	HIS
1	B	779	GLN
1	B	935	GLN
1	B	1083	HIS
1	B	1108	ASN
1	B	1119	ASN
1	C	30	ASN
1	C	66	HIS
1	C	69	HIS
1	C	164	ASN
1	C	196	ASN
1	C	207	HIS
1	C	239	GLN
1	C	354	ASN
1	C	414	GLN
1	C	437	ASN
1	C	655	HIS
1	C	779	GLN
1	C	1108	ASN
1	C	1119	ASN
2	D	36	GLN
2	D	99	GLN
2	F	6	GLN
2	F	10	GLN
2	F	88	GLN

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Mol	Chain	Res	Type
3	G	31	ASN
2	H	36	GLN
3	I	35	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

30 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
4	NAG	J	1	1,4	14,14,15	1.42	2 (14%)	17,19,21	1.44	2 (11%)
4	NAG	J	2	4	14,14,15	0.37	0	17,19,21	0.80	1 (5%)
4	NAG	K	1	1,4	14,14,15	1.19	2 (14%)	17,19,21	0.61	0
4	NAG	K	2	4	14,14,15	0.67	1 (7%)	17,19,21	0.62	0
4	NAG	L	1	1,4	14,14,15	0.85	1 (7%)	17,19,21	0.69	0
4	NAG	L	2	4	14,14,15	1.03	1 (7%)	17,19,21	0.74	0
4	NAG	M	1	1,4	14,14,15	1.12	2 (14%)	17,19,21	0.80	0
4	NAG	M	2	4	14,14,15	0.35	0	17,19,21	0.46	0
4	NAG	N	1	1,4	14,14,15	1.31	2 (14%)	17,19,21	0.52	0
4	NAG	N	2	4	14,14,15	0.59	0	17,19,21	0.60	0
4	NAG	O	1	1,4	14,14,15	1.41	2 (14%)	17,19,21	1.44	2 (11%)
4	NAG	O	2	4	14,14,15	0.38	0	17,19,21	0.81	1 (5%)
4	NAG	P	1	1,4	14,14,15	1.21	2 (14%)	17,19,21	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	P	2	4	14,14,15	0.67	1 (7%)	17,19,21	0.62	0
4	NAG	Q	1	1,4	14,14,15	0.86	1 (7%)	17,19,21	0.68	0
4	NAG	Q	2	4	14,14,15	1.03	1 (7%)	17,19,21	0.74	0
4	NAG	R	1	1,4	14,14,15	1.11	2 (14%)	17,19,21	0.80	0
4	NAG	R	2	4	14,14,15	0.34	0	17,19,21	0.46	0
4	NAG	S	1	1,4	14,14,15	1.31	2 (14%)	17,19,21	0.52	0
4	NAG	S	2	4	14,14,15	0.59	0	17,19,21	0.60	0
4	NAG	T	1	1,4	14,14,15	1.42	2 (14%)	17,19,21	1.44	2 (11%)
4	NAG	T	2	4	14,14,15	0.37	0	17,19,21	0.82	1 (5%)
4	NAG	U	1	1,4	14,14,15	1.20	2 (14%)	17,19,21	0.62	0
4	NAG	U	2	4	14,14,15	0.66	1 (7%)	17,19,21	0.63	0
4	NAG	V	1	1,4	14,14,15	0.85	1 (7%)	17,19,21	0.68	0
4	NAG	V	2	4	14,14,15	1.02	1 (7%)	17,19,21	0.74	0
4	NAG	W	1	1,4	14,14,15	1.11	2 (14%)	17,19,21	0.80	0
4	NAG	W	2	4	14,14,15	0.34	0	17,19,21	0.46	0
4	NAG	X	1	1,4	14,14,15	1.31	2 (14%)	17,19,21	0.52	0
4	NAG	X	2	4	14,14,15	0.59	0	17,19,21	0.61	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
4	NAG	J	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1
4	NAG	K	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	K	2	4	-	2/6/23/26	0/1/1/1
4	NAG	L	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	L	2	4	-	2/6/23/26	0/1/1/1
4	NAG	M	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	M	2	4	-	1/6/23/26	0/1/1/1
4	NAG	N	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	N	2	4	-	2/6/23/26	0/1/1/1
4	NAG	O	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	O	2	4	-	2/6/23/26	0/1/1/1
4	NAG	P	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	P	2	4	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	Q	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	2/6/23/26	0/1/1/1
4	NAG	R	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	R	2	4	-	1/6/23/26	0/1/1/1
4	NAG	S	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	S	2	4	-	2/6/23/26	0/1/1/1
4	NAG	T	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	T	2	4	-	2/6/23/26	0/1/1/1
4	NAG	U	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	U	2	4	-	2/6/23/26	0/1/1/1
4	NAG	V	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	V	2	4	-	2/6/23/26	0/1/1/1
4	NAG	W	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	W	2	4	-	1/6/23/26	0/1/1/1
4	NAG	X	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	X	2	4	-	2/6/23/26	0/1/1/1

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	1	NAG	O5-C1	-4.55	1.36	1.43
4	T	1	NAG	O5-C1	-4.55	1.36	1.43
4	O	1	NAG	O5-C1	-4.54	1.36	1.43
4	S	1	NAG	O5-C1	-4.10	1.36	1.43
4	X	1	NAG	O5-C1	-4.09	1.36	1.43
4	N	1	NAG	O5-C1	-4.09	1.36	1.43
4	L	2	NAG	O5-C1	-3.71	1.37	1.43
4	Q	2	NAG	O5-C1	-3.70	1.37	1.43
4	V	2	NAG	O5-C1	-3.67	1.37	1.43
4	U	1	NAG	O5-C1	-3.36	1.38	1.43
4	K	1	NAG	O5-C1	-3.36	1.38	1.43
4	P	1	NAG	O5-C1	-3.34	1.38	1.43
4	M	1	NAG	C1-C2	-2.86	1.48	1.52
4	R	1	NAG	C1-C2	-2.81	1.48	1.52
4	W	1	NAG	C1-C2	-2.80	1.48	1.52
4	M	1	NAG	O5-C1	-2.60	1.39	1.43
4	R	1	NAG	O5-C1	-2.59	1.39	1.43
4	W	1	NAG	O5-C1	-2.58	1.39	1.43
4	P	1	NAG	C1-C2	-2.54	1.48	1.52
4	U	1	NAG	C1-C2	-2.47	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	X	1	NAG	C1-C2	-2.45	1.49	1.52
4	T	1	NAG	C1-C2	-2.44	1.49	1.52
4	N	1	NAG	C1-C2	-2.43	1.49	1.52
4	S	1	NAG	C1-C2	-2.43	1.49	1.52
4	J	1	NAG	C1-C2	-2.43	1.49	1.52
4	K	1	NAG	C1-C2	-2.41	1.49	1.52
4	K	2	NAG	O5-C1	-2.36	1.39	1.43
4	O	1	NAG	C1-C2	-2.36	1.49	1.52
4	P	2	NAG	O5-C1	-2.36	1.39	1.43
4	U	2	NAG	O5-C1	-2.33	1.39	1.43
4	L	1	NAG	O5-C1	-2.25	1.39	1.43
4	Q	1	NAG	O5-C1	-2.22	1.40	1.43
4	V	1	NAG	O5-C1	-2.21	1.40	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	1	NAG	C3-C4-C5	4.45	118.30	110.23
4	O	1	NAG	C3-C4-C5	4.45	118.30	110.23
4	T	1	NAG	C3-C4-C5	4.44	118.29	110.23
4	T	2	NAG	C1-O5-C5	2.84	115.99	112.19
4	O	2	NAG	C1-O5-C5	2.81	115.96	112.19
4	J	2	NAG	C1-O5-C5	2.78	115.92	112.19
4	T	1	NAG	O4-C4-C5	-2.10	104.14	109.32
4	O	1	NAG	O4-C4-C5	-2.10	104.16	109.32
4	J	1	NAG	O4-C4-C5	-2.09	104.18	109.32

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	J	1	NAG	O5-C5-C6-O6
4	O	1	NAG	O5-C5-C6-O6
4	T	1	NAG	O5-C5-C6-O6
4	K	2	NAG	O5-C5-C6-O6
4	P	2	NAG	O5-C5-C6-O6
4	U	2	NAG	O5-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6
4	O	2	NAG	O5-C5-C6-O6
4	T	2	NAG	O5-C5-C6-O6
4	X	2	NAG	O5-C5-C6-O6
4	J	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	O	2	NAG	C4-C5-C6-O6
4	T	2	NAG	C4-C5-C6-O6
4	N	2	NAG	O5-C5-C6-O6
4	S	2	NAG	O5-C5-C6-O6
4	L	1	NAG	O5-C5-C6-O6
4	Q	1	NAG	O5-C5-C6-O6
4	V	1	NAG	O5-C5-C6-O6
4	K	2	NAG	C4-C5-C6-O6
4	L	1	NAG	C4-C5-C6-O6
4	N	2	NAG	C4-C5-C6-O6
4	P	2	NAG	C4-C5-C6-O6
4	Q	1	NAG	C4-C5-C6-O6
4	S	2	NAG	C4-C5-C6-O6
4	U	2	NAG	C4-C5-C6-O6
4	V	1	NAG	C4-C5-C6-O6
4	X	2	NAG	C4-C5-C6-O6
4	J	1	NAG	C4-C5-C6-O6
4	O	1	NAG	C4-C5-C6-O6
4	T	1	NAG	C4-C5-C6-O6
4	L	2	NAG	C4-C5-C6-O6
4	Q	2	NAG	C4-C5-C6-O6
4	V	2	NAG	C4-C5-C6-O6
4	L	2	NAG	O5-C5-C6-O6
4	Q	2	NAG	O5-C5-C6-O6
4	V	2	NAG	O5-C5-C6-O6
4	M	2	NAG	O5-C5-C6-O6
4	R	2	NAG	O5-C5-C6-O6
4	W	2	NAG	O5-C5-C6-O6
4	R	1	NAG	C4-C5-C6-O6
4	M	1	NAG	C4-C5-C6-O6
4	W	1	NAG	C4-C5-C6-O6

There are no ring outliers.

10 monomers are involved in 11 short contacts:

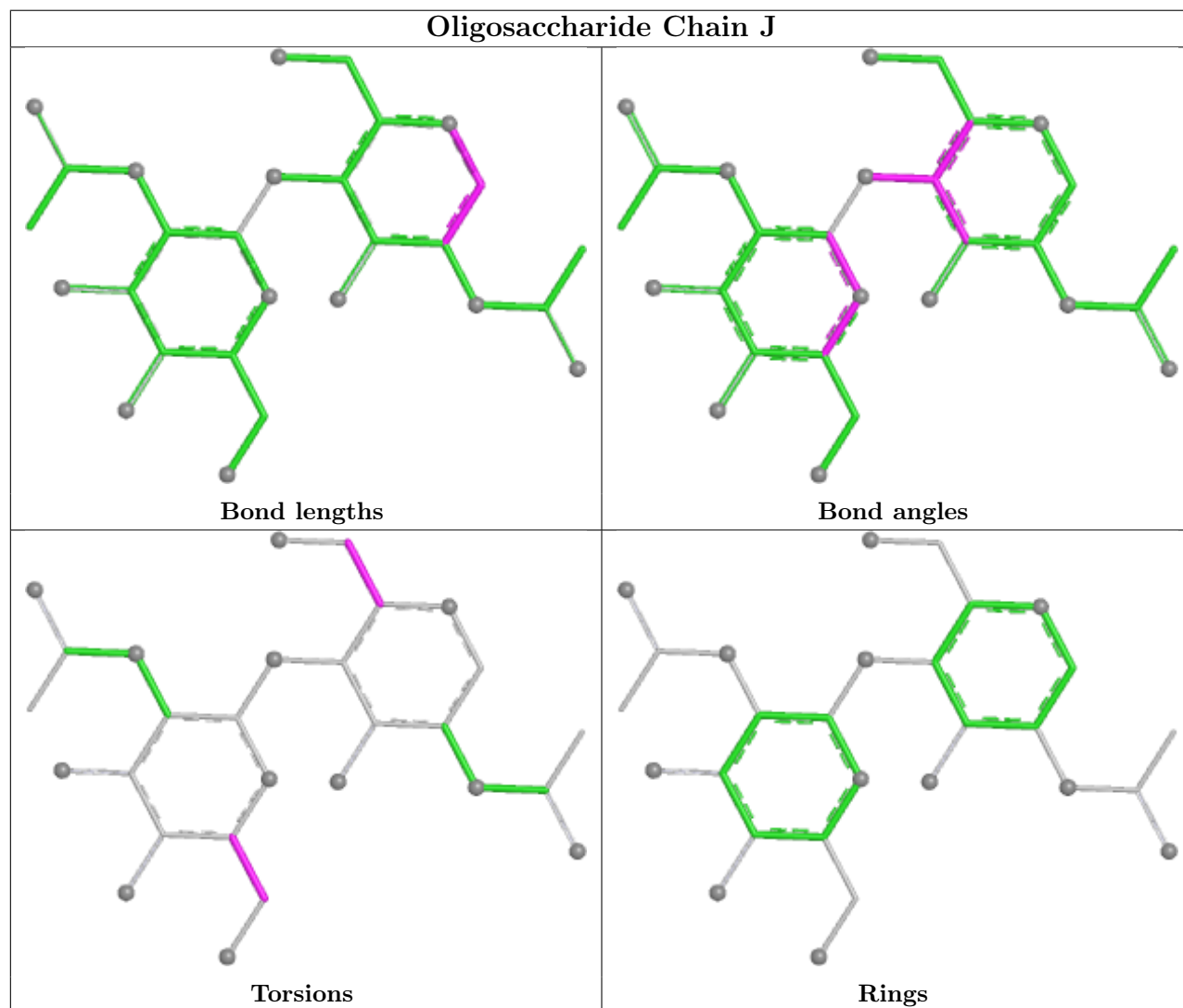
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	X	1	NAG	1	0
4	X	2	NAG	1	0
4	V	1	NAG	2	0
4	L	1	NAG	2	0
4	J	1	NAG	1	0
4	Q	1	NAG	2	0

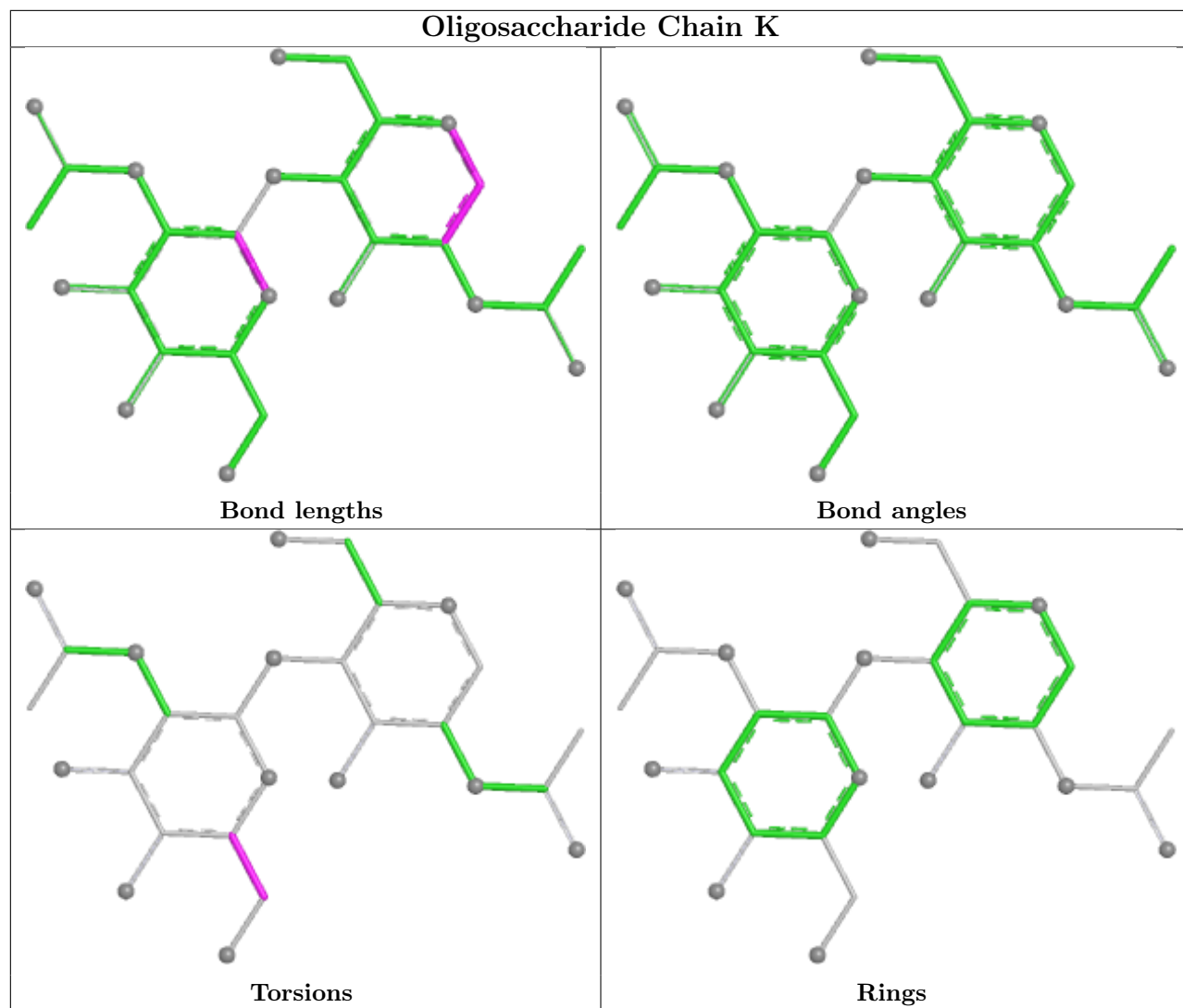
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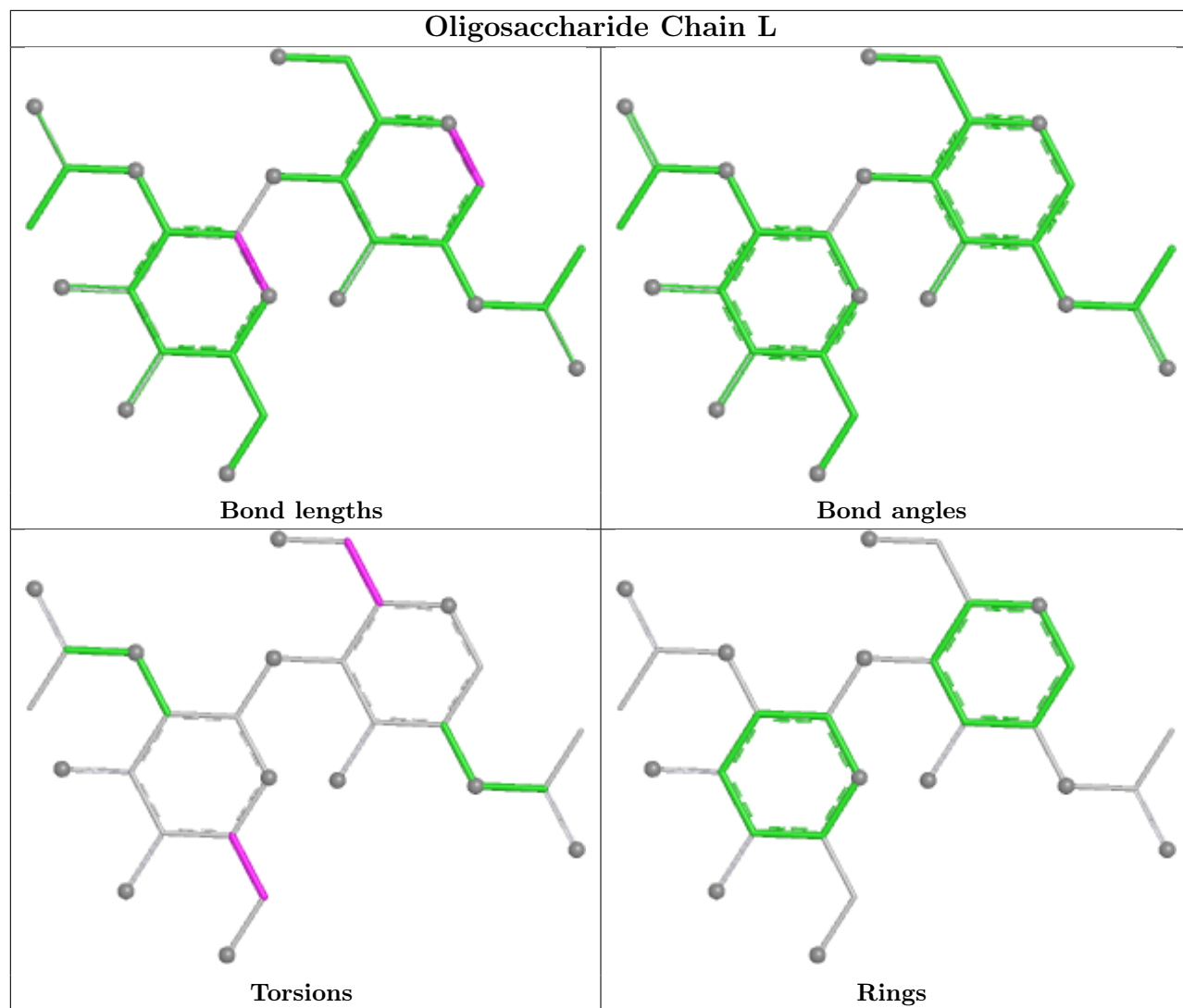
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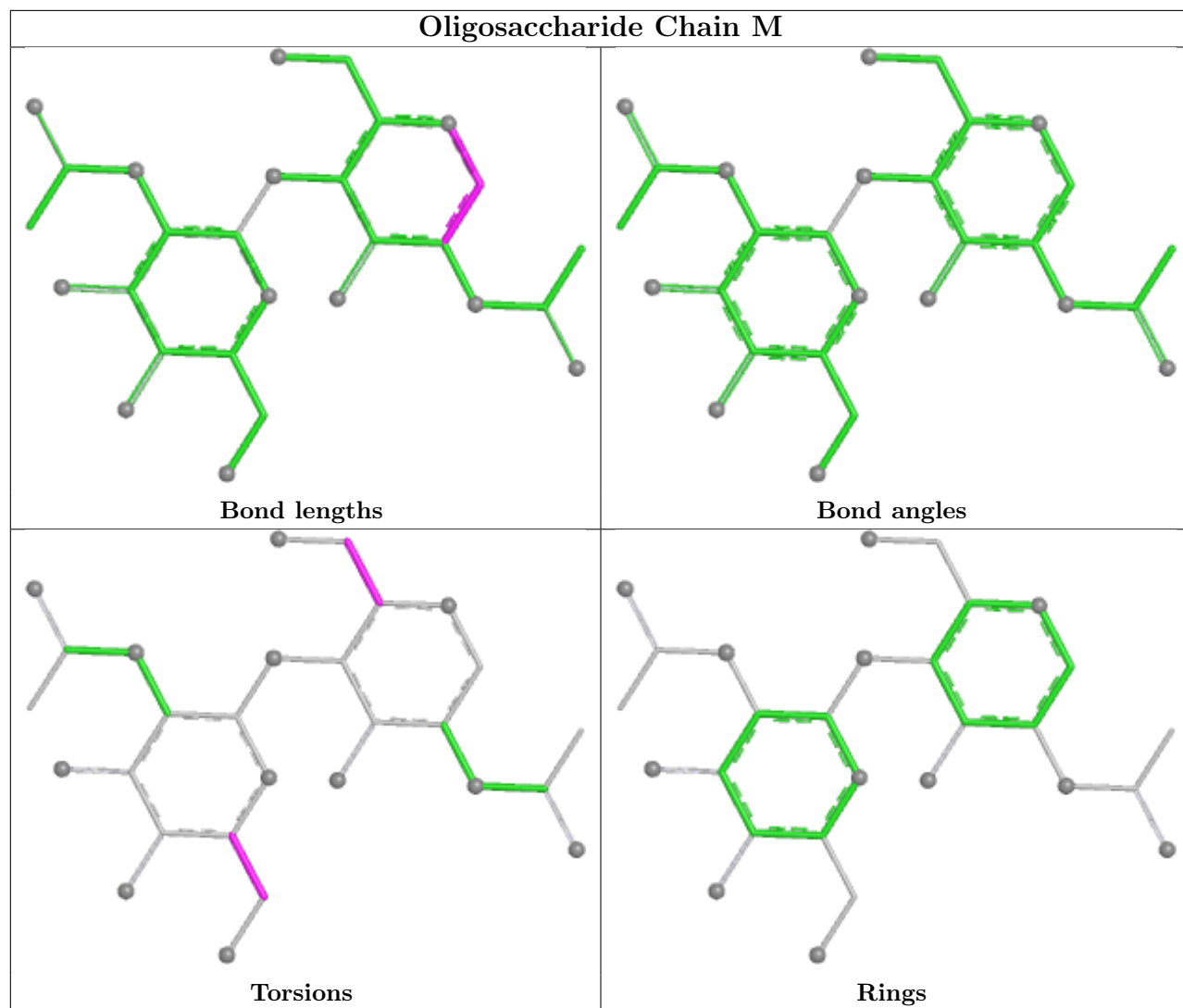
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	S	1	NAG	1	0
4	O	1	NAG	1	0
4	T	1	NAG	1	0
4	S	2	NAG	1	0

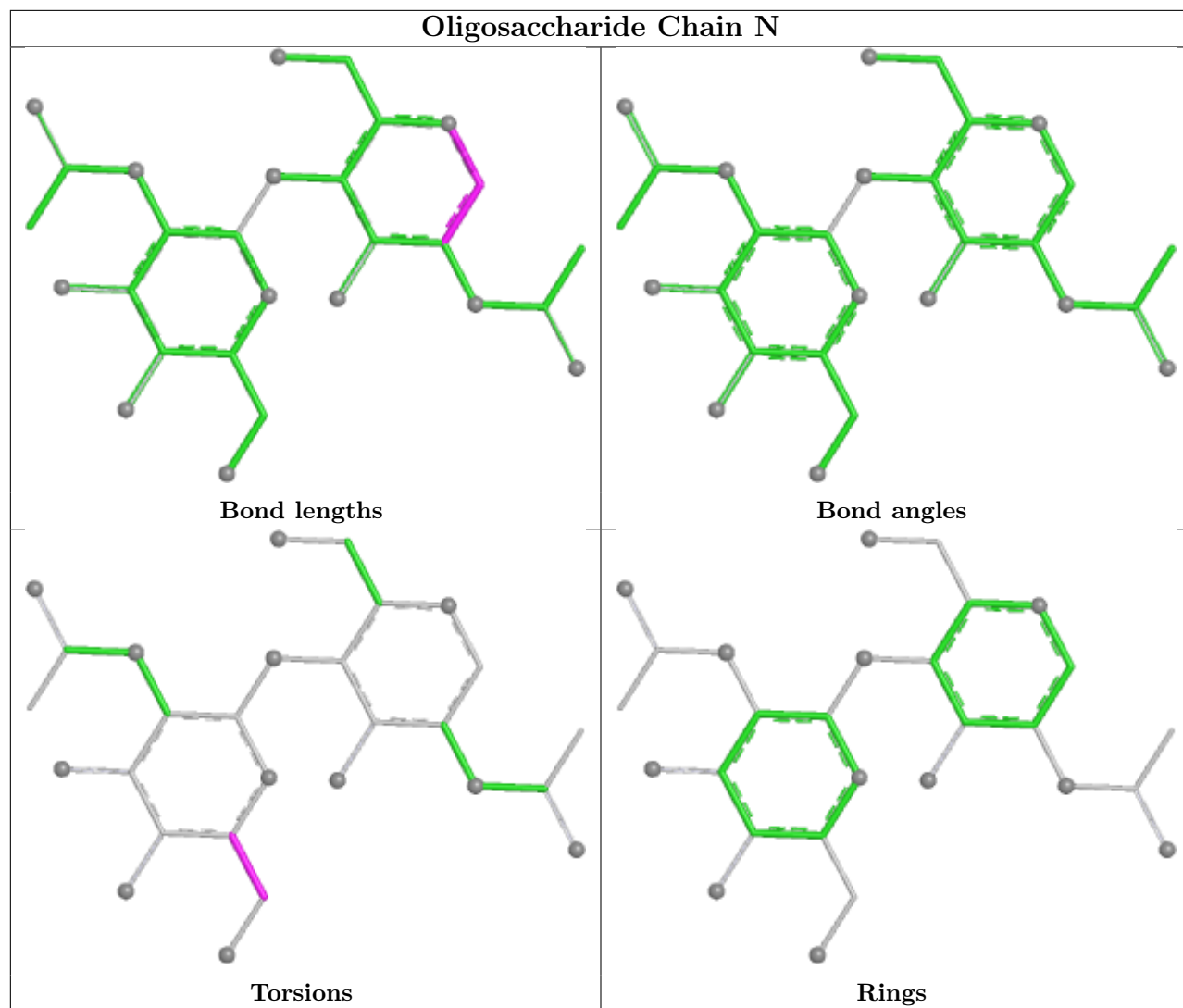
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

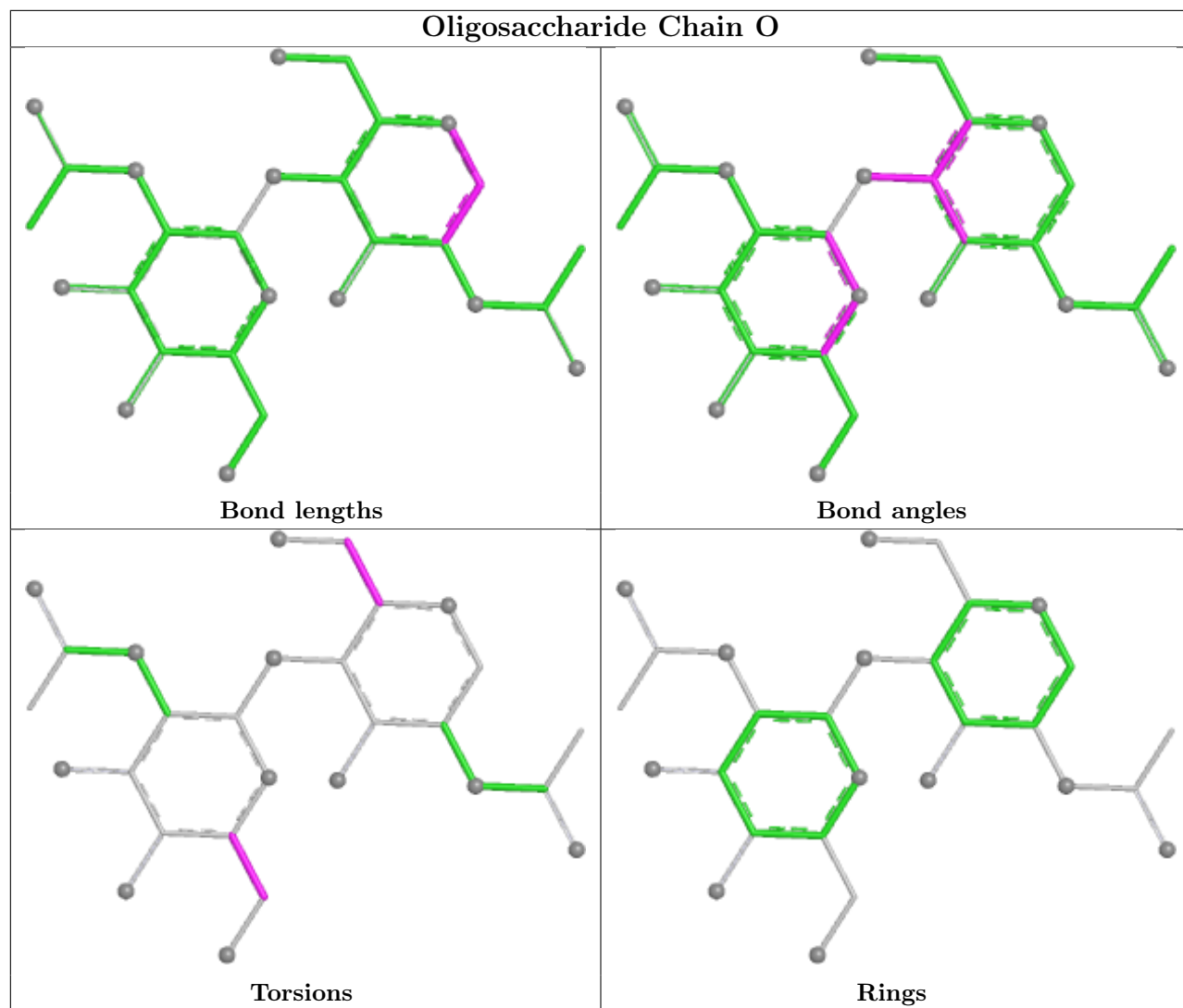


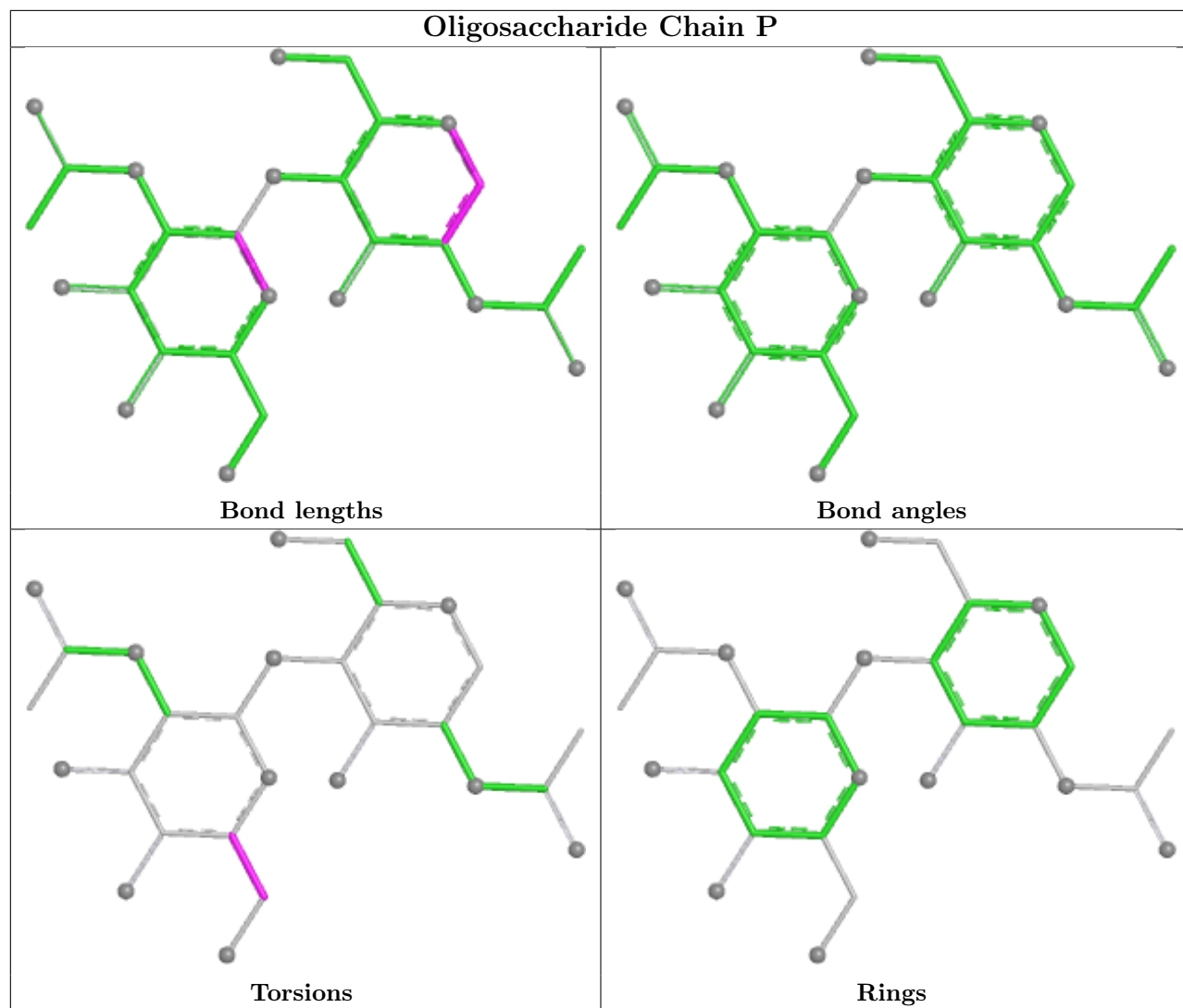


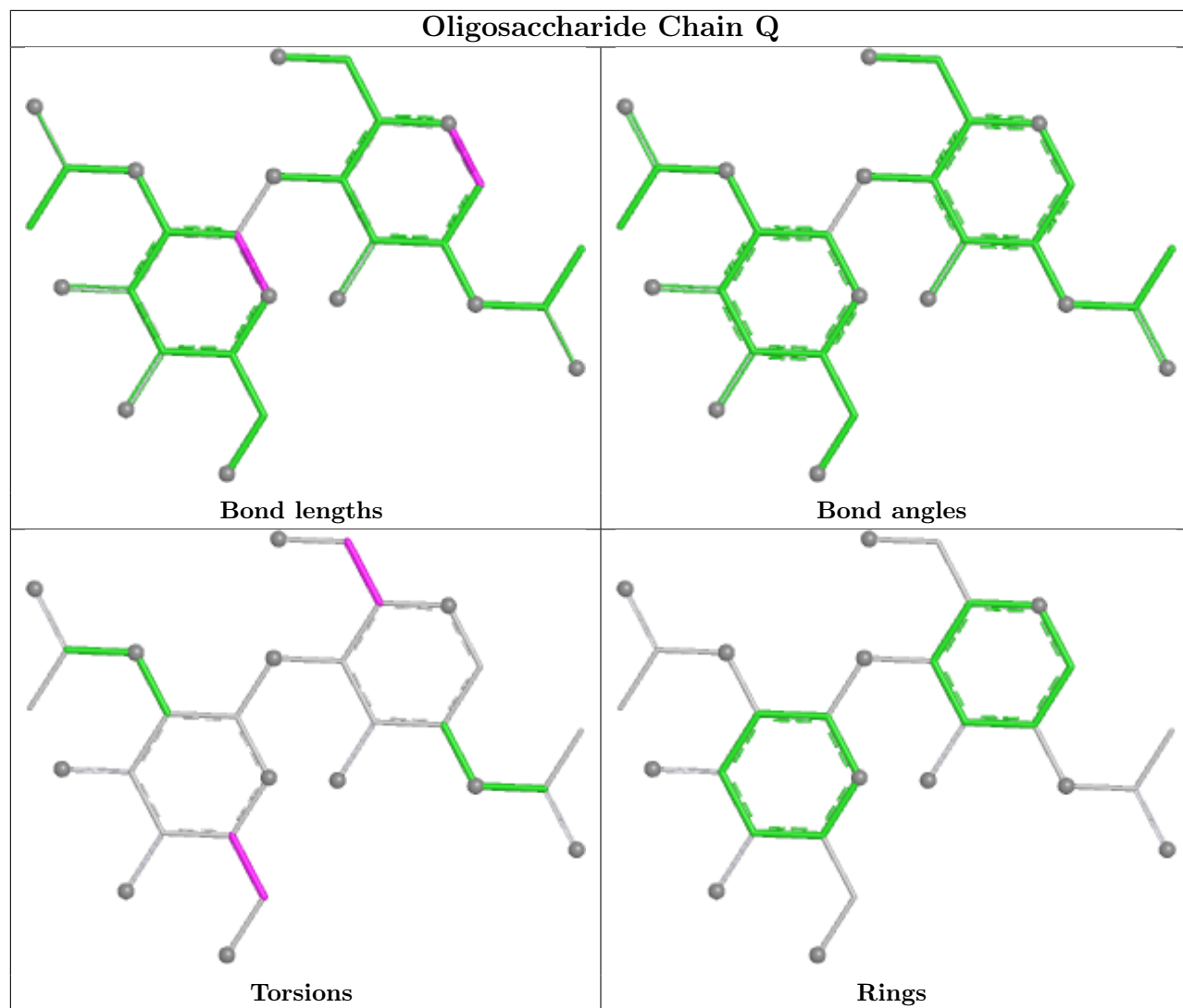


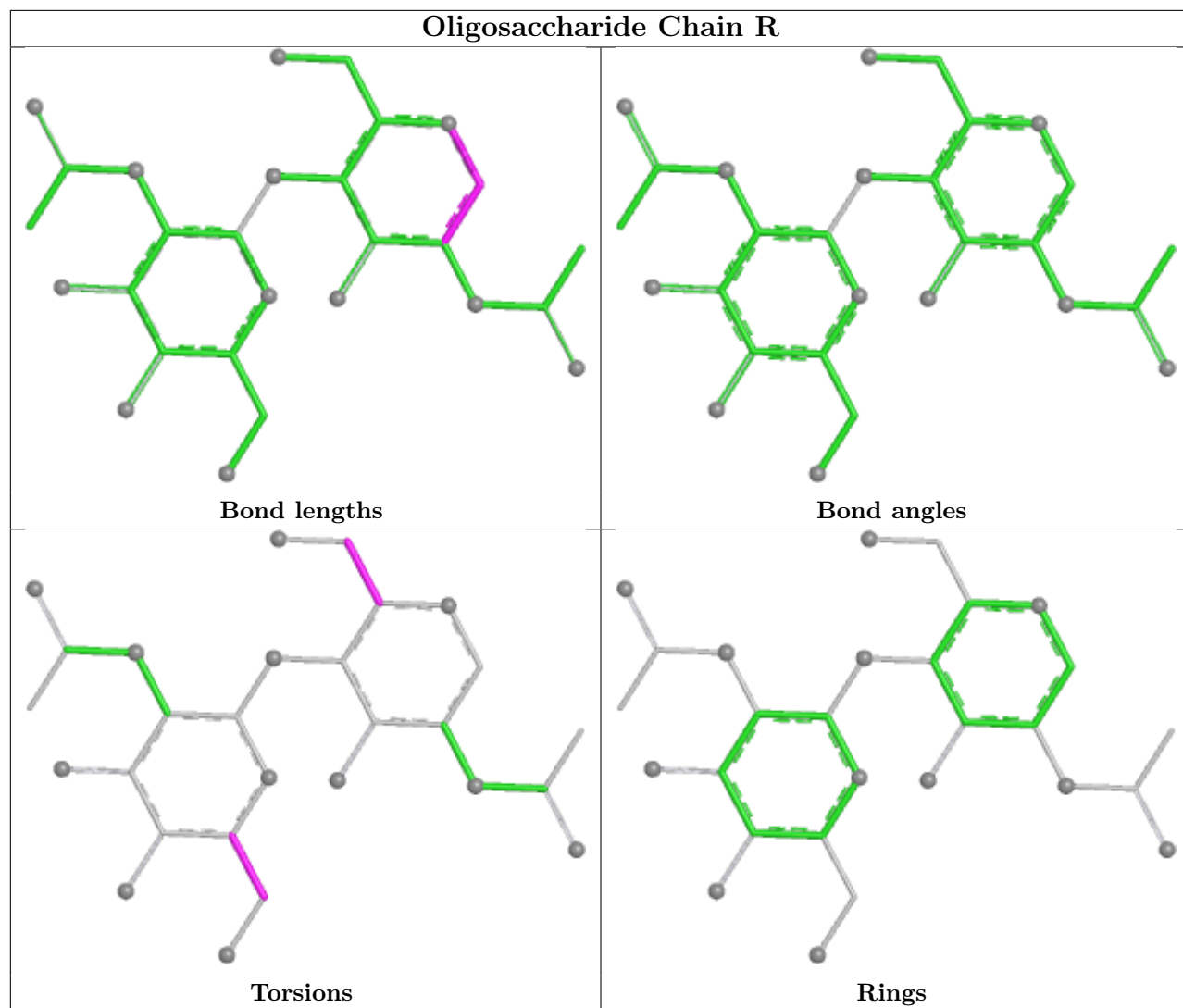


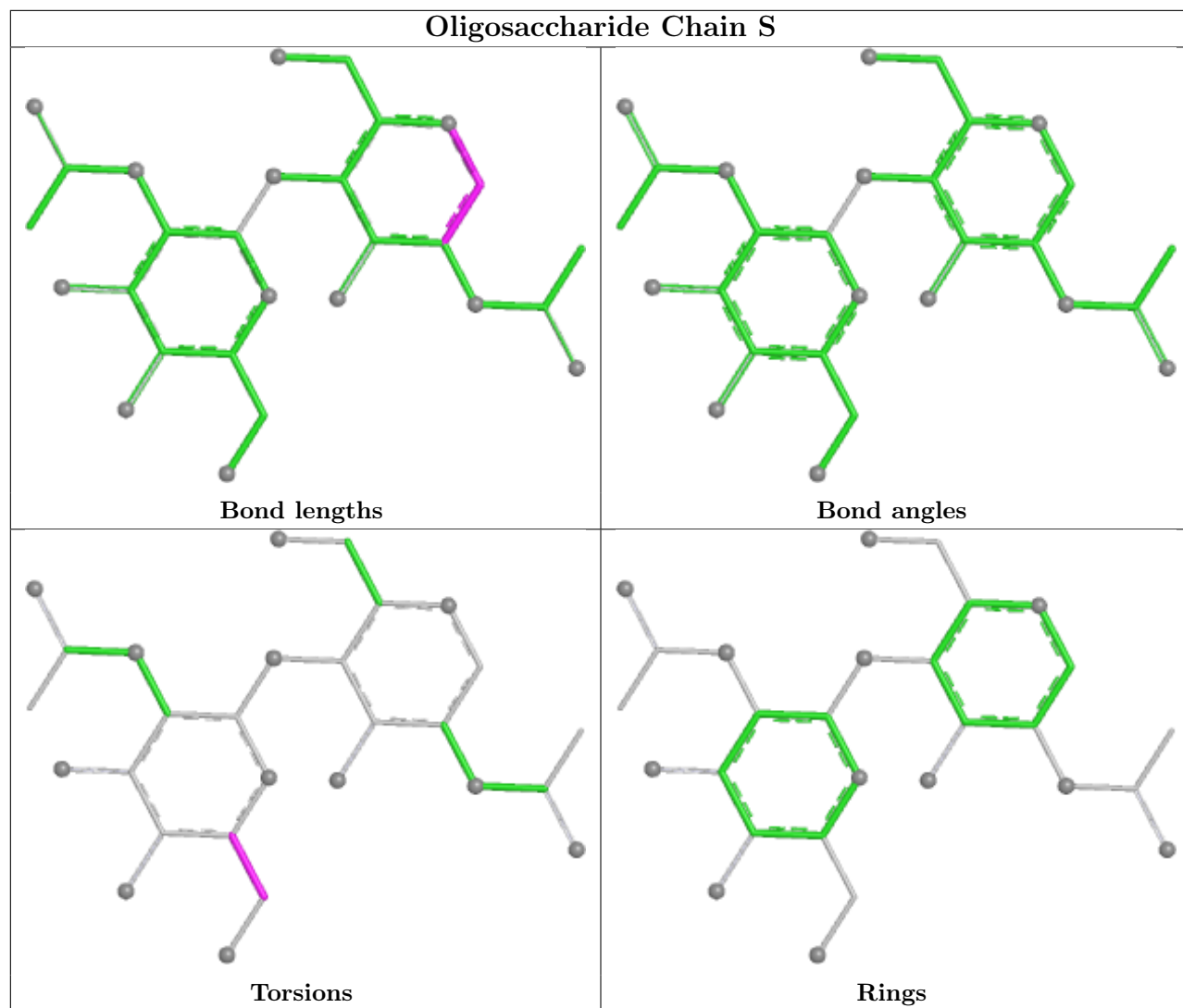


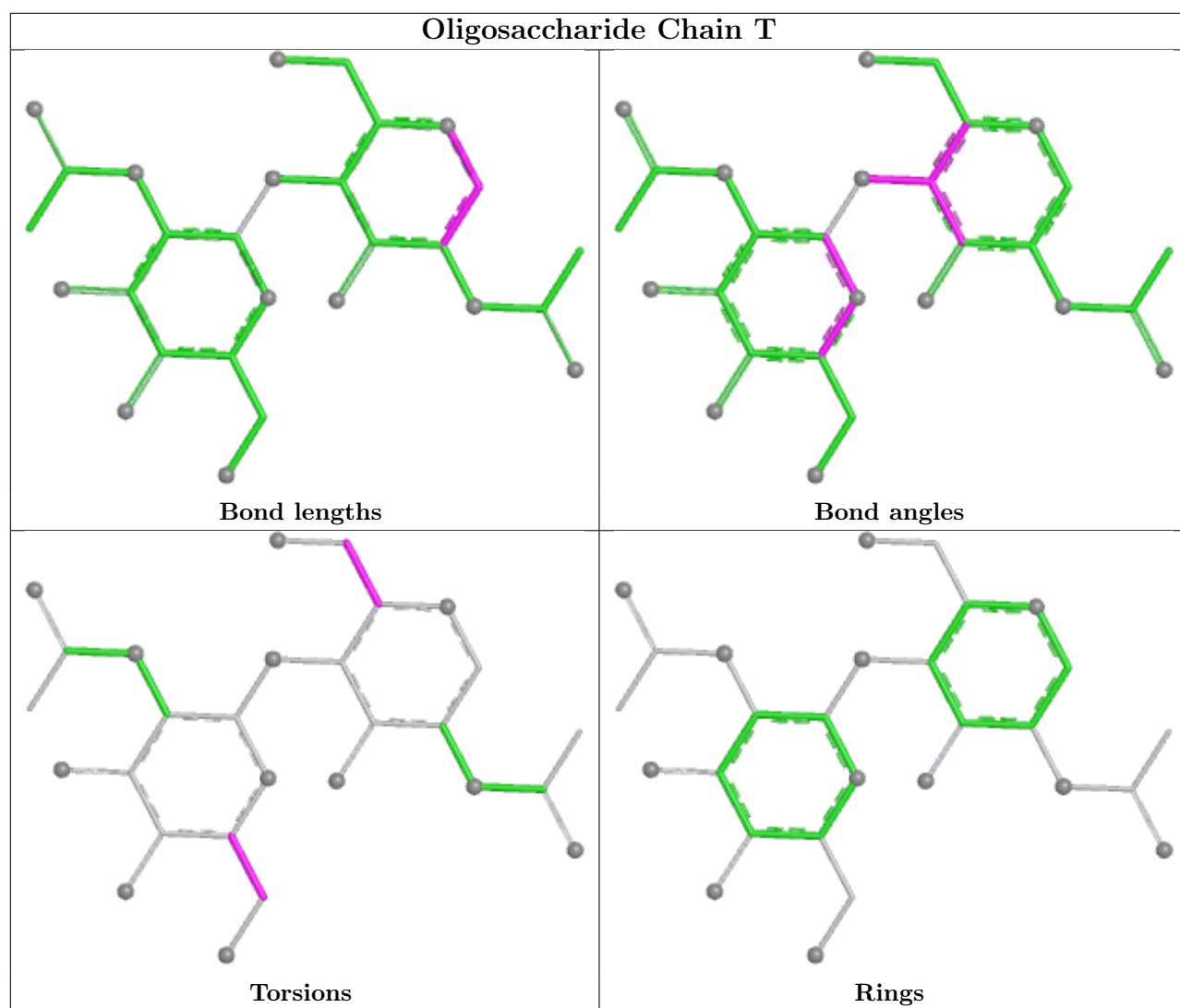


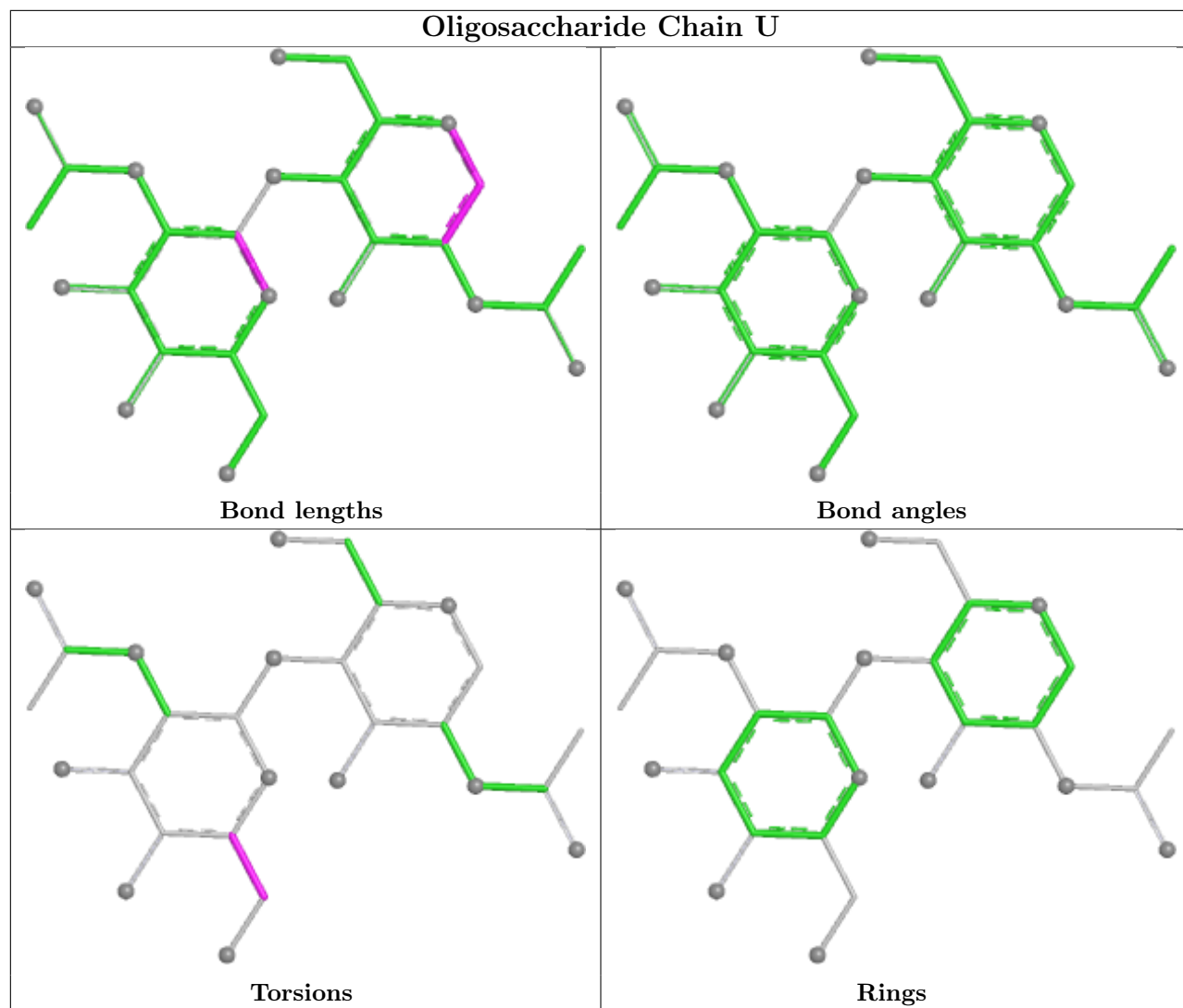


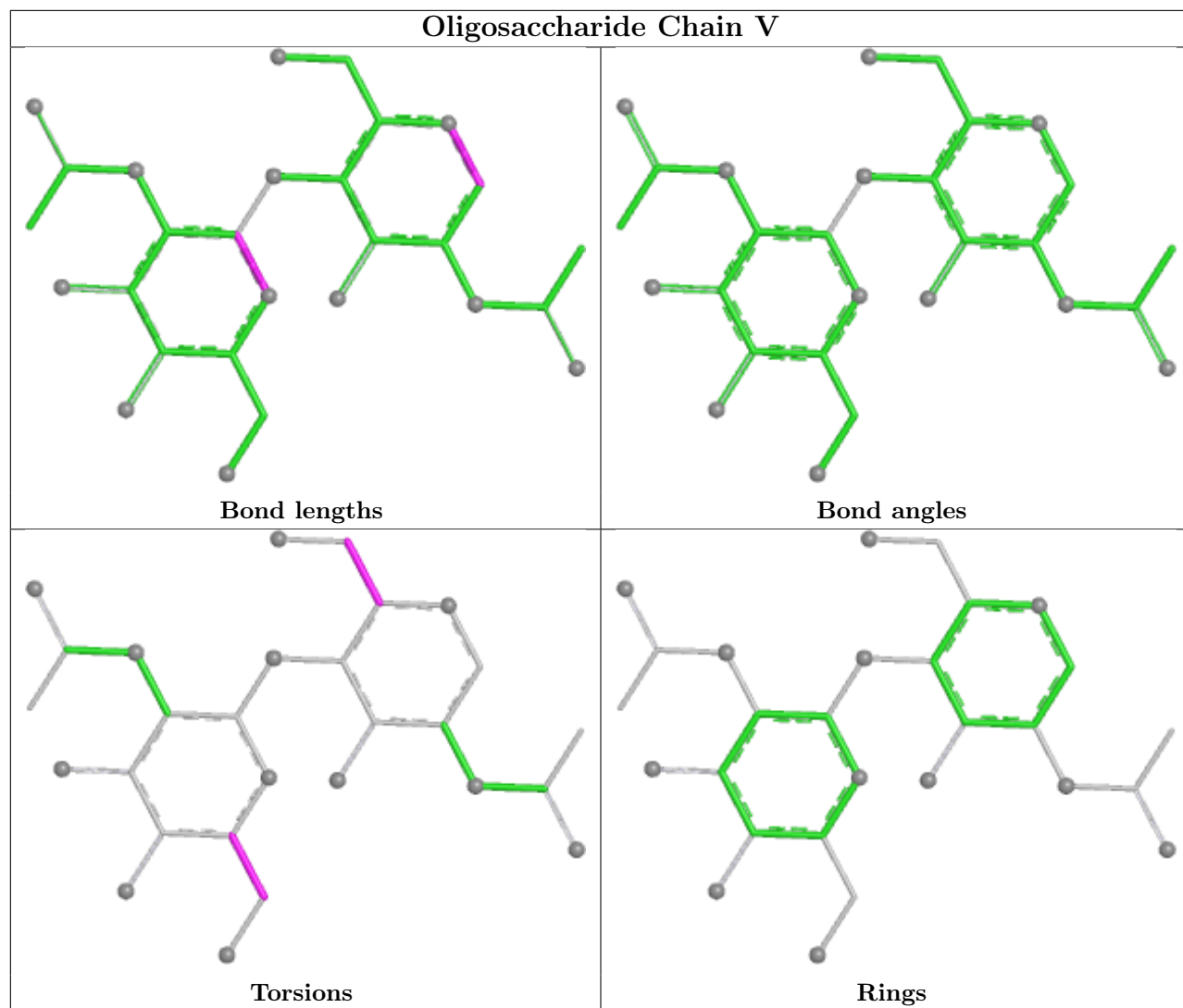


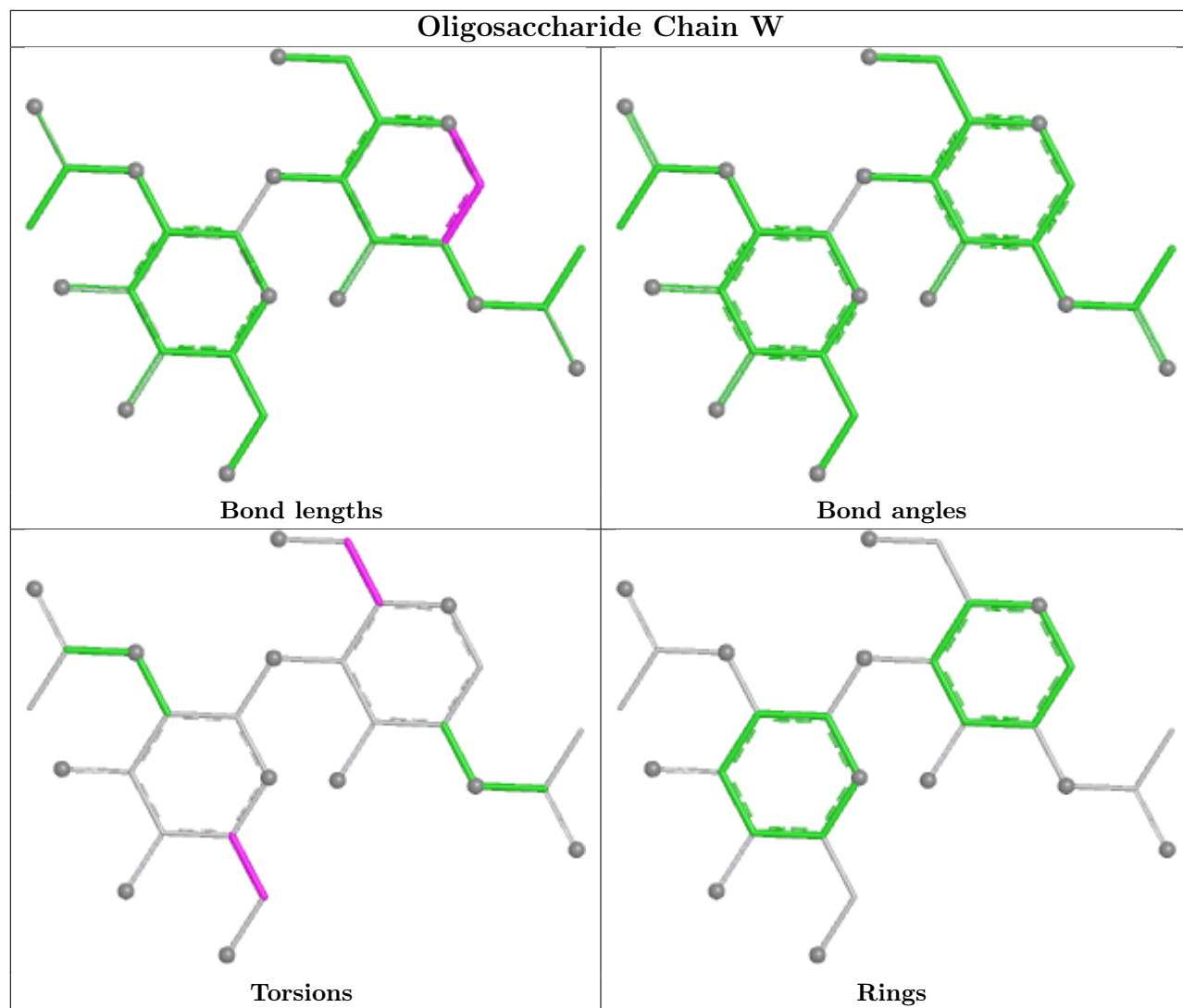


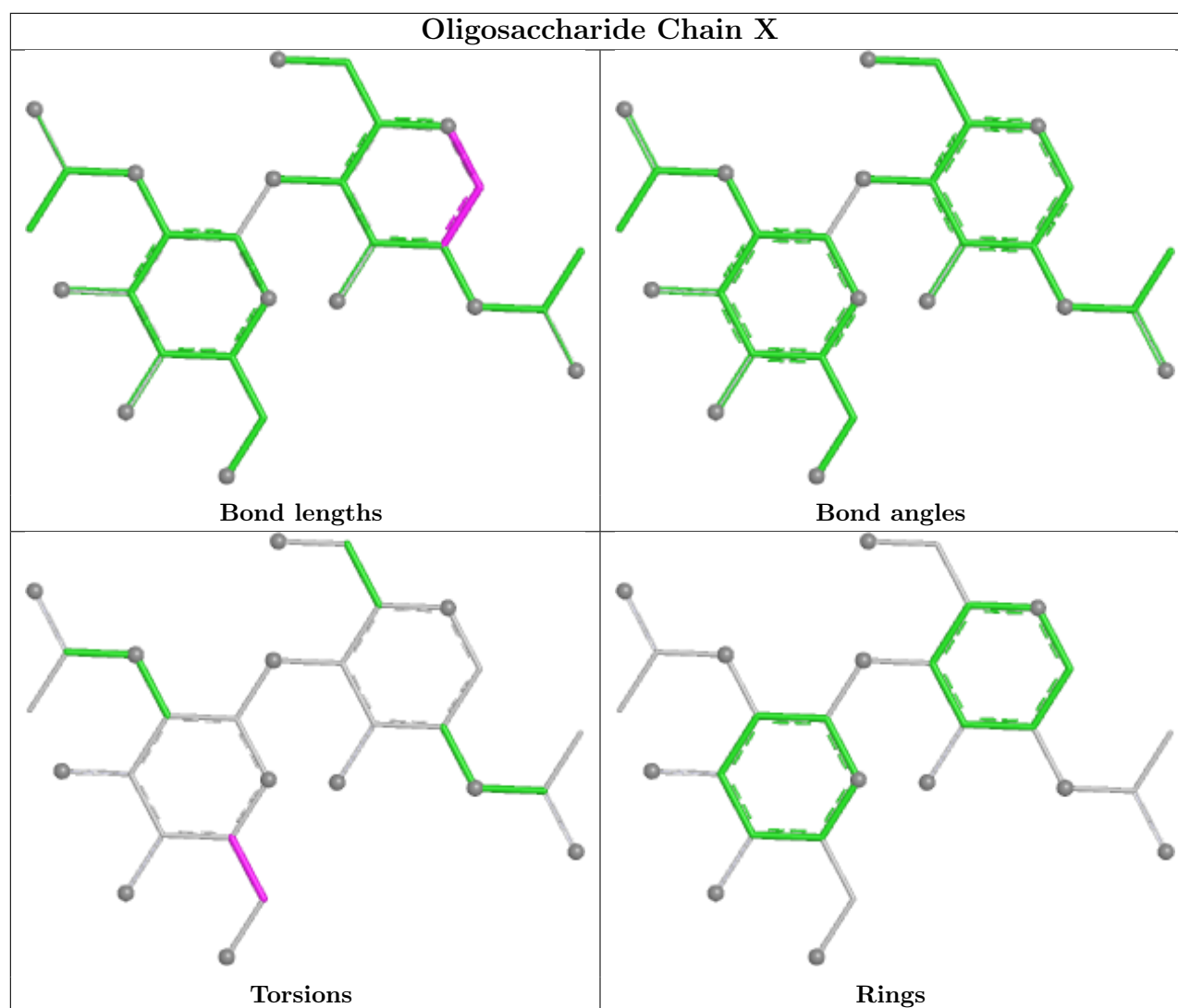












5.6 Ligand geometry [i](#)

30 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	$\# Z > 2$
5	NAG	C	1304	1	14,14,15	0.32	0	17,19,21	1.07	1 (5%)
5	NAG	A	1307	1	14,14,15	0.43	0	17,19,21	0.64	0
5	NAG	A	1309	1	14,14,15	0.85	1 (7%)	17,19,21	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	1304	1	14,14,15	0.32	0	17,19,21	1.08	1 (5%)
5	NAG	C	1302	1	14,14,15	0.22	0	17,19,21	0.50	0
5	NAG	A	1302	1	14,14,15	0.21	0	17,19,21	0.51	0
5	NAG	C	1306	1	14,14,15	0.90	1 (7%)	17,19,21	2.15	1 (5%)
5	NAG	C	1308	1	14,14,15	0.72	1 (7%)	17,19,21	1.02	1 (5%)
5	NAG	C	1310	1	14,14,15	0.50	0	17,19,21	0.66	0
5	NAG	B	1304	1	14,14,15	0.33	0	17,19,21	1.07	1 (5%)
5	NAG	A	1310	1	14,14,15	0.49	0	17,19,21	0.66	0
5	NAG	B	1301	1	14,14,15	0.73	1 (7%)	17,19,21	0.62	0
5	NAG	C	1309	1	14,14,15	0.83	1 (7%)	17,19,21	0.50	0
5	NAG	B	1302	1	14,14,15	0.21	0	17,19,21	0.51	0
5	NAG	A	1303	1	14,14,15	0.40	0	17,19,21	0.63	0
5	NAG	A	1308	1	14,14,15	0.69	1 (7%)	17,19,21	0.68	0
5	NAG	B	1307	1	14,14,15	0.41	0	17,19,21	0.64	0
5	NAG	B	1308	1	14,14,15	0.79	1 (7%)	17,19,21	1.14	1 (5%)
5	NAG	C	1301	1	14,14,15	0.73	1 (7%)	17,19,21	0.61	0
5	NAG	B	1310	1	14,14,15	0.49	0	17,19,21	0.66	0
5	NAG	C	1305	1	14,14,15	0.40	0	17,19,21	0.34	0
5	NAG	B	1306	1	14,14,15	1.54	1 (7%)	17,19,21	0.92	1 (5%)
5	NAG	B	1309	1	14,14,15	0.84	1 (7%)	17,19,21	0.49	0
5	NAG	B	1303	1	14,14,15	0.40	0	17,19,21	0.63	0
5	NAG	A	1301	1	14,14,15	0.74	1 (7%)	17,19,21	0.61	0
5	NAG	A	1305	1	14,14,15	0.40	0	17,19,21	0.34	0
5	NAG	A	1306	1	14,14,15	1.56	1 (7%)	17,19,21	0.89	1 (5%)
5	NAG	B	1305	1	14,14,15	0.39	0	17,19,21	0.34	0
5	NAG	C	1303	1	14,14,15	0.40	0	17,19,21	0.63	0
5	NAG	C	1307	1	14,14,15	0.43	0	17,19,21	0.63	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
5	NAG	C	1304	1	-	1/6/23/26	0/1/1/1
5	NAG	A	1307	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1309	1	-	3/6/23/26	0/1/1/1
5	NAG	A	1304	1	-	1/6/23/26	0/1/1/1
5	NAG	C	1302	1	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	1302	1	-	3/6/23/26	0/1/1/1
5	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1308	1	-	3/6/23/26	0/1/1/1
5	NAG	C	1310	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1304	1	-	1/6/23/26	0/1/1/1
5	NAG	A	1310	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1301	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1309	1	-	3/6/23/26	0/1/1/1
5	NAG	B	1302	1	-	3/6/23/26	0/1/1/1
5	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1308	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1307	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1308	1	-	3/6/23/26	0/1/1/1
5	NAG	C	1301	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1310	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1305	1	-	3/6/23/26	0/1/1/1
5	NAG	B	1306	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1309	1	-	3/6/23/26	0/1/1/1
5	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1305	1	-	3/6/23/26	0/1/1/1
5	NAG	A	1306	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1305	1	-	3/6/23/26	0/1/1/1
5	NAG	C	1303	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1307	1	-	2/6/23/26	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1306	NAG	O5-C1	-5.76	1.34	1.43
5	B	1306	NAG	O5-C1	-5.73	1.34	1.43
5	A	1309	NAG	O5-C1	-2.89	1.38	1.43
5	B	1309	NAG	O5-C1	-2.88	1.38	1.43
5	C	1309	NAG	O5-C1	-2.85	1.38	1.43
5	C	1306	NAG	O5-C1	2.79	1.48	1.43
5	B	1308	NAG	O5-C1	-2.70	1.39	1.43
5	A	1301	NAG	O5-C1	-2.55	1.39	1.43
5	C	1301	NAG	O5-C1	-2.52	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1301	NAG	O5-C1	-2.51	1.39	1.43
5	C	1308	NAG	O5-C1	-2.47	1.39	1.43
5	A	1308	NAG	O5-C1	-2.42	1.39	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1306	NAG	C1-O5-C5	8.59	123.69	112.19
5	B	1308	NAG	C1-O5-C5	4.23	117.86	112.19
5	A	1304	NAG	C1-O5-C5	3.64	117.06	112.19
5	C	1304	NAG	C1-O5-C5	3.63	117.05	112.19
5	B	1304	NAG	C1-O5-C5	3.61	117.02	112.19
5	C	1308	NAG	C1-O5-C5	3.25	116.54	112.19
5	B	1306	NAG	C1-O5-C5	-3.07	108.08	112.19
5	A	1306	NAG	C1-O5-C5	-2.60	108.70	112.19

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1308	NAG	O5-C5-C6-O6
5	C	1306	NAG	O5-C5-C6-O6
5	C	1308	NAG	O5-C5-C6-O6
5	A	1310	NAG	O5-C5-C6-O6
5	B	1310	NAG	O5-C5-C6-O6
5	C	1310	NAG	O5-C5-C6-O6
5	B	1308	NAG	C4-C5-C6-O6
5	C	1306	NAG	C4-C5-C6-O6
5	A	1303	NAG	O5-C5-C6-O6
5	B	1303	NAG	O5-C5-C6-O6
5	C	1303	NAG	O5-C5-C6-O6
5	C	1308	NAG	C4-C5-C6-O6
5	A	1305	NAG	O5-C5-C6-O6
5	B	1305	NAG	O5-C5-C6-O6
5	C	1305	NAG	O5-C5-C6-O6
5	A	1309	NAG	O5-C5-C6-O6
5	B	1309	NAG	O5-C5-C6-O6
5	C	1309	NAG	O5-C5-C6-O6
5	A	1309	NAG	C4-C5-C6-O6
5	B	1309	NAG	C4-C5-C6-O6
5	C	1309	NAG	C4-C5-C6-O6
5	A	1305	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	B	1305	NAG	C4-C5-C6-O6
5	C	1305	NAG	C4-C5-C6-O6
5	A	1310	NAG	C4-C5-C6-O6
5	B	1310	NAG	C4-C5-C6-O6
5	C	1310	NAG	C4-C5-C6-O6
5	A	1302	NAG	O5-C5-C6-O6
5	B	1302	NAG	O5-C5-C6-O6
5	C	1302	NAG	O5-C5-C6-O6
5	A	1303	NAG	C4-C5-C6-O6
5	B	1303	NAG	C4-C5-C6-O6
5	C	1303	NAG	C4-C5-C6-O6
5	A	1304	NAG	O5-C5-C6-O6
5	B	1304	NAG	O5-C5-C6-O6
5	C	1304	NAG	O5-C5-C6-O6
5	A	1308	NAG	C4-C5-C6-O6
5	A	1307	NAG	C4-C5-C6-O6
5	C	1307	NAG	C4-C5-C6-O6
5	B	1307	NAG	C4-C5-C6-O6
5	A	1302	NAG	C3-C2-N2-C7
5	B	1302	NAG	C3-C2-N2-C7
5	C	1302	NAG	C3-C2-N2-C7
5	A	1307	NAG	O5-C5-C6-O6
5	B	1307	NAG	O5-C5-C6-O6
5	C	1307	NAG	O5-C5-C6-O6
5	A	1308	NAG	O5-C5-C6-O6
5	A	1302	NAG	C1-C2-N2-C7
5	A	1305	NAG	C1-C2-N2-C7
5	A	1309	NAG	C1-C2-N2-C7
5	B	1302	NAG	C1-C2-N2-C7
5	B	1305	NAG	C1-C2-N2-C7
5	B	1309	NAG	C1-C2-N2-C7
5	C	1302	NAG	C1-C2-N2-C7
5	C	1305	NAG	C1-C2-N2-C7
5	C	1308	NAG	C1-C2-N2-C7
5	C	1309	NAG	C1-C2-N2-C7
5	B	1308	NAG	C3-C2-N2-C7

There are no ring outliers.

19 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1304	NAG	1	0

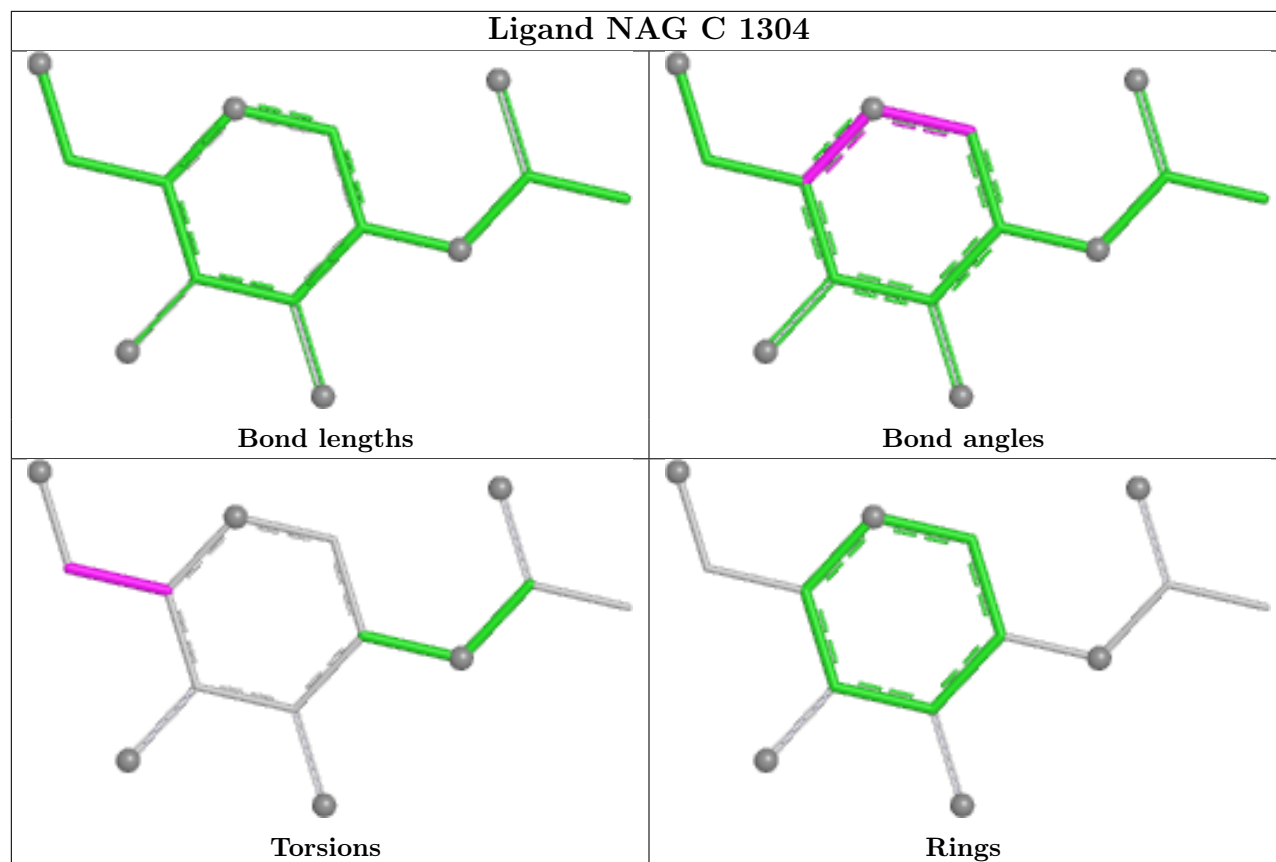
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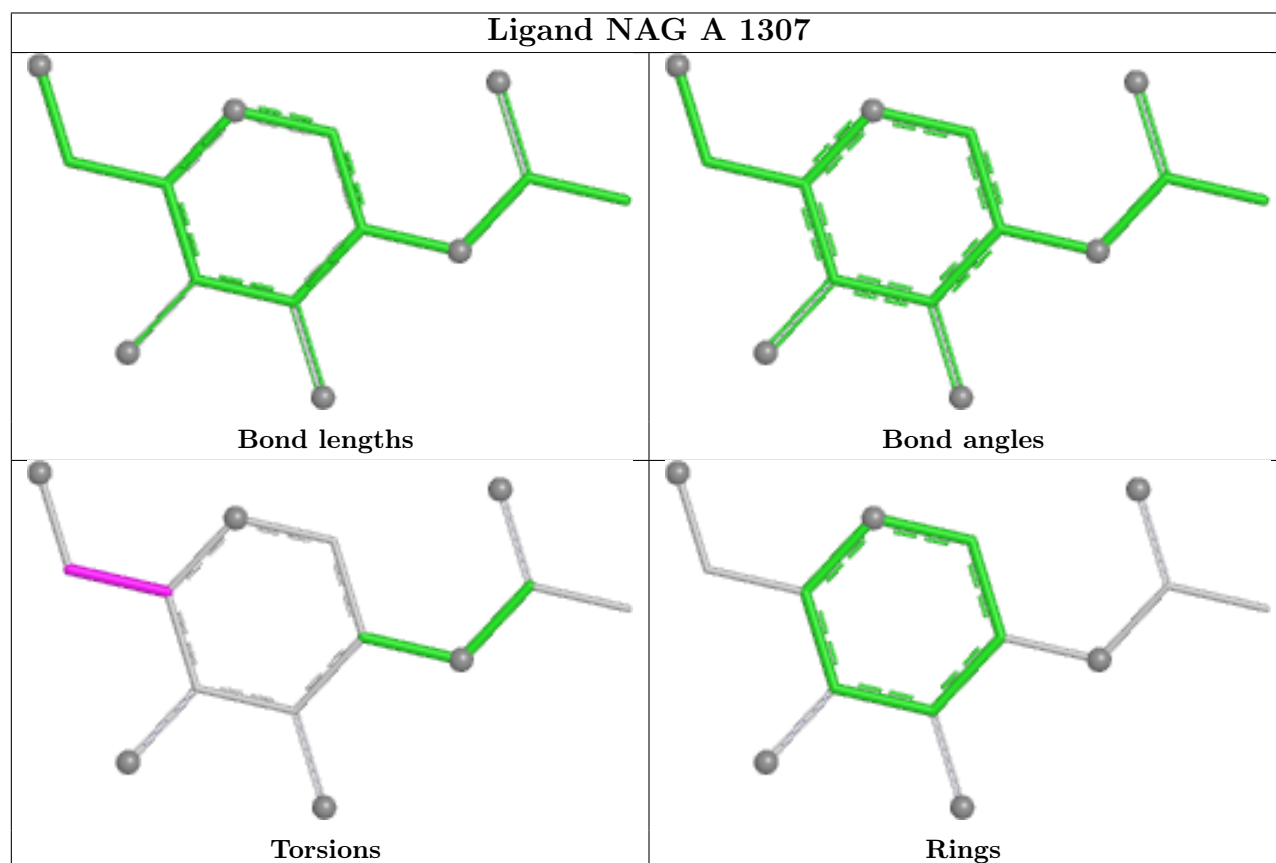
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1307	NAG	1	0
5	A	1309	NAG	2	0
5	A	1304	NAG	1	0
5	C	1302	NAG	5	0
5	A	1302	NAG	5	0
5	B	1304	NAG	1	0
5	C	1309	NAG	2	0
5	B	1302	NAG	5	0
5	A	1303	NAG	1	0
5	B	1307	NAG	1	0
5	C	1305	NAG	3	0
5	B	1309	NAG	2	0
5	B	1303	NAG	1	0
5	A	1305	NAG	3	0
5	A	1306	NAG	1	0
5	B	1305	NAG	3	0
5	C	1303	NAG	1	0
5	C	1307	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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

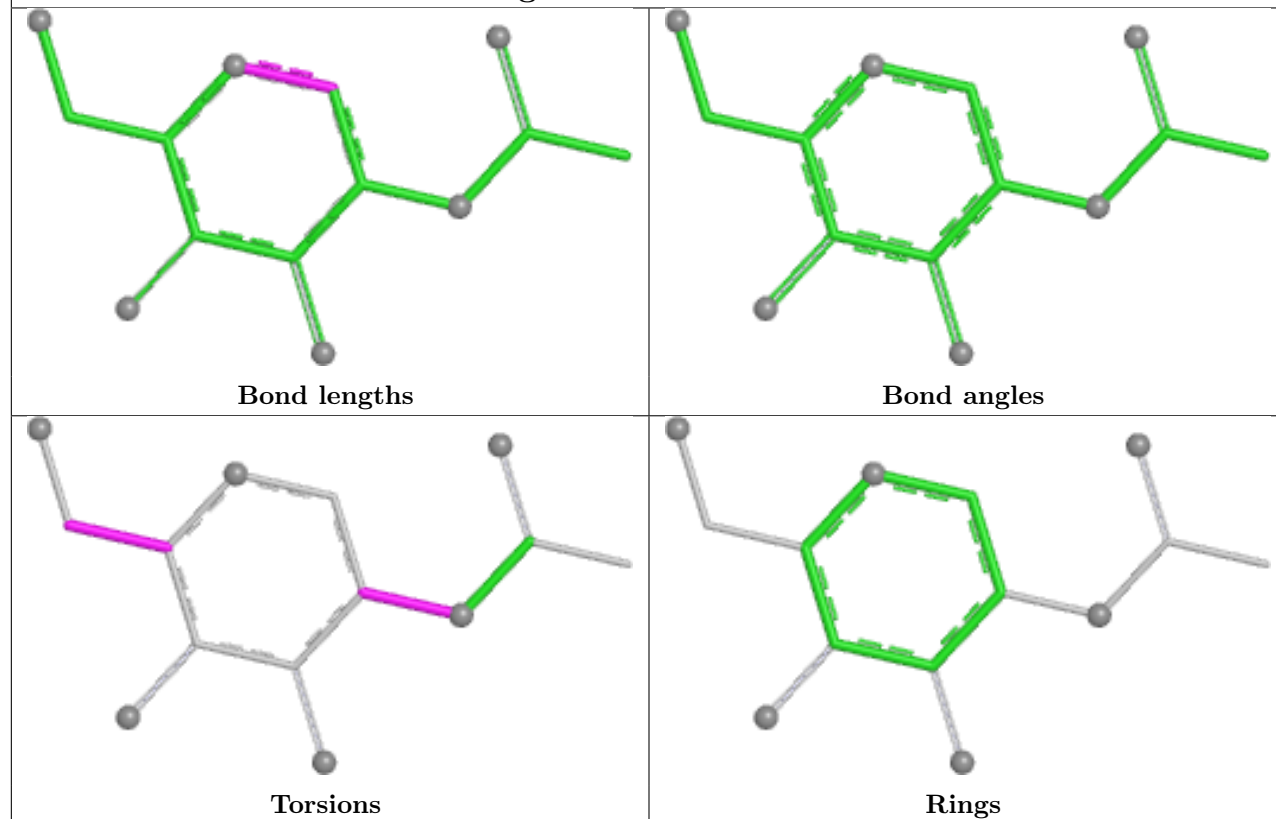
Ligand NAG C 1304



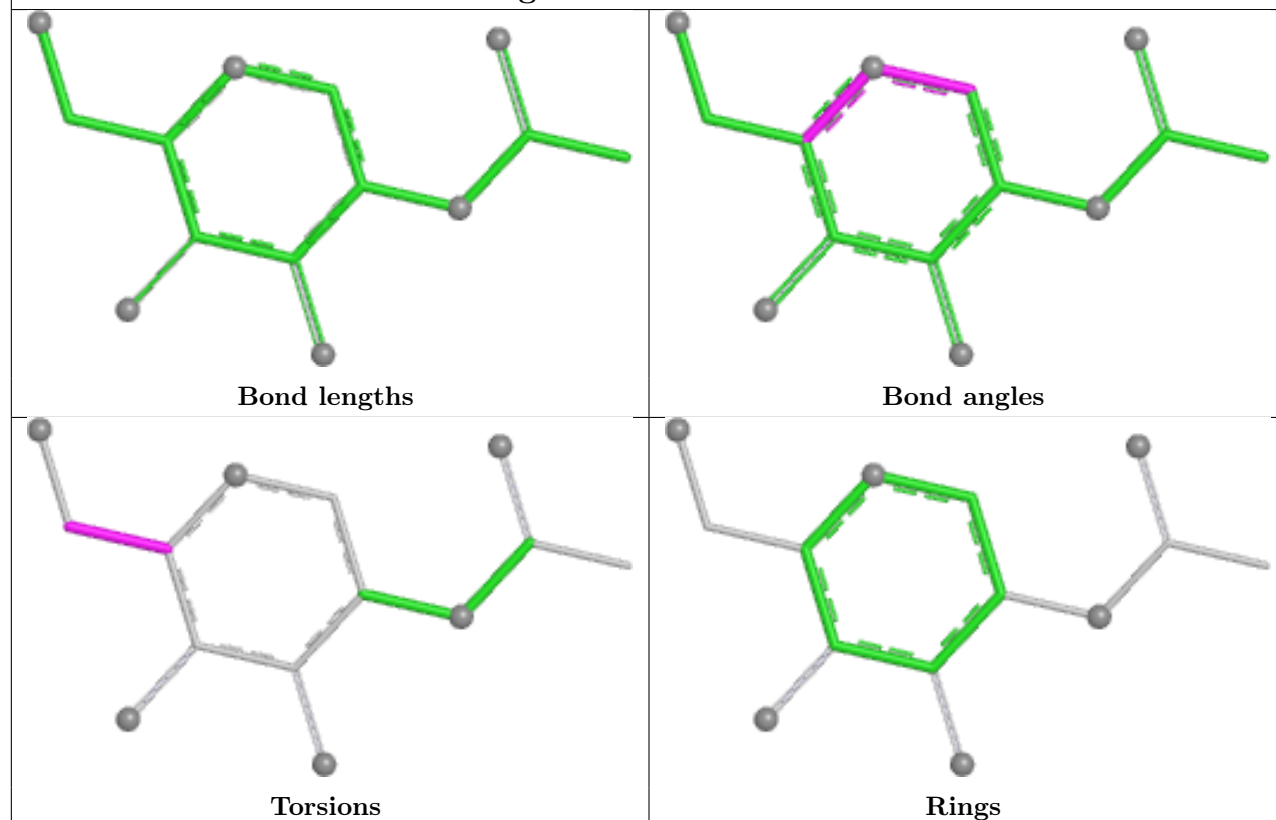
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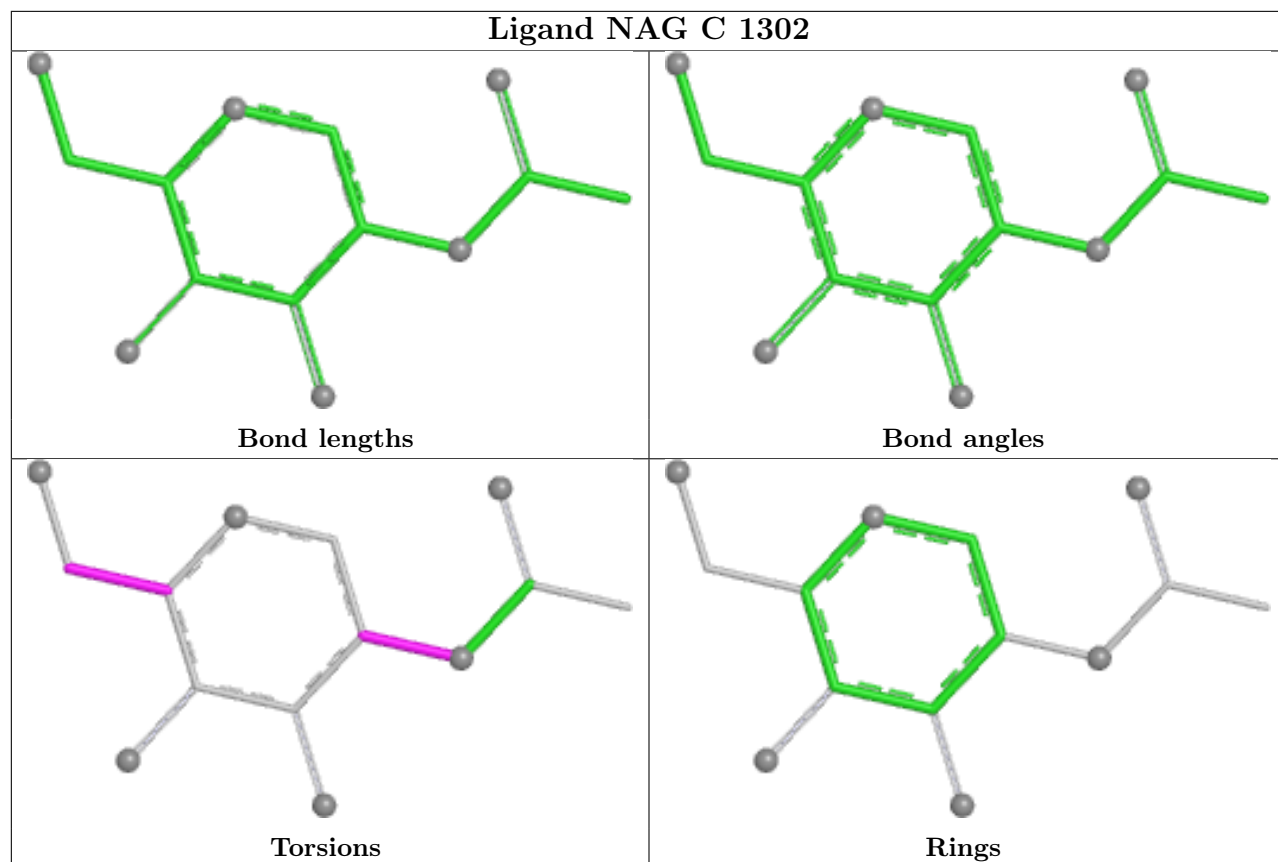
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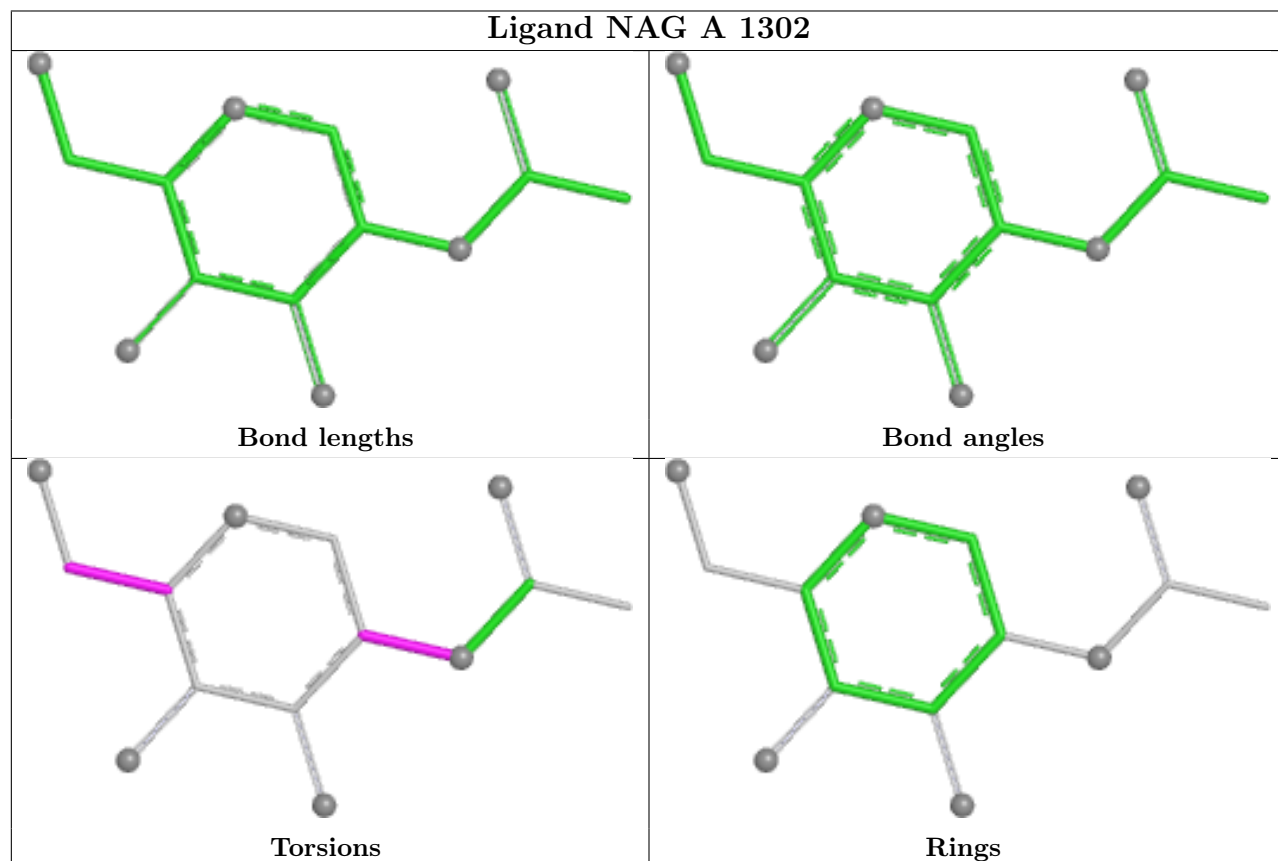
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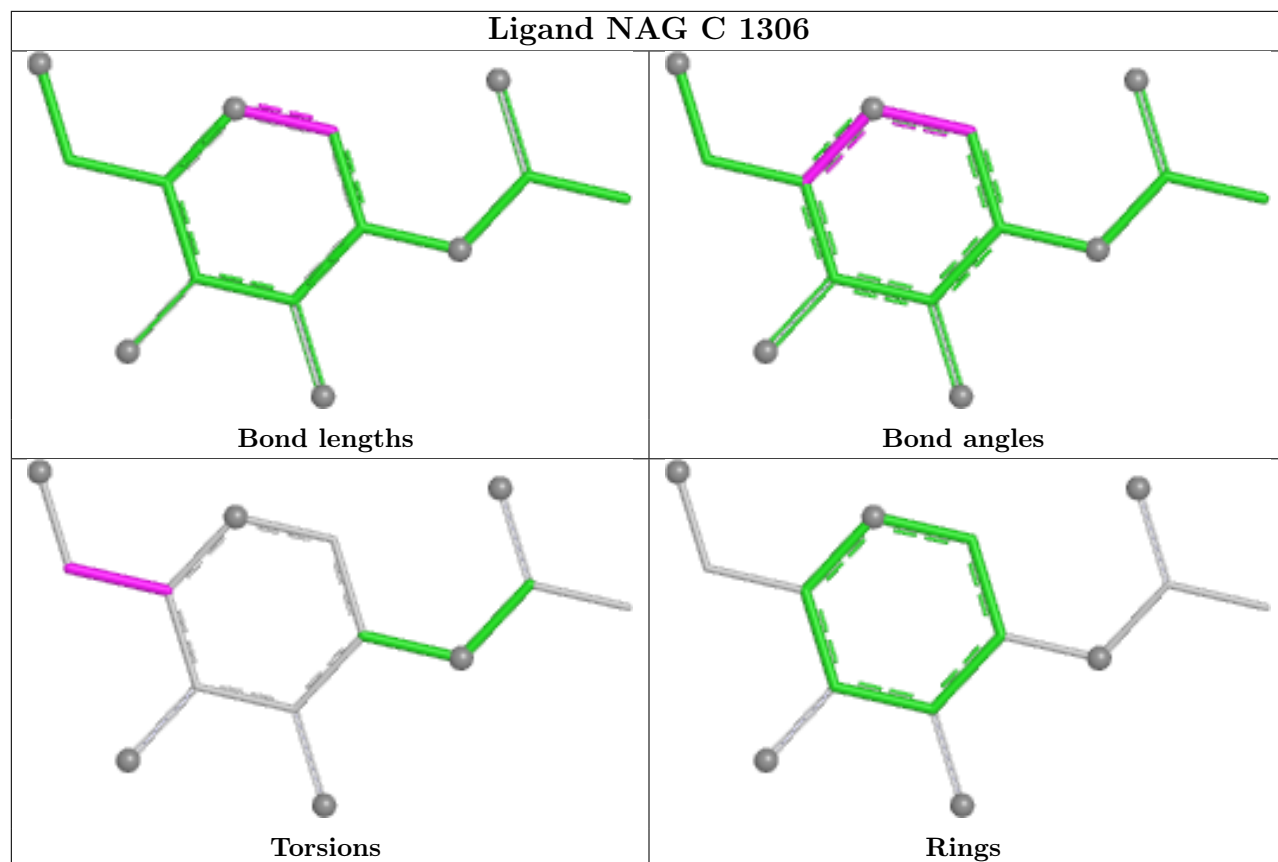
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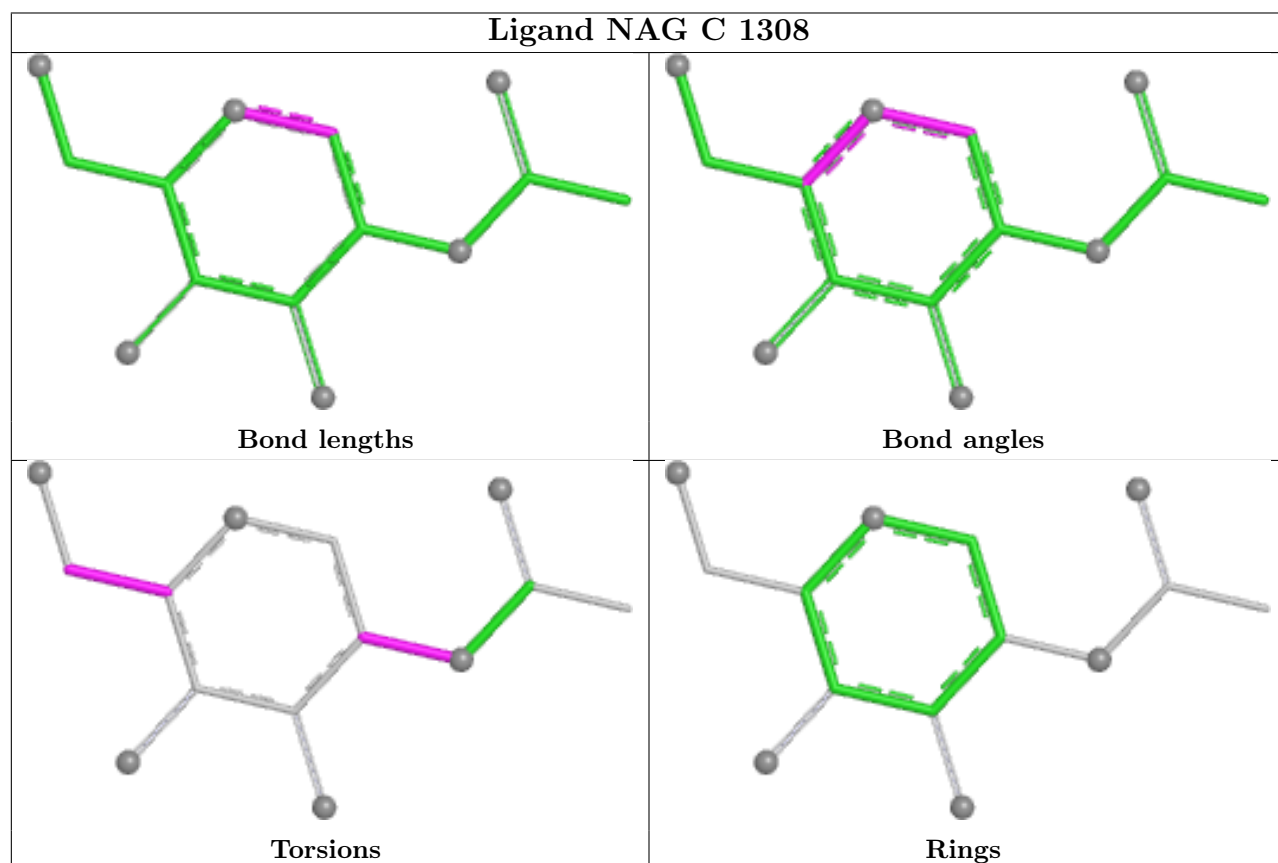
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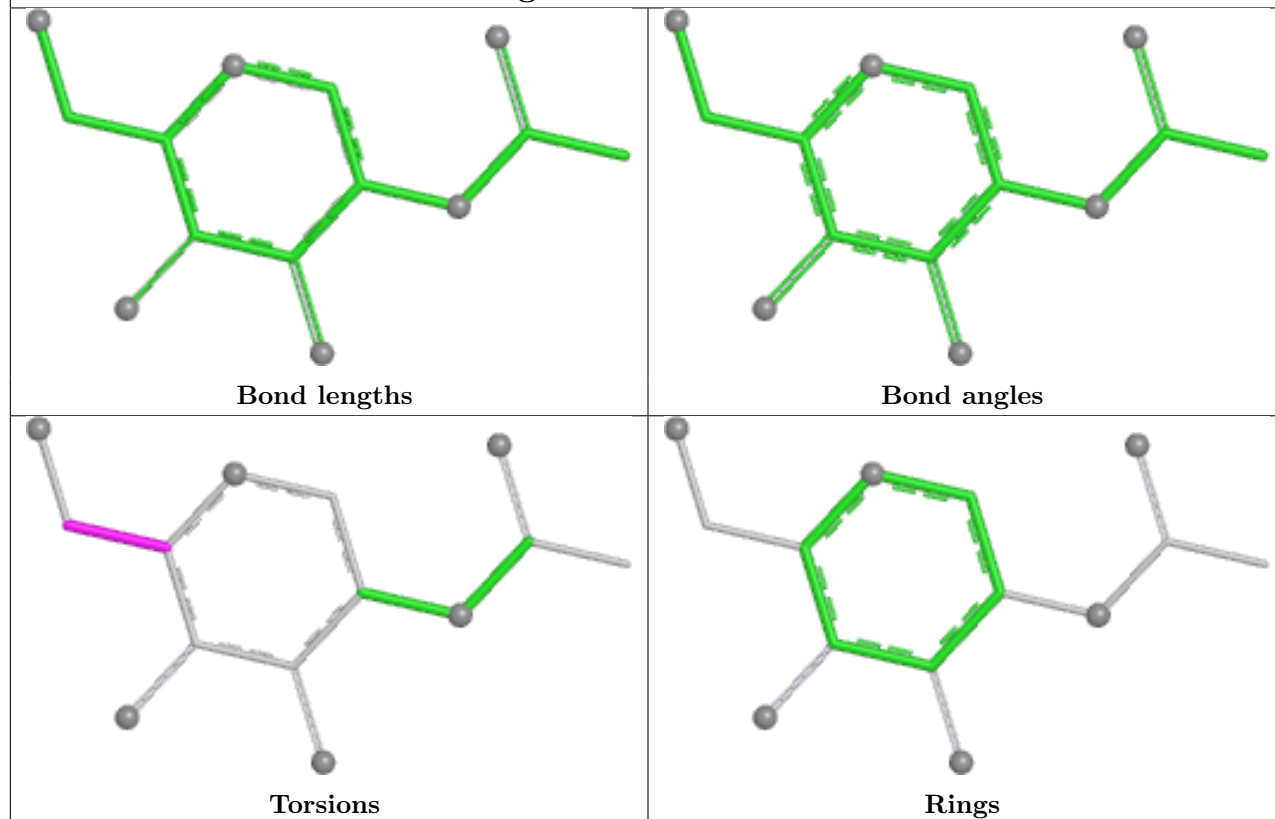
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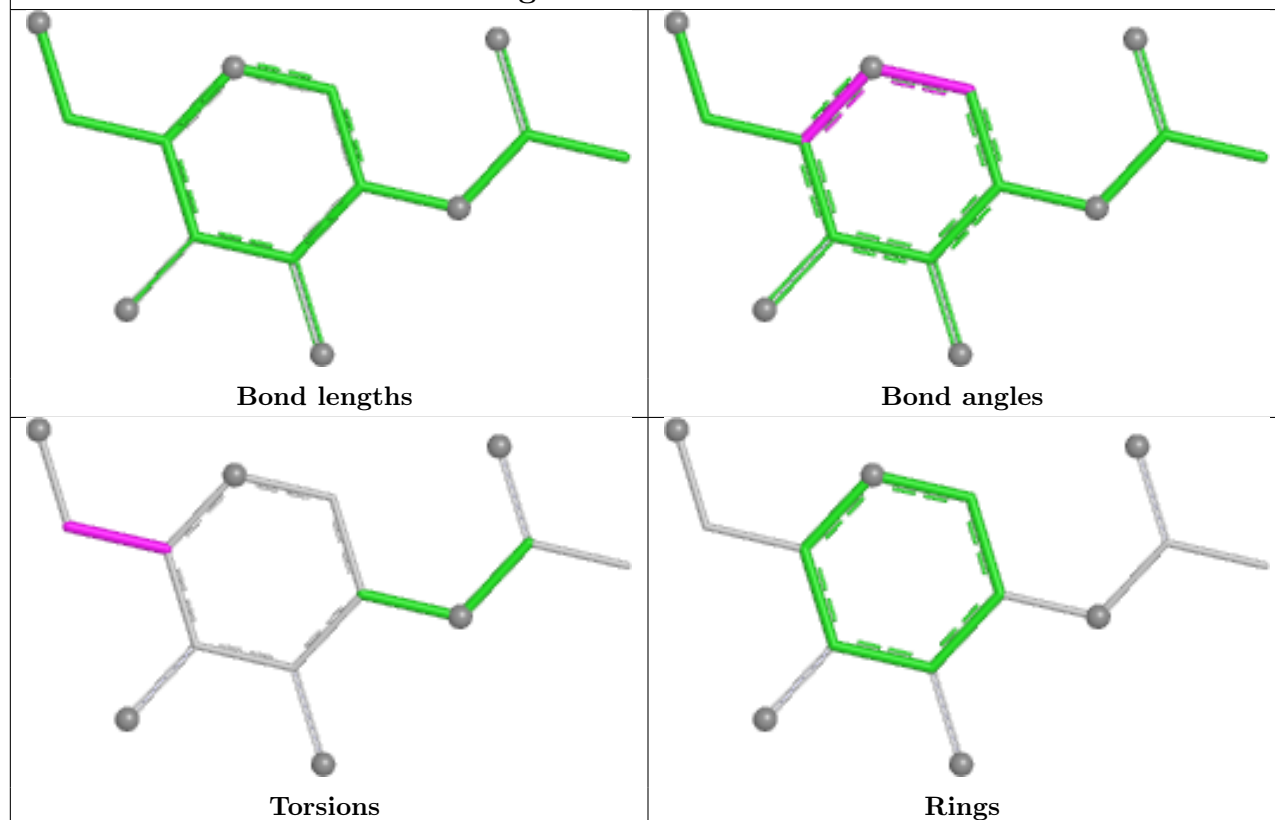
Ligand NAG C 1308



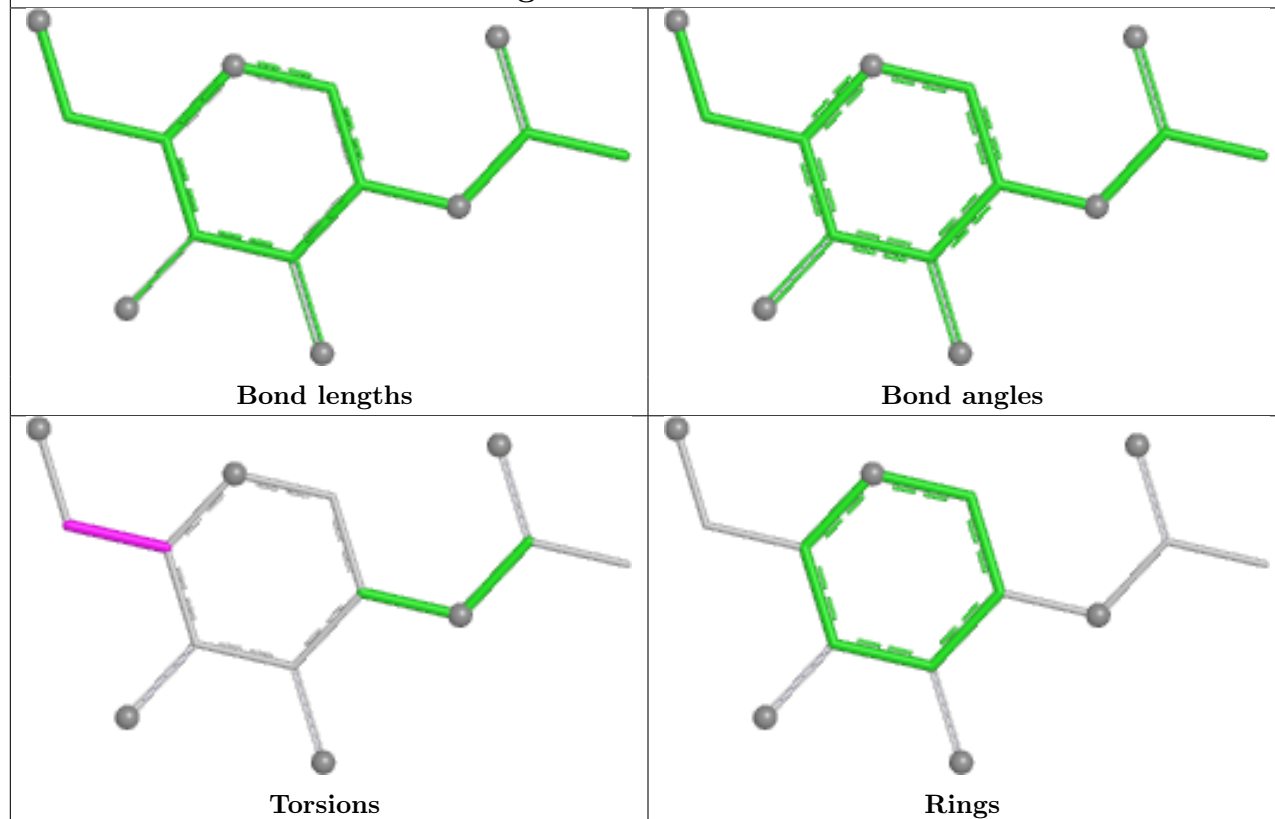
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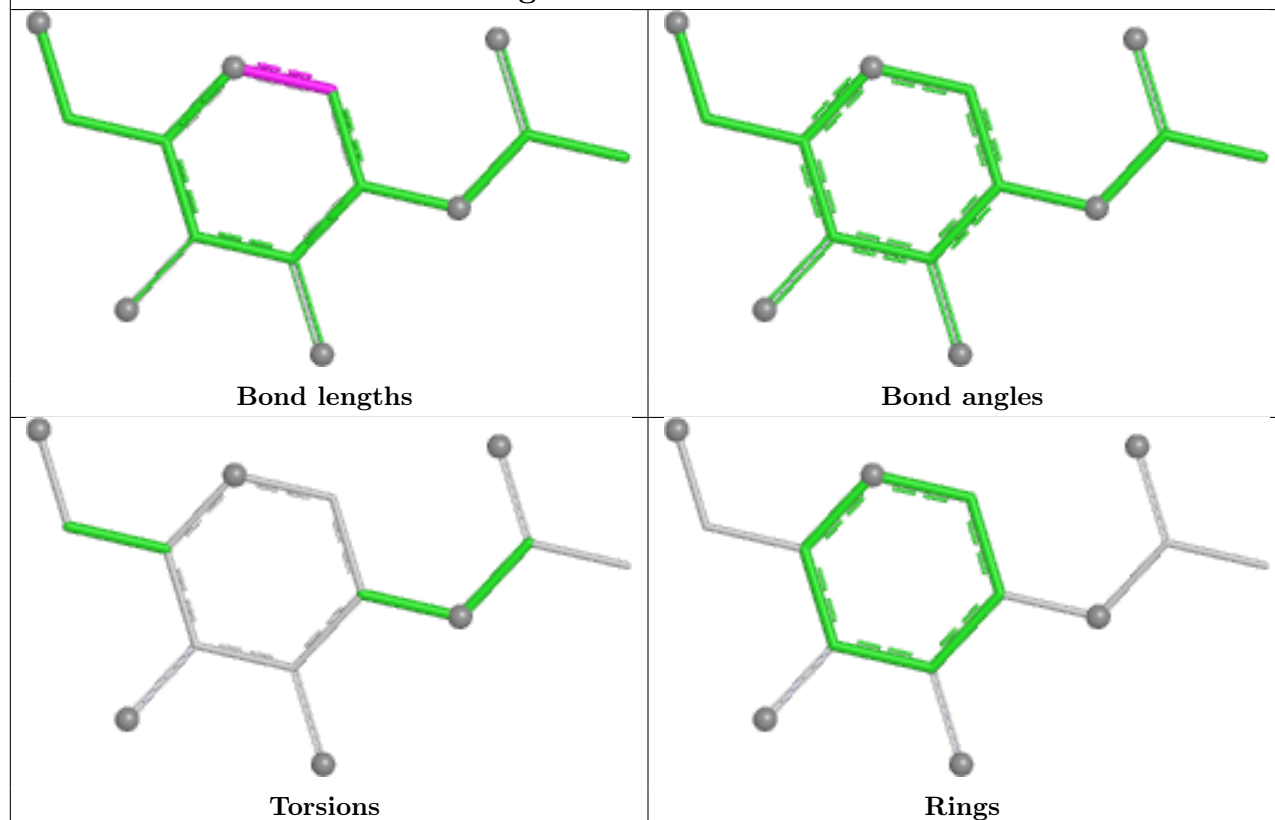
Ligand NAG B 1304



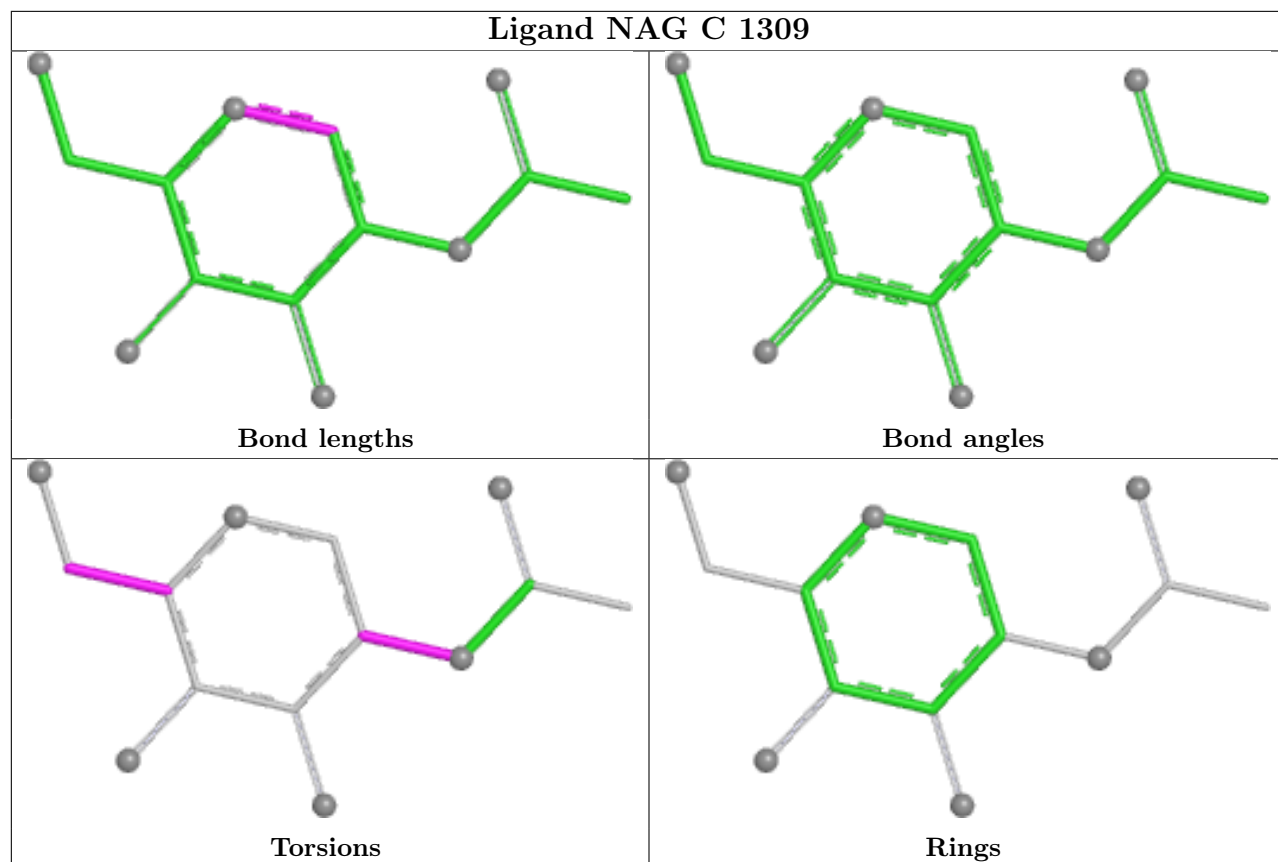
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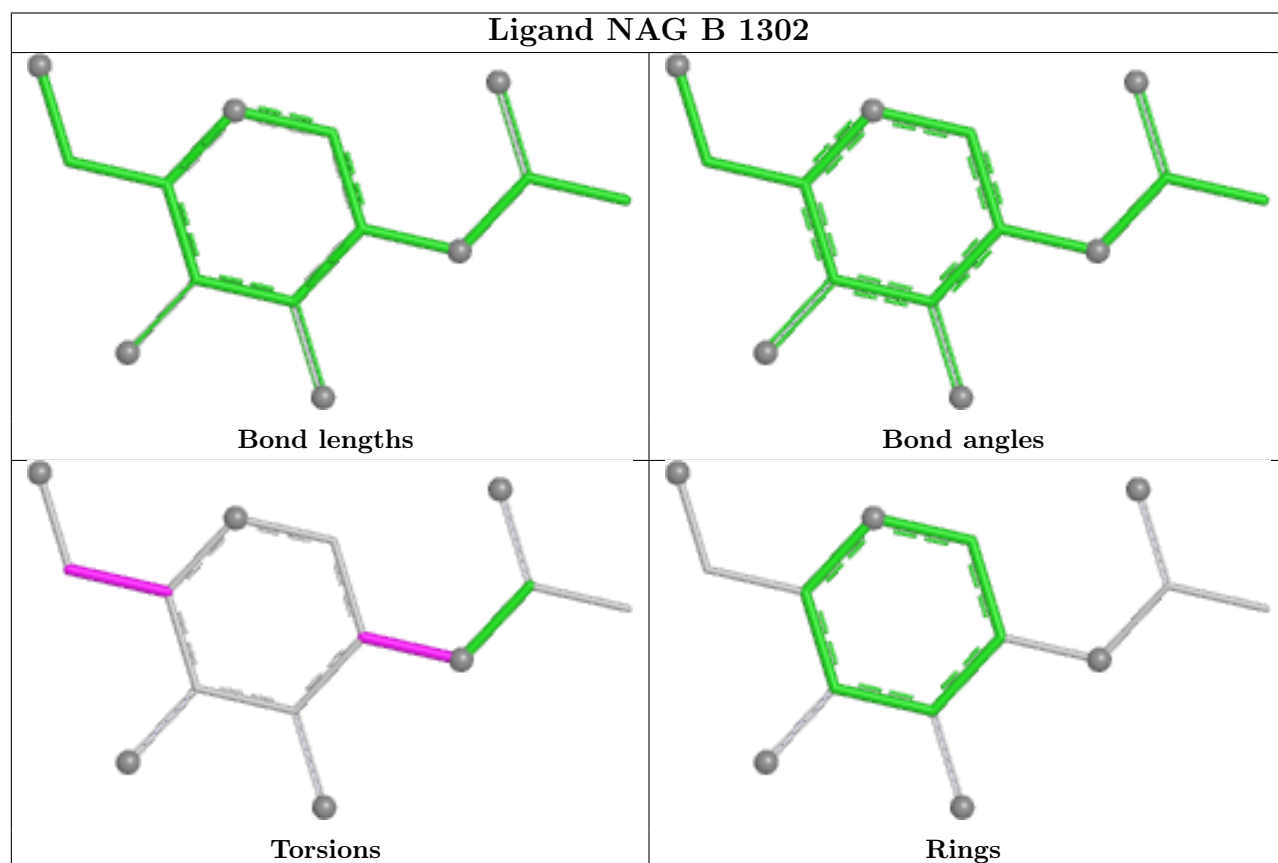
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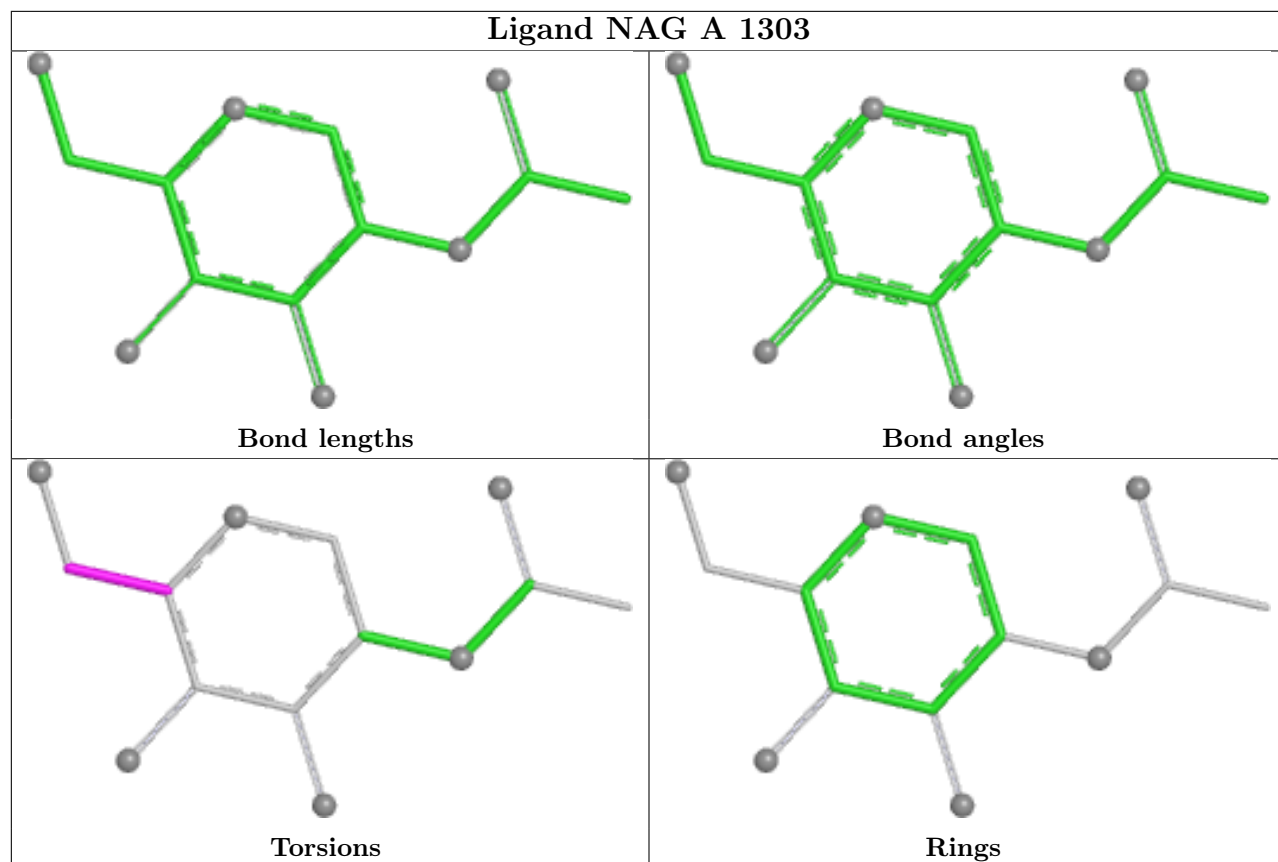
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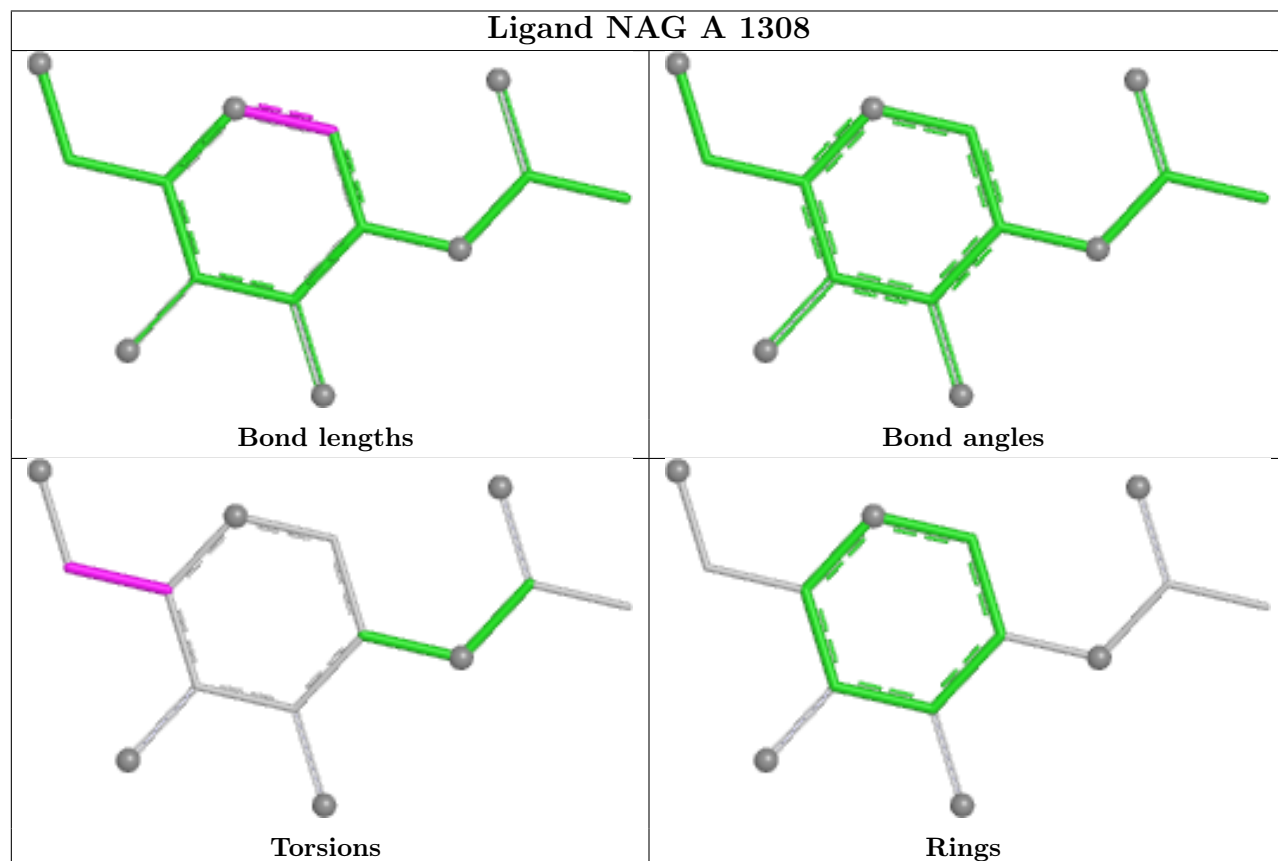
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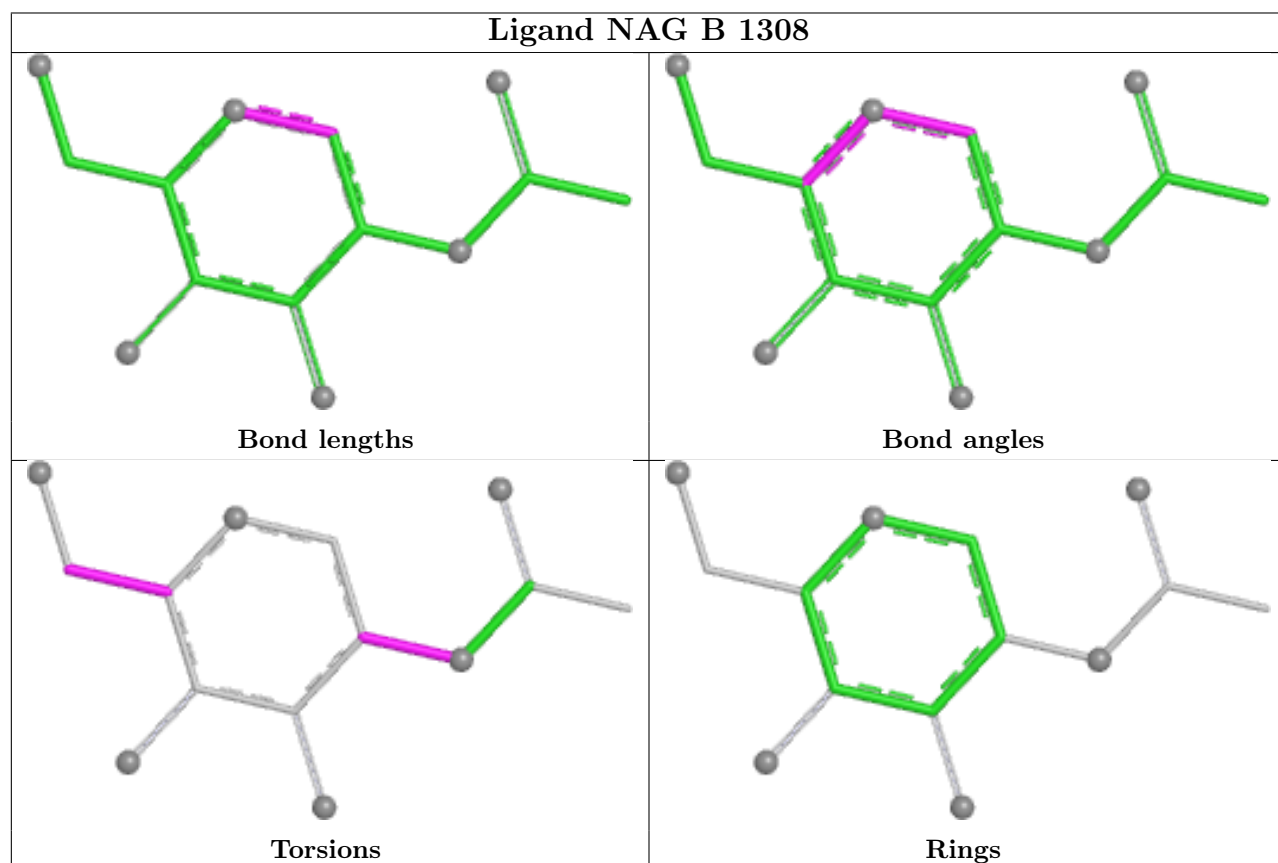
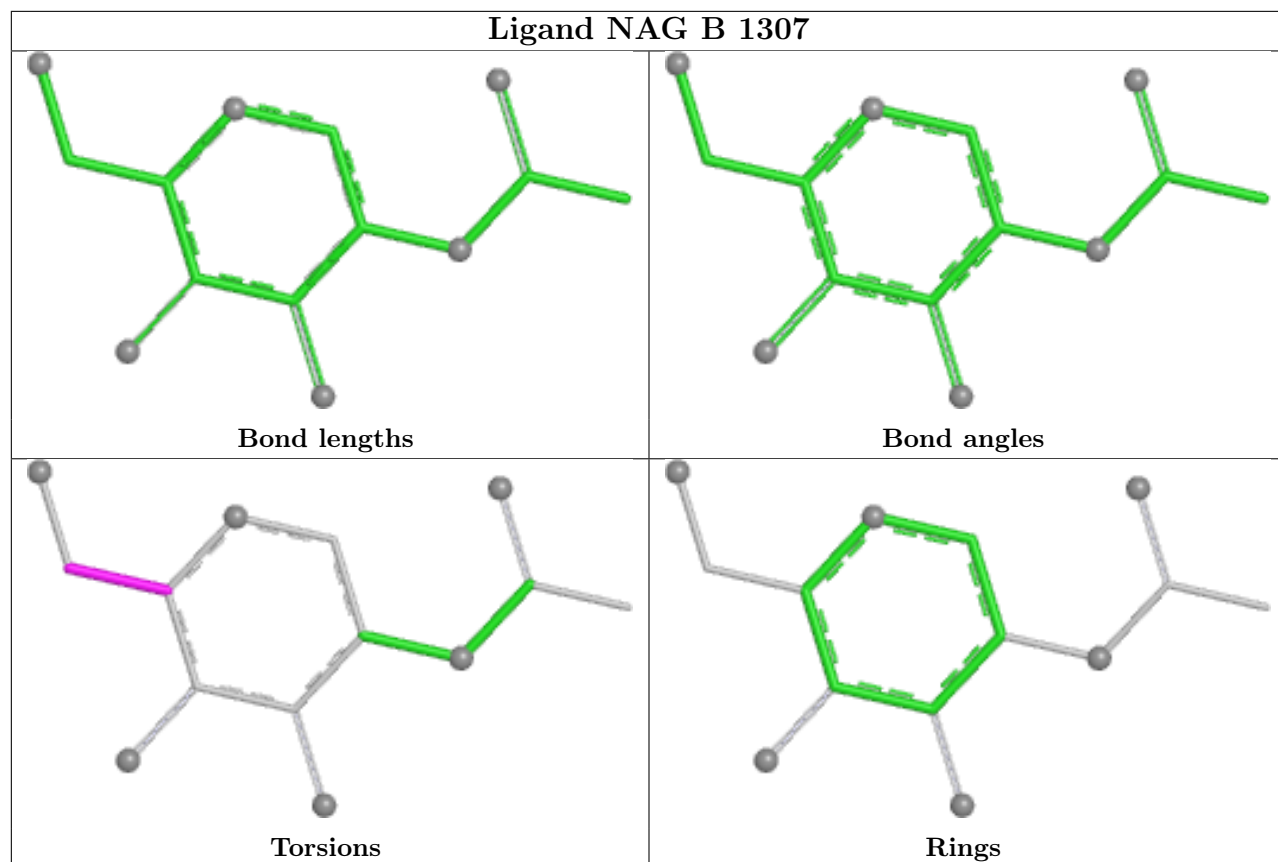


Ligand NAG A 1303

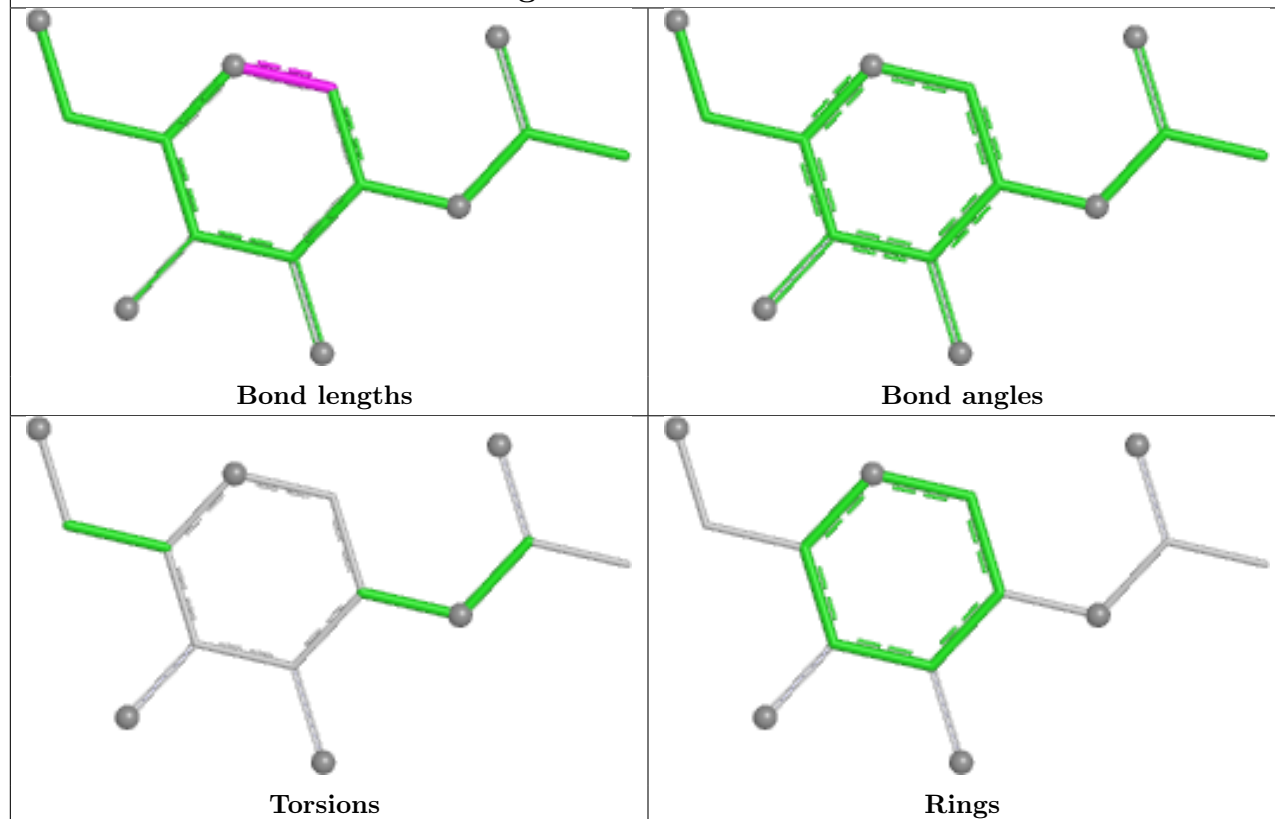


Ligand NAG A 1308

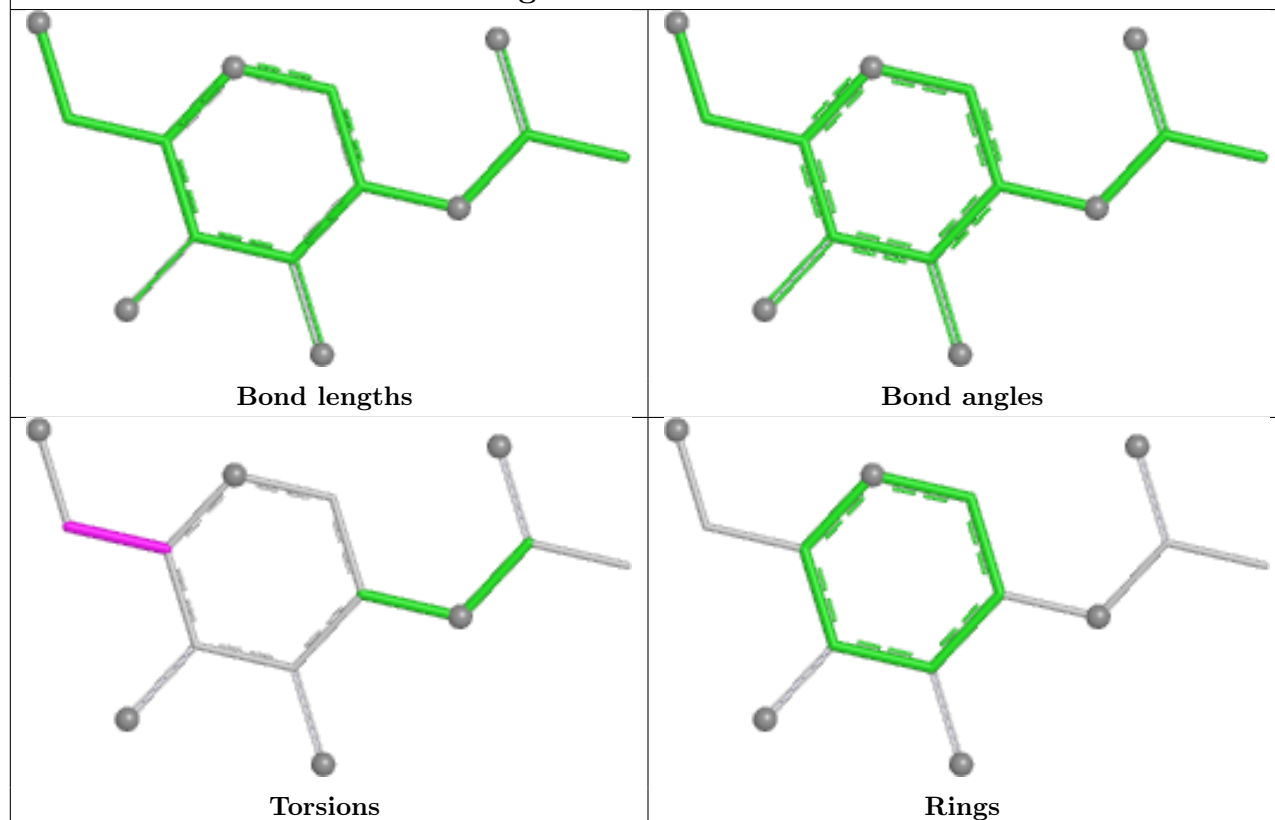




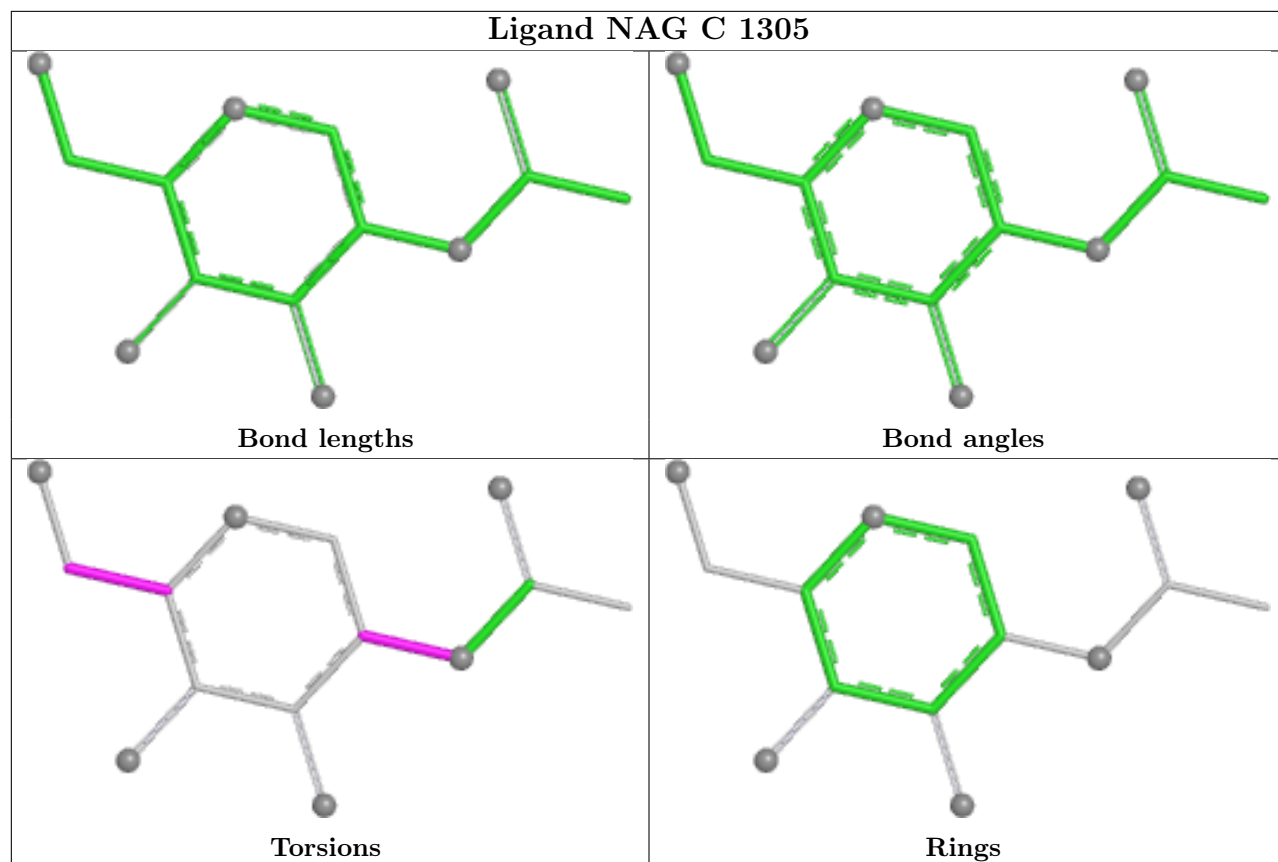
Ligand NAG C 1301



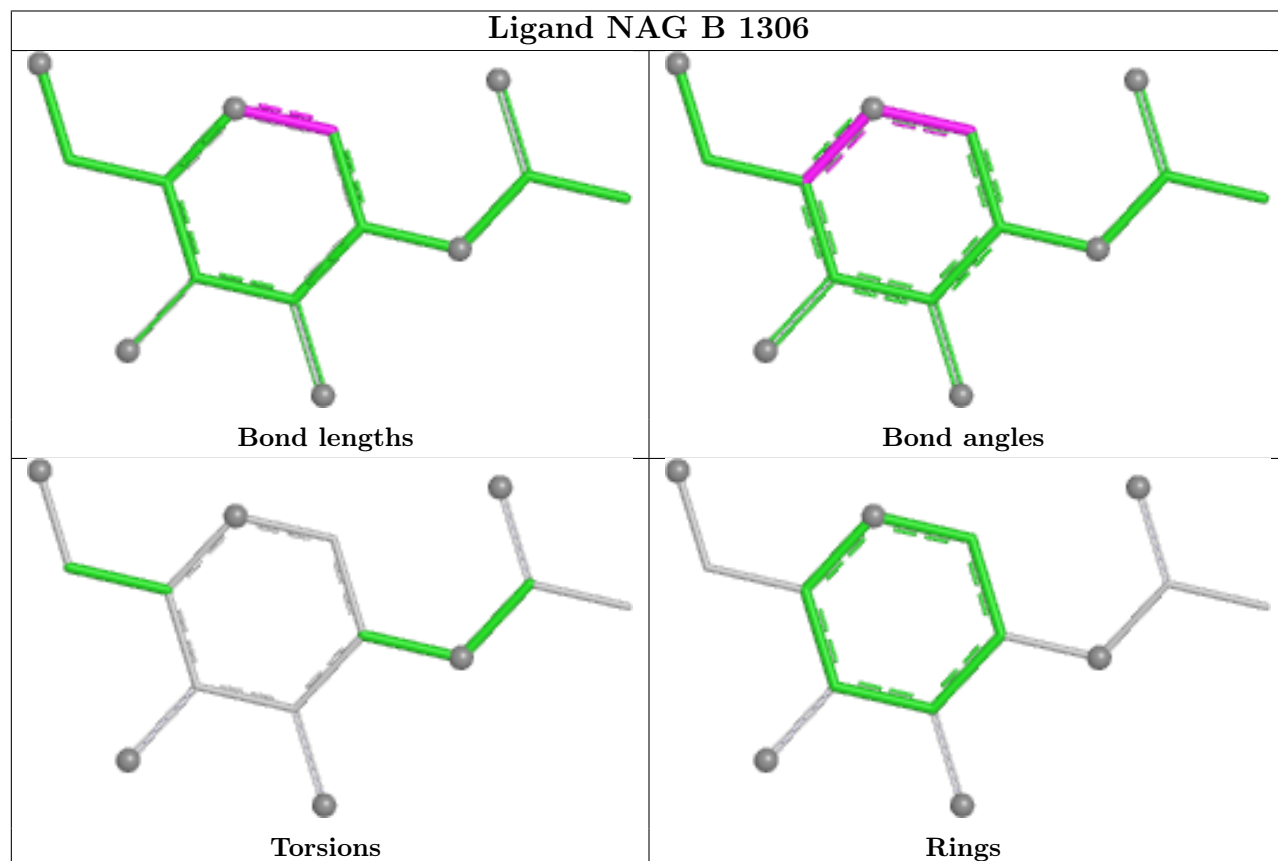
Ligand NAG B 1310

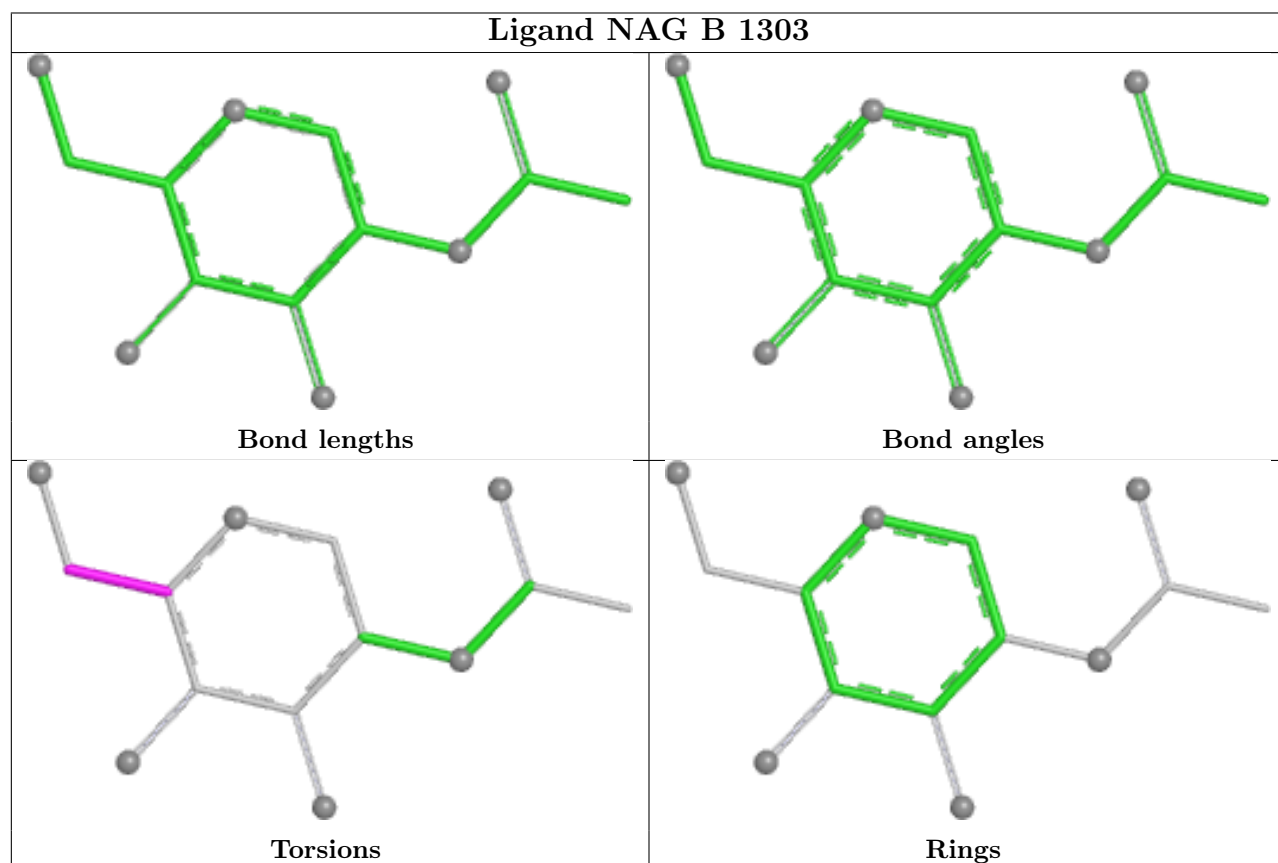
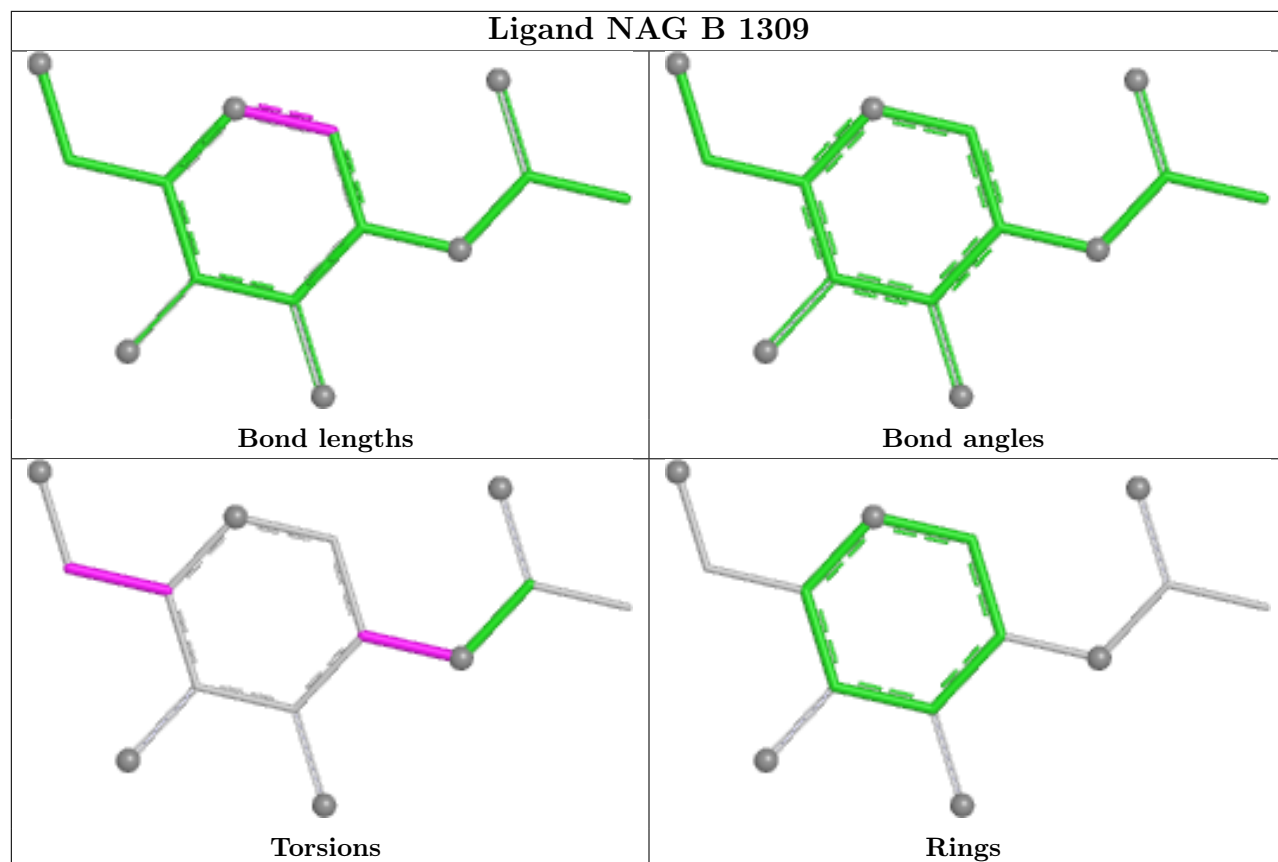


Ligand NAG C 1305

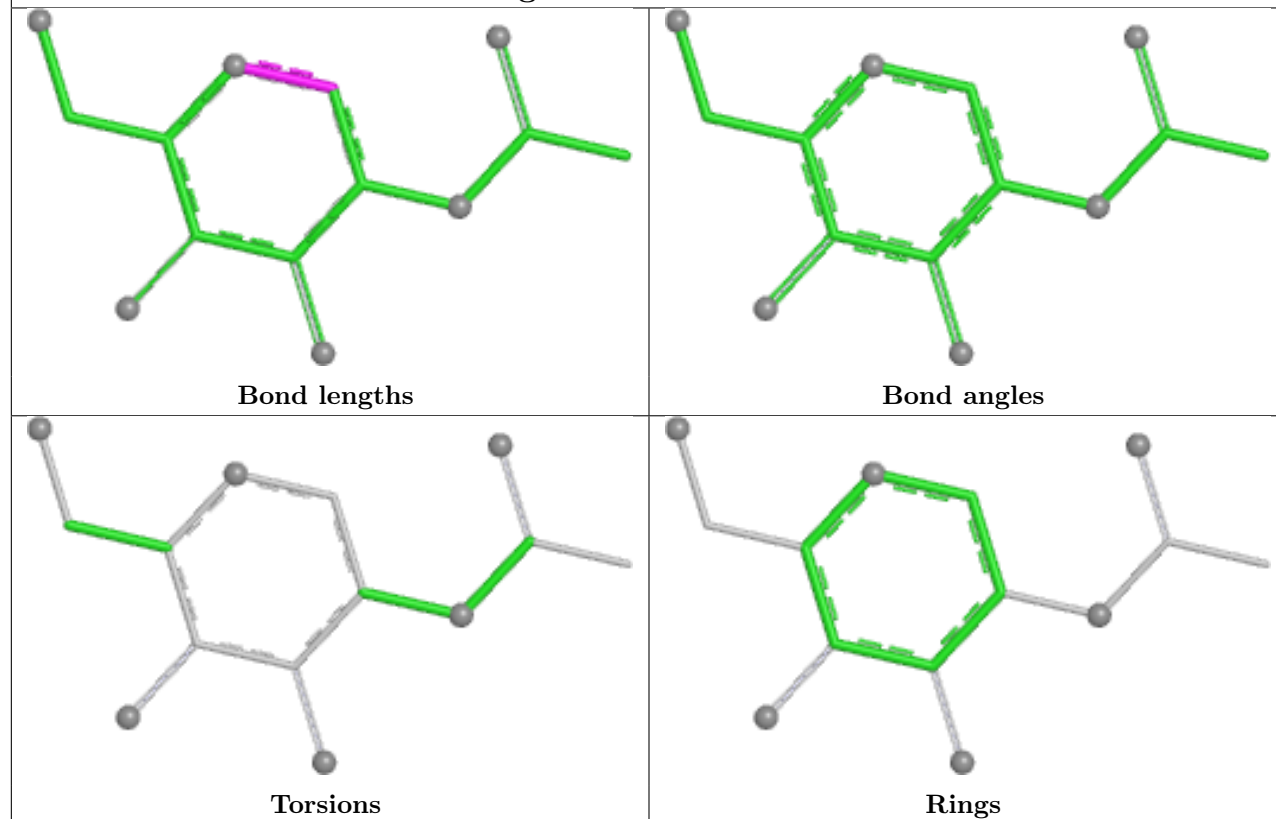


Ligand NAG B 1306

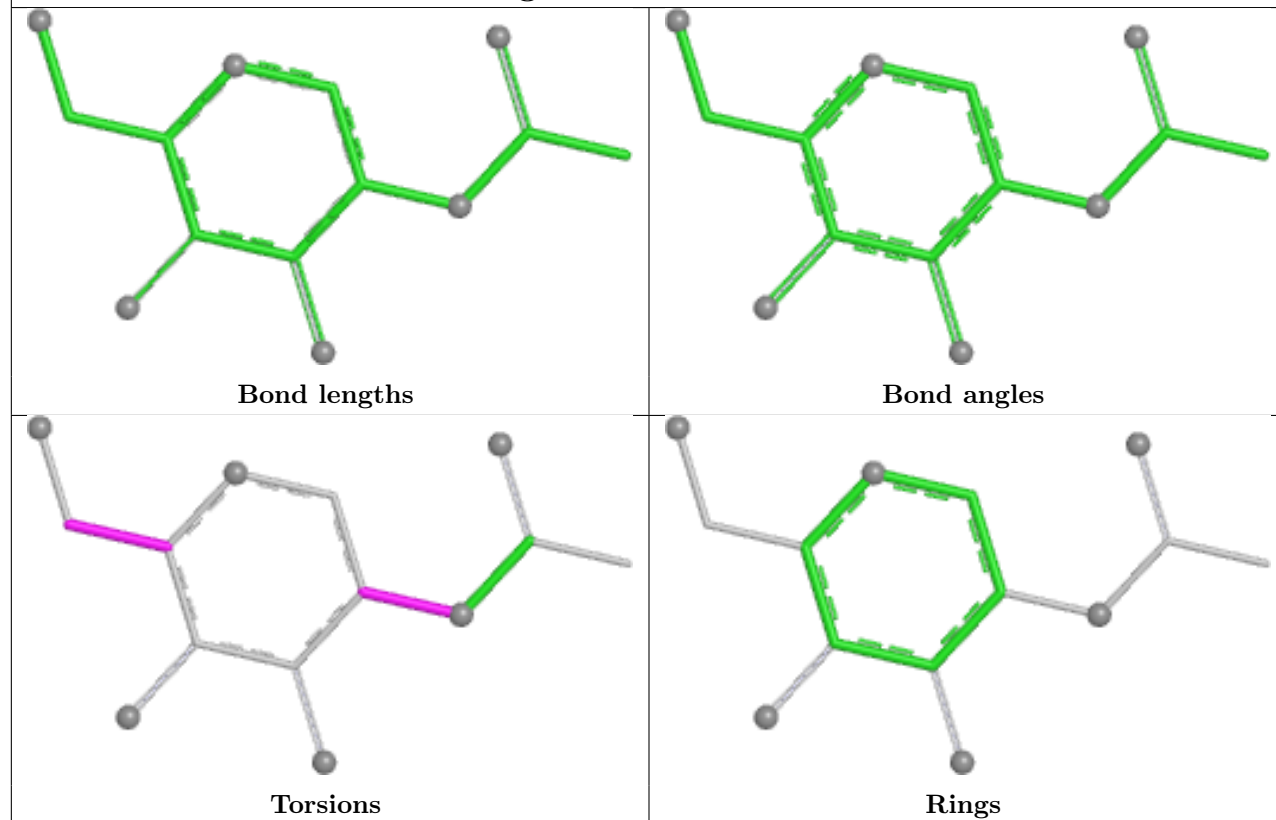




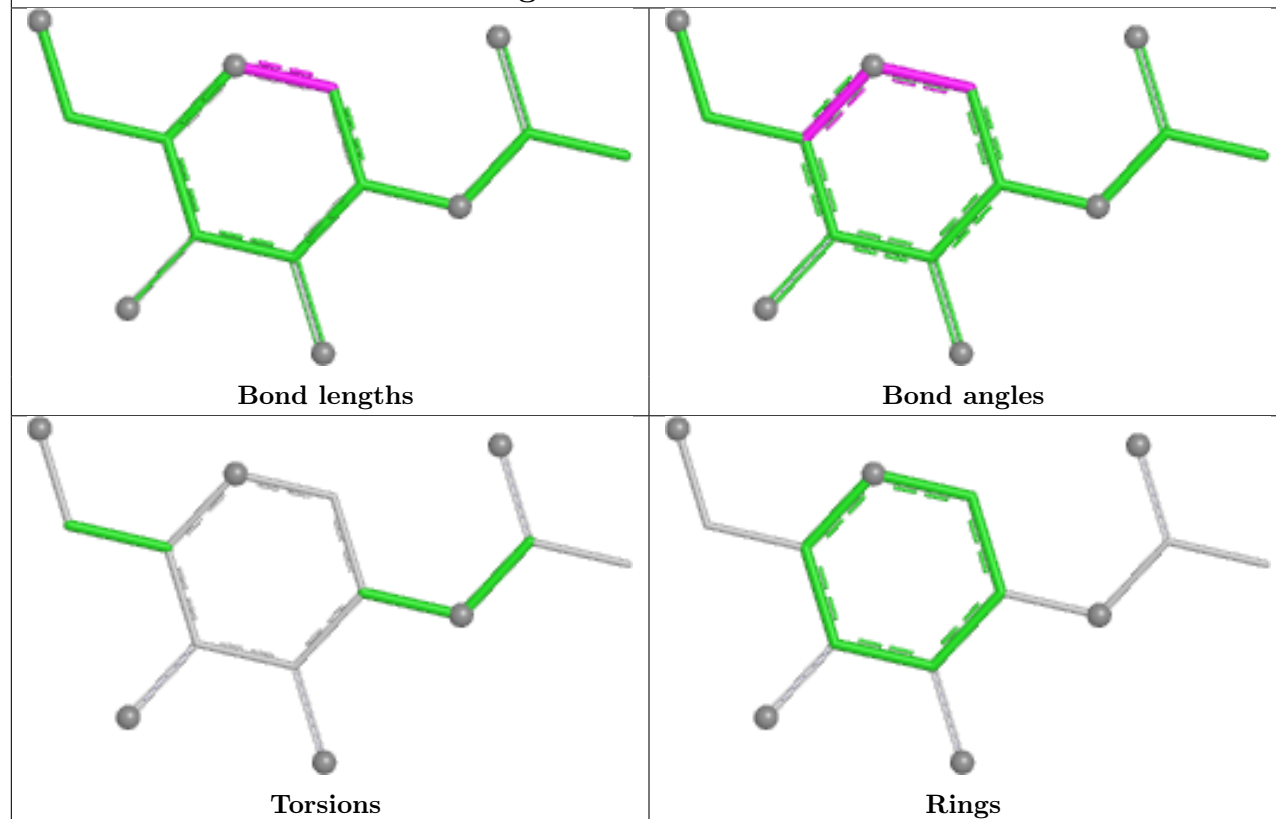
Ligand NAG A 1301



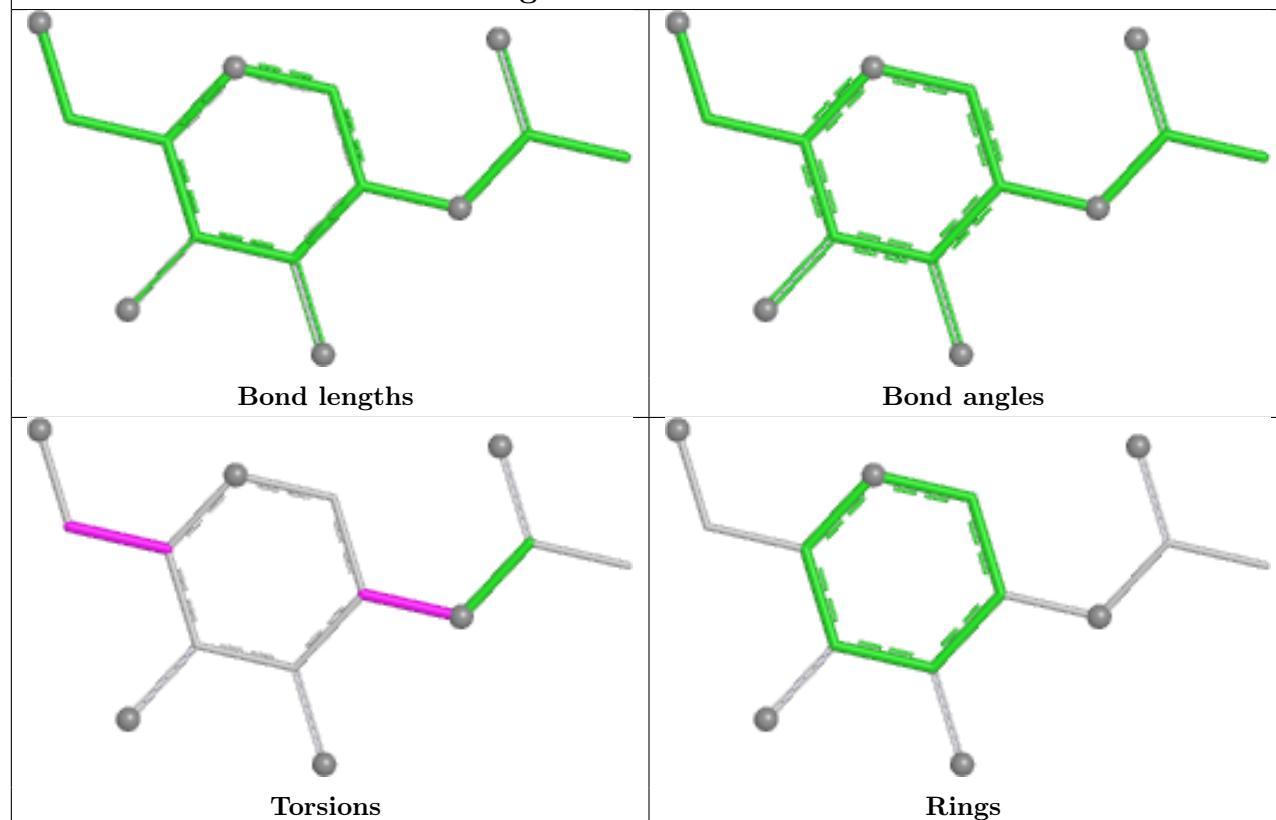
Ligand NAG A 1305

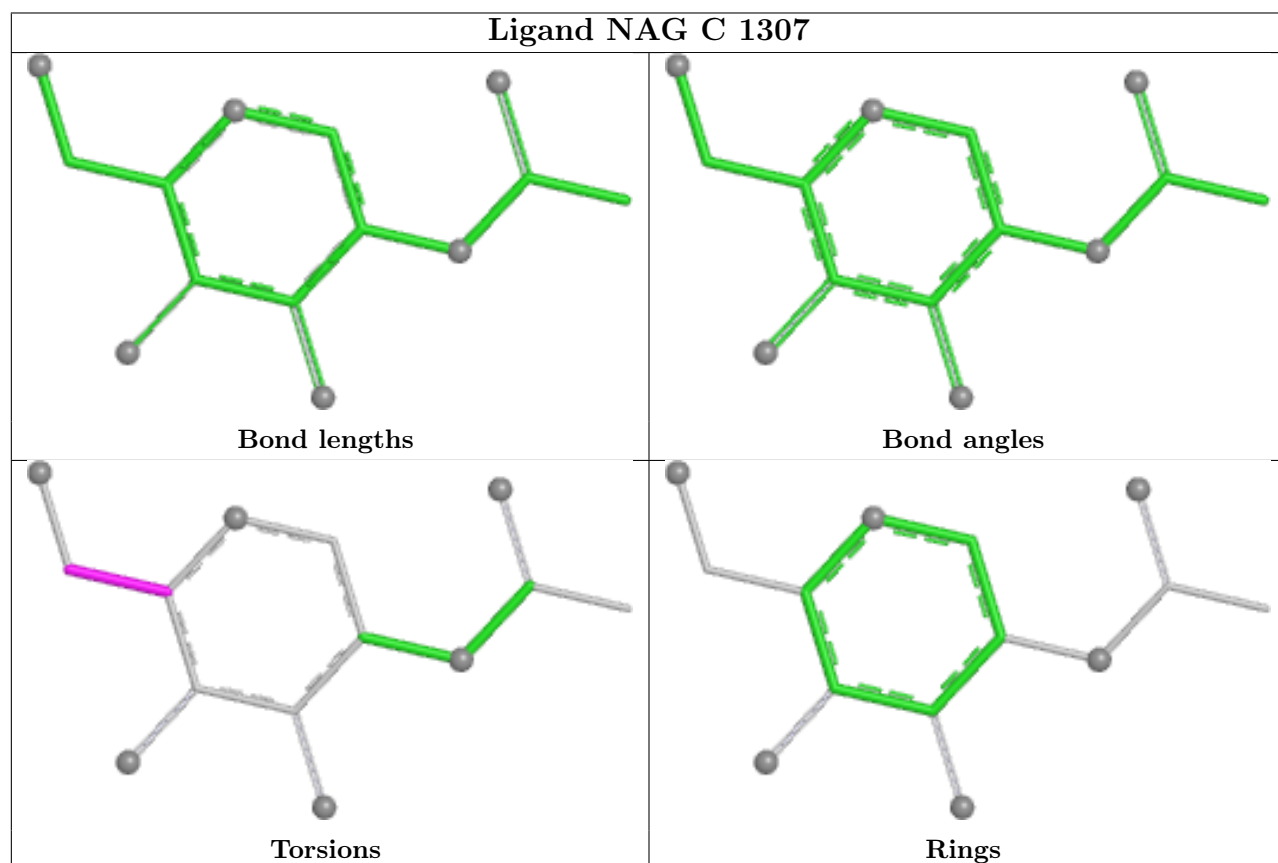
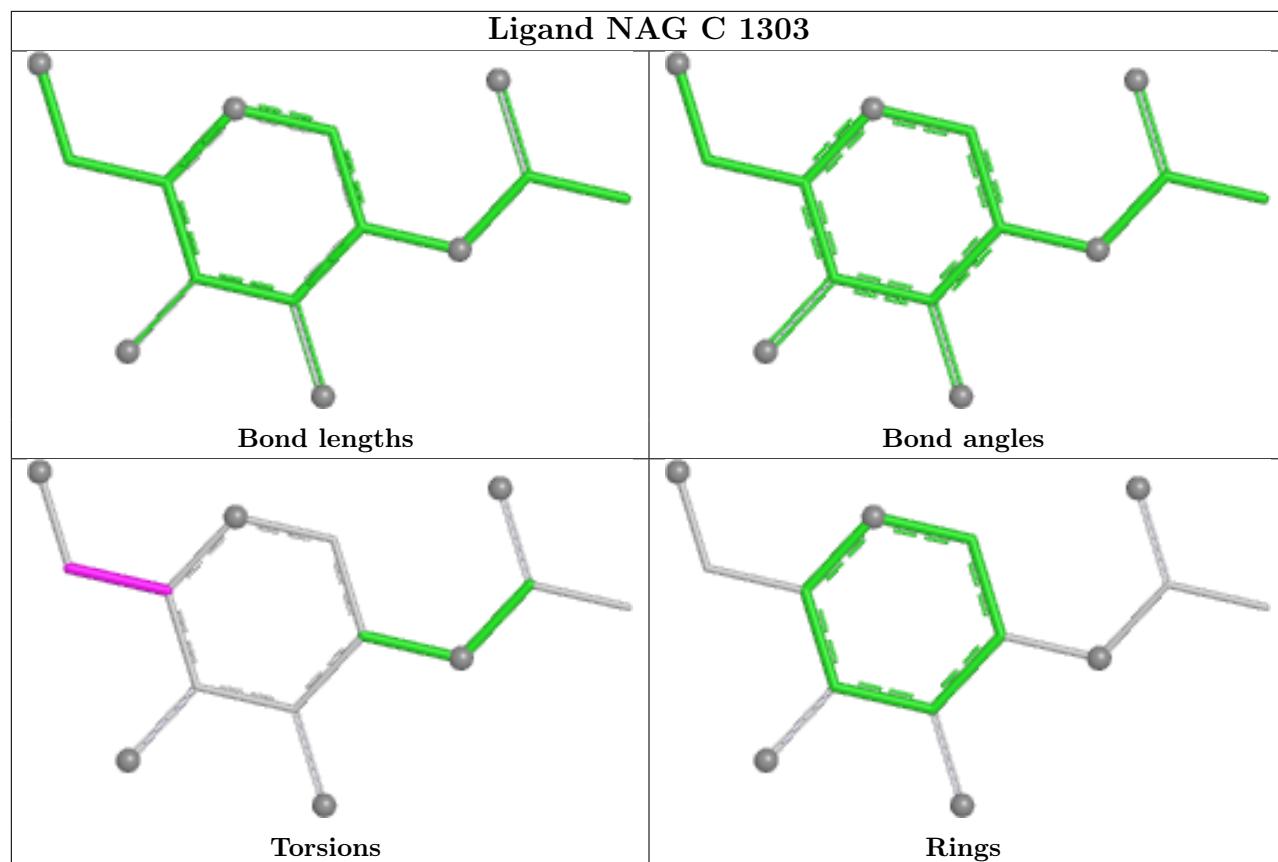


Ligand NAG A 1306



Ligand NAG B 1305





5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

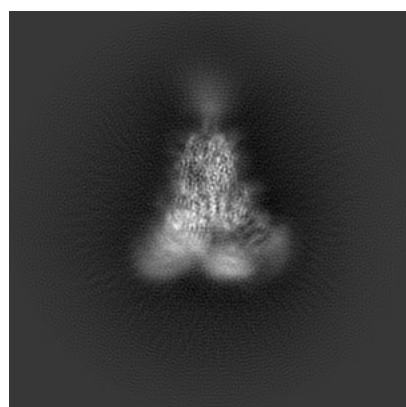
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30333. These allow visual inspection of the internal detail of the map and identification of artifacts.

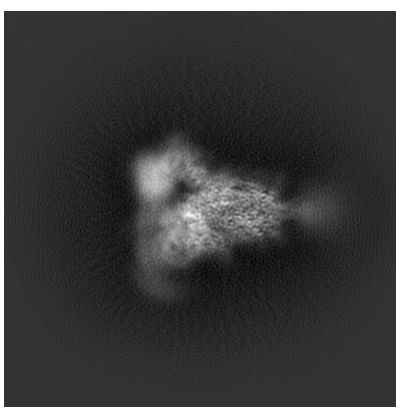
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

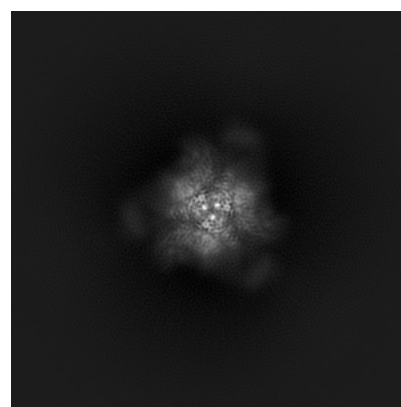
6.1.1 Primary map



X



Y

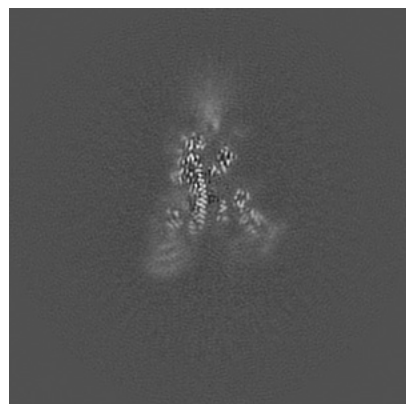


Z

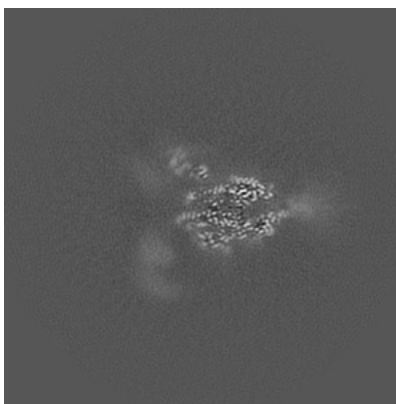
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

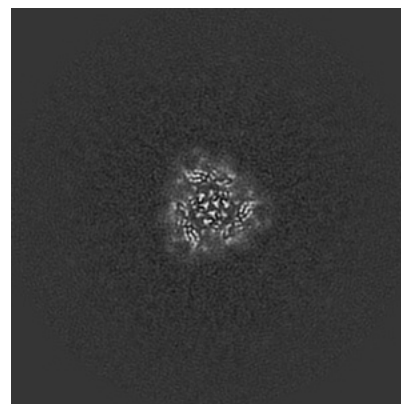
6.2.1 Primary map



X Index: 200



Y Index: 200

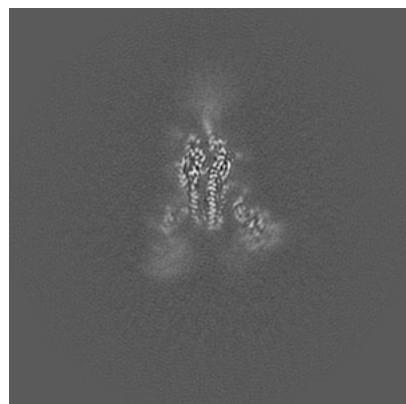


Z Index: 200

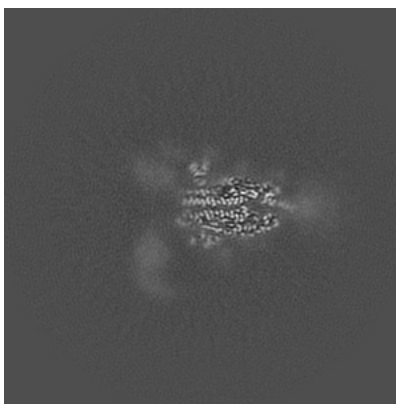
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

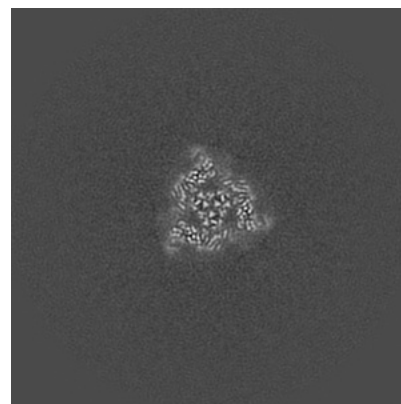
6.3.1 Primary map



X Index: 193



Y Index: 205

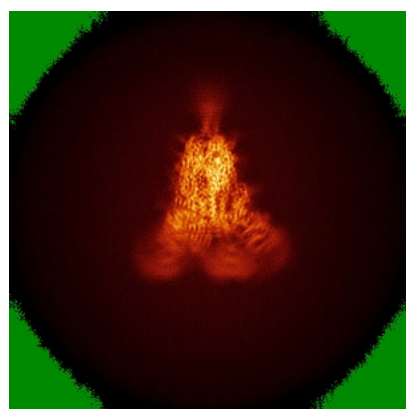


Z Index: 196

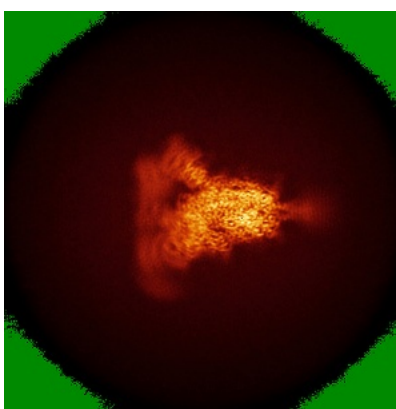
The images above show the largest variance slices of the map in three orthogonal directions.

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

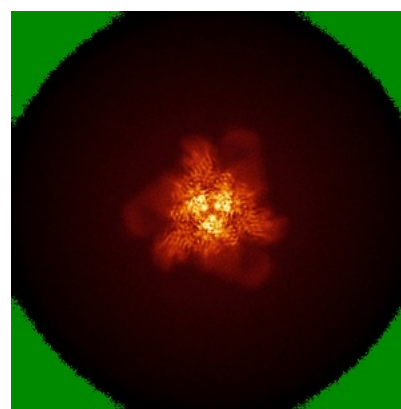
6.4.1 Primary map



X



Y

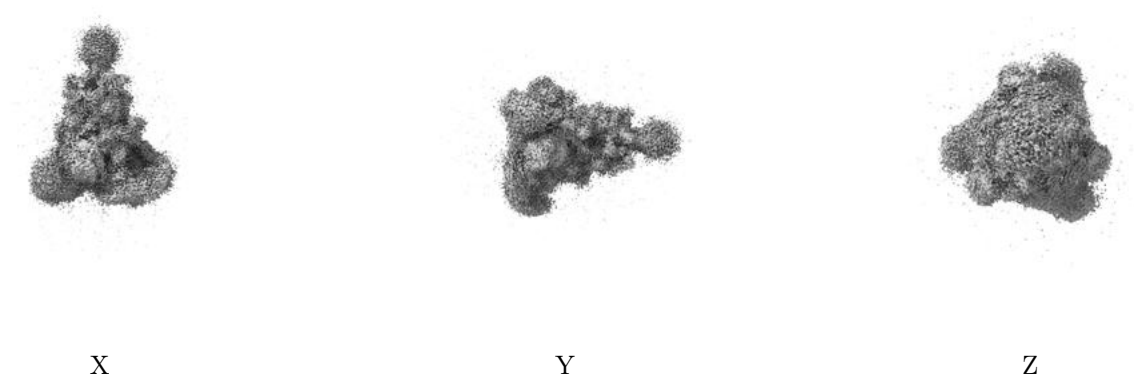


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.0045. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

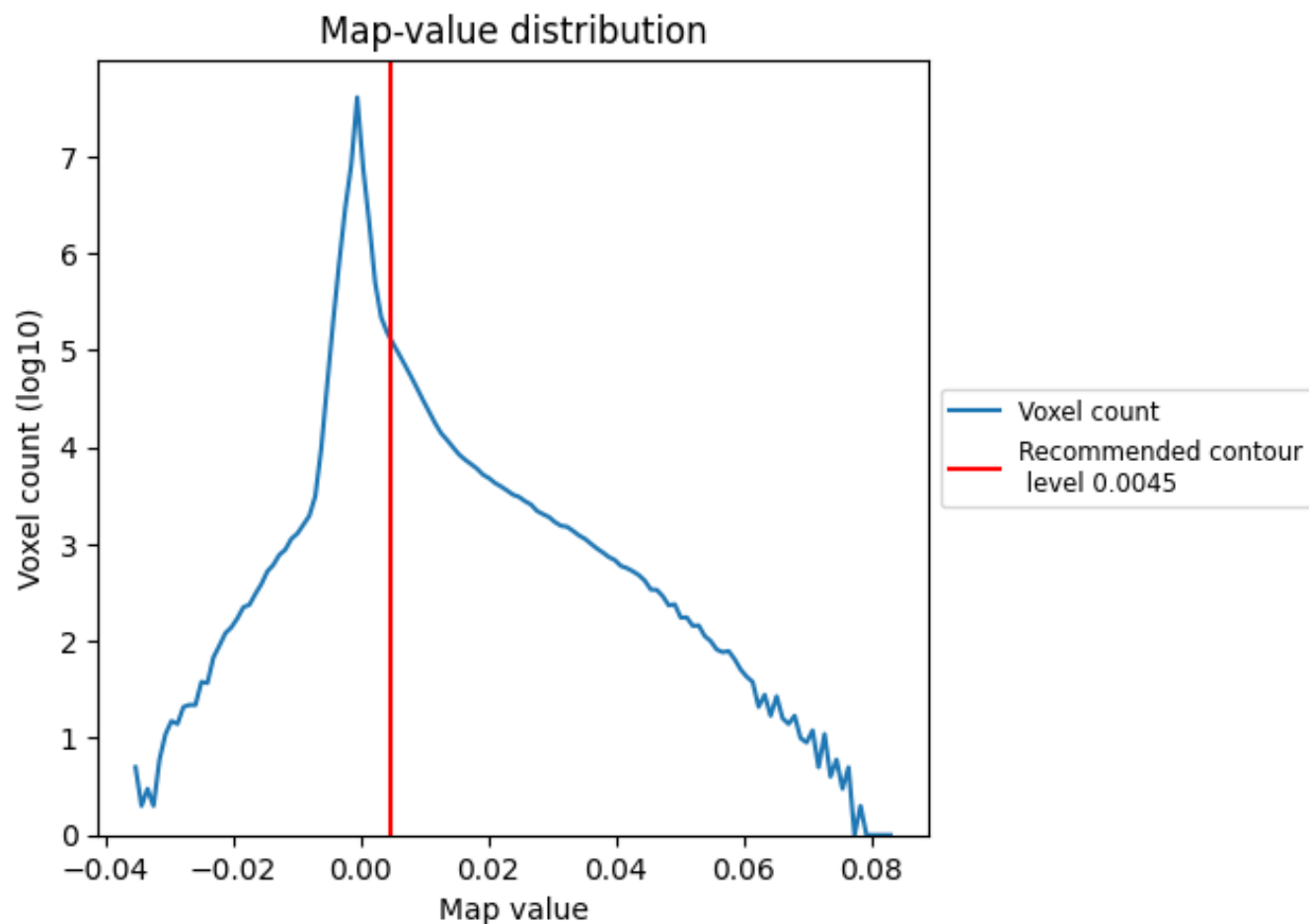
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

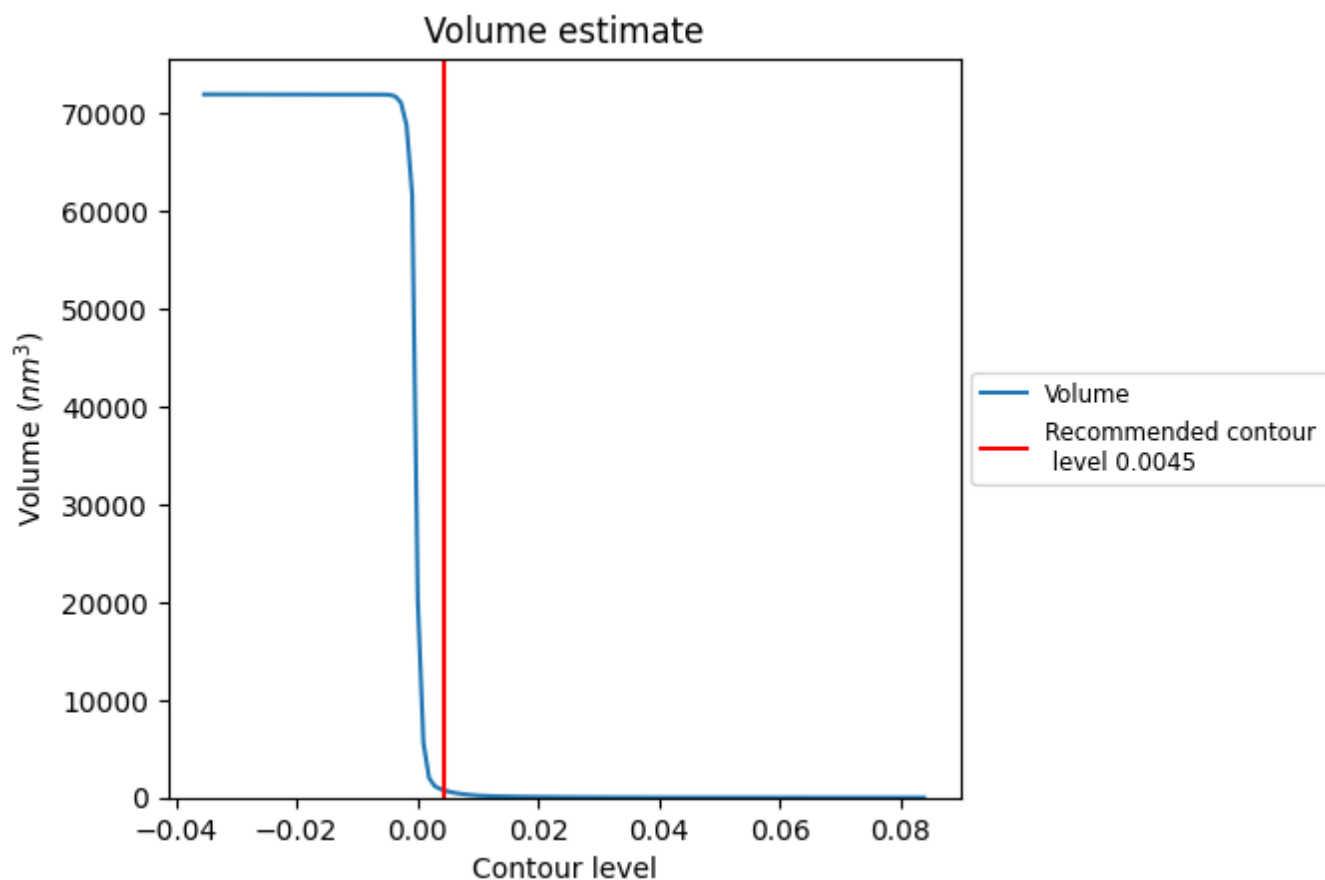
This section contains the results of statistical analysis of the map.

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.

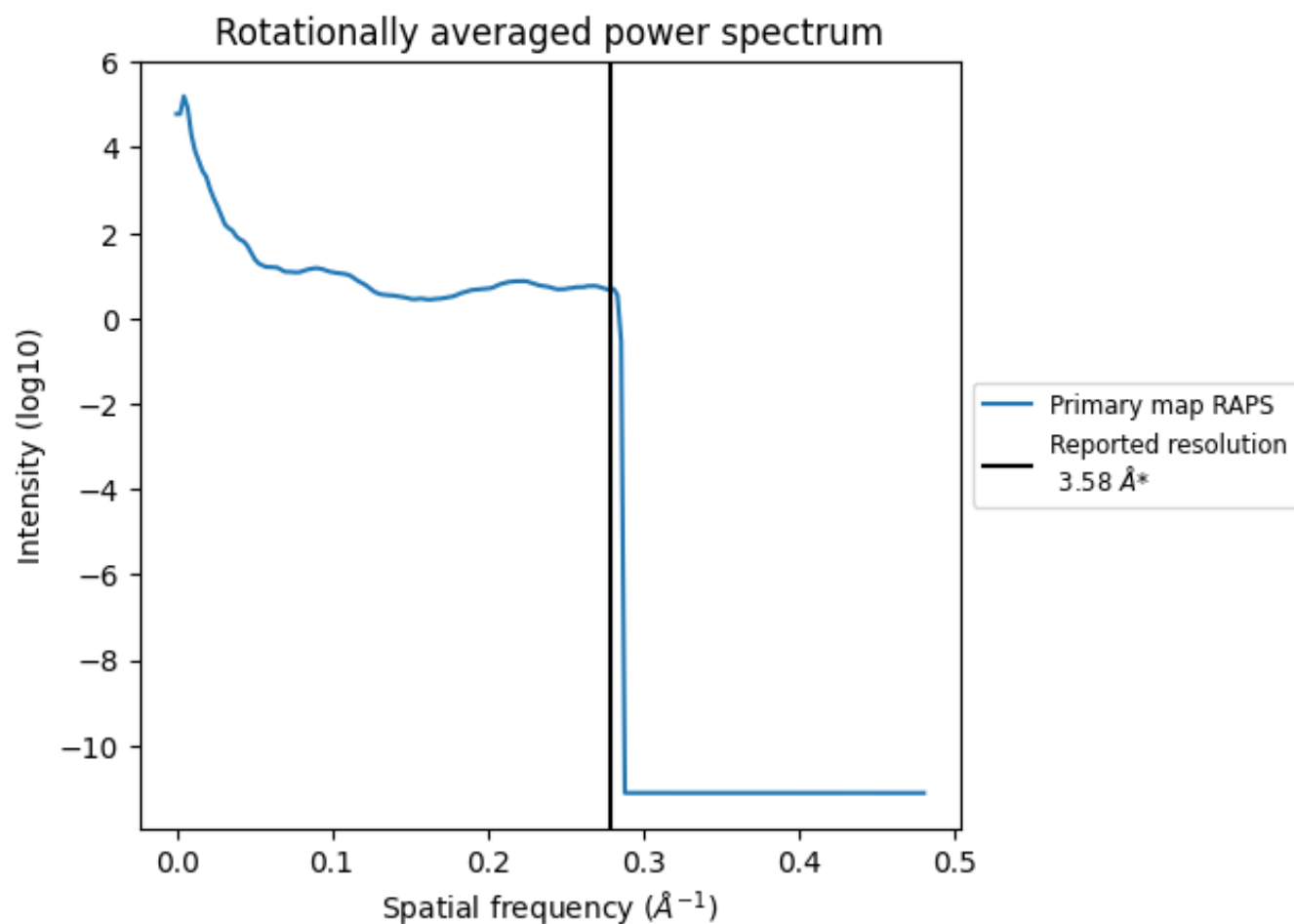
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 742 nm^3 ; this corresponds to an approximate mass of 670 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 0.279 Å⁻¹

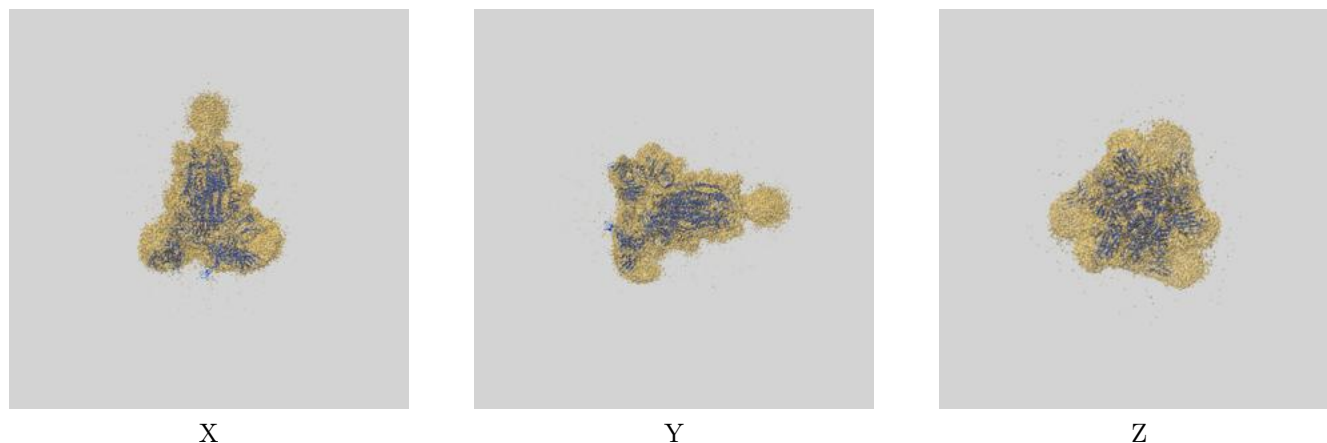
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

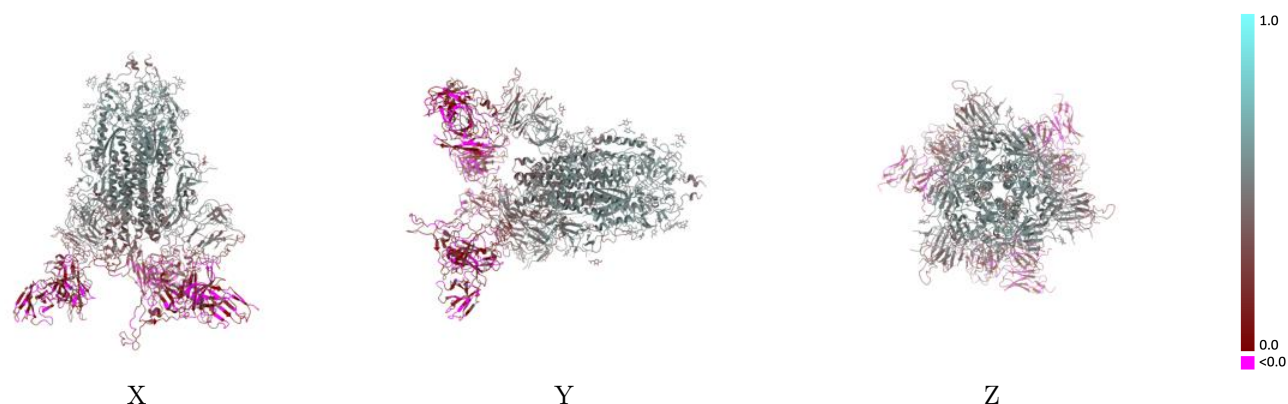
This section contains information regarding the fit between EMDB map EMD-30333 and PDB model 7CAK. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

9.1 Map-model overlay [i](#)



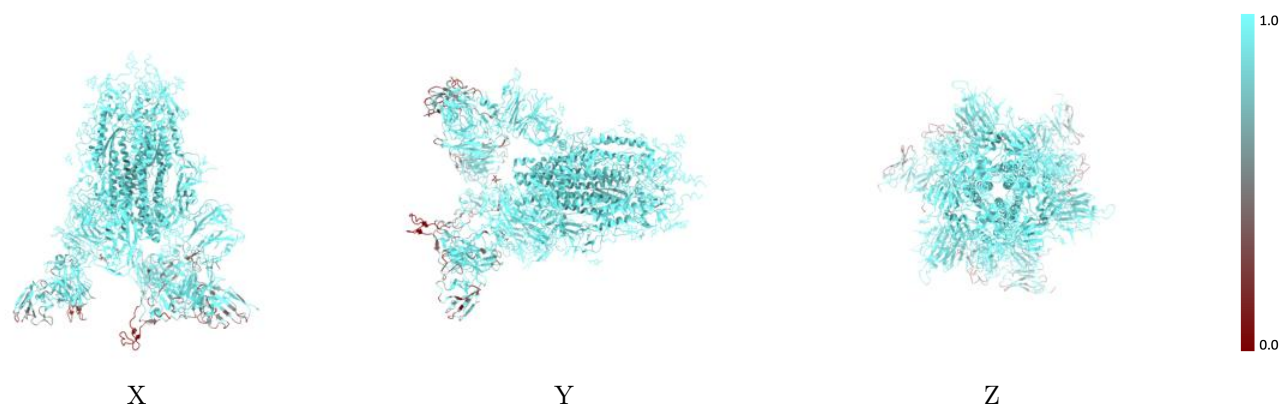
The images above show the 3D surface view of the map at the recommended contour level 0.0045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



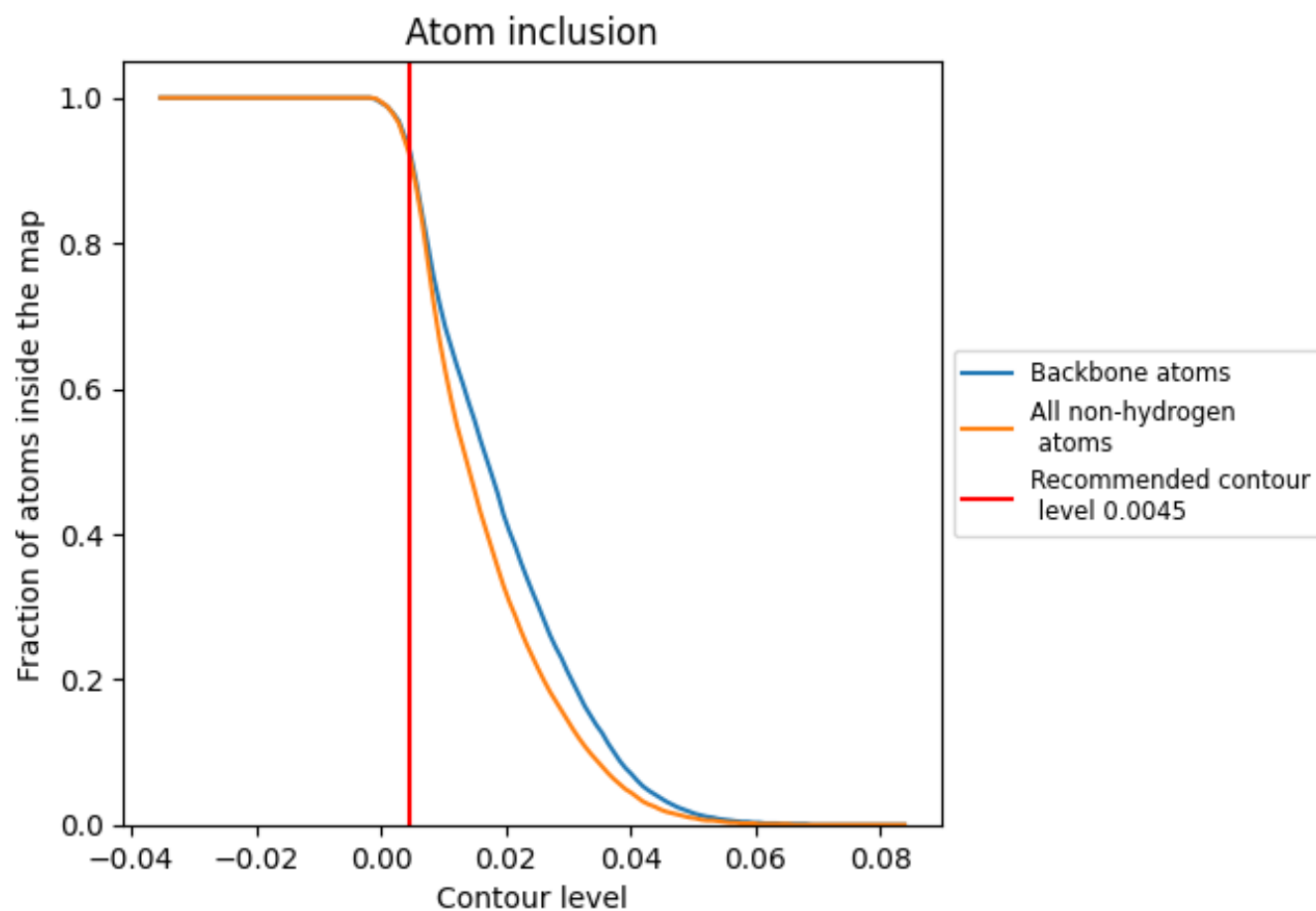
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0045).

9.4 Atom inclusion ⓘ



At the recommended contour level, 93% of all backbone atoms, 92% 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 (0.0045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9250	 0.3620
A	 0.9470	 0.4240
B	 0.9480	 0.4230
C	 0.9480	 0.4230
D	 0.7530	 0.0360
E	 0.8960	 0.0620
F	 0.7350	 0.0980
G	 0.8990	 0.0700
H	 0.7370	 0.0670
I	 0.8990	 0.1020
J	 0.5000	 0.2390
K	 1.0000	 0.5040
L	 1.0000	 0.4490
M	 1.0000	 0.4810
N	 1.0000	 0.4540
O	 0.5000	 0.2330
P	 1.0000	 0.5150
Q	 1.0000	 0.4440
R	 1.0000	 0.4770
S	 1.0000	 0.4570
T	 0.5000	 0.2470
U	 1.0000	 0.4940
V	 1.0000	 0.4460
W	 1.0000	 0.4700
X	 1.0000	 0.4660

