Full wwPDB EM Validation Report ⓘ

Feb 26, 2024 – 07:15 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*
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:

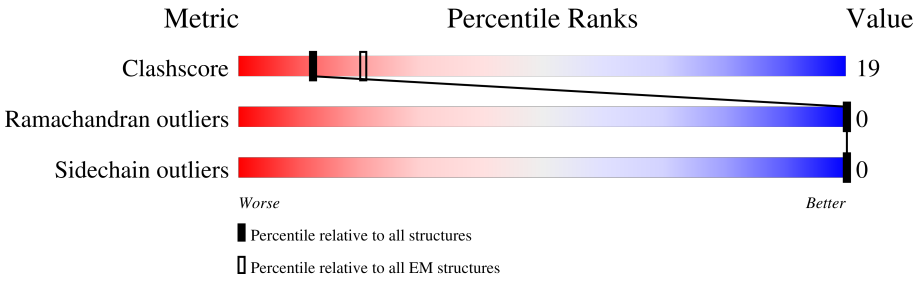
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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 >=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 <=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	64% 35%
1	B	1046	67% 32%
1	C	1046	68% 31%

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 (i)

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:

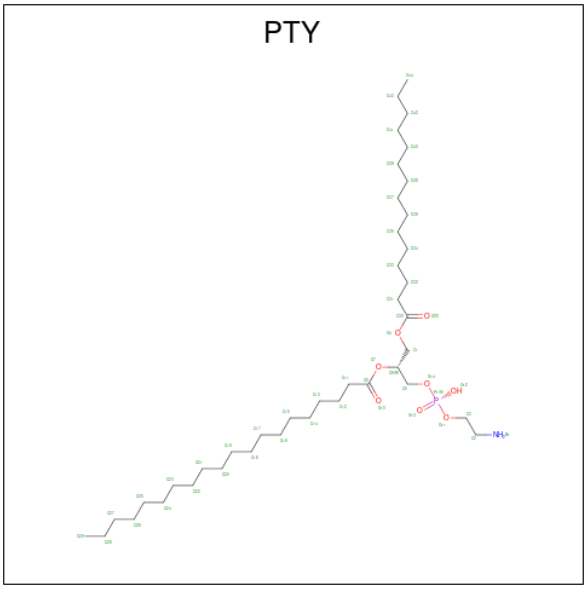
Chain	Residue	Modelled	Actual	Comment	Reference
A	738	VAL	ILE	conflict	UNP A0A4T9VBR9
A	774	GLY	GLU	conflict	UNP A0A4T9VBR9
A	791	SER	LYS	conflict	UNP A0A4T9VBR9
A	794	ILE	VAL	conflict	UNP A0A4T9VBR9
A	800	SER	THR	conflict	UNP A0A4T9VBR9
A	807	GLN	GLU	conflict	UNP A0A4T9VBR9
A	808	MET	ASN	conflict	UNP 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: $C_{40}H_{80}NO_8P$).



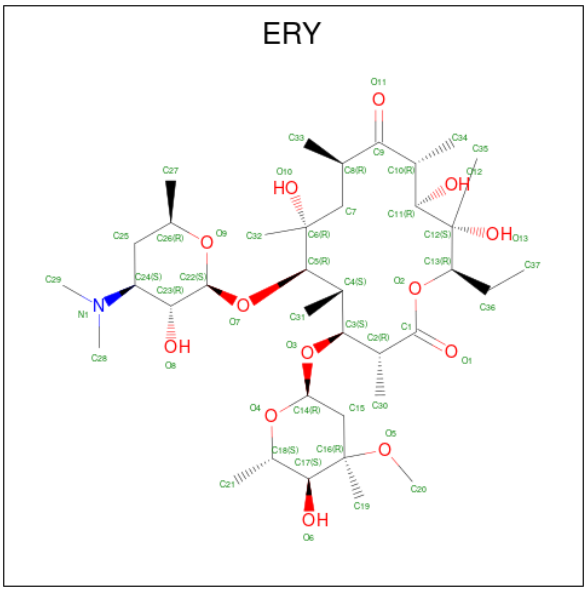
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			48	38	1	8	1	
2	A	1	Total	C	N	O	P	0
			45	35	1	8	1	
2	A	1	Total	C	N	O	P	0
			45	35	1	8	1	
2	A	1	Total	C	N	O	P	0
			41	31	1	8	1	
2	A	1	Total	C	N	O	P	0
			44	34	1	8	1	
2	A	1	Total	C	N	O	P	0
			41	31	1	8	1	
2	B	1	Total	C	N	O	P	0
			37	27	1	8	1	
2	B	1	Total	C	N	O	P	0
			36	26	1	8	1	
2	B	1	Total	C	N	O	P	0
			41	31	1	8	1	
2	B	1	Total	C	N	O	P	0
			44	34	1	8	1	
2	B	1	Total	C	N	O	P	0
			35	25	1	8	1	
2	B	1	Total	C	N	O	P	0
			50	40	1	8	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
2	B	1	Total	C	N	O	P	0
			35	25	1	8	1	
2	B	1	Total	C	N	O	P	0
			44	34	1	8	1	
2	C	1	Total	C	N	O	P	0
			46	36	1	8	1	
2	C	1	Total	C	N	O	P	0
			41	31	1	8	1	
2	C	1	Total	C	N	O	P	0
			41	31	1	8	1	
2	C	1	Total	C	N	O	P	0
			32	22	1	8	1	
2	C	1	Total	C	N	O	P	0
			35	25	1	8	1	
2	C	1	Total	C	O			0
			38	34	4			
2	C	1	Total	C	N	O	P	0
			50	40	1	8	1	
2	C	1	Total	C	O			0
			16	14	2			
2	C	1	Total	C	O			0
			15	13	2			

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



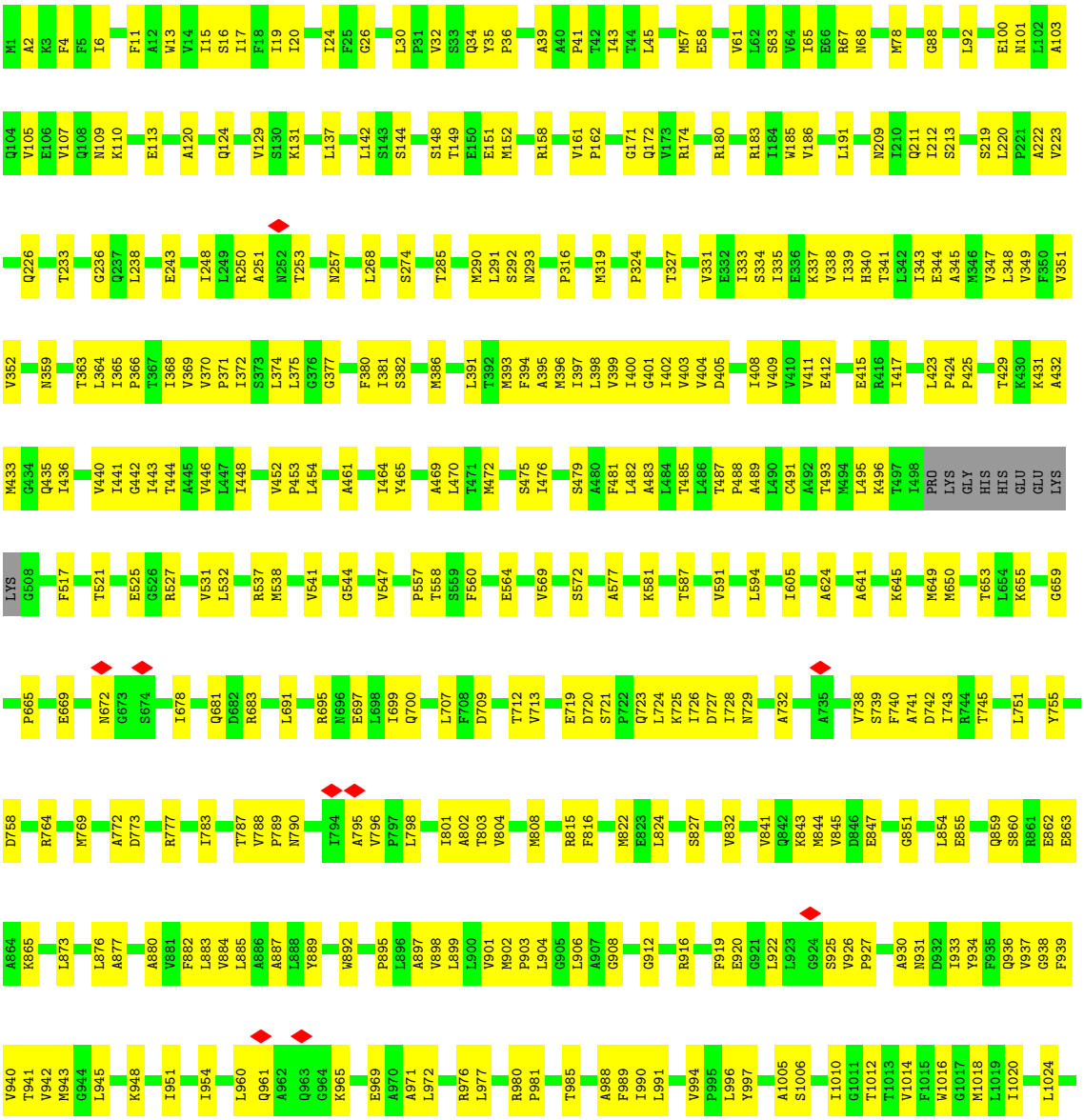
Mol	Chain	Residues	Atoms				AltConf
3	B	1	Total	C	N	O	0
			51	37	1	13	

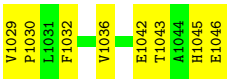
3 Residue-property plots (i)

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

- Molecule 1: Efflux pump membrane transporter

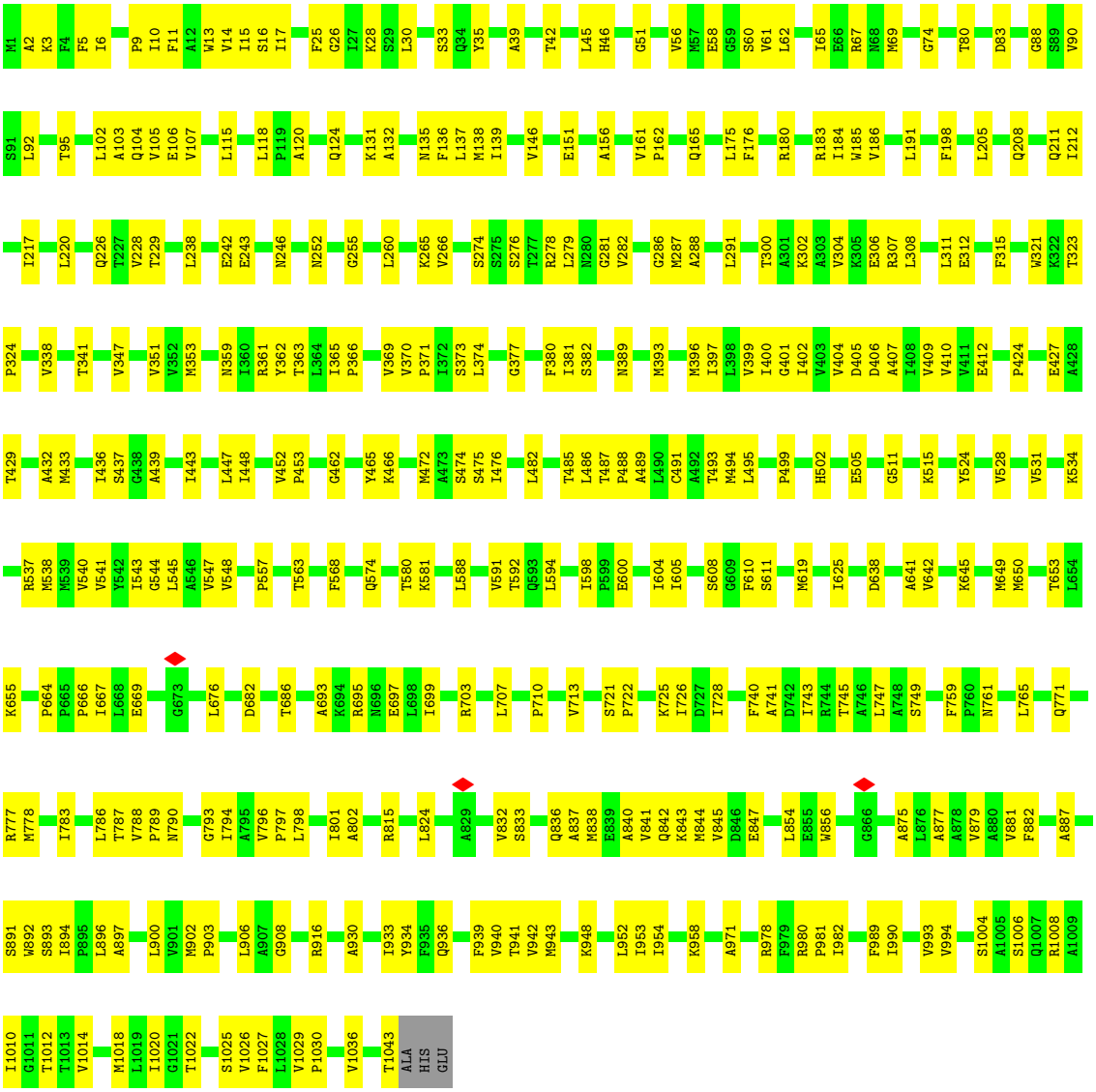
Chain A:





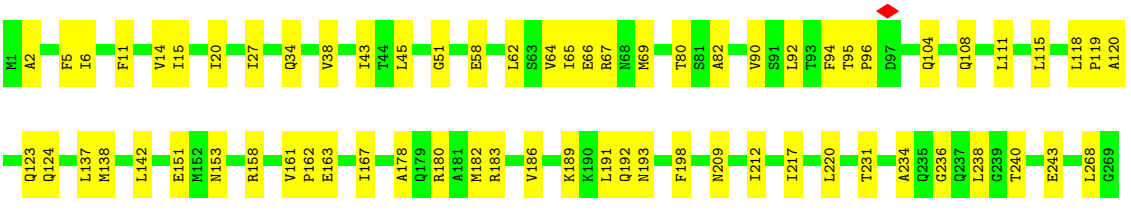
• Molecule 1: Efflux pump membrane transporter

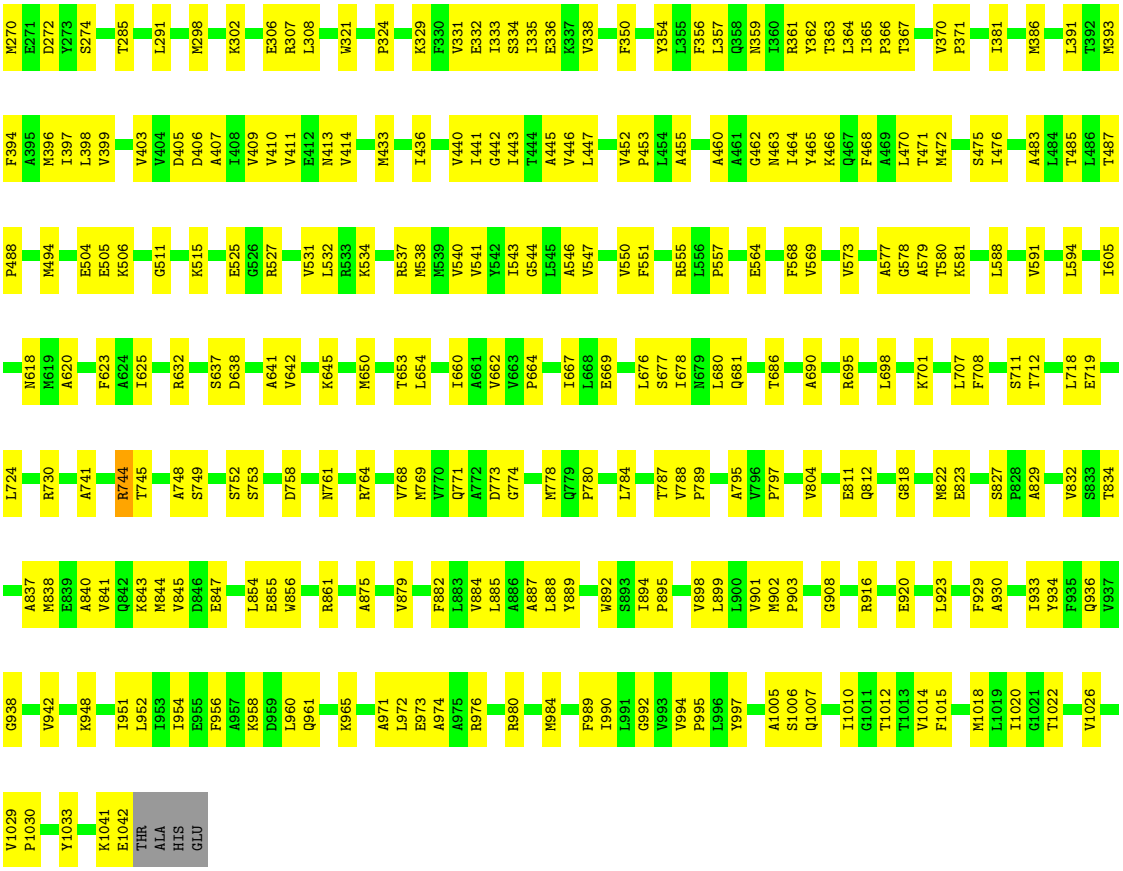
Chain B:



• Molecule 1: Efflux pump membrane transporter

Chain C:




M270 E271 D272 Y273 S274 T285 L291 M298 K302 E306 R307 L308 W321 P324 K329 F330 V331 E332 I333 S334 I335 E336 K337 V338 F350 Y354 L355 F356 L357 Q358 N359 I360 R361 Y362 T363 L364 I365 P366 T367 V370 P371 I381 M386 L391 T392 M393
F394 A395 M396 I397 L398 V399 V403 V404 D405 D406 A407 I408 V409 V410 V411 E412 N413 V414 M433 I436 V440 I441 G442 I443 T444 A445 V446 L447 V452 P453 L454 A455 A460 A461 G462 N463 I464 Y465 K466 Q467 F468 A469 L470 T471 M472 S475 I476 A483 L484 T485 L486 T487
P488 M494 E504 E505 K506 G511 K515 E525 G526 R527 V531 L532 R533 K534 R537 M538 M539 V540 V541 Y542 I543 G544 L545 A546 V547 V550 F551 R555 L556 P557 E564 F568 V569 V573 A577 G578 A579 T580 K581 L588 V591 L594 I605
N618 M619 A620 F623 A624 I625 R632 S637 D638 A641 V642 K645 M650 T653 L654 I660 A661 V662 V663 P664 I667 L668 E669 L676 S677 I678 N679 L680 Q681 T686 A690 R695 L698 K701 L707 F708 S711 T712 L718 E719
L724 R730 A741 R744 T745 A748 S749 S752 S753 D758 N761 R764 V768 M769 V770 Q771 A772 D773 G774 M778 Q779 P780 L784 T787 V788 P789 A795 V796 P797 V804 E811 Q812 G818 M822 E823 S827 P828 A829 V832 S833 T834
A837 M838 E839 A840 V841 Q842 K843 M844 V845 D846 E847 L854 E855 W856 R861 A875 V879 F882 L883 V884 L885 A886 A887 L888 Y889 W892 S893 I894 P895 V898 L899 L900 V901 M902 P903 G908 R916 E920 L923 F929 A930 I933 Y934 F935 Q936 V937
Q938 V942 K948 I951 L952 I953 I954 E955 F956 A957 K958 D959 L960 Q961 K965 A971 L972 E973 A974 A975 R976 R980 M984 F989 I990 L991 G992 Y993 V994 P995 L996 Y997 A1005 S1006 Q1007 I1010 G1011 T1012 T1013 V1014 F1015 M1018 L1019 I1020 G1021 T1022 V1026
V1029 P1030 Y1033 K1041 E1042 THR ALA HIS GLU

4 Experimental information (i)

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 ($e^-/Å^2$)	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 (Å)	378.0, 378.0, 378.0	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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 (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	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

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PTY	A	1102	-	-	10/48/48/53	-
2	PTY	C	1109	-	-	5/12/12/53	-
2	PTY	C	1101	-	-	16/49/49/53	-
2	PTY	B	1105	-	-	15/47/47/53	-
2	PTY	B	1109	-	-	21/47/47/53	-

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	A	1104	-	-	19/44/44/53	-
2	PTY	B	1104	-	-	17/44/44/53	-
2	PTY	C	1103	-	-	9/44/44/53	-
2	PTY	B	1102	-	-	15/40/40/53	-
3	ERY	B	1101	-	-	38/72/107/107	0/3/3/3
2	PTY	C	1106	-	-	12/38/38/53	-
2	PTY	C	1108	-	-	2/12/12/53	-
2	PTY	C	1107	-	-	17/53/53/53	-
2	PTY	C	1104	-	-	9/35/35/53	-
2	PTY	B	1103	-	-	9/39/39/53	-
2	PTY	A	1106	-	-	12/44/44/53	-
2	PTY	C	1105	-	-	16/38/38/53	-
2	PTY	B	1108	-	-	18/38/38/53	-
2	PTY	C	1102	-	-	13/44/44/53	-
2	PTY	A	1101	-	-	17/51/51/53	-
2	PTY	A	1105	-	-	19/47/47/53	-
2	PTY	A	1103	-	-	19/48/48/53	-
2	PTY	B	1106	-	-	7/38/38/53	-

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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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.

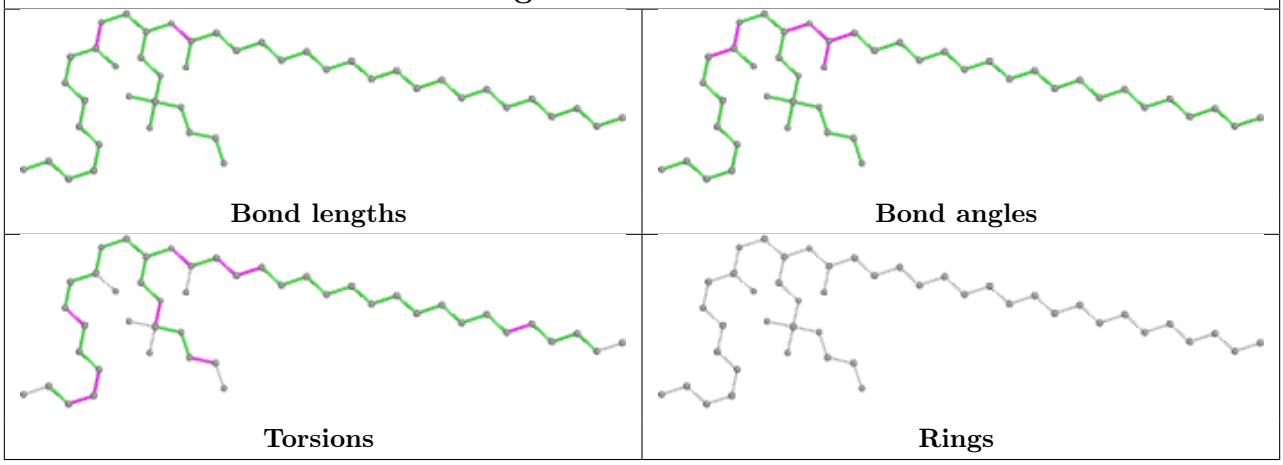
24 monomers are involved in 157 short contacts:

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

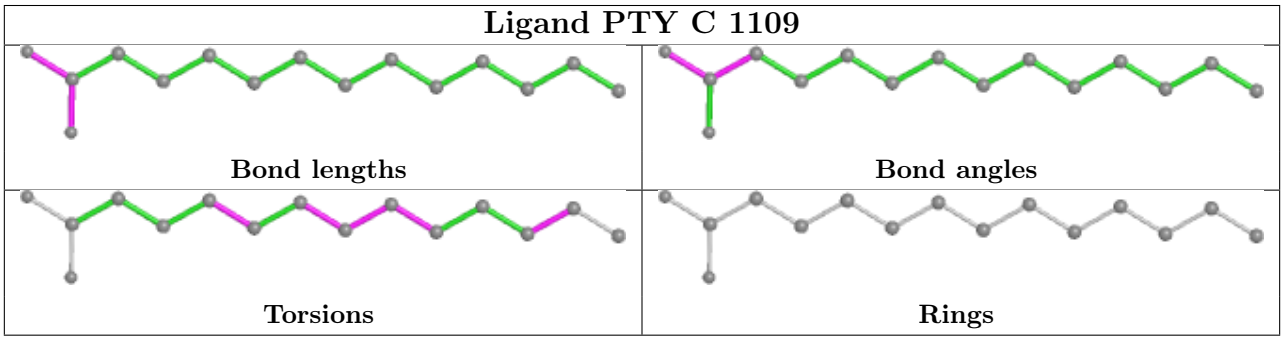
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less then 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.

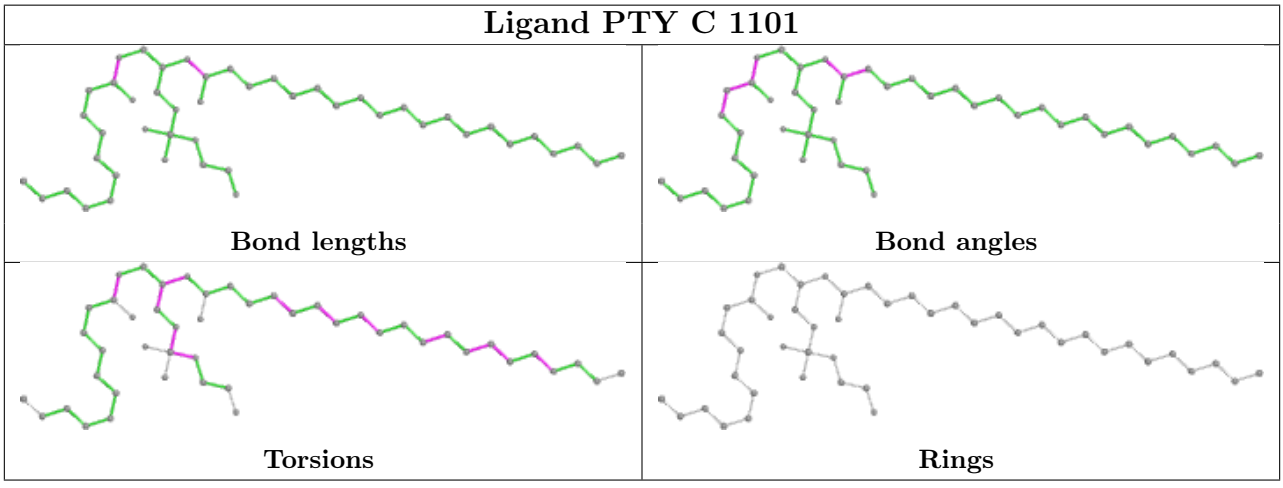
Ligand PTY A 1102



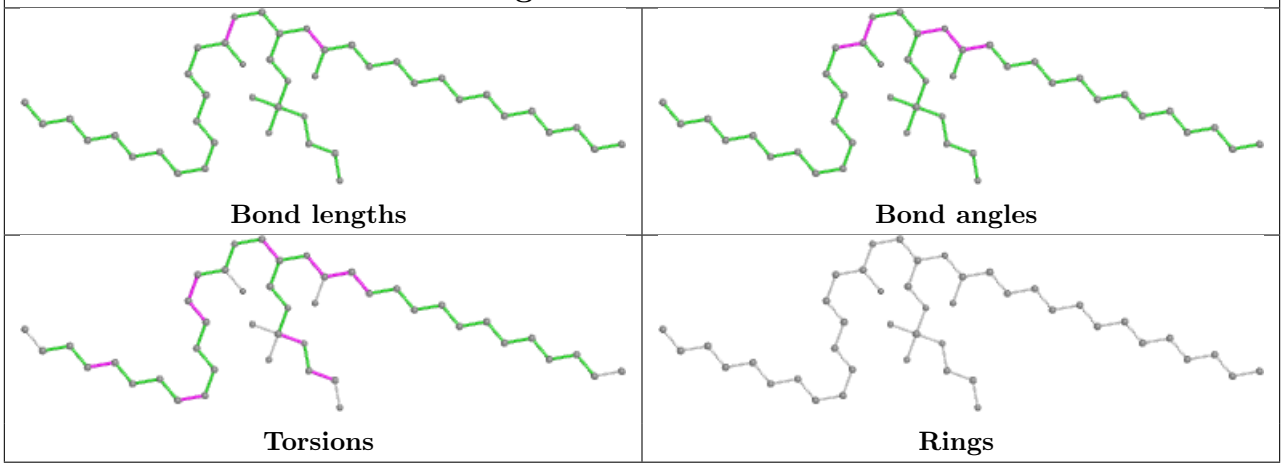
Ligand PTY C 1109



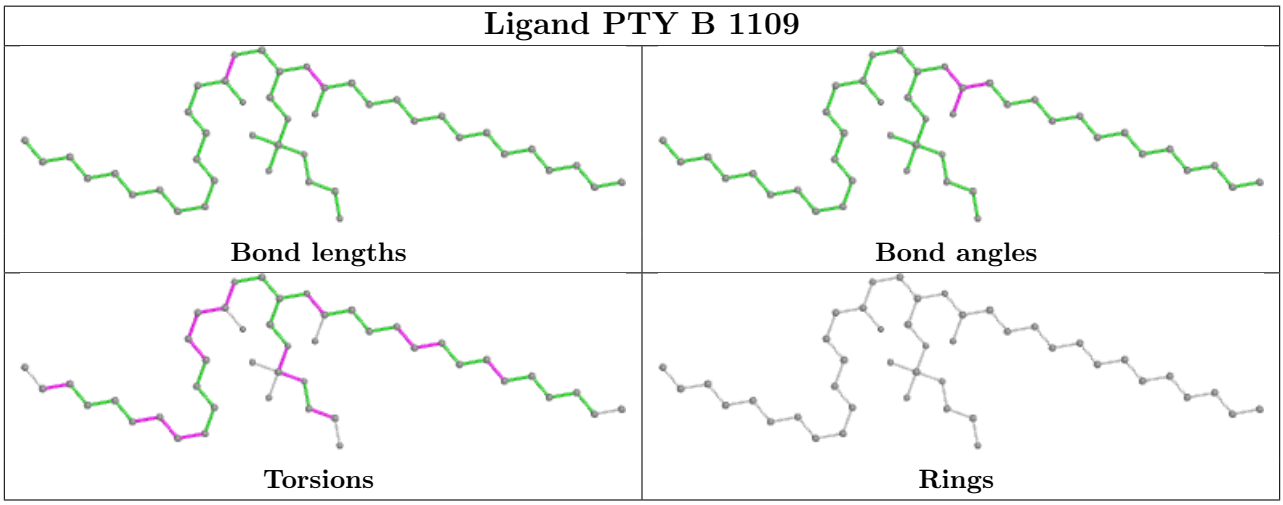
Ligand PTY C 1101



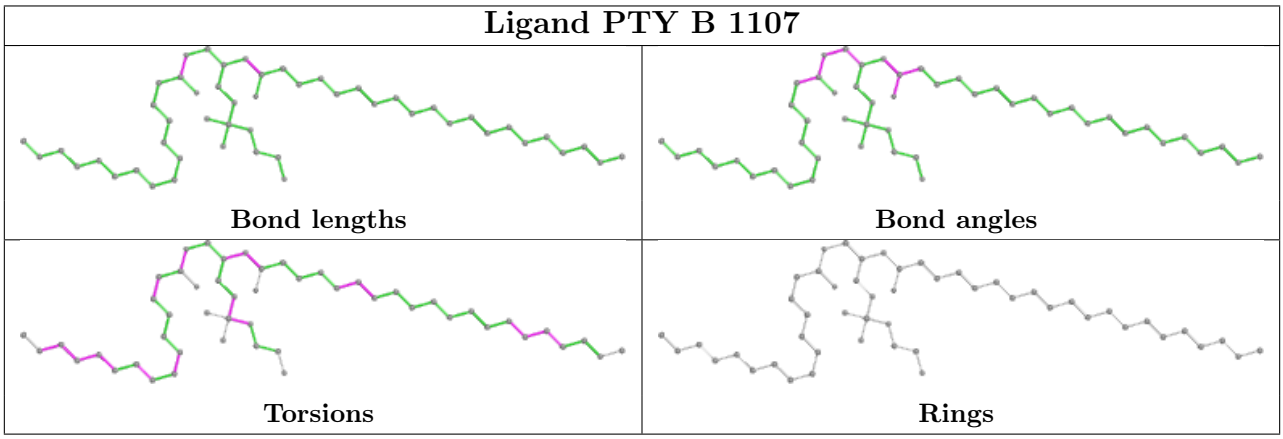
Ligand PTY B 1105



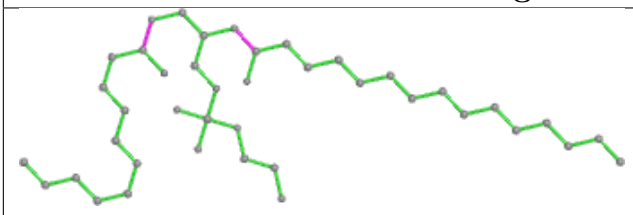
Ligand PTY B 1109



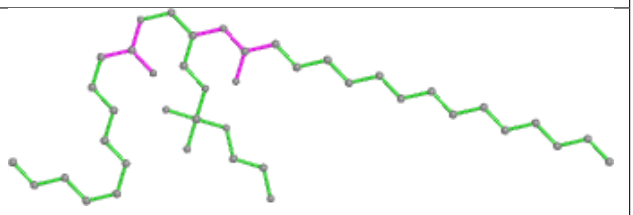
Ligand PTY B 1107



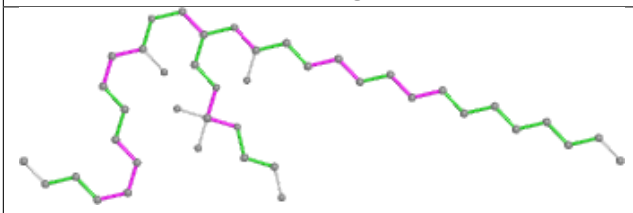
Ligand PTY A 1104



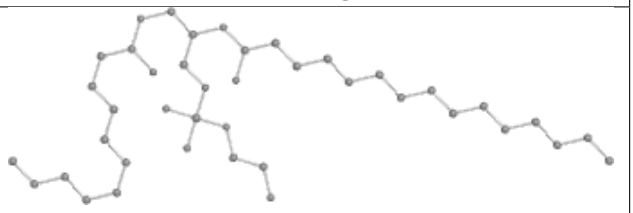
Bond lengths



Bond angles

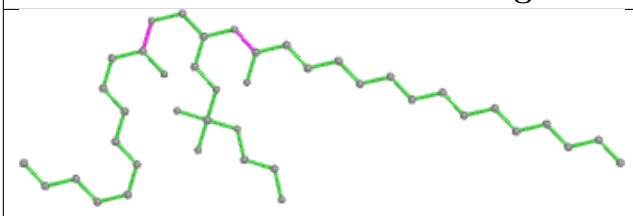


Torsions

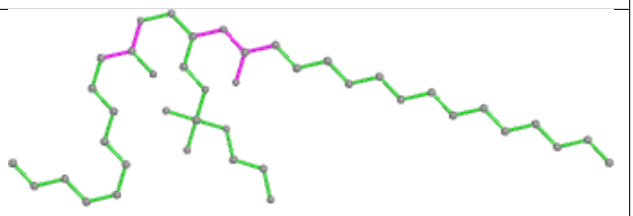


Rings

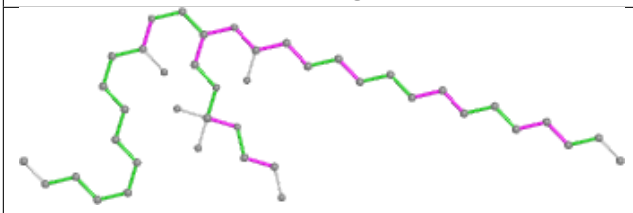
Ligand PTY B 1104



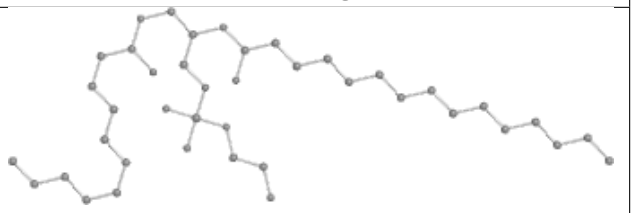
Bond lengths



Bond angles

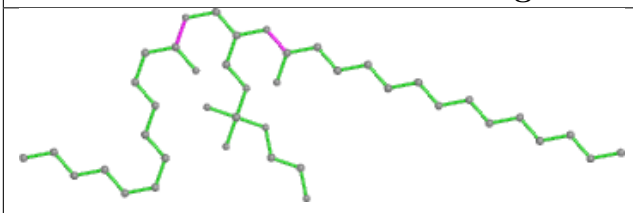


Torsions

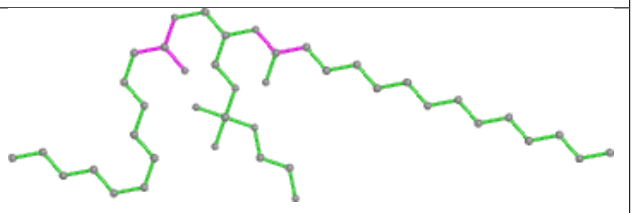


Rings

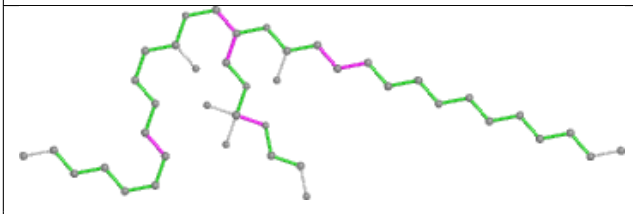
Ligand PTY C 1103



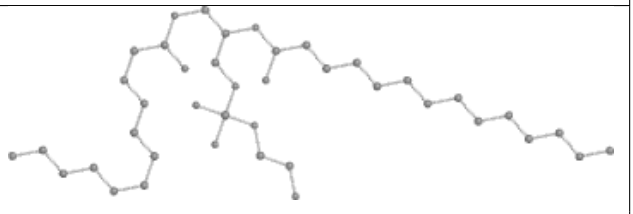
Bond lengths



Bond angles

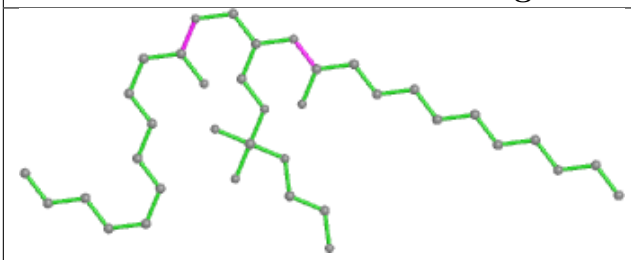


Torsions

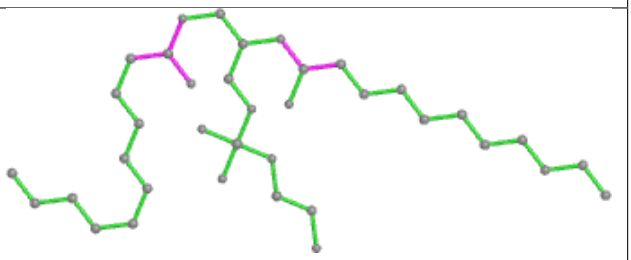


Rings

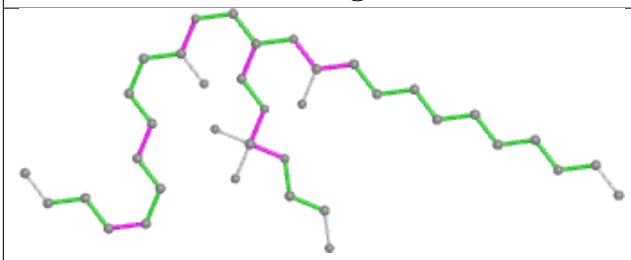
Ligand PTY B 1102



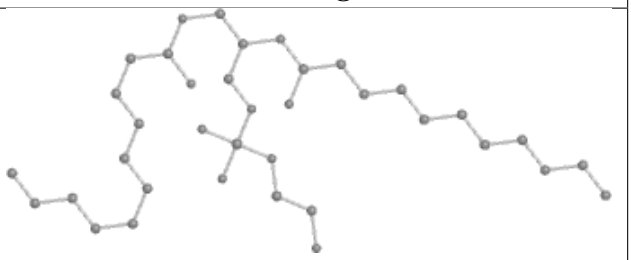
Bond lengths



Bond angles

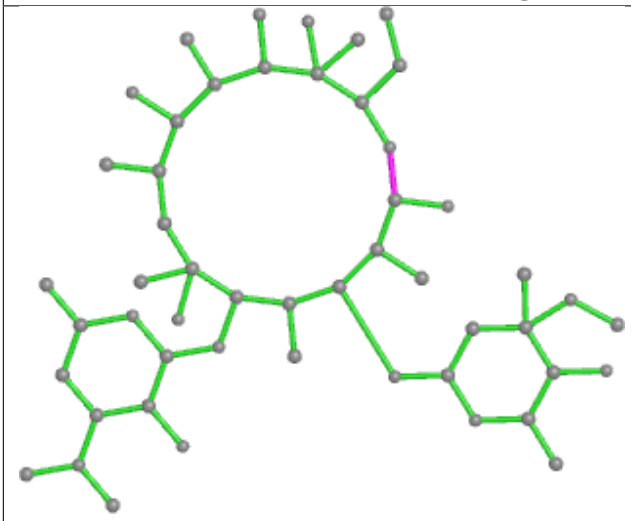


Torsions

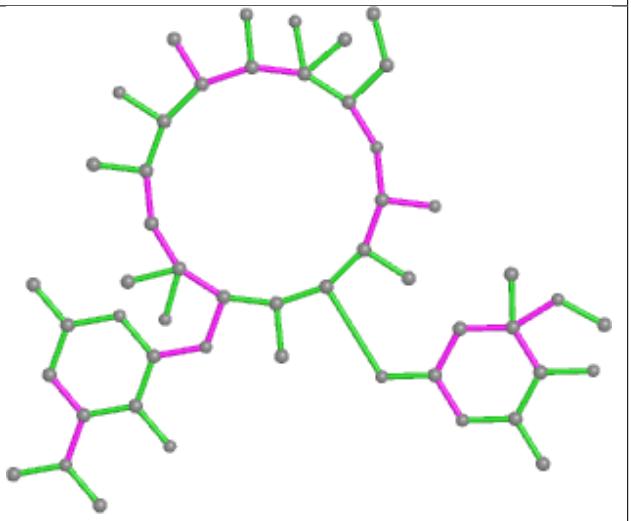


Rings

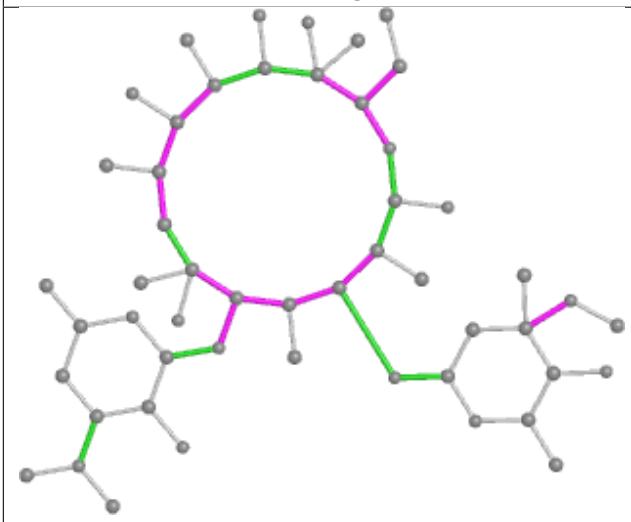
Ligand ERY B 1101



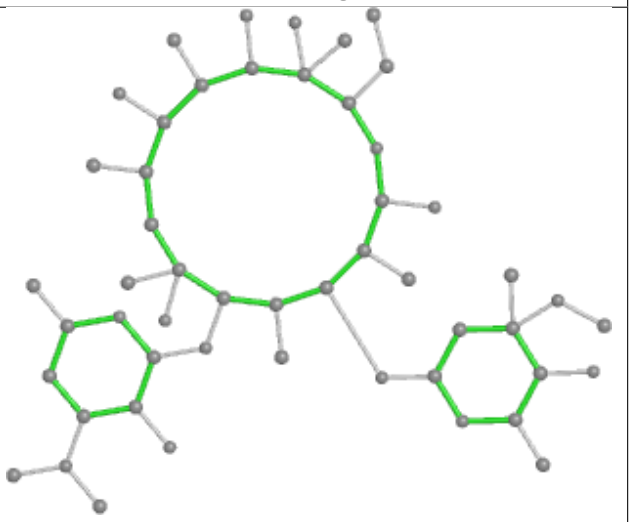
Bond lengths



Bond angles

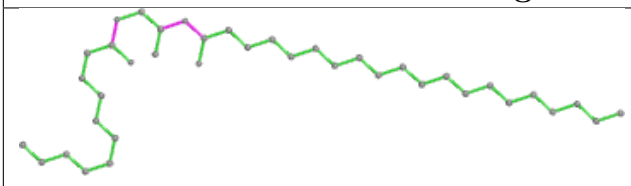


Torsions

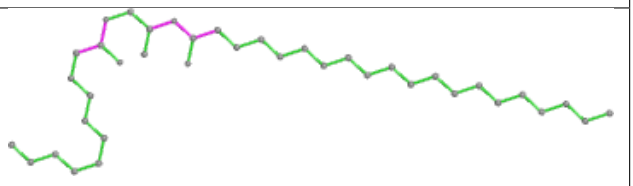


Rings

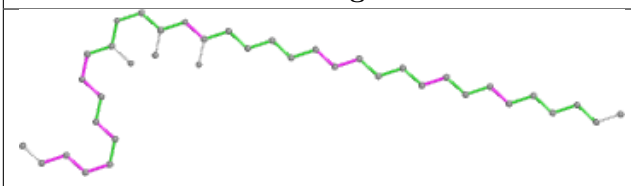
Ligand PTY C 1106



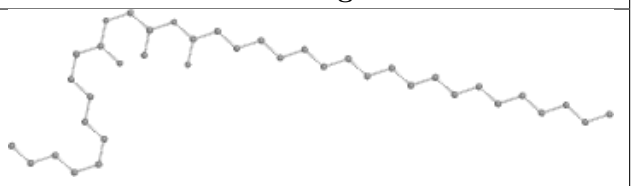
Bond lengths



Bond angles

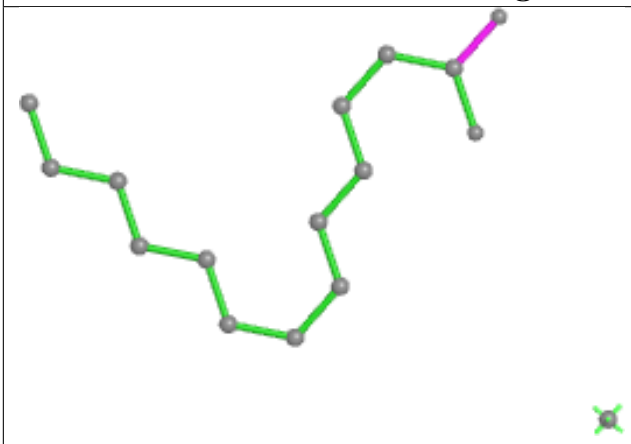


Torsions

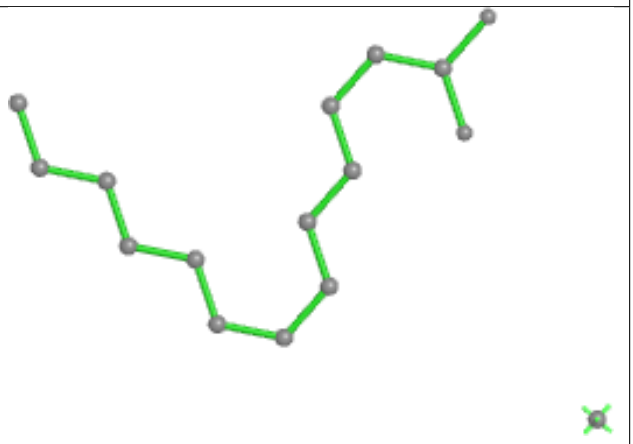


Rings

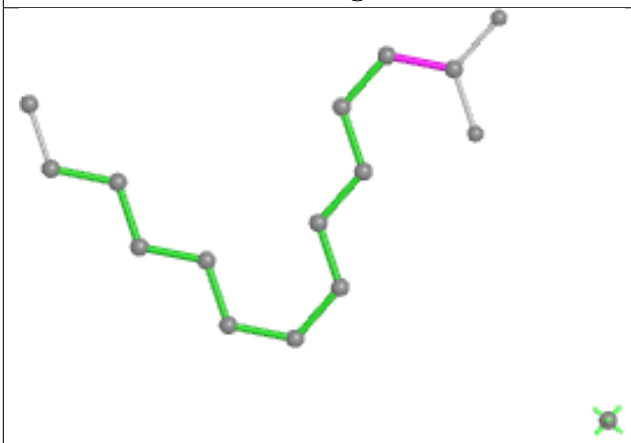
Ligand PTY C 1108



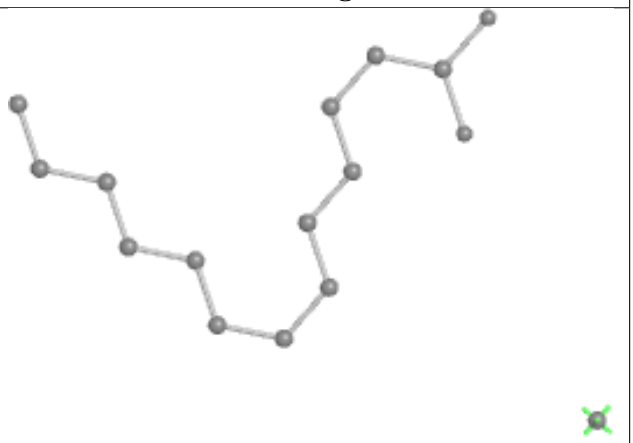
Bond lengths



Bond angles

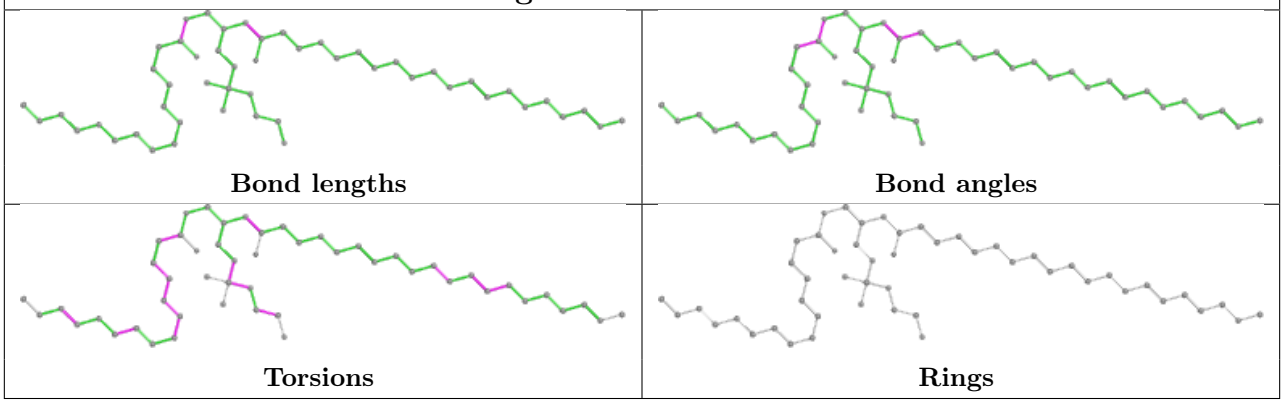


Torsions

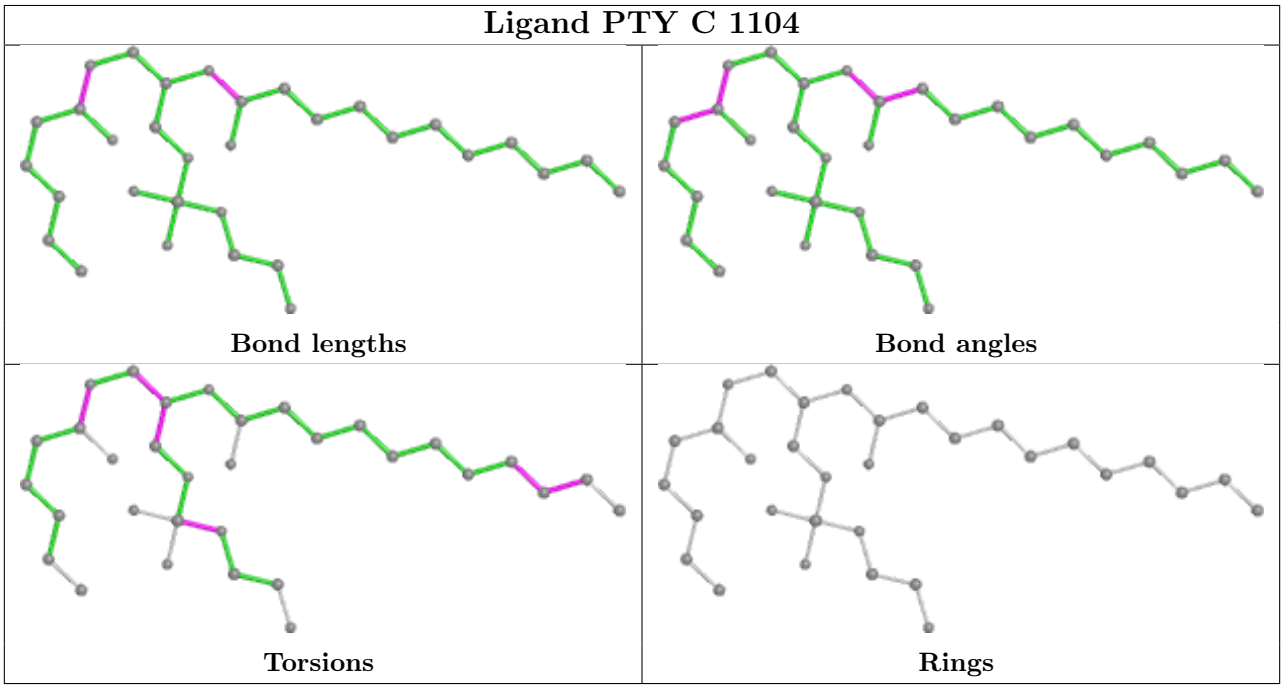


Rings

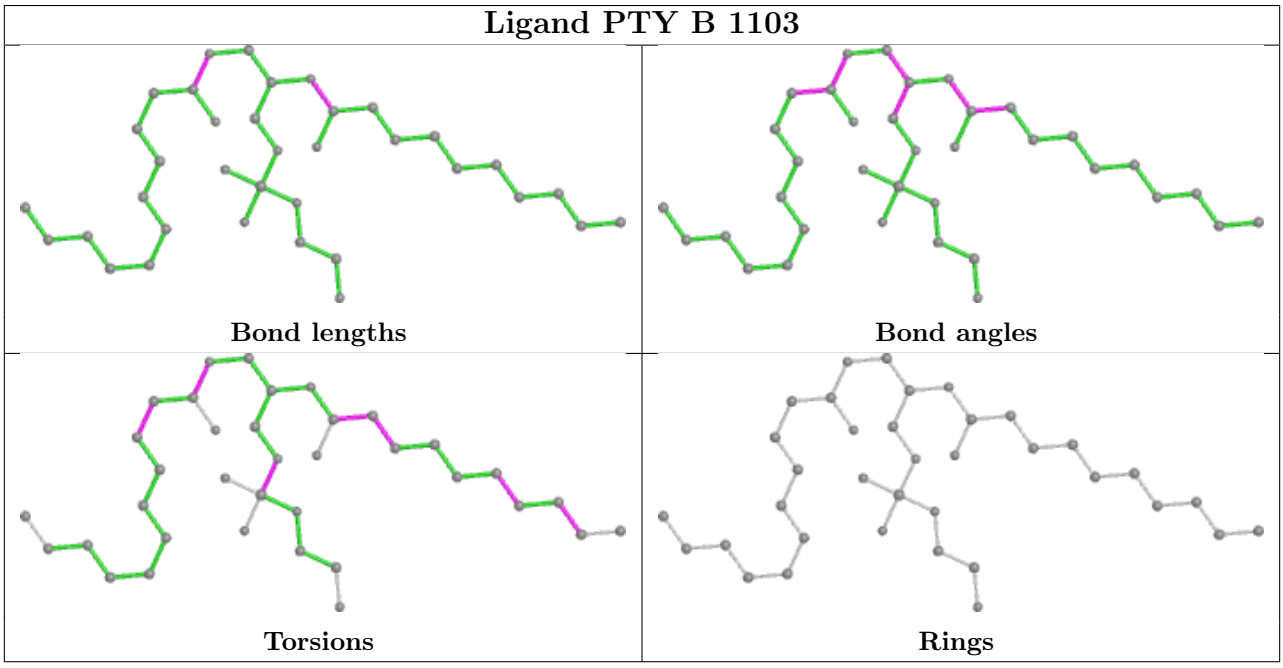
Ligand PTY C 1107

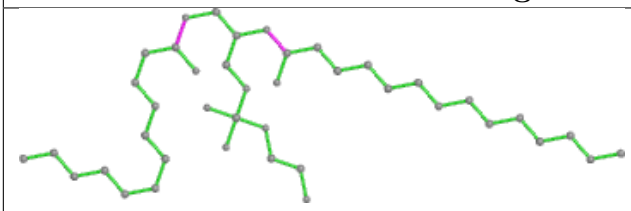
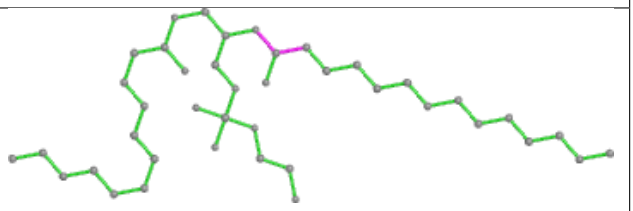
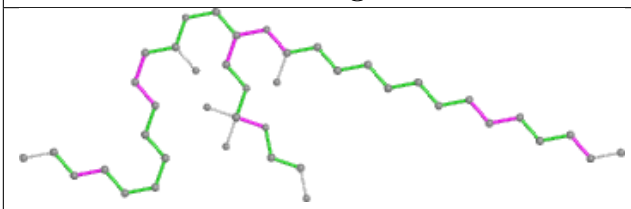
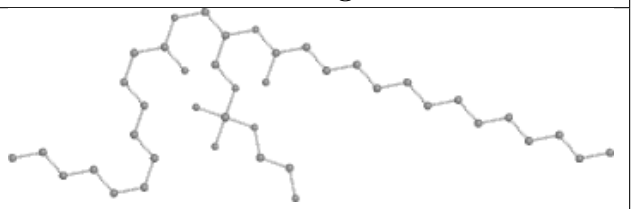


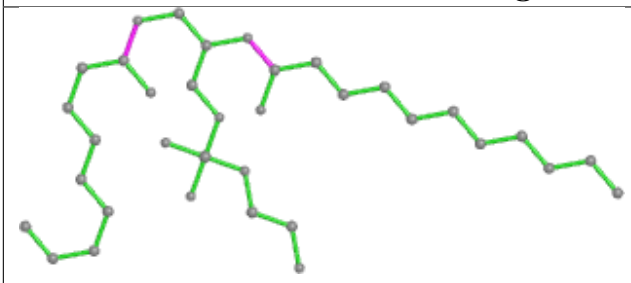
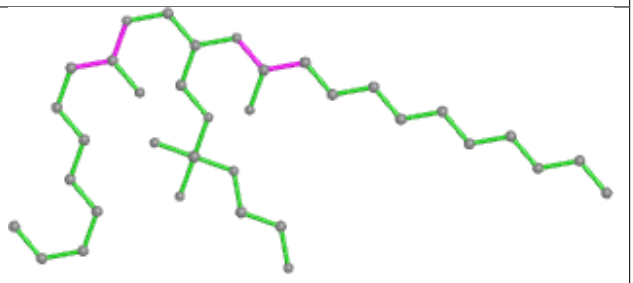
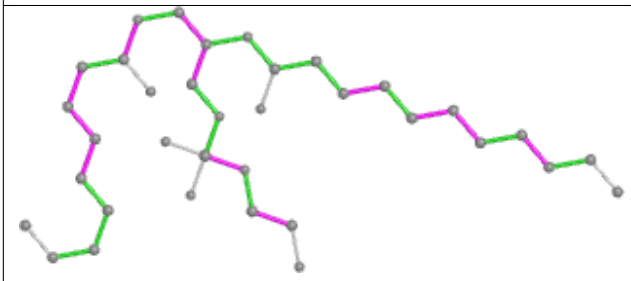
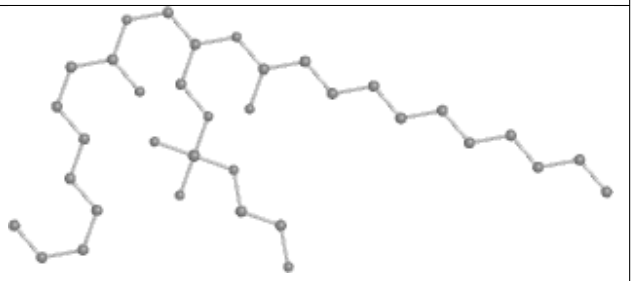
Ligand PTY C 1104



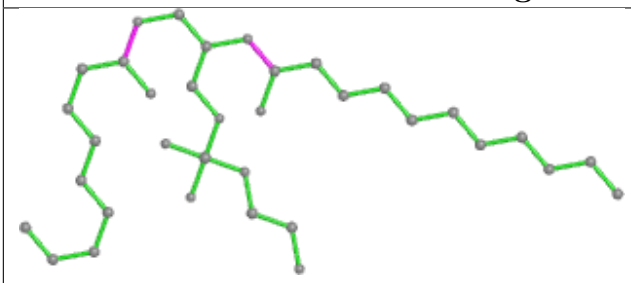
Ligand PTY B 1103



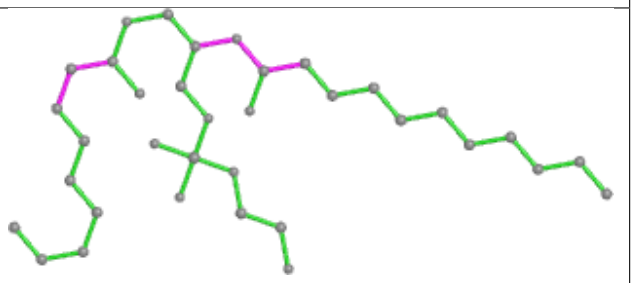
Ligand PTY A 1106	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PTY C 1105	
 Bond lengths	 Bond angles
 Torsions	 Rings

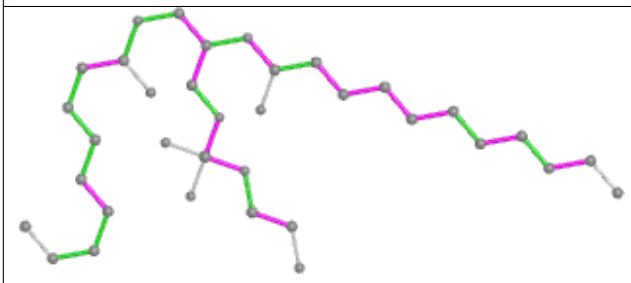
Ligand PTY B 1108



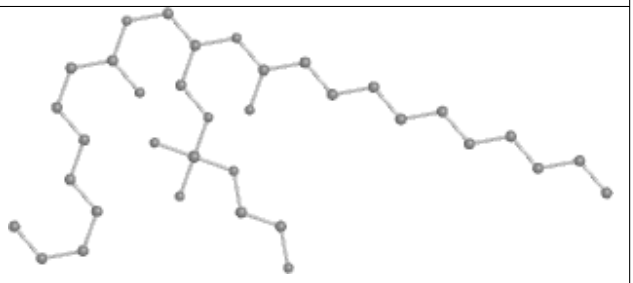
Bond lengths



Bond angles

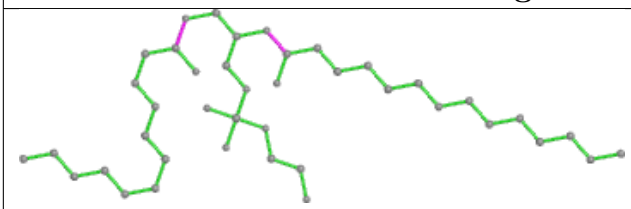


Torsions

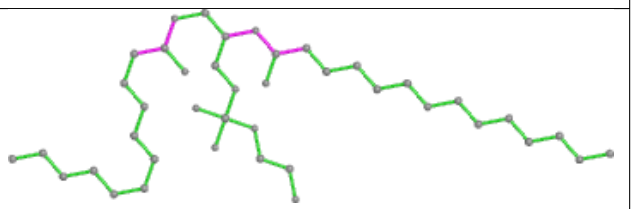


Rings

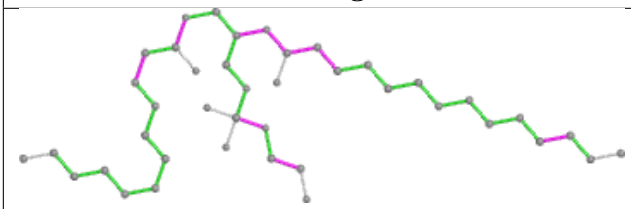
Ligand PTY C 1102



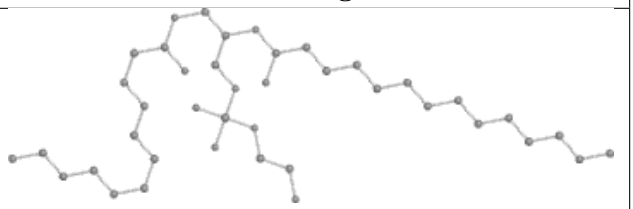
Bond lengths



Bond angles

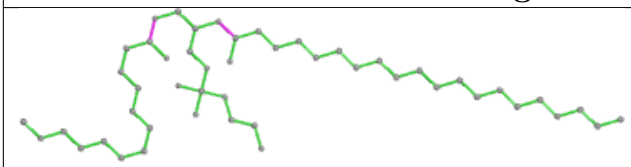


Torsions

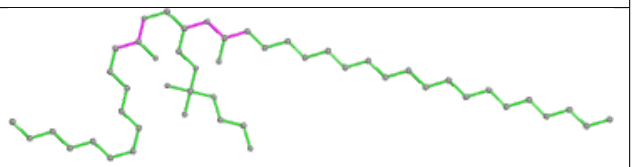


Rings

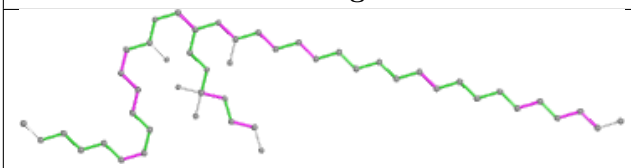
Ligand PTY A 1101



Bond lengths



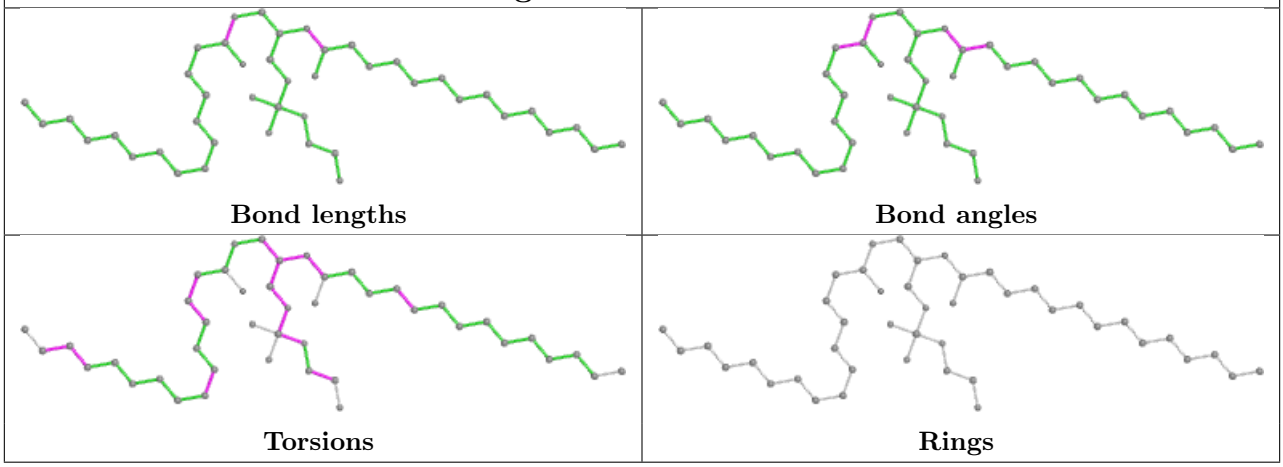
Bond angles



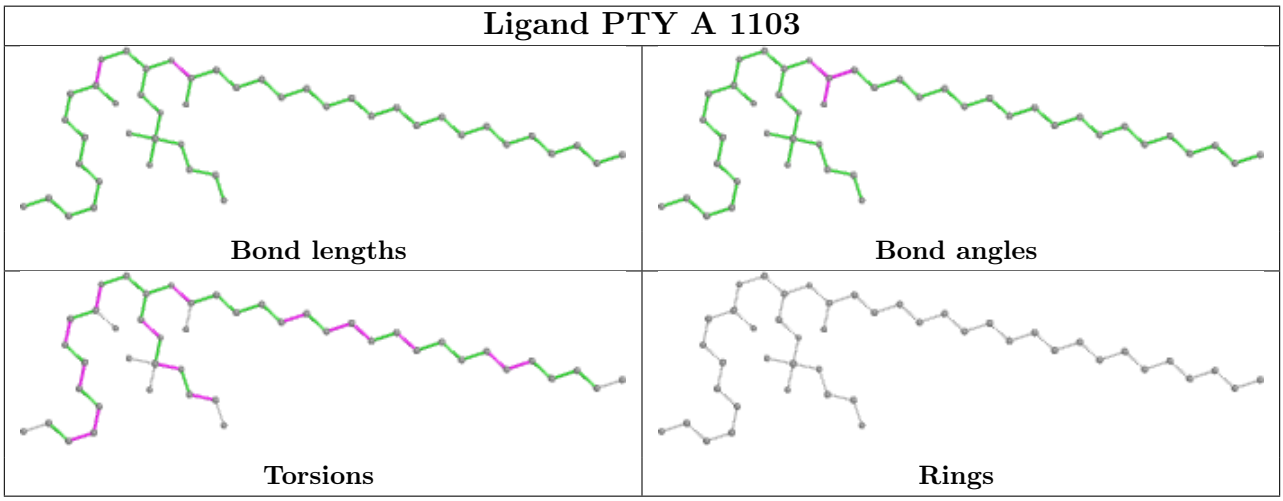
Torsions

Rings

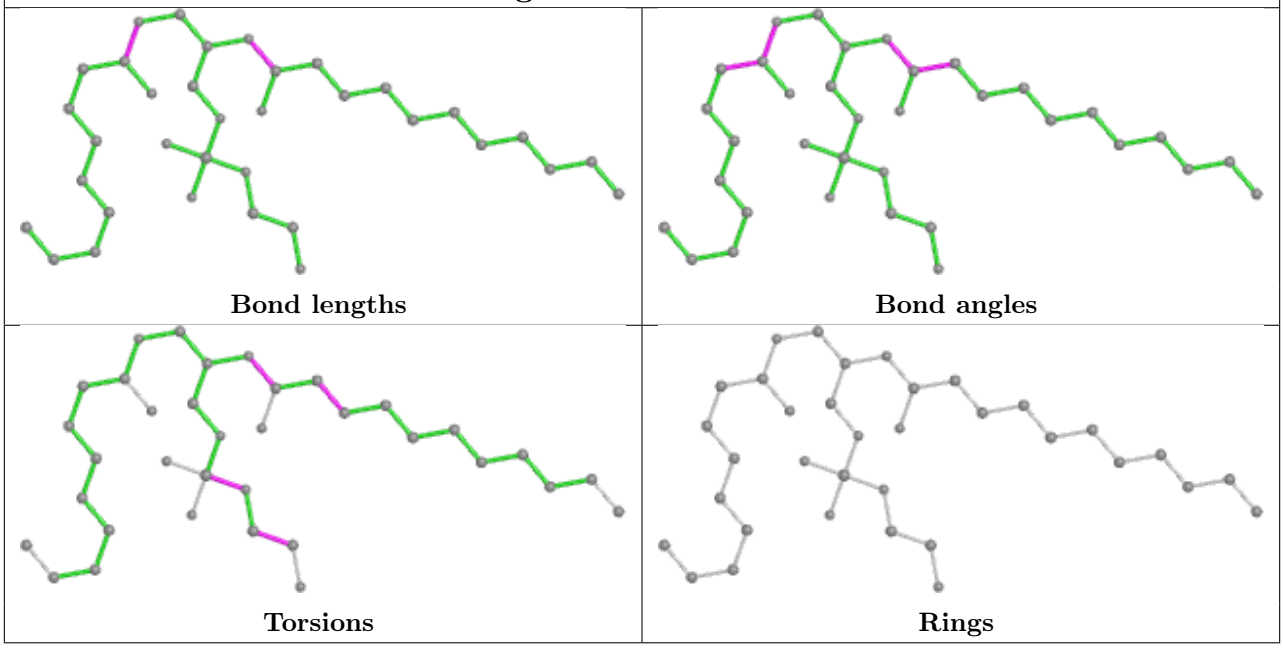
Ligand PTY A 1105



Ligand PTY A 1103



Ligand PTY B 1106



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

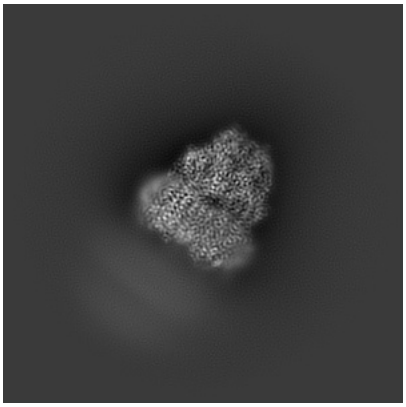
6 Map visualisation

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

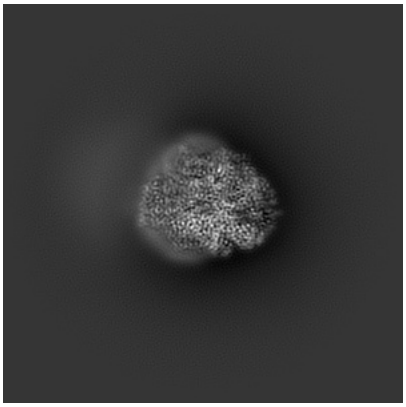
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

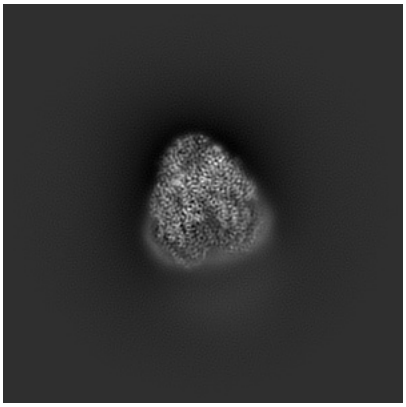
6.1.1 Primary map



X



Y

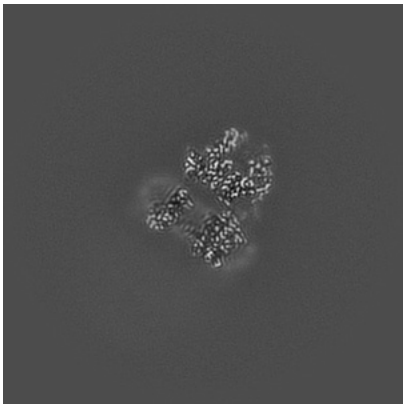


Z

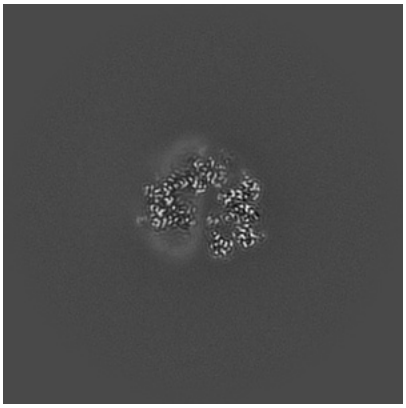
The images above show the map projected in three orthogonal directions.

6.2 Central slices

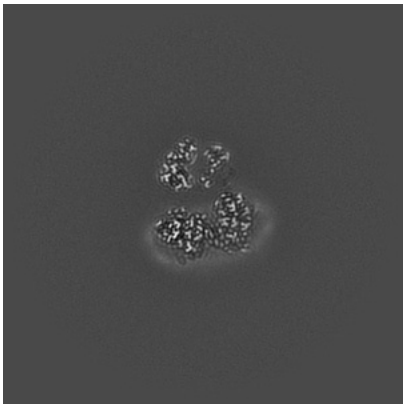
6.2.1 Primary map



X Index: 175



Y Index: 175

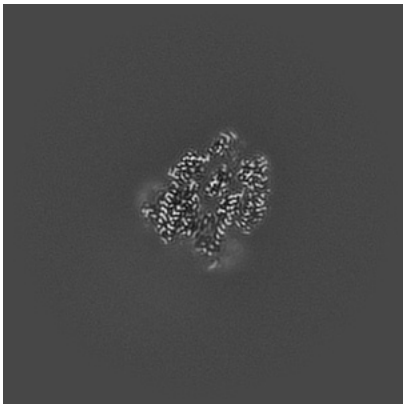


Z Index: 175

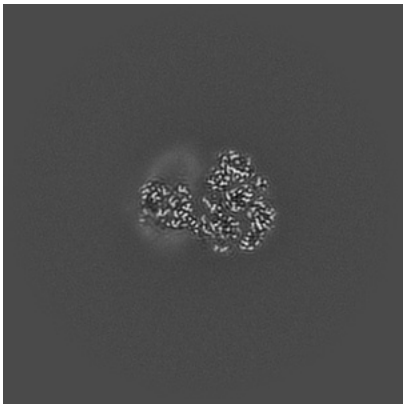
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

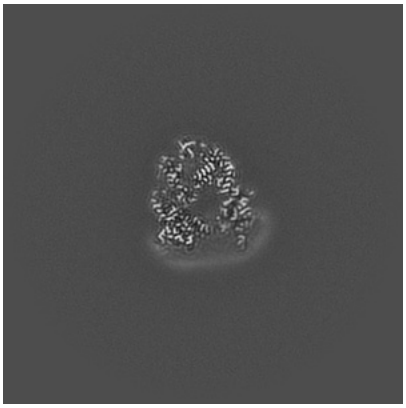
6.3.1 Primary map



X Index: 155



Y Index: 190

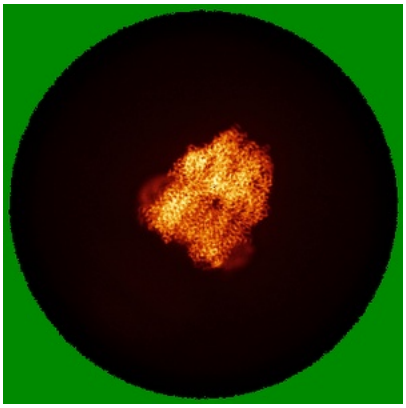


Z Index: 183

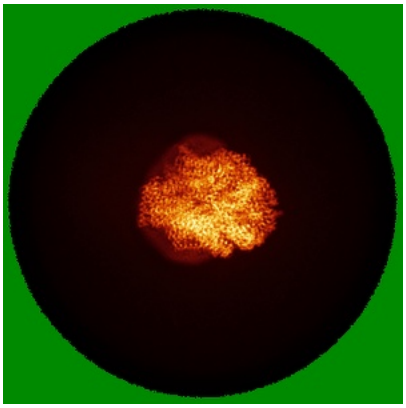
The images above show the largest variance slices of the map in three orthogonal directions.

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

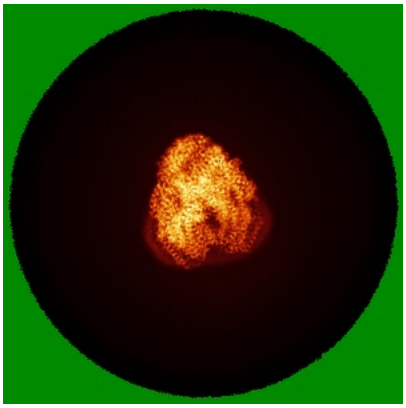
6.4.1 Primary map



X



Y

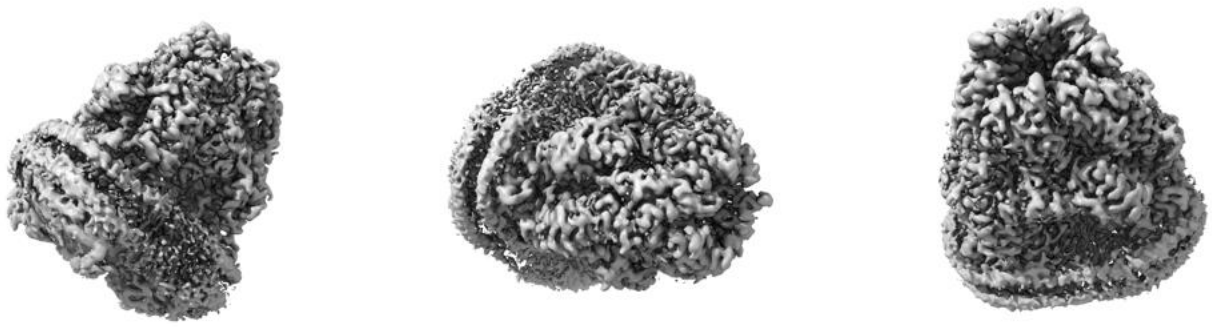


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

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

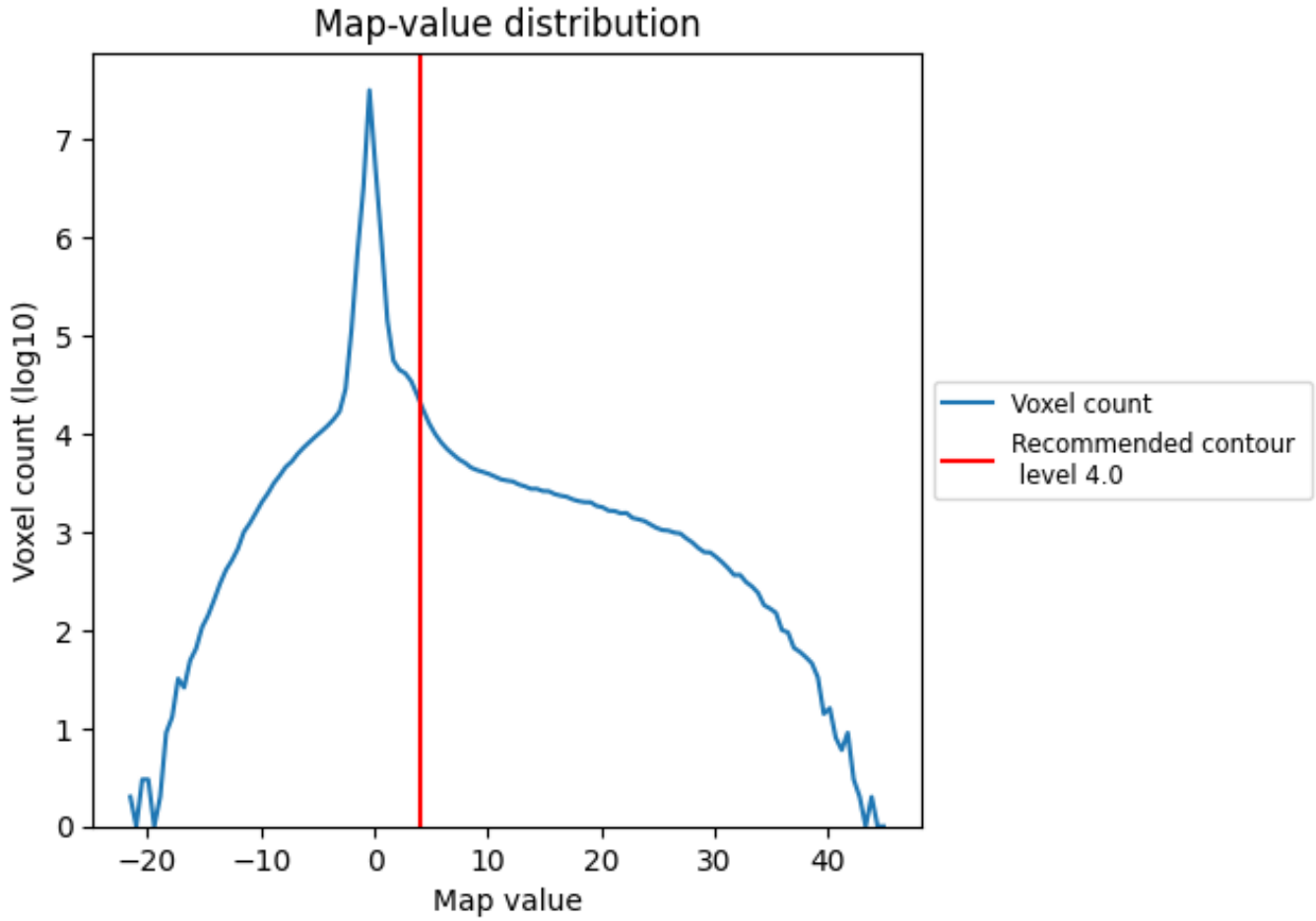
6.6 Mask visualisation (i)

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

7 Map analysis

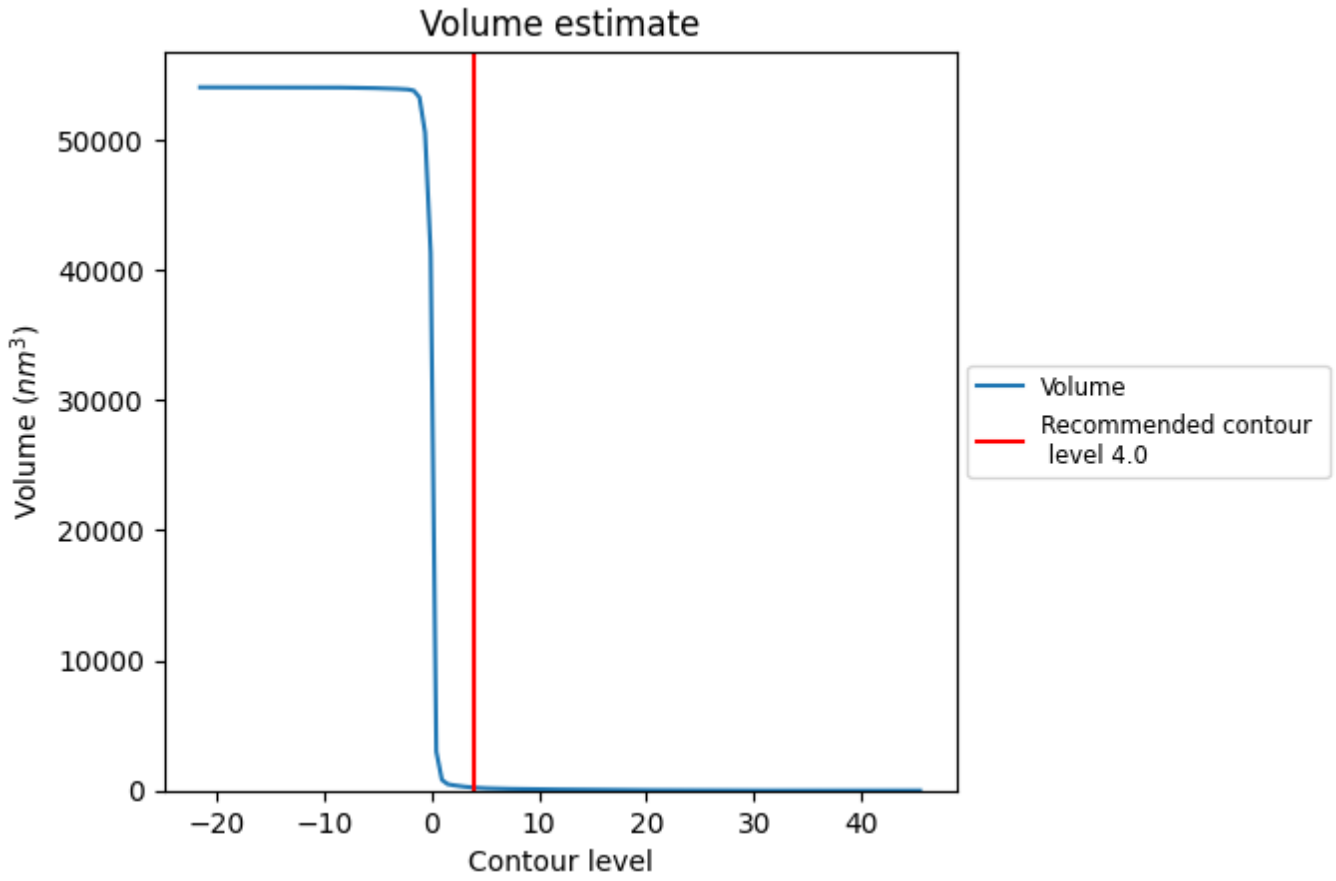
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

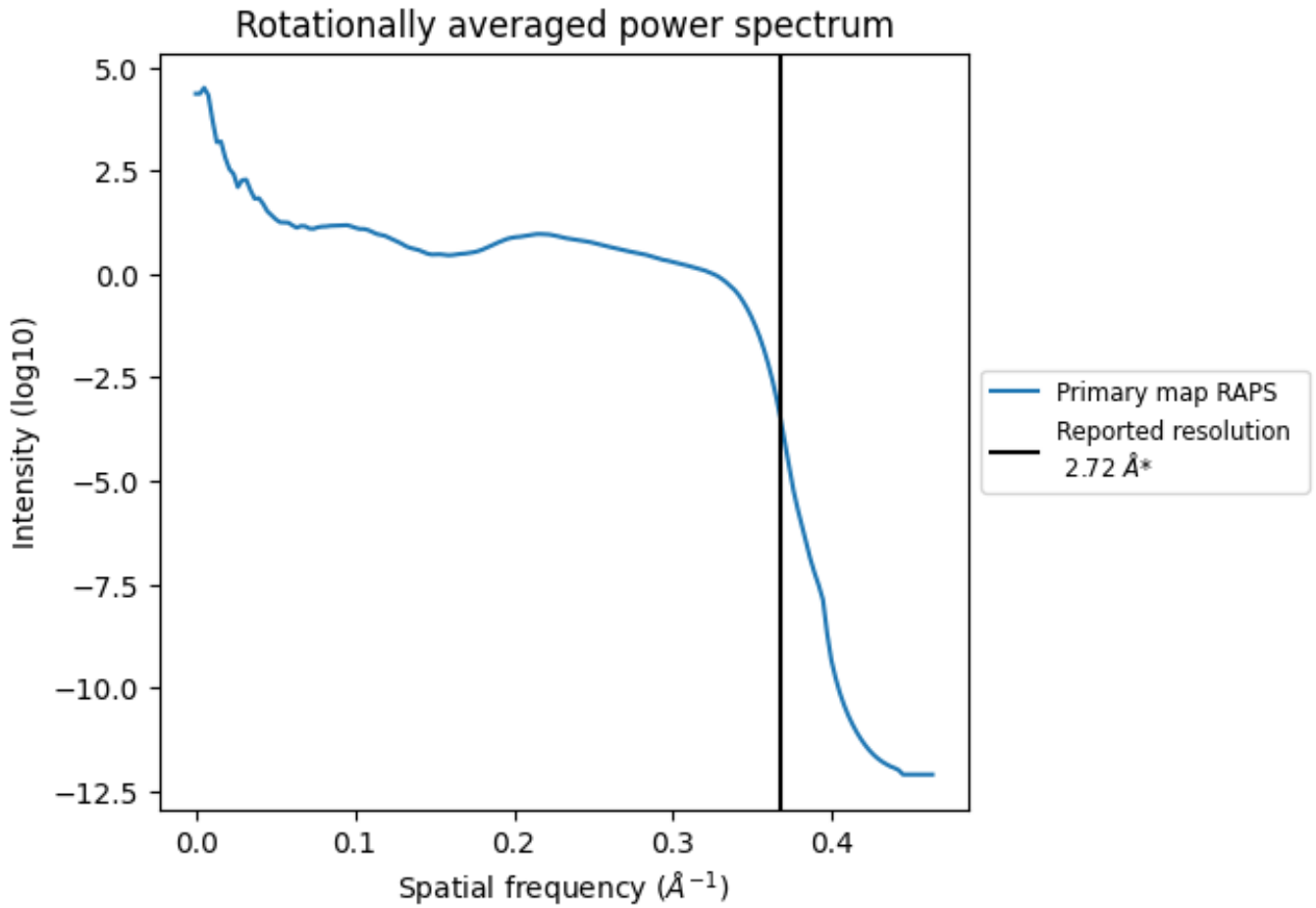
7.2 Volume estimate



The volume at the recommended contour level is 224 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 (i)



*Reported resolution corresponds to spatial frequency of 0.368 $Å^{-1}$

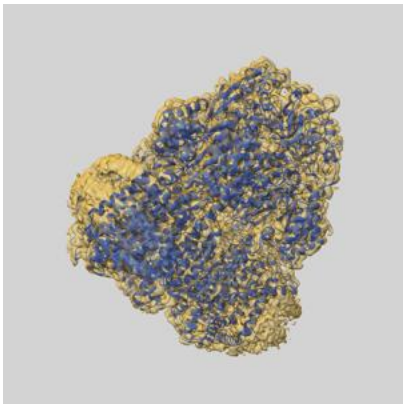
8 Fourier-Shell correlation (i)

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

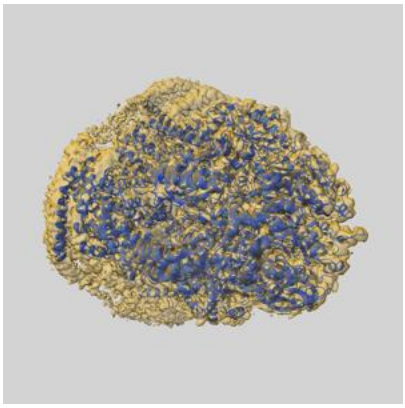
9 Map-model fit

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.

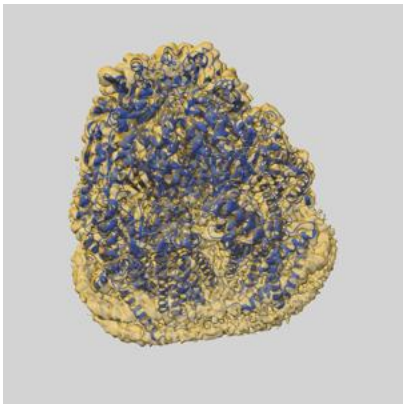
9.1 Map-model overlay



X



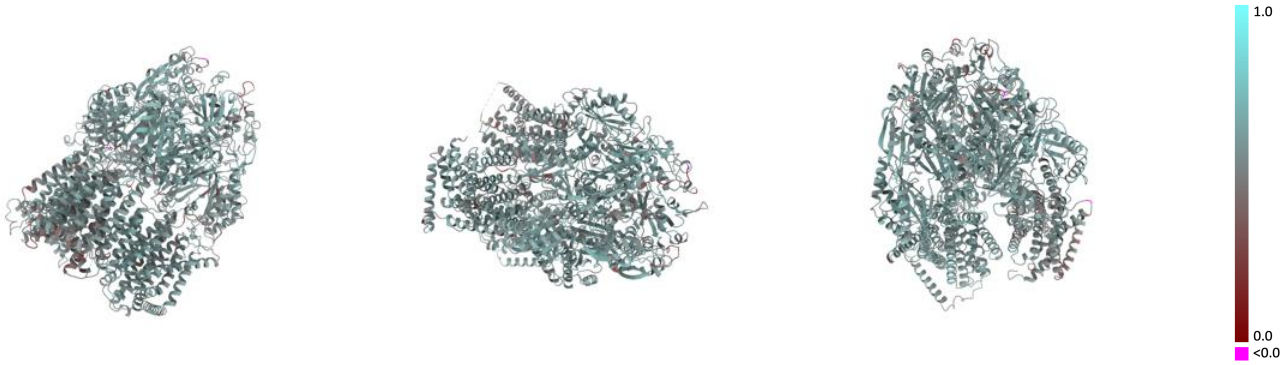
Y



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.

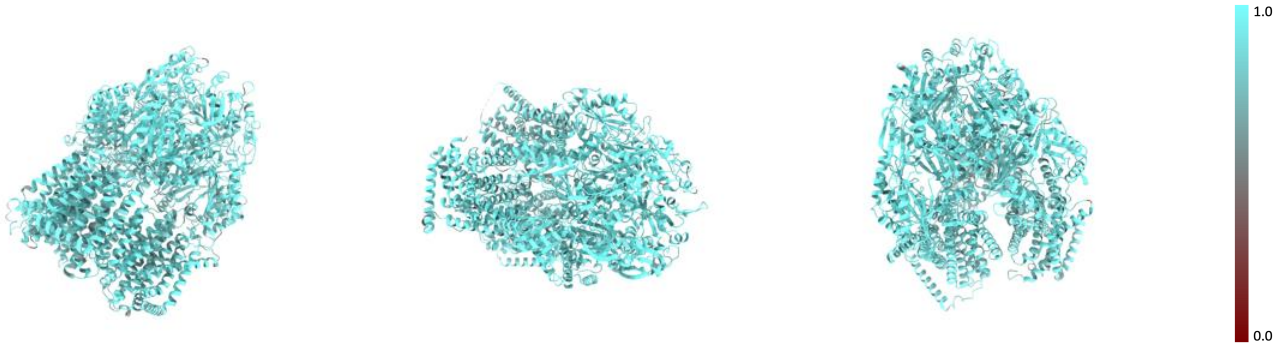
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

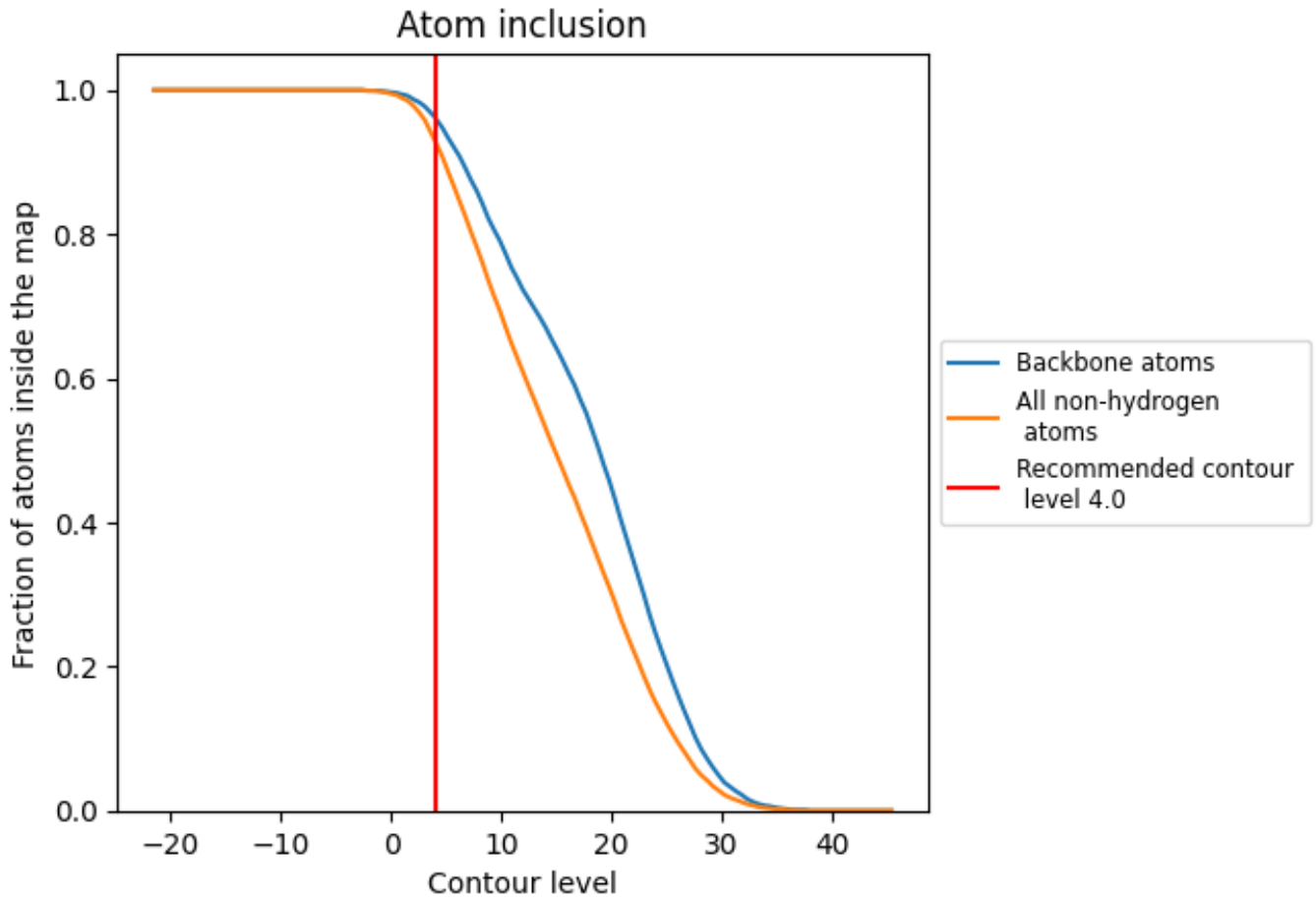
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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	0.9290	0.5660
A	0.9170	0.5510
B	0.9270	0.5650
C	0.9430	0.5840