



## Full wwPDB EM Validation Report ⓘ

Nov 7, 2023 – 10:16 AM JST

PDB ID : 5GJW  
EMDB ID : EMD-9515  
Title : Structure of the mammalian voltage-gated calcium channel Cav1.1 complex for ClassII map  
Authors : Wu, J.P.; Yan, Z.; Li, Z.Q.; Zhou, Q.; Yan, N.  
Deposited on : 2016-07-02  
Resolution : 3.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

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

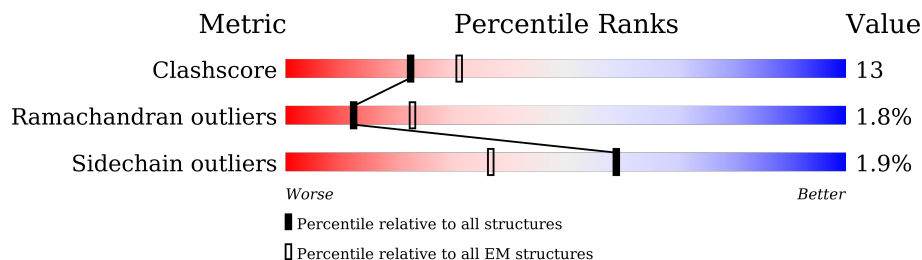
EMDB validation analysis : 0.0.1.dev70  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

# 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 3.90 Å.

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



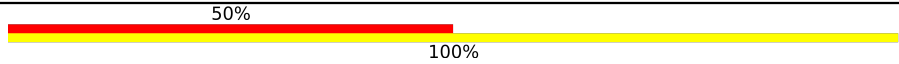



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	1873	
2	B	106	
3	C	199	
4	E	222	
5	F	1106	
6	D	2	
6	G	2	
6	J	2	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
6	K	2	 50% 100%
7	H	3	 33% 33% 67%
7	I	3	 33% 67%
8	L	3	 33% 33% 67%

## 2 Entry composition i

There are 10 unique types of molecules in this entry. The entry contains 21561 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 Voltage-dependent L-type calcium channel subunit alpha-1S.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1291	10261	6745	1687	1759	70	0	0

- Molecule 2 is a protein called Voltage-dependent L-type calcium channel subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	100	710	455	125	129	1	0	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	69	SER	-	expression tag	UNP P19517
B	70	LEU	-	expression tag	UNP P19517
B	71	GLU	-	expression tag	UNP P19517
B	72	VAL	-	expression tag	UNP P19517
B	73	LEU	-	expression tag	UNP P19517
B	74	PHE	-	expression tag	UNP P19517
B	75	GLN	-	expression tag	UNP P19517
B	76	GLY	-	expression tag	UNP P19517
B	77	PRO	-	expression tag	UNP P19517
B	78	HIS	-	expression tag	UNP P19517
B	79	MET	-	expression tag	UNP P19517

- Molecule 3 is a protein called Voltage-dependent L-type calcium channel subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	178	1367	876	232	254	5	0	0

- Molecule 4 is a protein called Voltage-dependent calcium channel gamma-1 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	166	1304	860	213	213	18	0	0

- Molecule 5 is a protein called Voltage-dependent calcium channel subunit alpha-2/delta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	942	7572	4812	1278	1452	30	2	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	1075	ETA	GLY	See sequence details	UNP P13806

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



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	D	2	28	16	2	10	0	0
6	G	2	28	16	2	10	0	0
6	J	2	28	16	2	10	0	0
6	K	2	28	16	2	10	0	0

- Molecule 7 is an oligosaccharide called 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
			Total	C	N	O		
7	H	3	39	22	2	15	0	0

*Continued on next page...*

Continued from previous page...

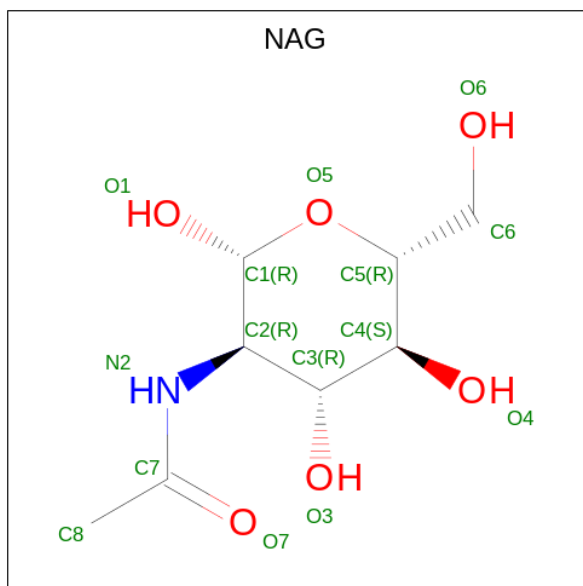
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	I	3	39	22	2	15	0	0

- Molecule 8 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	L	3	42	24	3	15	0	0

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

Continued on next page...

*Continued from previous page...*

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

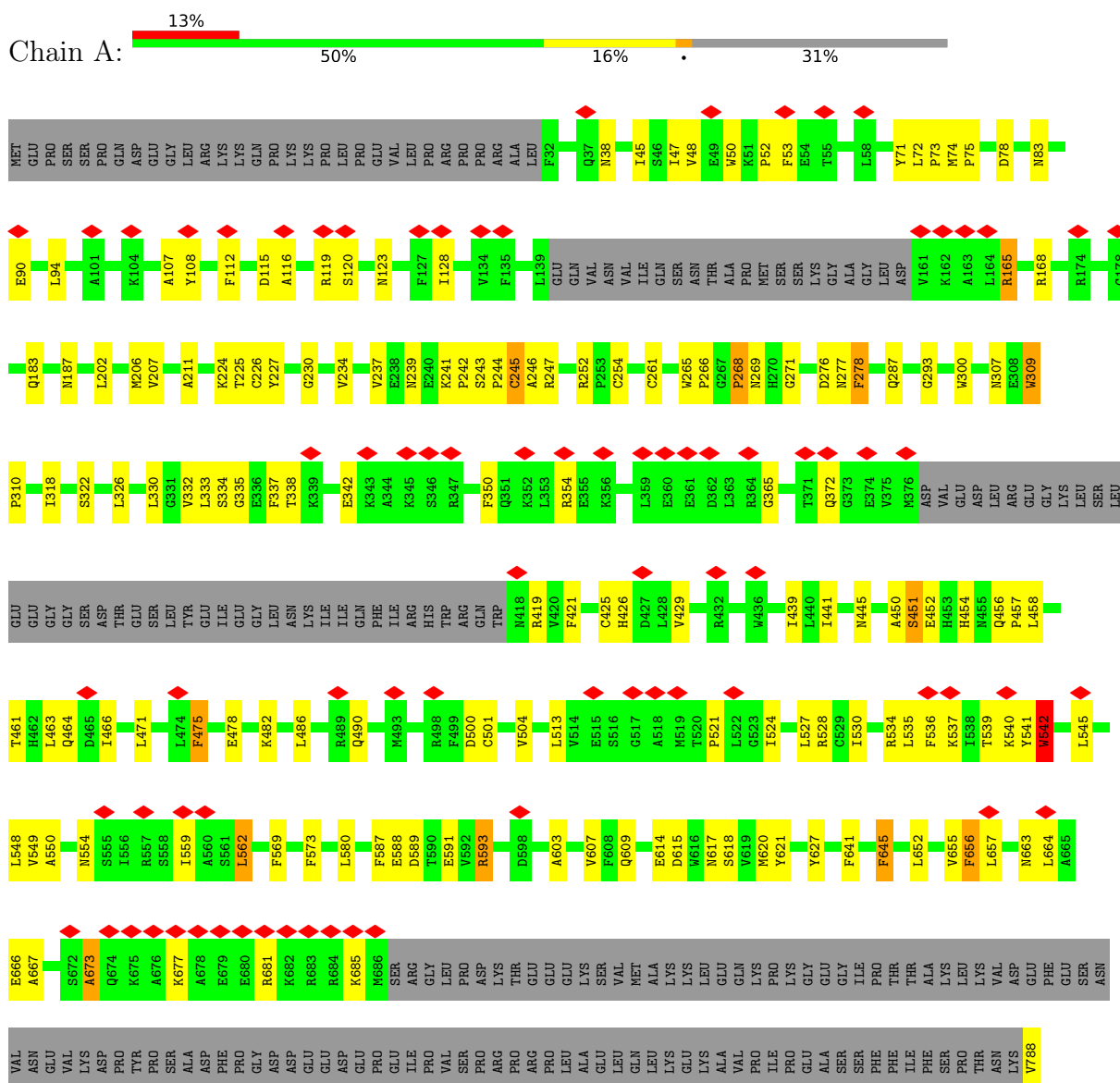
- Molecule 10 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
10	A	2	Total	Ca	0
			2	2	
10	F	1	Total	Ca	0
			1	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.

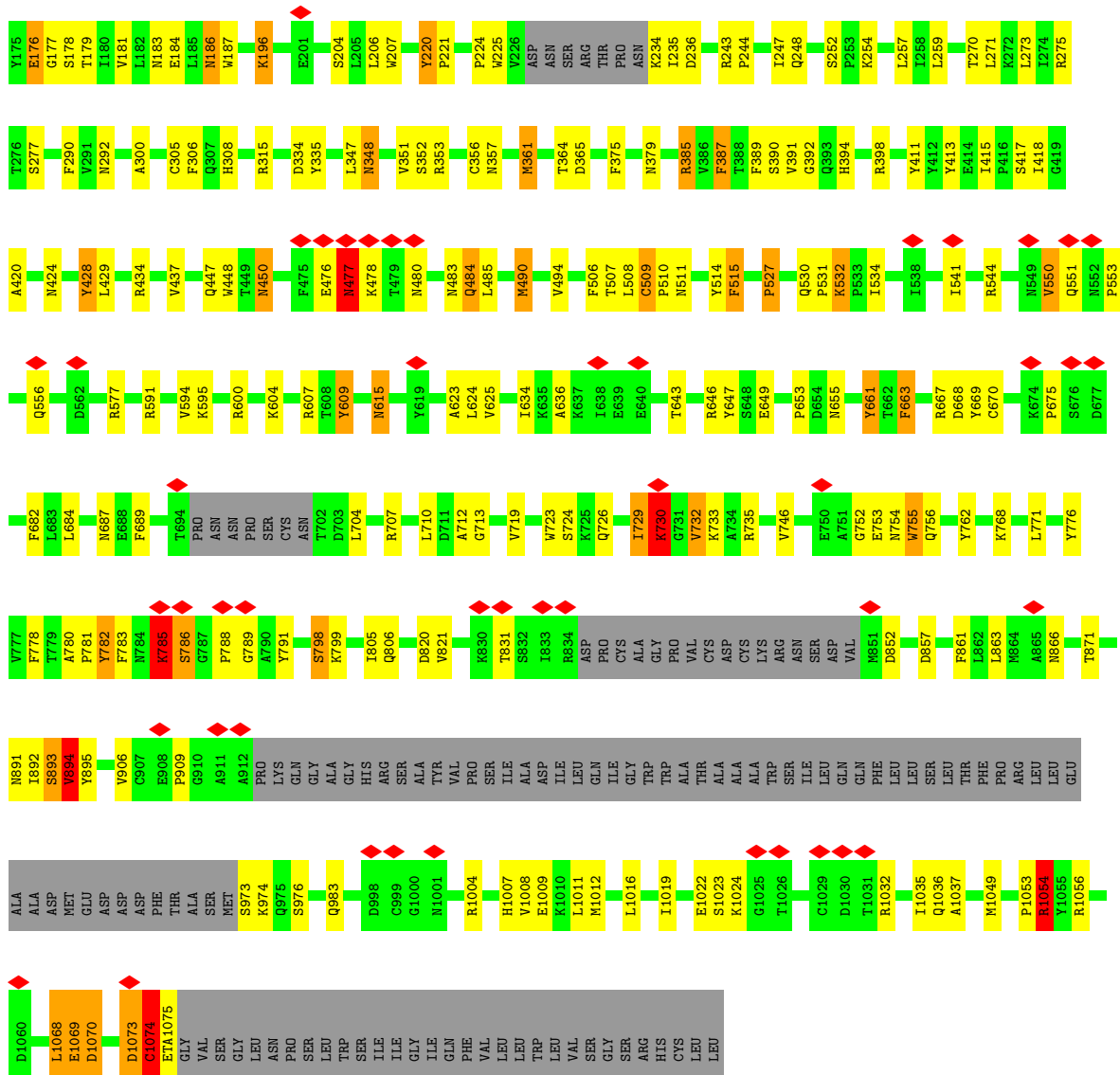
- Molecule 1: Voltage-dependent L-type calcium channel subunit alpha-1S











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



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



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

Chain J:  100%


  
MAG1  
MAG2

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

Chain K:  50%  
100%

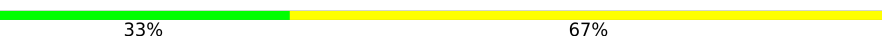
  
MAG1  
MAG2

- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  33%  
33% 67%

  
MAG1  
MAG2  
BMA3

- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  33% 67%

  
MAG1  
MAG2  
BMA3

- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  33%  
33% 67%

  
MAG1  
MAG2  
MAG3

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	123274	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1.3	Depositor
Maximum defocus (nm)	2.9	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.205	Depositor
Minimum map value	-0.107	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	337.92, 337.92, 337.92	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.32, 1.32, 1.32	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, ETA, CA, 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	0.55	4/10507 (0.0%)	0.69	9/14255 (0.1%)
2	B	0.31	0/723	0.52	0/979
3	C	0.31	0/1394	0.49	0/1892
4	E	0.40	0/1336	0.69	3/1802 (0.2%)
5	F	0.67	4/7729 (0.1%)	0.87	30/10474 (0.3%)
All	All	0.57	8/21689 (0.0%)	0.75	42/29402 (0.1%)

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	16
3	C	0	2
4	E	0	2
5	F	0	18
All	All	0	38

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	527	PRO	N-CD	6.29	1.56	1.47
1	A	1339	ASP	C-N	-6.17	1.22	1.34
1	A	242	PRO	N-CD	5.98	1.56	1.47
5	F	515	PHE	CB-CG	-5.76	1.41	1.51
1	A	1017	PRO	N-CD	5.42	1.55	1.47
5	F	781	PRO	N-CD	5.32	1.55	1.47
5	F	207	TRP	CB-CG	-5.28	1.40	1.50
1	A	1396	PRO	N-CD	5.03	1.54	1.47

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	33	ALA	CB-CA-C	-9.85	95.32	110.10
5	F	413	TYR	CB-CA-C	-9.32	91.77	110.40
5	F	661	TYR	N-CA-C	-9.06	86.55	111.00
5	F	390	SER	CB-CA-C	8.99	127.17	110.10
5	F	300	ALA	CB-CA-C	8.87	123.40	110.10
4	E	176	TYR	N-CA-C	-8.71	87.47	111.00
4	E	176	TYR	CB-CA-C	8.58	127.56	110.40
5	F	161	VAL	CB-CA-C	-8.12	95.97	111.40
5	F	385	ARG	CB-CA-C	-8.04	94.31	110.40
1	A	618	SER	CB-CA-C	7.98	125.26	110.10
5	F	259	LEU	CB-CA-C	-7.96	95.07	110.20
5	F	447	GLN	N-CA-C	-7.96	89.51	111.00
5	F	390	SER	N-CA-C	-7.93	89.60	111.00
5	F	663	PHE	CB-CA-C	-7.87	94.67	110.40
5	F	661	TYR	CB-CA-C	7.86	126.12	110.40
5	F	447	GLN	CB-CA-C	7.18	124.77	110.40
5	F	798	SER	CB-CA-C	-7.14	96.53	110.10
5	F	609	TYR	CA-CB-CG	6.81	126.33	113.40
5	F	550	VAL	C-N-CA	6.75	138.57	121.70
5	F	389	PHE	CB-CA-C	-6.74	96.93	110.40
1	A	1316	LEU	CB-CA-C	6.63	122.79	110.20
5	F	387	PHE	N-CA-C	-6.59	93.20	111.00
1	A	673	ALA	CB-CA-C	-6.57	100.24	110.10
5	F	387	PHE	CB-CA-C	6.49	123.37	110.40
1	A	1395	GLY	C-N-CD	6.03	141.07	128.40
5	F	177	GLY	N-CA-C	-5.81	98.57	113.10
5	F	361	MET	CB-CA-C	-5.80	98.80	110.40
1	A	1399	LEU	CA-CB-CG	-5.70	102.18	115.30
5	F	300	ALA	N-CA-C	-5.68	95.66	111.00
5	F	206	LEU	CA-CB-CG	-5.68	102.24	115.30
1	A	1016	TRP	C-N-CD	5.57	140.10	128.40
5	F	780	ALA	C-N-CD	5.56	140.07	128.40
5	F	305	CYS	CA-CB-SG	5.54	123.98	114.00
5	F	783	PHE	C-N-CA	5.51	135.48	121.70
1	A	645	PHE	CB-CA-C	-5.46	99.48	110.40
1	A	241	LYS	C-N-CD	5.27	139.47	128.40
5	F	556	GLN	C-N-CA	5.27	134.88	121.70
5	F	389	PHE	CB-CG-CD1	5.22	124.45	120.80
5	F	729	ILE	C-N-CA	5.20	134.69	121.70
5	F	490	MET	CB-CA-C	-5.19	100.02	110.40
1	A	1310	PRO	CB-CA-C	5.10	124.75	112.00
5	F	247	ILE	CB-CA-C	-5.01	101.57	111.60

There are no chirality outliers.

All (38) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1141	HIS	Peptide
1	A	1173	LYS	Peptide
1	A	1293	ALA	Peptide
1	A	1344	TYR	Peptide
1	A	1346	PRO	Peptide
1	A	1382	ASP	Peptide
1	A	1441	HIS	Peptide
1	A	268	PRO	Peptide
1	A	276	ASP	Peptide
1	A	309	TRP	Peptide
1	A	38	ASN	Peptide
1	A	450	ALA	Peptide
1	A	820	ASP	Peptide
1	A	976	LYS	Peptide
1	A	977	ASP	Peptide
1	A	993	ASN	Peptide
3	C	280	VAL	Peptide
3	C	281	GLY	Peptide
4	E	207	MET	Peptide
4	E	208	PRO	Peptide
5	F	1022	GLU	Peptide
5	F	1074	CYS	Peptide,Mainchain
5	F	176	GLU	Peptide
5	F	220	TYR	Peptide
5	F	476	GLU	Peptide
5	F	477	ASN	Peptide
5	F	484	GLN	Peptide
5	F	527	PRO	Peptide
5	F	534	ILE	Peptide
5	F	600	ARG	Peptide
5	F	730	LYS	Peptide
5	F	785	LYS	Peptide
5	F	786	SER	Peptide
5	F	805	ILE	Peptide
5	F	892	ILE	Peptide
5	F	893	SER	Peptide
5	F	894	VAL	Peptide



## 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	10261	0	10238	316	0
2	B	710	0	633	6	0
3	C	1367	0	1343	17	0
4	E	1304	0	1330	33	0
5	F	7572	0	7406	185	0
6	D	28	0	25	0	0
6	G	28	0	25	2	0
6	J	28	0	25	0	0
6	K	28	0	25	0	0
7	H	39	0	34	0	0
7	I	39	0	34	0	0
8	L	42	0	37	0	0
9	A	14	0	13	0	0
9	F	98	0	91	0	0
10	A	2	0	0	0	0
10	F	1	0	0	0	0
All	All	21561	0	21259	543	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 13.

All (543) 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:269:ASN:ND2	1:A:621:TYR:CE2	1.84	1.43
1:A:1380:ILE:CG2	1:A:1384:PHE:CE2	2.14	1.31
5:F:531:PRO:O	5:F:532:LYS:HG3	1.14	1.25
1:A:664:LEU:CD2	1:A:1065:ILE:HD12	1.69	1.23
1:A:1380:ILE:HG21	1:A:1384:PHE:CE2	1.75	1.17
1:A:475:PHE:CE2	1:A:537:LYS:HE3	1.78	1.17
1:A:1005:MET:CE	1:A:1362:ILE:CD1	2.26	1.13
1:A:1380:ILE:HG22	1:A:1384:PHE:CD2	1.83	1.12
1:A:475:PHE:HE2	1:A:537:LYS:HE3	1.09	1.10
1:A:1005:MET:HE1	1:A:1362:ILE:CD1	1.81	1.08
1:A:562:LEU:HD12	1:A:655:VAL:HG22	1.33	1.07

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:ARG:CG	1:A:168:ARG:NH2	2.18	1.07
1:A:1005:MET:CE	1:A:1362:ILE:HD11	1.85	1.05
1:A:165:ARG:HG2	1:A:168:ARG:NH2	1.72	1.05
1:A:992:HIS:NE2	1:A:996:HIS:CD2	2.24	1.04
5:F:531:PRO:O	5:F:532:LYS:CG	2.06	1.04
1:A:664:LEU:HD23	1:A:1065:ILE:HD12	1.36	1.03
1:A:269:ASN:ND2	1:A:621:TYR:CZ	2.26	1.02
1:A:1380:ILE:CG2	1:A:1384:PHE:CD2	2.40	1.02
5:F:661:TYR:CD2	5:F:663:PHE:CZ	2.48	1.00
1:A:269:ASN:ND2	1:A:621:TYR:CD2	2.33	0.97
1:A:664:LEU:HD21	1:A:1065:ILE:HD12	1.45	0.97
5:F:243:ARG:HG3	5:F:244:PRO:HD2	1.47	0.96
5:F:661:TYR:CE2	5:F:663:PHE:CZ	2.52	0.96
1:A:1389:ARG:HD3	1:A:1391:TRP:CH2	2.03	0.94
5:F:347:LEU:O	5:F:348:ASN:HB2	1.67	0.92
1:A:938:LEU:HD22	1:A:1055:PHE:HE2	1.34	0.92
1:A:165:ARG:HG2	1:A:168:ARG:HH21	1.26	0.92
1:A:1005:MET:HE2	1:A:1362:ILE:HD11	1.52	0.91
1:A:1005:MET:HE2	1:A:1362:ILE:CD1	1.95	0.90
1:A:1045:PHE:O	1:A:1049:ILE:HG13	1.70	0.90
1:A:1091:TYR:CE1	4:E:212:TRP:HB3	2.06	0.89
5:F:290:PHE:CE2	5:F:353:ARG:HA	2.07	0.88
1:A:1091:TYR:HE1	4:E:212:TRP:HB3	1.38	0.88
1:A:1386:TYR:HA	1:A:1389:ARG:HH21	1.39	0.87
1:A:1390:ASP:HB2	1:A:1393:ILE:HD12	1.56	0.85
1:A:664:LEU:CD2	1:A:1065:ILE:CD1	2.52	0.85
1:A:165:ARG:HG3	1:A:168:ARG:NH2	1.88	0.85
1:A:587:PHE:CG	1:A:593:ARG:NH1	2.45	0.85
1:A:656:PHE:HB2	1:A:1057:MET:SD	2.16	0.84
5:F:661:TYR:HD2	5:F:663:PHE:CZ	1.94	0.84
5:F:1049:MET:SD	5:F:1054:ARG:NH2	2.50	0.83
1:A:475:PHE:CE2	1:A:537:LYS:CE	2.60	0.83
5:F:428:TYR:CE1	5:F:429:LEU:CD2	2.62	0.83
5:F:290:PHE:HE2	5:F:353:ARG:HA	1.44	0.83
5:F:290:PHE:HE2	5:F:353:ARG:CA	1.92	0.82
5:F:531:PRO:C	5:F:532:LYS:HG3	1.98	0.82
1:A:1005:MET:CE	1:A:1362:ILE:HD13	2.08	0.81
1:A:337:PHE:HD2	1:A:1068:PHE:CZ	1.99	0.81
5:F:271:LEU:HD21	5:F:275:ARG:NH2	1.95	0.81
1:A:820:ASP:OD1	1:A:828:ARG:HD3	1.82	0.79
5:F:661:TYR:CE2	5:F:663:PHE:CE1	2.70	0.79

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:664:LEU:HD21	1:A:1065:ILE:CD1	2.10	0.79
1:A:225:THR:HA	1:A:266:PRO:HG3	1.64	0.79
1:A:603:ALA:O	1:A:607:VAL:HG23	1.83	0.79
5:F:661:TYR:HE2	5:F:663:PHE:CE1	2.00	0.78
5:F:1036:GLN:HG2	5:F:1037:ALA:H	1.47	0.78
1:A:337:PHE:CD2	1:A:1068:PHE:CE2	2.72	0.78
1:A:1091:TYR:HD2	1:A:1399:LEU:HD13	1.48	0.77
1:A:71:TYR:OH	1:A:165:ARG:NH2	2.17	0.77
5:F:428:TYR:CE1	5:F:429:LEU:HD21	2.19	0.77
1:A:562:LEU:CD1	1:A:655:VAL:HG22	2.13	0.77
1:A:45:ILE:HG12	1:A:107:ALA:HA	1.68	0.76
1:A:593:ARG:H	1:A:593:ARG:HD2	1.50	0.76
1:A:1040:GLU:O	1:A:1043:ILE:HG12	1.86	0.75
1:A:942:PHE:HE2	1:A:1051:LEU:HD12	1.52	0.74
5:F:661:TYR:HE2	5:F:663:PHE:CZ	2.03	0.73
1:A:337:PHE:CD2	1:A:1068:PHE:CZ	2.76	0.73
5:F:428:TYR:HE1	5:F:429:LEU:HD21	1.52	0.73
1:A:1380:ILE:HG22	1:A:1384:PHE:CE2	2.06	0.73
1:A:942:PHE:CE2	1:A:1051:LEU:HD12	2.24	0.73
1:A:452:GLU:HA	1:A:456:GLN:HE21	1.53	0.72
5:F:428:TYR:CD1	5:F:429:LEU:HG	2.24	0.72
5:F:174:ILE:HD13	5:F:174:ILE:O	1.89	0.72
1:A:1386:TYR:O	1:A:1389:ARG:HG3	1.90	0.71
1:A:429:VAL:HG13	1:A:482:LYS:HE2	1.73	0.71
5:F:243:ARG:CG	5:F:244:PRO:HD2	2.20	0.71
5:F:1069:GLU:O	5:F:1070:ASP:HB2	1.90	0.71
1:A:1068:PHE:HE1	1:A:1384:PHE:CG	2.09	0.70
1:A:1005:MET:HE2	1:A:1362:ILE:HD13	1.69	0.70
1:A:938:LEU:HD22	1:A:1055:PHE:CE2	2.22	0.69
5:F:733:LYS:HE3	5:F:820:ASP:CG	2.13	0.69
5:F:161:VAL:HG23	5:F:161:VAL:O	1.93	0.68
1:A:1005:MET:HE1	1:A:1362:ILE:HD12	1.75	0.68
1:A:1370:PHE:CE1	1:A:1374:ASN:ND2	2.58	0.68
1:A:1380:ILE:CG2	1:A:1384:PHE:CZ	2.77	0.68
5:F:116:ARG:NH1	5:F:118:ASP:O	2.26	0.68
1:A:1391:TRP:HZ3	1:A:1396:PRO:HD3	1.58	0.67
5:F:428:TYR:HE1	5:F:429:LEU:CD2	2.06	0.67
1:A:992:HIS:NE2	1:A:996:HIS:HD2	1.86	0.67
1:A:1231:SER:HA	1:A:1234:PHE:HB3	1.76	0.67
5:F:254:LYS:HE3	5:F:428:TYR:OH	1.94	0.67
5:F:661:TYR:HD2	5:F:663:PHE:CE2	2.12	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:PHE:CZ	1:A:1064:VAL:HG12	2.30	0.66
5:F:428:TYR:CE1	5:F:429:LEU:HG	2.30	0.66
1:A:1396:PRO:HD2	1:A:1397:HIS:H	1.60	0.66
1:A:425:CYS:SG	1:A:426:HIS:N	2.68	0.66
5:F:257:LEU:HD12	5:F:292:ASN:O	1.96	0.66
1:A:429:VAL:CG1	1:A:482:LYS:HE2	2.26	0.66
1:A:1389:ARG:HD3	1:A:1391:TRP:HH2	1.60	0.66
5:F:852:ASP:HA	5:F:866:ASN:HD21	1.61	0.66
1:A:1091:TYR:CE2	1:A:1399:LEU:HB3	2.30	0.66
1:A:419:ARG:HG3	1:A:421:PHE:H	1.61	0.65
1:A:789:ARG:O	1:A:792:CYS:SG	2.43	0.65
1:A:1394:LEU:O	1:A:1394:LEU:HD12	1.96	0.65
1:A:795:ILE:HG21	1:A:849:LEU:HD13	1.79	0.65
1:A:1091:TYR:CE2	1:A:1399:LEU:CB	2.81	0.64
1:A:1091:TYR:HE2	1:A:1399:LEU:HB2	1.63	0.64
1:A:912:LYS:HG3	1:A:915:LYS:HD2	1.80	0.63
5:F:290:PHE:CD2	5:F:353:ARG:HA	2.32	0.63
1:A:441:ILE:HG23	1:A:471:LEU:HD22	1.80	0.63
4:E:207:MET:SD	4:E:207:MET:N	2.71	0.63
5:F:243:ARG:HG3	5:F:244:PRO:CD	2.27	0.63
1:A:893:VAL:HG13	1:A:896:LEU:HD12	1.80	0.63
1:A:1391:TRP:CZ3	1:A:1396:PRO:HD3	2.34	0.63
1:A:1293:ALA:HB2	1:A:1339:ASP:H	1.63	0.62
1:A:793:HIS:HA	1:A:796:VAL:HG22	1.82	0.62
3:C:313:ARG:HA	3:C:367:ASP:HB3	1.81	0.62
1:A:486:LEU:O	1:A:490:GLN:NE2	2.33	0.62
1:A:243:SER:OG	1:A:252:ARG:NH1	2.33	0.62
5:F:174:ILE:HD11	5:F:181:VAL:CG2	2.30	0.62
1:A:788:VAL:CG1	1:A:790:VAL:HG23	2.28	0.62
1:A:1380:ILE:HG21	1:A:1384:PHE:CZ	2.32	0.62
1:A:287:GLN:NE2	1:A:621:TYR:OH	2.31	0.62
1:A:992:HIS:CD2	1:A:996:HIS:HD2	2.17	0.62
5:F:1074:CYS:SG	5:F:1075:ETA:N	2.73	0.61
1:A:429:VAL:HG13	1:A:482:LYS:CE	2.30	0.61
5:F:754:ASN:O	5:F:756:GLN:HG3	2.01	0.61
1:A:90:GLU:OE1	1:A:168:ARG:NH1	2.33	0.61
1:A:1380:ILE:HG23	1:A:1384:PHE:CE2	2.31	0.61
5:F:56:VAL:HG11	5:F:799:LYS:HD3	1.83	0.61
3:C:303:HIS:HA	3:C:306:ASP:HB2	1.83	0.61
1:A:451:SER:OG	1:A:464:GLN:NE2	2.35	0.60
1:A:925:ILE:HA	1:A:928:ILE:HG22	1.83	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1418:LYS:HG3	1:A:1419:HIS:N	2.15	0.60
2:B:140:TYR:HB2	2:B:146:ILE:HG13	1.83	0.60
1:A:1068:PHE:CE1	1:A:1384:PHE:CE2	2.90	0.60
5:F:271:LEU:CD2	5:F:275:ARG:NH2	2.63	0.60
5:F:352:SER:OG	5:F:353:ARG:N	2.34	0.60
1:A:969:ARG:NH1	5:F:176:GLU:OE2	2.34	0.60
1:A:372:GLN:NE2	3:C:299:ASP:OD2	2.32	0.60
1:A:588:GLU:OE2	5:F:275:ARG:NH1	2.33	0.59
1:A:953:LYS:HD3	1:A:1026:SER:HB2	1.82	0.59
4:E:120:MET:HG3	4:E:143:PHE:CE2	2.37	0.59
1:A:72:LEU:O	1:A:83:ASN:ND2	2.36	0.59
1:A:1442:ARG:HG2	1:A:1446:LYS:HB2	1.83	0.59
2:B:125:ALA:HA	2:B:158:PHE:H	1.67	0.59
4:E:57:CYS:HA	4:E:80:CYS:HA	1.83	0.59
1:A:365:GLY:HA3	3:C:437:ASN:HB2	1.85	0.59
1:A:1393:ILE:HG22	1:A:1394:LEU:HD23	1.84	0.59
4:E:146:PHE:HA	4:E:149:LEU:HD12	1.85	0.59
4:E:210:ASN:CB	4:E:212:TRP:HE1	2.15	0.59
5:F:609:TYR:HB3	5:F:625:VAL:HA	1.85	0.59
5:F:732:VAL:HG21	5:F:735:ARG:HH21	1.68	0.59
1:A:1390:ASP:OD1	1:A:1390:ASP:N	2.33	0.58
3:C:388:TYR:HE1	3:C:422:LEU:HB3	1.67	0.58
1:A:74:MET:HB2	1:A:78:ASP:O	2.03	0.58
5:F:669:TYR:CD2	5:F:670:CYS:N	2.72	0.58
1:A:244:PRO:O	1:A:252:ARG:NH1	2.37	0.58
1:A:1068:PHE:HE1	1:A:1384:PHE:CD1	2.21	0.58
1:A:1175:ARG:NH2	1:A:1175:ARG:HG3	2.17	0.58
1:A:1068:PHE:CE1	1:A:1384:PHE:CZ	2.92	0.58
1:A:452:GLU:OE2	1:A:528:ARG:NH2	2.37	0.57
5:F:30:PRO:HG2	5:F:35:ILE:HD11	1.85	0.57
5:F:252:SER:OG	5:F:357:ASN:OD1	2.21	0.57
1:A:247:ARG:HB3	1:A:261:CYS:HB2	1.85	0.57
1:A:580:LEU:O	1:A:627:TYR:OH	2.21	0.57
1:A:1386:TYR:O	1:A:1389:ARG:CG	2.53	0.57
4:E:208:PRO:HG3	4:E:213:GLU:HB3	1.86	0.57
1:A:609:GLN:HA	1:A:1016:TRP:HZ2	1.68	0.57
1:A:969:ARG:HD3	5:F:176:GLU:HG3	1.86	0.57
1:A:1262:LYS:O	1:A:1262:LYS:HG2	2.04	0.57
5:F:591:ARG:HB3	5:F:604:LYS:HE3	1.86	0.57
4:E:56:ILE:N	4:E:81:SER:O	2.35	0.57
5:F:417:SER:OG	5:F:418:ILE:N	2.37	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1262:LYS:HE3	4:E:209:GLN:O	2.04	0.57
1:A:1091:TYR:CD2	1:A:1399:LEU:HD13	2.35	0.57
1:A:1386:TYR:HA	1:A:1389:ARG:NH2	2.17	0.57
5:F:669:TYR:CD2	5:F:670:CYS:HB2	2.40	0.57
1:A:820:ASP:OD2	1:A:828:ARG:HB2	2.06	0.56
1:A:1068:PHE:HE1	1:A:1384:PHE:CD2	2.23	0.56
5:F:391:VAL:HG12	5:F:415:ILE:HB	1.86	0.56
5:F:428:TYR:CE1	5:F:429:LEU:CG	2.89	0.56
1:A:230:GLY:O	5:F:544:ARG:NH1	2.38	0.56
5:F:1007:HIS:NE2	5:F:1009:GLU:OE2	2.39	0.56
1:A:119:ARG:O	1:A:123:ASN:ND2	2.38	0.56
1:A:1233:ALA:HA	1:A:1236:ARG:HE	1.70	0.56
5:F:515:PHE:HD2	5:F:623:ALA:HB3	1.69	0.56
1:A:1068:PHE:CE1	1:A:1384:PHE:CD2	2.94	0.56
1:A:1273:LEU:HB3	1:A:1371:LEU:HD21	1.88	0.56
5:F:161:VAL:O	5:F:161:VAL:CG2	2.54	0.56
4:E:210:ASN:HB2	4:E:212:TRP:HE1	1.70	0.56
1:A:1488:GLU:O	1:A:1492:ALA:N	2.39	0.55
5:F:270:THR:HG22	5:F:392:GLY:HA3	1.88	0.55
1:A:165:ARG:HG3	1:A:168:ARG:CZ	2.35	0.55
5:F:643:THR:HA	5:F:646:ARG:HE	1.71	0.55
1:A:1094:LYS:HB3	4:E:212:TRP:CE3	2.42	0.55
5:F:667:ARG:NH1	5:F:668:ASP:O	2.40	0.55
1:A:1396:PRO:CD	1:A:1397:HIS:H	2.20	0.55
5:F:1036:GLN:O	5:F:1037:ALA:HB3	2.06	0.55
5:F:753:GLU:O	5:F:753:GLU:HG2	2.07	0.55
5:F:510:PRO:HB2	5:F:768:LYS:HG2	1.89	0.55
3:C:370:THR:O	3:C:376:GLN:NE2	2.37	0.55
5:F:352:SER:O	5:F:353:ARG:HB2	2.07	0.55
5:F:507:THR:H	5:F:508:LEU:HD23	1.71	0.55
5:F:647:TYR:HB3	5:F:712:ALA:HB3	1.89	0.55
1:A:542:TRP:HE3	1:A:542:TRP:H	1.55	0.54
1:A:793:HIS:HA	1:A:796:VAL:CG2	2.37	0.54
1:A:1175:ARG:HG3	1:A:1175:ARG:HH21	1.71	0.54
1:A:439:ILE:HD13	1:A:541:TYR:HE2	1.73	0.54
5:F:594:VAL:HG21	5:F:607:ARG:HH21	1.72	0.54
5:F:595:LYS:HE3	5:F:983:GLN:HE22	1.73	0.54
1:A:475:PHE:HZ	1:A:537:LYS:HD2	1.73	0.54
5:F:113:HIS:NE2	5:F:183:ASN:OD1	2.29	0.54
5:F:420:ALA:O	5:F:424:ASN:ND2	2.41	0.54
1:A:807:LEU:O	1:A:811:LEU:N	2.41	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:732:VAL:O	5:F:733:LYS:HB3	2.08	0.53
1:A:318:ILE:O	1:A:322:SER:N	2.36	0.53
1:A:333:LEU:HD21	1:A:1064:VAL:HG11	1.90	0.53
4:E:37:PRO:HA	4:E:174:ILE:HA	1.91	0.53
1:A:1091:TYR:CD2	1:A:1399:LEU:HB3	2.43	0.53
5:F:782:TYR:CD1	5:F:782:TYR:N	2.74	0.53
1:A:441:ILE:O	1:A:445:ASN:N	2.41	0.53
4:E:32:TRP:HE1	4:E:53:LEU:HG	1.73	0.53
5:F:225:TRP:NE1	5:F:236:ASP:OD2	2.41	0.53
1:A:562:LEU:HD12	1:A:655:VAL:CG2	2.24	0.53
4:E:5:GLU:OE1	4:E:10:ARG:NH2	2.41	0.53
4:E:210:ASN:HB2	4:E:212:TRP:NE1	2.23	0.53
1:A:569:PHE:CE2	1:A:573:PHE:HE2	2.26	0.53
1:A:788:VAL:HG13	1:A:790:VAL:CG2	2.39	0.53
1:A:334:SER:OG	1:A:335:GLY:N	2.43	0.52
1:A:1150:SER:O	1:A:1154:ASN:ND2	2.41	0.52
5:F:531:PRO:C	5:F:532:LYS:CG	2.68	0.52
1:A:48:VAL:HA	1:A:53:PHE:HE2	1.73	0.52
1:A:120:SER:HA	1:A:123:ASN:ND2	2.24	0.52
1:A:656:PHE:HA	1:A:1057:MET:SD	2.50	0.52
5:F:684:LEU:HD23	5:F:687:ASN:HD22	1.74	0.52
1:A:971:TYR:O	1:A:988:ARG:NH2	2.35	0.52
1:A:337:PHE:CE1	1:A:664:LEU:HD11	2.45	0.52
1:A:1313:VAL:O	1:A:1317:PHE:N	2.40	0.52
1:A:535:LEU:HD13	1:A:941:MET:HG2	1.92	0.52
2:B:148:ARG:NH2	2:B:151:LYS:O	2.42	0.52
5:F:75:ASN:C	5:F:77:ALA:H	2.13	0.52
1:A:542:TRP:CE3	1:A:542:TRP:N	2.78	0.51
5:F:636:ALA:HA	5:F:710:LEU:HD13	1.91	0.51
5:F:669:TYR:CE2	5:F:670:CYS:HB2	2.45	0.51
1:A:919:GLN:HA	1:A:922:PHE:HB2	1.91	0.51
5:F:375:PHE:HD1	5:F:379:ASN:HD22	1.59	0.51
1:A:542:TRP:CE3	1:A:542:TRP:CA	2.94	0.51
1:A:835:PHE:O	1:A:839:PHE:N	2.38	0.51
1:A:1068:PHE:CE1	1:A:1384:PHE:CE1	2.99	0.51
5:F:477:ASN:HB3	5:F:480:ASN:HD21	1.76	0.51
5:F:32:ALA:HA	5:F:35:ILE:HD12	1.91	0.51
5:F:78:ARG:NH1	5:F:78:ARG:HG3	2.26	0.51
5:F:113:HIS:O	5:F:114:GLN:HB2	2.10	0.51
5:F:798:SER:OG	5:F:799:LYS:N	2.42	0.51
1:A:475:PHE:CZ	1:A:537:LYS:HD2	2.45	0.51

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:821:PRO:HG3	1:A:1286:MET:HG2	1.93	0.51
1:A:1386:TYR:CD1	1:A:1389:ARG:HD2	2.46	0.51
1:A:72:LEU:HD12	1:A:73:PRO:HD2	1.93	0.51
1:A:977:ASP:O	1:A:979:ASP:N	2.43	0.51
5:F:114:GLN:O	5:F:115:TRP:HB3	2.11	0.51
5:F:1036:GLN:HG2	5:F:1037:ALA:N	2.21	0.51
1:A:1143:SER:O	1:A:1147:ASN:ND2	2.45	0.50
1:A:245:CYS:SG	1:A:246:ALA:N	2.84	0.50
1:A:475:PHE:CZ	1:A:537:LYS:CE	2.93	0.50
1:A:1005:MET:HE1	1:A:1362:ILE:HD13	1.78	0.50
1:A:183:GLN:O	1:A:187:ASN:ND2	2.45	0.50
1:A:1418:LYS:HA	1:A:1460:THR:HA	1.92	0.50
5:F:184:GLU:HG3	5:F:187:TRP:HE1	1.76	0.50
5:F:113:HIS:HE1	5:F:186:ASN:HB3	1.74	0.50
1:A:120:SER:HA	1:A:123:ASN:HD22	1.75	0.50
1:A:326:LEU:HD21	1:A:1379:VAL:HG21	1.94	0.50
1:A:569:PHE:CE2	1:A:573:PHE:CE2	3.00	0.50
1:A:788:VAL:HG12	1:A:790:VAL:HG23	1.94	0.50
1:A:475:PHE:CZ	1:A:537:LYS:CD	2.95	0.50
1:A:1199:LEU:HD23	1:A:1202:ILE:HD12	1.94	0.50
3:C:283:SER:OG	3:C:284:LEU:N	2.45	0.50
3:C:388:TYR:HB3	3:C:433:ILE:HA	1.94	0.50
1:A:94:LEU:HD22	1:A:128:ILE:HG22	1.94	0.50
1:A:559:ILE:HA	1:A:562:LEU:HB2	1.93	0.50
1:A:820:ASP:CG	1:A:828:ARG:HB2	2.31	0.50
1:A:1091:TYR:CD1	4:E:212:TRP:HB3	2.44	0.50
3:C:388:TYR:HD2	3:C:433:ILE:HG23	1.77	0.50
1:A:1016:TRP:N	1:A:1017:PRO:CD	2.75	0.50
5:F:97:LYS:O	5:F:100:VAL:N	2.45	0.50
1:A:656:PHE:CD1	1:A:656:PHE:C	2.85	0.49
5:F:95:ARG:NH2	5:F:204:SER:O	2.45	0.49
5:F:394:HIS:CE1	5:F:398:ARG:HE	2.30	0.49
1:A:820:ASP:OD1	1:A:828:ARG:HB2	2.12	0.49
1:A:1167:LEU:HD23	1:A:1170:LEU:HD12	1.94	0.49
3:C:426:PRO:HG2	3:C:429:MET:HB2	1.94	0.49
4:E:117:PHE:O	4:E:121:GLY:N	2.41	0.49
1:A:338:THR:O	1:A:342:GLU:N	2.45	0.49
5:F:50:ALA:O	5:F:54:SER:OG	2.21	0.49
5:F:906:VAL:HA	5:F:976:SER:HA	1.94	0.49
1:A:569:PHE:CZ	1:A:573:PHE:HE2	2.31	0.49
1:A:501:CYS:HA	1:A:504:VAL:HG12	1.94	0.49

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:550:ALA:O	1:A:554:ASN:ND2	2.46	0.49
1:A:1196:ASP:OD2	1:A:1239:ARG:NH1	2.46	0.49
1:A:207:VAL:O	1:A:211:ALA:N	2.44	0.49
5:F:159:ARG:NH2	5:F:224:PRO:O	2.45	0.49
5:F:174:ILE:HD11	5:F:181:VAL:HG21	1.95	0.49
1:A:1068:PHE:CD1	1:A:1384:PHE:CE2	3.00	0.49
5:F:428:TYR:CD1	5:F:428:TYR:C	2.85	0.49
1:A:656:PHE:CB	1:A:1057:MET:SD	2.95	0.48
1:A:826:SER:OG	1:A:827:VAL:N	2.46	0.48
5:F:95:ARG:HD3	5:F:494:VAL:HG22	1.95	0.48
5:F:746:VAL:HG11	5:F:752:GLY:HA2	1.95	0.48
5:F:776:TYR:HE1	5:F:799:LYS:HD2	1.78	0.48
1:A:1431:PRO:HB3	1:A:1436:GLY:HA2	1.95	0.48
5:F:1073:ASP:O	5:F:1074:CYS:C	2.52	0.48
1:A:542:TRP:CE3	1:A:542:TRP:HA	2.48	0.48
1:A:293:GLY:HA3	1:A:617:ASN:HD21	1.78	0.48
1:A:1175:ARG:HH21	1:A:1175:ARG:CG	2.27	0.48
1:A:1505:LEU:O	1:A:1509:VAL:N	2.42	0.48
5:F:43:GLN:NE2	5:F:1012:MET:O	2.46	0.48
4:E:35:LEU:HG	4:E:37:PRO:HD3	1.96	0.48
5:F:634:ILE:HB	5:F:707:ARG:HH12	1.78	0.48
1:A:617:ASN:HB3	1:A:621:TYR:CE2	2.49	0.48
1:A:1097:PRO:HB3	1:A:1463:PHE:CE2	2.49	0.48
2:B:139:LYS:HG3	2:B:145:TRP:CD1	2.48	0.48
5:F:306:PHE:O	5:F:308:HIS:ND1	2.47	0.48
1:A:1097:PRO:HB3	1:A:1463:PHE:HE2	1.78	0.47
1:A:1333:SER:OG	1:A:1334:TYR:N	2.46	0.47
1:A:1104:LYS:HG3	1:A:1105:ASN:H	1.78	0.47
5:F:782:TYR:HB2	5:F:785:LYS:HB3	1.96	0.47
1:A:50:TRP:HB3	1:A:52:PRO:HD2	1.96	0.47
5:F:428:TYR:HD1	5:F:429:LEU:HG	1.75	0.47
1:A:1005:MET:HG3	1:A:1005:MET:O	2.13	0.47
5:F:92:LEU:O	5:F:96:SER:CB	2.63	0.47
5:F:127:VAL:HG12	5:F:147:ILE:HD11	1.96	0.47
1:A:542:TRP:HE3	1:A:542:TRP:N	2.13	0.47
1:A:1173:LYS:O	1:A:1175:ARG:N	2.47	0.47
1:A:1390:ASP:HB2	1:A:1393:ILE:CD1	2.37	0.47
5:F:347:LEU:O	5:F:348:ASN:CB	2.47	0.47
1:A:1391:TRP:HZ3	1:A:1396:PRO:CD	2.26	0.47
5:F:273:LEU:O	5:F:277:SER:N	2.45	0.47
5:F:719:VAL:HA	5:F:723:TRP:HB2	1.96	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:LEU:HD12	1:A:548:LEU:HB2	1.96	0.47
1:A:1083:LYS:HA	1:A:1086:ARG:HB3	1.97	0.47
4:E:131:LYS:HG2	4:E:133:ARG:HH21	1.79	0.47
5:F:43:GLN:HE22	5:F:1012:MET:HB3	1.79	0.47
5:F:661:TYR:CD2	5:F:663:PHE:CE2	2.93	0.47
1:A:681:ARG:O	1:A:685:LYS:N	2.47	0.47
5:F:102:LEU:O	5:F:106:ALA:HB2	2.14	0.47
5:F:243:ARG:CD	5:F:244:PRO:HD2	2.45	0.47
1:A:475:PHE:HZ	1:A:537:LYS:CD	2.28	0.47
2:B:107:THR:OG1	2:B:132:ASP:N	2.43	0.47
5:F:643:THR:HG23	5:F:646:ARG:HH21	1.80	0.47
1:A:1282:ALA:O	1:A:1286:MET:N	2.43	0.46
5:F:315[B]:ARG:HH21	5:F:1049:MET:HG2	1.80	0.46
1:A:224:LYS:HB2	1:A:245:CYS:O	2.15	0.46
1:A:1323:GLU:OE1	1:A:1323:GLU:HA	2.14	0.46
5:F:515:PHE:HB3	5:F:623:ALA:O	2.15	0.46
1:A:265:TRP:CZ2	1:A:271:GLY:HA2	2.50	0.46
1:A:1094:LYS:HB3	4:E:212:TRP:CZ3	2.50	0.46
1:A:1292:ILE:HD12	1:A:1300:ILE:HG21	1.97	0.46
5:F:509:CYS:O	5:F:511:ASN:N	2.48	0.46
1:A:47:ILE:HA	1:A:50:TRP:HD1	1.80	0.46
1:A:202:LEU:O	1:A:206:MET:N	2.49	0.46
1:A:614:GLU:HG2	1:A:1017:PRO:HD3	1.97	0.46
1:A:877:ALA:HA	1:A:896:LEU:HD13	1.98	0.46
1:A:1251:GLU:H	1:A:1251:GLU:HG3	1.56	0.46
1:A:1339:ASP:O	1:A:1341:GLU:N	2.42	0.46
5:F:973:SER:OG	5:F:974:LYS:N	2.48	0.46
4:E:210:ASN:HB3	4:E:212:TRP:HE1	1.81	0.46
1:A:1091:TYR:HE2	1:A:1399:LEU:CB	2.20	0.46
3:C:373:HIS:HB3	3:C:376:GLN:HB2	1.98	0.46
5:F:151:PHE:HB3	5:F:160:GLN:HB3	1.98	0.46
1:A:587:PHE:CD1	1:A:593:ARG:NH1	2.70	0.46
1:A:1417:ILE:O	1:A:1461:VAL:N	2.45	0.46
5:F:506:PHE:HA	5:F:762:TYR:HE2	1.81	0.46
1:A:458:LEU:O	1:A:461:THR:OG1	2.34	0.46
1:A:1172:PHE:O	1:A:1177:TYR:N	2.49	0.46
1:A:1302:ARG:H	1:A:1302:ARG:HD3	1.81	0.46
5:F:785:LYS:HD3	5:F:789:GLY:HA3	1.98	0.46
1:A:350:PHE:HB3	1:A:354:ARG:HH12	1.81	0.45
1:A:545:LEU:HG	1:A:549:VAL:HG23	1.98	0.45
5:F:729:ILE:HG22	5:F:730:LYS:H	1.81	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:PHE:CE2	1:A:1064:VAL:HG12	2.51	0.45
1:A:1068:PHE:CE1	1:A:1384:PHE:CD1	3.03	0.45
1:A:1494:ILE:O	1:A:1498:TRP:N	2.41	0.45
5:F:55:GLY:O	5:F:59:LEU:N	2.46	0.45
1:A:589:ASP:OD2	1:A:593:ARG:NH2	2.49	0.45
1:A:1131:ASN:HD22	1:A:1242:ARG:HD2	1.80	0.45
5:F:551:GLN:HE22	5:F:553:PRO:HG3	1.81	0.45
1:A:1430:GLN:HG3	1:A:1432:PRO:HD2	1.97	0.45
5:F:154:ASP:OD1	5:F:155:ALA:N	2.49	0.45
1:A:478:GLU:O	1:A:482:LYS:HG3	2.17	0.45
1:A:545:LEU:HA	1:A:548:LEU:HB2	1.99	0.45
1:A:554:ASN:ND2	1:A:666:GLU:OE2	2.49	0.45
1:A:965:GLU:OE1	1:A:990:TRP:NE1	2.49	0.45
3:C:311:ILE:HG12	3:C:365:ALA:HB3	1.97	0.45
5:F:95:ARG:HH11	5:F:494:VAL:HG22	1.81	0.45
5:F:162:SER:OG	5:F:163:TYR:N	2.50	0.45
6:G:1:NAG:O6	6:G:2:NAG:H82	2.16	0.45
1:A:995:PHE:HE2	1:A:1326:GLN:HG3	1.81	0.45
1:A:1309:PHE:O	1:A:1312:ALA:N	2.50	0.45
1:A:1418:LYS:HG3	1:A:1419:HIS:H	1.82	0.45
5:F:1049:MET:CE	5:F:1054:ARG:NH2	2.80	0.45
5:F:1068:LEU:HD23	5:F:1068:LEU:HA	1.70	0.45
4:E:36:SER:HB3	4:E:175:GLU:HB2	1.99	0.45
5:F:361:MET:HA	5:F:387:PHE:O	2.16	0.45
5:F:515:PHE:CD2	5:F:623:ALA:HB3	2.51	0.45
1:A:500:ASP:OD2	1:A:540:LYS:NZ	2.41	0.45
1:A:609:GLN:HE21	1:A:615:ASP:HB3	1.82	0.45
5:F:78:ARG:HH11	5:F:78:ARG:CG	2.30	0.45
1:A:992:HIS:NE2	1:A:996:HIS:CG	2.82	0.44
1:A:1139:HIS:H	1:A:1142:GLN:HE21	1.65	0.44
1:A:656:PHE:CA	1:A:1057:MET:SD	3.05	0.44
4:E:17:LEU:HD23	4:E:20:ILE:HD12	1.98	0.44
5:F:428:TYR:HE1	5:F:429:LEU:CG	2.29	0.44
1:A:1309:PHE:O	1:A:1312:ALA:HB3	2.18	0.44
1:A:337:PHE:CZ	1:A:1064:VAL:CG1	3.00	0.44
1:A:930:ASN:O	1:A:934:VAL:N	2.51	0.44
5:F:102:LEU:HB3	5:F:490:MET:SD	2.58	0.44
1:A:1178:PHE:O	4:E:138:ARG:NH1	2.37	0.44
5:F:791:TYR:HA	5:F:821:VAL:HG11	2.00	0.44
1:A:656:PHE:CD1	1:A:657:LEU:N	2.86	0.44
5:F:78:ARG:HG3	5:F:78:ARG:HH11	1.83	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:364:THR:OG1	5:F:365:ASP:N	2.50	0.44
5:F:719:VAL:O	5:F:724:SER:N	2.51	0.44
5:F:778:PHE:HE2	5:F:1016:LEU:HD11	1.83	0.44
1:A:899:LEU:HD22	1:A:902:LEU:HD11	1.99	0.44
1:A:1393:ILE:O	1:A:1394:LEU:HB3	2.17	0.44
5:F:450:ASN:OD1	5:F:450:ASN:N	2.48	0.44
5:F:1004:ARG:NH1	5:F:1023:SER:O	2.51	0.44
1:A:237:VAL:O	1:A:239:ASN:N	2.46	0.43
1:A:921:VAL:O	1:A:925:ILE:N	2.51	0.43
1:A:227:TYR:HE1	1:A:234:VAL:HG22	1.83	0.43
1:A:591:GLU:O	1:A:593:ARG:HD2	2.17	0.43
1:A:617:ASN:O	1:A:620:MET:N	2.51	0.43
5:F:290:PHE:CE2	5:F:353:ARG:CA	2.76	0.43
1:A:912:LYS:O	1:A:916:HIS:N	2.49	0.43
1:A:1419:HIS:HB3	1:A:1455:LEU:HD11	2.00	0.43
3:C:312:THR:HG21	3:C:353:ARG:HH12	1.83	0.43
5:F:733:LYS:HB2	5:F:820:ASP:HB2	1.99	0.43
5:F:58:GLN:O	5:F:61:ASP:HB2	2.19	0.43
5:F:428:TYR:CD1	5:F:429:LEU:N	2.87	0.43
1:A:445:ASN:HD21	1:A:534:ARG:HD2	1.82	0.43
1:A:928:ILE:HA	1:A:931:ILE:HB	2.01	0.43
5:F:1008:VAL:HG22	5:F:1019:ILE:HG12	1.99	0.43
1:A:562:LEU:CD1	1:A:655:VAL:CG2	2.91	0.43
1:A:562:LEU:HD22	1:A:562:LEU:HA	1.74	0.43
1:A:1135:LEU:HD21	1:A:1239:ARG:HE	1.83	0.43
5:F:541:ILE:HD12	5:F:909:PRO:HG3	2.00	0.43
5:F:649:GLU:O	5:F:655:ASN:ND2	2.51	0.43
3:C:398:GLN:HA	3:C:401:ILE:HD12	2.01	0.43
1:A:463:LEU:HA	1:A:466:ILE:HG12	2.01	0.43
1:A:1440:PRO:HB3	1:A:1444:ALA:HB3	2.01	0.43
5:F:290:PHE:HZ	5:F:1056:ARG:HH21	1.67	0.43
2:B:145:TRP:HB2	2:B:159:ILE:HB	2.01	0.43
4:E:35:LEU:HB3	4:E:49:ALA:H	1.83	0.43
1:A:656:PHE:HD1	1:A:657:LEU:N	2.17	0.42
1:A:1258:TRP:CH2	4:E:211:PRO:HB3	2.54	0.42
5:F:38:TRP:HE1	5:F:831:THR:HB	1.83	0.42
1:A:792:CYS:HA	1:A:795:ILE:HD12	2.01	0.42
1:A:332:VAL:HG22	1:A:657:LEU:HD21	2.00	0.42
1:A:536:PHE:O	1:A:539:THR:OG1	2.28	0.42
1:A:788:VAL:HG13	1:A:790:VAL:HG23	1.95	0.42
1:A:1091:TYR:HE1	4:E:212:TRP:CB	2.22	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:32:TRP:HD1	4:E:52:GLY:HA2	1.84	0.42
1:A:521:PRO:HA	1:A:524:ILE:HG22	2.01	0.42
1:A:673:ALA:O	1:A:677:LYS:HG3	2.19	0.42
5:F:196:LYS:HG3	5:F:220:TYR:OH	2.20	0.42
1:A:1052:ILE:O	1:A:1056:MET:N	2.45	0.42
5:F:114:GLN:O	5:F:115:TRP:CB	2.66	0.42
5:F:356:CYS:SG	5:F:357:ASN:N	2.93	0.42
1:A:1139:HIS:N	1:A:1142:GLN:HE21	2.18	0.42
1:A:1263:SER:HB3	1:A:1383:ASN:HD21	1.85	0.42
5:F:669:TYR:HD2	5:F:670:CYS:H	1.63	0.42
1:A:429:VAL:HG11	1:A:486:LEU:HD12	2.01	0.42
1:A:645:PHE:O	1:A:645:PHE:CG	2.71	0.42
1:A:908:ILE:HD12	1:A:914:LEU:HD11	2.02	0.42
1:A:947:VAL:O	1:A:951:LYS:HG3	2.20	0.42
5:F:726:GLN:HB3	5:F:729:ILE:HD11	2.02	0.42
1:A:820:ASP:O	1:A:822:ILE:N	2.51	0.42
1:A:1399:LEU:HD23	1:A:1399:LEU:HA	1.83	0.42
3:C:426:PRO:HA	3:C:427:PRO:HD3	1.83	0.42
4:E:210:ASN:CB	4:E:212:TRP:NE1	2.79	0.42
5:F:113:HIS:O	5:F:114:GLN:CB	2.68	0.42
5:F:704:LEU:HA	5:F:704:LEU:HD23	1.89	0.42
5:F:857:ASP:OD1	5:F:861:PHE:N	2.47	0.42
5:F:434:ARG:HA	5:F:437:VAL:HG12	2.01	0.42
1:A:1314:LEU:HD23	1:A:1314:LEU:HA	1.91	0.41
4:E:19:GLY:HA2	4:E:22:LEU:HB3	2.01	0.41
4:E:32:TRP:NE1	4:E:53:LEU:HG	2.34	0.41
5:F:653:PRO:HG3	5:F:684:LEU:HD21	2.02	0.41
5:F:771:LEU:HD23	5:F:771:LEU:HA	1.87	0.41
1:A:277:ASN:O	1:A:278:PHE:C	2.58	0.41
1:A:307:ASN:OD1	1:A:307:ASN:N	2.45	0.41
1:A:663:ASN:O	1:A:667:ALA:N	2.50	0.41
1:A:933:LEU:HD23	1:A:933:LEU:HA	1.89	0.41
1:A:1197:VAL:O	1:A:1200:SER:OG	2.30	0.41
5:F:43:GLN:HB2	5:F:1011:LEU:HD23	2.03	0.41
5:F:64:GLU:O	5:F:67:GLN:NE2	2.40	0.41
5:F:615:ASN:OD1	6:G:1:NAG:O5	2.37	0.41
1:A:454:HIS:HA	1:A:951:LYS:HD2	2.02	0.41
1:A:1078:ASN:OD1	1:A:1078:ASN:N	2.54	0.41
5:F:92:LEU:O	5:F:96:SER:HB3	2.20	0.41
1:A:836:ASP:HA	1:A:839:PHE:HB2	2.02	0.41
5:F:130:ASN:O	5:F:132:LYS:N	2.49	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:234:LYS:HG3	5:F:235:ILE:HD12	2.02	0.41
1:A:513:LEU:HD23	1:A:527:LEU:HD11	2.03	0.41
1:A:942:PHE:HD2	1:A:1048:TYR:HD1	1.67	0.41
1:A:1015:GLY:C	1:A:1017:PRO:HD2	2.40	0.41
1:A:1132:THR:O	1:A:1136:GLY:N	2.53	0.41
3:C:435:ASP:N	3:C:435:ASP:OD1	2.54	0.41
5:F:863:LEU:HD23	5:F:863:LEU:HA	1.87	0.41
1:A:116:ALA:HA	1:A:119:ARG:HB3	2.02	0.41
1:A:527:LEU:HA	1:A:530:ILE:HD12	2.02	0.41
1:A:652:LEU:HD23	1:A:652:LEU:HA	1.79	0.41
5:F:129:TYR:HE1	5:F:149:PRO:HD2	1.86	0.41
1:A:108:TYR:HB3	1:A:112:PHE:HB2	2.03	0.41
5:F:92:LEU:HD22	5:F:448:TRP:CH2	2.56	0.41
5:F:480:ASN:HB3	5:F:483:ASN:ND2	2.36	0.41
5:F:647:TYR:CE1	5:F:713:GLY:HA3	2.56	0.41
1:A:627:TYR:HD1	1:A:627:TYR:HA	1.58	0.41
1:A:965:GLU:HA	1:A:990:TRP:HE1	1.85	0.41
1:A:1396:PRO:CD	1:A:1397:HIS:N	2.83	0.41
1:A:1414:LYS:NZ	1:A:1416:ARG:O	2.54	0.41
4:E:120:MET:HG3	4:E:143:PHE:CD2	2.56	0.41
5:F:102:LEU:HB3	5:F:490:MET:HE3	2.01	0.41
5:F:385:ARG:NH2	5:F:1069:GLU:OE2	2.54	0.41
5:F:894:VAL:HG12	5:F:895:TYR:HB3	2.03	0.41
1:A:793:HIS:HE1	1:A:854:TYR:CZ	2.39	0.41
1:A:962:LYS:HE3	1:A:988:ARG:HH12	1.86	0.41
1:A:268:PRO:HB3	1:A:300:TRP:CZ3	2.55	0.40
5:F:411:TYR:CD1	5:F:1074:CYS:HA	2.56	0.40
5:F:514:TYR:CE1	5:F:624:LEU:HD13	2.56	0.40
1:A:115:ASP:O	1:A:119:ARG:N	2.53	0.40
1:A:1091:TYR:HD1	1:A:1091:TYR:HA	1.76	0.40
1:A:330:LEU:HB3	1:A:1387:LEU:HD11	2.03	0.40
1:A:1392:SER:O	1:A:1393:ILE:HG13	2.21	0.40
5:F:675:PRO:HB3	5:F:682:PHE:HB2	2.04	0.40
1:A:620:MET:HG3	1:A:641:PHE:HD2	1.87	0.40
5:F:791:TYR:OH	5:F:871:THR:O	2.28	0.40
3:C:285:LYS:HD3	3:C:369:ASP:HA	2.04	0.40
5:F:243:ARG:NE	5:F:244:PRO:HD2	2.36	0.40
5:F:290:PHE:HE2	5:F:353:ARG:C	2.23	0.40
5:F:334:ASP:OD1	5:F:335:TYR:N	2.55	0.40
5:F:1035:ILE:HG22	5:F:1036:GLN:O	2.21	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	1279/1873 (68%)	1099 (86%)	163 (13%)	17 (1%)	12	48
2	B	98/106 (92%)	91 (93%)	7 (7%)	0	100	100
3	C	174/199 (87%)	168 (97%)	6 (3%)	0	100	100
4	E	156/222 (70%)	143 (92%)	13 (8%)	0	100	100
5	F	930/1106 (84%)	752 (81%)	148 (16%)	30 (3%)	4	32
All	All	2637/3506 (75%)	2253 (85%)	337 (13%)	47 (2%)	12	42

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	F	348	ASN
5	F	351	VAL
5	F	477	ASN
5	F	478	LYS
5	F	532	LYS
5	F	785	LYS
5	F	893	SER
5	F	894	VAL
1	A	978	GLY
1	A	1293	ALA
1	A	1394	LEU
1	A	1458	ASP
5	F	178	SER
5	F	730	LYS
5	F	732	VAL
5	F	806	GLN
5	F	1053	PRO
5	F	1054	ARG
5	F	1068	LEU
5	F	1073	ASP
5	F	1074	CYS

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	310	PRO
1	A	542	TRP
1	A	821	PRO
1	A	908	ILE
5	F	484	GLN
5	F	485	LEU
1	A	1142	GLN
1	A	1396	PRO
5	F	77	ALA
5	F	450	ASN
5	F	786	SER
5	F	1069	GLU
1	A	278	PHE
1	A	309	TRP
1	A	451	SER
5	F	755	TRP
5	F	1070	ASP
1	A	75	PRO
1	A	1105	ASN
5	F	509	CYS
1	A	457	PRO
5	F	221	PRO
5	F	530	GLN
5	F	550	VAL
5	F	788	PRO
1	A	1440	PRO

### 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	1081/1628 (66%)	1059 (98%)	22 (2%)	55 74
2	B	59/91 (65%)	58 (98%)	1 (2%)	60 78
3	C	143/179 (80%)	143 (100%)	0	100 100
4	E	141/192 (73%)	140 (99%)	1 (1%)	84 90

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	F	838/974 (86%)	818 (98%)	20 (2%)	49 69
All	All	2262/3064 (74%)	2218 (98%)	44 (2%)	59 75

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	165	ARG
1	A	226	CYS
1	A	245	CYS
1	A	254	CYS
1	A	475	PHE
1	A	542	TRP
1	A	562	LEU
1	A	593	ARG
1	A	656	PHE
1	A	790	VAL
1	A	995	PHE
1	A	1005	MET
1	A	1051	LEU
1	A	1056	MET
1	A	1068	PHE
1	A	1091	TYR
1	A	1175	ARG
1	A	1251	GLU
1	A	1262	LYS
1	A	1302	ARG
1	A	1384	PHE
1	A	1409	TYR
2	B	115	PRO
4	E	207	MET
5	F	78	ARG
5	F	95	ARG
5	F	116	ARG
5	F	148	LYS
5	F	174	ILE
5	F	179	THR
5	F	186	ASN
5	F	196	LYS
5	F	248	GLN
5	F	428	TYR
5	F	577	ARG
5	F	615	ASN

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	F	689	PHE
5	F	755	TRP
5	F	782	TYR
5	F	891	ASN
5	F	1024	LYS
5	F	1032	ARG
5	F	1054	ARG
5	F	1074	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	80	ASN
1	A	123	ASN
1	A	187	ASN
1	A	445	ASN
1	A	456	GLN
1	A	464	GLN
1	A	554	ASN
1	A	602	GLN
1	A	793	HIS
1	A	996	HIS
1	A	1142	GLN
1	A	1147	ASN
1	A	1154	ASN
1	A	1299	GLN
1	A	1326	GLN
1	A	1383	ASN
4	E	160	GLN
5	F	43	GLN
5	F	130	ASN
5	F	311	GLN
5	F	313	ASN
5	F	316	ASN
5	F	325	ASN
5	F	379	ASN
5	F	424	ASN
5	F	480	ASN
5	F	644	GLN
5	F	655	ASN
5	F	679	ASN
5	F	687	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
5	F	716	ASN
5	F	866	ASN
5	F	1036	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	ETA	F	1075	5	3,3,3	0.45	0	2,2,2	0.54	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	ETA	F	1075	5	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	1075	ETA	O-C-CA-N

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	1075	ETA	1	0

## 5.5 Carbohydrates [i](#)

17 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	D	1	5,6	14,14,15	0.43	0	17,19,21	1.08	1 (5%)
6	NAG	D	2	6	14,14,15	0.38	0	17,19,21	0.70	1 (5%)
6	NAG	G	1	5,6	14,14,15	0.76	1 (7%)	17,19,21	0.86	0
6	NAG	G	2	6	14,14,15	0.59	0	17,19,21	0.60	0
7	NAG	H	1	5,7	14,14,15	0.71	1 (7%)	17,19,21	0.55	0
7	NAG	H	2	7	14,14,15	0.42	0	17,19,21	0.58	0
7	BMA	H	3	7	11,11,12	0.73	0	15,15,17	1.12	2 (13%)
7	NAG	I	1	5,7	14,14,15	0.38	0	17,19,21	1.06	1 (5%)
7	NAG	I	2	7	14,14,15	0.33	0	17,19,21	0.46	0
7	BMA	I	3	7	11,11,12	1.13	2 (18%)	15,15,17	1.31	2 (13%)
6	NAG	J	1	5,6	14,14,15	0.41	0	17,19,21	0.63	0
6	NAG	J	2	6	14,14,15	0.50	0	17,19,21	0.48	0
6	NAG	K	1	5,6	14,14,15	0.27	0	17,19,21	1.08	1 (5%)
6	NAG	K	2	6	14,14,15	0.62	0	17,19,21	0.95	1 (5%)
8	NAG	L	1	5,8	14,14,15	0.41	0	17,19,21	0.70	0
8	NAG	L	2	8	14,14,15	0.92	1 (7%)	17,19,21	2.26	3 (17%)
8	NAG	L	3	8	14,14,15	0.31	0	17,19,21	0.69	1 (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
6	NAG	D	1	5,6	-	3/6/23/26	0/1/1/1
6	NAG	D	2	6	-	0/6/23/26	0/1/1/1
6	NAG	G	1	5,6	-	0/6/23/26	0/1/1/1
6	NAG	G	2	6	-	0/6/23/26	0/1/1/1
7	NAG	H	1	5,7	-	0/6/23/26	0/1/1/1
7	NAG	H	2	7	-	2/6/23/26	0/1/1/1
7	BMA	H	3	7	-	2/2/19/22	0/1/1/1
7	NAG	I	1	5,7	-	1/6/23/26	0/1/1/1
7	NAG	I	2	7	-	1/6/23/26	0/1/1/1
7	BMA	I	3	7	-	2/2/19/22	0/1/1/1
6	NAG	J	1	5,6	-	1/6/23/26	0/1/1/1
6	NAG	J	2	6	-	2/6/23/26	0/1/1/1
6	NAG	K	1	5,6	-	2/6/23/26	0/1/1/1
6	NAG	K	2	6	-	2/6/23/26	0/1/1/1
8	NAG	L	1	5,8	-	2/6/23/26	0/1/1/1
8	NAG	L	2	8	-	5/6/23/26	0/1/1/1
8	NAG	L	3	8	-	2/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	2	NAG	O5-C1	-2.99	1.38	1.43
7	I	3	BMA	C1-C2	2.87	1.58	1.52
6	G	1	NAG	C1-C2	2.52	1.56	1.52
7	H	1	NAG	O5-C1	-2.36	1.39	1.43
7	I	3	BMA	C2-C3	2.04	1.55	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L	2	NAG	C2-N2-C7	7.99	134.28	122.90
6	K	1	NAG	C1-O5-C5	3.89	117.46	112.19
7	I	1	NAG	C1-O5-C5	3.79	117.33	112.19
8	L	2	NAG	C1-C2-N2	2.93	115.50	110.49
6	D	1	NAG	C2-N2-C7	2.93	127.07	122.90
6	K	2	NAG	C2-N2-C7	2.92	127.06	122.90
7	H	3	BMA	C1-O5-C5	2.83	116.03	112.19
7	I	3	BMA	C1-O5-C5	2.72	115.87	112.19
7	I	3	BMA	C1-C2-C3	2.52	112.76	109.67
8	L	3	NAG	C1-O5-C5	2.40	115.44	112.19
6	D	2	NAG	C1-O5-C5	2.38	115.42	112.19

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L	2	NAG	C8-C7-N2	2.28	119.95	116.10
7	H	3	BMA	O2-C2-C3	-2.11	105.91	110.14

There are no chirality outliers.

All (27) torsion outliers are listed below:

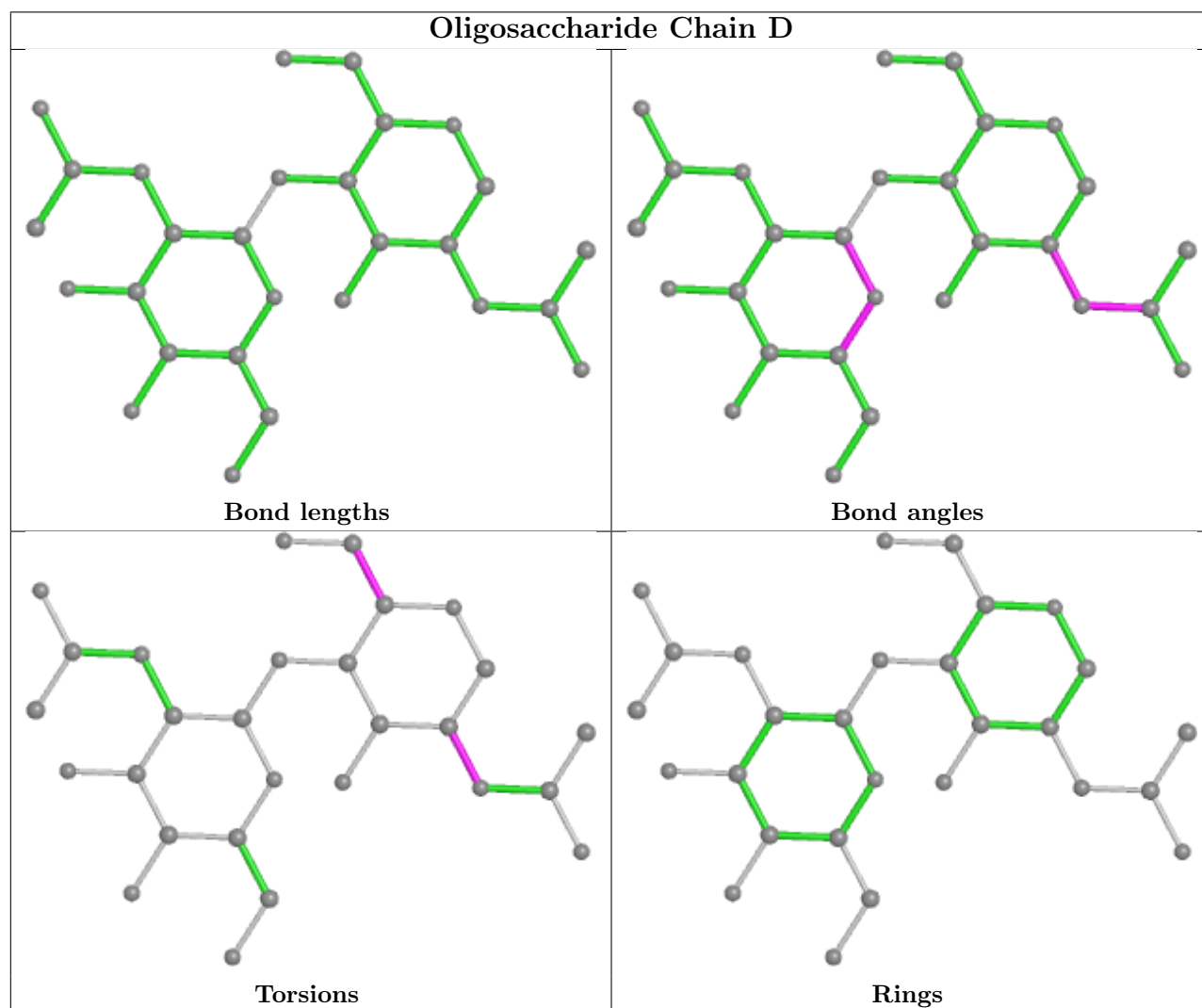
Mol	Chain	Res	Type	Atoms
8	L	2	NAG	O5-C5-C6-O6
7	H	2	NAG	O5-C5-C6-O6
6	K	1	NAG	O5-C5-C6-O6
6	K	1	NAG	C4-C5-C6-O6
7	H	2	NAG	C4-C5-C6-O6
8	L	2	NAG	C4-C5-C6-O6
6	J	2	NAG	O5-C5-C6-O6
7	I	3	BMA	O5-C5-C6-O6
6	D	1	NAG	C4-C5-C6-O6
6	J	2	NAG	C4-C5-C6-O6
8	L	1	NAG	C4-C5-C6-O6
8	L	2	NAG	C8-C7-N2-C2
8	L	2	NAG	O7-C7-N2-C2
8	L	3	NAG	O5-C5-C6-O6
7	H	3	BMA	C4-C5-C6-O6
6	D	1	NAG	O5-C5-C6-O6
8	L	3	NAG	C4-C5-C6-O6
6	J	1	NAG	O5-C5-C6-O6
8	L	1	NAG	O5-C5-C6-O6
7	H	3	BMA	O5-C5-C6-O6
7	I	1	NAG	O5-C5-C6-O6
7	I	2	NAG	O5-C5-C6-O6
7	I	3	BMA	C4-C5-C6-O6
6	D	1	NAG	C3-C2-N2-C7
6	K	2	NAG	O5-C5-C6-O6
6	K	2	NAG	C3-C2-N2-C7
8	L	2	NAG	C3-C2-N2-C7

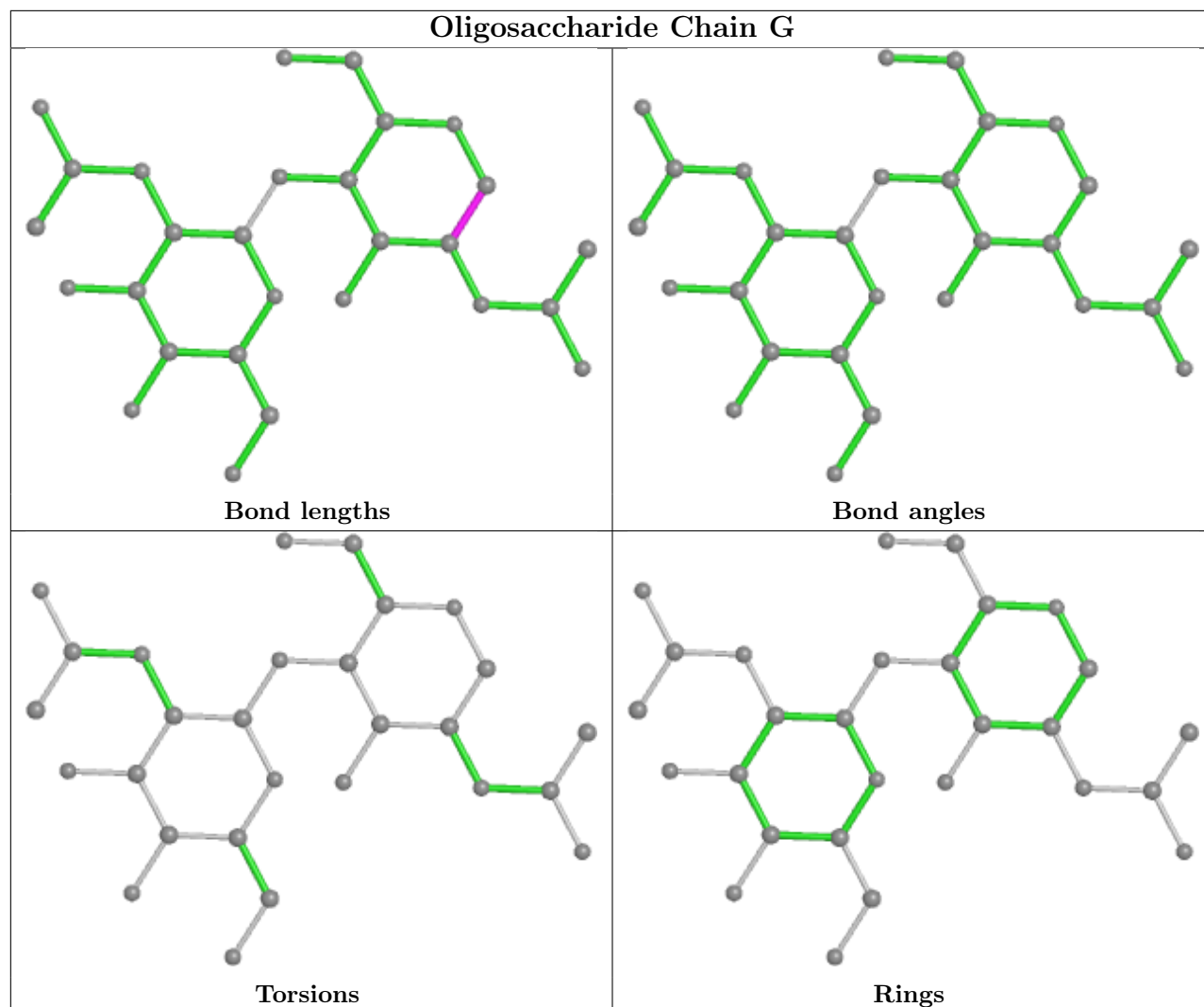
There are no ring outliers.

2 monomers are involved in 2 short contacts:

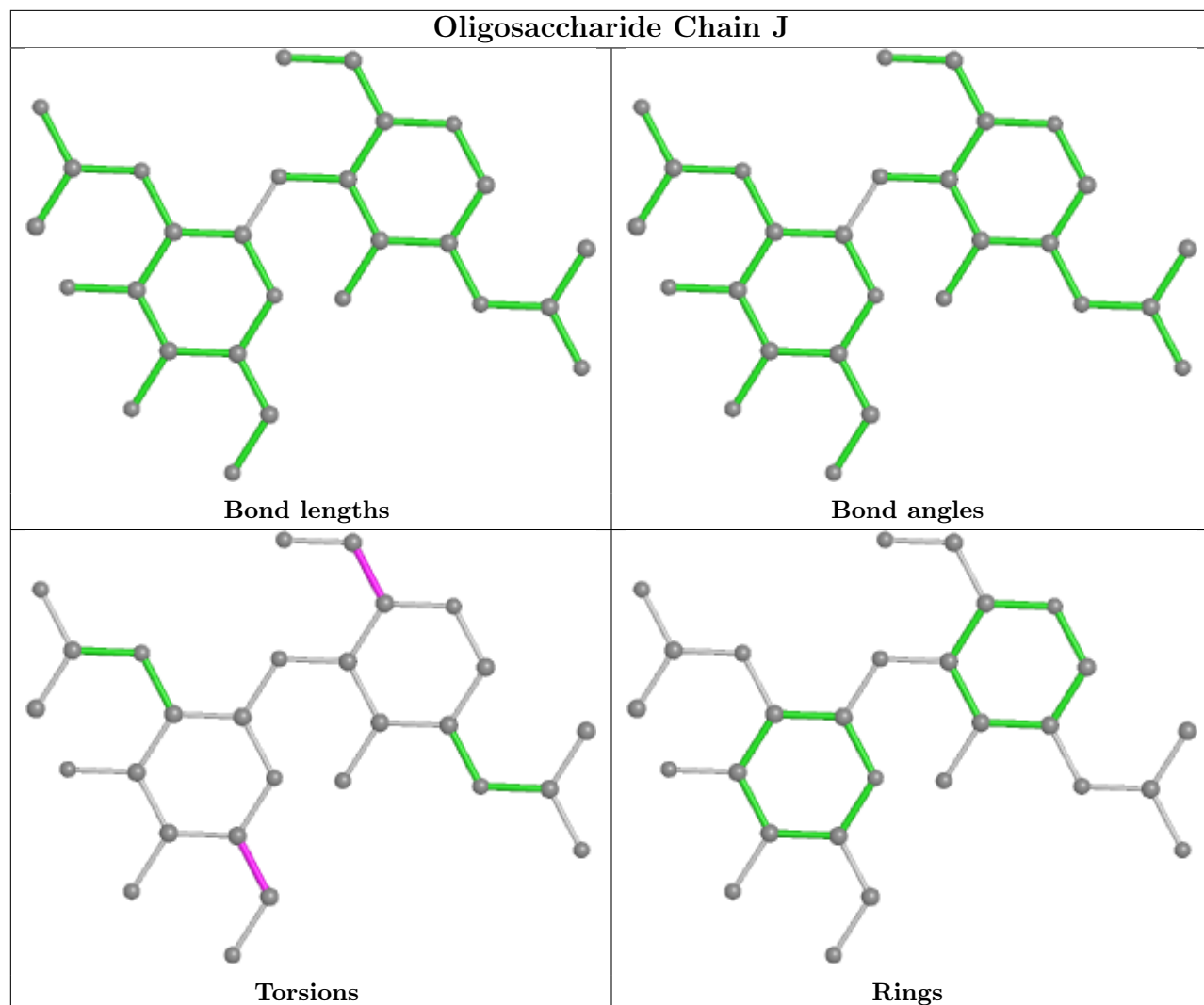
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	1	NAG	2	0
6	G	2	NAG	1	0

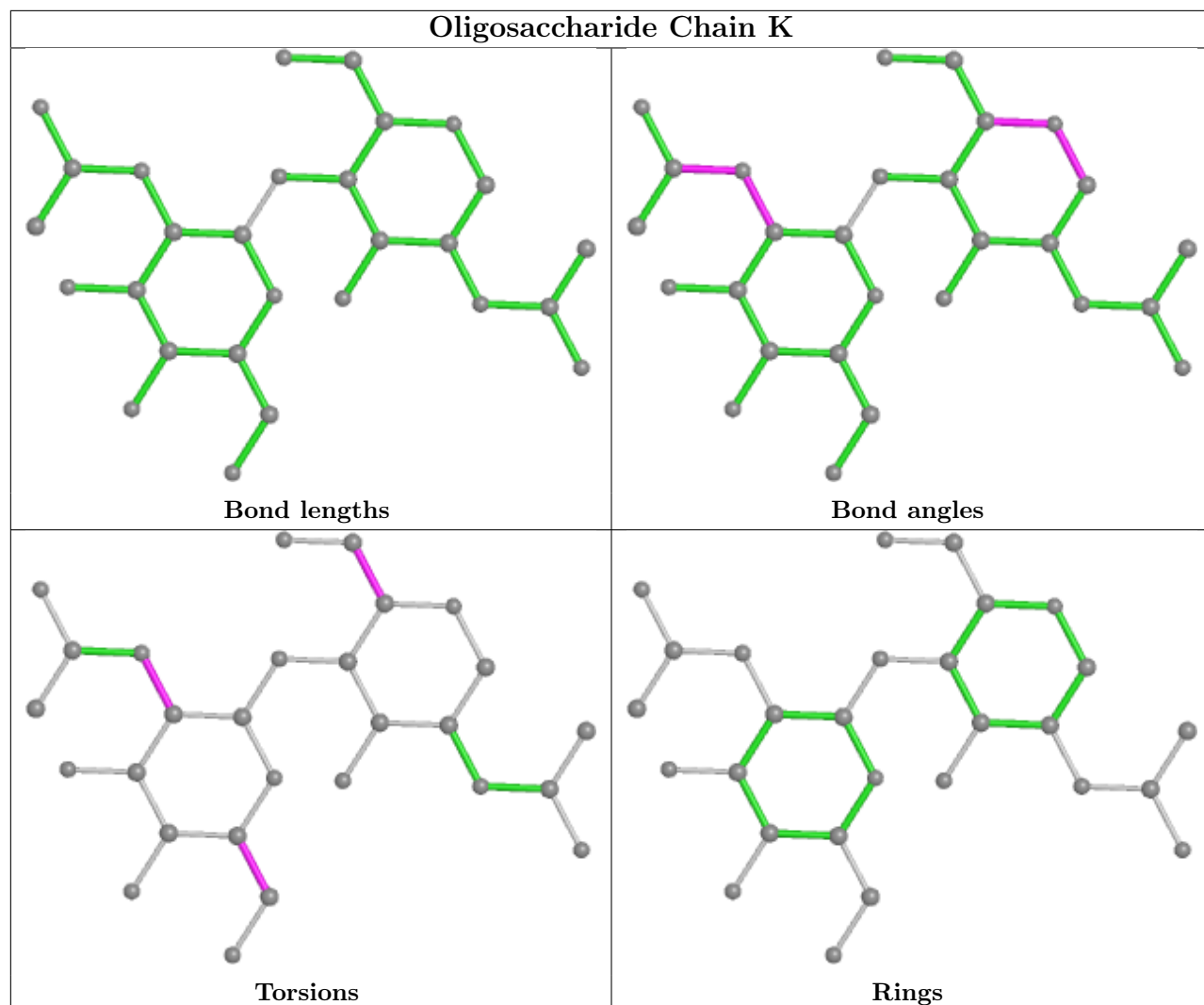
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

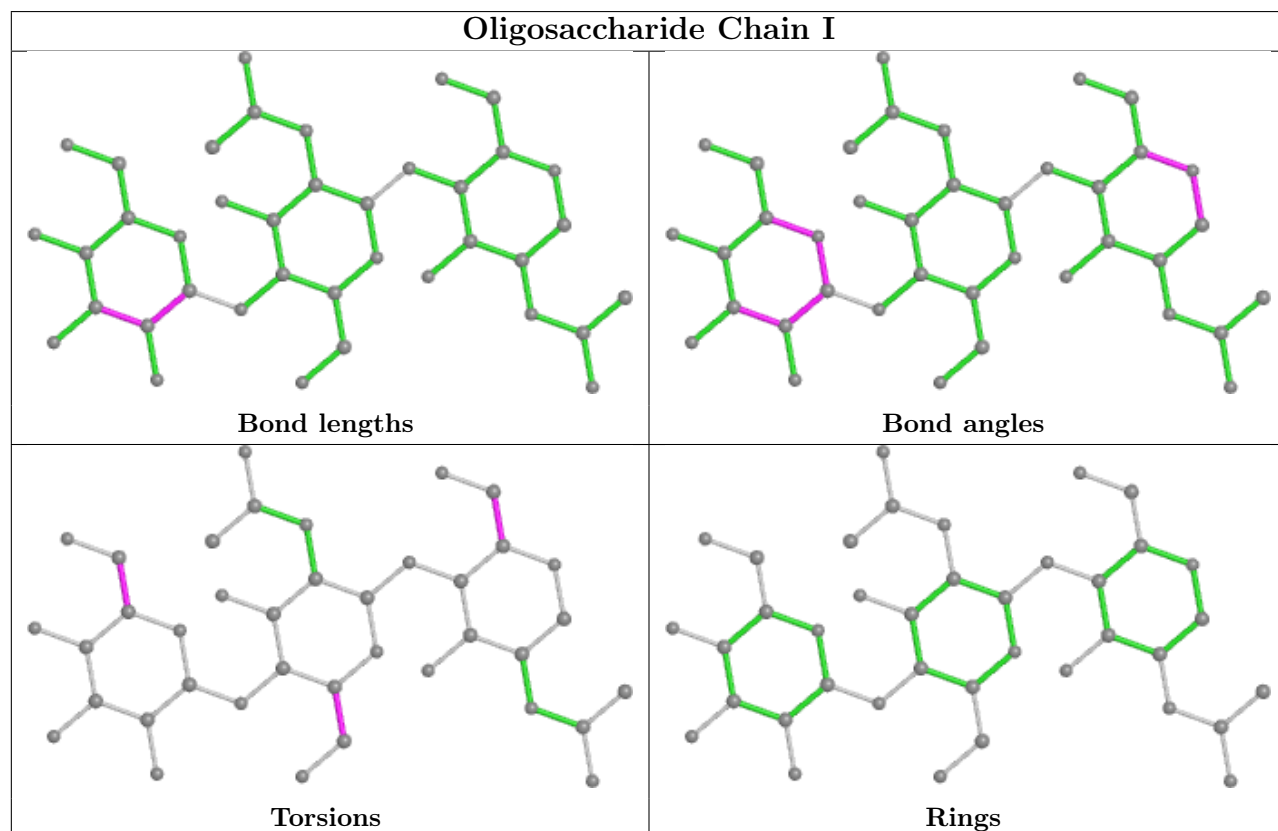
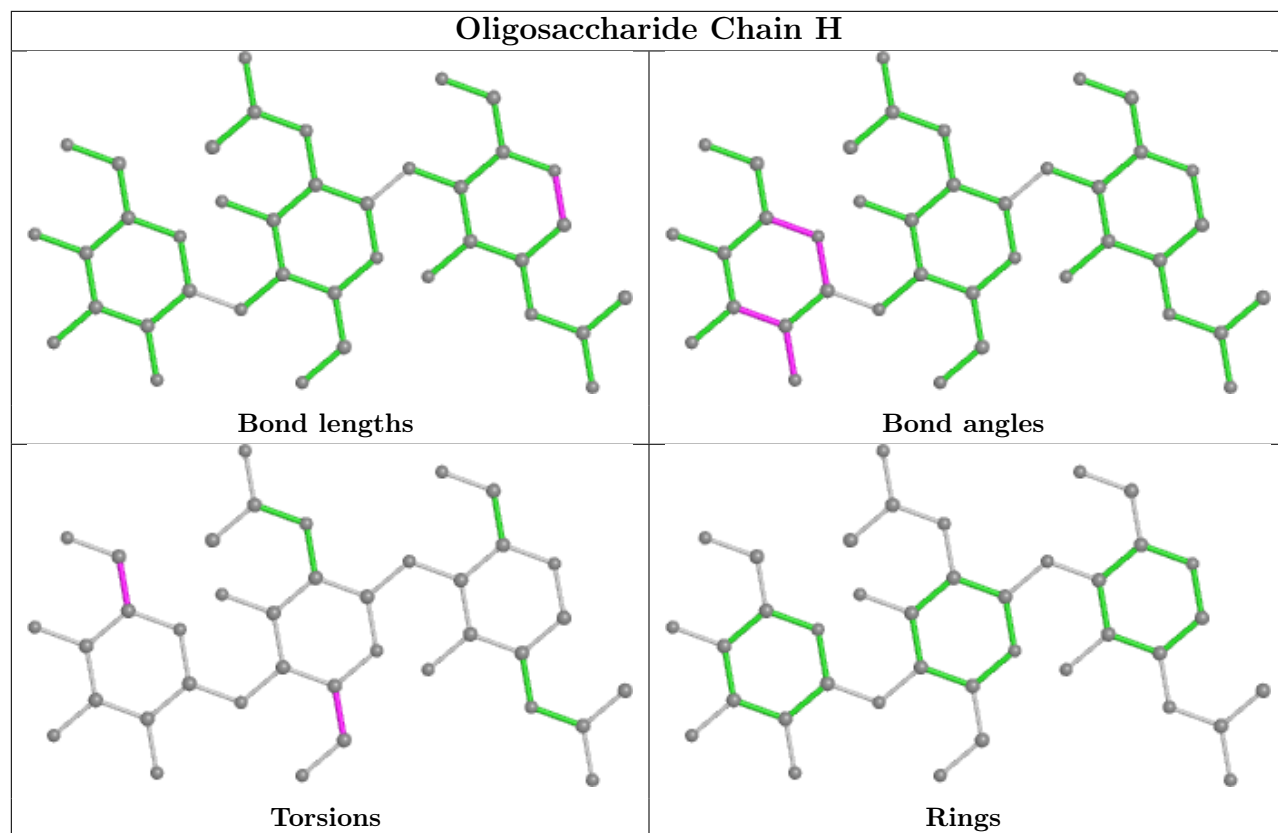


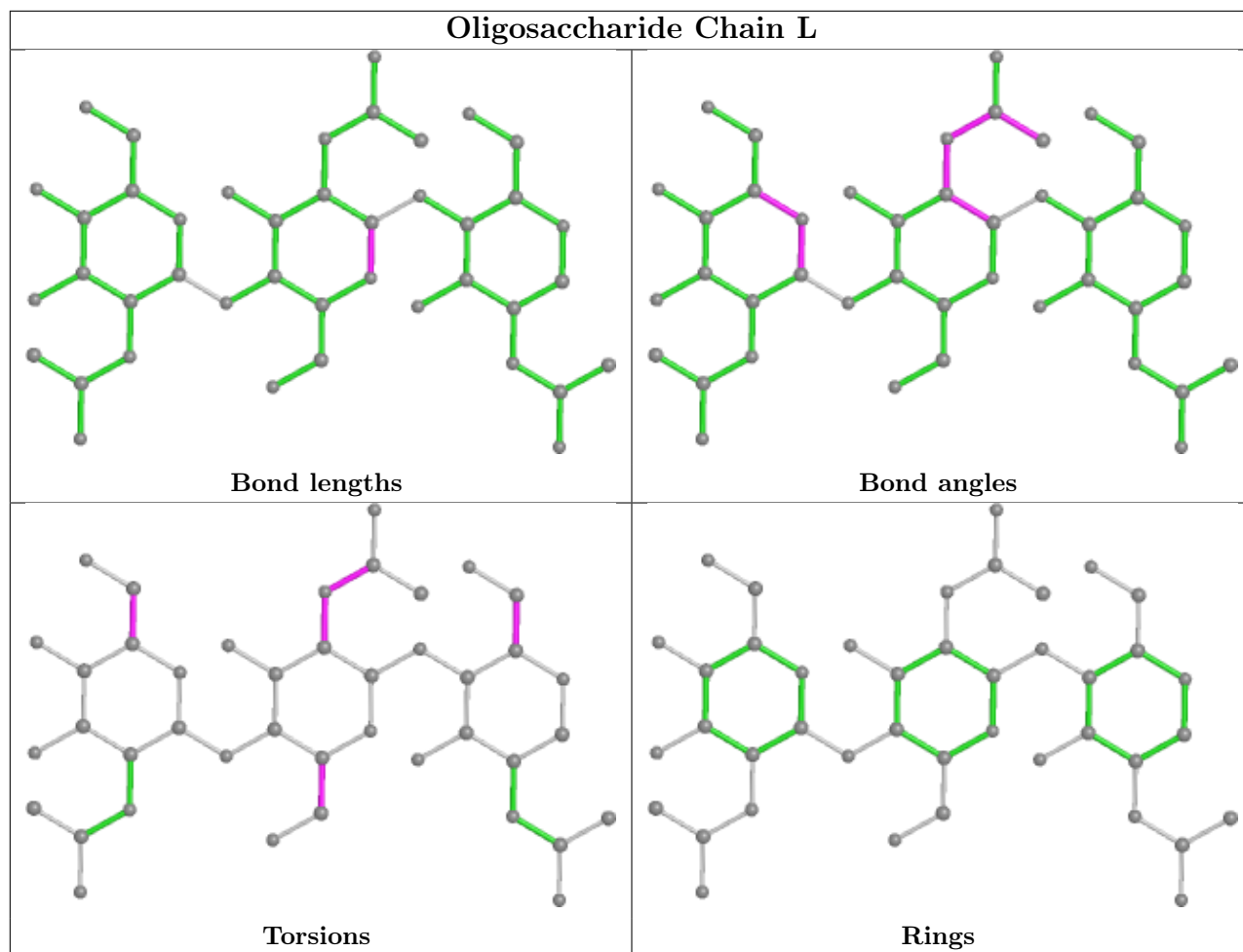












## 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 3 are monoatomic - leaving 8 for Mogul analysis.

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	$\# Z  > 2$
9	NAG	F	1222	5	14,14,15	0.48	0	17,19,21	0.72	1 (5%)
9	NAG	F	1220	5	14,14,15	0.36	0	17,19,21	0.37	0
9	NAG	F	1215	5	14,14,15	0.27	0	17,19,21	0.42	0
9	NAG	F	1214	5	14,14,15	0.24	0	17,19,21	0.53	0
9	NAG	F	1207	5	14,14,15	0.53	0	17,19,21	0.40	0
9	NAG	F	1204	5	14,14,15	0.22	0	17,19,21	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	NAG	A	1901	1	14,14,15	0.33	0	17,19,21	0.97	1 (5%)
9	NAG	F	1221	5	14,14,15	0.43	0	17,19,21	0.43	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
9	NAG	F	1222	5	-	2/6/23/26	0/1/1/1
9	NAG	F	1220	5	-	2/6/23/26	0/1/1/1
9	NAG	F	1215	5	-	2/6/23/26	0/1/1/1
9	NAG	F	1214	5	-	2/6/23/26	0/1/1/1
9	NAG	F	1207	5	-	2/6/23/26	0/1/1/1
9	NAG	F	1204	5	-	0/6/23/26	0/1/1/1
9	NAG	A	1901	1	-	0/6/23/26	0/1/1/1
9	NAG	F	1221	5	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	1901	NAG	C1-O5-C5	2.62	115.75	112.19
9	F	1222	NAG	C1-O5-C5	2.58	115.69	112.19

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	F	1220	NAG	O5-C5-C6-O6
9	F	1207	NAG	O5-C5-C6-O6
9	F	1220	NAG	C4-C5-C6-O6
9	F	1215	NAG	O5-C5-C6-O6
9	F	1215	NAG	C4-C5-C6-O6
9	F	1222	NAG	O5-C5-C6-O6
9	F	1214	NAG	O5-C5-C6-O6
9	F	1214	NAG	C4-C5-C6-O6
9	F	1222	NAG	C4-C5-C6-O6
9	F	1207	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

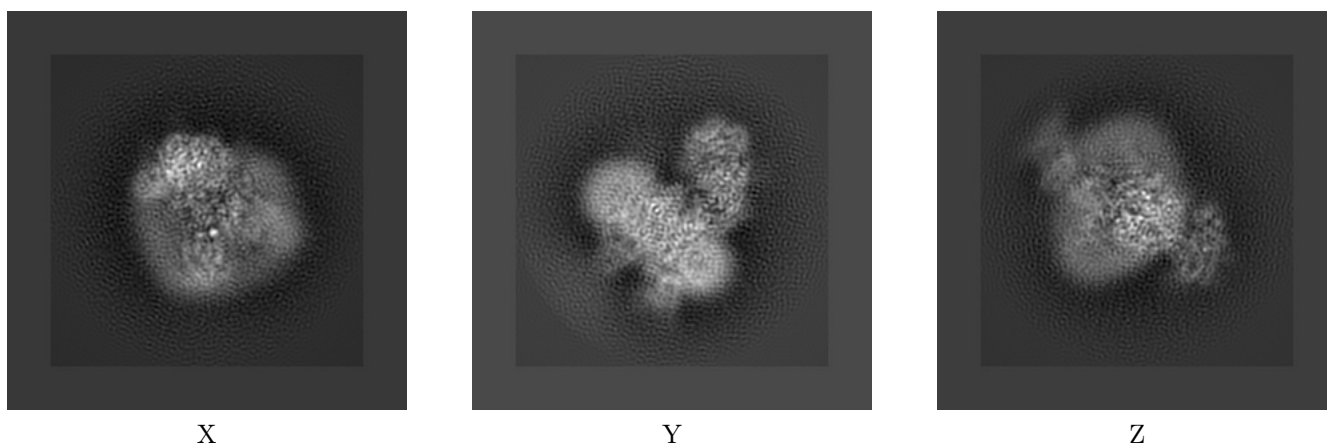
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9515. 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](#)

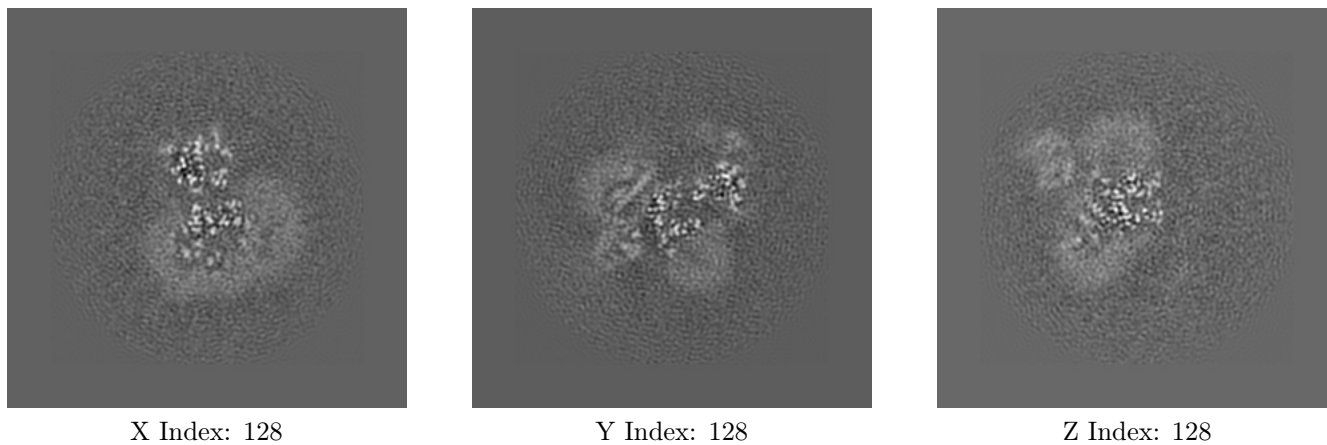
#### 6.1.1 Primary map



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

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

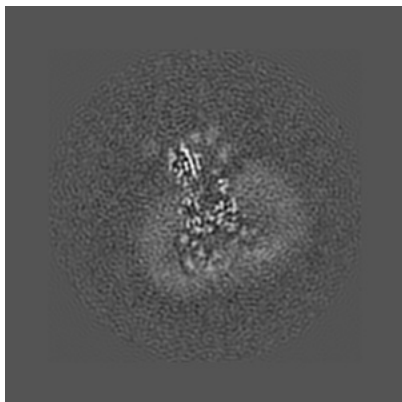
#### 6.2.1 Primary map



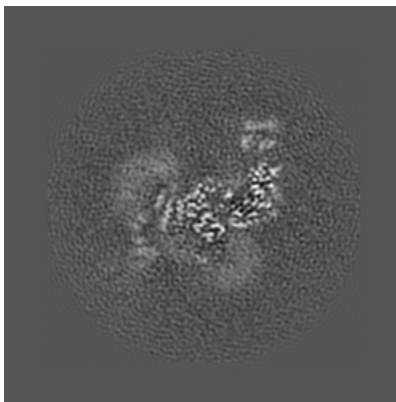
The images above show central slices of the map in three orthogonal directions.

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

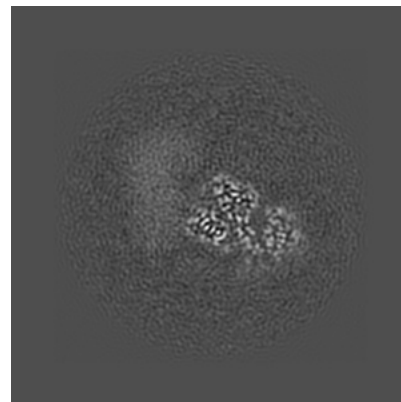
### 6.3.1 Primary map



X Index: 123



Y Index: 121

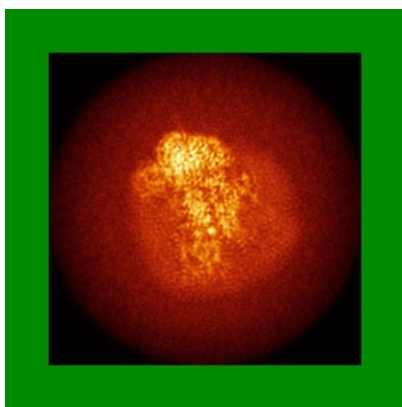


Z Index: 159

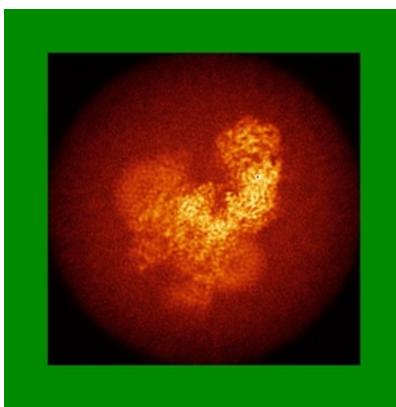
The images above show the largest variance slices of the map in three orthogonal directions.

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

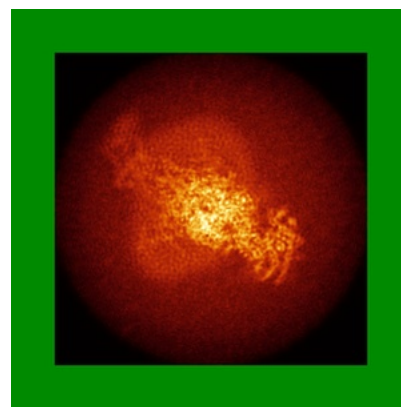
### 6.4.1 Primary map



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](#)

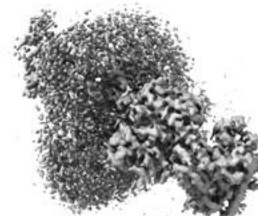
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

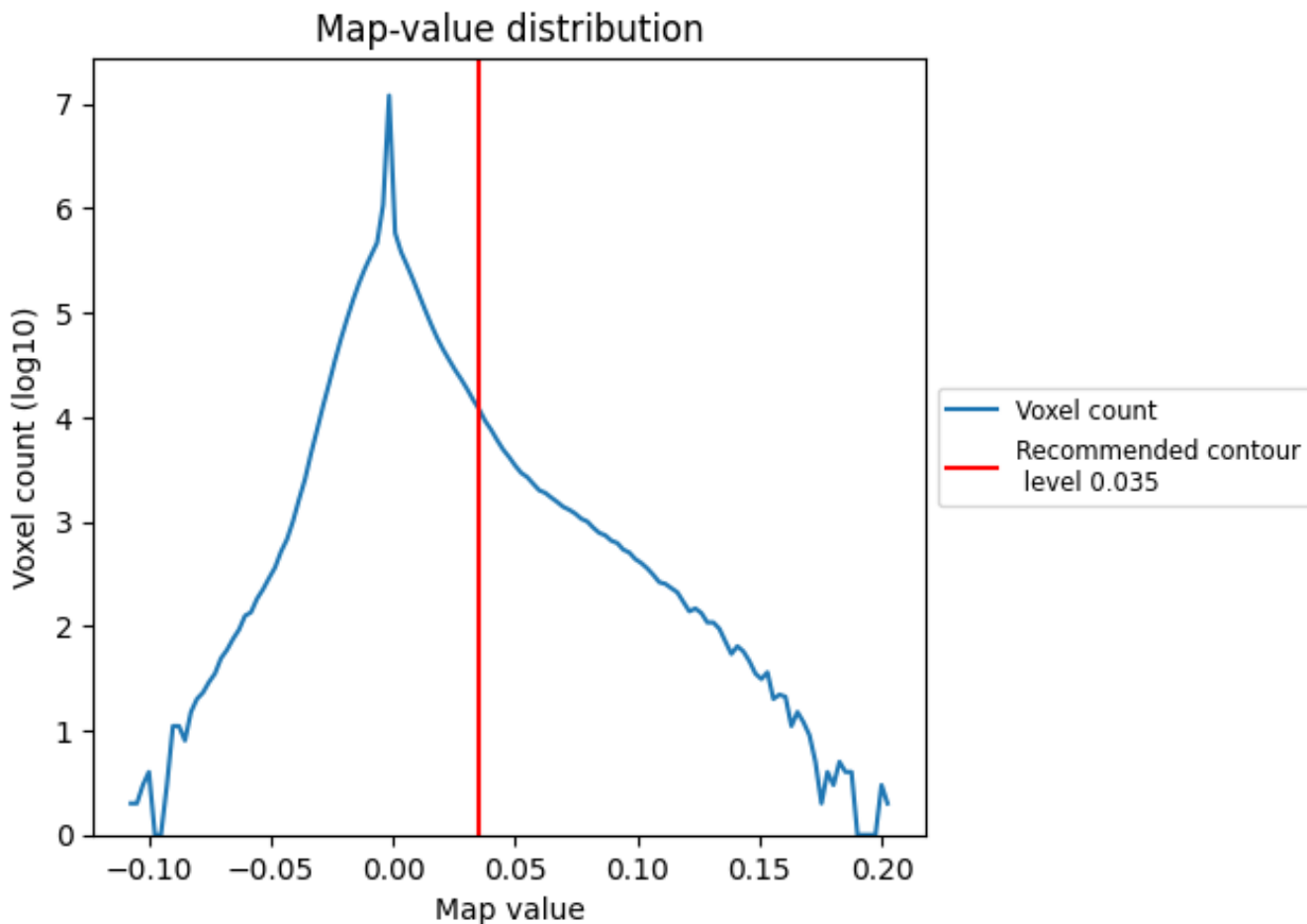
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

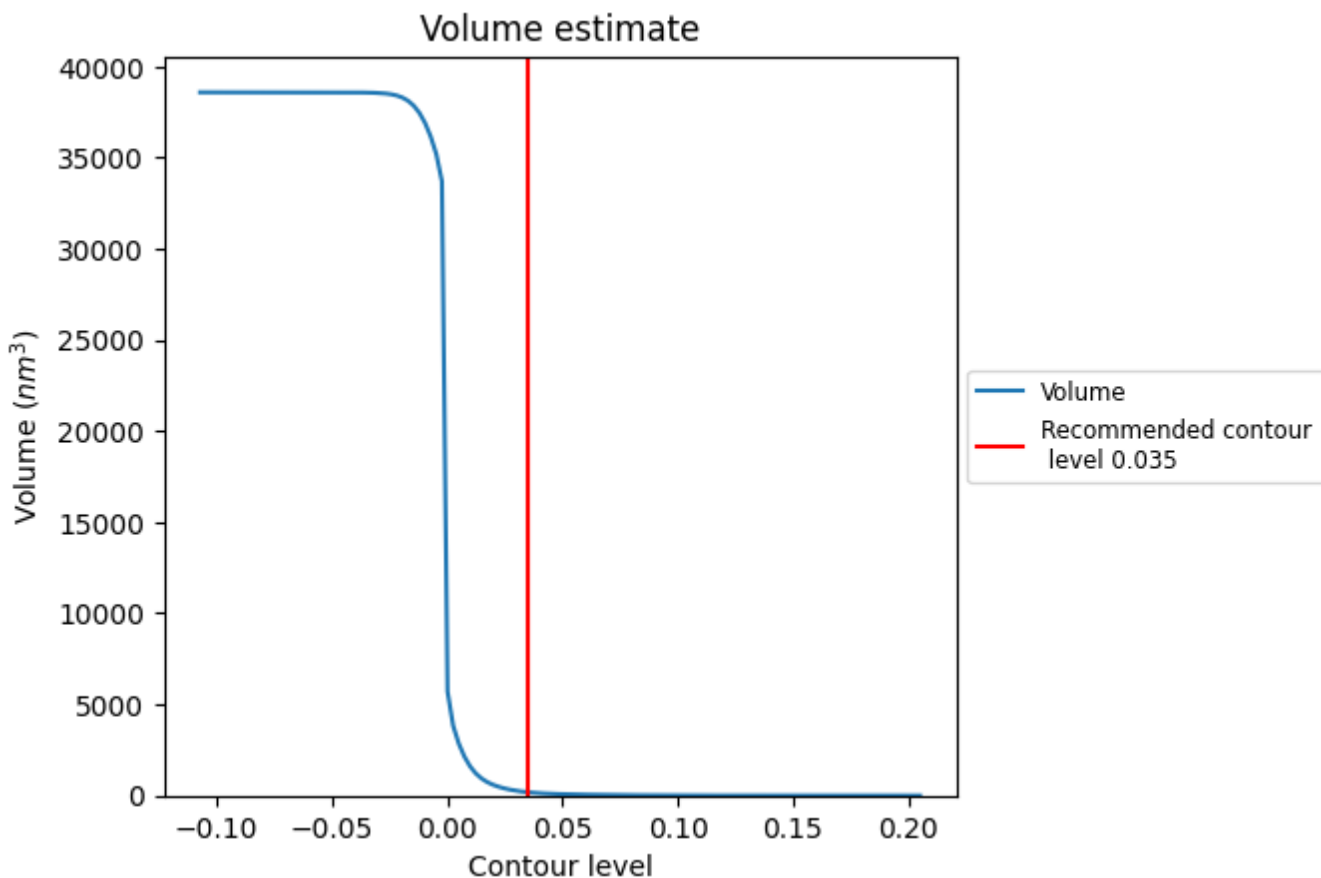
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

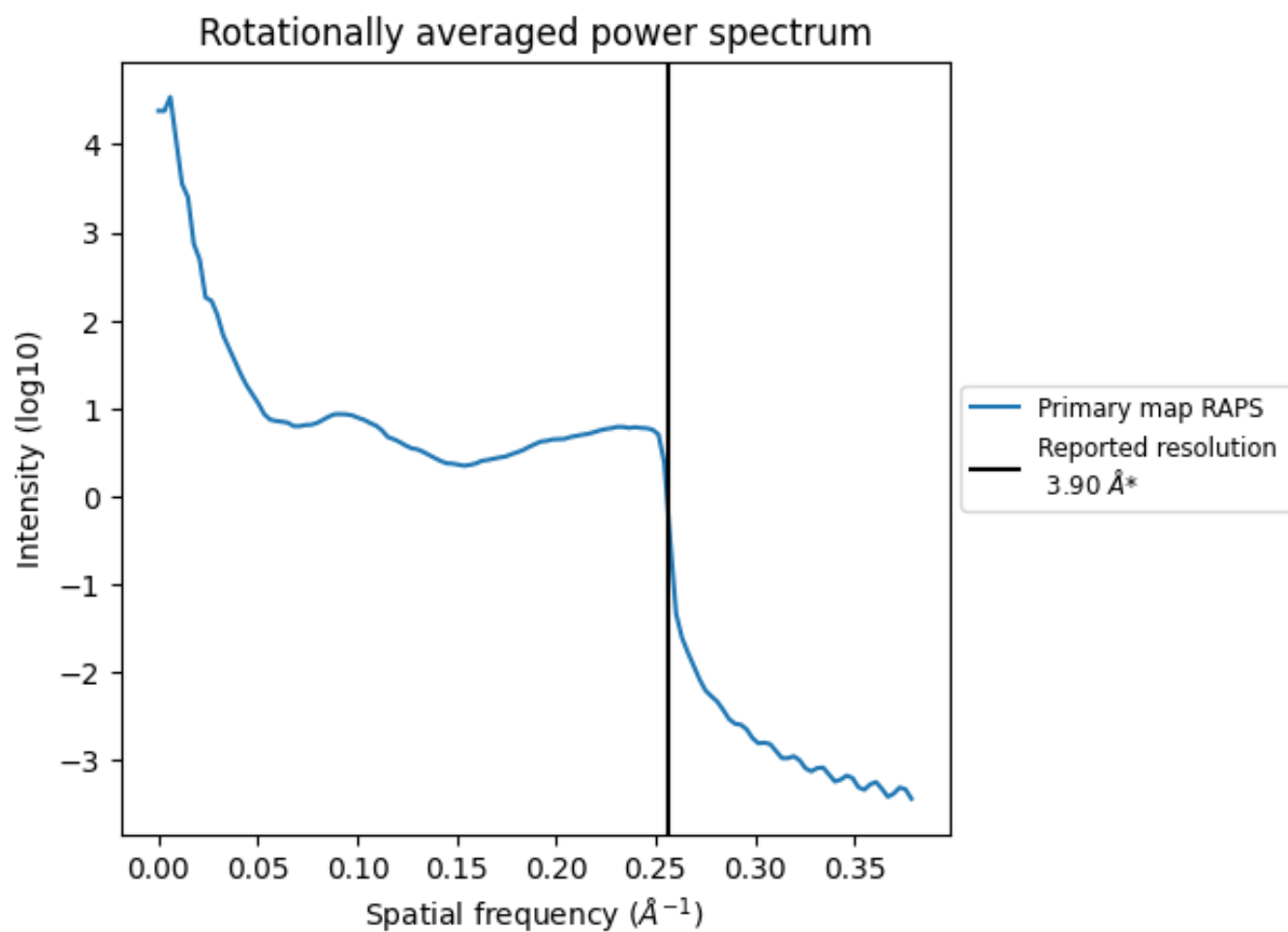
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 181 nm<sup>3</sup>; this corresponds to an approximate mass of 163 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  $0.256 \text{\AA}^{-1}$

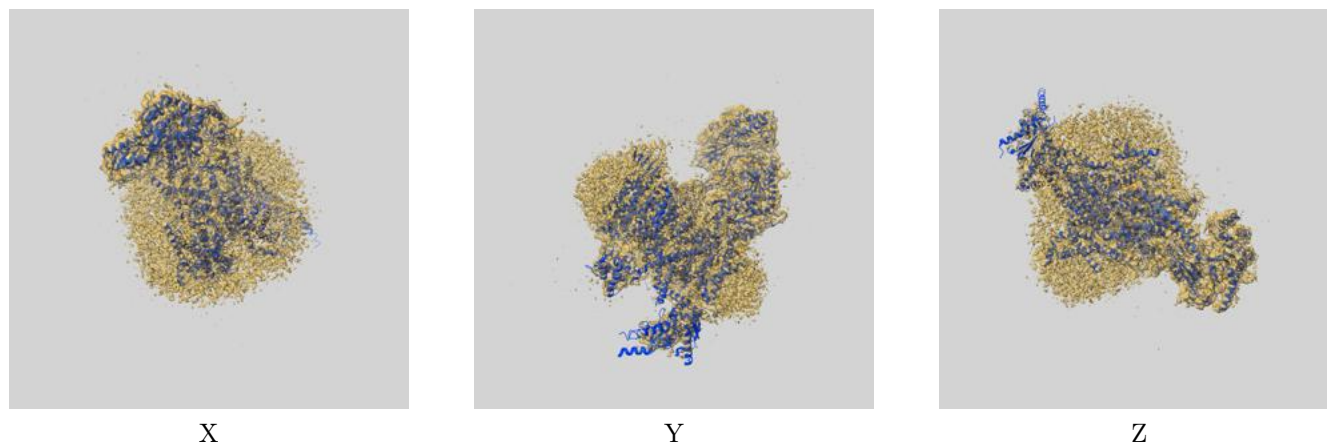
## 8 Fourier-Shell correlation

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

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

This section contains information regarding the fit between EMDB map EMD-9515 and PDB model 5GJW. Per-residue inclusion information can be found in section [3](#) on page [8](#).

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



The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



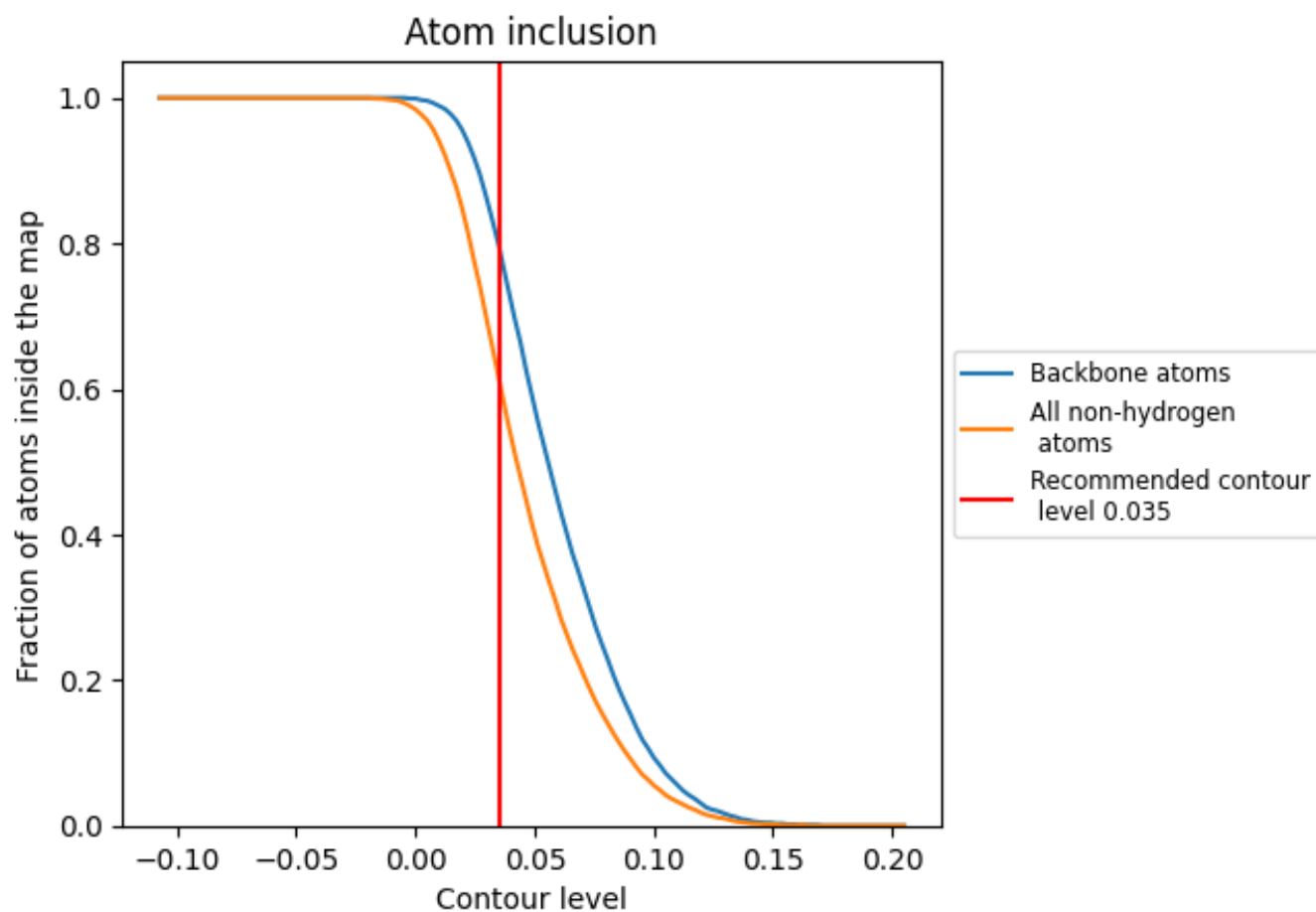
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.035).

## 9.4 Atom inclusion [i](#)





























At the recommended contour level, 80% of all backbone atoms, 61% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6140	 0.3600
A	 0.6090	 0.3670
B	 0.0970	 0.1650
C	 0.2710	 0.1860
D	 0.2500	 0.3260
E	 0.5380	 0.2950
F	 0.7480	 0.4120
G	 0.2860	 0.2700
H	 0.4620	 0.3530
I	 0.7180	 0.4350
J	 0.6430	 0.3820
K	 0.5360	 0.4070
L	 0.5000	 0.2400

