



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 06:53 PM UTC

PDB ID : 7CWN / pdb_00007cwn
EMDB ID : EMD-30484
Title : P17-H014 Fab cocktail in complex with SARS-CoV-2 spike protein
Authors : Wang, N.; Wang, X.
Deposited on : 2020-08-29
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

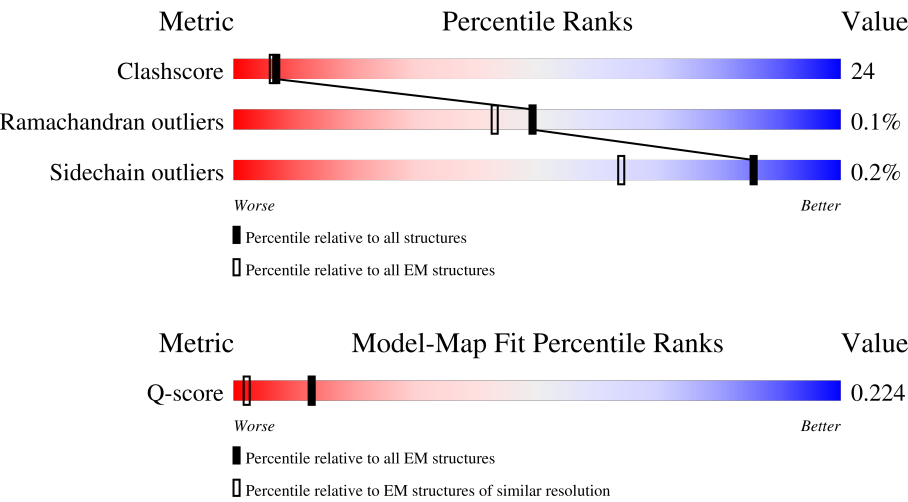
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	1273	
1	B	1273	
1	C	1273	
2	G	213	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	K	213	
2	L	213	
3	F	209	
3	I	209	
3	J	209	
4	D	207	
4	M	207	
4	N	207	
5	E	214	
5	H	214	
5	O	214	
6	P	2	
6	Q	2	
6	R	2	
6	S	2	
6	T	2	
6	U	2	
6	V	2	
6	W	2	
6	X	2	
6	Y	2	
6	Z	2	
6	a	2	
6	b	2	
6	c	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	d	2	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	NAG	Z	1	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 36191 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	1072	Total	C	N	O	S	0	0
			8348	5330	1392	1587	39		
1	B	1070	Total	C	N	O	S	0	0
			8339	5324	1392	1584	39		
1	C	1072	Total	C	N	O	S	0	0
			8351	5330	1395	1587	39		

- Molecule 2 is a protein called heavy chain of P17 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	K	120	Total	C	N	O	S	0	0
			918	574	165	175	4		
2	L	120	Total	C	N	O	S	0	0
			918	574	165	175	4		
2	G	120	Total	C	N	O	S	0	0
			918	574	165	175	4		

- Molecule 3 is a protein called light chain of P17 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	108	Total	C	N	O	S	0	0
			817	511	137	167	2		
3	J	107	Total	C	N	O	S	0	0
			813	509	136	166	2		
3	F	107	Total	C	N	O	S	0	0
			813	509	136	166	2		

- Molecule 4 is a protein called light chain of H014 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	107	Total	C	N	O	S	0	0
			844	540	140	162	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
4	N	107	Total	C	N	O	S	0	0
			844	540	140	162	2		
4	M	107	Total	C	N	O	S	0	0
			844	540	140	162	2		

- Molecule 5 is a protein called heavy chain of H014 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	122	Total	C	N	O	S	0	0
			929	589	147	189	4		
5	H	122	Total	C	N	O	S	0	0
			922	583	147	188	4		
5	O	122	Total	C	N	O	S	0	0
			929	589	147	189	4		

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



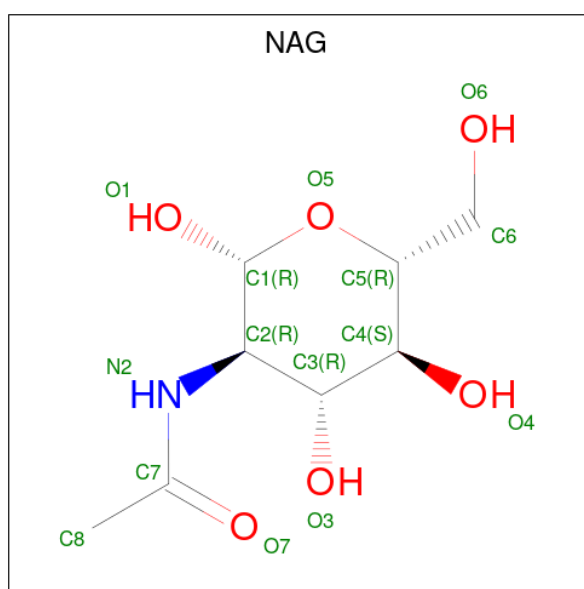
Mol	Chain	Residues	Atoms				AltConf	Trace
6	P	2	Total	C	N	O	0	0
			28	16	2	10		
6	Q	2	Total	C	N	O	0	0
			28	16	2	10		
6	R	2	Total	C	N	O	0	0
			28	16	2	10		
6	S	2	Total	C	N	O	0	0
			28	16	2	10		
6	T	2	Total	C	N	O	0	0
			28	16	2	10		
6	U	2	Total	C	N	O	0	0
			28	16	2	10		
6	V	2	Total	C	N	O	0	0
			28	16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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
6	Y	2	Total	C	N	O	0	0
			28	16	2	10		
6	Z	2	Total	C	N	O	0	0
			28	16	2	10		
6	a	2	Total	C	N	O	0	0
			28	16	2	10		
6	b	2	Total	C	N	O	0	0
			28	16	2	10		
6	c	2	Total	C	N	O	0	0
			28	16	2	10		
6	d	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

Continued on next page...

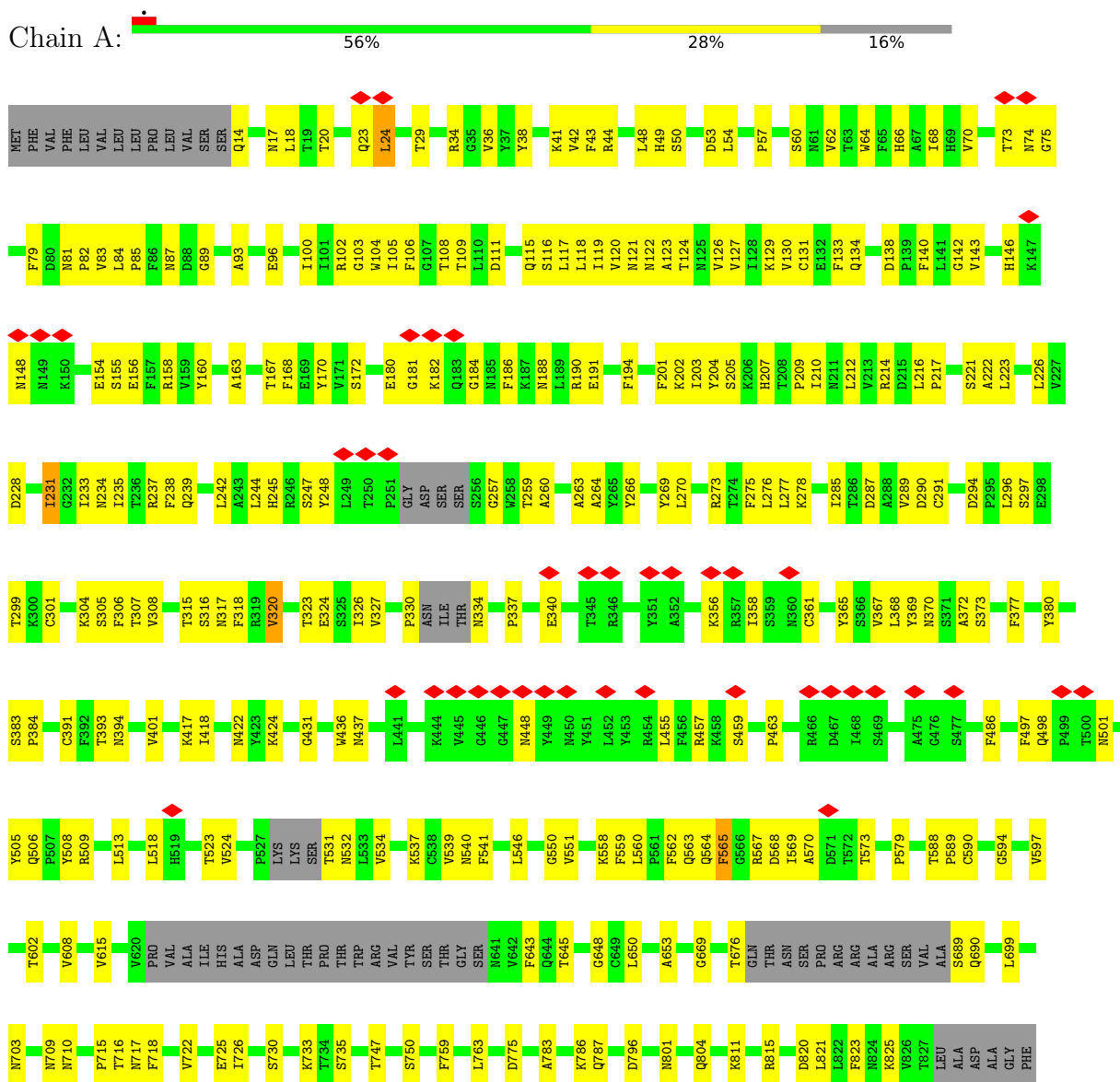
Continued from previous page...

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

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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

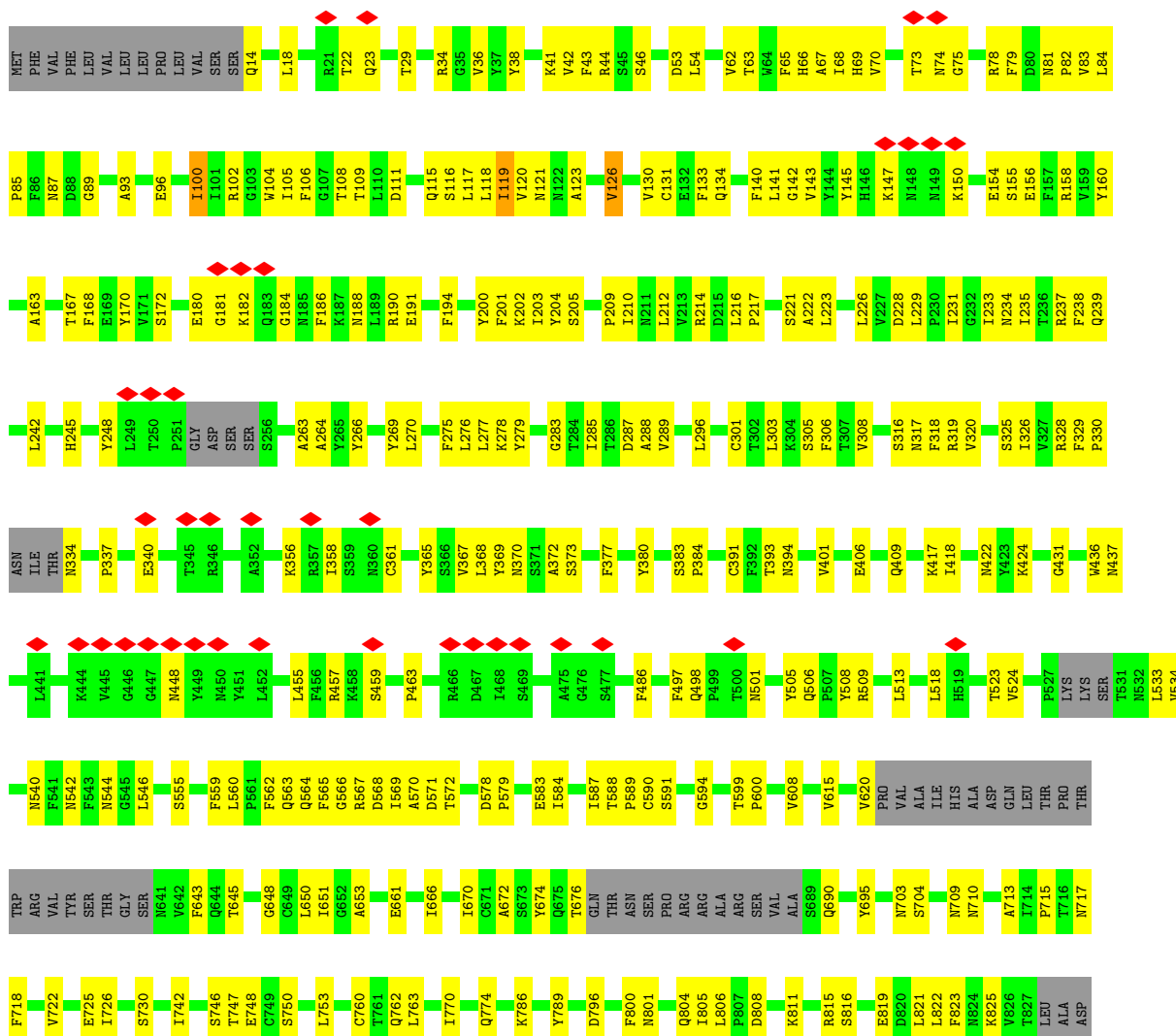


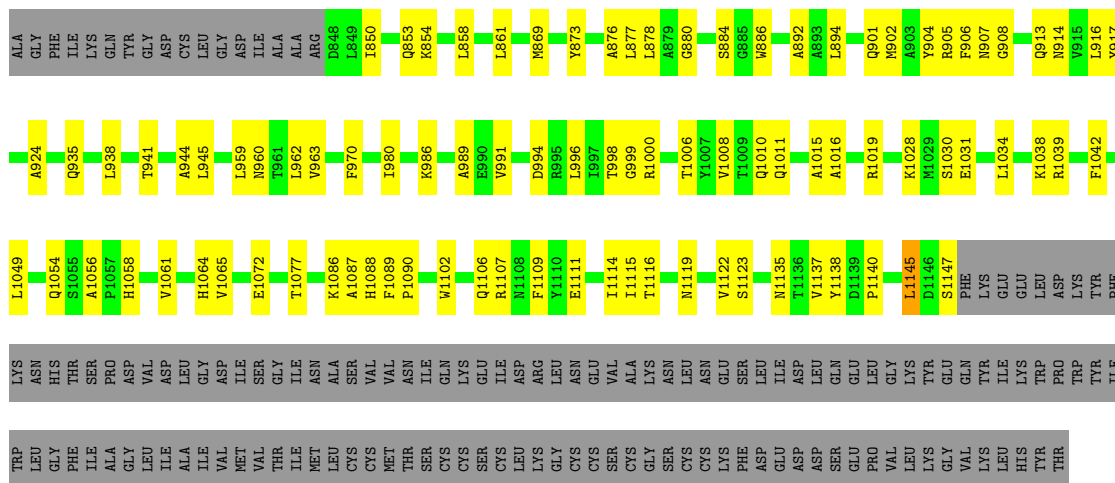
ILE	ASP	H1064	S937	ILE
ALA	LEU	V1065	L938	LYS
ILE	GLY	V1065	S939	GLN
VAL	ASP	E1072		TYR
MET	ILE		L945	GLY
VAL	SER	T1077	G946	ASP
THR	GLY			CYS
ILE	ILE	A1080	D950	LEU
MET	ASN			GLY
LEU	ALA	K1086	N953	ASP
CYS	SER	A1087		ILE
CYS	VAL	H1088	Q957	ALA
MET	VAL	F1089	A958	ALA
THR	ASN	P1090	L959	ARG
SER	ILE	R1091	N960	D848
CYS	GLN	E1092	T961	D849
CYS	LYS	G1093	L962	
SER	GLU		V963	A852
CYS	ILE	R1107	K964	Q853
LEU	ASP		Q965	K854
LYS	ARG	Y1110		F855
GLY	LEU		F970	N856
CYS	ASN	I1115		G857
CYS	GLU	T1116	G999	L858
SER	VAL	T1117	R1000	
CYS	ALA	D1118	L1001	T859
GLY	LYS			
SER	ASN	V1122	T1006	L864
CYS	LEU		Y1007	L865
CYS	ASN	V1129	V1008	M869
LYS	GLU		V1008	
PHE	SER	I1132	T1009	Y873
ASP	LEU		Q1010	T874
GLU	ILE	V1137	R1019	S875
ASP	ASP	Y1138		
LEU	LEU	D1139	M1023	A879
SER	GLN	P1140		
GLU	GLU	L1141	K1028	I882
PRO	LEU	Q1142		
VAL	GLY		E1031	L894
LEU	LYS	L1145	C1032	Q895
LYS	TYR	D1146		
GLY	GLU	S1147	K1038	F898
VAL	GLN	PHE	R1039	
LYS	TYR	LYS	F1042	Q901
LEU	ILE	GLU		N902
LYS	LYS	GLU		
TYR	TRP	LEU		
THR	PRO	ASP		R905
	TRP	LEU	H1048	F906
	TRP	LYS	L1049	N907
	ILE	PHE	F1052	G908
	TRP	LYS	P1053	
	LEU	ASN	Q1054	N914
	GLY	HIS		V915
	PHE	THR	P1057	L916
	ILE	SER	H1058	
	ALA	PRO	V1061	F927
	GLY	ASP	F1062	Q935
	LEU	VAL	L1062	D936

• Molecule 1: Spike glycoprotein

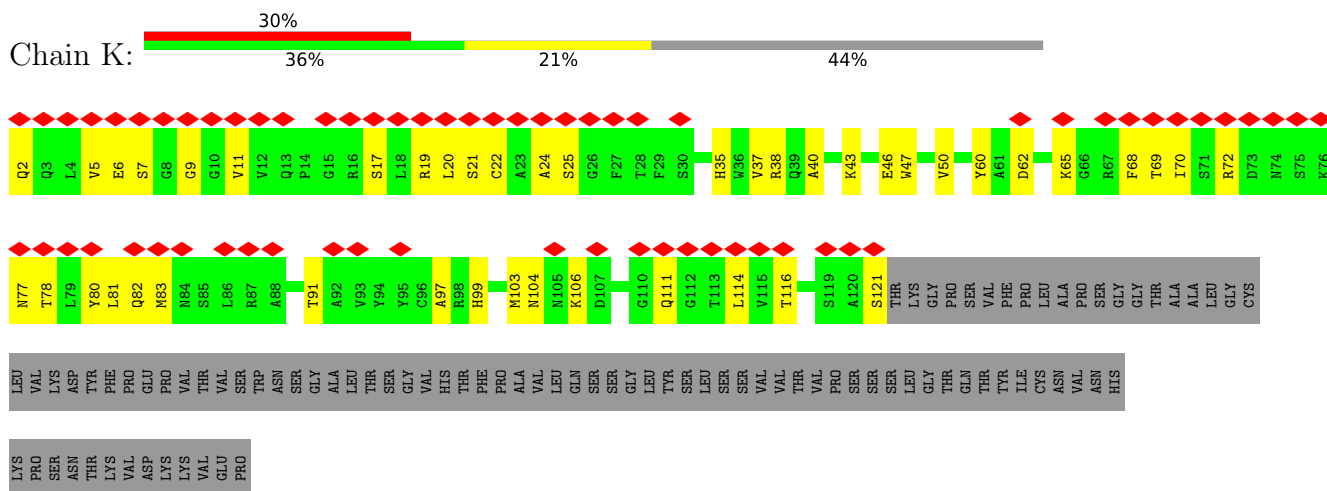


N709	V597	N606	V615	V620	T531	N532	V534	ALA	ILE	HIS	ASP	GLU	LEU	THR	PRO	TRP	ARG	VAL	TYR	SER	THR	SER	GLY	SER	N641	F643	Q644	T645	G648	C649	L650	A653	G669	T676	GLN	THR	ASN	SER	PRO	D820	L821	F823	N824	K825	V826	T827	ALA	LEU	ASP	ALA	GLY
N710	G526	PRO	LYS	SER	T531	N532	V534	ALA	ILE	HIS	ASP	GLU	LEU	THR	PRO	TRP	ARG	VAL	TYR	SER	THR	SER	GLY	SER	N641	F643	Q644	T645	G648	C649	L650	A653	G669	T676	GLN	THR	ASN	SER	PRO	D820	L821	F823	N824	K825	V826	T827	ALA	LEU	ASP	ALA	GLY
A713	N597	N606	V615	V620	T531	N532	V534	ALA	ILE	HIS	ASP	GLU	LEU	THR	PRO	TRP	ARG	VAL	TYR	SER	THR	SER	GLY	SER	N641	F643	Q644	T645	G648	C649	L650	A653	G669	T676	GLN	THR	ASN	SER	PRO	D820	L821	F823	N824	K825	V826	T827	ALA	LEU	ASP	ALA	GLY
P715	G526	PRO	LYS	SER	T531	N532	V534	ALA	ILE	HIS	ASP	GLU	LEU	THR	PRO	TRP	ARG	VAL	TYR	SER	THR	SER	GLY	SER	N641	F643	Q644	T645	G648	C649	L650	A653	G669	T676	GLN	THR	ASN	SER	PRO	D820	L821	F823	N824	K825	V826	T827	ALA	LEU	ASP	ALA	GLY
T716	G526	PRO	LYS	SER	T531	N532	V534	ALA	ILE	HIS	ASP	GLU	LEU	THR	PRO	TRP	ARG	VAL	TYR	SER	THR	SER	GLY	SER	N641	F643	Q644	T645	G648	C649	L650	A653	G669	T676	GLN	THR	ASN	SER	PRO	D820	L821	F823	N824	K825	V826	T827	ALA	LEU	ASP	ALA	GLY
F718	G526	PRO	LYS	SER	T531	N532	V534	ALA	ILE	HIS	ASP	GLU	LEU	THR	PRO	TRP	ARG	VAL	TYR	SER	THR	SER	GLY	SER	N641	F643	Q644	T645	G648	C649	L650	A653	G669	T676	GLN	THR	ASN	SER	PRO	D820	L821	F823	N824	K825	V826	T827	ALA	LEU	ASP	ALA	GLY
V722	G526	PRO	LYS	SER	T531	N532	V534	ALA	ILE	HIS	ASP	GLU	LEU	THR	PRO	TRP	ARG	VAL	TYR	SER	THR	SER	GLY	SER	N641	F643	Q644	T645	G648	C649	L650	A653	G669	T676	GLN	THR	ASN	SER	PRO	D820	L821	F823	N824	K825	V826	T827	ALA	LEU	ASP	ALA	GLY
E725	G526	PRO	LYS	SER	T531	N532	V534	ALA	ILE	HIS	ASP	GLU	LEU	THR	PRO	TRP	ARG	VAL	TYR	SER	THR	SER	GLY	SER	N641	F643	Q644	T645	G648	C649	L650	A653	G669	T676	GLN	THR	ASN	SER	PRO	D820	L821	F823	N824	K825	V826	T827	ALA	LEU	ASP	ALA	GLY
I726	G526	PRO	LYS	SER	T531	N532	V534	ALA	ILE	HIS	ASP	GLU	LEU	THR	PRO	TRP	ARG	VAL	TYR	SER	THR	SER	GLY	SER	N641	F643	Q644	T645	G648	C649	L650	A653	G669	T676	GLN	THR	ASN	SER	PRO	D820	L821	F823	N824	K825	V826	T827	ALA	LEU	ASP	ALA	GLY
K733	G526	PRO	LYS	SER	T531	N532	V534	ALA	ILE	HIS	ASP	GLU	LEU	THR	PRO	TRP	ARG	VAL	TYR	SER	THR	SER	GLY	SER	N641	F643	Q644	T645	G648	C649	L650	A653	G669	T676	GLN	THR	ASN	SER	PRO	D820	L821	F823	N824	K825	V826	T827	ALA	LEU	ASP	ALA	GLY
T734	G526	PRO	LYS	SER	T531	N532	V534	ALA	ILE	HIS	ASP	GLU	LEU	THR	PRO	TRP	ARG	VAL	TYR	SER	THR	SER	GLY	SER	N641	F643	Q644	T645	G648	C649	L650	A653	G669	T676	GLN	THR	ASN	SER	PRO	D820	L821	F823	N824	K825	V826	T827	ALA	LEU	ASP	ALA	GLY
S735	G526	PRO	LYS	SER	T531	N532	V534	ALA	ILE	HIS	ASP	GLU	LEU	THR	PRO	TRP	ARG	VAL	TYR	SER	THR	SER	GLY	SER	N641	F643	Q644	T645	G648	C649	L650	A653	G669	T676	GLN	THR	ASN	SER	PRO	D820	L821	F823	N824	K825	V826	T827	ALA	LEU	ASP	ALA	GLY
D745	G526	PRO	LYS	SER	T531	N532	V534	ALA	ILE	HIS	ASP	GLU	LEU	THR	PRO	TRP	ARG	VAL	TYR	SER	THR	SER	GLY	SER	N641	F643	Q644	T645	G648	C649	L650	A653	G669	T676	GLN	THR	ASN	SER	PRO	D820	L821	F823	N824	K825	V826	T827	ALA	LEU	ASP	ALA	GLY
S746	G526	PRO	LYS	SER	T531	N532	V534	ALA	ILE	HIS	ASP	GLU	LEU	THR	PRO	TRP	ARG	VAL	TYR	SER	THR	SER	GLY	SER	N641	F643	Q644	T645	G648	C649	L650	A653	G669	T676	GLN	THR	ASN	SER	PRO	D820	L821	F823	N824	K825	V826	T827	ALA	LEU	ASP	ALA	GLY
T747	G526	PRO	LYS	SER	T531	N532	V534	ALA	ILE	HIS	ASP	GLU	LEU	THR	PRO	TRP	ARG	VAL	TYR	SER	THR	SER	GLY	SER	N641	F643	Q644	T645	G648	C649	L650	A653	G669	T676	GLN	THR	ASN	SER	PRO	D820	L821	F823	N824	K825	V826	T827	ALA	LEU	ASP	ALA	GLY
S750	G526	PRO	LYS	SER	T531	N532	V534	ALA	ILE	HIS	ASP	GLU	LEU	THR	PRO	TRP	ARG	VAL	TYR	SER	THR	SER	GLY	SER	N641	F643	Q644	T645	G648	C649	L650	A653	G669	T676	GLN	THR	ASN	SER	PRO	D820	L821	F823	N824	K825	V826	T827	ALA	LEU	ASP	ALA	GLY
F759	G526	PRO	LYS	SER	T531	N532	V534	ALA	ILE	HIS	ASP	GLU	LEU	THR	PRO	TRP	ARG	VAL	TYR	SER	THR	SER	GLY	SER	N641	F643	Q644	T645	G648	C649	L650	A653	G669	T676	GLN	THR	ASN	SER	PRO	D820	L821	F823	N824	K825	V826	T827	ALA	LEU	ASP	ALA	GLY
L763	G526	PRO	LYS	SER	T531	N532	V534	ALA	ILE	HIS	ASP	GLU	LEU	THR	PRO	TRP	ARG	VAL	TYR	SER	THR	SER	GLY	SER	N641	F643	Q644	T645	G648	C649	L650	A653	G669	T676	GLN	THR	ASN	SER	PRO	D820	L821	F823	N824	K825	V826	T827	ALA	LEU	ASP	ALA	GLY
D775	G526	PRO	LYS	SER	T531	N532	V534	ALA	ILE	HIS	ASP	GLU	LEU	THR	PRO	TRP	ARG	VAL	TYR	SER	THR	SER	GLY	SER	N641	F643	Q644	T645	G648	C649	L650	A653	G669	T676	GLN	THR	ASN	SER	PRO	D820	L821	F823	N824	K825	V826	T827	ALA	LEU	ASP	ALA	GLY
A783	G526	PRO	LYS	SER	T531	N532	V534	ALA	ILE	HIS	ASP	GLU	LEU	THR	PRO	TRP	ARG	VAL	TYR	SER	THR	SER	GLY	SER	N641	F643	Q644	T645	G648	C649	L650	A653	G669	T676	GLN	THR	ASN	SER	PRO	D820	L821	F823	N824	K825	V826	T827	ALA	LEU	ASP	ALA	GLY
K786	G526	PRO	LYS	SER	T531	N532	V534	ALA	ILE	HIS	ASP	GLU	LEU	THR	PRO	TRP	ARG	VAL	TYR	SER	THR	SER	GLY	SER	N641	F643	Q644	T645	G648	C649	L650	A653	G669	T676	GLN	THR	ASN	SER	PRO	D820	L821	F823	N824	K825	V826	T827	ALA	LEU	ASP	ALA	GLY
Q787	G526	PRO	LYS	SER	T531	N532	V534	ALA	ILE	HIS	ASP	GLU	LEU	THR	PRO	TRP	ARG	VAL	TYR	SER	THR	SER	GLY	SER	N641	F643	Q644	T645	G648	C649	L650	A653	G669	T676	GLN	THR	ASN	SER	PRO	D820	L821	F823	N824	K825	V826	T827	ALA	LEU	ASP	ALA	GLY
D796	G526	PRO	LYS	SER	T531	N532	V534	ALA	ILE	HIS	ASP	GLU	LEU	THR	PRO	TRP	ARG	VAL	TYR	SER	THR	SER	GLY	SER	N641	F643	Q644	T645	G648	C649	L650	A653	G669	T676	GLN	THR	ASN	SER	PRO	D820	L821	F823	N824	K825	V826	T827	ALA	LEU	ASP	ALA	GLY
F800	G526	PRO	LYS	SER	T531	N532	V534	ALA	ILE	HIS	ASP	GLU	LEU	THR	PRO	TRP	ARG	VAL	TYR	SER	THR	SER	GLY	SER	N641	F643	Q644	T645	G648	C649	L650	A653	G669	T676	GLN	THR	ASN	SER	PRO	D820	L821	F823	N824	K825	V826	T827	ALA	LEU	ASP	ALA	GLY
N801	G526	PRO	LYS	SER	T531	N532	V534	ALA	ILE	HIS	ASP	GLU	LEU	THR	PRO	TRP	ARG	VAL	TYR	SER	THR	SER	GLY	SER	N641	F643	Q644	T645	G648	C649	L650	A653	G669	T676	GLN	THR	ASN	SER	PRO	D820	L821	F823	N824	K825	V826	T827	ALA	LEU	ASP	ALA	GLY
Q804	G526	PRO	LYS	SER	T531	N532	V534	ALA	ILE	HIS	ASP	GLU	LEU	THR	PRO	TRP	ARG	VAL	TYR	SER	THR	SER	GLY	SER	N641	F643	Q644	T645	G648	C649	L650	A653	G669	T676	GLN	THR	ASN	SER	PRO	D820	L821	F823	N824	K825	V826	T827	ALA	LEU	ASP	ALA	GLY
K811	G526	PRO	LYS	SER	T531	N532	V534	ALA	ILE	HIS	ASP	GLU	LEU	THR	PRO	TRP	ARG	VAL	TYR	SER	THR	SER	GLY	SER	N641	F643	Q644	T645	G648	C649	L650	A653	G669	T676	GLN	THR	ASN	SER	PRO	D820	L821	F823	N824	K825	V826	T827	ALA	LEU	ASP	ALA	GLY
R815	G526	PRO	LYS	SER	T531	N532	V534	ALA	ILE	HIS	ASP	GLU	LEU	THR	PRO	TRP	ARG	VAL	TYR	SER	THR	SER	GLY	SER	N641	F643	Q644	T645	G648	C649	L650	A653	G669	T676	GLN	THR	ASN	SER	PRO	D820	L821	F823	N824	K825	V826	T827	ALA	LEU	ASP	ALA	GLY
D820	G526	PRO	LYS	SER	T531	N532	V534	ALA	ILE	HIS	ASP	GLU	LEU	THR	PRO	TRP	ARG	VAL	TYR	SER	THR	SER	GLY	SER	N641	F643	Q644	T645	G648	C649	L650	A653	G669	T676	GLN	THR	ASN	SER	PRO	D820	L821	F823	N824	K825	V826	T827	ALA	LEU	ASP	ALA	GLY
L821	G526	PRO	LYS	SER	T531	N532	V534	ALA	ILE	HIS	ASP	GLU	LEU	THR	PRO	TRP	ARG	VAL	TYR	SER	THR	SER	GLY	SER	N641	F643	Q644	T645	G648	C649	L650	A653	G669	T676	GLN	THR	ASN	SER	PRO	D820	L821	F823	N824	K825	V826	T827	ALA	LEU	ASP	ALA	GLY
F823	G526	PRO	LYS	SER	T531	N532	V534	ALA	ILE	HIS	ASP	GLU	LEU	THR	PRO	TRP	ARG	VAL	TYR	SER	THR	SER	GLY	SER	N641	F643	Q644	T645	G648	C649	L650	A653	G669	T676	GLN	THR	ASN	SER	PRO	D820	L821	F823	N824	K825	V826	T827	ALA	LEU	ASP	ALA	GLY
N824	G526	PRO	LYS	SER	T531	N532	V534	ALA	ILE	HIS	ASP	GLU	LEU	THR	PRO	TRP	ARG	VAL	TYR	SER	THR	SER	GLY	SER	N641	F643	Q644	T645	G648	C649	L650	A653	G669	T676	GLN	THR	ASN	SER	PRO	D820	L821	F823	N824	K825	V826	T827	ALA	LEU	ASP	ALA	GLY
K825	G526	PRO	LYS	SER	T531	N532	V534	ALA	ILE	HIS	ASP	GLU	LEU	THR	PRO	TRP	ARG	VAL	TYR	SER	THR	SER	GLY	SER	N641	F643	Q644	T645	G648	C649	L650	A653	G669	T676	GLN	THR	ASN	SER	PRO	D820	L821	F823	N824	K825	V826	T827	ALA	LEU	ASP	ALA	GLY
V826	G526	PRO	LYS	SER	T531	N532	V534	ALA	ILE	HIS	ASP	GLU	LEU	THR	PRO	TRP	ARG	VAL	TYR	SER	THR	SER	GLY	SER	N641	F643	Q644																								

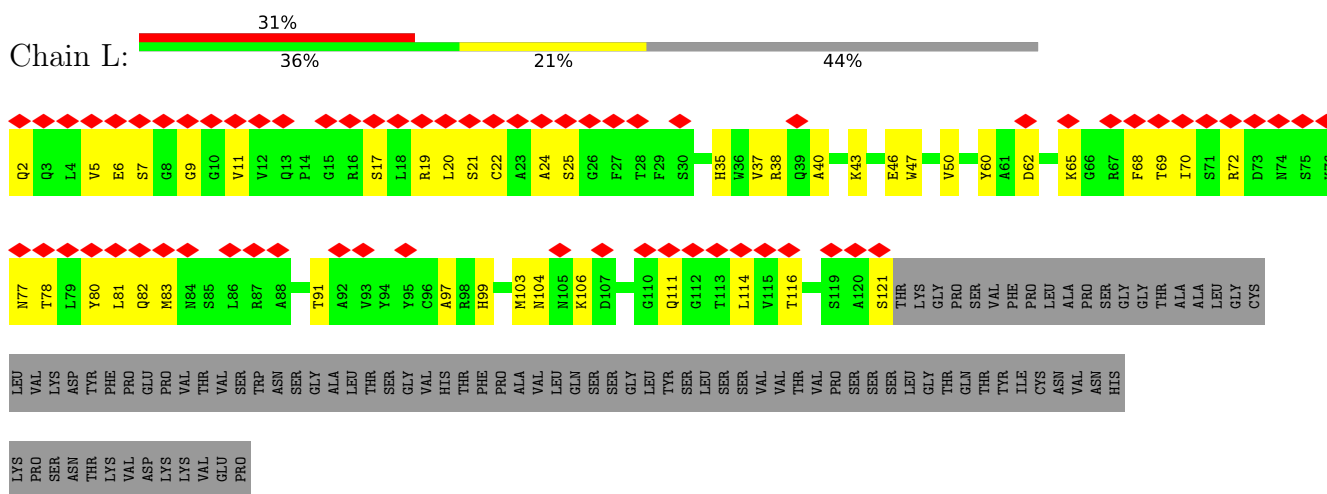




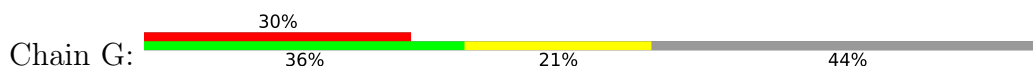
- Molecule 2: heavy chain of P17 Fab

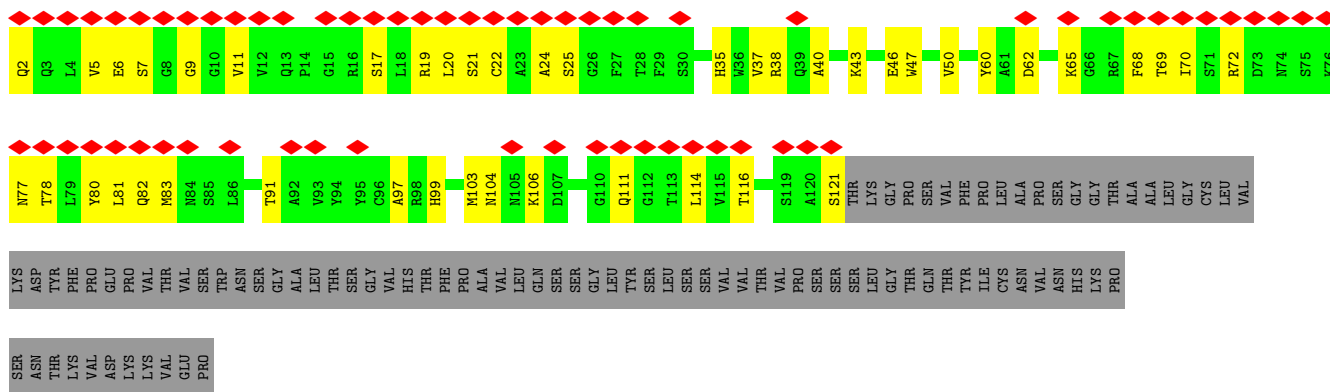


- Molecule 2: heavy chain of P17 Fab

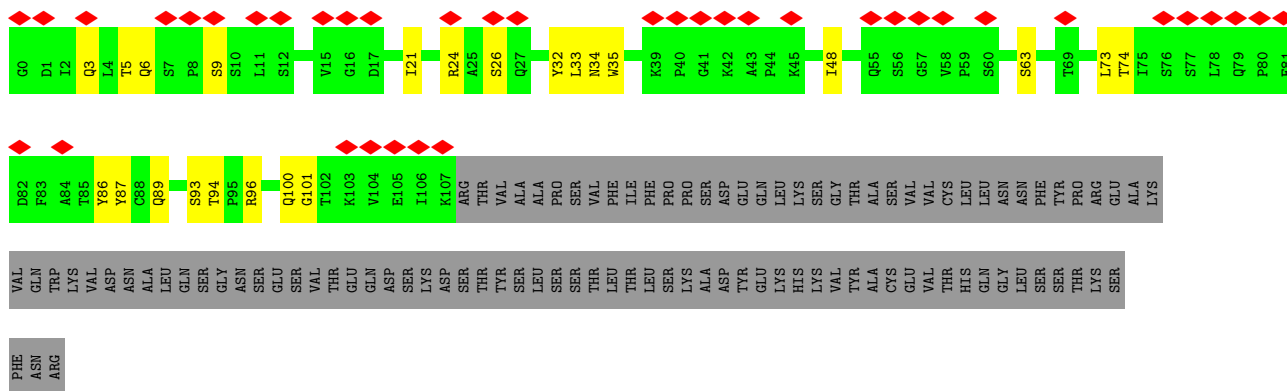


- Molecule 2: heavy chain of P17 Fab

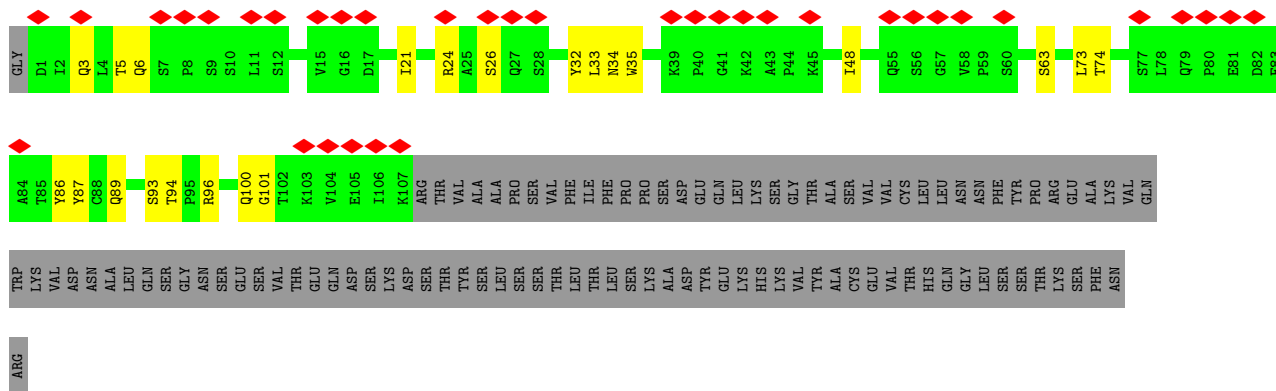
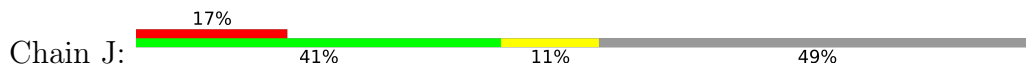




- Molecule 3: light chain of P17 Fab

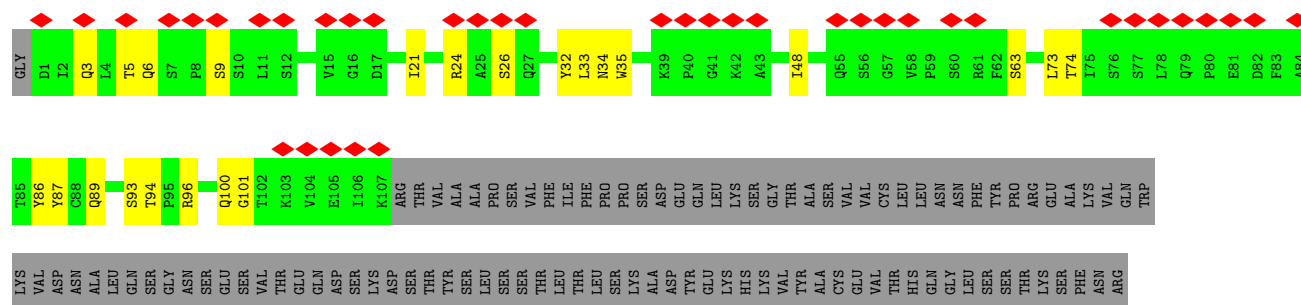


- Molecule 3: light chain of P17 Fab

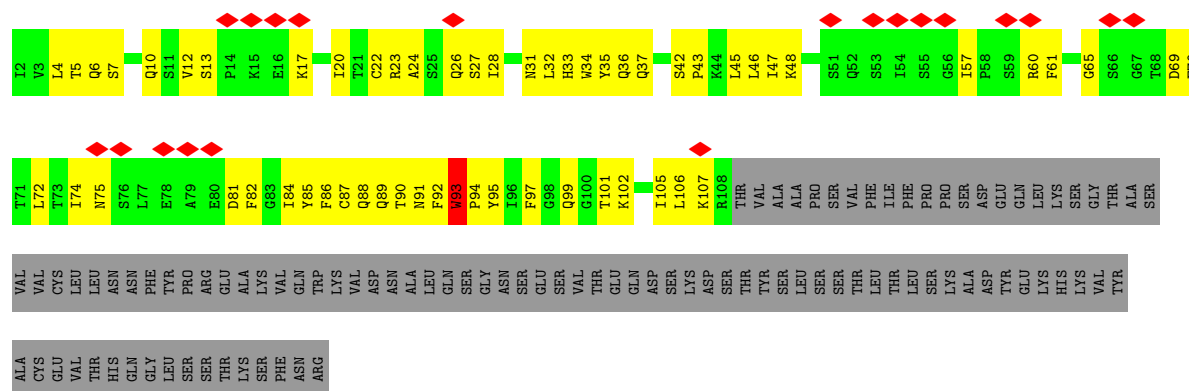
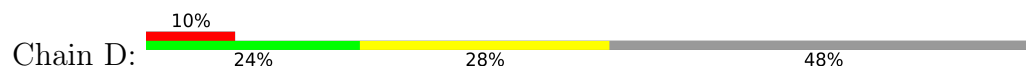


- Molecule 3: light chain of P17 Fab

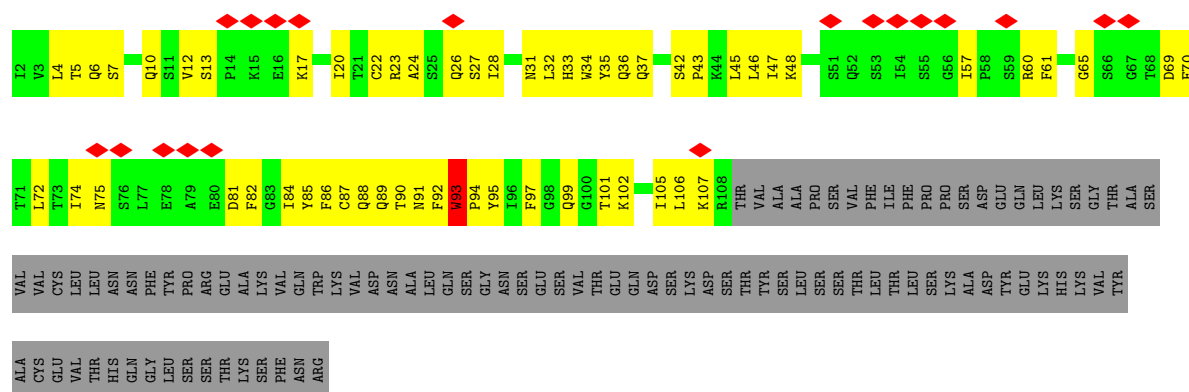
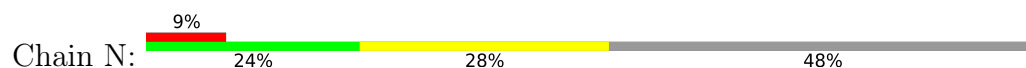




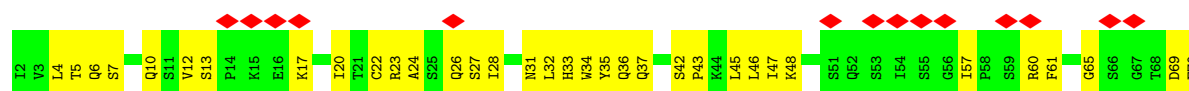
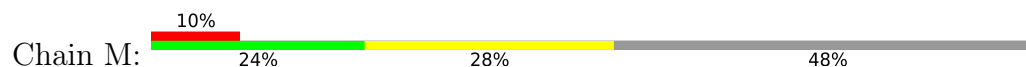
• Molecule 4: light chain of H014 Fab



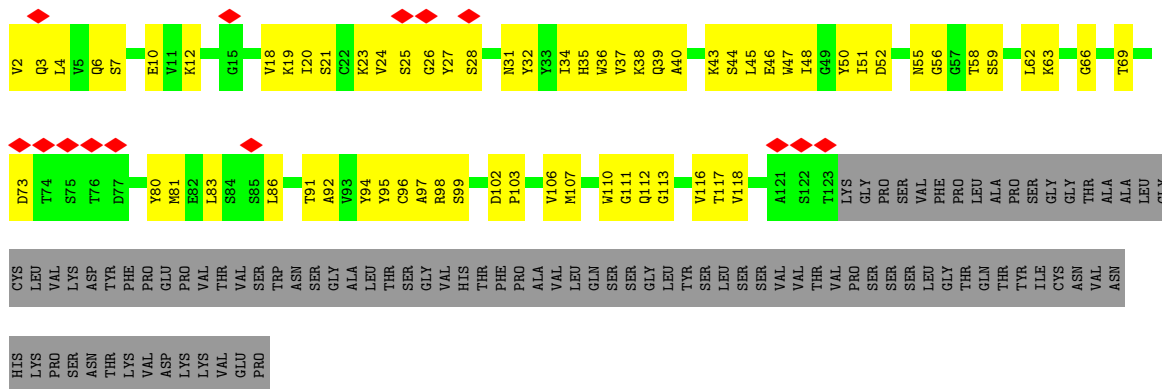
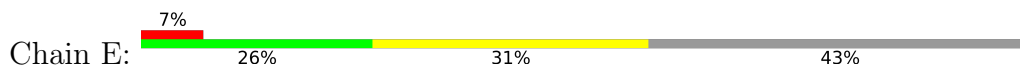
• Molecule 4: light chain of H014 Fab



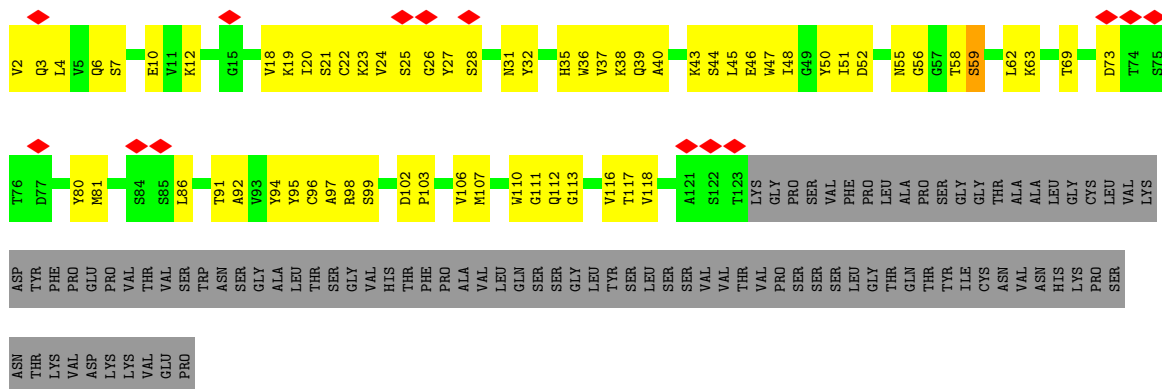
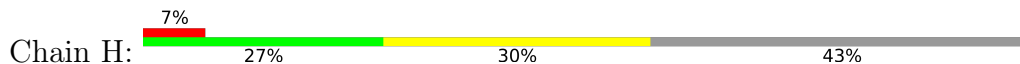
• Molecule 4: light chain of H014 Fab



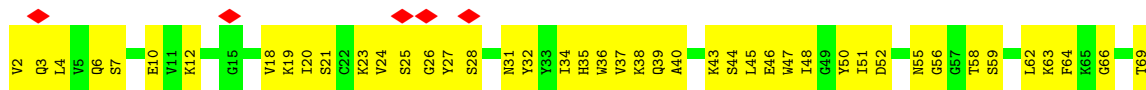
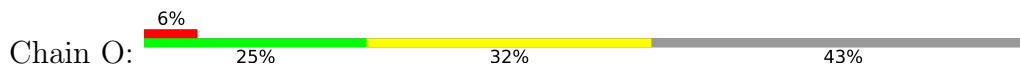
- Molecule 5: heavy chain of H014 Fab

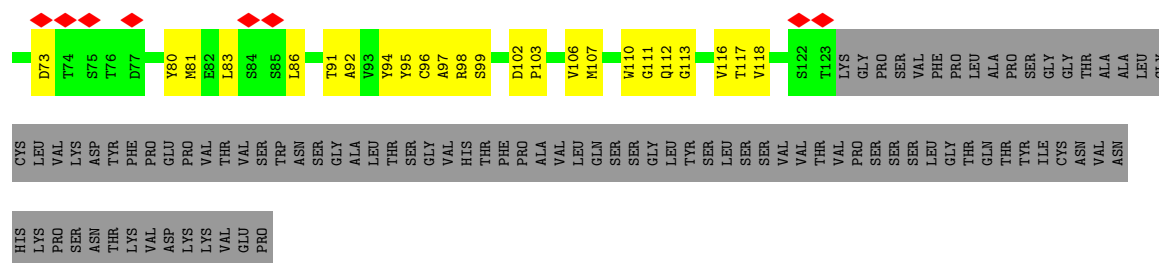


- Molecule 5: heavy chain of H014 Fab



- Molecule 5: heavy chain of H014 Fab





- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:  50% 50%



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:  100%



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:  50% 100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	175063	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	0.058	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00538	Depositor
Map size (Å)	416.0, 416.0, 416.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.44	0/8539	0.66	4/11622 (0.0%)
1	B	0.46	0/8529	0.70	5/11606 (0.0%)
1	C	0.49	0/8542	0.72	3/11625 (0.0%)
2	G	0.32	0/937	0.64	0/1269
2	K	0.32	0/937	0.64	0/1269
2	L	0.32	0/937	0.64	0/1269
3	F	0.33	0/830	0.63	0/1126
3	I	0.33	0/834	0.63	0/1131
3	J	0.33	0/830	0.63	0/1126
4	D	0.53	0/865	0.88	2/1171 (0.2%)
4	M	0.53	0/865	0.88	2/1171 (0.2%)
4	N	0.54	0/865	0.88	2/1171 (0.2%)
5	E	0.54	0/952	0.84	0/1298
5	H	0.54	0/944	0.84	1/1287 (0.1%)
5	O	0.54	0/952	0.84	0/1298
All	All	0.46	0/36358	0.71	19/49439 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	5
1	C	0	3
2	G	0	1
2	K	0	1
2	L	0	1
All	All	0	15

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	100	ILE	N-CA-C	-10.82	102.81	113.20
1	C	100	ILE	N-CA-C	-10.78	102.85	113.20
1	A	301	CYS	N-CA-C	-8.72	102.41	113.23
4	M	93	TRP	CB-CA-C	6.99	123.93	110.17
4	N	93	TRP	CB-CA-C	6.99	123.93	110.17
4	D	93	TRP	CB-CA-C	6.97	123.91	110.17
4	D	93	TRP	CA-CB-CG	6.22	125.42	113.60
4	M	93	TRP	CA-CB-CG	6.20	125.38	113.60
4	N	93	TRP	CA-CB-CG	6.17	125.33	113.60
1	B	283	GLY	CA-C-O	-6.07	116.31	122.56
1	B	849	LEU	N-CA-C	-5.69	106.10	113.16
1	A	849	LEU	N-CA-C	-5.65	106.15	113.16
1	A	320	VAL	N-CA-C	-5.37	100.63	109.12
1	A	231	ILE	N-CA-C	-5.33	106.97	111.56
1	C	119	ILE	CA-C-O	-5.24	118.07	122.63
1	C	329	PHE	CB-CA-C	5.05	117.40	109.27
1	B	231	ILE	N-CA-C	-5.04	107.22	111.56
1	B	122	ASN	N-CA-C	-5.04	107.49	113.38
5	H	59	SER	N-CA-C	-5.01	100.34	109.56

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1145	LEU	Peptide
1	A	248	TYR	Peptide
1	A	391	CYS	Peptide
1	A	565	PHE	Peptide
1	B	1145	LEU	Peptide
1	B	248	TYR	Peptide
1	B	278	LYS	Mainchain
1	B	391	CYS	Peptide
1	B	565	PHE	Peptide
1	C	1145	LEU	Peptide
1	C	248	TYR	Peptide
1	C	391	CYS	Peptide
2	G	72	ARG	Peptide
2	K	72	ARG	Peptide
2	L	72	ARG	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	8348	0	8120	437	0
1	B	8339	0	8119	403	0
1	C	8351	0	8123	429	0
2	G	918	0	885	27	0
2	K	918	0	885	27	0
2	L	918	0	885	28	0
3	F	813	0	797	17	0
3	I	817	0	800	17	0
3	J	813	0	797	15	0
4	D	844	0	827	116	0
4	M	844	0	827	117	0
4	N	844	0	827	116	0
5	E	929	0	873	81	0
5	H	922	0	866	80	0
5	O	929	0	873	83	0
6	P	28	0	25	1	0
6	Q	28	0	25	0	0
6	R	28	0	25	1	0
6	S	28	0	25	0	0
6	T	28	0	25	0	0
6	U	28	0	25	1	0
6	V	28	0	25	0	0
6	W	28	0	25	1	0
6	X	28	0	25	0	0
6	Y	28	0	25	2	0
6	Z	28	0	25	7	0
6	a	28	0	25	0	0
6	b	28	0	25	1	0
6	c	28	0	25	0	0
6	d	28	0	25	5	0
7	A	84	0	78	1	0
7	B	70	0	65	1	0
7	C	70	0	65	0	0
All	All	36191	0	35087	1706	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 24.

All (1706) 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:C:234:ASN:HD22	6:Z:1:NAG:C1	1.10	1.63
1:A:276:LEU:HD11	1:A:306:PHE:CE1	1.32	1.59
1:C:22:THR:CG2	1:C:78:ARG:HD2	1.28	1.58
1:C:63:THR:HG21	1:C:65:PHE:CZ	1.36	1.57
1:A:234:ASN:HD22	6:P:1:NAG:C1	1.03	1.56
1:C:63:THR:CG2	1:C:65:PHE:CZ	1.85	1.53
1:A:64:TRP:CZ2	1:A:66:HIS:CE1	1.95	1.52
1:A:296:LEU:HD12	1:A:608:VAL:CG1	1.40	1.52
1:B:372:ALA:HA	4:D:93:TRP:CB	1.40	1.52
1:A:64:TRP:CZ2	1:A:66:HIS:HE1	1.28	1.49
1:C:372:ALA:HA	4:N:93:TRP:CB	1.40	1.49
1:C:63:THR:HB	1:C:65:PHE:CE2	1.49	1.48
1:A:276:LEU:CD1	1:A:306:PHE:HE1	1.23	1.48
1:A:372:ALA:HA	4:M:93:TRP:CB	1.40	1.47
1:B:234:ASN:HD22	6:U:1:NAG:C1	1.27	1.44
1:A:296:LEU:CD1	1:A:608:VAL:HG13	1.45	1.42
1:A:296:LEU:CD1	1:A:608:VAL:CG1	1.97	1.38
1:C:296:LEU:HD13	1:C:608:VAL:CG1	1.53	1.38
1:B:372:ALA:CA	4:D:93:TRP:HB3	1.54	1.37
1:B:372:ALA:HB2	4:D:93:TRP:CD1	1.59	1.36
1:A:372:ALA:HB2	4:M:93:TRP:CD1	1.59	1.36
1:C:372:ALA:HB2	4:N:93:TRP:CD1	1.59	1.36
1:C:66:HIS:CD2	1:C:69:HIS:HB2	1.59	1.35
1:C:372:ALA:CA	4:N:93:TRP:HB3	1.54	1.35
1:A:372:ALA:CA	4:M:93:TRP:HB3	1.54	1.35
1:C:296:LEU:CD1	1:C:608:VAL:HG11	1.55	1.34
1:C:303:LEU:CD2	1:C:305:SER:HB3	1.58	1.32
1:A:276:LEU:CD1	1:A:306:PHE:CE1	2.00	1.32
1:B:372:ALA:CB	4:D:93:TRP:HD1	1.44	1.30
1:C:372:ALA:CB	4:N:93:TRP:HD1	1.44	1.29
1:A:372:ALA:CB	4:M:93:TRP:HD1	1.44	1.29
4:M:91:ASN:N	4:M:95:TYR:CE1	2.01	1.28
1:A:48:LEU:CD1	1:A:304:LYS:O	1.80	1.28
4:D:91:ASN:N	4:D:95:TYR:CE1	2.01	1.28
4:N:91:ASN:N	4:N:95:TYR:CE1	2.02	1.27
1:A:18:LEU:HD12	1:A:18:LEU:O	1.24	1.25
1:A:48:LEU:HD13	1:A:304:LYS:O	1.10	1.25
1:A:372:ALA:CB	4:M:93:TRP:CD1	2.20	1.25
1:B:372:ALA:O	4:D:92:PHE:O	1.54	1.25
1:C:372:ALA:CB	4:N:93:TRP:CD1	2.20	1.25

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:372:ALA:O	4:N:92:PHE:O	1.54	1.24
1:A:324:GLU:OE2	1:A:534:VAL:CG2	1.85	1.24
1:A:372:ALA:CA	4:M:93:TRP:CD1	2.21	1.23
1:C:372:ALA:HA	4:N:93:TRP:CG	1.75	1.22
1:A:372:ALA:HA	4:M:93:TRP:CG	1.75	1.22
1:B:372:ALA:CA	4:D:93:TRP:CD1	2.21	1.22
1:C:372:ALA:CA	4:N:93:TRP:CD1	2.21	1.21
1:A:287:ASP:HB3	1:A:306:PHE:CE2	1.75	1.21
1:C:22:THR:CG2	1:C:78:ARG:CD	2.19	1.20
1:B:372:ALA:HA	4:D:93:TRP:CG	1.75	1.20
1:A:372:ALA:O	4:M:92:PHE:O	1.54	1.20
1:A:121:ASN:CG	1:A:126:VAL:HG22	1.66	1.18
1:A:324:GLU:OE2	1:A:534:VAL:HG21	1.38	1.18
1:B:372:ALA:CB	4:D:93:TRP:CD1	2.20	1.18
1:A:287:ASP:HB3	1:A:306:PHE:HE2	1.06	1.17
1:A:64:TRP:CE2	1:A:66:HIS:CE1	2.32	1.17
1:C:63:THR:CB	1:C:65:PHE:CE2	2.27	1.15
1:A:565:PHE:HB2	1:C:42:VAL:HG22	1.24	1.15
1:A:372:ALA:CA	4:M:93:TRP:HD1	1.58	1.14
1:C:66:HIS:CD2	1:C:69:HIS:CB	2.30	1.14
1:A:296:LEU:HD11	1:A:608:VAL:HG13	1.20	1.14
1:C:372:ALA:CA	4:N:93:TRP:HD1	1.58	1.13
1:A:42:VAL:HG22	1:B:565:PHE:HB2	1.19	1.12
1:B:104:TRP:CE3	1:B:119:ILE:HD11	1.83	1.12
1:B:372:ALA:CA	4:D:93:TRP:HD1	1.58	1.12
1:C:22:THR:HG21	1:C:78:ARG:HB3	1.20	1.11
1:B:104:TRP:HE3	1:B:119:ILE:HD11	0.96	1.10
1:B:372:ALA:O	4:D:92:PHE:C	1.95	1.09
1:C:372:ALA:O	4:N:92:PHE:C	1.95	1.09
1:A:372:ALA:O	4:M:92:PHE:C	1.95	1.09
1:B:42:VAL:HA	1:C:565:PHE:O	1.53	1.08
1:A:299:THR:HG22	1:A:315:THR:OG1	1.54	1.08
1:B:328:ARG:N	1:B:542:ASN:O	1.86	1.07
1:C:63:THR:HG22	1:C:65:PHE:CZ	1.86	1.07
1:A:296:LEU:CD1	1:A:608:VAL:HG11	1.83	1.07
1:B:853:GLN:NE2	1:B:959:LEU:HB3	1.70	1.06
1:B:278:LYS:HB2	1:B:306:PHE:CZ	1.90	1.05
1:C:22:THR:HG22	1:C:78:ARG:HD2	1.06	1.04
1:A:66:HIS:ND1	1:A:264:ALA:HB2	1.72	1.04
1:C:18:LEU:HD12	1:C:18:LEU:O	1.56	1.04
1:A:201:PHE:HB3	1:A:231:ILE:HG13	1.40	1.03

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:ASN:CG	1:A:126:VAL:CG2	2.30	1.03
1:A:853:GLN:NE2	1:A:959:LEU:HB3	1.72	1.03
1:C:22:THR:HG21	1:C:78:ARG:CB	1.88	1.03
1:B:853:GLN:NE2	1:B:959:LEU:CB	2.22	1.03
1:A:853:GLN:NE2	1:A:959:LEU:CB	2.23	1.02
1:A:296:LEU:HD12	1:A:608:VAL:CG2	1.89	1.01
1:B:372:ALA:HA	4:D:93:TRP:CD1	1.91	1.01
1:A:373:SER:HA	4:M:92:PHE:HA	1.43	1.01
1:B:42:VAL:HG22	1:C:565:PHE:HB2	1.41	1.01
4:N:91:ASN:N	4:N:95:TYR:HE1	1.47	1.01
4:M:91:ASN:N	4:M:95:TYR:HE1	1.47	1.00
1:B:201:PHE:HB3	1:B:231:ILE:HG13	1.41	1.00
1:B:536:ASN:OD1	1:B:553:THR:HG22	1.58	1.00
1:C:63:THR:CG2	1:C:65:PHE:CE2	2.45	0.99
1:C:372:ALA:HA	4:N:93:TRP:CD1	1.91	0.99
1:C:22:THR:HG23	1:C:78:ARG:HD2	1.42	0.98
1:A:287:ASP:CB	1:A:306:PHE:CE2	2.46	0.98
1:A:44:ARG:NH2	1:B:567:ARG:HD2	1.77	0.98
1:A:296:LEU:HD12	1:A:608:VAL:CB	1.93	0.98
1:A:64:TRP:CE2	1:A:66:HIS:HE1	1.76	0.97
1:B:373:SER:HA	4:D:92:PHE:HA	1.43	0.97
2:L:17:SER:HA	2:L:83:MET:O	1.64	0.97
1:C:373:SER:HA	4:N:92:PHE:HA	1.43	0.97
2:G:17:SER:HA	2:G:83:MET:O	1.65	0.97
1:A:18:LEU:O	1:A:18:LEU:CD1	2.13	0.96
1:C:63:THR:O	1:C:65:PHE:CD2	2.18	0.96
2:K:17:SER:HA	2:K:83:MET:O	1.65	0.96
1:A:299:THR:HG22	1:A:315:THR:HG1	1.28	0.96
4:N:10:GLN:HG3	4:N:20:ILE:HG12	1.47	0.96
1:B:328:ARG:CB	1:B:543:PHE:CD1	2.49	0.95
1:A:41:LYS:HB3	1:B:564:GLN:N	1.80	0.95
4:D:91:ASN:N	4:D:95:TYR:HE1	1.47	0.95
1:A:296:LEU:HD12	1:A:608:VAL:HG11	1.44	0.95
4:N:35:TYR:HB2	4:N:86:PHE:HB2	1.49	0.95
4:M:35:TYR:HB2	4:M:86:PHE:HB2	1.49	0.94
1:A:372:ALA:HA	4:M:93:TRP:CD1	1.91	0.94
1:C:22:THR:HG21	1:C:78:ARG:HD2	1.50	0.94
4:D:90:THR:HA	4:D:95:TYR:CE1	2.02	0.94
1:C:380:TYR:HE1	5:H:56:GLY:H	0.98	0.94
4:M:90:THR:HA	4:M:95:TYR:CE1	2.02	0.94
4:M:10:GLN:HG3	4:M:20:ILE:HG12	1.47	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:380:TYR:HE1	5:E:56:GLY:H	0.98	0.94
1:C:66:HIS:HD2	1:C:69:HIS:CB	1.74	0.93
1:C:63:THR:CB	1:C:65:PHE:CZ	2.48	0.93
4:D:35:TYR:HB2	4:D:86:PHE:HB2	1.49	0.93
4:N:90:THR:HA	4:N:95:TYR:CE1	2.02	0.93
1:B:328:ARG:HB2	1:B:543:PHE:CD1	2.02	0.93
1:A:853:GLN:HE21	1:A:959:LEU:HB3	1.32	0.92
1:B:38:TYR:HD2	1:C:562:PHE:CZ	1.88	0.92
1:B:380:TYR:HE1	5:E:56:GLY:N	1.68	0.92
1:A:64:TRP:CH2	1:A:66:HIS:NE2	2.37	0.92
5:O:10:GLU:HB2	5:O:116:VAL:HG22	1.51	0.92
1:A:380:TYR:HE1	5:O:56:GLY:H	0.98	0.92
4:D:10:GLN:HG3	4:D:20:ILE:HG12	1.47	0.92
1:B:853:GLN:HE21	1:B:959:LEU:HB3	1.32	0.92
1:A:380:TYR:HE1	5:O:56:GLY:N	1.68	0.91
5:H:35:HIS:HB2	5:H:97:ALA:HB3	1.53	0.91
1:C:380:TYR:HE1	5:H:56:GLY:N	1.68	0.91
5:E:35:HIS:HB2	5:E:97:ALA:HB3	1.53	0.91
1:A:564:GLN:N	1:C:41:LYS:HB3	1.85	0.90
1:A:66:HIS:ND1	1:A:264:ALA:CB	2.32	0.90
1:A:121:ASN:OD1	1:A:126:VAL:HG22	1.71	0.90
5:H:10:GLU:HB2	5:H:116:VAL:HG22	1.51	0.90
5:O:35:HIS:HB2	5:O:97:ALA:HB3	1.53	0.90
1:A:118:LEU:CD2	1:A:120:VAL:HG23	2.03	0.89
5:E:10:GLU:HB2	5:E:116:VAL:HG22	1.51	0.89
1:B:38:TYR:CD2	1:C:562:PHE:HZ	1.91	0.89
3:F:33:LEU:HA	3:F:89:GLN:O	1.74	0.88
1:A:64:TRP:CH2	1:A:66:HIS:CE1	2.61	0.88
1:A:287:ASP:OD2	1:A:306:PHE:CD2	2.26	0.88
1:C:303:LEU:HD21	1:C:305:SER:HB3	1.52	0.88
3:I:33:LEU:HA	3:I:89:GLN:O	1.74	0.88
1:B:41:LYS:HB3	1:C:564:GLN:N	1.87	0.88
1:C:22:THR:HG22	1:C:78:ARG:CD	1.93	0.87
1:C:63:THR:HB	1:C:65:PHE:HE2	1.05	0.87
1:B:327:VAL:HG12	1:B:542:ASN:HB3	1.57	0.87
1:C:296:LEU:HD13	1:C:608:VAL:HG11	0.87	0.87
1:A:563:GLN:HB3	1:C:41:LYS:O	1.73	0.87
1:B:299:THR:HG21	1:B:597:VAL:HB	1.56	0.87
1:C:63:THR:CG2	1:C:65:PHE:CE1	2.58	0.87
1:A:64:TRP:CZ2	1:A:66:HIS:NE2	2.43	0.87
1:A:567:ARG:HD2	1:C:44:ARG:NH2	1.90	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:THR:HG22	1:C:78:ARG:HH11	1.38	0.86
1:A:287:ASP:CG	1:A:306:PHE:CE2	2.53	0.86
1:B:42:VAL:CA	1:C:565:PHE:O	2.22	0.86
1:B:1102:TRP:CZ2	1:B:1133:VAL:HG21	2.10	0.86
1:C:588:THR:HG23	1:C:589:PRO:HD2	1.57	0.86
3:J:33:LEU:HA	3:J:89:GLN:O	1.74	0.86
1:A:43:PHE:HB3	1:B:559:PHE:CE1	2.11	0.85
1:B:104:TRP:HE3	1:B:119:ILE:CD1	1.84	0.85
1:C:303:LEU:HD22	1:C:305:SER:HB3	1.59	0.85
1:B:372:ALA:HB1	4:D:94:PRO:HD2	1.57	0.85
1:C:303:LEU:HD23	1:C:305:SER:HB3	1.55	0.85
1:A:121:ASN:HA	1:A:126:VAL:HG22	1.59	0.84
1:A:372:ALA:HB1	4:M:94:PRO:HD2	1.58	0.84
1:B:328:ARG:HB3	1:B:543:PHE:CD1	2.11	0.84
1:C:372:ALA:HB1	4:N:94:PRO:HD2	1.57	0.84
1:A:563:GLN:CB	1:C:41:LYS:O	2.26	0.84
1:B:853:GLN:HE22	1:B:959:LEU:CD1	1.89	0.84
1:A:853:GLN:HE22	1:A:959:LEU:CD1	1.88	0.84
1:B:324:GLU:OE2	1:B:534:VAL:HG21	1.76	0.84
1:A:299:THR:CG2	1:A:315:THR:OG1	2.26	0.84
4:N:91:ASN:H	4:N:95:TYR:HE1	1.04	0.84
1:A:534:VAL:HG11	1:A:539:VAL:CG1	2.07	0.84
1:B:372:ALA:C	4:D:93:TRP:HB3	2.03	0.83
4:N:90:THR:C	4:N:95:TYR:HE1	1.87	0.83
1:C:1102:TRP:CD1	1:C:1135:ASN:ND2	2.47	0.83
1:A:559:PHE:CE1	1:C:43:PHE:HB3	2.14	0.83
4:D:90:THR:C	4:D:95:TYR:HE1	1.87	0.83
1:B:328:ARG:CB	1:B:543:PHE:HD1	1.90	0.83
1:A:372:ALA:N	4:M:93:TRP:CD1	2.47	0.83
4:D:89:GLN:O	4:D:95:TYR:HD1	1.62	0.83
1:A:296:LEU:CG	1:A:608:VAL:HG11	2.09	0.83
4:M:90:THR:C	4:M:95:TYR:HE1	1.87	0.82
4:D:90:THR:HA	4:D:95:TYR:HE1	1.38	0.82
1:A:372:ALA:C	4:M:93:TRP:HB3	2.03	0.82
1:C:303:LEU:CD2	1:C:305:SER:CB	2.53	0.82
4:N:90:THR:HA	4:N:95:TYR:HE1	1.38	0.82
1:B:278:LYS:HB2	1:B:306:PHE:HZ	1.44	0.82
4:M:89:GLN:O	4:M:95:TYR:HD1	1.62	0.82
1:A:42:VAL:HG11	1:B:567:ARG:HG3	1.61	0.82
1:A:273:ARG:NH1	1:A:290:ASP:OD2	2.13	0.82
1:B:273:ARG:NH1	1:B:290:ASP:OD2	2.13	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:90:THR:HA	4:M:95:TYR:HE1	1.38	0.82
1:A:121:ASN:OD1	1:A:126:VAL:CG2	2.26	0.82
1:B:372:ALA:N	4:D:93:TRP:CD1	2.47	0.82
1:C:234:ASN:HD22	6:Z:1:NAG:C2	1.93	0.82
1:C:372:ALA:N	4:N:93:TRP:CD1	2.47	0.82
1:C:278:LYS:HB2	1:C:306:PHE:CE2	2.14	0.81
1:C:372:ALA:C	4:N:93:TRP:HB3	2.03	0.81
4:N:89:GLN:O	4:N:95:TYR:HD1	1.62	0.81
4:D:90:THR:CA	4:D:95:TYR:HE1	1.93	0.81
1:B:42:VAL:HG11	1:C:567:ARG:HG3	1.60	0.81
1:A:44:ARG:HH21	1:B:567:ARG:HD2	1.44	0.81
1:A:41:LYS:O	1:B:563:GLN:HB3	1.79	0.81
1:A:118:LEU:HD23	1:A:120:VAL:HG23	1.63	0.80
1:B:299:THR:CG2	1:B:597:VAL:HB	2.11	0.80
1:A:534:VAL:CB	1:A:539:VAL:HG11	2.10	0.80
1:B:804:GLN:OE1	1:B:935:GLN:NE2	2.14	0.80
1:C:63:THR:HG22	1:C:65:PHE:CE1	2.17	0.80
4:M:90:THR:CA	4:M:95:TYR:HE1	1.93	0.80
1:C:373:SER:CA	4:N:92:PHE:HA	2.12	0.80
1:A:804:GLN:OE1	1:A:935:GLN:NE2	2.14	0.80
1:C:287:ASP:HB3	1:C:306:PHE:CE2	2.17	0.80
1:B:380:TYR:CE1	5:E:56:GLY:N	2.46	0.80
1:A:41:LYS:HB3	1:B:564:GLN:H	1.45	0.79
1:B:41:LYS:O	1:C:563:GLN:HB3	1.81	0.79
1:B:373:SER:CA	4:D:92:PHE:HA	2.12	0.79
1:A:373:SER:CA	4:M:92:PHE:HA	2.12	0.79
4:N:90:THR:CA	4:N:95:TYR:HE1	1.93	0.79
1:A:324:GLU:OE2	1:A:534:VAL:HG22	1.83	0.79
1:C:588:THR:CG2	1:C:589:PRO:HD2	2.12	0.79
1:B:901:GLN:HE21	1:B:905:ARG:HE	1.31	0.79
1:A:64:TRP:HZ2	1:A:66:HIS:HE1	1.23	0.79
4:N:6:GLN:O	4:N:99:GLN:NE2	2.16	0.79
4:M:6:GLN:O	4:M:99:GLN:NE2	2.16	0.78
4:M:90:THR:C	4:M:95:TYR:CE1	2.61	0.78
4:D:6:GLN:O	4:D:99:GLN:NE2	2.17	0.78
1:C:66:HIS:HD2	1:C:69:HIS:HB2	1.01	0.78
1:B:853:GLN:HE21	1:B:959:LEU:CB	1.92	0.78
1:C:296:LEU:CD1	1:C:608:VAL:CG1	2.33	0.78
1:B:299:THR:HG21	1:B:597:VAL:CB	2.13	0.78
4:M:93:TRP:CG	4:M:94:PRO:HD3	2.19	0.77
6:d:1:NAG:H3	6:d:1:NAG:H82	1.65	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:ARG:NH2	1:C:567:ARG:HD2	2.00	0.77
3:F:63:SER:O	3:F:74:THR:HB	1.85	0.77
1:C:380:TYR:CE1	5:H:56:GLY:N	2.46	0.77
4:M:6:GLN:NE2	4:M:87:CYS:SG	2.58	0.77
4:M:97:PHE:HD2	5:O:45:LEU:HB3	1.49	0.77
1:A:380:TYR:CE1	5:O:56:GLY:N	2.46	0.77
1:A:901:GLN:HE21	1:A:905:ARG:HE	1.31	0.77
4:D:97:PHE:HD2	5:E:45:LEU:HB3	1.50	0.77
4:D:6:GLN:NE2	4:D:87:CYS:SG	2.58	0.77
4:D:93:TRP:CG	4:D:94:PRO:HD3	2.19	0.77
4:N:22:CYS:N	4:N:70:PHE:O	2.18	0.77
4:N:97:PHE:HD2	5:H:45:LEU:HB3	1.50	0.77
1:A:377:PHE:O	5:O:59:SER:HB2	1.85	0.77
1:A:853:GLN:NE2	1:A:959:LEU:HD13	2.00	0.77
1:C:914:ASN:ND2	1:C:1111:GLU:OE2	2.18	0.76
4:N:6:GLN:NE2	4:N:87:CYS:SG	2.58	0.76
4:N:93:TRP:CG	4:N:94:PRO:HD3	2.19	0.76
1:B:42:VAL:CG1	1:C:567:ARG:HG3	2.15	0.76
1:B:377:PHE:O	5:E:59:SER:HB2	1.85	0.76
1:C:118:LEU:HG	1:C:120:VAL:HG23	1.66	0.76
4:N:90:THR:C	4:N:95:TYR:CE1	2.61	0.76
1:A:550:GLY:HA2	1:A:589:PRO:HA	1.66	0.76
1:B:372:ALA:HA	4:D:93:TRP:HB3	0.77	0.76
3:I:63:SER:O	3:I:74:THR:HB	1.85	0.76
4:N:24:ALA:HB3	4:N:28:ILE:HG22	1.68	0.76
4:D:90:THR:C	4:D:95:TYR:CE1	2.61	0.76
3:J:63:SER:O	3:J:74:THR:HB	1.85	0.76
1:C:276:LEU:HD13	1:C:289:VAL:O	1.86	0.76
1:C:372:ALA:HA	4:N:93:TRP:HB3	0.77	0.76
1:A:287:ASP:OD2	1:A:306:PHE:CE2	2.39	0.76
4:D:24:ALA:HB3	4:D:28:ILE:HG22	1.68	0.76
1:B:41:LYS:O	1:C:563:GLN:CB	2.34	0.76
1:B:380:TYR:CE1	5:E:55:ASN:HB3	2.21	0.76
1:C:303:LEU:HD13	1:C:308:VAL:HG22	1.67	0.76
2:G:69:THR:O	2:G:81:LEU:HA	1.86	0.76
1:A:534:VAL:HB	1:A:539:VAL:HG11	1.67	0.75
1:B:550:GLY:HA2	1:B:589:PRO:HA	1.67	0.75
2:L:69:THR:O	2:L:81:LEU:HA	1.86	0.75
4:N:89:GLN:O	4:N:95:TYR:CD1	2.40	0.75
1:A:853:GLN:NE2	1:A:959:LEU:CD1	2.48	0.75
1:C:377:PHE:O	5:H:59:SER:HB2	1.85	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:89:GLN:O	4:M:95:TYR:CD1	2.40	0.75
1:C:1102:TRP:HB2	1:C:1135:ASN:ND2	2.02	0.75
5:E:91:THR:HG23	5:E:117:THR:HA	1.69	0.75
4:M:22:CYS:N	4:M:70:PHE:O	2.18	0.75
1:A:372:ALA:HA	4:M:93:TRP:HB3	0.77	0.75
1:B:853:GLN:NE2	1:B:959:LEU:CD1	2.49	0.75
2:K:69:THR:O	2:K:81:LEU:HA	1.86	0.75
1:A:42:VAL:HG22	1:B:565:PHE:CB	2.09	0.75
1:A:380:TYR:CE1	5:O:55:ASN:HB3	2.21	0.75
1:A:534:VAL:CG1	1:A:539:VAL:HG11	2.17	0.75
4:D:89:GLN:O	4:D:95:TYR:CD1	2.40	0.75
4:D:22:CYS:N	4:D:70:PHE:O	2.18	0.74
1:B:369:TYR:HB3	4:D:93:TRP:CZ2	2.23	0.74
1:A:564:GLN:H	1:C:41:LYS:HB3	1.49	0.74
1:C:380:TYR:CE1	5:H:55:ASN:HB3	2.21	0.74
1:B:327:VAL:HG12	1:B:542:ASN:CB	2.17	0.74
5:H:91:THR:HG23	5:H:117:THR:HA	1.69	0.74
6:d:1:NAG:H3	6:d:1:NAG:C8	2.17	0.74
1:A:369:TYR:HB3	4:M:93:TRP:CZ2	2.23	0.74
1:C:369:TYR:HB3	4:N:93:TRP:CZ2	2.23	0.74
4:M:24:ALA:HB3	4:M:28:ILE:HG22	1.68	0.74
1:B:853:GLN:NE2	1:B:959:LEU:HD13	2.01	0.74
5:O:91:THR:HG23	5:O:117:THR:HA	1.69	0.73
1:A:299:THR:HG21	1:A:597:VAL:HB	1.70	0.73
1:B:328:ARG:HB2	1:B:543:PHE:CE1	2.23	0.73
1:C:108:THR:HG21	6:Z:1:NAG:H61	1.70	0.73
1:C:383:SER:HG	5:H:69:THR:HG1	1.31	0.73
1:A:48:LEU:HD12	1:A:304:LYS:O	1.87	0.73
1:A:908:GLY:O	1:A:1038:LYS:NZ	2.22	0.73
1:B:43:PHE:N	1:C:565:PHE:O	2.21	0.73
1:B:48:LEU:HD11	1:B:306:PHE:CD2	2.21	0.73
1:A:317:ASN:HD22	1:A:594:GLY:HA2	1.54	0.73
1:A:372:ALA:C	4:M:92:PHE:C	2.57	0.73
1:A:567:ARG:HD2	1:C:44:ARG:HH21	1.53	0.73
1:B:317:ASN:HD22	1:B:594:GLY:HA2	1.54	0.73
1:C:567:ARG:NH1	1:C:571:ASP:O	2.22	0.73
1:A:299:THR:CG2	1:A:597:VAL:HG21	2.19	0.73
1:B:908:GLY:O	1:B:1038:LYS:NZ	2.21	0.73
1:C:204:TYR:HB3	1:C:223:LEU:HB3	1.71	0.73
1:A:296:LEU:HG	1:A:608:VAL:HG11	1.71	0.72
1:A:853:GLN:HE21	1:A:959:LEU:CB	1.93	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:LYS:O	1:B:563:GLN:CB	2.36	0.72
1:C:372:ALA:C	4:N:92:PHE:C	2.57	0.72
1:A:43:PHE:CB	1:B:559:PHE:CE1	2.73	0.72
1:C:650:LEU:HD21	1:C:653:ALA:HB3	1.71	0.72
1:C:143:VAL:HG22	1:C:154:GLU:HG2	1.72	0.72
1:A:559:PHE:CD1	1:C:43:PHE:CB	2.73	0.72
1:B:372:ALA:C	4:D:92:PHE:C	2.57	0.72
1:A:143:VAL:HG22	1:A:154:GLU:HG2	1.72	0.71
1:A:669:GLY:HA3	1:C:869:MET:HE1	1.72	0.71
1:B:299:THR:HG23	1:B:597:VAL:HG21	1.71	0.71
4:D:91:ASN:N	4:D:95:TYR:CZ	2.52	0.71
1:B:299:THR:CG2	1:B:597:VAL:CB	2.69	0.71
1:C:22:THR:HG21	1:C:78:ARG:CG	2.19	0.71
1:B:327:VAL:HA	1:B:542:ASN:HB3	1.72	0.71
1:A:43:PHE:CB	1:B:559:PHE:CD1	2.74	0.71
1:A:204:TYR:HB3	1:A:223:LEU:HB3	1.71	0.71
1:B:143:VAL:HG22	1:B:154:GLU:HG2	1.72	0.71
1:A:726:ILE:HD13	1:A:945:LEU:HD23	1.73	0.71
1:A:380:TYR:HE1	5:O:55:ASN:HB3	1.56	0.71
1:A:963:VAL:HG11	1:B:570:ALA:HB1	1.73	0.71
1:B:130:VAL:HB	1:B:168:PHE:HB3	1.72	0.71
1:C:63:THR:HG21	1:C:65:PHE:CE1	2.17	0.71
1:B:380:TYR:HE1	5:E:55:ASN:HB3	1.56	0.71
1:B:100:ILE:HG21	1:B:263:ALA:HB2	1.72	0.71
1:A:534:VAL:HG11	1:A:539:VAL:HG11	1.71	0.70
1:C:380:TYR:HE1	5:H:55:ASN:HB3	1.56	0.70
1:C:63:THR:O	1:C:65:PHE:CE2	2.44	0.70
1:A:130:VAL:HB	1:A:168:PHE:HB3	1.72	0.70
1:A:34:ARG:NH1	1:A:221:SER:OG	2.25	0.70
1:C:34:ARG:NH1	1:C:221:SER:OG	2.25	0.70
4:M:93:TRP:CD1	4:M:94:PRO:HD3	2.26	0.70
1:A:815:ARG:HD2	1:A:823:PHE:HE2	1.57	0.70
1:B:204:TYR:HB3	1:B:223:LEU:HB3	1.71	0.70
4:D:93:TRP:CD1	4:D:94:PRO:HD3	2.26	0.70
4:N:93:TRP:CD1	4:N:94:PRO:HD3	2.26	0.70
1:C:121:ASN:HA	1:C:126:VAL:HA	1.74	0.70
1:A:73:THR:HG23	1:A:74:ASN:H	1.57	0.70
1:A:102:ARG:NH1	1:A:154:GLU:OE2	2.25	0.70
1:B:815:ARG:HD2	1:B:823:PHE:HE2	1.57	0.70
1:C:63:THR:HG21	1:C:65:PHE:HZ	0.89	0.70
1:A:276:LEU:CD1	1:A:306:PHE:CZ	2.71	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:ARG:NH1	1:C:154:GLU:OE2	2.25	0.69
1:C:544:ASN:HD21	1:C:579:PRO:HB3	1.57	0.69
4:D:90:THR:CA	4:D:95:TYR:CE1	2.71	0.69
4:N:91:ASN:N	4:N:95:TYR:CZ	2.52	0.69
1:B:180:GLU:HG3	1:B:181:GLY:H	1.58	0.69
1:B:102:ARG:NH1	1:B:154:GLU:OE2	2.25	0.69
1:B:536:ASN:HA	1:B:551:VAL:CG1	2.23	0.69
4:M:22:CYS:HB3	4:M:70:PHE:HB2	1.74	0.69
1:B:104:TRP:CE3	1:B:119:ILE:CD1	2.68	0.69
1:A:118:LEU:HD21	1:A:120:VAL:HG23	1.71	0.69
1:A:180:GLU:HG3	1:A:181:GLY:H	1.58	0.69
1:B:534:VAL:HG11	1:B:537:LYS:HE2	1.73	0.69
1:B:726:ILE:HD13	1:B:945:LEU:HD23	1.73	0.69
1:C:180:GLU:HG3	1:C:181:GLY:H	1.58	0.69
1:C:73:THR:HG23	1:C:74:ASN:H	1.57	0.69
5:O:35:HIS:O	5:O:97:ALA:N	2.26	0.69
5:H:35:HIS:O	5:H:97:ALA:N	2.25	0.69
1:C:22:THR:HG21	1:C:78:ARG:CD	2.08	0.69
1:C:372:ALA:HB2	4:N:93:TRP:HD1	1.03	0.69
5:E:35:HIS:O	5:E:97:ALA:N	2.26	0.69
1:A:296:LEU:HD12	1:A:608:VAL:HG22	1.75	0.69
1:A:296:LEU:HD11	1:A:608:VAL:CG1	1.92	0.69
5:H:38:LYS:O	5:H:46:GLU:N	2.26	0.69
1:B:42:VAL:HG13	1:C:565:PHE:O	1.93	0.68
1:B:1031:GLU:OE2	1:C:1039:ARG:NE	2.23	0.68
1:C:901:GLN:HE21	1:C:905:ARG:HE	1.39	0.68
1:A:118:LEU:HD21	1:A:120:VAL:CG2	2.22	0.68
1:A:276:LEU:HD13	1:A:306:PHE:CE1	2.21	0.68
1:B:34:ARG:NH1	1:B:221:SER:OG	2.25	0.68
1:B:372:ALA:N	4:D:93:TRP:HD1	1.87	0.68
1:C:130:VAL:HB	1:C:168:PHE:HB3	1.72	0.68
4:N:90:THR:CA	4:N:95:TYR:CE1	2.71	0.68
1:B:299:THR:HG21	1:B:597:VAL:CG1	2.23	0.68
1:C:100:ILE:HG21	1:C:263:ALA:HB2	1.76	0.68
4:M:90:THR:CA	4:M:95:TYR:CE1	2.71	0.68
1:A:42:VAL:CG2	1:B:565:PHE:HB2	2.12	0.68
4:D:22:CYS:HB3	4:D:70:PHE:HB2	1.74	0.68
1:A:372:ALA:N	4:M:93:TRP:HD1	1.87	0.68
1:A:567:ARG:HG3	1:C:42:VAL:HG11	1.75	0.68
1:A:369:TYR:HB3	4:M:93:TRP:HZ2	1.59	0.67
1:A:38:TYR:HD2	1:B:562:PHE:CZ	2.13	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:38:LYS:O	5:E:46:GLU:N	2.26	0.67
1:C:81:ASN:O	1:C:239:GLN:NE2	2.27	0.67
1:A:383:SER:HG	5:O:69:THR:HG1	1.33	0.67
1:B:73:THR:HG23	1:B:74:ASN:H	1.57	0.67
1:B:81:ASN:O	1:B:239:GLN:NE2	2.27	0.67
1:B:431:GLY:HA3	1:B:513:LEU:O	1.95	0.67
4:N:22:CYS:HB3	4:N:70:PHE:HB2	1.74	0.67
1:A:1039:ARG:NE	1:C:1031:GLU:OE2	2.26	0.67
1:C:431:GLY:HA3	1:C:513:LEU:O	1.95	0.67
1:A:100:ILE:HG21	1:A:263:ALA:HB2	1.77	0.67
1:A:676:THR:H	1:A:690:GLN:HG2	1.59	0.67
1:C:201:PHE:HB3	1:C:231:ILE:HG13	1.77	0.67
4:M:91:ASN:H	4:M:95:TYR:HE1	1.04	0.67
5:O:38:LYS:O	5:O:46:GLU:N	2.26	0.67
1:A:296:LEU:HB2	1:A:608:VAL:HG21	1.76	0.67
1:B:38:TYR:CD2	1:C:562:PHE:CZ	2.72	0.67
1:B:853:GLN:NE2	1:B:959:LEU:HB2	2.08	0.67
1:C:703:ASN:OD1	1:C:704:SER:N	2.28	0.67
1:A:42:VAL:HA	1:B:565:PHE:O	1.95	0.67
1:B:327:VAL:CG1	1:B:542:ASN:HB3	2.25	0.67
4:D:91:ASN:H	4:D:95:TYR:HE1	1.04	0.67
1:B:676:THR:H	1:B:690:GLN:HG2	1.60	0.66
1:A:431:GLY:HA3	1:A:513:LEU:O	1.95	0.66
1:A:81:ASN:O	1:A:239:GLN:NE2	2.27	0.66
4:M:32:LEU:HD21	4:M:87:CYS:HB2	1.77	0.66
1:B:645:THR:OG1	1:B:648:GLY:O	2.12	0.66
1:C:372:ALA:O	4:N:92:PHE:CA	2.44	0.66
4:N:37:GLN:HB2	4:N:43:PRO:HG3	1.77	0.66
1:A:42:VAL:CG1	1:B:567:ARG:HG3	2.26	0.66
1:A:320:VAL:HB	1:A:590:CYS:HB2	1.77	0.66
1:A:546:LEU:HD21	1:A:573:THR:HG21	1.77	0.66
1:A:565:PHE:O	1:C:42:VAL:HA	1.95	0.66
1:C:372:ALA:N	4:N:93:TRP:HD1	1.87	0.66
1:B:148:ASN:C	1:B:150:LYS:H	2.02	0.66
4:D:37:GLN:HB2	4:D:43:PRO:HG3	1.77	0.66
1:B:369:TYR:HB3	4:D:93:TRP:HZ2	1.59	0.66
4:N:32:LEU:HD21	4:N:87:CYS:HB2	1.77	0.66
1:B:277:LEU:HD23	1:B:285:ILE:HD11	1.78	0.66
1:C:369:TYR:HB3	4:N:93:TRP:HZ2	1.59	0.66
1:A:299:THR:HG21	1:A:597:VAL:CB	2.26	0.66
1:A:559:PHE:CE1	1:C:43:PHE:CB	2.79	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:THR:HG23	1:A:597:VAL:HG21	1.78	0.66
1:B:42:VAL:HG11	1:C:567:ARG:CG	2.25	0.66
4:D:32:LEU:HD21	4:D:87:CYS:HB2	1.77	0.66
5:O:6:GLN:NE2	5:O:96:CYS:H	1.94	0.66
1:A:121:ASN:CB	1:A:126:VAL:HG22	2.26	0.65
1:A:372:ALA:O	4:M:92:PHE:CA	2.44	0.65
1:B:372:ALA:O	4:D:92:PHE:CA	2.44	0.65
1:A:42:VAL:HG11	1:B:567:ARG:CG	2.26	0.65
1:B:116:SER:N	1:B:131:CYS:O	2.29	0.65
1:B:725:GLU:OE1	1:B:1064:HIS:NE2	2.30	0.65
5:E:6:GLN:NE2	5:E:96:CYS:H	1.94	0.65
1:A:116:SER:N	1:A:131:CYS:O	2.29	0.65
1:C:725:GLU:OE1	1:C:1064:HIS:NE2	2.29	0.65
4:M:37:GLN:HB2	4:M:43:PRO:HG3	1.77	0.65
1:A:121:ASN:CA	1:A:126:VAL:HG22	2.26	0.65
5:E:2:VAL:HB	5:E:26:GLY:HA3	1.79	0.65
5:H:97:ALA:HB1	5:H:107:MET:HB3	1.78	0.65
1:A:725:GLU:OE1	1:A:1064:HIS:NE2	2.30	0.65
1:B:121:ASN:HA	1:B:126:VAL:HA	1.79	0.65
1:B:1091:ARG:NH1	1:B:1118:ASP:O	2.29	0.65
1:B:811:LYS:NZ	1:B:820:ASP:OD2	2.30	0.65
1:C:726:ILE:HG12	1:C:1061:VAL:HG22	1.79	0.65
5:H:6:GLN:NE2	5:H:96:CYS:H	1.94	0.65
1:A:1091:ARG:NH1	1:A:1118:ASP:O	2.29	0.65
5:O:2:VAL:HB	5:O:26:GLY:HA3	1.79	0.65
2:K:6:GLU:H	2:K:111:GLN:HE22	1.46	0.64
4:M:91:ASN:N	4:M:95:TYR:CZ	2.52	0.64
1:B:68:ILE:HG23	1:B:259:THR:HB	1.78	0.64
1:B:111:ASP:OD1	1:B:134:GLN:NE2	2.29	0.64
1:C:66:HIS:CD2	1:C:69:HIS:HB3	2.32	0.64
1:C:116:SER:N	1:C:131:CYS:O	2.29	0.64
1:C:805:ILE:HD12	1:C:878:LEU:HD11	1.78	0.64
5:O:97:ALA:HB1	5:O:107:MET:HB3	1.78	0.64
1:A:811:LYS:NZ	1:A:820:ASP:OD2	2.30	0.64
1:C:22:THR:HG22	1:C:78:ARG:NH1	2.10	0.64
1:A:38:TYR:HD2	1:B:562:PHE:HZ	1.46	0.64
1:B:326:ILE:HA	1:B:531:THR:OG1	1.97	0.64
1:B:546:LEU:HD21	1:B:573:THR:HG21	1.77	0.64
1:C:373:SER:HA	4:N:92:PHE:CA	2.25	0.64
1:C:1102:TRP:HD1	1:C:1135:ASN:ND2	1.95	0.64
5:H:2:VAL:HB	5:H:26:GLY:HA3	1.79	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:20:LEU:O	2:G:80:TYR:HA	1.98	0.64
1:A:853:GLN:NE2	1:A:959:LEU:HB2	2.09	0.64
1:A:326:ILE:HD11	1:A:534:VAL:HG23	1.79	0.64
1:B:373:SER:HA	4:D:92:PHE:CA	2.26	0.64
5:E:97:ALA:HB1	5:E:107:MET:HB3	1.78	0.64
1:A:276:LEU:HD12	1:A:306:PHE:CE1	2.25	0.64
1:A:372:ALA:HB2	4:M:93:TRP:HD1	1.03	0.64
1:A:372:ALA:C	4:M:92:PHE:O	2.41	0.64
1:C:296:LEU:HD13	1:C:608:VAL:HG13	1.69	0.64
1:C:303:LEU:HD13	1:C:308:VAL:HA	1.80	0.64
1:C:746:SER:OG	1:C:748:GLU:OE1	2.15	0.64
2:L:6:GLU:H	2:L:111:GLN:HE22	1.45	0.64
2:G:6:GLU:H	2:G:111:GLN:HE22	1.46	0.64
1:A:43:PHE:N	1:B:565:PHE:O	2.25	0.63
1:B:44:ARG:HH21	1:C:567:ARG:HD2	1.63	0.63
6:d:2:NAG:O7	6:d:2:NAG:O3	2.14	0.63
1:A:111:ASP:OD1	1:A:134:GLN:NE2	2.29	0.63
1:B:372:ALA:HB2	4:D:93:TRP:HD1	1.03	0.63
5:O:6:GLN:NE2	5:O:96:CYS:SG	2.59	0.63
2:L:20:LEU:O	2:L:80:TYR:HA	1.98	0.63
4:N:69:ASP:OD1	4:N:70:PHE:N	2.32	0.63
1:C:763:LEU:HD22	1:C:1008:VAL:HG21	1.81	0.63
4:N:4:LEU:HA	4:N:24:ALA:HA	1.81	0.63
4:N:88:GLN:HG2	4:N:97:PHE:CD1	2.34	0.63
2:K:20:LEU:O	2:K:80:TYR:HA	1.98	0.63
4:D:69:ASP:OD1	4:D:70:PHE:N	2.32	0.63
1:A:373:SER:HA	4:M:92:PHE:CA	2.25	0.62
1:B:1115:ILE:HG22	1:B:1137:VAL:HG13	1.81	0.62
1:C:140:PHE:HB2	1:C:242:LEU:HB2	1.82	0.62
4:D:4:LEU:HA	4:D:24:ALA:HA	1.81	0.62
1:A:563:GLN:HG2	1:C:41:LYS:O	1.99	0.62
1:A:570:ALA:HB1	1:C:963:VAL:HG11	1.81	0.62
5:E:6:GLN:NE2	5:E:96:CYS:SG	2.59	0.62
1:C:908:GLY:O	1:C:1038:LYS:NZ	2.32	0.62
1:C:1086:LYS:HD2	1:C:1122:VAL:HG11	1.81	0.62
5:E:102:ASP:HB3	5:E:103:PRO:HD2	1.81	0.62
5:H:102:ASP:HB3	5:H:103:PRO:HD2	1.81	0.62
1:C:1116:THR:HB	1:C:1140:PRO:HD3	1.81	0.62
1:A:140:PHE:HB2	1:A:242:LEU:HB2	1.81	0.62
1:A:1115:ILE:HG22	1:A:1137:VAL:HG13	1.82	0.62
1:B:372:ALA:C	4:D:92:PHE:O	2.41	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1086:LYS:HD2	1:B:1122:VAL:HG11	1.80	0.62
4:M:88:GLN:HG2	4:M:97:PHE:CD1	2.34	0.62
1:B:276:LEU:CD1	1:B:306:PHE:CE1	2.82	0.62
1:C:372:ALA:C	4:N:92:PHE:O	2.41	0.62
4:M:69:ASP:OD1	4:M:70:PHE:N	2.32	0.62
1:C:18:LEU:O	1:C:18:LEU:CD1	2.41	0.62
4:D:88:GLN:HG2	4:D:97:PHE:CD1	2.34	0.62
1:A:121:ASN:ND2	1:A:126:VAL:HG21	2.15	0.62
1:A:372:ALA:O	4:M:92:PHE:HB3	2.00	0.62
1:A:1086:LYS:HD2	1:A:1122:VAL:HG11	1.80	0.62
4:N:34:TRP:HD1	4:N:47:ILE:HB	1.65	0.62
1:A:93:ALA:HB3	1:A:266:TYR:HB2	1.82	0.62
1:B:140:PHE:HB2	1:B:242:LEU:HB2	1.81	0.62
4:M:4:LEU:HA	4:M:24:ALA:HA	1.81	0.62
4:M:20:ILE:HD12	4:M:85:TYR:HD2	1.64	0.62
1:B:726:ILE:HG12	1:B:1061:VAL:HG22	1.82	0.61
1:C:372:ALA:O	4:N:92:PHE:HB3	2.00	0.61
1:C:886:TRP:HB2	1:C:1034:LEU:O	1.99	0.61
4:D:20:ILE:HD12	4:D:85:TYR:HD2	1.64	0.61
4:N:20:ILE:HD12	4:N:85:TYR:HD2	1.64	0.61
1:A:726:ILE:HG12	1:A:1061:VAL:HG22	1.82	0.61
4:D:7:SER:O	4:D:101:THR:OG1	2.14	0.61
1:C:278:LYS:HD3	1:C:306:PHE:CD2	2.35	0.61
1:A:43:PHE:CG	1:B:559:PHE:CD1	2.89	0.61
1:A:43:PHE:HB2	1:B:559:PHE:CD1	2.36	0.61
4:M:35:TYR:CZ	4:M:45:LEU:HD13	2.36	0.61
1:C:455:LEU:HD23	2:L:103:MET:HE1	1.82	0.61
5:O:102:ASP:HB3	5:O:103:PRO:HD2	1.81	0.61
4:N:35:TYR:CZ	4:N:45:LEU:HD13	2.36	0.61
1:A:853:GLN:HE22	1:A:959:LEU:HD12	1.65	0.61
1:B:93:ALA:HB3	1:B:266:TYR:HB2	1.82	0.61
1:B:455:LEU:HD23	2:K:103:MET:HE1	1.82	0.61
1:C:676:THR:HG23	1:C:690:GLN:HG2	1.82	0.61
1:A:559:PHE:CD1	1:C:43:PHE:HB2	2.36	0.60
1:A:853:GLN:CD	1:A:959:LEU:HD13	2.26	0.60
4:D:34:TRP:HD1	4:D:47:ILE:HB	1.65	0.60
4:M:34:TRP:HD1	4:M:47:ILE:HB	1.65	0.60
1:A:455:LEU:HD23	2:G:103:MET:HE1	1.82	0.60
1:A:563:GLN:CG	1:C:41:LYS:O	2.49	0.60
1:B:372:ALA:O	4:D:92:PHE:HB3	2.00	0.60
1:C:276:LEU:N	1:C:276:LEU:HD12	2.16	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:666:ILE:HD12	1:C:670:ILE:HG22	1.83	0.60
1:C:111:ASP:OD1	1:C:134:GLN:NE2	2.29	0.60
1:C:93:ALA:HB3	1:C:266:TYR:HB2	1.82	0.60
1:A:66:HIS:ND1	1:A:264:ALA:HB1	2.16	0.60
1:A:121:ASN:ND2	1:A:126:VAL:CG2	2.65	0.60
1:B:327:VAL:HA	1:B:542:ASN:O	2.01	0.60
1:C:44:ARG:O	1:C:283:GLY:HA2	2.02	0.60
1:C:853:GLN:NE2	1:C:959:LEU:HB3	2.16	0.60
4:D:35:TYR:CZ	4:D:45:LEU:HD13	2.36	0.60
1:C:276:LEU:HD11	1:C:301:CYS:SG	2.42	0.60
1:A:299:THR:CG2	1:A:597:VAL:CG2	2.79	0.59
1:B:328:ARG:HB3	1:B:543:PHE:HD1	1.56	0.59
1:B:986:LYS:O	1:B:987:VAL:C	2.45	0.59
1:B:853:GLN:HE22	1:B:959:LEU:HD12	1.66	0.59
1:B:853:GLN:CD	1:B:959:LEU:HD13	2.26	0.59
1:A:326:ILE:HD12	1:A:532:ASN:O	2.02	0.59
1:A:299:THR:HG21	1:A:597:VAL:CG2	2.32	0.59
1:B:1028:LYS:NZ	1:B:1042:PHE:O	2.35	0.59
1:A:38:TYR:CD2	1:B:562:PHE:HZ	2.20	0.59
1:A:1028:LYS:NZ	1:A:1042:PHE:O	2.35	0.59
1:B:745:ASP:OD1	1:C:319:ARG:NH1	2.36	0.59
4:M:12:VAL:O	4:M:105:ILE:HA	2.03	0.59
1:C:119:ILE:HG22	1:C:119:ILE:O	2.03	0.59
4:D:17:LYS:HG2	4:D:75:ASN:HA	1.85	0.59
4:N:7:SER:O	4:N:101:THR:OG1	2.14	0.59
1:B:326:ILE:HG22	1:B:326:ILE:O	2.01	0.59
1:C:555:SER:OG	1:C:584:ILE:O	2.19	0.59
5:E:6:GLN:OE1	5:E:113:GLY:N	2.31	0.59
1:B:231:ILE:HG22	1:B:233:ILE:HG22	1.85	0.58
4:N:12:VAL:O	4:N:105:ILE:HA	2.03	0.58
4:M:89:GLN:HE21	4:M:92:PHE:HD2	1.51	0.58
4:D:12:VAL:O	4:D:105:ILE:HA	2.02	0.58
1:A:540:ASN:OD1	1:A:541:PHE:N	2.37	0.58
1:A:645:THR:OG1	1:A:648:GLY:O	2.13	0.58
4:M:7:SER:O	4:M:101:THR:OG1	2.14	0.58
1:B:327:VAL:CB	1:B:542:ASN:HB3	2.33	0.58
1:C:804:GLN:OE1	1:C:935:GLN:NE2	2.28	0.58
5:H:6:GLN:OE1	5:H:113:GLY:N	2.31	0.58
1:C:287:ASP:HB3	1:C:306:PHE:HE2	1.68	0.58
2:G:7:SER:HB3	2:G:21:SER:HB3	1.85	0.58
1:A:1129:VAL:HG13	1:C:917:TYR:HB3	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:540:ASN:OD1	1:B:541:PHE:N	2.37	0.58
2:L:7:SER:HB3	2:L:21:SER:HB3	1.85	0.58
5:H:6:GLN:NE2	5:H:96:CYS:SG	2.59	0.58
1:A:1089:PHE:HE2	1:C:914:ASN:HA	1.69	0.58
1:C:661:GLU:O	1:C:695:TYR:OH	2.19	0.58
1:C:726:ILE:HD13	1:C:945:LEU:HD23	1.86	0.58
2:K:19:ARG:HA	2:K:82:GLN:HA	1.86	0.58
4:D:89:GLN:HE21	4:D:92:PHE:HD2	1.52	0.58
3:J:86:TYR:O	3:J:101:GLY:HA2	2.04	0.58
4:N:17:LYS:HG2	4:N:75:ASN:HA	1.85	0.58
1:B:105:ILE:HG12	1:B:239:GLN:H	1.69	0.58
1:B:902:MET:HE1	1:B:1049:LEU:HD13	1.86	0.58
4:M:43:PRO:HD2	5:O:110:TRP:HZ3	1.68	0.58
1:A:558:LYS:O	1:C:43:PHE:CE1	2.56	0.58
1:C:326:ILE:HD11	1:C:534:VAL:HB	1.84	0.58
1:A:1031:GLU:OE2	1:B:1039:ARG:NE	2.36	0.57
4:D:34:TRP:O	4:D:46:LEU:N	2.36	0.57
5:H:73:ASP:HB2	5:H:80:TYR:HE2	1.69	0.57
4:M:17:LYS:HG2	4:M:75:ASN:HA	1.85	0.57
3:I:86:TYR:O	3:I:101:GLY:HA2	2.04	0.57
4:N:43:PRO:HD2	5:H:110:TRP:HZ3	1.68	0.57
4:N:89:GLN:HE21	4:N:92:PHE:HD2	1.52	0.57
5:H:4:LEU:HD23	5:H:24:VAL:HG22	1.87	0.57
4:M:34:TRP:CD1	4:M:47:ILE:HB	2.39	0.57
5:O:4:LEU:HD23	5:O:24:VAL:HG22	1.86	0.57
1:C:815:ARG:HD2	1:C:823:PHE:HE2	1.69	0.57
2:K:7:SER:HB3	2:K:21:SER:HB3	1.85	0.57
4:N:33:HIS:HA	4:N:47:ILE:O	2.05	0.57
4:N:34:TRP:O	4:N:46:LEU:N	2.36	0.57
3:F:86:TYR:O	3:F:101:GLY:HA2	2.04	0.57
5:O:38:LYS:HD2	5:O:92:ALA:HB3	1.87	0.57
1:A:105:ILE:HG12	1:A:239:GLN:H	1.69	0.57
1:B:84:LEU:N	1:B:238:PHE:O	2.29	0.57
1:B:326:ILE:HD12	1:B:532:ASN:O	2.04	0.57
1:C:902:MET:HE1	1:C:1049:LEU:HD13	1.87	0.57
2:L:19:ARG:HA	2:L:82:GLN:HA	1.86	0.57
1:A:563:GLN:HA	1:C:41:LYS:HB3	1.87	0.57
5:O:73:ASP:HB2	5:O:80:TYR:HE2	1.70	0.57
1:A:853:GLN:HE22	1:A:959:LEU:CB	2.17	0.57
5:E:73:ASP:HB2	5:E:80:TYR:HE2	1.70	0.57
1:A:534:VAL:HG11	1:A:539:VAL:HG13	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:587:ILE:O	1:C:588:THR:OG1	2.23	0.57
4:D:43:PRO:HD2	5:E:110:TRP:HZ3	1.68	0.57
2:L:2:GLN:N	2:L:25:SER:O	2.38	0.57
4:N:5:THR:N	4:N:23:ARG:O	2.36	0.57
4:M:34:TRP:O	4:M:46:LEU:N	2.36	0.57
1:A:212:LEU:HD23	1:A:214:ARG:H	1.70	0.56
1:A:534:VAL:CG1	1:A:539:VAL:CG1	2.78	0.56
1:C:303:LEU:CD1	1:C:308:VAL:HG13	2.34	0.56
2:G:19:ARG:HA	2:G:82:GLN:HA	1.86	0.56
1:A:57:PRO:O	1:A:60:SER:HB2	2.05	0.56
1:A:905:ARG:NH1	1:A:1049:LEU:O	2.37	0.56
1:A:936:ASP:HA	1:A:939:SER:HB2	1.87	0.56
1:B:115:GLN:HB2	1:B:233:ILE:HD12	1.87	0.56
1:C:66:HIS:HA	1:C:264:ALA:HA	1.88	0.56
4:D:5:THR:N	4:D:23:ARG:O	2.37	0.56
4:D:33:HIS:HA	4:D:47:ILE:O	2.05	0.56
4:D:34:TRP:CD1	4:D:47:ILE:HB	2.39	0.56
4:N:22:CYS:SG	4:N:32:LEU:HD11	2.45	0.56
1:A:29:THR:HG22	1:A:62:VAL:O	2.05	0.56
1:A:115:GLN:HB2	1:A:233:ILE:HD12	1.86	0.56
1:B:320:VAL:HB	1:B:590:CYS:HB2	1.86	0.56
1:B:536:ASN:HA	1:B:551:VAL:HG13	1.87	0.56
4:D:22:CYS:SG	4:D:32:LEU:HD11	2.45	0.56
4:M:22:CYS:SG	4:M:32:LEU:HD11	2.45	0.56
1:A:53:ASP:OD1	1:A:54:LEU:N	2.37	0.56
1:A:559:PHE:CD1	1:C:43:PHE:CG	2.94	0.56
1:B:905:ARG:NH1	1:B:1049:LEU:O	2.37	0.56
1:C:115:GLN:HB2	1:C:233:ILE:HD12	1.87	0.56
2:K:2:GLN:N	2:K:25:SER:O	2.38	0.56
2:K:47:TRP:HZ2	2:K:50:VAL:HG13	1.71	0.56
4:N:34:TRP:CD1	4:N:47:ILE:HB	2.39	0.56
1:A:563:GLN:C	1:C:41:LYS:HB3	2.30	0.56
1:B:41:LYS:HB3	1:C:564:GLN:H	1.64	0.56
1:B:936:ASP:HA	1:B:939:SER:HB2	1.88	0.56
1:C:105:ILE:HG12	1:C:239:GLN:H	1.69	0.56
2:K:91:THR:HG23	2:K:116:THR:HA	1.88	0.56
4:M:90:THR:HA	4:M:95:TYR:CD1	2.41	0.56
1:A:417:LYS:HE2	1:A:455:LEU:HD12	1.88	0.56
4:M:33:HIS:HA	4:M:47:ILE:O	2.05	0.56
1:C:1102:TRP:HB2	1:C:1135:ASN:HD21	1.68	0.56
2:L:47:TRP:HZ2	2:L:50:VAL:HG13	1.71	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:40:ALA:HB3	5:H:43:LYS:HB2	1.88	0.56
1:A:23:GLN:O	1:A:24:LEU:HB2	2.06	0.56
1:B:106:PHE:HB3	1:B:235:ILE:HD13	1.88	0.56
1:B:383:SER:HG	5:E:69:THR:HG1	1.33	0.56
1:C:212:LEU:HD23	1:C:214:ARG:H	1.70	0.56
5:E:38:LYS:HD2	5:E:92:ALA:HB3	1.87	0.56
1:A:650:LEU:HD21	1:A:653:ALA:HB3	1.89	0.56
1:B:1102:TRP:CE2	1:B:1133:VAL:HG21	2.41	0.56
1:C:18:LEU:HD11	1:C:79:PHE:CG	2.41	0.56
5:E:4:LEU:HD23	5:E:24:VAL:HG22	1.87	0.56
1:C:303:LEU:HD23	1:C:305:SER:CB	2.28	0.55
1:C:367:VAL:HA	1:C:370:ASN:HB2	1.88	0.55
4:D:34:TRP:O	4:D:45:LEU:HD12	2.06	0.55
5:E:112:GLN:OE1	5:E:112:GLN:N	2.36	0.55
2:G:2:GLN:N	2:G:25:SER:O	2.38	0.55
2:G:91:THR:HG23	2:G:116:THR:HA	1.88	0.55
1:A:709:ASN:OD1	1:A:709:ASN:N	2.37	0.55
1:B:106:PHE:HB3	1:B:235:ILE:HG21	1.89	0.55
1:B:118:LEU:HD12	1:B:135:PHE:CE1	2.41	0.55
1:B:709:ASN:N	1:B:709:ASN:OD1	2.37	0.55
1:C:53:ASP:OD1	1:C:54:LEU:N	2.37	0.55
5:O:6:GLN:OE1	5:O:113:GLY:N	2.31	0.55
1:A:106:PHE:HB3	1:A:235:ILE:HG21	1.88	0.55
1:A:902:MET:HE1	1:A:1049:LEU:HD13	1.86	0.55
1:B:42:VAL:CG1	1:C:565:PHE:O	2.54	0.55
1:B:212:LEU:HD23	1:B:214:ARG:H	1.70	0.55
2:K:104:ASN:HB3	2:K:106:LYS:HG2	1.87	0.55
4:D:90:THR:HA	4:D:95:TYR:CD1	2.41	0.55
2:G:104:ASN:HB3	2:G:106:LYS:HG2	1.87	0.55
1:B:417:LYS:HE2	1:B:455:LEU:HD12	1.88	0.55
1:B:650:LEU:HD21	1:B:653:ALA:HB3	1.89	0.55
1:C:106:PHE:HB3	1:C:235:ILE:HG21	1.88	0.55
2:L:104:ASN:HB3	2:L:106:LYS:HG2	1.87	0.55
4:N:90:THR:HA	4:N:95:TYR:CD1	2.40	0.55
5:O:40:ALA:HB3	5:O:43:LYS:HB2	1.88	0.55
1:A:106:PHE:HB3	1:A:235:ILE:HD13	1.88	0.55
1:A:1019:ARG:NH2	1:A:1023:ASN:OD1	2.35	0.55
5:E:6:GLN:HE22	5:E:96:CYS:H	1.55	0.55
2:L:91:THR:HG23	2:L:116:THR:HA	1.88	0.55
1:B:299:THR:HG21	1:B:597:VAL:HG11	1.88	0.55
1:B:1019:ARG:NH2	1:B:1023:ASN:OD1	2.34	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:318:PHE:HZ	1:C:615:VAL:HG11	1.71	0.55
1:A:384:PRO:HD3	5:O:58:THR:OG1	2.07	0.55
1:A:546:LEU:HD22	1:A:565:PHE:CE1	2.42	0.55
1:C:437:ASN:ND2	1:C:506:GLN:OE1	2.40	0.55
5:H:6:GLN:HE22	5:H:96:CYS:H	1.55	0.55
5:H:38:LYS:HD2	5:H:92:ALA:HB3	1.87	0.55
2:G:47:TRP:HZ2	2:G:50:VAL:HG13	1.71	0.55
1:A:367:VAL:HA	1:A:370:ASN:HB2	1.88	0.55
1:C:904:TYR:O	1:C:907:ASN:N	2.40	0.55
4:N:34:TRP:O	4:N:45:LEU:HD12	2.07	0.55
1:A:43:PHE:CG	1:B:559:PHE:HD1	2.24	0.55
1:B:148:ASN:C	1:B:150:LYS:N	2.64	0.55
1:B:546:LEU:HD22	1:B:565:PHE:CE1	2.42	0.55
1:B:759:PHE:HD2	1:B:1001:LEU:HD21	1.71	0.54
1:C:747:THR:HA	1:C:750:SER:HB3	1.88	0.54
4:M:34:TRP:O	4:M:45:LEU:HD12	2.06	0.54
1:A:703:ASN:HD22	1:C:789:TYR:HE1	1.55	0.54
1:B:67:ALA:O	1:B:68:ILE:C	2.50	0.54
1:B:1087:ALA:HB1	1:B:1089:PHE:HE1	1.72	0.54
1:C:417:LYS:HE2	1:C:455:LEU:HD12	1.88	0.54
1:C:941:THR:HG22	1:C:944:ALA:H	1.72	0.54
1:A:103:GLY:HA3	1:A:119:ILE:O	2.08	0.54
1:C:278:LYS:CB	1:C:306:PHE:CE2	2.87	0.54
1:C:317:ASN:HD22	1:C:594:GLY:HA2	1.72	0.54
1:A:437:ASN:ND2	1:A:506:GLN:OE1	2.40	0.54
1:B:457:ARG:NH1	1:B:459:SER:OG	2.41	0.54
5:E:40:ALA:HB3	5:E:43:LYS:HB2	1.88	0.54
1:A:1087:ALA:HB1	1:A:1089:PHE:HE1	1.72	0.54
1:B:437:ASN:ND2	1:B:506:GLN:OE1	2.40	0.54
4:M:5:THR:N	4:M:23:ARG:O	2.37	0.54
5:O:28:SER:OG	5:O:31:ASN:ND2	2.40	0.54
1:A:562:PHE:CZ	1:C:38:TYR:HD2	2.26	0.54
1:B:19:THR:HG23	1:B:138:ASP:OD2	2.08	0.54
5:H:28:SER:OG	5:H:31:ASN:ND2	2.41	0.54
5:O:112:GLN:OE1	5:O:112:GLN:N	2.36	0.54
1:A:66:HIS:HA	1:A:264:ALA:HA	1.90	0.54
1:B:365:TYR:HA	1:B:368:LEU:HD13	1.90	0.54
1:B:367:VAL:HA	1:B:370:ASN:HB2	1.88	0.54
1:B:858:LEU:HD23	1:B:959:LEU:HD22	1.90	0.54
1:C:384:PRO:HD3	5:H:58:THR:OG1	2.07	0.54
2:K:37:VAL:HG12	2:K:47:TRP:HA	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:37:VAL:HG12	2:G:47:TRP:HA	1.90	0.54
1:A:118:LEU:HD22	1:A:129:LYS:HD2	1.90	0.54
1:A:759:PHE:HD2	1:A:1001:LEU:HD21	1.71	0.54
1:C:303:LEU:HD13	1:C:308:VAL:HG13	1.88	0.54
5:E:28:SER:OG	5:E:31:ASN:ND2	2.41	0.54
5:O:6:GLN:HE22	5:O:96:CYS:H	1.55	0.54
1:A:457:ARG:NH1	1:A:459:SER:OG	2.41	0.54
1:B:384:PRO:HD3	5:E:58:THR:OG1	2.07	0.54
1:C:106:PHE:HB3	1:C:235:ILE:HD13	1.89	0.54
1:C:906:PHE:CE2	1:C:916:LEU:HB2	2.42	0.54
2:L:62:ASP:HA	2:L:65:LYS:HB2	1.90	0.54
4:M:22:CYS:O	4:M:70:PHE:N	2.41	0.54
1:B:108:THR:O	1:B:237:ARG:NH2	2.41	0.54
1:C:372:ALA:HB1	4:N:94:PRO:CD	2.36	0.54
5:E:27:TYR:CE2	5:E:98:ARG:HD3	2.43	0.54
1:B:875:SER:O	1:B:879:ALA:N	2.41	0.53
2:K:62:ASP:HA	2:K:65:LYS:HB2	1.90	0.53
4:M:34:TRP:CE3	4:M:72:LEU:HB2	2.43	0.53
1:A:875:SER:O	1:A:879:ALA:N	2.41	0.53
1:C:372:ALA:CA	4:N:93:TRP:CB	2.35	0.53
4:N:34:TRP:CE3	4:N:72:LEU:HB2	2.43	0.53
1:C:365:TYR:HA	1:C:368:LEU:HD13	1.90	0.53
4:D:34:TRP:CE3	4:D:72:LEU:HB2	2.43	0.53
1:A:108:THR:O	1:A:237:ARG:NH2	2.41	0.53
5:O:35:HIS:N	5:O:97:ALA:O	2.35	0.53
1:A:372:ALA:HB1	4:M:94:PRO:CD	2.36	0.53
1:A:559:PHE:HD1	1:C:43:PHE:CG	2.26	0.53
5:H:27:TYR:CE2	5:H:98:ARG:HD3	2.43	0.53
1:B:170:TYR:CE2	1:B:172:SER:HB2	2.44	0.53
1:C:457:ARG:NH1	1:C:459:SER:OG	2.41	0.53
1:A:858:LEU:HD23	1:A:959:LEU:HD22	1.90	0.53
1:C:34:ARG:NE	1:C:216:LEU:HD23	2.24	0.53
1:C:276:LEU:N	1:C:276:LEU:CD1	2.72	0.53
2:K:11:VAL:HA	2:K:116:THR:HB	1.91	0.53
2:L:11:VAL:HA	2:L:116:THR:HB	1.91	0.53
5:H:112:GLN:OE1	5:H:112:GLN:N	2.36	0.53
2:G:11:VAL:HA	2:G:116:THR:HB	1.91	0.53
1:B:372:ALA:HB1	4:D:94:PRO:CD	2.36	0.53
1:C:709:ASN:N	1:C:709:ASN:OD1	2.40	0.53
1:C:825:LYS:HE3	1:C:938:LEU:O	2.08	0.53
5:H:4:LEU:HD12	5:H:110:TRP:HA	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:ARG:NE	1:A:216:LEU:HD23	2.24	0.53
1:A:43:PHE:CE1	1:B:558:LYS:O	2.62	0.53
1:A:334:ASN:HB2	1:A:361:CYS:HA	1.91	0.53
1:C:170:TYR:CE2	1:C:172:SER:HB2	2.44	0.53
1:C:202:LYS:HG2	1:C:228:ASP:HA	1.91	0.53
1:C:980:ILE:HD12	1:C:996:LEU:HD11	1.89	0.53
5:O:27:TYR:CE2	5:O:98:ARG:HD3	2.43	0.53
1:A:373:SER:C	4:M:92:PHE:HA	2.34	0.53
1:C:108:THR:O	1:C:237:ARG:NH2	2.41	0.53
1:C:210:ILE:HD12	1:C:217:PRO:HD3	1.92	0.53
1:C:373:SER:C	4:N:92:PHE:HA	2.33	0.53
1:B:373:SER:C	4:D:92:PHE:HA	2.33	0.52
1:C:84:LEU:N	1:C:238:PHE:O	2.29	0.52
1:C:278:LYS:CB	1:C:306:PHE:HE2	2.22	0.52
5:E:4:LEU:HD12	5:E:110:TRP:HA	1.91	0.52
1:A:276:LEU:HD11	1:A:306:PHE:HE1	0.39	0.52
1:A:565:PHE:CB	1:C:42:VAL:HG22	2.17	0.52
1:B:53:ASP:OD1	1:B:54:LEU:N	2.37	0.52
1:B:202:LYS:HG2	1:B:228:ASP:HA	1.91	0.52
4:D:97:PHE:CZ	5:E:47:TRP:HB2	2.44	0.52
5:O:4:LEU:HD12	5:O:110:TRP:HA	1.91	0.52
1:A:689:SER:OG	1:A:690:GLN:N	2.42	0.52
1:B:131:CYS:HB2	1:B:133:PHE:CE2	2.44	0.52
2:K:70:ILE:HB	2:K:81:LEU:HD12	1.91	0.52
4:N:97:PHE:HD2	5:H:45:LEU:CB	2.20	0.52
2:G:62:ASP:HA	2:G:65:LYS:HB2	1.90	0.52
1:A:324:GLU:CD	1:A:534:VAL:HG21	2.27	0.52
1:B:299:THR:CG2	1:B:597:VAL:HG21	2.39	0.52
1:B:914:ASN:HA	1:C:1089:PHE:HE2	1.73	0.52
3:I:63:SER:O	3:I:74:THR:CB	2.57	0.52
1:A:131:CYS:HB2	1:A:133:PHE:CE2	2.44	0.52
1:B:786:LYS:HG3	1:B:787:GLN:HG3	1.91	0.52
1:B:913:GLN:HE21	1:C:1089:PHE:HB3	1.74	0.52
4:M:97:PHE:CZ	5:O:47:TRP:HB2	2.44	0.52
1:B:29:THR:HG22	1:B:62:VAL:O	2.09	0.52
1:C:131:CYS:HB2	1:C:133:PHE:CE2	2.44	0.52
1:A:567:ARG:CG	1:C:42:VAL:HG11	2.40	0.52
1:A:869:MET:HE1	1:B:669:GLY:HA3	1.92	0.52
4:D:22:CYS:O	4:D:70:PHE:N	2.41	0.52
1:A:365:TYR:HA	1:A:368:LEU:HD13	1.90	0.52
1:C:66:HIS:CD2	1:C:69:HIS:CG	2.95	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:334:ASN:HB2	1:C:361:CYS:HA	1.91	0.52
2:L:37:VAL:HG12	2:L:47:TRP:HA	1.90	0.52
1:A:244:LEU:HD22	1:A:259:THR:HA	1.92	0.52
1:B:186:PHE:CD1	1:B:209:PRO:HB3	2.45	0.52
1:B:210:ILE:HD12	1:B:217:PRO:HD3	1.92	0.52
4:N:97:PHE:CZ	5:H:47:TRP:HB2	2.44	0.52
4:M:6:GLN:HE22	4:M:87:CYS:N	2.08	0.52
1:A:170:TYR:CE2	1:A:172:SER:HB2	2.44	0.52
1:B:34:ARG:NE	1:B:216:LEU:HD23	2.24	0.52
1:C:186:PHE:CD1	1:C:209:PRO:HB3	2.45	0.52
5:H:37:VAL:O	5:H:95:TYR:N	2.38	0.52
1:A:202:LYS:HG2	1:A:228:ASP:HA	1.91	0.51
1:A:1089:PHE:CE2	1:C:914:ASN:HA	2.44	0.51
1:B:201:PHE:CB	1:B:231:ILE:HG13	2.29	0.51
1:B:327:VAL:CA	1:B:542:ASN:HB3	2.39	0.51
1:C:22:THR:CG2	1:C:78:ARG:CG	2.80	0.51
5:E:35:HIS:N	5:E:97:ALA:O	2.35	0.51
1:A:210:ILE:HD12	1:A:217:PRO:HD3	1.92	0.51
1:A:564:GLN:H	1:C:41:LYS:CB	2.21	0.51
1:B:328:ARG:HB3	1:B:543:PHE:HA	1.92	0.51
1:C:666:ILE:HD11	1:C:672:ALA:HB2	1.92	0.51
4:D:6:GLN:HE22	4:D:87:CYS:N	2.08	0.51
1:A:186:PHE:CD1	1:A:209:PRO:HB3	2.45	0.51
2:L:70:ILE:HB	2:L:81:LEU:HD12	1.91	0.51
4:N:22:CYS:O	4:N:70:PHE:N	2.41	0.51
3:F:94:THR:OG1	3:F:96:ARG:NH1	2.44	0.51
1:B:38:TYR:OH	1:B:284:THR:HA	2.11	0.51
1:B:643:PHE:CE2	1:B:645:THR:HG22	2.45	0.51
1:C:858:LEU:HD21	1:C:962:LEU:HD23	1.93	0.51
1:A:565:PHE:O	1:C:43:PHE:N	2.37	0.51
1:A:717:ASN:OD1	1:A:718:PHE:N	2.43	0.51
1:A:786:LYS:HG3	1:A:787:GLN:HG3	1.91	0.51
1:B:296:LEU:HD11	1:B:606:ASN:O	2.11	0.51
1:B:689:SER:OG	1:B:690:GLN:N	2.42	0.51
1:B:717:ASN:OD1	1:B:718:PHE:N	2.43	0.51
1:C:29:THR:CG2	1:C:62:VAL:HB	2.41	0.51
4:D:42:SER:HB2	5:E:110:TRP:CE3	2.46	0.51
4:N:6:GLN:HE22	4:N:87:CYS:N	2.08	0.51
2:G:11:VAL:HG11	2:G:121:SER:HA	1.93	0.51
5:O:35:HIS:NE2	5:O:99:SER:HB2	2.26	0.51
1:B:328:ARG:HG3	1:B:579:PRO:HG2	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:94:THR:OG1	3:J:96:ARG:NH1	2.44	0.51
5:O:20:ILE:HD12	5:O:94:TYR:HD2	1.76	0.51
1:B:904:TYR:CE1	1:C:1107:ARG:HD3	2.45	0.51
3:I:94:THR:OG1	3:I:96:ARG:NH1	2.44	0.51
5:E:35:HIS:NE2	5:E:99:SER:HB2	2.26	0.51
5:H:20:ILE:HD12	5:H:94:TYR:HD2	1.76	0.51
4:M:42:SER:HB2	5:O:110:TRP:CE3	2.46	0.51
4:M:84:ILE:HG12	4:M:102:LYS:HA	1.93	0.51
5:O:51:ILE:HG12	5:O:52:ASP:N	2.26	0.51
1:A:84:LEU:N	1:A:238:PHE:O	2.29	0.51
1:A:122:ASN:ND2	1:A:127:VAL:HG12	2.25	0.51
1:A:122:ASN:HD21	1:A:127:VAL:HG12	1.76	0.51
4:N:42:SER:HB2	5:H:110:TRP:CE3	2.46	0.51
1:A:115:GLN:HE21	1:A:167:THR:HG21	1.76	0.51
1:A:245:HIS:CD2	1:A:260:ALA:HB2	2.46	0.51
1:B:551:VAL:N	1:B:588:THR:O	2.42	0.51
5:E:6:GLN:H	5:E:112:GLN:HE22	1.59	0.51
5:E:38:LYS:N	5:E:46:GLU:O	2.31	0.51
4:N:84:ILE:HG12	4:N:102:LYS:HA	1.93	0.51
4:M:97:PHE:HD2	5:O:45:LEU:CB	2.20	0.51
1:A:41:LYS:HB3	1:B:563:GLN:C	2.34	0.51
1:B:46:SER:HB3	1:B:281:GLU:HA	1.93	0.51
1:B:914:ASN:HA	1:C:1089:PHE:CE2	2.46	0.51
1:C:1028:LYS:NZ	1:C:1042:PHE:O	2.43	0.51
5:E:51:ILE:HG12	5:E:52:ASP:N	2.26	0.51
1:A:643:PHE:CE2	1:A:645:THR:HG22	2.45	0.50
1:C:401:VAL:HG22	1:C:509:ARG:HG2	1.93	0.50
5:E:20:ILE:HD12	5:E:94:TYR:HD2	1.76	0.50
5:E:47:TRP:HZ2	5:E:50:TYR:CD2	2.29	0.50
5:O:47:TRP:HZ2	5:O:50:TYR:CD2	2.29	0.50
3:J:5:THR:HB	3:J:24:ARG:HB2	1.94	0.50
1:B:119:ILE:HG13	1:B:119:ILE:O	2.12	0.50
1:C:337:PRO:HB2	1:C:340:GLU:HB2	1.93	0.50
2:G:70:ILE:HB	2:G:81:LEU:HD12	1.91	0.50
1:B:48:LEU:CD1	1:B:306:PHE:CD2	2.93	0.50
1:C:18:LEU:HD12	1:C:18:LEU:C	2.32	0.50
1:C:786:LYS:NZ	1:C:892:ALA:HA	2.26	0.50
2:K:35:HIS:HB2	2:K:97:ALA:HB3	1.94	0.50
4:D:26:GLN:HG3	4:D:27:SER:H	1.76	0.50
3:J:63:SER:O	3:J:74:THR:CB	2.57	0.50
5:H:35:HIS:NE2	5:H:99:SER:HB2	2.26	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:6:GLN:H	5:O:112:GLN:HE22	1.59	0.50
1:A:401:VAL:HG22	1:A:509:ARG:HG2	1.93	0.50
1:A:735:SER:O	1:A:859:THR:OG1	2.27	0.50
2:L:38:ARG:NH2	2:L:46:GLU:OE1	2.38	0.50
5:O:73:ASP:HB2	5:O:80:TYR:CE2	2.46	0.50
1:A:276:LEU:HD12	1:A:306:PHE:CZ	2.43	0.50
1:A:855:PHE:HD2	1:B:572:THR:HG21	1.75	0.50
1:B:17:ASN:HD22	1:B:137:ASN:HD21	1.60	0.50
1:C:318:PHE:CZ	1:C:615:VAL:HG11	2.47	0.50
2:L:35:HIS:HB2	2:L:97:ALA:HB3	1.94	0.50
2:L:40:ALA:HB3	2:L:43:LYS:HB2	1.94	0.50
5:H:47:TRP:HZ2	5:H:50:TYR:CD2	2.29	0.50
2:G:35:HIS:HB2	2:G:97:ALA:HB3	1.94	0.50
3:F:63:SER:O	3:F:74:THR:CB	2.57	0.50
1:A:337:PRO:HB2	1:A:340:GLU:HB2	1.93	0.50
3:I:5:THR:HB	3:I:24:ARG:HB2	1.94	0.50
5:E:73:ASP:HB2	5:E:80:TYR:CE2	2.46	0.50
5:H:51:ILE:HG12	5:H:52:ASP:N	2.26	0.50
1:B:19:THR:CG2	1:B:138:ASP:OD2	2.60	0.50
1:C:115:GLN:HE21	1:C:167:THR:HG21	1.77	0.50
1:C:372:ALA:O	4:N:92:PHE:CB	2.60	0.50
5:H:73:ASP:HB2	5:H:80:TYR:CE2	2.46	0.50
5:O:35:HIS:CD2	5:O:99:SER:HB2	2.47	0.50
1:A:914:ASN:HA	1:B:1089:PHE:HE2	1.76	0.49
1:C:29:THR:HG23	1:C:62:VAL:HB	1.94	0.49
1:C:710:ASN:O	1:C:1077:THR:HG22	2.12	0.49
2:K:11:VAL:HG11	2:K:121:SER:HA	1.93	0.49
4:N:20:ILE:HD12	4:N:85:TYR:CD2	2.47	0.49
1:A:759:PHE:CD2	1:A:1001:LEU:HD21	2.46	0.49
2:K:40:ALA:HB3	2:K:43:LYS:HB2	1.94	0.49
4:D:82:PHE:HB3	4:D:105:ILE:HD12	1.94	0.49
4:D:84:ILE:HG12	4:D:102:LYS:HA	1.93	0.49
4:N:82:PHE:HB3	4:N:105:ILE:HD12	1.94	0.49
5:H:35:HIS:ND1	5:H:50:TYR:HB3	2.28	0.49
3:F:5:THR:HB	3:F:24:ARG:HB2	1.94	0.49
1:A:935:GLN:O	1:A:939:SER:N	2.40	0.49
5:H:10:GLU:HG3	5:H:18:VAL:HG23	1.95	0.49
2:G:24:ALA:HB3	2:G:77:ASN:HB3	1.95	0.49
1:A:372:ALA:O	4:M:92:PHE:CB	2.60	0.49
1:B:326:ILE:CA	1:B:531:THR:OG1	2.60	0.49
1:C:1114:ILE:O	1:C:1119:ASN:ND2	2.46	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:6:GLN:H	5:H:112:GLN:HE22	1.59	0.49
2:G:40:ALA:HB3	2:G:43:LYS:HB2	1.94	0.49
4:M:26:GLN:HG3	4:M:27:SER:H	1.76	0.49
6:Y:1:NAG:H4	6:Y:2:NAG:N2	2.27	0.49
1:B:118:LEU:HD12	1:B:135:PHE:CZ	2.47	0.49
1:B:401:VAL:HG22	1:B:509:ARG:HG2	1.93	0.49
1:B:759:PHE:CD2	1:B:1001:LEU:HD21	2.47	0.49
1:C:276:LEU:O	1:C:288:ALA:HA	2.12	0.49
1:C:1102:TRP:CG	1:C:1135:ASN:ND2	2.81	0.49
5:E:35:HIS:CD2	5:E:99:SER:HB2	2.47	0.49
2:L:11:VAL:HG11	2:L:121:SER:HA	1.93	0.49
4:N:26:GLN:HG3	4:N:27:SER:H	1.76	0.49
4:M:31:ASN:CG	4:M:90:THR:HG21	2.38	0.49
5:O:35:HIS:ND1	5:O:50:TYR:HB3	2.27	0.49
1:A:448:ASN:HB3	1:A:497:PHE:HB2	1.95	0.49
1:B:115:GLN:HE21	1:B:167:THR:HG21	1.77	0.49
2:L:24:ALA:HB3	2:L:77:ASN:HB3	1.95	0.49
5:O:19:LYS:HA	5:O:81:MET:O	2.12	0.49
6:d:2:NAG:HO3	6:d:2:NAG:C7	2.20	0.49
1:B:89:GLY:HA3	1:B:270:LEU:HD12	1.95	0.49
1:B:118:LEU:HD22	1:B:129:LYS:HD2	1.93	0.49
1:B:722:VAL:HG22	1:B:1065:VAL:HG22	1.94	0.49
1:C:46:SER:HA	1:C:279:TYR:O	2.13	0.49
1:C:108:THR:HG21	6:Z:1:NAG:C6	2.42	0.49
1:C:303:LEU:HD13	1:C:308:VAL:CG2	2.41	0.49
1:C:393:THR:O	1:C:523:THR:OG1	2.31	0.49
2:K:38:ARG:NH2	2:K:46:GLU:OE1	2.38	0.49
5:E:10:GLU:HG3	5:E:18:VAL:HG23	1.95	0.49
1:A:276:LEU:HG	1:A:289:VAL:HB	1.95	0.49
1:A:290:ASP:O	1:A:297:SER:HB3	2.12	0.49
1:A:551:VAL:N	1:A:588:THR:O	2.43	0.49
1:B:245:HIS:CD2	1:B:260:ALA:HB2	2.47	0.49
1:B:337:PRO:HB2	1:B:340:GLU:HB2	1.93	0.49
1:B:894:LEU:CD2	1:C:1072:GLU:HG2	2.42	0.49
1:C:328:ARG:CZ	1:C:533:LEU:HB2	2.42	0.49
1:C:1054:GLN:N	1:C:1061:VAL:O	2.45	0.49
5:E:19:LYS:HA	5:E:81:MET:O	2.12	0.49
5:H:35:HIS:CD2	5:H:99:SER:HB2	2.47	0.49
4:M:20:ILE:HD12	4:M:85:TYR:CD2	2.47	0.49
1:A:393:THR:O	1:A:523:THR:OG1	2.31	0.49
1:A:567:ARG:HG3	1:C:42:VAL:CG1	2.41	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:GLY:C	1:B:186:PHE:H	2.21	0.49
1:B:853:GLN:HE22	1:B:959:LEU:CB	2.15	0.49
1:B:855:PHE:HE1	1:C:589:PRO:HD3	1.78	0.49
1:C:717:ASN:OD1	1:C:718:PHE:N	2.44	0.49
3:J:93:SER:OG	3:J:94:THR:N	2.46	0.49
4:N:31:ASN:CG	4:N:90:THR:HG21	2.38	0.49
5:H:35:HIS:N	5:H:97:ALA:O	2.35	0.49
4:M:65:GLY:HA2	4:M:70:PHE:HA	1.95	0.49
5:O:10:GLU:HG3	5:O:18:VAL:HG23	1.95	0.49
1:A:287:ASP:CG	1:A:306:PHE:CZ	2.91	0.49
1:A:1139:ASP:CG	1:A:1142:GLN:H	2.21	0.49
1:B:182:LYS:HG3	1:B:186:PHE:CD2	2.48	0.49
1:B:299:THR:CG2	1:B:597:VAL:CG2	2.91	0.49
1:B:369:TYR:CB	4:D:93:TRP:CZ2	2.95	0.49
1:C:303:LEU:CD1	1:C:308:VAL:HA	2.42	0.49
4:N:65:GLY:HA2	4:N:70:PHE:HA	1.95	0.49
4:M:82:PHE:HB3	4:M:105:ILE:HD12	1.93	0.49
1:C:808:ASP:OD2	1:C:811:LYS:HG2	2.13	0.48
4:D:20:ILE:HD12	4:D:85:TYR:CD2	2.47	0.48
4:D:65:GLY:HA2	4:D:70:PHE:HA	1.95	0.48
5:E:4:LEU:CD2	5:E:24:VAL:HG22	2.43	0.48
5:O:37:VAL:O	5:O:95:TYR:N	2.38	0.48
1:A:180:GLU:HG3	1:A:181:GLY:N	2.27	0.48
1:B:372:ALA:O	4:D:92:PHE:CB	2.60	0.48
5:E:35:HIS:ND1	5:E:50:TYR:HB3	2.27	0.48
5:E:112:GLN:H	5:E:112:GLN:CD	2.21	0.48
1:B:276:LEU:HG	1:B:289:VAL:HB	1.95	0.48
1:B:1139:ASP:CG	1:B:1142:GLN:H	2.21	0.48
1:C:89:GLY:HA3	1:C:270:LEU:HD12	1.95	0.48
5:H:4:LEU:CD2	5:H:24:VAL:HG22	2.43	0.48
1:A:231:ILE:HG22	1:A:233:ILE:HG22	1.95	0.48
1:A:722:VAL:HG22	1:A:1065:VAL:HG22	1.94	0.48
1:C:108:THR:CG2	6:Z:1:NAG:O6	2.61	0.48
1:C:1145:LEU:O	1:C:1147:SER:N	2.46	0.48
4:D:97:PHE:HD2	5:E:45:LEU:CB	2.20	0.48
1:A:89:GLY:HA3	1:A:270:LEU:HD12	1.95	0.48
1:A:182:LYS:HG3	1:A:186:PHE:CD2	2.48	0.48
1:B:41:LYS:O	1:C:563:GLN:CA	2.62	0.48
1:C:184:GLY:C	1:C:186:PHE:H	2.21	0.48
5:O:4:LEU:CD2	5:O:24:VAL:HG22	2.43	0.48
1:A:20:THR:OG1	1:A:79:PHE:HB3	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1032:CYS:SG	1:B:1048:HIS:NE2	2.86	0.48
1:C:180:GLU:HG3	1:C:181:GLY:N	2.27	0.48
5:O:47:TRP:CZ2	5:O:50:TYR:HD2	2.32	0.48
1:A:184:GLY:C	1:A:186:PHE:H	2.21	0.48
1:B:796:ASP:OD1	1:B:796:ASP:N	2.46	0.48
1:C:182:LYS:HG3	1:C:186:PHE:CD2	2.48	0.48
1:A:716:THR:HA	1:A:1110:TYR:HB3	1.96	0.48
1:B:120:VAL:HG13	1:B:141:LEU:HD11	1.95	0.48
1:B:1145:LEU:O	1:B:1147:SER:N	2.47	0.48
1:C:620:VAL:HG11	1:C:651:ILE:HD11	1.96	0.48
4:D:31:ASN:CG	4:D:90:THR:HG21	2.38	0.48
5:E:47:TRP:CZ2	5:E:50:TYR:HD2	2.32	0.48
2:L:68:PHE:HB3	2:L:81:LEU:HD21	1.96	0.48
5:H:19:LYS:HA	5:H:81:MET:O	2.12	0.48
1:A:562:PHE:HZ	1:C:38:TYR:HD2	1.61	0.48
1:A:1032:CYS:SG	1:A:1048:HIS:NE2	2.87	0.48
1:B:716:THR:HA	1:B:1110:TYR:HB3	1.96	0.48
1:C:369:TYR:CB	4:N:93:TRP:CZ2	2.95	0.48
4:D:32:LEU:HD13	4:D:70:PHE:CG	2.48	0.48
3:F:93:SER:OG	3:F:94:THR:N	2.46	0.48
5:O:3:GLN:HB2	5:O:25:SER:OG	2.14	0.48
1:A:41:LYS:CB	1:B:564:GLN:H	2.19	0.48
1:A:709:ASN:ND2	7:A:1305:NAG:O7	2.47	0.48
1:A:953:ASN:O	1:A:957:GLN:N	2.39	0.48
1:C:330:PRO:HA	1:C:579:PRO:HB2	1.96	0.48
2:K:24:ALA:HB3	2:K:77:ASN:HB3	1.95	0.48
3:I:93:SER:OG	3:I:94:THR:N	2.46	0.48
4:N:32:LEU:HD13	4:N:70:PHE:CG	2.48	0.48
5:H:38:LYS:N	5:H:46:GLU:O	2.31	0.48
1:A:763:LEU:HD22	1:A:1008:VAL:HG21	1.96	0.47
1:B:763:LEU:HD22	1:B:1008:VAL:HG21	1.96	0.47
4:D:32:LEU:HD21	4:D:87:CYS:CB	2.43	0.47
5:H:3:GLN:HB2	5:H:25:SER:OG	2.14	0.47
5:H:47:TRP:CZ2	5:H:50:TYR:HD2	2.32	0.47
4:M:32:LEU:HD13	4:M:70:PHE:CG	2.48	0.47
1:A:14:GLN:HB3	1:A:158:ARG:HD3	1.96	0.47
1:A:64:TRP:HZ2	1:A:66:HIS:CE1	2.06	0.47
1:A:156:GLU:OE1	1:A:156:GLU:N	2.44	0.47
1:A:369:TYR:CB	5:O:62:LEU:HD21	2.45	0.47
1:B:23:GLN:HG2	1:B:24:LEU:N	2.30	0.47
1:B:194:PHE:HB3	1:B:201:PHE:CZ	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:535:LYS:HA	1:B:552:LEU:O	2.13	0.47
1:C:815:ARG:HD2	1:C:823:PHE:CE2	2.49	0.47
5:E:3:GLN:HB2	5:E:25:SER:OG	2.14	0.47
6:Y:1:NAG:H4	6:Y:2:NAG:C7	2.43	0.47
1:A:146:HIS:C	1:A:148:ASN:H	2.22	0.47
1:B:121:ASN:HD22	1:B:176:LEU:HB2	1.78	0.47
1:B:327:VAL:C	1:B:542:ASN:O	2.53	0.47
1:C:278:LYS:HE3	1:C:287:ASP:HB3	1.95	0.47
1:C:742:ILE:O	1:C:1000:ARG:NH1	2.44	0.47
2:K:68:PHE:HB3	2:K:81:LEU:HD21	1.95	0.47
1:A:278:LYS:HE3	1:A:287:ASP:HB3	1.95	0.47
1:C:23:GLN:O	1:C:23:GLN:HG2	2.15	0.47
1:C:156:GLU:OE1	1:C:156:GLU:N	2.44	0.47
1:C:287:ASP:OD2	1:C:306:PHE:CD2	2.67	0.47
1:C:1102:TRP:CB	1:C:1135:ASN:ND2	2.75	0.47
1:A:109:THR:HG22	1:A:111:ASP:HB3	1.97	0.47
1:A:796:ASP:OD1	1:A:796:ASP:N	2.46	0.47
1:A:1145:LEU:O	1:A:1147:SER:N	2.46	0.47
1:B:168:PHE:CZ	1:B:170:TYR:HB2	2.50	0.47
1:B:783:ALA:HB2	1:B:873:TYR:CZ	2.50	0.47
1:C:186:PHE:C	1:C:188:ASN:H	2.22	0.47
1:C:448:ASN:HB3	1:C:497:PHE:HB2	1.95	0.47
5:E:47:TRP:HZ2	5:E:50:TYR:HD2	1.61	0.47
5:O:47:TRP:HZ2	5:O:50:TYR:HD2	1.61	0.47
1:A:123:ALA:HA	1:A:124:THR:HA	1.68	0.47
1:A:194:PHE:HB3	1:A:201:PHE:CZ	2.49	0.47
1:B:186:PHE:C	1:B:188:ASN:H	2.22	0.47
1:B:283:GLY:O	1:B:284:THR:HB	2.14	0.47
1:B:328:ARG:HD2	1:B:580:GLN:HG3	1.97	0.47
1:B:448:ASN:HB3	1:B:497:PHE:HB2	1.95	0.47
1:B:709:ASN:ND2	7:B:1304:NAG:O7	2.47	0.47
1:B:1088:HIS:C	1:B:1089:PHE:HD1	2.23	0.47
3:J:35:TRP:HA	3:J:87:TYR:O	2.15	0.47
2:G:38:ARG:NH2	2:G:46:GLU:OE1	2.38	0.47
4:M:35:TYR:CE1	4:M:88:GLN:HG3	2.50	0.47
1:A:38:TYR:CD1	1:A:285:ILE:HD12	2.50	0.47
1:A:121:ASN:HA	1:A:126:VAL:CG2	2.39	0.47
1:A:180:GLU:O	1:A:182:LYS:HG2	2.15	0.47
1:A:699:LEU:HD23	1:C:873:TYR:CZ	2.50	0.47
1:A:783:ALA:HB2	1:A:873:TYR:CZ	2.50	0.47
1:B:14:GLN:HB3	1:B:158:ARG:HD3	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:VAL:C	1:C:565:PHE:O	2.57	0.47
1:B:369:TYR:CB	5:E:62:LEU:HD21	2.45	0.47
1:C:120:VAL:HG13	1:C:141:LEU:HD11	1.96	0.47
1:C:180:GLU:O	1:C:182:LYS:HG2	2.15	0.47
1:C:194:PHE:HB3	1:C:201:PHE:CZ	2.49	0.47
4:N:32:LEU:HD21	4:N:87:CYS:CB	2.43	0.47
4:N:35:TYR:CE1	4:N:88:GLN:HG3	2.50	0.47
5:H:47:TRP:HZ2	5:H:50:TYR:HD2	1.60	0.47
4:M:32:LEU:HD21	4:M:87:CYS:CB	2.43	0.47
5:O:112:GLN:H	5:O:112:GLN:CD	2.21	0.47
1:A:418:ILE:HA	1:A:422:ASN:HB2	1.97	0.47
1:A:486:PHE:HA	3:F:32:TYR:HE2	1.80	0.47
1:C:722:VAL:HG22	1:C:1065:VAL:HG22	1.97	0.47
2:K:60:TYR:HE1	2:K:70:ILE:HG22	1.80	0.47
5:H:112:GLN:H	5:H:112:GLN:CD	2.21	0.47
2:G:68:PHE:HB3	2:G:81:LEU:HD21	1.95	0.47
5:O:38:LYS:N	5:O:46:GLU:O	2.31	0.47
5:H:12:LYS:O	5:H:118:VAL:HA	2.15	0.47
5:O:12:LYS:O	5:O:118:VAL:HA	2.15	0.47
5:O:97:ALA:HB1	5:O:107:MET:CB	2.44	0.47
1:B:21:ARG:HG3	1:B:22:THR:N	2.30	0.47
1:B:41:LYS:HB3	1:C:563:GLN:C	2.38	0.47
1:B:180:GLU:HG3	1:B:181:GLY:N	2.27	0.47
1:C:14:GLN:HB3	1:C:158:ARG:HD3	1.96	0.47
1:C:591:SER:HB3	1:C:615:VAL:HG12	1.97	0.47
4:N:28:ILE:HD13	4:N:70:PHE:CZ	2.50	0.47
3:F:35:TRP:HA	3:F:87:TYR:O	2.15	0.47
1:B:418:ILE:HA	1:B:422:ASN:HB2	1.97	0.46
1:C:328:ARG:HD3	1:C:328:ARG:HA	1.78	0.46
1:C:369:TYR:CB	5:H:62:LEU:HD21	2.45	0.46
1:C:850:ILE:HB	1:C:854:LYS:HE3	1.97	0.46
4:M:28:ILE:HD13	4:M:70:PHE:CZ	2.50	0.46
4:M:89:GLN:C	4:M:95:TYR:HD1	2.23	0.46
1:A:715:PRO:HD3	1:C:894:LEU:HD13	1.98	0.46
1:B:953:ASN:O	1:B:957:GLN:N	2.39	0.46
1:C:486:PHE:HA	3:J:32:TYR:HE2	1.80	0.46
1:C:1016:ALA:HA	1:C:1019:ARG:HB3	1.98	0.46
4:D:13:SER:OG	4:D:106:LEU:HB2	2.16	0.46
4:D:35:TYR:CE1	4:D:88:GLN:HG3	2.50	0.46
1:A:168:PHE:CZ	1:A:170:TYR:HB2	2.50	0.46
1:A:710:ASN:O	1:A:1077:THR:HG22	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:961:THR:O	1:A:965:GLN:HG2	2.15	0.46
1:B:188:ASN:O	1:B:190:ARG:HG3	2.16	0.46
1:B:1088:HIS:CE1	1:B:1122:VAL:HG22	2.50	0.46
1:C:188:ASN:O	1:C:190:ARG:HG3	2.16	0.46
5:E:86:LEU:HB3	5:E:118:VAL:HG21	1.97	0.46
5:H:97:ALA:HB1	5:H:107:MET:CB	2.44	0.46
4:M:12:VAL:HG12	4:M:13:SER:H	1.81	0.46
1:A:906:PHE:CE2	1:A:916:LEU:HB2	2.50	0.46
1:B:393:THR:HG21	1:B:518:LEU:H	1.81	0.46
1:B:486:PHE:HA	3:I:32:TYR:HE2	1.80	0.46
1:C:145:TYR:HE1	1:C:150:LYS:HA	1.80	0.46
4:N:31:ASN:OD1	4:N:32:LEU:N	2.49	0.46
1:A:372:ALA:CB	4:M:94:PRO:HD2	2.39	0.46
1:B:43:PHE:HD1	1:C:563:GLN:OE1	1.99	0.46
1:B:1028:LYS:O	1:B:1032:CYS:N	2.46	0.46
1:C:168:PHE:CZ	1:C:170:TYR:HB2	2.50	0.46
1:C:600:PRO:HG3	1:C:674:TYR:CD1	2.51	0.46
4:D:12:VAL:HG12	4:D:13:SER:H	1.81	0.46
4:D:31:ASN:OD1	4:D:32:LEU:N	2.49	0.46
4:N:13:SER:OG	4:N:106:LEU:HB2	2.16	0.46
4:N:33:HIS:ND1	5:H:106:VAL:HG12	2.31	0.46
1:A:17:ASN:HB2	1:A:138:ASP:OD2	2.15	0.46
1:A:48:LEU:CD1	1:A:305:SER:HA	2.46	0.46
1:A:186:PHE:C	1:A:188:ASN:H	2.22	0.46
1:A:188:ASN:O	1:A:190:ARG:HG3	2.16	0.46
1:A:1088:HIS:CE1	1:A:1122:VAL:HG22	2.50	0.46
1:A:1116:THR:HB	1:A:1140:PRO:HD3	1.97	0.46
1:B:536:ASN:N	1:B:552:LEU:O	2.39	0.46
1:B:1116:THR:HB	1:B:1140:PRO:HD3	1.97	0.46
1:C:1006:THR:O	1:C:1010:GLN:HG2	2.15	0.46
4:D:33:HIS:ND1	5:E:106:VAL:HG12	2.31	0.46
5:E:12:LYS:O	5:E:118:VAL:HA	2.15	0.46
1:A:559:PHE:HA	1:C:43:PHE:CD1	2.51	0.46
1:B:23:GLN:O	1:B:24:LEU:HB2	2.15	0.46
1:B:327:VAL:HA	1:B:542:ASN:CB	2.45	0.46
1:B:855:PHE:CE1	1:C:589:PRO:HD3	2.51	0.46
1:C:109:THR:HG22	1:C:111:ASP:HB3	1.97	0.46
1:C:1115:ILE:HG22	1:C:1137:VAL:HG13	1.97	0.46
2:K:5:VAL:O	2:K:22:CYS:HA	2.16	0.46
4:D:28:ILE:HD13	4:D:70:PHE:CZ	2.50	0.46
5:E:6:GLN:CD	5:E:111:GLY:HA3	2.41	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:60:TYR:HE1	2:G:70:ILE:HG22	1.80	0.46
4:M:13:SER:OG	4:M:106:LEU:HB2	2.16	0.46
1:A:326:ILE:HA	1:A:531:THR:OG1	2.16	0.46
1:A:1088:HIS:C	1:A:1089:PHE:HD1	2.23	0.46
1:B:180:GLU:O	1:B:182:LYS:HG2	2.15	0.46
1:C:418:ILE:HA	1:C:422:ASN:HB2	1.96	0.46
1:C:801:ASN:ND2	6:b:1:NAG:O7	2.49	0.46
3:I:35:TRP:HA	3:I:87:TYR:O	2.15	0.46
5:O:6:GLN:CD	5:O:111:GLY:HA3	2.41	0.46
5:O:86:LEU:HB3	5:O:118:VAL:CG2	2.46	0.46
1:A:369:TYR:CB	4:M:93:TRP:CZ2	2.95	0.46
1:B:106:PHE:HB2	1:B:117:LEU:HB3	1.98	0.46
1:B:906:PHE:CE2	1:B:916:LEU:HB2	2.51	0.46
1:C:275:PHE:C	1:C:276:LEU:HD12	2.40	0.46
1:C:568:ASP:OD1	1:C:569:ILE:N	2.44	0.46
4:M:31:ASN:OD1	4:M:32:LEU:N	2.49	0.46
1:C:87:ASN:HB2	1:C:269:TYR:CD1	2.51	0.46
1:C:104:TRP:HB2	1:C:106:PHE:CE2	2.51	0.46
5:E:37:VAL:O	5:E:95:TYR:N	2.38	0.46
5:O:86:LEU:HB3	5:O:118:VAL:HG21	1.97	0.46
6:d:1:NAG:C8	6:d:1:NAG:C3	2.86	0.46
1:A:563:GLN:CA	1:C:41:LYS:HB3	2.46	0.45
1:B:106:PHE:HB2	1:B:117:LEU:HD23	1.99	0.45
2:L:5:VAL:O	2:L:22:CYS:HA	2.16	0.45
3:J:35:TRP:HD1	3:J:48:ILE:HB	1.81	0.45
5:H:86:LEU:HB3	5:H:118:VAL:HG21	1.97	0.45
1:A:1072:GLU:N	1:A:1072:GLU:OE1	2.50	0.45
1:B:104:TRP:HB2	1:B:106:PHE:CE2	2.51	0.45
1:B:109:THR:HG22	1:B:111:ASP:HB3	1.96	0.45
1:B:327:VAL:CA	1:B:542:ASN:O	2.63	0.45
5:E:20:ILE:HD11	5:E:116:VAL:CG2	2.46	0.45
4:N:12:VAL:HG12	4:N:13:SER:H	1.81	0.45
2:G:5:VAL:O	2:G:22:CYS:HA	2.16	0.45
3:F:35:TRP:HD1	3:F:48:ILE:HB	1.81	0.45
5:O:20:ILE:HD11	5:O:116:VAL:CG2	2.46	0.45
1:A:104:TRP:HB2	1:A:106:PHE:CE2	2.51	0.45
1:A:393:THR:HG21	1:A:518:LEU:H	1.81	0.45
1:A:562:PHE:HZ	1:C:38:TYR:CD2	2.34	0.45
1:B:156:GLU:OE1	1:B:156:GLU:N	2.44	0.45
1:B:961:THR:O	1:B:965:GLN:HG2	2.15	0.45
2:L:60:TYR:HE1	2:L:70:ILE:HG22	1.80	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:91:ASN:HA	4:N:95:TYR:OH	2.16	0.45
5:O:27:TYR:CD1	5:O:32:TYR:HD2	2.34	0.45
1:A:87:ASN:HB2	1:A:269:TYR:CD1	2.51	0.45
1:A:100:ILE:HD13	1:A:263:ALA:HB2	1.98	0.45
1:C:591:SER:HB3	1:C:615:VAL:CG1	2.46	0.45
1:C:1115:ILE:HA	1:C:1119:ASN:HD22	1.81	0.45
3:F:34:ASN:HB2	3:F:89:GLN:HB3	1.98	0.45
1:A:43:PHE:CD1	1:B:559:PHE:HA	2.52	0.45
1:A:66:HIS:CE1	1:A:264:ALA:CB	2.98	0.45
1:A:568:ASP:OD1	1:A:569:ILE:N	2.45	0.45
1:A:1089:PHE:HB3	1:C:913:GLN:HE21	1.81	0.45
1:B:710:ASN:O	1:B:1077:THR:HG22	2.15	0.45
1:B:864:LEU:HG	1:B:865:LEU:HD12	1.99	0.45
1:B:882:ILE:O	1:B:898:PHE:HD1	2.00	0.45
1:B:1102:TRP:CH2	1:B:1133:VAL:HG21	2.52	0.45
1:C:43:PHE:CE1	1:C:283:GLY:HA3	2.52	0.45
1:C:106:PHE:HB2	1:C:117:LEU:HB3	1.98	0.45
1:C:816:SER:OG	1:C:819:GLU:HG3	2.16	0.45
3:I:9:SER:HG	3:I:100:GLN:HE21	1.61	0.45
3:I:34:ASN:HB2	3:I:89:GLN:HB3	1.98	0.45
5:E:27:TYR:CD1	5:E:32:TYR:HD2	2.34	0.45
5:E:86:LEU:HB3	5:E:118:VAL:CG2	2.46	0.45
4:M:33:HIS:ND1	5:O:106:VAL:HG12	2.31	0.45
1:A:106:PHE:HB2	1:A:117:LEU:HB3	1.98	0.45
1:C:393:THR:HG21	1:C:518:LEU:H	1.81	0.45
1:C:1016:ALA:O	1:C:1019:ARG:HB3	2.17	0.45
5:H:20:ILE:HD11	5:H:116:VAL:CG2	2.46	0.45
5:H:86:LEU:HB3	5:H:118:VAL:CG2	2.46	0.45
1:A:882:ILE:O	1:A:898:PHE:HD1	2.00	0.45
1:B:247:SER:H	1:B:257:GLY:HA3	1.81	0.45
1:B:356:LYS:HE3	1:B:358:ILE:HD11	1.99	0.45
1:C:83:VAL:HA	1:C:239:GLN:HB2	1.99	0.45
1:C:106:PHE:HB2	1:C:117:LEU:HD23	1.99	0.45
1:C:145:TYR:CE2	1:C:147:LYS:HA	2.52	0.45
3:J:34:ASN:HB2	3:J:89:GLN:HB3	1.98	0.45
5:H:4:LEU:O	5:H:111:GLY:HA2	2.16	0.45
1:A:1093:GLY:HA2	1:A:1107:ARG:HG3	1.99	0.45
1:B:83:VAL:HA	1:B:239:GLN:HB2	1.99	0.45
1:C:356:LYS:HE3	1:C:358:ILE:HD11	1.99	0.45
1:C:986:LYS:O	1:C:989:ALA:N	2.50	0.45
4:N:12:VAL:HG12	4:N:13:SER:N	2.32	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:91:ASN:HA	4:M:95:TYR:OH	2.16	0.45
1:A:142:GLY:O	1:A:155:SER:N	2.50	0.45
1:A:815:ARG:HD2	1:A:823:PHE:CE2	2.45	0.45
1:B:815:ARG:HD2	1:B:823:PHE:CE2	2.45	0.45
1:B:1054:GLN:N	1:B:1061:VAL:O	2.50	0.45
1:C:142:GLY:O	1:C:155:SER:N	2.50	0.45
5:E:4:LEU:HA	5:E:23:LYS:O	2.17	0.45
3:F:9:SER:HG	3:F:100:GLN:HE21	1.61	0.45
1:A:41:LYS:O	1:B:563:GLN:HG2	2.17	0.45
1:A:106:PHE:HB2	1:A:117:LEU:HD23	1.99	0.45
1:A:563:GLN:HA	1:C:41:LYS:CB	2.47	0.45
1:A:747:THR:HA	1:A:750:SER:HB3	1.99	0.45
1:B:41:LYS:C	1:C:564:GLN:H	2.25	0.45
1:B:299:THR:CG2	1:B:597:VAL:HG11	2.47	0.45
1:B:1072:GLU:OE1	1:B:1072:GLU:N	2.50	0.45
1:C:276:LEU:HD22	1:C:289:VAL:HB	1.98	0.45
1:C:850:ILE:O	1:C:854:LYS:HG3	2.17	0.45
4:N:43:PRO:HD2	5:H:110:TRP:CZ3	2.51	0.45
5:H:6:GLN:CD	5:H:111:GLY:HA3	2.41	0.45
5:H:27:TYR:CD1	5:H:32:TYR:HD2	2.34	0.45
1:B:747:THR:HA	1:B:750:SER:HB3	1.99	0.44
1:B:1093:GLY:HA2	1:B:1107:ARG:HG3	1.99	0.44
1:C:497:PHE:HA	1:C:501:ASN:HD21	1.83	0.44
1:C:1106:GLN:HE21	1:C:1109:PHE:HB3	1.82	0.44
3:I:35:TRP:HD1	3:I:48:ILE:HB	1.81	0.44
4:D:89:GLN:C	4:D:95:TYR:HD1	2.23	0.44
5:E:4:LEU:O	5:E:111:GLY:HA2	2.16	0.44
4:N:34:TRP:CD2	4:N:72:LEU:HB2	2.53	0.44
1:A:970:PHE:CD2	1:A:999:GLY:HA3	2.53	0.44
1:B:87:ASN:HB2	1:B:269:TYR:CD1	2.51	0.44
1:C:800:PHE:CE1	1:C:924:ALA:HA	2.52	0.44
4:M:33:HIS:CE1	5:O:106:VAL:HG12	2.53	0.44
1:A:356:LYS:HE3	1:A:358:ILE:HD11	1.99	0.44
1:A:560:LEU:N	1:A:563:GLN:OE1	2.43	0.44
4:D:12:VAL:HG12	4:D:13:SER:N	2.32	0.44
5:O:4:LEU:O	5:O:111:GLY:HA2	2.16	0.44
5:O:4:LEU:HA	5:O:23:LYS:O	2.17	0.44
1:A:83:VAL:HA	1:A:239:GLN:HB2	1.99	0.44
1:B:142:GLY:O	1:B:155:SER:N	2.50	0.44
1:B:393:THR:O	1:B:523:THR:OG1	2.31	0.44
1:C:143:VAL:O	1:C:245:HIS:HA	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1011:GLN:O	1:C:1015:ALA:N	2.38	0.44
4:D:34:TRP:CD2	4:D:72:LEU:HB2	2.52	0.44
4:D:82:PHE:HB3	4:D:105:ILE:CD1	2.48	0.44
4:D:91:ASN:HA	4:D:95:TYR:OH	2.16	0.44
1:B:315:THR:HG22	1:B:316:SER:N	2.33	0.44
1:C:877:LEU:HD22	1:C:1034:LEU:HD11	1.98	0.44
4:N:33:HIS:CE1	5:H:106:VAL:HG12	2.53	0.44
4:M:12:VAL:HG12	4:M:13:SER:N	2.32	0.44
5:O:10:GLU:O	5:O:116:VAL:HA	2.18	0.44
1:C:145:TYR:CE1	1:C:150:LYS:HA	2.53	0.44
5:E:10:GLU:O	5:E:116:VAL:HA	2.18	0.44
5:H:10:GLU:O	5:H:116:VAL:HA	2.18	0.44
3:F:6:GLN:O	3:F:100:GLN:NE2	2.51	0.44
4:M:36:GLN:OE1	4:M:46:LEU:HD21	2.18	0.44
4:M:82:PHE:HB3	4:M:105:ILE:CD1	2.48	0.44
5:O:39:GLN:HG3	5:O:44:SER:C	2.43	0.44
1:A:296:LEU:CD1	1:A:608:VAL:CG2	2.79	0.44
1:A:323:THR:OG1	1:A:537:LYS:HE3	2.18	0.44
1:A:895:GLN:NE2	1:B:713:ALA:HB2	2.33	0.44
1:B:328:ARG:HA	1:B:328:ARG:HD3	1.71	0.44
1:B:970:PHE:CD2	1:B:999:GLY:HA3	2.53	0.44
1:C:34:ARG:HE	1:C:216:LEU:HD23	1.83	0.44
1:C:200:TYR:HA	1:C:229:LEU:O	2.18	0.44
5:H:4:LEU:HA	5:H:23:LYS:O	2.18	0.44
1:A:497:PHE:HA	1:A:501:ASN:HD21	1.82	0.44
1:B:733:LYS:NZ	1:B:775:ASP:OD2	2.40	0.44
1:B:735:SER:O	1:B:859:THR:OG1	2.27	0.44
1:C:67:ALA:O	1:C:79:PHE:HA	2.17	0.44
1:C:542:ASN:HA	1:C:546:LEU:O	2.18	0.44
5:E:32:TYR:CD2	5:E:98:ARG:HD2	2.53	0.44
4:M:34:TRP:CD2	4:M:72:LEU:HB2	2.52	0.44
1:A:864:LEU:HG	1:A:865:LEU:HD12	1.99	0.44
1:A:914:ASN:HA	1:B:1089:PHE:CE2	2.53	0.44
1:B:555:SER:OG	1:B:584:ILE:O	2.34	0.44
1:C:578:ASP:HB3	1:C:583:GLU:HG2	1.99	0.44
1:C:905:ARG:HD3	1:C:1049:LEU:O	2.18	0.44
3:I:6:GLN:O	3:I:100:GLN:NE2	2.51	0.44
5:E:97:ALA:HB1	5:E:107:MET:CB	2.44	0.44
4:N:45:LEU:HD21	4:N:48:LYS:HB3	2.00	0.44
5:H:7:SER:HB3	5:H:21:SER:OG	2.18	0.44
5:H:39:GLN:HG3	5:H:44:SER:O	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:TRP:CZ3	1:A:66:HIS:NE2	2.69	0.43
1:A:143:VAL:O	1:A:245:HIS:HA	2.18	0.43
1:A:759:PHE:O	1:A:763:LEU:HG	2.18	0.43
1:C:96:GLU:HB2	1:C:190:ARG:NH1	2.34	0.43
1:C:277:LEU:HD23	1:C:285:ILE:HD11	2.00	0.43
1:C:436:TRP:O	1:C:508:TYR:HA	2.18	0.43
1:C:564:GLN:HG3	1:C:565:PHE:CD1	2.53	0.43
1:C:676:THR:HG23	1:C:690:GLN:CG	2.46	0.43
1:C:994:ASP:O	1:C:998:THR:N	2.44	0.43
4:D:43:PRO:HD2	5:E:110:TRP:CZ3	2.51	0.43
5:E:39:GLN:HG3	5:E:44:SER:O	2.18	0.43
5:O:32:TYR:CD2	5:O:98:ARG:HD2	2.53	0.43
1:A:34:ARG:HE	1:A:216:LEU:HD23	1.83	0.43
1:A:436:TRP:O	1:A:508:TYR:HA	2.18	0.43
1:B:143:VAL:O	1:B:245:HIS:HA	2.18	0.43
1:B:759:PHE:O	1:B:763:LEU:HG	2.18	0.43
1:C:29:THR:HG22	1:C:62:VAL:O	2.18	0.43
1:C:806:LEU:HD23	1:C:806:LEU:HA	1.85	0.43
5:E:39:GLN:HG3	5:E:44:SER:C	2.43	0.43
4:N:82:PHE:HB3	4:N:105:ILE:CD1	2.48	0.43
2:G:99:HIS:CG	3:F:89:GLN:HE22	2.36	0.43
1:A:315:THR:HG22	1:A:316:SER:N	2.33	0.43
1:A:565:PHE:HB2	1:C:42:VAL:CG2	2.18	0.43
1:A:894:LEU:HD13	1:B:715:PRO:HD3	1.99	0.43
1:A:1054:GLN:N	1:A:1061:VAL:O	2.50	0.43
2:K:99:HIS:CG	3:I:89:GLN:HE22	2.36	0.43
4:D:33:HIS:CE1	5:E:106:VAL:HG12	2.53	0.43
5:O:39:GLN:HG3	5:O:44:SER:O	2.18	0.43
1:A:70:VAL:HG23	1:A:75:GLY:O	2.18	0.43
1:A:318:PHE:HZ	1:A:615:VAL:HG11	1.84	0.43
1:B:935:GLN:O	1:B:939:SER:N	2.39	0.43
1:B:1032:CYS:SG	1:B:1051:SER:OG	2.77	0.43
1:C:287:ASP:CB	1:C:306:PHE:CE2	2.96	0.43
1:C:501:ASN:HB3	1:C:505:TYR:HB2	2.00	0.43
3:I:21:ILE:HD12	3:I:73:LEU:HD23	2.00	0.43
1:A:41:LYS:O	1:B:563:GLN:CG	2.66	0.43
1:A:294:ASP:OD1	1:A:297:SER:N	2.45	0.43
1:A:1080:ALA:C	1:A:1132:ILE:HG13	2.44	0.43
1:B:205:SER:HB3	1:B:226:LEU:HD11	1.99	0.43
1:B:497:PHE:HA	1:B:501:ASN:HD21	1.83	0.43
1:C:70:VAL:HG23	1:C:75:GLY:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:822:LEU:HD13	1:C:1056:ALA:HB2	1.99	0.43
5:E:81:MET:HE1	5:E:94:TYR:CG	2.54	0.43
2:L:99:HIS:CG	3:J:89:GLN:HE22	2.36	0.43
3:J:21:ILE:HD12	3:J:73:LEU:HD23	2.00	0.43
4:N:36:GLN:OE1	4:N:46:LEU:HD21	2.18	0.43
5:H:10:GLU:HG3	5:H:18:VAL:CG2	2.48	0.43
5:H:39:GLN:HG3	5:H:44:SER:C	2.43	0.43
1:A:330:PRO:HA	1:A:579:PRO:HB2	2.01	0.43
1:B:100:ILE:HD13	1:B:263:ALA:HB2	1.99	0.43
1:B:436:TRP:O	1:B:508:TYR:HA	2.18	0.43
4:D:10:GLN:HG2	4:D:101:THR:HG21	2.00	0.43
4:D:36:GLN:OE1	4:D:46:LEU:HD21	2.18	0.43
4:M:37:GLN:HB2	4:M:86:PHE:HE2	1.84	0.43
1:B:115:GLN:NE2	1:B:167:THR:HG21	2.34	0.43
1:B:120:VAL:HG12	1:B:122:ASN:N	2.34	0.43
1:B:821:LEU:O	1:B:825:LYS:HG2	2.19	0.43
1:B:894:LEU:HD13	1:C:715:PRO:HD3	2.00	0.43
1:C:753:LEU:HD21	1:C:760:CYS:SG	2.59	0.43
4:D:45:LEU:HD21	4:D:48:LYS:HB3	2.00	0.43
3:J:6:GLN:O	3:J:100:GLN:NE2	2.51	0.43
1:A:287:ASP:OD2	1:A:306:PHE:CG	2.68	0.43
1:A:380:TYR:OH	5:O:55:ASN:HB3	2.19	0.43
1:B:70:VAL:HG23	1:B:75:GLY:O	2.18	0.43
1:B:676:THR:HG23	1:B:690:GLN:HG2	2.01	0.43
1:C:205:SER:HB3	1:C:226:LEU:HD11	1.99	0.43
1:C:296:LEU:HB2	1:C:608:VAL:HG21	1.99	0.43
4:D:37:GLN:HB2	4:D:86:PHE:HE2	1.84	0.43
5:H:32:TYR:CD2	5:H:98:ARG:HD2	2.53	0.43
3:F:21:ILE:HD12	3:F:73:LEU:HD23	2.00	0.43
4:M:45:LEU:HD21	4:M:48:LYS:HB3	2.00	0.43
4:M:57:ILE:CG2	4:M:61:PHE:HD2	2.32	0.43
5:O:10:GLU:HG3	5:O:18:VAL:CG2	2.48	0.43
1:A:34:ARG:HD2	1:A:191:GLU:OE2	2.19	0.43
1:A:327:VAL:O	1:A:531:THR:N	2.52	0.43
1:B:42:VAL:HG11	1:C:567:ARG:CD	2.49	0.43
1:B:96:GLU:HB2	1:B:190:ARG:NH1	2.33	0.43
1:C:599:THR:HB	1:C:608:VAL:HG12	2.01	0.43
4:D:20:ILE:CD1	4:D:85:TYR:HD2	2.31	0.43
4:N:10:GLN:HG2	4:N:101:THR:HG21	2.00	0.43
4:N:57:ILE:CG2	4:N:61:PHE:HD2	2.32	0.43
1:B:852:ALA:HA	1:B:855:PHE:CE2	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:22:CYS:O	2:K:78:THR:HA	2.19	0.43
5:O:7:SER:HB3	5:O:21:SER:OG	2.18	0.43
1:A:64:TRP:CE2	1:A:66:HIS:NE2	2.79	0.42
1:A:96:GLU:HB2	1:A:190:ARG:NH1	2.34	0.42
1:A:296:LEU:HD12	1:A:608:VAL:HG13	1.19	0.42
1:A:699:LEU:HD21	1:C:869:MET:HB3	2.01	0.42
1:C:1088:HIS:CE1	1:C:1122:VAL:HG22	2.53	0.42
5:E:10:GLU:HG3	5:E:18:VAL:CG2	2.48	0.42
2:G:22:CYS:O	2:G:78:THR:HA	2.19	0.42
5:O:81:MET:HE1	5:O:94:TYR:CG	2.54	0.42
1:B:276:LEU:HD11	1:B:306:PHE:CE1	2.53	0.42
1:C:231:ILE:HG22	1:C:233:ILE:HG22	2.02	0.42
1:C:380:TYR:CZ	5:H:55:ASN:HB3	2.54	0.42
4:D:57:ILE:CG2	4:D:61:PHE:HD2	2.32	0.42
1:A:49:HIS:O	1:A:277:LEU:N	2.43	0.42
1:A:205:SER:HB3	1:A:226:LEU:HD11	1.99	0.42
1:A:307:THR:HA	1:A:602:THR:HG21	2.01	0.42
1:A:825:LYS:HE3	1:A:938:LEU:O	2.19	0.42
1:B:34:ARG:HD2	1:B:191:GLU:OE2	2.19	0.42
1:B:380:TYR:CZ	5:E:55:ASN:HB3	2.53	0.42
1:B:394:ASN:N	1:B:394:ASN:OD1	2.52	0.42
1:B:568:ASP:OD1	1:B:569:ILE:N	2.45	0.42
1:B:1080:ALA:C	1:B:1132:ILE:HG13	2.44	0.42
1:C:18:LEU:CD1	1:C:79:PHE:CD2	3.01	0.42
1:C:34:ARG:HD2	1:C:191:GLU:OE2	2.19	0.42
1:C:108:THR:HG23	6:Z:1:NAG:O6	2.19	0.42
5:E:7:SER:HB3	5:E:21:SER:OG	2.18	0.42
2:L:22:CYS:O	2:L:78:THR:HA	2.19	0.42
1:A:85:PRO:HA	1:A:237:ARG:HA	2.01	0.42
1:A:864:LEU:O	1:B:669:GLY:N	2.51	0.42
1:A:869:MET:HB3	1:B:699:LEU:HD21	2.01	0.42
1:A:1006:THR:O	1:A:1010:GLN:HG2	2.19	0.42
1:B:380:TYR:OH	5:E:55:ASN:HB3	2.19	0.42
1:C:380:TYR:OH	5:H:55:ASN:HB3	2.19	0.42
1:C:560:LEU:N	1:C:563:GLN:OE1	2.46	0.42
1:C:1116:THR:HA	1:C:1138:TYR:O	2.19	0.42
4:D:33:HIS:O	4:D:88:GLN:N	2.52	0.42
4:N:33:HIS:O	4:N:88:GLN:N	2.52	0.42
1:A:115:GLN:NE2	1:A:167:THR:HG21	2.34	0.42
1:A:380:TYR:CZ	5:O:55:ASN:HB3	2.53	0.42
1:B:501:ASN:HB3	1:B:505:TYR:HB2	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:825:LYS:HE3	1:B:938:LEU:O	2.19	0.42
5:E:47:TRP:CZ2	5:E:50:TYR:CD2	3.08	0.42
4:N:37:GLN:HB2	4:N:86:PHE:HE2	1.84	0.42
1:A:160:TYR:HE1	1:A:163:ALA:HB2	1.85	0.42
1:A:501:ASN:HB3	1:A:505:TYR:HB2	2.00	0.42
1:B:1006:THR:O	1:B:1010:GLN:HG2	2.19	0.42
4:D:4:LEU:HD23	4:D:89:GLN:HB2	2.01	0.42
4:N:60:ARG:HH21	4:N:81:ASP:CG	2.28	0.42
5:H:81:MET:HE1	5:H:94:TYR:CG	2.54	0.42
4:M:10:GLN:HG2	4:M:101:THR:HG21	2.00	0.42
1:A:369:TYR:CA	4:M:93:TRP:CZ2	3.03	0.42
1:A:558:LYS:O	1:C:43:PHE:CZ	2.73	0.42
1:A:901:GLN:NE2	1:A:905:ARG:HE	2.08	0.42
1:B:34:ARG:HE	1:B:216:LEU:HD23	1.83	0.42
1:B:323:THR:OG1	1:B:539:VAL:HG12	2.20	0.42
1:C:115:GLN:NE2	1:C:167:THR:HG21	2.34	0.42
1:C:570:ALA:C	1:C:572:THR:H	2.27	0.42
1:C:960:ASN:O	1:C:963:VAL:N	2.52	0.42
4:N:89:GLN:C	4:N:95:TYR:HD1	2.23	0.42
4:M:43:PRO:HD2	5:O:110:TRP:CZ3	2.51	0.42
5:O:47:TRP:CZ2	5:O:50:TYR:CD2	3.07	0.42
1:A:733:LYS:NZ	1:A:775:ASP:OD2	2.40	0.42
4:D:6:GLN:HE22	4:D:87:CYS:H	1.68	0.42
5:O:91:THR:HA	5:O:116:VAL:O	2.20	0.42
1:A:821:LEU:O	1:A:825:LYS:HG2	2.19	0.42
1:A:1028:LYS:O	1:A:1032:CYS:N	2.46	0.42
1:B:398:ASP:OD1	1:B:398:ASP:N	2.51	0.42
1:C:85:PRO:HA	1:C:237:ARG:HA	2.01	0.42
4:D:60:ARG:HG3	4:D:61:PHE:CD1	2.55	0.42
4:D:60:ARG:HH21	4:D:81:ASP:CG	2.28	0.42
4:M:4:LEU:HD23	4:M:89:GLN:HB2	2.01	0.42
5:O:36:TRP:O	5:O:48:ILE:HG22	2.20	0.42
5:O:62:LEU:O	5:O:63:LYS:C	2.63	0.42
1:A:852:ALA:HA	1:A:855:PHE:CE2	2.54	0.42
1:B:121:ASN:C	1:B:123:ALA:H	2.27	0.42
1:B:369:TYR:CA	4:D:93:TRP:CZ2	3.03	0.42
1:B:717:ASN:O	1:B:1070:ALA:N	2.46	0.42
1:C:645:THR:OG1	1:C:648:GLY:O	2.20	0.42
5:E:62:LEU:O	5:E:63:LYS:C	2.63	0.42
5:E:91:THR:HA	5:E:116:VAL:O	2.20	0.42
4:N:84:ILE:HA	4:N:102:LYS:HA	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:801:ASN:ND2	6:R:1:NAG:O7	2.53	0.41
1:B:160:TYR:HE1	1:B:163:ALA:HB2	1.85	0.41
1:C:160:TYR:HE1	1:C:163:ALA:HB2	1.85	0.41
1:C:970:PHE:CD2	1:C:999:GLY:HA3	2.55	0.41
4:D:60:ARG:HB2	4:D:75:ASN:O	2.20	0.41
4:M:33:HIS:O	4:M:88:GLN:N	2.52	0.41
5:O:63:LYS:HB3	5:O:64:PHE:H	1.67	0.41
1:A:394:ASN:N	1:A:394:ASN:OD1	2.52	0.41
1:A:676:THR:HG23	1:A:690:GLN:HG2	2.01	0.41
1:B:42:VAL:HG13	1:C:567:ARG:HG3	1.97	0.41
1:C:369:TYR:CA	4:N:93:TRP:CZ2	3.03	0.41
1:C:804:GLN:CD	1:C:935:GLN:HE22	2.20	0.41
4:D:43:PRO:HB2	5:E:110:TRP:CH2	2.56	0.41
4:N:60:ARG:O	4:N:74:ILE:HA	2.20	0.41
5:O:27:TYR:CE1	5:O:32:TYR:HD2	2.38	0.41
1:A:201:PHE:CB	1:A:231:ILE:HG13	2.30	0.41
1:A:203:ILE:HG22	1:A:226:LEU:HD12	2.03	0.41
1:B:200:TYR:HA	1:B:229:LEU:O	2.20	0.41
1:B:291:CYS:O	1:B:298:GLU:HG3	2.19	0.41
1:B:318:PHE:HZ	1:B:615:VAL:HG11	1.84	0.41
1:B:326:ILE:C	1:B:531:THR:OG1	2.63	0.41
1:C:770:ILE:O	1:C:774:GLN:HG2	2.21	0.41
1:C:861:LEU:H	1:C:861:LEU:HG	1.68	0.41
4:N:4:LEU:HD23	4:N:89:GLN:HB2	2.01	0.41
5:H:47:TRP:CZ2	5:H:50:TYR:CD2	3.07	0.41
4:M:60:ARG:HH21	4:M:81:ASP:CG	2.28	0.41
1:A:36:VAL:O	1:A:222:ALA:HA	2.21	0.41
1:A:730:SER:O	1:A:1058:HIS:HB3	2.20	0.41
1:B:41:LYS:HD3	1:C:564:GLN:HB2	2.02	0.41
1:B:801:ASN:ND2	6:W:1:NAG:O7	2.54	0.41
1:C:63:THR:HG22	1:C:65:PHE:CE2	2.33	0.41
1:C:203:ILE:HG22	1:C:226:LEU:HD12	2.03	0.41
5:E:27:TYR:CE1	5:E:32:TYR:HD2	2.38	0.41
2:L:68:PHE:HD1	2:L:83:MET:HA	1.86	0.41
4:N:60:ARG:HG3	4:N:61:PHE:CD1	2.55	0.41
4:N:106:LEU:O	4:N:107:LYS:HB3	2.21	0.41
4:M:60:ARG:HB2	4:M:75:ASN:O	2.20	0.41
5:O:34:ILE:HB	5:O:51:ILE:HG22	2.03	0.41
1:A:50:SER:HA	1:A:275:PHE:O	2.21	0.41
1:A:857:GLY:HA2	1:B:592:PHE:CE1	2.55	0.41
1:B:43:PHE:O	1:C:566:GLY:HA2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:PRO:HA	1:B:237:ARG:HA	2.02	0.41
1:C:320:VAL:HB	1:C:590:CYS:HB3	2.01	0.41
1:C:643:PHE:CE2	1:C:645:THR:HG22	2.55	0.41
2:K:9:GLY:HA3	2:K:114:LEU:O	2.20	0.41
3:F:21:ILE:HB	3:F:73:LEU:HB3	2.03	0.41
4:M:106:LEU:O	4:M:107:LYS:HB3	2.21	0.41
1:A:855:PHE:CD2	1:B:572:THR:HG21	2.54	0.41
1:B:82:PRO:HG2	1:B:84:LEU:HD21	2.03	0.41
1:B:323:THR:HG1	1:B:539:VAL:HG12	1.84	0.41
1:B:557:LYS:O	1:B:584:ILE:HG13	2.21	0.41
1:C:234:ASN:ND2	6:Z:1:NAG:N2	2.69	0.41
1:C:278:LYS:HD3	1:C:306:PHE:CE2	2.55	0.41
1:C:1087:ALA:HB3	1:C:1123:SER:O	2.21	0.41
5:E:34:ILE:HB	5:E:51:ILE:HG22	2.03	0.41
5:E:36:TRP:O	5:E:48:ILE:HG22	2.20	0.41
5:E:66:GLY:HA3	5:E:83:LEU:HD12	2.03	0.41
4:N:43:PRO:HB2	5:H:110:TRP:CH2	2.55	0.41
1:A:372:ALA:H	4:M:93:TRP:CD1	2.33	0.41
1:B:36:VAL:O	1:B:222:ALA:HA	2.21	0.41
1:B:84:LEU:O	1:B:238:PHE:N	2.51	0.41
1:B:100:ILE:HG21	1:B:263:ALA:CB	2.46	0.41
1:B:800:PHE:N	1:B:800:PHE:CD1	2.88	0.41
1:C:326:ILE:O	1:C:542:ASN:N	2.26	0.41
4:D:60:ARG:O	4:D:74:ILE:HA	2.21	0.41
4:N:6:GLN:HE22	4:N:87:CYS:H	1.68	0.41
5:H:36:TRP:O	5:H:48:ILE:HG22	2.20	0.41
1:A:82:PRO:HG2	1:A:84:LEU:HD21	2.03	0.41
1:B:424:LYS:HB3	1:B:463:PRO:HA	2.03	0.41
1:C:786:LYS:HZ1	1:C:892:ALA:HA	1.86	0.41
3:J:3:GLN:HB2	3:J:26:SER:HB3	2.03	0.41
4:N:60:ARG:HB2	4:N:75:ASN:O	2.20	0.41
2:G:68:PHE:HD1	2:G:83:MET:HA	1.86	0.41
1:A:41:LYS:HB3	1:B:563:GLN:HA	2.03	0.41
1:A:64:TRP:CZ2	1:A:214:ARG:HD2	2.56	0.41
1:A:424:LYS:HB3	1:A:463:PRO:HA	2.03	0.41
1:A:498:GLN:H	1:A:501:ASN:ND2	2.19	0.41
1:A:669:GLY:HA3	1:C:869:MET:CE	2.48	0.41
1:A:1006:THR:HG21	1:C:762:GLN:HE22	1.85	0.41
1:B:118:LEU:CD2	1:B:129:LYS:HD2	2.51	0.41
1:B:895:GLN:NE2	1:C:713:ALA:HB2	2.35	0.41
1:B:978:ASN:O	1:B:982:SER:N	2.52	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1052:PHE:HB2	1:B:1063:LEU:HB2	2.03	0.41
1:C:36:VAL:O	1:C:222:ALA:HA	2.21	0.41
1:C:82:PRO:HG2	1:C:84:LEU:HD21	2.03	0.41
1:C:205:SER:O	1:C:223:LEU:HG	2.21	0.41
1:C:796:ASP:OD1	1:C:796:ASP:N	2.54	0.41
1:C:853:GLN:HE21	1:C:959:LEU:HB3	1.82	0.41
4:D:84:ILE:HA	4:D:102:LYS:HA	2.02	0.41
4:D:106:LEU:O	4:D:107:LYS:HB3	2.21	0.41
5:H:62:LEU:O	5:H:63:LYS:C	2.63	0.41
5:H:91:THR:HA	5:H:116:VAL:O	2.20	0.41
4:M:60:ARG:HG3	4:M:61:PHE:CD1	2.55	0.41
4:M:84:ILE:HA	4:M:102:LYS:HA	2.02	0.41
1:A:290:ASP:OD1	1:A:291:CYS:N	2.55	0.41
1:A:1089:PHE:N	1:A:1089:PHE:CD1	2.89	0.41
1:A:1139:ASP:OD1	1:A:1141:LEU:N	2.47	0.41
1:B:190:ARG:HG2	1:B:207:HIS:ND1	2.36	0.41
1:B:203:ILE:HG22	1:B:226:LEU:HD12	2.03	0.41
1:B:327:VAL:HG12	1:B:542:ASN:HB2	1.99	0.41
2:K:68:PHE:HD1	2:K:83:MET:HA	1.86	0.41
3:F:3:GLN:HB2	3:F:26:SER:HB3	2.03	0.41
4:M:20:ILE:CD1	4:M:85:TYR:HD2	2.31	0.41
4:M:43:PRO:HB2	5:O:110:TRP:CH2	2.56	0.41
1:A:205:SER:O	1:A:223:LEU:HG	2.21	0.40
1:A:247:SER:HB3	1:A:257:GLY:HA3	2.02	0.40
1:B:1139:ASP:OD1	1:B:1141:LEU:N	2.47	0.40
1:C:102:ARG:NH1	1:C:123:ALA:HB2	2.36	0.40
1:C:424:LYS:HB3	1:C:463:PRO:HA	2.03	0.40
3:I:3:GLN:HB2	3:I:26:SER:HB3	2.03	0.40
1:A:18:LEU:O	1:A:18:LEU:CG	2.69	0.40
1:A:308:VAL:H	1:A:602:THR:CG2	2.34	0.40
1:B:19:THR:HG22	1:B:138:ASP:OD1	2.21	0.40
1:B:536:ASN:OD1	1:B:553:THR:CG2	2.48	0.40
1:C:894:LEU:HD23	1:C:894:LEU:HA	1.88	0.40
1:C:991:VAL:O	1:C:994:ASP:HB2	2.21	0.40
2:L:7:SER:N	2:L:21:SER:O	2.54	0.40
5:H:22:CYS:HB2	5:H:36:TRP:CH2	2.57	0.40
4:M:60:ARG:O	4:M:74:ILE:HA	2.20	0.40
1:A:369:TYR:HB2	5:O:62:LEU:HD21	2.04	0.40
1:A:725:GLU:OE2	1:A:1028:LYS:HE3	2.22	0.40
1:A:823:PHE:CD1	1:A:1057:PRO:HG3	2.57	0.40
1:A:946:GLY:O	1:A:950:ASP:N	2.44	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1052:PHE:HB2	1:A:1063:LEU:HB2	2.03	0.40
1:B:560:LEU:N	1:B:563:GLN:OE1	2.43	0.40
1:B:725:GLU:OE2	1:B:1028:LYS:HE3	2.22	0.40
1:C:394:ASN:OD1	1:C:394:ASN:N	2.52	0.40
1:C:498:GLN:H	1:C:501:ASN:ND2	2.19	0.40
1:C:730:SER:O	1:C:1058:HIS:HB3	2.21	0.40
2:L:9:GLY:HA3	2:L:114:LEU:O	2.20	0.40
5:H:27:TYR:CE1	5:H:32:TYR:HD2	2.38	0.40
5:O:66:GLY:HA3	5:O:83:LEU:HD12	2.02	0.40
1:A:190:ARG:HG2	1:A:207:HIS:ND1	2.36	0.40
1:A:927:PHE:HE1	1:A:1065:VAL:HG21	1.86	0.40
1:B:43:PHE:CD1	1:C:559:PHE:HA	2.57	0.40
1:B:853:GLN:NE2	1:B:959:LEU:CG	2.82	0.40
1:B:913:GLN:HE22	1:C:1090:PRO:HD2	1.86	0.40
1:C:316:SER:OG	1:C:317:ASN:N	2.54	0.40
1:C:325:SER:HA	1:C:540:ASN:O	2.21	0.40
1:C:406:GLU:O	1:C:409:GLN:HB2	2.21	0.40
1:C:587:ILE:HG22	1:C:588:THR:N	2.36	0.40
1:C:873:TYR:O	1:C:876:ALA:N	2.54	0.40
1:A:853:GLN:NE2	1:A:959:LEU:CG	2.82	0.40
1:B:205:SER:O	1:B:223:LEU:HG	2.21	0.40
1:C:821:LEU:O	1:C:825:LYS:HG2	2.22	0.40
1:C:880:GLY:O	1:C:884:SER:OG	2.34	0.40
1:C:1030:SER:O	1:C:1034:LEU:HB2	2.21	0.40
3:I:21:ILE:HB	3:I:73:LEU:HB3	2.03	0.40
2:G:9:GLY:HA3	2:G:114:LEU:O	2.21	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	1058/1273 (83%)	985 (93%)	72 (7%)	1 (0%)	48	79
1	B	1056/1273 (83%)	976 (92%)	80 (8%)	0	100	100
1	C	1058/1273 (83%)	977 (92%)	81 (8%)	0	100	100
2	G	118/213 (55%)	106 (90%)	12 (10%)	0	100	100
2	K	118/213 (55%)	106 (90%)	12 (10%)	0	100	100
2	L	118/213 (55%)	106 (90%)	12 (10%)	0	100	100
3	F	105/209 (50%)	96 (91%)	9 (9%)	0	100	100
3	I	106/209 (51%)	97 (92%)	9 (8%)	0	100	100
3	J	105/209 (50%)	96 (91%)	9 (9%)	0	100	100
4	D	105/207 (51%)	99 (94%)	5 (5%)	1 (1%)	12	45
4	M	105/207 (51%)	99 (94%)	5 (5%)	1 (1%)	12	45
4	N	105/207 (51%)	99 (94%)	5 (5%)	1 (1%)	12	45
5	E	120/214 (56%)	114 (95%)	6 (5%)	0	100	100
5	H	120/214 (56%)	114 (95%)	6 (5%)	0	100	100
5	O	120/214 (56%)	114 (95%)	6 (5%)	0	100	100
All	All	4517/6348 (71%)	4184 (93%)	329 (7%)	4 (0%)	49	79

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	93	TRP
4	N	93	TRP
4	M	93	TRP
1	A	24	LEU

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	928/1112 (84%)	926 (100%)	2 (0%)	87	89
1	B	927/1112 (83%)	925 (100%)	2 (0%)	87	89

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	928/1112 (84%)	925 (100%)	3 (0%)	86	88
2	G	96/178 (54%)	96 (100%)	0	100	100
2	K	96/178 (54%)	96 (100%)	0	100	100
2	L	96/178 (54%)	96 (100%)	0	100	100
3	F	93/184 (50%)	93 (100%)	0	100	100
3	I	93/184 (50%)	93 (100%)	0	100	100
3	J	93/184 (50%)	93 (100%)	0	100	100
4	D	96/187 (51%)	96 (100%)	0	100	100
4	M	96/187 (51%)	96 (100%)	0	100	100
4	N	96/187 (51%)	96 (100%)	0	100	100
5	E	99/181 (55%)	99 (100%)	0	100	100
5	H	98/181 (54%)	98 (100%)	0	100	100
5	O	99/181 (55%)	99 (100%)	0	100	100
All	All	3934/5526 (71%)	3927 (100%)	7 (0%)	85	89

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	ILE
1	A	524	VAL
1	B	524	VAL
1	B	533	LEU
1	C	68	ILE
1	C	126	VAL
1	C	524	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (82) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	HIS
1	A	115	GLN
1	A	122	ASN
1	A	148	ASN
1	A	165	ASN
1	A	234	ASN
1	A	239	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	317	ASN
1	A	370	ASN
1	A	501	ASN
1	A	779	GLN
1	A	784	GLN
1	A	804	GLN
1	A	853	GLN
1	A	901	GLN
1	A	935	GLN
1	B	115	GLN
1	B	121	ASN
1	B	148	ASN
1	B	165	ASN
1	B	211	ASN
1	B	234	ASN
1	B	239	GLN
1	B	317	ASN
1	B	370	ASN
1	B	501	ASN
1	B	779	GLN
1	B	784	GLN
1	B	804	GLN
1	B	853	GLN
1	B	901	GLN
1	B	913	GLN
1	B	935	GLN
1	C	61	ASN
1	C	66	HIS
1	C	69	HIS
1	C	165	ASN
1	C	234	ASN
1	C	239	GLN
1	C	282	ASN
1	C	317	ASN
1	C	370	ASN
1	C	501	ASN
1	C	564	GLN
1	C	655	HIS
1	C	784	GLN
1	C	901	GLN
1	C	913	GLN
1	C	955	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	992	GLN
1	C	1058	HIS
1	C	1119	ASN
1	C	1135	ASN
2	K	84	ASN
3	I	38	GLN
3	I	79	GLN
3	I	90	GLN
4	D	6	GLN
4	D	10	GLN
4	D	88	GLN
4	D	89	GLN
5	E	31	ASN
5	E	55	ASN
2	L	84	ASN
3	J	38	GLN
3	J	79	GLN
3	J	90	GLN
4	N	6	GLN
4	N	10	GLN
4	N	88	GLN
4	N	89	GLN
5	H	31	ASN
5	H	55	ASN
2	G	84	ASN
3	F	38	GLN
3	F	90	GLN
4	M	6	GLN
4	M	10	GLN
4	M	88	GLN
4	M	89	GLN
5	O	31	ASN
5	O	55	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	$\# Z > 2$
6	NAG	P	1	1,6	14,14,15	1.58	1 (7%)	17,19,21	1.40	3 (17%)
6	NAG	P	2	6	14,14,15	0.20	0	17,19,21	0.54	0
6	NAG	Q	1	1,6	14,14,15	0.32	0	17,19,21	0.51	0
6	NAG	Q	2	6	14,14,15	0.31	0	17,19,21	0.42	0
6	NAG	R	1	1,6	14,14,15	0.48	0	17,19,21	0.46	0
6	NAG	R	2	6	14,14,15	0.18	0	17,19,21	0.47	0
6	NAG	S	1	1,6	14,14,15	0.50	0	17,19,21	0.53	0
6	NAG	S	2	6	14,14,15	0.25	0	17,19,21	0.39	0
6	NAG	T	1	1,6	14,14,15	0.47	0	17,19,21	0.41	0
6	NAG	T	2	6	14,14,15	0.23	0	17,19,21	0.46	0
6	NAG	U	1	1,6	14,14,15	1.59	1 (7%)	17,19,21	1.40	2 (11%)
6	NAG	U	2	6	14,14,15	0.22	0	17,19,21	0.52	0
6	NAG	V	1	1,6	14,14,15	0.35	0	17,19,21	0.48	0
6	NAG	V	2	6	14,14,15	0.29	0	17,19,21	0.41	0
6	NAG	W	1	1,6	14,14,15	0.49	0	17,19,21	0.46	0
6	NAG	W	2	6	14,14,15	0.21	0	17,19,21	0.48	0
6	NAG	X	1	1,6	14,14,15	0.44	0	17,19,21	0.42	0
6	NAG	X	2	6	14,14,15	0.29	0	17,19,21	0.44	0
6	NAG	Y	1	1,6	14,14,15	0.32	0	17,19,21	0.99	1 (5%)
6	NAG	Y	2	6	14,14,15	0.50	0	17,19,21	1.23	2 (11%)
6	NAG	Z	1	1,6	14,14,15	1.18	2 (14%)	17,19,21	1.11	2 (11%)
6	NAG	Z	2	6	14,14,15	0.34	0	17,19,21	0.45	0
6	NAG	a	1	1,6	14,14,15	0.51	0	17,19,21	0.48	0
6	NAG	a	2	6	14,14,15	0.32	0	17,19,21	0.41	0
6	NAG	b	1	1,6	14,14,15	0.44	0	17,19,21	0.47	0
6	NAG	b	2	6	14,14,15	0.26	0	17,19,21	0.37	0
6	NAG	c	1	1,6	14,14,15	0.42	0	17,19,21	0.48	0
6	NAG	c	2	6	14,14,15	0.27	0	17,19,21	0.39	0
6	NAG	d	1	1,6	14,14,15	0.27	0	17,19,21	0.66	0
6	NAG	d	2	6	14,14,15	0.26	0	17,19,21	0.66	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
6	NAG	P	1	1,6	-	3/6/23/26	0/1/1/1
6	NAG	P	2	6	-	0/6/23/26	0/1/1/1
6	NAG	Q	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	Q	2	6	-	2/6/23/26	0/1/1/1
6	NAG	R	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	R	2	6	-	2/6/23/26	0/1/1/1
6	NAG	S	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	S	2	6	-	1/6/23/26	0/1/1/1
6	NAG	T	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	T	2	6	-	2/6/23/26	0/1/1/1
6	NAG	U	1	1,6	-	3/6/23/26	0/1/1/1
6	NAG	U	2	6	-	0/6/23/26	0/1/1/1
6	NAG	V	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	V	2	6	-	2/6/23/26	0/1/1/1
6	NAG	W	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	W	2	6	-	2/6/23/26	0/1/1/1
6	NAG	X	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	X	2	6	-	2/6/23/26	0/1/1/1
6	NAG	Y	1	1,6	-	3/6/23/26	0/1/1/1
6	NAG	Y	2	6	-	0/6/23/26	0/1/1/1
6	NAG	Z	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	Z	2	6	-	2/6/23/26	0/1/1/1
6	NAG	a	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	a	2	6	-	2/6/23/26	0/1/1/1
6	NAG	b	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	b	2	6	-	2/6/23/26	0/1/1/1
6	NAG	c	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	c	2	6	-	2/6/23/26	0/1/1/1
6	NAG	d	1	1,6	-	3/6/23/26	0/1/1/1
6	NAG	d	2	6	-	1/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	P	1	NAG	O5-C1	-5.68	1.34	1.43
6	U	1	NAG	O5-C1	-5.68	1.34	1.43
6	Z	1	NAG	O5-C1	-3.69	1.37	1.43
6	Z	1	NAG	C1-C2	-2.11	1.49	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Y	2	NAG	C1-O5-C5	3.77	117.24	112.19
6	P	1	NAG	C3-C4-C5	3.60	116.76	110.23
6	U	1	NAG	C3-C4-C5	3.60	116.76	110.23
6	Z	1	NAG	C3-C4-C5	3.18	116.00	110.23
6	Y	2	NAG	C1-C2-N2	2.69	114.67	110.43
6	Y	1	NAG	C4-C3-C2	-2.59	107.22	111.02
6	U	1	NAG	C1-O5-C5	-2.32	109.08	112.19
6	P	1	NAG	C1-O5-C5	-2.31	109.09	112.19
6	Z	1	NAG	O4-C4-C5	-2.06	104.25	109.32
6	P	1	NAG	O4-C4-C5	-2.00	104.39	109.32

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	Y	1	NAG	C8-C7-N2-C2
6	Y	1	NAG	O7-C7-N2-C2
6	d	1	NAG	C1-C2-N2-C7
6	d	1	NAG	C8-C7-N2-C2
6	d	1	NAG	O7-C7-N2-C2
6	Q	2	NAG	O5-C5-C6-O6
6	V	2	NAG	O5-C5-C6-O6
6	b	1	NAG	O5-C5-C6-O6
6	Q	2	NAG	C4-C5-C6-O6
6	V	2	NAG	C4-C5-C6-O6
6	Z	1	NAG	C4-C5-C6-O6
6	Q	1	NAG	O5-C5-C6-O6
6	V	1	NAG	O5-C5-C6-O6
6	c	2	NAG	O5-C5-C6-O6
6	b	1	NAG	C4-C5-C6-O6
6	R	2	NAG	O5-C5-C6-O6
6	W	2	NAG	O5-C5-C6-O6
6	R	2	NAG	C4-C5-C6-O6
6	W	2	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	Q	1	NAG	C4-C5-C6-O6
6	V	1	NAG	C4-C5-C6-O6
6	W	1	NAG	O5-C5-C6-O6
6	Z	1	NAG	O5-C5-C6-O6
6	R	1	NAG	O5-C5-C6-O6
6	Z	2	NAG	C4-C5-C6-O6
6	Z	2	NAG	O5-C5-C6-O6
6	X	2	NAG	C4-C5-C6-O6
6	T	2	NAG	C4-C5-C6-O6
6	U	1	NAG	C4-C5-C6-O6
6	P	1	NAG	C4-C5-C6-O6
6	c	2	NAG	C4-C5-C6-O6
6	R	1	NAG	C4-C5-C6-O6
6	W	1	NAG	C4-C5-C6-O6
6	a	2	NAG	C4-C5-C6-O6
6	b	2	NAG	C4-C5-C6-O6
6	T	2	NAG	O5-C5-C6-O6
6	X	2	NAG	O5-C5-C6-O6
6	S	2	NAG	O5-C5-C6-O6
6	d	2	NAG	C3-C2-N2-C7
6	Y	1	NAG	O5-C5-C6-O6
6	c	1	NAG	C4-C5-C6-O6
6	b	2	NAG	O5-C5-C6-O6
6	U	1	NAG	O5-C5-C6-O6
6	a	2	NAG	O5-C5-C6-O6
6	P	1	NAG	O5-C5-C6-O6
6	c	1	NAG	O5-C5-C6-O6
6	P	1	NAG	C3-C2-N2-C7
6	U	1	NAG	C3-C2-N2-C7

There are no ring outliers.

10 monomers are involved in 19 short contacts:

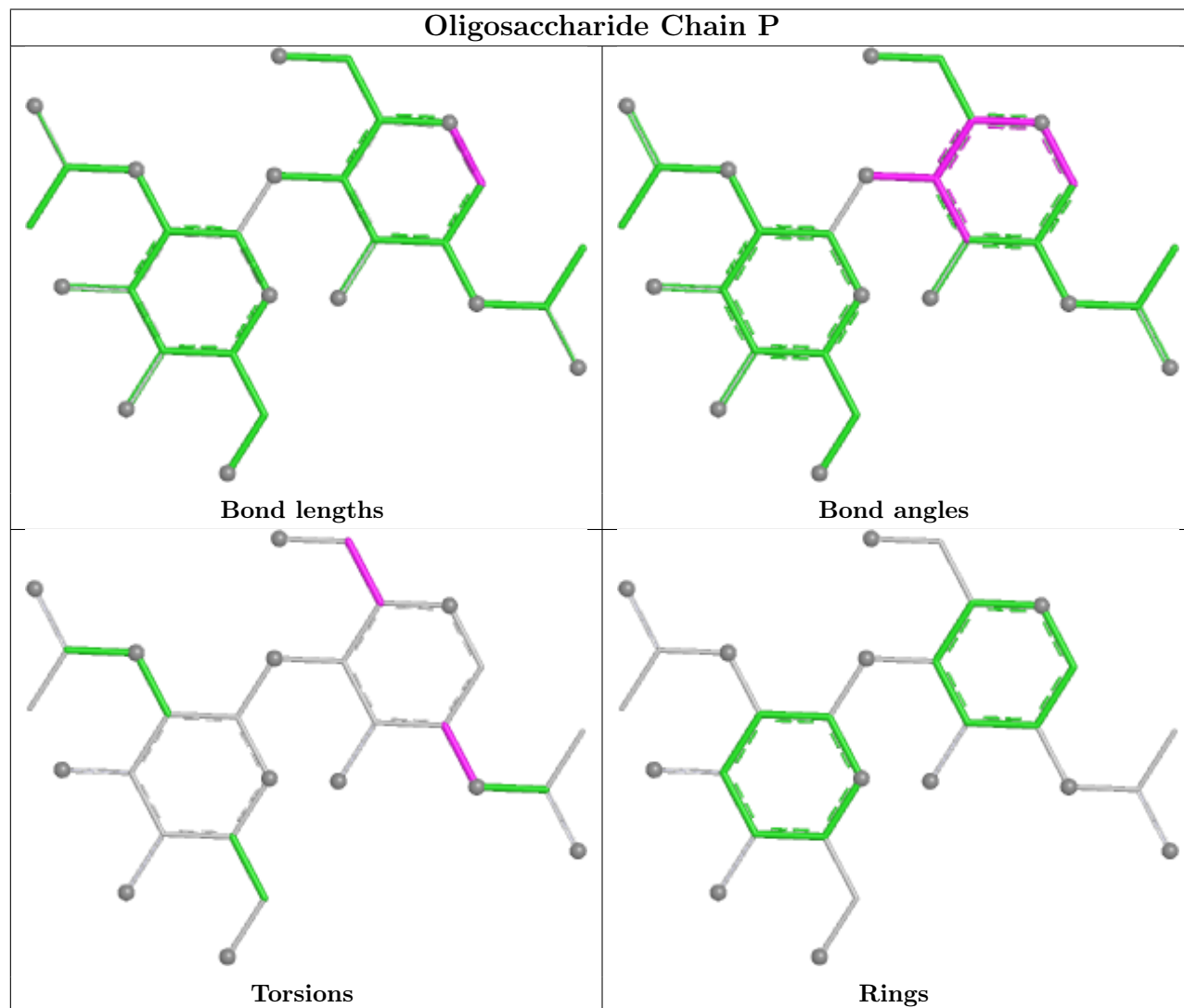
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	U	1	NAG	1	0
6	Y	1	NAG	2	0
6	R	1	NAG	1	0
6	d	2	NAG	2	0
6	Z	1	NAG	7	0
6	Y	2	NAG	2	0
6	P	1	NAG	1	0
6	W	1	NAG	1	0

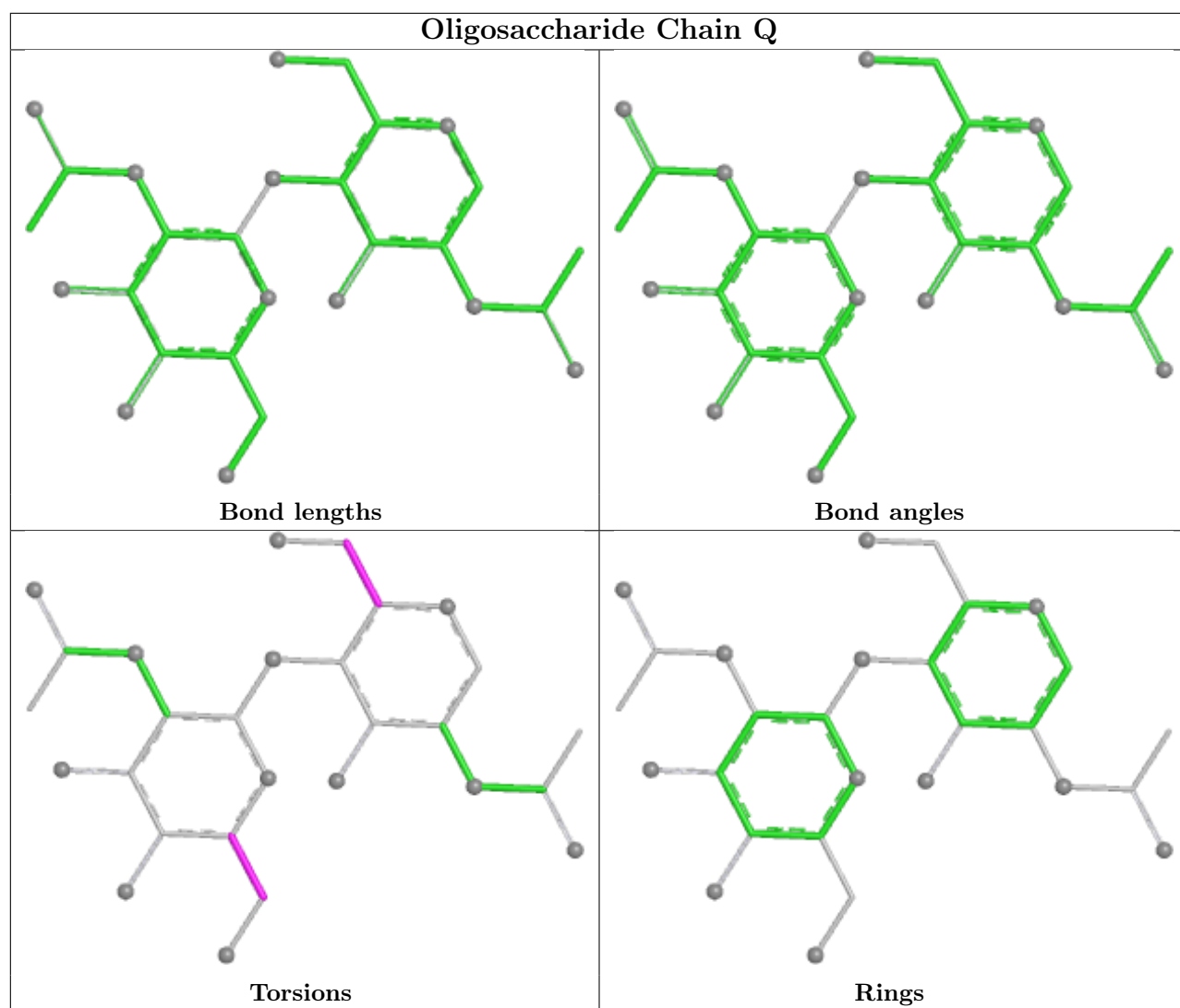
Continued on next page...

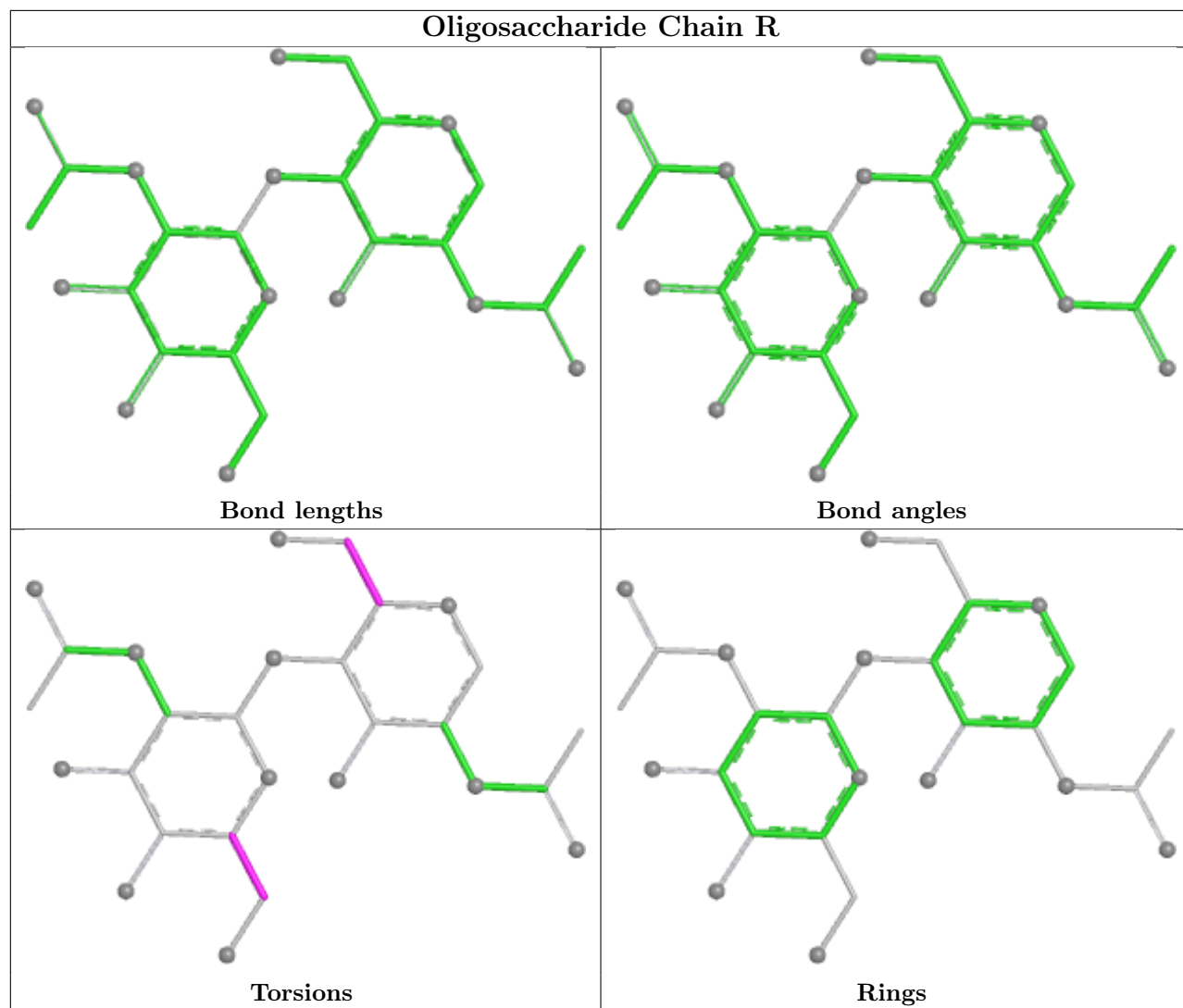
Continued from previous page...

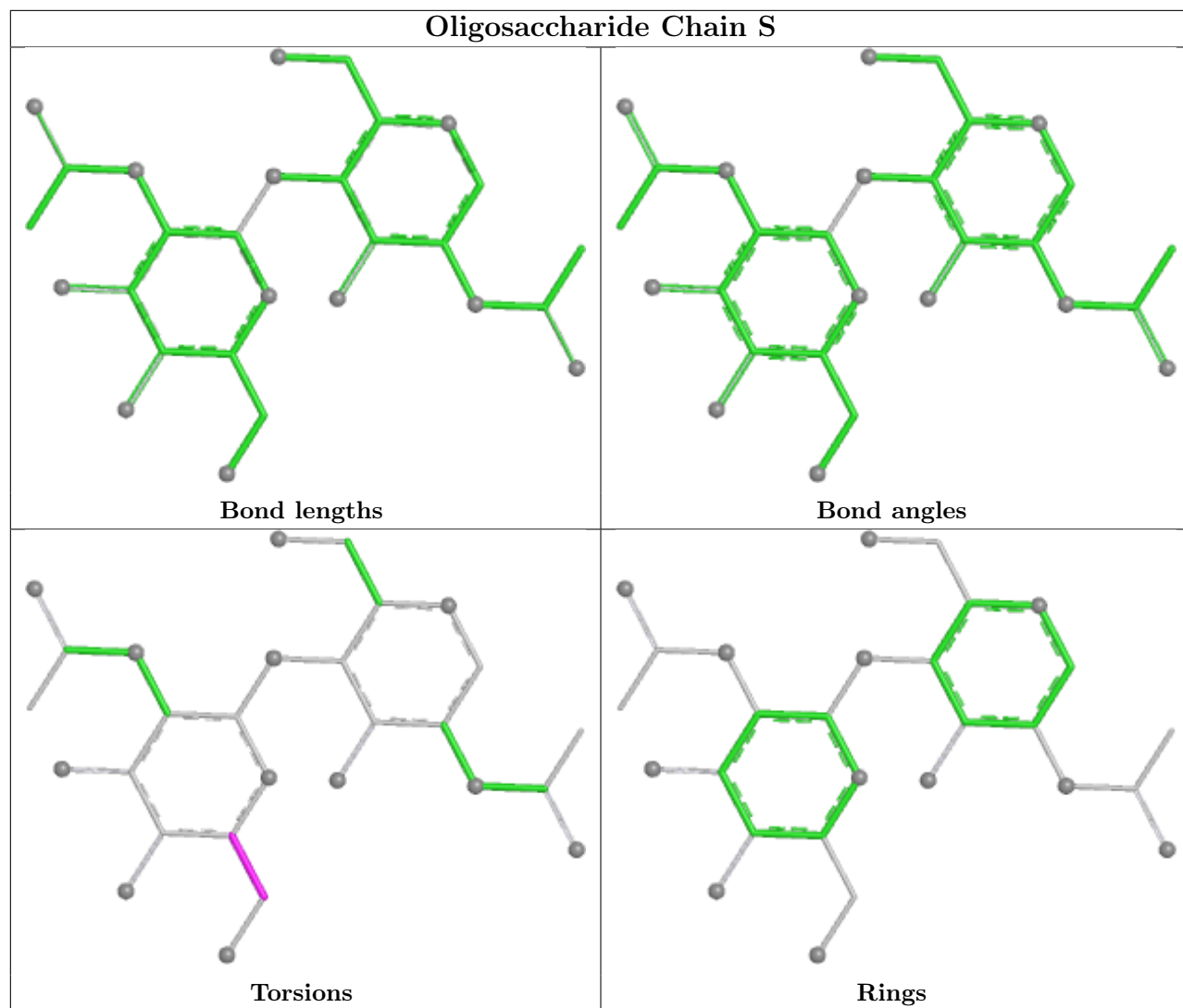
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	b	1	NAG	1	0
6	d	1	NAG	3	0

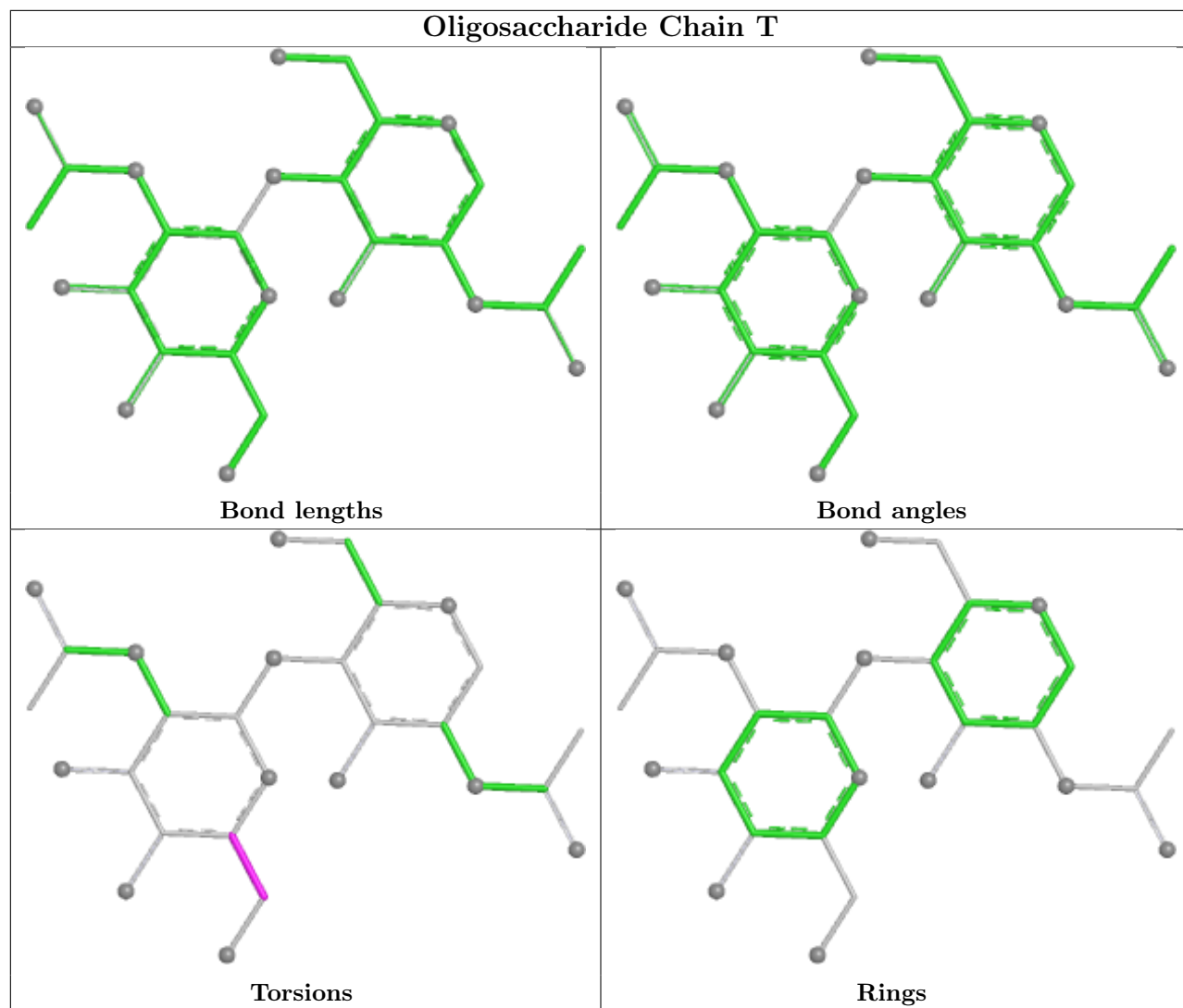
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

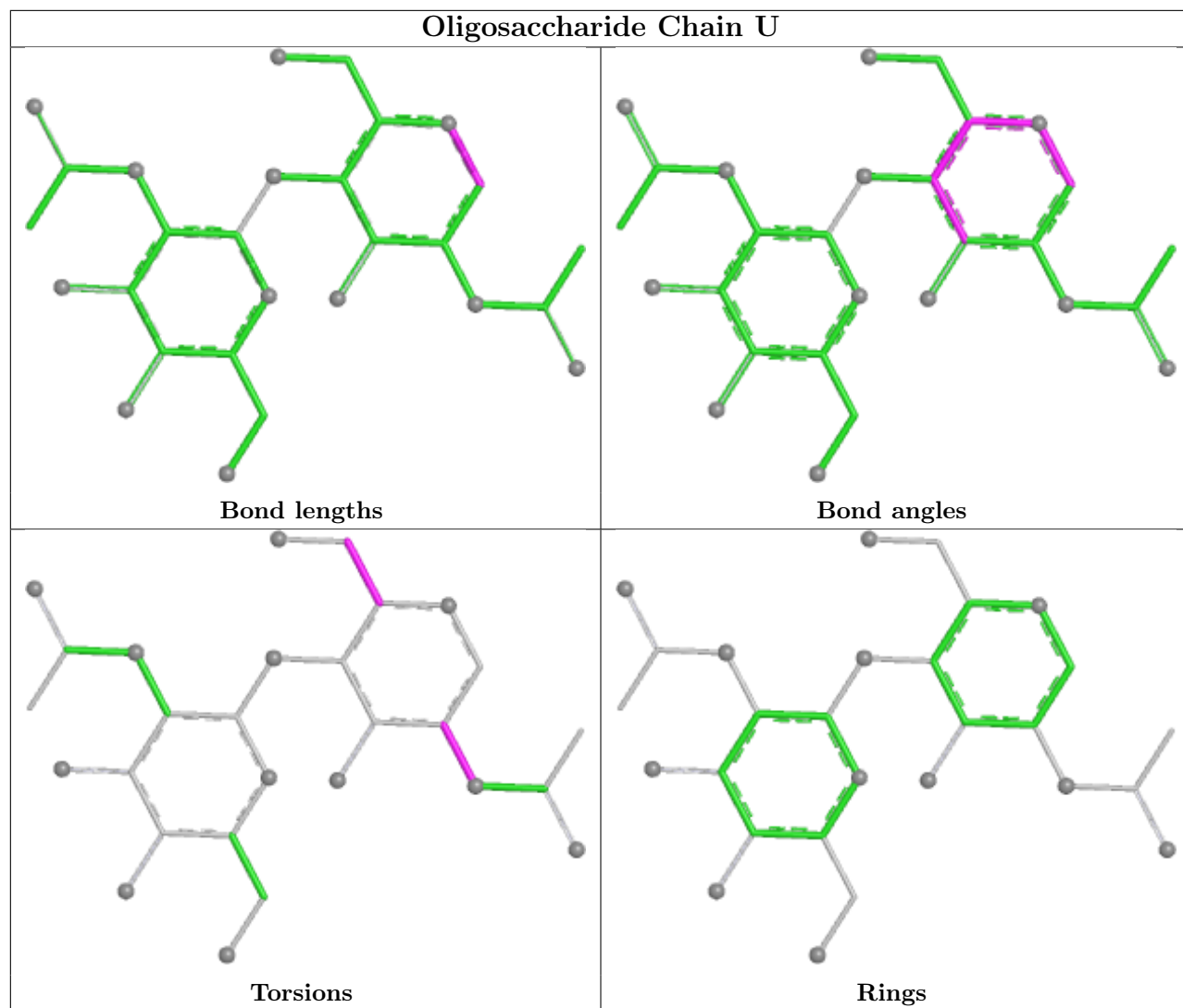


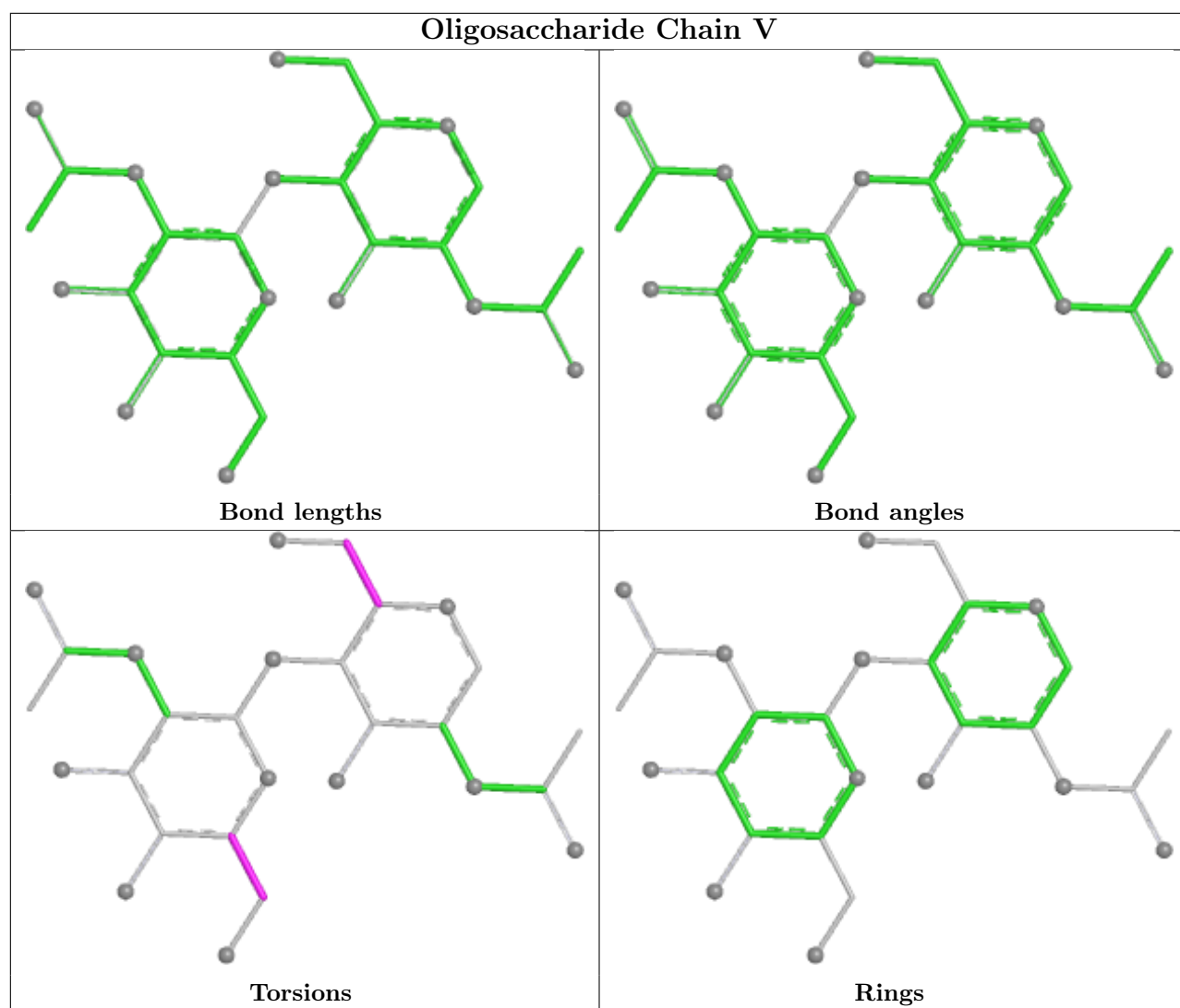


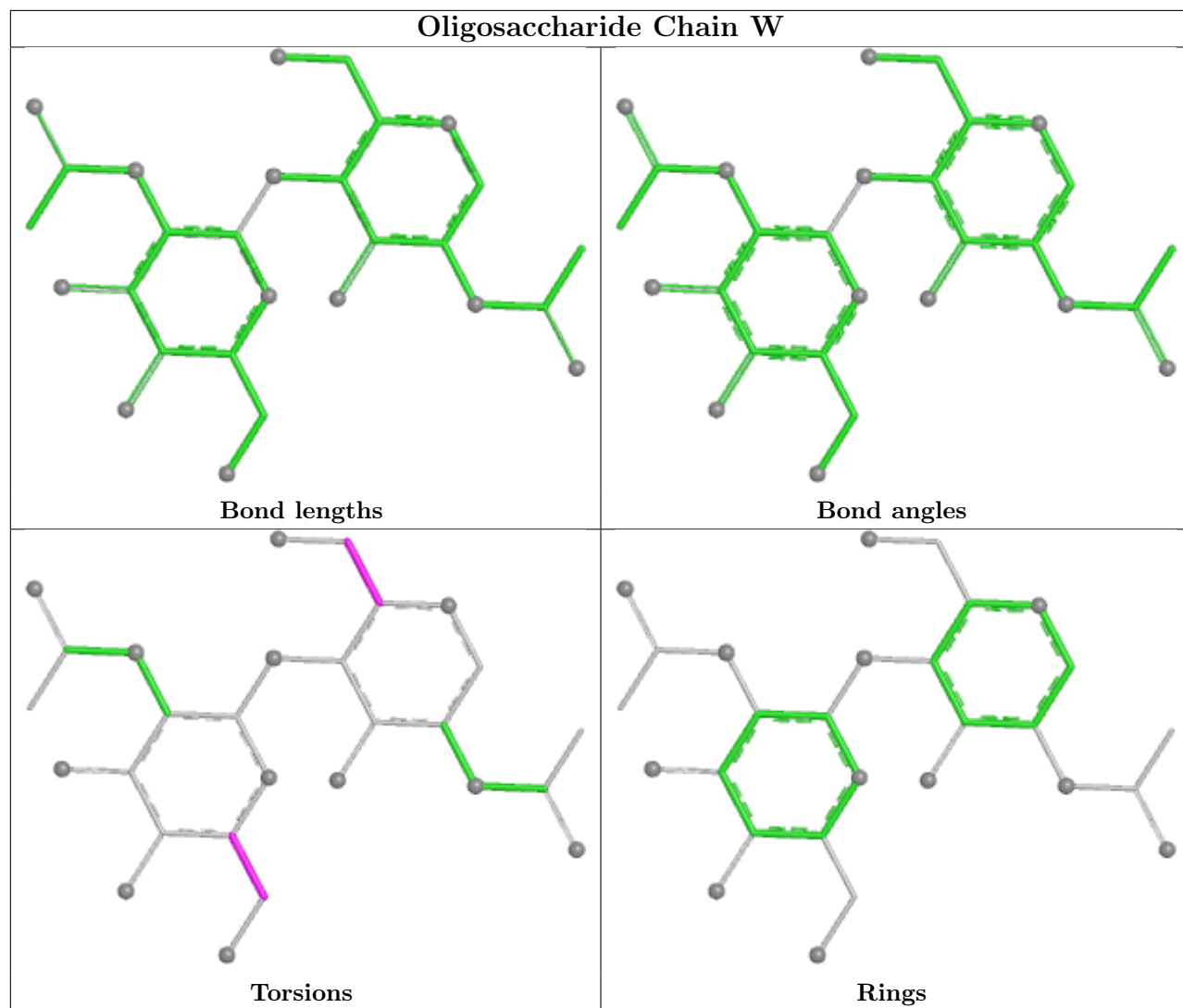


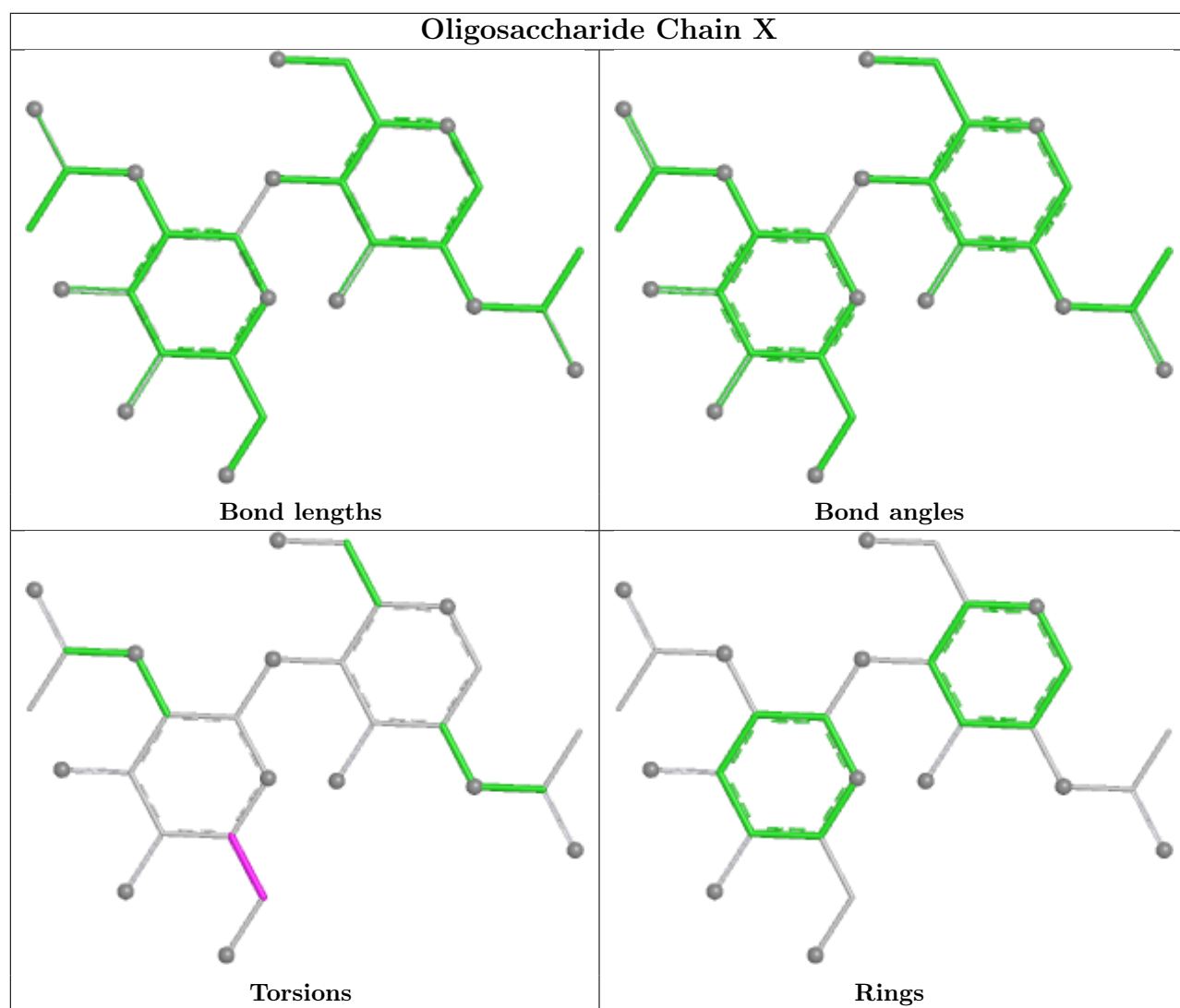


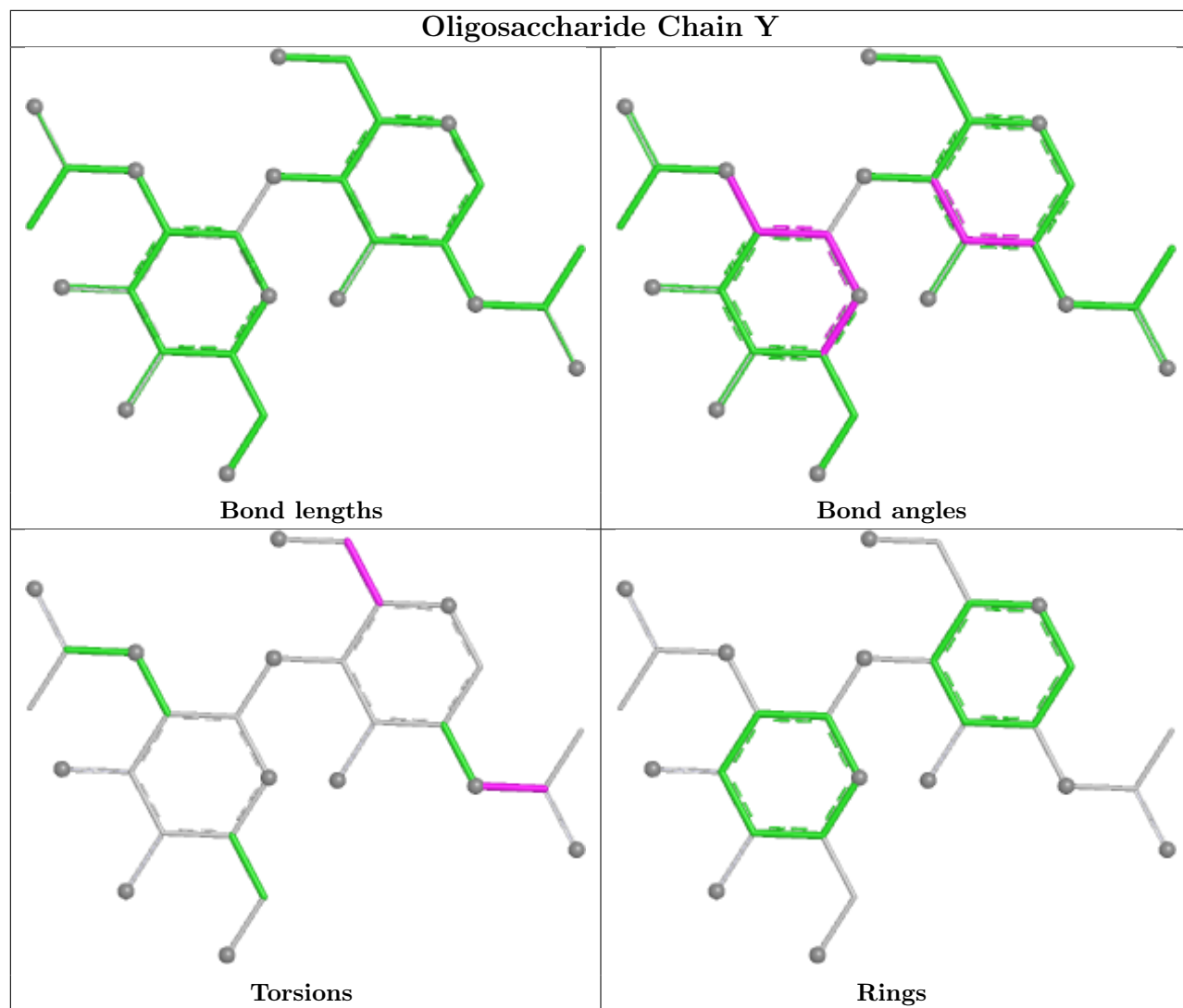


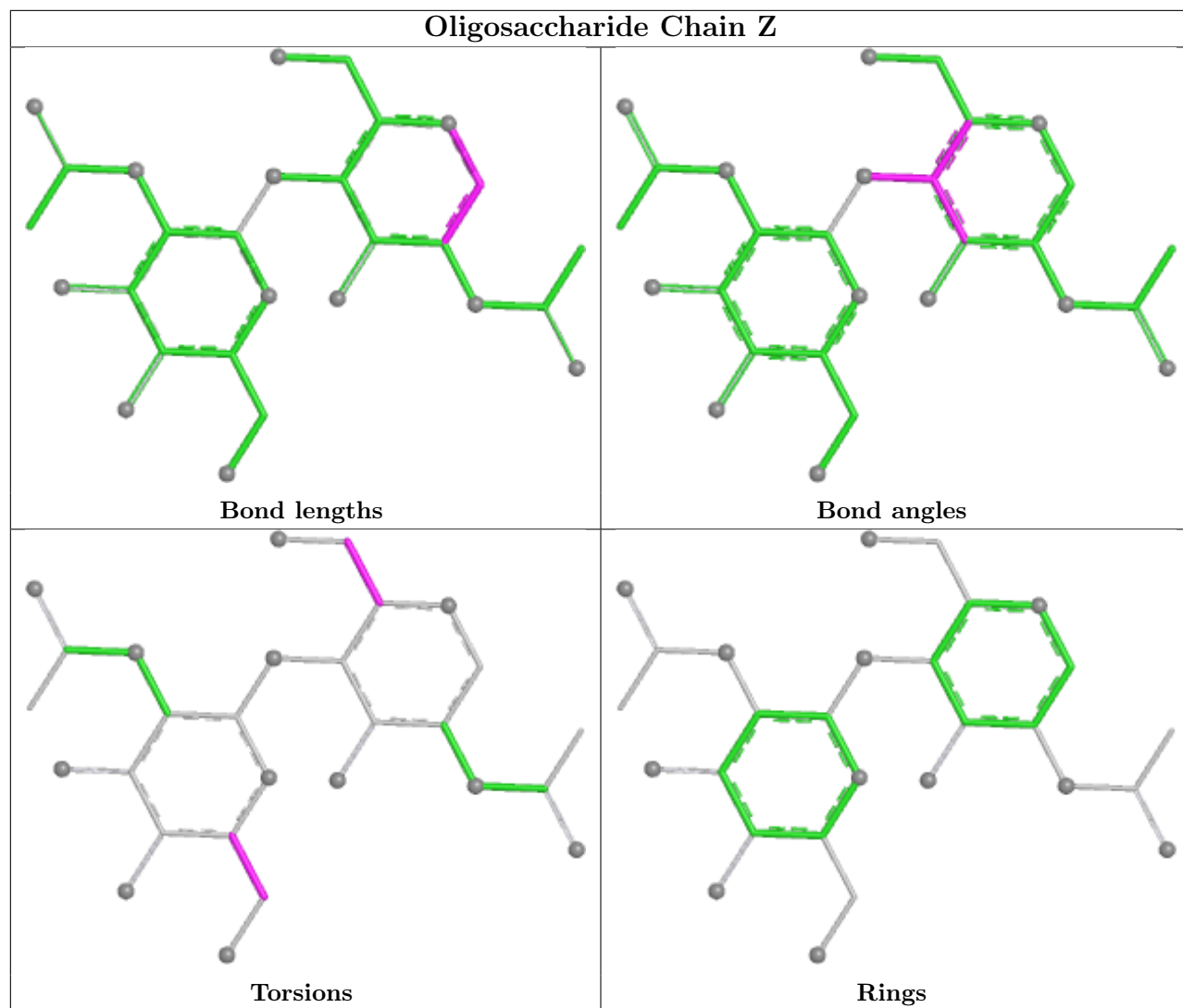


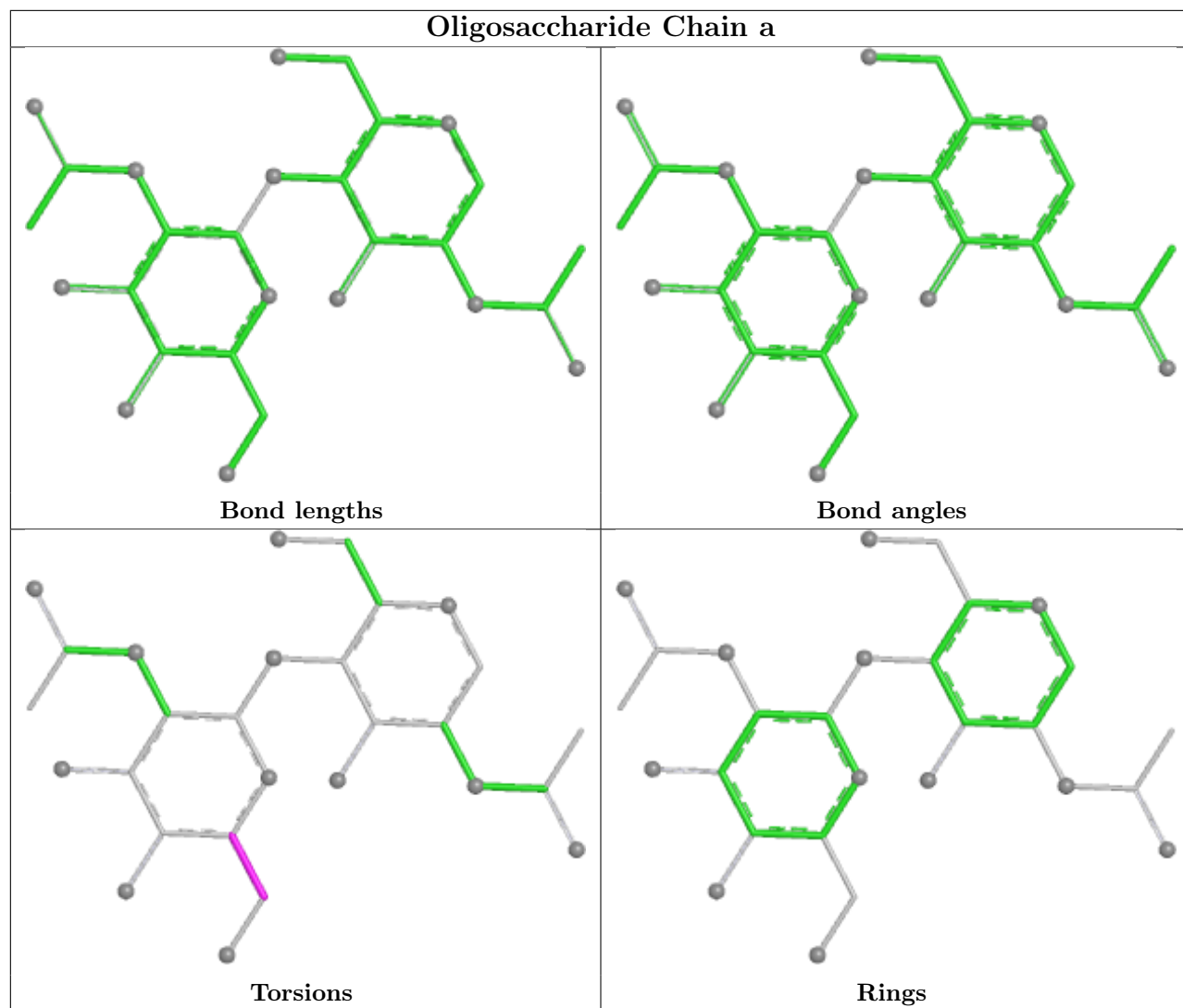


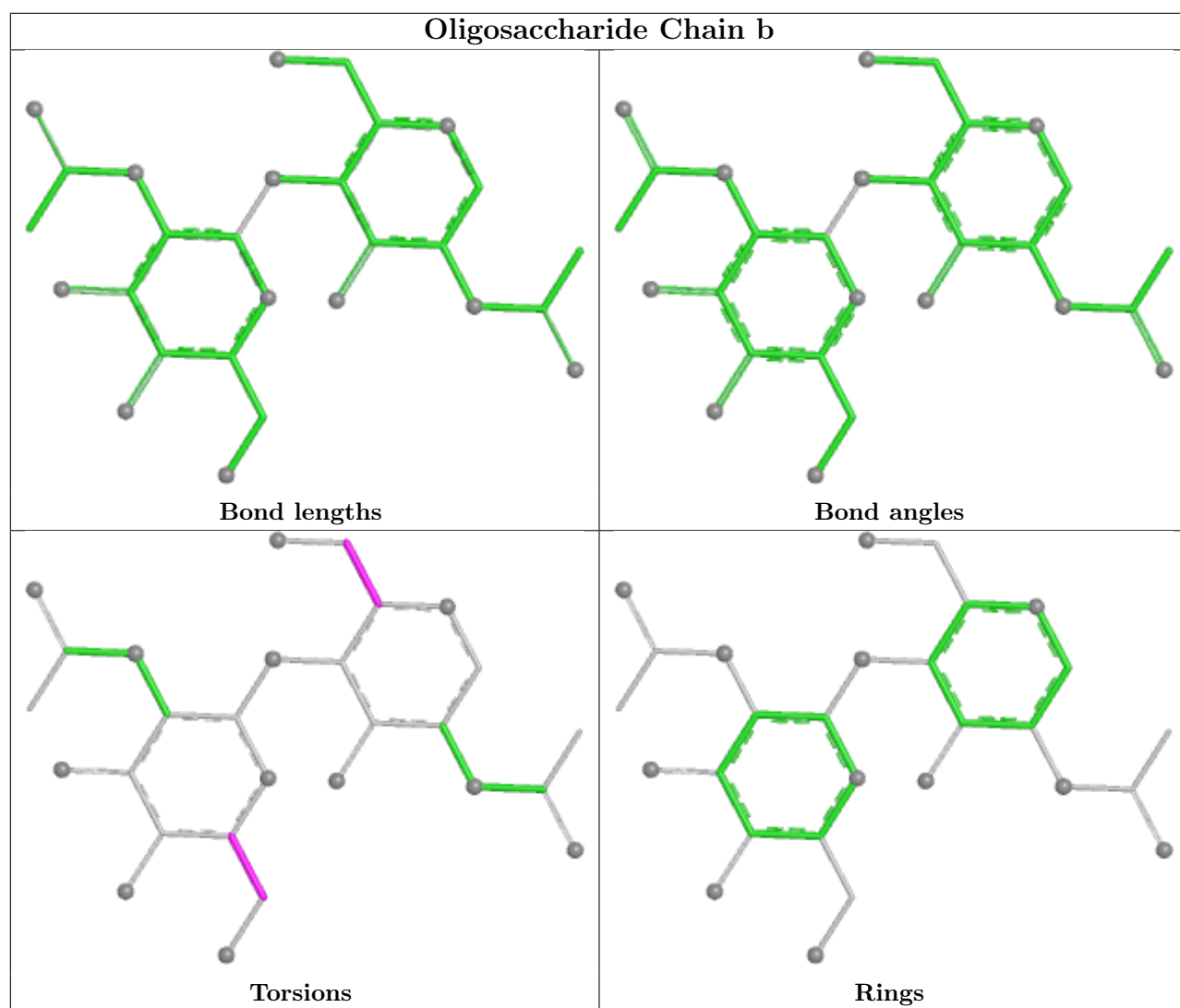


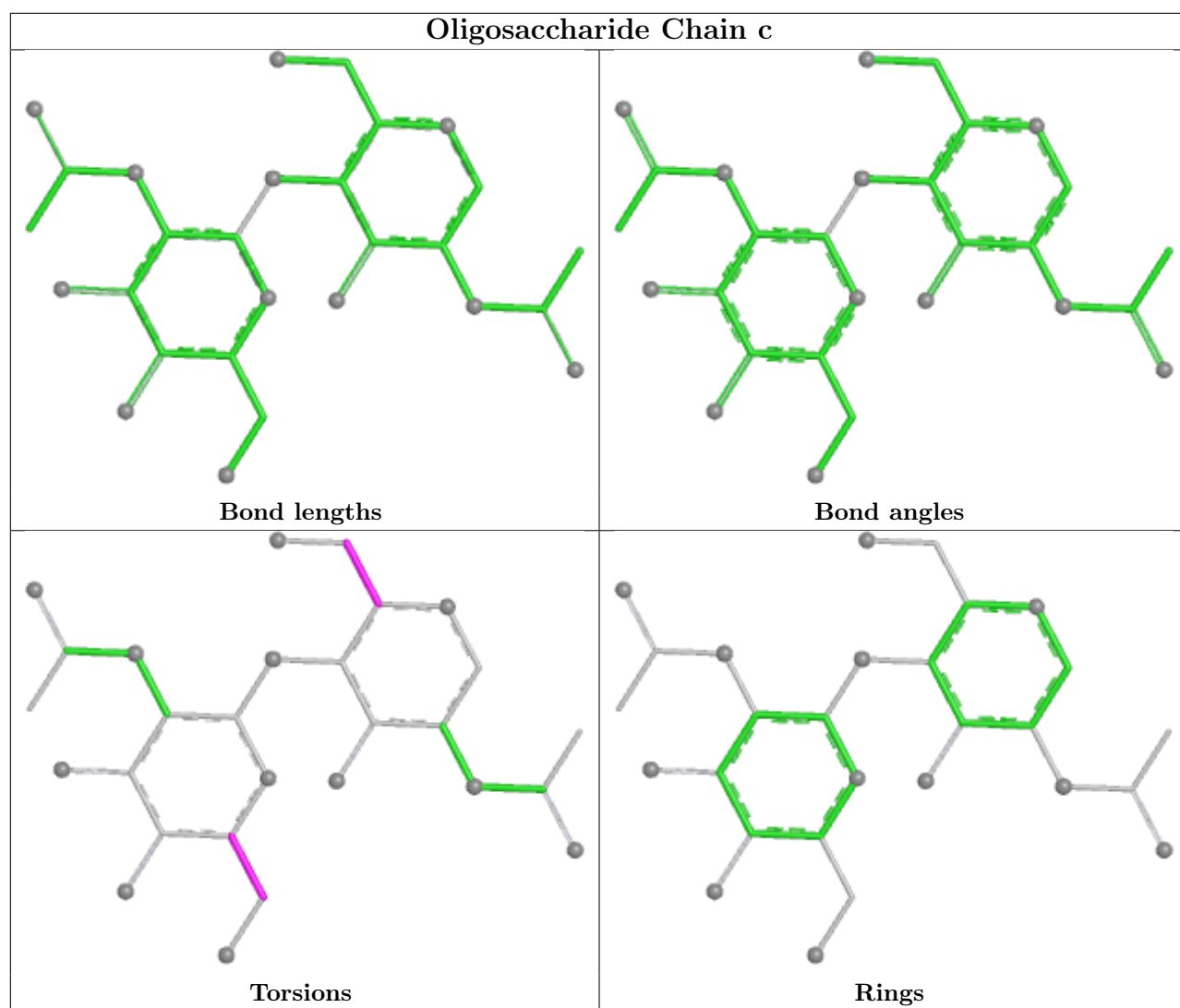


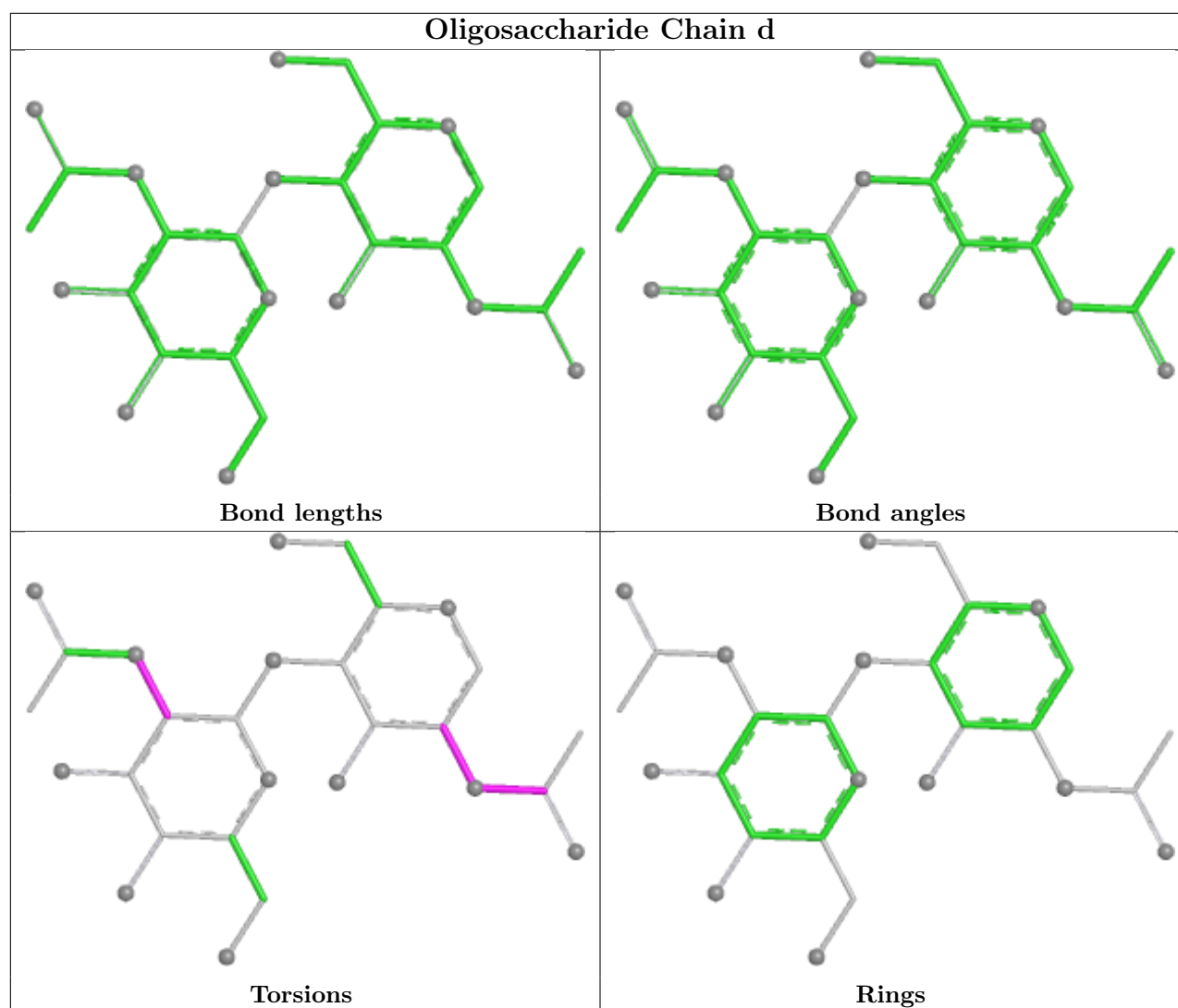












5.6 Ligand geometry [i](#)

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	NAG	A	1303	1	14,14,15	0.46	0	17,19,21	0.50	0
7	NAG	B	1304	1	14,14,15	0.56	0	17,19,21	0.37	0
7	NAG	A	1306	1	14,14,15	0.21	0	17,19,21	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	C	1303	1	14,14,15	0.33	0	17,19,21	0.38	0
7	NAG	C	1301	1	14,14,15	0.41	0	17,19,21	0.43	0
7	NAG	A	1301	1	14,14,15	0.36	0	17,19,21	0.40	0
7	NAG	A	1305	1	14,14,15	0.55	0	17,19,21	0.37	0
7	NAG	C	1302	1	14,14,15	0.67	0	17,19,21	0.46	0
7	NAG	B	1305	1	14,14,15	0.23	0	17,19,21	0.64	0
7	NAG	A	1304	1	14,14,15	0.22	0	17,19,21	0.46	0
7	NAG	B	1301	1	14,14,15	0.21	0	17,19,21	0.36	0
7	NAG	B	1303	1	14,14,15	0.19	0	17,19,21	0.45	0
7	NAG	A	1302	1	14,14,15	0.22	0	17,19,21	0.37	0
7	NAG	C	1304	1	14,14,15	0.46	0	17,19,21	0.52	0
7	NAG	B	1302	1	14,14,15	0.47	0	17,19,21	0.51	0
7	NAG	C	1305	1	14,14,15	0.25	0	17,19,21	0.53	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
7	NAG	A	1303	1	-	1/6/23/26	0/1/1/1
7	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1306	1	-	1/6/23/26	0/1/1/1
7	NAG	C	1303	1	-	0/6/23/26	0/1/1/1
7	NAG	C	1301	1	-	0/6/23/26	0/1/1/1
7	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
7	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
7	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
7	NAG	B	1305	1	-	1/6/23/26	0/1/1/1
7	NAG	A	1304	1	-	0/6/23/26	0/1/1/1
7	NAG	B	1301	1	-	0/6/23/26	0/1/1/1
7	NAG	B	1303	1	-	0/6/23/26	0/1/1/1
7	NAG	A	1302	1	-	0/6/23/26	0/1/1/1
7	NAG	C	1304	1	-	2/6/23/26	0/1/1/1
7	NAG	B	1302	1	-	1/6/23/26	0/1/1/1
7	NAG	C	1305	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	1302	NAG	O5-C5-C6-O6
7	A	1305	NAG	C4-C5-C6-O6
7	B	1304	NAG	C4-C5-C6-O6
7	A	1305	NAG	O5-C5-C6-O6
7	B	1304	NAG	O5-C5-C6-O6
7	C	1304	NAG	C4-C5-C6-O6
7	C	1302	NAG	C4-C5-C6-O6
7	C	1304	NAG	O5-C5-C6-O6
7	C	1305	NAG	O5-C5-C6-O6
7	A	1306	NAG	O5-C5-C6-O6
7	B	1305	NAG	O5-C5-C6-O6
7	A	1303	NAG	O5-C5-C6-O6
7	B	1302	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	1304	NAG	1	0
7	A	1305	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

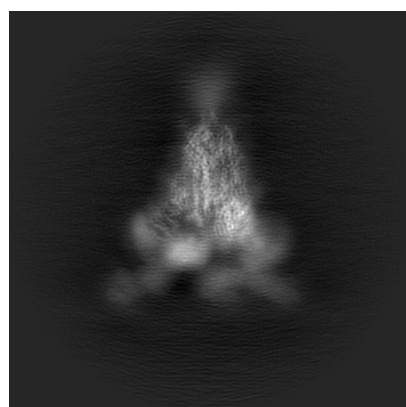
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30484. These allow visual inspection of the internal detail of the map and identification of artifacts.

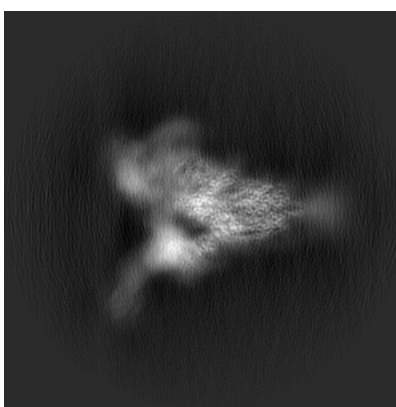
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

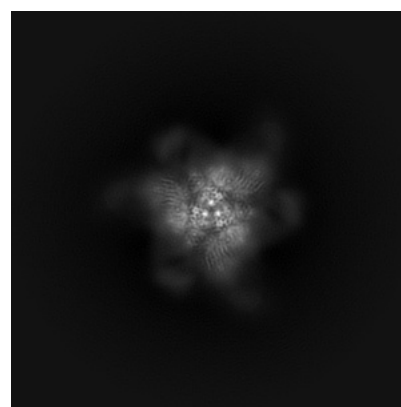
6.1.1 Primary map



X



Y

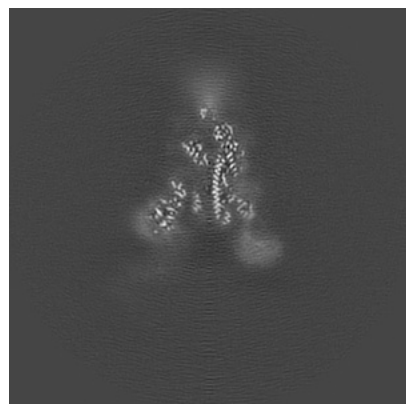


Z

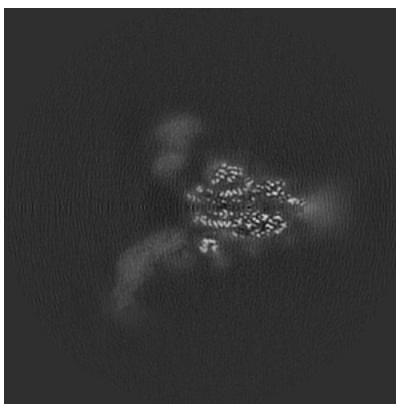
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

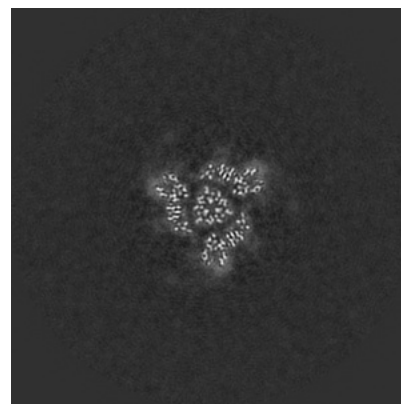
6.2.1 Primary map



X Index: 200



Y Index: 200

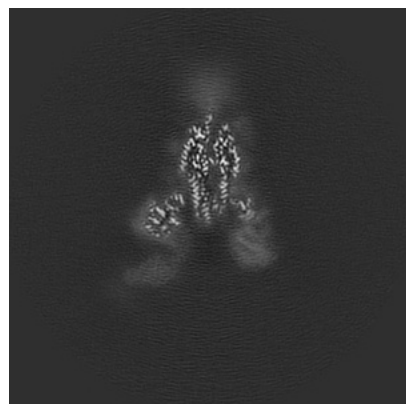


Z Index: 200

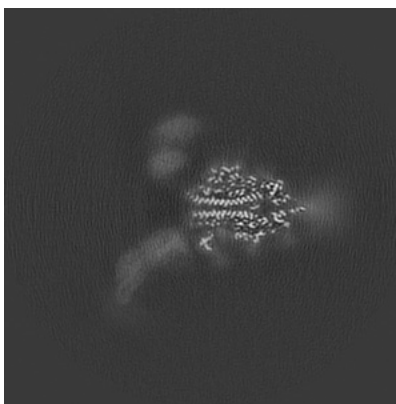
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

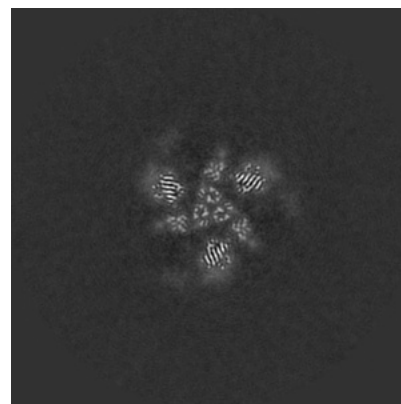
6.3.1 Primary map



X Index: 209



Y Index: 196

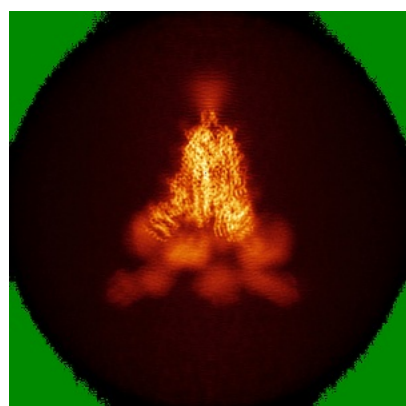


Z Index: 194

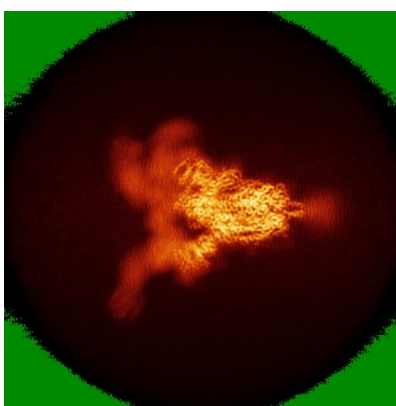
The images above show the largest variance slices of the map in three orthogonal directions.

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

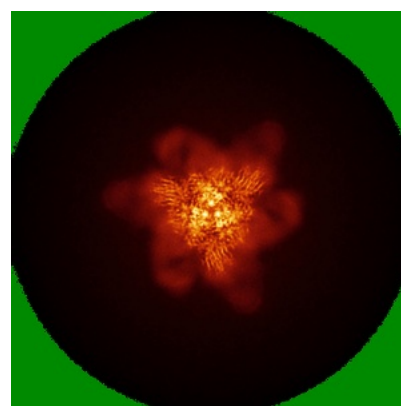
6.4.1 Primary map



X



Y

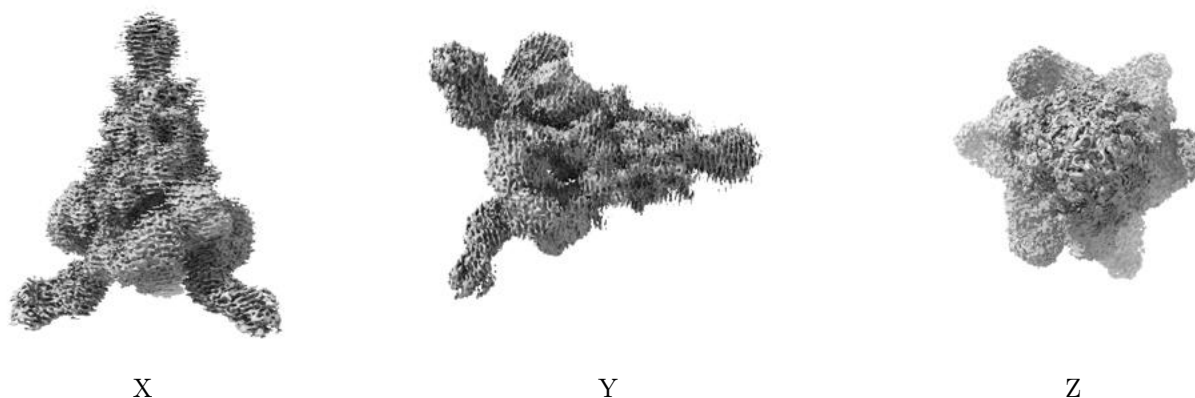


Z

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 0.00538. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

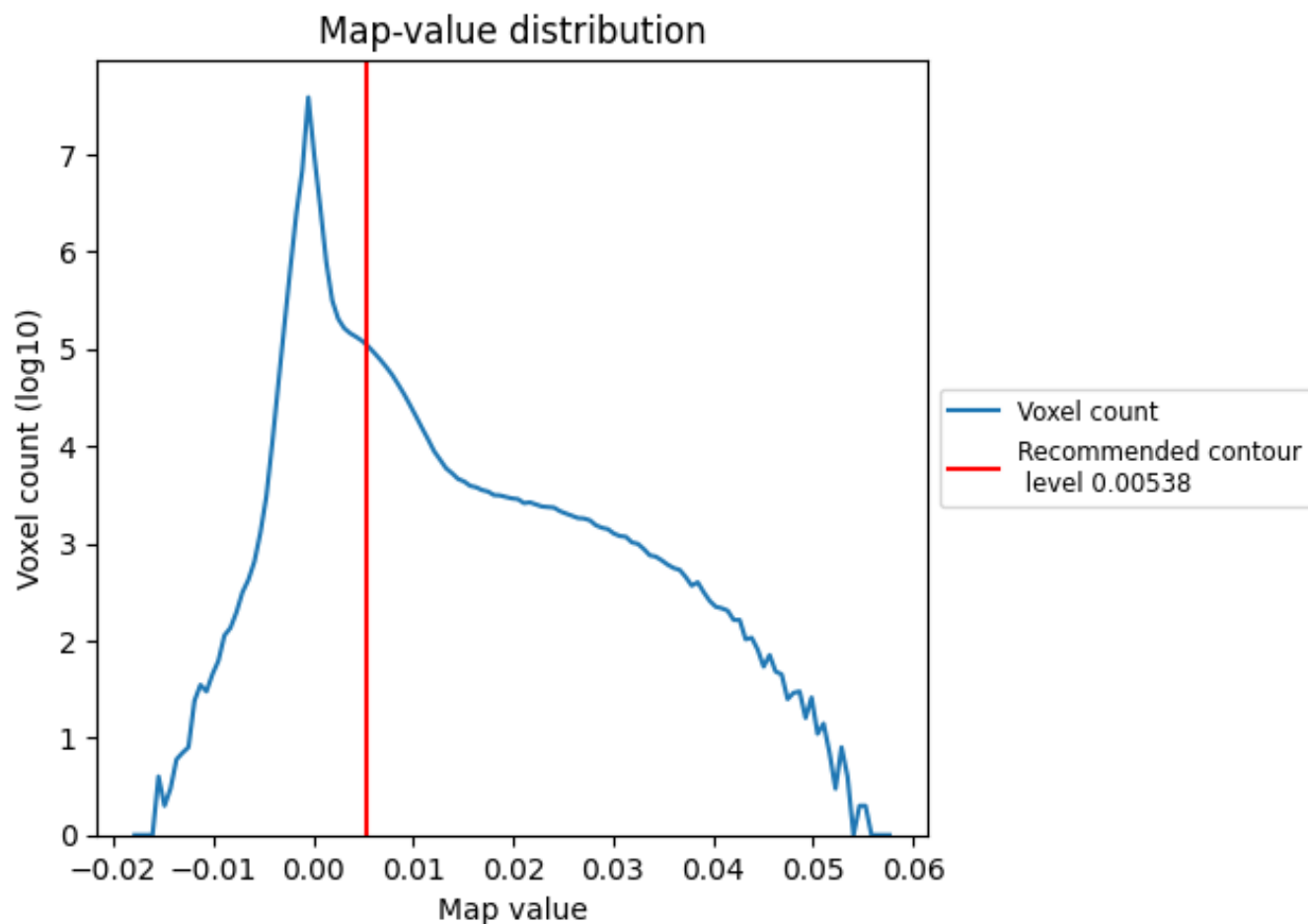
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

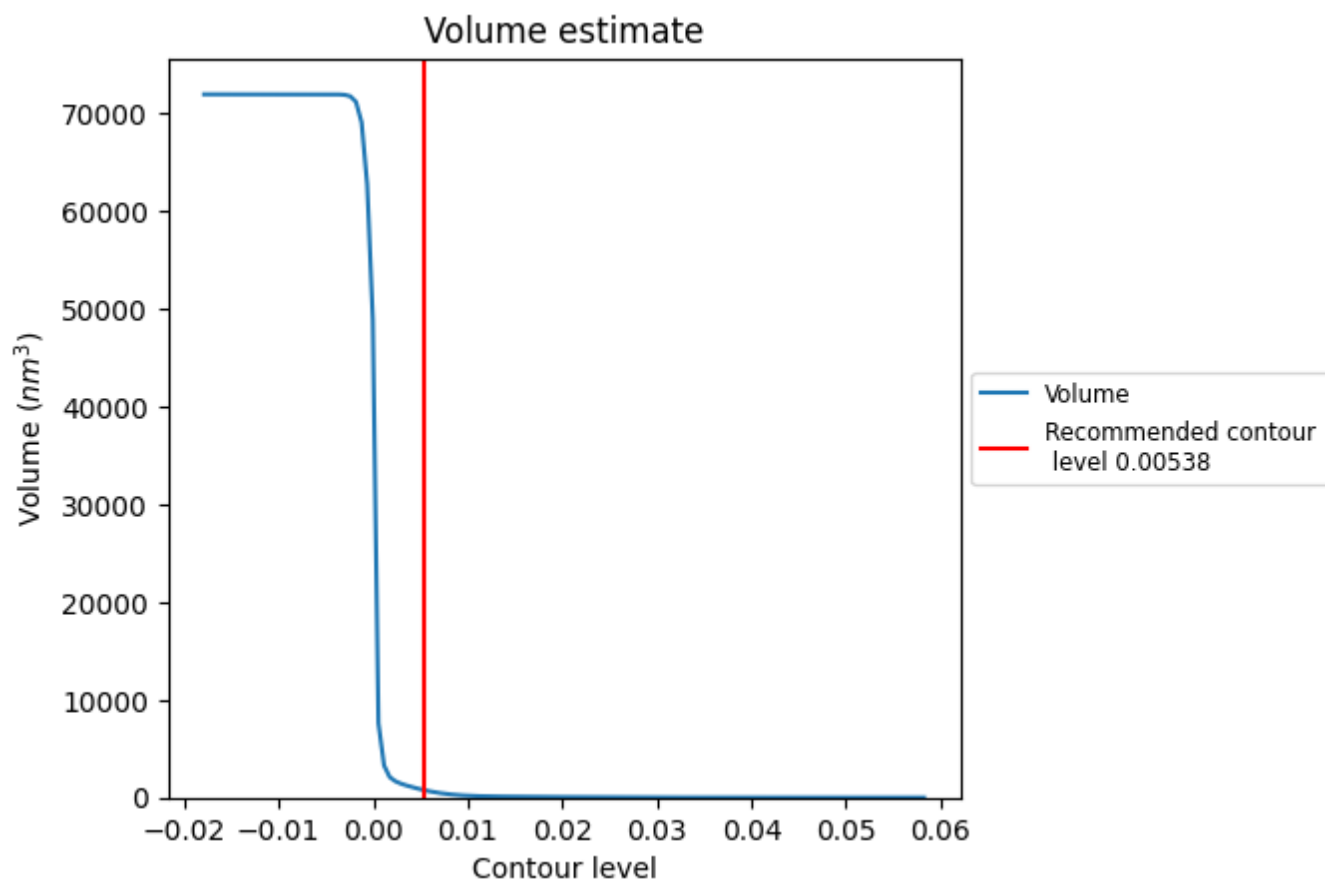
This section contains the results of statistical analysis of the map.

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.

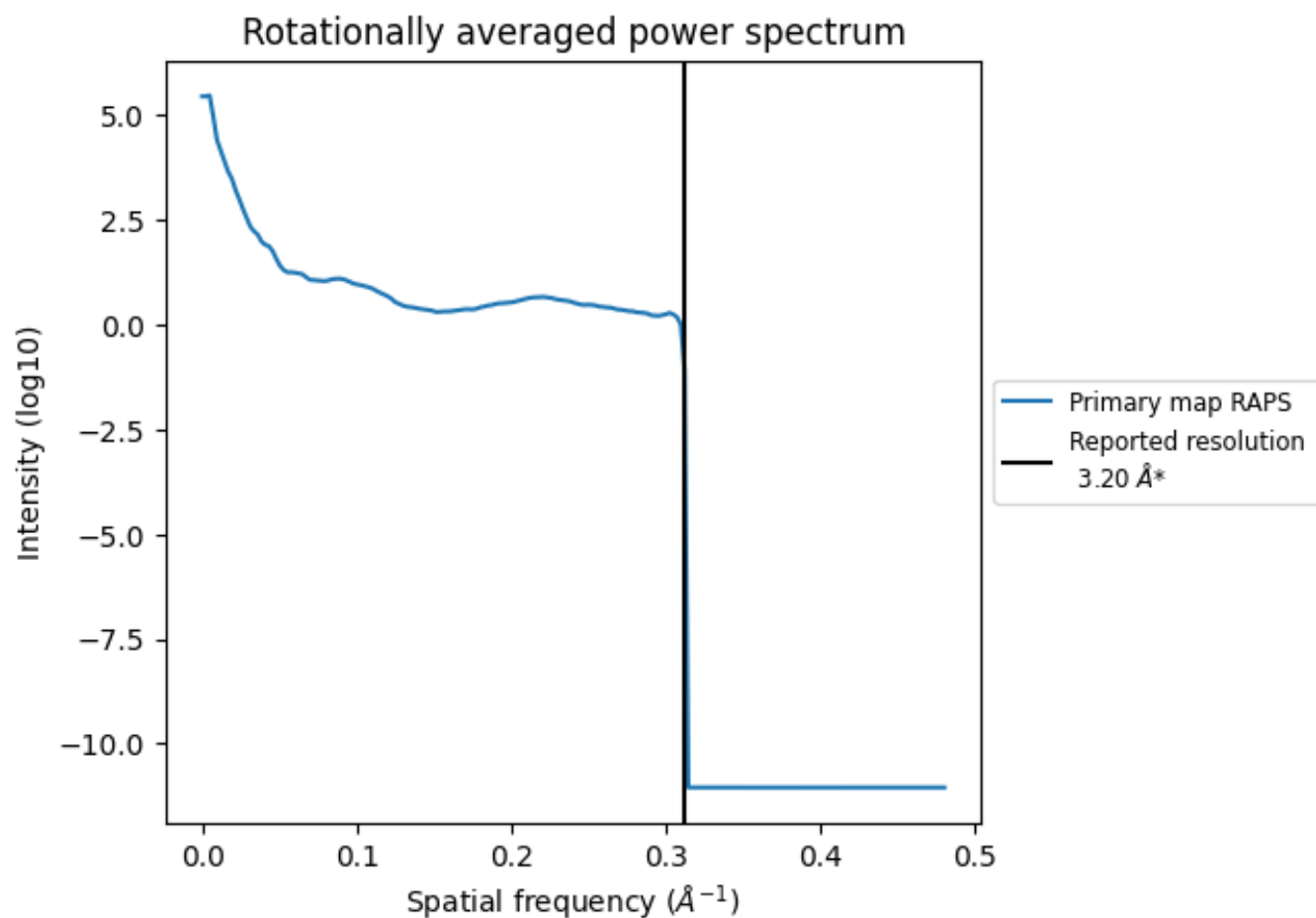
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 763 nm³; this corresponds to an approximate mass of 689 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 0.312 $\text{\AA}^{-1}$

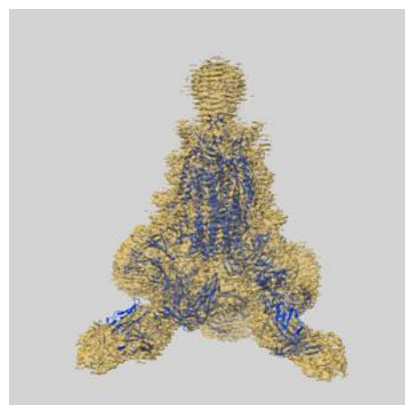
8 Fourier-Shell correlation ⓘ

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

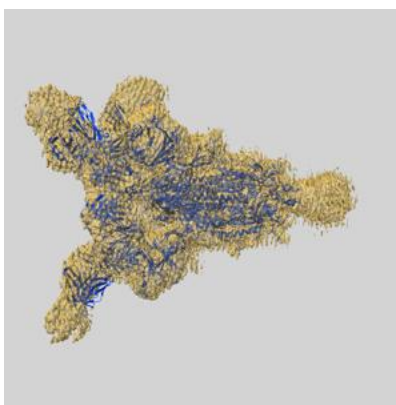
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30484 and PDB model 7CWN. Per-residue inclusion information can be found in section [3](#) on page [9](#).

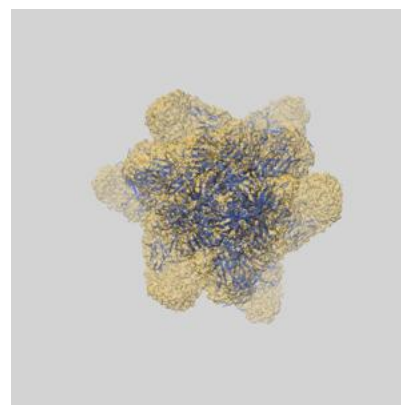
9.1 Map-model overlay [i](#)



X



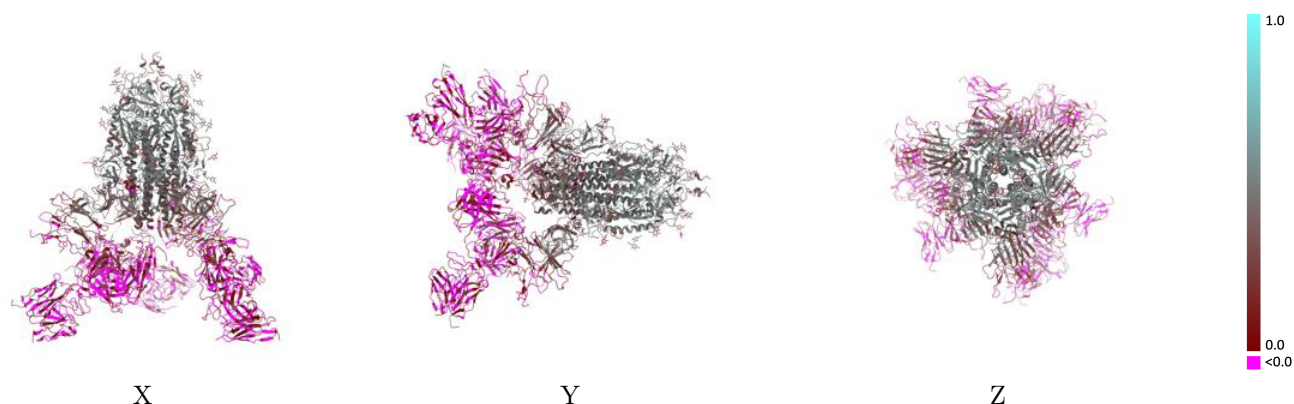
Y



Z

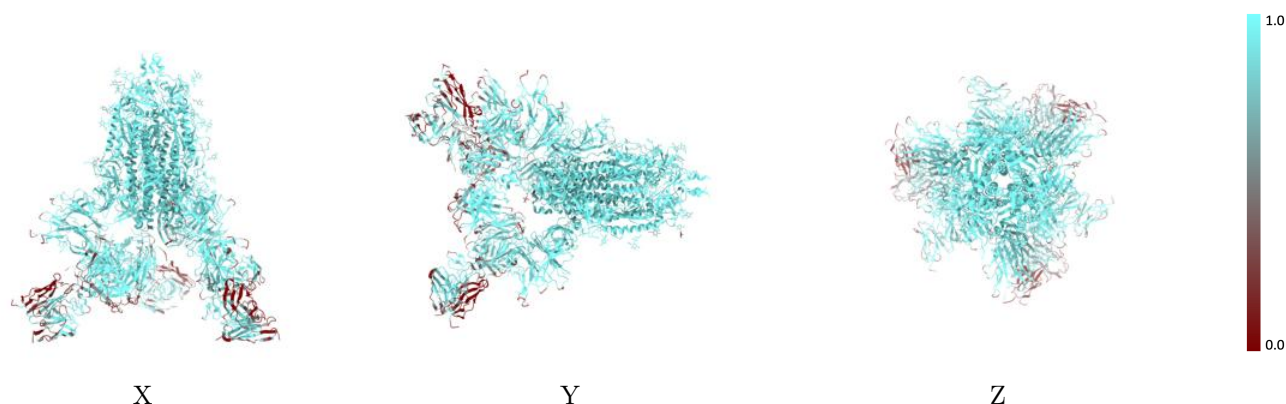
The images above show the 3D surface view of the map at the recommended contour level 0.00538 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



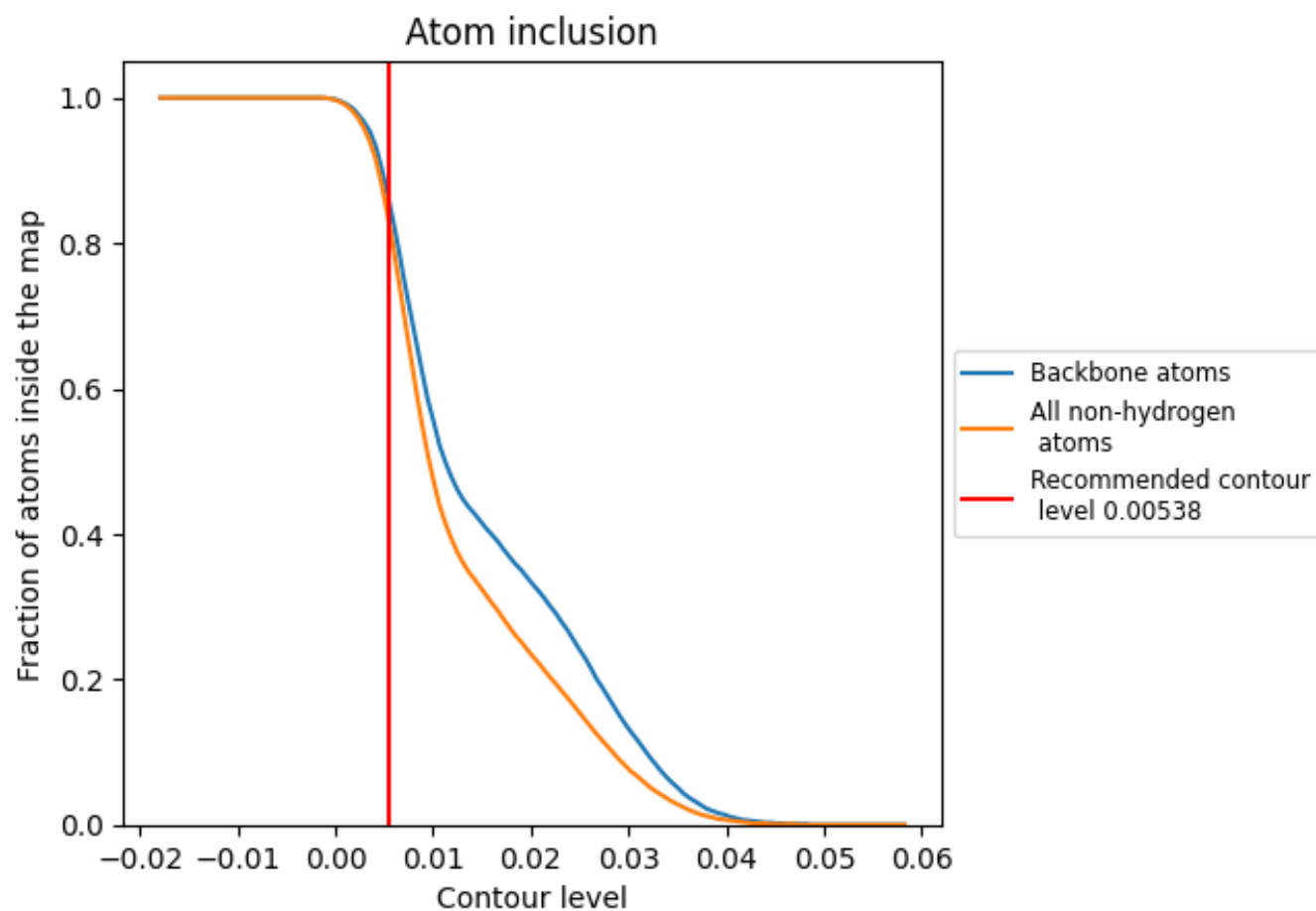
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00538).

9.4 Atom inclusion ⓘ



At the recommended contour level, 86% of all backbone atoms, 84% 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 (0.00538) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8370	 0.2240
A	 0.9070	 0.3080
B	 0.9090	 0.3100
C	 0.9100	 0.3100
D	 0.7790	 0.0090
E	 0.8550	 0.0200
F	 0.6080	 -0.0030
G	 0.4180	 0.0440
H	 0.8550	 0.0110
I	 0.6010	 -0.0000
J	 0.6330	 0.0040
K	 0.4280	 0.0490
L	 0.4320	 0.0470
M	 0.7730	 0.0070
N	 0.7840	 0.0120
O	 0.8540	 0.0150
P	 0.2860	 0.0240
Q	 0.7860	 0.3560
R	 0.9290	 0.3420
S	 0.8210	 0.3320
T	 0.8210	 0.3530
U	 0.2860	 0.0060
V	 0.7860	 0.3830
W	 0.9290	 0.3460
X	 0.8210	 0.3750
Y	 0.7860	 0.2490
Z	 0.3210	 0.0990
a	 0.7860	 0.3580
b	 0.8930	 0.3670
c	 0.7860	 0.2380
d	 0.5710	 0.1250

