



Full wwPDB EM Validation Report ⓘ

May 17, 2025 – 05:00 PM EDT

PDB ID : 6WQZ / pdb_00006wqz
EMDB ID : EMD-21874
Title : Structure of human ATG9A, the only transmembrane protein of the core autophagy machinery
Authors : Guardia, C.M.; Tan, X.; Lian, T.; Rana, M.S.; Zhou, W.; Christenson, E.T.; Lowry, A.J.; Faraldo-Gomez, J.D.; Bonifacino, J.S.; Jiang, J.; Banerjee, A.
Deposited on : 2020-04-29
Resolution : 2.80 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.dev118
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

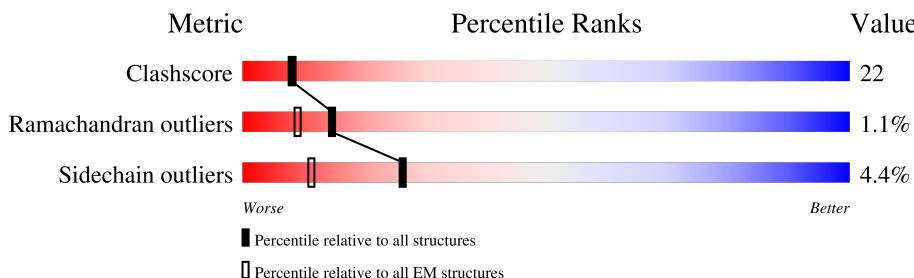
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	724	<div> <div>9%</div> <div>50%</div> <div>21%</div> <div>26%</div> </div>
1	B	724	<div> <div>9%</div> <div>49%</div> <div>21%</div> <div>26%</div> </div>
1	C	724	<div> <div>9%</div> <div>51%</div> <div>20%</div> <div>26%</div> </div>
1	D	724	<div> <div>95%</div> </div>
1	E	724	<div> <div>95%</div> </div>
1	F	724	<div> <div>95%</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	LMN	A	802	-	-	X	-

2 Entry composition ⓘ

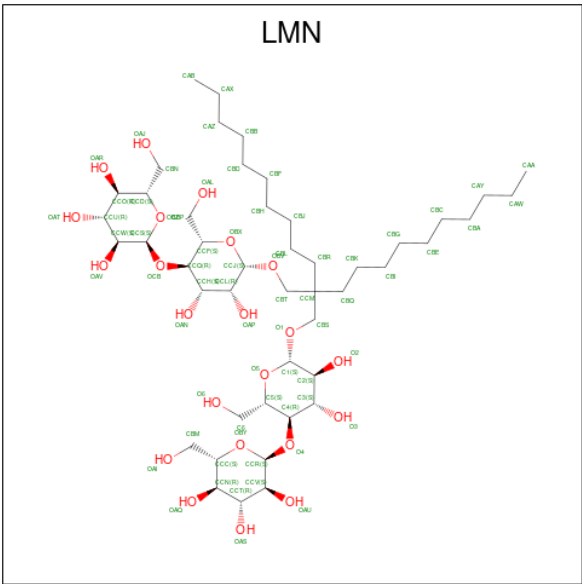
There are 2 unique types of molecules in this entry. The entry contains 14128 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Autophagy-related protein 9A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	536	Total	C	N	O	S	0	0
			4393	2885	739	745	24		
1	F	35	Total	C	N	O		0	0
			175	105	35	35			
1	B	536	Total	C	N	O	S	0	0
			4393	2885	739	745	24		
1	A	536	Total	C	N	O	S	0	0
			4393	2885	739	745	24		
1	E	36	Total	C	N	O		0	0
			180	108	36	36			
1	D	36	Total	C	N	O		0	0
			180	108	36	36			

- Molecule 2 is Lauryl Maltose Neopentyl Glycol (CCD ID: LMN) (formula: C₄₇H₈₈O₂₂).



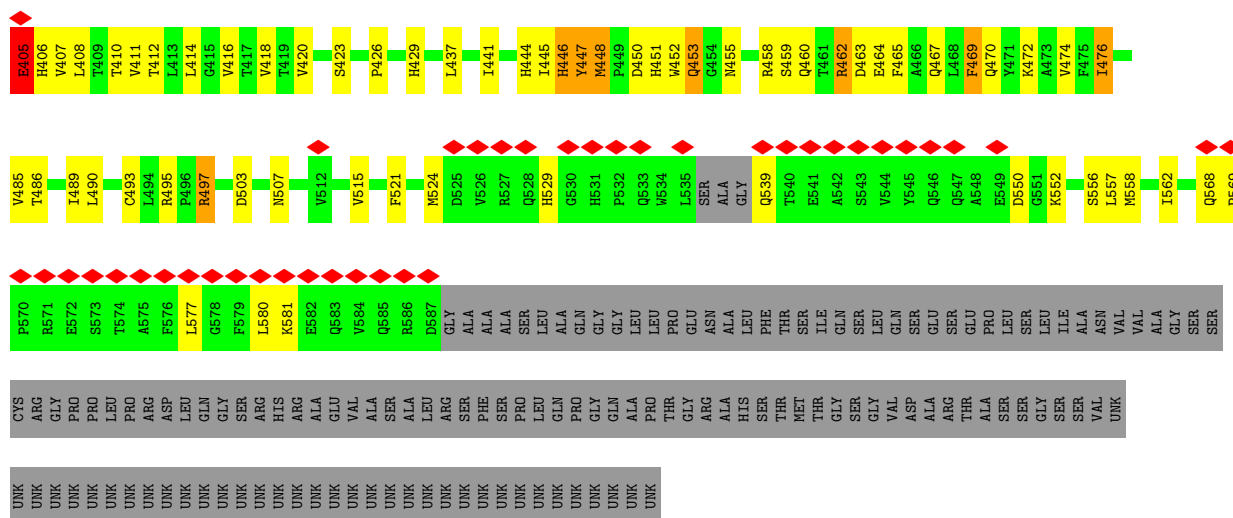
Mol	Chain	Residues	Atoms			AltConf
2	C	1	Total	C	O	0
			69	47	22	

Continued on next page...

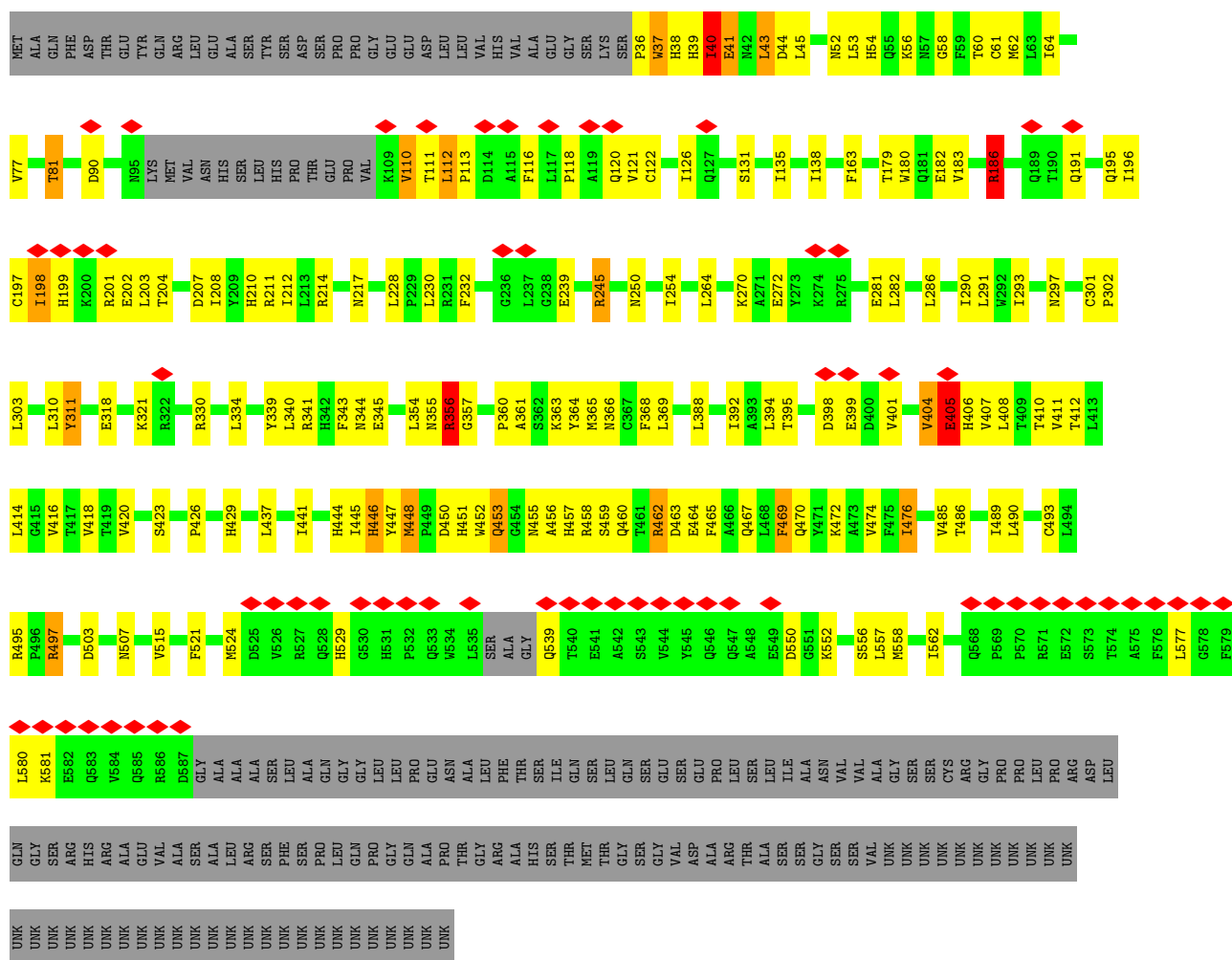
Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
2	C	1	Total	C	O	0
			69	47	22	
2	B	1	Total	C	O	0
			69	47	22	
2	B	1	Total	C	O	0
			69	47	22	
2	A	1	Total	C	O	0
			69	47	22	
2	A	1	Total	C	O	0
			69	47	22	

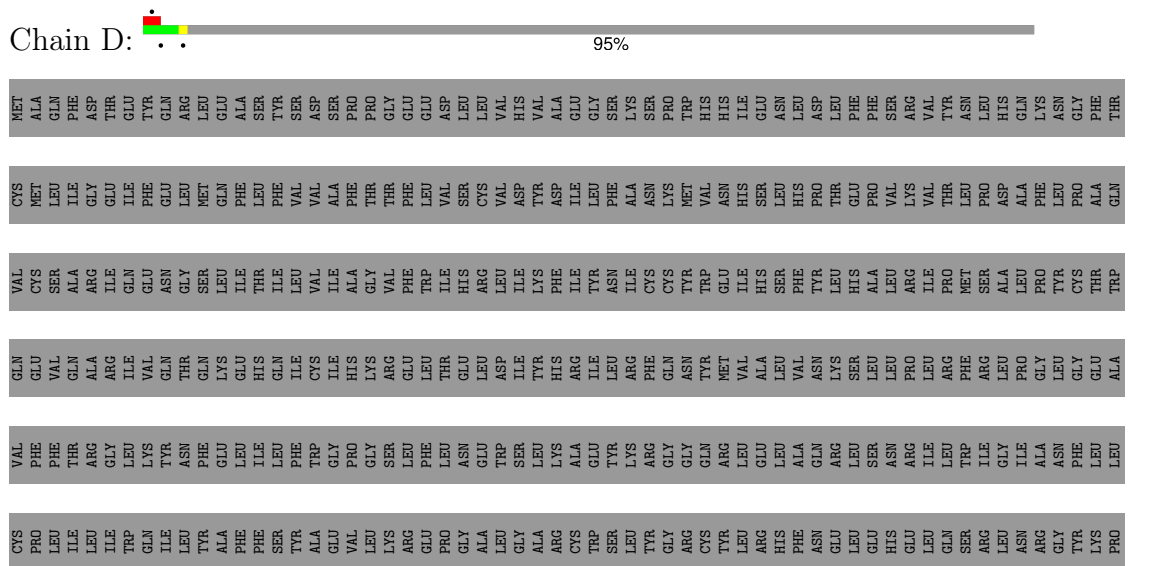
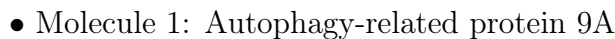




• Molecule 1: Autophagy-related protein 9A



• Molecule 1: Autophagy-related protein 9A





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	593720	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	57	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	7.258	Depositor
Minimum map value	-4.383	Depositor
Average map value	0.010	Depositor
Map value standard deviation	0.172	Depositor
Recommended contour level	0.453	Depositor
Map size (\AA)	203.51999, 203.51999, 203.51999	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.06, 1.06, 1.06	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: LMN

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	0.70	12/4516 (0.3%)	0.72	14/6135 (0.2%)
1	B	0.92	29/4516 (0.6%)	0.88	12/6135 (0.2%)
1	C	0.69	11/4516 (0.2%)	0.85	12/6135 (0.2%)
All	All	0.78	52/13548 (0.4%)	0.82	38/18405 (0.2%)

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	2
1	B	0	4
1	C	0	4
1	D	0	1
1	E	0	1
1	F	0	1
All	All	0	13

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	311	TYR	C-O	-17.61	1.03	1.24
1	C	311	TYR	C-O	-15.70	1.05	1.24
1	A	311	TYR	C-O	-15.41	1.06	1.24
1	B	314	PHE	C-O	-14.62	1.04	1.24
1	C	447	TYR	C-O	-14.22	1.08	1.24
1	B	310	LEU	C-O	-13.83	1.08	1.24
1	B	447	TYR	C-O	-13.61	1.08	1.24
1	B	312	ALA	C-O	-13.43	1.08	1.24
1	B	310	LEU	CA-C	-13.19	1.36	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	311	TYR	N-CA	-12.79	1.30	1.46
1	A	447	TYR	C-O	-12.78	1.09	1.24
1	B	313	PHE	C-O	-10.84	1.10	1.24
1	C	311	TYR	N-CA	-10.80	1.33	1.46
1	B	311	TYR	CA-C	-10.78	1.38	1.52
1	A	311	TYR	CA-C	-10.30	1.39	1.52
1	A	310	LEU	C-N	-10.08	1.20	1.33
1	C	310	LEU	C-N	-9.71	1.21	1.33
1	B	312	ALA	CA-C	-9.55	1.40	1.52
1	B	314	PHE	C-N	-9.15	1.20	1.33
1	B	311	TYR	N-CA	-9.14	1.35	1.46
1	C	311	TYR	CA-C	-9.10	1.41	1.52
1	B	309	ILE	C-O	-8.51	1.14	1.24
1	B	311	TYR	CB-CG	-8.23	1.33	1.51
1	C	367	CYS	C-N	8.21	1.45	1.33
1	A	447	TYR	CA-C	-7.53	1.43	1.52
1	B	309	ILE	CA-CB	-7.50	1.44	1.54
1	B	447	TYR	CZ-OH	-7.41	1.22	1.38
1	B	311	TYR	CA-CB	-7.25	1.41	1.53
1	A	311	TYR	CB-CG	-6.98	1.36	1.51
1	B	313	PHE	N-CA	-6.85	1.37	1.46
1	C	447	TYR	CZ-OH	-6.66	1.24	1.38
1	B	314	PHE	CA-C	-6.63	1.42	1.52
1	B	309	ILE	N-CA	-6.50	1.38	1.46
1	C	311	TYR	CA-CB	-6.45	1.43	1.53
1	C	311	TYR	CB-CG	-6.44	1.37	1.51
1	B	447	TYR	CA-CB	6.34	1.65	1.53
1	C	447	TYR	CA-CB	6.32	1.63	1.53
1	B	310	LEU	C-N	-6.25	1.25	1.33
1	A	311	TYR	CA-CB	-6.25	1.43	1.53
1	B	367	CYS	C-N	6.13	1.42	1.33
1	A	447	TYR	CZ-OH	-6.04	1.25	1.38
1	B	447	TYR	CA-C	-5.74	1.45	1.52
1	A	448	MET	SD-CE	-5.73	1.65	1.79
1	B	311	TYR	CZ-OH	-5.71	1.26	1.38
1	B	447	TYR	CB-CG	-5.66	1.39	1.51
1	C	447	TYR	CB-CG	-5.38	1.39	1.51
1	B	314	PHE	CG-CD1	-5.34	1.27	1.38
1	A	448	MET	CA-C	-5.27	1.46	1.52
1	B	310	LEU	CA-CB	-5.25	1.45	1.53
1	B	308	GLN	C-N	-5.22	1.27	1.33
1	A	366	ASN	C-N	-5.18	1.26	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	313	PHE	CA-CB	-5.13	1.44	1.53

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	367	CYS	O-C-N	-37.88	81.96	122.12
1	B	367	CYS	O-C-N	-37.68	82.18	122.12
1	A	311	TYR	CA-C-O	-10.13	109.81	120.55
1	A	366	ASN	O-C-N	-9.75	108.56	122.41
1	A	366	ASN	CA-C-N	8.96	137.53	122.65
1	A	366	ASN	C-N-CA	8.96	137.53	122.65
1	C	311	TYR	CA-C-O	-8.31	111.74	120.55
1	C	40	ILE	N-CA-C	8.11	126.21	109.34
1	B	40	ILE	N-CA-C	8.07	126.13	109.34
1	A	40	ILE	N-CA-C	8.05	126.09	109.34
1	B	309	ILE	N-CA-C	7.78	118.57	110.72
1	B	446	HIS	O-C-N	-6.70	113.68	122.59
1	A	356	ARG	N-CA-C	-6.68	103.99	111.28
1	B	356	ARG	N-CA-C	-6.67	104.01	111.28
1	C	356	ARG	N-CA-C	-6.66	104.02	111.28
1	B	404	VAL	N-CA-C	-6.31	98.65	107.80
1	A	404	VAL	N-CA-C	-6.26	98.72	107.80
1	C	446	HIS	O-C-N	-6.19	114.36	122.59
1	C	404	VAL	N-CA-C	-6.17	98.86	107.80
1	A	311	TYR	CA-C-N	6.09	128.44	120.28
1	A	311	TYR	C-N-CA	6.09	128.44	120.28
1	B	311	TYR	CA-C-O	-6.07	113.99	120.42
1	C	405	GLU	N-CA-C	5.98	123.53	110.80
1	A	405	GLU	N-CA-C	5.97	123.51	110.80
1	B	405	GLU	N-CA-C	5.94	123.45	110.80
1	B	311	TYR	CA-C-N	5.92	128.70	120.29
1	B	311	TYR	C-N-CA	5.92	128.70	120.29
1	C	447	TYR	CB-CA-C	-5.83	100.81	110.14
1	A	37	TRP	N-CA-C	5.29	117.95	110.50
1	C	37	TRP	N-CA-C	5.24	117.89	110.50
1	B	37	TRP	N-CA-C	5.24	117.88	110.50
1	C	448	MET	CB-CG-SD	5.20	128.31	112.70
1	A	446	HIS	O-C-N	-5.13	115.77	122.59
1	C	40	ILE	CB-CA-C	-5.08	102.95	111.29
1	A	40	ILE	CB-CA-C	-5.07	102.97	111.29
1	A	186	ARG	N-CA-C	-5.06	105.66	111.07
1	B	40	ILE	CB-CA-C	-5.05	103.01	111.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	186	ARG	N-CA-C	-5.03	105.68	111.07

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	197	CYS	Peptide
1	A	469	PHE	Peptide
1	B	197	CYS	Peptide
1	B	367	CYS	Mainchain
1	B	447	TYR	Sidechain
1	B	469	PHE	Peptide
1	C	197	CYS	Peptide
1	C	311	TYR	Mainchain
1	C	367	CYS	Mainchain
1	C	469	PHE	Peptide
1	D	701	UNK	Peptide
1	E	701	UNK	Peptide
1	F	702	UNK	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	4393	0	4391	176	0
1	B	4393	0	4391	178	0
1	C	4393	0	4391	178	0
1	D	180	0	39	8	0
1	E	180	0	39	9	0
1	F	175	0	37	10	0
2	A	138	0	176	30	0
2	B	138	0	176	27	0
2	C	138	0	176	29	0
All	All	14128	0	13816	605	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 22.

All (605) 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:40:ILE:HD11	1:A:196:ILE:CD1	1.35	1.56
1:B:40:ILE:HD11	1:B:196:ILE:CD1	1.35	1.55
1:C:40:ILE:HD11	1:C:196:ILE:CD1	1.35	1.51
1:A:40:ILE:CD1	1:A:196:ILE:HD11	1.53	1.38
1:B:40:ILE:CD1	1:B:196:ILE:HD11	1.53	1.37
1:C:40:ILE:CD1	1:C:196:ILE:HD11	1.53	1.34
1:A:404:VAL:CG1	1:A:407:VAL:HG23	1.56	1.34
1:B:404:VAL:CG1	1:B:407:VAL:HG23	1.56	1.33
1:C:404:VAL:CG1	1:C:407:VAL:HG23	1.56	1.33
1:B:404:VAL:CG1	1:B:407:VAL:CG2	2.07	1.33
1:A:404:VAL:CG1	1:A:407:VAL:CG2	2.07	1.32
1:C:404:VAL:CG1	1:C:407:VAL:CG2	2.07	1.32
1:C:40:ILE:HD11	1:C:196:ILE:CG1	1.63	1.28
1:B:40:ILE:HD11	1:B:196:ILE:CG1	1.63	1.27
1:A:40:ILE:HD11	1:A:196:ILE:CG1	1.63	1.26
1:B:40:ILE:CD1	1:B:196:ILE:CD1	2.16	1.17
1:A:40:ILE:CD1	1:A:196:ILE:CD1	2.17	1.16
1:C:40:ILE:CD1	1:C:196:ILE:CD1	2.17	1.15
1:A:40:ILE:CG1	1:A:196:ILE:HD11	1.79	1.12
1:C:40:ILE:CG1	1:C:196:ILE:HD11	1.79	1.12
1:B:40:ILE:CG1	1:B:196:ILE:HD11	1.79	1.11
1:C:356:ARG:HD3	1:F:703:UNK:O	1.48	1.11
1:A:404:VAL:HG11	1:A:407:VAL:HG21	1.32	1.10
1:B:404:VAL:HG11	1:B:407:VAL:CG2	1.82	1.10
1:C:404:VAL:HG11	1:C:407:VAL:HG21	1.32	1.08
1:A:245:ARG:HD3	1:A:334:LEU:CD1	1.84	1.07
1:C:245:ARG:HD3	1:C:334:LEU:CD1	1.84	1.06
1:B:404:VAL:HG11	1:B:407:VAL:HG21	1.31	1.06
1:B:245:ARG:HD3	1:B:334:LEU:CD1	1.84	1.06
1:A:497:ARG:HH11	1:A:497:ARG:HG2	1.21	1.06
1:B:497:ARG:HG2	1:B:497:ARG:HH11	1.21	1.04
1:C:404:VAL:HG12	1:C:407:VAL:CG2	1.85	1.04
1:C:497:ARG:HG2	1:C:497:ARG:HH11	1.21	1.03
1:C:404:VAL:HG11	1:C:407:VAL:CG2	1.82	1.02
1:A:404:VAL:HG12	1:A:407:VAL:CG2	1.85	1.02
1:E:697:UNK:O	1:E:701:UNK:O	1.77	1.02
1:B:404:VAL:HG12	1:B:407:VAL:CG2	1.85	1.02
1:C:404:VAL:HG13	1:C:407:VAL:HG23	1.41	1.01
1:A:404:VAL:HG11	1:A:407:VAL:CG2	1.82	1.01
1:A:404:VAL:HG13	1:A:407:VAL:HG23	1.41	1.01

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:ILE:HD11	1:B:196:ILE:HD11	1.03	0.97
1:B:404:VAL:HG13	1:B:407:VAL:HG23	1.41	0.97
1:C:40:ILE:HD11	1:C:196:ILE:HD11	1.03	0.96
1:C:340:LEU:HD22	1:C:445:ILE:CG2	1.97	0.94
1:F:704:UNK:O	1:F:705:UNK:C	2.12	0.94
1:A:40:ILE:HD11	1:A:196:ILE:HG13	1.48	0.94
1:B:340:LEU:HD22	1:B:445:ILE:CG2	1.99	0.92
1:C:54:HIS:HD2	1:C:183:VAL:HG21	1.35	0.92
1:B:40:ILE:HD11	1:B:196:ILE:HG13	1.49	0.92
1:A:340:LEU:HD22	1:A:445:ILE:CG2	1.98	0.91
1:A:40:ILE:HD11	1:A:196:ILE:HD11	1.03	0.91
1:A:404:VAL:CG1	1:A:407:VAL:HG21	1.88	0.91
1:A:446:HIS:HD2	1:E:713:UNK:CB	1.83	0.91
1:C:40:ILE:HD11	1:C:196:ILE:HG13	1.49	0.91
1:B:54:HIS:HD2	1:B:183:VAL:HG21	1.35	0.90
1:B:404:VAL:CG1	1:B:407:VAL:HG21	1.88	0.90
1:A:54:HIS:HD2	1:A:183:VAL:HG21	1.35	0.89
1:B:446:HIS:HD2	1:D:713:UNK:CB	1.85	0.89
1:C:39:HIS:NE2	1:C:198:ILE:O	2.06	0.89
1:C:446:HIS:HD2	1:F:712:UNK:CB	1.86	0.89
1:B:39:HIS:NE2	1:B:198:ILE:O	2.06	0.88
1:A:39:HIS:NE2	1:A:198:ILE:O	2.06	0.88
1:B:120:GLN:O	1:B:120:GLN:NE2	2.08	0.87
1:C:120:GLN:O	1:C:120:GLN:NE2	2.08	0.87
1:A:120:GLN:O	1:A:120:GLN:NE2	2.08	0.87
1:C:404:VAL:CG1	1:C:407:VAL:HG21	1.88	0.86
2:B:801:LMN:HCL	2:B:801:LMN:H1	1.57	0.86
2:C:801:LMN:HCL	2:C:801:LMN:H1	1.57	0.86
2:A:801:LMN:HCL	2:A:801:LMN:H1	1.57	0.86
1:D:705:UNK:O	1:D:706:UNK:C	2.23	0.86
1:C:356:ARG:HD3	1:F:703:UNK:C	2.06	0.84
1:A:77:VAL:O	1:A:81:THR:CG2	2.25	0.84
1:B:77:VAL:O	1:B:81:THR:CG2	2.25	0.84
1:C:77:VAL:O	1:C:81:THR:HG23	1.76	0.84
1:A:77:VAL:O	1:A:81:THR:HG23	1.76	0.84
1:C:77:VAL:O	1:C:81:THR:CG2	2.25	0.83
1:B:40:ILE:CG1	1:B:196:ILE:CD1	2.53	0.83
1:C:40:ILE:HD13	1:C:43:LEU:CD1	2.08	0.83
1:A:40:ILE:HD13	1:A:43:LEU:CD1	2.08	0.83
1:C:40:ILE:CG1	1:C:196:ILE:CD1	2.53	0.83
1:C:356:ARG:CD	1:F:703:UNK:O	2.26	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:ARG:HG2	1:A:497:ARG:NH1	1.92	0.83
1:C:361:ALA:HA	1:C:441:ILE:HD11	1.59	0.83
1:B:77:VAL:O	1:B:81:THR:HG23	1.77	0.83
1:B:40:ILE:HD13	1:B:43:LEU:CD1	2.08	0.83
1:B:448:MET:HG2	1:B:452:TRP:CE3	2.13	0.83
1:E:705:UNK:O	1:E:706:UNK:C	2.23	0.83
1:C:245:ARG:HD3	1:C:334:LEU:HD11	1.61	0.82
1:B:52:ASN:ND2	1:B:62:MET:CE	2.42	0.82
1:C:52:ASN:ND2	1:C:62:MET:CE	2.42	0.82
1:A:52:ASN:ND2	1:A:62:MET:CE	2.43	0.82
1:A:40:ILE:CG1	1:A:196:ILE:CD1	2.53	0.82
1:B:245:ARG:HD3	1:B:334:LEU:HD11	1.61	0.81
1:A:361:ALA:HA	1:A:441:ILE:HD11	1.61	0.81
1:B:356:ARG:HD3	1:D:704:UNK:C	2.09	0.81
1:B:361:ALA:HA	1:B:441:ILE:HD11	1.60	0.81
1:A:245:ARG:HD3	1:A:334:LEU:HD11	1.61	0.80
2:A:801:LMN:OBY	2:A:801:LMN:H6	1.82	0.80
2:C:801:LMN:H6	2:C:801:LMN:OBY	1.82	0.79
1:C:448:MET:HG2	1:C:452:TRP:CE3	2.18	0.79
2:B:801:LMN:H6	2:B:801:LMN:OBY	1.82	0.79
1:A:40:ILE:HD13	1:A:43:LEU:HD11	1.65	0.79
1:C:40:ILE:HD13	1:C:43:LEU:HD11	1.65	0.79
1:A:446:HIS:CD2	1:E:713:UNK:CB	2.65	0.79
1:B:446:HIS:CD2	1:D:713:UNK:CB	2.66	0.78
1:B:40:ILE:HD13	1:B:43:LEU:HD11	1.65	0.78
1:C:40:ILE:HG12	1:C:196:ILE:HD11	1.66	0.77
1:A:40:ILE:HG12	1:A:196:ILE:HD11	1.66	0.77
1:C:446:HIS:CD2	1:F:712:UNK:CB	2.67	0.76
1:B:245:ARG:HD3	1:B:334:LEU:HD12	1.68	0.76
1:C:52:ASN:ND2	1:C:62:MET:HE1	2.00	0.76
1:C:497:ARG:HG2	1:C:497:ARG:NH1	1.92	0.76
1:A:52:ASN:ND2	1:A:62:MET:HE1	2.00	0.76
1:C:404:VAL:HG12	1:C:407:VAL:HG23	1.54	0.75
1:B:40:ILE:HG12	1:B:196:ILE:HD11	1.66	0.75
1:A:245:ARG:HD3	1:A:334:LEU:HD12	1.68	0.75
1:B:52:ASN:ND2	1:B:62:MET:HE1	2.00	0.75
1:C:245:ARG:CD	1:C:334:LEU:HD11	2.17	0.74
1:C:361:ALA:HA	1:C:441:ILE:CD1	2.18	0.74
1:B:497:ARG:HG2	1:B:497:ARG:NH1	1.92	0.74
1:A:245:ARG:CD	1:A:334:LEU:HD11	2.17	0.74
1:B:361:ALA:HA	1:B:441:ILE:CD1	2.18	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:802:LMN:CBQ	2:C:802:LMN:HBEA	2.19	0.73
1:B:44:ASP:CG	1:B:214:ARG:HH11	1.97	0.73
1:C:245:ARG:HD3	1:C:334:LEU:HD12	1.67	0.73
1:A:462:ARG:HG2	1:A:462:ARG:HH11	1.54	0.73
1:B:245:ARG:CD	1:B:334:LEU:HD11	2.17	0.73
2:B:802:LMN:HBK	2:B:802:LMN:CBJ	2.18	0.73
1:B:462:ARG:HG2	1:B:462:ARG:HH11	1.54	0.73
1:A:361:ALA:HA	1:A:441:ILE:CD1	2.18	0.73
2:A:802:LMN:HBK	2:A:802:LMN:CBJ	2.18	0.73
2:A:802:LMN:CBQ	2:A:802:LMN:HBEA	2.19	0.73
2:C:802:LMN:HBK	2:C:802:LMN:CBJ	2.18	0.72
2:B:802:LMN:HBEA	2:B:802:LMN:CBQ	2.19	0.72
1:B:451:HIS:NE2	1:B:464:GLU:OE2	2.22	0.72
1:A:451:HIS:NE2	1:A:464:GLU:OE2	2.22	0.72
1:A:44:ASP:CG	1:A:214:ARG:HH11	1.97	0.72
1:A:40:ILE:CD1	1:A:196:ILE:CG1	2.57	0.72
1:C:44:ASP:CG	1:C:214:ARG:HH11	1.97	0.72
1:C:462:ARG:HH11	1:C:462:ARG:HG2	1.54	0.72
1:A:394:LEU:HB3	1:A:401:VAL:HG21	1.73	0.71
1:B:388:LEU:HD11	1:B:411:VAL:HG13	1.72	0.71
1:C:394:LEU:HB3	1:C:401:VAL:HG21	1.73	0.71
2:C:801:LMN:H6	2:C:801:LMN:CCR	2.21	0.71
1:B:112:LEU:HB3	1:B:113:PRO:HD3	1.73	0.71
2:B:801:LMN:H6	2:B:801:LMN:CCR	2.21	0.71
2:A:801:LMN:H6	2:A:801:LMN:CCR	2.21	0.71
1:C:451:HIS:NE2	1:C:464:GLU:OE2	2.22	0.71
1:B:40:ILE:CD1	1:B:196:ILE:CG1	2.57	0.71
1:B:40:ILE:HG22	1:B:41:GLU:HG2	1.72	0.70
1:B:54:HIS:CD2	1:B:183:VAL:HG21	2.24	0.70
1:A:356:ARG:HD3	1:E:704:UNK:C	2.21	0.70
1:A:388:LEU:HD11	1:A:411:VAL:HG13	1.72	0.70
1:C:388:LEU:HD11	1:C:411:VAL:HG13	1.72	0.70
1:B:394:LEU:HB3	1:B:401:VAL:HG21	1.73	0.70
1:A:39:HIS:CD2	1:A:198:ILE:HA	2.27	0.70
2:C:802:LMN:HBK	2:C:802:LMN:CBL	2.22	0.70
2:B:802:LMN:HBK	2:B:802:LMN:CBL	2.22	0.69
1:C:464:GLU:HA	1:C:467:GLN:HG2	1.74	0.69
1:C:112:LEU:HB3	1:C:113:PRO:HD3	1.73	0.69
2:B:802:LMN:OAN	2:B:802:LMN:HCS	1.91	0.69
1:C:39:HIS:CD2	1:C:198:ILE:HA	2.28	0.69
1:A:112:LEU:HB3	1:A:113:PRO:HD3	1.73	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:ILE:HG22	1:C:41:GLU:HG2	1.72	0.69
1:C:40:ILE:CD1	1:C:196:ILE:CG1	2.57	0.69
2:C:802:LMN:HCS	2:C:802:LMN:OAN	1.91	0.69
1:B:464:GLU:HA	1:B:467:GLN:HG2	1.74	0.69
1:A:40:ILE:HG22	1:A:41:GLU:HG2	1.72	0.69
1:B:40:ILE:CD1	1:B:196:ILE:HG13	2.21	0.69
1:A:40:ILE:CD1	1:A:196:ILE:HG13	2.21	0.69
2:A:802:LMN:OAN	2:A:802:LMN:HCS	1.91	0.69
1:A:464:GLU:HA	1:A:467:GLN:HG2	1.74	0.68
1:C:40:ILE:CD1	1:C:196:ILE:HG13	2.21	0.68
2:A:802:LMN:HBK	2:A:802:LMN:CBL	2.22	0.68
1:B:503:ASP:O	1:B:507:ASN:ND2	2.27	0.68
1:A:340:LEU:HD22	1:A:445:ILE:HG23	1.75	0.68
2:C:802:LMN:HBL	2:C:802:LMN:CBK	2.24	0.68
1:B:39:HIS:CD2	1:B:198:ILE:HA	2.28	0.68
1:C:503:ASP:O	1:C:507:ASN:ND2	2.27	0.67
1:B:552:LYS:O	1:B:556:SER:HB2	1.94	0.67
1:A:54:HIS:CD2	1:A:183:VAL:HG21	2.24	0.67
1:C:245:ARG:CD	1:C:334:LEU:CD1	2.69	0.67
1:A:503:ASP:O	1:A:507:ASN:ND2	2.27	0.67
1:C:448:MET:HG2	1:C:452:TRP:HE3	1.58	0.67
2:A:802:LMN:CBK	2:A:802:LMN:HBL	2.24	0.67
1:A:404:VAL:HG12	1:A:407:VAL:HG23	1.54	0.67
1:A:552:LYS:O	1:A:556:SER:HB2	1.94	0.66
1:C:54:HIS:CD2	1:C:183:VAL:HG21	2.24	0.66
1:F:696:UNK:O	1:F:700:UNK:N	2.28	0.66
1:B:340:LEU:HD22	1:B:445:ILE:HG23	1.77	0.66
1:C:404:VAL:HG12	1:C:407:VAL:CB	2.26	0.66
1:C:552:LYS:O	1:C:556:SER:HB2	1.94	0.66
1:B:404:VAL:HG12	1:B:407:VAL:CB	2.26	0.66
1:B:44:ASP:OD2	1:B:214:ARG:NH1	2.26	0.65
1:A:245:ARG:CD	1:A:334:LEU:CD1	2.69	0.65
2:B:802:LMN:HBL	2:B:802:LMN:CBK	2.24	0.65
1:B:356:ARG:HD3	1:D:704:UNK:O	1.96	0.65
1:C:340:LEU:HD22	1:C:445:ILE:HG23	1.75	0.65
1:A:404:VAL:HG12	1:A:407:VAL:CB	2.26	0.65
1:C:497:ARG:HH11	1:C:497:ARG:CG	2.06	0.65
1:B:448:MET:HG2	1:B:452:TRP:HE3	1.63	0.63
2:B:802:LMN:HBK	2:B:802:LMN:HBL	1.81	0.63
2:C:802:LMN:HBEA	2:C:802:LMN:HBQA	1.81	0.62
1:A:44:ASP:OD2	1:A:214:ARG:NH1	2.26	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:802:LMN:HBK	2:C:802:LMN:HBL	1.81	0.62
2:B:802:LMN:HBEA	2:B:802:LMN:HBQA	1.81	0.62
2:A:802:LMN:HBK	2:A:802:LMN:HBL	1.81	0.62
1:E:695:UNK:O	1:E:699:UNK:N	2.32	0.62
1:D:695:UNK:O	1:D:699:UNK:N	2.32	0.61
2:B:802:LMN:OAU	2:B:802:LMN:H5	2.00	0.61
2:A:802:LMN:HBEA	2:A:802:LMN:HBQA	1.81	0.61
2:C:802:LMN:HBEA	2:C:802:LMN:HBQ	1.83	0.61
2:C:802:LMN:OAU	2:C:802:LMN:H5	2.00	0.61
1:C:44:ASP:OD2	1:C:214:ARG:NH1	2.26	0.61
2:A:802:LMN:HBPA	2:A:802:LMN:HOAR	1.65	0.61
2:A:802:LMN:OAU	2:A:802:LMN:H5	2.00	0.61
1:C:405:GLU:HB2	1:A:111:THR:HA	1.83	0.60
1:C:455:ASN:HB2	1:C:458:ARG:HG3	1.84	0.60
1:D:696:UNK:O	1:D:700:UNK:N	2.34	0.60
1:B:111:THR:HA	1:A:405:GLU:HB2	1.83	0.60
1:C:341:ARG:O	1:C:552:LYS:NZ	2.31	0.60
1:A:455:ASN:HB2	1:A:458:ARG:HG3	1.84	0.60
1:B:455:ASN:HB2	1:B:458:ARG:HG3	1.83	0.60
1:C:414:LEU:O	1:C:418:VAL:HG23	2.02	0.60
1:B:414:LEU:O	1:B:418:VAL:HG23	2.02	0.60
1:A:414:LEU:O	1:A:418:VAL:HG23	2.02	0.60
1:B:38:HIS:HA	1:B:195:GLN:O	2.02	0.60
1:A:38:HIS:HA	1:A:195:GLN:O	2.02	0.60
2:A:802:LMN:HBEA	2:A:802:LMN:HBQ	1.83	0.60
1:C:111:THR:HA	1:B:405:GLU:HB2	1.83	0.59
2:B:802:LMN:HBEA	2:B:802:LMN:HBQ	1.83	0.59
1:B:341:ARG:NH2	1:B:345:GLU:O	2.36	0.59
1:B:245:ARG:CD	1:B:334:LEU:CD1	2.69	0.59
1:C:341:ARG:NH2	1:C:345:GLU:O	2.36	0.59
1:B:40:ILE:CD1	1:B:43:LEU:HD11	2.33	0.59
1:A:341:ARG:NH2	1:A:345:GLU:O	2.36	0.59
2:C:802:LMN:OAU	2:C:802:LMN:H3	2.03	0.58
2:A:802:LMN:OCB	2:A:802:LMN:OAR	2.19	0.58
1:E:696:UNK:O	1:E:700:UNK:N	2.36	0.58
2:B:802:LMN:OAU	2:B:802:LMN:H3	2.03	0.58
1:C:38:HIS:HA	1:C:195:GLN:O	2.02	0.58
1:A:448:MET:HG2	1:A:452:TRP:CE3	2.37	0.58
1:C:40:ILE:CD1	1:C:43:LEU:HD11	2.33	0.58
1:A:369:LEU:HD13	1:A:426:PRO:HB3	1.85	0.58
2:C:802:LMN:OCB	2:C:802:LMN:OAR	2.19	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:369:LEU:HD13	1:B:426:PRO:HB3	1.85	0.58
1:B:407:VAL:O	1:B:411:VAL:HG23	2.04	0.58
2:A:802:LMN:OAU	2:A:802:LMN:H3	2.03	0.58
1:A:40:ILE:CD1	1:A:43:LEU:HD11	2.33	0.57
2:B:802:LMN:OCB	2:B:802:LMN:OAR	2.19	0.57
1:C:369:LEU:HD13	1:C:426:PRO:HB3	1.85	0.57
1:A:407:VAL:O	1:A:411:VAL:HG23	2.04	0.57
1:C:407:VAL:O	1:C:411:VAL:HG23	2.04	0.57
1:B:250:ASN:OD1	1:B:297:ASN:ND2	2.34	0.57
1:A:462:ARG:HH11	1:A:462:ARG:CG	2.17	0.57
1:C:250:ASN:OD1	1:C:297:ASN:ND2	2.34	0.56
1:C:462:ARG:HH11	1:C:462:ARG:CG	2.17	0.56
1:F:695:UNK:O	1:F:699:UNK:N	2.37	0.56
1:A:250:ASN:OD1	1:A:297:ASN:ND2	2.34	0.56
1:C:286:LEU:O	1:C:290:ILE:HG22	2.06	0.56
1:B:286:LEU:O	1:B:290:ILE:HG22	2.06	0.56
1:A:341:ARG:O	1:A:552:LYS:NZ	2.31	0.56
1:B:112:LEU:HD12	1:B:112:LEU:O	2.06	0.56
1:C:77:VAL:O	1:C:81:THR:HG22	2.04	0.56
1:A:112:LEU:HD12	1:A:112:LEU:O	2.06	0.55
1:A:286:LEU:O	1:A:290:ILE:HG22	2.06	0.55
2:B:801:LMN:CCR	2:B:801:LMN:C6	2.85	0.55
1:A:77:VAL:O	1:A:81:THR:HG22	2.04	0.55
1:A:37:TRP:HA	1:A:37:TRP:CE3	2.42	0.55
1:B:37:TRP:HA	1:B:37:TRP:CE3	2.42	0.55
2:A:801:LMN:CCR	2:A:801:LMN:C6	2.85	0.55
1:C:112:LEU:O	1:C:112:LEU:HD12	2.06	0.55
1:C:340:LEU:HD22	1:C:445:ILE:HG21	1.87	0.54
1:C:116:PHE:CD1	1:C:116:PHE:N	2.73	0.54
1:C:404:VAL:HG23	1:A:110:VAL:HG22	1.90	0.54
1:A:339:TYR:OH	1:A:550:ASP:OD2	2.21	0.54
1:C:37:TRP:CE3	1:C:37:TRP:HA	2.42	0.54
1:C:356:ARG:CD	1:F:703:UNK:C	2.81	0.54
1:B:77:VAL:O	1:B:81:THR:HG22	2.04	0.54
1:A:131:SER:O	1:A:135:ILE:HG13	2.08	0.54
1:C:291:LEU:HD12	1:C:495:ARG:CZ	2.38	0.54
1:A:365:MET:HE3	1:A:465:PHE:CD1	2.43	0.54
1:C:365:MET:HE3	1:C:465:PHE:CD1	2.43	0.53
1:C:201:ARG:NH2	1:C:207:ASP:OD2	2.42	0.53
2:B:802:LMN:OAR	2:B:802:LMN:HBPA	2.09	0.53
1:C:52:ASN:HD22	1:C:62:MET:HE1	1.73	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:801:LMN:CCR	2:C:801:LMN:C6	2.85	0.53
1:B:291:LEU:HD12	1:B:495:ARG:CZ	2.38	0.53
1:B:131:SER:O	1:B:135:ILE:HG13	2.08	0.53
1:B:201:ARG:NH2	1:B:207:ASP:OD2	2.42	0.53
1:A:404:VAL:HG12	1:A:407:VAL:HB	1.90	0.53
1:A:497:ARG:HH11	1:A:497:ARG:CG	2.06	0.53
2:C:802:LMN:OAR	2:C:802:LMN:HBPA	2.09	0.53
1:C:404:VAL:HG12	1:C:407:VAL:HB	1.90	0.53
1:B:116:PHE:CD1	1:B:116:PHE:N	2.72	0.53
1:B:52:ASN:HD22	1:B:62:MET:HE1	1.73	0.53
2:A:802:LMN:HBPA	2:A:802:LMN:OAR	2.09	0.53
1:C:131:SER:O	1:C:135:ILE:HG13	2.08	0.53
1:A:290:ILE:HG23	1:A:495:ARG:HG2	1.91	0.53
2:A:801:LMN:OAN	2:A:801:LMN:HCS	2.09	0.53
2:A:802:LMN:CBL	2:A:802:LMN:CBK	2.85	0.53
1:C:392:ILE:HA	1:C:395:THR:HG22	1.91	0.53
1:B:80:THR:HG21	1:B:310:LEU:HD13	1.90	0.53
2:B:801:LMN:OAN	2:B:801:LMN:HCS	2.09	0.53
1:C:110:VAL:HG22	1:B:404:VAL:HG23	1.90	0.52
1:C:436:GLN:NE2	1:E:701:UNK:CB	2.72	0.52
1:A:201:ARG:NH2	1:A:207:ASP:OD2	2.41	0.52
1:C:290:ILE:HG23	1:C:495:ARG:HG2	1.91	0.52
1:B:340:LEU:HD22	1:B:445:ILE:HG21	1.89	0.52
1:B:365:MET:HE3	1:B:465:PHE:CD1	2.44	0.52
1:A:291:LEU:HD12	1:A:495:ARG:CZ	2.38	0.52
1:C:254:ILE:HG12	1:C:293:ILE:HD12	1.91	0.52
2:B:802:LMN:H3	2:B:802:LMN:CCV	2.39	0.52
1:B:404:VAL:HG12	1:B:407:VAL:HB	1.90	0.52
1:C:118:PRO:HG2	1:C:121:VAL:HG23	1.92	0.52
1:A:392:ILE:HA	1:A:395:THR:HG22	1.92	0.52
1:C:111:THR:HA	1:B:405:GLU:CG	2.40	0.52
1:B:110:VAL:HG22	1:A:404:VAL:HG23	1.90	0.52
1:A:521:PHE:CE1	1:A:529:HIS:HD2	2.28	0.51
1:C:521:PHE:CE1	1:C:529:HIS:HD2	2.28	0.51
1:B:392:ILE:HA	1:B:395:THR:HG22	1.92	0.51
1:A:52:ASN:HD22	1:A:62:MET:HE1	1.73	0.51
1:A:254:ILE:HG12	1:A:293:ILE:HD12	1.91	0.51
1:B:305:LEU:O	1:B:309:ILE:HD12	2.10	0.51
1:B:290:ILE:HG23	1:B:495:ARG:HG2	1.91	0.51
2:C:801:LMN:H6	2:C:801:LMN:HBM	1.93	0.51
1:B:521:PHE:CE1	1:B:529:HIS:HD2	2.28	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:ILE:HG12	1:B:293:ILE:HD12	1.91	0.51
1:C:138:ILE:HD13	1:C:303:LEU:HD21	1.93	0.51
2:C:802:LMN:H3	2:C:802:LMN:CCV	2.39	0.51
1:A:40:ILE:CD1	1:A:43:LEU:CD1	2.86	0.51
1:A:558:MET:HE3	1:A:580:LEU:HD21	1.92	0.51
1:C:330:ARG:HB3	1:C:469:PHE:O	2.11	0.51
1:C:405:GLU:CG	1:A:111:THR:HA	2.40	0.51
1:B:111:THR:HA	1:A:405:GLU:CG	2.40	0.51
1:B:404:VAL:HG12	1:B:407:VAL:HG23	1.54	0.51
2:A:801:LMN:H6	2:A:801:LMN:HBM	1.93	0.51
1:B:330:ARG:HB3	1:B:469:PHE:O	2.11	0.50
1:A:118:PRO:HG2	1:A:121:VAL:HG23	1.92	0.50
2:C:801:LMN:OAN	2:C:801:LMN:HCS	2.09	0.50
2:B:802:LMN:CBQ	2:B:802:LMN:CBE	2.86	0.50
1:A:330:ARG:HB3	1:A:469:PHE:O	2.11	0.50
1:C:558:MET:HE3	1:C:580:LEU:HD21	1.92	0.50
1:B:138:ILE:HD13	1:B:303:LEU:HD21	1.93	0.50
1:B:462:ARG:CG	1:B:462:ARG:NH1	2.73	0.50
1:A:116:PHE:N	1:A:116:PHE:CD1	2.73	0.50
1:A:217:ASN:ND2	1:A:343:PHE:O	2.44	0.50
1:A:138:ILE:HD13	1:A:303:LEU:HD21	1.93	0.50
1:A:340:LEU:HD22	1:A:445:ILE:HG21	1.89	0.50
1:B:217:ASN:ND2	1:B:343:PHE:O	2.44	0.50
2:A:802:LMN:H3	2:A:802:LMN:CCV	2.39	0.50
1:C:217:ASN:ND2	1:C:343:PHE:O	2.44	0.50
2:C:802:LMN:CBQ	2:C:802:LMN:CBE	2.86	0.50
1:B:118:PRO:HG2	1:B:121:VAL:HG23	1.92	0.50
1:C:361:ALA:CA	1:C:441:ILE:HD11	2.38	0.50
1:B:360:PRO:HB2	1:B:441:ILE:HG12	1.94	0.50
2:A:801:LMN:H6	2:A:801:LMN:HCR	1.94	0.50
2:C:802:LMN:HBQA	2:C:802:LMN:CBE	2.40	0.49
1:A:552:LYS:O	1:A:556:SER:CB	2.60	0.49
1:C:552:LYS:O	1:C:556:SER:CB	2.60	0.49
1:B:356:ARG:CD	1:D:704:UNK:C	2.89	0.49
1:A:52:ASN:ND2	1:A:62:MET:HE2	2.25	0.49
2:C:802:LMN:CBL	2:C:802:LMN:CBK	2.85	0.49
1:B:462:ARG:HH11	1:B:462:ARG:CG	2.17	0.49
2:B:801:LMN:H6	2:B:801:LMN:HBM	1.93	0.49
2:C:801:LMN:H6	2:C:801:LMN:HCR	1.94	0.49
1:A:460:GLN:O	1:A:464:GLU:HG2	2.13	0.49
1:A:37:TRP:HA	1:A:37:TRP:HE3	1.78	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:355:ASN:CB	1:B:429:HIS:HA	2.43	0.49
1:B:558:MET:HE3	1:B:580:LEU:HD21	1.93	0.48
2:B:802:LMN:HBQA	2:B:802:LMN:CBE	2.40	0.48
1:A:462:ARG:CG	1:A:462:ARG:NH1	2.73	0.48
1:C:40:ILE:CD1	1:C:43:LEU:CD1	2.87	0.48
1:A:360:PRO:HB2	1:A:441:ILE:HG12	1.96	0.48
1:C:37:TRP:HA	1:C:37:TRP:HE3	1.78	0.48
1:C:460:GLN:O	1:C:464:GLU:HG2	2.13	0.48
1:B:552:LYS:O	1:B:556:SER:CB	2.60	0.48
2:B:801:LMN:H6	2:B:801:LMN:HCR	1.94	0.48
1:C:429:HIS:HA	1:A:355:ASN:CB	2.43	0.48
1:A:361:ALA:CA	1:A:441:ILE:HD11	2.40	0.48
1:B:112:LEU:HD12	1:B:112:LEU:C	2.39	0.48
2:C:802:LMN:HBPA	2:C:802:LMN:HOAR	1.79	0.48
1:B:355:ASN:CB	1:A:429:HIS:HA	2.43	0.48
1:A:40:ILE:HG13	1:A:196:ILE:CD1	2.44	0.48
1:B:341:ARG:O	1:B:552:LYS:NZ	2.31	0.48
1:B:460:GLN:O	1:B:464:GLU:HG2	2.12	0.48
1:C:52:ASN:ND2	1:C:62:MET:HE2	2.25	0.47
1:C:239:GLU:O	1:C:239:GLU:HG3	2.15	0.47
1:C:357:GLY:HA2	1:C:444:HIS:ND1	2.29	0.47
1:B:54:HIS:C	1:B:54:HIS:ND1	2.73	0.47
1:B:208:ILE:O	1:B:212:ILE:HG13	2.15	0.47
1:A:54:HIS:ND1	1:A:54:HIS:C	2.73	0.47
1:A:364:TYR:OH	1:A:456:ALA:O	2.26	0.47
1:A:272:GLU:HG3	1:A:282:LEU:HD21	1.97	0.47
1:C:199:HIS:O	1:C:199:HIS:ND1	2.48	0.47
1:B:412:THR:O	1:B:416:VAL:HG23	2.15	0.47
2:A:802:LMN:HBL	2:A:802:LMN:HBQA	1.75	0.47
1:C:360:PRO:HB2	1:C:441:ILE:HG12	1.96	0.47
1:A:199:HIS:O	1:A:199:HIS:ND1	2.48	0.47
1:C:54:HIS:ND1	1:C:54:HIS:C	2.72	0.47
1:C:272:GLU:HG3	1:C:282:LEU:HD21	1.97	0.47
1:B:37:TRP:HA	1:B:37:TRP:HE3	1.78	0.47
1:B:52:ASN:ND2	1:B:62:MET:HE2	2.25	0.47
1:B:344:ASN:HB2	1:B:524:MET:HE1	1.97	0.47
2:B:802:LMN:HBPA	2:B:802:LMN:HOAR	1.79	0.47
1:A:357:GLY:HA2	1:A:444:HIS:ND1	2.30	0.47
1:A:524:MET:HB3	1:A:557:LEU:HB2	1.97	0.47
1:C:245:ARG:HD2	1:C:245:ARG:HA	1.50	0.47
1:B:524:MET:HB3	1:B:557:LEU:HB2	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:801:LMN:HBLA	2:B:801:LMN:HBQ	1.76	0.47
1:A:112:LEU:HD12	1:A:112:LEU:C	2.39	0.47
1:A:122:CYS:O	1:A:126:ILE:HG22	2.15	0.47
1:C:472:LYS:O	1:C:476:ILE:HG23	2.15	0.47
1:B:539:GLN:OE1	1:B:539:GLN:N	2.48	0.47
1:A:239:GLU:O	1:A:239:GLU:HG3	2.15	0.47
1:C:112:LEU:HD12	1:C:112:LEU:C	2.38	0.47
1:A:412:THR:O	1:A:416:VAL:HG23	2.15	0.47
1:C:539:GLN:N	1:C:539:GLN:OE1	2.48	0.46
1:B:179:THR:O	1:B:182:GLU:N	2.48	0.46
1:B:199:HIS:O	1:B:199:HIS:ND1	2.48	0.46
1:B:239:GLU:HG3	1:B:239:GLU:O	2.14	0.46
1:A:311:TYR:CD1	1:A:311:TYR:C	2.93	0.46
1:C:52:ASN:HD22	1:C:62:MET:CE	2.25	0.46
1:C:201:ARG:HH21	1:C:204:THR:HG23	1.81	0.46
1:F:704:UNK:O	1:F:706:UNK:N	2.47	0.46
1:B:122:CYS:O	1:B:126:ILE:HG22	2.16	0.46
1:A:208:ILE:O	1:A:212:ILE:HG13	2.15	0.46
2:A:802:LMN:CBQ	2:A:802:LMN:CBE	2.86	0.46
1:C:56:LYS:O	1:C:58:GLY:N	2.49	0.46
1:B:56:LYS:O	1:B:58:GLY:N	2.48	0.46
1:B:245:ARG:HD2	1:B:245:ARG:HA	1.50	0.46
1:C:344:ASN:HB2	1:C:524:MET:HE1	1.97	0.46
1:C:412:THR:O	1:C:416:VAL:HG23	2.15	0.46
1:B:344:ASN:HB2	1:B:524:MET:CE	2.46	0.46
1:A:118:PRO:HG2	1:A:121:VAL:CG2	2.46	0.46
1:C:388:LEU:HD23	1:A:318:GLU:OE1	2.15	0.46
1:B:313:PHE:O	1:B:313:PHE:CG	2.69	0.46
1:C:39:HIS:CG	1:C:198:ILE:HG23	2.51	0.46
1:C:76:VAL:O	1:C:80:THR:OG1	2.26	0.46
1:C:118:PRO:HG2	1:C:121:VAL:CG2	2.46	0.46
1:C:208:ILE:O	1:C:212:ILE:HG13	2.15	0.46
1:B:357:GLY:HA2	1:B:444:HIS:ND1	2.31	0.46
1:B:472:LYS:O	1:B:476:ILE:HG23	2.15	0.46
1:A:420:VAL:O	1:A:423:SER:OG	2.29	0.46
1:A:539:GLN:N	1:A:539:GLN:OE1	2.48	0.46
1:B:195:GLN:NE2	1:B:196:ILE:O	2.49	0.46
1:B:318:GLU:OE1	1:A:388:LEU:HD23	2.15	0.46
1:B:497:ARG:HH11	1:B:497:ARG:CG	2.06	0.46
1:A:344:ASN:HB2	1:A:524:MET:HE1	1.97	0.46
1:C:40:ILE:HG13	1:C:196:ILE:CD1	2.44	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:318:GLU:OE1	1:B:388:LEU:HD23	2.15	0.46
1:A:43:LEU:HD12	1:A:43:LEU:HA	1.72	0.46
1:C:179:THR:O	1:C:182:GLU:N	2.48	0.46
1:C:330:ARG:HB2	1:C:469:PHE:CE2	2.51	0.46
1:A:330:ARG:HB2	1:A:469:PHE:CE2	2.51	0.46
1:C:122:CYS:O	1:C:126:ILE:HG22	2.16	0.45
1:C:524:MET:HB3	1:C:557:LEU:HB2	1.97	0.45
1:B:118:PRO:HG2	1:B:121:VAL:CG2	2.46	0.45
1:B:201:ARG:HH21	1:B:204:THR:HG23	1.81	0.45
1:B:330:ARG:HB2	1:B:469:PHE:CE2	2.51	0.45
1:B:361:ALA:CA	1:B:441:ILE:HD11	2.39	0.45
1:C:462:ARG:CG	1:C:462:ARG:NH1	2.73	0.45
1:B:272:GLU:HG3	1:B:282:LEU:HD21	1.97	0.45
1:A:39:HIS:CG	1:A:198:ILE:HG23	2.51	0.45
1:A:179:THR:O	1:A:182:GLU:N	2.49	0.45
1:A:195:GLN:NE2	1:A:196:ILE:O	2.49	0.45
1:C:111:THR:HA	1:B:405:GLU:CB	2.47	0.45
1:C:195:GLN:NE2	1:C:196:ILE:O	2.49	0.45
1:C:420:VAL:O	1:C:423:SER:OG	2.28	0.45
1:A:56:LYS:O	1:A:58:GLY:N	2.48	0.45
2:A:801:LMN:HBLA	2:A:801:LMN:HBQ	1.76	0.45
2:A:802:LMN:HBQA	2:A:802:LMN:CBE	2.40	0.45
1:A:311:TYR:O	1:A:311:TYR:CG	2.69	0.45
1:C:43:LEU:HD12	1:C:43:LEU:HA	1.72	0.45
1:C:340:LEU:O	1:C:353:ARG:NH2	2.43	0.45
1:A:472:LYS:O	1:A:476:ILE:HG23	2.15	0.45
1:C:452:TRP:CZ2	1:C:464:GLU:HG3	2.51	0.45
1:B:301:CYS:HB3	1:B:302:PRO:HD3	1.99	0.45
1:A:201:ARG:HH21	1:A:204:THR:HG23	1.81	0.45
2:C:801:LMN:C6	2:C:801:LMN:HCR	2.47	0.45
1:C:311:TYR:O	1:C:311:TYR:CG	2.70	0.45
1:C:398:ASP:O	1:C:399:GLU:HG2	2.17	0.45
1:C:493:CYS:O	1:C:497:ARG:HD2	2.17	0.45
1:B:311:TYR:CD2	1:B:311:TYR:C	2.92	0.45
1:B:363:LYS:HE2	1:B:437:LEU:HD21	1.99	0.45
1:B:453:GLN:HE21	1:B:453:GLN:HA	1.82	0.45
1:A:356:ARG:HD2	1:E:704:UNK:HA	1.99	0.45
1:A:452:TRP:CZ2	1:A:464:GLU:HG3	2.52	0.45
1:B:39:HIS:CG	1:B:198:ILE:HG23	2.51	0.45
1:B:398:ASP:O	1:B:399:GLU:HG2	2.17	0.45
1:A:344:ASN:HB2	1:A:524:MET:CE	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:CYS:O	1:A:497:ARG:HD2	2.17	0.45
1:B:452:TRP:CZ2	1:B:464:GLU:HG3	2.51	0.45
1:A:398:ASP:O	1:A:399:GLU:HG2	2.17	0.45
1:A:301:CYS:HB3	1:A:302:PRO:HD3	1.99	0.44
1:C:344:ASN:HB2	1:C:524:MET:CE	2.46	0.44
1:B:406:HIS:O	1:B:410:THR:OG1	2.23	0.44
1:A:486:THR:O	1:A:490:LEU:HB2	2.18	0.44
2:A:801:LMN:C6	2:A:801:LMN:HCR	2.47	0.44
1:A:264:LEU:HD23	1:A:270:LYS:HA	1.99	0.44
1:A:311:TYR:CD1	1:A:311:TYR:O	2.70	0.44
1:B:186:ARG:HD2	1:B:186:ARG:HA	1.55	0.44
1:C:264:LEU:HD23	1:C:270:LYS:HA	1.99	0.44
1:C:486:THR:O	1:C:490:LEU:HB2	2.18	0.44
1:B:52:ASN:HD22	1:B:62:MET:CE	2.25	0.44
1:B:111:THR:HA	1:A:405:GLU:CB	2.47	0.44
1:C:210:HIS:HB3	1:C:515:VAL:HG11	2.00	0.44
1:C:363:LYS:HE2	1:C:437:LEU:HD21	1.99	0.44
1:A:186:ARG:HA	1:A:186:ARG:HD2	1.55	0.44
1:C:453:GLN:HE21	1:C:453:GLN:HA	1.82	0.44
1:C:462:ARG:HG2	1:C:462:ARG:NH1	2.28	0.44
1:B:40:ILE:CD1	1:B:43:LEU:CD1	2.87	0.44
1:B:493:CYS:O	1:B:497:ARG:HD2	2.16	0.44
1:C:301:CYS:HB3	1:C:302:PRO:HD3	1.99	0.43
1:A:210:HIS:HB3	1:A:515:VAL:HG11	2.00	0.43
1:C:311:TYR:CD2	1:C:311:TYR:C	2.96	0.43
2:C:802:LMN:HAZA	2:C:802:LMN:HBFA	1.74	0.43
1:B:340:LEU:O	1:B:353:ARG:NH2	2.43	0.43
1:B:408:LEU:HD12	1:B:408:LEU:HA	1.84	0.43
1:B:558:MET:O	1:B:562:ILE:HG12	2.19	0.43
1:C:311:TYR:O	1:C:311:TYR:CD2	2.71	0.43
1:C:405:GLU:CB	1:A:111:THR:HA	2.47	0.43
1:B:486:THR:O	1:B:490:LEU:HB2	2.18	0.43
1:B:264:LEU:HD23	1:B:270:LYS:HA	2.00	0.43
1:B:355:ASN:HB3	1:A:429:HIS:HA	2.01	0.43
2:C:802:LMN:HBK	2:C:802:LMN:HBJA	2.00	0.43
1:C:429:HIS:HA	1:A:355:ASN:HB3	2.01	0.43
2:B:801:LMN:C6	2:B:801:LMN:HCR	2.47	0.43
2:A:802:LMN:HBK	2:A:802:LMN:HBJA	2.00	0.43
1:C:355:ASN:HB3	1:B:429:HIS:HA	2.01	0.43
1:C:577:LEU:O	1:C:581:LYS:HD3	2.19	0.43
1:A:36:PRO:HA	1:A:163:PHE:HD1	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:558:MET:O	1:A:562:ILE:HG12	2.19	0.42
1:C:558:MET:O	1:C:562:ILE:HG12	2.19	0.42
1:A:54:HIS:C	1:A:54:HIS:HD1	2.27	0.42
1:C:459:SER:O	1:C:463:ASP:HB2	2.20	0.42
1:B:210:HIS:HB3	1:B:515:VAL:HG11	2.00	0.42
1:B:459:SER:O	1:B:463:ASP:HB2	2.20	0.42
1:A:459:SER:O	1:A:463:ASP:HB2	2.20	0.42
1:C:445:ILE:HD13	1:C:445:ILE:HA	1.82	0.42
1:B:36:PRO:HA	1:B:163:PHE:HD1	1.85	0.42
1:B:40:ILE:HG13	1:B:196:ILE:CD1	2.44	0.42
1:B:339:TYR:OH	1:B:550:ASP:OD2	2.21	0.42
1:B:568:GLN:HA	1:B:569:PRO:HD3	1.90	0.42
1:B:485:VAL:O	1:B:489:ILE:HG22	2.20	0.42
1:A:453:GLN:HE21	1:A:453:GLN:HA	1.82	0.42
1:B:321:LYS:HG2	1:A:392:ILE:HD13	2.01	0.42
1:B:577:LEU:O	1:B:581:LYS:HD3	2.19	0.42
1:C:54:HIS:ND1	1:C:54:HIS:O	2.53	0.42
1:C:281:GLU:HG3	1:C:282:LEU:N	2.35	0.42
1:B:228:LEU:O	1:B:230:LEU:HG	2.20	0.42
1:A:203:LEU:HD23	1:A:203:LEU:HA	1.91	0.42
1:A:363:LYS:HE2	1:A:437:LEU:HD21	2.01	0.42
1:C:36:PRO:HA	1:C:163:PHE:HD1	1.85	0.42
2:C:801:LMN:HBLA	2:C:801:LMN:HBQ	1.77	0.42
1:C:321:LYS:HG2	1:B:392:ILE:HD13	2.02	0.42
1:B:232:PHE:CZ	1:B:489:ILE:HD12	2.55	0.42
1:B:445:ILE:HD13	1:B:445:ILE:HA	1.83	0.42
1:A:408:LEU:HD12	1:A:408:LEU:HA	1.84	0.42
1:A:577:LEU:O	1:A:581:LYS:HD3	2.20	0.42
1:C:228:LEU:O	1:C:230:LEU:HG	2.20	0.42
2:B:802:LMN:HAZA	2:B:802:LMN:HBFA	1.73	0.42
2:A:802:LMN:HBB	2:A:802:LMN:HABB	1.84	0.42
1:B:54:HIS:ND1	1:B:54:HIS:O	2.53	0.41
1:A:228:LEU:O	1:A:230:LEU:HG	2.20	0.41
1:C:485:VAL:O	1:C:489:ILE:HG22	2.19	0.41
1:A:281:GLU:HG3	1:A:282:LEU:N	2.35	0.41
1:C:364:TYR:N	1:C:437:LEU:HD13	2.36	0.41
1:A:52:ASN:HD22	1:A:62:MET:CE	2.26	0.41
1:A:54:HIS:ND1	1:A:54:HIS:O	2.53	0.41
1:A:406:HIS:O	1:A:410:THR:OG1	2.23	0.41
1:B:191:GLN:HG2	1:B:196:ILE:HG22	2.03	0.41
2:B:802:LMN:HBB	2:B:802:LMN:HABB	1.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:ILE:CD1	1:C:196:ILE:HD12	2.36	0.41
1:C:207:ASP:O	1:C:211:ARG:HG2	2.21	0.41
1:B:80:THR:HG21	1:B:310:LEU:CD1	2.51	0.41
1:B:281:GLU:HG3	1:B:282:LEU:N	2.35	0.41
1:B:388:LEU:HA	1:B:388:LEU:HD12	1.76	0.41
1:A:191:GLN:HG2	1:A:196:ILE:HG22	2.03	0.41
1:C:232:PHE:CZ	1:C:489:ILE:HD12	2.56	0.41
1:C:392:ILE:HD13	1:A:321:LYS:HG2	2.02	0.41
1:C:404:VAL:CG1	1:C:404:VAL:O	2.69	0.41
1:B:40:ILE:HD13	1:B:43:LEU:HD13	1.98	0.41
1:B:110:VAL:HG22	1:B:110:VAL:O	2.21	0.41
1:B:204:THR:C	1:B:206:LEU:H	2.29	0.41
1:A:462:ARG:HG2	1:A:462:ARG:NH1	2.27	0.41
1:A:485:VAL:O	1:A:489:ILE:HG22	2.20	0.41
2:A:802:LMN:HAZA	2:A:802:LMN:HBFA	1.74	0.41
1:B:450:ASP:OD1	1:B:450:ASP:N	2.49	0.41
1:C:450:ASP:N	1:C:450:ASP:OD1	2.49	0.40
1:C:110:VAL:HG22	1:C:110:VAL:O	2.21	0.40
1:C:186:ARG:HA	1:C:186:ARG:HD2	1.55	0.40
1:C:568:GLN:HA	1:C:569:PRO:HD3	1.90	0.40
2:C:802:LMN:OCB	2:C:802:LMN:CCO	2.69	0.40
1:A:201:ARG:HG2	1:A:202:GLU:H	1.87	0.40
1:A:232:PHE:CZ	1:A:489:ILE:HD12	2.55	0.40
1:B:420:VAL:O	1:B:423:SER:OG	2.28	0.40
1:A:207:ASP:O	1:A:211:ARG:HG2	2.21	0.40
1:C:404:VAL:O	1:C:406:HIS:N	2.55	0.40
1:B:207:ASP:O	1:B:211:ARG:HG2	2.21	0.40
1:A:110:VAL:HG22	1:A:110:VAL:O	2.21	0.40
1:A:368:PHE:HZ	1:A:457:HIS:HA	1.86	0.40
1:A:404:VAL:O	1:A:406:HIS:N	2.55	0.40
1:A:450:ASP:OD1	1:A:450:ASP:N	2.49	0.40
1:A:452:TRP:HZ2	1:A:464:GLU:HG3	1.86	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	530/724 (73%)	480 (91%)	44 (8%)	6 (1%)	12	37
1	B	530/724 (73%)	478 (90%)	46 (9%)	6 (1%)	12	37
1	C	530/724 (73%)	478 (90%)	46 (9%)	6 (1%)	12	37
All	All	1590/2172 (73%)	1436 (90%)	136 (9%)	18 (1%)	15	37

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	40	ILE
1	C	405	GLU
1	B	40	ILE
1	B	405	GLU
1	A	40	ILE
1	A	405	GLU
1	C	180	TRP
1	B	180	TRP
1	A	180	TRP
1	C	41	GLU
1	C	198	ILE
1	C	470	GLN
1	B	41	GLU
1	B	198	ILE
1	B	470	GLN
1	A	41	GLU
1	A	198	ILE
1	A	470	GLN

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	473/595 (80%)	453 (96%)	20 (4%)	25	58
1	B	473/595 (80%)	452 (96%)	21 (4%)	24	56
1	C	473/595 (80%)	452 (96%)	21 (4%)	24	56
All	All	1419/1785 (80%)	1357 (96%)	62 (4%)	26	56

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	40	ILE
1	C	43	LEU
1	C	45	LEU
1	C	53	LEU
1	C	60	THR
1	C	61	CYS
1	C	64	ILE
1	C	81	THR
1	C	90	ASP
1	C	110	VAL
1	C	112	LEU
1	C	186	ARG
1	C	245	ARG
1	C	354	LEU
1	C	356	ARG
1	C	448	MET
1	C	453	GLN
1	C	462	ARG
1	C	474	VAL
1	C	476	ILE
1	C	497	ARG
1	B	40	ILE
1	B	43	LEU
1	B	45	LEU
1	B	53	LEU
1	B	60	THR
1	B	61	CYS
1	B	64	ILE
1	B	81	THR
1	B	90	ASP
1	B	110	VAL
1	B	112	LEU
1	B	186	ARG
1	B	245	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	354	LEU
1	B	356	ARG
1	B	448	MET
1	B	453	GLN
1	B	462	ARG
1	B	474	VAL
1	B	476	ILE
1	B	497	ARG
1	A	40	ILE
1	A	43	LEU
1	A	45	LEU
1	A	53	LEU
1	A	60	THR
1	A	61	CYS
1	A	64	ILE
1	A	81	THR
1	A	90	ASP
1	A	110	VAL
1	A	112	LEU
1	A	186	ARG
1	A	245	ARG
1	A	354	LEU
1	A	356	ARG
1	A	453	GLN
1	A	462	ARG
1	A	474	VAL
1	A	476	ILE
1	A	497	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	54	HIS
1	C	55	GLN
1	C	57	ASN
1	C	189	GLN
1	C	217	ASN
1	C	308	GLN
1	C	342	HIS
1	C	366	ASN
1	C	379	ASN
1	C	428	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	436	GLN
1	C	446	HIS
1	C	453	GLN
1	C	457	HIS
1	C	529	HIS
1	C	559	HIS
1	C	564	ASN
1	B	54	HIS
1	B	55	GLN
1	B	57	ASN
1	B	189	GLN
1	B	217	ASN
1	B	308	GLN
1	B	342	HIS
1	B	366	ASN
1	B	379	ASN
1	B	428	GLN
1	B	446	HIS
1	B	453	GLN
1	B	457	HIS
1	B	529	HIS
1	B	559	HIS
1	B	564	ASN
1	A	54	HIS
1	A	57	ASN
1	A	72	GLN
1	A	189	GLN
1	A	217	ASN
1	A	308	GLN
1	A	342	HIS
1	A	366	ASN
1	A	379	ASN
1	A	428	GLN
1	A	446	HIS
1	A	453	GLN
1	A	457	HIS
1	A	529	HIS
1	A	559	HIS
1	A	564	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	LMN	B	802	-	72,72,72	1.64	9 (12%)	92,98,98	1.45	11 (11%)
2	LMN	B	801	-	72,72,72	1.60	11 (15%)	92,98,98	1.45	12 (13%)
2	LMN	A	802	-	72,72,72	1.65	10 (13%)	92,98,98	1.45	10 (10%)
2	LMN	C	802	-	72,72,72	1.64	8 (11%)	92,98,98	1.45	11 (11%)
2	LMN	C	801	-	72,72,72	1.60	10 (13%)	92,98,98	1.45	13 (14%)
2	LMN	A	801	-	72,72,72	1.60	10 (13%)	92,98,98	1.45	12 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LMN	B	802	-	-	32/50/130/130	0/4/4/4
2	LMN	B	801	-	-	27/50/130/130	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LMN	A	802	-	-	32/50/130/130	0/4/4/4
2	LMN	C	802	-	-	32/50/130/130	0/4/4/4
2	LMN	C	801	-	-	27/50/130/130	0/4/4/4
2	LMN	A	801	-	-	27/50/130/130	0/4/4/4

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	LMN	O1-C1	-5.28	1.31	1.40
2	C	801	LMN	O1-C1	-5.24	1.31	1.40
2	B	801	LMN	O1-C1	-5.22	1.31	1.40
2	C	802	LMN	O5-C1	5.02	1.54	1.41
2	A	802	LMN	O5-C1	4.96	1.54	1.41
2	B	802	LMN	O5-C1	4.90	1.54	1.41
2	C	801	LMN	O5-C1	4.67	1.53	1.41
2	A	801	LMN	O5-C1	4.64	1.53	1.41
2	B	801	LMN	O5-C1	4.61	1.53	1.41
2	A	802	LMN	O1-C1	-4.51	1.32	1.40
2	B	802	LMN	O1-C1	-4.46	1.32	1.40
2	C	802	LMN	O1-C1	-4.43	1.32	1.40
2	A	802	LMN	CBT-CCM	4.11	1.62	1.53
2	C	802	LMN	CBT-CCM	4.06	1.62	1.53
2	B	802	LMN	CBT-CCM	4.02	1.62	1.53
2	A	801	LMN	CBT-CCM	3.87	1.62	1.53
2	B	801	LMN	CBT-CCM	3.86	1.62	1.53
2	C	801	LMN	CBT-CCM	3.81	1.62	1.53
2	B	801	LMN	CBS-CCM	3.79	1.62	1.53
2	A	801	LMN	CBS-CCM	3.78	1.62	1.53
2	B	802	LMN	CBS-CCM	3.78	1.62	1.53
2	C	802	LMN	CBS-CCM	3.77	1.62	1.53
2	A	802	LMN	CBS-CCM	3.73	1.61	1.53
2	C	801	LMN	CBS-CCM	3.72	1.61	1.53
2	B	802	LMN	O4-C4	3.42	1.52	1.43
2	C	802	LMN	O4-C4	3.42	1.52	1.43
2	A	802	LMN	O4-C4	3.39	1.52	1.43
2	A	802	LMN	CBQ-CCM	3.27	1.60	1.54
2	B	802	LMN	CBQ-CCM	3.27	1.60	1.54
2	C	802	LMN	CBQ-CCM	3.15	1.59	1.54
2	C	801	LMN	OBY-CCR	3.04	1.49	1.41
2	C	802	LMN	OBY-CCR	3.03	1.49	1.41
2	B	802	LMN	OBY-CCR	3.03	1.49	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	LMN	OBY-CCR	3.01	1.49	1.41
2	A	802	LMN	OBY-CCR	3.01	1.49	1.41
2	A	801	LMN	OBY-CCR	2.97	1.49	1.41
2	C	801	LMN	O4-C4	2.81	1.51	1.43
2	B	801	LMN	O4-C4	2.81	1.51	1.43
2	A	801	LMN	O4-C4	2.78	1.50	1.43
2	C	801	LMN	CBQ-CCM	2.66	1.59	1.54
2	A	801	LMN	CBQ-CCM	2.61	1.59	1.54
2	B	801	LMN	CBQ-CCM	2.59	1.58	1.54
2	A	802	LMN	CCH-CCQ	-2.23	1.46	1.52
2	B	802	LMN	CCH-CCQ	-2.22	1.46	1.52
2	A	801	LMN	OBY-CCC	2.22	1.49	1.44
2	C	802	LMN	CCH-CCQ	-2.21	1.46	1.52
2	A	801	LMN	C3-C4	-2.19	1.46	1.52
2	B	801	LMN	C3-C4	-2.17	1.46	1.52
2	C	801	LMN	OBY-CCC	2.16	1.49	1.44
2	C	801	LMN	C3-C4	-2.16	1.46	1.52
2	B	801	LMN	OBY-CCC	2.14	1.49	1.44
2	A	801	LMN	OBZ-CCS	2.08	1.47	1.41
2	C	801	LMN	OBZ-CCS	2.07	1.47	1.41
2	B	802	LMN	OAN-CCH	2.05	1.48	1.43
2	B	801	LMN	OBZ-CCS	2.04	1.47	1.41
2	B	801	LMN	OBZ-CCD	2.03	1.49	1.44
2	A	802	LMN	OAN-CCH	2.03	1.48	1.43
2	A	802	LMN	OBZ-CCS	2.02	1.47	1.41

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	LMN	CCJ-OBX-CCF	-5.50	102.98	113.72
2	A	801	LMN	CCJ-OBX-CCF	-5.49	103.00	113.72
2	C	801	LMN	CCJ-OBX-CCF	-5.47	103.03	113.72
2	B	801	LMN	OBV-CCJ-CCL	3.97	114.31	108.27
2	C	801	LMN	OBV-CCJ-CCL	3.91	114.22	108.27
2	A	801	LMN	OBV-CCJ-CCL	3.91	114.21	108.27
2	B	802	LMN	OBV-CCJ-CCL	3.87	114.15	108.27
2	A	802	LMN	C2-C3-C4	3.87	118.45	109.68
2	C	802	LMN	OBV-CCJ-CCL	3.86	114.14	108.27
2	B	802	LMN	C2-C3-C4	3.85	118.41	109.68
2	A	802	LMN	OBV-CCJ-CCL	3.84	114.11	108.27
2	C	802	LMN	C2-C3-C4	3.82	118.36	109.68
2	B	802	LMN	CCJ-CCL-CCH	3.48	117.34	110.01

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	802	LMN	CCJ-CCL-CCH	3.46	117.29	110.01
2	A	802	LMN	CCJ-CCL-CCH	3.46	117.29	110.01
2	C	802	LMN	CCJ-OBX-CCF	-3.34	107.19	113.72
2	A	802	LMN	CCJ-OBX-CCF	-3.30	107.27	113.72
2	B	802	LMN	CCJ-OBX-CCF	-3.28	107.32	113.72
2	A	802	LMN	OBZ-CCD-CCO	3.07	115.22	109.70
2	B	802	LMN	OBZ-CCD-CCO	3.03	115.17	109.70
2	C	802	LMN	OBZ-CCD-CCO	3.01	115.12	109.70
2	C	802	LMN	CCL-CCH-CCQ	2.96	116.40	109.68
2	B	802	LMN	CCL-CCH-CCQ	2.95	116.38	109.68
2	A	802	LMN	CCL-CCH-CCQ	2.94	116.36	109.68
2	A	801	LMN	OBZ-CCD-CCO	2.90	114.93	109.70
2	B	801	LMN	OBZ-CCD-CCO	2.87	114.88	109.70
2	C	801	LMN	OBZ-CCD-CCO	2.87	114.87	109.70
2	C	802	LMN	C1-C2-C3	2.79	115.89	110.01
2	A	802	LMN	C1-C2-C3	2.78	115.86	110.01
2	B	802	LMN	C1-C2-C3	2.74	115.78	110.01
2	C	801	LMN	CCT-CCN-CCC	2.55	114.85	110.23
2	A	801	LMN	CCT-CCN-CCC	2.52	114.80	110.23
2	B	801	LMN	CCT-CCN-CCC	2.50	114.76	110.23
2	A	801	LMN	CBL-CBR-CCM	-2.47	109.68	117.19
2	B	801	LMN	CBL-CBR-CCM	-2.47	109.69	117.19
2	C	801	LMN	CBL-CBR-CCM	-2.45	109.75	117.19
2	C	801	LMN	CBK-CBQ-CCM	-2.33	110.10	117.19
2	A	801	LMN	CBK-CBQ-CCM	-2.33	110.12	117.19
2	B	801	LMN	CBK-CBQ-CCM	-2.32	110.16	117.19
2	C	801	LMN	CCU-CCO-CCD	2.30	114.41	110.23
2	A	801	LMN	CCU-CCO-CCD	2.29	114.39	110.23
2	B	801	LMN	OCB-CCQ-CCH	2.26	112.98	107.23
2	B	801	LMN	CCU-CCO-CCD	2.26	114.33	110.23
2	A	801	LMN	OCB-CCQ-CCH	2.26	112.97	107.23
2	C	801	LMN	OCB-CCQ-CCH	2.25	112.95	107.23
2	A	801	LMN	OAR-CCO-CCU	-2.22	105.14	110.38
2	C	801	LMN	OAR-CCO-CCU	-2.20	105.20	110.38
2	B	801	LMN	OAR-CCO-CCU	-2.19	105.20	110.38
2	A	801	LMN	O2-C2-C1	-2.19	104.85	110.08
2	C	801	LMN	O2-C2-C1	-2.17	104.90	110.08
2	B	801	LMN	O2-C2-C1	-2.16	104.92	110.08
2	A	802	LMN	O5-C1-C2	-2.13	106.00	110.37
2	A	801	LMN	CCR-O4-C4	-2.12	112.96	117.98
2	B	801	LMN	CCR-O4-C4	-2.11	112.97	117.98
2	C	801	LMN	CCR-O4-C4	-2.11	112.98	117.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	802	LMN	C3-C4-C5	2.07	115.52	110.93
2	C	802	LMN	O5-C1-C2	-2.07	106.12	110.37
2	B	802	LMN	C3-C4-C5	2.07	115.51	110.93
2	B	802	LMN	O5-C1-C2	-2.07	106.13	110.37
2	C	801	LMN	CBR-CCM-CBQ	-2.06	106.13	109.96
2	B	801	LMN	C1-C2-C3	2.05	114.32	110.01
2	A	801	LMN	C1-C2-C3	2.05	114.31	110.01
2	C	801	LMN	C1-C2-C3	2.04	114.30	110.01
2	C	802	LMN	CCU-CCO-CCD	2.04	113.92	110.23
2	C	802	LMN	CBL-CBR-CCM	-2.03	111.03	117.19
2	B	802	LMN	CBL-CBR-CCM	-2.03	111.03	117.19
2	A	802	LMN	CBL-CBR-CCM	-2.02	111.06	117.19
2	A	802	LMN	C3-C4-C5	2.00	115.37	110.93
2	B	802	LMN	CCU-CCO-CCD	2.00	113.86	110.23

There are no chirality outliers.

All (177) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	801	LMN	CBK-CBQ-CCM-CBR
2	C	801	LMN	CBK-CBQ-CCM-CBS
2	C	801	LMN	CBK-CBQ-CCM-CBT
2	C	801	LMN	CBL-CBR-CCM-CBT
2	C	801	LMN	O1-CBS-CCM-CBQ
2	C	801	LMN	O1-CBS-CCM-CBR
2	C	801	LMN	OBV-CBT-CCM-CBQ
2	C	801	LMN	OBV-CBT-CCM-CBR
2	C	802	LMN	C2-C1-O1-CBS
2	C	802	LMN	O5-C1-O1-CBS
2	C	802	LMN	CBL-CBR-CCM-CBQ
2	C	802	LMN	CBL-CBR-CCM-CBS
2	C	802	LMN	CBL-CBR-CCM-CBT
2	C	802	LMN	O1-CBS-CCM-CBQ
2	C	802	LMN	O1-CBS-CCM-CBR
2	C	802	LMN	OBV-CBT-CCM-CBQ
2	C	802	LMN	OBV-CBT-CCM-CBR
2	B	801	LMN	CBK-CBQ-CCM-CBR
2	B	801	LMN	CBK-CBQ-CCM-CBS
2	B	801	LMN	CBK-CBQ-CCM-CBT
2	B	801	LMN	CBL-CBR-CCM-CBT
2	B	801	LMN	O1-CBS-CCM-CBQ
2	B	801	LMN	O1-CBS-CCM-CBR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	801	LMN	OBV-CBT-CCM-CBQ
2	B	801	LMN	OBV-CBT-CCM-CBR
2	B	802	LMN	C2-C1-O1-CBS
2	B	802	LMN	O5-C1-O1-CBS
2	B	802	LMN	CBL-CBR-CCM-CBQ
2	B	802	LMN	CBL-CBR-CCM-CBS
2	B	802	LMN	CBL-CBR-CCM-CBT
2	B	802	LMN	O1-CBS-CCM-CBQ
2	B	802	LMN	O1-CBS-CCM-CBR
2	B	802	LMN	OBV-CBT-CCM-CBQ
2	B	802	LMN	OBV-CBT-CCM-CBR
2	A	801	LMN	CBK-CBQ-CCM-CBR
2	A	801	LMN	CBK-CBQ-CCM-CBS
2	A	801	LMN	CBK-CBQ-CCM-CBT
2	A	801	LMN	CBL-CBR-CCM-CBT
2	A	801	LMN	O1-CBS-CCM-CBQ
2	A	801	LMN	O1-CBS-CCM-CBR
2	A	801	LMN	OBV-CBT-CCM-CBQ
2	A	801	LMN	OBV-CBT-CCM-CBR
2	A	802	LMN	C2-C1-O1-CBS
2	A	802	LMN	O5-C1-O1-CBS
2	A	802	LMN	CBL-CBR-CCM-CBQ
2	A	802	LMN	CBL-CBR-CCM-CBS
2	A	802	LMN	CBL-CBR-CCM-CBT
2	A	802	LMN	O1-CBS-CCM-CBQ
2	A	802	LMN	O1-CBS-CCM-CBR
2	A	802	LMN	OBV-CBT-CCM-CBQ
2	A	802	LMN	OBV-CBT-CCM-CBR
2	C	802	LMN	C3-C4-O4-CCR
2	B	802	LMN	C3-C4-O4-CCR
2	A	802	LMN	C3-C4-O4-CCR
2	C	801	LMN	OBV-CBT-CCM-CBS
2	B	801	LMN	OBV-CBT-CCM-CBS
2	A	801	LMN	OBV-CBT-CCM-CBS
2	C	802	LMN	CCH-CCQ-OCB-CCS
2	B	802	LMN	CCH-CCQ-OCB-CCS
2	A	802	LMN	CCH-CCQ-OCB-CCS
2	C	802	LMN	CCV-CCR-O4-C4
2	B	802	LMN	CCV-CCR-O4-C4
2	A	802	LMN	CCV-CCR-O4-C4
2	C	801	LMN	O1-CBS-CCM-CBT
2	B	801	LMN	O1-CBS-CCM-CBT

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	801	LMN	O1-CBS-CCM-CBT
2	C	801	LMN	OAI-CBM-CCC-OBV
2	B	801	LMN	OAI-CBM-CCC-OBV
2	C	801	LMN	OAI-CBM-CCC-CCN
2	B	801	LMN	OAI-CBM-CCC-CCN
2	A	801	LMN	OAI-CBM-CCC-CCN
2	A	801	LMN	OAI-CBM-CCC-OBV
2	C	802	LMN	OBV-CCR-O4-C4
2	B	802	LMN	OBV-CCR-O4-C4
2	A	802	LMN	OBV-CCR-O4-C4
2	C	802	LMN	OAJ-CBN-CCD-OBZ
2	B	802	LMN	OAJ-CBN-CCD-OBZ
2	A	802	LMN	OAJ-CBN-CCD-OBZ
2	C	802	LMN	OBX-CCJ-OBV-CBT
2	B	802	LMN	OBX-CCJ-OBV-CBT
2	A	802	LMN	OBX-CCJ-OBV-CBT
2	C	802	LMN	O1-CBS-CCM-CBT
2	B	802	LMN	O1-CBS-CCM-CBT
2	A	802	LMN	O1-CBS-CCM-CBT
2	C	802	LMN	OAI-CBM-CCC-CCN
2	B	802	LMN	OAI-CBM-CCC-CCN
2	A	802	LMN	OAI-CBM-CCC-CCN
2	C	802	LMN	CBJ-CBL-CBR-CCM
2	B	802	LMN	CBJ-CBL-CBR-CCM
2	A	802	LMN	CBJ-CBL-CBR-CCM
2	C	802	LMN	OAI-CBM-CCC-OBV
2	B	802	LMN	OAI-CBM-CCC-OBV
2	A	802	LMN	OAI-CBM-CCC-OBV
2	C	801	LMN	CCF-CCQ-OCB-CCS
2	B	801	LMN	CCF-CCQ-OCB-CCS
2	A	801	LMN	CCF-CCQ-OCB-CCS
2	C	802	LMN	CAZ-CBB-CBD-CBF
2	B	802	LMN	CAZ-CBB-CBD-CBF
2	A	802	LMN	CAZ-CBB-CBD-CBF
2	B	801	LMN	C3-C4-O4-CCR
2	A	801	LMN	C3-C4-O4-CCR
2	C	801	LMN	C3-C4-O4-CCR
2	C	801	LMN	CCH-CCQ-OCB-CCS
2	B	801	LMN	CCH-CCQ-OCB-CCS
2	A	801	LMN	CCH-CCQ-OCB-CCS
2	C	802	LMN	OBV-CBT-CCM-CBS
2	B	802	LMN	OBV-CBT-CCM-CBS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	802	LMN	OBV-CBT-CCM-CBS
2	C	802	LMN	CBG-CBI-CBK-CBQ
2	B	802	LMN	CBG-CBI-CBK-CBQ
2	A	802	LMN	CBG-CBI-CBK-CBQ
2	C	801	LMN	C5-C4-O4-CCR
2	B	801	LMN	C5-C4-O4-CCR
2	A	801	LMN	C5-C4-O4-CCR
2	A	801	LMN	CAY-CBA-CBC-CBE
2	B	802	LMN	CBA-CBC-CBE-CBG
2	C	801	LMN	CAY-CBA-CBC-CBE
2	C	802	LMN	CBA-CBC-CBE-CBG
2	B	801	LMN	CAY-CBA-CBC-CBE
2	A	802	LMN	CBA-CBC-CBE-CBG
2	C	801	LMN	CBL-CBR-CCM-CBS
2	B	801	LMN	CBL-CBR-CCM-CBS
2	A	801	LMN	CBL-CBR-CCM-CBS
2	B	801	LMN	CBI-CBK-CBQ-CCM
2	C	801	LMN	CBI-CBK-CBQ-CCM
2	A	801	LMN	CBI-CBK-CBQ-CCM
2	C	801	LMN	CBA-CBC-CBE-CBG
2	B	801	LMN	CBA-CBC-CBE-CBG
2	A	801	LMN	CBA-CBC-CBE-CBG
2	C	802	LMN	CBH-CBJ-CBL-CBR
2	B	802	LMN	CBH-CBJ-CBL-CBR
2	A	802	LMN	CBH-CBJ-CBL-CBR
2	A	802	LMN	CAB-CAX-CAZ-CBB
2	C	802	LMN	CAB-CAX-CAZ-CBB
2	B	802	LMN	CAB-CAX-CAZ-CBB
2	C	802	LMN	CBF-CBH-CBJ-CBL
2	B	802	LMN	CBF-CBH-CBJ-CBL
2	A	802	LMN	CBF-CBH-CBJ-CBL
2	C	801	LMN	CBL-CBR-CCM-CBQ
2	B	801	LMN	CBL-CBR-CCM-CBQ
2	A	801	LMN	CBL-CBR-CCM-CBQ
2	C	802	LMN	OAJ-CBN-CCD-CCO
2	B	802	LMN	OAJ-CBN-CCD-CCO
2	A	802	LMN	OAJ-CBN-CCD-CCO
2	C	802	LMN	O5-C5-C6-O6
2	B	802	LMN	O5-C5-C6-O6
2	B	801	LMN	CBH-CBJ-CBL-CBR
2	C	801	LMN	CBH-CBJ-CBL-CBR
2	A	801	LMN	CBH-CBJ-CBL-CBR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	802	LMN	O5-C5-C6-O6
2	C	802	LMN	CAA-CAW-CAY-CBA
2	B	802	LMN	CAA-CAW-CAY-CBA
2	A	802	LMN	CAA-CAW-CAY-CBA
2	C	801	LMN	CAX-CAZ-CBB-CBD
2	A	801	LMN	CAX-CAZ-CBB-CBD
2	B	801	LMN	CAX-CAZ-CBB-CBD
2	A	802	LMN	CBE-CBG-CBI-CBK
2	C	802	LMN	CBE-CBG-CBI-CBK
2	B	802	LMN	CBE-CBG-CBI-CBK
2	B	802	LMN	CAX-CAZ-CBB-CBD
2	A	802	LMN	CAX-CAZ-CBB-CBD
2	C	802	LMN	CAX-CAZ-CBB-CBD
2	B	802	LMN	CCF-CCQ-OCB-CCS
2	C	802	LMN	CCF-CCQ-OCB-CCS
2	A	802	LMN	CCF-CCQ-OCB-CCS
2	C	801	LMN	CAA-CAW-CAY-CBA
2	A	801	LMN	CAA-CAW-CAY-CBA
2	B	801	LMN	CAA-CAW-CAY-CBA
2	C	801	LMN	CBG-CBI-CBK-CBQ
2	B	801	LMN	CBG-CBI-CBK-CBQ
2	A	801	LMN	CBG-CBI-CBK-CBQ
2	B	801	LMN	CAW-CAY-CBA-CBC
2	C	801	LMN	CAW-CAY-CBA-CBC
2	A	801	LMN	CAW-CAY-CBA-CBC
2	A	801	LMN	CBE-CBG-CBI-CBK
2	C	801	LMN	CBE-CBG-CBI-CBK
2	B	801	LMN	CBE-CBG-CBI-CBK

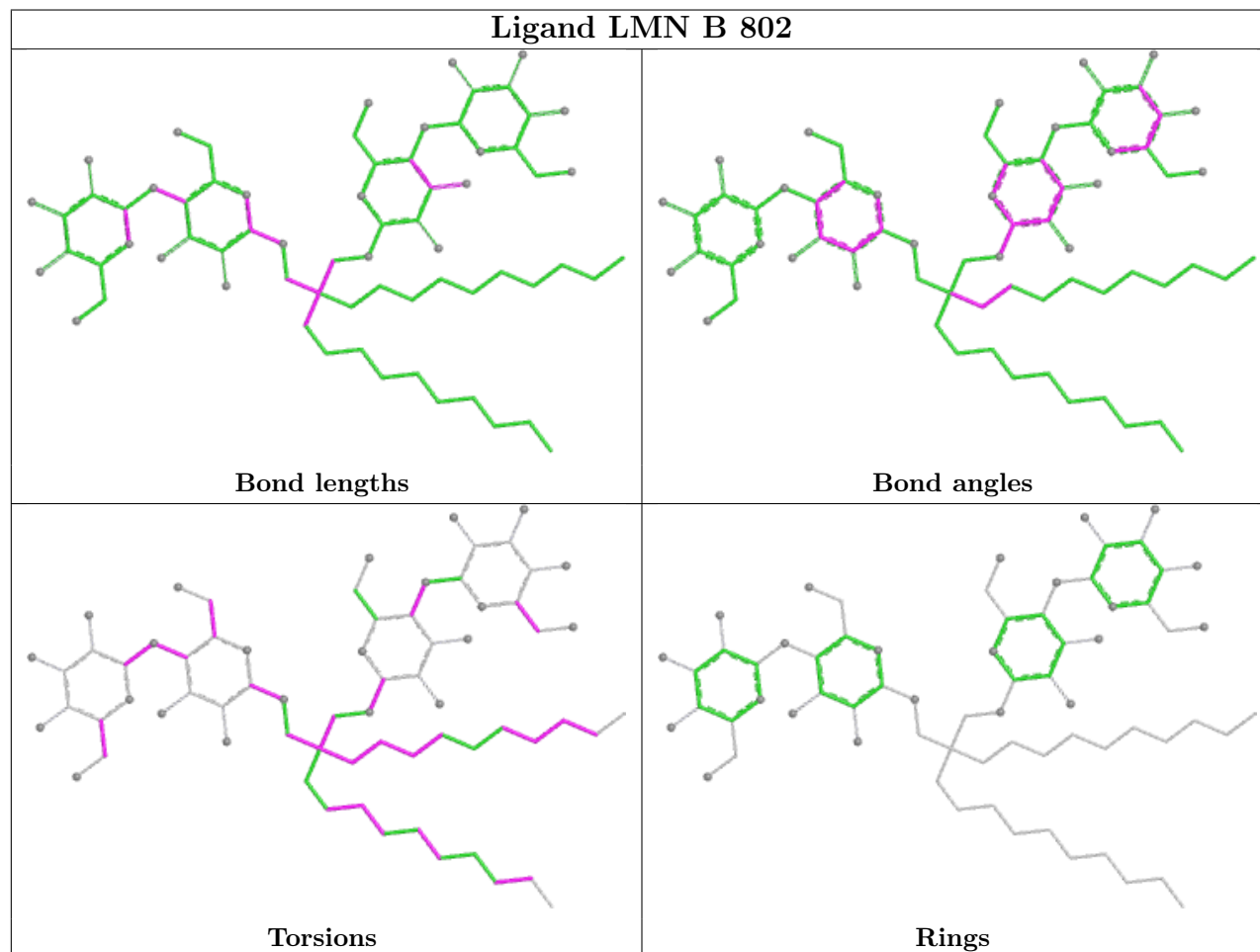
There are no ring outliers.

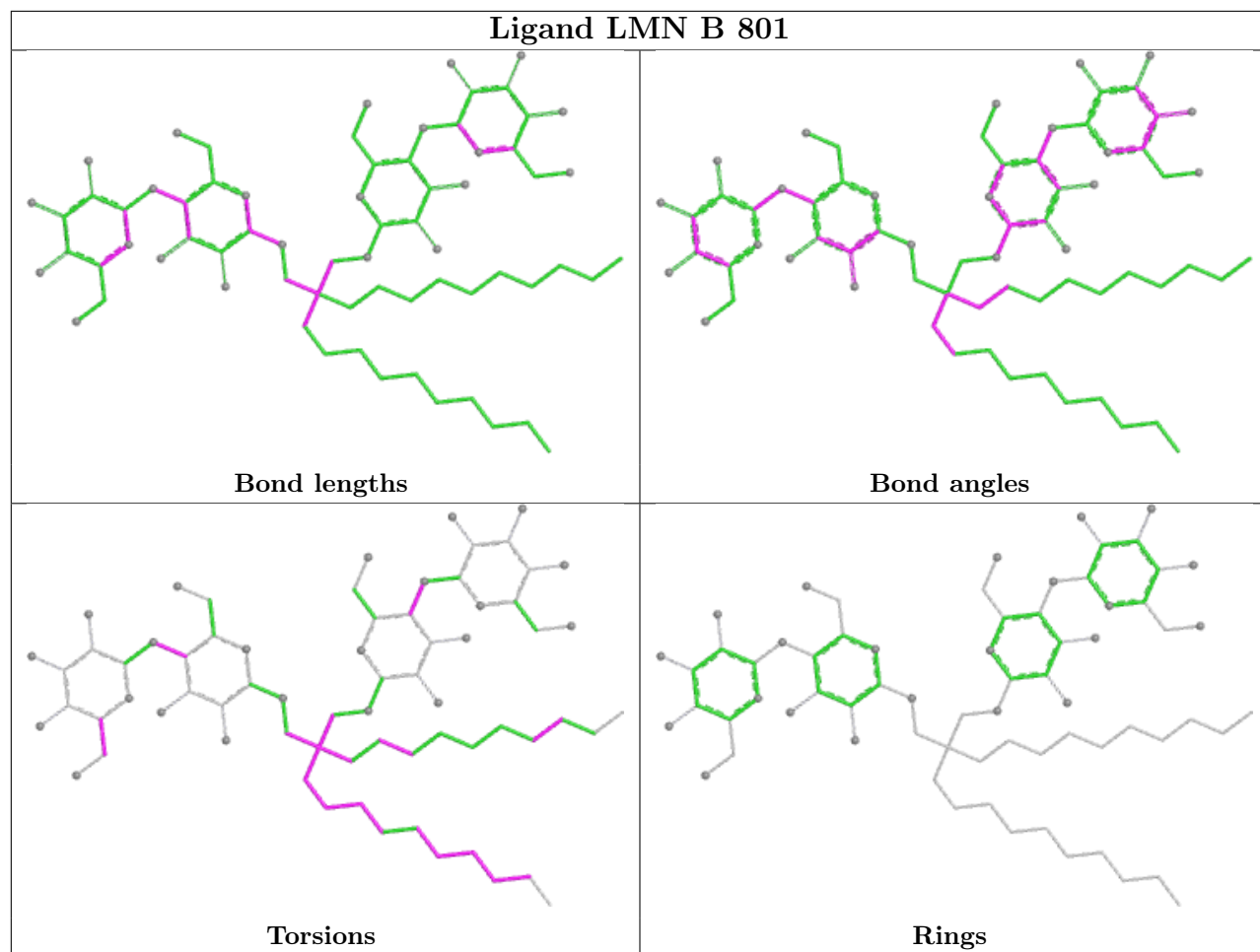
6 monomers are involved in 86 short contacts:

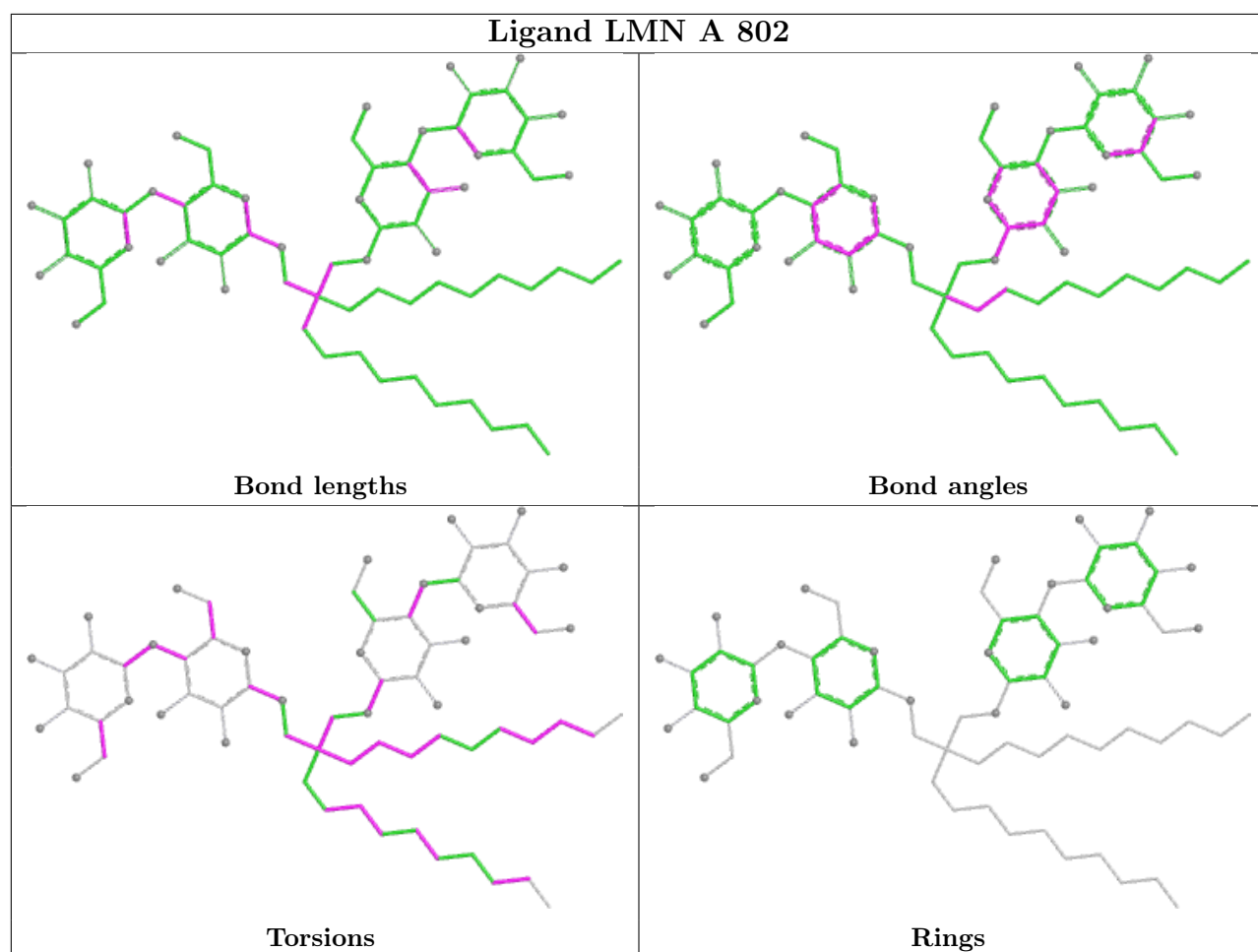
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	802	LMN	18	0
2	B	801	LMN	9	0
2	A	802	LMN	21	0
2	C	802	LMN	20	0
2	C	801	LMN	9	0
2	A	801	LMN	9	0

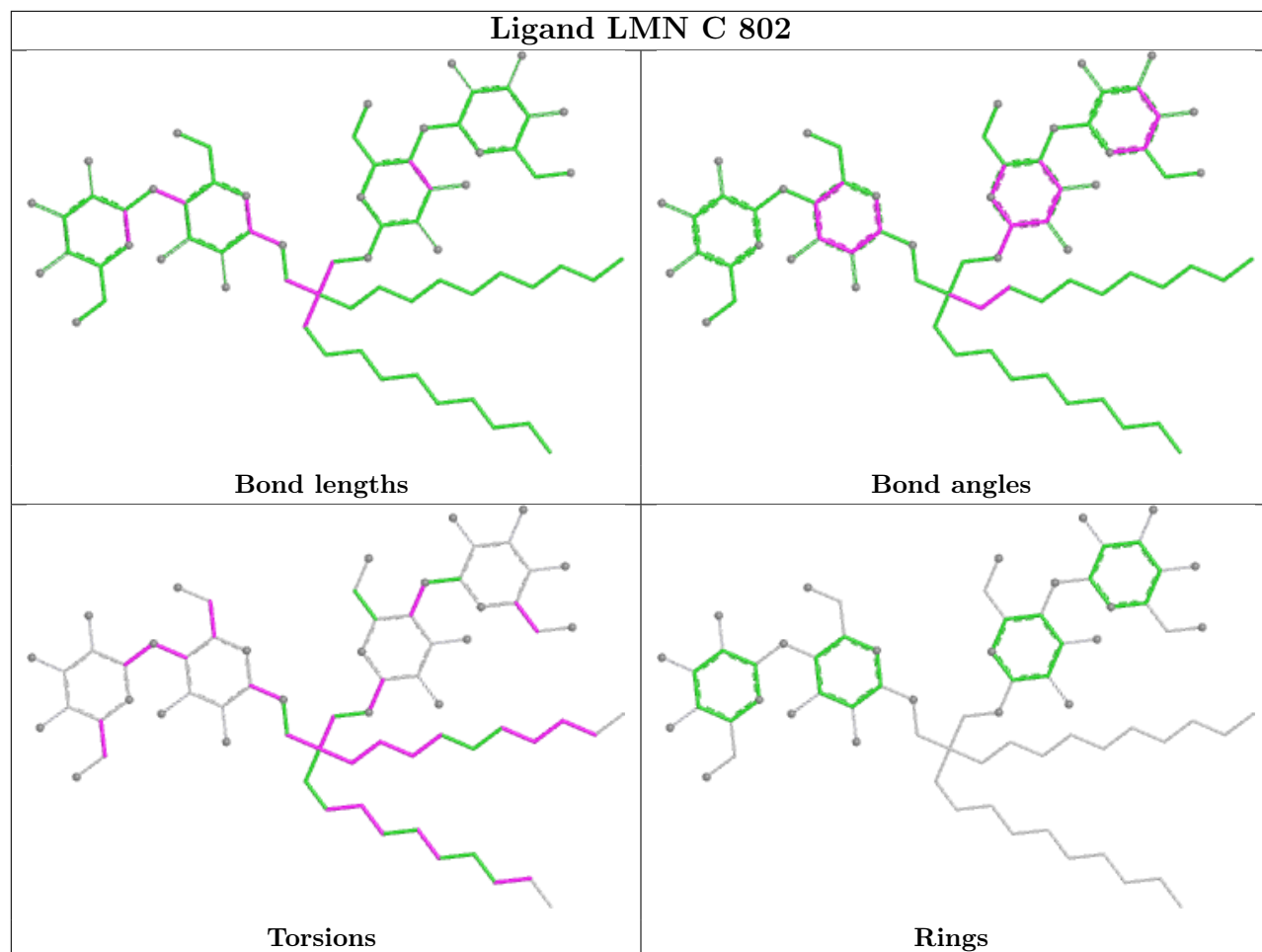
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

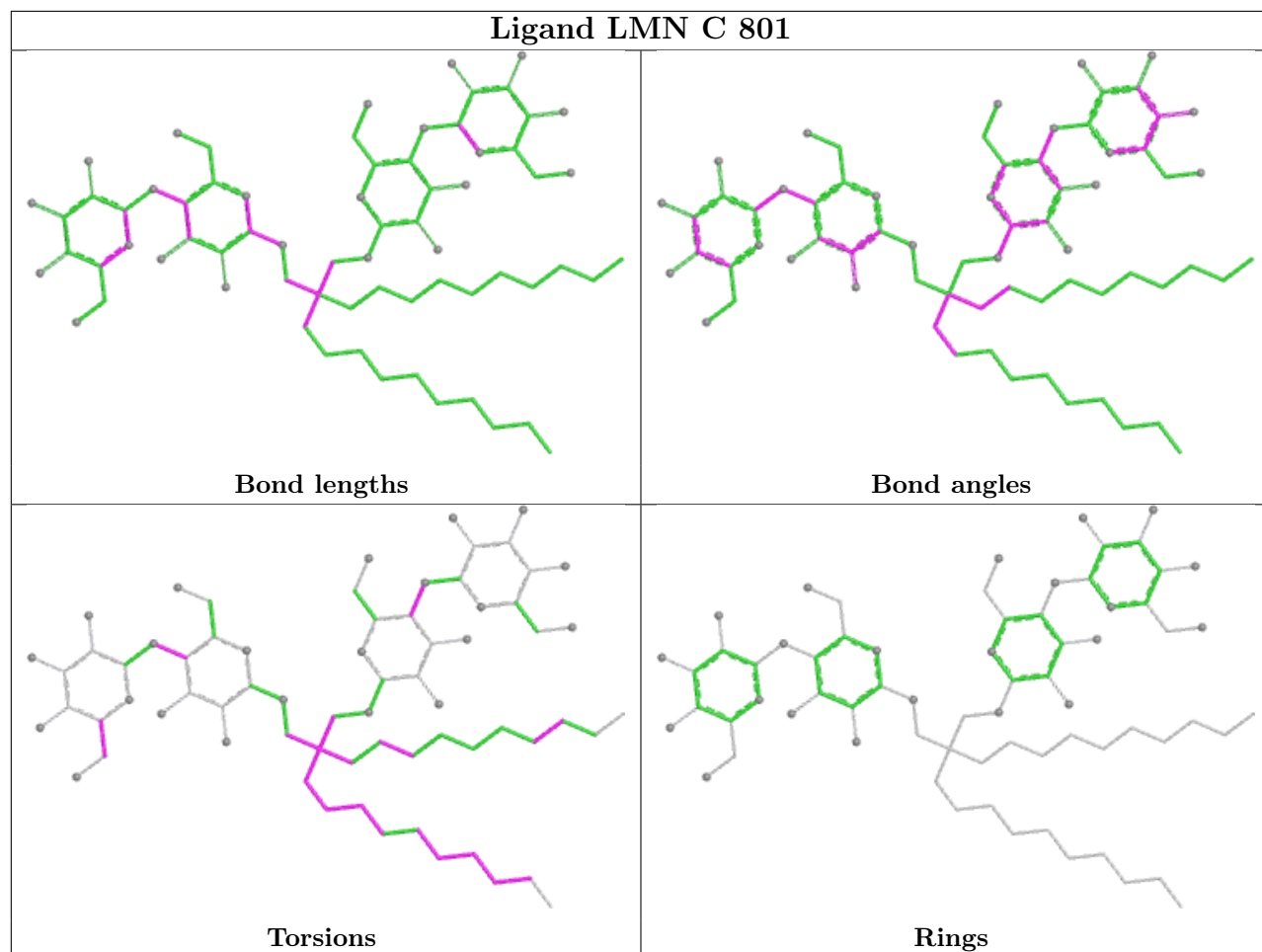
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

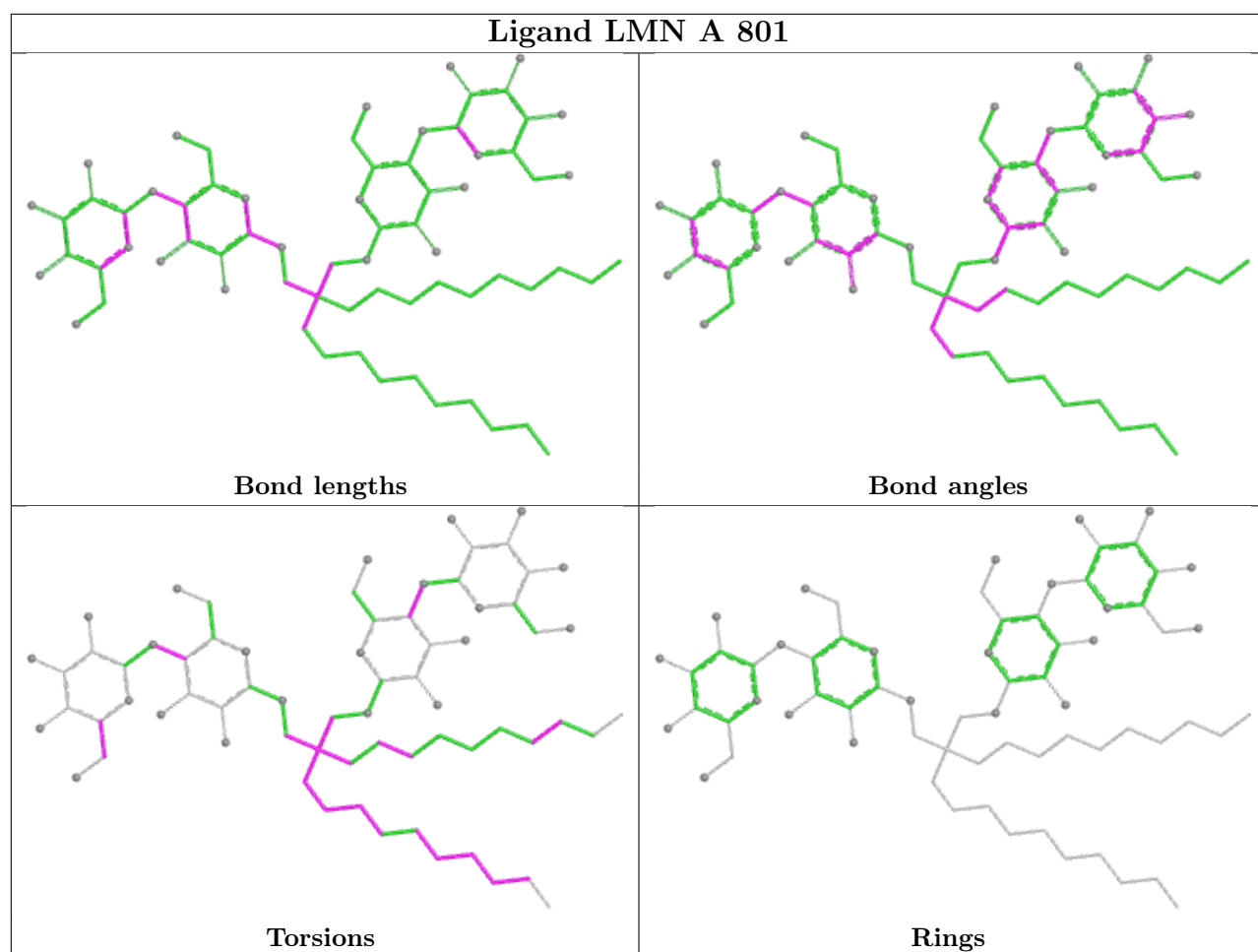












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

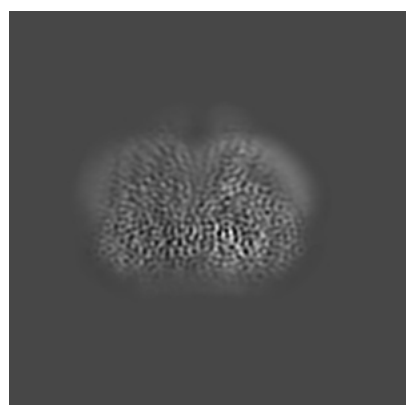
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21874. These allow visual inspection of the internal detail of the map and identification of artifacts.

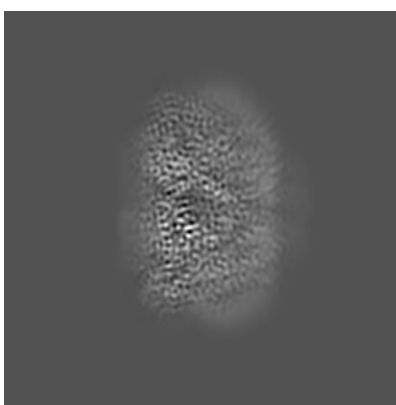
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

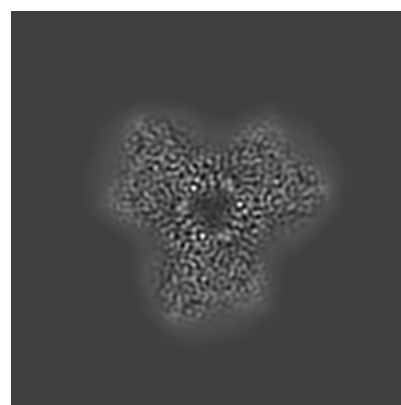
6.1.1 Primary map



X



Y

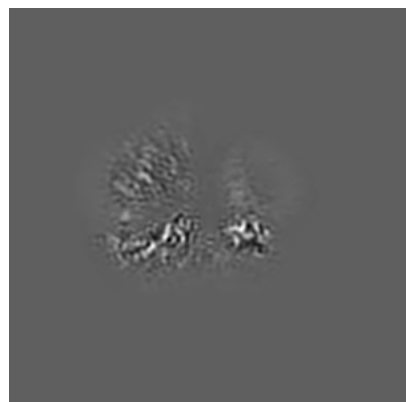


Z

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

6.2 Central slices [i](#)

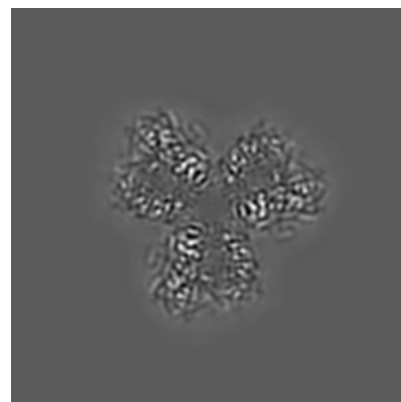
6.2.1 Primary map



X Index: 96



Y Index: 96

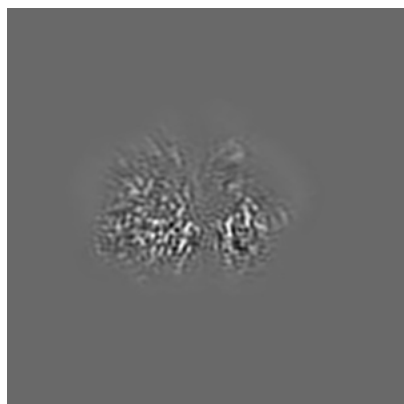


Z Index: 96

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

6.3 Largest variance slices [i](#)

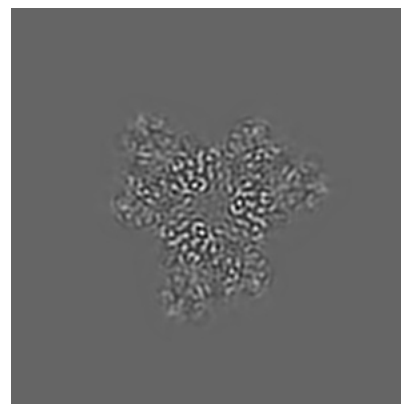
6.3.1 Primary map



X Index: 87



Y Index: 106

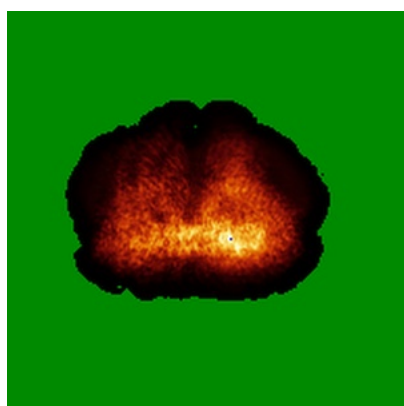


Z Index: 84

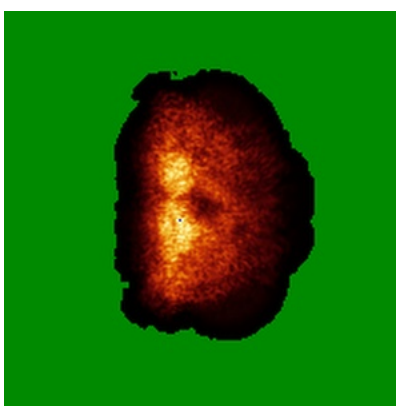
The images above show the largest variance slices of the map in three orthogonal directions.

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

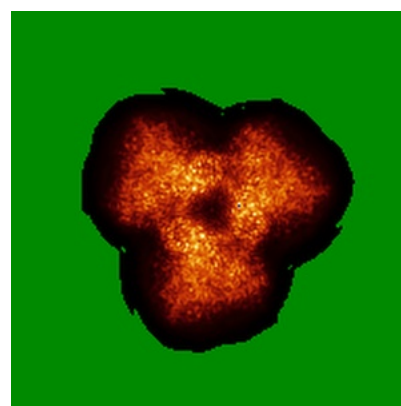
6.4.1 Primary map



X



Y

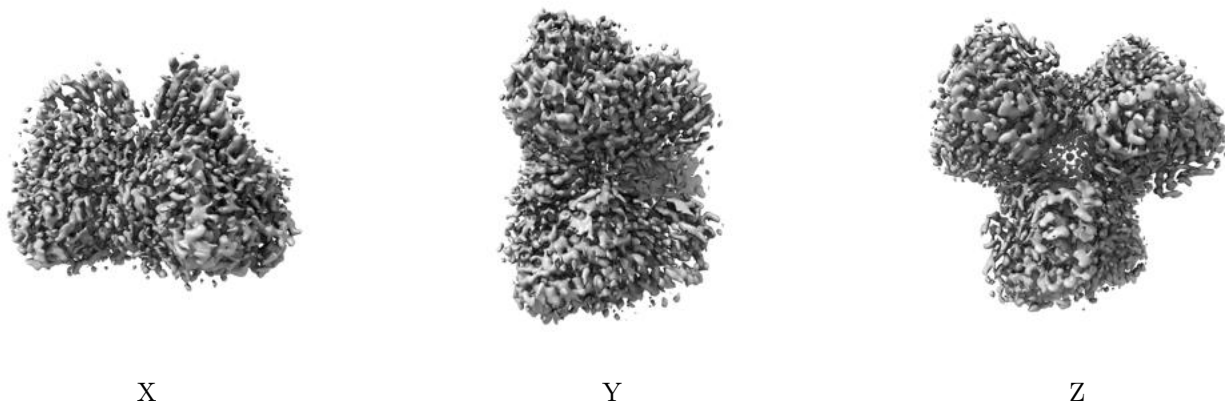


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.453. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

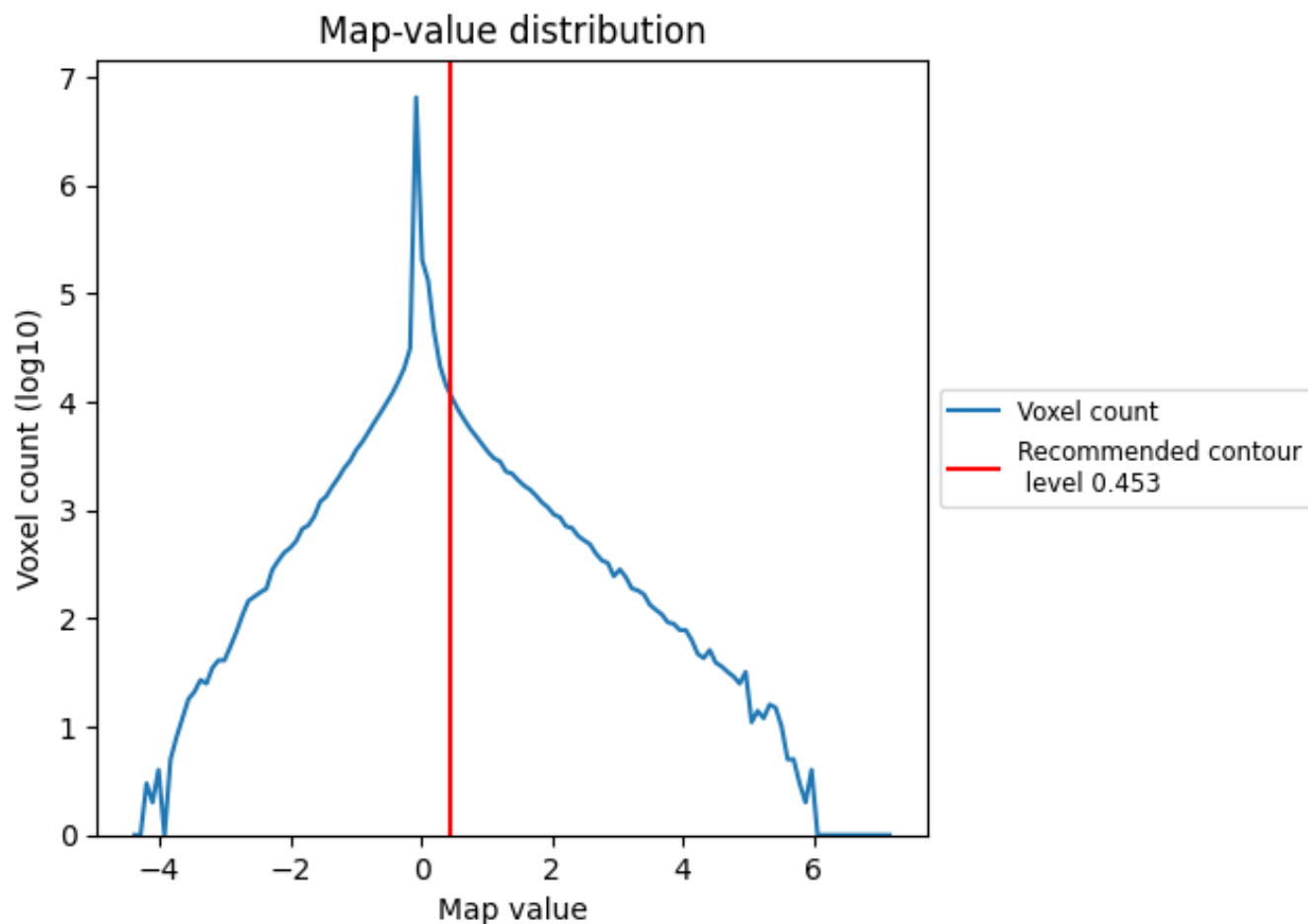
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

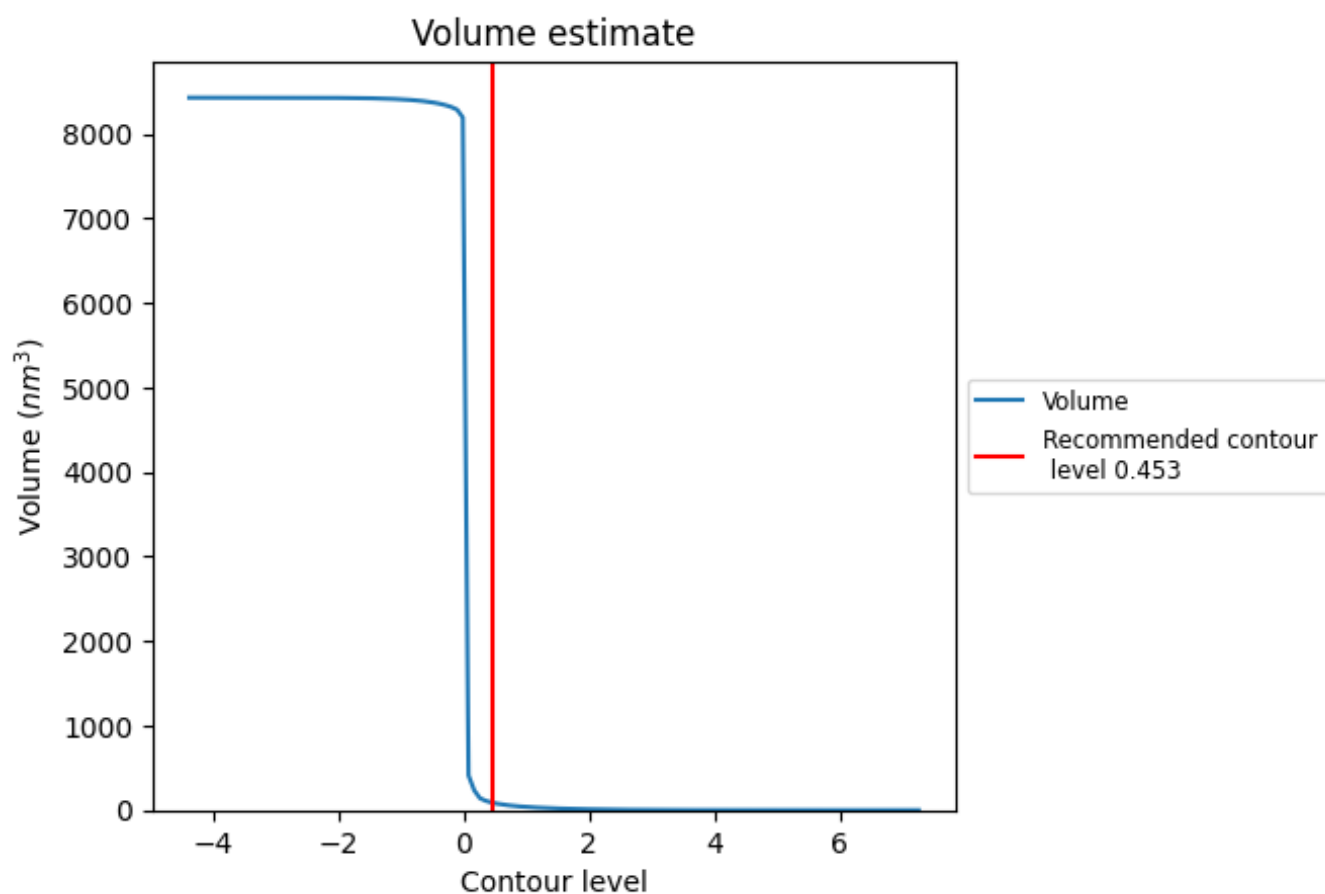
This section contains the results of statistical analysis of the map.

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.

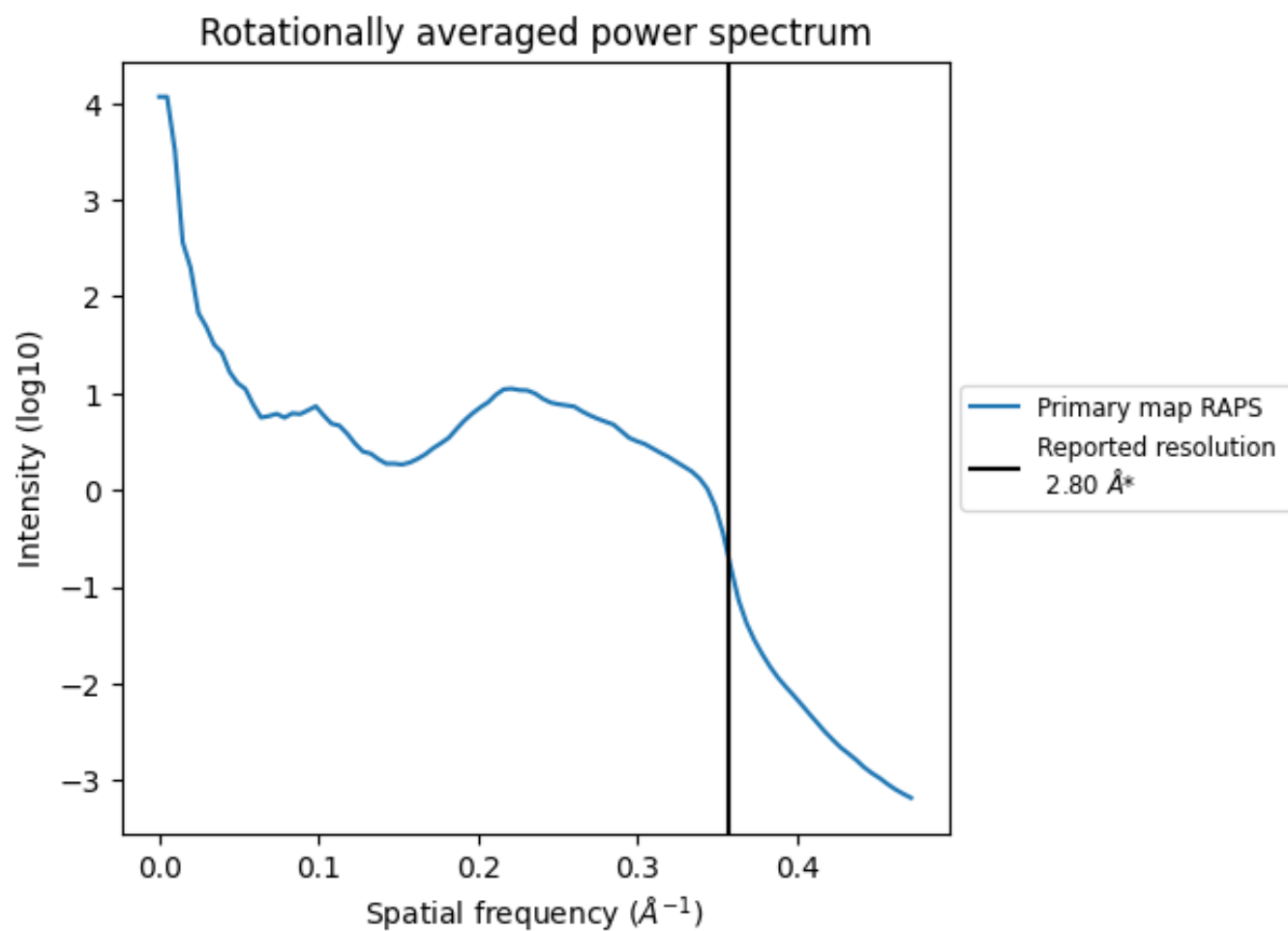
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 89 nm^3 ; this corresponds to an approximate mass of 80 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 0.357 Å⁻¹

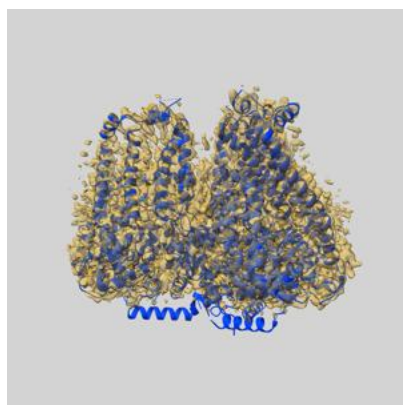
8 Fourier-Shell correlation

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

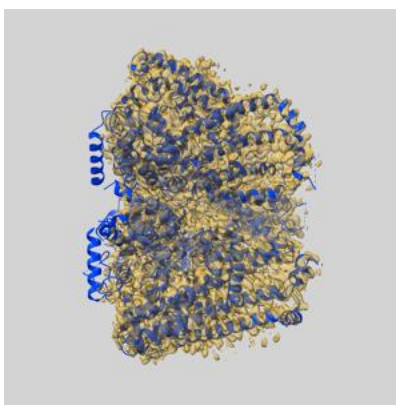
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21874 and PDB model 6WQZ. Per-residue inclusion information can be found in section [3](#) on page [6](#).

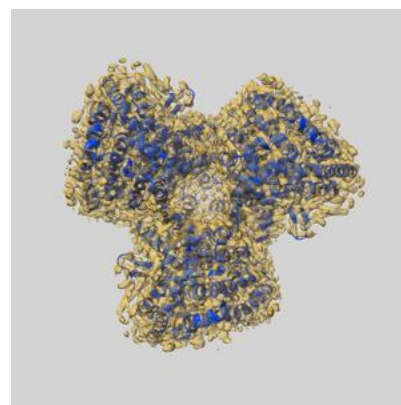
9.1 Map-model overlay [i](#)



X



Y



Z

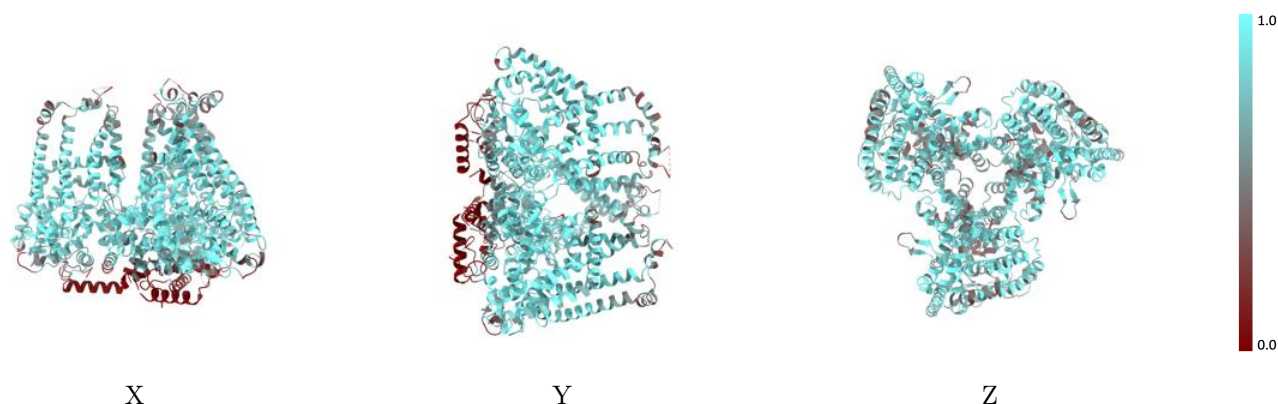
The images above show the 3D surface view of the map at the recommended contour level 0.453 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



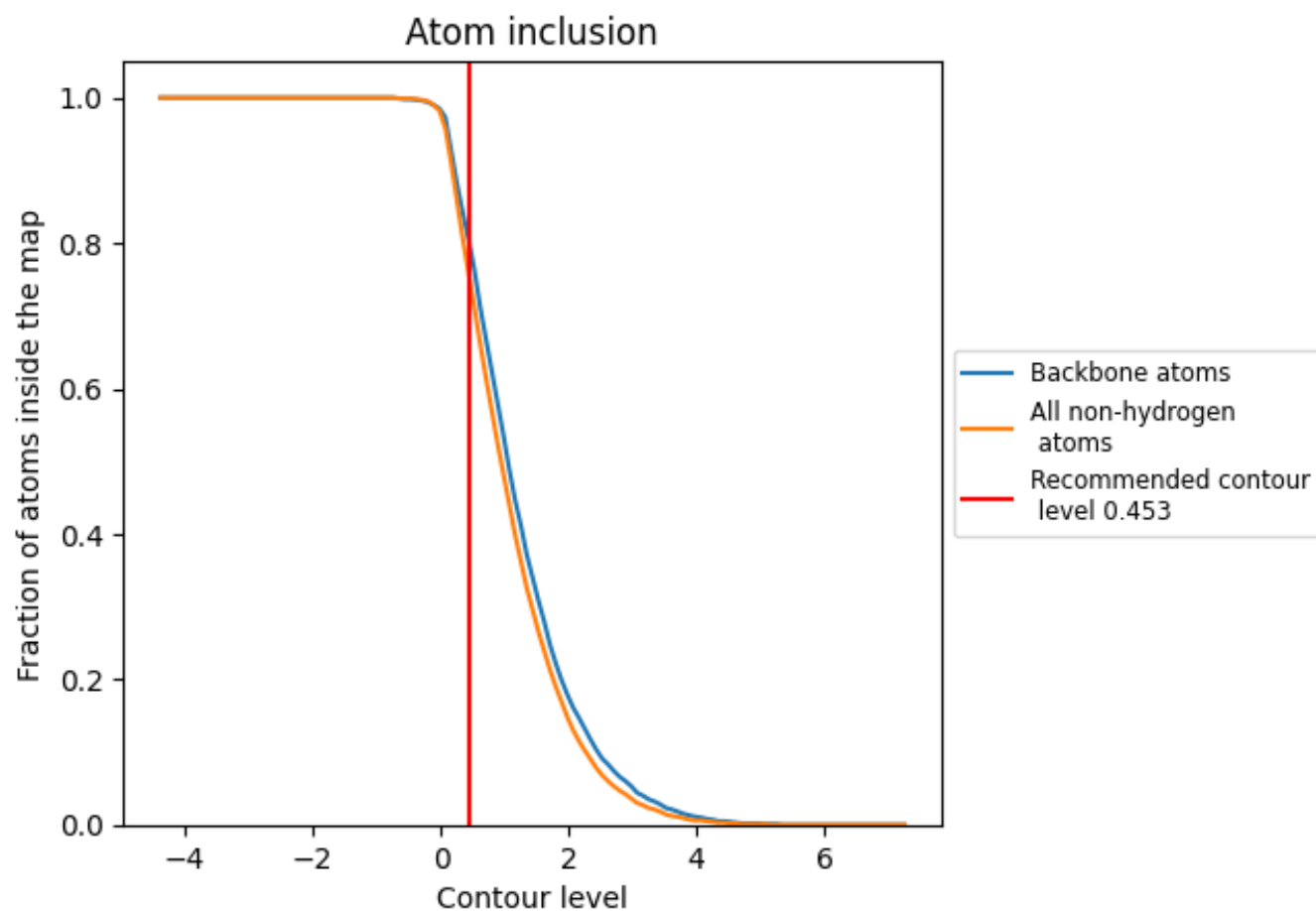
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.453).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 75% 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 (0.453) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.7510</div>	<div><div></div>0.5000</div>
A	<div><div></div>0.7610</div>	<div><div></div>0.5040</div>
B	<div><div></div>0.7620</div>	<div><div></div>0.5030</div>
C	<div><div></div>0.7620</div>	<div><div></div>0.5060</div>
D	<div><div></div>0.4720</div>	<div><div></div>0.3860</div>
E	<div><div></div>0.4780</div>	<div><div></div>0.3920</div>
F	<div><div></div>0.5090</div>	<div><div></div>0.4040</div>

1.0

0.0

<0.0