



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 11:53 PM UTC

PDB ID : 5A63 / pdb_00005a63
EMDB ID : EMD-3061
Title : Cryo-EM structure of the human gamma-secretase complex at 3.4 angstrom resolution.
Authors : Bai, X.; Yan, C.; Yang, G.; Lu, P.; Ma, D.; Sun, L.; Zhou, R.; Scheres, S.H.W.; Shi, Y.
Deposited on : 2015-06-24
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

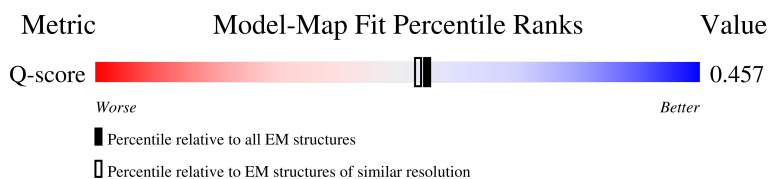
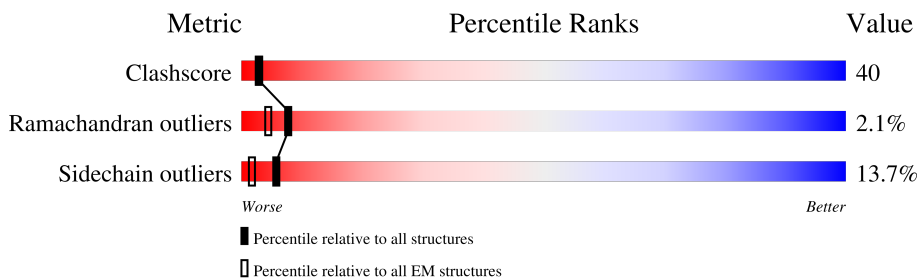
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	709	
2	B	467	
3	C	265	
4	D	101	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	2	100%
5	G	2	100%
5	H	2	50% 100%
5	I	2	50% 100%
5	J	2	50% 50%
6	F	5	40% 60%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 10003 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 Nicastrin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	665	Total	C	N	O	S	0	0
			5222	3312	888	1001	21		

- Molecule 2 is a protein called Presenilin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	215	Total	C	N	O	S	0	0
			1702	1170	249	274	9		

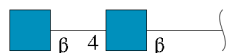
- Molecule 3 is a protein called Gamma-secretase subunit APH-1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	243	Total	C	N	O	S	0	0
			1872	1254	299	315	4		

- Molecule 4 is a protein called Gamma-secretase subunit PEN-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	100	Total	C	N	O	S	0	0
			850	580	134	135	1		

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



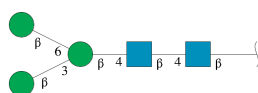
Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	2	Total	C	N	O	0	0
			28	16	2	10		
5	G	2	Total	C	N	O	0	0
			28	16	2	10		

Continued on next page...

Continued from previous page...

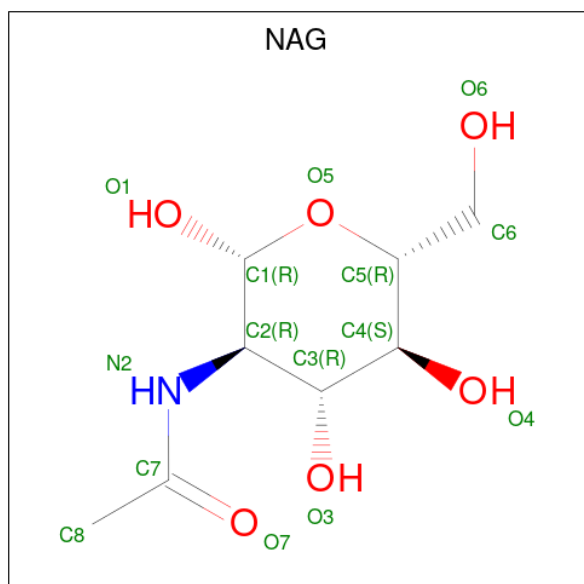
Mol	Chain	Residues	Atoms				AltConf	Trace
5	H	2	Total	C	N	O	0	0
			28	16	2	10		
5	I	2	Total	C	N	O	0	0
			28	16	2	10		
5	J	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is an oligosaccharide called beta-D-mannopyranose-(1-3)-[beta-D-mannopyranos e-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
6	F	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



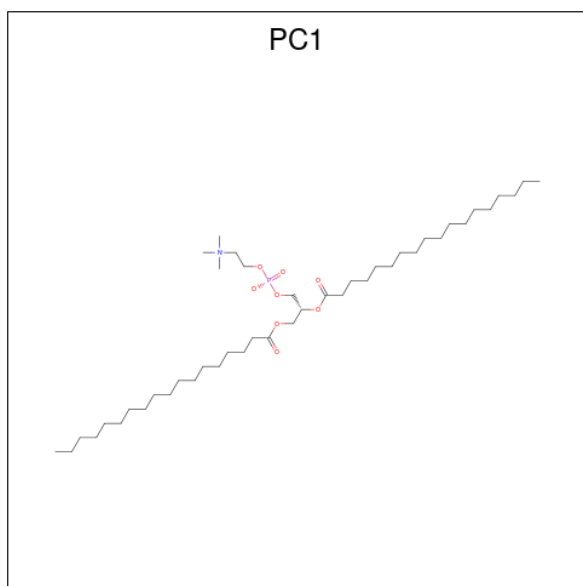
Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	N	O	0
			14	8	1	5	

Continued on next page...

Continued from previous page...

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

- Molecule 8 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).

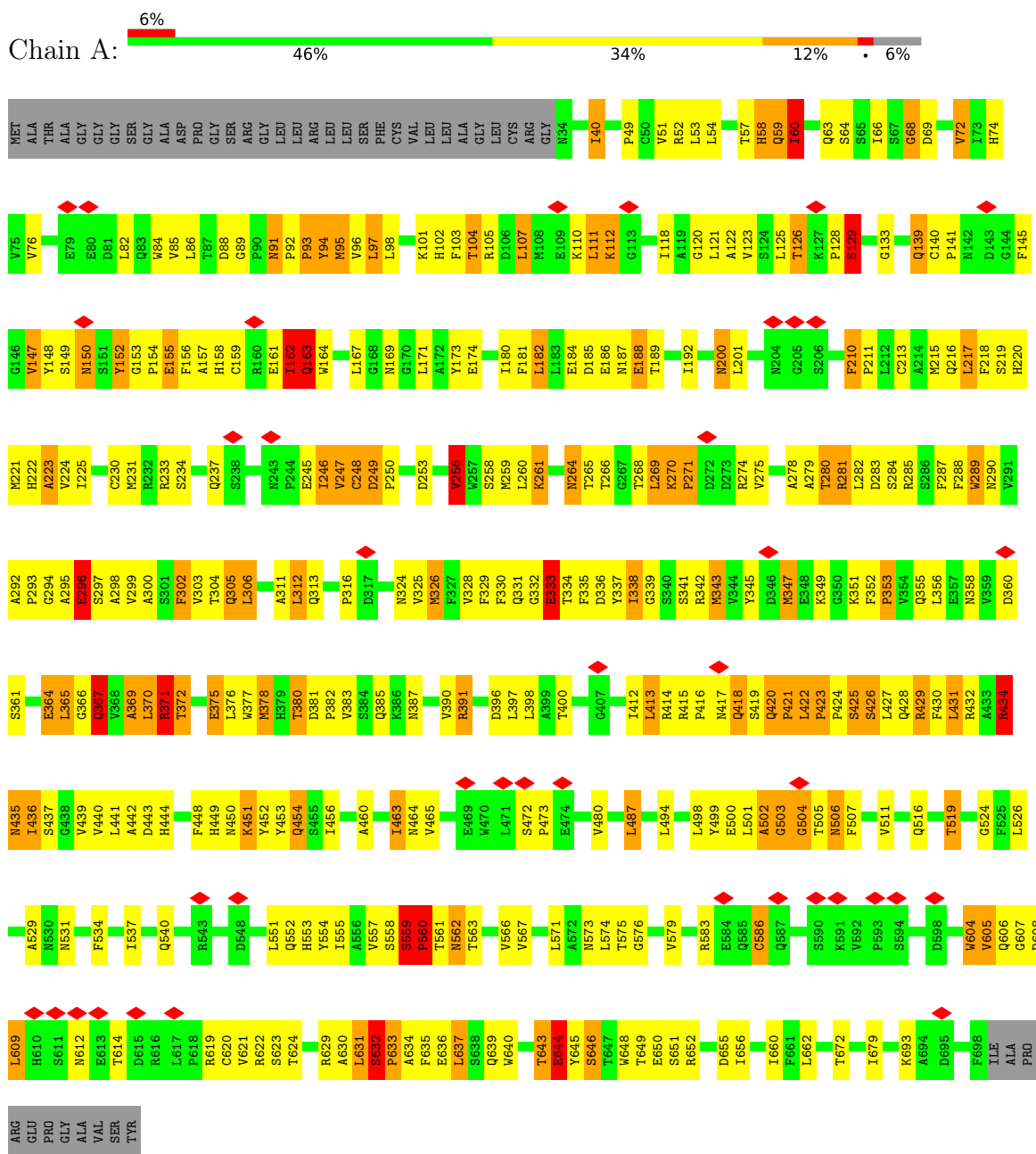


Mol	Chain	Residues	Atoms					AltConf
8	B	1	Total	C	N	O	P	0
			43	33	1	8	1	
8	C	1	Total	C	N	O	P	0
			43	33	1	8	1	

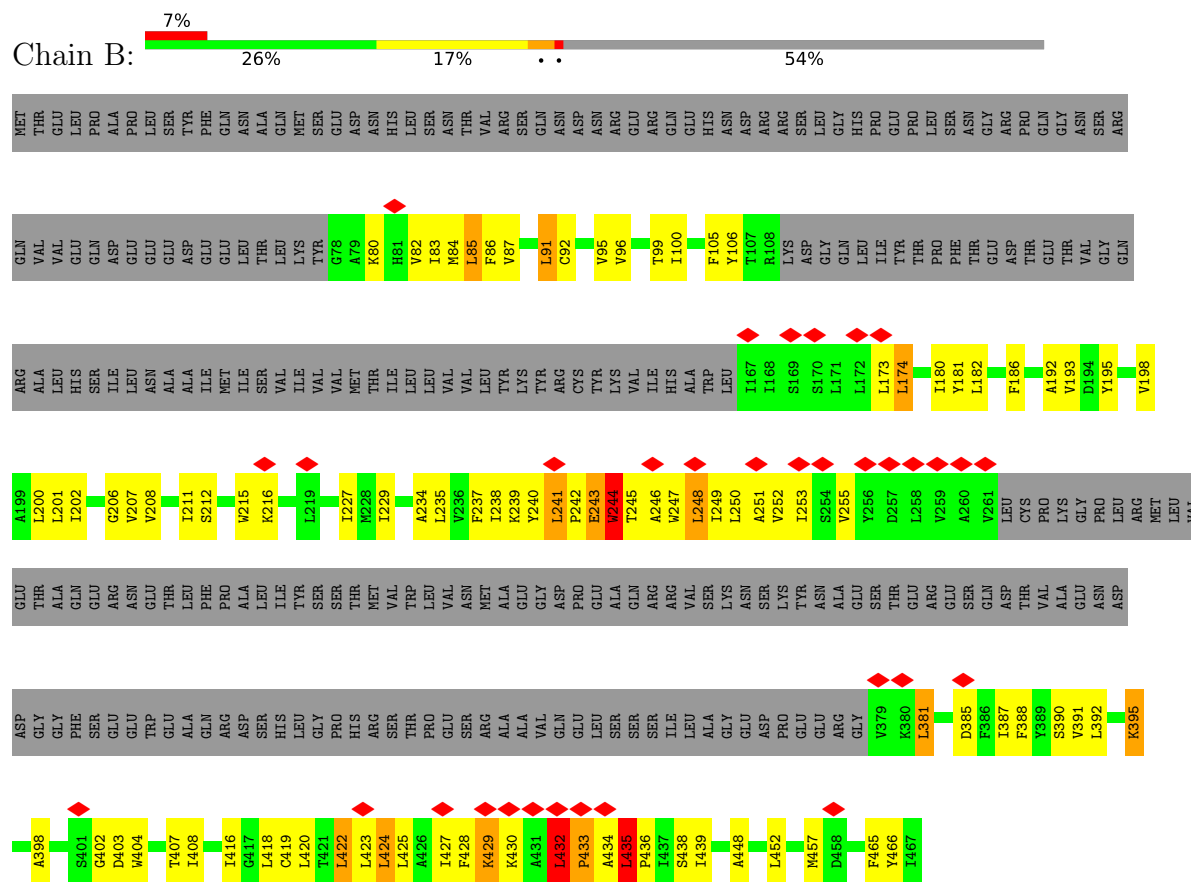
3 Residue-property plots

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

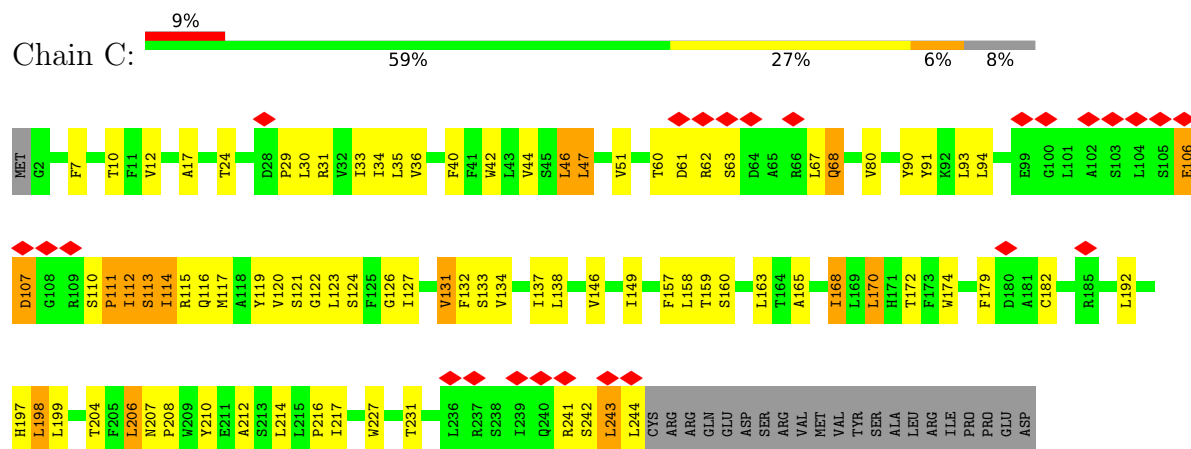
• Molecule 1: Nicastrin



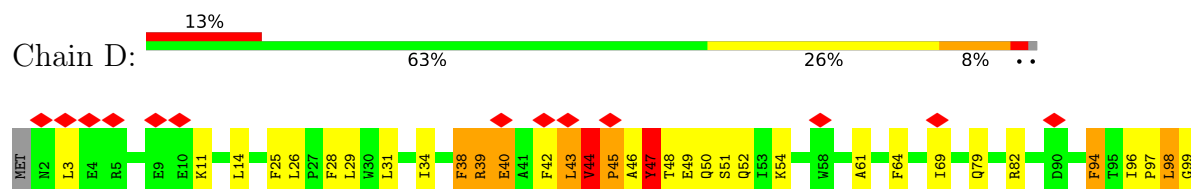
- Molecule 2: Presenilin-1



- Molecule 3: Gamma-secretase subunit APH-1A



- Molecule 4: Gamma-secretase subunit PEN-2





- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



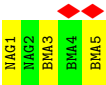
- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



- Molecule 6: beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	159549	Depositor
Resolution determination method	Not provided	
CTF correction method	EACH PARTICLE	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	38	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	3200	Depositor
Magnification	35714	Depositor
Image detector	GATAN K2 (4k x 4k)	Depositor
Maximum map value	0.447	Depositor
Minimum map value	-0.272	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.08	Depositor
Map size ($\text{\AA}$)	252.0, 252.0, 252.0	wwPDB
Map dimensions	180, 180, 180	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.4, 1.4, 1.4	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PC1, BMA, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.73	11/5345 (0.2%)	1.13	46/7284 (0.6%)
2	B	0.59	1/1748 (0.1%)	1.23	8/2385 (0.3%)
3	C	0.61	2/1924 (0.1%)	1.26	5/2624 (0.2%)
4	D	0.63	3/883 (0.3%)	1.12	4/1205 (0.3%)
All	All	0.68	17/9900 (0.2%)	1.18	63/13498 (0.5%)

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	3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	422	LEU	C-N	6.48	1.41	1.33
1	A	423	PRO	C-N	6.09	1.40	1.33
1	A	292	ALA	C-N	5.89	1.41	1.34
1	A	420	GLN	C-N	5.51	1.40	1.33
1	A	607	GLY	C-N	5.48	1.40	1.33
1	A	632	SER	C-N	5.38	1.40	1.33
1	A	293	PRO	N-CD	5.36	1.55	1.47
1	A	608	PRO	N-CD	5.35	1.55	1.47
1	A	421	PRO	N-CD	5.30	1.55	1.47
4	D	44	VAL	C-N	5.29	1.41	1.34
3	C	111	PRO	N-CD	5.25	1.55	1.47
4	D	101	PRO	N-CD	5.20	1.55	1.47
3	C	110	SER	C-N	5.13	1.41	1.34
2	B	433	PRO	N-CD	5.08	1.54	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	271	PRO	N-CD	5.06	1.54	1.47
1	A	633	PRO	N-CD	5.06	1.54	1.47
4	D	45	PRO	N-CD	5.03	1.54	1.47

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	372	THR	N-CA-C	10.88	122.90	111.14
1	A	370	LEU	N-CA-C	10.35	122.32	111.14
1	A	161	GLU	N-CA-C	10.06	122.01	111.14
1	A	92	PRO	N-CA-C	7.44	119.78	110.70
1	A	644	GLU	N-CA-C	7.42	122.45	112.88
2	B	434	ALA	N-CA-C	7.22	118.94	111.14
1	A	423	PRO	CA-C-N	-6.91	112.37	119.83
1	A	423	PRO	C-N-CA	-6.91	112.37	119.83
1	A	426	SER	N-CA-C	-6.85	103.04	111.33
3	C	199	LEU	CA-C-O	-6.80	113.34	120.55
1	A	422	LEU	CA-C-N	-6.67	113.51	120.38
1	A	422	LEU	C-N-CA	-6.67	113.51	120.38
1	A	607	GLY	CA-C-N	-6.62	113.14	119.76
1	A	607	GLY	C-N-CA	-6.62	113.14	119.76
1	A	420	GLN	CA-C-N	-6.61	113.17	119.85
1	A	420	GLN	C-N-CA	-6.61	113.17	119.85
1	A	506	ASN	N-CA-C	6.59	118.54	111.36
1	A	367	GLN	N-CA-C	6.45	120.30	111.39
1	A	503	GLY	N-CA-C	6.40	124.46	115.43
1	A	643	THR	N-CA-C	6.39	118.25	111.28
2	B	87	VAL	O-C-N	6.31	124.46	120.42
1	A	60	ILE	N-CA-C	-6.30	98.55	108.95
1	A	296	GLU	N-CA-C	6.26	118.18	111.36
1	A	632	SER	CA-C-N	-6.24	113.20	119.56
1	A	632	SER	C-N-CA	-6.24	113.20	119.56
1	A	434	ARG	N-CA-C	6.21	120.44	112.12
1	A	162	ILE	N-CA-C	6.14	122.11	109.34
1	A	247	VAL	N-CA-C	6.08	116.86	110.72
2	B	227	ILE	N-CA-CB	6.00	118.70	110.54
1	A	502	ALA	N-CA-C	-5.99	104.75	111.28
1	A	369	ALA	N-CA-C	5.93	117.74	111.28
1	A	640	TRP	N-CA-C	5.89	117.70	111.28
1	A	560	PRO	CA-N-CD	-5.72	103.99	112.00
4	D	38	PHE	N-CA-C	-5.69	105.00	111.14
4	D	44	VAL	CA-C-N	-5.63	112.80	119.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	44	VAL	C-N-CA	-5.63	112.80	119.05
1	A	40	ILE	N-CA-C	5.62	115.86	110.74
3	C	63	SER	N-CA-C	5.59	117.37	111.28
1	A	200	ASN	N-CA-C	5.56	119.16	112.93
1	A	91	ASN	CA-C-N	5.53	126.07	120.38
1	A	91	ASN	C-N-CA	5.53	126.07	120.38
2	B	244	TRP	N-CA-C	5.48	117.33	111.36
3	C	110	SER	CA-C-N	-5.43	113.02	119.05
3	C	110	SER	C-N-CA	-5.43	113.02	119.05
1	A	417	ASN	N-CA-C	5.38	117.15	111.28
2	B	432	LEU	CA-C-N	-5.34	114.06	119.83
2	B	432	LEU	C-N-CA	-5.34	114.06	119.83
3	C	168	ILE	N-CA-CB	5.34	116.80	110.55
1	A	381	ASP	CA-C-N	5.29	124.92	119.05
1	A	381	ASP	C-N-CA	5.29	124.92	119.05
1	A	292	ALA	CA-C-N	-5.26	113.61	119.19
1	A	292	ALA	C-N-CA	-5.26	113.61	119.19
1	A	246	ILE	CB-CA-C	-5.23	106.25	111.80
1	A	93	PRO	N-CA-C	-5.23	101.70	112.47
4	D	47	TYR	N-CA-C	-5.21	101.37	109.24
1	A	40	ILE	CB-CA-C	-5.18	105.09	111.94
1	A	289	TRP	N-CA-C	5.13	116.56	111.07
2	B	398	ALA	N-CA-C	5.11	116.54	110.97
1	A	504	GLY	N-CA-C	5.07	118.38	112.50
1	A	302	PHE	N-CA-C	5.06	116.88	111.36
1	A	559	SER	CA-C-N	-5.06	113.52	119.84
1	A	559	SER	C-N-CA	-5.06	113.52	119.84
2	B	243	GLU	N-CA-C	-5.04	105.78	111.28

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	210	PHE	Peptide
1	A	256	VAL	Peptide
1	A	68	GLY	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5222	0	5113	572	0
2	B	1702	0	1793	112	0
3	C	1872	0	1911	93	0
4	D	850	0	840	52	0
5	E	28	0	25	0	0
5	G	28	0	25	0	0
5	H	28	0	25	1	0
5	I	28	0	25	0	0
5	J	28	0	25	2	0
6	F	61	0	52	0	0
7	A	70	0	65	3	0
8	B	43	0	60	0	0
8	C	43	0	60	1	0
All	All	10003	0	10019	792	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 40.

All (792) 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:316:PRO:HG2	1:A:507:PHE:CD2	1.52	1.42
1:A:152:TYR:CE1	1:A:383:VAL:HG21	1.61	1.36
1:A:279:ALA:O	1:A:364:GLU:HG2	1.29	1.28
1:A:633:PRO:HB2	1:A:645:TYR:CD2	1.66	1.28
1:A:155:GLU:HG3	1:A:156:PHE:CE1	1.71	1.24
1:A:95:MET:CE	1:A:217:LEU:HD11	1.69	1.20
4:D:47:TYR:CB	4:D:50:GLN:HB2	1.72	1.19
4:D:50:GLN:OE1	4:D:54:LYS:HD2	1.43	1.19
1:A:260:LEU:HD22	1:A:312:LEU:HD22	1.23	1.17
1:A:95:MET:CE	1:A:215:MET:HE3	1.75	1.17
1:A:268:THR:CG2	1:A:355:GLN:HG3	1.73	1.17
1:A:156:PHE:CD2	1:A:421:PRO:HB3	1.82	1.14
1:A:223:ALA:HB2	1:A:247:VAL:HG22	1.14	1.13
3:C:34:ILE:HD11	3:C:120:VAL:HB	1.30	1.13
4:D:47:TYR:HB2	4:D:50:GLN:CB	1.79	1.13
1:A:378:MET:HE2	1:A:398:LEU:HD22	1.32	1.11
1:A:586:CYS:CB	1:A:620:CYS:SG	2.39	1.10
4:D:40:GLU:O	4:D:44:VAL:HG23	1.51	1.10

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:82:VAL:HG22	2:B:422:LEU:HD22	1.15	1.09
1:A:316:PRO:CG	1:A:507:PHE:CD2	2.35	1.09
1:A:299:VAL:O	1:A:303:VAL:HG23	1.55	1.07
1:A:95:MET:HE3	1:A:217:LEU:HD11	1.28	1.06
1:A:604:TRP:HD1	1:A:620:CYS:SG	1.76	1.06
1:A:540:GLN:CG	1:A:606:GLN:HE21	1.68	1.05
1:A:316:PRO:HG2	1:A:507:PHE:CE2	1.92	1.05
1:A:282:LEU:HD13	1:A:329:PHE:HB3	1.08	1.04
1:A:249:ASP:HB3	1:A:557:VAL:CG2	1.88	1.04
1:A:311:ALA:O	1:A:511:VAL:HG23	1.55	1.04
1:A:540:GLN:HG2	1:A:606:GLN:NE2	1.73	1.04
1:A:422:LEU:HD23	1:A:423:PRO:HD2	1.38	1.03
1:A:378:MET:CE	1:A:398:LEU:HD22	1.88	1.02
1:A:152:TYR:O	1:A:154:PRO:HD3	1.60	1.02
1:A:365:LEU:H	1:A:365:LEU:HD12	1.24	1.02
1:A:432:ARG:HH12	1:A:644:GLU:HB2	1.21	1.02
1:A:95:MET:HE2	1:A:215:MET:HE3	1.04	1.02
1:A:378:MET:O	1:A:416:PRO:HD3	1.61	1.00
1:A:422:LEU:HD23	1:A:423:PRO:CD	1.90	1.00
1:A:245:GLU:OE2	4:D:98:LEU:HD21	1.62	1.00
1:A:156:PHE:HB3	1:A:421:PRO:HB3	1.40	0.99
1:A:223:ALA:HB2	1:A:247:VAL:CG2	1.91	0.99
1:A:279:ALA:HB2	1:A:328:VAL:CG1	1.93	0.99
1:A:282:LEU:HD23	1:A:331:GLN:NE2	1.77	0.99
1:A:586:CYS:SG	1:A:620:CYS:SG	1.12	0.99
1:A:367:GLN:O	1:A:443:ASP:HB3	1.63	0.98
4:D:44:VAL:HG11	4:D:47:TYR:CD1	1.97	0.98
1:A:152:TYR:CE1	1:A:383:VAL:CG2	2.47	0.98
1:A:250:PRO:HB3	1:A:635:PHE:CD2	1.97	0.98
1:A:250:PRO:HB3	1:A:635:PHE:CE2	1.98	0.98
1:A:280:THR:OG1	1:A:305:GLN:HG2	1.63	0.97
1:A:311:ALA:C	1:A:511:VAL:HG23	1.89	0.97
1:A:268:THR:HG23	1:A:355:GLN:HG3	1.40	0.97
1:A:260:LEU:CD2	1:A:312:LEU:HD22	1.94	0.97
1:A:424:PRO:HA	1:A:428:GLN:NE2	1.80	0.97
2:B:429:LYS:H	2:B:429:LYS:HD2	1.30	0.96
1:A:140:CYS:HG	1:A:159:CYS:CB	1.79	0.96
1:A:147:VAL:HG11	1:A:431:LEU:HB3	1.44	0.96
1:A:223:ALA:CB	1:A:247:VAL:HG22	1.97	0.95
1:A:633:PRO:CB	1:A:645:TYR:HD2	1.78	0.95
2:B:244:TRP:CE3	2:B:247:TRP:HD1	1.84	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:ASP:HB3	1:A:557:VAL:HG21	1.48	0.94
1:A:230:CYS:SG	1:A:247:VAL:HG13	2.06	0.94
1:A:268:THR:HG21	1:A:355:GLN:HG3	1.50	0.93
1:A:224:VAL:HG21	4:D:101:PRO:HA	1.49	0.93
1:A:152:TYR:HE1	1:A:383:VAL:CG2	1.79	0.93
1:A:281:ARG:HG3	1:A:281:ARG:HH11	1.35	0.92
3:C:34:ILE:HD11	3:C:120:VAL:CB	1.99	0.92
1:A:152:TYR:HE1	1:A:383:VAL:HG21	1.10	0.92
1:A:139:GLN:HG2	1:A:163:GLN:HG2	1.51	0.92
3:C:90:TYR:CE2	3:C:94:LEU:HD11	2.05	0.91
1:A:279:ALA:CB	1:A:328:VAL:CG1	2.49	0.91
1:A:633:PRO:HB2	1:A:645:TYR:HD2	1.04	0.90
1:A:224:VAL:CG2	4:D:101:PRO:HA	2.02	0.89
1:A:540:GLN:HG2	1:A:606:GLN:HE21	1.33	0.89
1:A:622:ARG:HG2	1:A:622:ARG:HH11	1.35	0.89
1:A:397:LEU:CD2	1:A:439:VAL:HG23	2.02	0.89
1:A:156:PHE:CB	1:A:421:PRO:HB3	2.02	0.89
2:B:239:LYS:CG	2:B:240:TYR:CE1	2.55	0.89
1:A:300:ALA:O	1:A:304:THR:HG23	1.71	0.89
1:A:95:MET:HE2	1:A:215:MET:CE	1.98	0.88
1:A:152:TYR:HD1	1:A:153:GLY:N	1.72	0.88
1:A:282:LEU:CD1	1:A:329:PHE:HB3	1.99	0.88
1:A:156:PHE:CG	1:A:421:PRO:HB3	2.08	0.88
1:A:224:VAL:HG21	4:D:100:THR:O	1.73	0.87
1:A:633:PRO:CB	1:A:645:TYR:CD2	2.51	0.87
1:A:586:CYS:SG	1:A:620:CYS:CB	2.62	0.87
2:B:82:VAL:HG22	2:B:422:LEU:CD2	2.03	0.87
1:A:249:ASP:CB	1:A:557:VAL:HG21	2.04	0.87
1:A:316:PRO:HG2	1:A:507:PHE:HD2	1.05	0.87
1:A:361:SER:OG	1:A:501:LEU:HD13	1.74	0.87
2:B:239:LYS:HG2	2:B:240:TYR:CE1	2.10	0.87
1:A:152:TYR:CZ	1:A:383:VAL:HG11	2.10	0.86
1:A:96:VAL:HG22	1:A:118:ILE:HD11	1.57	0.86
1:A:604:TRP:CD1	1:A:620:CYS:SG	2.66	0.86
1:A:162:ILE:HG21	1:A:420:GLN:OE1	1.74	0.85
1:A:378:MET:HE2	1:A:398:LEU:CD2	2.06	0.85
1:A:156:PHE:HD2	1:A:421:PRO:HB3	1.39	0.85
1:A:371:ARG:CB	1:A:371:ARG:HH11	1.88	0.85
1:A:156:PHE:HB3	1:A:421:PRO:CB	2.06	0.85
1:A:156:PHE:CD2	1:A:421:PRO:CB	2.59	0.85
1:A:279:ALA:HB1	1:A:330:PHE:CE2	2.11	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:LEU:HD22	1:A:312:LEU:CD2	2.05	0.84
1:A:635:PHE:HZ	1:A:649:THR:HG23	1.43	0.84
1:A:155:GLU:HG3	1:A:156:PHE:CD1	2.13	0.83
1:A:378:MET:CE	1:A:398:LEU:CD2	2.55	0.83
1:A:140:CYS:SG	1:A:159:CYS:HB3	2.19	0.83
1:A:451:LYS:HB2	1:A:451:LYS:NZ	1.94	0.83
1:A:259:MET:SD	1:A:326:MET:CB	2.66	0.83
1:A:259:MET:SD	1:A:326:MET:HB2	2.19	0.83
1:A:260:LEU:CD2	1:A:312:LEU:CD2	2.56	0.83
2:B:86:PHE:CZ	2:B:419:CYS:SG	2.71	0.83
1:A:128:PRO:O	1:A:129:SER:HB2	1.78	0.83
2:B:198:VAL:HG21	4:D:94:PHE:CE1	2.14	0.82
4:D:3:LEU:HD23	4:D:40:GLU:OE1	1.79	0.82
1:A:268:THR:HG21	1:A:355:GLN:CG	2.10	0.82
1:A:563:THR:O	1:A:567:VAL:HG23	1.78	0.82
1:A:418:GLN:HE21	1:A:419:SER:H	1.28	0.82
1:A:540:GLN:HG3	1:A:606:GLN:HE21	1.42	0.82
2:B:245:THR:O	2:B:249:ILE:HG13	1.80	0.82
1:A:279:ALA:HB1	1:A:330:PHE:HE2	1.45	0.81
3:C:17:ALA:HB2	3:C:168:ILE:HG21	1.62	0.81
1:A:324:ASN:OD1	1:A:325:VAL:N	2.12	0.81
2:B:243:GLU:O	2:B:247:TRP:CD1	2.33	0.81
1:A:68:GLY:HA2	1:A:218:PHE:CD1	2.16	0.81
2:B:96:VAL:HG21	2:B:390:SER:HB3	1.62	0.81
1:A:279:ALA:CB	1:A:328:VAL:HG13	2.11	0.81
1:A:311:ALA:O	1:A:511:VAL:CG2	2.28	0.81
1:A:299:VAL:CG2	1:A:553:HIS:NE2	2.44	0.80
2:B:244:TRP:CZ3	2:B:247:TRP:HD1	2.00	0.80
1:A:586:CYS:HG	1:A:620:CYS:CB	1.91	0.80
1:A:147:VAL:CG1	1:A:431:LEU:HB3	2.12	0.80
1:A:397:LEU:HD23	1:A:439:VAL:HG23	1.64	0.80
1:A:311:ALA:C	1:A:511:VAL:CG2	2.56	0.79
1:A:316:PRO:CG	1:A:507:PHE:HD2	1.82	0.79
1:A:68:GLY:CA	1:A:218:PHE:CE1	2.66	0.79
1:A:432:ARG:NH1	1:A:644:GLU:HB2	1.97	0.78
1:A:96:VAL:HG23	1:A:121:LEU:HB3	1.66	0.78
2:B:99:THR:HG21	2:B:181:TYR:HE1	1.49	0.78
1:A:280:THR:OG1	1:A:305:GLN:CG	2.30	0.78
1:A:245:GLU:OE2	4:D:98:LEU:CD2	2.31	0.77
2:B:244:TRP:CZ3	2:B:247:TRP:CD1	2.72	0.77
1:A:152:TYR:C	1:A:154:PRO:HD3	2.10	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:MET:O	1:A:347:MET:HG2	1.84	0.77
1:A:281:ARG:HG3	1:A:281:ARG:NH1	1.98	0.77
1:A:605:VAL:CG1	1:A:621:VAL:HG23	2.15	0.76
2:B:435:LEU:H	2:B:436:PRO:HD3	1.50	0.76
1:A:95:MET:CE	1:A:217:LEU:CD1	2.59	0.76
1:A:152:TYR:CD1	1:A:153:GLY:N	2.53	0.76
3:C:60:THR:HG21	3:C:67:LEU:HD21	1.67	0.76
1:A:269:LEU:HB3	1:A:358:ASN:HD21	1.48	0.76
2:B:237:PHE:O	2:B:241:LEU:HB2	1.85	0.76
2:B:435:LEU:CD1	2:B:439:ILE:CD1	2.64	0.76
1:A:223:ALA:CA	1:A:247:VAL:HG21	2.17	0.75
2:B:448:ALA:HB1	3:C:47:LEU:HD21	1.68	0.75
1:A:250:PRO:HA	1:A:649:THR:HG22	1.67	0.75
1:A:635:PHE:CZ	1:A:649:THR:HG23	2.22	0.74
2:B:239:LYS:HG3	2:B:240:TYR:CE1	2.23	0.74
1:A:279:ALA:O	1:A:364:GLU:CG	2.24	0.74
1:A:637:LEU:CB	1:A:639:GLN:HE21	2.01	0.73
4:D:47:TYR:HB2	4:D:50:GLN:HB2	0.83	0.73
1:A:278:ALA:C	1:A:305:GLN:HE22	1.97	0.73
1:A:64:SER:CB	1:A:219:SER:H	2.01	0.73
1:A:637:LEU:HB3	1:A:639:GLN:HE21	1.52	0.73
1:A:139:GLN:CG	1:A:163:GLN:HG2	2.18	0.73
1:A:269:LEU:HB3	1:A:358:ASN:ND2	2.04	0.73
2:B:85:LEU:HD22	2:B:418:LEU:HD21	1.70	0.73
2:B:435:LEU:N	2:B:436:PRO:CD	2.52	0.73
2:B:435:LEU:HD12	2:B:439:ILE:HG13	1.70	0.73
2:B:429:LYS:HD2	2:B:429:LYS:N	2.03	0.73
1:A:397:LEU:HG	1:A:439:VAL:HG21	1.69	0.73
1:A:282:LEU:HD13	1:A:329:PHE:CB	2.04	0.72
1:A:299:VAL:HG22	1:A:553:HIS:NE2	2.04	0.72
1:A:633:PRO:HB2	1:A:645:TYR:CE2	2.23	0.72
1:A:266:THR:HB	7:A:1714:NAG:O7	1.88	0.72
1:A:418:GLN:HE21	1:A:419:SER:N	1.87	0.72
2:B:241:LEU:HG	2:B:245:THR:HG22	1.70	0.72
1:A:418:GLN:HE21	1:A:418:GLN:CA	2.03	0.72
2:B:174:LEU:HG	2:B:229:ILE:HD11	1.71	0.72
1:A:422:LEU:HD23	1:A:423:PRO:N	2.03	0.72
1:A:140:CYS:SG	1:A:159:CYS:CB	2.74	0.72
1:A:418:GLN:NE2	1:A:419:SER:H	1.86	0.72
1:A:453:TYR:O	1:A:454:GLN:C	2.32	0.72
1:A:259:MET:SD	1:A:326:MET:HB3	2.30	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:504:GLY:O	1:A:505:THR:OG1	2.08	0.71
3:C:112:ILE:HD13	3:C:112:ILE:H	1.56	0.71
1:A:290:ASN:O	1:A:552:GLN:HG3	1.88	0.71
1:A:299:VAL:O	1:A:303:VAL:CG2	2.34	0.71
1:A:64:SER:HB3	1:A:219:SER:C	2.15	0.71
1:A:224:VAL:HG21	4:D:101:PRO:CA	2.20	0.71
1:A:64:SER:HB3	1:A:219:SER:H	1.56	0.70
2:B:239:LYS:CG	2:B:240:TYR:HE1	2.01	0.70
1:A:253:ASP:HB3	1:A:559:SER:O	1.91	0.70
1:A:261:LYS:O	1:A:324:ASN:ND2	2.24	0.70
1:A:451:LYS:HB2	1:A:451:LYS:HZ2	1.55	0.70
1:A:249:ASP:HB3	1:A:557:VAL:HG23	1.73	0.70
1:A:279:ALA:CB	1:A:330:PHE:HE2	2.05	0.70
1:A:367:GLN:O	1:A:443:ASP:CB	2.38	0.70
3:C:34:ILE:CG1	3:C:120:VAL:HG11	2.21	0.69
1:A:133:GLY:HA2	1:A:452:TYR:HE1	1.56	0.69
1:A:171:LEU:HD23	1:A:287:PHE:CE2	2.26	0.69
1:A:66:ILE:HD13	1:A:220:HIS:ND1	2.07	0.69
1:A:316:PRO:CG	1:A:507:PHE:CE2	2.72	0.69
1:A:150:ASN:O	1:A:154:PRO:HG3	1.91	0.69
1:A:424:PRO:HA	1:A:428:GLN:HE22	1.57	0.69
1:A:279:ALA:HB2	1:A:328:VAL:HG11	1.73	0.69
2:B:239:LYS:HG2	2:B:240:TYR:HE1	1.55	0.69
4:D:3:LEU:HG	4:D:11:LYS:HE2	1.75	0.69
1:A:233:ARG:O	1:A:237:GLN:HG2	1.92	0.69
1:A:397:LEU:CD2	1:A:439:VAL:CG2	2.71	0.69
1:A:164:TRP:CE2	1:A:423:PRO:HA	2.28	0.68
1:A:372:THR:HG23	1:A:449:HIS:CD2	2.28	0.68
1:A:94:TYR:O	1:A:118:ILE:HG13	1.94	0.68
1:A:95:MET:HG2	1:A:120:GLY:O	1.94	0.68
1:A:223:ALA:N	1:A:247:VAL:CG2	2.57	0.68
1:A:300:ALA:HB2	1:A:463:ILE:HD12	1.76	0.68
1:A:311:ALA:HB1	1:A:511:VAL:CG2	2.24	0.68
1:A:171:LEU:HD23	1:A:287:PHE:HE2	1.59	0.68
1:A:300:ALA:HB1	1:A:369:ALA:HB2	1.76	0.68
1:A:633:PRO:O	1:A:637:LEU:HD22	1.94	0.68
3:C:179:PHE:O	3:C:182:CYS:SG	2.52	0.68
1:A:141:PRO:HG2	1:A:424:PRO:HG3	1.75	0.68
1:A:223:ALA:CA	1:A:247:VAL:CG2	2.72	0.68
1:A:256:VAL:HG22	1:A:329:PHE:HB2	1.76	0.68
1:A:68:GLY:N	1:A:218:PHE:CD1	2.62	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:VAL:HG23	1:A:121:LEU:CB	2.24	0.67
1:A:111:LEU:HD21	1:A:118:ILE:HD13	1.76	0.67
1:A:311:ALA:HB1	1:A:511:VAL:HG22	1.76	0.67
1:A:281:ARG:HB2	1:A:333:GLU:HB2	1.75	0.67
1:A:68:GLY:N	1:A:218:PHE:CE1	2.63	0.67
2:B:182:LEU:HD21	2:B:201:LEU:HD23	1.76	0.67
1:A:54:LEU:HD12	1:A:248:CYS:SG	2.35	0.67
2:B:435:LEU:HD11	2:B:439:ILE:CD1	2.24	0.67
3:C:163:LEU:HD11	3:C:217:ILE:HD13	1.75	0.67
1:A:72:VAL:HG13	1:A:94:TYR:CD1	2.29	0.67
1:A:256:VAL:HG21	1:A:567:VAL:HG12	1.77	0.67
1:A:605:VAL:HG11	1:A:621:VAL:CG2	2.24	0.67
1:A:64:SER:N	1:A:219:SER:O	2.28	0.67
1:A:224:VAL:HG11	4:D:99:GLY:O	1.94	0.66
1:A:268:THR:HG21	1:A:355:GLN:CD	2.21	0.66
2:B:435:LEU:CD1	2:B:439:ILE:HD11	2.26	0.66
1:A:223:ALA:HA	1:A:247:VAL:HG21	1.77	0.66
3:C:34:ILE:CD1	3:C:120:VAL:HB	2.18	0.66
1:A:68:GLY:CA	1:A:218:PHE:CD1	2.77	0.66
1:A:299:VAL:HG11	1:A:526:LEU:HD21	1.76	0.66
1:A:529:ALA:HB2	1:A:551:LEU:CD1	2.24	0.66
1:A:369:ALA:HB2	1:A:463:ILE:HD11	1.77	0.66
1:A:282:LEU:HD23	1:A:331:GLN:HE21	1.61	0.66
1:A:378:MET:O	1:A:416:PRO:CD	2.43	0.66
1:A:559:SER:CB	1:A:560:PRO:HD3	2.25	0.66
3:C:163:LEU:HD21	3:C:204:THR:HG22	1.76	0.66
1:A:95:MET:HE3	1:A:217:LEU:CD1	2.17	0.65
1:A:305:GLN:HB2	1:A:365:LEU:HD11	1.78	0.65
1:A:249:ASP:OD1	1:A:652:ARG:NH2	2.29	0.65
1:A:171:LEU:CD2	1:A:287:PHE:HE2	2.09	0.65
1:A:385:GLN:HB3	1:A:391:ARG:HD3	1.78	0.65
3:C:112:ILE:HG12	3:C:117:MET:HG3	1.76	0.65
1:A:68:GLY:HA2	1:A:218:PHE:CE1	2.31	0.65
2:B:85:LEU:CD1	2:B:422:LEU:HD11	2.27	0.65
1:A:162:ILE:HD12	1:A:164:TRP:CH2	2.33	0.64
1:A:397:LEU:HD21	1:A:439:VAL:HG23	1.78	0.64
1:A:162:ILE:HD11	1:A:164:TRP:CZ2	2.32	0.64
2:B:435:LEU:H	2:B:436:PRO:CD	2.09	0.64
1:A:68:GLY:CA	1:A:218:PHE:HE1	2.08	0.64
1:A:418:GLN:HE21	1:A:418:GLN:HA	1.63	0.64
1:A:434:ARG:O	1:A:435:ASN:HB2	1.95	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:LEU:HD12	1:A:365:LEU:N	2.03	0.64
1:A:579:VAL:HG12	1:A:620:CYS:O	1.98	0.64
2:B:249:ILE:O	2:B:253:ILE:HG22	1.97	0.64
3:C:112:ILE:H	3:C:112:ILE:CD1	2.10	0.64
1:A:223:ALA:CB	1:A:247:VAL:CG2	2.64	0.64
3:C:159:THR:HG21	3:C:210:TYR:CD1	2.33	0.64
3:C:112:ILE:CG1	3:C:117:MET:HG3	2.28	0.63
1:A:499:TYR:O	1:A:503:GLY:N	2.31	0.63
1:A:156:PHE:HD2	1:A:421:PRO:CB	2.05	0.63
1:A:185:ASP:OD1	1:A:187:ASN:N	2.29	0.63
1:A:260:LEU:HD21	1:A:312:LEU:CD2	2.27	0.63
1:A:559:SER:HB2	1:A:560:PRO:HD3	1.79	0.63
1:A:576:GLY:HA3	1:A:623:SER:HB3	1.81	0.63
1:A:622:ARG:HG2	1:A:622:ARG:NH1	2.04	0.63
1:A:260:LEU:HD12	1:A:313:GLN:HE22	1.63	0.62
1:A:524:GLY:HA2	1:A:531:ASN:HD21	1.64	0.62
1:A:95:MET:CG	1:A:120:GLY:O	2.47	0.62
1:A:268:THR:HG21	1:A:355:GLN:OE1	1.99	0.62
2:B:100:ILE:HD11	2:B:238:ILE:HD13	1.81	0.62
1:A:500:GLU:O	1:A:503:GLY:HA2	1.98	0.62
2:B:99:THR:HG21	2:B:181:TYR:CE1	2.34	0.62
3:C:61:ASP:O	3:C:62:ARG:HB2	1.98	0.62
1:A:95:MET:HE1	1:A:217:LEU:HD11	1.77	0.61
1:A:249:ASP:OD1	1:A:652:ARG:NE	2.33	0.61
1:A:605:VAL:HG22	1:A:606:GLN:O	2.00	0.61
1:A:95:MET:SD	1:A:217:LEU:HD11	2.39	0.61
1:A:305:GLN:HB2	1:A:365:LEU:CD1	2.30	0.61
1:A:371:ARG:HH11	1:A:371:ARG:HB3	1.63	0.61
1:A:385:GLN:CA	1:A:391:ARG:HD3	2.30	0.61
1:A:152:TYR:CD1	1:A:383:VAL:HG21	2.27	0.61
1:A:422:LEU:CD2	1:A:423:PRO:HD2	2.22	0.61
1:A:511:VAL:O	1:A:511:VAL:HG13	2.01	0.61
1:A:150:ASN:ND2	1:A:150:ASN:H	1.98	0.61
2:B:85:LEU:HD13	2:B:422:LEU:HD11	1.82	0.61
2:B:424:LEU:O	2:B:428:PHE:HB2	2.00	0.61
1:A:337:TYR:HB3	1:A:429:ARG:HG3	1.83	0.60
2:B:207:VAL:CG1	4:D:26:LEU:HD21	2.31	0.60
1:A:54:LEU:HD23	1:A:59:GLN:HB2	1.82	0.60
1:A:155:GLU:CG	1:A:156:PHE:CE1	2.65	0.60
1:A:300:ALA:HB2	1:A:463:ILE:CD1	2.31	0.60
1:A:605:VAL:HG11	1:A:621:VAL:HG23	1.80	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:SER:CB	1:A:429:ARG:HH11	2.14	0.60
2:B:241:LEU:CD1	2:B:245:THR:HG21	2.31	0.60
1:A:260:LEU:CD1	1:A:313:GLN:NE2	2.64	0.60
1:A:371:ARG:HH11	1:A:371:ARG:CG	2.13	0.60
2:B:247:TRP:CE3	2:B:247:TRP:HA	2.36	0.60
1:A:66:ILE:HD13	1:A:220:HIS:CE1	2.36	0.60
1:A:95:MET:HE1	1:A:217:LEU:HD21	1.83	0.60
1:A:96:VAL:CG2	1:A:121:LEU:HB3	2.32	0.60
1:A:304:THR:HG22	1:A:487:LEU:HG	1.83	0.60
1:A:98:LEU:HD13	1:A:107:LEU:HD21	1.84	0.60
1:A:133:GLY:HA2	1:A:452:TYR:CE1	2.35	0.60
1:A:260:LEU:HD12	1:A:313:GLN:NE2	2.17	0.60
1:A:347:MET:HE2	1:A:430:PHE:CE2	2.35	0.60
2:B:435:LEU:HD12	2:B:439:ILE:CD1	2.32	0.60
4:D:45:PRO:HG2	4:D:46:ALA:H	1.66	0.60
2:B:244:TRP:CE3	2:B:247:TRP:CD1	2.76	0.60
1:A:97:LEU:HD13	1:A:192:ILE:HG21	1.84	0.59
3:C:112:ILE:HD13	3:C:112:ILE:O	2.02	0.59
1:A:66:ILE:HB	1:A:220:HIS:CE1	2.37	0.59
2:B:86:PHE:HZ	2:B:419:CYS:SG	2.21	0.59
3:C:159:THR:HG21	3:C:210:TYR:CE1	2.38	0.59
1:A:463:ILE:HG23	1:A:465:VAL:HG23	1.84	0.59
1:A:385:GLN:HB3	1:A:391:ARG:CD	2.32	0.59
1:A:82:LEU:HD23	1:A:110:LYS:HZ2	1.68	0.59
1:A:162:ILE:CD1	1:A:164:TRP:CZ2	2.85	0.59
1:A:224:VAL:HG21	4:D:100:THR:C	2.28	0.59
3:C:163:LEU:HD13	3:C:214:LEU:HD12	1.84	0.59
1:A:341:SER:HB2	1:A:429:ARG:HD2	1.85	0.58
1:A:101:LYS:CG	1:A:126:THR:HG21	2.33	0.58
1:A:279:ALA:HB1	1:A:328:VAL:HG13	1.85	0.58
1:A:313:GLN:HG2	1:A:575:THR:O	2.03	0.58
2:B:96:VAL:HG21	2:B:390:SER:CB	2.34	0.58
1:A:148:TYR:HE2	1:A:422:LEU:N	2.01	0.58
1:A:529:ALA:HB2	1:A:551:LEU:HD11	1.84	0.58
2:B:239:LYS:HG3	2:B:240:TYR:CD1	2.37	0.58
4:D:48:THR:OG1	4:D:49:GLU:HG2	2.03	0.58
1:A:250:PRO:HB3	1:A:635:PHE:HE2	1.66	0.58
4:D:51:SER:O	4:D:54:LYS:HG2	2.04	0.58
3:C:114:ILE:O	3:C:114:ILE:HD12	2.03	0.58
1:A:148:TYR:HE2	1:A:422:LEU:H	1.50	0.58
1:A:250:PRO:CB	1:A:635:PHE:CE2	2.83	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:ALA:O	1:A:300:ALA:N	2.34	0.57
1:A:434:ARG:HH11	1:A:434:ARG:CG	2.15	0.57
1:A:586:CYS:SG	1:A:604:TRP:HD1	2.26	0.57
1:A:559:SER:OG	1:A:560:PRO:HD3	2.04	0.57
1:A:96:VAL:CG2	1:A:118:ILE:HD11	2.31	0.57
1:A:123:VAL:HG23	1:A:123:VAL:O	2.03	0.57
1:A:430:PHE:HB3	1:A:436:ILE:HD11	1.87	0.57
3:C:30:LEU:O	3:C:34:ILE:HG23	2.04	0.57
4:D:40:GLU:O	4:D:44:VAL:CG2	2.41	0.57
3:C:34:ILE:CG1	3:C:120:VAL:CG1	2.83	0.57
1:A:186:GLU:OE1	1:A:189:THR:OG1	2.21	0.57
4:D:39:ARG:O	4:D:43:LEU:HB2	2.05	0.57
1:A:95:MET:HE1	1:A:217:LEU:CG	2.35	0.56
1:A:156:PHE:HD2	1:A:421:PRO:CD	2.18	0.56
1:A:304:THR:OG1	1:A:365:LEU:HD22	2.05	0.56
1:A:378:MET:HE3	1:A:398:LEU:CD2	2.35	0.56
2:B:241:LEU:HG	2:B:245:THR:CG2	2.34	0.56
1:A:97:LEU:CD1	1:A:192:ILE:HG21	2.36	0.56
1:A:279:ALA:HB2	1:A:328:VAL:HG12	1.85	0.56
1:A:418:GLN:NE2	1:A:418:GLN:HA	2.20	0.56
2:B:244:TRP:CE3	2:B:244:TRP:HA	2.41	0.56
2:B:435:LEU:HD12	2:B:439:ILE:CG1	2.35	0.56
2:B:435:LEU:HD11	2:B:439:ILE:HD12	1.86	0.56
1:A:605:VAL:CG2	1:A:606:GLN:N	2.68	0.56
3:C:34:ILE:HD11	3:C:120:VAL:CG1	2.35	0.56
1:A:335:PHE:O	1:A:337:TYR:N	2.38	0.56
2:B:85:LEU:HD13	2:B:422:LEU:CD1	2.35	0.56
1:A:278:ALA:O	1:A:305:GLN:NE2	2.39	0.56
1:A:364:GLU:OE1	1:A:426:SER:N	2.38	0.56
1:A:156:PHE:CD2	1:A:421:PRO:CA	2.89	0.56
2:B:247:TRP:HA	2:B:247:TRP:HE3	1.71	0.56
1:A:222:HIS:O	1:A:651:SER:OG	2.23	0.55
1:A:296:GLU:OE1	1:A:450:ASN:HB2	2.05	0.55
1:A:95:MET:CE	1:A:217:LEU:HD21	2.36	0.55
1:A:101:LYS:HD3	1:A:126:THR:HG21	1.88	0.55
4:D:96:ILE:HG22	4:D:97:PRO:HD2	1.88	0.55
1:A:171:LEU:CG	1:A:287:PHE:HE2	2.19	0.55
1:A:339:GLY:HA2	1:A:630:ALA:HB1	1.87	0.55
1:A:516:GLN:O	1:A:519:THR:HG22	2.05	0.55
1:A:223:ALA:O	1:A:224:VAL:HG13	2.07	0.55
1:A:233:ARG:HB2	4:D:96:ILE:CD1	2.36	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:ARG:NH1	1:A:434:ARG:HG2	2.20	0.55
1:A:397:LEU:HD13	1:A:501:LEU:HD11	1.88	0.55
1:A:450:ASN:OD1	1:A:453:TYR:HA	2.07	0.55
1:A:633:PRO:CG	1:A:645:TYR:CD2	2.89	0.55
1:A:586:CYS:HG	1:A:604:TRP:HD1	1.54	0.55
3:C:34:ILE:HG13	3:C:120:VAL:CG1	2.37	0.55
1:A:54:LEU:CD2	1:A:59:GLN:HB2	2.37	0.55
1:A:299:VAL:HG11	1:A:526:LEU:CD2	2.37	0.55
1:A:506:ASN:C	1:A:507:PHE:CD1	2.85	0.55
2:B:241:LEU:CD1	2:B:245:THR:CG2	2.86	0.54
3:C:111:PRO:HG2	3:C:112:ILE:HD12	1.90	0.54
1:A:294:GLY:HA3	1:A:553:HIS:HD2	1.72	0.54
1:A:605:VAL:HG23	1:A:606:GLN:N	2.22	0.54
3:C:62:ARG:HG2	3:C:68:GLN:OE1	2.07	0.54
1:A:385:GLN:O	1:A:391:ARG:HB2	2.07	0.54
1:A:540:GLN:HG2	1:A:606:GLN:HE22	1.67	0.54
2:B:408:ILE:HD13	3:C:131:VAL:HG11	1.90	0.54
1:A:347:MET:SD	1:A:352:PHE:CE2	3.01	0.54
2:B:457:MET:HE2	3:C:132:PHE:HB3	1.90	0.54
1:A:51:VAL:HA	1:A:221:MET:HE3	1.90	0.54
1:A:152:TYR:C	1:A:152:TYR:CD1	2.86	0.54
1:A:260:LEU:CD1	1:A:313:GLN:HE22	2.20	0.54
1:A:281:ARG:HH11	1:A:281:ARG:CG	2.13	0.54
1:A:369:ALA:HB1	1:A:463:ILE:CG1	2.38	0.54
1:A:422:LEU:HD22	1:A:423:PRO:O	2.07	0.54
1:A:337:TYR:OH	1:A:428:GLN:NE2	2.41	0.54
1:A:378:MET:HE3	1:A:398:LEU:HD23	1.90	0.54
1:A:559:SER:CB	1:A:560:PRO:CD	2.86	0.53
3:C:90:TYR:HE2	3:C:121:SER:HB2	1.74	0.53
1:A:156:PHE:HD2	1:A:421:PRO:HD3	1.72	0.53
1:A:552:GLN:OE1	1:A:552:GLN:HA	2.09	0.53
1:A:529:ALA:CB	1:A:551:LEU:HD11	2.38	0.53
3:C:40:PHE:O	3:C:44:VAL:HG23	2.09	0.53
1:A:506:ASN:O	1:A:507:PHE:HD1	1.91	0.53
4:D:31:LEU:HD13	4:D:64:PHE:CZ	2.43	0.53
1:A:289:TRP:NE1	1:A:650:GLU:OE2	2.40	0.53
1:A:341:SER:HB2	1:A:429:ARG:HH11	1.73	0.53
1:A:152:TYR:CE1	1:A:383:VAL:CB	2.91	0.53
1:A:385:GLN:CB	1:A:391:ARG:HD3	2.39	0.53
2:B:241:LEU:HD11	2:B:245:THR:HG21	1.91	0.53
1:A:200:ASN:HD21	1:A:213:CYS:HB3	1.74	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:1:NAG:O3	5:H:2:NAG:H83	2.09	0.53
1:A:288:PHE:CE2	1:A:456:ILE:HD11	2.44	0.53
1:A:633:PRO:CG	1:A:645:TYR:HD2	2.20	0.53
1:A:443:ASP:OD1	1:A:444:HIS:ND1	2.41	0.52
1:A:164:TRP:CZ2	1:A:423:PRO:HA	2.43	0.52
2:B:242:PRO:HD2	2:B:245:THR:HB	1.90	0.52
1:A:40:ILE:HD11	3:C:157:PHE:HZ	1.74	0.52
1:A:369:ALA:CB	1:A:463:ILE:HD11	2.39	0.52
1:A:268:THR:CG2	1:A:355:GLN:CG	2.60	0.52
3:C:34:ILE:HG12	3:C:120:VAL:HG11	1.91	0.52
3:C:34:ILE:HB	3:C:90:TYR:OH	2.09	0.52
1:A:68:GLY:HA2	1:A:218:PHE:HD1	1.74	0.52
3:C:126:GLY:O	3:C:168:ILE:HG12	2.09	0.52
3:C:137:ILE:HD11	3:C:160:SER:OG	2.10	0.52
1:A:104:THR:HG22	1:A:105:ARG:H	1.75	0.52
1:A:645:TYR:O	1:A:646:SER:OG	2.23	0.52
1:A:155:GLU:CG	1:A:156:PHE:CD1	2.89	0.52
1:A:162:ILE:CG2	1:A:420:GLN:OE1	2.55	0.52
1:A:182:LEU:HD13	1:A:288:PHE:CE2	2.44	0.52
2:B:241:LEU:CG	2:B:245:THR:HG22	2.38	0.52
1:A:91:ASN:O	1:A:93:PRO:HD2	2.10	0.51
1:A:40:ILE:HD11	3:C:157:PHE:CZ	2.45	0.51
1:A:64:SER:HB3	1:A:219:SER:N	2.23	0.51
1:A:66:ILE:HB	1:A:220:HIS:NE2	2.26	0.51
1:A:162:ILE:O	1:A:163:GLN:HB2	2.08	0.51
1:A:222:HIS:O	1:A:223:ALA:HB3	2.09	0.51
1:A:326:MET:HG3	1:A:326:MET:O	2.09	0.51
2:B:106:TYR:CG	2:B:235:LEU:HD22	2.45	0.51
4:D:97:PRO:HG2	4:D:100:THR:OG1	2.11	0.51
1:A:82:LEU:HD23	1:A:110:LYS:NZ	2.25	0.51
1:A:269:LEU:HD13	1:A:358:ASN:HD22	1.76	0.51
1:A:443:ASP:OD1	1:A:444:HIS:N	2.43	0.51
1:A:605:VAL:HG11	1:A:621:VAL:HG21	1.92	0.51
2:B:435:LEU:CD1	2:B:439:ILE:HD12	2.41	0.51
1:A:249:ASP:OD1	1:A:652:ARG:CZ	2.59	0.51
1:A:562:ASN:OD1	1:A:562:ASN:N	2.43	0.51
1:A:224:VAL:CG1	4:D:99:GLY:O	2.58	0.51
1:A:372:THR:CG2	1:A:449:HIS:CD2	2.93	0.51
3:C:90:TYR:CE2	3:C:94:LEU:CD1	2.87	0.51
3:C:170:LEU:HG	3:C:174:TRP:CZ2	2.46	0.51
4:D:44:VAL:CG1	4:D:47:TYR:CD1	2.86	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:THR:CG2	1:A:365:LEU:HD13	2.41	0.51
1:A:390:VAL:CG2	7:A:1705:NAG:H82	2.41	0.51
2:B:250:LEU:O	2:B:439:ILE:HG21	2.10	0.51
1:A:60:ILE:HG12	1:A:648:TRP:CZ3	2.46	0.51
1:A:343:MET:CE	1:A:347:MET:SD	2.98	0.51
1:A:559:SER:HB2	1:A:560:PRO:CD	2.40	0.51
3:C:106:GLU:OE1	3:C:106:GLU:HA	2.10	0.51
1:A:102:HIS:O	1:A:107:LEU:HD23	2.11	0.50
1:A:283:ASP:HA	1:A:553:HIS:HB3	1.93	0.50
1:A:425:SER:O	1:A:428:GLN:N	2.44	0.50
1:A:635:PHE:CZ	1:A:649:THR:CG2	2.93	0.50
1:A:693:LYS:NZ	3:C:242:SER:O	2.44	0.50
1:A:364:GLU:O	1:A:440:VAL:HA	2.11	0.50
2:B:402:GLY:O	2:B:404:TRP:N	2.44	0.50
2:B:448:ALA:CB	3:C:47:LEU:HD21	2.40	0.50
1:A:633:PRO:CB	1:A:645:TYR:CE2	2.89	0.50
2:B:82:VAL:HB	3:C:33:ILE:HD11	1.93	0.50
2:B:416:ILE:CD1	3:C:40:PHE:HB2	2.42	0.50
1:A:540:GLN:CG	1:A:606:GLN:NE2	2.39	0.50
1:A:633:PRO:HD2	1:A:645:TYR:CD2	2.47	0.50
2:B:240:TYR:CD1	2:B:240:TYR:N	2.77	0.50
1:A:145:PHE:CG	1:A:336:ASP:HB3	2.47	0.50
2:B:435:LEU:HD11	2:B:439:ILE:HD11	1.89	0.50
1:A:162:ILE:CD1	1:A:164:TRP:CH2	2.95	0.50
1:A:171:LEU:HG	1:A:287:PHE:HE2	1.75	0.50
1:A:270:LYS:HG3	1:A:271:PRO:CD	2.42	0.50
1:A:631:LEU:HD23	1:A:635:PHE:HB2	1.94	0.50
2:B:253:ILE:HD13	2:B:388:PHE:CZ	2.46	0.50
1:A:622:ARG:NH1	1:A:622:ARG:CG	2.73	0.50
1:A:58:HIS:ND1	1:A:58:HIS:N	2.60	0.49
1:A:152:TYR:CZ	1:A:383:VAL:CG1	2.89	0.49
1:A:633:PRO:CD	1:A:645:TYR:HD2	2.25	0.49
1:A:223:ALA:N	1:A:247:VAL:HG21	2.25	0.49
1:A:250:PRO:HB3	1:A:635:PHE:HD2	1.64	0.49
1:A:557:VAL:HG13	1:A:558:SER:N	2.26	0.49
1:A:68:GLY:H	1:A:218:PHE:HD1	1.55	0.49
1:A:230:CYS:SG	1:A:247:VAL:CG1	2.91	0.49
1:A:280:THR:HG23	1:A:365:LEU:HD13	1.93	0.49
2:B:244:TRP:O	2:B:248:LEU:N	2.34	0.49
4:D:96:ILE:CG2	4:D:97:PRO:HD2	2.42	0.49
1:A:49:PRO:HD3	1:A:656:ILE:HD13	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:605:VAL:CG2	1:A:606:GLN:O	2.61	0.49
2:B:466:TYR:CZ	3:C:163:LEU:HD23	2.47	0.49
3:C:24:THR:HG21	3:C:119:TYR:CE1	2.47	0.49
3:C:42:TRP:CH2	3:C:46:LEU:HD12	2.47	0.49
1:A:152:TYR:CE1	1:A:383:VAL:HG11	2.47	0.49
1:A:418:GLN:CA	1:A:418:GLN:NE2	2.73	0.49
3:C:10:THR:CB	3:C:138:LEU:HD21	2.43	0.49
3:C:80:VAL:HG11	3:C:198:LEU:HD12	1.94	0.49
1:A:347:MET:HE2	1:A:430:PHE:HE2	1.75	0.49
3:C:122:GLY:HA3	3:C:172:THR:HA	1.94	0.49
1:A:385:GLN:HA	1:A:391:ARG:HB2	1.93	0.49
3:C:227:TRP:O	3:C:231:THR:HG23	2.13	0.49
1:A:74:HIS:N	1:A:95:MET:O	2.45	0.49
1:A:152:TYR:O	1:A:154:PRO:CD	2.47	0.49
1:A:222:HIS:N	1:A:222:HIS:CD2	2.78	0.49
1:A:274:ARG:HD2	1:A:360:ASP:OD2	2.13	0.49
2:B:211:ILE:O	2:B:215:TRP:N	2.45	0.49
1:A:72:VAL:HG13	1:A:94:TYR:CE1	2.48	0.49
1:A:222:HIS:HB3	1:A:247:VAL:HG23	1.95	0.49
1:A:231:MET:HE3	1:A:248:CYS:HB3	1.95	0.49
1:A:378:MET:SD	1:A:413:LEU:CD2	3.01	0.48
1:A:425:SER:O	1:A:426:SER:C	2.56	0.48
2:B:385:ASP:OD1	2:B:435:LEU:HD22	2.12	0.48
1:A:121:LEU:O	1:A:180:ILE:HA	2.13	0.48
1:A:224:VAL:O	1:A:225:ILE:HB	2.13	0.48
2:B:250:LEU:HD13	2:B:392:LEU:HD12	1.93	0.48
1:A:57:THR:HG22	1:A:58:HIS:ND1	2.28	0.48
1:A:101:LYS:CD	1:A:126:THR:HG21	2.42	0.48
1:A:152:TYR:OH	1:A:383:VAL:HB	2.13	0.48
1:A:365:LEU:H	1:A:365:LEU:CD1	2.08	0.48
1:A:629:ARG:CZ	1:A:631:LEU:HD12	2.43	0.48
3:C:80:VAL:CG1	3:C:198:LEU:HD12	2.43	0.48
1:A:367:GLN:O	1:A:443:ASP:CG	2.56	0.48
3:C:115:ARG:CB	3:C:115:ARG:HH11	2.27	0.48
2:B:182:LEU:HD22	2:B:202:ILE:CD1	2.44	0.48
2:B:239:LYS:CG	2:B:240:TYR:CD1	2.93	0.48
1:A:186:GLU:OE1	1:A:186:GLU:HA	2.13	0.48
1:A:311:ALA:CA	1:A:511:VAL:HG23	2.44	0.48
2:B:387:ILE:O	2:B:391:VAL:HG23	2.13	0.48
1:A:290:ASN:O	1:A:552:GLN:CG	2.59	0.48
1:A:419:SER:O	1:A:419:SER:OG	2.30	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:609:LEU:CD2	1:A:614:THR:HA	2.44	0.47
2:B:91:LEU:O	2:B:95:VAL:HG23	2.14	0.47
3:C:62:ARG:CG	3:C:68:GLN:OE1	2.61	0.47
3:C:206:LEU:HD23	3:C:212:ALA:HB1	1.95	0.47
1:A:269:LEU:CD1	1:A:358:ASN:HD22	2.27	0.47
1:A:294:GLY:O	1:A:299:VAL:HG23	2.14	0.47
1:A:341:SER:OG	1:A:429:ARG:NH1	2.47	0.47
1:A:679:ILE:HG21	3:C:12:VAL:HA	1.96	0.47
1:A:385:GLN:O	1:A:391:ARG:HD3	2.14	0.47
1:A:451:LYS:HB2	1:A:451:LYS:HZ3	1.76	0.47
3:C:61:ASP:O	3:C:62:ARG:CB	2.63	0.47
4:D:39:ARG:O	4:D:43:LEU:CB	2.62	0.47
1:A:122:ALA:HA	1:A:181:PHE:O	2.15	0.47
1:A:432:ARG:HH12	1:A:644:GLU:CB	2.09	0.47
1:A:60:ILE:HG22	1:A:173:TYR:O	2.15	0.47
1:A:157:ALA:C	1:A:158:HIS:ND1	2.73	0.47
1:A:371:ARG:HD3	1:A:376:LEU:CD1	2.45	0.47
1:A:385:GLN:C	1:A:391:ARG:HD3	2.40	0.47
4:D:47:TYR:CB	4:D:50:GLN:CB	2.63	0.47
1:A:349:LYS:HB3	1:A:351:LYS:HD2	1.97	0.47
1:A:369:ALA:CB	1:A:463:ILE:CG1	2.92	0.47
1:A:552:GLN:HG2	5:J:1:NAG:C8	2.45	0.47
1:A:66:ILE:CD1	1:A:220:HIS:ND1	2.76	0.47
1:A:98:LEU:CD1	1:A:107:LEU:HD21	2.45	0.47
1:A:369:ALA:CB	1:A:463:ILE:HG13	2.45	0.47
1:A:427:LEU:HD12	1:A:427:LEU:O	2.15	0.47
2:B:208:VAL:HG21	4:D:28:PHE:CD1	2.50	0.47
2:B:208:VAL:O	2:B:211:ILE:HG13	2.15	0.47
3:C:62:ARG:HG2	3:C:68:GLN:CD	2.38	0.47
1:A:633:PRO:HD2	1:A:645:TYR:HD2	1.80	0.47
2:B:211:ILE:HD12	2:B:212:SER:N	2.30	0.47
3:C:112:ILE:CD1	3:C:112:ILE:N	2.73	0.47
1:A:68:GLY:HA3	1:A:218:PHE:HE1	1.81	0.46
1:A:95:MET:HE1	1:A:217:LEU:CD2	2.44	0.46
4:D:38:PHE:CD1	4:D:38:PHE:C	2.92	0.46
1:A:304:THR:OG1	1:A:365:LEU:CD2	2.63	0.46
1:A:164:TRP:HB3	1:A:448:PHE:CE1	2.50	0.46
1:A:269:LEU:HA	1:A:269:LEU:HD23	1.79	0.46
3:C:90:TYR:CE2	3:C:121:SER:HB2	2.50	0.46
3:C:174:TRP:CZ2	3:C:197:HIS:HA	2.50	0.46
1:A:76:VAL:HB	1:A:98:LEU:HD23	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:GLY:O	1:A:505:THR:HG23	2.15	0.46
1:A:253:ASP:O	1:A:630:ALA:HB3	2.16	0.46
1:A:377:TRP:CE3	1:A:415:ARG:O	2.69	0.46
2:B:80:LYS:O	2:B:83:ILE:HG22	2.15	0.46
1:A:53:LEU:HD21	1:A:554:TYR:OH	2.16	0.46
1:A:63:GLN:HG3	1:A:221:MET:HB2	1.98	0.46
2:B:207:VAL:HG11	4:D:26:LEU:HD21	1.97	0.46
4:D:3:LEU:O	4:D:11:LYS:HE2	2.16	0.46
1:A:152:TYR:OH	1:A:383:VAL:CG1	2.64	0.46
1:A:281:ARG:HD3	1:A:297:SER:O	2.15	0.46
1:A:378:MET:HE1	1:A:415:ARG:HE	1.79	0.46
4:D:97:PRO:HB2	4:D:100:THR:OG1	2.15	0.46
1:A:233:ARG:HB2	4:D:96:ILE:HD13	1.97	0.45
2:B:241:LEU:HD11	2:B:245:THR:CG2	2.46	0.45
4:D:44:VAL:HG11	4:D:47:TYR:HD1	1.66	0.45
1:A:268:THR:HA	1:A:353:PRO:HA	1.97	0.45
1:A:285:ARG:HG2	1:A:334:THR:OG1	2.16	0.45
1:A:306:LEU:HD23	1:A:306:LEU:O	2.17	0.45
2:B:234:ALA:HA	2:B:391:VAL:HG22	1.98	0.45
1:A:300:ALA:CB	1:A:369:ALA:HB2	2.44	0.45
1:A:253:ASP:OD1	1:A:555:ILE:HG23	2.17	0.45
1:A:253:ASP:CB	1:A:559:SER:O	2.61	0.45
1:A:275:VAL:HG12	1:A:324:ASN:HB3	1.98	0.45
1:A:644:GLU:HG2	1:A:645:TYR:HD1	1.80	0.45
1:A:397:LEU:HD21	1:A:439:VAL:CG2	2.42	0.45
1:A:128:PRO:O	1:A:129:SER:CB	2.56	0.45
1:A:279:ALA:CA	1:A:328:VAL:HG13	2.46	0.45
1:A:367:GLN:HE21	1:A:367:GLN:HB3	1.58	0.45
3:C:106:GLU:O	3:C:107:ASP:HB2	2.15	0.45
4:D:31:LEU:HD13	4:D:64:PHE:CE2	2.52	0.45
1:A:223:ALA:HB1	1:A:230:CYS:SG	2.57	0.45
1:A:583:ARG:HB2	1:A:604:TRP:CZ2	2.51	0.45
3:C:113:SER:OG	3:C:116:GLN:CD	2.60	0.45
1:A:283:ASP:CG	1:A:555:ILE:HD11	2.42	0.45
3:C:34:ILE:HG13	3:C:120:VAL:HG12	1.98	0.45
1:A:157:ALA:O	1:A:158:HIS:ND1	2.50	0.45
1:A:164:TRP:CZ2	1:A:423:PRO:CA	3.00	0.45
1:A:418:GLN:HE21	1:A:418:GLN:C	2.25	0.45
1:A:96:VAL:O	1:A:121:LEU:HB2	2.17	0.45
1:A:280:THR:OG1	1:A:305:GLN:CB	2.64	0.45
1:A:341:SER:HB2	1:A:429:ARG:NH1	2.32	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:LEU:HD12	1:A:431:LEU:HA	1.83	0.45
1:A:57:THR:CG2	1:A:58:HIS:CE1	3.00	0.44
1:A:216:GLN:CD	1:A:218:PHE:CZ	2.95	0.44
1:A:283:ASP:OD2	1:A:555:ILE:HD11	2.17	0.44
4:D:44:VAL:HG12	4:D:46:ALA:O	2.17	0.44
1:A:634:ALA:HB2	1:A:645:TYR:HB2	2.00	0.44
1:A:637:LEU:CB	1:A:639:GLN:HG2	2.47	0.44
1:A:156:PHE:CD2	1:A:421:PRO:HD3	2.52	0.44
1:A:311:ALA:CB	1:A:511:VAL:CG2	2.95	0.44
2:B:83:ILE:HG21	3:C:29:PRO:HB3	1.99	0.44
3:C:34:ILE:HG13	3:C:35:LEU:N	2.32	0.44
1:A:371:ARG:CG	1:A:371:ARG:NH1	2.73	0.44
1:A:397:LEU:CG	1:A:439:VAL:HG21	2.43	0.44
1:A:498:LEU:O	1:A:502:ALA:N	2.32	0.44
2:B:92:CYS:O	2:B:96:VAL:HG23	2.17	0.44
2:B:248:LEU:HD23	2:B:248:LEU:HA	1.81	0.44
3:C:12:VAL:O	3:C:165:ALA:HB2	2.18	0.44
1:A:51:VAL:HG22	1:A:221:MET:HE1	1.98	0.44
1:A:302:PHE:CD1	1:A:302:PHE:C	2.95	0.44
1:A:377:TRP:HA	1:A:414:ARG:O	2.17	0.44
2:B:416:ILE:CD1	3:C:36:VAL:HG12	2.48	0.44
1:A:264:ASN:O	1:A:265:THR:CB	2.66	0.44
1:A:586:CYS:HB2	1:A:620:CYS:SG	2.46	0.44
2:B:85:LEU:HD21	2:B:381:LEU:HD23	1.98	0.44
1:A:182:LEU:HD23	1:A:184:GLU:HG3	1.99	0.44
1:A:338:ILE:C	1:A:338:ILE:HD12	2.43	0.44
3:C:42:TRP:CZ3	3:C:46:LEU:HD12	2.52	0.44
1:A:139:GLN:HG2	1:A:163:GLN:CG	2.35	0.44
1:A:284:SER:OG	1:A:553:HIS:HB2	2.17	0.44
1:A:68:GLY:N	1:A:218:PHE:HD1	2.11	0.44
1:A:95:MET:HG3	1:A:120:GLY:O	2.17	0.43
1:A:632:SER:HB3	1:A:645:TYR:O	2.17	0.43
2:B:250:LEU:CD1	2:B:392:LEU:HG	2.48	0.43
1:A:185:ASP:HB3	1:A:188:GLU:OE2	2.18	0.43
1:A:298:ALA:O	1:A:302:PHE:CD2	2.71	0.43
2:B:239:LYS:C	2:B:240:TYR:HD1	2.25	0.43
3:C:90:TYR:HE2	3:C:94:LEU:HD11	1.72	0.43
1:A:103:PHE:O	1:A:103:PHE:CG	2.70	0.43
1:A:223:ALA:C	1:A:224:VAL:HG13	2.43	0.43
1:A:337:TYR:CB	1:A:429:ARG:HG3	2.47	0.43
1:A:441:LEU:HD12	1:A:494:LEU:HD12	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:416:ILE:HD11	3:C:36:VAL:HG12	1.98	0.43
3:C:7:PHE:O	3:C:10:THR:HG22	2.19	0.43
3:C:80:VAL:HG13	3:C:197:HIS:CG	2.54	0.43
4:D:34:ILE:CD1	4:D:61:ALA:HA	2.48	0.43
1:A:192:ILE:HG12	1:A:660:ILE:HD12	2.01	0.43
1:A:102:HIS:O	1:A:104:THR:N	2.50	0.43
1:A:366:GLY:O	1:A:442:ALA:HA	2.18	0.43
1:A:534:PHE:CE2	1:A:566:VAL:HG11	2.53	0.43
2:B:100:ILE:CD1	2:B:238:ILE:HD13	2.48	0.43
2:B:241:LEU:HD21	2:B:249:ILE:HD12	2.00	0.43
1:A:156:PHE:CD2	1:A:421:PRO:CD	2.99	0.43
1:A:390:VAL:HG23	7:A:1705:NAG:H82	2.00	0.43
1:A:506:ASN:C	1:A:507:PHE:HD1	2.26	0.43
3:C:31:ARG:O	3:C:34:ILE:HG12	2.19	0.43
4:D:26:LEU:HB3	4:D:29:LEU:HB2	2.00	0.43
1:A:68:GLY:N	1:A:218:PHE:HE1	2.12	0.43
1:A:311:ALA:HB1	1:A:511:VAL:HG23	1.98	0.43
1:A:662:LEU:HD13	3:C:149:ILE:HA	2.01	0.43
1:A:224:VAL:CG2	4:D:100:THR:O	2.57	0.43
2:B:452:LEU:HD13	3:C:51:VAL:CG2	2.48	0.43
3:C:91:TYR:CE1	3:C:182:CYS:SG	3.11	0.43
4:D:97:PRO:HG2	4:D:100:THR:HG1	1.84	0.43
1:A:279:ALA:O	1:A:364:GLU:HA	2.18	0.43
1:A:299:VAL:CG2	1:A:553:HIS:CD2	3.02	0.43
1:A:343:MET:HE2	1:A:347:MET:SD	2.58	0.43
2:B:432:LEU:N	2:B:433:PRO:HD3	2.34	0.43
1:A:97:LEU:HD13	1:A:192:ILE:CG2	2.49	0.42
1:A:112:LYS:HB3	1:A:112:LYS:HE2	1.82	0.42
3:C:112:ILE:HG13	3:C:117:MET:HG3	2.01	0.42
1:A:583:ARG:HA	1:A:604:TRP:NE1	2.35	0.42
1:A:605:VAL:HG13	1:A:619:ARG:O	2.19	0.42
1:A:306:LEU:HG	1:A:329:PHE:CE2	2.55	0.42
1:A:334:THR:HG23	1:A:335:PHE:CD2	2.55	0.42
1:A:341:SER:CB	1:A:429:ARG:HD2	2.49	0.42
1:A:356:LEU:HA	1:A:356:LEU:HD12	1.75	0.42
1:A:396:ASP:O	1:A:400:THR:HG23	2.19	0.42
1:A:558:SER:O	1:A:559:SER:C	2.62	0.42
2:B:465:PHE:HA	3:C:204:THR:HB	2.01	0.42
3:C:60:THR:HG21	3:C:67:LEU:CD2	2.45	0.42
3:C:242:SER:O	3:C:243:LEU:C	2.62	0.42
1:A:312:LEU:HD11	1:A:498:LEU:CB	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:552:GLN:HG2	5:J:1:NAG:H81	2.00	0.42
2:B:174:LEU:HD22	2:B:206:GLY:HA2	2.00	0.42
3:C:243:LEU:O	3:C:243:LEU:HD22	2.18	0.42
1:A:296:GLU:OE1	1:A:367:GLN:NE2	2.48	0.42
1:A:54:LEU:CD1	1:A:248:CYS:SG	3.06	0.42
1:A:74:HIS:O	1:A:96:VAL:HA	2.18	0.42
1:A:296:GLU:HG3	1:A:370:LEU:HD21	2.01	0.42
1:A:345:TYR:CE2	1:A:349:LYS:HE2	2.55	0.42
2:B:244:TRP:CE3	2:B:244:TRP:CA	3.03	0.42
3:C:17:ALA:CB	3:C:168:ILE:HG21	2.41	0.42
3:C:60:THR:O	3:C:61:ASP:HB3	2.20	0.42
2:B:186:PHE:CD1	2:B:193:VAL:HG21	2.55	0.42
4:D:25:PHE:C	4:D:26:LEU:HD12	2.45	0.42
1:A:279:ALA:HA	1:A:328:VAL:HG13	2.02	0.41
2:B:235:LEU:HD23	2:B:235:LEU:HA	1.91	0.41
2:B:247:TRP:CH2	2:B:395:LYS:HB3	2.53	0.41
3:C:34:ILE:CD1	3:C:120:VAL:CG1	2.98	0.41
3:C:163:LEU:HD21	3:C:204:THR:CG2	2.47	0.41
4:D:34:ILE:HD11	4:D:61:ALA:HA	2.01	0.41
4:D:45:PRO:HG2	4:D:46:ALA:N	2.34	0.41
1:A:234:SER:OG	1:A:246:ILE:HG23	2.19	0.41
2:B:195:TYR:CZ	4:D:94:PHE:HB2	2.55	0.41
1:A:158:HIS:O	1:A:159:CYS:SG	2.79	0.41
1:A:162:ILE:HD11	1:A:421:PRO:HG2	2.03	0.41
1:A:185:ASP:OD1	1:A:186:GLU:N	2.53	0.41
1:A:222:HIS:CB	1:A:247:VAL:HG23	2.50	0.41
1:A:279:ALA:HB1	1:A:330:PHE:CD2	2.53	0.41
1:A:429:ARG:NH2	1:A:432:ARG:NH1	2.68	0.41
2:B:433:PRO:HB3	2:B:436:PRO:HG3	2.02	0.41
1:A:162:ILE:HD12	1:A:164:TRP:CZ2	2.54	0.41
1:A:672:THR:HG23	3:C:158:LEU:HD13	2.03	0.41
2:B:193:VAL:HG12	2:B:198:VAL:HG23	2.02	0.41
3:C:207:ASN:O	3:C:208:PRO:C	2.61	0.41
1:A:68:GLY:CA	1:A:218:PHE:HD1	2.30	0.41
1:A:453:TYR:CD2	1:A:454:GLN:HG2	2.55	0.41
1:A:553:HIS:HD1	1:A:563:THR:HG21	1.85	0.41
3:C:115:ARG:NH1	8:C:1245:PC1:O12	2.48	0.41
1:A:258:SER:HB2	1:A:571:LEU:HD21	2.03	0.41
1:A:375:GLU:HA	1:A:412:ILE:HG23	2.02	0.41
1:A:451:LYS:NZ	1:A:451:LYS:CB	2.73	0.41
2:B:242:PRO:O	2:B:243:GLU:C	2.61	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:CYS:SG	1:A:159:CYS:O	2.79	0.41
2:B:251:ALA:O	2:B:255:VAL:HG23	2.21	0.41
4:D:82:ARG:NH2	4:D:97:PRO:HG3	2.35	0.41
1:A:57:THR:CG2	1:A:58:HIS:ND1	2.83	0.41
1:A:234:SER:HB2	1:A:247:VAL:HG12	2.02	0.41
1:A:352:PHE:CD1	1:A:353:PRO:HD2	2.56	0.41
1:A:672:THR:HG23	3:C:158:LEU:CD1	2.50	0.41
2:B:239:LYS:C	2:B:240:TYR:CD1	2.99	0.41
2:B:246:ALA:HB1	2:B:395:LYS:HG3	2.02	0.41
1:A:64:SER:HB3	1:A:219:SER:O	2.20	0.41
1:A:101:LYS:HG2	1:A:126:THR:HG21	2.02	0.41
1:A:167:LEU:HD22	1:A:451:LYS:HG2	2.02	0.41
1:A:304:THR:HG22	1:A:487:LEU:CG	2.51	0.41
1:A:361:SER:CB	1:A:501:LEU:HD13	2.48	0.41
1:A:52:ARG:HG2	1:A:54:LEU:HD21	2.03	0.40
1:A:256:VAL:HG21	1:A:567:VAL:CG1	2.48	0.40
1:A:349:LYS:HB3	1:A:351:LYS:CD	2.50	0.40
1:A:125:LEU:HD12	1:A:125:LEU:HA	1.85	0.40
1:A:140:CYS:CB	1:A:159:CYS:HG	2.33	0.40
2:B:241:LEU:HD12	2:B:241:LEU:HA	1.76	0.40
2:B:432:LEU:O	2:B:433:PRO:C	2.64	0.40
1:A:245:GLU:CD	4:D:98:LEU:HD21	2.40	0.40
1:A:460:ALA:HB1	1:A:465:VAL:HB	2.03	0.40
2:B:192:ALA:HB3	4:D:79:GLN:HE22	1.86	0.40
2:B:248:LEU:HD22	2:B:252:VAL:HG23	2.03	0.40
1:A:53:LEU:HB2	1:A:60:ILE:HD11	2.02	0.40
1:A:60:ILE:HG12	1:A:648:TRP:HZ3	1.85	0.40
1:A:169:ASN:HD22	1:A:171:LEU:HB2	1.85	0.40
1:A:332:GLY:HA2	1:A:555:ILE:HG12	2.03	0.40
1:A:378:MET:HA	1:A:440:VAL:O	2.21	0.40
3:C:35:LEU:HA	3:C:124:SER:HB2	2.03	0.40
1:A:60:ILE:O	1:A:60:ILE:HG13	2.22	0.40
1:A:91:ASN:C	1:A:93:PRO:HD2	2.45	0.40
1:A:380:THR:O	1:A:382:PRO:HD3	2.21	0.40
3:C:119:TYR:CD1	3:C:119:TYR:C	2.99	0.40
3:C:241:ARG:O	3:C:242:SER:C	2.63	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	663/709 (94%)	589 (89%)	54 (8%)	20 (3%)	3	18
2	B	209/467 (45%)	196 (94%)	8 (4%)	5 (2%)	4	22
3	C	241/265 (91%)	228 (95%)	12 (5%)	1 (0%)	30	59
4	D	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
All	All	1211/1542 (78%)	1108 (92%)	77 (6%)	26 (2%)	8	24

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	472	SER
1	A	559	SER
1	A	210	PHE
1	A	333	GLU
1	A	371	ARG
1	A	435	ASN
1	A	454	GLN
1	A	473	PRO
2	B	216	LYS
2	B	403	ASP
1	A	211	PRO
1	A	612	ASN
2	B	105	PHE
1	A	88	ASP
1	A	560	PRO
1	A	163	GLN
1	A	223	ALA
1	A	353	PRO
2	B	435	LEU
3	C	107	ASP
1	A	89	GLY
1	A	646	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	655	ASP
1	A	480	VAL
2	B	432	LEU
1	A	129	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	583/612 (95%)	495 (85%)	88 (15%)	3	11
2	B	184/408 (45%)	160 (87%)	24 (13%)	4	16
3	C	193/214 (90%)	172 (89%)	21 (11%)	6	22
4	D	88/89 (99%)	77 (88%)	11 (12%)	4	18
All	All	1048/1323 (79%)	904 (86%)	144 (14%)	6	14

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	HIS
1	A	59	GLN
1	A	60	ILE
1	A	69	ASP
1	A	72	VAL
1	A	84	TRP
1	A	85	VAL
1	A	86	LEU
1	A	94	TYR
1	A	95	MET
1	A	97	LEU
1	A	104	THR
1	A	107	LEU
1	A	111	LEU
1	A	112	LYS
1	A	126	THR
1	A	129	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	139	GLN
1	A	147	VAL
1	A	149	SER
1	A	150	ASN
1	A	152	TYR
1	A	155	GLU
1	A	162	ILE
1	A	163	GLN
1	A	174	GLU
1	A	182	LEU
1	A	188	GLU
1	A	201	LEU
1	A	217	LEU
1	A	248	CYS
1	A	249	ASP
1	A	256	VAL
1	A	261	LYS
1	A	264	ASN
1	A	269	LEU
1	A	270	LYS
1	A	280	THR
1	A	281	ARG
1	A	296	GLU
1	A	305	GLN
1	A	306	LEU
1	A	312	LEU
1	A	326	MET
1	A	333	GLU
1	A	338	ILE
1	A	342	ARG
1	A	343	MET
1	A	347	MET
1	A	364	GLU
1	A	365	LEU
1	A	367	GLN
1	A	371	ARG
1	A	375	GLU
1	A	378	MET
1	A	380	THR
1	A	387	ASN
1	A	391	ARG
1	A	413	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	418	GLN
1	A	425	SER
1	A	429	ARG
1	A	431	LEU
1	A	434	ARG
1	A	436	ILE
1	A	437	SER
1	A	451	LYS
1	A	463	ILE
1	A	464	ASN
1	A	487	LEU
1	A	519	THR
1	A	537	ILE
1	A	559	SER
1	A	561	THR
1	A	562	ASN
1	A	573	ASN
1	A	574	LEU
1	A	586	CYS
1	A	604	TRP
1	A	605	VAL
1	A	609	LEU
1	A	624	THR
1	A	631	LEU
1	A	632	SER
1	A	636	GLU
1	A	637	LEU
1	A	643	THR
1	A	644	GLU
2	B	84	MET
2	B	85	LEU
2	B	91	LEU
2	B	173	LEU
2	B	174	LEU
2	B	180	ILE
2	B	200	LEU
2	B	241	LEU
2	B	244	TRP
2	B	248	LEU
2	B	381	LEU
2	B	395	LYS
2	B	407	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	420	LEU
2	B	422	LEU
2	B	423	LEU
2	B	424	LEU
2	B	425	LEU
2	B	427	ILE
2	B	429	LYS
2	B	430	LYS
2	B	432	LEU
2	B	435	LEU
2	B	438	SER
3	C	46	LEU
3	C	47	LEU
3	C	68	GLN
3	C	93	LEU
3	C	106	GLU
3	C	112	ILE
3	C	113	SER
3	C	114	ILE
3	C	123	LEU
3	C	127	ILE
3	C	131	VAL
3	C	133	SER
3	C	134	VAL
3	C	146	VAL
3	C	170	LEU
3	C	192	LEU
3	C	198	LEU
3	C	206	LEU
3	C	216	PRO
3	C	243	LEU
3	C	244	LEU
4	D	14	LEU
4	D	39	ARG
4	D	40	GLU
4	D	42	PHE
4	D	43	LEU
4	D	44	VAL
4	D	47	TYR
4	D	52	GLN
4	D	69	ILE
4	D	94	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	98	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	HIS
1	A	139	GLN
1	A	142	ASN
1	A	150	ASN
1	A	163	GLN
1	A	194	GLN
1	A	222	HIS
1	A	305	GLN
1	A	313	GLN
1	A	331	GLN
1	A	358	ASN
1	A	418	GLN
1	A	428	GLN
1	A	516	GLN
1	A	531	ASN
1	A	535	GLN
1	A	568	GLN
1	A	606	GLN
1	A	639	GLN
2	B	81	HIS
3	C	116	GLN
3	C	136	ASN
3	C	207	ASN
4	D	79	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 ⓘ

15 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
5	NAG	E	1	5,1	14,14,15	0.57	0	17,19,21	1.07	1 (5%)
5	NAG	E	2	5	14,14,15	0.50	0	17,19,21	1.31	2 (11%)
6	NAG	F	1	6,1	14,14,15	0.49	0	17,19,21	1.53	3 (17%)
6	NAG	F	2	6	14,14,15	0.47	0	17,19,21	0.87	0
6	BMA	F	3	6	11,11,12	0.38	0	15,15,17	0.82	1 (6%)
6	BMA	F	4	6	11,11,12	0.31	0	15,15,17	0.58	0
6	BMA	F	5	6	11,11,12	0.41	0	15,15,17	1.55	2 (13%)
5	NAG	G	1	5,1	14,14,15	0.64	0	17,19,21	1.39	1 (5%)
5	NAG	G	2	5	14,14,15	0.56	0	17,19,21	1.38	4 (23%)
5	NAG	H	1	5,1	14,14,15	0.49	0	17,19,21	1.12	2 (11%)
5	NAG	H	2	5	14,14,15	0.53	0	17,19,21	1.24	3 (17%)
5	NAG	I	1	5,1	14,14,15	0.51	0	17,19,21	1.10	2 (11%)
5	NAG	I	2	5	14,14,15	0.73	0	17,19,21	2.29	5 (29%)
5	NAG	J	1	5,1	14,14,15	0.68	0	17,19,21	1.18	1 (5%)
5	NAG	J	2	5	14,14,15	0.47	0	17,19,21	0.73	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	E	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	E	2	5	-	2/6/23/26	0/1/1/1
6	NAG	F	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	F	2	6	-	1/6/23/26	0/1/1/1
6	BMA	F	3	6	-	0/2/19/22	0/1/1/1
6	BMA	F	4	6	-	1/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BMA	F	5	6	-	0/2/19/22	0/1/1/1
5	NAG	G	1	5,1	-	3/6/23/26	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	0/1/1/1
5	NAG	H	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	H	2	5	-	3/6/23/26	0/1/1/1
5	NAG	I	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	I	2	5	-	4/6/23/26	0/1/1/1
5	NAG	J	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	J	2	5	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	2	NAG	C2-N2-C7	4.91	129.48	122.90
6	F	5	BMA	C1-O5-C5	4.74	118.53	112.19
6	F	1	NAG	C1-O5-C5	4.63	118.39	112.19
5	G	1	NAG	C1-O5-C5	4.54	118.27	112.19
5	I	2	NAG	C8-C7-N2	4.17	123.03	116.12
5	I	2	NAG	C4-C3-C2	4.07	116.98	111.02
5	I	2	NAG	C3-C4-C5	3.53	116.62	110.23
5	E	2	NAG	C8-C7-N2	2.92	120.97	116.12
5	I	2	NAG	O7-C7-C8	-2.88	116.93	122.05
5	E	1	NAG	C4-C3-C2	2.79	115.11	111.02
5	J	1	NAG	O5-C5-C4	-2.71	104.23	110.83
5	G	2	NAG	C8-C7-N2	2.64	120.50	116.12
5	H	2	NAG	C8-C7-N2	2.60	120.42	116.12
5	E	2	NAG	C2-N2-C7	2.57	126.34	122.90
6	F	5	BMA	C3-C4-C5	2.56	114.87	110.23
5	I	1	NAG	C4-C3-C2	2.36	114.48	111.02
5	H	2	NAG	C2-N2-C7	2.30	125.98	122.90
6	F	1	NAG	C8-C7-N2	2.24	119.83	116.12
5	H	1	NAG	O4-C4-C5	2.23	114.83	109.32
5	H	2	NAG	C1-O5-C5	2.22	115.16	112.19
5	G	2	NAG	C4-C3-C2	2.19	114.23	111.02
6	F	1	NAG	C2-N2-C7	2.15	125.79	122.90
5	G	2	NAG	C3-C4-C5	2.14	114.11	110.23
5	H	1	NAG	C4-C3-C2	-2.13	107.90	111.02
6	F	3	BMA	C3-C4-C5	2.09	114.02	110.23
5	I	1	NAG	O5-C1-C2	-2.04	108.13	111.29
5	G	2	NAG	O5-C1-C2	-2.03	108.14	111.29

There are no chirality outliers.

All (23) torsion outliers are listed below:

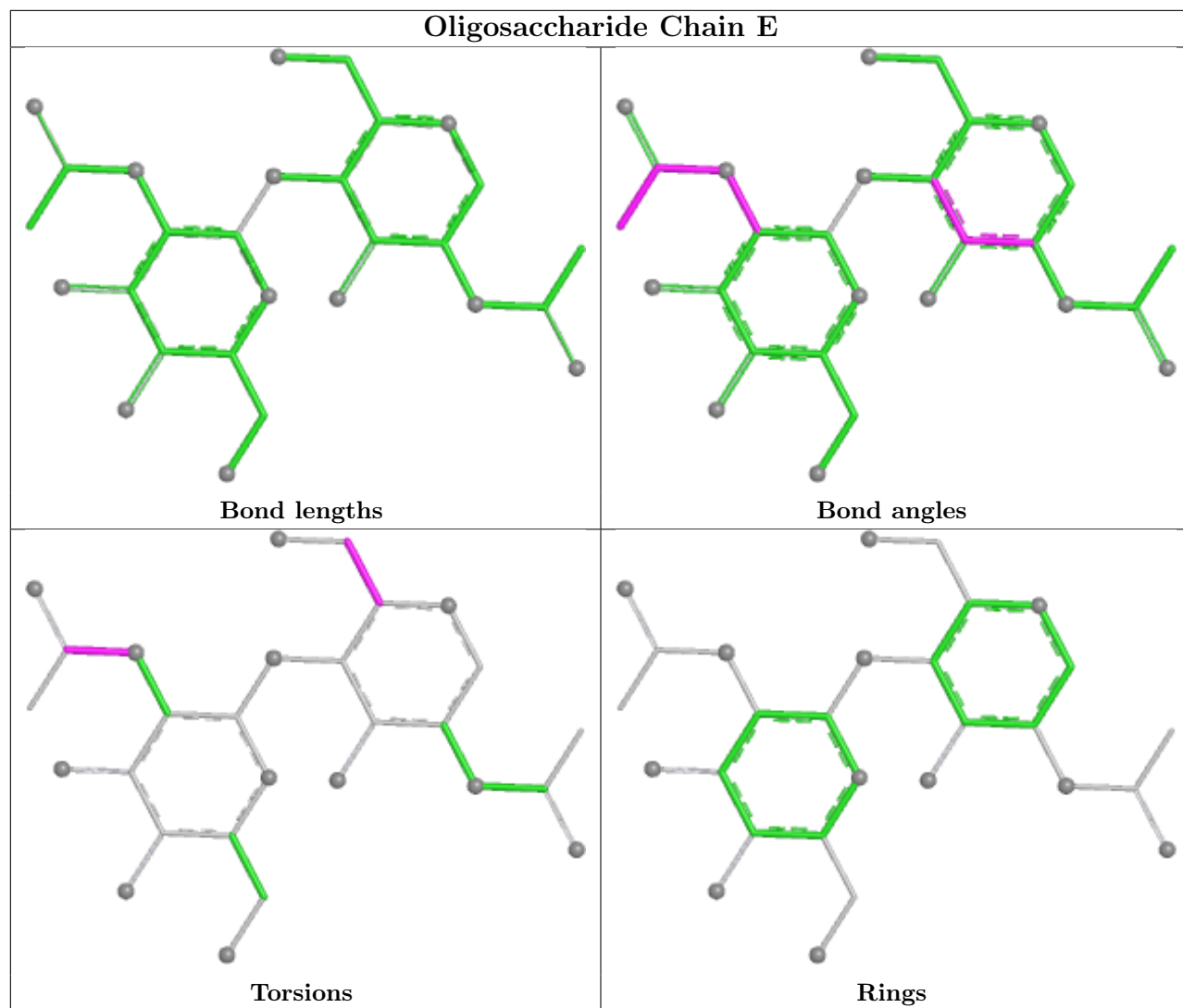
Mol	Chain	Res	Type	Atoms
5	E	1	NAG	O5-C5-C6-O6
5	E	1	NAG	C4-C5-C6-O6
5	H	1	NAG	C4-C5-C6-O6
5	E	2	NAG	C8-C7-N2-C2
5	E	2	NAG	O7-C7-N2-C2
5	G	2	NAG	C8-C7-N2-C2
5	G	2	NAG	O7-C7-N2-C2
5	H	2	NAG	C8-C7-N2-C2
5	H	2	NAG	O7-C7-N2-C2
5	I	2	NAG	C8-C7-N2-C2
5	I	2	NAG	O7-C7-N2-C2
6	F	1	NAG	C8-C7-N2-C2
6	F	1	NAG	O7-C7-N2-C2
5	H	1	NAG	O5-C5-C6-O6
5	H	2	NAG	O5-C5-C6-O6
5	G	1	NAG	O5-C5-C6-O6
6	F	2	NAG	O5-C5-C6-O6
6	F	4	BMA	O5-C5-C6-O6
5	G	1	NAG	C1-C2-N2-C7
5	I	1	NAG	C1-C2-N2-C7
5	I	2	NAG	C1-C2-N2-C7
5	G	1	NAG	C3-C2-N2-C7
5	I	2	NAG	C3-C2-N2-C7

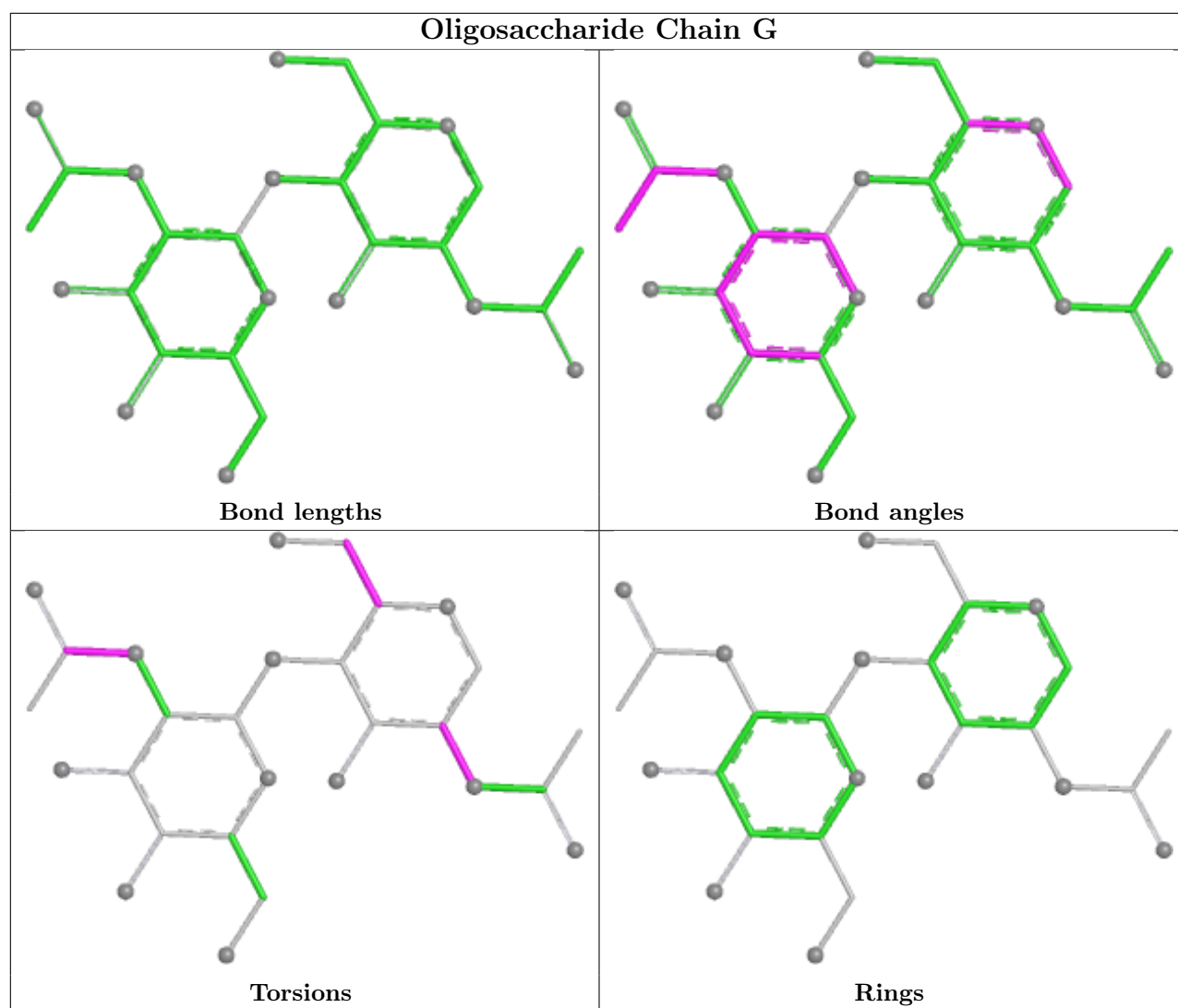
There are no ring outliers.

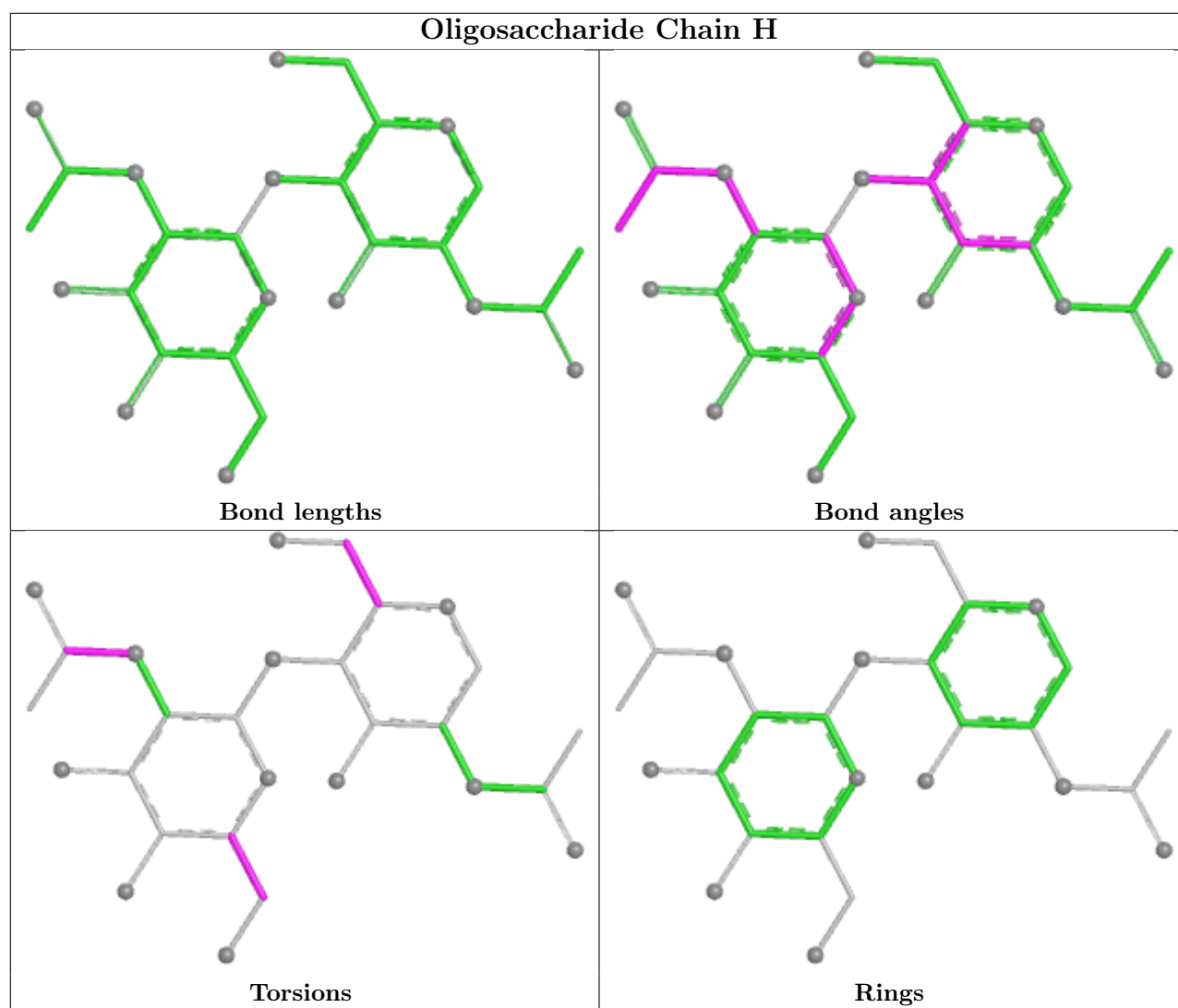
3 monomers are involved in 3 short contacts:

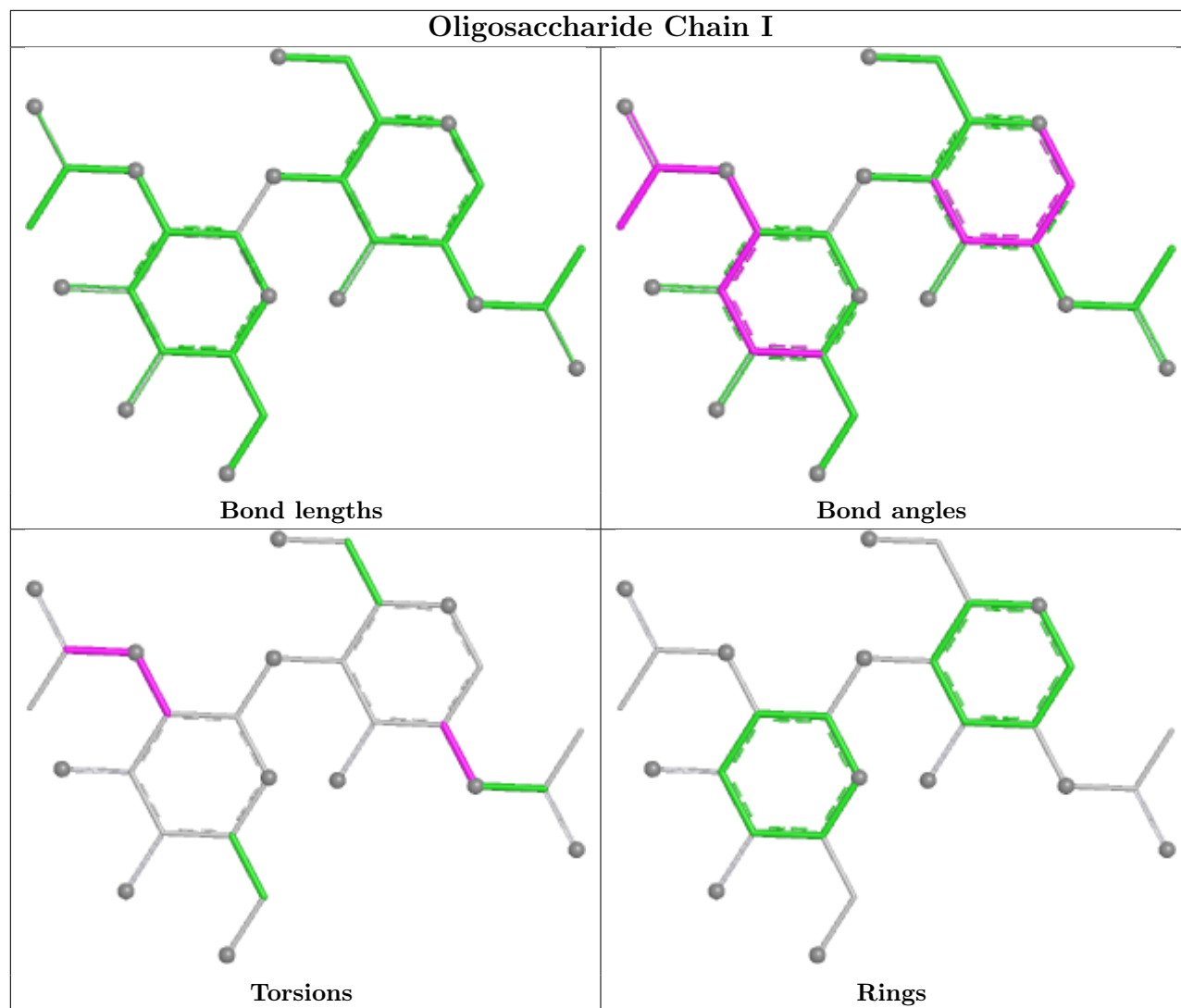
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	J	1	NAG	2	0
5	H	2	NAG	1	0
5	H	1	NAG	1	0

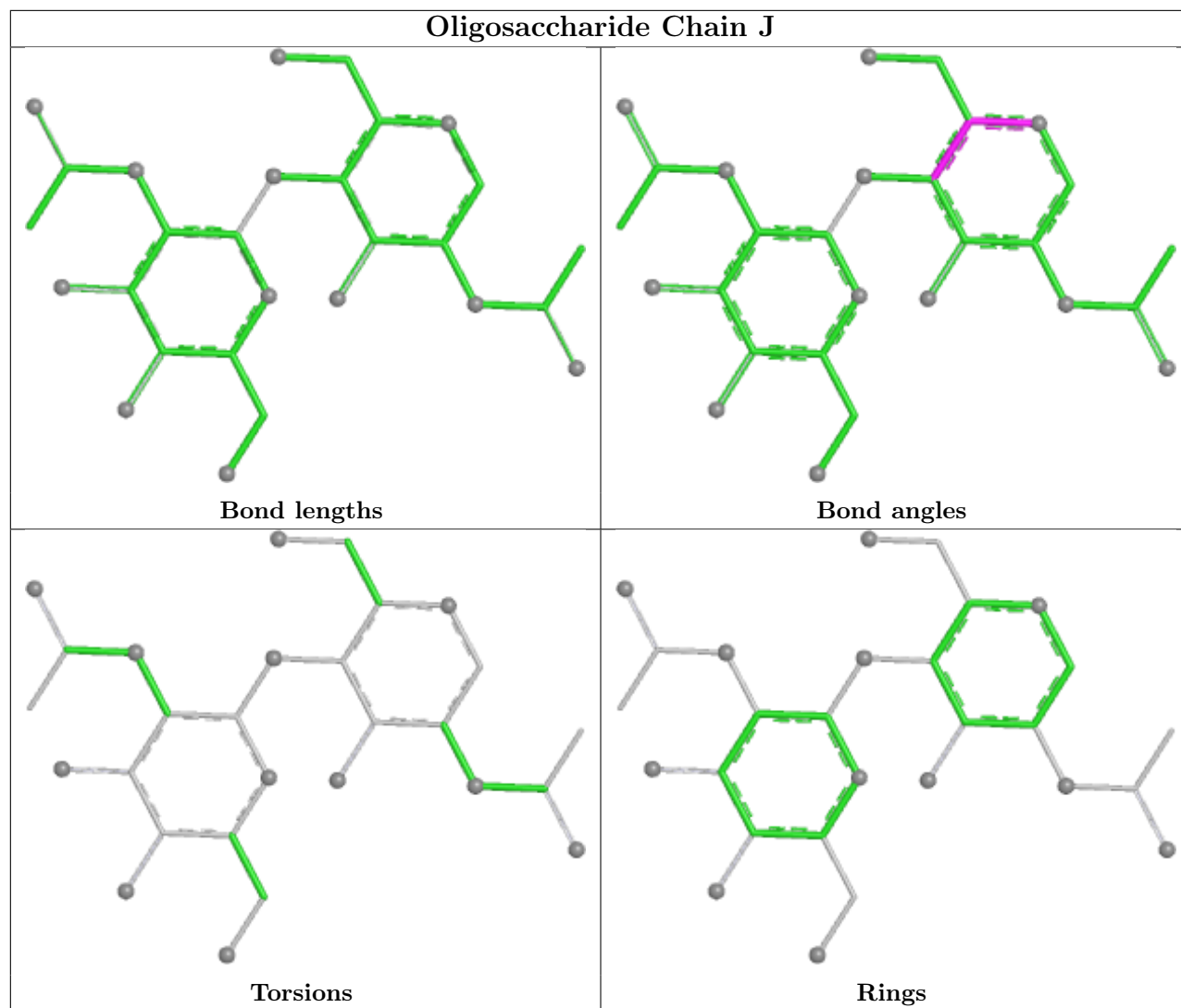
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

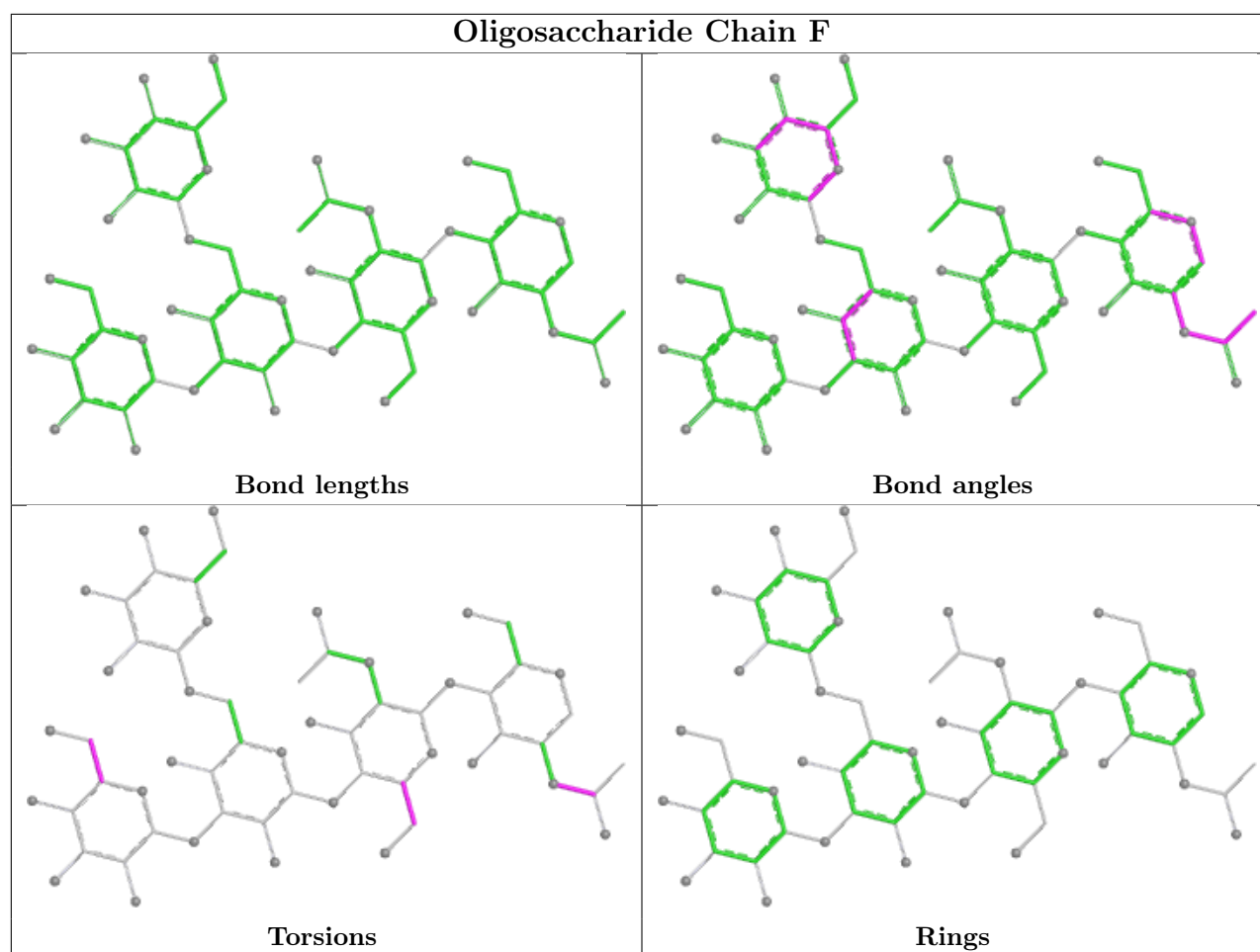












5.6 Ligand geometry [i](#)

7 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	NAG	A	1714	1	14,14,15	0.48	0	17,19,21	0.74	0
8	PC1	B	1468	-	42,42,53	1.06	2 (4%)	48,50,61	1.02	2 (4%)
7	NAG	A	1705	1	14,14,15	0.54	0	17,19,21	0.98	1 (5%)
7	NAG	A	1713	1	14,14,15	0.53	0	17,19,21	1.09	1 (5%)
7	NAG	A	1715	1	14,14,15	0.47	0	17,19,21	0.87	0
7	NAG	A	1712	1	14,14,15	0.44	0	17,19,21	0.98	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	PC1	C	1245	-	42,42,53	1.07	2 (4%)	48,50,61	0.98	3 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	A	1714	1	-	0/6/23/26	0/1/1/1
8	PC1	B	1468	-	-	19/46/46/57	-
7	NAG	A	1705	1	-	1/6/23/26	0/1/1/1
7	NAG	A	1713	1	-	1/6/23/26	0/1/1/1
7	NAG	A	1715	1	-	0/6/23/26	0/1/1/1
7	NAG	A	1712	1	-	0/6/23/26	0/1/1/1
8	PC1	C	1245	-	-	19/46/46/57	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	1245	PC1	O31-C31	4.44	1.46	1.33
8	C	1245	PC1	O21-C21	4.39	1.46	1.34
8	B	1468	PC1	O31-C31	4.34	1.46	1.33
8	B	1468	PC1	O21-C21	4.29	1.46	1.34

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	1468	PC1	O21-C21-C22	4.06	120.27	111.48
8	C	1245	PC1	O21-C21-C22	3.97	120.08	111.48
7	A	1713	NAG	O5-C1-C2	-2.92	106.78	111.29
7	A	1712	NAG	O5-C1-C2	-2.78	107.00	111.29
8	C	1245	PC1	O31-C31-C32	2.78	120.30	111.83
8	B	1468	PC1	O31-C31-C32	2.64	119.87	111.83
7	A	1705	NAG	O5-C1-C2	-2.29	107.75	111.29
8	C	1245	PC1	O31-C31-O32	-2.11	118.34	123.63

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	1245	PC1	C11-O13-P-O11

Continued on next page...

Continued from previous page...

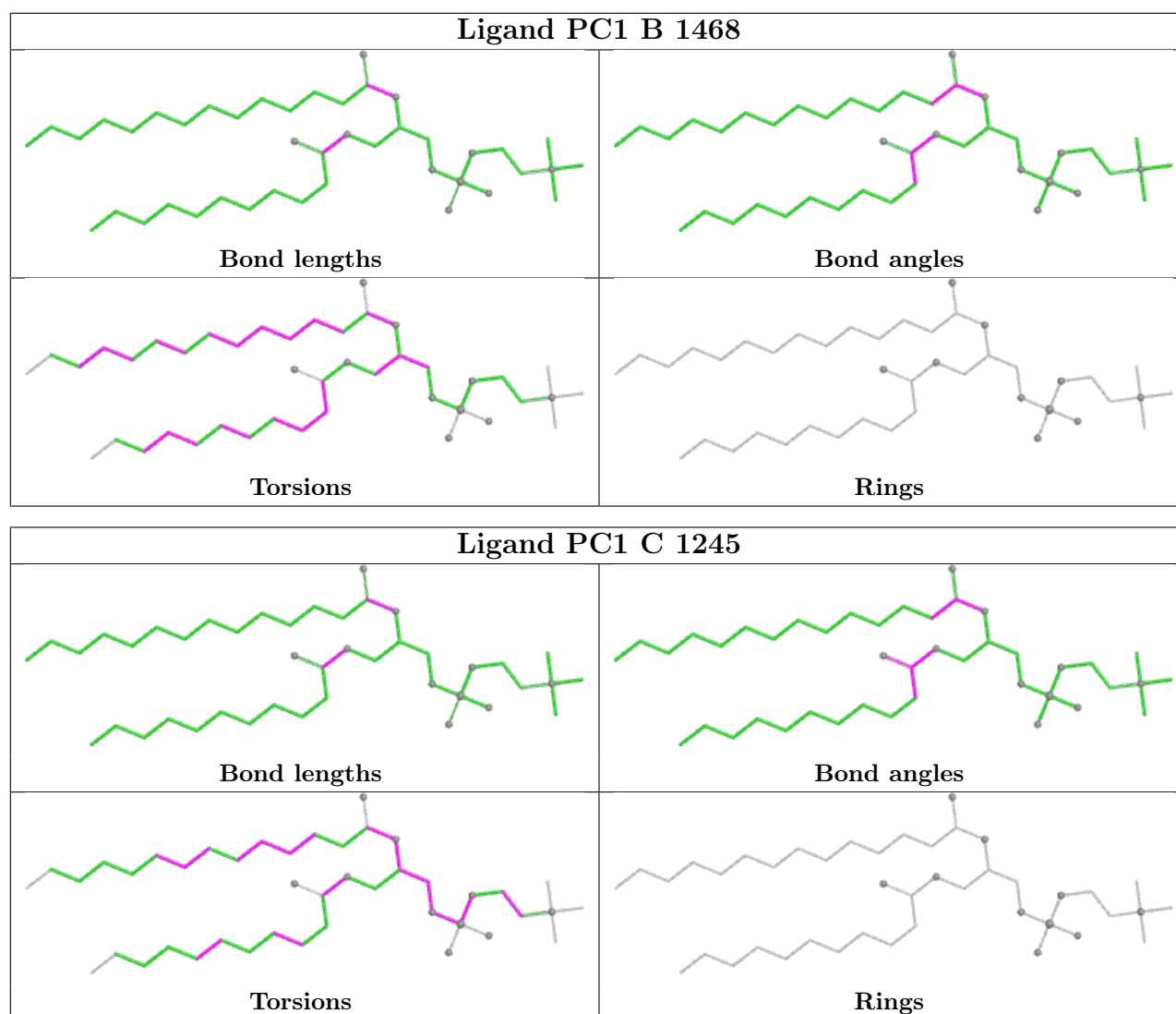
Mol	Chain	Res	Type	Atoms
8	C	1245	PC1	C1-O11-P-O14
8	C	1245	PC1	C1-O11-P-O13
8	C	1245	PC1	O13-C11-C12-N
8	C	1245	PC1	C22-C21-O21-C2
8	B	1468	PC1	O22-C21-O21-C2
8	C	1245	PC1	O22-C21-O21-C2
8	B	1468	PC1	C22-C21-O21-C2
8	B	1468	PC1	C23-C24-C25-C26
8	B	1468	PC1	C27-C28-C29-C2A
8	B	1468	PC1	C34-C35-C36-C37
8	C	1245	PC1	C32-C31-O31-C3
8	B	1468	PC1	C24-C25-C26-C27
8	C	1245	PC1	C22-C23-C24-C25
8	C	1245	PC1	O32-C31-O31-C3
8	C	1245	PC1	C32-C33-C34-C35
8	B	1468	PC1	C36-C37-C38-C39
8	C	1245	PC1	C35-C36-C37-C38
8	C	1245	PC1	C24-C25-C26-C27
7	A	1705	NAG	O5-C5-C6-O6
8	B	1468	PC1	C22-C23-C24-C25
8	B	1468	PC1	C21-C22-C23-C24
8	B	1468	PC1	C31-C32-C33-C34
8	B	1468	PC1	C25-C26-C27-C28
8	B	1468	PC1	C29-C2A-C2B-C2C
8	C	1245	PC1	C1-C2-O21-C21
8	B	1468	PC1	O21-C2-C3-O31
8	B	1468	PC1	C2A-C2B-C2C-C2D
8	C	1245	PC1	O11-C1-C2-C3
8	C	1245	PC1	C11-O13-P-O14
8	C	1245	PC1	C2-C1-O11-P
8	B	1468	PC1	C37-C38-C39-C3A
8	B	1468	PC1	C32-C33-C34-C35
8	C	1245	PC1	C26-C27-C28-C29
8	C	1245	PC1	C23-C24-C25-C26
7	A	1713	NAG	C4-C5-C6-O6
8	B	1468	PC1	O11-C1-C2-O21
8	B	1468	PC1	O31-C31-C32-C33
8	C	1245	PC1	C27-C28-C29-C2A
8	B	1468	PC1	O32-C31-C32-C33

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1714	NAG	1	0
7	A	1705	NAG	2	0
8	C	1245	PC1	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

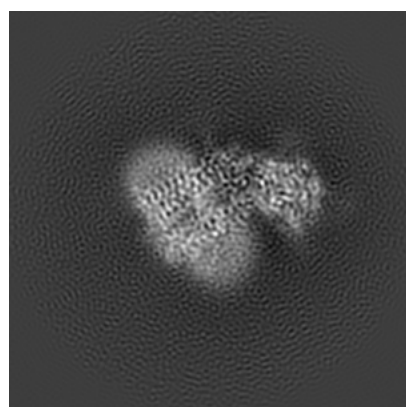
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3061. These allow visual inspection of the internal detail of the map and identification of artifacts.

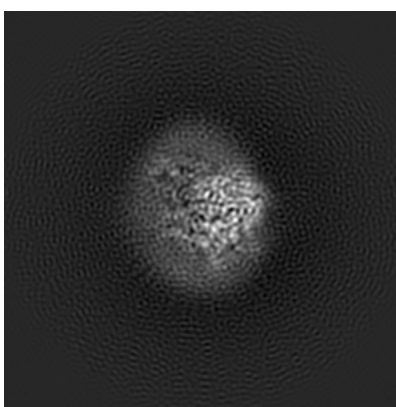
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

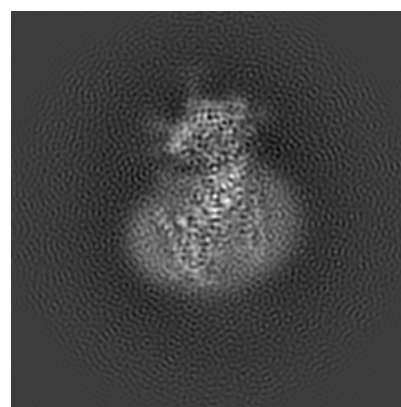
6.1.1 Primary map



X



Y

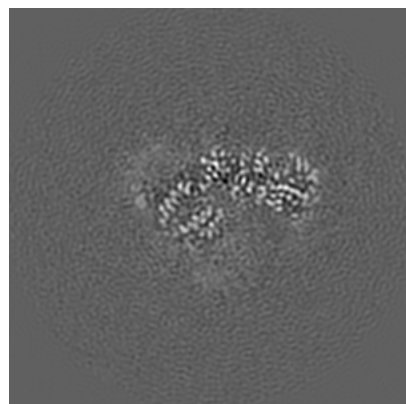


Z

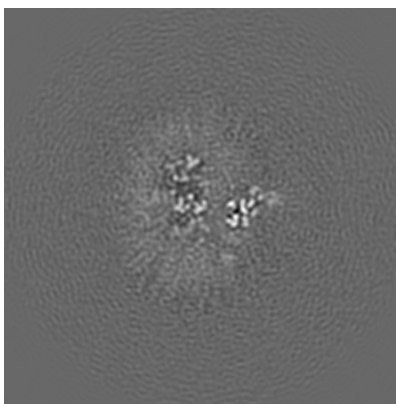
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

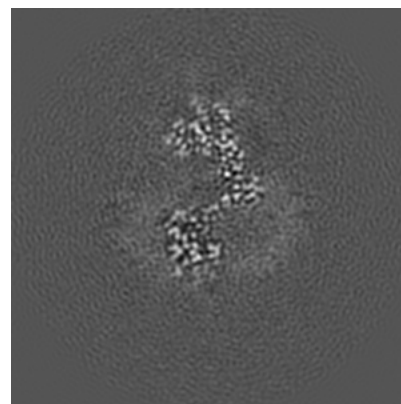
6.2.1 Primary map



X Index: 90



Y Index: 90

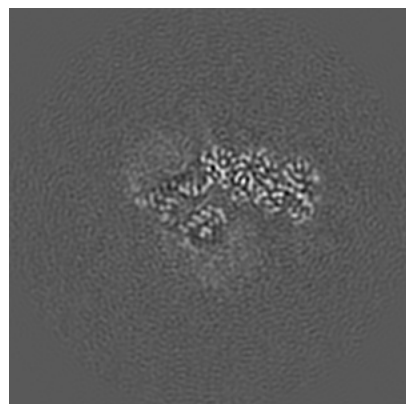


Z Index: 90

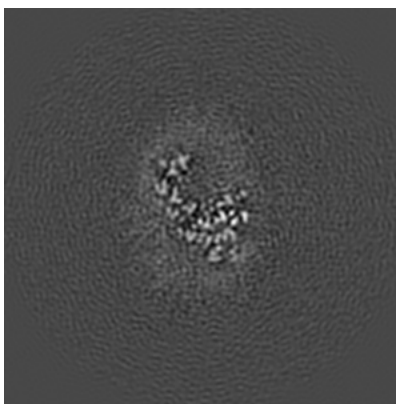
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

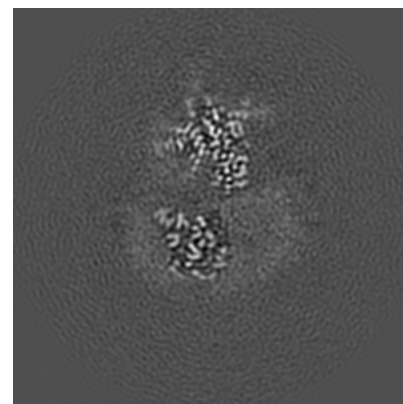
6.3.1 Primary map



X Index: 91



Y Index: 84

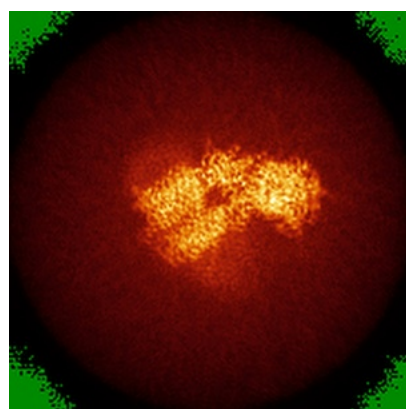


Z Index: 95

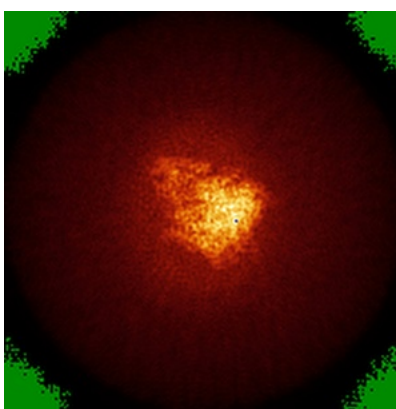
The images above show the largest variance slices of the map in three orthogonal directions.

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

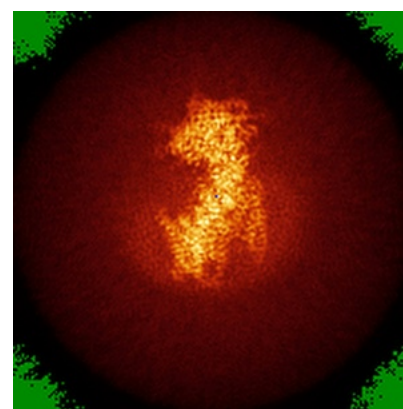
6.4.1 Primary map



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

This section was not generated.

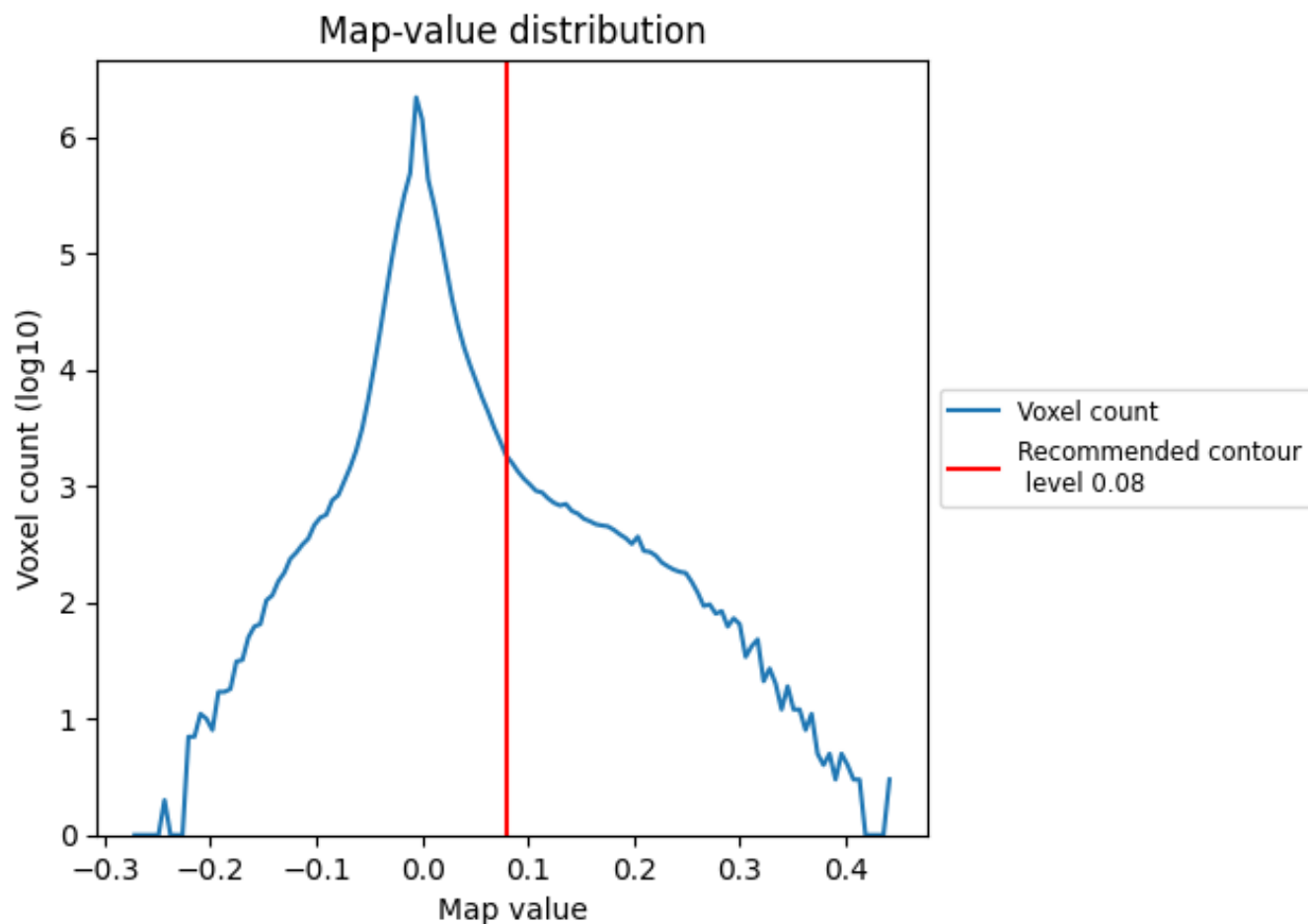
6.6 Mask visualisation

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

7 Map analysis [i](#)

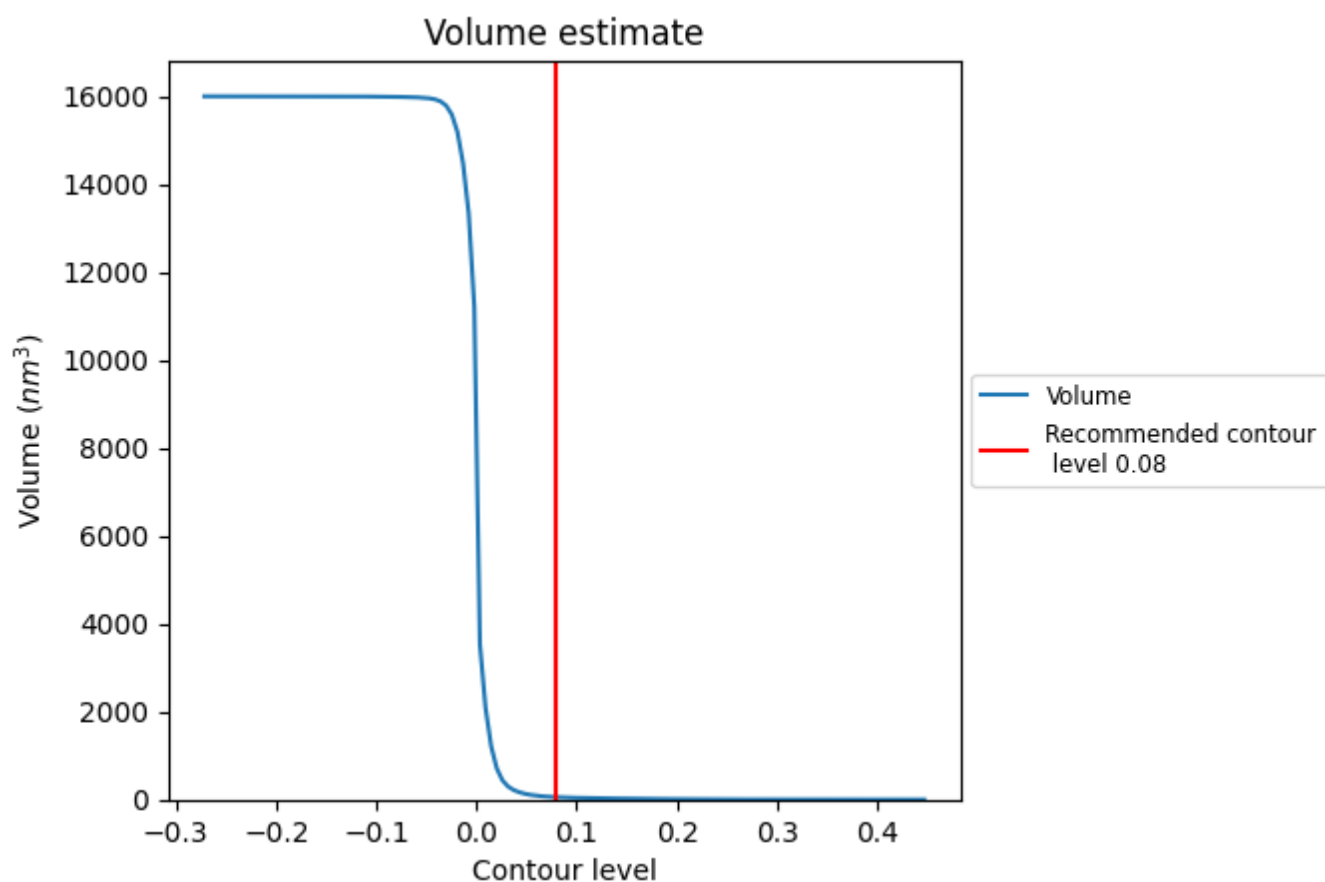
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

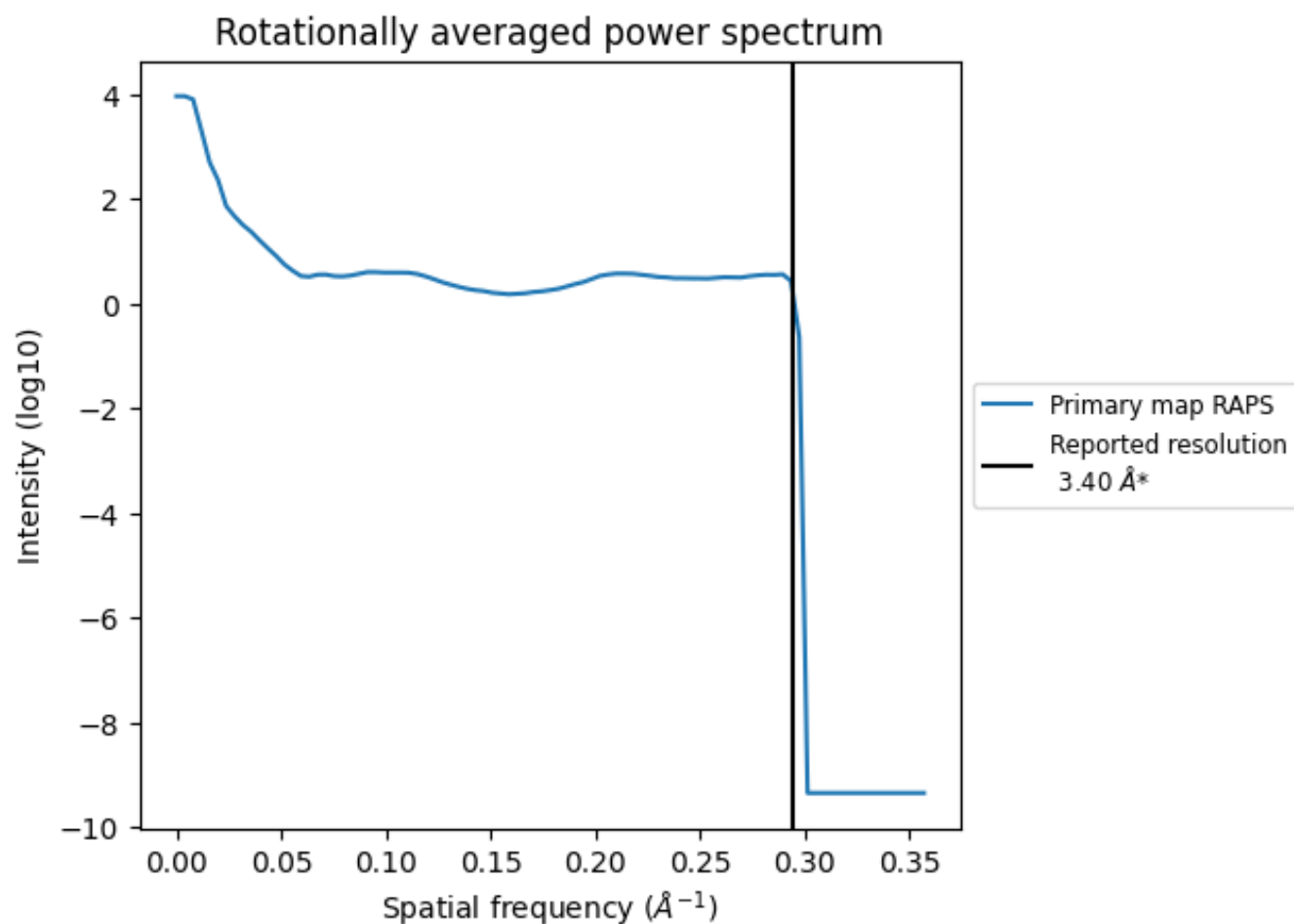
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 54 nm³; this corresponds to an approximate mass of 49 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

8 Fourier-Shell correlation ⓘ

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

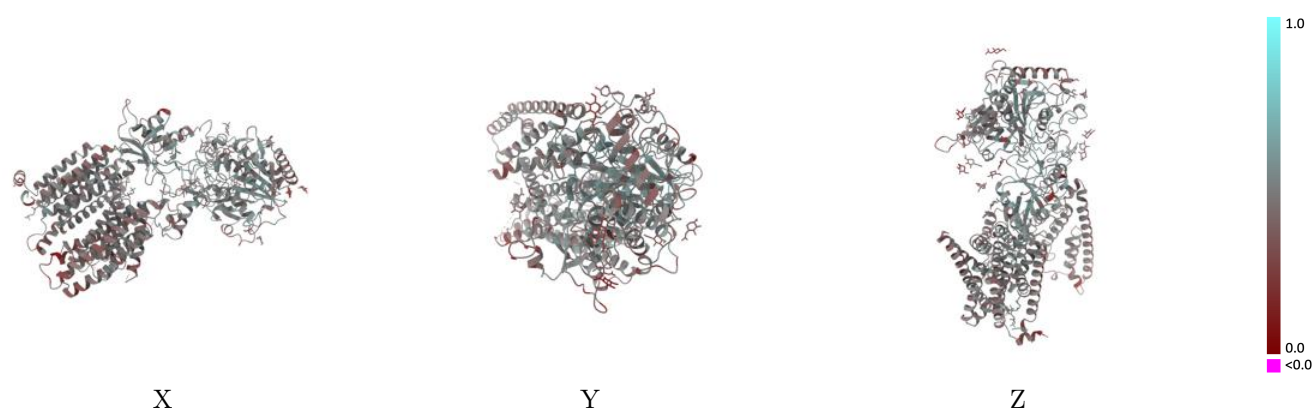
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3061 and PDB model 5A63. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)

This section was not generated.

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

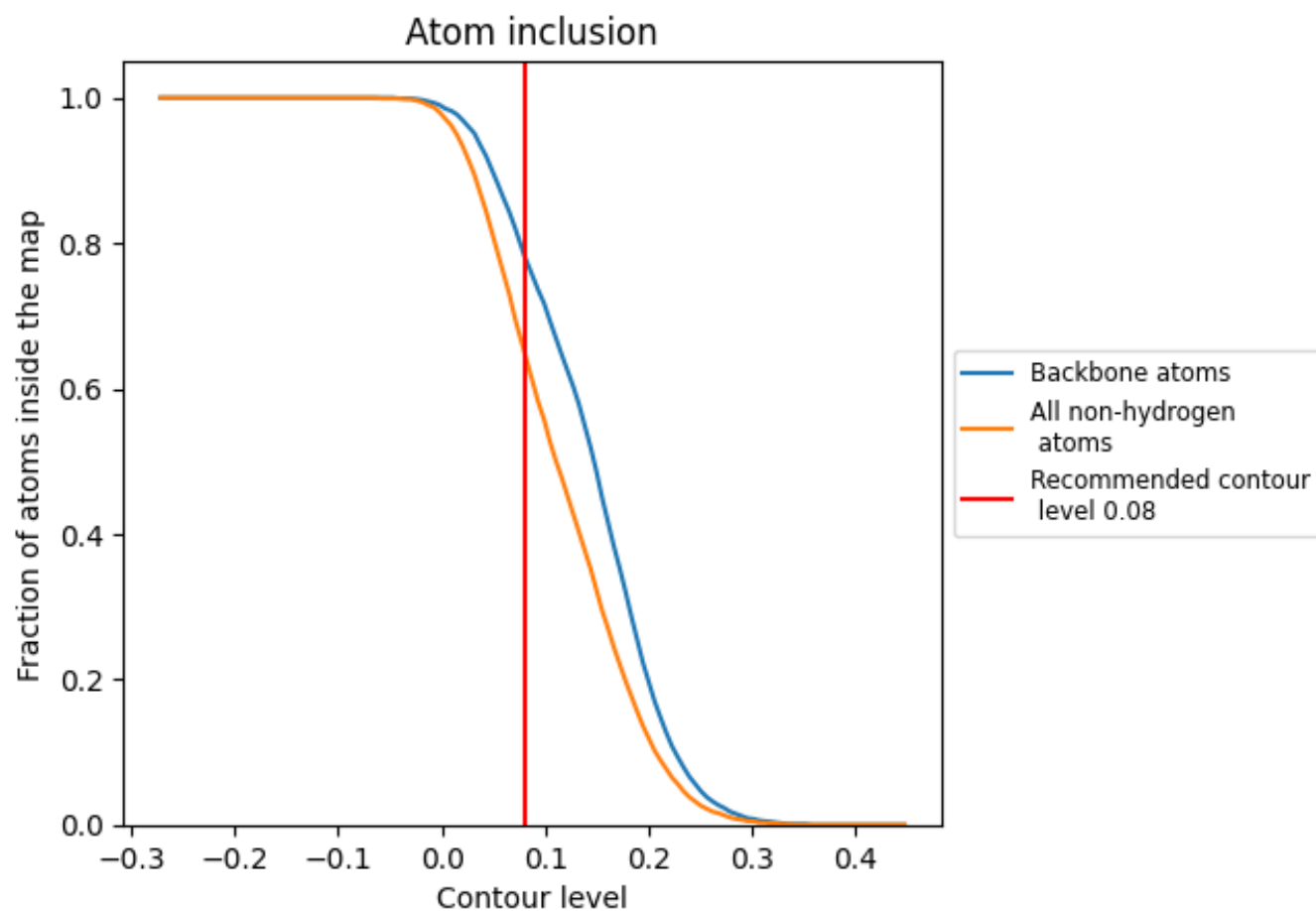


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 65% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6490	0.4570
A	0.6990	0.4780
B	0.5730	0.4410
C	0.6220	0.4480
D	0.5970	0.3980
E	0.5000	0.4230
F	0.5250	0.4320
G	0.6430	0.4040
H	0.5000	0.2720
I	0.2140	0.3160
J	0.3570	0.3160

1.0

0.0

<0.0