



## Full wwPDB EM Validation Report ⓘ

Nov 12, 2022 – 08:44 PM EST

PDB ID : 6VKT  
EMDB ID : EMD-21229  
Title : Cryo-electron microscopy structures of a gonococcal multidrug efflux pump illuminate a mechanism of erythromycin drug recognition  
Authors : Lyu, M.; Moseng, M.A.  
Deposited on : 2020-01-22  
Resolution : 2.72 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

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

EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

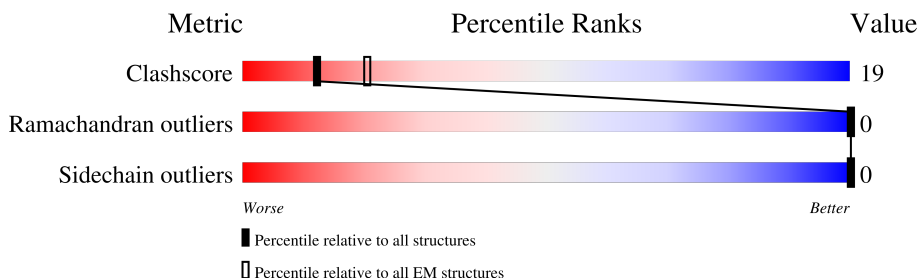
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.72 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	1046	
1	B	1046	
1	C	1046	

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
2	PTY	C	1106	-	-	X	-
3	ERY	B	1101	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24331 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 Efflux pump membrane transporter.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1037	Total	C	N	O	S	0	0
			7761	4977	1288	1451	45		
1	B	1043	Total	C	N	O	S	0	0
			7813	5010	1299	1459	45		
1	C	1042	Total	C	N	O	S	0	0
			7806	5006	1298	1457	45		

There are 66 discrepancies between the modelled and reference sequences:

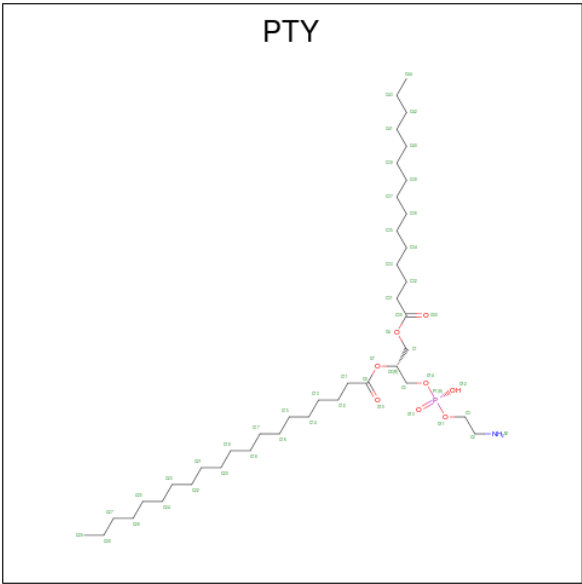
Chain	Residue	Modelled	Actual	Comment	Reference
A	738	VAL	ILE	conflict	UNP A0A4T9VBR9
A	774	GLY	GLU	conflict	UNP A0A4T9VBR9
A	791	SER	LYS	conflict	UNP A0A4T9VBR9
A	794	ILE	VAL	conflict	UNP A0A4T9VBR9
A	800	SER	THR	conflict	UNP A0A4T9VBR9
A	807	GLN	GLU	conflict	UNP A0A4T9VBR9
A	808	MET	ASN	conflict	UNP A0A4T9VBR9
A	821	ALA	SER	conflict	UNP A0A4T9VBR9
A	823	GLU	LYS	conflict	UNP A0A4T9VBR9
A	826	GLY	ALA	conflict	UNP A0A4T9VBR9
A	839	GLU	ALA	conflict	UNP A0A4T9VBR9
A	850	SER	GLY	conflict	UNP A0A4T9VBR9
A	854	LEU	PHE	conflict	UNP A0A4T9VBR9
A	871	ILE	LEU	conflict	UNP A0A4T9VBR9
A	872	ALA	ILE	conflict	UNP A0A4T9VBR9
A	875	ALA	GLY	conflict	UNP A0A4T9VBR9
A	878	ALA	VAL	conflict	UNP A0A4T9VBR9
A	879	VAL	ALA	conflict	UNP A0A4T9VBR9
A	899	LEU	ILE	conflict	UNP A0A4T9VBR9
A	902	MET	ILE	conflict	UNP A0A4T9VBR9
A	907	ALA	ILE	conflict	UNP A0A4T9VBR9
A	1000	GLY	ALA	conflict	UNP A0A4T9VBR9
B	738	VAL	ILE	conflict	UNP A0A4T9VBR9
B	774	GLY	GLU	conflict	UNP A0A4T9VBR9

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	791	SER	LYS	conflict	UNP A0A4T9VBR9
B	794	ILE	VAL	conflict	UNP A0A4T9VBR9
B	800	SER	THR	conflict	UNP A0A4T9VBR9
B	807	GLN	GLU	conflict	UNP A0A4T9VBR9
B	808	MET	ASN	conflict	UNP A0A4T9VBR9
B	821	ALA	SER	conflict	UNP A0A4T9VBR9
B	823	GLU	LYS	conflict	UNP A0A4T9VBR9
B	826	GLY	ALA	conflict	UNP A0A4T9VBR9
B	839	GLU	ALA	conflict	UNP A0A4T9VBR9
B	850	SER	GLY	conflict	UNP A0A4T9VBR9
B	854	LEU	PHE	conflict	UNP A0A4T9VBR9
B	871	ILE	LEU	conflict	UNP A0A4T9VBR9
B	872	ALA	ILE	conflict	UNP A0A4T9VBR9
B	875	ALA	GLY	conflict	UNP A0A4T9VBR9
B	878	ALA	VAL	conflict	UNP A0A4T9VBR9
B	879	VAL	ALA	conflict	UNP A0A4T9VBR9
B	899	LEU	ILE	conflict	UNP A0A4T9VBR9
B	902	MET	ILE	conflict	UNP A0A4T9VBR9
B	907	ALA	ILE	conflict	UNP A0A4T9VBR9
B	1000	GLY	ALA	conflict	UNP A0A4T9VBR9
C	738	VAL	ILE	conflict	UNP A0A4T9VBR9
C	774	GLY	GLU	conflict	UNP A0A4T9VBR9
C	791	SER	LYS	conflict	UNP A0A4T9VBR9
C	794	ILE	VAL	conflict	UNP A0A4T9VBR9
C	800	SER	THR	conflict	UNP A0A4T9VBR9
C	807	GLN	GLU	conflict	UNP A0A4T9VBR9
C	808	MET	ASN	conflict	UNP A0A4T9VBR9
C	821	ALA	SER	conflict	UNP A0A4T9VBR9
C	823	GLU	LYS	conflict	UNP A0A4T9VBR9
C	826	GLY	ALA	conflict	UNP A0A4T9VBR9
C	839	GLU	ALA	conflict	UNP A0A4T9VBR9
C	850	SER	GLY	conflict	UNP A0A4T9VBR9
C	854	LEU	PHE	conflict	UNP A0A4T9VBR9
C	871	ILE	LEU	conflict	UNP A0A4T9VBR9
C	872	ALA	ILE	conflict	UNP A0A4T9VBR9
C	875	ALA	GLY	conflict	UNP A0A4T9VBR9
C	878	ALA	VAL	conflict	UNP A0A4T9VBR9
C	879	VAL	ALA	conflict	UNP A0A4T9VBR9
C	899	LEU	ILE	conflict	UNP A0A4T9VBR9
C	902	MET	ILE	conflict	UNP A0A4T9VBR9
C	907	ALA	ILE	conflict	UNP A0A4T9VBR9
C	1000	GLY	ALA	conflict	UNP A0A4T9VBR9

- Molecule 2 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: C<sub>40</sub>H<sub>80</sub>NO<sub>8</sub>P).



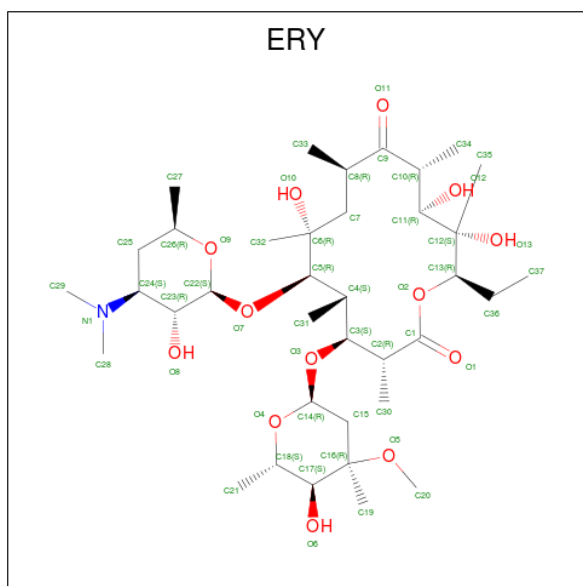
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			264	204	6	48	6	
			Total	C	N	O	P	
			264	204	6	48	6	
			Total	C	N	O	P	
2	A	1	264	204	6	48	6	0
			Total	C	N	O	P	
			264	204	6	48	6	
			Total	C	N	O	P	
			264	204	6	48	6	
2	A	1	Total	C	N	O	P	0
			264	204	6	48	6	
			Total	C	N	O	P	
			264	204	6	48	6	
			Total	C	N	O	P	
2	B	1	322	242	8	64	8	0
			Total	C	N	O	P	
			322	242	8	64	8	
			Total	C	N	O	P	
			322	242	8	64	8	
2	B	1	Total	C	N	O	P	0
			322	242	8	64	8	
			Total	C	N	O	P	
			322	242	8	64	8	
			Total	C	N	O	P	
2	B	1	322	242	8	64	8	0
			Total	C	N	O	P	
			322	242	8	64	8	
			Total	C	N	O	P	
			322	242	8	64	8	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
2	B	1	Total	C	N	O	P	0
			322	242	8	64	8	
2	B	1	Total	C	N	O	P	0
			322	242	8	64	8	
2	C	1	Total	C	N	O	P	0
			314	246	6	56	6	
2	C	1	Total	C	N	O	P	0
			314	246	6	56	6	
2	C	1	Total	C	N	O	P	0
			314	246	6	56	6	
2	C	1	Total	C	N	O	P	0
			314	246	6	56	6	
2	C	1	Total	C	N	O	P	0
			314	246	6	56	6	
2	C	1	Total	C	N	O	P	0
			314	246	6	56	6	
2	C	1	Total	C	N	O	P	0
			314	246	6	56	6	
2	C	1	Total	C	N	O	P	0
			314	246	6	56	6	

- Molecule 3 is ERYTHROMYCIN A (three-letter code: ERY) (formula:  $C_{37}H_{67}NO_{13}$ ) (labeled as "Ligand of Interest" by depositor).

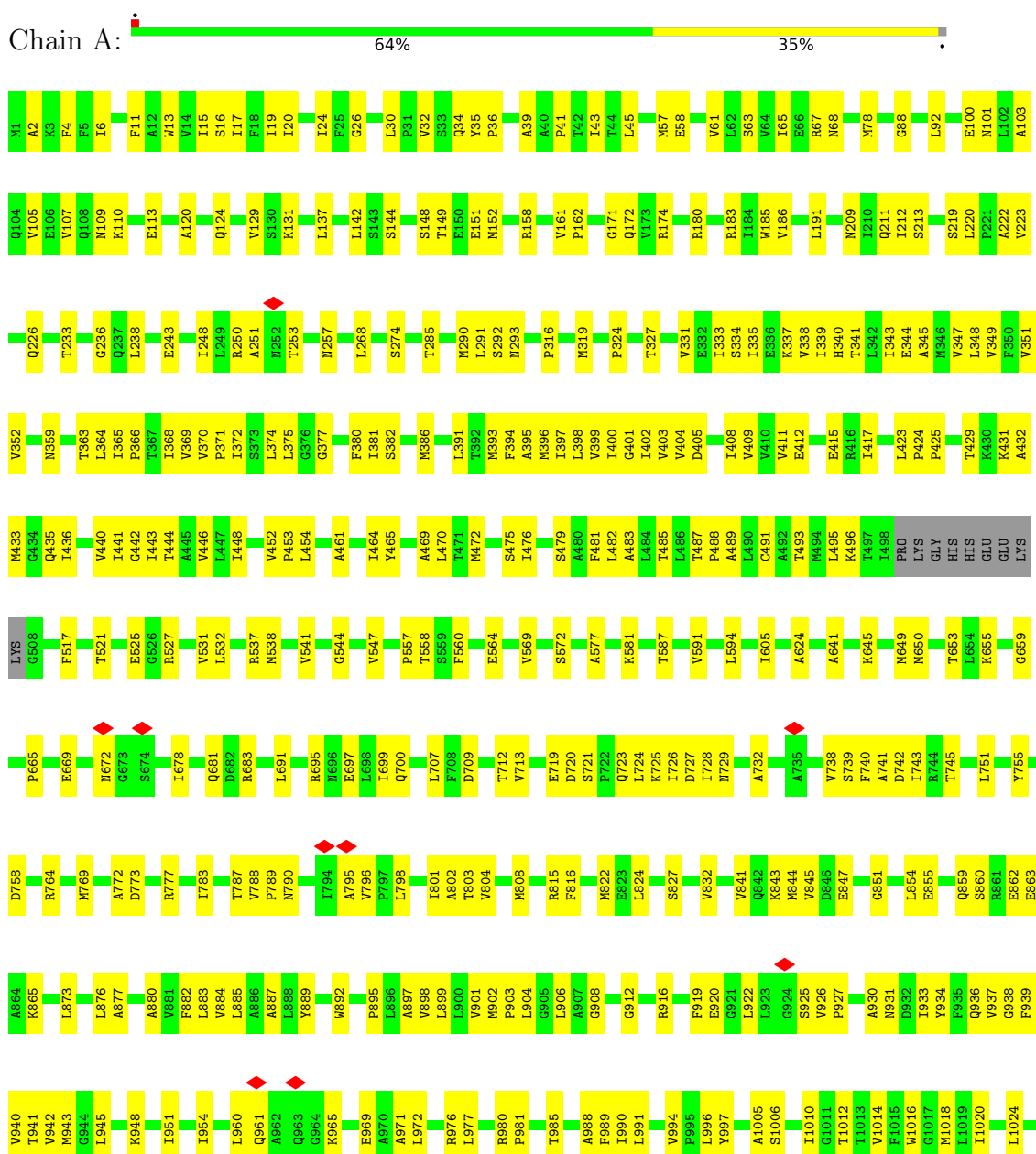


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
3	B	1	51	37	1	13	0

### 3 Residue-property plots

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

#### • Molecule 1: Efflux pump membrane transporter







V1029	G938	A837	L724	P488	F394	M270
P1030	Y942	M838	R730	M494	A395	E271
Y1033	K948	E839	A741	E504	M396	D272
K1041	A840	A841	R744	E505	I397	Y273
E1042	I951	Q842	T745	K506	L398	S274
THR	L952	K843	A748	G511	V399	T285
ALA	I953	M844	S749	K515	V403	L291
HIS	I954	D846	A752	K525	V404	M298
GLU	E955	E847	S753	G526	D405	K302
	F956	L854	D758	R527	D406	E306
	A957	E855	N761	V531	A407	R307
	K958	W856	R764	L532	T408	L308
	D959	R861	V768	R533	V409	W321
	L960	A875	M769	K534	V410	P324
	Q961	R879	I770	R537	V411	K329
	K965	F882	Q771	M539	E412	F330
	A971	V883	A772	V540	N413	V331
	L972	W884	D774	V541	V414	E332
	E973	L885	M778	I543		I333
	A974	A886	Q779	G544		S334
	A975	A887	P780	L545		I335
	R976	L888	L686	A546		E336
	R980	Y889	E669	V547		K337
	N984	W892	L676			V338
	F989	S893	I677	V550		F350
	I990	I894	S677	F551		F354
	L991	P895	I678	R555		I355
	G992	V898	Q679	L556		F356
	V993	L899	L680	P557		L357
	V994	L900	Q681	E564		Q358
	P995	V901	T686	F568		N359
	L996	M902	A690	V569		R361
	Y997	P903	R695	V573		T363
	A1005	G908	E811	A577		L364
	S1006	R916	Q812	G578		I365
	Q1007	E920	G818	A579		Y362
	T1010	L923	M822	T580		T366
	G1011	F929	E823	K581		T367
	T1012	A930	S827	L588		V370
	T1013	I933	P828	V591		P371
	V1014	Y934	A829	L594		I381
	F1015	F935	V832	T605		M386
	M1018	Q936	T834			L391
	L1019	V937				T392
	I1020					M393
	G1021					
	T1022					
	V1026					

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1507208	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	45.425	Depositor
Minimum map value	-21.501	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	4.0	Depositor
Map size ( $\text{\AA}$ )	378.0, 378.0, 378.0	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.08, 1.08, 1.08	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.25	0/7900	0.41	0/10719
1	B	0.25	0/7955	0.40	0/10792
1	C	0.25	0/7948	0.40	0/10782
All	All	0.25	0/23803	0.41	0/32293

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	916	ARG	Sidechain
1	B	67	ARG	Sidechain
1	C	744	ARG	Sidechain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7761	0	7927	324	0
1	B	7813	0	7986	297	0
1	C	7806	0	7979	259	0
2	A	264	0	378	36	0
2	B	322	0	440	45	0
2	C	314	0	441	46	0
3	B	51	0	67	41	0
All	All	24331	0	25218	945	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 19.

All (945) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:961:GLN:HG3	1:A:1046:GLU:OE2	1.33	1.26
2:C:1101:PTY:HC11	2:C:1106:PTY:C1	1.71	1.18
2:C:1101:PTY:HC11	2:C:1106:PTY:HC11	1.24	1.14
1:B:176:PHE:CG	3:B:1101:ERY:H26	1.85	1.11
1:B:176:PHE:CD2	3:B:1101:ERY:H26	1.85	1.11
1:A:1043:THR:HG21	2:A:1106:PTY:N1	1.69	1.08
1:B:136:PHE:CD2	3:B:1101:ERY:H373	1.90	1.06
2:C:1101:PTY:HC51	2:C:1106:PTY:HC6	1.08	1.04
1:B:176:PHE:HE1	3:B:1101:ERY:H213	1.21	1.02
2:A:1102:PTY:HC51	2:A:1102:PTY:HC32	1.37	1.02
3:B:1101:ERY:H321	3:B:1101:ERY:H333	1.39	1.00
1:C:443:ILE:HG23	1:C:948:LYS:HG3	1.46	0.98
2:C:1101:PTY:O13	2:C:1106:PTY:O10	1.82	0.97
2:B:1106:PTY:C31	2:C:1106:PTY:H332	1.95	0.96
1:B:176:PHE:CE1	3:B:1101:ERY:H213	2.01	0.95
1:A:30:LEU:O	2:A:1105:PTY:HC22	1.66	0.95
1:C:405:ASP:OD2	1:C:948:LYS:HE2	1.67	0.94
1:B:443:ILE:HD13	1:B:948:LYS:HG3	1.49	0.93
1:A:1042:GLU:CG	1:A:1043:THR:H	1.78	0.93
1:A:324:PRO:HG2	1:A:605:ILE:HD11	1.47	0.93

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:LEU:HD11	1:A:400:ILE:HD11	1.48	0.93
1:A:408:ILE:HD11	1:A:985:THR:HG22	1.49	0.92
1:C:577:ALA:HB2	1:C:719:GLU:HG3	1.49	0.92
1:B:568:PHE:CE2	3:B:1101:ERY:H341	2.05	0.92
2:C:1101:PTY:H321	2:C:1101:PTY:HC12	1.52	0.91
2:C:1101:PTY:HC51	2:C:1106:PTY:C6	2.00	0.90
1:B:28:LYS:CG	2:B:1108:PTY:HC21	2.02	0.89
1:C:324:PRO:HG2	1:C:605:ILE:HD11	1.55	0.89
1:C:894:ILE:HD11	1:C:958:LYS:HD2	1.53	0.89
2:C:1101:PTY:C5	2:C:1106:PTY:HC6	2.00	0.89
1:B:534:LYS:HD2	1:B:537:ARG:HD2	1.55	0.87
1:B:28:LYS:HG3	2:B:1108:PTY:HC21	1.57	0.86
1:B:220:LEU:HD11	1:C:581:LYS:HD2	1.56	0.86
1:A:882:PHE:HB2	1:A:899:LEU:HD11	1.56	0.85
1:B:568:PHE:CE2	3:B:1101:ERY:C34	2.59	0.85
2:C:1101:PTY:H312	2:C:1107:PTY:O10	1.76	0.85
1:A:366:PRO:HA	1:A:369:VAL:HG22	1.55	0.85
1:A:742:ASP:HB3	1:A:789:PRO:HD2	1.59	0.84
1:C:845:VAL:HG21	1:C:854:LEU:HD12	1.59	0.84
1:C:787:THR:HG22	1:C:797:PRO:HA	1.59	0.83
1:A:248:ILE:HG21	1:A:251:ALA:HB2	1.61	0.82
1:A:398:LEU:HD13	1:A:941:THR:HG21	1.60	0.82
2:A:1101:PTY:H291	2:C:1108:PTY:C2	2.11	0.81
2:C:1101:PTY:C1	2:C:1106:PTY:HC11	2.07	0.81
2:A:1103:PTY:HC31	2:A:1104:PTY:N1	1.95	0.81
1:B:176:PHE:CE1	3:B:1101:ERY:C21	2.63	0.81
1:A:443:ILE:HG23	1:A:948:LYS:HG2	1.62	0.81
1:B:136:PHE:HD2	3:B:1101:ERY:H373	1.41	0.81
1:C:443:ILE:HG23	1:C:948:LYS:CG	2.11	0.80
1:B:176:PHE:CD2	3:B:1101:ERY:C26	2.65	0.80
3:B:1101:ERY:H321	3:B:1101:ERY:C33	2.11	0.80
1:B:25:PHE:HD1	2:B:1107:PTY:O10	1.64	0.80
2:C:1105:PTY:HC32	2:C:1109:PTY:H111	1.62	0.79
1:C:391:LEU:HD13	1:C:464:ILE:HG23	1.65	0.78
1:A:417:ILE:HG21	1:A:431:LYS:HE3	1.64	0.78
1:B:499:PRO:HG2	1:B:502:HIS:HB2	1.65	0.78
2:C:1105:PTY:HC32	2:C:1109:PTY:C11	2.13	0.78
1:A:1042:GLU:CG	1:A:1043:THR:N	2.47	0.78
2:C:1105:PTY:HC52	2:C:1105:PTY:HC31	1.64	0.78
1:A:220:LEU:HD23	1:B:274:SER:HA	1.66	0.78
2:B:1106:PTY:H311	2:C:1106:PTY:H332	1.63	0.78

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:961:GLN:CG	1:A:1046:GLU:OE2	2.27	0.77
1:A:1043:THR:CG2	2:A:1106:PTY:N1	2.48	0.77
1:B:726:ILE:HD11	1:B:783:ILE:HD12	1.67	0.77
1:C:564:GLU:OE2	1:C:1005:ALA:HB3	1.85	0.76
1:B:897:ALA:HB2	1:B:1036:VAL:HG21	1.67	0.76
1:A:965:LYS:HB3	1:A:969:GLU:HB2	1.66	0.76
2:C:1101:PTY:HC12	2:C:1101:PTY:C32	2.14	0.76
1:A:1042:GLU:HG2	1:A:1043:THR:H	1.51	0.76
2:B:1106:PTY:H312	2:C:1106:PTY:H332	1.68	0.76
2:B:1103:PTY:O30	2:B:1103:PTY:HC21	1.86	0.75
3:B:1101:ERY:O1	3:B:1101:ERY:H4	1.84	0.75
1:B:137:LEU:HG	1:B:138:MET:HG3	1.68	0.75
1:A:408:ILE:HA	1:A:411:VAL:HG12	1.65	0.74
1:B:45:LEU:HD12	1:B:90:VAL:HB	1.69	0.74
1:B:176:PHE:HB3	3:B:1101:ERY:H252	1.69	0.74
2:B:1103:PTY:H322	2:B:1103:PTY:HC11	1.68	0.74
1:C:398:LEU:HD11	1:C:1010:ILE:HD11	1.70	0.74
1:A:976:ARG:NH1	1:A:977:LEU:HG	2.03	0.74
1:A:391:LEU:HG	1:A:464:ILE:HG23	1.69	0.74
1:A:581:LYS:HD2	1:C:220:LEU:HD11	1.70	0.73
2:C:1101:PTY:H321	2:C:1101:PTY:C1	2.18	0.73
2:C:1101:PTY:C31	2:C:1107:PTY:O10	2.37	0.71
1:A:423:LEU:HD12	1:A:424:PRO:HD2	1.71	0.71
2:A:1102:PTY:HC32	2:A:1102:PTY:C5	2.18	0.71
1:B:2:ALA:HB1	1:B:433:MET:HB3	1.70	0.71
1:C:398:LEU:HD12	1:C:468:PHE:HZ	1.56	0.71
1:C:365:ILE:HB	1:C:366:PRO:HD3	1.73	0.70
1:A:898:VAL:O	1:A:901:VAL:HG12	1.91	0.70
1:A:220:LEU:HD11	1:B:581:LYS:HD3	1.72	0.70
1:A:707:LEU:HD12	1:A:832:VAL:HG21	1.73	0.70
1:B:176:PHE:CG	3:B:1101:ERY:C26	2.71	0.70
2:A:1102:PTY:HC51	2:A:1102:PTY:C3	2.16	0.69
1:B:30:LEU:HD21	1:B:382:SER:HA	1.73	0.69
1:C:409:VAL:HG12	1:C:436:ILE:HD12	1.73	0.69
1:C:443:ILE:HD11	1:C:952:LEU:HD21	1.73	0.69
1:A:572:SER:O	1:A:659:GLY:HA2	1.93	0.69
1:B:366:PRO:HA	1:B:369:VAL:HG22	1.75	0.69
1:C:701:LYS:HE3	1:C:844:MET:HB3	1.75	0.69
1:B:695:ARG:HG2	1:B:824:LEU:HD11	1.75	0.68
2:B:1104:PTY:H312	2:B:1105:PTY:H322	1.73	0.68
1:B:146:VAL:HG12	1:B:146:VAL:O	1.91	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:465:TYR:OH	1:C:936:GLN:OE1	2.11	0.68
1:B:25:PHE:CD1	2:B:1107:PTY:O10	2.47	0.68
1:C:399:VAL:HG22	1:C:403:VAL:HG13	1.75	0.68
1:A:226:GLN:HG3	1:B:580:THR:HG21	1.74	0.68
1:A:1042:GLU:HG3	1:A:1043:THR:H	1.57	0.68
1:A:699:ILE:HG23	1:A:713:VAL:HG12	1.76	0.68
3:B:1101:ERY:H311	3:B:1101:ERY:H72	1.75	0.68
3:B:1101:ERY:O9	3:B:1101:ERY:H323	1.93	0.68
1:C:443:ILE:HG23	1:C:948:LYS:CD	2.24	0.67
1:A:148:SER:OG	1:A:151:GLU:OE1	2.11	0.67
1:A:725:LYS:O	1:A:804:VAL:HA	1.95	0.67
2:C:1105:PTY:HC31	2:C:1105:PTY:C5	2.25	0.67
1:A:1043:THR:HG21	2:A:1106:PTY:C2	2.24	0.67
1:B:184:ILE:HG13	1:B:266:VAL:HG13	1.75	0.67
1:C:192:GLN:NE2	1:C:193:ASN:OD1	2.27	0.67
1:C:741:ALA:O	1:C:745:THR:HG23	1.95	0.67
2:C:1101:PTY:HC11	2:C:1106:PTY:C6	2.25	0.67
1:C:338:VAL:HG21	1:C:393:MET:HG3	1.76	0.66
1:A:212:ILE:HG21	1:B:747:LEU:HD12	1.77	0.66
1:A:441:ILE:HD11	2:A:1104:PTY:H141	1.78	0.66
2:C:1103:PTY:O12	2:C:1104:PTY:O10	2.14	0.66
1:B:993:VAL:HG11	1:B:1014:VAL:HG23	1.78	0.66
1:A:396:MET:HA	1:A:399:VAL:HG22	1.77	0.66
1:A:901:VAL:HG22	1:A:901:VAL:O	1.96	0.66
1:A:720:ASP:HB3	1:A:808:MET:HG3	1.78	0.66
1:B:971:ALA:HB1	1:B:1030:PRO:HB3	1.78	0.66
3:B:1101:ERY:H311	3:B:1101:ERY:C7	2.25	0.65
2:B:1103:PTY:H322	2:B:1103:PTY:C1	2.26	0.65
1:A:32:VAL:HG23	2:A:1105:PTY:HC21	1.78	0.65
1:A:1042:GLU:HG3	1:A:1043:THR:N	2.10	0.65
1:C:916:ARG:NH1	1:C:1012:THR:OG1	2.29	0.65
1:A:843:LYS:O	1:A:847:GLU:HG3	1.97	0.65
1:A:30:LEU:HD13	1:A:382:SER:HA	1.79	0.65
1:A:43:ILE:HD13	1:A:131:LYS:HB3	1.78	0.64
1:A:1043:THR:HG23	1:A:1045:HIS:H	1.61	0.64
1:B:399:VAL:HG21	1:B:475:SER:HB2	1.80	0.64
1:C:350:PHE:HD1	1:C:367:THR:HG21	1.63	0.64
1:B:176:PHE:HE1	3:B:1101:ERY:C21	1.99	0.64
1:C:357:LEU:HD12	1:C:363:THR:HG22	1.80	0.64
1:C:531:VAL:HG13	1:C:538:MET:HG3	1.78	0.64
1:C:718:LEU:HD23	1:C:811:GLU:HB3	1.80	0.64

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:738:VAL:HG13	1:A:788:VAL:HG21	1.80	0.63
1:B:374:LEU:HG	1:B:396:MET:HE3	1.80	0.63
1:C:1041:LYS:O	1:C:1042:GLU:CB	2.45	0.63
1:B:28:LYS:HG2	2:B:1108:PTY:HC21	1.79	0.63
1:A:396:MET:O	1:A:400:ILE:HG12	1.97	0.63
3:B:1101:ERY:O1	3:B:1101:ERY:H11	1.98	0.63
1:B:11:PHE:HD1	1:C:887:ALA:HB1	1.63	0.63
1:C:443:ILE:CG2	1:C:948:LYS:HG3	2.23	0.63
1:B:568:PHE:CZ	3:B:1101:ERY:C34	2.82	0.63
1:C:588:LEU:HD21	1:C:620:ALA:HB1	1.80	0.63
1:B:26:GLY:O	1:B:30:LEU:HG	1.98	0.63
1:B:324:PRO:HB2	1:B:625:ILE:HD12	1.80	0.62
1:A:683:ARG:HB2	1:A:851:GLY:HA2	1.80	0.62
1:A:902:MET:HB2	1:A:903:PRO:HD3	1.82	0.62
1:C:455:ALA:HA	1:C:466:LYS:HG2	1.82	0.62
1:C:712:THR:HG21	1:C:827:SER:HB2	1.82	0.62
1:C:960:LEU:HD13	1:C:973:GLU:HB3	1.81	0.62
1:C:212:ILE:HB	1:C:234:ALA:HB3	1.82	0.62
1:C:892:TRP:N	2:C:1102:PTY:O13	2.25	0.62
1:B:934:TYR:HB3	1:B:1010:ILE:HG23	1.80	0.62
1:A:898:VAL:HG22	1:A:954:ILE:HD12	1.82	0.62
1:B:138:MET:HE3	1:B:323:THR:HG21	1.81	0.61
1:B:208:GLN:O	1:C:730:ARG:NH2	2.33	0.61
2:A:1103:PTY:HC51	2:A:1103:PTY:O10	2.00	0.61
1:B:990:ILE:O	1:B:994:VAL:HG23	2.01	0.61
2:C:1106:PTY:H232	2:C:1106:PTY:H191	1.81	0.61
1:A:365:ILE:HB	1:A:366:PRO:HD3	1.82	0.61
1:A:374:LEU:HD11	1:A:400:ILE:CD1	2.28	0.61
1:C:120:ALA:O	1:C:124:GLN:HG3	2.00	0.61
2:C:1101:PTY:O13	2:C:1106:PTY:C5	2.49	0.61
1:A:976:ARG:HH12	1:A:977:LEU:HG	1.64	0.61
1:B:845:VAL:HG21	1:B:854:LEU:HD13	1.83	0.61
1:C:115:LEU:HD12	1:C:118:LEU:HD12	1.83	0.61
1:C:405:ASP:OD2	1:C:948:LYS:CE	2.47	0.60
1:A:491:CYS:HA	1:A:495:LEU:HG	1.83	0.60
1:B:370:VAL:HG21	1:B:404:VAL:HG12	1.84	0.60
3:B:1101:ERY:O8	3:B:1101:ERY:H292	2.02	0.60
1:A:408:ILE:HA	1:A:411:VAL:CG1	2.30	0.60
1:A:883:LEU:HB3	1:C:14:VAL:HG13	1.82	0.60
2:B:1104:PTY:C1	2:B:1105:PTY:HC21	2.32	0.60
1:A:403:VAL:HG22	1:A:479:SER:HB2	1.84	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:945:LEU:HD22	1:A:1018:MET:HE1	1.83	0.60
1:A:1042:GLU:O	2:A:1106:PTY:O13	2.20	0.60
1:B:176:PHE:CD2	3:B:1101:ERY:C27	2.84	0.60
1:C:948:LYS:O	1:C:951:ILE:HG22	2.01	0.60
1:A:213:SER:HB3	1:B:51:GLY:O	2.01	0.60
1:A:220:LEU:CD2	1:B:274:SER:HA	2.32	0.60
1:A:343:ILE:HD11	2:A:1105:PTY:H182	1.84	0.60
1:B:707:LEU:HD13	1:B:832:VAL:HG21	1.84	0.60
1:A:30:LEU:O	2:A:1105:PTY:C2	2.45	0.60
1:B:563:THR:HA	1:B:666:PRO:HD3	1.82	0.60
1:C:961:GLN:HA	1:C:965:LYS:HB2	1.84	0.60
1:B:728:ILE:HD13	1:B:743:ILE:HG21	1.84	0.60
1:B:796:VAL:HG11	1:B:801:ILE:HG13	1.84	0.60
1:A:724:LEU:HD12	1:C:217:ILE:HD11	1.84	0.59
1:B:833:SER:H	1:B:836:GLN:HE21	1.49	0.59
1:A:887:ALA:HB1	1:C:11:PHE:HD1	1.67	0.59
2:A:1103:PTY:HC31	2:A:1104:PTY:HN11	1.65	0.59
1:C:579:ALA:HB3	1:C:618:ASN:HB3	1.85	0.59
1:A:537:ARG:O	1:A:541:VAL:HG13	2.02	0.59
1:A:423:LEU:CD1	1:A:424:PRO:HD2	2.32	0.59
1:A:472:MET:O	1:A:476:ILE:HG12	2.01	0.59
1:B:11:PHE:CD1	1:C:887:ALA:HB1	2.38	0.59
1:A:345:ALA:O	1:A:349:VAL:HG23	2.02	0.59
1:B:161:VAL:HG21	1:B:175:LEU:HD11	1.85	0.59
1:C:525:GLU:OE2	1:C:976:ARG:HD2	2.02	0.59
1:C:724:LEU:HD11	1:C:780:PRO:HB3	1.85	0.59
1:C:1041:LYS:O	1:C:1042:GLU:HB2	2.02	0.58
2:C:1103:PTY:HC52	2:C:1104:PTY:H111	1.85	0.58
1:A:171:GLY:CA	1:A:292:SER:HB2	2.33	0.58
1:A:394:PHE:O	1:A:398:LEU:HG	2.02	0.58
1:A:448:ILE:O	1:A:452:VAL:HG13	2.03	0.58
1:A:980:ARG:HB3	1:A:981:PRO:HD3	1.85	0.58
1:B:370:VAL:HB	1:B:371:PRO:HD3	1.85	0.58
1:C:399:VAL:HG21	1:C:475:SER:HB2	1.84	0.58
1:B:279:LEU:HD13	1:B:605:ILE:HG12	1.84	0.58
1:C:357:LEU:HD13	1:C:362:TYR:HB3	1.86	0.58
1:C:898:VAL:HG22	1:C:954:ILE:HD12	1.84	0.58
1:B:891:SER:HA	2:B:1104:PTY:HC21	1.84	0.58
2:B:1106:PTY:H332	2:B:1106:PTY:O30	2.04	0.58
1:A:274:SER:HA	1:C:220:LEU:CD2	2.34	0.58
1:A:665:PRO:HB3	1:A:672:ASN:ND2	2.19	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1103:PTY:HC32	2:B:1103:PTY:HC51	1.84	0.58
2:B:1104:PTY:HC12	2:B:1105:PTY:HC21	1.85	0.58
1:C:137:LEU:HG	1:C:138:MET:HG3	1.84	0.58
1:A:790:ASN:ND2	1:A:796:VAL:HG21	2.18	0.58
1:B:74:GLY:O	1:B:95:THR:N	2.32	0.58
1:C:186:VAL:HG11	1:C:191:LEU:HD11	1.86	0.58
1:C:961:GLN:NE2	1:C:1033:TYR:OH	2.35	0.58
1:A:569:VAL:HG22	1:A:624:ALA:HB3	1.86	0.58
1:B:135:ASN:O	1:B:291:LEU:N	2.32	0.58
1:C:370:VAL:HB	1:C:371:PRO:HD3	1.86	0.58
1:A:898:VAL:CG2	1:A:954:ILE:HD12	2.33	0.58
1:A:989:PHE:CD2	1:A:1018:MET:HG3	2.39	0.58
1:B:361:ARG:NH1	1:B:494:MET:O	2.37	0.57
1:A:892:TRP:HB2	2:A:1106:PTY:HC52	1.86	0.57
1:B:741:ALA:O	1:B:745:THR:HG23	2.04	0.57
1:C:787:THR:HB	1:C:795:ALA:O	2.03	0.57
1:A:442:GLY:O	1:A:446:VAL:HG13	2.04	0.57
1:A:885:LEU:HB2	1:A:895:PRO:HB3	1.87	0.57
1:B:359:ASN:HB3	1:B:362:TYR:HD2	1.68	0.57
1:B:1029:VAL:HB	1:B:1030:PRO:HD3	1.85	0.57
3:B:1101:ERY:H11	3:B:1101:ERY:H71	1.87	0.57
1:A:399:VAL:HG11	1:A:475:SER:HB2	1.87	0.57
1:B:465:TYR:CE1	1:B:933:ILE:HG23	2.40	0.57
3:B:1101:ERY:H203	3:B:1101:ERY:O6	2.03	0.57
1:C:20:ILE:HD12	2:C:1105:PTY:H191	1.85	0.57
1:A:904:LEU:HD13	1:A:1024:LEU:CB	2.35	0.57
2:C:1105:PTY:HC32	2:C:1109:PTY:H112	1.86	0.57
1:A:873:LEU:HD12	1:A:876:LEU:HD12	1.86	0.57
1:A:100:GLU:OE2	1:A:293:ASN:ND2	2.38	0.57
1:A:349:VAL:HA	1:A:352:VAL:HG12	1.86	0.57
1:B:183:ARG:HG2	1:B:185:TRP:CZ2	2.39	0.57
1:C:447:LEU:HB3	1:C:476:ILE:HD13	1.86	0.57
1:A:370:VAL:HB	1:A:371:PRO:HD3	1.87	0.57
2:B:1103:PTY:HC11	2:B:1103:PTY:C32	2.33	0.57
1:B:789:PRO:HB3	1:B:794:ILE:HG12	1.86	0.56
3:B:1101:ERY:H372	3:B:1101:ERY:O13	2.04	0.56
1:A:248:ILE:HD12	1:A:257:ASN:HB3	1.87	0.56
1:A:740:PHE:HZ	1:C:236:GLY:HA3	1.70	0.56
1:B:324:PRO:HB2	1:B:625:ILE:CD1	2.35	0.56
1:B:359:ASN:HB3	1:B:362:TYR:CD2	2.40	0.56
1:B:543:ILE:O	1:B:547:VAL:HG13	2.04	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:577:ALA:HB1	1:A:721:SER:OG	2.05	0.56
1:A:697:GLU:O	1:A:700:GLN:HG3	2.06	0.56
1:A:1046:GLU:O	1:A:1046:GLU:CD	2.44	0.56
2:B:1102:PTY:H111	2:B:1106:PTY:HC12	1.87	0.56
1:C:366:PRO:O	1:C:370:VAL:HG23	2.06	0.56
1:A:250:ARG:HG2	1:A:253:THR:HG23	1.88	0.56
1:A:557:PRO:O	1:A:930:ALA:HB1	2.05	0.56
1:B:162:PRO:HB3	1:C:67:ARG:HD2	1.88	0.56
1:B:176:PHE:HB2	3:B:1101:ERY:H273	1.87	0.56
1:C:543:ILE:O	1:C:547:VAL:HG13	2.06	0.56
1:A:152:MET:HB2	1:A:285:THR:HG21	1.88	0.56
1:A:443:ILE:CG2	1:A:948:LYS:HG2	2.36	0.56
1:A:709:ASP:OD1	1:A:712:THR:OG1	2.19	0.56
1:C:885:LEU:HD11	1:C:898:VAL:HG11	1.87	0.56
1:A:729:ASN:OD1	1:A:732:ALA:N	2.36	0.56
1:A:897:ALA:HB2	1:A:1036:VAL:HG21	1.88	0.56
1:B:211:GLN:NE2	1:C:51:GLY:O	2.39	0.56
1:C:361:ARG:HD3	1:C:494:MET:O	2.06	0.56
1:A:436:ILE:HG22	1:A:440:VAL:HG23	1.88	0.55
1:A:569:VAL:CG2	1:A:624:ALA:HB3	2.36	0.55
1:B:531:VAL:HG13	1:B:538:MET:HG3	1.88	0.55
1:B:591:VAL:HG13	1:B:650:MET:HE1	1.88	0.55
1:C:956:PHE:HD2	1:C:974:ALA:HA	1.72	0.55
1:A:433:MET:SD	1:A:488:PRO:HG3	2.47	0.55
1:A:532:LEU:HD21	1:A:972:LEU:CD1	2.36	0.55
1:B:198:PHE:CD1	1:B:749:SER:HB2	2.41	0.55
1:A:41:PRO:HB3	1:A:100:GLU:HG2	1.87	0.55
1:A:185:TRP:HB3	1:A:773:ASP:HA	1.88	0.55
2:A:1106:PTY:HC51	2:A:1106:PTY:O10	2.07	0.55
1:B:162:PRO:HA	1:B:165:GLN:HE21	1.72	0.55
1:B:787:THR:HG22	1:B:797:PRO:HA	1.89	0.55
1:A:372:ILE:HG22	1:A:482:LEU:HD11	1.89	0.55
1:B:896:LEU:HD11	2:B:1104:PTY:H132	1.89	0.55
1:A:798:LEU:HG	1:A:802:ALA:HB3	1.88	0.55
1:B:638:ASP:O	1:B:642:VAL:HG23	2.07	0.55
1:B:1006:SER:O	1:B:1010:ILE:HG12	2.06	0.55
1:B:146:VAL:O	1:B:146:VAL:CG1	2.55	0.55
1:B:676:LEU:HD21	1:B:856:TRP:HZ3	1.72	0.55
2:C:1101:PTY:HC11	2:C:1106:PTY:O4	2.06	0.55
1:A:137:LEU:HD22	1:A:291:LEU:HD13	1.88	0.55
1:B:365:ILE:HB	1:B:366:PRO:HD3	1.89	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:ARG:NH1	1:C:769:MET:SD	2.80	0.55
1:C:443:ILE:CG2	1:C:948:LYS:CD	2.85	0.55
1:A:365:ILE:O	1:A:369:VAL:HG13	2.07	0.54
2:A:1101:PTY:H411	2:C:1107:PTY:H421	1.89	0.54
1:C:678:ILE:HG12	1:C:841:VAL:HG11	1.89	0.54
2:B:1108:PTY:C20	2:B:1108:PTY:C38	2.86	0.54
1:C:447:LEU:HD11	1:C:948:LYS:HD3	1.87	0.54
1:A:934:TYR:HA	1:A:937:VAL:HG22	1.89	0.54
1:A:936:GLN:O	1:A:940:VAL:HG13	2.07	0.54
1:B:695:ARG:CG	1:B:824:LEU:HD11	2.38	0.54
2:C:1105:PTY:C5	2:C:1105:PTY:C3	2.86	0.54
2:A:1104:PTY:HC32	2:C:1108:PTY:O30	2.07	0.54
2:B:1108:PTY:C38	2:B:1108:PTY:H191	2.38	0.54
1:B:42:THR:HB	1:B:132:ALA:HB3	1.90	0.54
1:B:242:GLU:O	1:B:246:ASN:ND2	2.35	0.54
1:C:990:ILE:O	1:C:994:VAL:HG23	2.07	0.54
1:B:568:PHE:CZ	3:B:1101:ERY:H343	2.42	0.54
3:B:1101:ERY:H333	3:B:1101:ERY:C32	2.24	0.54
2:B:1103:PTY:HC21	2:B:1103:PTY:C30	2.37	0.54
1:A:347:VAL:O	1:A:351:VAL:HG13	2.08	0.54
1:A:436:ILE:O	1:A:440:VAL:HG23	2.08	0.54
1:B:226:GLN:HG3	1:C:580:THR:HG21	1.89	0.54
1:B:592:THR:HG23	1:B:604:ILE:HG21	1.88	0.54
1:B:676:LEU:HD21	1:B:856:TRP:CZ3	2.43	0.54
1:C:364:LEU:HA	1:C:367:THR:OG1	2.08	0.54
1:C:829:ALA:HB3	1:C:832:VAL:HG23	1.88	0.54
1:C:875:ALA:O	1:C:879:VAL:HG13	2.08	0.54
1:A:402:ILE:HG21	1:A:476:ILE:HD12	1.90	0.53
1:B:453:PRO:HG2	1:B:877:ALA:HB2	1.89	0.53
1:B:489:ALA:O	1:B:493:THR:HG23	2.08	0.53
2:B:1108:PTY:C38	2:B:1108:PTY:C19	2.86	0.53
1:C:95:THR:HG23	1:C:96:PRO:O	2.08	0.53
1:A:236:GLY:HA2	1:B:740:PHE:HZ	1.73	0.53
1:A:859:GLN:O	1:A:863:GLU:OE1	2.26	0.53
1:C:676:LEU:HD12	1:C:708:PHE:HZ	1.73	0.53
1:C:748:ALA:O	1:C:752:SER:HB3	2.08	0.53
1:C:898:VAL:O	1:C:901:VAL:HG22	2.08	0.53
1:B:703:ARG:HG3	1:B:710:PRO:HB3	1.89	0.53
1:B:728:ILE:CD1	1:B:743:ILE:HG21	2.38	0.53
1:A:483:ALA:HA	1:A:487:THR:OG1	2.09	0.53
1:A:1043:THR:HG23	1:A:1045:HIS:N	2.23	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:LEU:HD21	1:B:382:SER:CA	2.38	0.53
1:C:34:GLN:HB2	1:C:331:VAL:HG22	1.91	0.53
1:C:45:LEU:HD23	1:C:111:LEU:HD22	1.90	0.53
1:A:691:LEU:CD2	1:A:822:MET:HG3	2.39	0.53
1:A:990:ILE:O	1:A:994:VAL:HG23	2.08	0.53
1:A:465:TYR:CE1	1:A:933:ILE:HD12	2.44	0.53
1:A:945:LEU:HD22	1:A:1018:MET:CE	2.39	0.53
1:B:377:GLY:O	1:B:381:ILE:HG23	2.08	0.53
1:C:774:GLY:O	1:C:778:MET:HG2	2.09	0.53
1:C:856:TRP:HB2	1:C:861:ARG:HG2	1.90	0.53
1:C:971:ALA:HB1	1:C:1030:PRO:HB3	1.91	0.53
1:A:738:VAL:HG11	1:A:801:ILE:HD13	1.91	0.53
1:B:302:LYS:O	1:B:306:GLU:HG3	2.08	0.53
1:B:896:LEU:HD11	2:B:1104:PTY:C13	2.39	0.53
2:C:1101:PTY:O13	2:C:1106:PTY:HC6	2.08	0.53
1:A:36:PRO:HG2	1:A:464:ILE:HA	1.91	0.53
1:A:393:MET:O	1:A:397:ILE:HG13	2.08	0.53
1:A:738:VAL:HG11	1:A:801:ILE:CD1	2.38	0.53
1:A:981:PRO:O	1:A:985:THR:HG23	2.09	0.53
1:C:989:PHE:CD2	1:C:1018:MET:HG3	2.44	0.53
1:B:252:ASN:HB2	1:B:255:GLY:O	2.09	0.53
1:C:660:ILE:HD12	1:C:711:SER:O	2.09	0.53
1:A:971:ALA:HB1	1:A:1030:PRO:HB3	1.91	0.53
1:B:902:MET:HB2	1:B:903:PRO:HD3	1.90	0.53
1:B:1025:SER:O	1:B:1029:VAL:HG23	2.09	0.53
2:C:1101:PTY:O13	2:C:1106:PTY:C6	2.56	0.53
1:A:724:LEU:CD1	1:C:217:ILE:HD11	2.38	0.52
1:A:594:LEU:HD11	1:A:653:THR:HB	1.91	0.52
1:B:104:GLN:OE1	1:B:131:LYS:NZ	2.36	0.52
1:B:980:ARG:HB3	1:B:981:PRO:HD3	1.90	0.52
1:A:211:GLN:OE1	1:B:60:SER:OG	2.25	0.52
1:A:920:GLU:OE2	1:A:927:PRO:HA	2.10	0.52
1:B:62:LEU:HD13	1:B:80:THR:HG23	1.90	0.52
1:B:537:ARG:HA	1:B:540:VAL:HG22	1.89	0.52
1:C:386:MET:CE	1:C:470:LEU:HD22	2.39	0.52
1:A:1029:VAL:HB	1:A:1030:PRO:HD3	1.91	0.52
1:B:102:LEU:O	1:B:106:GLU:HG3	2.09	0.52
1:B:58:GLU:OE2	1:B:815:ARG:HD2	2.09	0.52
1:C:158:ARG:CZ	1:C:764:ARG:HD3	2.39	0.52
1:C:569:VAL:HG13	1:C:662:VAL:O	2.10	0.52
1:C:894:ILE:CD1	1:C:958:LYS:HD2	2.33	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:SER:O	1:A:338:VAL:HG23	2.10	0.52
2:A:1103:PTY:H321	2:B:1106:PTY:H131	1.91	0.52
1:A:787:THR:HA	1:A:796:VAL:O	2.10	0.52
1:C:158:ARG:NH2	1:C:761:ASN:O	2.40	0.52
1:A:481:PHE:O	1:A:485:THR:HG23	2.10	0.52
1:B:433:MET:O	1:B:437:SER:OG	2.18	0.52
1:B:594:LEU:HD11	1:B:653:THR:HB	1.92	0.52
1:C:487:THR:HB	1:C:488:PRO:HD3	1.92	0.52
1:A:20:ILE:HG23	1:A:375:LEU:CD1	2.40	0.52
1:A:772:ALA:HB3	1:A:777:ARG:HG2	1.91	0.52
1:A:845:VAL:HG21	1:A:854:LEU:HD12	1.91	0.52
1:B:369:VAL:HG21	1:B:407:ALA:HB2	1.92	0.52
1:B:568:PHE:CE2	3:B:1101:ERY:H343	2.43	0.52
1:B:568:PHE:CE2	1:B:664:PRO:HG3	2.44	0.52
1:B:1010:ILE:O	1:B:1014:VAL:HG22	2.10	0.52
1:C:960:LEU:CD1	1:C:973:GLU:HB3	2.39	0.52
1:B:728:ILE:HA	1:B:802:ALA:HB2	1.92	0.52
1:C:650:MET:HA	1:C:654:LEU:HD13	1.92	0.52
1:C:680:LEU:HD23	1:C:822:MET:O	2.09	0.52
2:A:1105:PTY:HC6	2:A:1105:PTY:O13	2.10	0.51
1:B:39:ALA:HB2	1:B:669:GLU:HG2	1.92	0.51
1:B:278:ARG:NH1	1:B:281:GLY:O	2.43	0.51
1:C:359:ASN:HB3	1:C:362:TYR:HD1	1.75	0.51
1:C:534:LYS:HE2	1:C:537:ARG:HH21	1.74	0.51
1:A:57:MET:HE2	1:A:88:GLY:HA3	1.92	0.51
1:A:862:GLU:HA	1:A:865:LYS:HE2	1.91	0.51
1:B:432:ALA:O	1:B:436:ILE:HG12	2.10	0.51
1:B:790:ASN:HD21	1:B:796:VAL:HG23	1.75	0.51
1:B:934:TYR:HB3	1:B:1010:ILE:CG2	2.41	0.51
1:C:452:VAL:CG1	1:C:453:PRO:HD3	2.39	0.51
1:C:708:PHE:CZ	1:C:837:ALA:HB1	2.45	0.51
1:A:26:GLY:O	1:A:30:LEU:HB2	2.11	0.51
1:A:538:MET:HA	1:A:541:VAL:HG22	1.92	0.51
1:A:712:THR:OG1	1:A:827:SER:HB3	2.10	0.51
1:B:544:GLY:O	1:B:548:VAL:HG23	2.11	0.51
1:B:845:VAL:HG11	1:B:854:LEU:HD22	1.93	0.51
1:B:893:SER:OG	2:B:1104:PTY:O12	2.17	0.51
1:B:1022:THR:O	1:B:1026:VAL:HG13	2.10	0.51
1:C:180:ARG:HD2	1:C:268:LEU:HB3	1.92	0.51
1:A:20:ILE:HG23	1:A:375:LEU:HD13	1.92	0.51
1:B:771:GLN:O	1:B:777:ARG:NH1	2.44	0.51

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:816:PHE:CE1	1:A:855:GLU:HG2	2.46	0.51
1:B:115:LEU:HD12	1:B:118:LEU:HD12	1.93	0.51
1:C:2:ALA:O	1:C:6:ILE:HG13	2.10	0.51
2:C:1101:PTY:O10	2:C:1101:PTY:HC52	2.09	0.51
1:A:149:THR:HA	1:A:152:MET:HE3	1.92	0.51
1:B:338:VAL:HG22	1:B:397:ILE:HG13	1.92	0.51
1:C:920:GLU:OE1	1:C:923:LEU:HD21	2.09	0.51
1:A:377:GLY:O	1:A:381:ILE:HG23	2.11	0.51
1:B:703:ARG:CG	1:B:710:PRO:HB3	2.41	0.51
1:C:452:VAL:HG12	1:C:453:PRO:HD3	1.93	0.51
1:A:527:ARG:O	1:A:531:VAL:HG23	2.11	0.51
1:A:904:LEU:HD13	1:A:1024:LEU:HB2	1.93	0.51
1:B:610:PHE:CD2	3:B:1101:ERY:H292	2.46	0.51
1:B:765:LEU:HD12	1:C:119:PRO:HG3	1.93	0.51
2:B:1106:PTY:O13	2:C:1106:PTY:HC12	2.11	0.51
1:C:594:LEU:HD11	1:C:653:THR:HB	1.93	0.51
1:A:544:GLY:HA2	1:A:547:VAL:HG12	1.93	0.51
1:A:960:LEU:HG	1:A:961:GLN:OE1	2.11	0.51
1:A:2:ALA:O	1:A:6:ILE:HG13	2.11	0.50
1:A:34:GLN:HG2	1:A:35:TYR:CD2	2.46	0.50
1:A:906:LEU:HB2	1:A:939:PHE:CE1	2.46	0.50
2:A:1101:PTY:C29	2:C:1108:PTY:C2	2.84	0.50
1:B:136:PHE:CZ	1:B:139:ILE:HG12	2.46	0.50
1:B:176:PHE:CE1	3:B:1101:ERY:H211	2.46	0.50
1:B:370:VAL:CG2	1:B:404:VAL:HG12	2.41	0.50
1:C:332:GLU:O	1:C:336:GLU:HG3	2.11	0.50
1:C:410:VAL:HA	1:C:436:ILE:HD11	1.91	0.50
1:A:223:VAL:HG22	1:B:778:MET:SD	2.51	0.50
1:C:788:VAL:HB	1:C:789:PRO:HD2	1.93	0.50
1:C:1022:THR:O	1:C:1026:VAL:HG13	2.11	0.50
1:A:58:GLU:OE2	1:A:815:ARG:HD2	2.11	0.50
1:B:35:TYR:CD1	1:B:667:ILE:HD11	2.46	0.50
1:B:35:TYR:CG	1:B:667:ILE:HD11	2.47	0.50
1:B:568:PHE:CD2	3:B:1101:ERY:H341	2.46	0.50
1:B:897:ALA:HB2	1:B:1036:VAL:CG2	2.41	0.50
1:C:396:MET:HA	1:C:399:VAL:HG12	1.93	0.50
1:C:908:GLY:HA3	1:C:1020:ILE:HB	1.93	0.50
1:A:359:ASN:O	1:A:363:THR:HG23	2.10	0.50
1:A:887:ALA:HB1	1:C:11:PHE:CD1	2.46	0.50
1:B:228:VAL:HA	1:C:578:GLY:O	2.11	0.50
1:B:534:LYS:CD	1:B:537:ARG:HD2	2.36	0.50

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:391:LEU:CD1	1:C:464:ILE:HG23	2.40	0.50
1:C:433:MET:SD	1:C:488:PRO:HG3	2.51	0.50
1:A:43:ILE:CD1	1:A:131:LYS:HB3	2.42	0.50
1:B:424:PRO:HG2	1:B:427:GLU:OE1	2.12	0.50
1:C:104:GLN:HG2	1:C:108:GLN:HE21	1.77	0.50
1:C:483:ALA:HA	1:C:487:THR:OG1	2.12	0.50
1:A:386:MET:CE	1:A:470:LEU:HD12	2.42	0.50
1:A:751:LEU:HD11	1:A:783:ILE:HD11	1.93	0.50
1:C:119:PRO:O	1:C:123:GLN:HG3	2.11	0.50
1:C:363:THR:O	1:C:367:THR:HG23	2.12	0.50
1:C:381:ILE:HD11	1:C:471:THR:OG1	2.11	0.50
1:B:238:LEU:HD22	1:B:243:GLU:HB3	1.94	0.50
1:A:453:PRO:HG2	1:A:877:ALA:HB2	1.93	0.50
1:B:447:LEU:HD13	1:B:476:ILE:HD13	1.94	0.50
1:B:796:VAL:HG12	1:B:798:LEU:H	1.76	0.50
1:C:885:LEU:CB	1:C:895:PRO:HG3	2.42	0.50
1:C:894:ILE:HG23	1:C:954:ILE:HG21	1.92	0.50
1:A:741:ALA:O	1:A:745:THR:HG23	2.11	0.49
1:A:919:PHE:O	1:A:922:LEU:HG	2.12	0.49
1:B:443:ILE:HG21	1:B:948:LYS:HE2	1.93	0.49
1:C:354:TYR:HA	1:C:363:THR:HG21	1.94	0.49
1:A:403:VAL:HG22	1:A:479:SER:CB	2.41	0.49
1:A:454:LEU:HB2	1:A:469:ALA:HB2	1.94	0.49
1:A:489:ALA:O	1:A:493:THR:HG23	2.11	0.49
1:B:276:SER:OG	1:B:608:SER:HB3	2.12	0.49
1:B:46:HIS:HA	1:B:88:GLY:O	2.12	0.49
1:A:645:LYS:O	1:A:649:MET:HG3	2.13	0.49
1:B:676:LEU:HD11	1:B:838:MET:HG2	1.93	0.49
1:B:487:THR:HB	1:B:488:PRO:HD3	1.94	0.49
1:C:38:VAL:HB	1:C:460:ALA:CB	2.43	0.49
1:C:104:GLN:O	1:C:108:GLN:HG3	2.12	0.49
1:A:172:GLN:HB3	1:A:290:MET:HE2	1.95	0.49
2:A:1105:PTY:O10	2:A:1105:PTY:HC52	2.12	0.49
2:B:1105:PTY:H121	2:B:1105:PTY:HC6	1.95	0.49
1:C:381:ILE:HG23	1:C:386:MET:HB2	1.95	0.49
1:C:894:ILE:HB	1:C:895:PRO:HD3	1.95	0.49
1:A:940:VAL:HA	1:A:943:MET:HG2	1.94	0.49
1:A:681:GLN:HE21	1:A:816:PHE:HB3	1.78	0.49
1:B:777:ARG:O	1:B:778:MET:HE2	2.12	0.49
1:B:894:ILE:HG23	1:B:954:ILE:HG21	1.94	0.49
1:C:62:LEU:HD13	1:C:80:THR:HG23	1.93	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:PHE:HB2	2:A:1103:PTY:HC52	1.95	0.49
1:A:938:GLY:O	1:A:942:VAL:HG13	2.13	0.49
1:B:940:VAL:O	1:B:943:MET:HG2	2.13	0.49
2:A:1103:PTY:O13	2:A:1104:PTY:N1	2.35	0.48
1:B:3:LYS:O	1:B:6:ILE:HG22	2.12	0.48
1:C:591:VAL:HG13	1:C:650:MET:HE1	1.95	0.48
1:B:374:LEU:HG	1:B:396:MET:CE	2.41	0.48
1:B:611:SER:HB3	1:B:619:MET:HB3	1.94	0.48
1:A:441:ILE:CD1	2:A:1104:PTY:H141	2.42	0.48
2:B:1108:PTY:O10	2:B:1108:PTY:HC52	2.12	0.48
1:B:728:ILE:HA	1:B:802:ALA:CB	2.44	0.48
1:A:412:GLU:HA	1:A:415:GLU:CG	2.44	0.48
1:A:787:THR:CG2	1:A:795:ALA:HA	2.44	0.48
1:C:363:THR:O	1:C:366:PRO:HD2	2.12	0.48
1:C:1029:VAL:HB	1:C:1030:PRO:HD3	1.94	0.48
1:A:412:GLU:O	1:A:415:GLU:HG3	2.14	0.48
1:A:461:ALA:HB2	1:A:560:PHE:CE2	2.49	0.48
1:B:427:GLU:OE1	1:B:427:GLU:N	2.47	0.48
1:C:399:VAL:HG21	1:C:475:SER:CB	2.44	0.48
1:A:236:GLY:HA2	1:B:740:PHE:CZ	2.49	0.48
1:A:372:ILE:CG2	1:A:482:LEU:HD11	2.43	0.48
1:A:650:MET:HE2	1:A:659:GLY:HA3	1.95	0.48
1:A:920:GLU:O	1:A:925:SER:HB3	2.13	0.48
2:A:1103:PTY:HC31	2:A:1104:PTY:HN12	1.75	0.48
1:B:401:GLY:HA3	1:B:989:PHE:CD1	2.49	0.48
1:B:789:PRO:HA	1:B:794:ILE:HG12	1.95	0.48
1:C:43:ILE:HD13	1:C:94:PHE:CE1	2.48	0.48
1:C:189:LYS:O	1:C:192:GLN:HG3	2.14	0.48
1:A:452:VAL:CG2	1:A:453:PRO:HD3	2.44	0.48
1:B:341:THR:HG21	1:B:397:ILE:HG23	1.94	0.48
1:B:448:ILE:O	1:B:452:VAL:HG23	2.14	0.48
1:B:699:ILE:HG23	1:B:713:VAL:HG12	1.94	0.48
1:A:36:PRO:HG2	1:A:464:ILE:HG12	1.95	0.48
1:A:650:MET:CE	1:A:659:GLY:HA3	2.43	0.48
2:A:1102:PTY:C5	2:A:1102:PTY:C3	2.85	0.48
1:B:102:LEU:HA	1:B:105:VAL:HG12	1.95	0.48
1:B:120:ALA:O	1:B:124:GLN:HG3	2.14	0.48
1:B:220:LEU:CD2	1:C:274:SER:HA	2.43	0.48
1:B:373:SER:OG	1:B:482:LEU:HD12	2.13	0.48
1:B:989:PHE:CD2	1:B:1018:MET:HG3	2.49	0.48
1:C:676:LEU:HD12	1:C:708:PHE:CZ	2.49	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:ALA:O	1:A:124:GLN:HG3	2.14	0.48
1:A:396:MET:HA	1:A:399:VAL:CG2	2.44	0.48
1:A:738:VAL:CG1	1:A:788:VAL:HG21	2.44	0.48
1:A:904:LEU:HD13	1:A:1024:LEU:HB3	1.95	0.48
1:C:551:PHE:O	1:C:555:ARG:HG2	2.14	0.48
1:C:787:THR:HG22	1:C:797:PRO:CA	2.38	0.48
1:C:1010:ILE:O	1:C:1014:VAL:HG22	2.14	0.48
1:A:101:ASN:O	1:A:105:VAL:HG23	2.14	0.47
1:A:364:LEU:HG	1:A:368:ILE:HD11	1.95	0.47
1:A:665:PRO:HB3	1:A:672:ASN:HD21	1.79	0.47
3:B:1101:ERY:C33	3:B:1101:ERY:C32	2.86	0.47
2:B:1104:PTY:H312	2:B:1105:PTY:C32	2.43	0.47
1:C:350:PHE:CD1	1:C:367:THR:HG21	2.45	0.47
1:A:912:GLY:HA3	1:A:1016:TRP:CG	2.49	0.47
1:C:992:GLY:O	1:C:995:PRO:HD2	2.14	0.47
1:A:399:VAL:O	1:A:403:VAL:HG23	2.14	0.47
1:A:425:PRO:O	1:A:429:THR:HG23	2.14	0.47
1:A:845:VAL:HG21	1:A:854:LEU:CD1	2.45	0.47
1:C:707:LEU:HA	1:C:832:VAL:HG21	1.95	0.47
1:A:68:ASN:ND2	1:A:110:LYS:O	2.47	0.47
1:B:312:GLU:HA	1:B:315:PHE:CD2	2.49	0.47
1:B:952:LEU:HD13	1:B:978:ARG:NH2	2.30	0.47
1:C:62:LEU:HD12	1:C:82:ALA:HB2	1.95	0.47
1:A:532:LEU:HD21	1:A:972:LEU:HD12	1.94	0.47
1:C:916:ARG:HG2	1:C:929:PHE:CE2	2.50	0.47
2:C:1101:PTY:C1	2:C:1101:PTY:C32	2.86	0.47
1:A:728:ILE:HD12	1:A:728:ILE:H	1.80	0.47
1:A:885:LEU:HD21	1:A:951:ILE:CD1	2.45	0.47
1:B:645:LYS:O	1:B:649:MET:HG3	2.14	0.47
1:C:638:ASP:O	1:C:642:VAL:HG23	2.14	0.47
1:A:11:PHE:HD1	1:B:887:ALA:HB1	1.80	0.47
1:A:24:ILE:HG23	2:A:1105:PTY:H311	1.97	0.47
1:A:45:LEU:HG	1:A:129:VAL:HG22	1.97	0.47
1:A:142:LEU:HB2	1:A:285:THR:OG1	2.15	0.47
1:A:412:GLU:HA	1:A:415:GLU:HG3	1.96	0.47
1:A:558:THR:HA	1:A:931:ASN:HB3	1.97	0.47
1:A:726:ILE:HA	1:A:804:VAL:HG22	1.97	0.47
1:A:885:LEU:HD21	1:A:951:ILE:HD11	1.97	0.47
1:B:13:TRP:O	1:B:17:ILE:HG13	2.15	0.47
1:C:27:ILE:O	2:C:1105:PTY:HC22	2.15	0.47
1:C:393:MET:O	1:C:397:ILE:HG13	2.15	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:407:ALA:O	1:C:411:VAL:HG23	2.14	0.47
1:C:667:ILE:HG22	1:C:669:GLU:HG2	1.97	0.47
1:C:882:PHE:HB2	1:C:899:LEU:HD11	1.97	0.47
1:C:956:PHE:CE2	1:C:960:LEU:HD11	2.49	0.47
1:A:180:ARG:HG2	1:A:268:LEU:HD22	1.96	0.47
1:A:274:SER:HA	1:C:220:LEU:HD23	1.97	0.47
1:A:403:VAL:HG13	1:A:479:SER:OG	2.14	0.47
1:C:445:ALA:HB1	1:C:884:VAL:HG11	1.97	0.47
1:A:366:PRO:HA	1:A:369:VAL:CG2	2.37	0.47
1:A:862:GLU:HA	1:A:865:LYS:CE	2.45	0.47
1:B:16:SER:OG	1:B:486:LEU:HD22	2.15	0.47
1:B:882:PHE:CE2	2:B:1104:PTY:H162	2.50	0.47
1:C:5:PHE:CD1	1:C:485:THR:HG23	2.50	0.47
1:C:167:ILE:HD11	1:C:307:ARG:HG3	1.97	0.47
1:C:329:LYS:O	1:C:333:ILE:HG12	2.15	0.47
1:C:680:LEU:HD23	1:C:680:LEU:H	1.79	0.47
1:A:333:ILE:O	1:A:337:LYS:HG2	2.14	0.47
1:A:444:THR:O	1:A:448:ILE:HG12	2.15	0.47
1:B:183:ARG:HD2	1:B:771:GLN:HB2	1.96	0.47
1:B:1004:SER:O	1:B:1008:ARG:HG3	2.15	0.47
1:C:142:LEU:HB2	1:C:285:THR:HB	1.97	0.47
1:C:698:LEU:HA	1:C:701:LYS:HE2	1.97	0.47
1:A:965:LYS:HD2	1:A:969:GLU:HB3	1.96	0.46
1:A:997:TYR:CE1	1:A:1012:THR:HA	2.50	0.46
1:B:892:TRP:HB3	2:B:1104:PTY:H112	1.97	0.46
1:C:386:MET:HE3	1:C:470:LEU:HD22	1.96	0.46
1:A:860:SER:HA	1:A:863:GLU:OE1	2.15	0.46
1:A:1010:ILE:O	1:A:1014:VAL:HG22	2.14	0.46
1:B:641:ALA:O	1:B:645:LYS:HG3	2.16	0.46
1:C:58:GLU:HA	1:C:62:LEU:HB2	1.98	0.46
1:A:727:ASP:HB3	1:A:803:THR:HG22	1.97	0.46
1:B:544:GLY:O	1:B:547:VAL:HG22	2.16	0.46
1:C:405:ASP:O	1:C:409:VAL:HG23	2.16	0.46
1:C:902:MET:HB2	1:C:903:PRO:HD3	1.97	0.46
1:A:171:GLY:HA3	1:A:292:SER:HB2	1.97	0.46
1:A:429:THR:O	1:A:433:MET:HG2	2.15	0.46
1:C:712:THR:HG21	1:C:827:SER:CB	2.46	0.46
1:A:349:VAL:HA	1:A:352:VAL:CG1	2.46	0.46
1:B:312:GLU:HA	1:B:315:PHE:CG	2.50	0.46
1:B:845:VAL:CG1	1:B:854:LEU:HD22	2.46	0.46
1:A:219:SER:O	1:A:222:ALA:HB2	2.15	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:406:ASP:O	1:C:410:VAL:HG23	2.16	0.46
1:A:11:PHE:CD1	1:B:887:ALA:HB1	2.50	0.46
1:A:250:ARG:HG2	1:A:253:THR:CG2	2.46	0.46
1:B:405:ASP:O	1:B:409:VAL:HG13	2.16	0.46
1:B:882:PHE:CZ	2:B:1104:PTY:H162	2.51	0.46
1:B:939:PHE:HA	1:B:942:VAL:HG22	1.98	0.46
1:B:5:PHE:CD1	1:B:485:THR:HG23	2.51	0.46
1:C:442:GLY:O	1:C:446:VAL:HG22	2.16	0.46
2:C:1107:PTY:H111	2:C:1107:PTY:HC6	1.82	0.46
1:A:39:ALA:HA	1:A:669:GLU:HG2	1.98	0.46
1:C:161:VAL:HB	1:C:162:PRO:HD3	1.98	0.46
1:C:834:THR:O	1:C:838:MET:HG3	2.16	0.46
1:A:727:ASP:HB3	1:A:803:THR:CG2	2.45	0.45
1:A:937:VAL:O	1:A:940:VAL:HG22	2.15	0.45
1:B:10:ILE:O	1:B:14:VAL:HG23	2.16	0.45
1:B:771:GLN:HG3	1:B:777:ARG:HH12	1.79	0.45
1:C:394:PHE:CE1	1:C:1007:GLN:HG2	2.51	0.45
1:A:908:GLY:HA3	1:A:1020:ILE:HB	1.98	0.45
1:B:693:ALA:O	1:B:697:GLU:HG3	2.16	0.45
1:B:45:LEU:HD13	1:B:65:ILE:HG21	1.97	0.45
1:B:45:LEU:CD1	1:B:65:ILE:HG21	2.47	0.45
1:B:703:ARG:O	1:B:710:PRO:HG3	2.17	0.45
1:C:178:ALA:HB2	1:C:272:ASP:OD1	2.16	0.45
1:B:61:VAL:O	1:B:65:ILE:HG13	2.17	0.45
1:C:686:THR:O	1:C:690:ALA:HB3	2.16	0.45
1:A:13:TRP:O	1:A:17:ILE:HG13	2.16	0.45
1:A:174:ARG:HG3	1:A:290:MET:HE1	1.98	0.45
1:A:755:TYR:OH	1:A:758:ASP:OD1	2.28	0.45
1:C:66:GLU:OE2	1:C:818:GLY:HA2	2.17	0.45
1:A:341:THR:HG21	1:A:996:LEU:CD2	2.47	0.45
1:C:527:ARG:O	1:C:531:VAL:HG23	2.16	0.45
1:C:934:TYR:CZ	1:C:1006:SER:HB3	2.52	0.45
1:A:144:SER:OG	1:A:152:MET:SD	2.68	0.45
1:A:404:VAL:O	1:A:408:ILE:HG23	2.17	0.45
1:A:901:VAL:O	1:A:901:VAL:CG2	2.64	0.45
1:B:406:ASP:O	1:B:410:VAL:HG23	2.17	0.45
1:C:753:SER:HB2	1:C:771:GLN:CD	2.37	0.45
1:B:156:ALA:O	1:B:161:VAL:HG23	2.16	0.45
1:B:837:ALA:O	1:B:841:VAL:HG23	2.17	0.45
1:B:908:GLY:HA3	1:B:1020:ILE:HB	1.99	0.45
1:C:178:ALA:HB3	1:C:270:MET:HB3	1.98	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:238:LEU:HD22	1:C:243:GLU:HB3	1.98	0.45
1:C:938:GLY:O	1:C:942:VAL:HG23	2.17	0.45
2:C:1105:PTY:HC52	2:C:1105:PTY:C3	2.39	0.45
1:B:465:TYR:CZ	1:B:933:ILE:HG23	2.52	0.45
1:B:942:VAL:HG12	1:B:1018:MET:HG2	1.99	0.45
3:B:1101:ERY:H352	3:B:1101:ERY:H312	1.99	0.44
1:C:38:VAL:HA	1:C:463:ASN:HD22	1.81	0.44
1:C:182:MET:HB3	1:C:768:VAL:HG22	2.00	0.44
1:A:340:HIS:O	1:A:344:GLU:HG3	2.18	0.44
1:A:348:LEU:O	1:A:351:VAL:HG22	2.16	0.44
1:B:366:PRO:HA	1:B:369:VAL:CG2	2.43	0.44
1:B:676:LEU:HD11	1:B:838:MET:CG	2.47	0.44
1:B:786:LEU:O	1:B:798:LEU:HB2	2.17	0.44
1:C:11:PHE:CE2	1:C:15:ILE:HD11	2.52	0.44
1:C:845:VAL:HG11	1:C:854:LEU:HB2	1.99	0.44
1:A:63:SER:O	1:A:67:ARG:HG3	2.16	0.44
1:A:521:THR:O	1:A:525:GLU:HG3	2.18	0.44
1:C:452:VAL:HG11	2:C:1106:PTY:H292	1.99	0.44
1:C:837:ALA:O	1:C:841:VAL:HG23	2.17	0.44
1:B:789:PRO:CB	1:B:794:ILE:HG12	2.47	0.44
3:B:1101:ERY:C7	3:B:1101:ERY:C31	2.86	0.44
1:C:137:LEU:HD22	1:C:291:LEU:HG	1.99	0.44
1:C:399:VAL:O	1:C:403:VAL:HG13	2.18	0.44
1:C:504:GLU:HG3	1:C:505:GLU:H	1.82	0.44
1:A:137:LEU:HD12	1:A:327:THR:OG1	2.18	0.44
1:A:538:MET:O	1:A:541:VAL:HG22	2.17	0.44
1:A:841:VAL:HA	1:A:844:MET:HE2	2.00	0.44
1:B:401:GLY:HA3	1:B:989:PHE:CE1	2.52	0.44
3:B:1101:ERY:H343	3:B:1101:ERY:H353	2.00	0.44
1:C:386:MET:HE1	1:C:470:LEU:HB2	1.99	0.44
1:C:889:TYR:CE2	1:C:951:ILE:HD11	2.52	0.44
1:A:161:VAL:HB	1:A:162:PRO:HD3	1.98	0.44
1:B:875:ALA:O	1:B:879:VAL:HG23	2.18	0.44
2:B:1104:PTY:HC11	2:B:1105:PTY:HC21	1.98	0.44
1:C:163:GLU:OE1	1:C:163:GLU:N	2.51	0.44
1:A:925:SER:OG	1:A:926:VAL:N	2.51	0.44
1:B:936:GLN:O	1:B:940:VAL:HG23	2.18	0.44
2:B:1106:PTY:H322	2:C:1106:PTY:C34	2.48	0.44
1:C:413:ASN:HB2	1:C:436:ILE:HD13	2.00	0.44
1:C:695:ARG:HD3	1:C:822:MET:HB3	2.00	0.44
1:C:956:PHE:CD2	1:C:974:ALA:HA	2.52	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:997:TYR:CD1	1:C:1012:THR:HA	2.51	0.44
1:A:889:TYR:OH	1:A:951:ILE:HG23	2.18	0.44
1:A:940:VAL:O	1:A:943:MET:HG2	2.16	0.44
1:B:452:VAL:HB	1:B:453:PRO:HD3	2.00	0.44
1:B:655:LYS:HA	1:B:655:LYS:HE2	1.99	0.44
1:B:1026:VAL:HG23	1:B:1027:PHE:CD2	2.53	0.44
1:C:506:LYS:O	1:C:511:GLY:HA3	2.18	0.44
1:A:401:GLY:HA2	1:A:404:VAL:HG12	1.98	0.44
1:A:564:GLU:OE2	1:A:1005:ALA:HB3	2.18	0.44
1:A:641:ALA:O	1:A:645:LYS:HG3	2.18	0.44
1:B:396:MET:O	1:B:400:ILE:HG13	2.18	0.44
1:B:534:LYS:HB2	1:B:537:ARG:HG2	1.99	0.44
1:C:209:ASN:ND2	1:C:758:ASP:O	2.48	0.44
1:C:465:TYR:CE1	1:C:933:ILE:HG23	2.53	0.44
1:C:472:MET:O	1:C:476:ILE:HG13	2.18	0.44
1:C:784:LEU:HD21	1:C:804:VAL:HB	2.00	0.44
1:A:209:ASN:ND2	1:A:758:ASP:O	2.51	0.43
1:A:402:ILE:HG21	1:A:476:ILE:CD1	2.48	0.43
1:A:587:THR:O	1:A:591:VAL:HG23	2.18	0.43
1:C:62:LEU:HD22	1:C:90:VAL:HG23	2.00	0.43
1:C:151:GLU:HG2	1:C:180:ARG:NH2	2.33	0.43
1:C:707:LEU:HD12	1:C:840:ALA:HB2	2.00	0.43
1:A:461:ALA:HB2	1:A:560:PHE:CZ	2.53	0.43
1:B:307:ARG:O	1:B:311:LEU:HG	2.18	0.43
1:B:353:MET:HB2	1:B:363:THR:HG22	2.00	0.43
1:B:721:SER:OG	1:B:722:PRO:HD2	2.18	0.43
1:B:790:ASN:N	1:B:793:GLY:O	2.43	0.43
1:B:845:VAL:HG11	1:B:854:LEU:HB3	2.00	0.43
1:C:331:VAL:O	1:C:335:ILE:HG12	2.17	0.43
1:C:398:LEU:HD12	1:C:468:PHE:CZ	2.44	0.43
1:C:632:ARG:HB3	1:C:637:SER:HB3	2.00	0.43
1:C:641:ALA:O	1:C:645:LYS:HG2	2.18	0.43
1:A:423:LEU:CG	1:A:424:PRO:HD2	2.47	0.43
1:A:885:LEU:HD13	1:A:898:VAL:HB	2.00	0.43
1:C:532:LEU:HD12	1:C:972:LEU:CD1	2.47	0.43
1:B:80:THR:HB	1:B:815:ARG:HB2	2.01	0.43
1:B:279:LEU:O	1:B:282:VAL:HG22	2.18	0.43
1:B:300:THR:O	1:B:304:VAL:HG23	2.19	0.43
1:B:462:GLY:O	1:B:466:LYS:HG3	2.19	0.43
1:B:33:SER:O	1:B:389:ASN:HA	2.18	0.43
1:B:541:VAL:O	1:B:545:LEU:HG	2.18	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1106:PTY:C3	2:B:1106:PTY:HC51	2.49	0.43
2:B:1109:PTY:C11	2:B:1109:PTY:HC52	2.48	0.43
1:C:557:PRO:O	1:C:930:ALA:HB1	2.18	0.43
1:A:15:ILE:O	1:A:19:ILE:HG13	2.17	0.43
1:A:183:ARG:NH1	1:A:769:MET:SD	2.91	0.43
1:A:405:ASP:O	1:A:409:VAL:HG23	2.19	0.43
1:B:906:LEU:HB2	1:B:939:PHE:CE1	2.54	0.43
1:C:334:SER:O	1:C:338:VAL:HG13	2.18	0.43
1:C:677:SER:OG	1:C:823:GLU:OE2	2.36	0.43
1:A:61:VAL:O	1:A:65:ILE:HG13	2.18	0.43
1:B:103:ALA:O	1:B:107:VAL:HG23	2.18	0.43
1:B:136:PHE:CE1	1:B:139:ILE:HG12	2.54	0.43
1:A:180:ARG:HD3	1:A:268:LEU:HD13	2.00	0.43
1:A:517:PHE:HZ	1:A:980:ARG:HA	1.83	0.43
1:B:798:LEU:O	1:B:798:LEU:HD23	2.18	0.43
1:A:78:MET:HB2	1:A:92:LEU:HD23	2.00	0.43
1:A:432:ALA:O	1:A:436:ILE:HG12	2.18	0.43
1:B:135:ASN:HB3	1:B:291:LEU:O	2.19	0.43
1:B:502:HIS:HA	1:B:505:GLU:OE2	2.19	0.43
1:B:842:GLN:NE2	1:B:854:LEU:HD21	2.34	0.43
1:C:773:ASP:OD1	1:C:774:GLY:N	2.50	0.43
1:A:39:ALA:HB2	1:A:669:GLU:OE2	2.19	0.43
1:A:316:PRO:HD2	1:A:319:MET:SD	2.59	0.43
1:A:348:LEU:O	1:A:352:VAL:HG12	2.19	0.43
1:A:897:ALA:HB3	1:A:954:ILE:HD13	1.99	0.43
1:B:11:PHE:CE2	1:B:15:ILE:HD11	2.54	0.43
1:B:186:VAL:HG11	1:B:191:LEU:HD11	2.01	0.43
1:C:240:THR:OG1	1:C:243:GLU:HG3	2.19	0.43
1:C:885:LEU:HB3	1:C:895:PRO:HG3	2.01	0.43
1:A:186:VAL:HG11	1:A:191:LEU:HD11	2.00	0.42
1:A:841:VAL:HA	1:A:844:MET:CE	2.49	0.42
1:B:433:MET:SD	1:B:488:PRO:HG3	2.59	0.42
1:C:511:GLY:O	1:C:515:LYS:HG3	2.19	0.42
1:C:667:ILE:CG2	1:C:669:GLU:HG2	2.48	0.42
1:C:840:ALA:O	1:C:844:MET:HG3	2.18	0.42
1:A:452:VAL:HG22	1:A:453:PRO:HD3	2.02	0.42
1:B:161:VAL:HG21	1:B:175:LEU:CD1	2.49	0.42
1:B:308:LEU:HD13	1:B:321:TRP:CE3	2.54	0.42
1:B:472:MET:O	1:B:476:ILE:HG13	2.19	0.42
1:C:406:ASP:CG	1:C:440:VAL:HG13	2.39	0.42
1:A:723:GLN:HB3	1:C:231:THR:O	2.18	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1032:PHE:O	1:A:1036:VAL:HG13	2.20	0.42
2:A:1103:PTY:C32	2:B:1106:PTY:H131	2.49	0.42
1:B:412:GLU:CD	1:B:981:PRO:HG3	2.39	0.42
1:B:877:ALA:O	1:B:881:VAL:HG23	2.19	0.42
1:C:64:VAL:HG22	1:C:67:ARG:HH21	1.84	0.42
1:C:298:MET:HB3	1:C:298:MET:HE3	1.88	0.42
1:C:568:PHE:CZ	1:C:664:PRO:HG3	2.54	0.42
1:A:109:ASN:O	1:A:113:GLU:HG3	2.19	0.42
1:A:695:ARG:O	1:A:699:ILE:HG13	2.20	0.42
1:B:511:GLY:O	1:B:515:LYS:HG2	2.18	0.42
1:C:843:LYS:O	1:C:847:GLU:HG3	2.19	0.42
1:A:20:ILE:HD13	2:A:1105:PTY:H411	2.00	0.42
1:B:400:ILE:O	1:B:404:VAL:HG13	2.20	0.42
1:B:574:GLN:HG2	1:B:619:MET:SD	2.60	0.42
2:B:1103:PTY:C1	2:B:1103:PTY:C32	2.95	0.42
1:C:198:PHE:CG	1:C:749:SER:HB2	2.54	0.42
1:C:681:GLN:NE2	1:C:855:GLU:HG3	2.34	0.42
1:A:395:ALA:O	1:A:399:VAL:HG13	2.19	0.42
1:B:598:ILE:HG22	1:B:600:GLU:H	1.83	0.42
1:B:838:MET:HE3	1:B:856:TRP:CE2	2.54	0.42
1:C:356:PHE:CD1	1:C:984:MET:HG2	2.54	0.42
1:C:829:ALA:HB3	1:C:832:VAL:CG2	2.49	0.42
1:B:151:GLU:HG2	1:B:180:ARG:HH22	1.84	0.42
1:B:402:ILE:HD11	1:B:941:THR:HG23	2.01	0.42
1:B:842:GLN:CD	1:B:854:LEU:HD21	2.40	0.42
1:A:691:LEU:HD23	1:A:822:MET:HG3	2.02	0.42
1:B:185:TRP:CE3	1:B:771:GLN:HB3	2.55	0.42
1:B:838:MET:HE3	1:B:856:TRP:CZ2	2.54	0.42
2:B:1106:PTY:C5	2:B:1106:PTY:HC32	2.50	0.42
1:C:180:ARG:CG	1:C:268:LEU:HD22	2.50	0.42
1:C:465:TYR:HE1	1:C:933:ILE:HG23	1.85	0.42
1:A:348:LEU:HD13	1:A:991:LEU:O	2.20	0.42
1:A:431:LYS:HB3	1:A:431:LYS:HE2	1.60	0.42
1:A:709:ASP:OD1	1:A:709:ASP:N	2.49	0.42
1:A:880:ALA:O	1:A:884:VAL:HG23	2.19	0.42
1:C:62:LEU:CD1	1:C:82:ALA:HB2	2.50	0.42
1:C:980:ARG:O	1:C:984:MET:HG3	2.20	0.42
1:A:219:SER:HB2	1:B:777:ARG:HE	1.84	0.42
1:A:487:THR:HB	1:A:488:PRO:HD3	2.02	0.42
1:A:719:GLU:N	1:A:719:GLU:OE1	2.52	0.42
1:B:69:MET:HB3	1:B:92:LEU:HD21	2.02	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:ASP:OD1	1:B:83:ASP:N	2.53	0.42
1:C:462:GLY:O	1:C:466:LYS:HG3	2.20	0.42
1:C:898:VAL:CG2	1:C:954:ILE:HD12	2.49	0.42
1:A:148:SER:O	1:A:152:MET:HG3	2.19	0.41
1:A:238:LEU:HD22	1:A:243:GLU:HB3	2.02	0.41
1:B:588:LEU:HD12	1:B:608:SER:HB2	2.01	0.41
1:A:339:ILE:O	1:A:343:ILE:HG12	2.20	0.41
1:B:2:ALA:CB	1:B:433:MET:HB3	2.43	0.41
1:B:366:PRO:O	1:B:370:VAL:HG23	2.21	0.41
1:B:389:ASN:O	1:B:393:MET:HG2	2.19	0.41
1:B:524:TYR:O	1:B:528:VAL:HG23	2.20	0.41
1:C:546:ALA:O	1:C:550:VAL:HG23	2.20	0.41
1:A:16:SER:O	1:A:20:ILE:HG13	2.20	0.41
2:A:1105:PTY:O10	2:A:1105:PTY:P1	2.79	0.41
1:B:205:LEU:HD21	1:B:260:LEU:HD22	2.02	0.41
1:A:180:ARG:HH11	1:A:268:LEU:HB3	1.84	0.41
1:A:386:MET:HE3	1:A:470:LEU:HD12	2.01	0.41
1:A:845:VAL:HG11	1:A:854:LEU:HB2	2.02	0.41
2:A:1101:PTY:O10	2:A:1101:PTY:HC52	2.19	0.41
1:B:9:PRO:HB3	1:B:489:ALA:HB1	2.02	0.41
1:B:893:SER:O	1:B:1036:VAL:HG11	2.19	0.41
2:B:1103:PTY:H332	2:B:1106:PTY:H312	2.02	0.41
2:B:1105:PTY:H121	2:B:1105:PTY:C6	2.50	0.41
1:A:158:ARG:CZ	1:A:764:ARG:HD3	2.51	0.41
1:A:364:LEU:O	1:A:368:ILE:HG13	2.20	0.41
1:A:368:ILE:O	1:A:372:ILE:HG13	2.21	0.41
1:A:417:ILE:HG21	1:A:431:LYS:CE	2.44	0.41
1:A:431:LYS:O	1:A:435:GLN:HG3	2.20	0.41
1:A:443:ILE:O	1:A:446:VAL:HG22	2.20	0.41
1:A:495:LEU:O	1:A:496:LYS:HE2	2.20	0.41
1:B:843:LYS:O	1:B:847:GLU:HG3	2.21	0.41
1:B:1043:THR:HG22	2:B:1105:PTY:HC22	2.02	0.41
1:C:69:MET:HG2	1:C:92:LEU:HD11	2.02	0.41
1:C:153:ASN:OD1	1:C:285:THR:HG23	2.20	0.41
1:C:573:VAL:HB	1:C:620:ALA:HB3	2.03	0.41
1:C:441:ILE:HG22	1:C:888:LEU:HD11	2.03	0.41
1:A:352:VAL:HG11	1:A:988:ALA:HA	2.03	0.41
1:A:404:VAL:O	1:A:408:ILE:HG12	2.19	0.41
1:B:217:ILE:O	1:B:229:THR:HA	2.20	0.41
1:B:537:ARG:O	1:B:541:VAL:HG23	2.21	0.41
1:B:833:SER:HB3	1:B:836:GLN:HG2	2.02	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:623:PHE:O	1:C:625:ILE:HD12	2.21	0.41
1:A:380:PHE:CE2	2:A:1103:PTY:H281	2.55	0.41
1:A:1006:SER:O	1:A:1010:ILE:HG22	2.21	0.41
1:B:175:LEU:HD23	1:B:287:MET:HG2	2.03	0.41
1:B:212:ILE:HG12	1:C:744:ARG:HG3	2.02	0.41
1:B:534:LYS:O	1:B:538:MET:HG2	2.21	0.41
1:B:759:PHE:CE2	1:B:761:ASN:HB2	2.55	0.41
2:C:1106:PTY:H382	2:C:1106:PTY:H171	2.01	0.41
1:A:152:MET:HE3	1:A:285:THR:HG23	2.02	0.41
1:A:335:ILE:O	1:A:339:ILE:HG13	2.21	0.41
1:A:739:SER:O	1:A:743:ILE:HG13	2.21	0.41
1:B:185:TRP:HD1	1:B:265:LYS:HG3	1.85	0.41
1:B:365:ILE:O	1:B:369:VAL:HG22	2.20	0.41
1:B:789:PRO:HA	1:B:794:ILE:HG23	2.02	0.41
1:B:840:ALA:O	1:B:844:MET:HG3	2.21	0.41
1:B:916:ARG:HD3	1:B:1012:THR:HG21	2.03	0.41
1:C:65:ILE:O	1:C:69:MET:HB2	2.21	0.41
1:C:443:ILE:HG23	1:C:948:LYS:HD3	2.01	0.41
1:C:588:LEU:HD21	1:C:620:ALA:CB	2.48	0.41
2:C:1106:PTY:H191	2:C:1106:PTY:C23	2.46	0.41
1:A:16:SER:HB3	1:A:372:ILE:HD13	2.02	0.41
1:A:211:GLN:NE2	1:B:56:VAL:HG13	2.36	0.41
1:A:882:PHE:HB2	1:A:899:LEU:CD1	2.39	0.41
1:A:997:TYR:CD1	1:A:1012:THR:HA	2.56	0.41
1:B:139:ILE:HG13	3:B:1101:ERY:H8	2.03	0.41
1:B:491:CYS:O	1:B:495:LEU:HB2	2.21	0.41
1:B:788:VAL:C	1:B:794:ILE:HG23	2.41	0.41
1:C:443:ILE:HD11	1:C:952:LEU:CD2	2.48	0.41
1:C:544:GLY:O	1:C:547:VAL:HG22	2.20	0.41
1:C:990:ILE:HG23	1:C:1015:PHE:CE1	2.55	0.41
1:A:331:VAL:O	1:A:335:ILE:HG12	2.21	0.40
1:A:655:LYS:HE2	1:A:655:LYS:HA	2.02	0.40
1:B:286:GLY:HA3	3:B:1101:ERY:C27	2.52	0.40
1:B:557:PRO:O	1:B:930:ALA:HB1	2.21	0.40
1:C:308:LEU:HD13	1:C:321:TRP:CE3	2.56	0.40
1:A:103:ALA:O	1:A:107:VAL:HG23	2.21	0.40
1:B:380:PHE:CD2	1:B:474:SER:HB2	2.56	0.40
1:B:439:ALA:O	1:B:443:ILE:HG13	2.21	0.40
1:B:743:ILE:O	1:B:747:LEU:HG	2.22	0.40
1:B:953:ILE:HD11	1:B:982:ILE:CD1	2.51	0.40
3:B:1101:ERY:H4	3:B:1101:ERY:H71	1.58	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:676:LEU:HD11	1:C:837:ALA:HB3	2.04	0.40
1:A:152:MET:HB2	1:A:152:MET:HE3	1.97	0.40
1:A:532:LEU:HD21	1:A:972:LEU:HD11	2.02	0.40
1:A:678:ILE:HB	1:A:824:LEU:CD2	2.52	0.40
1:B:6:ILE:HD11	1:B:429:THR:HB	2.03	0.40
3:B:1101:ERY:O13	3:B:1101:ERY:H343	2.21	0.40
2:B:1109:PTY:H411	2:B:1109:PTY:H381	1.90	0.40
1:C:302:LYS:O	1:C:306:GLU:HG3	2.21	0.40
1:C:537:ARG:O	1:C:540:VAL:HG22	2.22	0.40
1:C:718:LEU:HB2	1:C:812:GLN:HB2	2.03	0.40
1:A:965:LYS:HD2	1:A:969:GLU:CB	2.51	0.40
1:A:1043:THR:CG2	2:A:1106:PTY:HN11	2.31	0.40
1:B:682:ASP:OD2	1:B:686:THR:N	2.48	0.40
1:B:894:ILE:CD1	1:B:958:LYS:HD3	2.52	0.40
1:C:272:ASP:OD1	1:C:272:ASP:N	2.54	0.40
1:C:410:VAL:O	1:C:414:VAL:HG23	2.21	0.40
1:C:537:ARG:O	1:C:541:VAL:HG23	2.22	0.40
2:C:1101:PTY:H311	2:C:1107:PTY:O10	2.19	0.40
1:A:233:THR:O	1:B:725:LYS:HA	2.22	0.40
1:A:436:ILE:HG22	1:A:436:ILE:O	2.20	0.40
1:B:176:PHE:CE2	1:B:288:ALA:HB2	2.57	0.40
1:B:347:VAL:O	1:B:351:VAL:HG23	2.21	0.40
1:B:896:LEU:O	1:B:900:LEU:HG	2.22	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	1033/1046 (99%)	1002 (97%)	31 (3%)	0	100	100
1	B	1041/1046 (100%)	1018 (98%)	23 (2%)	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	1040/1046 (99%)	1013 (97%)	27 (3%)	0	100	100
All	All	3114/3138 (99%)	3033 (97%)	81 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	829/837 (99%)	829 (100%)	0	100	100
1	B	835/837 (100%)	835 (100%)	0	100	100
1	C	834/837 (100%)	834 (100%)	0	100	100
All	All	2498/2511 (100%)	2498 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	157	GLN
1	A	211	GLN
1	A	257	ASN
1	A	358	GLN
1	A	435	GLN
1	A	574	GLN
1	A	617	GLN
1	A	681	GLN
1	A	790	ASN
1	A	836	GLN
1	B	147	GLN
1	B	165	GLN
1	B	211	GLN
1	B	293	ASN
1	B	617	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	762	GLN
1	B	779	GLN
1	B	785	ASN
1	B	817	ASN
1	B	836	GLN
1	B	917	ASN
1	C	108	GLN
1	C	123	GLN
1	C	124	GLN
1	C	192	GLN
1	C	283	ASN
1	C	463	ASN
1	C	617	GLN
1	C	681	GLN
1	C	762	GLN
1	C	869	GLN
1	C	961	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

24 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
2	PTY	C	1109	-	14,14,49	2.04	2 (14%)	14,14,54	1.06	1 (7%)
2	PTY	C	1105	-	34,34,49	1.11	2 (5%)	37,39,54	1.08	2 (5%)
2	PTY	B	1109	-	43,43,49	0.98	2 (4%)	46,48,54	1.11	2 (4%)
2	PTY	C	1108	-	14,14,49	1.20	1 (7%)	14,14,54	1.05	0
3	ERY	B	1101	-	53,53,53	0.92	1 (1%)	82,82,82	1.52	13 (15%)
2	PTY	B	1107	-	49,49,49	0.97	2 (4%)	52,54,54	1.11	4 (7%)
2	PTY	C	1107	-	49,49,49	0.89	2 (4%)	52,54,54	1.02	2 (3%)
2	PTY	A	1103	-	44,44,49	0.94	2 (4%)	47,49,54	1.07	2 (4%)
2	PTY	B	1103	-	35,35,49	1.07	2 (5%)	38,40,54	1.21	3 (7%)
2	PTY	B	1106	-	34,34,49	1.10	2 (5%)	37,39,54	1.12	2 (5%)
2	PTY	C	1104	-	31,31,49	1.15	2 (6%)	34,36,54	1.12	2 (5%)
2	PTY	B	1108	-	34,34,49	1.11	2 (5%)	37,39,54	1.32	3 (8%)
2	PTY	C	1103	-	40,40,49	0.97	2 (5%)	43,45,54	1.20	3 (6%)
2	PTY	C	1106	-	37,37,49	1.08	3 (8%)	39,39,54	1.26	3 (7%)
2	PTY	A	1101	-	47,47,49	0.95	2 (4%)	50,52,54	1.05	3 (6%)
2	PTY	A	1105	-	43,43,49	0.97	2 (4%)	46,48,54	1.06	2 (4%)
2	PTY	B	1104	-	40,40,49	0.91	2 (5%)	43,45,54	1.27	4 (9%)
2	PTY	A	1102	-	44,44,49	0.93	2 (4%)	47,49,54	1.14	4 (8%)
2	PTY	A	1106	-	40,40,49	0.99	2 (5%)	43,45,54	1.10	1 (2%)
2	PTY	A	1104	-	40,40,49	1.00	2 (5%)	43,45,54	1.16	5 (11%)
2	PTY	B	1102	-	36,36,49	1.02	2 (5%)	39,41,54	1.07	3 (7%)
2	PTY	C	1101	-	45,45,49	0.94	2 (4%)	48,50,54	1.08	3 (6%)
2	PTY	B	1105	-	43,43,49	1.00	2 (4%)	46,48,54	1.15	3 (6%)
2	PTY	C	1102	-	40,40,49	0.98	2 (5%)	43,45,54	1.09	3 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PTY	C	1109	-	-	5/12/12/53	-
2	PTY	C	1105	-	-	16/38/38/53	-
2	PTY	B	1109	-	-	21/47/47/53	-
2	PTY	C	1108	-	-	2/12/12/53	-
3	ERY	B	1101	-	-	38/72/107/107	0/3/3/3

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PTY	B	1107	-	-	22/53/53/53	-
2	PTY	C	1107	-	-	17/53/53/53	-
2	PTY	A	1103	-	-	19/48/48/53	-
2	PTY	B	1103	-	-	9/39/39/53	-
2	PTY	B	1106	-	-	7/38/38/53	-
2	PTY	C	1104	-	-	9/35/35/53	-
2	PTY	B	1108	-	-	18/38/38/53	-
2	PTY	C	1103	-	-	9/44/44/53	-
2	PTY	C	1106	-	-	12/38/38/53	-
2	PTY	A	1101	-	-	17/51/51/53	-
2	PTY	A	1105	-	-	19/47/47/53	-
2	PTY	B	1104	-	-	17/44/44/53	-
2	PTY	A	1102	-	-	10/48/48/53	-
2	PTY	A	1106	-	-	12/44/44/53	-
2	PTY	A	1104	-	-	19/44/44/53	-
2	PTY	B	1102	-	-	15/40/40/53	-
2	PTY	C	1101	-	-	16/49/49/53	-
2	PTY	B	1105	-	-	15/47/47/53	-
2	PTY	C	1102	-	-	13/44/44/53	-

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1109	PTY	O10-C8	7.18	1.45	1.22
3	B	1101	ERY	O2-C1	4.99	1.45	1.34
2	B	1107	PTY	O4-C30	4.66	1.47	1.33
2	C	1108	PTY	O4-C30	4.45	1.45	1.30
2	B	1105	PTY	O4-C30	4.31	1.45	1.33
2	B	1108	PTY	O4-C30	4.30	1.45	1.33
2	A	1101	PTY	O4-C30	4.28	1.45	1.33
2	B	1109	PTY	O4-C30	4.26	1.45	1.33
2	C	1106	PTY	O4-C30	4.23	1.45	1.33
2	B	1108	PTY	O7-C8	4.21	1.46	1.34
2	C	1105	PTY	O7-C8	4.20	1.46	1.34
2	B	1107	PTY	O7-C8	4.20	1.46	1.34
2	A	1104	PTY	O4-C30	4.20	1.45	1.33
2	A	1106	PTY	O4-C30	4.19	1.45	1.33
2	B	1106	PTY	O7-C8	4.17	1.46	1.34

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1105	PTY	O7-C8	4.17	1.46	1.34
2	C	1104	PTY	O7-C8	4.16	1.46	1.34
2	C	1104	PTY	O4-C30	4.15	1.45	1.33
2	A	1105	PTY	O7-C8	4.14	1.46	1.34
2	B	1103	PTY	O4-C30	4.13	1.45	1.33
2	C	1105	PTY	O4-C30	4.13	1.45	1.33
2	C	1101	PTY	O4-C30	4.11	1.45	1.33
2	C	1107	PTY	O7-C8	4.10	1.45	1.34
2	B	1106	PTY	O4-C30	4.09	1.45	1.33
2	A	1101	PTY	O7-C8	4.09	1.45	1.34
2	C	1106	PTY	O7-C8	4.08	1.45	1.34
2	C	1101	PTY	O7-C8	4.05	1.45	1.34
2	C	1102	PTY	O4-C30	4.04	1.45	1.33
2	A	1105	PTY	O4-C30	4.02	1.45	1.33
2	C	1103	PTY	O4-C30	4.02	1.45	1.33
2	C	1107	PTY	O4-C30	4.00	1.45	1.33
2	B	1103	PTY	O7-C8	3.99	1.45	1.34
2	B	1109	PTY	O7-C8	3.97	1.45	1.34
2	B	1102	PTY	O7-C8	3.95	1.45	1.34
2	A	1103	PTY	O4-C30	3.95	1.44	1.33
2	A	1104	PTY	O7-C8	3.92	1.45	1.34
2	A	1102	PTY	O7-C8	3.92	1.45	1.34
2	A	1103	PTY	O7-C8	3.90	1.45	1.34
2	C	1102	PTY	O7-C8	3.89	1.45	1.34
2	C	1103	PTY	O7-C8	3.86	1.45	1.34
2	A	1106	PTY	O7-C8	3.83	1.45	1.34
2	B	1102	PTY	O4-C30	3.83	1.44	1.33
2	A	1102	PTY	O4-C30	3.80	1.44	1.33
2	B	1104	PTY	O4-C30	3.63	1.44	1.33
2	B	1104	PTY	O7-C8	3.53	1.44	1.34
2	C	1109	PTY	O7-C8	-2.48	1.22	1.30
2	C	1106	PTY	O7-C6	-2.41	1.42	1.47

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1104	PTY	O7-C8-C11	5.12	122.54	111.50
2	B	1107	PTY	O7-C8-C11	4.67	121.57	111.50
2	A	1103	PTY	O7-C8-C11	4.66	121.55	111.50
2	A	1102	PTY	O7-C8-C11	4.61	121.43	111.50
2	B	1109	PTY	O7-C8-C11	4.47	121.14	111.50
3	B	1101	ERY	C12-C11-C10	-4.47	110.82	116.43

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1103	PTY	O7-C8-C11	4.46	121.11	111.50
2	B	1108	PTY	O7-C8-C11	4.41	121.00	111.50
3	B	1101	ERY	O5-C16-C17	4.25	110.10	103.81
2	A	1106	PTY	O7-C8-C11	4.15	120.45	111.50
2	A	1104	PTY	O7-C8-C11	4.03	120.19	111.50
2	A	1101	PTY	O7-C8-C11	4.03	120.18	111.50
2	C	1105	PTY	O7-C8-C11	3.98	120.07	111.50
2	C	1107	PTY	O7-C8-C11	3.94	119.98	111.50
2	B	1105	PTY	O7-C8-C11	3.93	119.96	111.50
2	C	1104	PTY	O7-C8-C11	3.91	119.93	111.50
2	A	1105	PTY	O7-C8-C11	3.90	119.90	111.50
2	C	1106	PTY	C6-O7-C8	-3.90	112.86	117.88
2	C	1106	PTY	O7-C8-C11	3.87	119.83	111.50
2	C	1102	PTY	O7-C8-C11	3.81	119.70	111.50
2	C	1103	PTY	O7-C8-C11	3.76	119.61	111.50
2	C	1101	PTY	O7-C8-C11	3.74	119.56	111.50
3	B	1101	ERY	O7-C5-C6	3.66	110.90	106.39
2	B	1106	PTY	O7-C8-C11	3.65	119.36	111.50
3	B	1101	ERY	O2-C1-C2	3.60	119.45	111.56
2	C	1103	PTY	O4-C30-C31	3.57	123.10	111.91
2	B	1102	PTY	O7-C8-C11	3.53	119.12	111.50
3	B	1101	ERY	C16-C15-C14	-3.38	109.20	115.07
2	B	1105	PTY	C6-O7-C8	-3.24	109.81	117.79
2	A	1104	PTY	O4-C30-C31	3.07	121.55	111.91
2	B	1108	PTY	C6-O7-C8	-3.05	110.27	117.79
2	B	1106	PTY	O4-C30-C31	3.02	121.37	111.91
3	B	1101	ERY	C13-O2-C1	-3.00	112.85	118.18
2	B	1104	PTY	O7-C8-O10	-2.94	116.61	123.70
3	B	1101	ERY	O5-C16-C15	-2.85	108.39	112.96
2	B	1103	PTY	C5-C6-C1	-2.82	105.11	111.79
2	A	1105	PTY	O4-C30-C31	2.74	120.50	111.91
2	B	1102	PTY	O4-C30-C31	2.71	120.42	111.91
3	B	1101	ERY	C22-O7-C5	-2.65	111.65	116.25
3	B	1101	ERY	C34-C10-C11	-2.65	111.08	114.38
2	A	1101	PTY	O4-C30-C31	2.65	120.22	111.91
2	C	1107	PTY	O4-C30-C31	2.60	120.07	111.91
2	B	1105	PTY	O4-C30-C31	2.57	119.96	111.91
2	B	1107	PTY	O4-C30-C31	2.53	119.85	111.91
2	C	1105	PTY	O4-C30-C31	2.48	119.69	111.91
2	A	1104	PTY	O7-C8-O10	-2.43	117.84	123.70
2	A	1102	PTY	O4-C30-C31	2.42	119.50	111.91
3	B	1101	ERY	O4-C14-C15	-2.42	107.52	112.12

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1104	PTY	C6-O7-C8	-2.41	111.87	117.79
2	A	1101	PTY	C6-O7-C8	-2.39	111.90	117.79
2	C	1103	PTY	O4-C30-O30	-2.38	117.57	123.59
2	A	1103	PTY	O7-C8-O10	-2.36	117.99	123.70
2	C	1106	PTY	O4-C30-C31	2.34	119.24	111.91
2	B	1107	PTY	O4-C1-C6	2.32	115.20	108.43
3	B	1101	ERY	C6-C7-C8	-2.29	110.49	115.38
2	B	1104	PTY	O4-C30-C31	2.28	119.07	111.91
3	B	1101	ERY	O2-C1-O1	-2.28	119.68	123.94
2	B	1108	PTY	C32-C31-C30	-2.27	105.38	113.62
2	C	1102	PTY	O4-C30-C31	2.23	118.91	111.91
3	B	1101	ERY	C25-C24-N1	-2.19	109.49	115.67
2	C	1102	PTY	C6-O7-C8	-2.17	112.44	117.79
2	B	1109	PTY	O7-C8-O10	-2.17	118.47	123.70
2	A	1104	PTY	O4-C30-O30	-2.15	118.18	123.59
2	A	1102	PTY	C6-O7-C8	-2.13	112.54	117.79
2	C	1104	PTY	O4-C30-C31	2.09	118.45	111.91
2	B	1107	PTY	O7-C8-O10	-2.09	118.66	123.70
2	C	1101	PTY	O4-C30-C31	2.07	118.40	111.91
2	A	1104	PTY	C6-O7-C8	-2.06	112.71	117.79
2	C	1101	PTY	C32-C31-C30	-2.06	106.12	113.62
2	B	1102	PTY	O4-C30-O30	-2.06	118.39	123.59
2	C	1109	PTY	O7-C8-C11	2.06	120.65	114.03
2	B	1103	PTY	O4-C30-C31	2.04	118.30	111.91
2	A	1102	PTY	O7-C8-O10	-2.00	118.86	123.70

There are no chirality outliers.

All (357) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1101	PTY	N1-C2-C3-O11
2	A	1101	PTY	C3-O11-P1-O13
2	A	1103	PTY	N1-C2-C3-O11
2	A	1103	PTY	C3-O11-P1-O13
2	A	1104	PTY	O10-C8-O7-C6
2	A	1104	PTY	C3-O11-P1-O13
2	A	1104	PTY	C5-O14-P1-O12
2	A	1105	PTY	C3-O11-P1-O12
2	A	1105	PTY	C3-O11-P1-O13
2	A	1105	PTY	C3-O11-P1-O14
2	A	1106	PTY	C5-C6-O7-C8
2	A	1106	PTY	C3-O11-P1-O12

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	B	1102	PTY	C3-O11-P1-O12
2	B	1102	PTY	C3-O11-P1-O13
2	B	1102	PTY	C3-O11-P1-O14
2	B	1102	PTY	C5-O14-P1-O13
2	B	1104	PTY	N1-C2-C3-O11
2	B	1104	PTY	C11-C8-O7-C6
2	B	1104	PTY	C3-O11-P1-O13
2	B	1105	PTY	O10-C8-O7-C6
2	B	1105	PTY	C3-O11-P1-O12
2	B	1105	PTY	C3-O11-P1-O13
2	B	1105	PTY	C3-O11-P1-O14
2	B	1106	PTY	C3-O11-P1-O13
2	B	1107	PTY	O10-C8-O7-C6
2	B	1108	PTY	C5-O14-P1-O12
2	B	1109	PTY	N1-C2-C3-O11
2	B	1109	PTY	O10-C8-O7-C6
2	B	1109	PTY	C11-C8-O7-C6
2	B	1109	PTY	C3-O11-P1-O12
2	B	1109	PTY	C3-O11-P1-O13
2	B	1109	PTY	C5-O14-P1-O13
2	C	1101	PTY	C3-O11-P1-O13
2	C	1101	PTY	C5-O14-P1-O13
2	C	1102	PTY	N1-C2-C3-O11
2	C	1102	PTY	C11-C8-O7-C6
2	C	1102	PTY	C3-O11-P1-O12
2	C	1102	PTY	C3-O11-P1-O13
2	C	1102	PTY	C3-O11-P1-O14
2	C	1103	PTY	C3-O11-P1-O13
2	C	1104	PTY	C3-O11-P1-O13
2	C	1105	PTY	N1-C2-C3-O11
2	C	1107	PTY	N1-C2-C3-O11
2	C	1107	PTY	O10-C8-O7-C6
2	C	1107	PTY	C11-C8-O7-C6
2	C	1107	PTY	C3-O11-P1-O13
2	C	1107	PTY	C5-O14-P1-O12
3	B	1101	ERY	C1-C2-C3-C4
3	B	1101	ERY	C30-C2-C3-O3
3	B	1101	ERY	C3-C4-C5-C6
3	B	1101	ERY	C3-C4-C5-O7
3	B	1101	ERY	C4-C5-C6-C7
3	B	1101	ERY	C4-C5-C6-C32
3	B	1101	ERY	C4-C5-C6-O10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
3	B	1101	ERY	O7-C5-C6-C7
3	B	1101	ERY	O7-C5-C6-C32
3	B	1101	ERY	O7-C5-C6-O10
3	B	1101	ERY	C6-C7-C8-C9
3	B	1101	ERY	C7-C8-C9-C10
3	B	1101	ERY	C7-C8-C9-O11
3	B	1101	ERY	C17-C16-O5-C20
2	C	1101	PTY	C31-C30-O4-C1
2	B	1103	PTY	O30-C30-O4-C1
2	B	1107	PTY	O30-C30-O4-C1
2	C	1101	PTY	O30-C30-O4-C1
2	B	1104	PTY	O10-C8-O7-C6
2	B	1107	PTY	C31-C30-O4-C1
2	A	1104	PTY	C11-C8-O7-C6
2	B	1105	PTY	C11-C8-O7-C6
2	B	1107	PTY	C11-C8-O7-C6
2	B	1103	PTY	C31-C30-O4-C1
2	C	1102	PTY	O10-C8-O7-C6
2	A	1106	PTY	C11-C8-O7-C6
2	C	1106	PTY	C19-C20-C21-C22
2	A	1105	PTY	C6-C5-O14-P1
2	A	1106	PTY	O10-C8-O7-C6
2	C	1105	PTY	C31-C30-O4-C1
2	A	1103	PTY	C35-C36-C37-C38
2	B	1107	PTY	C24-C25-C26-C27
2	B	1107	PTY	C30-C31-C32-C33
2	C	1105	PTY	O30-C30-O4-C1
2	A	1101	PTY	C30-C31-C32-C33
2	A	1106	PTY	C30-C31-C32-C33
2	C	1105	PTY	C30-C31-C32-C33
2	B	1103	PTY	C8-C11-C12-C13
2	B	1105	PTY	C30-C31-C32-C33
2	C	1104	PTY	C31-C30-O4-C1
2	C	1104	PTY	O30-C30-O4-C1
3	B	1101	ERY	C2-C3-C4-C31
3	B	1101	ERY	C2-C3-C4-C5
2	A	1102	PTY	C31-C32-C33-C34
2	A	1102	PTY	C8-C11-C12-C13
2	B	1102	PTY	C11-C8-O7-C6
2	B	1107	PTY	C22-C23-C24-C25
2	A	1101	PTY	C3-O11-P1-O14
2	A	1103	PTY	C3-O11-P1-O14

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	A	1104	PTY	C5-O14-P1-O11
2	A	1106	PTY	C3-O11-P1-O14
2	B	1102	PTY	C5-O14-P1-O11
2	B	1104	PTY	C3-O11-P1-O14
2	B	1106	PTY	C3-O11-P1-O14
2	B	1107	PTY	C3-O11-P1-O14
2	B	1107	PTY	C5-O14-P1-O11
2	B	1108	PTY	C5-O14-P1-O11
2	B	1109	PTY	C3-O11-P1-O14
2	B	1109	PTY	C5-O14-P1-O11
2	C	1101	PTY	C5-O14-P1-O11
2	C	1104	PTY	C3-O11-P1-O14
2	C	1105	PTY	C3-O11-P1-O14
2	C	1107	PTY	C5-O14-P1-O11
2	B	1102	PTY	O10-C8-O7-C6
3	B	1101	ERY	O2-C13-C36-C37
2	B	1104	PTY	C19-C20-C21-C22
2	A	1102	PTY	C23-C24-C25-C26
2	B	1107	PTY	C34-C35-C36-C37
2	C	1101	PTY	C16-C17-C18-C19
3	B	1101	ERY	O3-C3-C4-C31
3	B	1101	ERY	O3-C3-C4-C5
2	A	1101	PTY	C11-C8-O7-C6
2	A	1102	PTY	N1-C2-C3-O11
2	A	1105	PTY	N1-C2-C3-O11
2	B	1106	PTY	N1-C2-C3-O11
2	B	1105	PTY	C8-C11-C12-C13
2	B	1108	PTY	C8-C11-C12-C13
2	A	1103	PTY	C16-C17-C18-C19
2	B	1102	PTY	C32-C33-C34-C35
2	C	1105	PTY	C32-C33-C34-C35
2	A	1103	PTY	C22-C23-C24-C25
3	B	1101	ERY	C15-C16-O5-C20
2	A	1104	PTY	C11-C12-C13-C14
2	B	1107	PTY	C14-C15-C16-C17
2	A	1101	PTY	C25-C26-C27-C28
2	A	1101	PTY	O10-C8-O7-C6
2	C	1101	PTY	C12-C13-C14-C15
2	C	1106	PTY	C36-C37-C38-C39
2	B	1106	PTY	C11-C8-O7-C6
3	B	1101	ERY	C31-C4-C5-C6
2	B	1107	PTY	C40-C41-C42-C43

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	A	1103	PTY	O10-C8-O7-C6
2	A	1104	PTY	C34-C35-C36-C37
2	C	1102	PTY	C30-C31-C32-C33
2	C	1103	PTY	C8-C11-C12-C13
2	A	1103	PTY	C11-C8-O7-C6
2	C	1106	PTY	C11-C8-O7-C6
2	A	1105	PTY	C40-C41-C42-C43
3	B	1101	ERY	C35-C12-C13-O2
3	B	1101	ERY	C35-C12-C13-C36
3	B	1101	ERY	O13-C12-C13-C36
2	C	1106	PTY	C30-C31-C32-C33
3	B	1101	ERY	C11-C12-C13-C36
2	B	1106	PTY	O10-C8-O7-C6
2	C	1106	PTY	O10-C8-O7-C6
2	A	1104	PTY	C3-O11-P1-O14
2	C	1107	PTY	C3-O11-P1-O14
2	B	1108	PTY	C12-C13-C14-C15
2	A	1105	PTY	O14-C5-C6-C1
2	C	1101	PTY	C22-C23-C24-C25
2	C	1106	PTY	C14-C15-C16-C17
2	B	1105	PTY	C31-C32-C33-C34
2	B	1108	PTY	O4-C1-C6-C5
2	C	1107	PTY	C32-C33-C34-C35
2	C	1103	PTY	C33-C34-C35-C36
2	A	1101	PTY	C31-C32-C33-C34
2	C	1106	PTY	C35-C36-C37-C38
2	C	1102	PTY	C8-C11-C12-C13
2	B	1103	PTY	C14-C15-C16-C17
2	B	1109	PTY	C30-C31-C32-C33
2	C	1106	PTY	C22-C23-C24-C25
2	B	1107	PTY	C13-C14-C15-C16
2	C	1109	PTY	C15-C16-C17-C18
2	C	1101	PTY	C14-C15-C16-C17
2	C	1107	PTY	C40-C41-C42-C43
2	C	1109	PTY	C19-C20-C21-C22
2	C	1102	PTY	C31-C30-O4-C1
2	B	1108	PTY	C11-C12-C13-C14
2	C	1103	PTY	O4-C1-C6-O7
2	C	1106	PTY	C31-C32-C33-C34
2	C	1107	PTY	C31-C32-C33-C34
2	C	1107	PTY	C37-C38-C39-C40
2	B	1102	PTY	O14-C5-C6-C1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	C	1103	PTY	O14-C5-C6-C1
2	C	1105	PTY	O14-C5-C6-C1
2	A	1105	PTY	C30-C31-C32-C33
2	B	1105	PTY	N1-C2-C3-O11
2	B	1104	PTY	C31-C30-O4-C1
2	A	1101	PTY	C8-C11-C12-C13
2	A	1106	PTY	C20-C21-C22-C23
2	A	1104	PTY	C14-C15-C16-C17
2	B	1105	PTY	O4-C1-C6-C5
2	C	1103	PTY	C11-C12-C13-C14
3	B	1101	ERY	C4-C5-O7-C22
2	A	1103	PTY	C15-C16-C17-C18
2	C	1103	PTY	C3-O11-P1-O14
2	B	1109	PTY	C37-C38-C39-C40
2	A	1105	PTY	O14-C5-C6-O7
2	C	1102	PTY	O30-C30-O4-C1
2	C	1104	PTY	C17-C18-C19-C20
2	A	1103	PTY	C23-C24-C25-C26
2	A	1103	PTY	C31-C30-O4-C1
2	B	1108	PTY	C11-C8-O7-C6
2	B	1104	PTY	C16-C17-C18-C19
2	B	1108	PTY	O10-C8-O7-C6
2	C	1104	PTY	C16-C17-C18-C19
2	A	1101	PTY	C12-C13-C14-C15
2	A	1103	PTY	C30-C31-C32-C33
2	C	1106	PTY	C33-C34-C35-C36
2	B	1104	PTY	O14-C5-C6-C1
2	A	1104	PTY	C35-C36-C37-C38
2	B	1108	PTY	C17-C18-C19-C20
2	C	1102	PTY	C19-C20-C21-C22
2	B	1109	PTY	C16-C17-C18-C19
2	B	1107	PTY	C38-C39-C40-C41
2	A	1106	PTY	C17-C18-C19-C20
2	C	1109	PTY	C16-C17-C18-C19
2	C	1105	PTY	C11-C12-C13-C14
2	C	1107	PTY	C21-C22-C23-C24
2	B	1109	PTY	C12-C13-C14-C15
2	A	1104	PTY	O4-C1-C6-C5
2	A	1105	PTY	O4-C1-C6-C5
2	B	1102	PTY	O14-C5-C6-O7
2	A	1103	PTY	O30-C30-O4-C1
2	B	1104	PTY	O30-C30-O4-C1

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	B	1107	PTY	C23-C24-C25-C26
2	A	1101	PTY	C23-C24-C25-C26
3	B	1101	ERY	C11-C12-C13-O2
2	A	1104	PTY	C30-C31-C32-C33
3	B	1101	ERY	C12-C13-O2-C1
2	B	1109	PTY	C36-C37-C38-C39
2	A	1104	PTY	C33-C34-C35-C36
2	C	1101	PTY	C3-O11-P1-O14
2	B	1103	PTY	C16-C17-C18-C19
2	B	1105	PTY	C39-C40-C41-C42
2	A	1101	PTY	C3-O11-P1-O12
2	A	1103	PTY	C3-O11-P1-O12
2	A	1104	PTY	C3-O11-P1-O12
2	B	1102	PTY	C5-O14-P1-O12
2	B	1104	PTY	C3-O11-P1-O12
2	B	1106	PTY	C3-O11-P1-O12
2	B	1107	PTY	C3-O11-P1-O13
2	B	1107	PTY	C5-O14-P1-O13
2	B	1109	PTY	C5-O14-P1-O12
2	C	1101	PTY	C5-O14-P1-O12
2	C	1104	PTY	C3-O11-P1-O12
2	C	1105	PTY	C3-O11-P1-O12
2	C	1105	PTY	C3-O11-P1-O13
2	B	1109	PTY	C13-C14-C15-C16
2	A	1104	PTY	C12-C13-C14-C15
2	C	1105	PTY	O14-C5-C6-O7
2	A	1101	PTY	C32-C33-C34-C35
2	A	1105	PTY	C31-C32-C33-C34
2	C	1106	PTY	C15-C16-C17-C18
2	B	1105	PTY	O4-C1-C6-O7
2	B	1108	PTY	O4-C1-C6-O7
3	B	1101	ERY	C6-C5-O7-C22
2	B	1108	PTY	C33-C34-C35-C36
2	A	1102	PTY	C11-C12-C13-C14
2	A	1102	PTY	C34-C35-C36-C37
2	C	1109	PTY	C12-C13-C14-C15
2	A	1105	PTY	O10-C8-O7-C6
2	B	1109	PTY	O30-C30-O4-C1
2	C	1102	PTY	C5-C6-O7-C8
3	B	1101	ERY	C6-C7-C8-C33
2	A	1103	PTY	C32-C33-C34-C35
2	A	1103	PTY	C18-C19-C20-C21

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	C	1109	PTY	C14-C15-C16-C17
2	B	1109	PTY	C31-C30-O4-C1
2	C	1103	PTY	O14-C5-C6-O7
3	B	1101	ERY	C12-C13-C36-C37
2	B	1102	PTY	C31-C30-O4-C1
2	A	1105	PTY	C5-O14-P1-O11
2	B	1108	PTY	C3-O11-P1-O14
2	C	1106	PTY	C37-C38-C39-C40
3	B	1101	ERY	C36-C13-O2-C1
2	C	1103	PTY	O4-C1-C6-C5
2	B	1108	PTY	C15-C16-C17-C18
2	B	1109	PTY	O4-C30-C31-C32
2	B	1102	PTY	O30-C30-O4-C1
2	C	1105	PTY	C14-C15-C16-C17
3	B	1101	ERY	C33-C8-C9-C10
2	B	1108	PTY	O14-C5-C6-O7
2	B	1109	PTY	C41-C42-C43-C44
2	C	1105	PTY	C16-C17-C18-C19
2	C	1104	PTY	O4-C1-C6-O7
2	B	1104	PTY	C12-C13-C14-C15
2	C	1105	PTY	C13-C14-C15-C16
2	A	1105	PTY	C41-C42-C43-C44
2	A	1103	PTY	C34-C35-C36-C37
2	C	1108	PTY	O30-C30-C31-C32
2	A	1101	PTY	C18-C19-C20-C21
2	B	1107	PTY	C41-C42-C43-C44
2	C	1107	PTY	C34-C35-C36-C37
2	B	1107	PTY	C1-C6-O7-C8
2	B	1107	PTY	C5-C6-O7-C8
2	B	1104	PTY	C8-C11-C12-C13
2	B	1107	PTY	C36-C37-C38-C39
2	C	1108	PTY	O4-C30-C31-C32
3	B	1101	ERY	C33-C8-C9-O11
2	A	1104	PTY	O4-C1-C6-O7
2	C	1105	PTY	O4-C1-C6-O7
3	B	1101	ERY	C31-C4-C5-O7
2	A	1103	PTY	C13-C14-C15-C16
2	A	1105	PTY	C34-C35-C36-C37
2	B	1104	PTY	C15-C16-C17-C18
2	B	1109	PTY	C31-C32-C33-C34
2	C	1101	PTY	C21-C22-C23-C24
2	B	1108	PTY	O4-C30-C31-C32

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	B	1102	PTY	C35-C36-C37-C38
2	B	1108	PTY	C13-C14-C15-C16
2	A	1101	PTY	C26-C27-C28-C29
2	A	1102	PTY	O10-C8-O7-C6
2	C	1107	PTY	C20-C21-C22-C23
2	B	1106	PTY	C8-C11-C12-C13
2	B	1105	PTY	C35-C36-C37-C38
2	A	1101	PTY	O4-C1-C6-O7
2	C	1101	PTY	C24-C25-C26-C27
2	A	1106	PTY	C31-C32-C33-C34
2	C	1105	PTY	C31-C32-C33-C34
2	C	1101	PTY	C19-C20-C21-C22
2	B	1105	PTY	C12-C11-C8-O7
2	A	1105	PTY	C1-C6-O7-C8
2	B	1104	PTY	C5-C6-O7-C8
2	B	1109	PTY	C35-C36-C37-C38
2	A	1101	PTY	C35-C36-C37-C38
2	A	1106	PTY	C37-C38-C39-C40
2	C	1107	PTY	C18-C19-C20-C21
2	C	1107	PTY	C33-C34-C35-C36
2	A	1104	PTY	C15-C16-C17-C18
2	A	1106	PTY	O14-C5-C6-O7
2	C	1104	PTY	O14-C5-C6-O7
2	B	1103	PTY	C12-C11-C8-O7
2	B	1104	PTY	C20-C21-C22-C23
2	A	1104	PTY	O4-C30-C31-C32
3	B	1101	ERY	O13-C12-C13-O2
2	B	1102	PTY	C12-C11-C8-O7
3	B	1101	ERY	C19-C16-O5-C20
2	A	1105	PTY	C12-C13-C14-C15
2	A	1102	PTY	C11-C8-O7-C6
2	A	1105	PTY	C11-C8-O7-C6
2	A	1102	PTY	C35-C36-C37-C38
2	B	1107	PTY	C39-C40-C41-C42
2	A	1104	PTY	O30-C30-C31-C32
2	B	1105	PTY	C12-C11-C8-O10
2	A	1103	PTY	C6-C5-O14-P1
2	B	1103	PTY	C12-C11-C8-O10
2	A	1102	PTY	C5-O14-P1-O13
2	B	1103	PTY	C5-O14-P1-O13
2	B	1108	PTY	C3-O11-P1-O13
2	C	1101	PTY	O14-C5-C6-C1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	B	1108	PTY	N1-C2-C3-O11
3	B	1101	ERY	C11-C10-C9-C8
2	C	1102	PTY	C12-C11-C8-O7
2	A	1105	PTY	C5-C6-O7-C8
2	C	1101	PTY	C1-C6-O7-C8
2	B	1103	PTY	C30-C31-C32-C33
2	B	1104	PTY	C12-C11-C8-O7
2	C	1107	PTY	O4-C30-C31-C32
2	A	1106	PTY	C16-C17-C18-C19

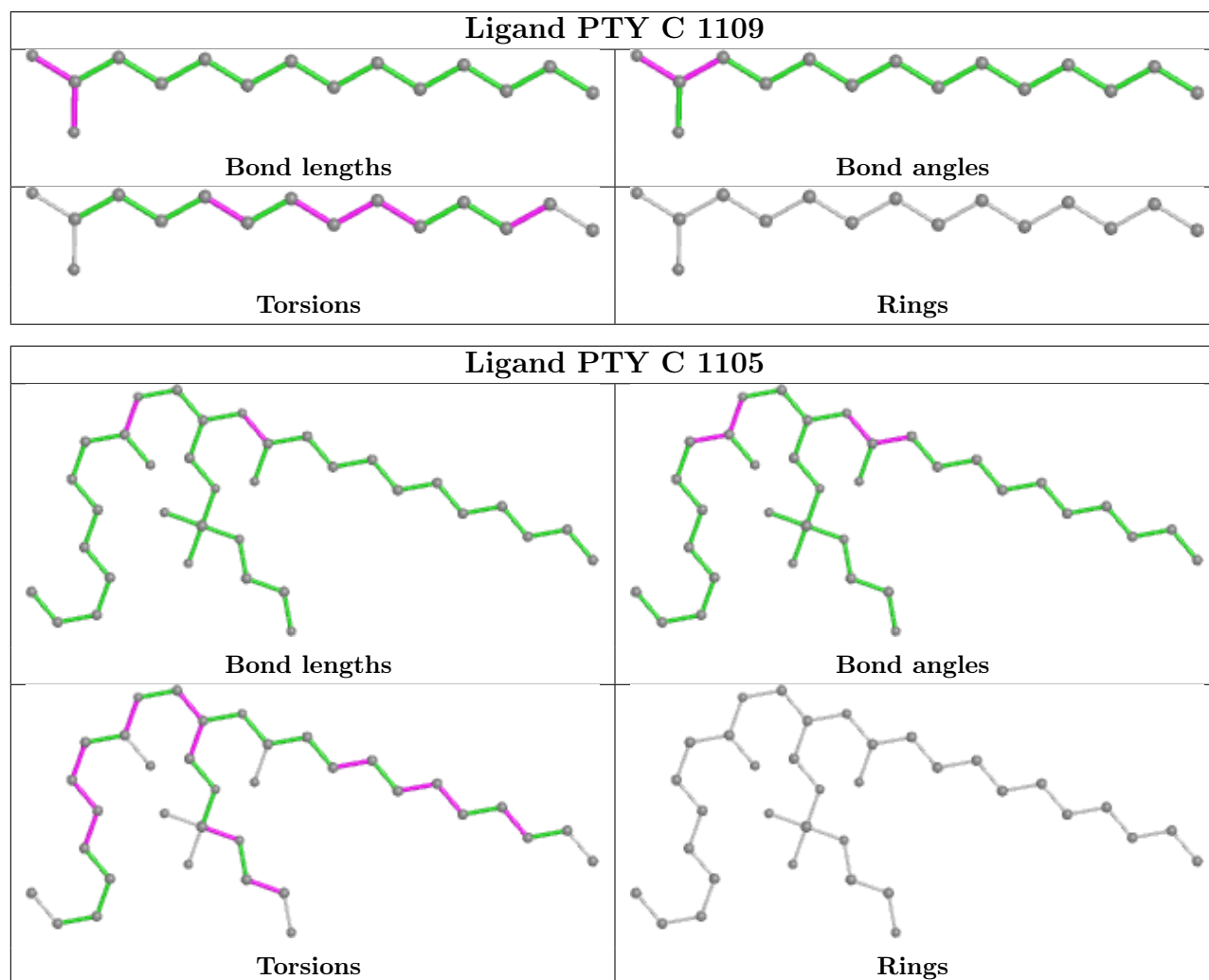
There are no ring outliers.

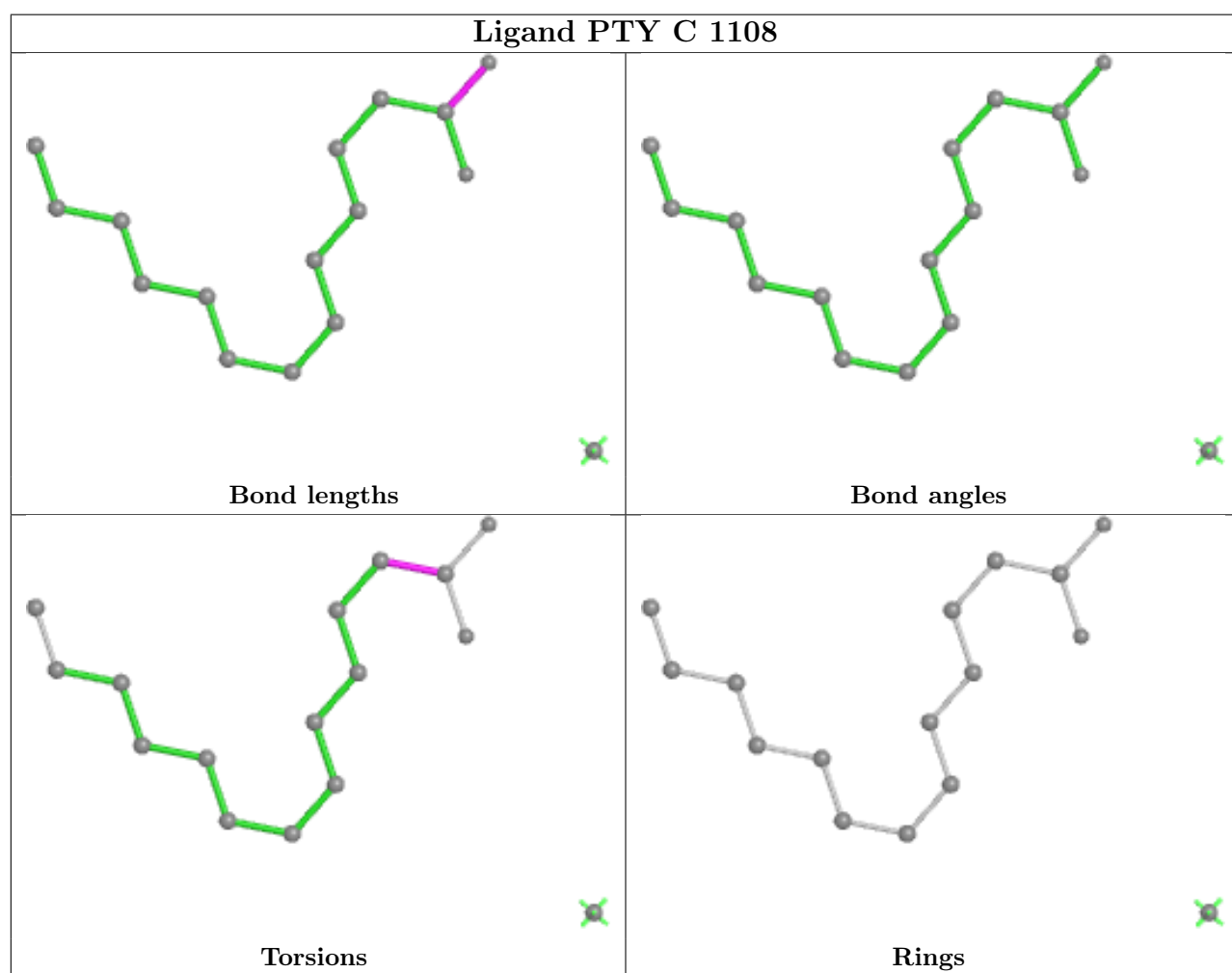
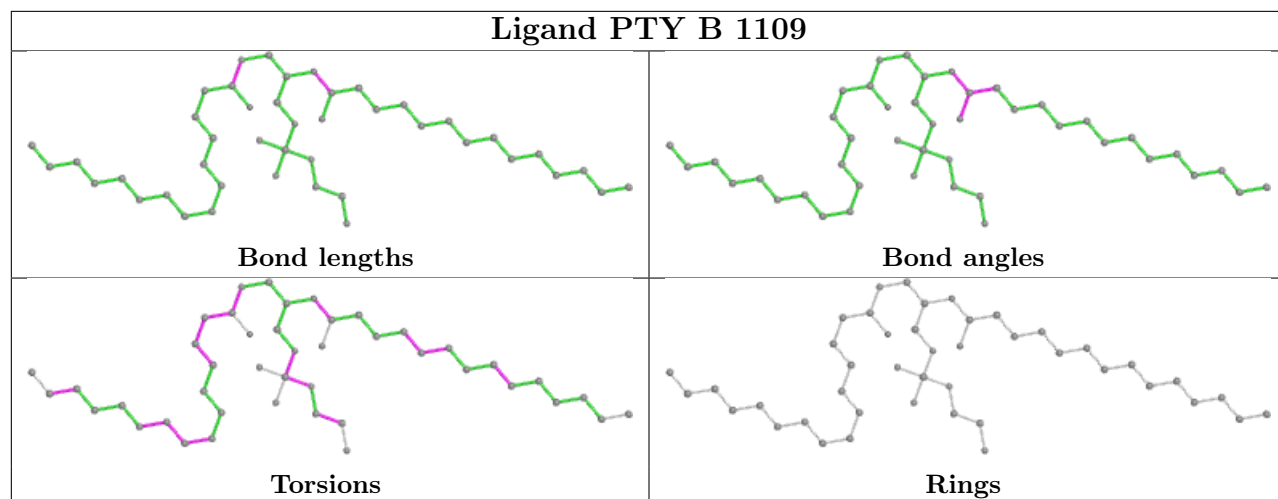
24 monomers are involved in 157 short contacts:

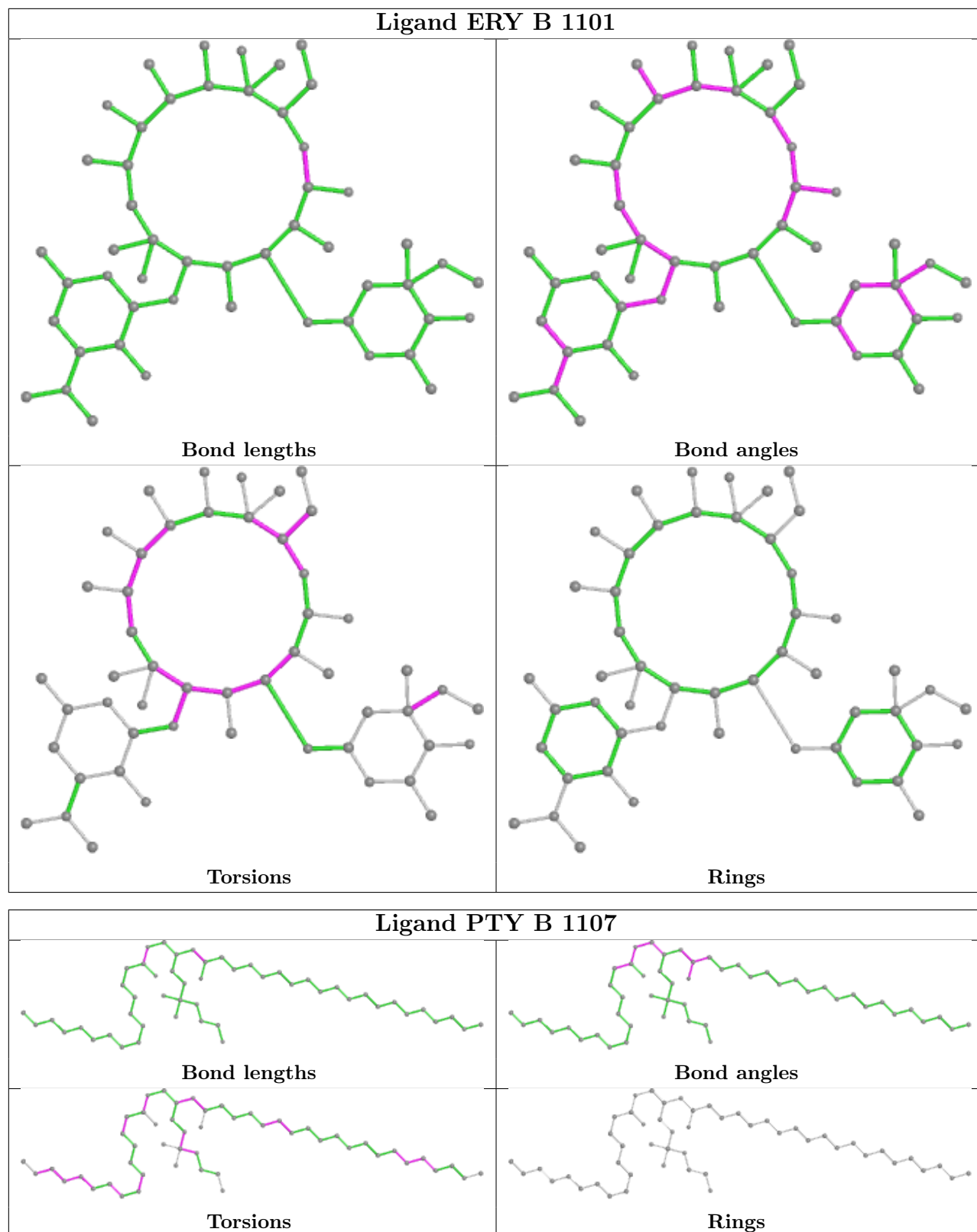
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1109	PTY	3	0
2	C	1105	PTY	9	0
2	B	1109	PTY	2	0
2	C	1108	PTY	3	0
3	B	1101	ERY	41	0
2	B	1107	PTY	2	0
2	C	1107	PTY	5	0
2	A	1103	PTY	9	0
2	B	1103	PTY	8	0
2	B	1106	PTY	12	0
2	C	1104	PTY	2	0
2	B	1108	PTY	7	0
2	C	1103	PTY	2	0
2	C	1106	PTY	21	0
2	A	1101	PTY	4	0
2	A	1105	PTY	9	0
2	B	1104	PTY	12	0
2	A	1102	PTY	4	0
2	A	1106	PTY	7	0
2	A	1104	PTY	7	0
2	B	1102	PTY	1	0
2	C	1101	PTY	20	0
2	B	1105	PTY	8	0
2	C	1102	PTY	1	0

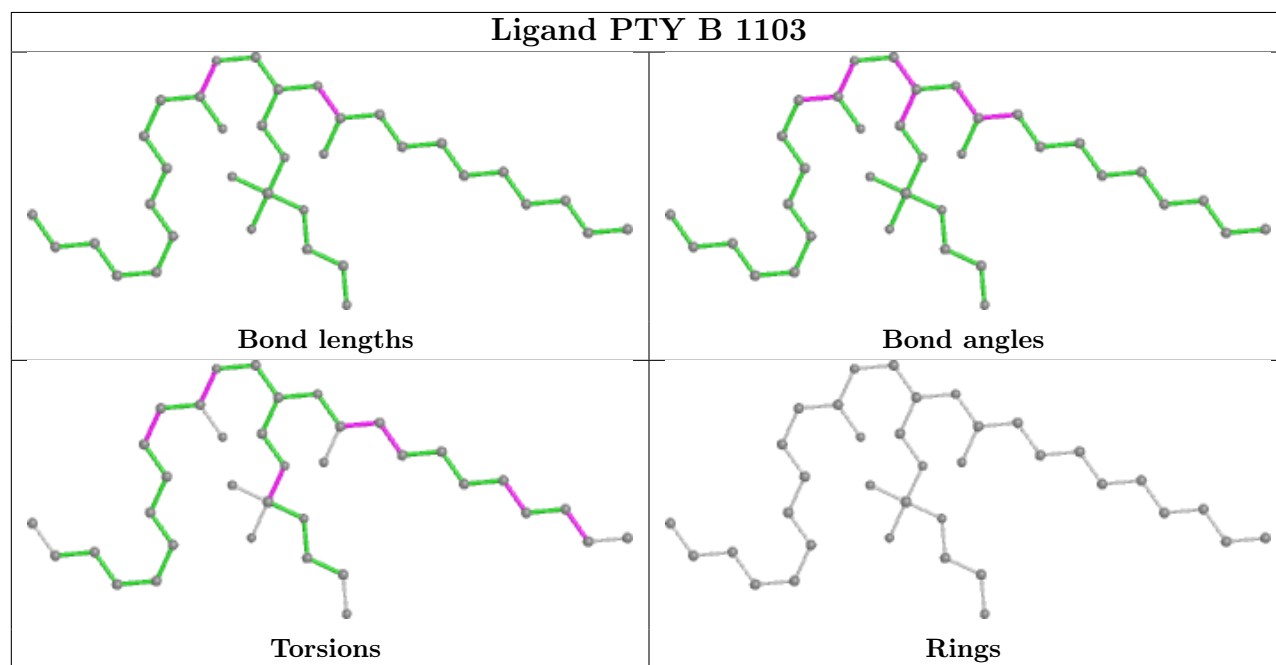
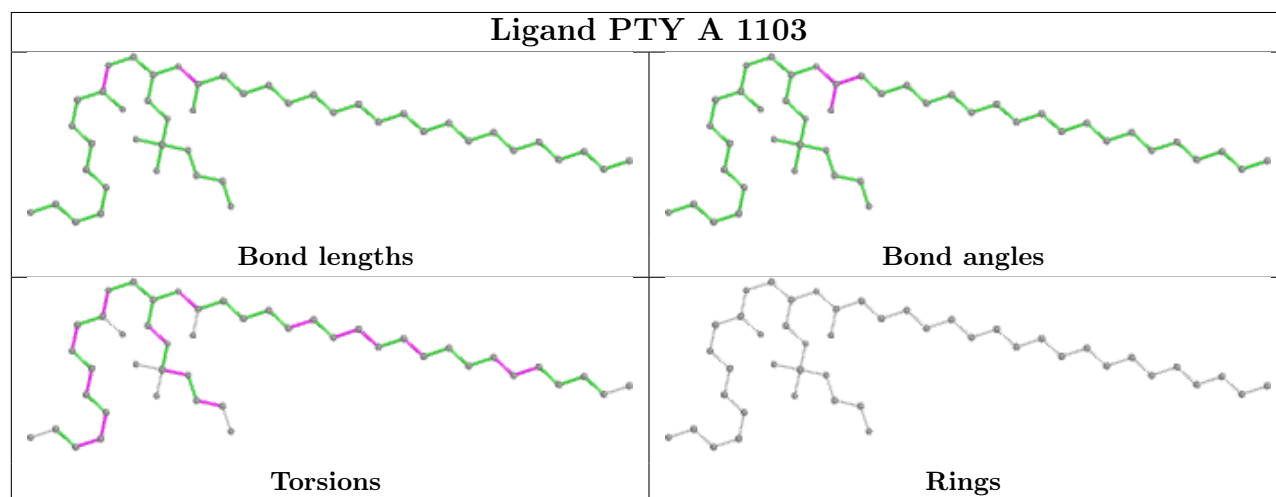
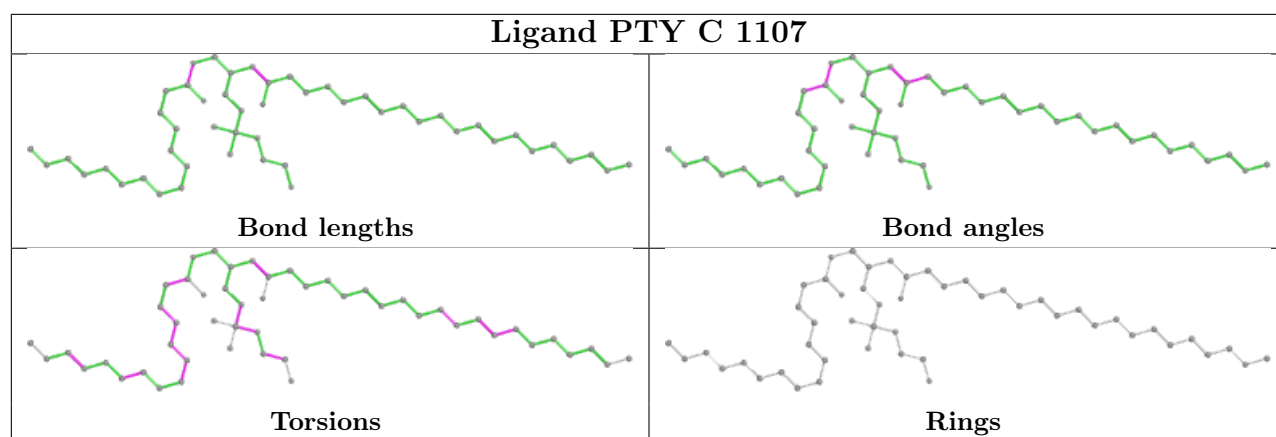
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

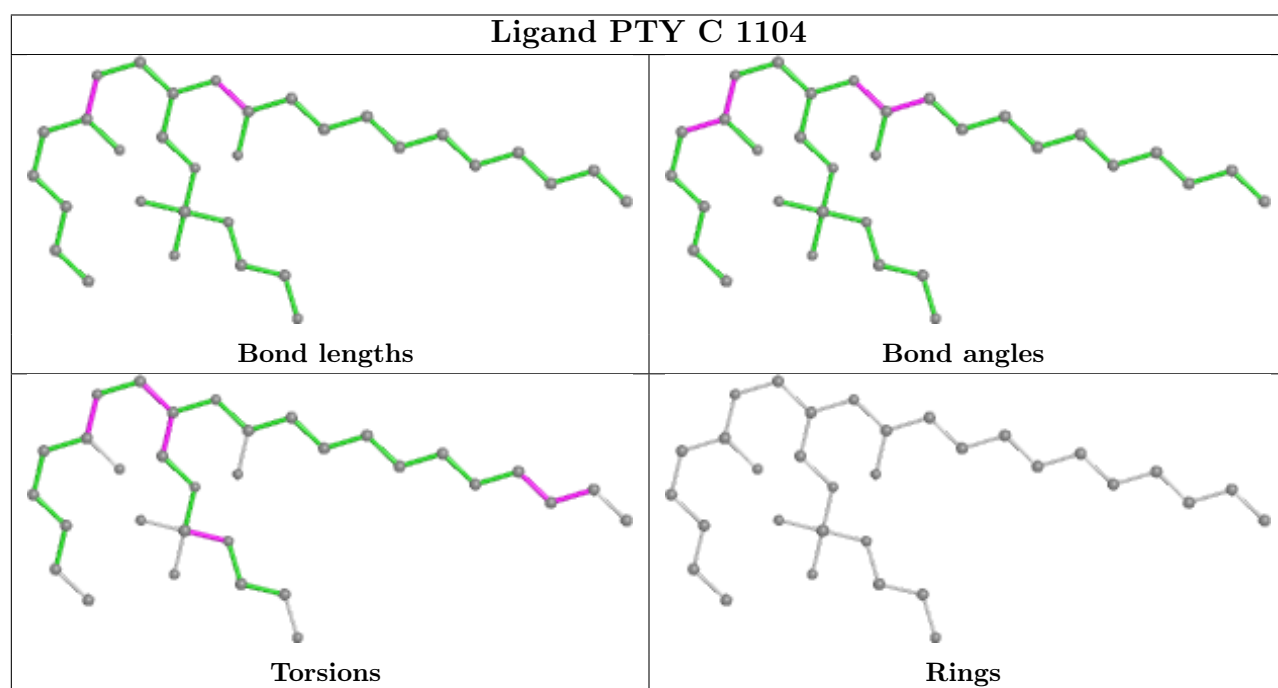
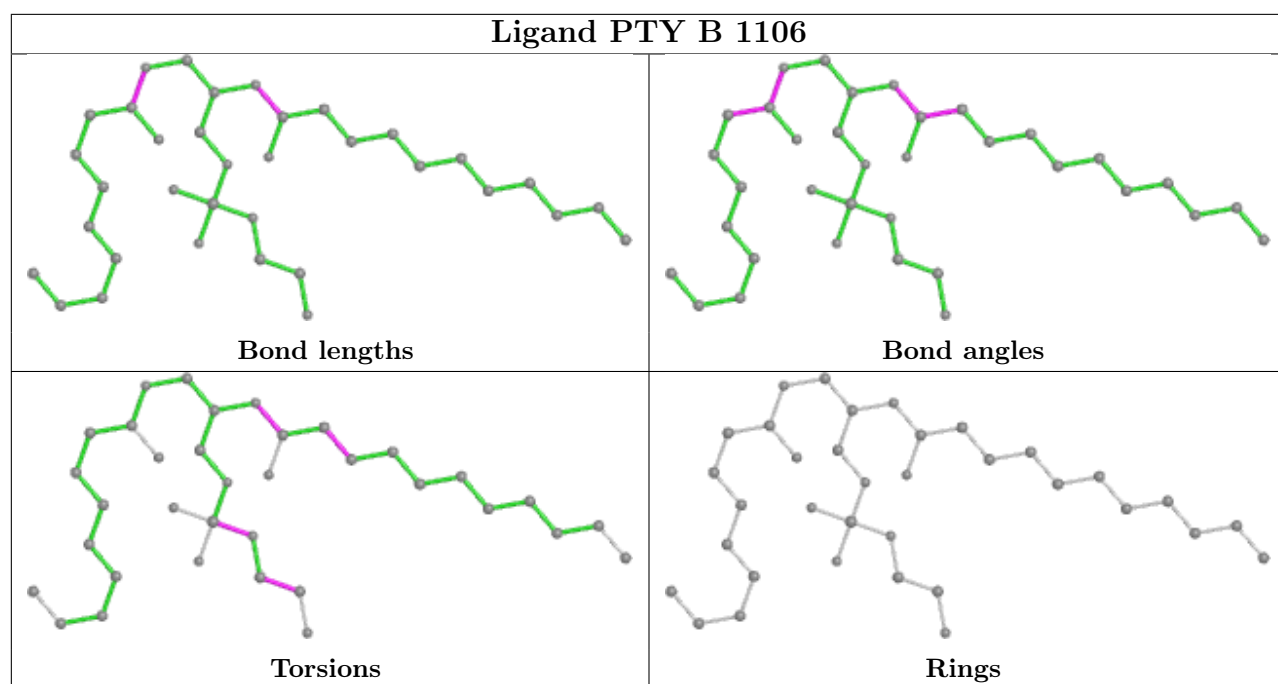


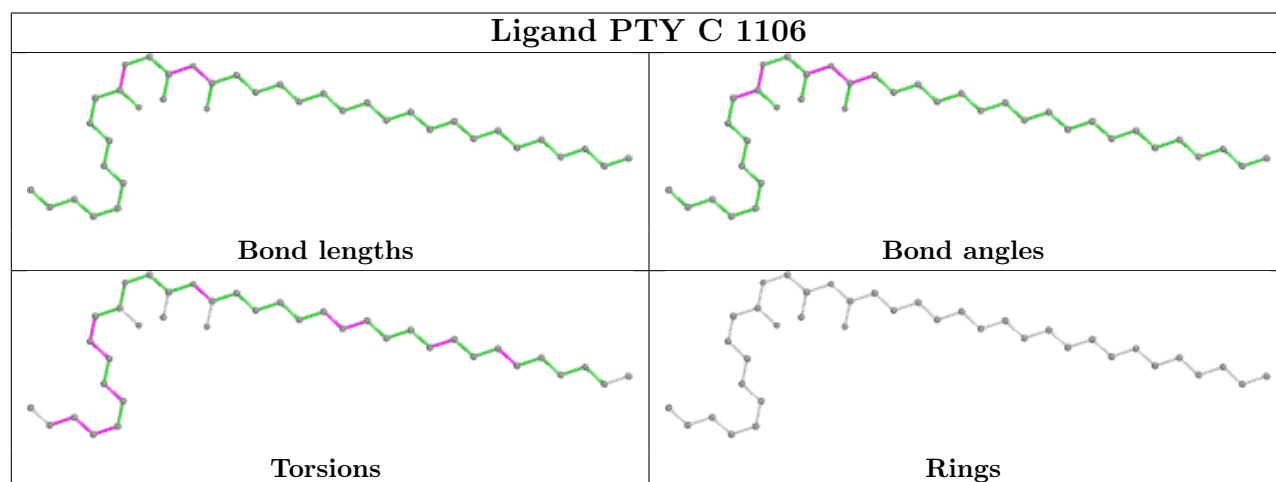
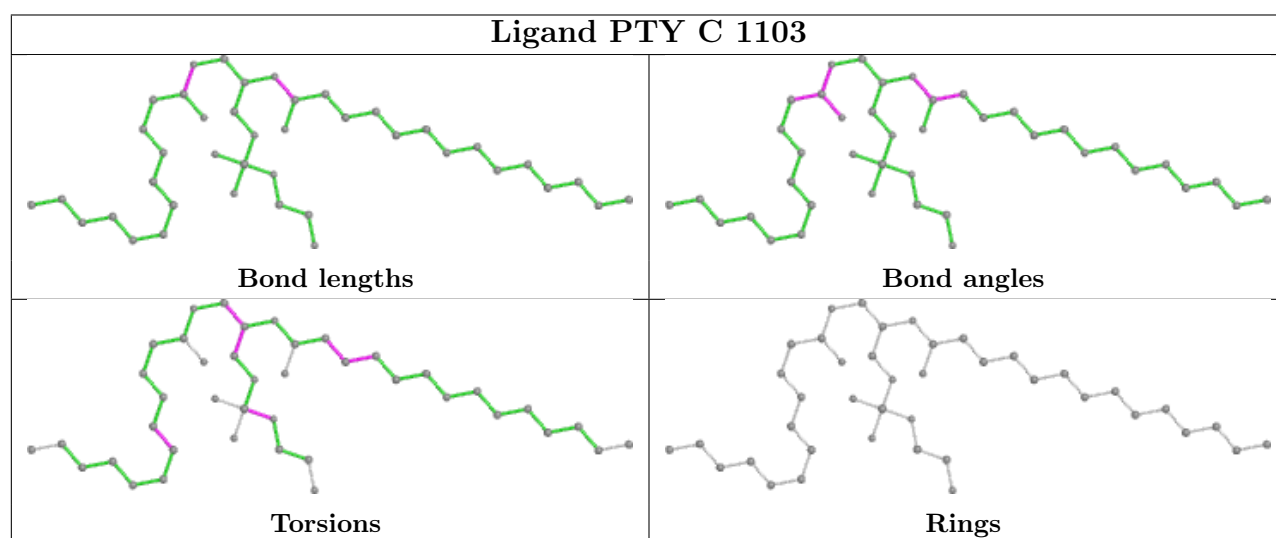
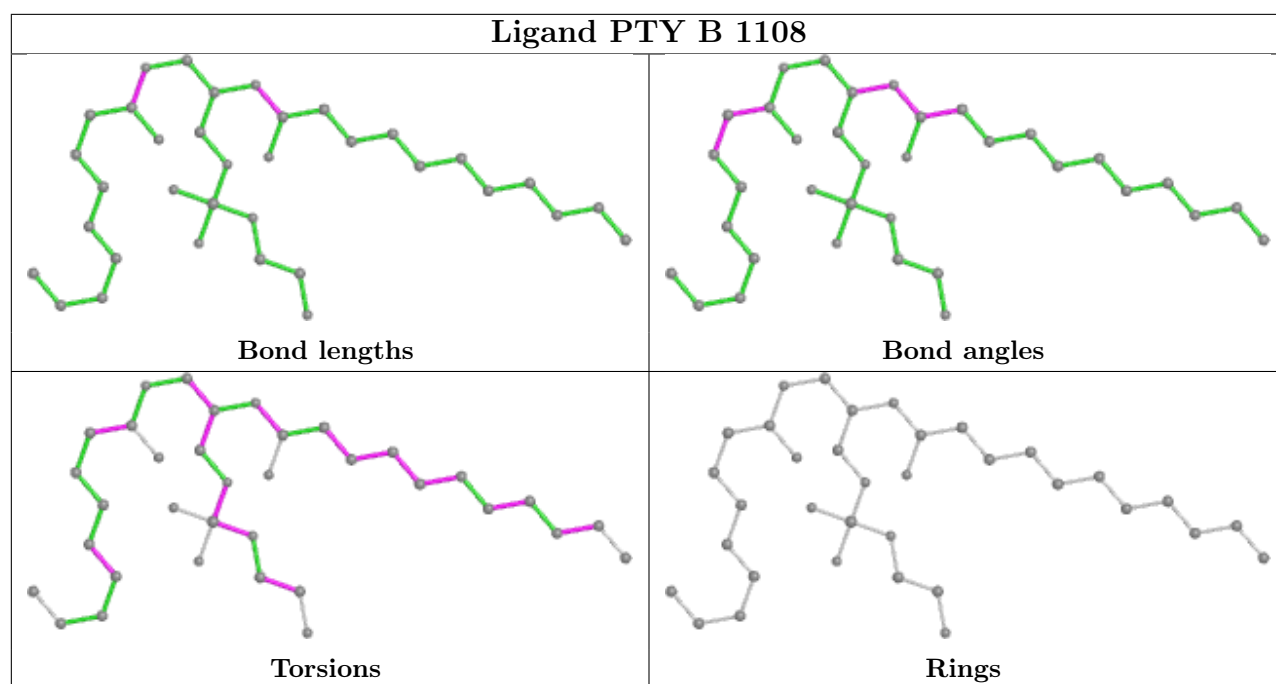


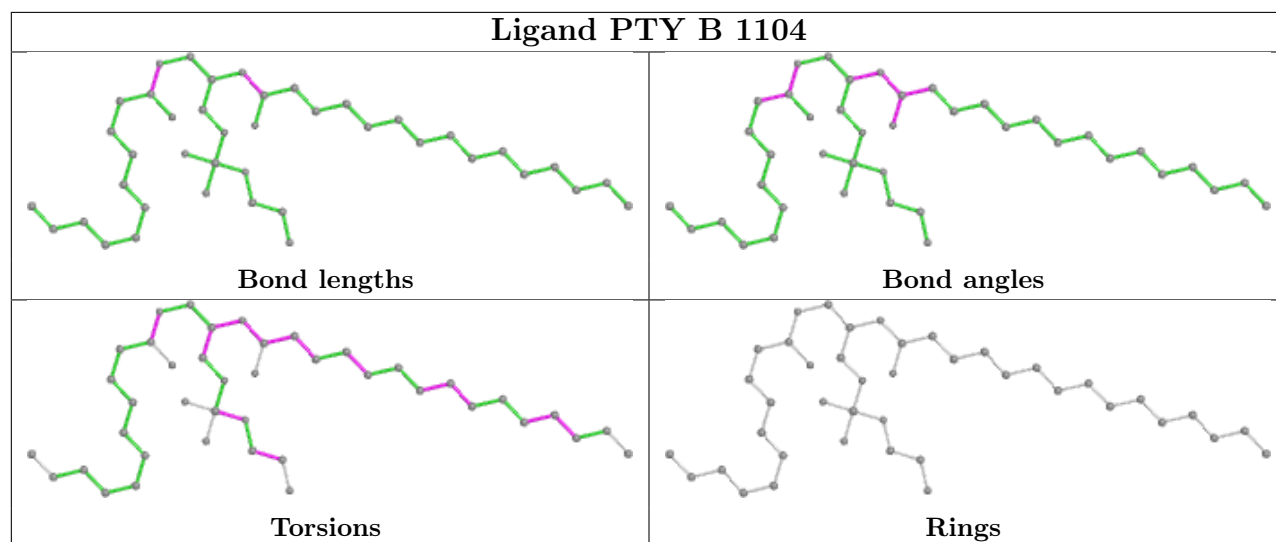
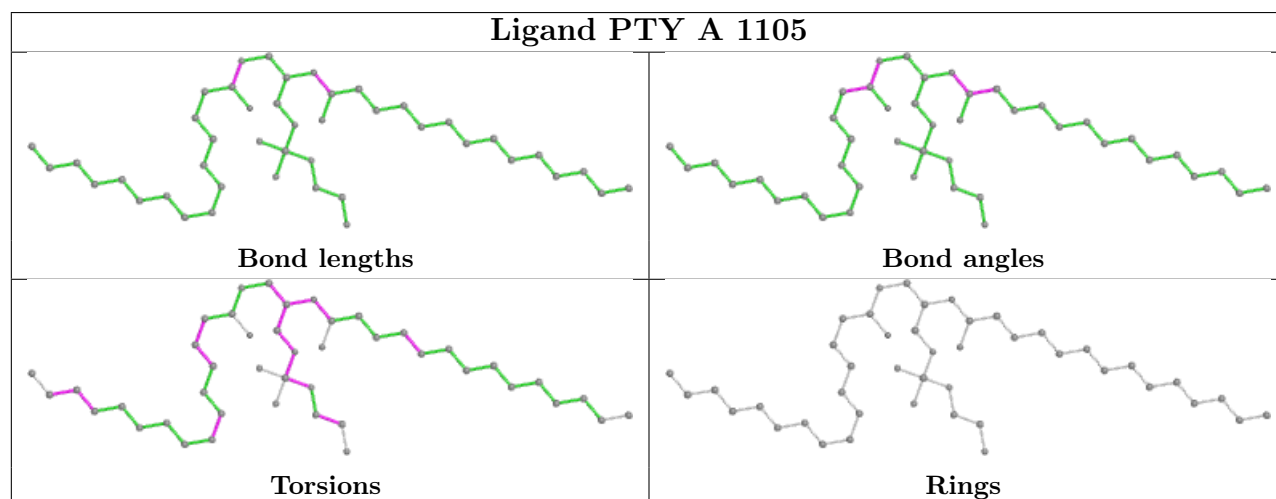
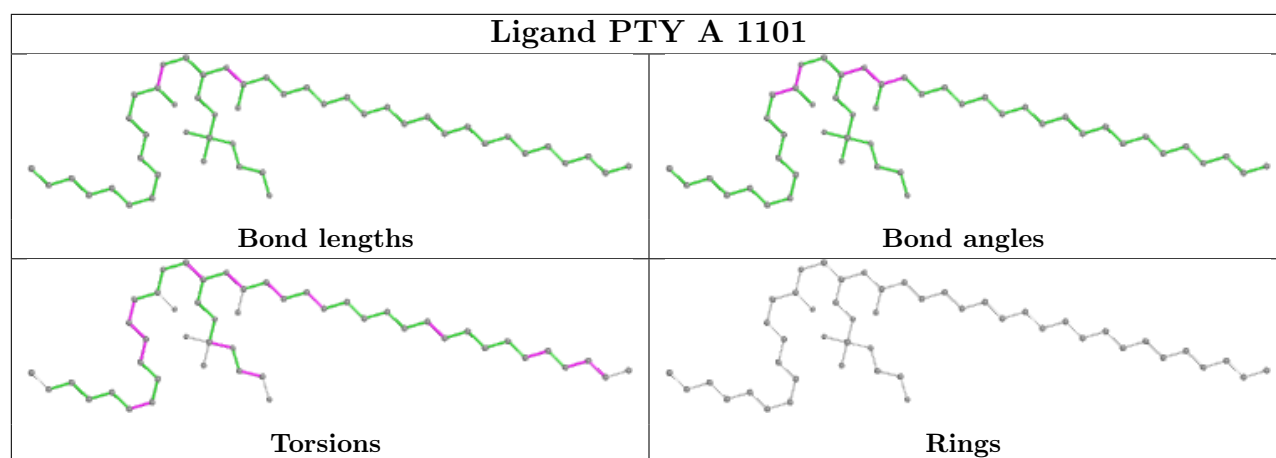




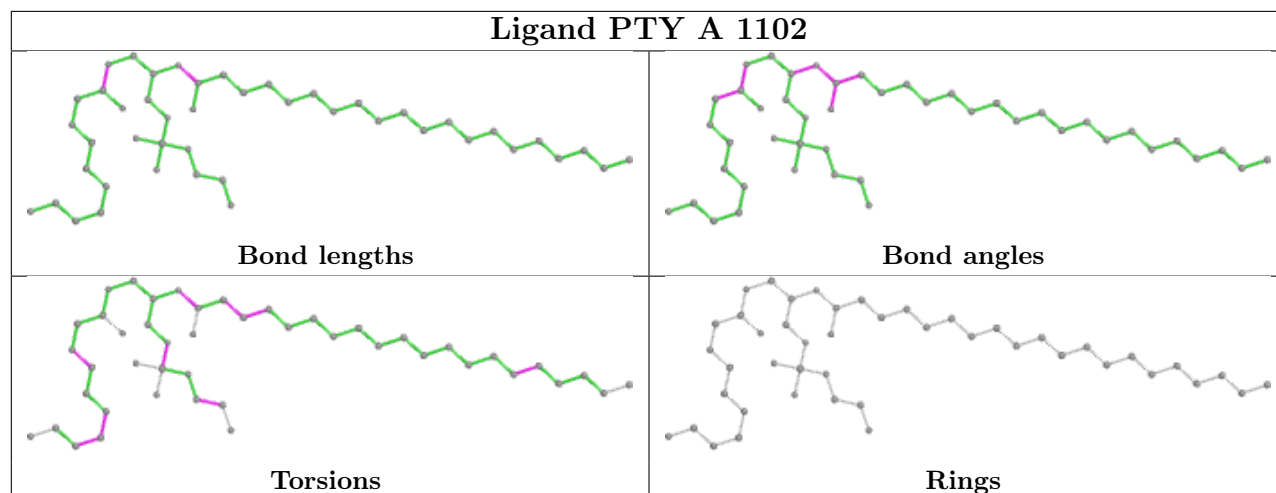




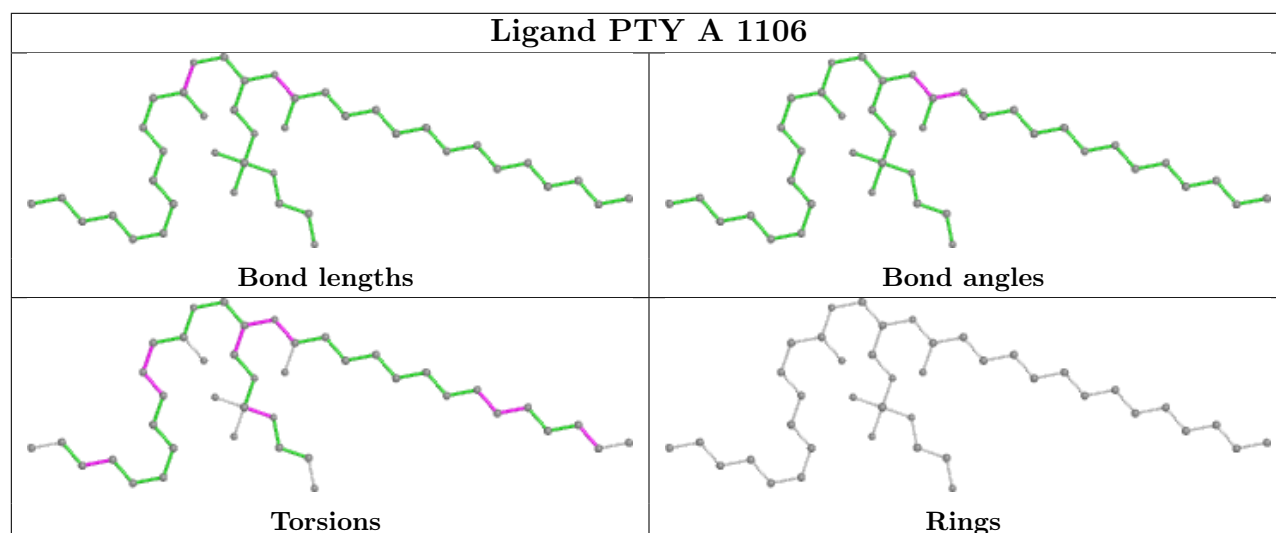




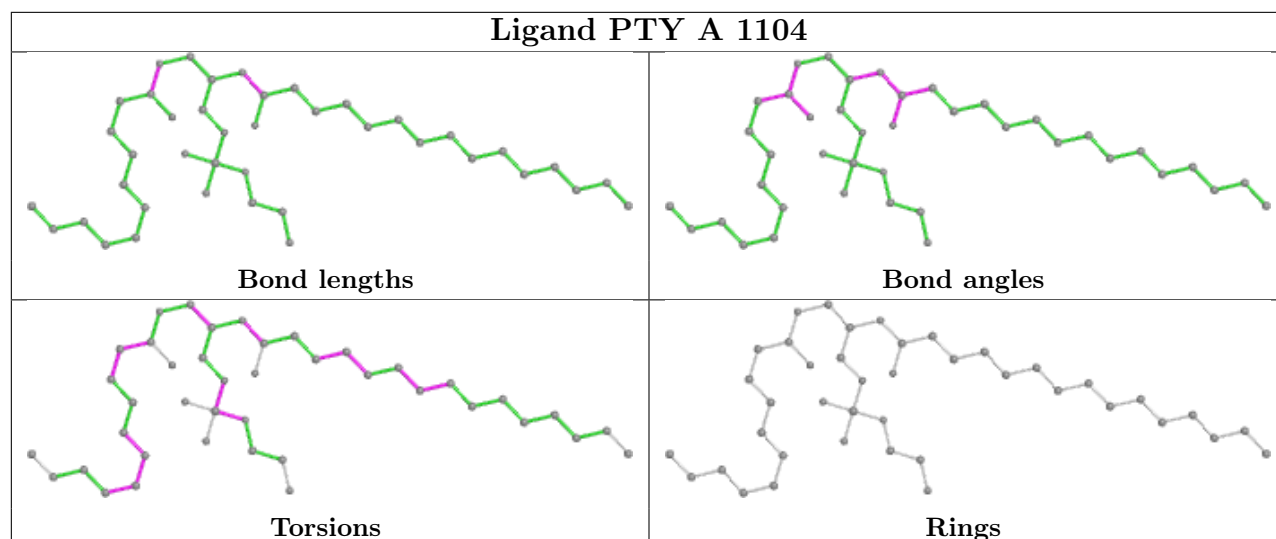
## Ligand PTY A 1102

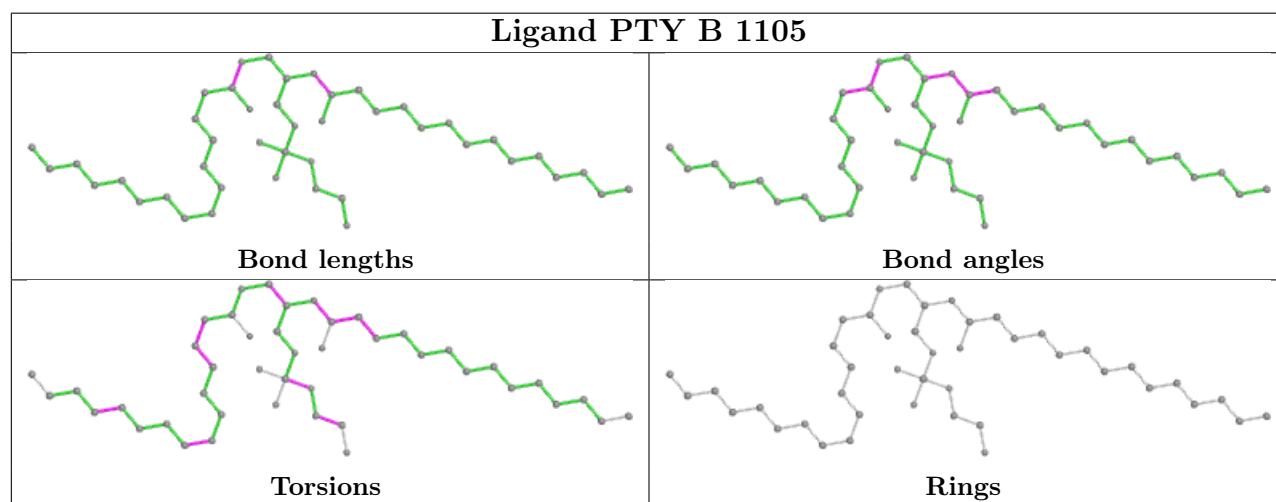
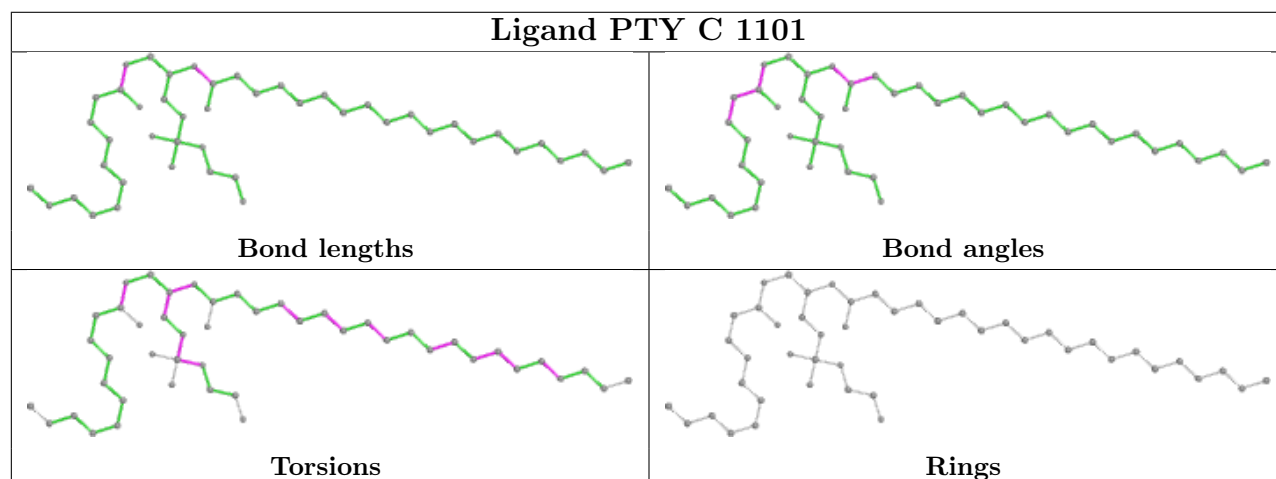
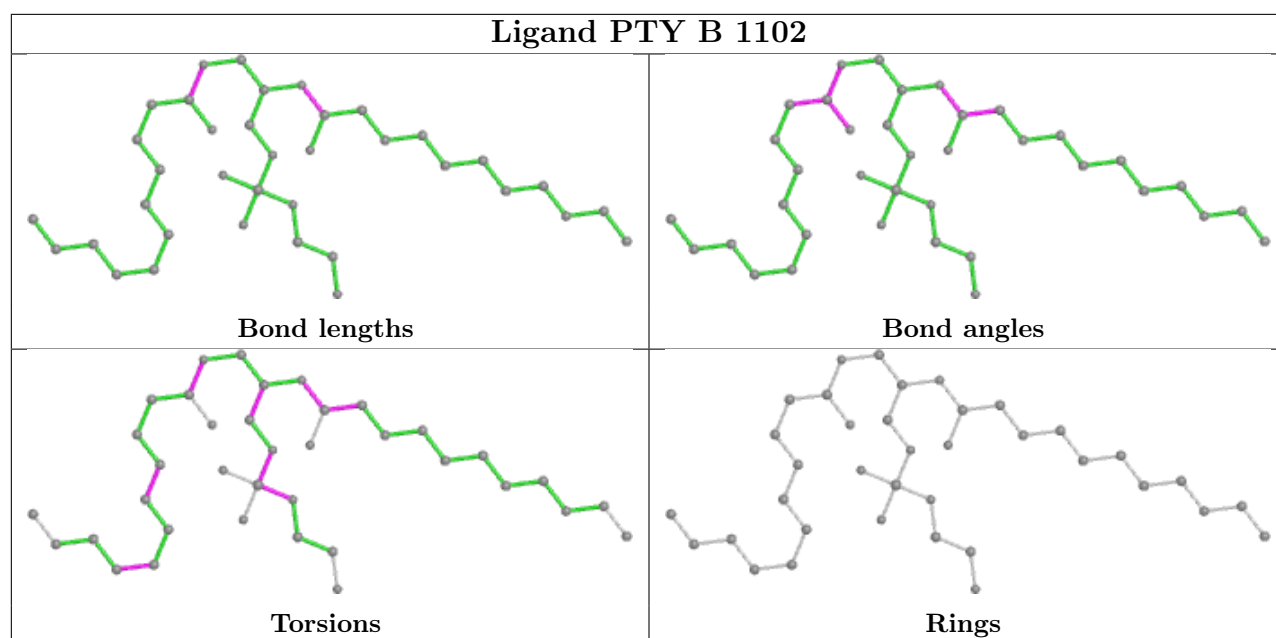


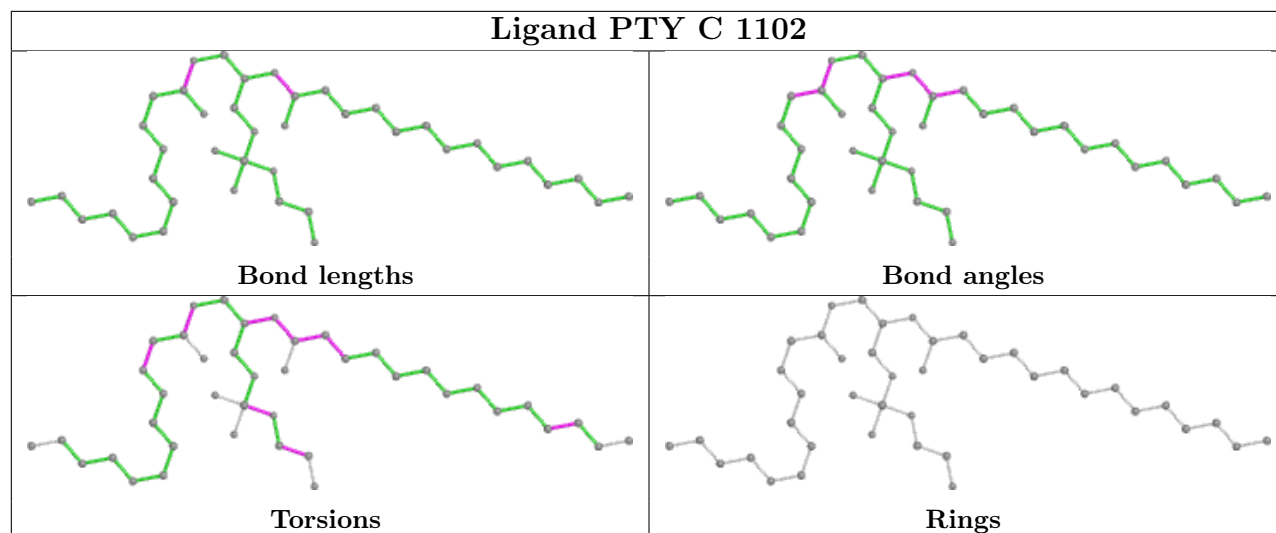
## Ligand PTY A 1106



## Ligand PTY A 1104







## 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.

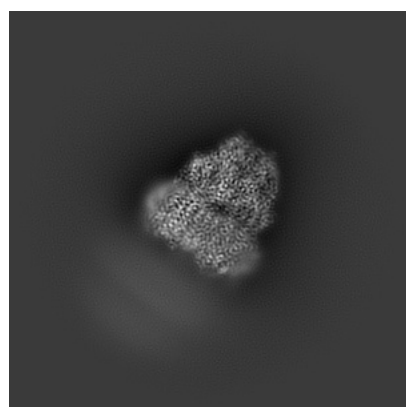
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21229. These allow visual inspection of the internal detail of the map and identification of artifacts.

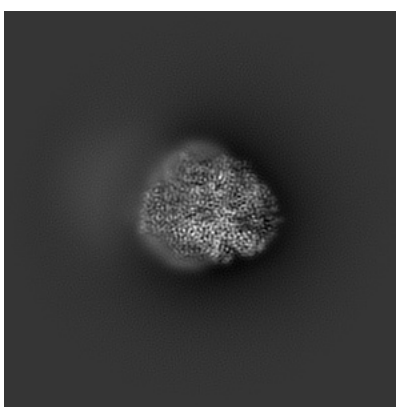
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

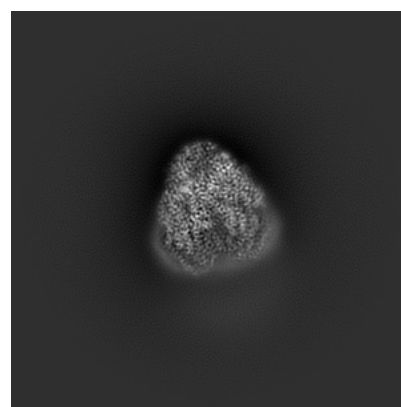
#### 6.1.1 Primary map



X



Y

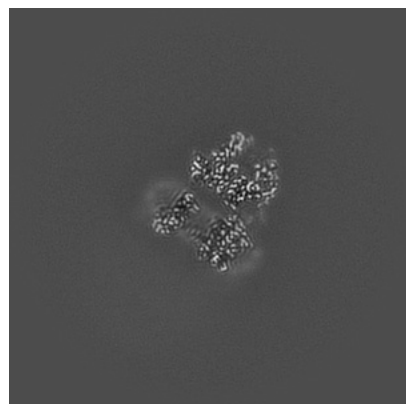


Z

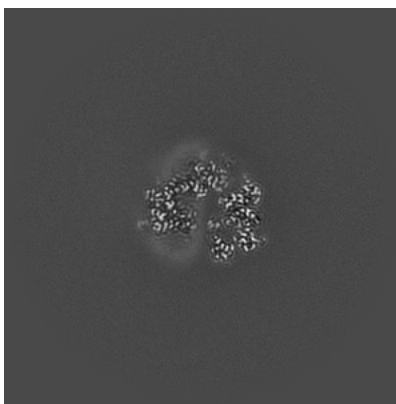
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

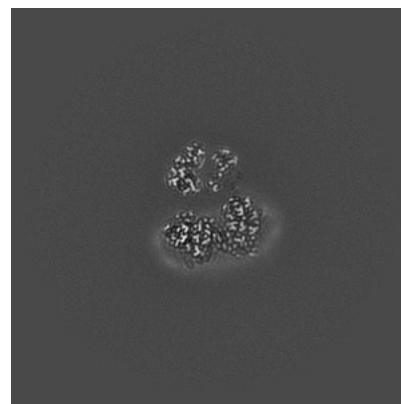
#### 6.2.1 Primary map



X Index: 175



Y Index: 175

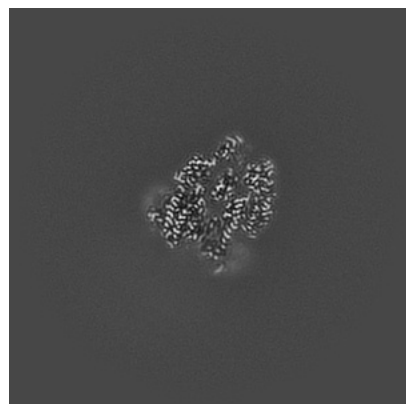


Z Index: 175

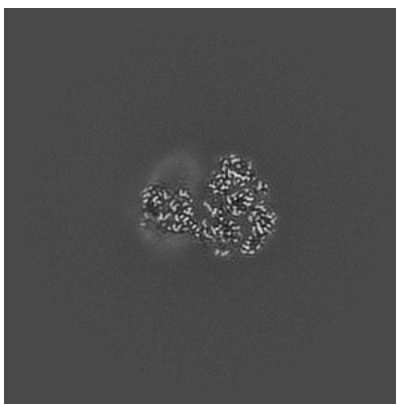
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

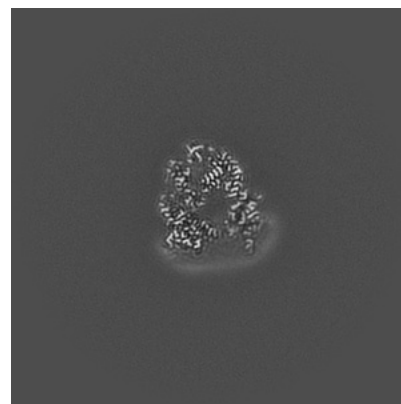
### 6.3.1 Primary map



X Index: 155



Y Index: 190

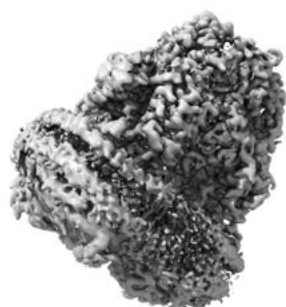


Z Index: 183

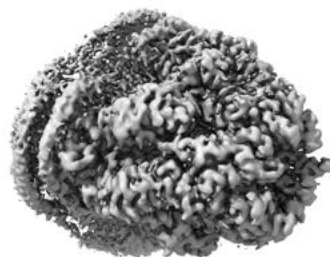
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

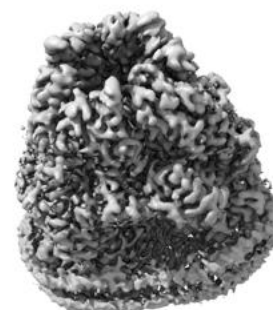
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.



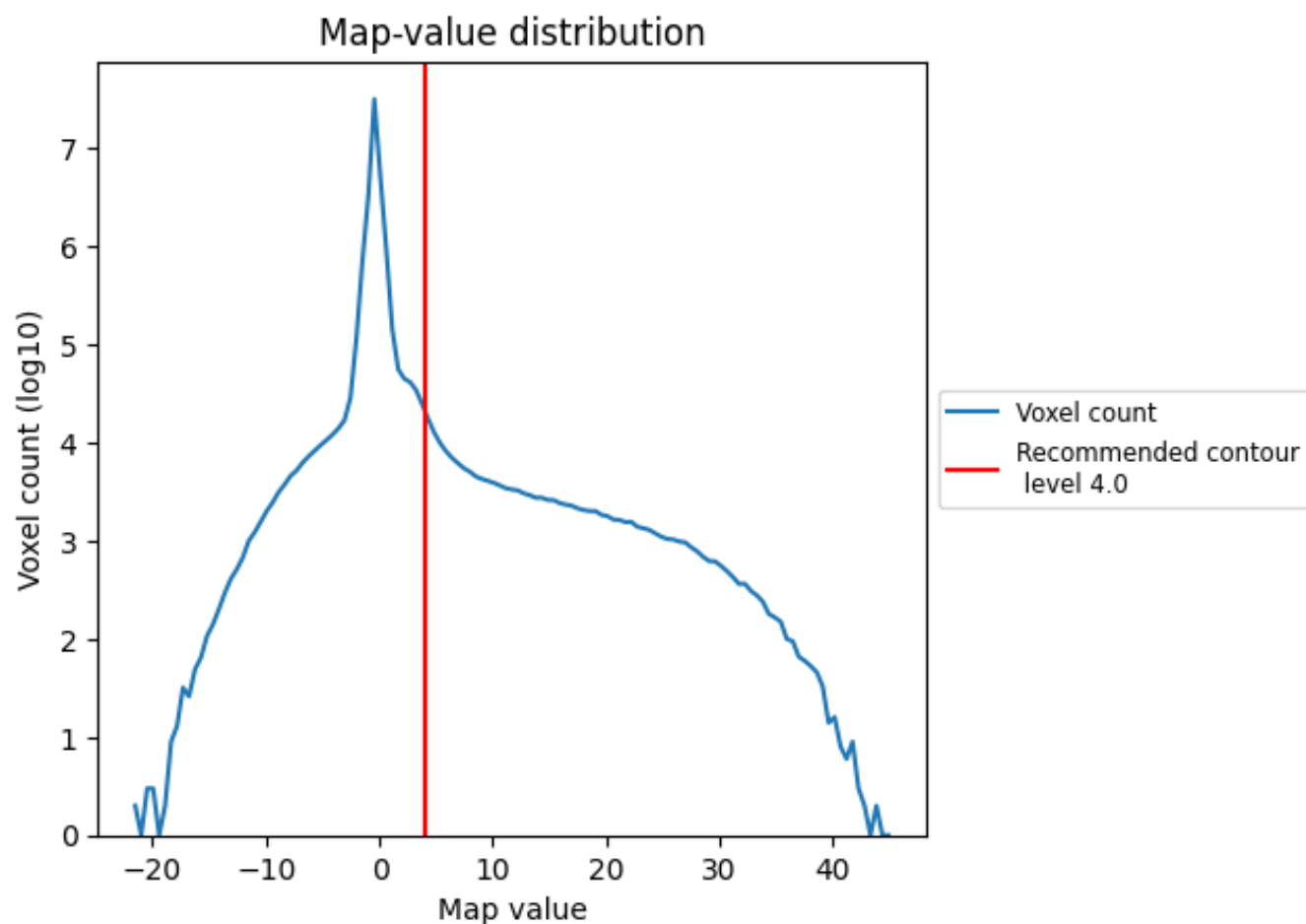
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

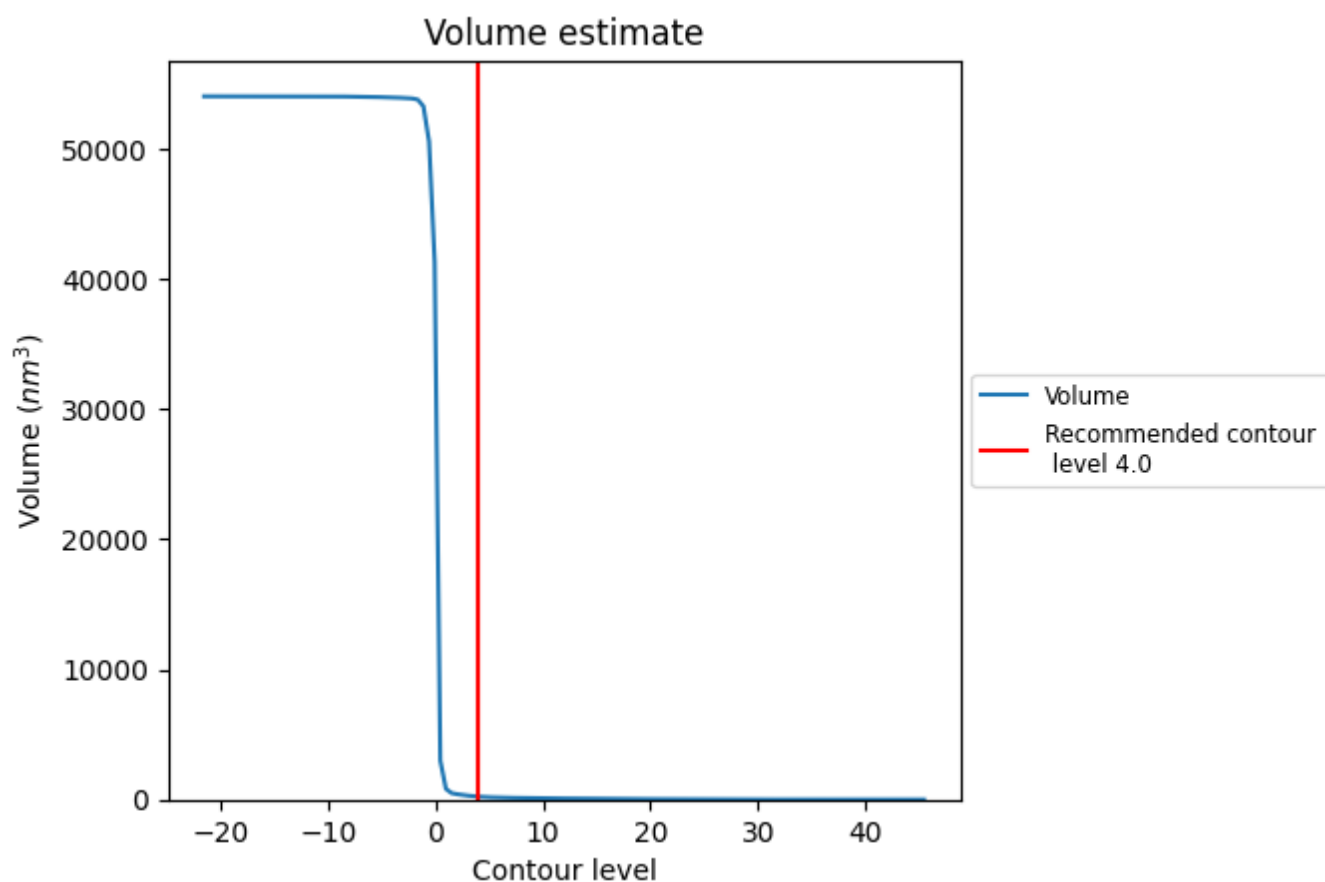
This section contains the results of statistical analysis of the map.

### 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.

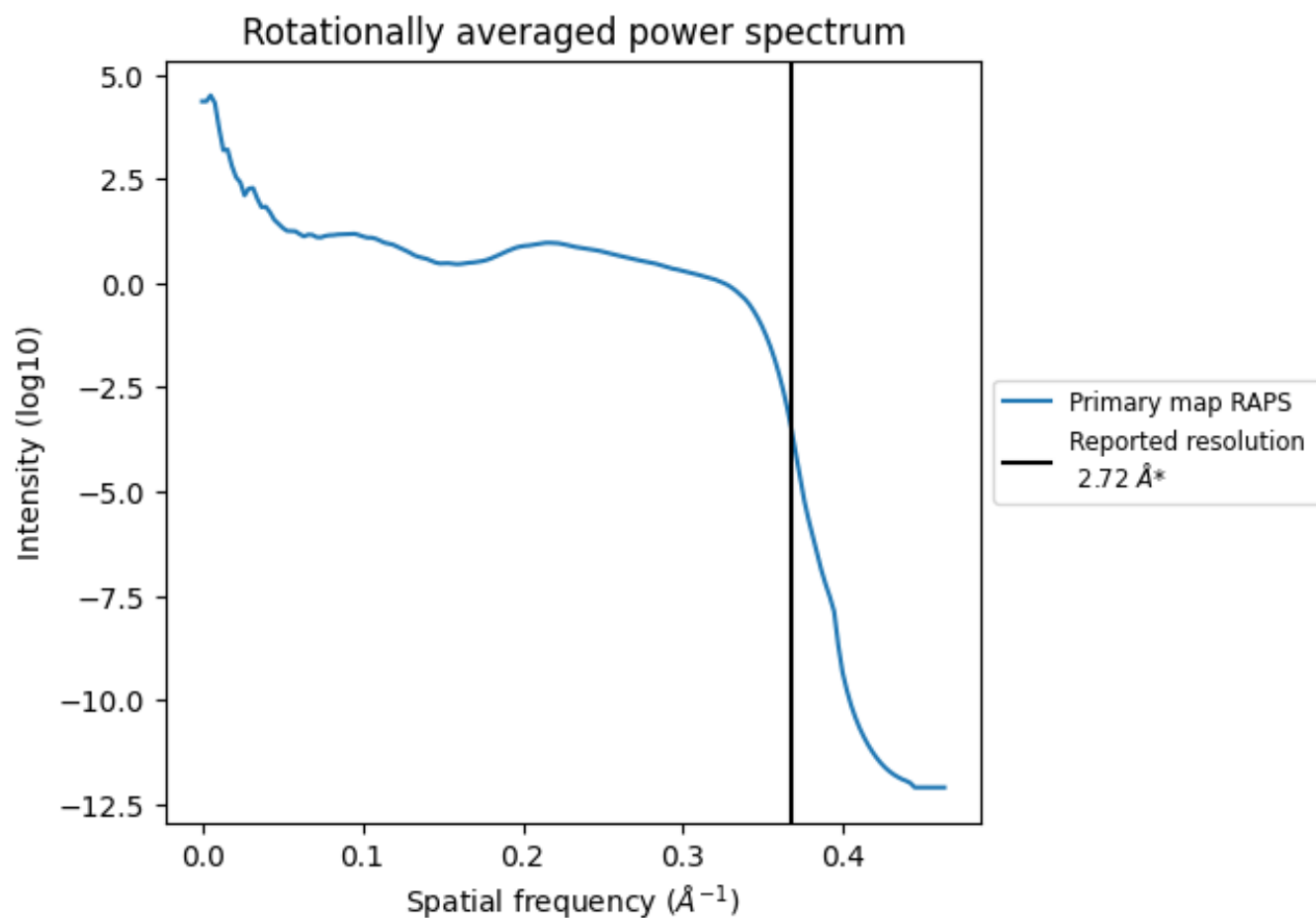
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 224  $\text{nm}^3$ ; this corresponds to an approximate mass of 202 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 0.368 Å<sup>-1</sup>

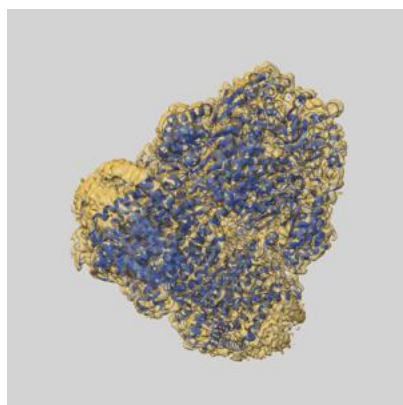
## 8 Fourier-Shell correlation

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

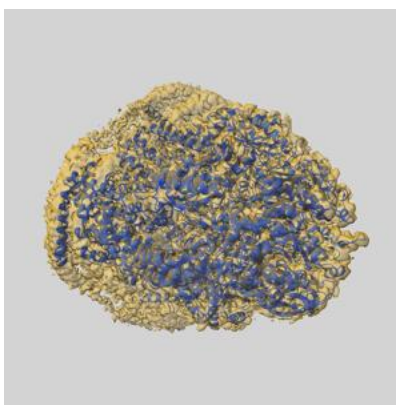
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21229 and PDB model 6VKT. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

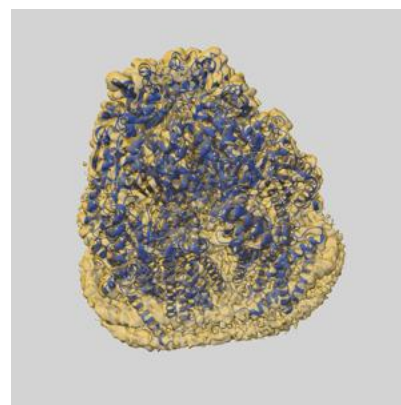
### 9.1 Map-model overlay [i](#)



X



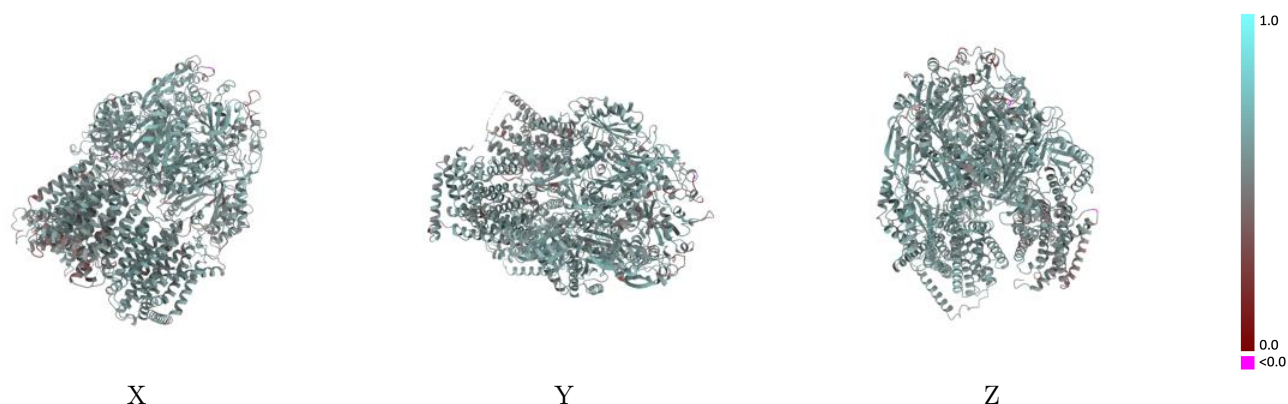
Y



Z

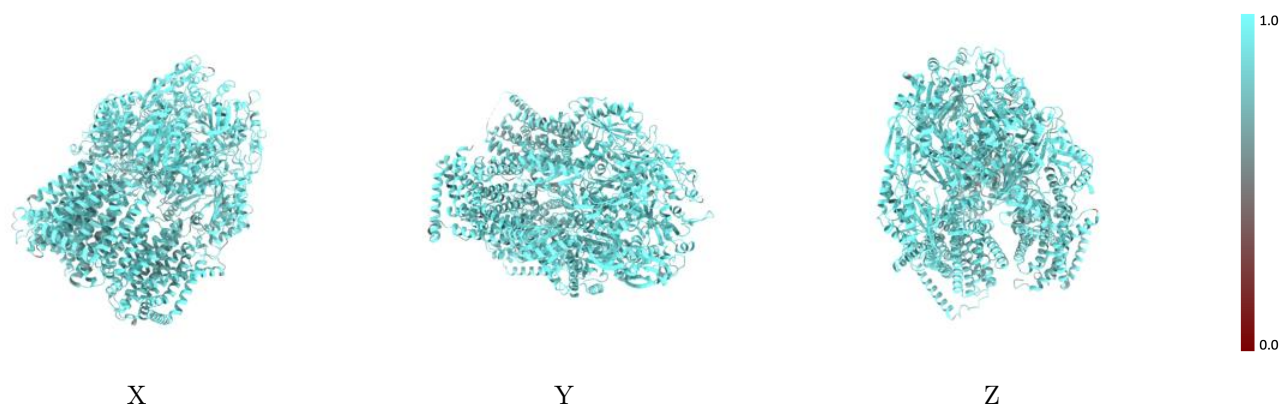
The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



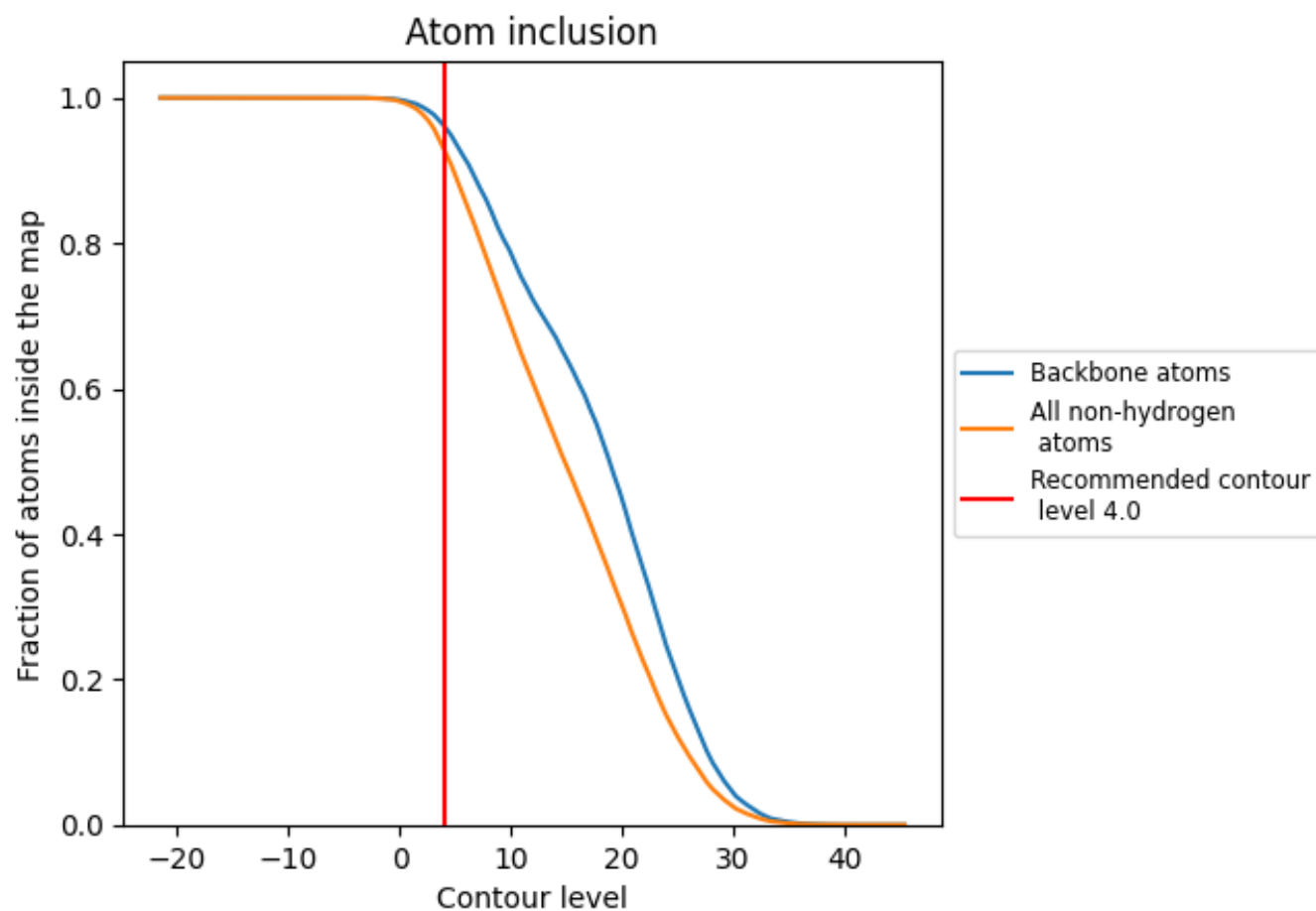
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4.0).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 93% 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 (4.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.9292	<div><div></div></div> 0.5660
A	<div><div></div></div> 0.9173	<div><div></div></div> 0.5510
B	<div><div></div></div> 0.9272	<div><div></div></div> 0.5650
C	<div><div></div></div> 0.9431	<div><div></div></div> 0.5840

