



Full wwPDB EM Validation Report ⓘ

Mar 15, 2026 – 01:00 AM UTC

PDB ID : 5OOD / pdb_00005ood
EMDB ID : EMD-3837
Title : Cryo-EM structure of jasplakinolide-stabilized F-actin in complex with ADP-Pi
Authors : Merino, F.; Pospich, S.; Funk, J.; Kuellmer, F.; Arndt, H.-D.; Bieling, P.; Raunser, S.
Deposited on : 2017-08-07
Resolution : 3.70 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

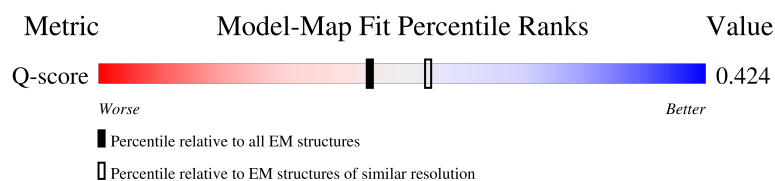
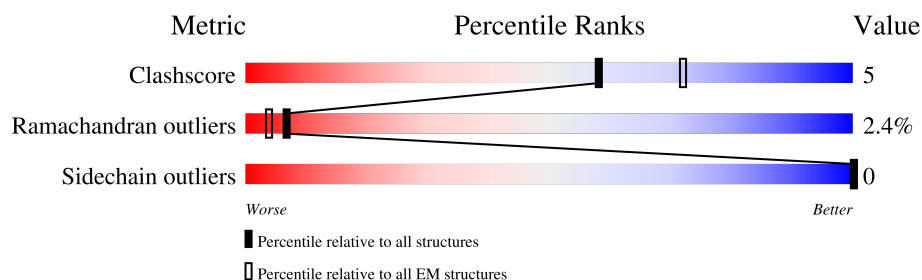
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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	11569 (3.20 - 4.20)

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	375	
1	B	375	
1	C	375	
1	D	375	

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Mol	Chain	Length	Quality of chain
1	E	375	

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
3	PO4	A	402	-	X	-	-
3	PO4	B	402	-	X	-	-
3	PO4	C	402	-	X	-	-
3	PO4	D	402	-	X	-	-
3	PO4	E	402	-	X	-	-

2 Entry composition [i](#)

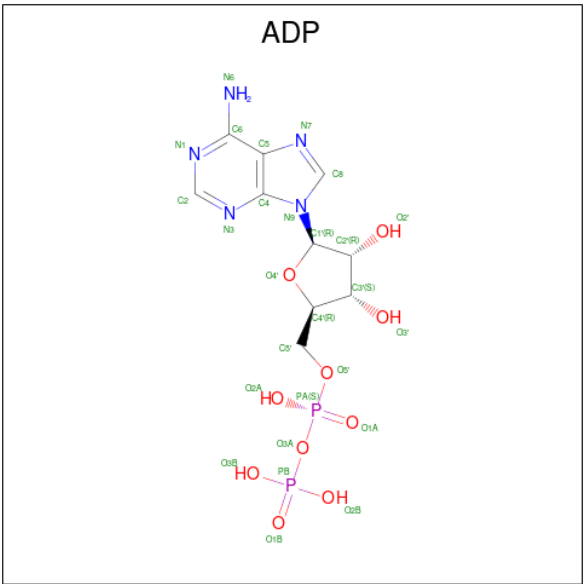
There are 5 unique types of molecules in this entry. The entry contains 14910 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	371	Total	C	N	O	S	0	0
			2900	1837	489	553	21		
1	B	371	Total	C	N	O	S	0	0
			2900	1837	489	553	21		
1	C	371	Total	C	N	O	S	0	0
			2900	1837	489	553	21		
1	D	371	Total	C	N	O	S	0	0
			2900	1837	489	553	21		
1	E	371	Total	C	N	O	S	0	0
			2900	1837	489	553	21		

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	B	1	Total	C	N	O	P	0
			27	10	5	10	2	

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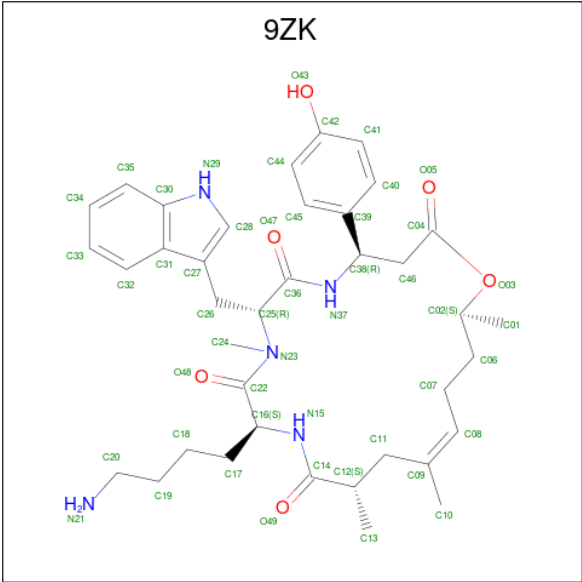
Mol	Chain	Residues	Atoms					AltConf
2	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	E	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	O	P	0
			5	4	1	
3	B	1	Total	O	P	0
			5	4	1	
3	C	1	Total	O	P	0
			5	4	1	
3	D	1	Total	O	P	0
			5	4	1	
3	E	1	Total	O	P	0
			5	4	1	

- Molecule 4 is (4 {R},7 {R},10 {S},13 {S},15 {E},19 {S})-10-(4-azanylbutyl)-4-(4-hydroxyphenyl)-7-(1 {H}-indol-3-ylmethyl)-8,13,15,19-tetramethyl-1-oxa-5,8,11-triazacyclononadec-15-ene-2,6,9,12-tetrone (CCD ID: 9ZK) (formula: C₃₈H₅₁N₅O₆).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			49	38	5	6	
4	A	1	Total	C	N	O	0
			49	38	5	6	
4	B	1	Total	C	N	O	0
			49	38	5	6	
4	C	1	Total	C	N	O	0
			49	38	5	6	
4	D	1	Total	C	N	O	0
			49	38	5	6	

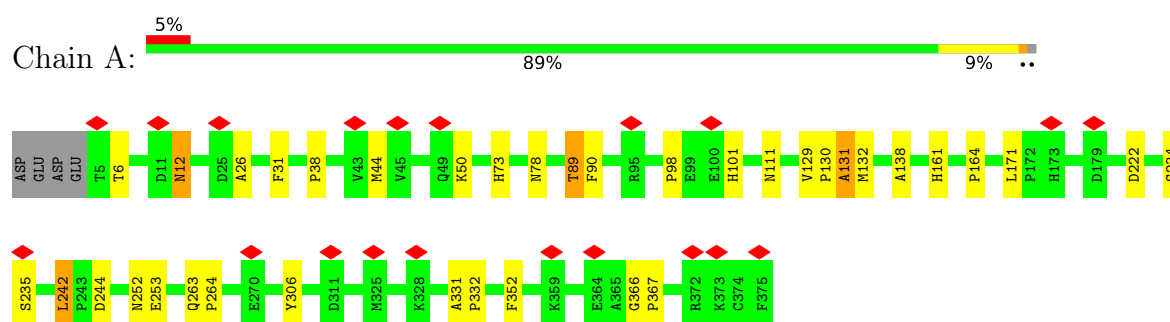
- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Mg	0
			1	1	
5	B	1	Total	Mg	0
			1	1	
5	C	1	Total	Mg	0
			1	1	
5	D	1	Total	Mg	0
			1	1	
5	E	1	Total	Mg	0
			1	1	

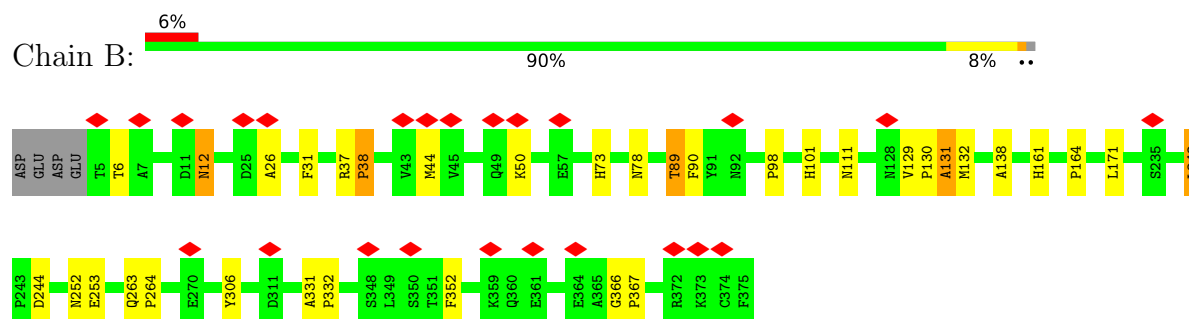
3 Residue-property plots [i](#)

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.

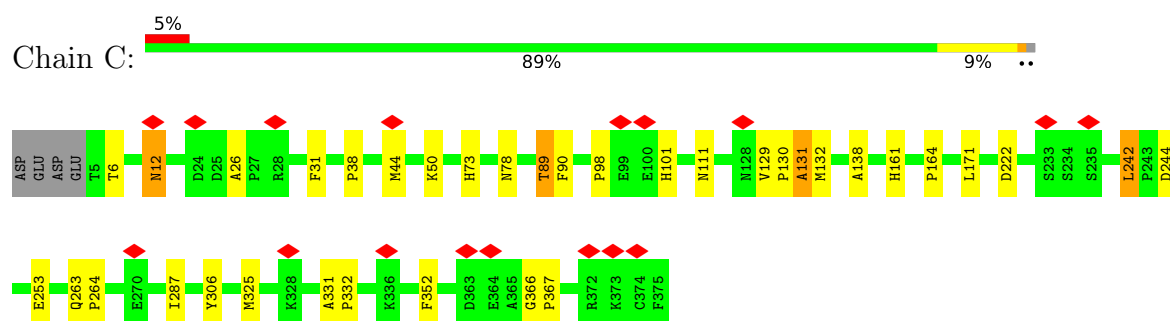
- Molecule 1: Actin, alpha skeletal muscle



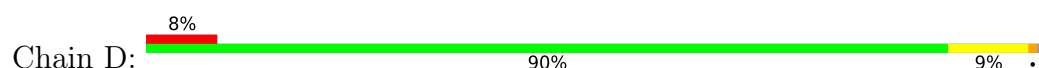
- Molecule 1: Actin, alpha skeletal muscle

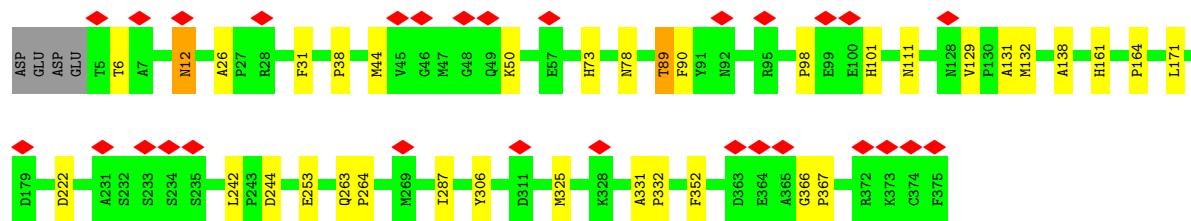


- Molecule 1: Actin, alpha skeletal muscle

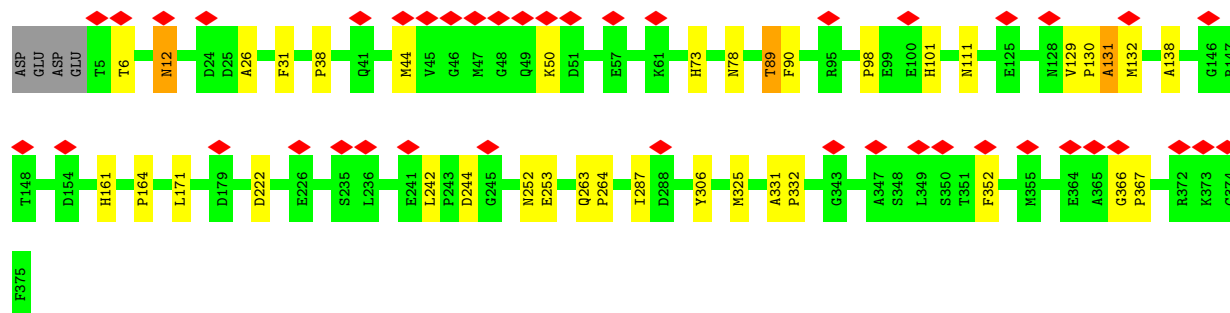
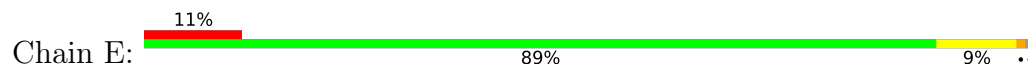


- Molecule 1: Actin, alpha skeletal muscle





- Molecule 1: Actin, alpha skeletal muscle



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	123716	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	78	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.157	Depositor
Minimum map value	-0.079	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.032	Depositor
Map size (Å)	313.92, 313.92, 313.92	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.09, 1.09, 1.09	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, HIC, MG, ADP, 9ZK

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	0.94	0/2950	1.14	26/3994 (0.7%)
1	B	0.94	0/2950	1.14	26/3994 (0.7%)
1	C	0.94	0/2950	1.14	26/3994 (0.7%)
1	D	0.94	0/2950	1.14	26/3994 (0.7%)
1	E	0.94	0/2950	1.14	26/3994 (0.7%)
All	All	0.94	0/14750	1.14	130/19970 (0.7%)

There are no bond length outliers.

All (130) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	101	HIS	CA-C-N	8.60	128.55	120.03
1	C	101	HIS	C-N-CA	8.60	128.55	120.03
1	B	101	HIS	CA-C-N	8.60	128.54	120.03
1	B	101	HIS	C-N-CA	8.60	128.54	120.03
1	A	101	HIS	CA-C-N	8.55	128.50	120.03
1	A	101	HIS	C-N-CA	8.55	128.50	120.03
1	D	101	HIS	CA-C-N	8.55	128.49	120.03
1	D	101	HIS	C-N-CA	8.55	128.49	120.03
1	E	101	HIS	CA-C-N	8.54	128.48	120.03
1	E	101	HIS	C-N-CA	8.54	128.48	120.03
1	B	129	VAL	CA-C-N	7.30	128.28	120.83
1	B	129	VAL	C-N-CA	7.30	128.28	120.83
1	D	129	VAL	CA-C-N	7.30	128.28	120.83
1	D	129	VAL	C-N-CA	7.30	128.28	120.83
1	A	129	VAL	CA-C-N	7.29	128.26	120.83
1	A	129	VAL	C-N-CA	7.29	128.26	120.83
1	C	129	VAL	CA-C-N	7.28	128.26	120.83
1	C	129	VAL	C-N-CA	7.28	128.26	120.83
1	E	366	GLY	CA-C-N	7.24	128.89	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	366	GLY	C-N-CA	7.24	128.89	119.84
1	D	366	GLY	CA-C-N	7.23	128.88	119.84
1	D	366	GLY	C-N-CA	7.23	128.88	119.84
1	B	366	GLY	CA-C-N	7.22	128.87	119.84
1	B	366	GLY	C-N-CA	7.22	128.87	119.84
1	C	366	GLY	CA-C-N	7.22	128.87	119.84
1	C	366	GLY	C-N-CA	7.22	128.87	119.84
1	E	129	VAL	CA-C-N	7.22	128.19	120.83
1	E	129	VAL	C-N-CA	7.22	128.19	120.83
1	A	366	GLY	CA-C-N	7.18	128.82	119.84
1	A	366	GLY	C-N-CA	7.18	128.82	119.84
1	A	26	ALA	CA-C-N	6.65	126.63	119.78
1	A	26	ALA	C-N-CA	6.65	126.63	119.78
1	B	26	ALA	CA-C-N	6.64	126.62	119.78
1	B	26	ALA	C-N-CA	6.64	126.62	119.78
1	D	26	ALA	CA-C-N	6.62	126.60	119.78
1	D	26	ALA	C-N-CA	6.62	126.60	119.78
1	E	26	ALA	CA-C-N	6.62	126.60	119.78
1	E	26	ALA	C-N-CA	6.62	126.60	119.78
1	C	26	ALA	CA-C-N	6.62	126.59	119.78
1	C	26	ALA	C-N-CA	6.62	126.59	119.78
1	C	331	ALA	CA-C-N	6.54	127.11	120.38
1	C	331	ALA	C-N-CA	6.54	127.11	120.38
1	E	331	ALA	CA-C-N	6.51	127.09	120.38
1	E	331	ALA	C-N-CA	6.51	127.09	120.38
1	D	331	ALA	CA-C-N	6.50	127.08	120.38
1	D	331	ALA	C-N-CA	6.50	127.08	120.38
1	B	331	ALA	CA-C-N	6.50	127.07	120.38
1	B	331	ALA	C-N-CA	6.50	127.07	120.38
1	A	331	ALA	CA-C-N	6.48	127.06	120.38
1	A	331	ALA	C-N-CA	6.48	127.06	120.38
1	E	263	GLN	CA-C-N	6.36	127.80	119.84
1	E	263	GLN	C-N-CA	6.36	127.80	119.84
1	E	332	PRO	CA-C-N	6.35	126.31	120.03
1	E	332	PRO	C-N-CA	6.35	126.31	120.03
1	B	263	GLN	CA-C-N	6.35	127.77	119.84
1	B	263	GLN	C-N-CA	6.35	127.77	119.84
1	C	263	GLN	CA-C-N	6.34	127.76	119.84
1	C	263	GLN	C-N-CA	6.34	127.76	119.84
1	A	332	PRO	CA-C-N	6.33	126.29	120.03
1	A	332	PRO	C-N-CA	6.33	126.29	120.03
1	D	332	PRO	CA-C-N	6.33	126.29	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	332	PRO	C-N-CA	6.33	126.29	120.03
1	B	332	PRO	CA-C-N	6.32	126.29	120.03
1	B	332	PRO	C-N-CA	6.32	126.29	120.03
1	D	263	GLN	CA-C-N	6.31	127.73	119.84
1	D	263	GLN	C-N-CA	6.31	127.73	119.84
1	C	332	PRO	CA-C-N	6.31	126.28	120.03
1	C	332	PRO	C-N-CA	6.31	126.28	120.03
1	A	263	GLN	CA-C-N	6.28	127.69	119.84
1	A	263	GLN	C-N-CA	6.28	127.69	119.84
1	B	6	THR	CB-CA-C	-6.28	109.32	116.54
1	D	12	ASN	CA-CB-CG	-6.27	106.33	112.60
1	B	12	ASN	CA-CB-CG	-6.26	106.34	112.60
1	B	31	PHE	CA-C-N	6.26	126.20	119.76
1	B	31	PHE	C-N-CA	6.26	126.20	119.76
1	C	31	PHE	CA-C-N	6.26	126.20	119.76
1	C	31	PHE	C-N-CA	6.26	126.20	119.76
1	E	6	THR	CB-CA-C	-6.25	109.35	116.54
1	C	12	ASN	CA-CB-CG	-6.25	106.35	112.60
1	C	6	THR	CB-CA-C	-6.25	109.36	116.54
1	D	6	THR	CB-CA-C	-6.25	109.36	116.54
1	D	31	PHE	CA-C-N	6.24	126.19	119.76
1	D	31	PHE	C-N-CA	6.24	126.19	119.76
1	A	12	ASN	CA-CB-CG	-6.24	106.36	112.60
1	A	31	PHE	CA-C-N	6.24	126.19	119.76
1	A	31	PHE	C-N-CA	6.24	126.19	119.76
1	E	12	ASN	CA-CB-CG	-6.23	106.37	112.60
1	A	6	THR	CB-CA-C	-6.22	109.39	116.54
1	E	31	PHE	CA-C-N	6.19	126.14	119.76
1	E	31	PHE	C-N-CA	6.19	126.14	119.76
1	C	171	LEU	CA-C-N	6.04	127.39	119.84
1	C	171	LEU	C-N-CA	6.04	127.39	119.84
1	A	171	LEU	CA-C-N	6.03	127.38	119.84
1	A	171	LEU	C-N-CA	6.03	127.38	119.84
1	B	171	LEU	CA-C-N	6.03	127.38	119.84
1	B	171	LEU	C-N-CA	6.03	127.38	119.84
1	E	171	LEU	CA-C-N	6.00	127.34	119.84
1	E	171	LEU	C-N-CA	6.00	127.34	119.84
1	D	171	LEU	CA-C-N	5.97	127.31	119.84
1	D	171	LEU	C-N-CA	5.97	127.31	119.84
1	C	306	TYR	CA-C-N	5.75	126.03	119.83
1	C	306	TYR	C-N-CA	5.75	126.03	119.83
1	B	306	TYR	CA-C-N	5.70	125.99	119.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	306	TYR	C-N-CA	5.70	125.99	119.83
1	D	306	TYR	CA-C-N	5.70	125.98	119.83
1	D	306	TYR	C-N-CA	5.70	125.98	119.83
1	E	306	TYR	CA-C-N	5.70	125.98	119.83
1	E	306	TYR	C-N-CA	5.70	125.98	119.83
1	A	306	TYR	CA-C-N	5.69	125.97	119.83
1	A	306	TYR	C-N-CA	5.69	125.97	119.83
1	A	242	LEU	CA-C-N	5.27	125.08	119.28
1	A	242	LEU	C-N-CA	5.27	125.08	119.28
1	B	242	LEU	CA-C-N	5.26	125.07	119.28
1	B	242	LEU	C-N-CA	5.26	125.07	119.28
1	C	242	LEU	CA-C-N	5.25	125.06	119.28
1	C	242	LEU	C-N-CA	5.25	125.06	119.28
1	E	242	LEU	CA-C-N	5.25	125.06	119.28
1	E	242	LEU	C-N-CA	5.25	125.06	119.28
1	D	242	LEU	CA-C-N	5.22	125.02	119.28
1	D	242	LEU	C-N-CA	5.22	125.02	119.28
1	D	111	ASN	CA-C-N	5.22	125.13	119.76
1	D	111	ASN	C-N-CA	5.22	125.13	119.76
1	C	111	ASN	CA-C-N	5.21	125.13	119.76
1	C	111	ASN	C-N-CA	5.21	125.13	119.76
1	A	111	ASN	CA-C-N	5.19	125.11	119.76
1	A	111	ASN	C-N-CA	5.19	125.11	119.76
1	B	111	ASN	CA-C-N	5.15	125.06	119.76
1	B	111	ASN	C-N-CA	5.15	125.06	119.76
1	E	111	ASN	CA-C-N	5.13	125.04	119.76
1	E	111	ASN	C-N-CA	5.13	125.04	119.76

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	2900	0	2872	15	0
1	B	2900	0	2872	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2900	0	2872	15	0
1	D	2900	0	2872	13	0
1	E	2900	0	2872	15	0
2	A	27	0	12	2	0
2	B	27	0	12	2	0
2	C	27	0	12	2	0
2	D	27	0	12	2	0
2	E	27	0	12	2	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
3	E	5	0	0	0	0
4	A	98	0	0	26	0
4	B	49	0	0	11	0
4	C	49	0	0	13	0
4	D	49	0	0	13	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
All	All	14910	0	14420	139	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 5.

All (139) 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)
4:D:404:9ZK:C14	4:D:404:9ZK:C10	2.55	0.84
4:D:404:9ZK:C27	4:D:404:9ZK:O48	2.26	0.84
4:B:404:9ZK:C10	4:B:404:9ZK:C14	2.55	0.84
4:B:404:9ZK:C27	4:B:404:9ZK:O48	2.25	0.84
4:A:403:9ZK:C10	4:A:403:9ZK:C14	2.55	0.84
4:A:405:9ZK:C27	4:A:405:9ZK:O48	2.25	0.83
4:A:403:9ZK:C27	4:A:403:9ZK:O48	2.25	0.83
4:C:404:9ZK:C10	4:C:404:9ZK:C14	2.55	0.82
4:A:405:9ZK:C10	4:A:405:9ZK:C14	2.55	0.82
4:C:404:9ZK:O48	4:C:404:9ZK:C27	2.25	0.82
4:A:405:9ZK:C10	4:A:405:9ZK:N15	2.46	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:404:9ZK:C10	4:C:404:9ZK:N15	2.45	0.79
4:A:403:9ZK:C10	4:A:403:9ZK:N15	2.46	0.78
4:B:404:9ZK:C10	4:B:404:9ZK:N15	2.46	0.78
4:D:404:9ZK:C10	4:D:404:9ZK:N15	2.46	0.78
1:B:253:GLU:H	1:B:253:GLU:CD	1.97	0.73
1:D:253:GLU:H	1:D:253:GLU:CD	1.97	0.73
1:E:253:GLU:CD	1:E:253:GLU:H	1.97	0.72
1:A:253:GLU:H	1:A:253:GLU:CD	1.97	0.71
1:C:253:GLU:H	1:C:253:GLU:CD	1.97	0.71
1:C:12:ASN:O	1:C:12:ASN:ND2	2.27	0.67
1:B:12:ASN:O	1:B:12:ASN:ND2	2.27	0.67
1:D:12:ASN:O	1:D:12:ASN:ND2	2.27	0.67
1:A:12:ASN:O	1:A:12:ASN:ND2	2.27	0.66
1:E:12:ASN:O	1:E:12:ASN:ND2	2.27	0.66
1:C:89:THR:OG1	1:C:90:PHE:N	2.32	0.60
4:A:405:9ZK:O48	4:A:405:9ZK:C28	2.50	0.60
4:D:404:9ZK:O48	4:D:404:9ZK:C28	2.50	0.59
4:B:404:9ZK:O48	4:B:404:9ZK:C28	2.50	0.59
4:A:403:9ZK:O48	4:A:403:9ZK:C28	2.50	0.59
1:D:244:ASP:OD1	1:D:244:ASP:C	2.47	0.58
4:C:404:9ZK:O48	4:C:404:9ZK:C28	2.50	0.58
1:B:89:THR:OG1	1:B:90:PHE:N	2.32	0.58
1:C:244:ASP:OD1	1:C:244:ASP:C	2.47	0.57
1:A:89:THR:OG1	1:A:90:PHE:N	2.32	0.57
1:B:244:ASP:C	1:B:244:ASP:OD1	2.47	0.56
2:B:401:ADP:H4'	2:B:401:ADP:O1A	2.06	0.56
2:D:401:ADP:H4'	2:D:401:ADP:O1A	2.06	0.56
1:D:89:THR:OG1	1:D:90:PHE:N	2.32	0.56
1:E:89:THR:OG1	1:E:90:PHE:N	2.32	0.56
2:A:401:ADP:H4'	2:A:401:ADP:O1A	2.06	0.55
2:C:401:ADP:O1A	2:C:401:ADP:H4'	2.06	0.55
4:D:404:9ZK:O48	4:D:404:9ZK:C26	2.54	0.55
2:E:401:ADP:H4'	2:E:401:ADP:O1A	2.06	0.55
4:A:403:9ZK:O48	4:A:403:9ZK:C26	2.54	0.55
4:C:404:9ZK:N37	4:C:404:9ZK:C24	2.71	0.54
4:C:404:9ZK:O48	4:C:404:9ZK:C26	2.54	0.54
1:A:138:ALA:HB2	1:A:161:HIS:CE1	2.43	0.54
4:A:403:9ZK:N37	4:A:403:9ZK:C24	2.71	0.54
4:A:405:9ZK:N37	4:A:405:9ZK:C24	2.71	0.53
1:D:138:ALA:HB2	1:D:161:HIS:CE1	2.43	0.53
1:E:244:ASP:OD1	1:E:244:ASP:C	2.47	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:405:9ZK:O48	4:A:405:9ZK:C26	2.54	0.53
1:B:138:ALA:HB2	1:B:161:HIS:CE1	2.44	0.53
1:C:138:ALA:HB2	1:C:161:HIS:CE1	2.43	0.53
1:A:244:ASP:OD1	1:A:244:ASP:C	2.47	0.53
1:E:138:ALA:HB2	1:E:161:HIS:CE1	2.44	0.53
4:B:404:9ZK:N37	4:B:404:9ZK:C24	2.71	0.53
4:D:404:9ZK:C24	4:D:404:9ZK:N37	2.71	0.52
4:C:404:9ZK:O48	4:C:404:9ZK:C18	2.56	0.52
4:B:404:9ZK:O48	4:B:404:9ZK:C26	2.54	0.52
4:C:404:9ZK:C10	4:C:404:9ZK:C13	2.88	0.50
1:D:138:ALA:HB2	1:D:161:HIS:HE1	1.77	0.50
4:B:404:9ZK:O48	4:B:404:9ZK:C18	2.56	0.50
4:A:403:9ZK:O48	4:A:403:9ZK:C18	2.56	0.49
1:B:352:PHE:O	1:B:352:PHE:CG	2.65	0.49
1:E:138:ALA:HB2	1:E:161:HIS:HE1	1.77	0.49
2:C:401:ADP:O1A	2:C:401:ADP:C4'	2.60	0.49
1:C:138:ALA:HB2	1:C:161:HIS:HE1	1.77	0.49
2:E:401:ADP:O1A	2:E:401:ADP:C4'	2.60	0.49
4:A:405:9ZK:C10	4:A:405:9ZK:C13	2.88	0.49
4:D:404:9ZK:O48	4:D:404:9ZK:C18	2.56	0.49
1:E:352:PHE:O	1:E:352:PHE:CG	2.65	0.49
2:A:401:ADP:O1A	2:A:401:ADP:C4'	2.60	0.49
2:B:401:ADP:O1A	2:B:401:ADP:C4'	2.60	0.49
2:D:401:ADP:O1A	2:D:401:ADP:C4'	2.60	0.49
1:B:138:ALA:HB2	1:B:161:HIS:HE1	1.77	0.49
4:A:405:9ZK:O48	4:A:405:9ZK:C18	2.56	0.48
1:D:352:PHE:O	1:D:352:PHE:CG	2.65	0.48
1:A:138:ALA:HB2	1:A:161:HIS:HE1	1.77	0.48
4:D:404:9ZK:C10	4:D:404:9ZK:C13	2.88	0.48
1:A:352:PHE:CG	1:A:352:PHE:O	2.65	0.48
1:C:352:PHE:CG	1:C:352:PHE:O	2.65	0.47
4:B:404:9ZK:C10	4:B:404:9ZK:C13	2.88	0.47
4:A:403:9ZK:C10	4:A:403:9ZK:C13	2.88	0.46
1:C:132:MET:HB3	1:C:132:MET:HE3	1.80	0.46
4:C:404:9ZK:C32	4:C:404:9ZK:C25	2.94	0.45
4:A:403:9ZK:C25	4:A:403:9ZK:C32	2.94	0.45
1:C:244:ASP:C	1:E:325:MET:SD	2.99	0.45
4:A:405:9ZK:N15	4:A:405:9ZK:C09	2.78	0.45
1:B:244:ASP:C	1:D:325:MET:SD	2.99	0.45
4:A:405:9ZK:C32	4:A:405:9ZK:C25	2.94	0.45
1:A:132:MET:HB3	1:A:132:MET:HE3	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:404:9ZK:C32	4:B:404:9ZK:C25	2.94	0.45
1:A:244:ASP:C	1:C:325:MET:SD	2.99	0.45
4:C:404:9ZK:N15	4:C:404:9ZK:C09	2.78	0.44
4:D:404:9ZK:C25	4:D:404:9ZK:C32	2.94	0.44
4:B:404:9ZK:C36	4:B:404:9ZK:C40	2.96	0.44
4:A:405:9ZK:C36	4:A:405:9ZK:C40	2.96	0.44
4:C:404:9ZK:C36	4:C:404:9ZK:C40	2.96	0.44
4:D:404:9ZK:C40	4:D:404:9ZK:C36	2.96	0.44
1:E:132:MET:HB3	1:E:132:MET:HE3	1.80	0.43
1:D:132:MET:HE3	1:D:132:MET:HB3	1.80	0.43
1:B:78:ASN:OD1	1:B:78:ASN:C	2.62	0.42
1:E:78:ASN:OD1	1:E:78:ASN:C	2.62	0.42
4:A:403:9ZK:C40	4:A:403:9ZK:C36	2.96	0.42
1:C:78:ASN:OD1	1:C:78:ASN:C	2.62	0.42
1:C:222:ASP:OD1	1:C:222:ASP:C	2.63	0.42
1:D:78:ASN:C	1:D:78:ASN:OD1	2.62	0.42
1:A:234:SER:OG	1:A:235:SER:N	2.53	0.42
4:C:404:9ZK:C10	4:C:404:9ZK:C06	2.98	0.41
4:A:405:9ZK:C10	4:A:405:9ZK:C06	2.98	0.41
1:E:222:ASP:OD1	1:E:222:ASP:C	2.63	0.41
1:A:222:ASP:OD1	1:A:222:ASP:C	2.63	0.41
1:A:78:ASN:OD1	1:A:78:ASN:C	2.62	0.41
4:D:404:9ZK:C10	4:D:404:9ZK:C06	2.98	0.41
4:A:403:9ZK:C10	4:A:403:9ZK:C06	2.98	0.41
4:B:404:9ZK:C10	4:B:404:9ZK:C06	2.98	0.41
1:B:37:ARG:HA	1:B:38:PRO:HD3	1.96	0.41
1:C:242:LEU:HB3	1:E:287:ILE:HD11	2.03	0.41
1:E:130:PRO:O	1:E:131:ALA:HB2	2.21	0.41
1:A:252:ASN:OD1	1:A:252:ASN:N	2.54	0.41
4:D:404:9ZK:N15	4:D:404:9ZK:C09	2.78	0.41
1:A:242:LEU:HB3	1:C:287:ILE:HD11	2.03	0.41
4:A:403:9ZK:C40	4:A:403:9ZK:O47	2.69	0.41
1:D:244:ASP:O	1:D:244:ASP:CG	2.63	0.41
1:A:130:PRO:O	1:A:131:ALA:HB2	2.21	0.40
1:B:242:LEU:HB3	1:D:287:ILE:HD11	2.03	0.40
1:B:252:ASN:OD1	1:B:252:ASN:N	2.54	0.40
4:D:404:9ZK:C40	4:D:404:9ZK:O47	2.69	0.40
1:E:252:ASN:OD1	1:E:252:ASN:N	2.54	0.40
4:A:405:9ZK:C40	4:A:405:9ZK:O47	2.69	0.40
1:B:130:PRO:O	1:B:131:ALA:HB2	2.21	0.40
1:B:132:MET:HE3	1:B:132:MET:HB3	1.80	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:PRO:O	1:C:131:ALA:HB2	2.21	0.40
4:C:404:9ZK:C40	4:C:404:9ZK:O47	2.69	0.40
1:D:222:ASP:OD1	1:D:222:ASP:C	2.63	0.40
1:E:244:ASP:O	1:E:244:ASP:CG	2.63	0.40
4:A:405:9ZK:O49	4:A:405:9ZK:C17	2.70	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	368/375 (98%)	339 (92%)	20 (5%)	9 (2%)	4	29
1	B	368/375 (98%)	338 (92%)	21 (6%)	9 (2%)	4	29
1	C	368/375 (98%)	339 (92%)	20 (5%)	9 (2%)	4	29
1	D	368/375 (98%)	339 (92%)	20 (5%)	9 (2%)	4	29
1	E	368/375 (98%)	339 (92%)	20 (5%)	9 (2%)	4	29
All	All	1840/1875 (98%)	1694 (92%)	101 (6%)	45 (2%)	7	29

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	LYS
1	A	89	THR
1	A	131	ALA
1	B	50	LYS
1	B	89	THR
1	B	131	ALA
1	C	50	LYS
1	C	89	THR
1	C	131	ALA

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Mol	Chain	Res	Type
1	D	50	LYS
1	D	89	THR
1	D	131	ALA
1	E	50	LYS
1	E	89	THR
1	E	131	ALA
1	A	44	MET
1	B	44	MET
1	C	44	MET
1	D	44	MET
1	E	44	MET
1	A	264	PRO
1	B	264	PRO
1	C	264	PRO
1	D	264	PRO
1	E	264	PRO
1	A	38	PRO
1	A	164	PRO
1	A	367	PRO
1	B	38	PRO
1	B	164	PRO
1	B	367	PRO
1	C	38	PRO
1	C	164	PRO
1	C	367	PRO
1	D	38	PRO
1	D	164	PRO
1	D	367	PRO
1	E	38	PRO
1	E	164	PRO
1	E	367	PRO
1	A	98	PRO
1	B	98	PRO
1	C	98	PRO
1	D	98	PRO
1	E	98	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	313/317 (99%)	313 (100%)	0	100	100
1	B	313/317 (99%)	313 (100%)	0	100	100
1	C	313/317 (99%)	313 (100%)	0	100	100
1	D	313/317 (99%)	313 (100%)	0	100	100
1	E	313/317 (99%)	313 (100%)	0	100	100
All	All	1565/1585 (99%)	1565 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	101	HIS
1	A	161	HIS
1	A	162	ASN
1	A	246	GLN
1	A	314	GLN
1	B	41	GLN
1	B	101	HIS
1	B	161	HIS
1	B	246	GLN
1	B	314	GLN
1	C	41	GLN
1	C	101	HIS
1	C	161	HIS
1	C	162	ASN
1	C	246	GLN
1	C	314	GLN
1	C	354	GLN
1	D	101	HIS
1	D	161	HIS
1	D	162	ASN
1	D	246	GLN
1	D	314	GLN
1	E	101	HIS
1	E	161	HIS
1	E	314	GLN

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Mol	Chain	Res	Type
1	E	354	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

5 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	HIC	C	73	1	10,11,12	1.09	1 (10%)	9,14,16	6.33	3 (33%)
1	HIC	D	73	1	10,11,12	1.08	1 (10%)	9,14,16	6.24	3 (33%)
1	HIC	E	73	1	10,11,12	1.09	1 (10%)	9,14,16	6.25	3 (33%)
1	HIC	B	73	1	10,11,12	1.09	1 (10%)	9,14,16	6.34	3 (33%)
1	HIC	A	73	1	10,11,12	1.10	1 (10%)	9,14,16	6.25	3 (33%)

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
1	HIC	C	73	1	-	0/5/6/8	0/1/1/1
1	HIC	D	73	1	-	0/5/6/8	0/1/1/1
1	HIC	E	73	1	-	0/5/6/8	0/1/1/1
1	HIC	B	73	1	-	0/5/6/8	0/1/1/1
1	HIC	A	73	1	-	0/5/6/8	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	73	HIC	CD2-NE2	-2.06	1.34	1.37
1	B	73	HIC	CD2-NE2	-2.05	1.34	1.37
1	D	73	HIC	CD2-NE2	-2.05	1.34	1.37
1	E	73	HIC	CD2-NE2	-2.05	1.34	1.37
1	C	73	HIC	CD2-NE2	-2.03	1.34	1.37

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	73	HIC	NE2-CE1-ND1	-15.83	106.60	112.66
1	C	73	HIC	NE2-CE1-ND1	-15.80	106.61	112.66
1	E	73	HIC	NE2-CE1-ND1	-15.62	106.68	112.66
1	A	73	HIC	NE2-CE1-ND1	-15.61	106.69	112.66
1	D	73	HIC	NE2-CE1-ND1	-15.60	106.69	112.66
1	C	73	HIC	CD2-NE2-CE1	9.60	110.50	106.71
1	B	73	HIC	CD2-NE2-CE1	9.58	110.50	106.71
1	A	73	HIC	CD2-NE2-CE1	9.44	110.44	106.71
1	D	73	HIC	CD2-NE2-CE1	9.41	110.43	106.71
1	E	73	HIC	CD2-NE2-CE1	9.39	110.42	106.71
1	B	73	HIC	CE1-ND1-CG	2.64	110.03	105.80
1	C	73	HIC	CE1-ND1-CG	2.63	110.01	105.80
1	D	73	HIC	CE1-ND1-CG	2.61	109.99	105.80
1	E	73	HIC	CE1-ND1-CG	2.61	109.98	105.80
1	A	73	HIC	CE1-ND1-CG	2.60	109.97	105.80

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 20 ligands modelled in this entry, 5 are monoatomic - leaving 15 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
2	ADP	C	401	5	28,29,29	2.86	11 (39%)	43,45,45	1.66	10 (23%)
4	9ZK	A	403	-	52,52,52	2.33	18 (34%)	68,71,71	1.99	19 (27%)
3	PO4	E	402	5	4,4,4	2.34	3 (75%)	6,6,6	2.00	3 (50%)
4	9ZK	C	404	-	52,52,52	2.33	18 (34%)	68,71,71	1.98	19 (27%)
2	ADP	E	401	5	28,29,29	2.87	11 (39%)	43,45,45	1.66	9 (20%)
4	9ZK	A	405	-	52,52,52	2.33	18 (34%)	68,71,71	1.99	19 (27%)
2	ADP	B	401	5	28,29,29	2.87	11 (39%)	43,45,45	1.66	9 (20%)
3	PO4	B	402	5	4,4,4	2.34	3 (75%)	6,6,6	2.00	3 (50%)
3	PO4	A	402	5	4,4,4	2.34	3 (75%)	6,6,6	2.00	3 (50%)
3	PO4	D	402	5	4,4,4	2.36	3 (75%)	6,6,6	2.01	3 (50%)
4	9ZK	D	404	-	52,52,52	2.33	18 (34%)	68,71,71	1.99	19 (27%)
4	9ZK	B	404	-	52,52,52	2.33	18 (34%)	68,71,71	1.99	19 (27%)
2	ADP	D	401	5	28,29,29	2.86	11 (39%)	43,45,45	1.66	10 (23%)
3	PO4	C	402	5	4,4,4	2.34	3 (75%)	6,6,6	2.00	3 (50%)
2	ADP	A	401	5	28,29,29	2.86	11 (39%)	43,45,45	1.66	10 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	C	401	5	-	4/16/32/32	0/3/3/3
4	9ZK	A	403	-	-	21/59/59/59	0/3/4/4
4	9ZK	C	404	-	-	21/59/59/59	0/3/4/4
2	ADP	E	401	5	-	4/16/32/32	0/3/3/3
4	9ZK	A	405	-	-	21/59/59/59	0/3/4/4
2	ADP	B	401	5	-	4/16/32/32	0/3/3/3
4	9ZK	D	404	-	-	21/59/59/59	0/3/4/4
4	9ZK	B	404	-	-	21/59/59/59	0/3/4/4
2	ADP	D	401	5	-	4/16/32/32	0/3/3/3
2	ADP	A	401	5	-	4/16/32/32	0/3/3/3

All (160) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	401	ADP	PA-O3A	-10.15	1.48	1.59
2	B	401	ADP	PA-O3A	-10.13	1.48	1.59
2	A	401	ADP	PA-O3A	-10.10	1.48	1.59
2	C	401	ADP	PA-O3A	-10.09	1.48	1.59
2	D	401	ADP	PA-O3A	-10.09	1.48	1.59
4	A	403	9ZK	C31-C30	-7.25	1.32	1.41
4	D	404	9ZK	C31-C30	-7.22	1.32	1.41
4	A	405	9ZK	C31-C30	-7.21	1.32	1.41
4	B	404	9ZK	C31-C30	-7.20	1.32	1.41
4	C	404	9ZK	C31-C30	-7.18	1.32	1.41
2	D	401	ADP	C4-N9	-5.41	1.26	1.37
2	B	401	ADP	C4-N9	-5.40	1.26	1.37
2	C	401	ADP	C4-N9	-5.39	1.26	1.37
2	E	401	ADP	C4-N9	-5.38	1.26	1.37
2	A	401	ADP	C4-N9	-5.37	1.26	1.37
4	A	403	9ZK	C31-C27	-5.09	1.35	1.44
4	B	404	9ZK	C31-C27	-5.09	1.35	1.44
4	C	404	9ZK	C31-C27	-5.07	1.35	1.44
4	D	404	9ZK	C31-C27	-5.03	1.35	1.44
4	A	405	9ZK	C31-C27	-5.00	1.35	1.44
4	A	405	9ZK	C14-N15	4.63	1.44	1.34
4	A	403	9ZK	C14-N15	4.61	1.43	1.34
4	D	404	9ZK	C14-N15	4.61	1.43	1.34
4	B	404	9ZK	C14-N15	4.60	1.43	1.34
4	C	404	9ZK	C14-N15	4.59	1.43	1.34
2	E	401	ADP	C5-N7	-4.32	1.31	1.39
2	C	401	ADP	C5-N7	-4.25	1.31	1.39
2	B	401	ADP	C5-N7	-4.25	1.31	1.39
2	A	401	ADP	C5-N7	-4.25	1.31	1.39
2	D	401	ADP	C5-N7	-4.24	1.31	1.39
4	D	404	9ZK	O47-C36	-4.19	1.15	1.23
4	A	405	9ZK	O47-C36	-4.18	1.15	1.23
4	A	403	9ZK	O47-C36	-4.16	1.15	1.23
4	B	404	9ZK	O47-C36	-4.14	1.15	1.23
4	C	404	9ZK	O47-C36	-4.14	1.15	1.23
4	A	403	9ZK	C25-N23	-3.97	1.41	1.47
4	B	404	9ZK	C25-N23	-3.96	1.41	1.47
4	C	404	9ZK	C25-N23	-3.95	1.41	1.47
4	D	404	9ZK	C25-N23	-3.94	1.41	1.47
4	A	405	9ZK	C25-N23	-3.94	1.41	1.47
3	E	402	PO4	P-O3	-3.46	1.44	1.54
3	C	402	PO4	P-O3	-3.45	1.44	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	402	PO4	P-O3	-3.45	1.44	1.54
4	A	405	9ZK	C28-N29	-3.44	1.31	1.37
4	A	405	9ZK	C36-N37	3.44	1.41	1.34
3	A	402	PO4	P-O3	-3.44	1.44	1.54
4	A	403	9ZK	C28-N29	-3.43	1.31	1.37
3	B	402	PO4	P-O3	-3.43	1.44	1.54
4	A	403	9ZK	C36-N37	3.41	1.41	1.34
4	B	404	9ZK	C36-N37	3.41	1.41	1.34
4	D	404	9ZK	C36-N37	3.40	1.41	1.34
4	D	404	9ZK	C28-N29	-3.40	1.31	1.37
4	C	404	9ZK	C36-N37	3.39	1.41	1.34
4	C	404	9ZK	C28-N29	-3.38	1.31	1.37
4	B	404	9ZK	C28-N29	-3.36	1.31	1.37
2	E	401	ADP	C8-N9	-3.31	1.31	1.37
2	A	401	ADP	C8-N9	-3.30	1.31	1.37
2	C	401	ADP	C8-N9	-3.30	1.31	1.37
2	D	401	ADP	C8-N9	-3.29	1.32	1.37
2	B	401	ADP	C8-N9	-3.28	1.32	1.37
4	A	403	9ZK	O49-C14	-3.23	1.17	1.23
4	A	405	9ZK	O49-C14	-3.20	1.17	1.23
4	C	404	9ZK	O49-C14	-3.19	1.17	1.23
4	B	404	9ZK	O49-C14	-3.19	1.17	1.23
4	D	404	9ZK	O49-C14	-3.13	1.17	1.23
2	C	401	ADP	C2'-C3'	-3.12	1.44	1.53
2	A	401	ADP	C2'-C3'	-3.12	1.44	1.53
2	B	401	ADP	C2'-C3'	-3.11	1.44	1.53
4	A	403	9ZK	C45-C39	-3.11	1.34	1.39
4	D	404	9ZK	O48-C22	-3.10	1.16	1.22
2	E	401	ADP	C2'-C3'	-3.10	1.45	1.53
4	A	405	9ZK	C45-C39	-3.10	1.34	1.39
4	D	404	9ZK	C45-C39	-3.10	1.34	1.39
4	A	405	9ZK	O48-C22	-3.08	1.16	1.22
4	B	404	9ZK	C45-C39	-3.08	1.34	1.39
2	D	401	ADP	C2'-C3'	-3.08	1.45	1.53
4	C	404	9ZK	O48-C22	-3.08	1.16	1.22
4	C	404	9ZK	C25-C36	-3.08	1.45	1.52
4	B	404	9ZK	C25-C36	-3.07	1.45	1.52
4	A	403	9ZK	O48-C22	-3.07	1.16	1.22
4	B	404	9ZK	O48-C22	-3.07	1.16	1.22
4	A	405	9ZK	C25-C36	-3.06	1.45	1.52
4	C	404	9ZK	C45-C39	-3.06	1.34	1.39
4	D	404	9ZK	C25-C36	-3.04	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	403	9ZK	C25-C36	-3.03	1.45	1.52
4	C	404	9ZK	C11-C12	-2.82	1.47	1.53
2	A	401	ADP	C4-N3	-2.81	1.29	1.34
2	D	401	ADP	C4-N3	-2.81	1.29	1.34
2	E	401	ADP	C4-N3	-2.80	1.29	1.34
4	D	404	9ZK	C11-C12	-2.80	1.47	1.53
2	C	401	ADP	C4-N3	-2.79	1.29	1.34
4	B	404	9ZK	C11-C12	-2.78	1.48	1.53
4	A	403	9ZK	C11-C12	-2.78	1.48	1.53
2	B	401	ADP	C4-N3	-2.78	1.29	1.34
4	C	404	9ZK	C40-C39	-2.76	1.34	1.39
4	A	405	9ZK	C11-C12	-2.76	1.48	1.53
4	B	404	9ZK	C40-C39	-2.74	1.34	1.39
4	A	403	9ZK	C40-C39	-2.73	1.34	1.39
4	C	404	9ZK	O03-C02	-2.72	1.42	1.47
4	B	404	9ZK	O03-C02	-2.71	1.42	1.47
4	A	405	9ZK	C40-C39	-2.71	1.34	1.39
4	A	405	9ZK	O03-C02	-2.71	1.42	1.47
4	D	404	9ZK	O03-C02	-2.71	1.42	1.47
4	A	403	9ZK	O03-C02	-2.71	1.42	1.47
4	A	403	9ZK	C34-C35	-2.69	1.34	1.38
4	D	404	9ZK	C34-C35	-2.68	1.34	1.38
4	D	404	9ZK	C40-C39	-2.67	1.34	1.39
4	C	404	9ZK	C34-C35	-2.67	1.34	1.38
4	B	404	9ZK	C34-C35	-2.66	1.34	1.38
4	A	405	9ZK	C34-C35	-2.66	1.34	1.38
2	C	401	ADP	C2-N3	-2.56	1.29	1.33
2	B	401	ADP	C5-C4	2.56	1.43	1.39
2	E	401	ADP	C5-C4	2.56	1.43	1.39
2	C	401	ADP	C5-C4	2.54	1.43	1.39
2	A	401	ADP	C2-N3	-2.53	1.29	1.33
2	A	401	ADP	C5-C4	2.53	1.43	1.39
2	B	401	ADP	C2-N3	-2.52	1.29	1.33
4	B	404	9ZK	C22-N23	2.51	1.41	1.35
2	D	401	ADP	C5-C4	2.51	1.43	1.39
2	E	401	ADP	C2-N3	-2.51	1.29	1.33
2	D	401	ADP	C2-N3	-2.49	1.29	1.33
4	D	404	9ZK	C22-N23	2.49	1.41	1.35
2	D	401	ADP	C2'-C1'	-2.49	1.45	1.53
4	A	405	9ZK	C22-N23	2.48	1.40	1.35
4	C	404	9ZK	C22-N23	2.47	1.40	1.35
4	A	403	9ZK	C22-N23	2.47	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	ADP	C2'-C1'	-2.47	1.45	1.53
2	B	401	ADP	C2'-C1'	-2.47	1.45	1.53
2	E	401	ADP	C2'-C1'	-2.46	1.45	1.53
2	A	401	ADP	C2'-C1'	-2.46	1.45	1.53
2	B	401	ADP	O4'-C4'	-2.45	1.39	1.45
2	A	401	ADP	O4'-C4'	-2.44	1.39	1.45
2	C	401	ADP	O4'-C4'	-2.44	1.39	1.45
2	E	401	ADP	O4'-C4'	-2.42	1.39	1.45
2	D	401	ADP	O4'-C4'	-2.39	1.39	1.45
4	C	404	9ZK	C32-C31	-2.23	1.36	1.39
4	A	405	9ZK	C32-C31	-2.23	1.36	1.39
3	D	402	PO4	P-O2	-2.22	1.48	1.54
3	B	402	PO4	P-O2	-2.22	1.48	1.54
4	D	404	9ZK	C32-C31	-2.21	1.36	1.39
4	A	403	9ZK	C32-C31	-2.21	1.36	1.39
3	D	402	PO4	P-O4	-2.20	1.48	1.54
3	A	402	PO4	P-O4	-2.19	1.48	1.54
4	B	404	9ZK	C32-C31	-2.18	1.36	1.39
3	A	402	PO4	P-O2	-2.18	1.48	1.54
3	E	402	PO4	P-O2	-2.18	1.48	1.54
3	C	402	PO4	P-O4	-2.18	1.48	1.54
3	B	402	PO4	P-O4	-2.18	1.48	1.54
3	E	402	PO4	P-O4	-2.18	1.48	1.54
3	C	402	PO4	P-O2	-2.17	1.48	1.54
4	A	405	9ZK	C33-C32	-2.17	1.35	1.38
4	A	403	9ZK	C33-C32	-2.17	1.35	1.38
4	D	404	9ZK	C33-C32	-2.14	1.35	1.38
4	B	404	9ZK	C33-C32	-2.14	1.35	1.38
4	C	404	9ZK	C33-C32	-2.11	1.35	1.38
2	E	401	ADP	C3'-C4'	-2.03	1.47	1.53
2	A	401	ADP	C3'-C4'	-2.03	1.47	1.53
2	C	401	ADP	C3'-C4'	-2.03	1.47	1.53
2	B	401	ADP	C3'-C4'	-2.02	1.47	1.53
2	D	401	ADP	C3'-C4'	-2.01	1.47	1.53

All (158) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	403	9ZK	C38-N37-C36	-8.53	111.14	122.98
4	D	404	9ZK	C38-N37-C36	-8.52	111.14	122.98
4	A	405	9ZK	C38-N37-C36	-8.52	111.14	122.98
4	B	404	9ZK	C38-N37-C36	-8.52	111.15	122.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	404	9ZK	C38-N37-C36	-8.46	111.23	122.98
4	A	405	9ZK	O03-C04-C46	5.97	122.13	111.43
4	C	404	9ZK	O03-C04-C46	5.97	122.12	111.43
4	A	403	9ZK	O03-C04-C46	5.96	122.10	111.43
4	B	404	9ZK	O03-C04-C46	5.94	122.07	111.43
4	D	404	9ZK	O03-C04-C46	5.94	122.07	111.43
2	B	401	ADP	C5-C4-N3	-4.36	120.71	126.72
2	A	401	ADP	C5-C4-N3	-4.35	120.73	126.72
2	C	401	ADP	C5-C4-N3	-4.34	120.74	126.72
2	D	401	ADP	C5-C4-N3	-4.33	120.75	126.72
2	E	401	ADP	C5-C4-N3	-4.31	120.78	126.72
2	B	401	ADP	C2'-C1'-N9	-3.68	104.17	113.30
2	A	401	ADP	C2'-C1'-N9	-3.66	104.22	113.30
2	C	401	ADP	C2'-C1'-N9	-3.65	104.22	113.30
2	E	401	ADP	C2'-C1'-N9	-3.65	104.22	113.30
2	D	401	ADP	C2'-C1'-N9	-3.65	104.24	113.30
3	D	402	PO4	O4-P-O2	3.27	118.08	107.91
3	E	402	PO4	O4-P-O2	3.25	118.04	107.91
3	C	402	PO4	O4-P-O2	3.25	118.03	107.91
3	A	402	PO4	O4-P-O2	3.25	118.01	107.91
3	B	402	PO4	O4-P-O2	3.24	117.99	107.91
4	B	404	9ZK	C27-C28-N29	-3.19	106.80	110.31
4	C	404	9ZK	C27-C28-N29	-3.19	106.81	110.31
4	A	405	9ZK	C27-C28-N29	-3.17	106.83	110.31
4	A	403	9ZK	C27-C28-N29	-3.16	106.83	110.31
4	D	404	9ZK	C27-C28-N29	-3.14	106.86	110.31
2	B	401	ADP	C4-C5-N7	-3.09	107.05	110.58
2	A	401	ADP	C4-C5-N7	-3.06	107.08	110.58
2	C	401	ADP	C4-C5-N7	-3.05	107.09	110.58
2	E	401	ADP	C4-C5-N7	-3.04	107.11	110.58
2	D	401	ADP	C4-C5-N7	-3.03	107.12	110.58
4	B	404	9ZK	C22-C16-N15	2.94	116.60	108.97
4	C	404	9ZK	C22-C16-N15	2.94	116.60	108.97
4	D	404	9ZK	C22-C16-N15	2.94	116.59	108.97
4	A	403	9ZK	C24-N23-C25	2.94	122.78	117.70
4	C	404	9ZK	C24-N23-C25	2.93	122.77	117.70
4	A	403	9ZK	C22-C16-N15	2.93	116.56	108.97
2	E	401	ADP	C4-N9-C8	2.92	108.81	105.74
4	B	404	9ZK	C24-N23-C25	2.92	122.76	117.70
4	A	405	9ZK	C24-N23-C25	2.92	122.75	117.70
4	A	405	9ZK	C22-C16-N15	2.92	116.54	108.97
4	D	404	9ZK	C24-N23-C25	2.92	122.74	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	ADP	C4-N9-C8	2.91	108.80	105.74
2	C	401	ADP	C4-N9-C8	2.91	108.79	105.74
2	B	401	ADP	C4-N9-C8	2.90	108.79	105.74
2	B	401	ADP	N3-C4-N9	2.90	132.09	127.17
2	C	401	ADP	N3-C4-N9	2.89	132.09	127.17
2	E	401	ADP	N3-C4-N9	2.89	132.09	127.17
2	A	401	ADP	N3-C4-N9	2.89	132.08	127.17
2	D	401	ADP	N3-C4-N9	2.88	132.06	127.17
2	A	401	ADP	C2-N3-C4	2.88	118.86	111.83
2	C	401	ADP	C2-N3-C4	2.88	118.86	111.83
2	D	401	ADP	C2-N3-C4	2.87	118.84	111.83
2	B	401	ADP	C2-N3-C4	2.86	118.83	111.83
2	A	401	ADP	C4-N9-C8	2.86	108.74	105.74
2	E	401	ADP	C2-N3-C4	2.86	118.82	111.83
4	A	403	9ZK	C10-C09-C08	-2.81	116.40	123.63
4	A	405	9ZK	C10-C09-C08	-2.81	116.42	123.63
4	B	404	9ZK	C10-C09-C08	-2.80	116.42	123.63
4	D	404	9ZK	C10-C09-C08	-2.79	116.47	123.63
4	C	404	9ZK	C10-C09-C08	-2.78	116.48	123.63
4	B	404	9ZK	C31-C27-C28	2.77	108.99	106.16
4	C	404	9ZK	C07-C08-C09	-2.73	121.36	127.62
4	A	405	9ZK	C07-C08-C09	-2.73	121.37	127.62
4	A	403	9ZK	C07-C08-C09	-2.73	121.38	127.62
4	B	404	9ZK	C07-C08-C09	-2.73	121.38	127.62
4	D	404	9ZK	C07-C08-C09	-2.73	121.38	127.62
4	C	404	9ZK	C31-C27-C28	2.72	108.94	106.16
4	A	403	9ZK	C31-C27-C28	2.72	108.94	106.16
4	A	405	9ZK	C31-C27-C28	2.71	108.93	106.16
4	D	404	9ZK	C31-C27-C28	2.70	108.92	106.16
4	A	405	9ZK	C35-C30-C31	-2.67	119.61	122.19
4	D	404	9ZK	C35-C30-C31	-2.63	119.64	122.19
4	A	403	9ZK	C35-C30-C31	-2.63	119.64	122.19
4	B	404	9ZK	C35-C30-C31	-2.61	119.67	122.19
4	C	404	9ZK	C35-C30-C31	-2.60	119.67	122.19
4	B	404	9ZK	C12-C11-C09	-2.53	109.38	114.82
2	C	401	ADP	O4'-C1'-N9	2.52	112.93	108.09
4	A	403	9ZK	C12-C11-C09	-2.52	109.41	114.82
4	A	405	9ZK	C12-C11-C09	-2.51	109.41	114.82
2	B	401	ADP	O4'-C1'-N9	2.51	112.91	108.09
2	A	401	ADP	O4'-C1'-N9	2.51	112.91	108.09
4	C	404	9ZK	C12-C11-C09	-2.51	109.42	114.82
4	D	404	9ZK	C12-C11-C09	-2.51	109.43	114.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	401	ADP	O4'-C1'-N9	2.50	112.89	108.09
2	D	401	ADP	O4'-C1'-N9	2.50	112.88	108.09
4	C	404	9ZK	C17-C16-C22	-2.49	103.58	109.75
4	D	404	9ZK	C17-C16-C22	-2.49	103.59	109.75
4	A	405	9ZK	C17-C16-C22	-2.48	103.60	109.75
4	B	404	9ZK	C17-C16-C22	-2.48	103.62	109.75
4	A	403	9ZK	C17-C16-C22	-2.47	103.62	109.75
3	B	402	PO4	O4-P-O3	-2.46	100.27	107.91
4	A	403	9ZK	O05-C04-C46	-2.45	118.95	124.65
3	E	402	PO4	O4-P-O3	-2.45	100.30	107.91
4	C	404	9ZK	O05-C04-C46	-2.44	118.98	124.65
3	D	402	PO4	O4-P-O3	-2.44	100.33	107.91
3	A	402	PO4	O4-P-O3	-2.44	100.33	107.91
4	A	405	9ZK	O05-C04-C46	-2.43	119.00	124.65
3	C	402	PO4	O4-P-O3	-2.43	100.34	107.91
4	B	404	9ZK	O48-C22-N23	-2.43	117.78	121.76
3	C	402	PO4	O4-P-O1	-2.42	102.40	110.95
3	D	402	PO4	O4-P-O1	-2.41	102.41	110.95
3	E	402	PO4	O4-P-O1	-2.41	102.42	110.95
4	D	404	9ZK	O05-C04-C46	-2.41	119.04	124.65
3	B	402	PO4	O4-P-O1	-2.41	102.42	110.95
3	A	402	PO4	O4-P-O1	-2.41	102.42	110.95
4	B	404	9ZK	O05-C04-C46	-2.41	119.05	124.65
4	D	404	9ZK	O48-C22-N23	-2.41	117.81	121.76
4	A	405	9ZK	O48-C22-N23	-2.41	117.81	121.76
4	A	403	9ZK	O48-C22-N23	-2.39	117.85	121.76
4	C	404	9ZK	O48-C22-N23	-2.37	117.88	121.76
2	C	401	ADP	C6-C5-N7	2.34	136.59	132.09
2	E	401	ADP	C6-C5-N7	2.33	136.59	132.09
2	A	401	ADP	C6-C5-N7	2.33	136.58	132.09
2	B	401	ADP	C6-C5-N7	2.33	136.58	132.09
2	D	401	ADP	C6-C5-N7	2.30	136.52	132.09
2	A	401	ADP	C3'-C2'-C1'	-2.21	97.29	101.46
2	D	401	ADP	C3'-C2'-C1'	-2.20	97.30	101.46
4	D	404	9ZK	C36-C25-N23	-2.20	104.11	109.97
4	A	403	9ZK	C36-C25-N23	-2.19	104.11	109.97
2	E	401	ADP	C3'-C2'-C1'	-2.19	97.31	101.46
4	D	404	9ZK	C26-C27-C31	-2.19	122.48	126.70
4	B	404	9ZK	C26-C27-C31	-2.19	122.49	126.70
4	A	405	9ZK	C36-C25-N23	-2.19	104.12	109.97
4	A	405	9ZK	C26-C27-C31	-2.19	122.49	126.70
2	B	401	ADP	C3'-C2'-C1'	-2.19	97.32	101.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	ADP	C3'-C2'-C1'	-2.19	97.32	101.46
4	A	403	9ZK	C01-C02-C06	-2.18	108.25	113.90
4	C	404	9ZK	C36-C25-N23	-2.18	104.15	109.97
4	B	404	9ZK	C01-C02-C06	-2.18	108.25	113.90
4	C	404	9ZK	C01-C02-C06	-2.18	108.26	113.90
4	D	404	9ZK	C01-C02-C06	-2.18	108.27	113.90
4	C	404	9ZK	C26-C27-C31	-2.17	122.52	126.70
4	B	404	9ZK	C36-C25-N23	-2.17	104.18	109.97
4	A	405	9ZK	C01-C02-C06	-2.17	108.29	113.90
4	A	403	9ZK	C26-C27-C31	-2.16	122.54	126.70
4	D	404	9ZK	C12-C14-N15	2.16	118.74	116.42
4	D	404	9ZK	O03-C02-C06	2.15	111.29	106.75
4	C	404	9ZK	O03-C02-C06	2.15	111.28	106.75
4	A	403	9ZK	O03-C02-C06	2.15	111.28	106.75
4	B	404	9ZK	O03-C02-C06	2.15	111.27	106.75
4	A	405	9ZK	O03-C02-C06	2.13	111.24	106.75
4	A	405	9ZK	C12-C14-N15	2.12	118.69	116.42
4	B	404	9ZK	C12-C14-N15	2.11	118.68	116.42
4	C	404	9ZK	C12-C14-N15	2.09	118.67	116.42
4	A	403	9ZK	C12-C14-N15	2.07	118.64	116.42
4	A	405	9ZK	O03-C04-O05	-2.07	118.88	123.70
4	B	404	9ZK	O03-C04-O05	-2.06	118.88	123.70
4	D	404	9ZK	O03-C04-O05	-2.06	118.89	123.70
4	C	404	9ZK	O03-C04-O05	-2.06	118.90	123.70
4	A	403	9ZK	O03-C04-O05	-2.04	118.94	123.70
2	D	401	ADP	N3-C2-N1	-2.03	125.50	128.58
2	A	401	ADP	N3-C2-N1	-2.02	125.52	128.58
2	C	401	ADP	N3-C2-N1	-2.01	125.54	128.58

There are no chirality outliers.

All (125) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	ADP	C4'-C5'-O5'-PA
2	B	401	ADP	C4'-C5'-O5'-PA
2	C	401	ADP	C4'-C5'-O5'-PA
2	D	401	ADP	C4'-C5'-O5'-PA
2	E	401	ADP	C4'-C5'-O5'-PA
4	A	403	9ZK	N23-C25-C26-C27
4	A	403	9ZK	C36-C25-N23-C24
4	A	403	9ZK	C36-C25-N23-C22
4	A	403	9ZK	C10-C09-C11-C12

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Mol	Chain	Res	Type	Atoms
4	A	403	9ZK	C08-C09-C11-C12
4	A	403	9ZK	C01-C02-C06-C07
4	A	403	9ZK	O03-C02-C06-C07
4	A	405	9ZK	N23-C25-C26-C27
4	A	405	9ZK	C36-C25-N23-C24
4	A	405	9ZK	C10-C09-C11-C12
4	A	405	9ZK	C08-C09-C11-C12
4	A	405	9ZK	C01-C02-C06-C07
4	A	405	9ZK	O03-C02-C06-C07
4	B	404	9ZK	N23-C25-C26-C27
4	B	404	9ZK	C36-C25-N23-C24
4	B	404	9ZK	C10-C09-C11-C12
4	B	404	9ZK	C08-C09-C11-C12
4	B	404	9ZK	C01-C02-C06-C07
4	B	404	9ZK	O03-C02-C06-C07
4	C	404	9ZK	N23-C25-C26-C27
4	C	404	9ZK	C36-C25-N23-C24
4	C	404	9ZK	C36-C25-N23-C22
4	C	404	9ZK	C10-C09-C11-C12
4	C	404	9ZK	C08-C09-C11-C12
4	C	404	9ZK	C01-C02-C06-C07
4	C	404	9ZK	O03-C02-C06-C07
4	D	404	9ZK	N23-C25-C26-C27
4	D	404	9ZK	C36-C25-N23-C24
4	D	404	9ZK	C36-C25-N23-C22
4	D	404	9ZK	C10-C09-C11-C12
4	D	404	9ZK	C08-C09-C11-C12
4	D	404	9ZK	C01-C02-C06-C07
4	D	404	9ZK	O03-C02-C06-C07
4	A	403	9ZK	C17-C16-N15-C14
4	A	405	9ZK	C17-C16-N15-C14
4	B	404	9ZK	C17-C16-N15-C14
4	C	404	9ZK	C17-C16-N15-C14
4	D	404	9ZK	C17-C16-N15-C14
4	A	403	9ZK	C25-C26-C27-C31
4	A	405	9ZK	C25-C26-C27-C31
4	B	404	9ZK	C25-C26-C27-C31
4	C	404	9ZK	C25-C26-C27-C31
4	D	404	9ZK	C25-C26-C27-C31
4	A	403	9ZK	C26-C25-N23-C24
4	A	405	9ZK	C26-C25-N23-C24
4	B	404	9ZK	C26-C25-N23-C24

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Mol	Chain	Res	Type	Atoms
4	C	404	9ZK	C26-C25-N23-C24
4	D	404	9ZK	C26-C25-N23-C24
4	A	403	9ZK	C46-C04-O03-C02
4	A	405	9ZK	C46-C04-O03-C02
4	B	404	9ZK	C46-C04-O03-C02
4	C	404	9ZK	C46-C04-O03-C02
4	D	404	9ZK	C46-C04-O03-C02
4	A	403	9ZK	C26-C25-N23-C22
4	A	405	9ZK	C26-C25-N23-C22
4	B	404	9ZK	C26-C25-N23-C22
4	C	404	9ZK	C26-C25-N23-C22
4	D	404	9ZK	C26-C25-N23-C22
4	A	405	9ZK	C36-C25-N23-C22
4	B	404	9ZK	C36-C25-N23-C22
4	A	403	9ZK	O05-C04-O03-C02
4	A	405	9ZK	O05-C04-O03-C02
4	B	404	9ZK	O05-C04-O03-C02
4	C	404	9ZK	O05-C04-O03-C02
4	D	404	9ZK	O05-C04-O03-C02
4	A	403	9ZK	C25-C26-C27-C28
4	A	405	9ZK	C25-C26-C27-C28
4	B	404	9ZK	C25-C26-C27-C28
4	C	404	9ZK	C25-C26-C27-C28
4	D	404	9ZK	C25-C26-C27-C28
4	A	403	9ZK	C16-C17-C18-C19
4	A	405	9ZK	C16-C17-C18-C19
4	B	404	9ZK	C16-C17-C18-C19
4	C	404	9ZK	C16-C17-C18-C19
4	D	404	9ZK	C16-C17-C18-C19
4	A	403	9ZK	C17-C18-C19-C20
4	A	405	9ZK	C17-C18-C19-C20
4	B	404	9ZK	C17-C18-C19-C20
4	C	404	9ZK	C17-C18-C19-C20
4	D	404	9ZK	C17-C18-C19-C20
4	A	403	9ZK	C18-C19-C20-N21
4	A	405	9ZK	C18-C19-C20-N21
4	B	404	9ZK	C18-C19-C20-N21
4	C	404	9ZK	C18-C19-C20-N21
4	D	404	9ZK	C18-C19-C20-N21
4	A	403	9ZK	C46-C38-C39-C40
4	A	403	9ZK	C46-C38-C39-C45
4	A	405	9ZK	C46-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
4	A	405	9ZK	C46-C38-C39-C45
4	B	404	9ZK	C46-C38-C39-C40
4	B	404	9ZK	C46-C38-C39-C45
4	C	404	9ZK	C46-C38-C39-C40
4	C	404	9ZK	C46-C38-C39-C45
4	D	404	9ZK	C46-C38-C39-C40
4	D	404	9ZK	C46-C38-C39-C45
4	A	403	9ZK	C39-C38-C46-C04
4	A	405	9ZK	C39-C38-C46-C04
4	B	404	9ZK	C39-C38-C46-C04
4	C	404	9ZK	C39-C38-C46-C04
4	D	404	9ZK	C39-C38-C46-C04
2	A	401	ADP	C5'-O5'-PA-O1A
2	B	401	ADP	C5'-O5'-PA-O1A
2	C	401	ADP	C5'-O5'-PA-O1A
2	D	401	ADP	C5'-O5'-PA-O1A
2	E	401	ADP	C5'-O5'-PA-O1A
2	A	401	ADP	PA-O3A-PB-O1B
2	B	401	ADP	PA-O3A-PB-O1B
2	C	401	ADP	PA-O3A-PB-O1B
2	D	401	ADP	PA-O3A-PB-O1B
2	E	401	ADP	PA-O3A-PB-O1B
4	A	403	9ZK	C06-C07-C08-C09
4	A	405	9ZK	C06-C07-C08-C09
4	B	404	9ZK	C06-C07-C08-C09
4	C	404	9ZK	C06-C07-C08-C09
4	D	404	9ZK	C06-C07-C08-C09
2	A	401	ADP	C3'-C4'-C5'-O5'
2	B	401	ADP	C3'-C4'-C5'-O5'
2	C	401	ADP	C3'-C4'-C5'-O5'
2	D	401	ADP	C3'-C4'-C5'-O5'
2	E	401	ADP	C3'-C4'-C5'-O5'

There are no ring outliers.

10 monomers are involved in 73 short contacts:

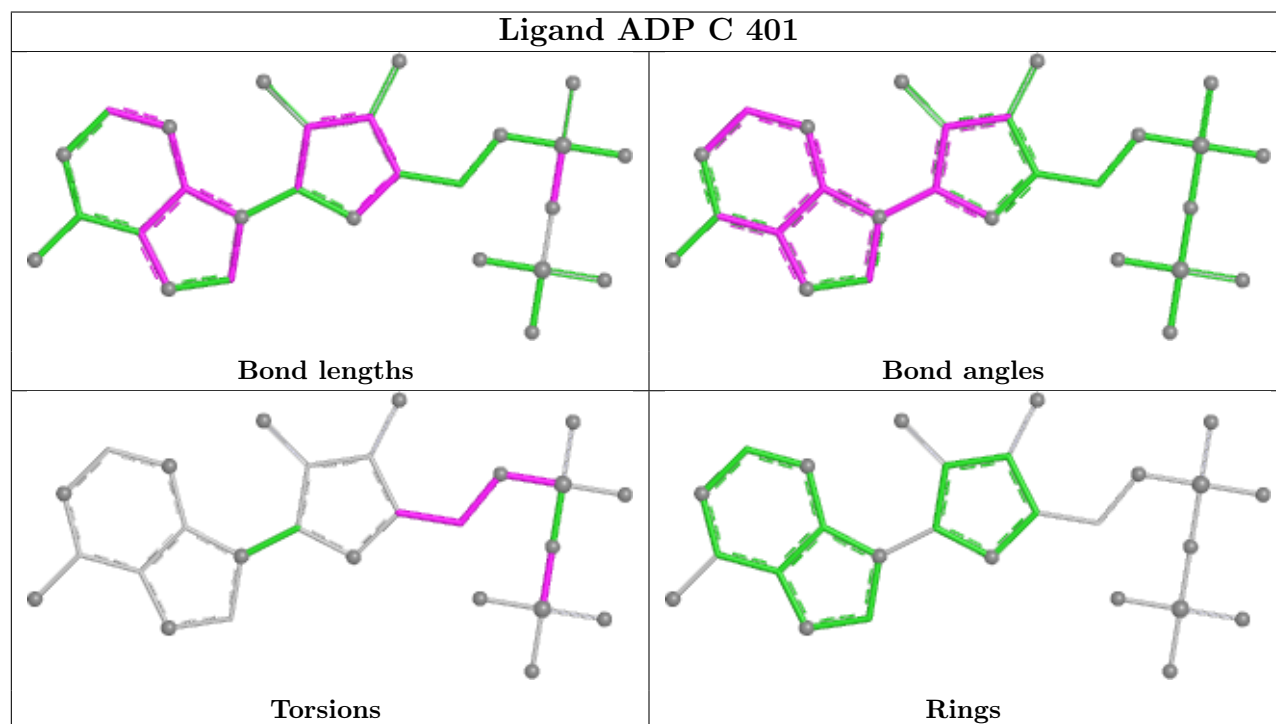
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	ADP	2	0
4	A	403	9ZK	12	0
4	C	404	9ZK	13	0
2	E	401	ADP	2	0
4	A	405	9ZK	14	0

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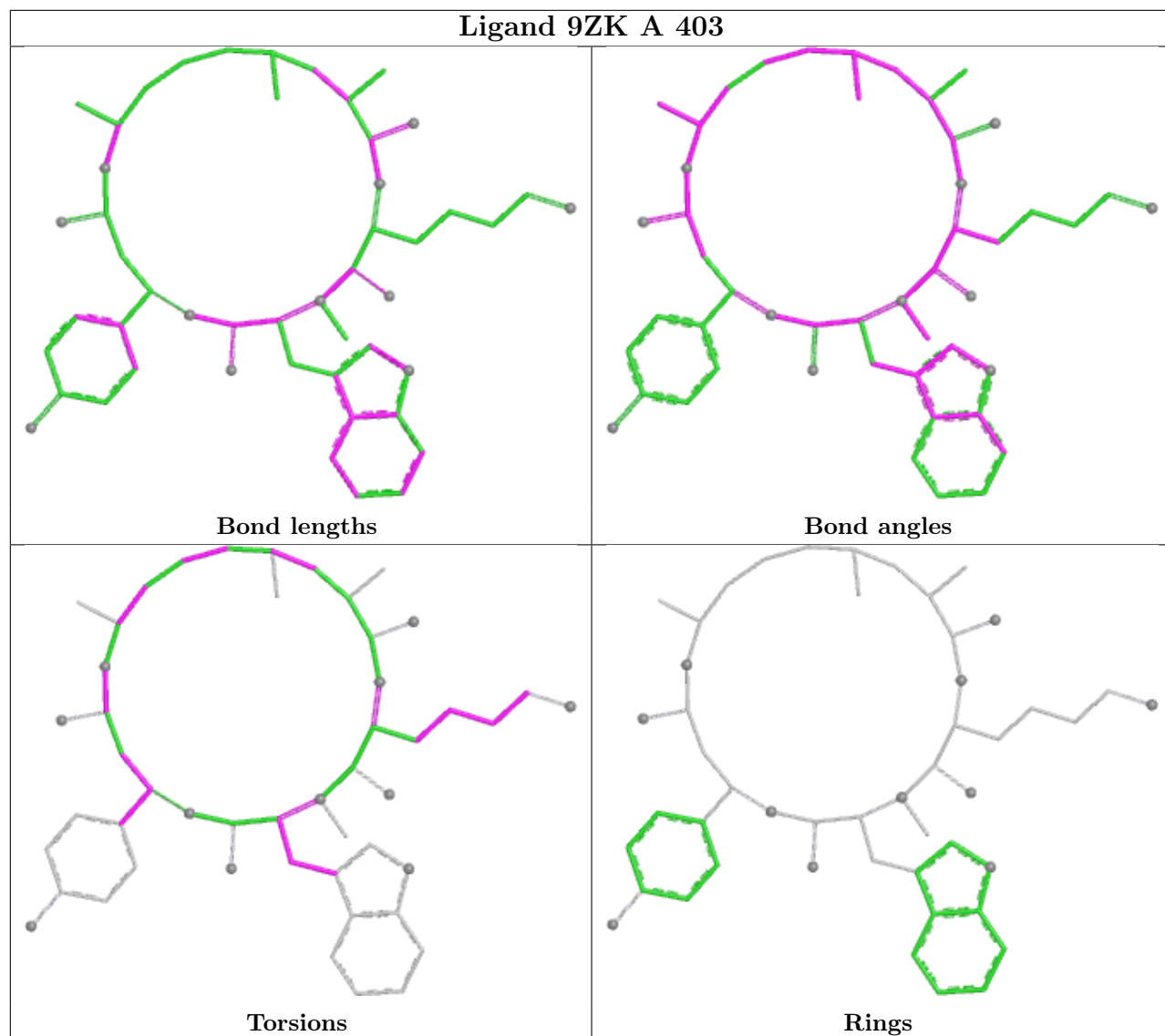
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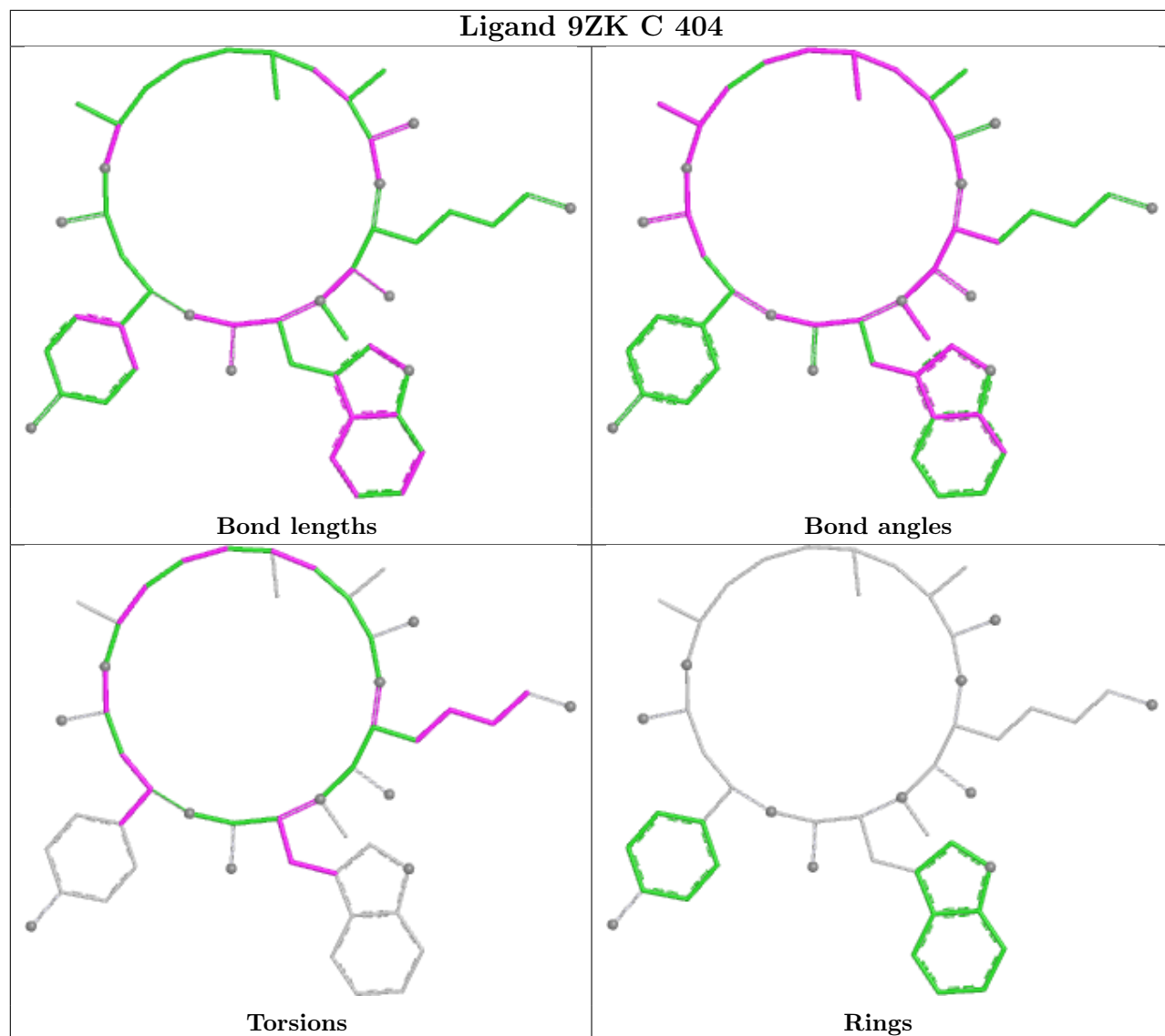
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	ADP	2	0
4	D	404	9ZK	13	0
4	B	404	9ZK	11	0
2	D	401	ADP	2	0
2	A	401	ADP	2	0

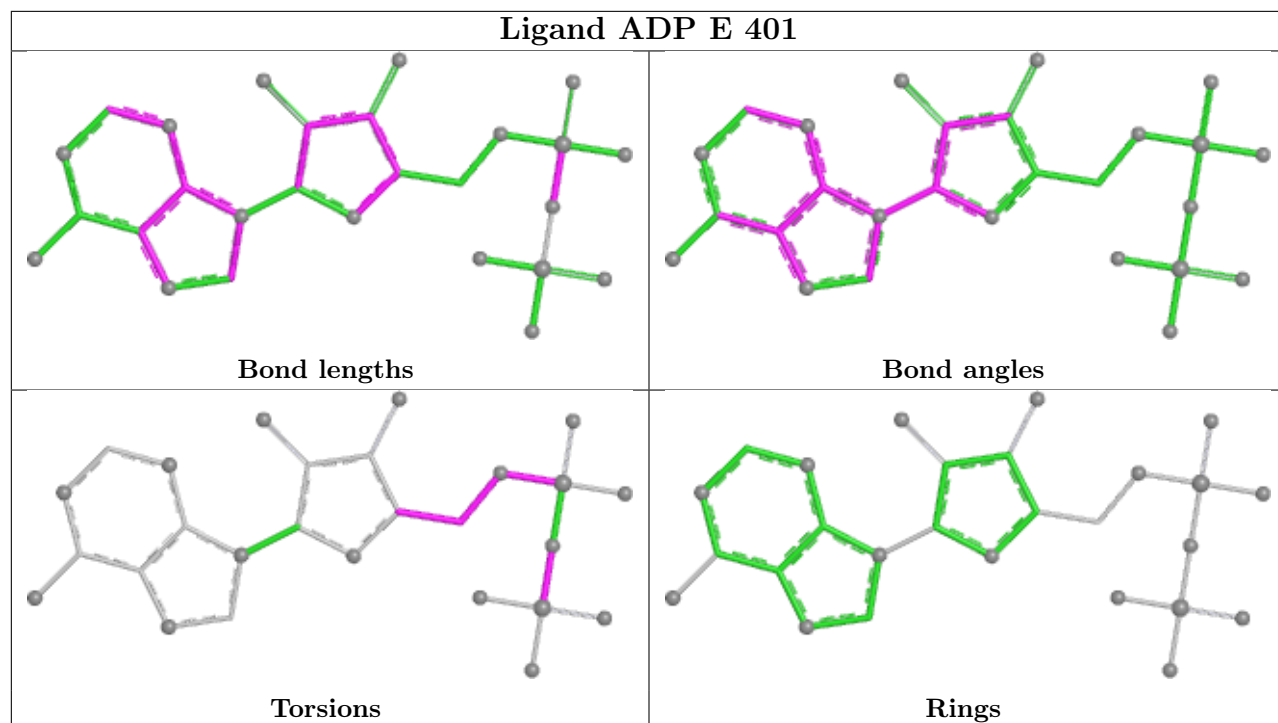
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



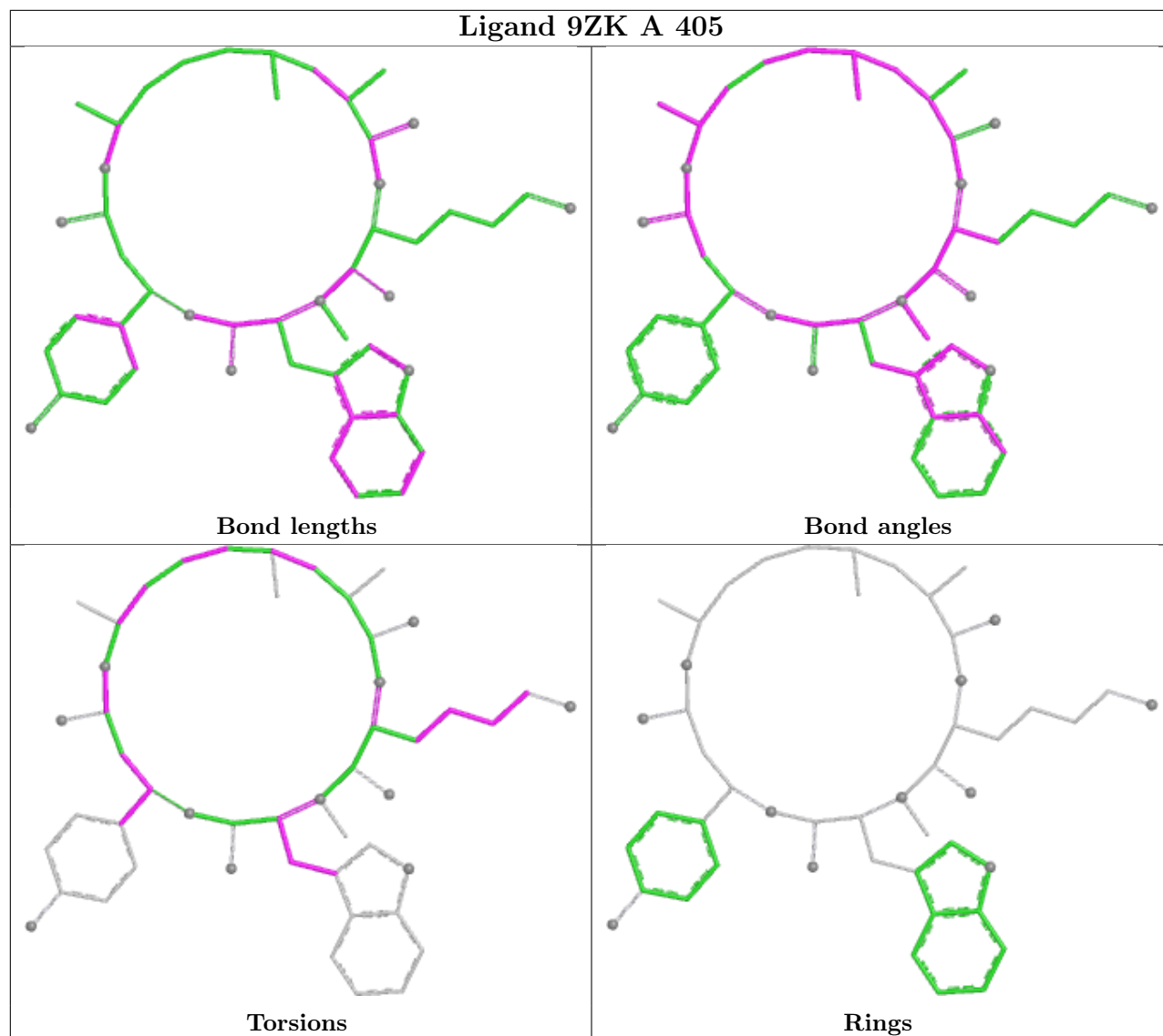
Ligand 9ZK A 403

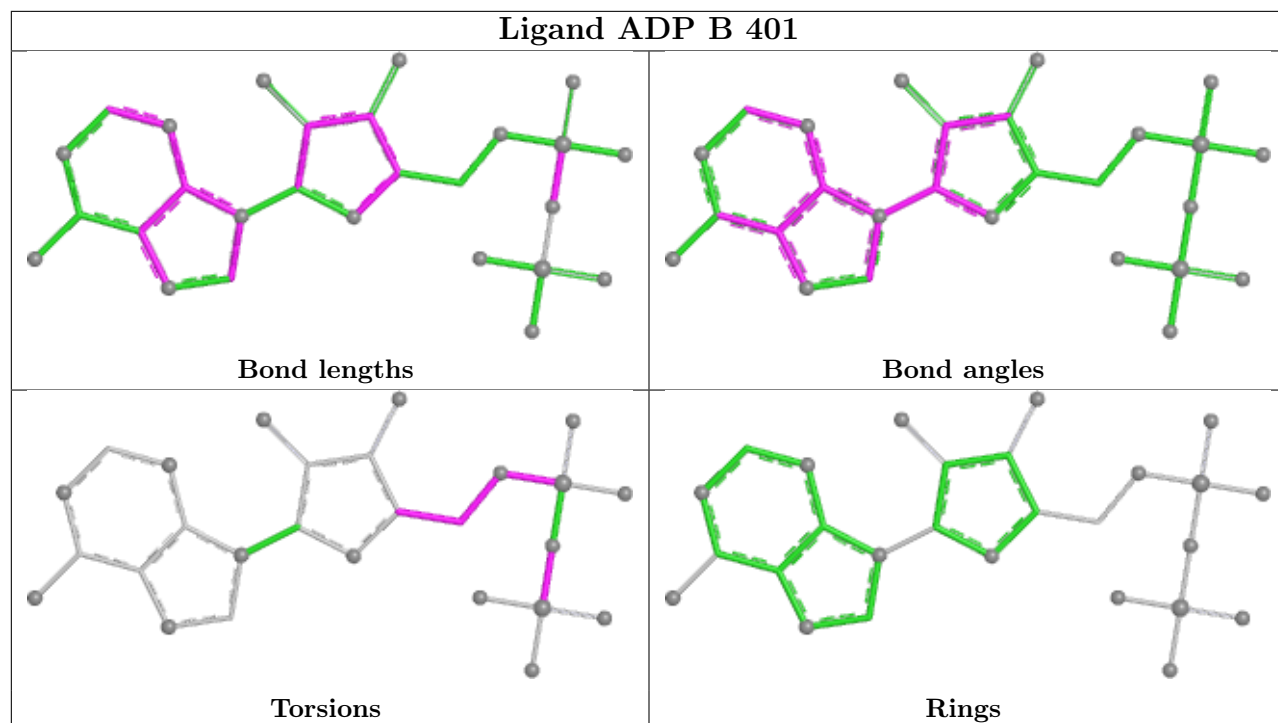


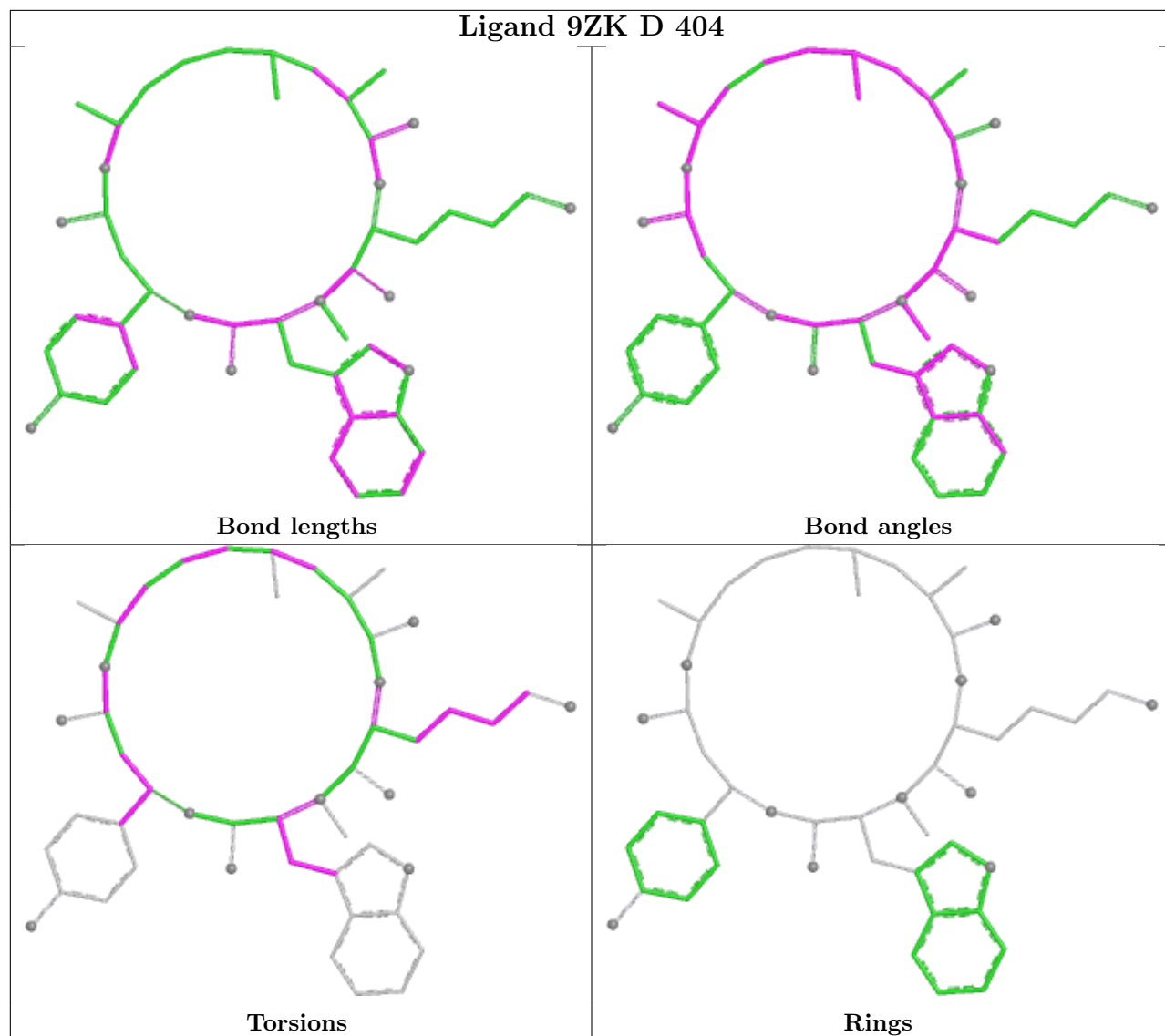




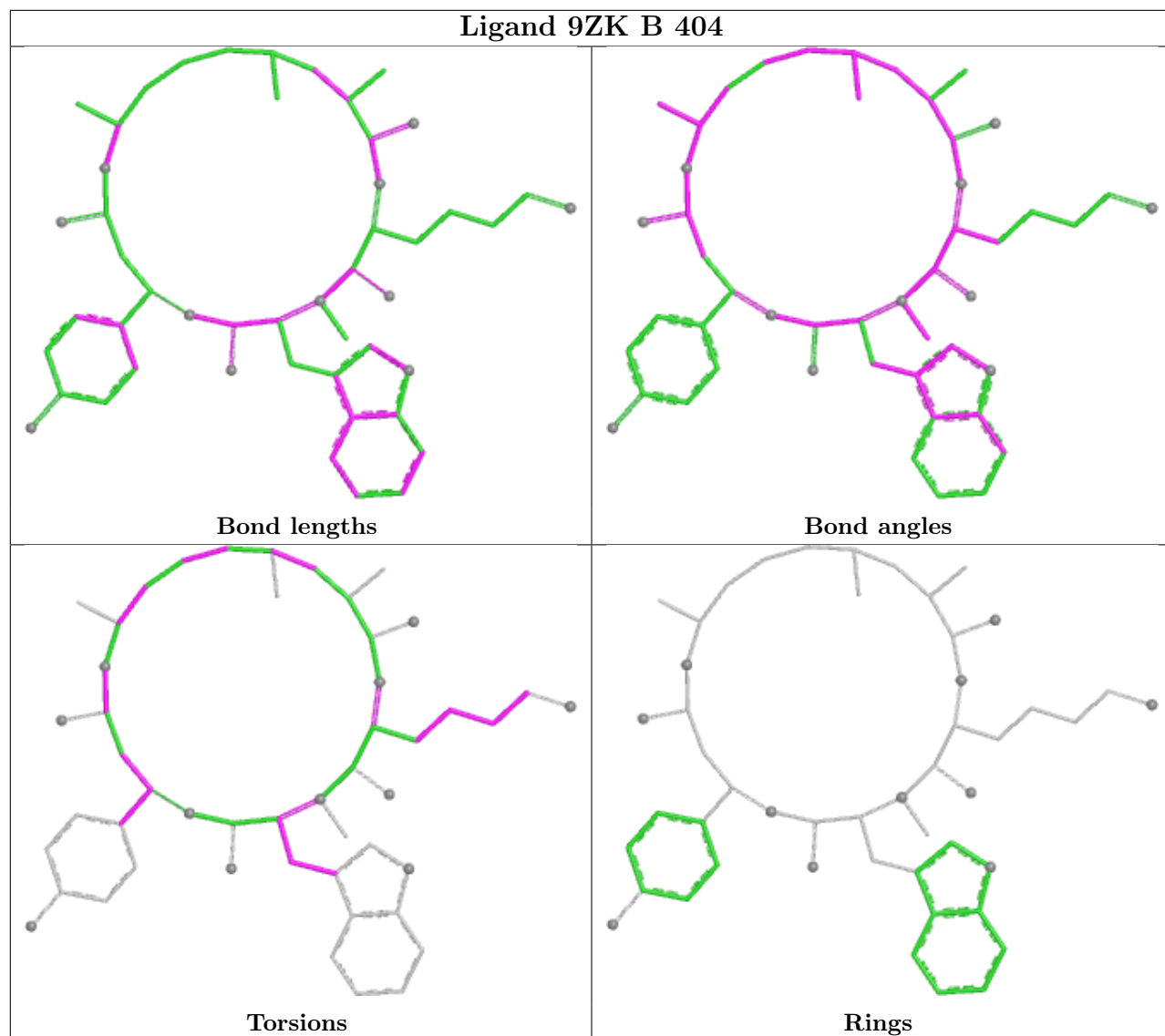
Ligand 9ZK A 405

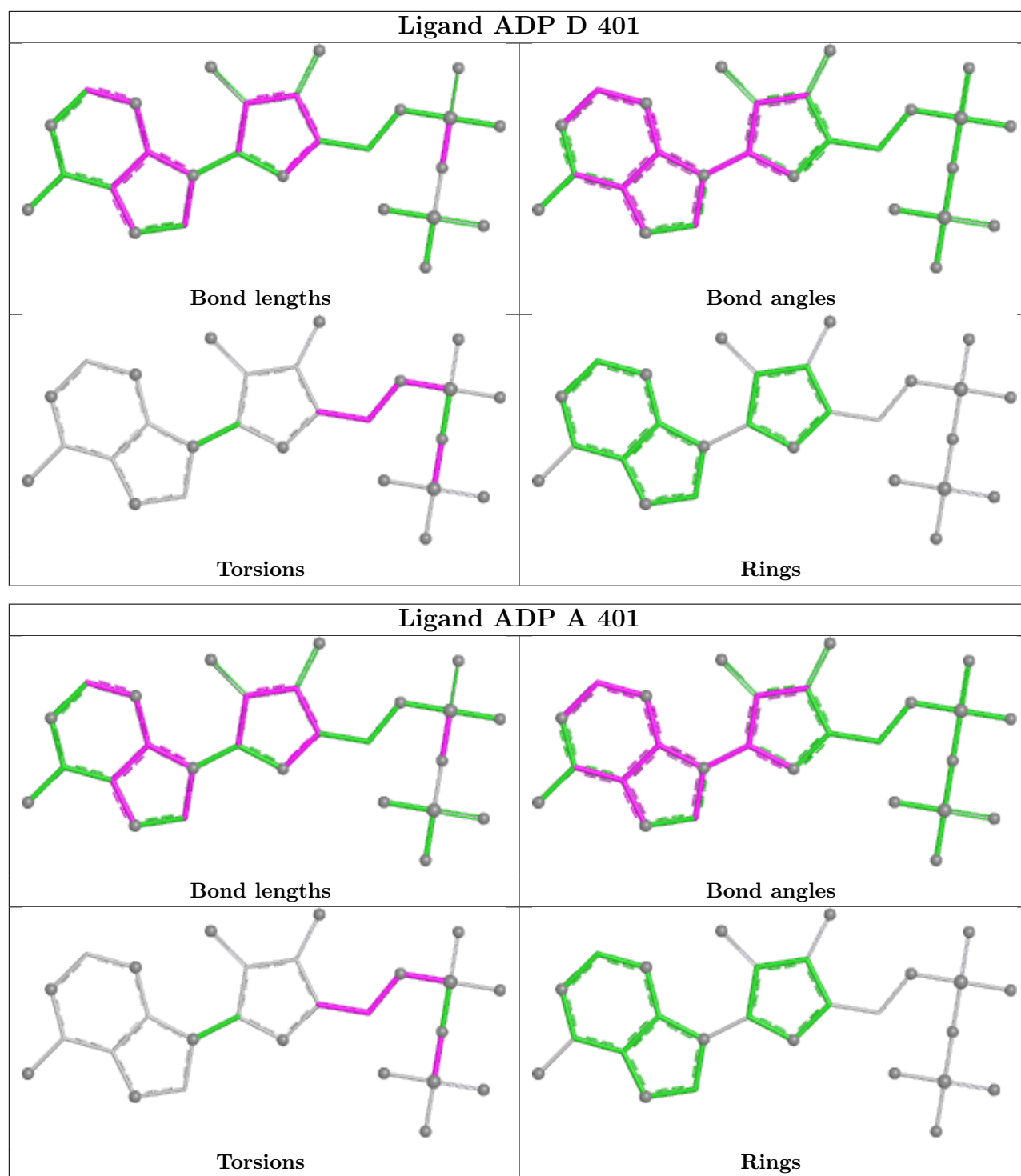






Ligand 9ZK B 404





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

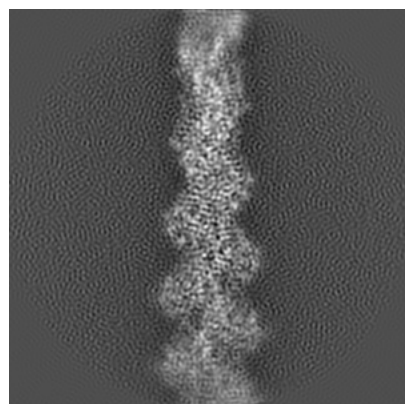
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3837. These allow visual inspection of the internal detail of the map and identification of artifacts.

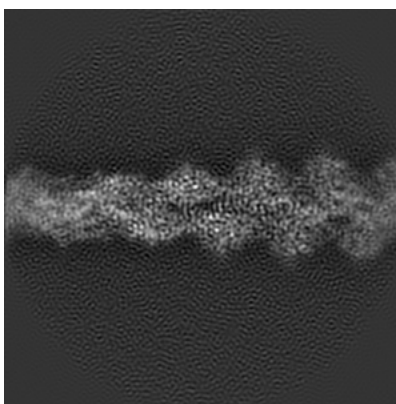
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

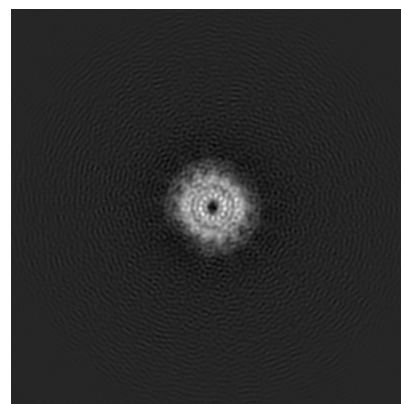
6.1.1 Primary map



X

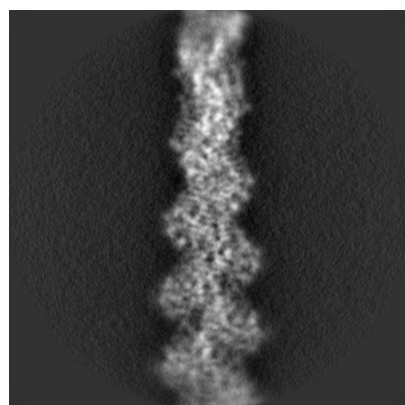


Y

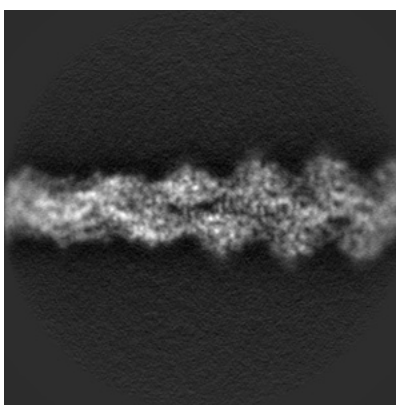


Z

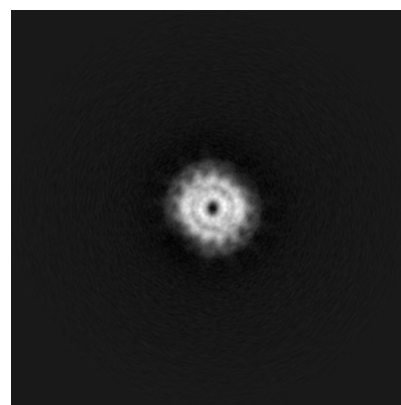
6.1.2 Raw map



X



Y

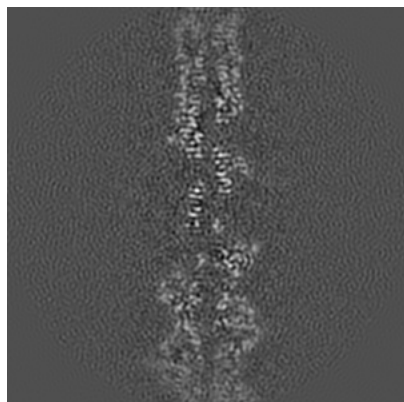


Z

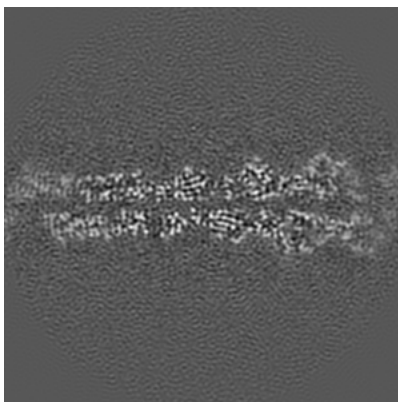
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

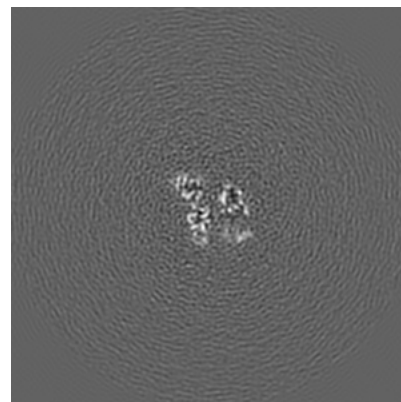
6.2.1 Primary map



X Index: 144

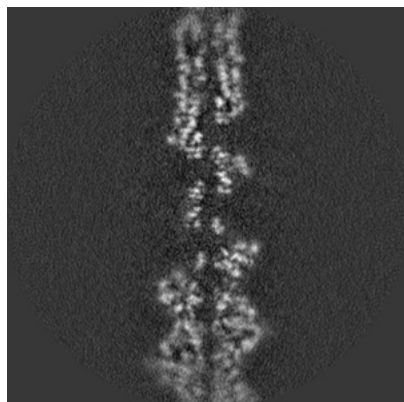


Y Index: 144

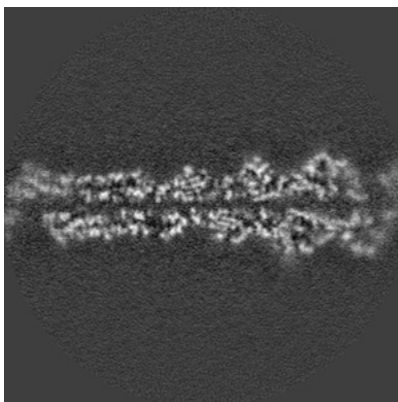


Z Index: 144

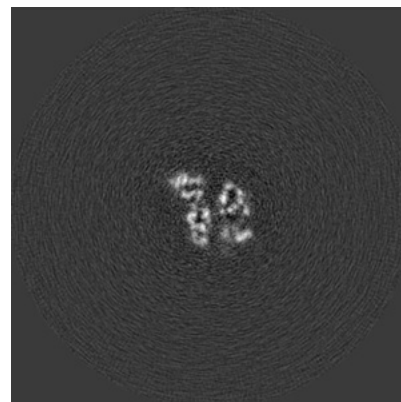
6.2.2 Raw map



X Index: 144



Y Index: 144

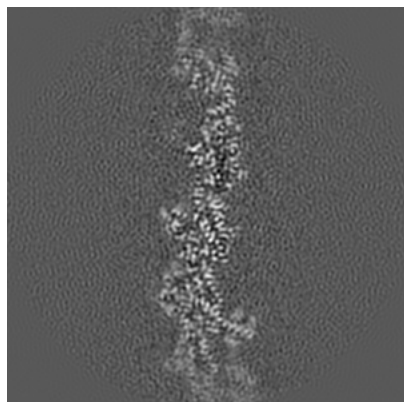


Z Index: 144

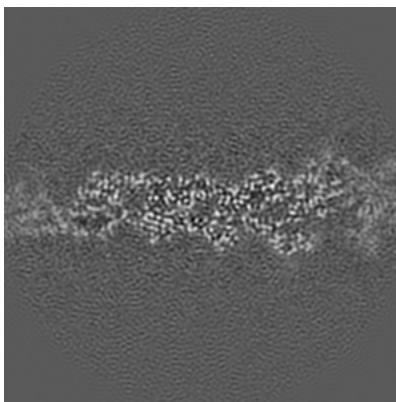
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

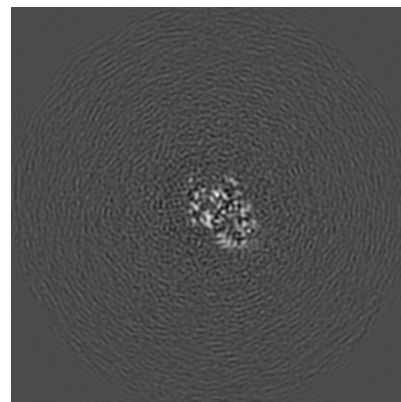
6.3.1 Primary map



X Index: 153

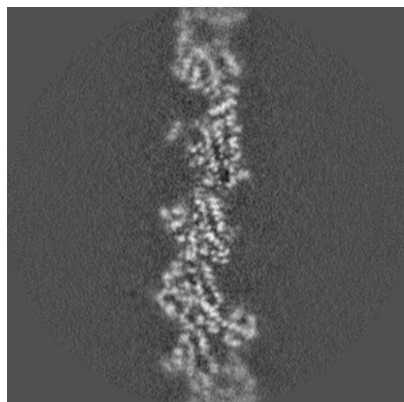


Y Index: 151

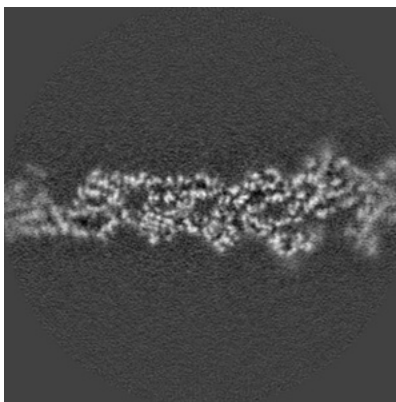


Z Index: 130

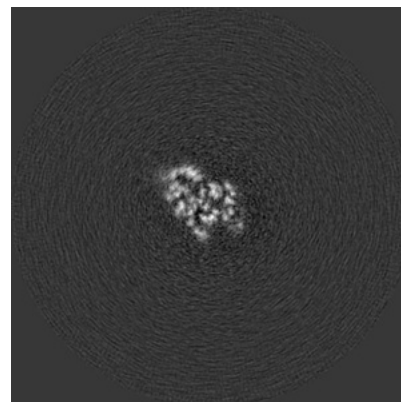
6.3.2 Raw map



X Index: 152



Y Index: 151

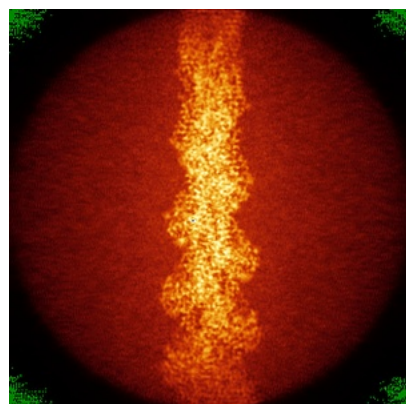


Z Index: 155

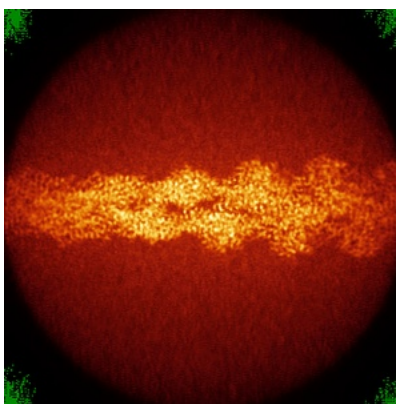
The images above show the largest variance slices of the map in three orthogonal directions.

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

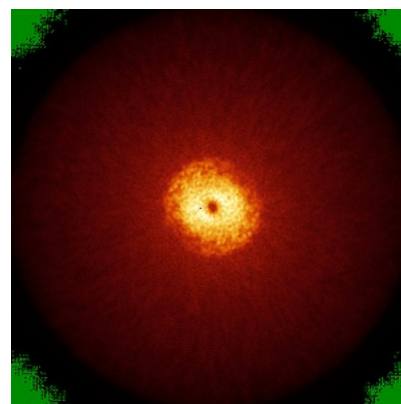
6.4.1 Primary map



X

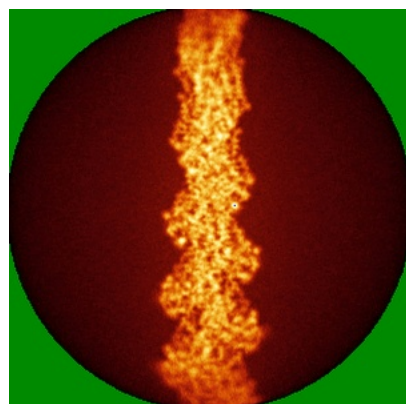


Y

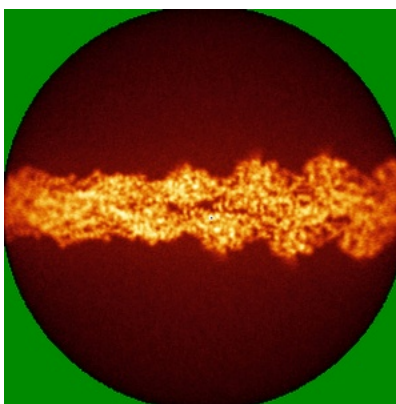


Z

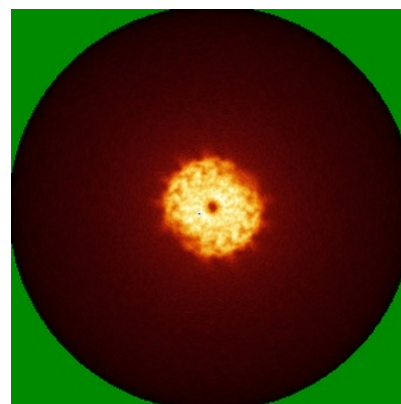
6.4.2 Raw map



X



Y

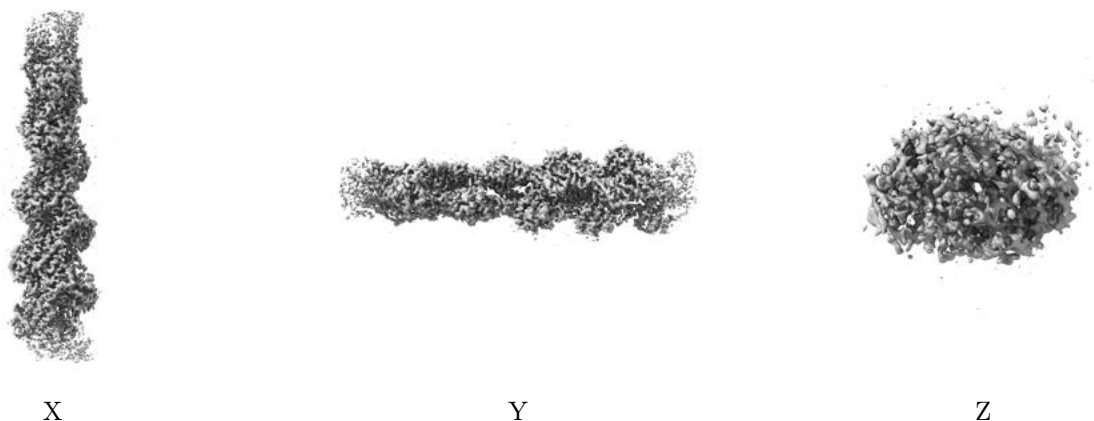


Z

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.

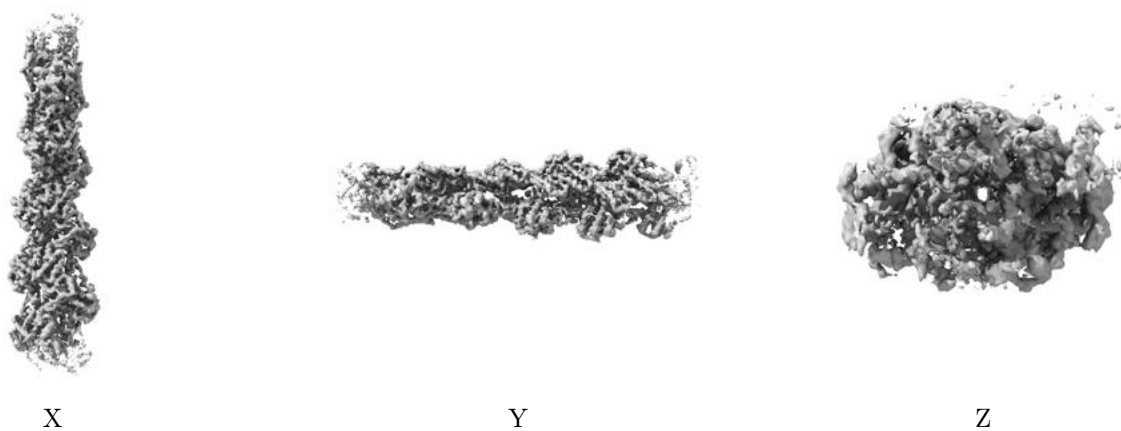
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.032. 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.

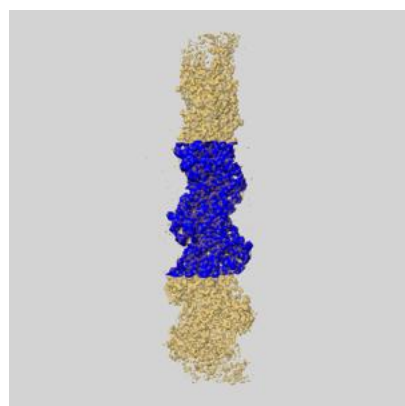
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

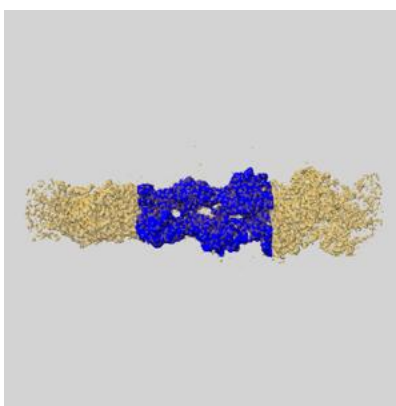
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

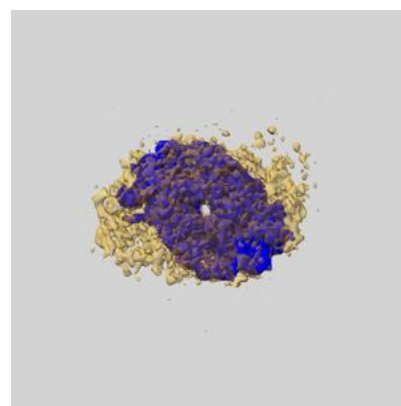
6.6.1 emd_3837_msk_1.map [i](#)



X



Y

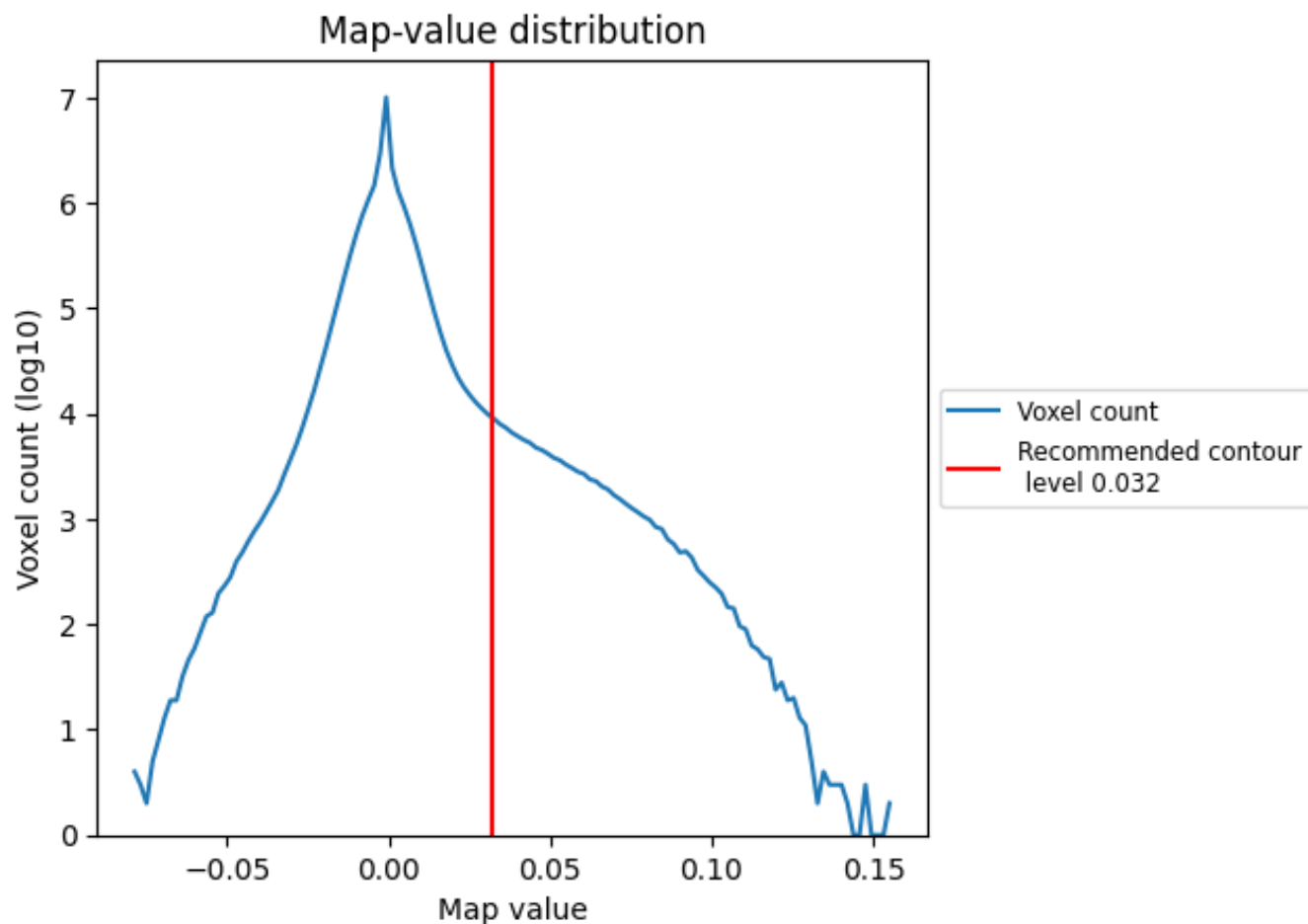


Z

7 Map analysis [i](#)

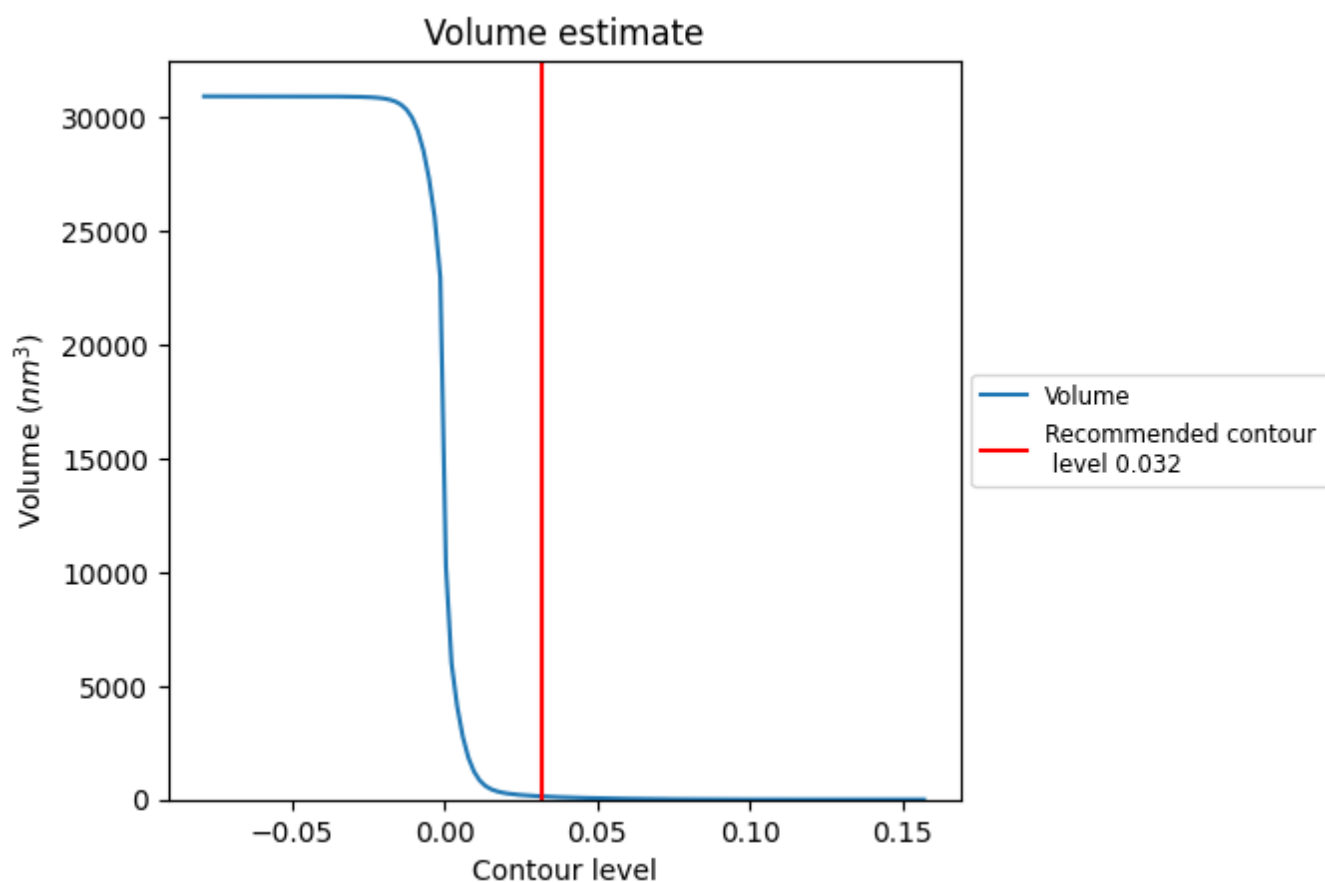
This section contains the results of statistical analysis of the map.

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.

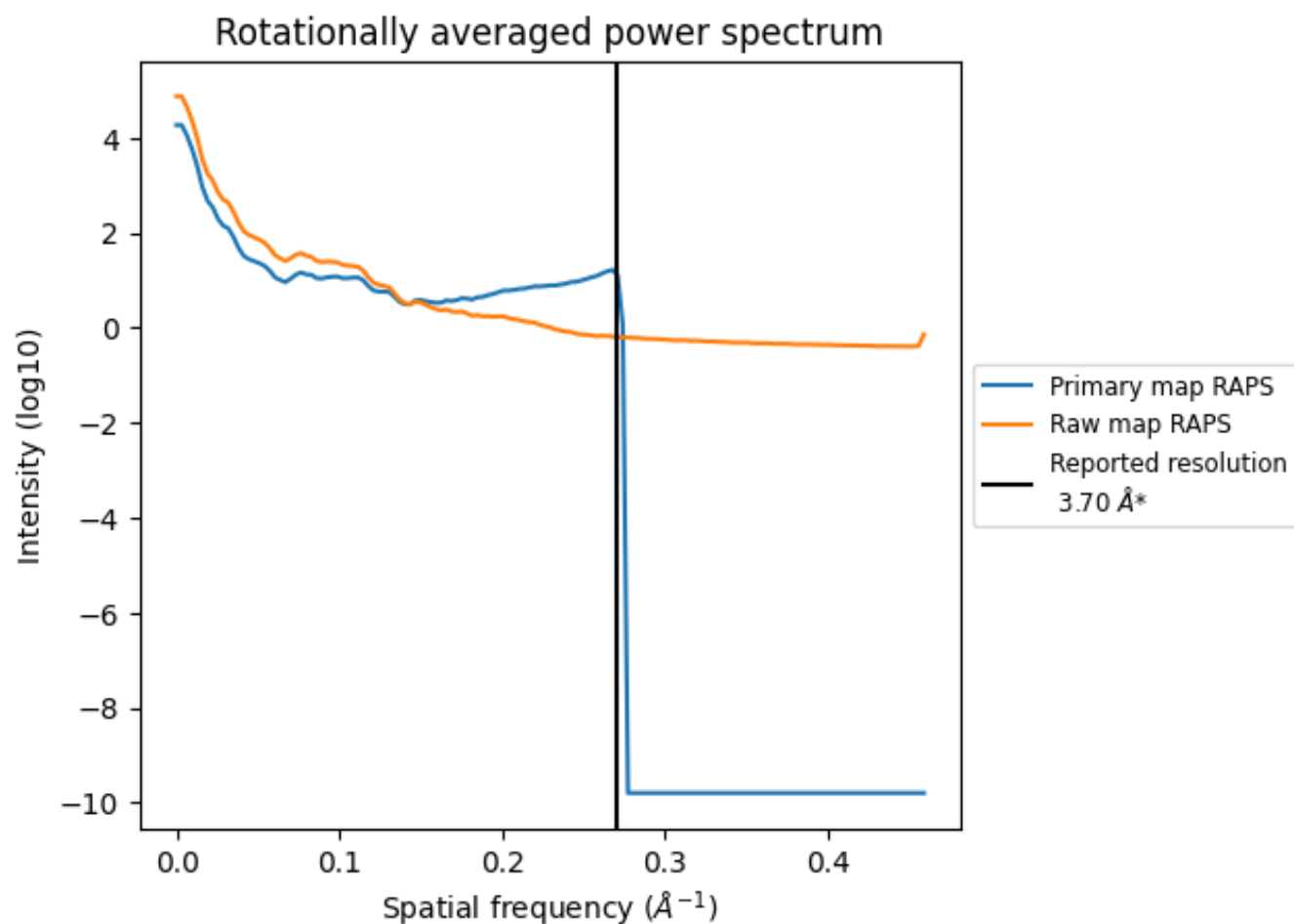
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 140 nm³; this corresponds to an approximate mass of 126 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 ⓘ

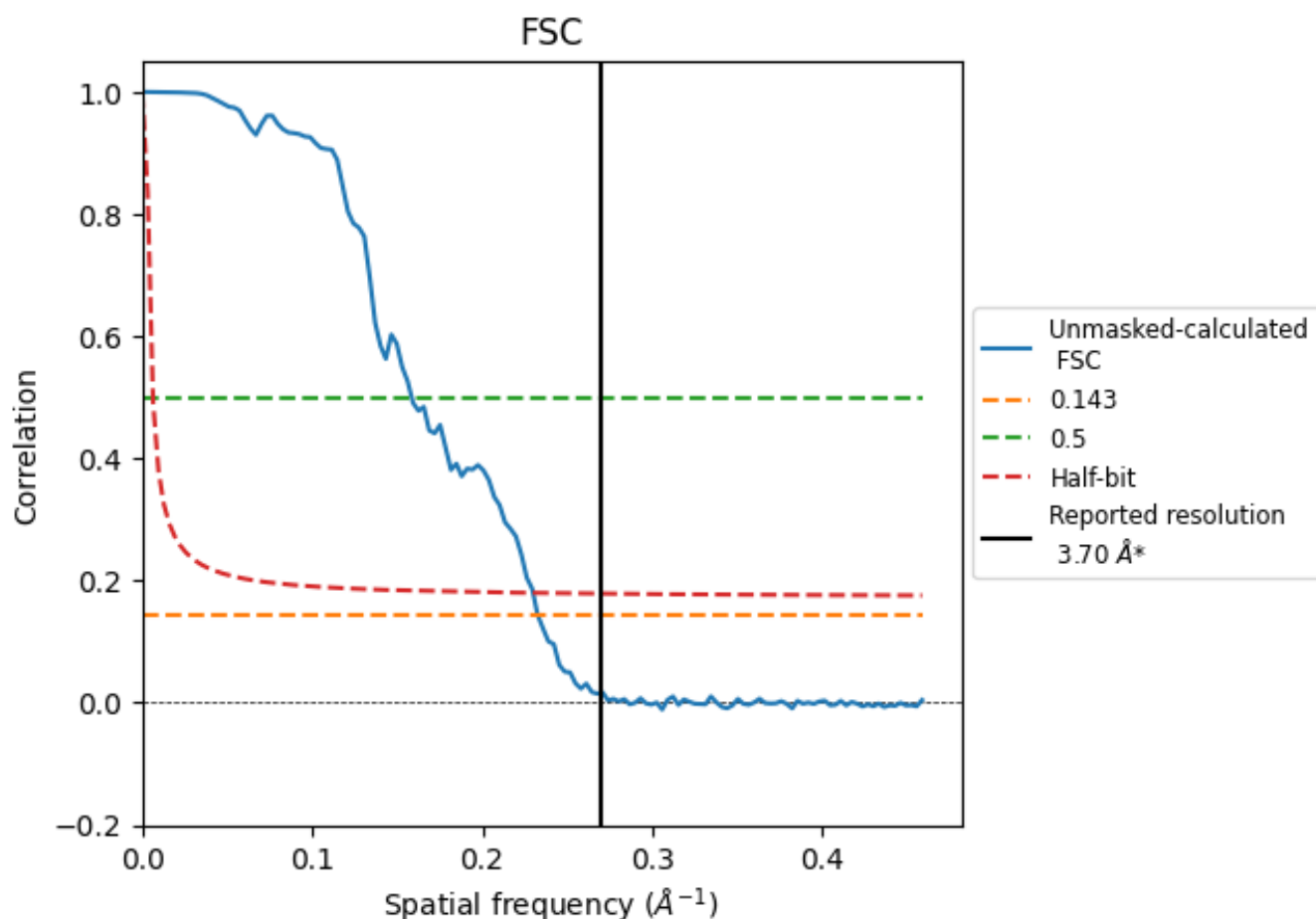


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

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 $0.270 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

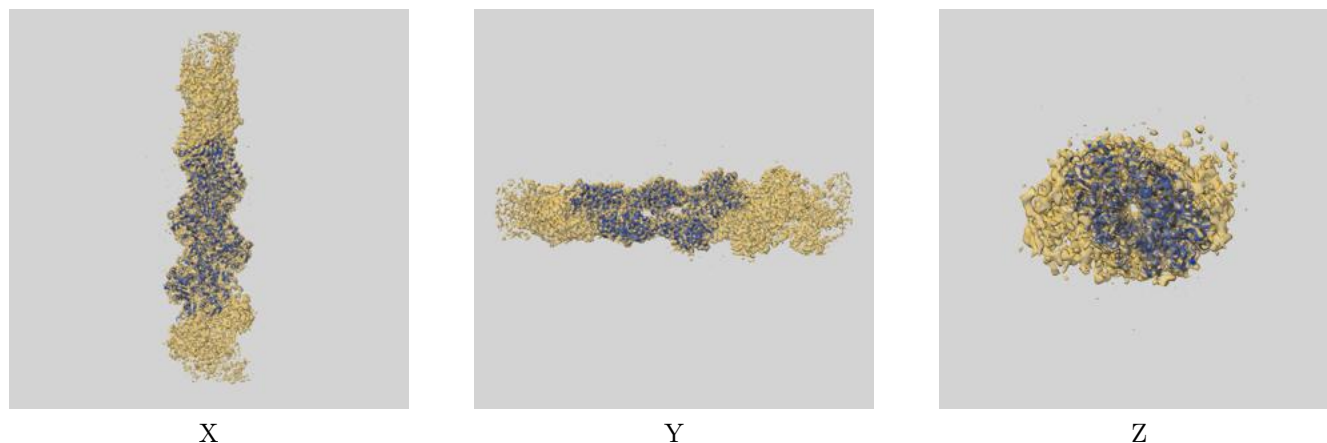
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.30	6.31	4.35

*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 4.30 differs from the reported value 3.7 by more than 10 %

9 Map-model fit [i](#)

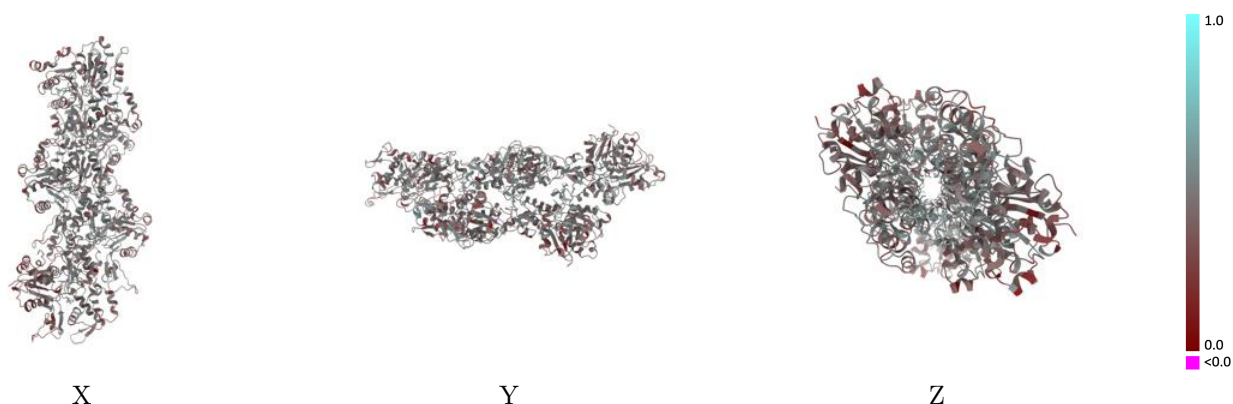
This section contains information regarding the fit between EMDB map EMD-3837 and PDB model 5OOD. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



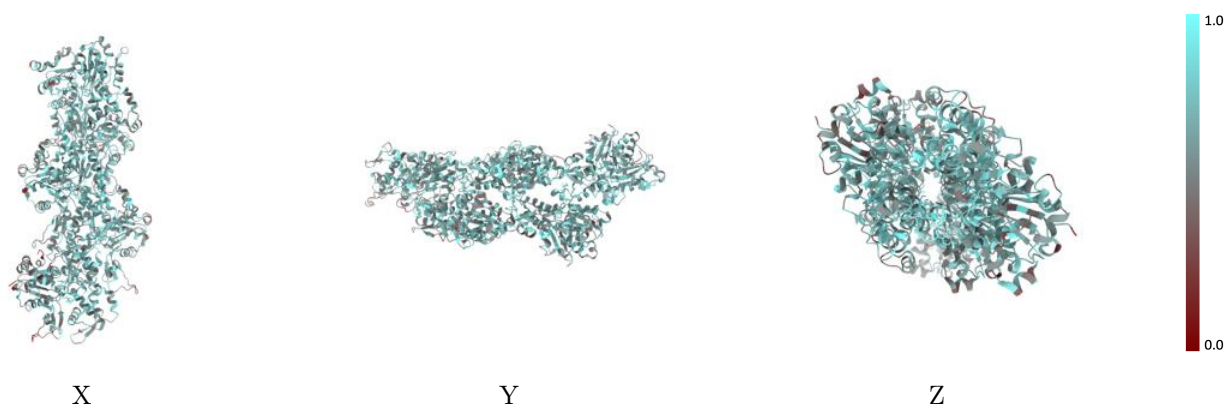
The images above show the 3D surface view of the map at the recommended contour level 0.032 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



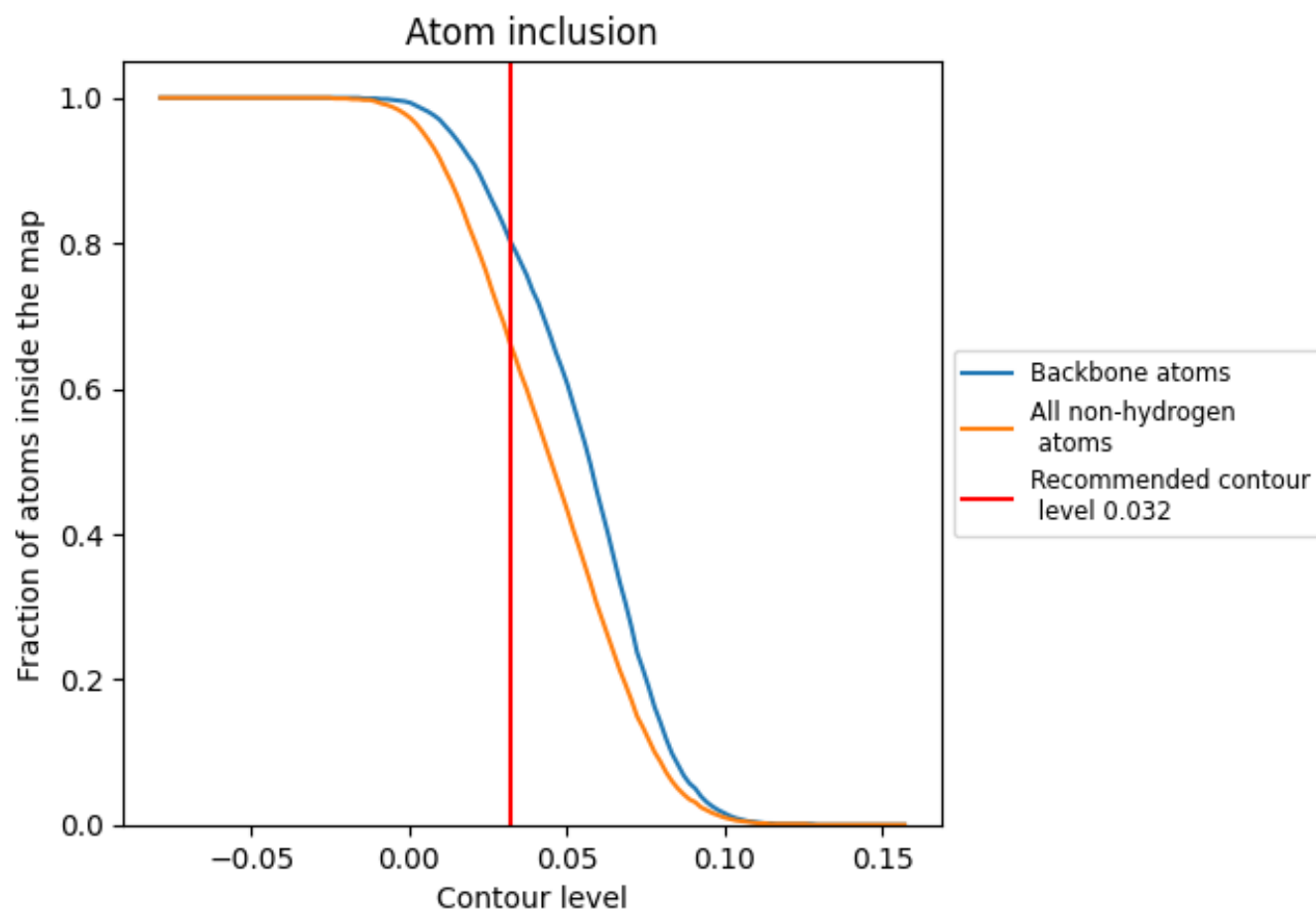
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.032).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 66% 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 (0.032) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6620	0.4240
A	0.6770	0.4270
B	0.6680	0.4220
C	0.6830	0.4440
D	0.6610	0.4260
E	0.6210	0.3990

