



Full wwPDB EM Validation Report ⓘ

Apr 15, 2026 – 02:23 AM UTC

PDB ID : 9LEG / pdb_00009leg
EMDB ID : EMD-63025
Title : AMO complex
Authors : Li, Z.Q.; Yang, X.Y.
Deposited on : 2025-01-07
Resolution : 2.36 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

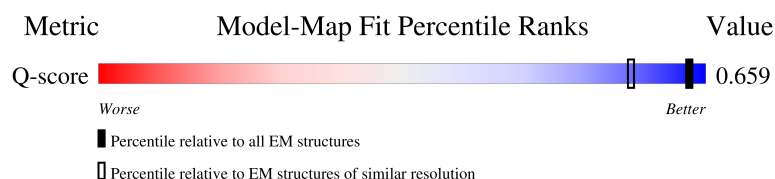
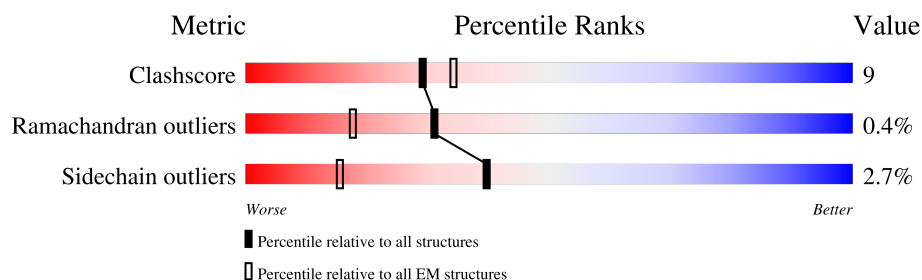
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.36 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4686 (1.86 - 2.86)

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	274	
1	L	274	
1	U	274	
2	B	420	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	M	420	
2	V	420	
3	C	271	
3	N	271	
3	W	271	
4	D	67	
4	O	67	
4	X	67	
5	E	45	
5	P	45	
5	Y	45	

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
7	DKA	A	310	-	-	X	-
7	DKA	A	311	-	-	X	-
7	DKA	L	310	-	-	X	-
7	DKA	L	311	-	-	X	-
7	DKA	U	302	-	-	X	-
7	DKA	U	303	-	-	X	-

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 28749 atoms, of which 2730 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 Ammonia monooxygenase subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	274	Total	C	N	O	S	0	0
			2248	1515	354	363	16		
1	L	274	Total	C	N	O	S	0	0
			2248	1515	354	363	16		
1	U	274	Total	C	N	O	S	0	0
			2248	1515	354	363	16		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	ILE	VAL	conflict	UNP A0A1H3PUN8
A	34	VAL	ILE	conflict	UNP A0A1H3PUN8
A	192	ILE	VAL	conflict	UNP A0A1H3PUN8
A	270	ALA	PRO	conflict	UNP A0A1H3PUN8
L	33	ILE	VAL	conflict	UNP A0A1H3PUN8
L	34	VAL	ILE	conflict	UNP A0A1H3PUN8
L	192	ILE	VAL	conflict	UNP A0A1H3PUN8
L	270	ALA	PRO	conflict	UNP A0A1H3PUN8
U	33	ILE	VAL	conflict	UNP A0A1H3PUN8
U	34	VAL	ILE	conflict	UNP A0A1H3PUN8
U	192	ILE	VAL	conflict	UNP A0A1H3PUN8
U	270	ALA	PRO	conflict	UNP A0A1H3PUN8

- Molecule 2 is a protein called Ammonia monooxygenase subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	383	Total	C	N	O	S	0	0
			3042	1961	529	540	12		
2	M	383	Total	C	N	O	S	0	0
			3042	1961	529	540	12		
2	V	383	Total	C	N	O	S	0	0
			3042	1961	529	540	12		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	73	THR	SER	conflict	UNP A0A1H3PUR7
B	88	ARG	LYS	conflict	UNP A0A1H3PUR7
B	233	LEU	ARG	conflict	UNP A0A1H3PUR7
B	366	VAL	ILE	conflict	UNP A0A1H3PUR7
M	73	THR	SER	conflict	UNP A0A1H3PUR7
M	88	ARG	LYS	conflict	UNP A0A1H3PUR7
M	233	LEU	ARG	conflict	UNP A0A1H3PUR7
M	366	VAL	ILE	conflict	UNP A0A1H3PUR7
V	73	THR	SER	conflict	UNP A0A1H3PUR7
V	88	ARG	LYS	conflict	UNP A0A1H3PUR7
V	233	LEU	ARG	conflict	UNP A0A1H3PUR7
V	366	VAL	ILE	conflict	UNP A0A1H3PUR7

- Molecule 3 is a protein called Ammonia monooxygenase subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	258	Total	C	N	O	S	0	0
			2160	1445	343	357	15		
3	N	258	Total	C	N	O	S	0	0
			2160	1445	343	357	15		
3	W	258	Total	C	N	O	S	0	0
			2160	1445	343	357	15		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	84	ILE	VAL	conflict	UNP A0A1H3PUB4
N	84	ILE	VAL	conflict	UNP A0A1H3PUB4
W	84	ILE	VAL	conflict	UNP A0A1H3PUB4

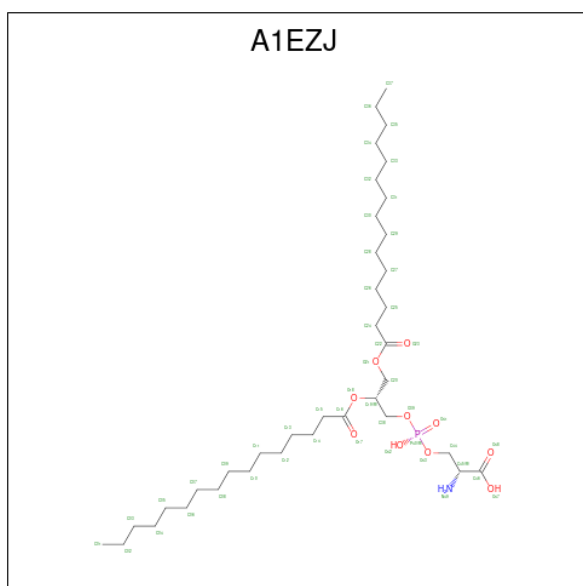
- Molecule 4 is a protein called Lipoprotein.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	19	Total	C	N	O	0	0
			151	95	25	31		
4	O	19	Total	C	N	O	0	0
			151	95	25	31		
4	X	19	Total	C	N	O	0	0
			151	95	25	31		

- Molecule 5 is a protein called AmoD.

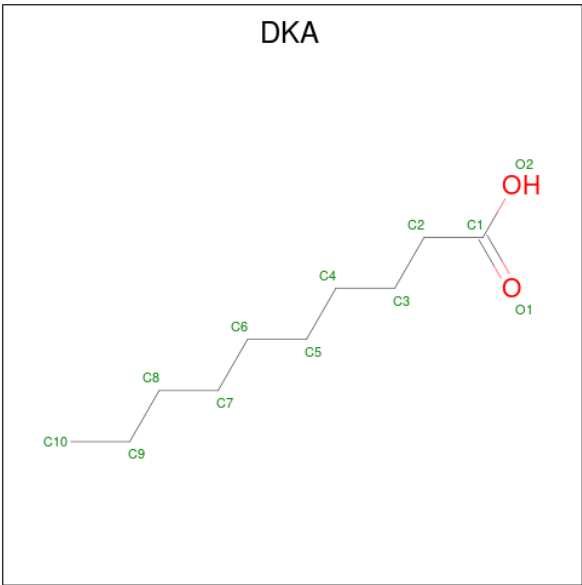
Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	39	Total	C	N	O	0	0
			309	200	50	59		
5	P	39	Total	C	N	O	0	0
			309	200	50	59		
5	Y	39	Total	C	N	O	0	0
			309	200	50	59		

- Molecule 6 is (2 {R})-2-azanyl-3-[[[(2 {R})-2-hexadecanoyloxy-3-pentadecanoyloxy-propoxy]-oxidanyl-phosphoryl]oxy-propanoic acid (CCD ID: A1EZJ) (formula: C₃₇H₇₂NO₁₀P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
6	A	1	Total	C	H	N	O	P	0
			119	37	70	1	10	1	
6	A	1	Total	C	H	N	O	P	0
			119	37	70	1	10	1	
6	C	1	Total	C	H	N	O	P	0
			119	37	70	1	10	1	
6	L	1	Total	C	H	N	O	P	0
			119	37	70	1	10	1	
6	L	1	Total	C	H	N	O	P	0
			119	37	70	1	10	1	
6	U	1	Total	C	H	N	O	P	0
			119	37	70	1	10	1	

- Molecule 7 is DECANOIC ACID (CCD ID: DKA) (formula: C₁₀H₂₀O₂).



Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	H	O	0
			31	10	19	2	
7	A	1	Total	C	H	O	0
			31	10	19	2	
7	A	1	Total	C	H	O	0
			31	10	19	2	
7	A	1	Total	C	H	O	0
			31	10	19	2	
7	A	1	Total	C	H	O	0
			31	10	19	2	
7	A	1	Total	C	H	O	0
			31	10	19	2	
7	A	1	Total	C	H	O	0
			31	10	19	2	
7	A	1	Total	C	H	O	0
			31	10	19	2	
7	B	1	Total	C	H	O	0
			31	10	19	2	
7	B	1	Total	C	H	O	0
			31	10	19	2	
7	B	1	Total	C	H	O	0
			31	10	19	2	
7	B	1	Total	C	H	O	0
			31	10	19	2	
7	C	1	Total	C	H	O	0
			31	10	19	2	

Continued on next page...

Continued from previous page...

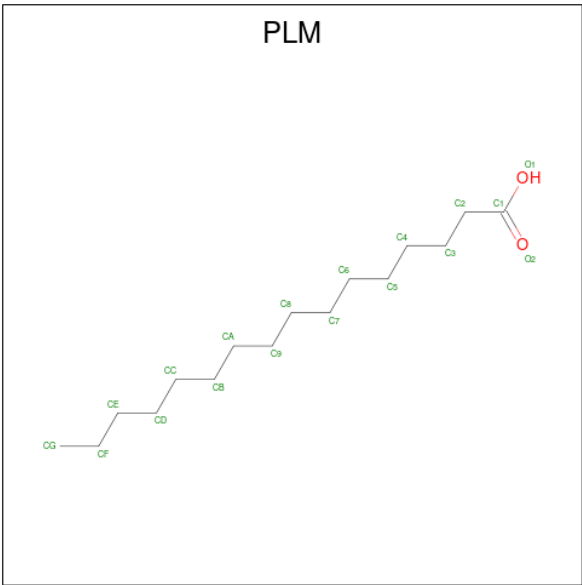
Mol	Chain	Residues	Atoms				AltConf
7	C	1	Total 31	C 10	H 19	O 2	0
7	C	1	Total 31	C 10	H 19	O 2	0
7	C	1	Total 31	C 10	H 19	O 2	0
7	L	1	Total 31	C 10	H 19	O 2	0
7	L	1	Total 31	C 10	H 19	O 2	0
7	L	1	Total 31	C 10	H 19	O 2	0
7	L	1	Total 31	C 10	H 19	O 2	0
7	L	1	Total 31	C 10	H 19	O 2	0
7	L	1	Total 31	C 10	H 19	O 2	0
7	L	1	Total 31	C 10	H 19	O 2	0
7	L	1	Total 31	C 10	H 19	O 2	0
7	L	1	Total 31	C 10	H 19	O 2	0
7	L	1	Total 31	C 10	H 19	O 2	0
7	M	1	Total 31	C 10	H 19	O 2	0
7	M	1	Total 31	C 10	H 19	O 2	0
7	M	1	Total 31	C 10	H 19	O 2	0
7	M	1	Total 31	C 10	H 19	O 2	0
7	N	1	Total 31	C 10	H 19	O 2	0
7	N	1	Total 31	C 10	H 19	O 2	0
7	N	1	Total 31	C 10	H 19	O 2	0
7	N	1	Total 31	C 10	H 19	O 2	0
7	U	1	Total 31	C 10	H 19	O 2	0

Continued on next page...

Continued from previous page...

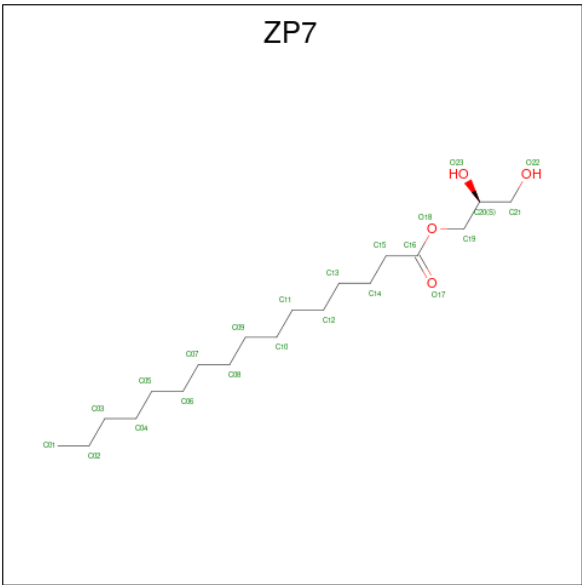
Mol	Chain	Residues	Atoms				AltConf
7	U	1	Total	C	H	O	0
			31	10	19	2	
7	U	1	Total	C	H	O	0
			31	10	19	2	
7	U	1	Total	C	H	O	0
			31	10	19	2	
7	U	1	Total	C	H	O	0
			31	10	19	2	
7	U	1	Total	C	H	O	0
			31	10	19	2	
7	U	1	Total	C	H	O	0
			31	10	19	2	
7	V	1	Total	C	H	O	0
			31	10	19	2	
7	V	1	Total	C	H	O	0
			31	10	19	2	
7	V	1	Total	C	H	O	0
			31	10	19	2	
7	V	1	Total	C	H	O	0
			31	10	19	2	
7	W	1	Total	C	H	O	0
			31	10	19	2	
7	W	1	Total	C	H	O	0
			31	10	19	2	
7	W	1	Total	C	H	O	0
			31	10	19	2	
7	W	1	Total	C	H	O	0
			31	10	19	2	

- Molecule 8 is PALMITIC ACID (CCD ID: PLM) (formula: C₁₆H₃₂O₂).



Mol	Chain	Residues	Atoms				AltConf
8	B	1	Total	C	H	O	0
			49	16	31	2	
8	B	1	Total	C	H	O	0
			49	16	31	2	
8	C	1	Total	C	H	O	0
			49	16	31	2	
8	M	1	Total	C	H	O	0
			49	16	31	2	
8	M	1	Total	C	H	O	0
			49	16	31	2	
8	N	1	Total	C	H	O	0
			49	16	31	2	
8	V	1	Total	C	H	O	0
			49	16	31	2	
8	V	1	Total	C	H	O	0
			49	16	31	2	
8	W	1	Total	C	H	O	0
			49	16	31	2	

- Molecule 9 is (2S)-2,3-dihydroxypropyl hexadecanoate (CCD ID: ZP7) (formula: C₁₉H₃₈O₄).

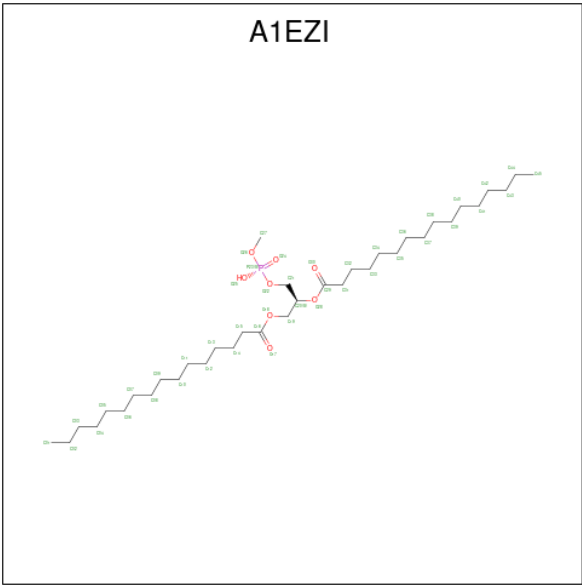


Mol	Chain	Residues	Atoms				AltConf
9	B	1	Total	C	H	O	0
			61	19	38	4	
9	C	1	Total	C	H	O	0
			61	19	38	4	
9	M	1	Total	C	H	O	0
			61	19	38	4	
9	N	1	Total	C	H	O	0
			61	19	38	4	
9	V	1	Total	C	H	O	0
			61	19	38	4	
9	W	1	Total	C	H	O	0
			61	19	38	4	

- Molecule 10 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

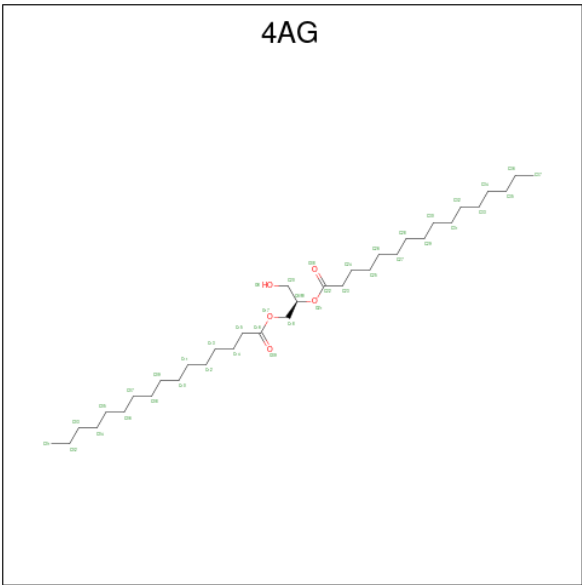
Mol	Chain	Residues	Atoms		AltConf
10	B	1	Total	Cu	0
			1	1	
10	C	2	Total	Cu	0
			2	2	
10	M	1	Total	Cu	0
			1	1	
10	N	2	Total	Cu	0
			2	2	
10	V	1	Total	Cu	0
			1	1	
10	W	2	Total	Cu	0
			2	2	

- Molecule 11 is [(2 {S})-2-hexadecanoyloxy-3-[methoxy(oxidanyl)phosphoryl]oxy-propyl] hexadecanoate (CCD ID: A1EZI) (formula: C₃₆H₇₁O₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
11	C	1	Total	C	H	O	P	0
			115	36	70	8	1	
11	C	1	Total	C	H	O	P	0
			115	36	70	8	1	
11	C	1	Total	C	H	O	P	0
			115	36	70	8	1	
11	N	1	Total	C	H	O	P	0
			115	36	70	8	1	
11	N	1	Total	C	H	O	P	0
			115	36	70	8	1	
11	N	1	Total	C	H	O	P	0
			115	36	70	8	1	
11	W	1	Total	C	H	O	P	0
			115	36	70	8	1	
11	W	1	Total	C	H	O	P	0
			115	36	70	8	1	
11	W	1	Total	C	H	O	P	0
			115	36	70	8	1	

- Molecule 12 is (2R)-3-HYDROXYPROPANE-1,2-DIYL DIHEXADECANOATE (CCD ID: 4AG) (formula: C₃₅H₆₈O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
12	C	1	Total	C	H	O	0
			108	35	68	5	
12	N	1	Total	C	H	O	0
			108	35	68	5	
12	W	1	Total	C	H	O	0
			108	35	68	5	

- Molecule 13 is water.

Mol	Chain	Residues	Atoms		AltConf
13	A	39	Total	O	0
			39	39	
13	B	125	Total	O	0
			125	125	
13	C	18	Total	O	0
			18	18	
13	D	1	Total	O	0
			1	1	
13	L	39	Total	O	0
			39	39	
13	M	125	Total	O	0
			125	125	
13	N	18	Total	O	0
			18	18	
13	O	1	Total	O	0
			1	1	
13	U	39	Total	O	0
			39	39	

Continued on next page...

Continued from previous page...

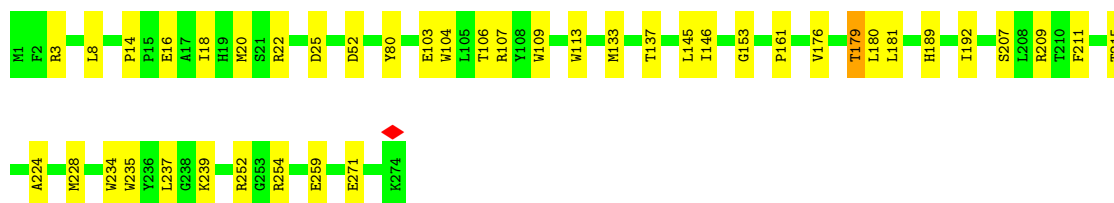
Mol	Chain	Residues	Atoms		AltConf
13	V	125	Total 125	O 125	0
13	W	18	Total 18	O 18	0
13	X	1	Total 1	O 1	0

3 Residue-property plots [i](#)

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

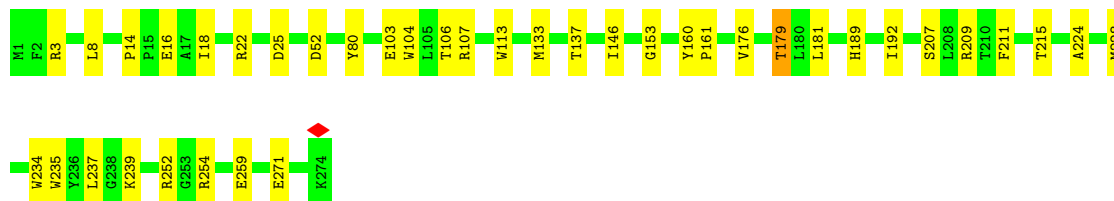
- Molecule 1: Ammonia monooxygenase subunit A

Chain A: 



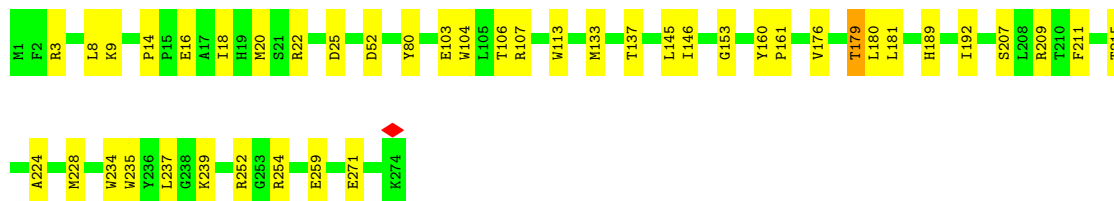
- Molecule 1: Ammonia monooxygenase subunit A

Chain L: 



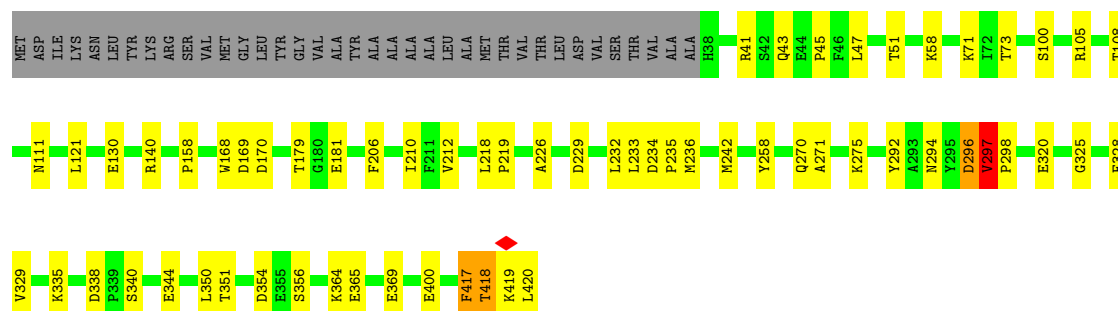
- Molecule 1: Ammonia monooxygenase subunit A

Chain U: 



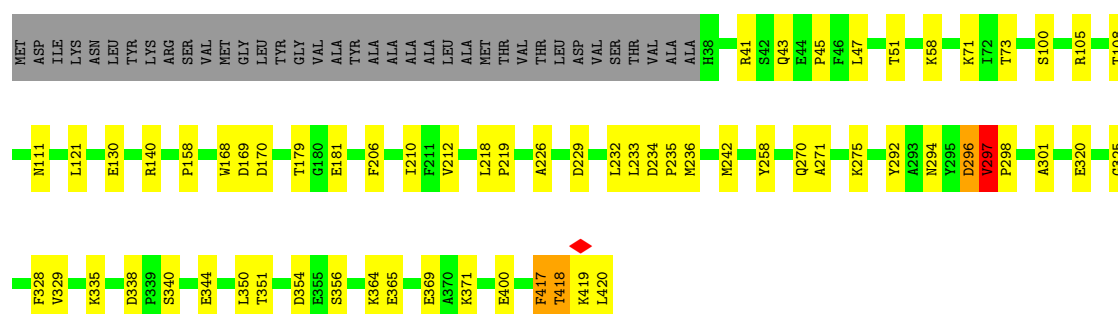
- Molecule 2: Ammonia monooxygenase subunit B

Chain B: 



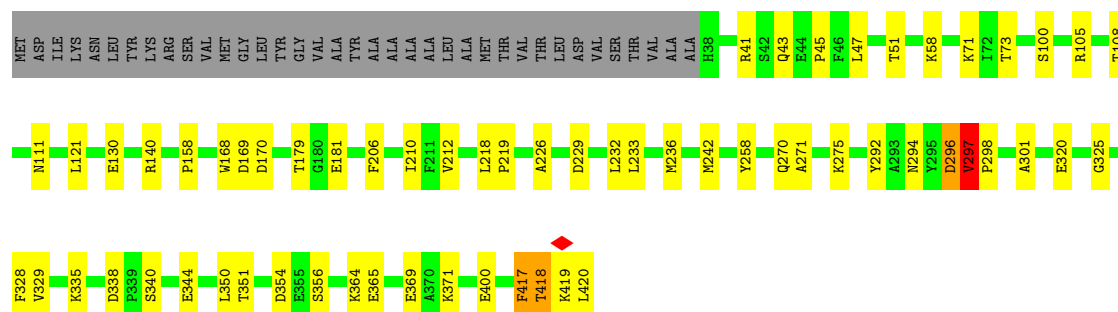
• Molecule 2: Ammonia monooxygenase subunit B

Chain M: 76% 15% 9%



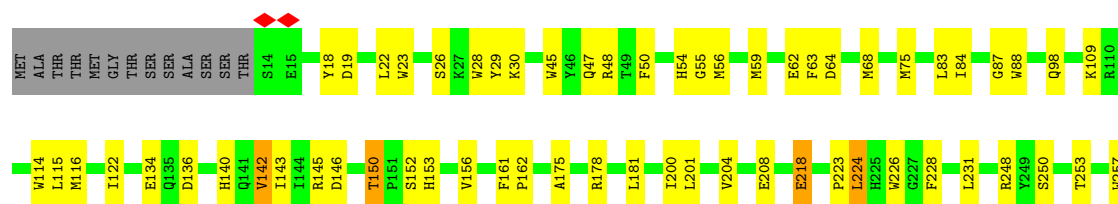
• Molecule 2: Ammonia monooxygenase subunit B

Chain V: 76% 14% 9%



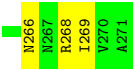
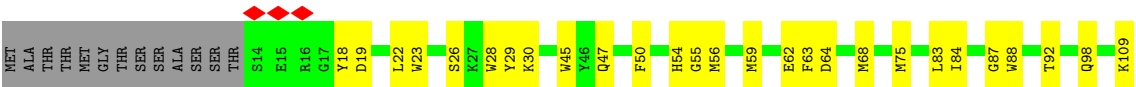
• Molecule 3: Ammonia monooxygenase subunit C

Chain C: 71% 23% 5%





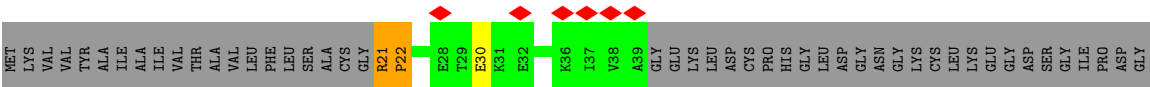
• Molecule 3: Ammonia monooxygenase subunit C



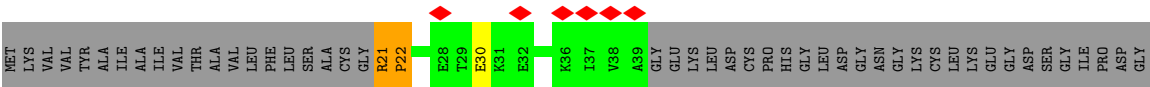
• Molecule 3: Ammonia monooxygenase subunit C



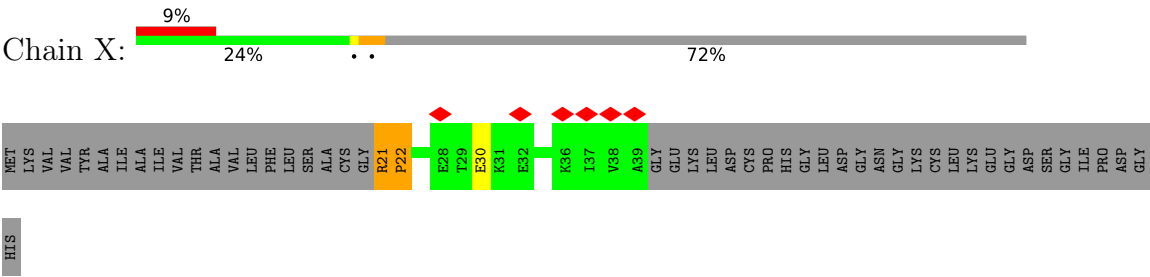
• Molecule 4: Lipoprotein



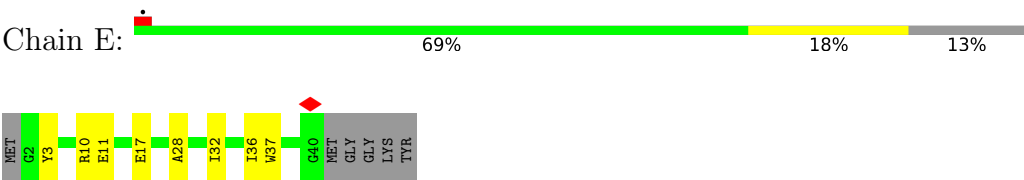
• Molecule 4: Lipoprotein



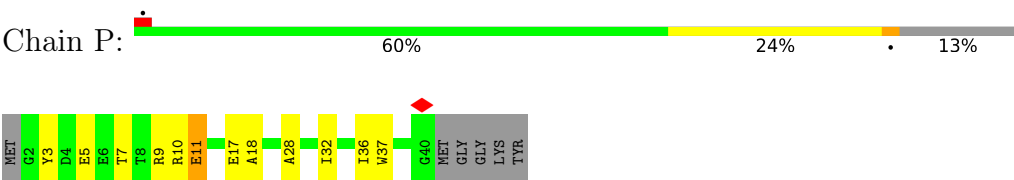
● Molecule 4: Lipoprotein



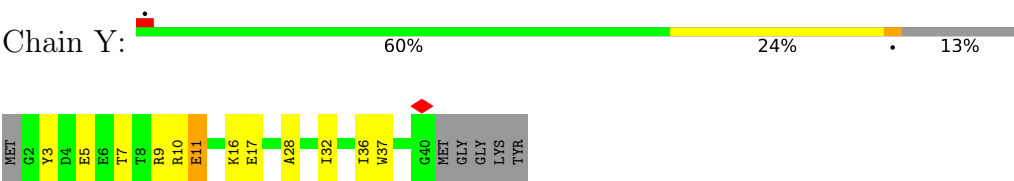
● Molecule 5: AmoD



● Molecule 5: AmoD



● Molecule 5: AmoD



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	94482	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.168	Depositor
Minimum map value	-1.135	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.059	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	299.26398, 299.26398, 299.26398	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.6679999, 0.6679999, 0.6679999	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 4AG, ZP7, A1EZI, A1EZJ, PLM, CU, DKA

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	0.27	0/2334	0.43	2/3184 (0.1%)
1	L	0.27	0/2334	0.43	2/3184 (0.1%)
1	U	0.27	0/2334	0.43	2/3184 (0.1%)
2	B	0.27	0/3133	0.41	1/4266 (0.0%)
2	M	0.27	0/3133	0.41	1/4266 (0.0%)
2	V	0.27	0/3133	0.41	1/4266 (0.0%)
3	C	0.27	0/2244	0.45	1/3059 (0.0%)
3	N	0.27	0/2244	0.45	1/3059 (0.0%)
3	W	0.27	0/2244	0.45	1/3059 (0.0%)
4	D	0.29	0/153	0.65	0/206
4	O	0.30	0/153	0.66	0/206
4	X	0.29	0/153	0.66	0/206
5	E	0.27	0/315	0.35	0/425
5	P	0.27	0/315	0.35	0/425
5	Y	0.27	0/315	0.35	0/425
All	All	0.27	0/24537	0.43	12/33420 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	U	192	ILE	N-CA-C	8.10	119.42	109.30
1	A	192	ILE	N-CA-C	8.09	119.41	109.30
1	L	192	ILE	N-CA-C	8.09	119.41	109.30
2	M	417	PHE	N-CA-C	6.09	119.97	112.54
2	B	417	PHE	N-CA-C	6.08	119.95	112.54
2	V	417	PHE	N-CA-C	6.08	119.95	112.54
1	L	271	GLU	N-CA-C	-5.76	106.79	113.88
1	U	271	GLU	N-CA-C	-5.76	106.79	113.88
1	A	271	GLU	N-CA-C	-5.75	106.81	113.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	218	GLU	N-CA-C	5.05	117.64	109.06
3	W	218	GLU	N-CA-C	5.04	117.63	109.06
3	N	218	GLU	N-CA-C	5.03	117.61	109.06

There are no chirality outliers.

There are no planarity outliers.

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	2248	0	2216	29	0
1	L	2248	0	2216	27	0
1	U	2248	0	2216	29	0
2	B	3042	0	3004	49	0
2	M	3042	0	3004	49	0
2	V	3042	0	3004	49	0
3	C	2160	0	2086	60	0
3	N	2160	0	2086	59	0
3	W	2160	0	2086	55	0
4	D	151	0	151	5	0
4	O	151	0	151	5	0
4	X	151	0	151	5	0
5	E	309	0	303	6	0
5	P	309	0	303	9	0
5	Y	309	0	303	9	0
6	A	98	140	0	1	0
6	C	49	70	0	0	0
6	L	98	140	0	2	0
6	U	49	70	0	2	0
7	A	108	171	171	25	0
7	B	48	76	76	3	0
7	C	48	76	76	3	0
7	L	108	171	171	26	0
7	M	48	76	76	3	0
7	N	48	76	76	3	0
7	U	108	171	171	24	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	V	48	76	76	3	0
7	W	48	76	76	4	0
8	B	36	62	62	4	0
8	C	18	31	31	1	0
8	M	36	62	62	4	0
8	N	18	31	31	1	0
8	V	36	62	62	4	0
8	W	18	31	31	1	0
9	B	23	38	0	3	0
9	C	23	38	0	0	0
9	M	23	38	0	3	0
9	N	23	38	0	0	0
9	V	23	38	0	3	0
9	W	23	38	0	0	0
10	B	1	0	0	0	0
10	C	2	0	0	0	0
10	M	1	0	0	0	0
10	N	2	0	0	0	0
10	V	1	0	0	0	0
10	W	2	0	0	0	0
11	C	135	210	0	18	0
11	N	135	210	0	17	0
11	W	135	210	0	17	0
12	C	40	68	68	4	0
12	N	40	68	68	4	0
12	W	40	68	68	4	0
13	A	39	0	0	2	0
13	B	125	0	0	10	0
13	C	18	0	0	1	0
13	D	1	0	0	0	0
13	L	39	0	0	1	0
13	M	125	0	0	10	0
13	N	18	0	0	1	0
13	O	1	0	0	0	0
13	U	39	0	0	2	0
13	V	125	0	0	10	0
13	W	18	0	0	1	0
13	X	1	0	0	0	0
All	All	26019	2730	24732	469	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 9.

All (469) 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)
7:L:310:DKA:H42	7:L:311:DKA:H31	1.18	1.16
7:A:310:DKA:H42	7:A:311:DKA:H31	1.18	1.15
3:C:178:ARG:NH1	11:C:301:A1EZI:O25	1.81	1.14
3:W:178:ARG:NH1	11:W:301:A1EZI:O25	1.81	1.14
7:A:309:DKA:H82	7:A:311:DKA:O2	1.50	1.12
3:N:178:ARG:NH1	11:N:301:A1EZI:O25	1.81	1.11
7:U:302:DKA:H42	7:U:303:DKA:H31	1.18	1.10
7:L:309:DKA:H82	7:L:311:DKA:O2	1.50	1.09
7:U:301:DKA:H82	7:U:303:DKA:O2	1.50	1.09
7:U:302:DKA:C4	7:U:303:DKA:H31	1.92	0.99
7:A:310:DKA:C4	7:A:311:DKA:H31	1.92	0.99
7:L:310:DKA:C4	7:L:311:DKA:H31	1.92	0.98
7:U:302:DKA:H51	7:U:303:DKA:C4	1.95	0.97
7:L:310:DKA:H51	7:L:311:DKA:C4	1.95	0.96
7:A:310:DKA:H51	7:A:311:DKA:C4	1.95	0.96
1:L:25:ASP:OD1	13:L:401:HOH:O	1.84	0.95
1:U:25:ASP:OD1	13:U:401:HOH:O	1.84	0.95
1:A:25:ASP:OD1	13:A:401:HOH:O	1.84	0.93
1:A:106:THR:HG21	3:C:134:GLU:HB3	1.53	0.91
1:U:106:THR:HG21	3:W:134:GLU:HB3	1.53	0.91
7:L:309:DKA:C8	7:L:311:DKA:O2	2.20	0.90
1:L:106:THR:HG21	3:N:134:GLU:HB3	1.53	0.88
7:A:309:DKA:C8	7:A:311:DKA:O2	2.20	0.88
7:U:301:DKA:C8	7:U:303:DKA:O2	2.20	0.87
7:U:302:DKA:C5	7:U:303:DKA:C4	2.53	0.87
3:C:28:TRP:HB2	11:C:301:A1EZI:O17	1.74	0.87
7:L:310:DKA:C5	7:L:311:DKA:C4	2.53	0.86
7:A:310:DKA:C5	7:A:311:DKA:C4	2.53	0.86
3:N:28:TRP:HB2	11:N:301:A1EZI:O17	1.74	0.86
7:W:308:DKA:H91	7:W:309:DKA:H91	1.58	0.86
3:W:28:TRP:HB2	11:W:301:A1EZI:O17	1.74	0.85
7:L:310:DKA:H51	7:L:311:DKA:H42	1.59	0.84
7:C:307:DKA:H91	7:C:308:DKA:H91	1.58	0.83
7:N:308:DKA:H91	7:N:309:DKA:H91	1.58	0.83
2:V:344:GLU:OE2	13:V:601:HOH:O	1.96	0.83
2:M:344:GLU:OE2	13:M:601:HOH:O	1.96	0.83
2:B:111:ASN:O	13:B:603:HOH:O	1.97	0.82
2:V:111:ASN:O	13:V:603:HOH:O	1.97	0.82
2:M:111:ASN:O	13:M:603:HOH:O	1.97	0.82
7:U:301:DKA:H82	7:U:303:DKA:C1	2.10	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:344:GLU:OE2	13:B:601:HOH:O	1.96	0.82
7:A:309:DKA:H82	7:A:311:DKA:C1	2.10	0.82
7:L:310:DKA:H42	7:L:311:DKA:C3	2.07	0.81
7:A:310:DKA:H51	7:A:311:DKA:H42	1.60	0.81
7:U:302:DKA:H51	7:U:303:DKA:H42	1.59	0.81
2:V:369:GLU:OE2	13:V:604:HOH:O	1.99	0.80
7:L:309:DKA:H82	7:L:311:DKA:C1	2.10	0.80
2:B:369:GLU:OE2	13:B:604:HOH:O	1.99	0.80
2:M:369:GLU:OE2	13:M:604:HOH:O	1.99	0.80
2:M:351:THR:OG1	13:M:602:HOH:O	1.96	0.79
2:V:351:THR:OG1	13:V:602:HOH:O	1.96	0.78
7:U:302:DKA:H42	7:U:303:DKA:C3	2.07	0.78
7:A:310:DKA:H42	7:A:311:DKA:C3	2.07	0.78
7:U:302:DKA:H51	7:U:303:DKA:H41	1.67	0.77
7:A:310:DKA:H51	7:A:311:DKA:H41	1.67	0.76
7:L:310:DKA:H51	7:L:311:DKA:H41	1.67	0.76
3:C:150:THR:HG22	3:C:153:HIS:H	1.51	0.76
12:W:307:4AG:H182	5:Y:37:TRP:CH2	2.21	0.76
12:C:306:4AG:H182	5:E:37:TRP:CH2	2.21	0.76
3:W:30:LYS:NZ	11:W:302:A1EZI:O25	2.19	0.76
3:N:150:THR:HG22	3:N:153:HIS:H	1.51	0.75
2:M:236:MET:HE1	9:M:503:ZP7:C19	2.17	0.75
3:N:30:LYS:NZ	11:N:302:A1EZI:O25	2.19	0.75
7:L:310:DKA:C5	7:L:311:DKA:H41	2.17	0.74
2:B:236:MET:HE1	9:B:502:ZP7:C19	2.17	0.74
12:N:307:4AG:H182	5:P:37:TRP:CH2	2.21	0.74
3:W:150:THR:HG22	3:W:153:HIS:H	1.51	0.74
2:V:236:MET:HE1	9:V:503:ZP7:C19	2.17	0.74
7:A:310:DKA:C5	7:A:311:DKA:H41	2.17	0.74
2:B:351:THR:OG1	13:B:602:HOH:O	1.96	0.74
2:V:354:ASP:OD2	2:V:364:LYS:NZ	2.20	0.73
3:C:30:LYS:NZ	11:C:302:A1EZI:O25	2.19	0.73
7:U:302:DKA:C5	7:U:303:DKA:H41	2.17	0.73
3:N:28:TRP:CB	11:N:301:A1EZI:O17	2.37	0.72
2:V:140:ARG:NH1	4:X:30:GLU:OE2	2.22	0.72
3:W:28:TRP:CB	11:W:301:A1EZI:O17	2.37	0.71
3:C:28:TRP:CB	11:C:301:A1EZI:O17	2.37	0.71
2:M:121:LEU:O	13:M:606:HOH:O	2.09	0.71
2:V:121:LEU:O	13:V:606:HOH:O	2.09	0.71
2:B:354:ASP:OD2	2:B:364:LYS:NZ	2.20	0.71
2:M:354:ASP:OD2	2:M:364:LYS:NZ	2.20	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:271:ALA:O	13:M:605:HOH:O	2.09	0.70
2:B:121:LEU:O	13:B:606:HOH:O	2.09	0.70
2:V:271:ALA:O	13:V:605:HOH:O	2.09	0.70
2:B:271:ALA:O	13:B:605:HOH:O	2.09	0.70
2:M:140:ARG:NH1	4:O:30:GLU:OE2	2.22	0.70
2:B:140:ARG:NH1	4:D:30:GLU:OE2	2.22	0.70
2:B:43:GLN:O	13:B:607:HOH:O	2.10	0.69
7:L:308:DKA:H21	8:M:502:PLM:H21	1.75	0.69
2:V:43:GLN:O	13:V:607:HOH:O	2.10	0.68
2:M:43:GLN:O	13:M:607:HOH:O	2.10	0.68
2:V:320:GLU:HG3	2:V:329:VAL:HG12	1.75	0.68
3:W:55:GLY:HA2	3:W:63:PHE:HD1	1.59	0.68
3:C:54:HIS:HD2	3:C:62:GLU:HB3	1.59	0.68
3:N:54:HIS:HD2	3:N:62:GLU:HB3	1.59	0.67
2:B:320:GLU:HG3	2:B:329:VAL:HG12	1.75	0.67
2:M:320:GLU:HG3	2:M:329:VAL:HG12	1.75	0.67
3:C:55:GLY:HA2	3:C:63:PHE:HD1	1.59	0.67
2:B:58:LYS:HE2	13:B:706:HOH:O	1.94	0.67
7:A:308:DKA:H21	8:B:501:PLM:H21	1.75	0.67
3:W:54:HIS:HD2	3:W:62:GLU:HB3	1.59	0.67
2:M:58:LYS:HE2	13:M:706:HOH:O	1.94	0.67
2:V:58:LYS:HE2	13:V:706:HOH:O	1.94	0.67
3:N:162:PRO:HG3	11:N:303:A1EZI:C05	2.25	0.66
7:U:310:DKA:H21	8:V:502:PLM:H21	1.75	0.66
7:U:305:DKA:H101	11:W:302:A1EZI:C36	2.26	0.66
3:W:162:PRO:HG3	11:W:303:A1EZI:C05	2.25	0.66
3:N:83:LEU:HD23	3:N:84:ILE:HD12	1.78	0.66
7:L:303:DKA:H101	11:N:302:A1EZI:C36	2.26	0.65
3:C:83:LEU:HD23	3:C:84:ILE:HD12	1.78	0.65
3:N:55:GLY:HA2	3:N:63:PHE:HD1	1.59	0.65
3:W:83:LEU:HD23	3:W:84:ILE:HD12	1.78	0.65
3:C:162:PRO:HG3	11:C:303:A1EZI:C05	2.25	0.65
7:A:303:DKA:H101	11:C:302:A1EZI:C36	2.26	0.65
1:A:176:VAL:O	1:A:179:THR:HG23	1.98	0.64
1:L:176:VAL:O	1:L:179:THR:HG23	1.98	0.64
1:U:176:VAL:O	1:U:179:THR:HG23	1.98	0.64
12:W:307:4AG:H182	5:Y:37:TRP:HH2	1.63	0.64
12:C:306:4AG:H182	5:E:37:TRP:HH2	1.63	0.63
3:N:75:MET:HE3	11:N:303:A1EZI:C10	2.29	0.63
3:C:75:MET:HE3	11:C:303:A1EZI:C10	2.29	0.63
3:W:75:MET:HE3	11:W:303:A1EZI:C10	2.29	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:310:DKA:C5	7:L:311:DKA:H31	2.30	0.62
3:N:29:TYR:CG	3:N:116:MET:HG2	2.35	0.62
7:L:310:DKA:C5	7:L:311:DKA:C3	2.78	0.62
3:C:75:MET:CE	11:C:303:A1EZI:C10	2.78	0.61
3:W:87:GLY:HA3	7:W:309:DKA:H103	1.83	0.61
7:A:310:DKA:C5	7:A:311:DKA:H31	2.30	0.61
7:U:302:DKA:C5	7:U:303:DKA:H31	2.30	0.61
7:U:302:DKA:C5	7:U:303:DKA:C3	2.78	0.61
3:W:75:MET:CE	11:W:303:A1EZI:C10	2.78	0.61
3:N:75:MET:CE	11:N:303:A1EZI:C10	2.78	0.60
7:U:305:DKA:H101	11:W:302:A1EZI:C37	2.31	0.60
7:A:303:DKA:H101	11:C:302:A1EZI:C37	2.31	0.60
3:C:29:TYR:CG	3:C:116:MET:HG2	2.35	0.60
7:L:303:DKA:H101	11:N:302:A1EZI:C37	2.31	0.60
12:N:307:4AG:H182	5:P:37:TRP:HH2	1.63	0.60
3:W:29:TYR:CG	3:W:116:MET:HG2	2.35	0.60
7:A:310:DKA:C5	7:A:311:DKA:C3	2.78	0.60
3:C:87:GLY:HA3	7:C:308:DKA:H103	1.83	0.60
3:N:87:GLY:HA3	7:N:309:DKA:H103	1.83	0.59
3:W:153:HIS:HA	3:W:156:VAL:HG12	1.85	0.58
1:A:189:HIS:O	2:B:105:ARG:NH1	2.36	0.58
3:C:153:HIS:HA	3:C:156:VAL:HG12	1.85	0.58
1:U:189:HIS:O	2:V:105:ARG:NH1	2.36	0.58
3:W:75:MET:CE	11:W:303:A1EZI:C11	2.82	0.58
2:B:297:VAL:HG11	13:V:724:HOH:O	2.03	0.57
1:L:189:HIS:O	2:M:105:ARG:NH1	2.36	0.57
2:M:100:SER:HA	3:N:142:VAL:HG22	1.86	0.57
3:N:75:MET:CE	11:N:303:A1EZI:C11	2.82	0.57
13:B:724:HOH:O	2:M:297:VAL:HG11	2.03	0.57
3:N:153:HIS:HA	3:N:156:VAL:HG12	1.85	0.57
7:U:301:DKA:C7	7:U:303:DKA:O2	2.53	0.57
2:B:179:THR:OG1	2:B:181:GLU:OE1	2.22	0.57
2:V:100:SER:HA	3:W:142:VAL:HG22	1.86	0.57
7:A:309:DKA:C7	7:A:311:DKA:O2	2.53	0.56
7:W:308:DKA:C9	7:W:309:DKA:H91	2.34	0.56
2:M:179:THR:OG1	2:M:181:GLU:OE1	2.22	0.56
1:L:133:MET:O	1:L:137:THR:HG22	2.06	0.56
3:C:75:MET:CE	11:C:303:A1EZI:C11	2.82	0.56
3:C:136:ASP:OD1	3:C:152:SER:OG	2.24	0.56
1:A:133:MET:O	1:A:137:THR:HG22	2.06	0.56
2:B:100:SER:HA	3:C:142:VAL:HG22	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:724:HOH:O	2:V:297:VAL:HG11	2.03	0.56
1:U:133:MET:O	1:U:137:THR:HG22	2.06	0.56
7:L:309:DKA:C7	7:L:311:DKA:O2	2.53	0.56
3:C:150:THR:HG21	13:C:403:HOH:O	2.06	0.55
1:U:234:TRP:HA	1:U:237:LEU:HB2	1.89	0.55
3:W:22:LEU:O	5:Y:3:TYR:OH	2.21	0.55
2:M:400:GLU:CD	2:M:400:GLU:H	2.15	0.55
2:V:179:THR:OG1	2:V:181:GLU:OE1	2.22	0.55
3:N:136:ASP:OD1	3:N:152:SER:OG	2.24	0.55
2:V:400:GLU:CD	2:V:400:GLU:H	2.15	0.55
2:B:400:GLU:CD	2:B:400:GLU:H	2.15	0.55
1:L:234:TRP:HA	1:L:237:LEU:HB2	1.89	0.55
1:A:234:TRP:HA	1:A:237:LEU:HB2	1.89	0.55
3:N:150:THR:HG21	13:N:403:HOH:O	2.06	0.55
3:C:22:LEU:O	5:E:3:TYR:OH	2.21	0.55
9:B:502:ZP7:C01	7:B:506:DKA:H92	2.37	0.54
9:V:503:ZP7:C01	7:V:507:DKA:H92	2.37	0.54
2:V:418:THR:HG23	2:V:419:LYS:HG2	1.89	0.54
9:M:503:ZP7:C01	7:M:507:DKA:H92	2.37	0.54
3:W:136:ASP:OD1	3:W:152:SER:OG	2.24	0.54
7:C:307:DKA:C9	7:C:308:DKA:H91	2.34	0.54
3:N:22:LEU:O	5:P:3:TYR:OH	2.21	0.54
3:W:150:THR:HG21	13:W:403:HOH:O	2.06	0.54
7:L:310:DKA:H52	7:L:311:DKA:H41	1.89	0.53
7:A:310:DKA:H52	7:A:311:DKA:H41	1.89	0.53
2:M:418:THR:HG23	2:M:419:LYS:HG2	1.89	0.53
1:A:252:ARG:NH1	2:V:226:ALA:O	2.42	0.53
2:B:418:THR:HG23	2:B:419:LYS:HG2	1.89	0.53
3:W:28:TRP:HB3	11:W:301:A1EZI:C12	2.39	0.53
3:N:28:TRP:HB3	11:N:301:A1EZI:C12	2.39	0.52
3:C:28:TRP:HB3	11:C:301:A1EZI:C12	2.39	0.52
2:M:226:ALA:O	1:U:252:ARG:NH1	2.43	0.52
2:V:292:TYR:HE2	2:V:294:ASN:HD22	1.58	0.52
3:C:55:GLY:HA2	3:C:63:PHE:CD1	2.43	0.52
7:L:310:DKA:C4	7:L:311:DKA:C3	2.78	0.52
2:M:292:TYR:HE2	2:M:294:ASN:HD22	1.58	0.52
2:B:292:TYR:HE2	2:B:294:ASN:HD22	1.58	0.52
7:N:308:DKA:C9	7:N:309:DKA:H91	2.34	0.52
2:B:226:ALA:O	1:L:252:ARG:NH1	2.43	0.51
7:U:302:DKA:H52	7:U:303:DKA:H41	1.89	0.51
1:U:14:PRO:HG3	3:W:257:TRP:HB3	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:50:PHE:HZ	12:C:306:4AG:H202	1.76	0.51
3:C:56:MET:HE3	3:C:143:ILE:HG22	1.93	0.51
3:N:55:GLY:HA2	3:N:63:PHE:CD1	2.43	0.51
2:V:296:ASP:O	2:V:297:VAL:HG23	2.11	0.51
2:V:140:ARG:HD3	4:X:30:GLU:HB3	1.93	0.50
3:N:50:PHE:HZ	12:N:307:4AG:H202	1.76	0.50
2:V:229:ASP:HA	2:V:232:LEU:HD12	1.94	0.50
1:A:14:PRO:HG3	3:C:257:TRP:HB3	1.93	0.50
2:B:419:LYS:O	2:B:420:LEU:HB2	2.12	0.50
2:B:296:ASP:O	2:B:297:VAL:HG23	2.11	0.50
2:M:47:LEU:O	2:M:51:THR:OG1	2.30	0.50
2:B:47:LEU:O	2:B:51:THR:OG1	2.30	0.50
2:B:71:LYS:HG2	2:B:73:THR:HG23	1.94	0.50
3:C:161:PHE:HB3	3:C:162:PRO:HD3	1.94	0.50
2:M:229:ASP:HA	2:M:232:LEU:HD12	1.94	0.50
2:V:47:LEU:O	2:V:51:THR:OG1	2.30	0.50
3:W:55:GLY:HA2	3:W:63:PHE:CD1	2.43	0.50
3:W:75:MET:CE	11:W:303:A1EZI:C12	2.90	0.50
3:W:98:GLN:OE1	5:Y:10:ARG:NH1	2.45	0.50
3:N:98:GLN:OE1	5:P:10:ARG:NH1	2.45	0.50
2:B:140:ARG:HD3	4:D:30:GLU:HB3	1.93	0.50
3:C:75:MET:CE	11:C:303:A1EZI:C12	2.90	0.50
3:W:50:PHE:HZ	12:W:307:4AG:H202	1.76	0.50
2:M:140:ARG:HD3	4:O:30:GLU:HB3	1.93	0.49
3:W:56:MET:HE3	3:W:143:ILE:HG22	1.93	0.49
1:L:52:ASP:OD2	1:L:107:ARG:NH2	2.43	0.49
1:U:103:GLU:O	1:U:107:ARG:HG2	2.12	0.49
2:V:71:LYS:HG2	2:V:73:THR:HG23	1.94	0.49
1:A:103:GLU:O	1:A:107:ARG:HG2	2.12	0.49
1:L:14:PRO:HG3	3:N:257:TRP:HB3	1.93	0.49
3:N:161:PHE:HB3	3:N:162:PRO:HD3	1.94	0.49
7:U:302:DKA:H52	7:U:303:DKA:C4	2.40	0.49
2:M:296:ASP:O	2:M:297:VAL:HG23	2.11	0.49
3:C:98:GLN:OE1	5:E:10:ARG:NH1	2.45	0.49
3:N:75:MET:CE	11:N:303:A1EZI:C12	2.90	0.49
3:N:56:MET:HE3	3:N:143:ILE:HG22	1.93	0.49
1:U:224:ALA:O	1:U:228:MET:HG3	2.13	0.49
2:V:169:ASP:HA	4:X:21:ARG:HH21	1.78	0.49
2:V:419:LYS:O	2:V:420:LEU:HB2	2.12	0.49
2:M:297:VAL:HB	2:M:298:PRO:HD3	1.95	0.49
3:N:114:TRP:NE1	3:N:175:ALA:HB2	2.28	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:258:TYR:CE2	8:V:505:PLM:H71	2.48	0.49
1:A:224:ALA:O	1:A:228:MET:HG3	2.13	0.49
2:B:297:VAL:HB	2:B:298:PRO:HD3	1.95	0.49
3:C:250:SER:O	3:C:253:THR:HG22	2.12	0.49
2:M:71:LYS:HG2	2:M:73:THR:HG23	1.94	0.49
3:W:161:PHE:HB3	3:W:162:PRO:HD3	1.94	0.49
1:A:153:GLY:HA2	1:A:224:ALA:HB1	1.95	0.48
1:L:103:GLU:O	1:L:107:ARG:HG2	2.12	0.48
2:M:258:TYR:CE2	8:M:505:PLM:H71	2.48	0.48
3:W:114:TRP:NE1	3:W:175:ALA:HB2	2.28	0.48
2:B:169:ASP:HA	4:D:21:ARG:HH21	1.78	0.48
1:A:209:ARG:HH21	2:M:45:PRO:HG2	1.78	0.48
2:M:58:LYS:NZ	2:M:338:ASP:OD2	2.43	0.48
1:U:3:ARG:NH1	2:V:233:LEU:O	2.46	0.48
3:W:23:TRP:HA	3:W:109:LYS:HB2	1.96	0.48
2:B:229:ASP:HA	2:B:232:LEU:HD12	1.94	0.48
1:L:209:ARG:HH21	2:V:45:PRO:HG2	1.78	0.48
3:N:250:SER:O	3:N:253:THR:HG22	2.12	0.48
3:C:23:TRP:HA	3:C:109:LYS:HB2	1.96	0.48
3:C:88:TRP:NE1	5:E:17:GLU:OE1	2.47	0.48
1:L:224:ALA:O	1:L:228:MET:HG3	2.13	0.48
2:M:419:LYS:O	2:M:420:LEU:HB2	2.12	0.48
1:U:153:GLY:HA2	1:U:224:ALA:HB1	1.95	0.48
2:V:297:VAL:HB	2:V:298:PRO:HD3	1.95	0.48
1:L:3:ARG:NH1	2:M:233:LEU:O	2.46	0.48
1:L:211:PHE:CZ	3:W:208:GLU:HG3	2.49	0.48
3:W:250:SER:O	3:W:253:THR:HG22	2.12	0.48
1:A:52:ASP:OD2	1:A:107:ARG:NH2	2.43	0.48
3:C:114:TRP:NE1	3:C:175:ALA:HB2	2.28	0.48
2:B:45:PRO:HG2	1:U:209:ARG:HH21	1.78	0.48
2:M:169:ASP:HA	4:O:21:ARG:HH21	1.78	0.48
7:L:310:DKA:H52	7:L:311:DKA:C3	2.44	0.48
2:B:258:TYR:CE2	8:B:504:PLM:H71	2.48	0.47
1:U:20:MET:HE3	1:U:20:MET:HB3	1.75	0.47
8:V:502:PLM:HB1	8:V:502:PLM:HG3	1.96	0.47
1:A:211:PHE:CZ	3:N:208:GLU:HG3	2.49	0.47
7:A:310:DKA:H52	7:A:311:DKA:C4	2.40	0.47
3:C:30:LYS:HG2	11:C:302:A1EZI:O17	2.15	0.47
3:N:23:TRP:HA	3:N:109:LYS:HB2	1.96	0.47
3:W:30:LYS:HG2	11:W:302:A1EZI:O17	2.14	0.47
1:A:3:ARG:NH1	2:B:233:LEU:O	2.46	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:75:MET:HE1	11:C:303:A1EZI:C10	2.44	0.47
3:C:208:GLU:HG3	1:U:211:PHE:CZ	2.49	0.47
7:L:310:DKA:H52	7:L:311:DKA:C4	2.40	0.47
7:V:508:DKA:H51	7:V:508:DKA:H103	1.97	0.47
2:B:236:MET:CE	9:B:502:ZP7:C19	2.91	0.47
3:N:30:LYS:HG2	11:N:302:A1EZI:O17	2.14	0.47
7:A:310:DKA:H52	7:A:311:DKA:C3	2.44	0.47
3:N:75:MET:HE1	11:N:303:A1EZI:C12	2.45	0.47
3:N:88:TRP:NE1	5:P:17:GLU:OE1	2.47	0.47
3:W:75:MET:HE1	11:W:303:A1EZI:C10	2.44	0.47
3:W:75:MET:HE1	11:W:303:A1EZI:C12	2.45	0.47
1:A:80:TYR:HD2	1:A:235:TRP:CE2	2.33	0.47
1:A:104:TRP:CE3	7:A:308:DKA:H52	2.50	0.47
3:N:75:MET:HE1	11:N:303:A1EZI:C10	2.44	0.47
1:U:80:TYR:HD2	1:U:235:TRP:CE2	2.33	0.47
3:C:75:MET:HE1	11:C:303:A1EZI:C12	2.45	0.47
7:M:508:DKA:H103	7:M:508:DKA:H51	1.97	0.47
7:U:302:DKA:H52	7:U:303:DKA:C3	2.44	0.47
3:W:45:TRP:CZ2	12:W:307:4AG:H261	2.50	0.47
2:B:212:VAL:HG11	7:B:505:DKA:H62	1.97	0.47
1:L:153:GLY:HA2	1:L:224:ALA:HB1	1.95	0.47
1:U:104:TRP:CE3	7:U:310:DKA:H52	2.50	0.47
2:M:236:MET:CE	9:M:503:ZP7:C19	2.91	0.46
1:L:80:TYR:HD2	1:L:235:TRP:CE2	2.33	0.46
2:M:212:VAL:HG11	7:M:506:DKA:H62	1.97	0.46
8:M:502:PLM:HG3	8:M:502:PLM:HB1	1.96	0.46
2:V:58:LYS:NZ	2:V:338:ASP:OD2	2.43	0.46
3:C:45:TRP:CZ2	12:C:306:4AG:H261	2.50	0.46
8:B:501:PLM:HB1	8:B:501:PLM:HG3	1.96	0.46
7:U:310:DKA:O2	8:V:502:PLM:O2	2.34	0.46
7:A:308:DKA:O2	8:B:501:PLM:O2	2.34	0.46
1:L:104:TRP:CE3	7:L:308:DKA:H52	2.50	0.46
3:N:45:TRP:CZ2	12:N:307:4AG:H261	2.50	0.46
2:V:236:MET:CE	9:V:503:ZP7:C19	2.91	0.46
2:V:296:ASP:HB3	2:V:297:VAL:H	1.39	0.46
3:C:29:TYR:HB2	3:C:116:MET:HG2	1.98	0.46
3:C:75:MET:HE3	11:C:303:A1EZI:C11	2.46	0.46
3:W:88:TRP:NE1	5:Y:17:GLU:OE1	2.47	0.46
1:A:161:PRO:HD3	6:A:307:A1EZJ:O23	2.16	0.46
7:B:507:DKA:H103	7:B:507:DKA:H51	1.97	0.46
1:L:161:PRO:HD3	6:L:307:A1EZJ:O23	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:170:ASP:OD1	2:B:170:ASP:N	2.49	0.45
3:W:75:MET:HE3	11:W:303:A1EZI:C11	2.46	0.45
2:M:206:PHE:O	2:M:210:ILE:HG23	2.17	0.45
3:W:204:VAL:HG12	3:W:228:PHE:HE1	1.82	0.45
1:A:8:LEU:HD22	1:A:18:ILE:HG12	1.99	0.45
3:N:29:TYR:HB2	3:N:116:MET:HG2	1.98	0.45
1:L:8:LEU:HD22	1:L:18:ILE:HG12	1.99	0.45
7:L:308:DKA:O2	8:M:502:PLM:O2	2.34	0.45
7:L:309:DKA:H72	7:L:311:DKA:O2	2.17	0.45
3:N:75:MET:HE3	11:N:303:A1EZI:C11	2.46	0.45
1:U:161:PRO:HD3	6:U:309:A1EZJ:O23	2.16	0.45
3:W:29:TYR:HB2	3:W:116:MET:HG2	1.98	0.45
2:M:170:ASP:OD1	2:M:170:ASP:N	2.49	0.45
3:N:200:ILE:O	3:N:204:VAL:HG13	2.17	0.45
3:N:114:TRP:CE2	3:N:175:ALA:HB2	2.52	0.45
3:N:204:VAL:HG12	3:N:228:PHE:HE1	1.82	0.45
2:V:170:ASP:N	2:V:170:ASP:OD1	2.49	0.45
2:V:212:VAL:HG11	7:V:506:DKA:H62	1.97	0.45
7:A:309:DKA:H72	7:A:311:DKA:O2	2.17	0.45
2:B:206:PHE:O	2:B:210:ILE:HG23	2.17	0.45
3:C:200:ILE:O	3:C:204:VAL:HG13	2.17	0.44
1:A:180:LEU:O	13:A:402:HOH:O	2.21	0.44
2:B:168:TRP:HZ3	4:D:22:PRO:HG2	1.83	0.44
3:W:114:TRP:CE2	3:W:175:ALA:HB2	2.52	0.44
3:C:268:ARG:HA	3:C:268:ARG:HD3	1.75	0.44
3:C:114:TRP:CE2	3:C:175:ALA:HB2	2.52	0.44
3:N:111:TYR:CZ	3:N:248:ARG:HG2	2.53	0.44
2:V:105:ARG:HD3	2:V:108:THR:OG1	2.18	0.44
2:V:168:TRP:HZ3	4:X:22:PRO:HG2	1.83	0.44
2:V:206:PHE:O	2:V:210:ILE:HG23	2.17	0.44
2:B:58:LYS:NZ	2:B:338:ASP:OD2	2.43	0.44
3:C:64:ASP:HA	3:C:68:MET:HB2	2.00	0.44
3:C:111:TYR:CZ	3:C:248:ARG:HG2	2.53	0.44
3:C:122:ILE:HD13	3:C:122:ILE:HA	1.84	0.44
2:M:105:ARG:HD3	2:M:108:THR:OG1	2.18	0.44
3:W:28:TRP:O	11:W:301:A1EZI:C13	2.66	0.44
1:L:146:ILE:HD11	7:L:310:DKA:H52	2.00	0.44
2:M:168:TRP:HZ3	4:O:22:PRO:HG2	1.83	0.44
1:U:146:ILE:HD11	7:U:302:DKA:H52	2.00	0.44
1:U:180:LEU:O	13:U:402:HOH:O	2.21	0.44
2:B:296:ASP:HB3	2:B:297:VAL:H	1.39	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:111:TYR:CZ	3:W:248:ARG:HG2	2.53	0.44
3:N:28:TRP:O	11:N:301:A1EZI:C13	2.66	0.44
3:C:28:TRP:O	11:C:301:A1EZI:C13	2.66	0.44
3:C:204:VAL:HG12	3:C:228:PHE:HE1	1.82	0.44
1:L:80:TYR:OH	1:L:239:LYS:HD3	2.18	0.44
3:W:200:ILE:O	3:W:204:VAL:HG13	2.17	0.44
3:W:268:ARG:HA	3:W:268:ARG:HD3	1.75	0.44
5:Y:28:ALA:O	5:Y:32:ILE:HG22	2.18	0.43
1:A:181:LEU:HA	2:B:270:GLN:HG3	2.00	0.43
2:B:105:ARG:HD3	2:B:108:THR:OG1	2.18	0.43
2:M:335:LYS:HB3	2:M:335:LYS:HE3	1.74	0.43
5:P:28:ALA:O	5:P:32:ILE:HG22	2.18	0.43
1:U:8:LEU:HD22	1:U:18:ILE:HG12	1.99	0.43
7:U:301:DKA:H72	7:U:303:DKA:O2	2.17	0.43
3:N:64:ASP:HA	3:N:68:MET:HB2	2.00	0.43
1:U:181:LEU:HA	2:V:270:GLN:HG3	2.00	0.43
1:A:113:TRP:CZ3	4:D:21:ARG:N	2.87	0.43
1:L:113:TRP:CZ3	4:O:21:ARG:N	2.87	0.43
1:L:181:LEU:HA	2:M:270:GLN:HG3	2.00	0.43
1:U:80:TYR:OH	1:U:239:LYS:HD3	2.18	0.43
1:U:113:TRP:CZ3	4:X:21:ARG:N	2.87	0.43
3:W:223:PRO:HA	3:W:226:TRP:CD2	2.54	0.43
1:A:146:ILE:HD11	7:A:310:DKA:H52	2.00	0.43
3:W:64:ASP:HA	3:W:68:MET:HB2	2.00	0.43
7:W:308:DKA:H91	7:W:309:DKA:C9	2.40	0.43
2:B:335:LYS:HE3	2:B:335:LYS:HB3	1.74	0.43
2:V:218:LEU:HB3	2:V:219:PRO:HD3	2.01	0.43
3:W:140:HIS:NE2	3:W:146:ASP:OD2	2.52	0.43
2:B:297:VAL:HG12	2:B:298:PRO:N	2.34	0.42
5:E:28:ALA:O	5:E:32:ILE:HG22	2.18	0.42
3:N:223:PRO:HA	3:N:226:TRP:CD2	2.54	0.42
3:C:140:HIS:NE2	3:C:146:ASP:OD2	2.52	0.42
3:C:223:PRO:HA	3:C:226:TRP:CD2	2.54	0.42
3:N:140:HIS:NE2	3:N:146:ASP:OD2	2.52	0.42
2:B:218:LEU:HB3	2:B:219:PRO:HD3	2.01	0.42
1:U:9:LYS:HE3	1:U:9:LYS:HB3	1.80	0.42
1:U:16:GLU:HG3	3:W:18:TYR:CD2	2.55	0.42
1:A:20:MET:HE3	1:A:20:MET:HB3	1.75	0.42
1:A:109:TRP:O	3:C:48:ARG:NH2	2.46	0.42
1:L:16:GLU:HG3	3:N:18:TYR:CD2	2.55	0.42
1:U:22:ARG:HD2	1:U:22:ARG:HA	1.82	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:335:LYS:HB3	2:V:335:LYS:HE3	1.73	0.42
2:V:275:LYS:HA	13:V:628:HOH:O	2.20	0.42
1:A:16:GLU:HG3	3:C:18:TYR:CD2	2.55	0.42
2:V:297:VAL:HG12	2:V:298:PRO:N	2.34	0.42
1:U:52:ASP:OD2	1:U:107:ARG:NH2	2.43	0.42
3:W:224:LEU:CD1	8:W:310:PLM:HB2	2.50	0.42
2:M:417:PHE:O	2:M:418:THR:HG22	2.20	0.41
3:W:201:LEU:O	3:W:204:VAL:HG22	2.21	0.41
5:Y:16:LYS:HZ3	5:Y:16:LYS:HG2	1.66	0.41
1:A:80:TYR:OH	1:A:239:LYS:HD3	2.18	0.41
3:C:224:LEU:CD1	8:C:309:PLM:HB2	2.50	0.41
3:N:201:LEU:O	3:N:204:VAL:HG22	2.20	0.41
3:N:224:LEU:CD1	8:N:310:PLM:HB2	2.50	0.41
2:B:417:PHE:O	2:B:418:THR:HG22	2.20	0.41
2:B:234:ASP:HA	2:B:235:PRO:HD3	1.95	0.41
5:Y:7:THR:O	5:Y:11:GLU:HG2	2.21	0.41
3:W:26:SER:O	3:W:30:LYS:HG3	2.20	0.41
5:Y:5:GLU:O	5:Y:9:ARG:HG3	2.21	0.41
2:M:41:ARG:HH21	3:N:59:MET:HB2	1.85	0.41
2:M:218:LEU:HB3	2:M:219:PRO:HD3	2.01	0.41
2:M:297:VAL:HG12	2:M:298:PRO:N	2.34	0.41
3:N:26:SER:O	3:N:30:LYS:HG3	2.20	0.41
3:N:145:ARG:HD3	3:N:145:ARG:HA	1.84	0.41
2:M:275:LYS:HA	13:M:628:HOH:O	2.20	0.41
3:N:47:GLN:HE21	3:N:152:SER:HA	1.86	0.41
5:P:5:GLU:O	5:P:9:ARG:HG3	2.21	0.41
2:V:158:PRO:HG3	2:V:325:GLY:HA3	2.03	0.41
2:V:301:ALA:HB2	2:V:371:LYS:HD2	2.02	0.41
2:B:328:PHE:HB3	2:B:350:LEU:HB2	2.02	0.41
1:L:237:LEU:HD23	1:L:237:LEU:HA	1.85	0.41
2:M:328:PHE:HB3	2:M:350:LEU:HB2	2.02	0.41
3:N:181:LEU:HD11	3:N:269:ILE:HG13	2.03	0.41
2:V:328:PHE:HB3	2:V:350:LEU:HB2	2.02	0.41
3:W:47:GLN:HE21	3:W:152:SER:HA	1.86	0.41
3:W:92:THR:OG1	3:W:178:ARG:NH2	2.54	0.41
1:A:22:ARG:CZ	7:A:303:DKA:H31	2.51	0.41
3:C:115:LEU:HD23	3:C:115:LEU:HA	1.91	0.41
1:L:22:ARG:CZ	7:L:303:DKA:H31	2.51	0.41
3:C:26:SER:O	3:C:30:LYS:HG3	2.20	0.40
2:M:301:ALA:HB2	2:M:371:LYS:HD2	2.02	0.40
1:U:160:TYR:HB3	6:U:309:A1EZJ:O23	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:417:PHE:O	2:V:418:THR:HG22	2.20	0.40
3:N:19:ASP:HB3	3:N:22:LEU:HD12	2.03	0.40
3:N:268:ARG:HA	3:N:268:ARG:HD3	1.75	0.40
5:P:7:THR:O	5:P:11:GLU:HG2	2.21	0.40
2:V:41:ARG:HH21	3:W:59:MET:HB2	1.85	0.40
2:B:158:PRO:HG3	2:B:325:GLY:HA3	2.03	0.40
3:C:181:LEU:HD11	3:C:269:ILE:HG13	2.03	0.40
1:L:160:TYR:HB3	6:L:307:A1EZJ:O23	2.22	0.40
3:N:88:TRP:CZ2	5:P:18:ALA:HB2	2.57	0.40
2:B:41:ARG:HH21	3:C:59:MET:HB2	1.85	0.40
3:C:19:ASP:HB3	3:C:22:LEU:HD12	2.03	0.40
2:M:158:PRO:HG3	2:M:325:GLY:HA3	2.03	0.40
2:M:234:ASP:HA	2:M:235:PRO:HD3	1.95	0.40
3:N:92:THR:OG1	3:N:178:ARG:NH2	2.54	0.40
1:A:80:TYR:CE1	1:A:239:LYS:HA	2.57	0.40
2:B:275:LYS:HA	13:B:628:HOH:O	2.20	0.40
3:C:28:TRP:HB3	11:C:301:A1EZI:O17	2.19	0.40
3:C:47:GLN:HE21	3:C:152:SER:HA	1.86	0.40
3:C:201:LEU:O	3:C:204:VAL:HG22	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	272/274 (99%)	266 (98%)	6 (2%)	0	100	100
1	L	272/274 (99%)	266 (98%)	6 (2%)	0	100	100
1	U	272/274 (99%)	266 (98%)	6 (2%)	0	100	100
2	B	381/420 (91%)	372 (98%)	7 (2%)	2 (0%)	24	27
2	M	381/420 (91%)	372 (98%)	7 (2%)	2 (0%)	24	27

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	V	381/420 (91%)	372 (98%)	7 (2%)	2 (0%)	24	27
3	C	256/271 (94%)	244 (95%)	11 (4%)	1 (0%)	30	34
3	N	256/271 (94%)	244 (95%)	11 (4%)	1 (0%)	30	34
3	W	256/271 (94%)	244 (95%)	11 (4%)	1 (0%)	30	34
4	D	17/67 (25%)	16 (94%)	0	1 (6%)	1	0
4	O	17/67 (25%)	16 (94%)	0	1 (6%)	1	0
4	X	17/67 (25%)	16 (94%)	0	1 (6%)	1	0
5	E	37/45 (82%)	37 (100%)	0	0	100	100
5	P	37/45 (82%)	37 (100%)	0	0	100	100
5	Y	37/45 (82%)	37 (100%)	0	0	100	100
All	All	2889/3231 (89%)	2805 (97%)	72 (2%)	12 (0%)	31	34

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	297	VAL
2	M	297	VAL
2	V	297	VAL
2	B	418	THR
2	V	418	THR
3	C	145	ARG
2	M	418	THR
3	N	145	ARG
3	W	145	ARG
4	D	22	PRO
4	O	22	PRO
4	X	22	PRO

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	229/229 (100%)	223 (97%)	6 (3%)	40	54
1	L	229/229 (100%)	224 (98%)	5 (2%)	45	59
1	U	229/229 (100%)	223 (97%)	6 (3%)	40	54
2	B	321/348 (92%)	314 (98%)	7 (2%)	45	59
2	M	321/348 (92%)	314 (98%)	7 (2%)	45	59
2	V	321/348 (92%)	314 (98%)	7 (2%)	45	59
3	C	223/233 (96%)	217 (97%)	6 (3%)	39	52
3	N	223/233 (96%)	217 (97%)	6 (3%)	39	52
3	W	223/233 (96%)	216 (97%)	7 (3%)	35	47
4	D	16/52 (31%)	15 (94%)	1 (6%)	16	19
4	O	16/52 (31%)	15 (94%)	1 (6%)	16	19
4	X	16/52 (31%)	15 (94%)	1 (6%)	16	19
5	E	30/34 (88%)	28 (93%)	2 (7%)	15	17
5	P	30/34 (88%)	28 (93%)	2 (7%)	15	17
5	Y	30/34 (88%)	28 (93%)	2 (7%)	15	17
All	All	2457/2688 (91%)	2391 (97%)	66 (3%)	40	52

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	145	LEU
1	A	179	THR
1	A	207	SER
1	A	215	THR
1	A	254	ARG
1	A	259	GLU
2	B	130	GLU
2	B	242	MET
2	B	296	ASP
2	B	297	VAL
2	B	340	SER
2	B	356	SER
2	B	365	GLU
3	C	142	VAL
3	C	150	THR
3	C	218	GLU
3	C	224	LEU
3	C	231	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	266	ASN
4	D	21	ARG
5	E	11	GLU
5	E	36	ILE
1	L	179	THR
1	L	207	SER
1	L	215	THR
1	L	254	ARG
1	L	259	GLU
2	M	130	GLU
2	M	242	MET
2	M	296	ASP
2	M	297	VAL
2	M	340	SER
2	M	356	SER
2	M	365	GLU
3	N	142	VAL
3	N	150	THR
3	N	218	GLU
3	N	224	LEU
3	N	231	LEU
3	N	266	ASN
4	O	21	ARG
5	P	11	GLU
5	P	36	ILE
1	U	145	LEU
1	U	179	THR
1	U	207	SER
1	U	215	THR
1	U	254	ARG
1	U	259	GLU
2	V	130	GLU
2	V	242	MET
2	V	296	ASP
2	V	297	VAL
2	V	340	SER
2	V	356	SER
2	V	365	GLU
3	W	142	VAL
3	W	150	THR
3	W	199	MET
3	W	218	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	W	224	LEU
3	W	231	LEU
3	W	266	ASN
4	X	21	ARG
5	Y	11	GLU
5	Y	36	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	189	ASN
2	B	263	HIS
2	B	311	ASN
2	B	403	ASN
3	C	203	ASN
3	C	238	GLN
3	C	258	ASN
3	C	260	GLN
1	L	214	HIS
2	M	189	ASN
2	M	263	HIS
2	M	311	ASN
2	M	403	ASN
3	N	203	ASN
3	N	238	GLN
3	N	258	ASN
3	N	260	GLN
1	U	214	HIS
2	V	189	ASN
2	V	263	HIS
2	V	311	ASN
2	V	403	ASN
3	W	203	ASN
3	W	238	GLN
3	W	258	ASN
3	W	260	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 93 ligands modelled in this entry, 9 are monoatomic - leaving 84 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
8	PLM	B	501	-	17,17,17	0.54	0	17,17,17	1.36	1 (5%)
7	DKA	V	508	-	11,11,11	0.71	0	11,11,11	0.83	0
12	4AG	W	307	-	39,39,39	0.85	4 (10%)	41,41,41	0.87	2 (4%)
7	DKA	M	504	-	11,11,11	0.65	0	11,11,11	1.48	1 (9%)
7	DKA	U	301	-	11,11,11	0.68	0	11,11,11	0.87	1 (9%)
7	DKA	U	304	-	11,11,11	0.68	0	11,11,11	0.83	0
7	DKA	W	312	-	11,11,11	0.67	0	11,11,11	0.91	0
6	A1EZJ	U	309	-	47,48,48	0.95	2 (4%)	49,55,55	1.11	4 (8%)
7	DKA	L	309	-	11,11,11	0.68	0	11,11,11	0.87	1 (9%)
7	DKA	C	307	-	11,11,11	0.64	0	11,11,11	0.97	1 (9%)
6	A1EZJ	L	307	-	47,48,48	0.95	2 (4%)	49,55,55	1.11	4 (8%)
6	A1EZJ	A	307	-	47,48,48	0.95	2 (4%)	49,55,55	1.11	4 (8%)
9	ZP7	C	305	-	22,22,22	0.83	2 (9%)	23,23,23	0.73	1 (4%)
7	DKA	A	309	-	11,11,11	0.68	0	11,11,11	0.87	1 (9%)
7	DKA	U	306	-	11,11,11	0.60	0	11,11,11	0.94	1 (9%)
11	A1EZI	N	302	-	44,44,44	0.92	4 (9%)	47,49,49	0.90	2 (4%)
7	DKA	L	305	-	11,11,11	0.67	0	11,11,11	0.92	1 (9%)
11	A1EZI	C	301	-	44,44,44	0.93	3 (6%)	47,49,49	0.94	2 (4%)
7	DKA	L	310	-	11,11,11	0.66	0	11,11,11	0.91	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	DKA	M	506	-	11,11,11	0.66	0	11,11,11	0.92	0
7	DKA	W	311	-	11,11,11	0.66	0	11,11,11	0.93	0
11	A1EZI	C	302	-	44,44,44	0.92	4 (9%)	47,49,49	0.90	2 (4%)
7	DKA	L	303	-	11,11,11	0.66	0	11,11,11	0.92	0
11	A1EZI	N	301	-	44,44,44	0.93	3 (6%)	47,49,49	0.94	2 (4%)
7	DKA	A	303	-	11,11,11	0.65	0	11,11,11	0.92	0
7	DKA	N	309	-	11,11,11	0.68	0	11,11,11	0.88	0
7	DKA	N	308	-	11,11,11	0.64	0	11,11,11	0.97	1 (9%)
8	PLM	M	505	-	17,17,17	0.55	0	17,17,17	0.79	0
7	DKA	C	310	-	11,11,11	0.66	0	11,11,11	0.93	0
7	DKA	L	308	-	11,11,11	0.66	0	11,11,11	0.82	0
7	DKA	U	305	-	11,11,11	0.66	0	11,11,11	0.92	0
7	DKA	V	504	-	11,11,11	0.65	0	11,11,11	1.48	1 (9%)
7	DKA	L	311	-	11,11,11	0.59	0	11,11,11	0.97	1 (9%)
7	DKA	A	311	-	11,11,11	0.59	0	11,11,11	0.97	1 (9%)
12	4AG	N	307	-	39,39,39	0.85	4 (10%)	41,41,41	0.87	2 (4%)
7	DKA	L	304	-	11,11,11	0.60	0	11,11,11	0.94	1 (9%)
9	ZP7	B	502	-	22,22,22	0.81	2 (9%)	23,23,23	0.79	1 (4%)
7	DKA	U	302	-	11,11,11	0.66	0	11,11,11	0.91	0
12	4AG	C	306	-	39,39,39	0.85	4 (10%)	41,41,41	0.87	2 (4%)
7	DKA	U	308	-	11,11,11	0.63	0	11,11,11	0.88	0
9	ZP7	V	503	-	22,22,22	0.81	2 (9%)	23,23,23	0.78	1 (4%)
7	DKA	L	306	-	11,11,11	0.63	0	11,11,11	0.89	0
7	DKA	V	506	-	11,11,11	0.67	0	11,11,11	0.92	0
7	DKA	W	308	-	11,11,11	0.64	0	11,11,11	0.97	1 (9%)
7	DKA	B	506	-	11,11,11	0.66	0	11,11,11	0.91	0
7	DKA	A	305	-	11,11,11	0.68	0	11,11,11	0.92	1 (9%)
7	DKA	U	307	-	11,11,11	0.68	0	11,11,11	0.92	1 (9%)
9	ZP7	N	306	-	22,22,22	0.83	2 (9%)	23,23,23	0.73	1 (4%)
8	PLM	B	504	-	17,17,17	0.55	0	17,17,17	0.79	0
11	A1EZI	W	302	-	44,44,44	0.92	4 (9%)	47,49,49	0.90	2 (4%)
7	DKA	N	311	-	11,11,11	0.65	0	11,11,11	0.93	0
8	PLM	W	310	-	17,17,17	0.53	0	17,17,17	0.86	1 (5%)
7	DKA	L	302	-	11,11,11	0.68	0	11,11,11	0.83	0
7	DKA	C	311	-	11,11,11	0.67	0	11,11,11	0.91	0
7	DKA	A	306	-	11,11,11	0.63	0	11,11,11	0.89	0
7	DKA	A	308	-	11,11,11	0.66	0	11,11,11	0.82	0
11	A1EZI	N	303	-	44,44,44	0.92	4 (9%)	47,49,49	0.84	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	DKA	A	304	-	11,11,11	0.61	0	11,11,11	0.95	1 (9%)
7	DKA	U	310	-	11,11,11	0.66	0	11,11,11	0.82	0
6	A1EZJ	C	304	-	47,48,48	0.93	4 (8%)	49,55,55	1.04	3 (6%)
7	DKA	A	302	-	11,11,11	0.68	0	11,11,11	0.83	0
8	PLM	M	502	-	17,17,17	0.54	0	17,17,17	1.36	1 (5%)
8	PLM	V	502	-	17,17,17	0.53	0	17,17,17	1.36	1 (5%)
7	DKA	M	508	-	11,11,11	0.70	0	11,11,11	0.82	0
7	DKA	N	312	-	11,11,11	0.67	0	11,11,11	0.91	0
7	DKA	B	505	-	11,11,11	0.66	0	11,11,11	0.91	0
6	A1EZJ	L	301	-	47,48,48	0.92	4 (8%)	49,55,55	1.04	3 (6%)
7	DKA	V	507	-	11,11,11	0.67	0	11,11,11	0.92	0
7	DKA	C	308	-	11,11,11	0.68	0	11,11,11	0.88	0
11	A1EZI	W	301	-	44,44,44	0.92	3 (6%)	47,49,49	0.94	2 (4%)
11	A1EZI	C	303	-	44,44,44	0.93	4 (9%)	47,49,49	0.84	2 (4%)
6	A1EZJ	A	301	-	47,48,48	0.92	4 (8%)	49,55,55	1.04	3 (6%)
9	ZP7	M	503	-	22,22,22	0.80	2 (9%)	23,23,23	0.79	1 (4%)
7	DKA	B	507	-	11,11,11	0.71	0	11,11,11	0.83	0
8	PLM	N	310	-	17,17,17	0.53	0	17,17,17	0.86	1 (5%)
7	DKA	W	309	-	11,11,11	0.68	0	11,11,11	0.88	0
8	PLM	V	505	-	17,17,17	0.55	0	17,17,17	0.79	0
8	PLM	C	309	-	17,17,17	0.53	0	17,17,17	0.86	1 (5%)
11	A1EZI	W	303	-	44,44,44	0.93	4 (9%)	47,49,49	0.84	2 (4%)
9	ZP7	W	306	-	22,22,22	0.84	2 (9%)	23,23,23	0.73	1 (4%)
7	DKA	M	507	-	11,11,11	0.65	0	11,11,11	0.91	0
7	DKA	B	503	-	11,11,11	0.65	0	11,11,11	1.48	1 (9%)
7	DKA	A	310	-	11,11,11	0.66	0	11,11,11	0.91	0
7	DKA	U	303	-	11,11,11	0.59	0	11,11,11	0.97	1 (9%)

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
8	PLM	B	501	-	-	10/15/15/15	-
7	DKA	V	508	-	-	7/9/9/9	-
12	4AG	W	307	-	-	17/41/41/41	-
7	DKA	M	504	-	-	6/9/9/9	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	DKA	U	301	-	-	4/9/9/9	-
7	DKA	U	304	-	-	1/9/9/9	-
7	DKA	W	312	-	-	4/9/9/9	-
6	A1EZJ	U	309	-	-	26/54/54/54	-
7	DKA	L	309	-	-	4/9/9/9	-
7	DKA	C	307	-	-	5/9/9/9	-
6	A1EZJ	L	307	-	-	26/54/54/54	-
6	A1EZJ	A	307	-	-	26/54/54/54	-
9	ZP7	C	305	-	-	8/22/22/22	-
7	DKA	A	309	-	-	4/9/9/9	-
7	DKA	U	306	-	-	3/9/9/9	-
11	A1EZI	N	302	-	-	29/48/48/48	-
7	DKA	L	305	-	-	5/9/9/9	-
11	A1EZI	C	301	-	-	22/48/48/48	-
7	DKA	L	310	-	-	6/9/9/9	-
7	DKA	M	506	-	-	6/9/9/9	-
7	DKA	W	311	-	-	4/9/9/9	-
11	A1EZI	C	302	-	-	29/48/48/48	-
7	DKA	L	303	-	-	6/9/9/9	-
11	A1EZI	N	301	-	-	22/48/48/48	-
7	DKA	A	303	-	-	6/9/9/9	-
7	DKA	N	309	-	-	3/9/9/9	-
7	DKA	N	308	-	-	5/9/9/9	-
8	PLM	M	505	-	-	10/15/15/15	-
7	DKA	C	310	-	-	4/9/9/9	-
7	DKA	L	308	-	-	6/9/9/9	-
7	DKA	U	305	-	-	6/9/9/9	-
7	DKA	V	504	-	-	6/9/9/9	-
7	DKA	L	311	-	-	6/9/9/9	-
7	DKA	A	311	-	-	6/9/9/9	-
12	4AG	N	307	-	-	17/41/41/41	-
7	DKA	L	304	-	-	3/9/9/9	-
9	ZP7	B	502	-	-	15/22/22/22	-
7	DKA	U	302	-	-	6/9/9/9	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	4AG	C	306	-	-	17/41/41/41	-
7	DKA	U	308	-	-	5/9/9/9	-
9	ZP7	V	503	-	-	15/22/22/22	-
7	DKA	L	306	-	-	5/9/9/9	-
7	DKA	V	506	-	-	6/9/9/9	-
7	DKA	W	308	-	-	5/9/9/9	-
7	DKA	B	506	-	-	5/9/9/9	-
7	DKA	A	305	-	-	5/9/9/9	-
7	DKA	U	307	-	-	5/9/9/9	-
9	ZP7	N	306	-	-	8/22/22/22	-
8	PLM	B	504	-	-	10/15/15/15	-
11	A1EZI	W	302	-	-	29/48/48/48	-
7	DKA	N	311	-	-	4/9/9/9	-
8	PLM	W	310	-	-	8/15/15/15	-
7	DKA	L	302	-	-	1/9/9/9	-
7	DKA	C	311	-	-	4/9/9/9	-
7	DKA	A	306	-	-	5/9/9/9	-
7	DKA	A	308	-	-	6/9/9/9	-
11	A1EZI	N	303	-	-	25/48/48/48	-
7	DKA	A	304	-	-	3/9/9/9	-
7	DKA	U	310	-	-	6/9/9/9	-
6	A1EZJ	C	304	-	-	30/54/54/54	-
7	DKA	A	302	-	-	1/9/9/9	-
8	PLM	M	502	-	-	10/15/15/15	-
8	PLM	V	502	-	-	10/15/15/15	-
7	DKA	M	508	-	-	7/9/9/9	-
7	DKA	N	312	-	-	4/9/9/9	-
7	DKA	B	505	-	-	6/9/9/9	-
6	A1EZJ	L	301	-	-	30/54/54/54	-
7	DKA	V	507	-	-	5/9/9/9	-
7	DKA	C	308	-	-	3/9/9/9	-
11	A1EZI	W	301	-	-	22/48/48/48	-
11	A1EZI	C	303	-	-	25/48/48/48	-
6	A1EZJ	A	301	-	-	30/54/54/54	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	ZP7	M	503	-	-	15/22/22/22	-
7	DKA	B	507	-	-	7/9/9/9	-
8	PLM	N	310	-	-	8/15/15/15	-
7	DKA	W	309	-	-	3/9/9/9	-
8	PLM	V	505	-	-	10/15/15/15	-
8	PLM	C	309	-	-	8/15/15/15	-
11	A1EZI	W	303	-	-	25/48/48/48	-
9	ZP7	W	306	-	-	8/22/22/22	-
7	DKA	M	507	-	-	5/9/9/9	-
7	DKA	B	503	-	-	6/9/9/9	-
7	DKA	A	310	-	-	6/9/9/9	-
7	DKA	U	303	-	-	6/9/9/9	-

All (75) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	307	A1EZJ	O18-C19	-3.47	1.38	1.46
6	L	307	A1EZJ	O18-C19	-3.47	1.38	1.46
6	U	309	A1EZJ	O18-C19	-3.47	1.38	1.46
11	W	302	A1EZI	O28-C20	-2.92	1.39	1.46
11	C	302	A1EZI	O28-C20	-2.92	1.39	1.46
11	N	302	A1EZI	O28-C20	-2.91	1.39	1.46
11	W	303	A1EZI	O28-C20	-2.78	1.40	1.46
11	N	301	A1EZI	O28-C20	-2.77	1.40	1.46
11	N	303	A1EZI	O28-C20	-2.76	1.40	1.46
11	C	301	A1EZI	O28-C20	-2.75	1.40	1.46
11	C	303	A1EZI	O28-C20	-2.74	1.40	1.46
11	W	301	A1EZI	O28-C20	-2.73	1.40	1.46
11	W	301	A1EZI	O18-C19	-2.70	1.39	1.45
11	C	301	A1EZI	O18-C19	-2.69	1.39	1.45
11	N	301	A1EZI	O18-C19	-2.67	1.39	1.45
12	W	307	4AG	O21-C6	-2.55	1.40	1.46
12	N	307	4AG	O21-C6	-2.55	1.40	1.46
12	C	306	4AG	O21-C6	-2.54	1.40	1.46
6	U	309	A1EZJ	O21-C20	-2.47	1.39	1.45
6	A	307	A1EZJ	O21-C20	-2.45	1.39	1.45
6	L	307	A1EZJ	O21-C20	-2.44	1.39	1.45
6	C	304	A1EZJ	O18-C19	-2.41	1.40	1.46
6	A	301	A1EZJ	O18-C19	-2.41	1.40	1.46
9	W	306	ZP7	O18-C16	2.39	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	301	A1EZJ	O18-C19	-2.39	1.41	1.46
9	W	306	ZP7	O18-C19	-2.38	1.39	1.45
9	C	305	ZP7	O18-C16	2.37	1.40	1.33
9	N	306	ZP7	O18-C19	-2.37	1.39	1.45
9	C	305	ZP7	O18-C19	-2.37	1.39	1.45
11	W	303	A1EZI	O18-C16	2.37	1.40	1.33
9	N	306	ZP7	O18-C16	2.37	1.40	1.33
11	N	302	A1EZI	O18-C19	-2.37	1.39	1.45
11	C	303	A1EZI	O18-C16	2.36	1.40	1.33
6	C	304	A1EZJ	O21-C20	-2.35	1.39	1.45
11	W	302	A1EZI	O18-C19	-2.35	1.39	1.45
11	C	303	A1EZI	O18-C19	-2.35	1.39	1.45
6	A	301	A1EZJ	O21-C20	-2.34	1.39	1.45
9	B	502	ZP7	O18-C19	-2.34	1.39	1.45
6	L	301	A1EZJ	O21-C20	-2.34	1.39	1.45
11	N	303	A1EZI	O18-C16	2.34	1.40	1.33
9	V	503	ZP7	O18-C19	-2.34	1.39	1.45
12	N	307	4AG	O17-C16	2.34	1.40	1.33
11	N	303	A1EZI	O18-C19	-2.34	1.39	1.45
11	C	302	A1EZI	O18-C19	-2.33	1.40	1.45
11	W	303	A1EZI	O18-C19	-2.33	1.40	1.45
12	C	306	4AG	O17-C16	2.33	1.40	1.33
9	M	503	ZP7	O18-C19	-2.31	1.40	1.45
12	W	307	4AG	O17-C16	2.31	1.40	1.33
12	W	307	4AG	O17-C18	-2.27	1.40	1.45
12	N	307	4AG	O17-C18	-2.27	1.40	1.45
12	C	306	4AG	O17-C18	-2.26	1.40	1.45
6	C	304	A1EZJ	O21-C22	2.23	1.39	1.33
6	A	301	A1EZJ	O21-C22	2.23	1.39	1.33
6	L	301	A1EZJ	O21-C22	2.22	1.39	1.33
9	V	503	ZP7	O18-C16	2.22	1.39	1.33
12	W	307	4AG	O21-C22	2.21	1.40	1.34
6	A	301	A1EZJ	O18-C16	2.21	1.40	1.34
6	L	301	A1EZJ	O18-C16	2.20	1.40	1.34
6	C	304	A1EZJ	O18-C16	2.20	1.40	1.34
9	B	502	ZP7	O18-C16	2.20	1.39	1.33
11	W	302	A1EZI	O18-C16	2.19	1.39	1.33
11	N	302	A1EZI	O18-C16	2.18	1.39	1.33
12	C	306	4AG	O21-C22	2.18	1.40	1.34
12	N	307	4AG	O21-C22	2.18	1.40	1.34
9	M	503	ZP7	O18-C16	2.18	1.39	1.33
11	C	302	A1EZI	O18-C16	2.18	1.39	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	W	302	A1EZI	O28-C29	2.16	1.40	1.34
11	N	302	A1EZI	O28-C29	2.15	1.40	1.34
11	C	302	A1EZI	O28-C29	2.14	1.40	1.34
11	W	301	A1EZI	O18-C16	2.10	1.39	1.33
11	C	301	A1EZI	O18-C16	2.09	1.39	1.33
11	N	301	A1EZI	O18-C16	2.09	1.39	1.33
11	C	303	A1EZI	P23-O26	2.05	1.65	1.58
11	N	303	A1EZI	P23-O26	2.03	1.65	1.58
11	W	303	A1EZI	P23-O26	2.03	1.65	1.58

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	502	PLM	C6-C5-C4	4.52	137.19	114.37
8	B	501	PLM	C6-C5-C4	4.51	137.18	114.37
8	V	502	PLM	C6-C5-C4	4.51	137.15	114.37
7	M	504	DKA	C8-C7-C6	3.87	133.94	114.37
7	B	503	DKA	C8-C7-C6	3.87	133.91	114.37
7	V	504	DKA	C8-C7-C6	3.87	133.91	114.37
6	A	307	A1EZJ	O18-C16-C15	3.71	119.52	111.48
6	U	309	A1EZJ	O18-C16-C15	3.71	119.51	111.48
11	C	302	A1EZI	O28-C29-C31	3.71	119.51	111.48
11	N	302	A1EZI	O28-C29-C31	3.70	119.48	111.48
6	L	307	A1EZJ	O18-C16-C15	3.70	119.48	111.48
11	W	302	A1EZI	O28-C29-C31	3.70	119.48	111.48
11	W	301	A1EZI	O28-C29-C31	3.60	119.26	111.48
11	N	301	A1EZI	O28-C29-C31	3.58	119.24	111.48
11	C	301	A1EZI	O28-C29-C31	3.58	119.23	111.48
11	N	303	A1EZI	O28-C29-C31	3.56	119.18	111.48
11	W	303	A1EZI	O28-C29-C31	3.55	119.17	111.48
11	C	303	A1EZI	O28-C29-C31	3.55	119.15	111.48
6	A	301	A1EZJ	O43-C44-C45	3.46	111.08	108.06
6	C	304	A1EZJ	O18-C16-C15	3.46	118.96	111.48
6	L	301	A1EZJ	O18-C16-C15	3.46	118.96	111.48
6	A	301	A1EZJ	O18-C16-C15	3.45	118.95	111.48
6	L	301	A1EZJ	O43-C44-C45	3.43	111.05	108.06
6	C	304	A1EZJ	O43-C44-C45	3.42	111.04	108.06
12	C	306	4AG	O21-C22-C23	3.38	118.78	111.48
12	W	307	4AG	O21-C22-C23	3.37	118.76	111.48
12	N	307	4AG	O21-C22-C23	3.36	118.75	111.48
6	U	309	A1EZJ	C19-O18-C16	-3.30	109.89	117.80
6	L	307	A1EZJ	C19-O18-C16	-3.30	109.90	117.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	307	A1EZJ	C19-O18-C16	-3.30	109.90	117.80
6	L	301	A1EZJ	O21-C22-C24	3.00	120.99	111.83
6	A	301	A1EZJ	O21-C22-C24	3.00	120.98	111.83
6	C	304	A1EZJ	O21-C22-C24	2.99	120.95	111.83
6	U	309	A1EZJ	O21-C22-C24	2.93	120.77	111.83
6	A	307	A1EZJ	O21-C22-C24	2.91	120.72	111.83
6	L	307	A1EZJ	O21-C22-C24	2.91	120.72	111.83
11	W	302	A1EZI	O18-C16-C15	2.87	120.58	111.83
11	C	301	A1EZI	O18-C16-C15	2.86	120.55	111.83
11	N	301	A1EZI	O18-C16-C15	2.86	120.54	111.83
11	N	302	A1EZI	O18-C16-C15	2.86	120.54	111.83
11	C	302	A1EZI	O18-C16-C15	2.85	120.54	111.83
11	W	301	A1EZI	O18-C16-C15	2.84	120.50	111.83
12	W	307	4AG	O17-C16-C15	2.44	119.26	111.83
12	C	306	4AG	O17-C16-C15	2.42	119.21	111.83
12	N	307	4AG	O17-C16-C15	2.41	119.19	111.83
9	B	502	ZP7	O18-C16-C15	2.41	119.17	111.83
9	M	503	ZP7	O18-C16-C15	2.39	119.13	111.83
9	V	503	ZP7	O18-C16-C15	2.38	119.09	111.83
11	C	303	A1EZI	O18-C16-C15	2.37	119.08	111.83
11	W	303	A1EZI	O18-C16-C15	2.37	119.06	111.83
11	N	303	A1EZI	O18-C16-C15	2.36	119.05	111.83
9	W	306	ZP7	O18-C16-C15	2.30	118.86	111.83
9	C	305	ZP7	O18-C16-C15	2.30	118.85	111.83
9	N	306	ZP7	O18-C16-C15	2.30	118.85	111.83
7	W	308	DKA	O2-C1-C2	2.08	120.59	114.00
7	N	308	DKA	O2-C1-C2	2.08	120.57	114.00
7	C	307	DKA	O2-C1-C2	2.08	120.56	114.00
8	W	310	PLM	O1-C1-C2	2.06	120.50	114.00
8	C	309	PLM	O1-C1-C2	2.05	120.49	114.00
7	L	311	DKA	O2-C1-C2	2.05	120.47	114.00
8	N	310	PLM	O1-C1-C2	2.05	120.47	114.00
6	U	309	A1EZJ	O21-C22-O23	-2.05	118.51	123.63
7	U	303	DKA	O2-C1-C2	2.05	120.46	114.00
7	A	311	DKA	O2-C1-C2	2.04	120.45	114.00
7	U	301	DKA	O2-C1-C2	2.03	120.42	114.00
7	L	309	DKA	O2-C1-C2	2.03	120.42	114.00
6	L	307	A1EZJ	O21-C22-O23	-2.03	118.55	123.63
6	A	307	A1EZJ	O21-C22-O23	-2.03	118.56	123.63
7	A	304	DKA	O2-C1-C2	2.02	120.39	114.00
7	A	309	DKA	O2-C1-C2	2.02	120.39	114.00
7	L	304	DKA	O2-C1-C2	2.02	120.38	114.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	305	DKA	O2-C1-C2	2.01	120.35	114.00
7	U	306	DKA	O2-C1-C2	2.01	120.35	114.00
7	A	305	DKA	O2-C1-C2	2.00	120.33	114.00
7	U	307	DKA	O2-C1-C2	2.00	120.33	114.00

There are no chirality outliers.

All (846) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	301	A1EZJ	C15-C16-O18-C19
6	A	301	A1EZJ	O17-C16-O18-C19
6	A	301	A1EZJ	C44-C45-C46-O47
6	A	301	A1EZJ	C44-C45-C46-O48
6	A	307	A1EZJ	C15-C16-O18-C19
6	A	307	A1EZJ	C44-O43-P40-O42
6	C	304	A1EZJ	C15-C16-O18-C19
6	C	304	A1EZJ	O17-C16-O18-C19
6	C	304	A1EZJ	C44-C45-C46-O47
6	C	304	A1EZJ	C44-C45-C46-O48
6	L	301	A1EZJ	C15-C16-O18-C19
6	L	301	A1EZJ	O17-C16-O18-C19
6	L	301	A1EZJ	C44-C45-C46-O47
6	L	301	A1EZJ	C44-C45-C46-O48
6	L	307	A1EZJ	C15-C16-O18-C19
6	L	307	A1EZJ	C44-O43-P40-O42
6	U	309	A1EZJ	C15-C16-O18-C19
6	U	309	A1EZJ	C44-O43-P40-O42
11	C	301	A1EZI	C31-C29-O28-C20
11	C	301	A1EZI	C21-O22-P23-O24
11	C	301	A1EZI	C21-O22-P23-O26
11	C	302	A1EZI	C21-O22-P23-O24
11	C	302	A1EZI	C21-O22-P23-O25
11	C	302	A1EZI	C21-O22-P23-O26
11	C	302	A1EZI	C27-O26-P23-O25
11	N	301	A1EZI	C31-C29-O28-C20
11	N	301	A1EZI	C21-O22-P23-O24
11	N	301	A1EZI	C21-O22-P23-O26
11	N	302	A1EZI	C21-O22-P23-O24
11	N	302	A1EZI	C21-O22-P23-O25
11	N	302	A1EZI	C21-O22-P23-O26
11	N	302	A1EZI	C27-O26-P23-O25
11	W	301	A1EZI	C31-C29-O28-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	W	301	A1EZI	C21-O22-P23-O24
11	W	301	A1EZI	C21-O22-P23-O26
11	W	302	A1EZI	C21-O22-P23-O24
11	W	302	A1EZI	C21-O22-P23-O25
11	W	302	A1EZI	C21-O22-P23-O26
11	W	302	A1EZI	C27-O26-P23-O25
11	C	301	A1EZI	O17-C16-O18-C19
11	N	301	A1EZI	O17-C16-O18-C19
11	W	301	A1EZI	O17-C16-O18-C19
11	C	301	A1EZI	C15-C16-O18-C19
11	N	301	A1EZI	C15-C16-O18-C19
11	W	301	A1EZI	C15-C16-O18-C19
6	A	301	A1EZJ	O23-C22-O21-C20
6	C	304	A1EZJ	O23-C22-O21-C20
6	L	301	A1EZJ	O23-C22-O21-C20
11	C	302	A1EZI	O17-C16-O18-C19
11	N	302	A1EZI	O17-C16-O18-C19
11	W	302	A1EZI	O17-C16-O18-C19
6	A	307	A1EZJ	O17-C16-O18-C19
6	L	307	A1EZJ	O17-C16-O18-C19
6	U	309	A1EZJ	O17-C16-O18-C19
11	C	301	A1EZI	O30-C29-O28-C20
11	C	303	A1EZI	O30-C29-O28-C20
11	N	301	A1EZI	O30-C29-O28-C20
11	N	303	A1EZI	O30-C29-O28-C20
11	W	301	A1EZI	O30-C29-O28-C20
11	W	303	A1EZI	O30-C29-O28-C20
11	C	302	A1EZI	C15-C16-O18-C19
11	N	302	A1EZI	C15-C16-O18-C19
11	W	302	A1EZI	C15-C16-O18-C19
11	C	303	A1EZI	C31-C29-O28-C20
11	N	303	A1EZI	C31-C29-O28-C20
11	W	303	A1EZI	C31-C29-O28-C20
6	A	301	A1EZJ	C24-C22-O21-C20
6	C	304	A1EZJ	C24-C22-O21-C20
6	L	301	A1EZJ	C24-C22-O21-C20
9	B	502	ZP7	C15-C16-O18-C19
9	M	503	ZP7	C15-C16-O18-C19
9	V	503	ZP7	C15-C16-O18-C19
11	C	303	A1EZI	C15-C16-O18-C19
11	N	303	A1EZI	C15-C16-O18-C19
11	W	303	A1EZI	C15-C16-O18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	B	502	ZP7	O17-C16-O18-C19
9	M	503	ZP7	O17-C16-O18-C19
9	V	503	ZP7	O17-C16-O18-C19
11	C	303	A1EZI	O17-C16-O18-C19
11	N	303	A1EZI	O17-C16-O18-C19
11	W	303	A1EZI	O17-C16-O18-C19
11	C	303	A1EZI	C20-C21-O22-P23
11	N	303	A1EZI	C20-C21-O22-P23
11	W	303	A1EZI	C20-C21-O22-P23
6	A	307	A1EZJ	C24-C22-O21-C20
6	L	307	A1EZJ	C24-C22-O21-C20
6	U	309	A1EZJ	C24-C22-O21-C20
6	A	307	A1EZJ	O23-C22-O21-C20
6	L	307	A1EZJ	O23-C22-O21-C20
6	U	309	A1EZJ	O23-C22-O21-C20
7	B	505	DKA	C1-C2-C3-C4
7	M	506	DKA	C1-C2-C3-C4
7	V	506	DKA	C1-C2-C3-C4
6	A	307	A1EZJ	C32-C33-C34-C35
6	L	307	A1EZJ	C32-C33-C34-C35
6	U	309	A1EZJ	C32-C33-C34-C35
9	B	502	ZP7	O18-C19-C20-O23
9	M	503	ZP7	O18-C19-C20-O23
9	V	503	ZP7	O18-C19-C20-O23
7	A	303	DKA	C1-C2-C3-C4
7	L	303	DKA	C1-C2-C3-C4
7	U	305	DKA	C1-C2-C3-C4
12	C	306	4AG	C22-C23-C24-C25
12	N	307	4AG	C22-C23-C24-C25
12	W	307	4AG	C22-C23-C24-C25
11	C	301	A1EZI	C12-C13-C14-C15
11	N	301	A1EZI	C12-C13-C14-C15
11	W	301	A1EZI	C12-C13-C14-C15
6	A	301	A1EZJ	C13-C14-C15-C16
6	C	304	A1EZJ	C13-C14-C15-C16
6	L	301	A1EZJ	C13-C14-C15-C16
9	B	502	ZP7	C19-C20-C21-O22
9	M	503	ZP7	C19-C20-C21-O22
9	V	503	ZP7	C19-C20-C21-O22
11	W	302	A1EZI	C04-C05-C06-C07
11	C	302	A1EZI	C04-C05-C06-C07
11	C	303	A1EZI	C03-C04-C05-C06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	N	302	A1EZI	C04-C05-C06-C07
11	N	303	A1EZI	C03-C04-C05-C06
11	W	303	A1EZI	C03-C04-C05-C06
7	B	503	DKA	C5-C6-C7-C8
7	M	504	DKA	C5-C6-C7-C8
8	B	501	PLM	C4-C5-C6-C7
8	V	502	PLM	C4-C5-C6-C7
7	V	504	DKA	C5-C6-C7-C8
8	M	502	PLM	C4-C5-C6-C7
12	C	306	4AG	C05-C06-C07-C08
12	N	307	4AG	C05-C06-C07-C08
12	W	307	4AG	C05-C06-C07-C08
7	A	309	DKA	C4-C5-C6-C7
7	L	309	DKA	C4-C5-C6-C7
7	U	301	DKA	C4-C5-C6-C7
8	B	504	PLM	CA-CB-CC-CD
8	M	505	PLM	CA-CB-CC-CD
8	V	505	PLM	CA-CB-CC-CD
9	B	502	ZP7	O23-C20-C21-O22
9	M	503	ZP7	O23-C20-C21-O22
9	V	503	ZP7	O23-C20-C21-O22
6	A	307	A1EZJ	C05-C06-C07-C08
6	L	307	A1EZJ	C05-C06-C07-C08
6	U	309	A1EZJ	C05-C06-C07-C08
11	C	302	A1EZI	C08-C09-C10-C11
11	C	303	A1EZI	C33-C34-C35-C36
11	N	302	A1EZI	C08-C09-C10-C11
11	N	303	A1EZI	C33-C34-C35-C36
11	W	302	A1EZI	C08-C09-C10-C11
11	W	303	A1EZI	C33-C34-C35-C36
7	A	304	DKA	C3-C4-C5-C6
7	L	304	DKA	C3-C4-C5-C6
7	U	306	DKA	C3-C4-C5-C6
11	C	301	A1EZI	C36-C37-C38-C39
11	N	301	A1EZI	C36-C37-C38-C39
6	A	301	A1EZJ	C29-C30-C31-C32
6	C	304	A1EZJ	C29-C30-C31-C32
6	L	301	A1EZJ	C29-C30-C31-C32
7	C	307	DKA	C3-C4-C5-C6
7	N	308	DKA	C3-C4-C5-C6
7	W	308	DKA	C6-C7-C8-C9
8	M	505	PLM	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	C	305	ZP7	C10-C11-C12-C13
9	W	306	ZP7	C10-C11-C12-C13
11	W	301	A1EZI	C36-C37-C38-C39
6	A	301	A1EZJ	C27-C28-C29-C30
6	C	304	A1EZJ	C27-C28-C29-C30
6	L	301	A1EZJ	C27-C28-C29-C30
7	C	307	DKA	C6-C7-C8-C9
7	N	308	DKA	C6-C7-C8-C9
7	W	308	DKA	C3-C4-C5-C6
8	B	504	PLM	C6-C7-C8-C9
8	V	505	PLM	C6-C7-C8-C9
9	N	306	ZP7	C10-C11-C12-C13
12	W	307	4AG	C29-C30-C31-C32
12	C	306	4AG	C02-C03-C04-C05
12	C	306	4AG	C29-C30-C31-C32
12	N	307	4AG	C02-C03-C04-C05
12	N	307	4AG	C29-C30-C31-C32
12	W	307	4AG	C02-C03-C04-C05
11	C	303	A1EZI	C39-C40-C41-C42
11	N	303	A1EZI	C39-C40-C41-C42
11	W	303	A1EZI	C39-C40-C41-C42
6	A	301	A1EZJ	C33-C34-C35-C36
6	C	304	A1EZJ	C33-C34-C35-C36
6	L	301	A1EZJ	C33-C34-C35-C36
11	C	301	A1EZI	C08-C09-C10-C11
7	B	503	DKA	C6-C7-C8-C9
7	M	504	DKA	C6-C7-C8-C9
7	V	504	DKA	C6-C7-C8-C9
11	C	302	A1EZI	C12-C13-C14-C15
11	N	301	A1EZI	C08-C09-C10-C11
11	N	302	A1EZI	C12-C13-C14-C15
11	W	301	A1EZI	C08-C09-C10-C11
11	W	302	A1EZI	C12-C13-C14-C15
12	C	306	4AG	C31-C32-C33-C34
12	N	307	4AG	C31-C32-C33-C34
12	W	307	4AG	C31-C32-C33-C34
7	N	311	DKA	C4-C5-C6-C7
7	C	310	DKA	C4-C5-C6-C7
7	W	311	DKA	C4-C5-C6-C7
11	C	301	A1EZI	C09-C10-C11-C12
11	N	301	A1EZI	C09-C10-C11-C12
11	W	301	A1EZI	C09-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	A	307	A1EZJ	C03-C04-C05-C06
6	L	307	A1EZJ	C03-C04-C05-C06
6	U	309	A1EZJ	C03-C04-C05-C06
11	N	301	A1EZI	C03-C04-C05-C06
11	C	302	A1EZI	C31-C29-O28-C20
11	N	302	A1EZI	C31-C29-O28-C20
11	W	302	A1EZI	C31-C29-O28-C20
11	C	301	A1EZI	C03-C04-C05-C06
11	W	301	A1EZI	C03-C04-C05-C06
7	C	311	DKA	C3-C4-C5-C6
7	W	312	DKA	C3-C4-C5-C6
7	N	312	DKA	C3-C4-C5-C6
11	C	301	A1EZI	C04-C05-C06-C07
11	C	301	A1EZI	C06-C07-C08-C09
11	N	301	A1EZI	C04-C05-C06-C07
11	N	301	A1EZI	C06-C07-C08-C09
11	W	301	A1EZI	C04-C05-C06-C07
11	W	301	A1EZI	C06-C07-C08-C09
11	C	303	A1EZI	C32-C33-C34-C35
11	N	301	A1EZI	C32-C33-C34-C35
11	N	303	A1EZI	C32-C33-C34-C35
11	W	301	A1EZI	C32-C33-C34-C35
11	W	303	A1EZI	C32-C33-C34-C35
9	C	305	ZP7	C13-C14-C15-C16
9	N	306	ZP7	C13-C14-C15-C16
9	W	306	ZP7	C13-C14-C15-C16
11	C	301	A1EZI	C32-C33-C34-C35
11	N	302	A1EZI	C39-C40-C41-C42
11	W	302	A1EZI	C39-C40-C41-C42
11	C	302	A1EZI	C39-C40-C41-C42
7	A	305	DKA	C2-C3-C4-C5
7	L	305	DKA	C2-C3-C4-C5
7	U	307	DKA	C2-C3-C4-C5
9	B	502	ZP7	C12-C13-C14-C15
9	M	503	ZP7	C12-C13-C14-C15
9	V	503	ZP7	C12-C13-C14-C15
11	C	302	A1EZI	C10-C11-C12-C13
11	N	302	A1EZI	C10-C11-C12-C13
11	W	302	A1EZI	C10-C11-C12-C13
7	A	302	DKA	C3-C4-C5-C6
7	L	302	DKA	C3-C4-C5-C6
7	U	304	DKA	C3-C4-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	B	502	ZP7	C13-C14-C15-C16
9	M	503	ZP7	C13-C14-C15-C16
8	C	309	PLM	CC-CD-CE-CF
8	N	310	PLM	CC-CD-CE-CF
8	W	310	PLM	CC-CD-CE-CF
9	V	503	ZP7	C13-C14-C15-C16
11	N	302	A1EZI	C40-C41-C42-C43
11	W	302	A1EZI	C40-C41-C42-C43
7	A	311	DKA	C3-C4-C5-C6
7	L	311	DKA	C3-C4-C5-C6
11	C	302	A1EZI	C40-C41-C42-C43
7	C	308	DKA	C2-C3-C4-C5
7	N	309	DKA	C2-C3-C4-C5
7	U	303	DKA	C3-C4-C5-C6
7	W	309	DKA	C2-C3-C4-C5
11	W	302	A1EZI	C29-C31-C32-C33
9	B	502	ZP7	C07-C08-C09-C10
9	M	503	ZP7	C07-C08-C09-C10
9	V	503	ZP7	C07-C08-C09-C10
7	B	503	DKA	C1-C2-C3-C4
7	M	504	DKA	C1-C2-C3-C4
7	V	504	DKA	C1-C2-C3-C4
11	C	301	A1EZI	C29-C31-C32-C33
11	C	302	A1EZI	C29-C31-C32-C33
11	N	301	A1EZI	C29-C31-C32-C33
11	N	302	A1EZI	C29-C31-C32-C33
11	W	301	A1EZI	C29-C31-C32-C33
12	C	306	4AG	C08-C09-C10-C11
12	N	307	4AG	C08-C09-C10-C11
12	W	307	4AG	C08-C09-C10-C11
8	B	501	PLM	CB-CC-CD-CE
8	M	502	PLM	CB-CC-CD-CE
8	V	502	PLM	C3-C4-C5-C6
6	A	301	A1EZJ	C08-C09-C10-C11
6	C	304	A1EZJ	C08-C09-C10-C11
6	L	301	A1EZJ	C08-C09-C10-C11
8	B	501	PLM	C3-C4-C5-C6
8	V	502	PLM	CB-CC-CD-CE
6	A	301	A1EZJ	C11-C12-C13-C14
6	C	304	A1EZJ	C11-C12-C13-C14
6	L	301	A1EZJ	C11-C12-C13-C14
8	M	502	PLM	C3-C4-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	A	306	DKA	C5-C6-C7-C8
7	L	306	DKA	C5-C6-C7-C8
7	U	308	DKA	C5-C6-C7-C8
7	W	309	DKA	C5-C6-C7-C8
7	C	308	DKA	C5-C6-C7-C8
7	N	309	DKA	C5-C6-C7-C8
8	M	502	PLM	C2-C3-C4-C5
8	B	501	PLM	C2-C3-C4-C5
8	V	502	PLM	C2-C3-C4-C5
11	N	302	A1EZI	C02-C03-C04-C05
11	W	302	A1EZI	C02-C03-C04-C05
6	A	301	A1EZJ	C05-C06-C07-C08
6	C	304	A1EZJ	C05-C06-C07-C08
6	L	301	A1EZJ	C05-C06-C07-C08
11	C	302	A1EZI	C02-C03-C04-C05
11	C	302	A1EZI	C13-C14-C15-C16
11	N	302	A1EZI	C13-C14-C15-C16
11	W	302	A1EZI	C13-C14-C15-C16
9	C	305	ZP7	C15-C16-O18-C19
9	N	306	ZP7	C15-C16-O18-C19
9	W	306	ZP7	C15-C16-O18-C19
9	B	502	ZP7	C10-C11-C12-C13
9	M	503	ZP7	C10-C11-C12-C13
9	V	503	ZP7	C10-C11-C12-C13
11	C	302	A1EZI	O30-C29-O28-C20
11	N	302	A1EZI	O30-C29-O28-C20
11	W	302	A1EZI	O30-C29-O28-C20
7	A	308	DKA	C1-C2-C3-C4
7	L	308	DKA	C1-C2-C3-C4
7	U	310	DKA	C1-C2-C3-C4
9	C	305	ZP7	O17-C16-O18-C19
9	N	306	ZP7	O17-C16-O18-C19
9	W	306	ZP7	O17-C16-O18-C19
7	L	303	DKA	C3-C4-C5-C6
7	A	303	DKA	C3-C4-C5-C6
7	U	305	DKA	C3-C4-C5-C6
11	C	301	A1EZI	C19-C20-O28-C29
11	N	301	A1EZI	C19-C20-O28-C29
11	W	301	A1EZI	C19-C20-O28-C29
9	M	503	ZP7	C04-C05-C06-C07
12	C	306	4AG	C32-C33-C34-C35
12	N	307	4AG	C32-C33-C34-C35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
12	W	307	4AG	C32-C33-C34-C35
9	B	502	ZP7	C04-C05-C06-C07
9	V	503	ZP7	C04-C05-C06-C07
6	A	307	A1EZJ	O18-C19-C38-O39
6	L	307	A1EZJ	O18-C19-C38-O39
6	U	309	A1EZJ	O18-C19-C38-O39
6	A	301	A1EZJ	C25-C26-C27-C28
6	C	304	A1EZJ	C25-C26-C27-C28
6	L	301	A1EZJ	C25-C26-C27-C28
7	A	305	DKA	C3-C4-C5-C6
7	L	305	DKA	C3-C4-C5-C6
7	A	308	DKA	C7-C8-C9-C10
7	L	308	DKA	C7-C8-C9-C10
7	U	310	DKA	C7-C8-C9-C10
7	U	307	DKA	C3-C4-C5-C6
8	N	310	PLM	C6-C7-C8-C9
6	A	301	A1EZJ	C01-C02-C03-C04
6	L	301	A1EZJ	C01-C02-C03-C04
7	L	306	DKA	C7-C8-C9-C10
7	U	308	DKA	C7-C8-C9-C10
8	C	309	PLM	C6-C7-C8-C9
6	C	304	A1EZJ	C01-C02-C03-C04
7	A	306	DKA	C7-C8-C9-C10
8	W	310	PLM	C6-C7-C8-C9
7	B	503	DKA	C3-C4-C5-C6
7	M	504	DKA	C3-C4-C5-C6
7	V	504	DKA	C3-C4-C5-C6
8	B	501	PLM	C9-CA-CB-CC
8	M	502	PLM	C9-CA-CB-CC
7	L	310	DKA	C7-C8-C9-C10
7	U	302	DKA	C7-C8-C9-C10
12	C	306	4AG	C23-C22-O21-C6
12	N	307	4AG	C23-C22-O21-C6
7	A	310	DKA	C7-C8-C9-C10
8	V	502	PLM	C9-CA-CB-CC
9	C	305	ZP7	C07-C08-C09-C10
9	N	306	ZP7	C07-C08-C09-C10
9	W	306	ZP7	C07-C08-C09-C10
11	N	303	A1EZI	C05-C06-C07-C08
11	C	303	A1EZI	C05-C06-C07-C08
11	W	303	A1EZI	C05-C06-C07-C08
6	C	304	A1EZJ	C34-C35-C36-C37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	A	301	A1EZJ	C34-C35-C36-C37
6	L	301	A1EZJ	C34-C35-C36-C37
6	A	301	A1EZJ	C09-C10-C11-C12
6	L	301	A1EZJ	C09-C10-C11-C12
6	C	304	A1EZJ	C09-C10-C11-C12
7	V	508	DKA	C7-C8-C9-C10
7	B	507	DKA	C7-C8-C9-C10
7	M	508	DKA	C7-C8-C9-C10
11	C	301	A1EZI	C01-C02-C03-C04
11	N	301	A1EZI	C01-C02-C03-C04
11	W	301	A1EZI	C01-C02-C03-C04
9	B	502	ZP7	C11-C12-C13-C14
9	M	503	ZP7	C11-C12-C13-C14
9	V	503	ZP7	C11-C12-C13-C14
11	C	301	A1EZI	C40-C41-C42-C43
11	N	301	A1EZI	C40-C41-C42-C43
11	W	301	A1EZI	C40-C41-C42-C43
7	A	311	DKA	C4-C5-C6-C7
7	L	311	DKA	C4-C5-C6-C7
7	U	303	DKA	C4-C5-C6-C7
8	B	504	PLM	C9-CA-CB-CC
8	V	505	PLM	C9-CA-CB-CC
11	C	303	A1EZI	C19-C20-C21-O22
11	N	303	A1EZI	C19-C20-C21-O22
11	W	303	A1EZI	C19-C20-C21-O22
12	W	307	4AG	C23-C22-O21-C6
8	M	505	PLM	C9-CA-CB-CC
11	C	303	A1EZI	C08-C09-C10-C11
11	C	301	A1EZI	C10-C11-C12-C13
11	N	301	A1EZI	C10-C11-C12-C13
11	W	303	A1EZI	C08-C09-C10-C11
11	N	303	A1EZI	C08-C09-C10-C11
11	W	301	A1EZI	C10-C11-C12-C13
6	A	307	A1EZJ	C30-C31-C32-C33
6	L	307	A1EZJ	C30-C31-C32-C33
6	U	309	A1EZJ	C30-C31-C32-C33
8	B	501	PLM	CD-CE-CF-CG
8	V	502	PLM	CD-CE-CF-CG
7	B	505	DKA	C5-C6-C7-C8
7	M	506	DKA	C5-C6-C7-C8
7	V	506	DKA	C5-C6-C7-C8
8	M	502	PLM	CD-CE-CF-CG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	C	302	A1EZI	C34-C35-C36-C37
11	W	302	A1EZI	C34-C35-C36-C37
11	N	302	A1EZI	C34-C35-C36-C37
11	C	302	A1EZI	C38-C39-C40-C41
11	N	302	A1EZI	C38-C39-C40-C41
11	W	302	A1EZI	C38-C39-C40-C41
11	C	303	A1EZI	C10-C11-C12-C13
11	N	303	A1EZI	C10-C11-C12-C13
11	W	303	A1EZI	C10-C11-C12-C13
7	U	302	DKA	C4-C5-C6-C7
7	L	310	DKA	C4-C5-C6-C7
7	A	310	DKA	C4-C5-C6-C7
6	C	304	A1EZJ	C28-C29-C30-C31
7	A	311	DKA	C7-C8-C9-C10
7	L	311	DKA	C7-C8-C9-C10
7	U	303	DKA	C7-C8-C9-C10
6	A	301	A1EZJ	C28-C29-C30-C31
6	L	301	A1EZJ	C28-C29-C30-C31
7	A	311	DKA	C5-C6-C7-C8
7	L	311	DKA	C5-C6-C7-C8
7	U	303	DKA	C5-C6-C7-C8
11	C	301	A1EZI	C33-C34-C35-C36
11	W	301	A1EZI	C33-C34-C35-C36
11	N	301	A1EZI	C33-C34-C35-C36
11	C	302	A1EZI	C32-C33-C34-C35
11	N	302	A1EZI	C32-C33-C34-C35
11	W	302	A1EZI	C32-C33-C34-C35
12	C	306	4AG	C26-C27-C28-C29
12	N	307	4AG	C26-C27-C28-C29
12	W	307	4AG	C26-C27-C28-C29
8	B	504	PLM	C1-C2-C3-C4
8	M	505	PLM	C1-C2-C3-C4
8	V	505	PLM	C1-C2-C3-C4
6	A	307	A1EZJ	C01-C02-C03-C04
6	L	307	A1EZJ	C01-C02-C03-C04
6	U	309	A1EZJ	C01-C02-C03-C04
7	A	308	DKA	C2-C3-C4-C5
7	L	308	DKA	C2-C3-C4-C5
7	U	310	DKA	C2-C3-C4-C5
8	C	309	PLM	C9-CA-CB-CC
8	N	310	PLM	C9-CA-CB-CC
8	W	310	PLM	C9-CA-CB-CC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	L	307	A1EZJ	C29-C30-C31-C32
6	U	309	A1EZJ	C29-C30-C31-C32
6	A	307	A1EZJ	C29-C30-C31-C32
6	A	301	A1EZJ	C20-C19-O18-C16
6	C	304	A1EZJ	C20-C19-O18-C16
6	L	301	A1EZJ	C20-C19-O18-C16
11	C	303	A1EZI	C21-C20-O28-C29
11	N	303	A1EZI	C21-C20-O28-C29
11	W	303	A1EZI	C21-C20-O28-C29
7	L	304	DKA	C7-C8-C9-C10
7	N	312	DKA	C7-C8-C9-C10
7	W	312	DKA	C7-C8-C9-C10
7	A	304	DKA	C7-C8-C9-C10
7	C	311	DKA	C7-C8-C9-C10
7	U	306	DKA	C7-C8-C9-C10
11	N	303	A1EZI	C37-C38-C39-C40
11	C	303	A1EZI	C37-C38-C39-C40
11	W	303	A1EZI	C37-C38-C39-C40
12	C	306	4AG	O38-C22-O21-C6
12	N	307	4AG	O38-C22-O21-C6
12	W	307	4AG	O38-C22-O21-C6
11	C	302	A1EZI	O28-C20-C21-O22
11	N	302	A1EZI	O28-C20-C21-O22
11	W	302	A1EZI	O28-C20-C21-O22
12	C	306	4AG	C10-C11-C12-C13
12	W	307	4AG	C10-C11-C12-C13
12	N	307	4AG	C10-C11-C12-C13
7	A	303	DKA	C5-C6-C7-C8
7	U	305	DKA	C5-C6-C7-C8
7	L	303	DKA	C5-C6-C7-C8
6	A	301	A1EZJ	C04-C05-C06-C07
6	C	304	A1EZJ	C04-C05-C06-C07
6	L	301	A1EZJ	C04-C05-C06-C07
8	V	505	PLM	C5-C6-C7-C8
8	B	504	PLM	C5-C6-C7-C8
8	M	505	PLM	C5-C6-C7-C8
9	C	305	ZP7	C03-C04-C05-C06
9	N	306	ZP7	C03-C04-C05-C06
9	W	306	ZP7	C03-C04-C05-C06
6	A	307	A1EZJ	C45-C44-O43-P40
6	L	307	A1EZJ	C45-C44-O43-P40
6	U	309	A1EZJ	C45-C44-O43-P40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	L	307	A1EZJ	C04-C05-C06-C07
6	U	309	A1EZJ	C04-C05-C06-C07
6	A	307	A1EZJ	C04-C05-C06-C07
8	M	505	PLM	CD-CE-CF-CG
7	B	505	DKA	C3-C4-C5-C6
8	B	504	PLM	CD-CE-CF-CG
8	V	505	PLM	CD-CE-CF-CG
7	V	506	DKA	C3-C4-C5-C6
7	M	506	DKA	C3-C4-C5-C6
7	A	310	DKA	C1-C2-C3-C4
7	L	310	DKA	C1-C2-C3-C4
7	U	302	DKA	C1-C2-C3-C4
7	B	507	DKA	C3-C4-C5-C6
7	M	508	DKA	C3-C4-C5-C6
7	V	508	DKA	C3-C4-C5-C6
6	A	307	A1EZJ	C20-C19-C38-O39
6	L	307	A1EZJ	C20-C19-C38-O39
6	U	309	A1EZJ	C20-C19-C38-O39
7	A	306	DKA	C2-C3-C4-C5
7	L	306	DKA	C2-C3-C4-C5
7	U	308	DKA	C2-C3-C4-C5
12	C	306	4AG	C23-C24-C25-C26
12	W	307	4AG	C23-C24-C25-C26
11	C	303	A1EZI	O28-C20-C21-O22
11	N	303	A1EZI	O28-C20-C21-O22
11	W	303	A1EZI	O28-C20-C21-O22
12	N	307	4AG	C23-C24-C25-C26
6	L	307	A1EZJ	C22-C24-C25-C26
9	B	502	ZP7	C01-C02-C03-C04
9	M	503	ZP7	C01-C02-C03-C04
9	V	503	ZP7	C01-C02-C03-C04
6	A	307	A1EZJ	C22-C24-C25-C26
6	U	309	A1EZJ	C22-C24-C25-C26
6	A	307	A1EZJ	C44-O43-P40-O39
6	A	307	A1EZJ	C44-O43-P40-O41
6	L	307	A1EZJ	C44-O43-P40-O39
6	L	307	A1EZJ	C44-O43-P40-O41
6	U	309	A1EZJ	C44-O43-P40-O39
6	U	309	A1EZJ	C44-O43-P40-O41
11	C	303	A1EZI	C21-O22-P23-O24
11	C	303	A1EZI	C21-O22-P23-O25
11	C	303	A1EZI	C21-O22-P23-O26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	N	303	A1EZI	C21-O22-P23-O24
11	N	303	A1EZI	C21-O22-P23-O25
11	N	303	A1EZI	C21-O22-P23-O26
11	W	303	A1EZI	C21-O22-P23-O24
11	W	303	A1EZI	C21-O22-P23-O25
11	W	303	A1EZI	C21-O22-P23-O26
6	A	301	A1EZJ	C32-C33-C34-C35
6	C	304	A1EZJ	C32-C33-C34-C35
6	L	301	A1EZJ	C32-C33-C34-C35
12	N	307	4AG	C12-C13-C14-C15
12	C	306	4AG	C12-C13-C14-C15
12	W	307	4AG	C12-C13-C14-C15
12	W	307	4AG	C13-C14-C15-C16
8	C	309	PLM	C3-C4-C5-C6
8	N	310	PLM	C3-C4-C5-C6
8	W	310	PLM	C3-C4-C5-C6
7	A	303	DKA	C7-C8-C9-C10
7	L	303	DKA	C7-C8-C9-C10
7	U	305	DKA	C7-C8-C9-C10
12	C	306	4AG	C13-C14-C15-C16
12	N	307	4AG	C13-C14-C15-C16
11	N	303	A1EZI	C13-C14-C15-C16
11	N	301	A1EZI	C35-C36-C37-C38
11	C	301	A1EZI	C35-C36-C37-C38
11	C	303	A1EZI	C13-C14-C15-C16
11	W	303	A1EZI	C13-C14-C15-C16
11	W	301	A1EZI	C35-C36-C37-C38
6	A	307	A1EZJ	C07-C08-C09-C10
6	U	309	A1EZJ	C07-C08-C09-C10
9	B	502	ZP7	C05-C06-C07-C08
9	V	503	ZP7	C05-C06-C07-C08
6	L	307	A1EZJ	C07-C08-C09-C10
9	M	503	ZP7	C05-C06-C07-C08
7	U	306	DKA	C5-C6-C7-C8
7	A	304	DKA	C5-C6-C7-C8
7	L	304	DKA	C5-C6-C7-C8
7	B	507	DKA	C1-C2-C3-C4
7	M	508	DKA	C1-C2-C3-C4
7	V	508	DKA	C1-C2-C3-C4
6	A	301	A1EZJ	C06-C07-C08-C09
6	L	301	A1EZJ	C06-C07-C08-C09
6	C	304	A1EZJ	C06-C07-C08-C09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	A	307	A1EZJ	C11-C12-C13-C14
6	L	307	A1EZJ	C11-C12-C13-C14
6	U	309	A1EZJ	C11-C12-C13-C14
11	N	302	A1EZI	C19-C20-C21-O22
11	W	302	A1EZI	C19-C20-C21-O22
7	B	505	DKA	C2-C3-C4-C5
7	M	506	DKA	C2-C3-C4-C5
7	V	506	DKA	C2-C3-C4-C5
11	C	302	A1EZI	C09-C10-C11-C12
7	W	309	DKA	C3-C4-C5-C6
11	N	302	A1EZI	C09-C10-C11-C12
11	W	302	A1EZI	C09-C10-C11-C12
7	C	308	DKA	C3-C4-C5-C6
7	N	309	DKA	C3-C4-C5-C6
9	W	306	ZP7	C12-C13-C14-C15
9	C	305	ZP7	C12-C13-C14-C15
9	N	306	ZP7	C12-C13-C14-C15
7	M	507	DKA	C3-C4-C5-C6
6	L	301	A1EZJ	C31-C32-C33-C34
7	B	506	DKA	C3-C4-C5-C6
7	V	507	DKA	C2-C3-C4-C5
6	C	304	A1EZJ	C31-C32-C33-C34
7	B	506	DKA	C2-C3-C4-C5
7	M	507	DKA	C2-C3-C4-C5
7	V	507	DKA	C3-C4-C5-C6
6	A	301	A1EZJ	C31-C32-C33-C34
8	V	502	PLM	C6-C7-C8-C9
8	B	501	PLM	C6-C7-C8-C9
7	A	308	DKA	C4-C5-C6-C7
7	U	310	DKA	C4-C5-C6-C7
7	V	507	DKA	C6-C7-C8-C9
8	M	502	PLM	C6-C7-C8-C9
7	B	506	DKA	C6-C7-C8-C9
7	L	308	DKA	C4-C5-C6-C7
7	M	507	DKA	C6-C7-C8-C9
7	U	307	DKA	C4-C5-C6-C7
7	A	305	DKA	C4-C5-C6-C7
7	L	305	DKA	C4-C5-C6-C7
7	A	306	DKA	O1-C1-C2-C3
7	L	306	DKA	O1-C1-C2-C3
7	M	506	DKA	O2-C1-C2-C3
7	U	308	DKA	O1-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	V	506	DKA	O2-C1-C2-C3
8	B	504	PLM	C8-C9-CA-CB
7	B	505	DKA	O2-C1-C2-C3
8	V	505	PLM	C8-C9-CA-CB
8	M	505	PLM	C8-C9-CA-CB
8	B	504	PLM	C2-C3-C4-C5
7	B	505	DKA	O1-C1-C2-C3
7	M	506	DKA	O1-C1-C2-C3
8	C	309	PLM	O2-C1-C2-C3
8	N	310	PLM	O2-C1-C2-C3
8	W	310	PLM	O2-C1-C2-C3
8	M	505	PLM	C2-C3-C4-C5
8	V	505	PLM	C2-C3-C4-C5
11	W	302	A1EZI	C05-C06-C07-C08
7	A	303	DKA	O1-C1-C2-C3
7	L	303	DKA	O1-C1-C2-C3
7	L	306	DKA	O2-C1-C2-C3
7	U	305	DKA	O1-C1-C2-C3
7	V	506	DKA	O1-C1-C2-C3
11	C	302	A1EZI	C05-C06-C07-C08
11	N	302	A1EZI	C05-C06-C07-C08
7	A	306	DKA	O2-C1-C2-C3
7	U	308	DKA	O2-C1-C2-C3
7	A	305	DKA	C7-C8-C9-C10
7	L	305	DKA	C7-C8-C9-C10
7	C	311	DKA	C6-C7-C8-C9
7	N	312	DKA	C6-C7-C8-C9
7	W	312	DKA	C6-C7-C8-C9
7	U	307	DKA	C7-C8-C9-C10
11	C	302	A1EZI	C19-C20-C21-O22
7	M	504	DKA	O1-C1-C2-C3
7	A	311	DKA	O1-C1-C2-C3
7	B	503	DKA	O1-C1-C2-C3
7	B	503	DKA	O2-C1-C2-C3
7	L	311	DKA	O1-C1-C2-C3
7	M	504	DKA	O2-C1-C2-C3
7	U	303	DKA	O1-C1-C2-C3
7	V	504	DKA	O2-C1-C2-C3
7	V	504	DKA	O1-C1-C2-C3
9	V	503	ZP7	C09-C10-C11-C12
9	B	502	ZP7	C09-C10-C11-C12
9	M	503	ZP7	C09-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	A	307	A1EZJ	C27-C28-C29-C30
6	L	307	A1EZJ	C27-C28-C29-C30
6	U	309	A1EZJ	C27-C28-C29-C30
7	A	311	DKA	O2-C1-C2-C3
7	L	311	DKA	O2-C1-C2-C3
7	U	303	DKA	O2-C1-C2-C3
11	N	302	A1EZI	C41-C42-C43-C44
11	C	302	A1EZI	C41-C42-C43-C44
11	W	302	A1EZI	C41-C42-C43-C44
7	A	303	DKA	O2-C1-C2-C3
7	L	303	DKA	O2-C1-C2-C3
7	U	305	DKA	O2-C1-C2-C3
7	B	507	DKA	O2-C1-C2-C3
7	M	508	DKA	O2-C1-C2-C3
7	V	508	DKA	O2-C1-C2-C3
8	B	501	PLM	O1-C1-C2-C3
8	M	502	PLM	O1-C1-C2-C3
8	V	502	PLM	O1-C1-C2-C3
7	L	310	DKA	O2-C1-C2-C3
7	U	302	DKA	O2-C1-C2-C3
9	M	503	ZP7	C02-C03-C04-C05
7	W	311	DKA	C7-C8-C9-C10
9	V	503	ZP7	C02-C03-C04-C05
7	C	310	DKA	C7-C8-C9-C10
9	B	502	ZP7	C02-C03-C04-C05
7	A	310	DKA	O2-C1-C2-C3
8	C	309	PLM	O1-C1-C2-C3
8	W	310	PLM	O1-C1-C2-C3
7	N	311	DKA	C7-C8-C9-C10
8	N	310	PLM	O1-C1-C2-C3
11	C	303	A1EZI	C01-C02-C03-C04
11	N	303	A1EZI	C01-C02-C03-C04
6	A	301	A1EZJ	C20-C19-C38-O39
6	C	304	A1EZJ	C20-C19-C38-O39
6	L	301	A1EZJ	C20-C19-C38-O39
7	M	508	DKA	C2-C3-C4-C5
7	B	507	DKA	C4-C5-C6-C7
7	M	508	DKA	C4-C5-C6-C7
11	W	303	A1EZI	C01-C02-C03-C04
7	B	507	DKA	C2-C3-C4-C5
7	V	508	DKA	C2-C3-C4-C5
7	V	508	DKA	C4-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	L	310	DKA	O1-C1-C2-C3
7	U	302	DKA	O1-C1-C2-C3
7	A	310	DKA	O1-C1-C2-C3
8	M	502	PLM	O2-C1-C2-C3
7	B	507	DKA	O1-C1-C2-C3
7	C	307	DKA	O2-C1-C2-C3
7	C	310	DKA	O1-C1-C2-C3
7	N	311	DKA	O1-C1-C2-C3
7	W	308	DKA	O2-C1-C2-C3
7	W	311	DKA	O1-C1-C2-C3
8	B	501	PLM	O2-C1-C2-C3
8	V	502	PLM	O2-C1-C2-C3
7	M	508	DKA	O1-C1-C2-C3
7	N	308	DKA	O2-C1-C2-C3
7	V	508	DKA	O1-C1-C2-C3
12	N	307	4AG	C24-C25-C26-C27
12	W	307	4AG	C24-C25-C26-C27
7	C	310	DKA	O2-C1-C2-C3
7	N	311	DKA	O2-C1-C2-C3
7	W	311	DKA	O2-C1-C2-C3
12	C	306	4AG	C24-C25-C26-C27
11	W	302	A1EZI	C42-C43-C44-C45
7	A	305	DKA	C6-C7-C8-C9
7	L	305	DKA	C6-C7-C8-C9
7	U	307	DKA	C6-C7-C8-C9
11	C	302	A1EZI	C42-C43-C44-C45
11	N	302	A1EZI	C42-C43-C44-C45
7	C	307	DKA	O1-C1-C2-C3
7	N	308	DKA	O1-C1-C2-C3
7	W	308	DKA	O1-C1-C2-C3
8	B	504	PLM	O2-C1-C2-C3
8	M	505	PLM	O2-C1-C2-C3
8	V	505	PLM	O2-C1-C2-C3
7	L	309	DKA	C2-C3-C4-C5
7	U	301	DKA	C2-C3-C4-C5
7	A	309	DKA	C2-C3-C4-C5
8	N	310	PLM	C4-C5-C6-C7
11	N	301	A1EZI	C41-C42-C43-C44
11	W	301	A1EZI	C41-C42-C43-C44
8	C	309	PLM	C4-C5-C6-C7
11	C	301	A1EZI	C41-C42-C43-C44
8	W	310	PLM	C4-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	U	301	DKA	C7-C8-C9-C10
7	A	309	DKA	C7-C8-C9-C10
7	L	309	DKA	C7-C8-C9-C10
11	C	302	A1EZI	O28-C29-C31-C32
11	W	302	A1EZI	O28-C29-C31-C32
8	B	504	PLM	O1-C1-C2-C3
8	M	505	PLM	O1-C1-C2-C3
8	V	505	PLM	O1-C1-C2-C3
11	N	302	A1EZI	O28-C29-C31-C32
7	C	307	DKA	C2-C3-C4-C5
7	N	308	DKA	C2-C3-C4-C5
7	W	308	DKA	C2-C3-C4-C5
8	N	310	PLM	CA-CB-CC-CD
8	C	309	PLM	CA-CB-CC-CD
8	W	310	PLM	CA-CB-CC-CD
11	C	303	A1EZI	O28-C29-C31-C32
11	N	303	A1EZI	O28-C29-C31-C32
11	W	303	A1EZI	O28-C29-C31-C32
6	A	307	A1EZJ	O43-C44-C45-N49
6	L	307	A1EZJ	O43-C44-C45-N49
6	U	309	A1EZJ	O43-C44-C45-N49
11	N	303	A1EZI	C35-C36-C37-C38
11	C	303	A1EZI	C35-C36-C37-C38
11	W	303	A1EZI	C35-C36-C37-C38
12	C	306	4AG	C09-C10-C11-C12
12	N	307	4AG	C09-C10-C11-C12
12	W	307	4AG	C09-C10-C11-C12
6	A	307	A1EZJ	O21-C22-C24-C25
6	L	307	A1EZJ	O21-C22-C24-C25
6	U	309	A1EZJ	O21-C22-C24-C25
7	A	308	DKA	O2-C1-C2-C3
7	L	308	DKA	O2-C1-C2-C3
7	U	310	DKA	O2-C1-C2-C3
12	W	307	4AG	C27-C28-C29-C30
12	C	306	4AG	C27-C28-C29-C30
12	N	307	4AG	C27-C28-C29-C30
6	A	301	A1EZJ	C19-C38-O39-P40
6	C	304	A1EZJ	C19-C38-O39-P40
6	L	301	A1EZJ	C19-C38-O39-P40
11	C	303	A1EZI	C06-C07-C08-C09
11	W	303	A1EZI	C06-C07-C08-C09
8	M	502	PLM	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	B	501	PLM	C5-C6-C7-C8
6	A	301	A1EZJ	C26-C27-C28-C29
8	V	502	PLM	C5-C6-C7-C8
9	W	306	ZP7	C11-C12-C13-C14
9	C	305	ZP7	C11-C12-C13-C14
11	N	303	A1EZI	C06-C07-C08-C09
6	C	304	A1EZJ	C26-C27-C28-C29
6	L	301	A1EZJ	C26-C27-C28-C29
9	N	306	ZP7	C11-C12-C13-C14
6	A	307	A1EZJ	C10-C11-C12-C13
6	L	307	A1EZJ	C10-C11-C12-C13
6	U	309	A1EZJ	C10-C11-C12-C13
6	A	301	A1EZJ	C10-C11-C12-C13
6	C	304	A1EZJ	C10-C11-C12-C13
6	L	301	A1EZJ	C10-C11-C12-C13
11	C	302	A1EZI	C19-C20-O28-C29
11	N	302	A1EZI	C19-C20-O28-C29
11	W	302	A1EZI	C19-C20-O28-C29
7	L	309	DKA	C6-C7-C8-C9
7	A	309	DKA	C6-C7-C8-C9
6	A	301	A1EZJ	C24-C25-C26-C27
6	L	301	A1EZJ	C24-C25-C26-C27
6	C	304	A1EZJ	C24-C25-C26-C27
7	U	301	DKA	C6-C7-C8-C9
7	A	310	DKA	C2-C3-C4-C5
7	U	302	DKA	C2-C3-C4-C5
7	L	310	DKA	C2-C3-C4-C5
7	A	308	DKA	O1-C1-C2-C3
7	L	308	DKA	O1-C1-C2-C3
7	U	310	DKA	O1-C1-C2-C3
6	L	307	A1EZJ	O23-C22-C24-C25
6	A	307	A1EZJ	O23-C22-C24-C25
6	U	309	A1EZJ	O23-C22-C24-C25
11	C	303	A1EZI	C09-C10-C11-C12
7	B	506	DKA	O1-C1-C2-C3
11	N	303	A1EZI	C09-C10-C11-C12
11	W	303	A1EZI	C09-C10-C11-C12
6	A	307	A1EZJ	O18-C19-C20-O21
6	L	307	A1EZJ	O18-C19-C20-O21
6	U	309	A1EZJ	O18-C19-C20-O21
7	M	507	DKA	O1-C1-C2-C3
7	V	507	DKA	O1-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	C	302	A1EZI	O30-C29-C31-C32
11	W	302	A1EZI	O30-C29-C31-C32
11	N	302	A1EZI	O30-C29-C31-C32
6	A	301	A1EZJ	N49-C45-C46-O47
6	C	304	A1EZJ	N49-C45-C46-O47
6	L	301	A1EZJ	N49-C45-C46-O47
7	M	507	DKA	C5-C6-C7-C8
6	A	301	A1EZJ	N49-C45-C46-O48
6	C	304	A1EZJ	N49-C45-C46-O48
6	L	301	A1EZJ	N49-C45-C46-O48
7	V	507	DKA	C5-C6-C7-C8
7	B	506	DKA	C5-C6-C7-C8
7	W	312	DKA	C5-C6-C7-C8
7	C	311	DKA	C5-C6-C7-C8
7	N	312	DKA	C5-C6-C7-C8

There are no ring outliers.

57 monomers are involved in 172 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	501	PLM	3	0
7	V	508	DKA	1	0
12	W	307	4AG	4	0
7	U	301	DKA	5	0
6	U	309	A1EZJ	2	0
7	L	309	DKA	5	0
7	C	307	DKA	2	0
6	L	307	A1EZJ	2	0
6	A	307	A1EZJ	1	0
7	A	309	DKA	5	0
11	N	302	A1EZI	4	0
11	C	301	A1EZI	6	0
7	L	310	DKA	15	0
7	M	506	DKA	1	0
11	C	302	A1EZI	4	0
7	L	303	DKA	3	0
11	N	301	A1EZI	5	0
7	A	303	DKA	3	0
7	N	309	DKA	3	0
7	N	308	DKA	2	0
8	M	505	PLM	1	0
7	L	308	DKA	3	0

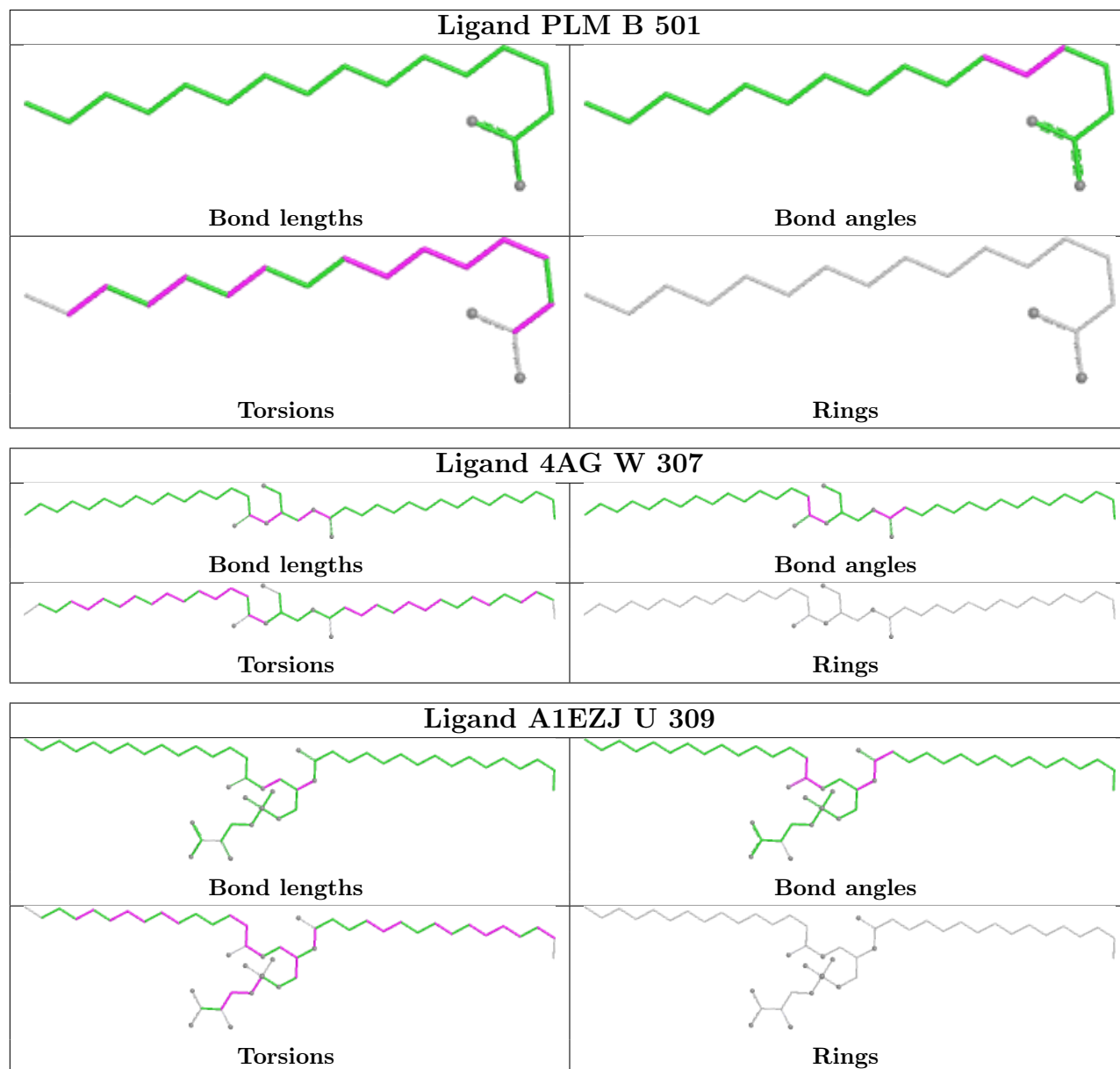
Continued on next page...

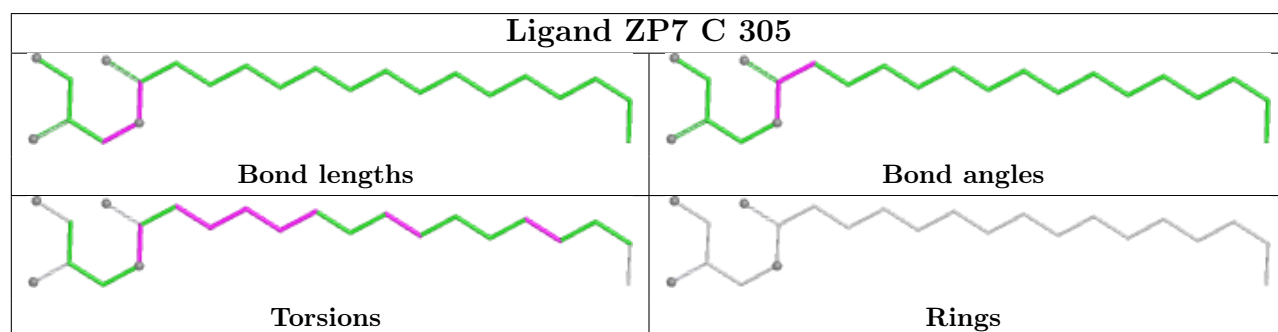
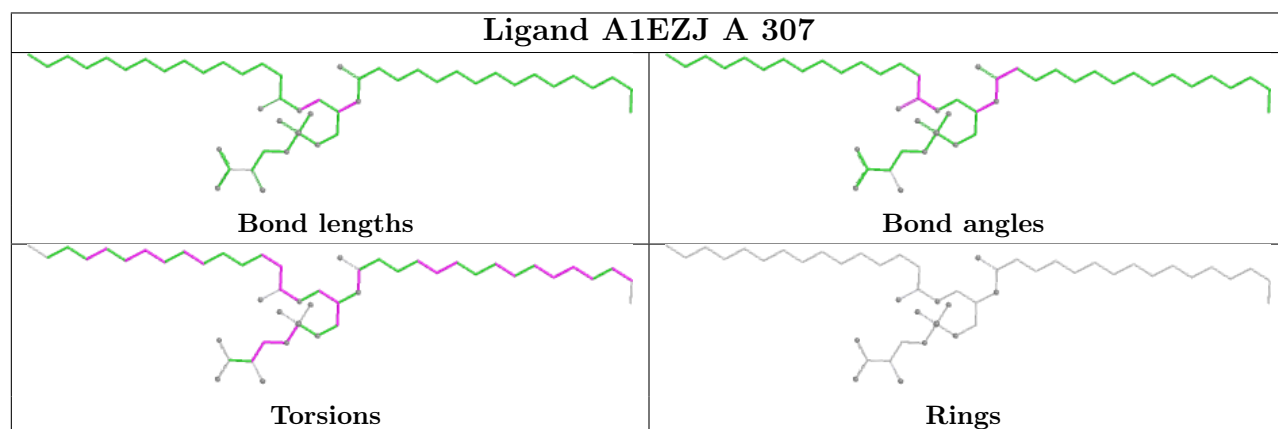
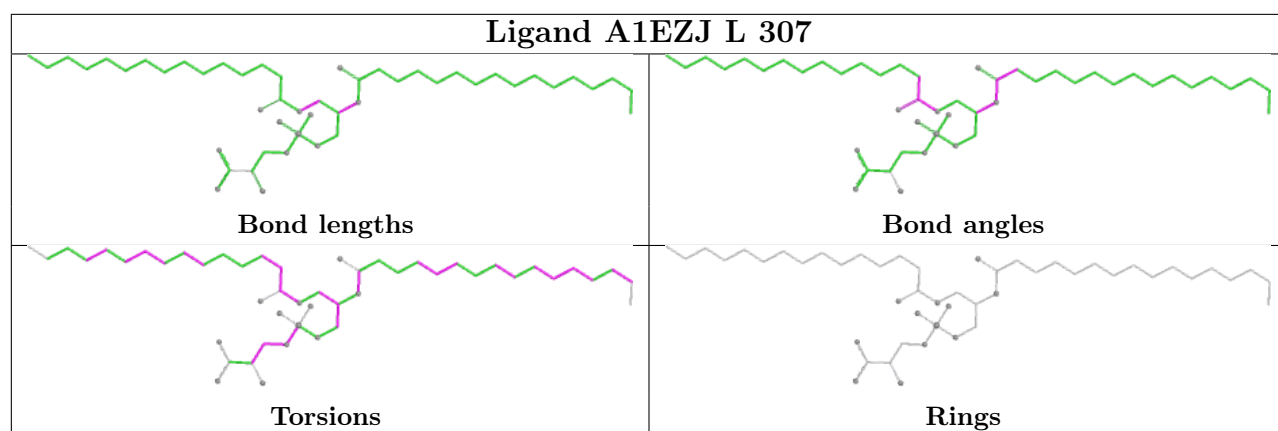
Continued from previous page...

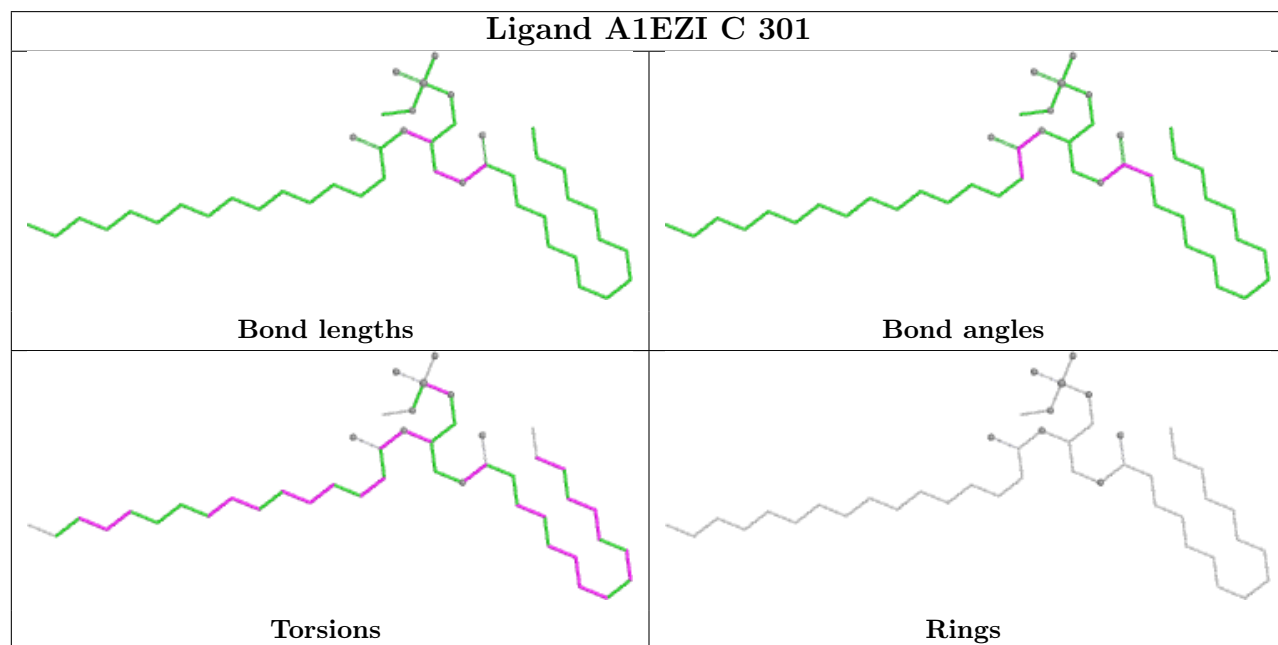
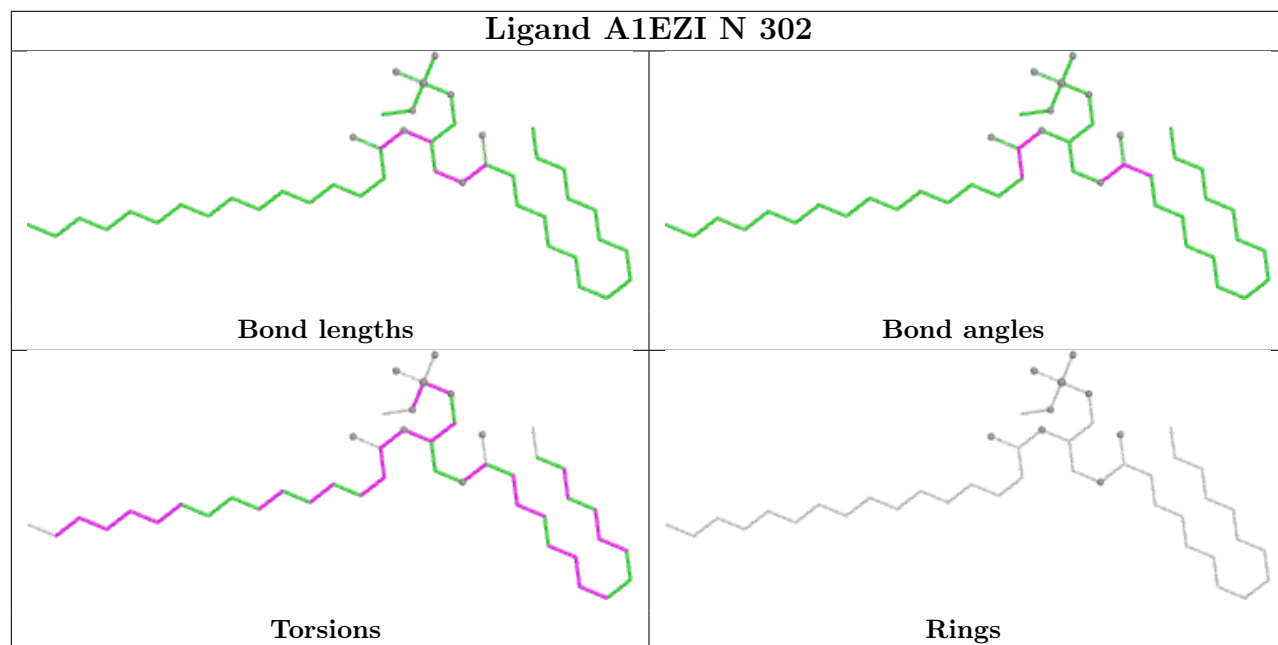
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	U	305	DKA	2	0
7	L	311	DKA	19	0
7	A	311	DKA	18	0
12	N	307	4AG	4	0
9	B	502	ZP7	3	0
7	U	302	DKA	14	0
12	C	306	4AG	4	0
9	V	503	ZP7	3	0
7	V	506	DKA	1	0
7	W	308	DKA	3	0
7	B	506	DKA	1	0
8	B	504	PLM	1	0
11	W	302	A1EZI	4	0
8	W	310	PLM	1	0
7	A	308	DKA	3	0
11	N	303	A1EZI	8	0
7	U	310	DKA	3	0
8	M	502	PLM	3	0
8	V	502	PLM	3	0
7	M	508	DKA	1	0
7	B	505	DKA	1	0
7	V	507	DKA	1	0
7	C	308	DKA	3	0
11	W	301	A1EZI	5	0
11	C	303	A1EZI	8	0
9	M	503	ZP7	3	0
7	B	507	DKA	1	0
8	N	310	PLM	1	0
7	W	309	DKA	4	0
8	V	505	PLM	1	0
8	C	309	PLM	1	0
11	W	303	A1EZI	8	0
7	M	507	DKA	1	0
7	A	310	DKA	14	0
7	U	303	DKA	18	0

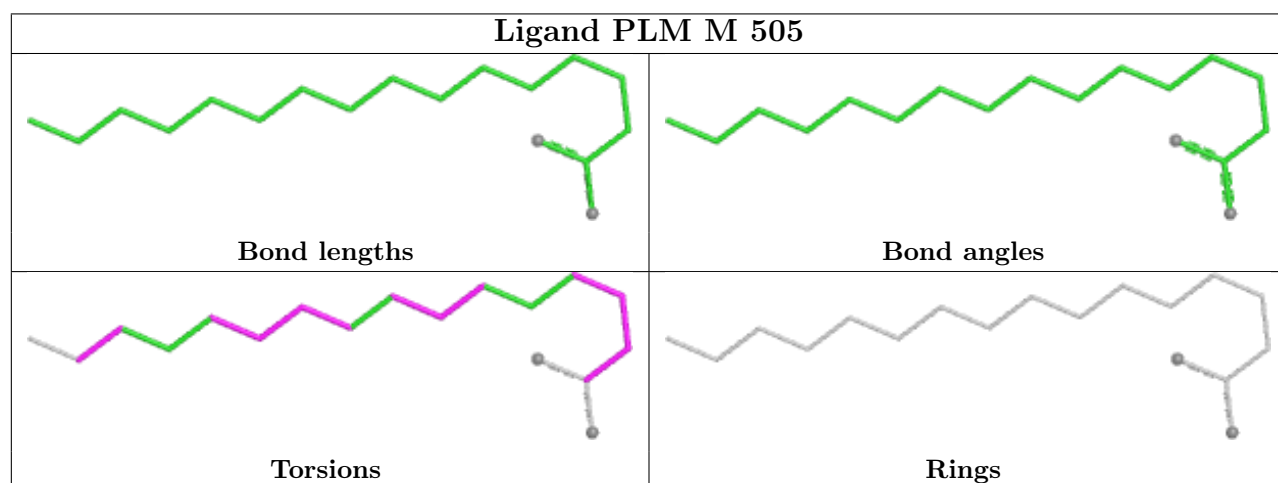
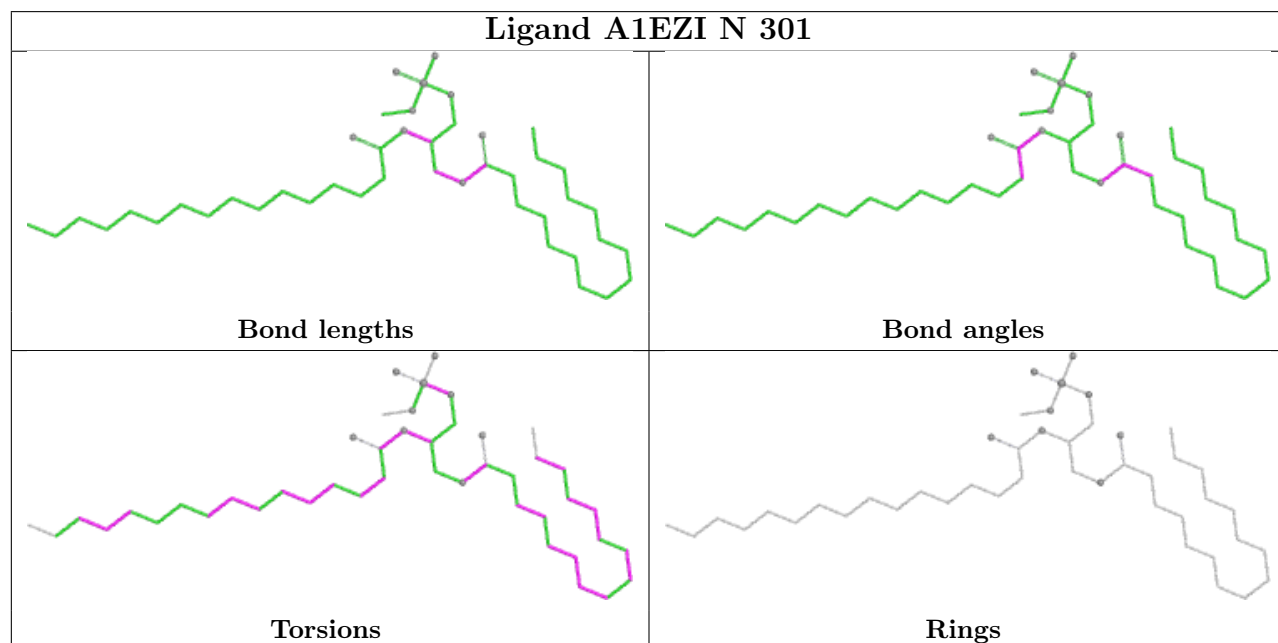
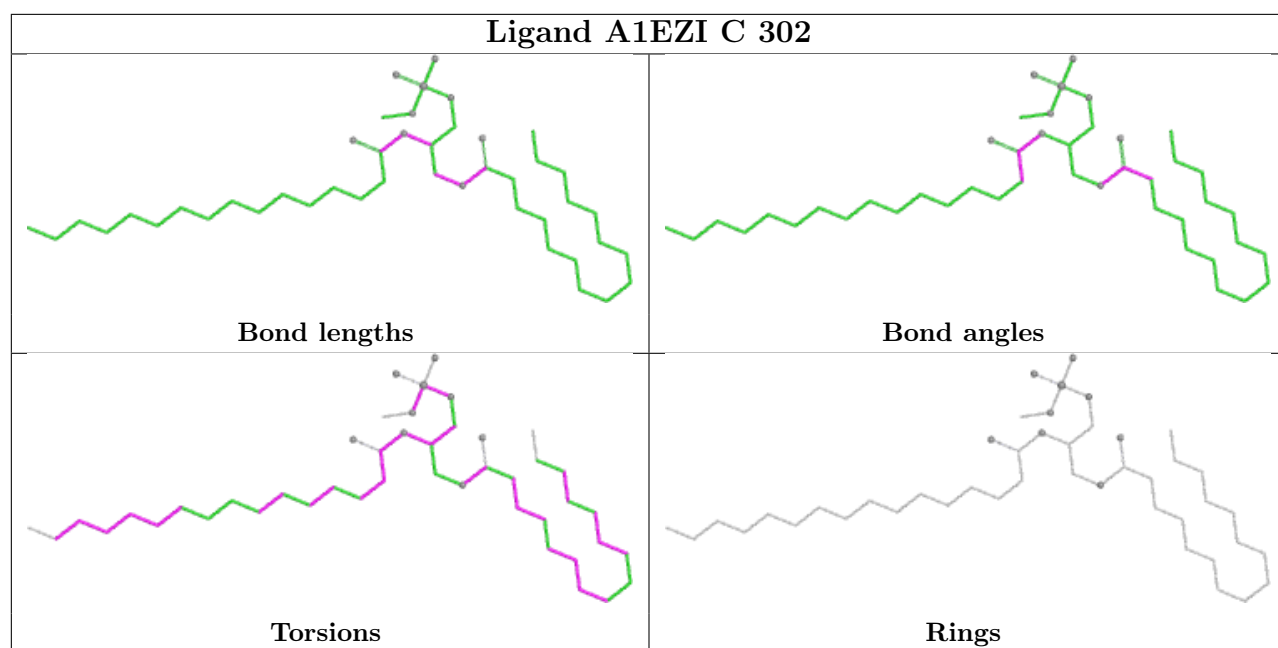
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

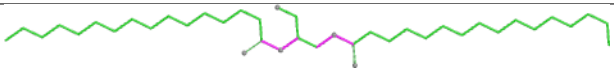
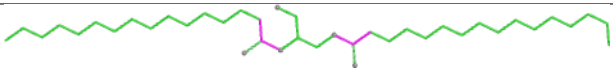
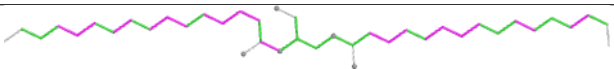
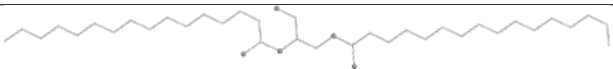
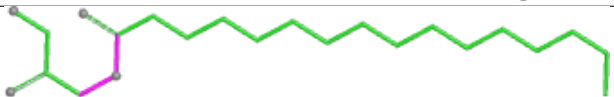
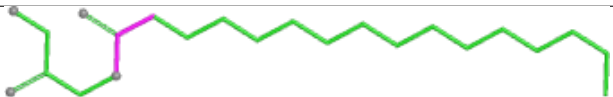
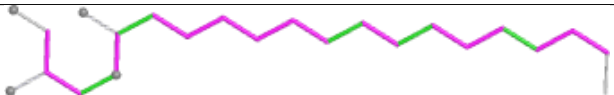
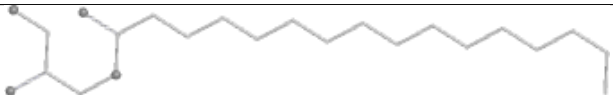
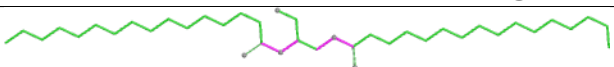
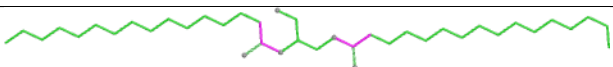
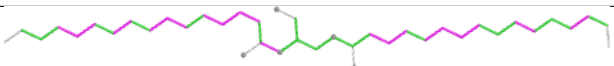
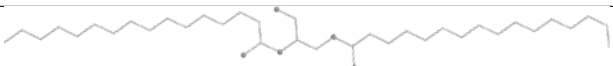
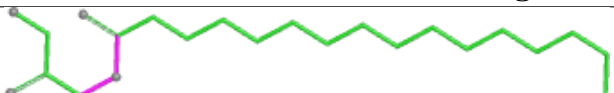
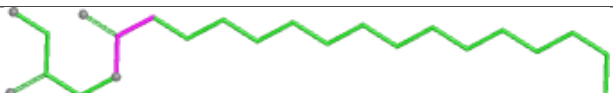
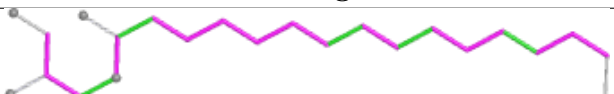
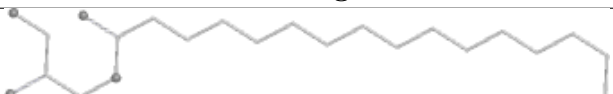
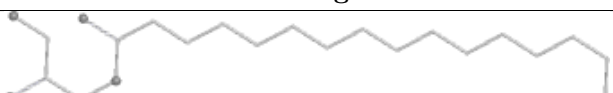
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

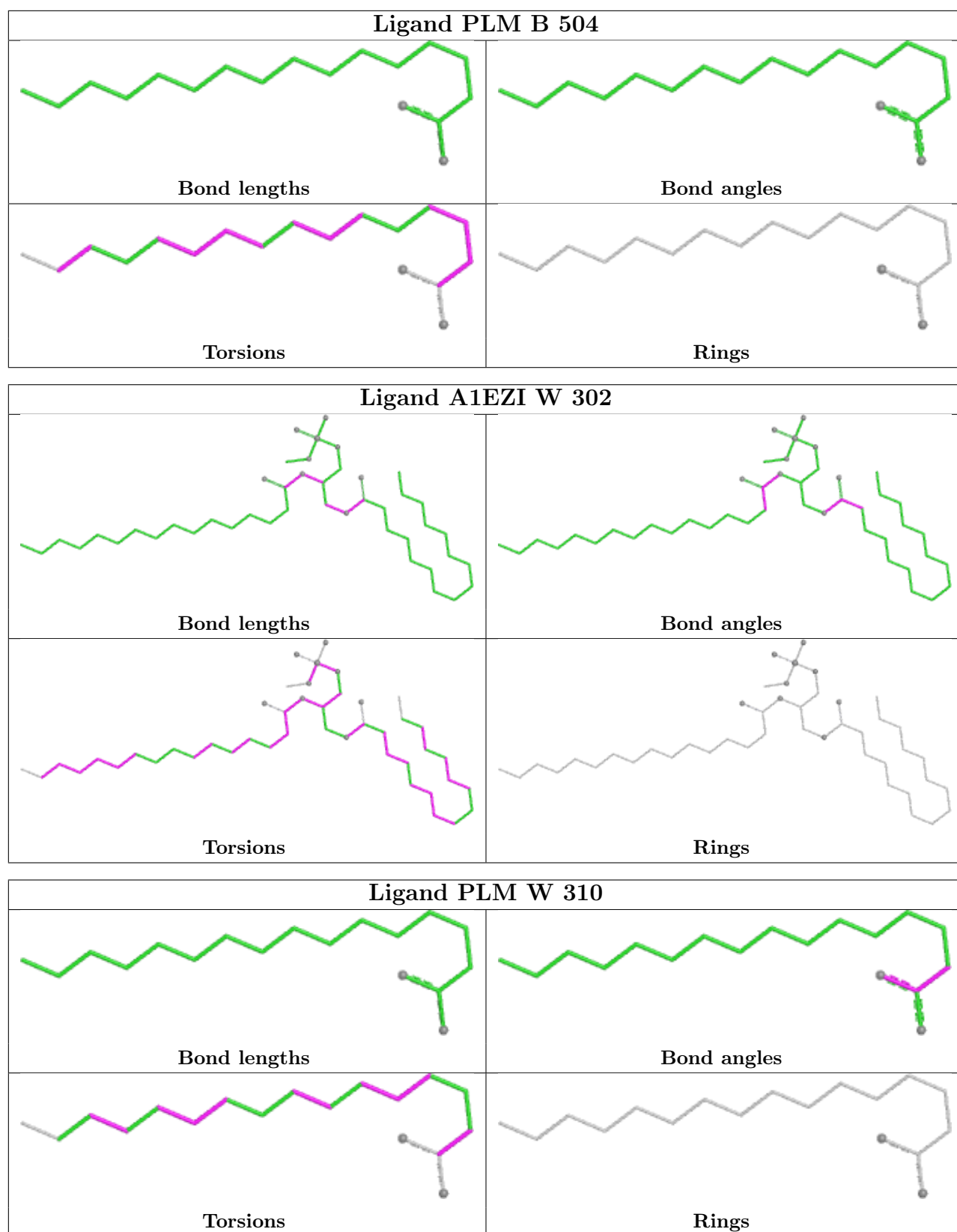


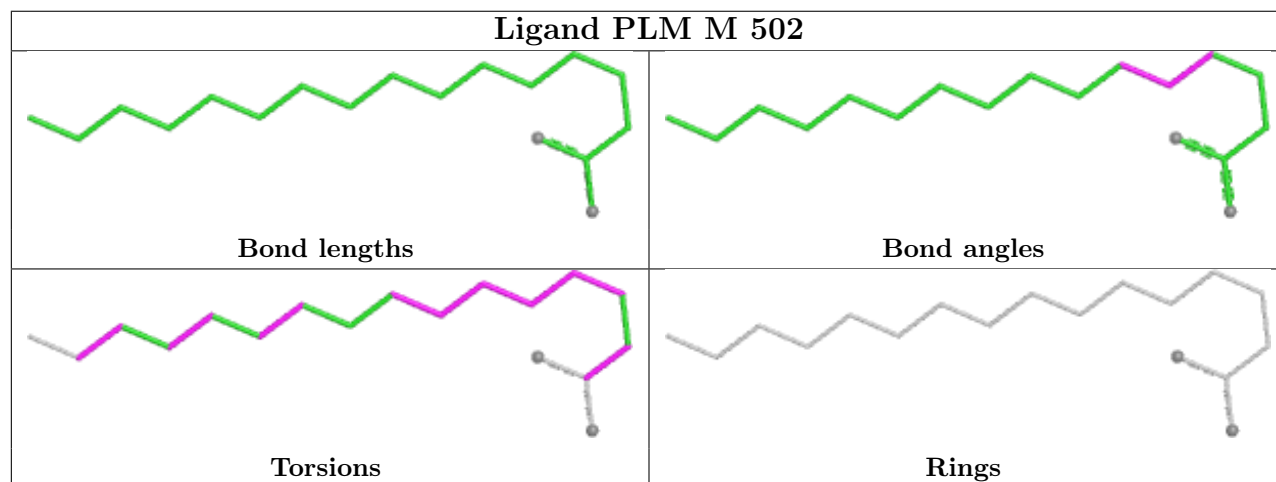
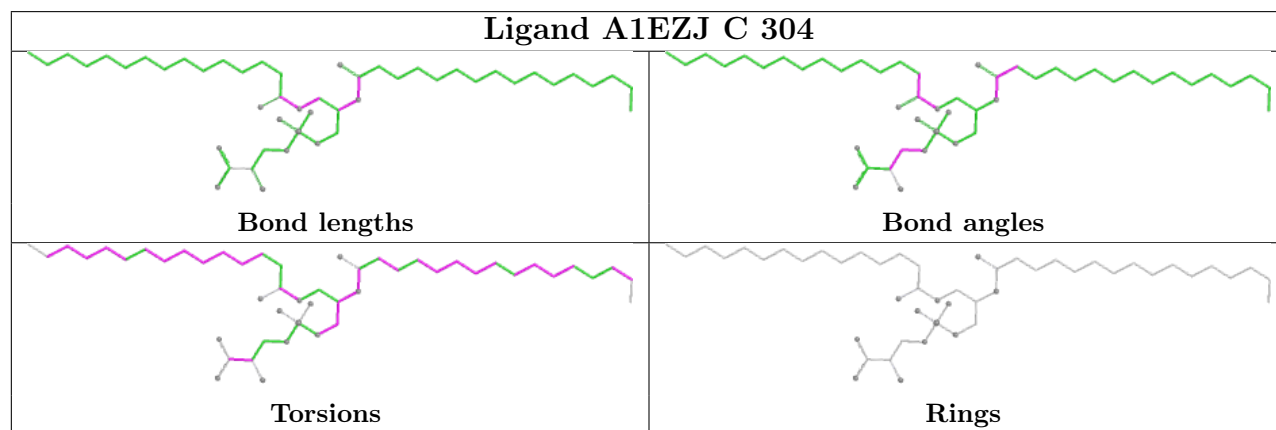
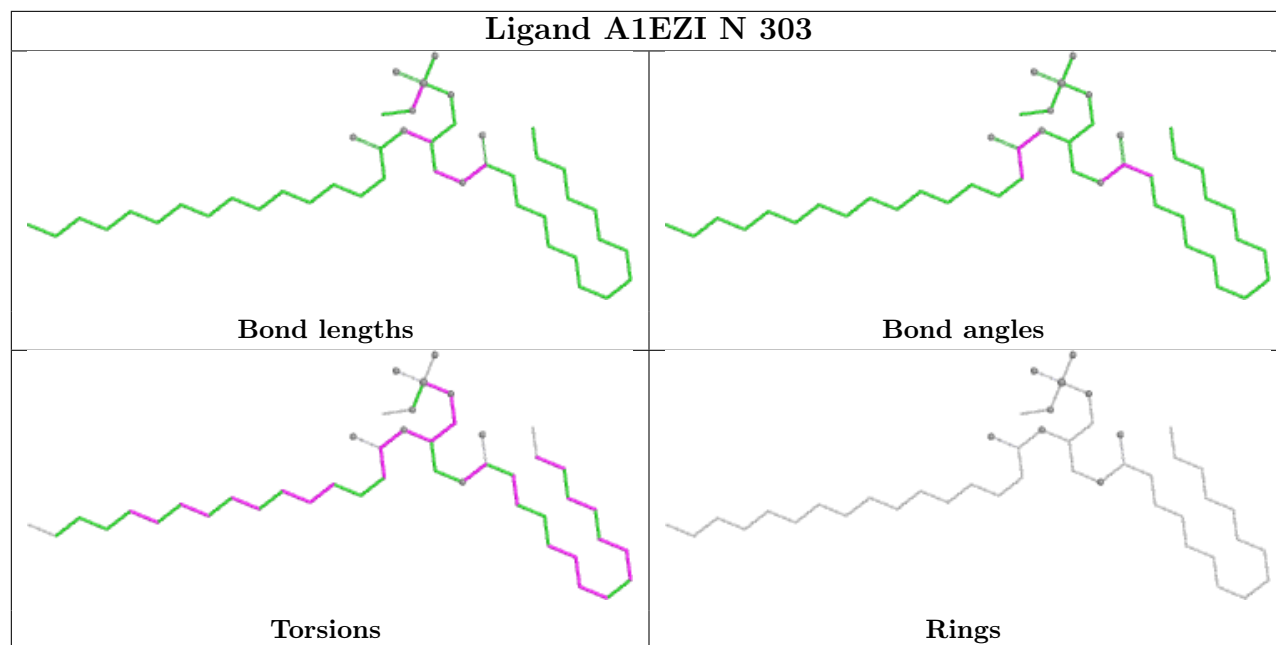


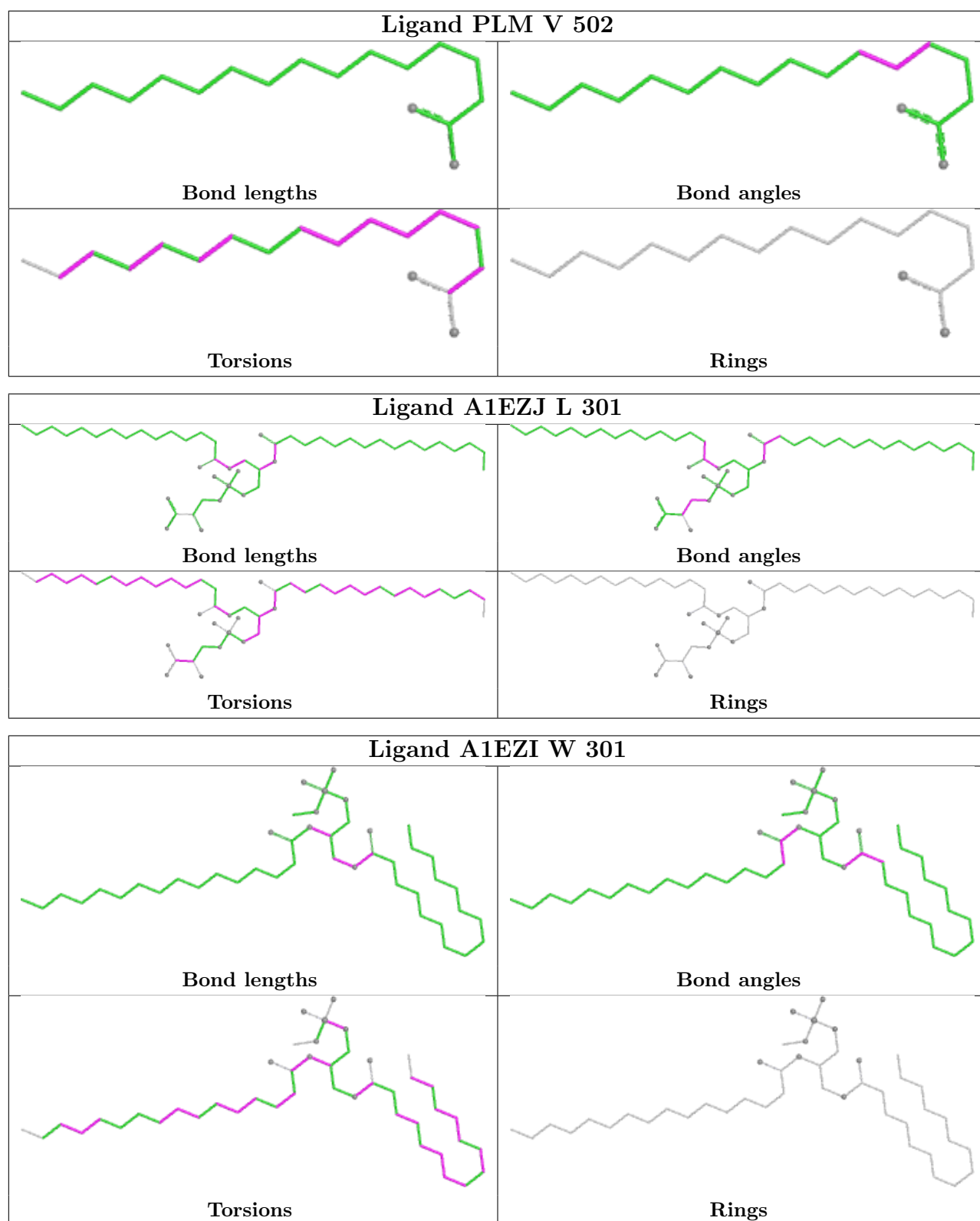


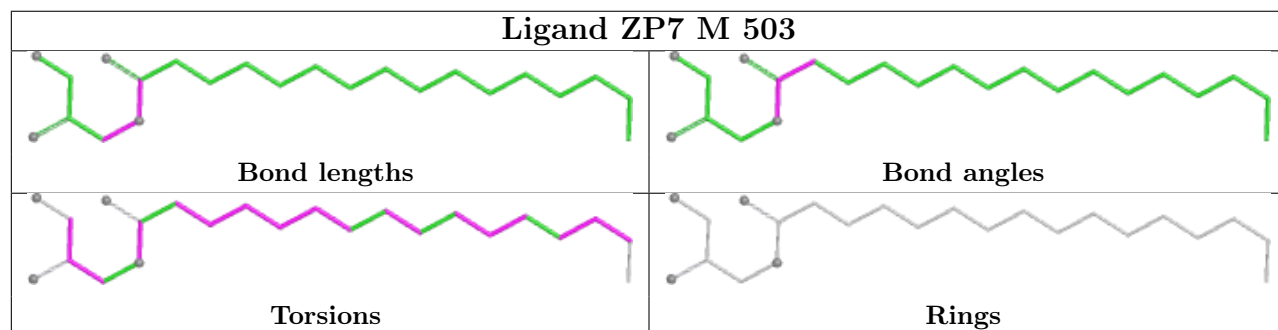
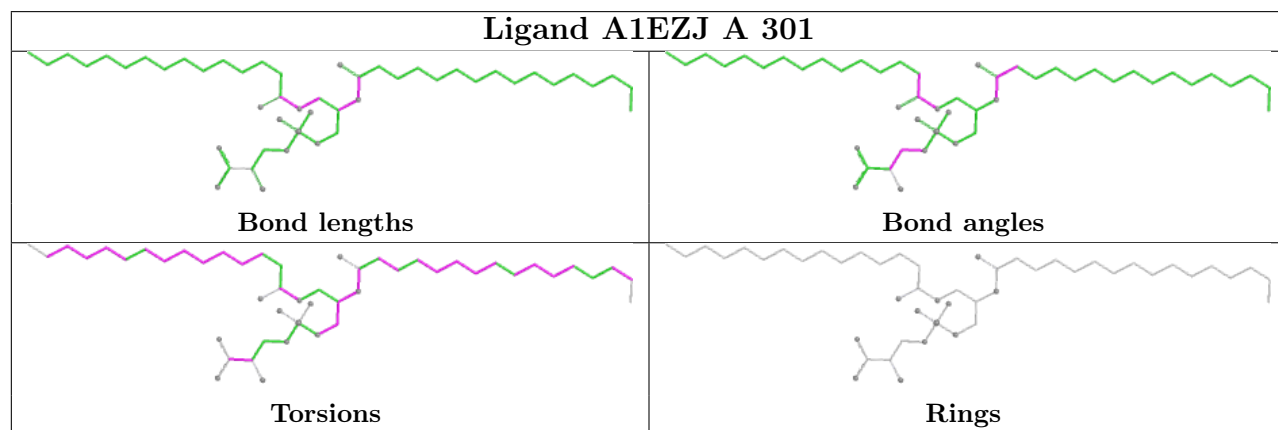
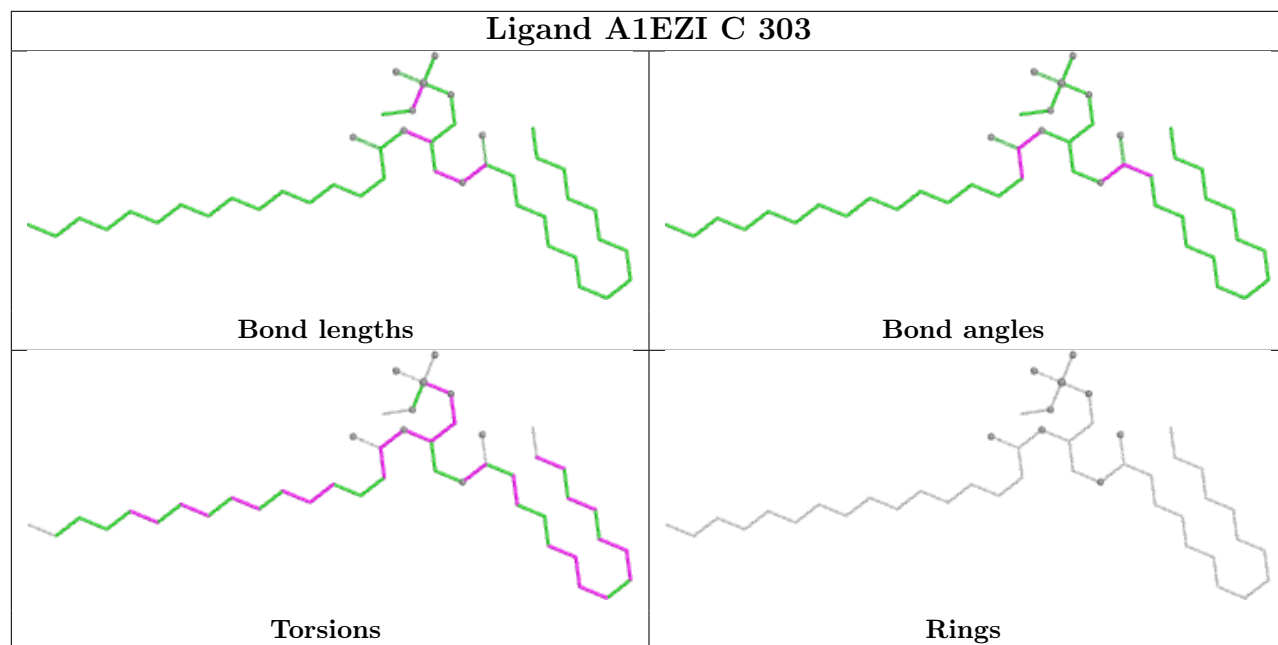


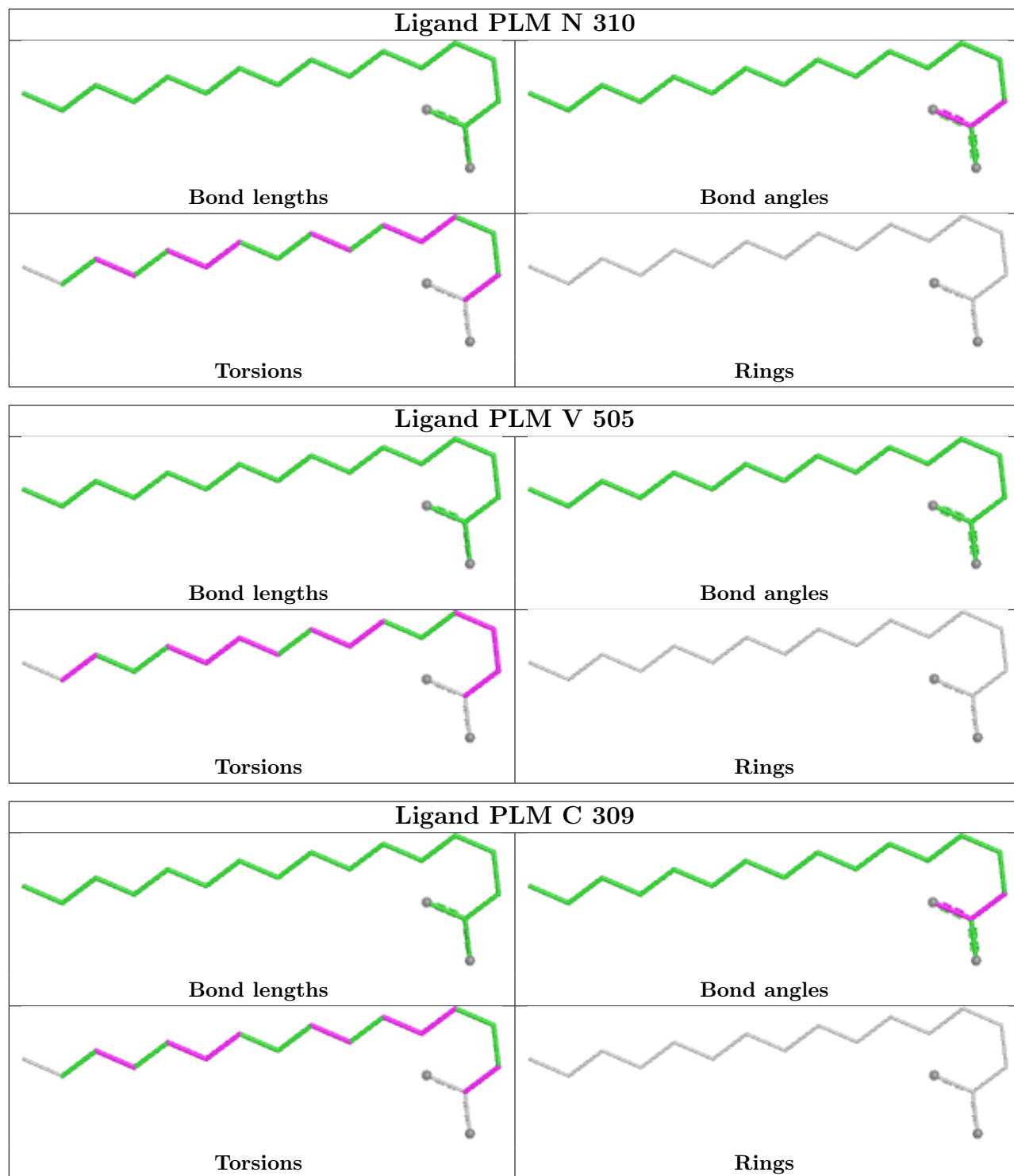
Ligand 4AG N 307			
 Bond lengths		 Bond angles	
 Torsions		 Rings	
Ligand ZP7 B 502			
 Bond lengths		 Bond angles	
 Torsions		 Rings	
Ligand 4AG C 306			
 Bond lengths		 Bond angles	
 Torsions		 Rings	
Ligand ZP7 V 503			
 Bond lengths		 Bond angles	
 Torsions		 Rings	
Ligand ZP7 N 306			
 Bond lengths		 Bond angles	
 Torsions		 Rings	

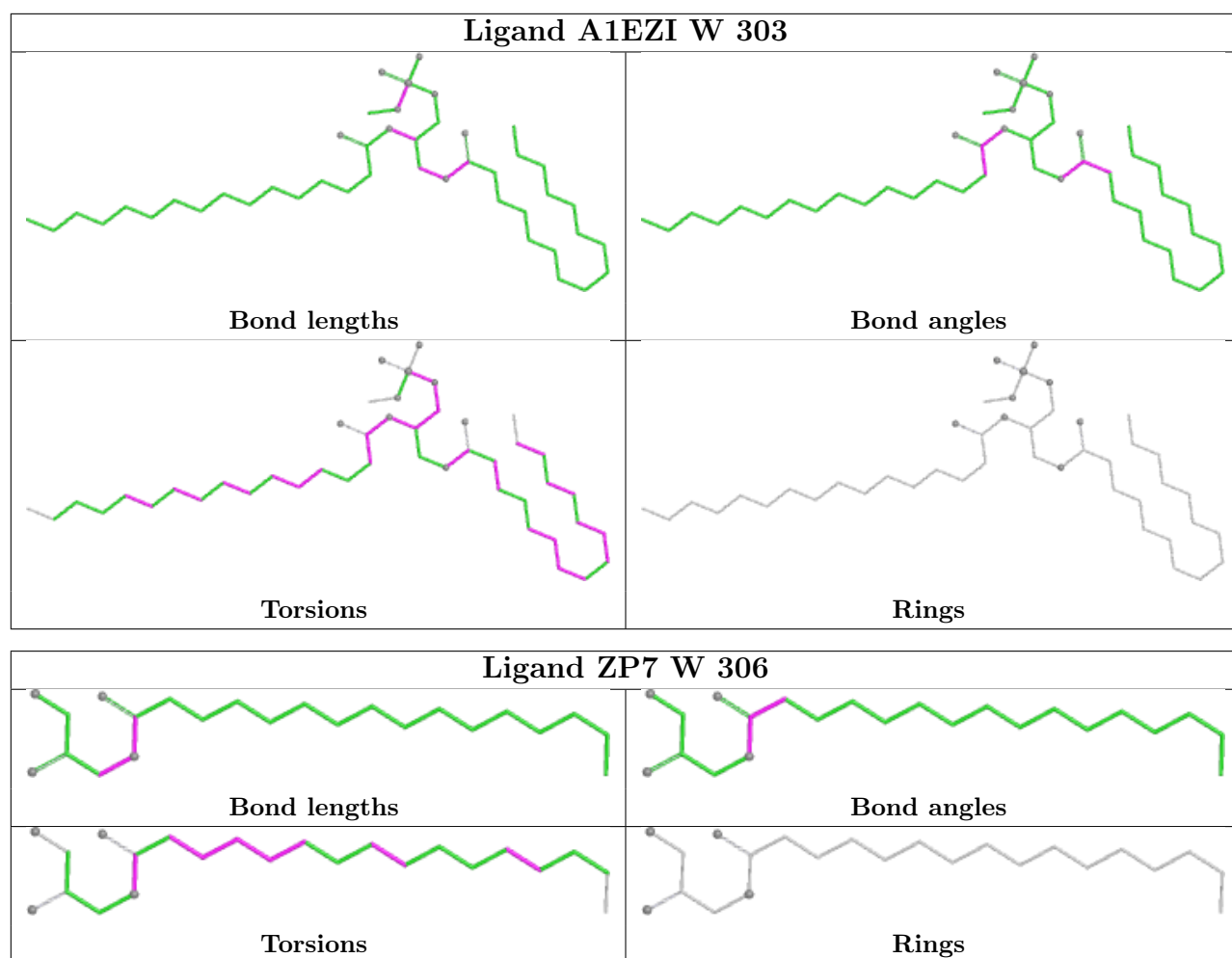












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

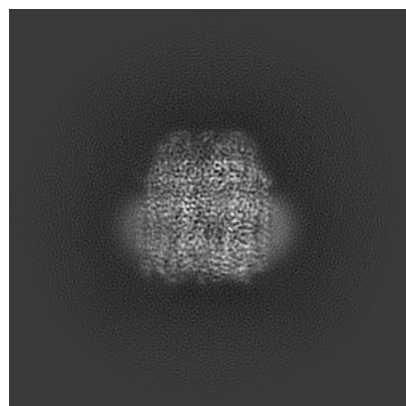
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63025. These allow visual inspection of the internal detail of the map and identification of artifacts.

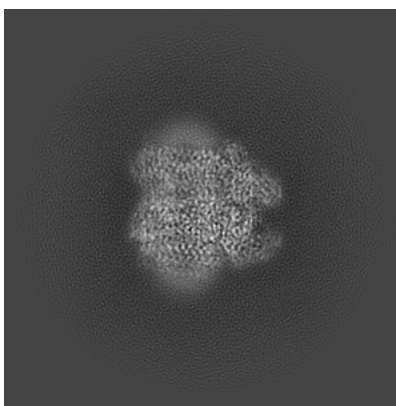
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

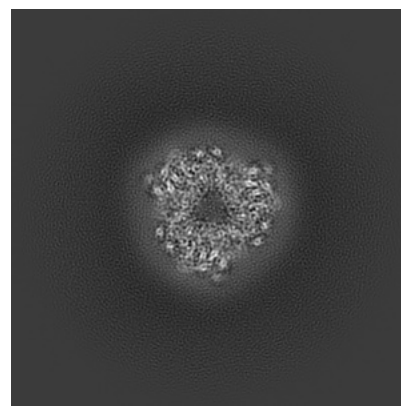
6.1.1 Primary map



X

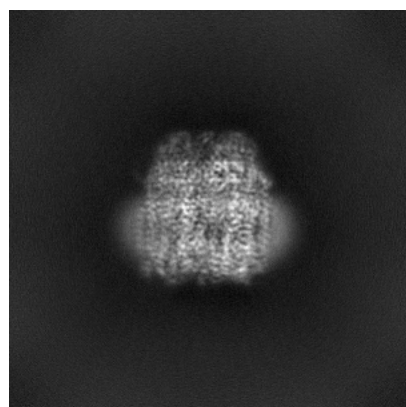


Y

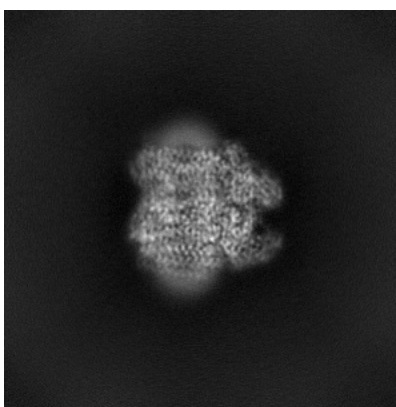


Z

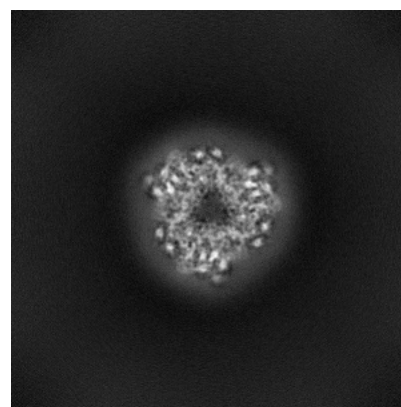
6.1.2 Raw map



X



Y

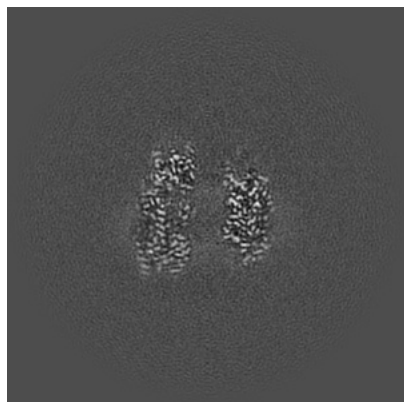


Z

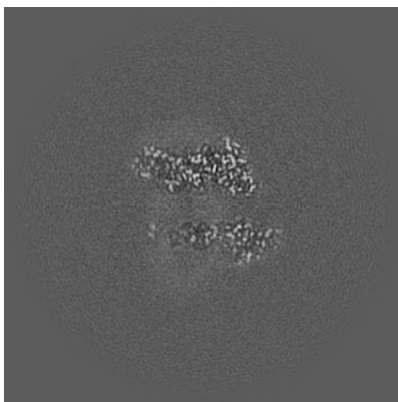
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

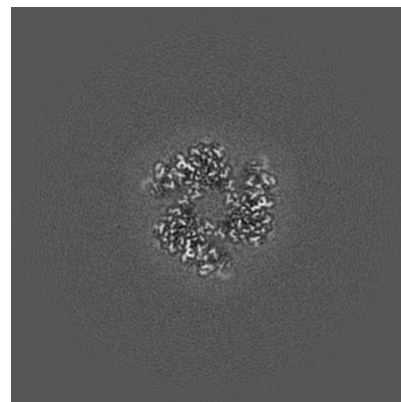
6.2.1 Primary map



X Index: 224

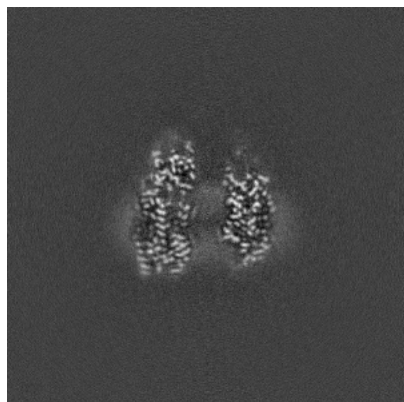


Y Index: 224

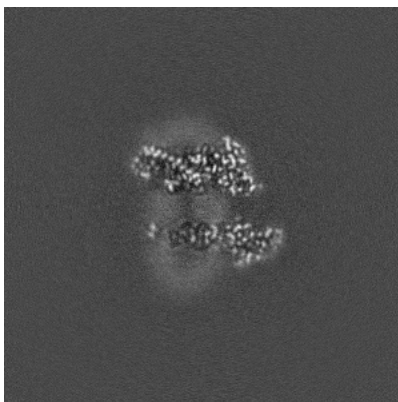


Z Index: 224

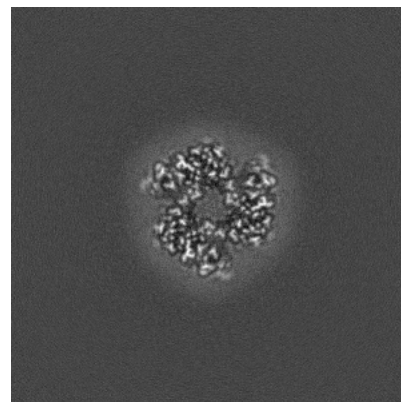
6.2.2 Raw map



X Index: 224



Y Index: 224

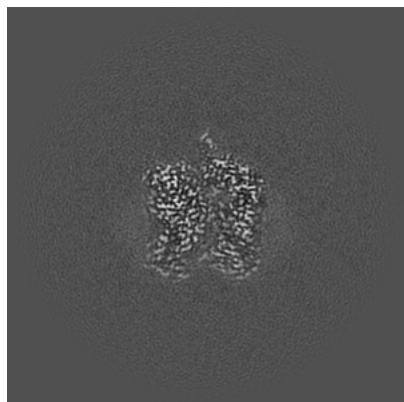


Z Index: 224

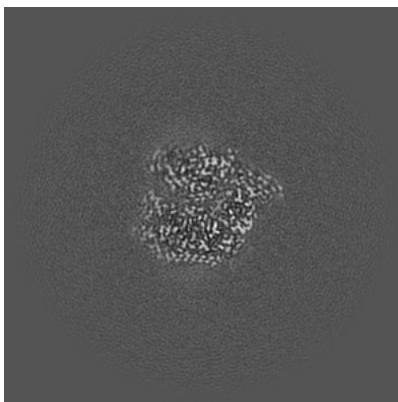
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

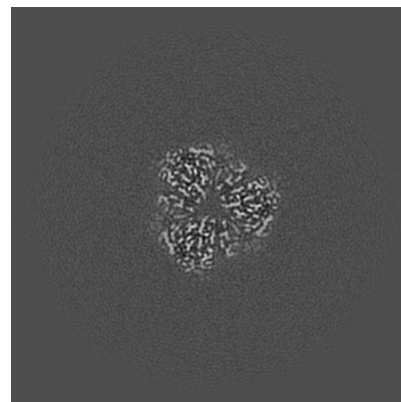
6.3.1 Primary map



X Index: 198

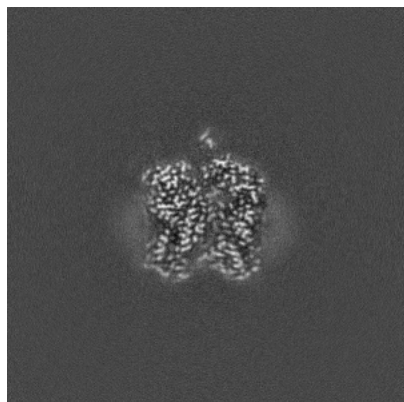


Y Index: 197

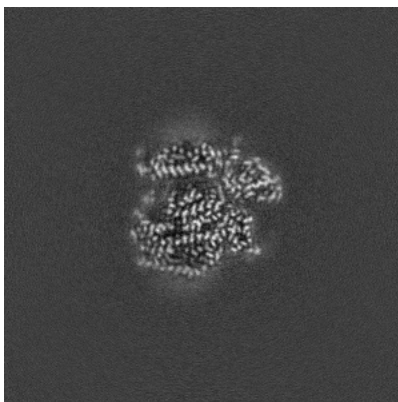


Z Index: 256

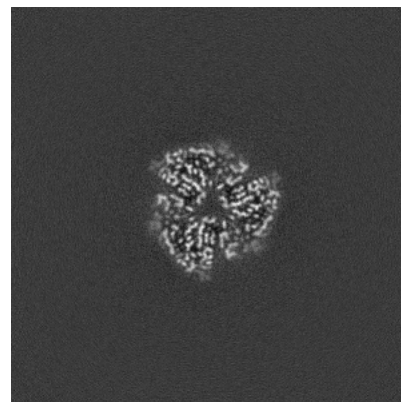
6.3.2 Raw map



X Index: 198



Y Index: 254

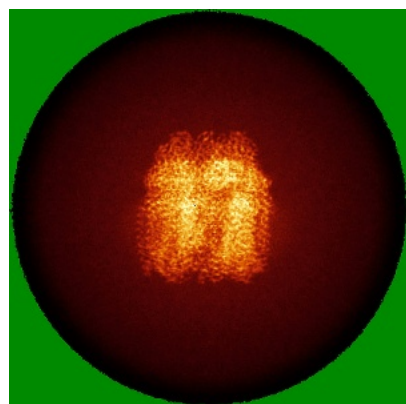


Z Index: 257

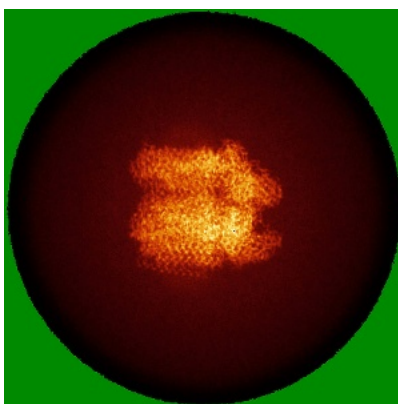
The images above show the largest variance slices of the map in three orthogonal directions.

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

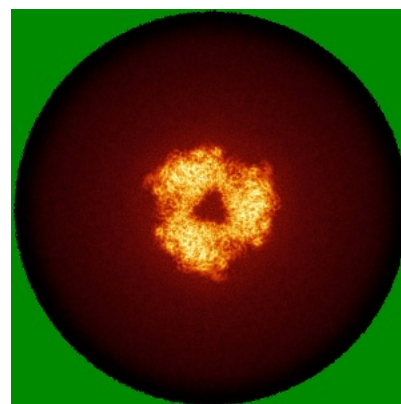
6.4.1 Primary map



X

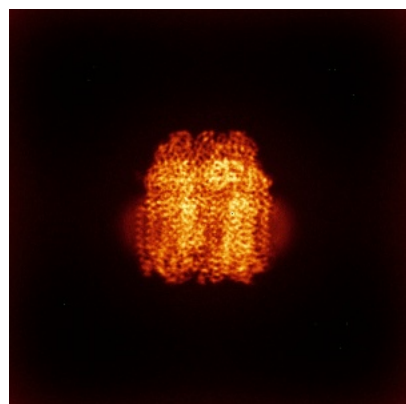


Y

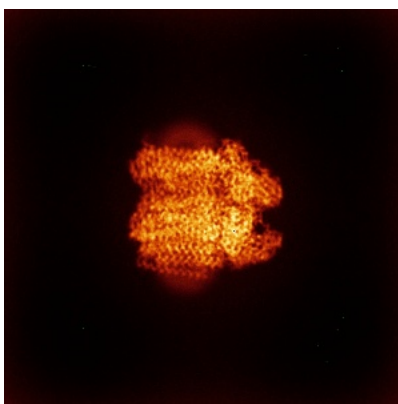


Z

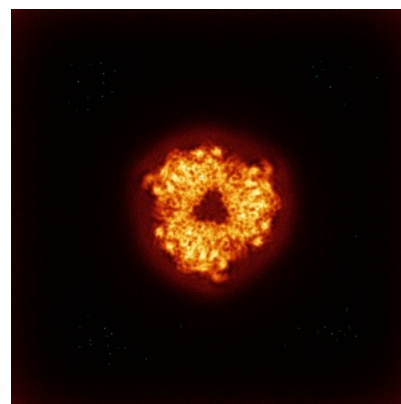
6.4.2 Raw map



X



Y

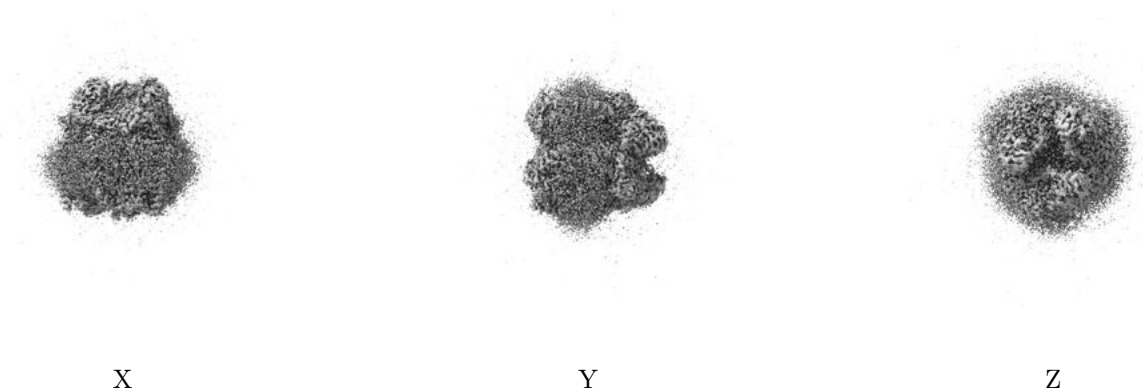


Z

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.

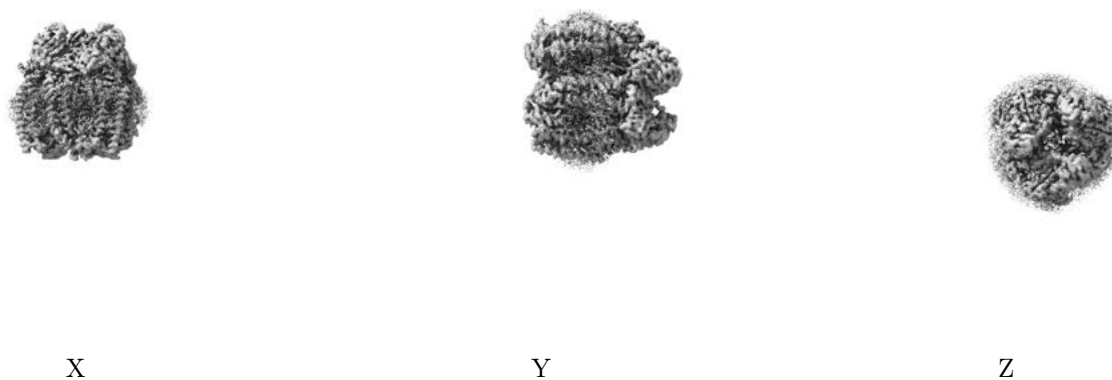
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

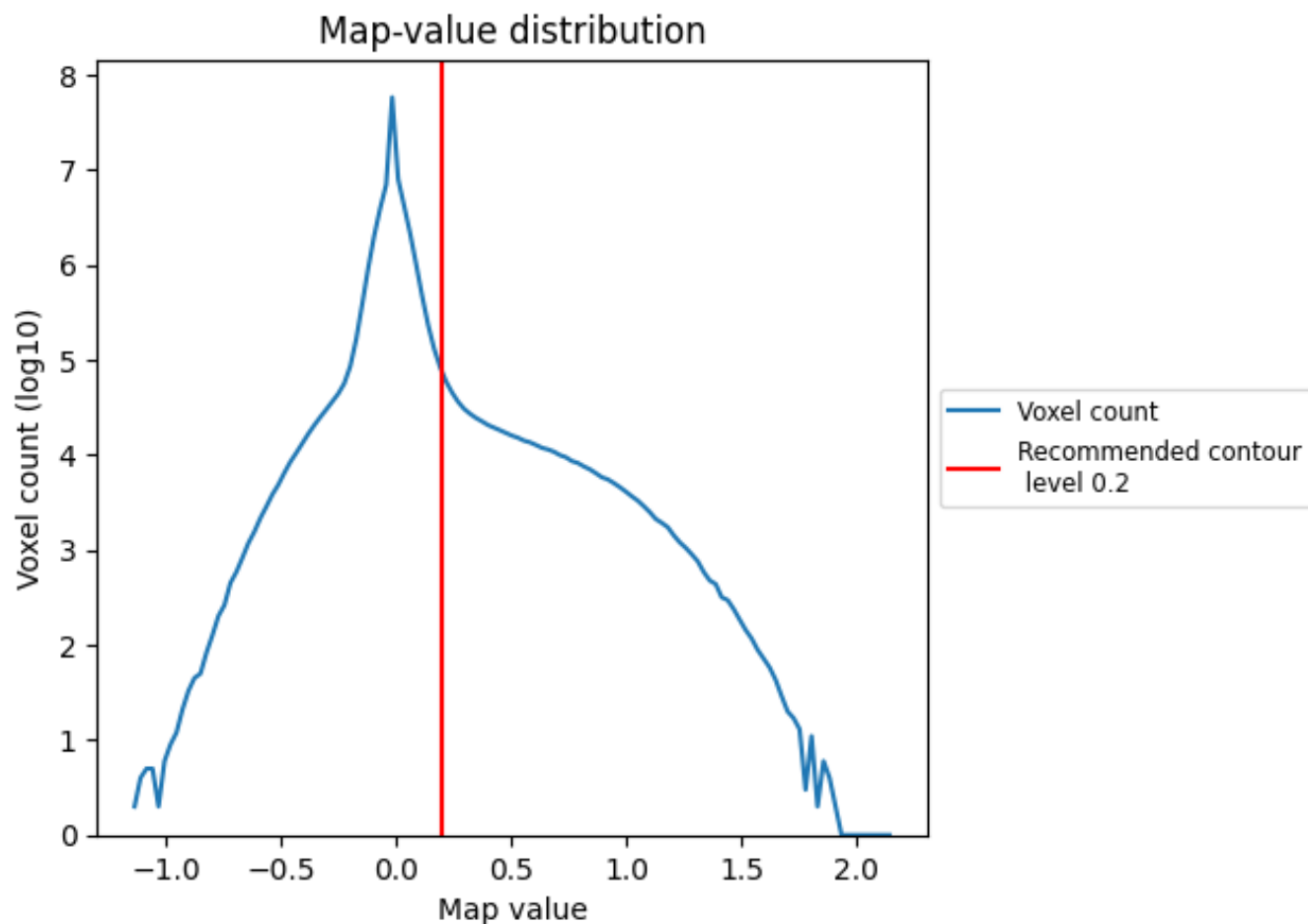
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

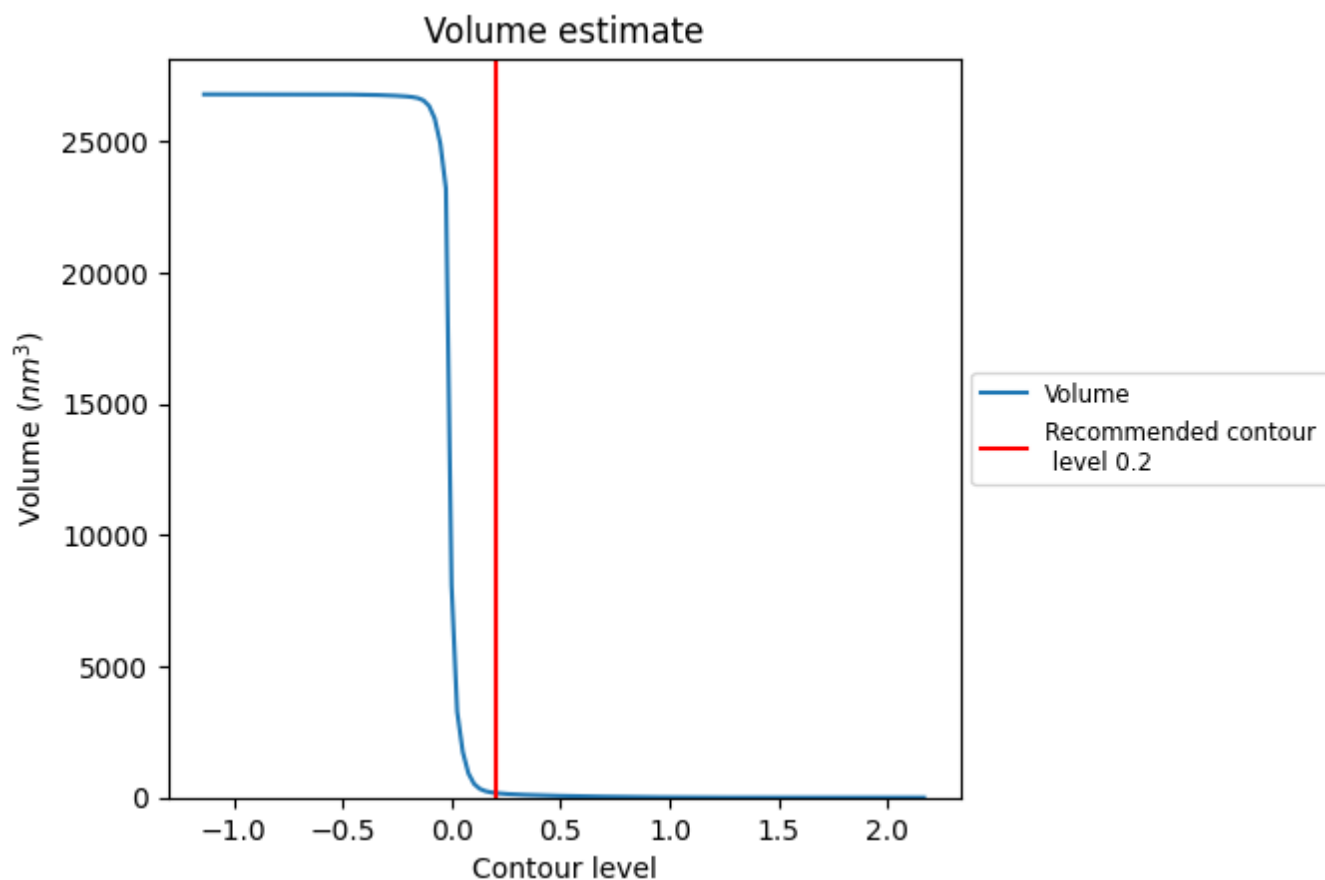
This section contains the results of statistical analysis of the map.

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.

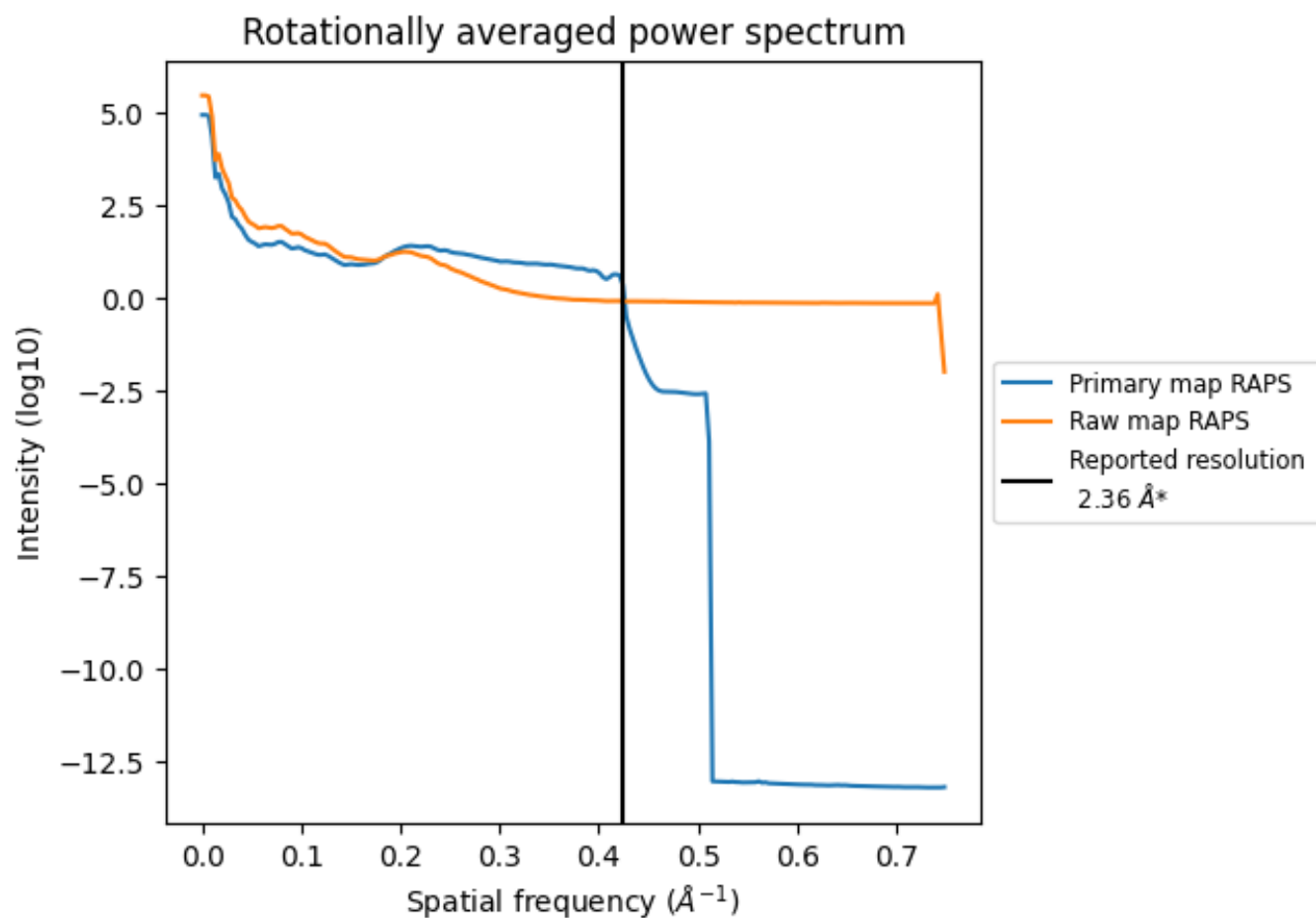
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 177 nm^3 ; this corresponds to an approximate mass of 160 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 ⓘ

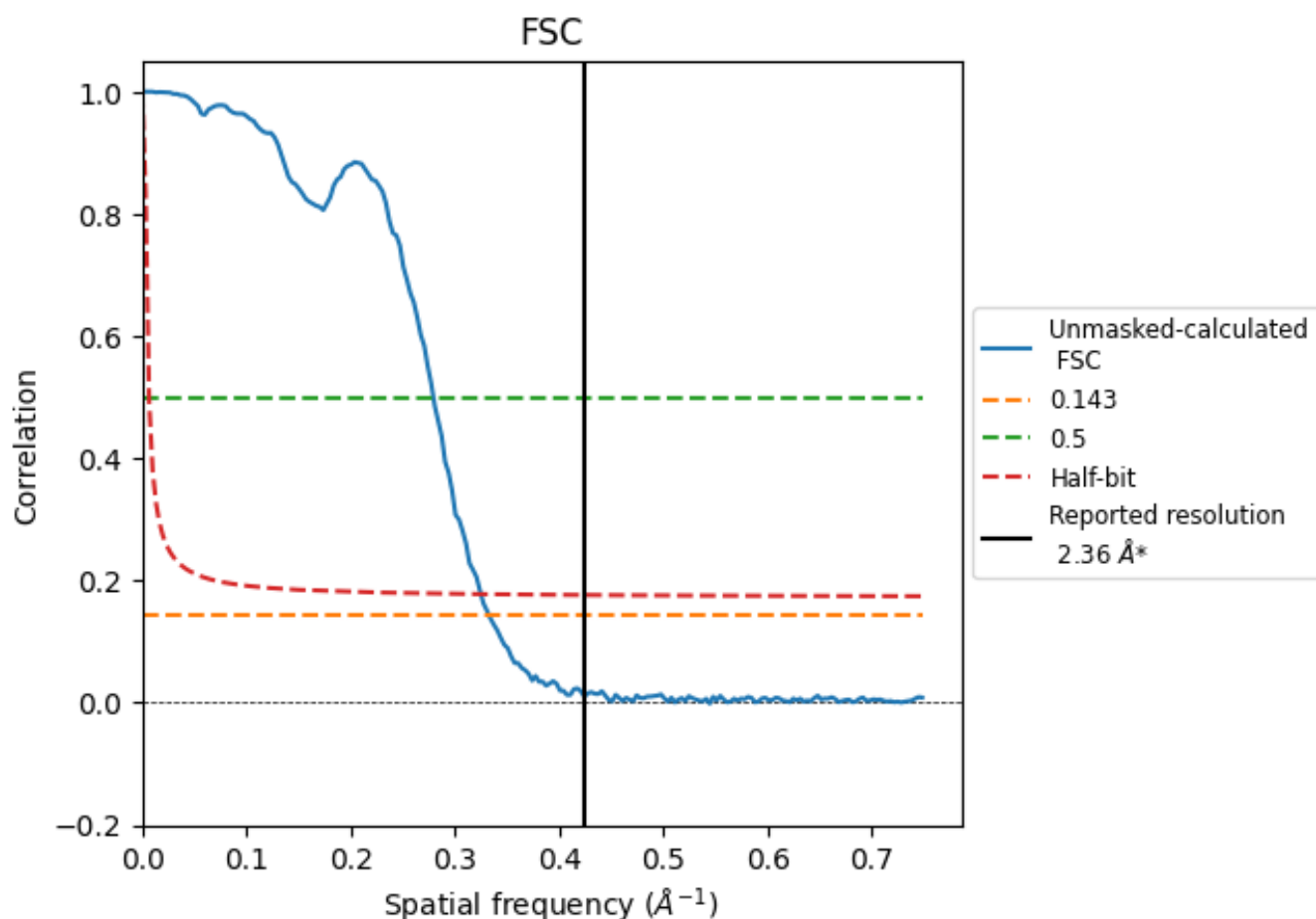


*Reported resolution corresponds to spatial frequency of 0.424 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.424 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

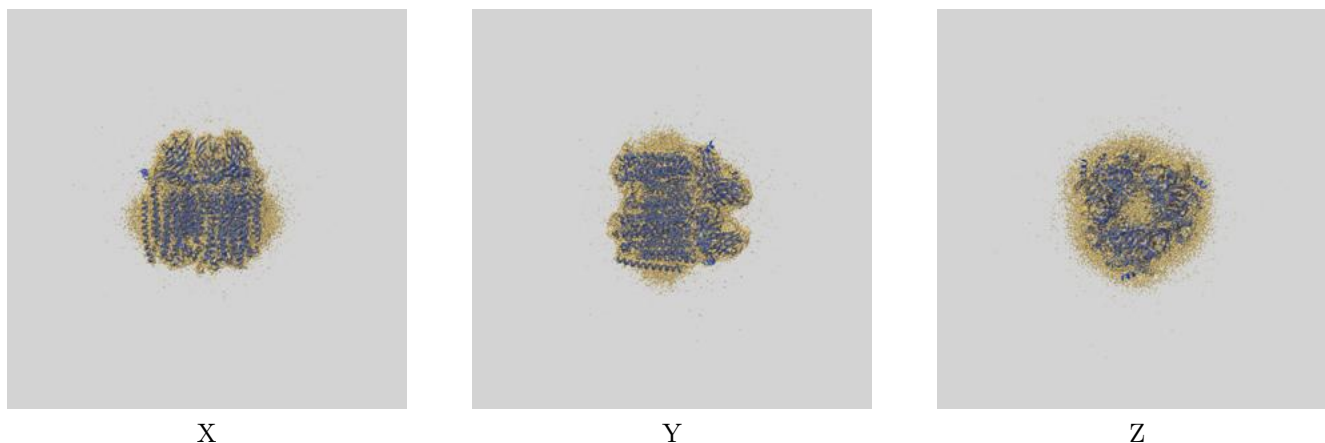
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.36	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.00	3.58	3.08

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.00 differs from the reported value 2.36 by more than 10 %

9 Map-model fit [i](#)

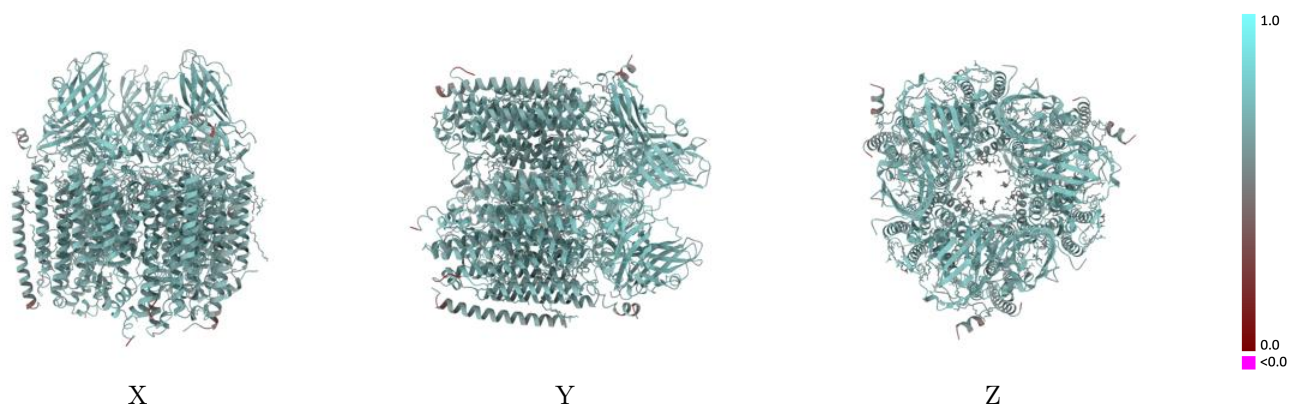
This section contains information regarding the fit between EMDB map EMD-63025 and PDB model 9LEG. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



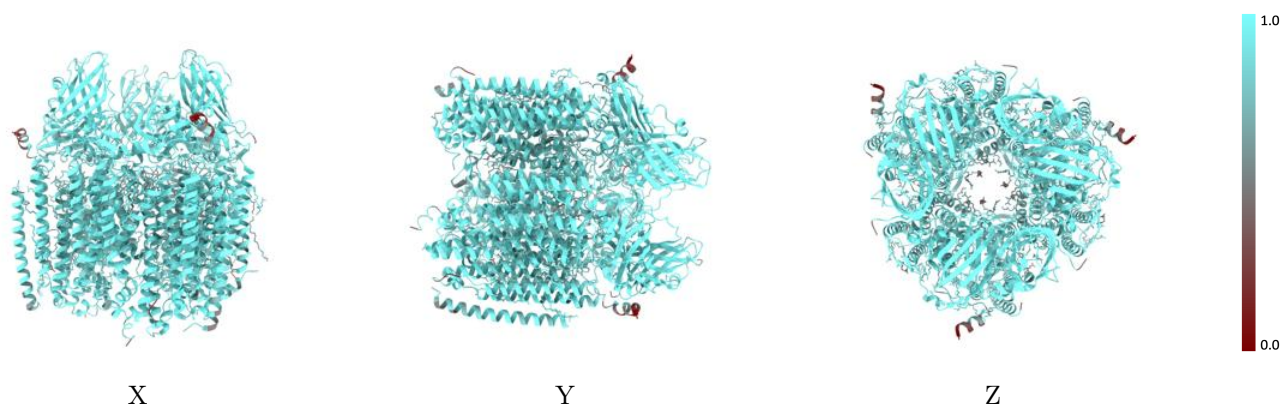
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



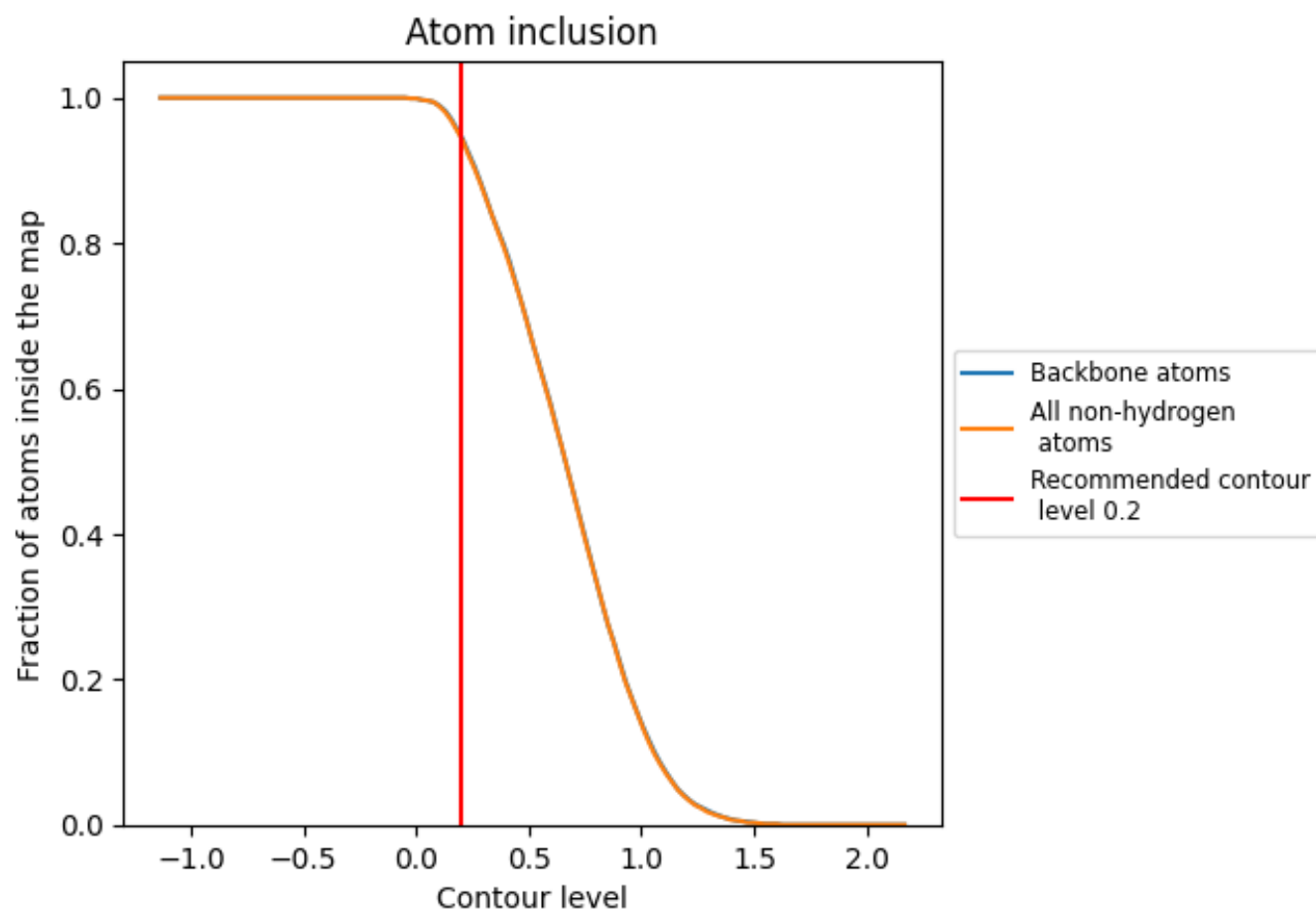
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 94% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9450	0.6590
A	0.9540	0.6760
B	0.9680	0.6710
C	0.9390	0.6440
D	0.5680	0.5350
E	0.8480	0.5530
L	0.9540	0.6750
M	0.9680	0.6710
N	0.9440	0.6470
O	0.5740	0.5350
P	0.8410	0.5520
U	0.9600	0.6790
V	0.9690	0.6710
W	0.9450	0.6480
X	0.5680	0.5410
Y	0.8410	0.5560

1.0

0.0

<0.0