



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 03:05 PM UTC

PDB ID : 8QZX / pdb_00008qzx
EMDB ID : EMD-18784
Title : CryoEM structure of DHS-eIF5A complex structure from *Trichomonas vaginalis*
Authors : Wator, E.; Wilk, P.; Grudnik, P.
Deposited on : 2023-10-30
Resolution : 3.01 Å(reported)
Based on initial model : 8A0E

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:

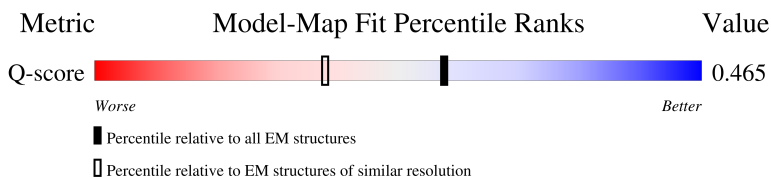
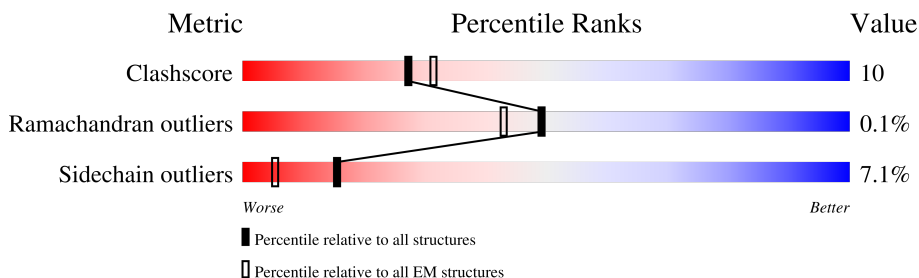
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.01 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	13882 (2.51 - 3.51)

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	364	
1	B	364	
1	C	364	
1	D	364	

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Mol	Chain	Length	Quality of chain
2	E	167	18% 47% 25% 9% • 19%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11708 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 Deoxyhypusine synthase related protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	333	Total	C	N	O	S	0	0
			2620	1684	435	485	16		
1	B	333	Total	C	N	O	S	0	0
			2618	1681	436	485	16		
1	C	334	Total	C	N	O	S	0	0
			2629	1688	438	487	16		
1	D	328	Total	C	N	O	S	0	0
			2580	1658	429	477	16		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	331	ALA	LYS	engineered mutation	UNP A2DTB8
B	331	ALA	LYS	engineered mutation	UNP A2DTB8
C	331	ALA	LYS	engineered mutation	UNP A2DTB8
D	331	ALA	LYS	engineered mutation	UNP A2DTB8

- Molecule 2 is a protein called Eukaryotic translation initiation factor 5A.

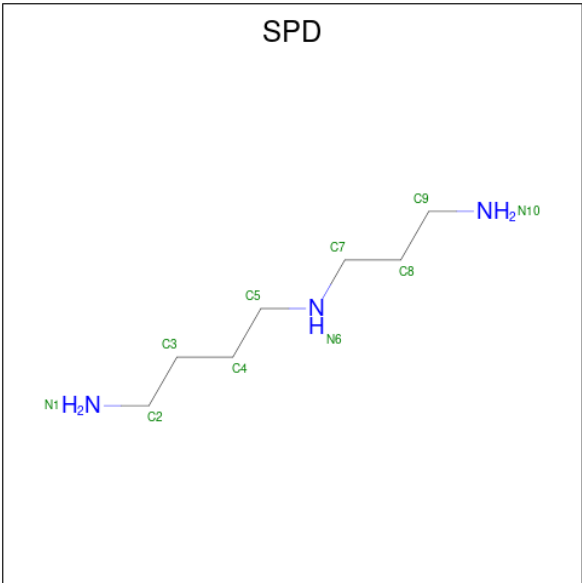
Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	136	Total	C	N	O	S	0	0
			1055	655	190	206	4		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			44	21	7	14	2	
3	B	1	Total	C	N	O	P	0
			44	21	7	14	2	
3	C	1	Total	C	N	O	P	0
			44	21	7	14	2	
3	D	1	Total	C	N	O	P	0
			44	21	7	14	2	

- Molecule 4 is SPERMIDINE (CCD ID: SPD) (formula: C₇H₁₉N₃) (labeled as "Ligand of Interest" by depositor).

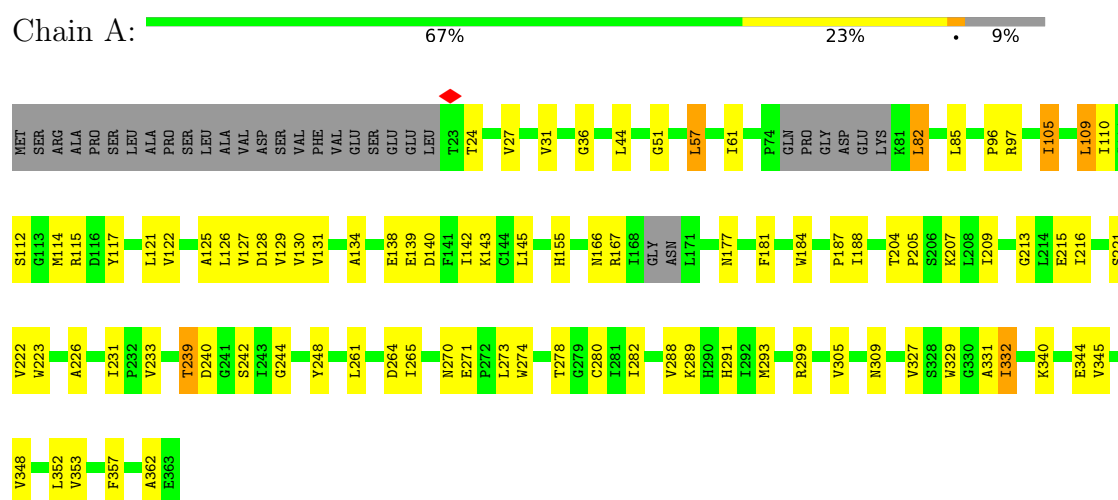


Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	C	N	0
			10	7	3	
4	C	1	Total	C	N	0
			10	7	3	
4	D	1	Total	C	N	0
			10	7	3	

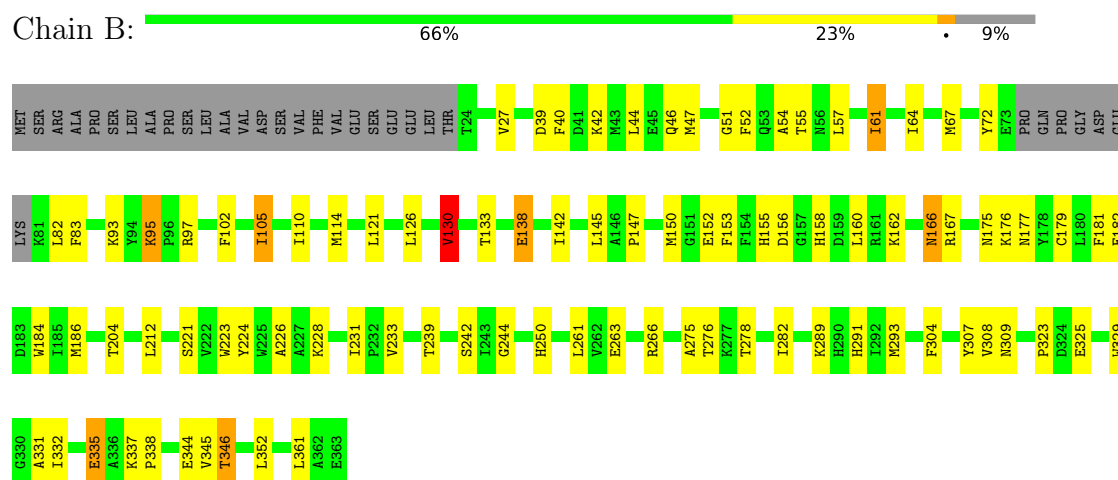
3 Residue-property plots

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

- Molecule 1: Deoxyhypusine synthase related protein, putative

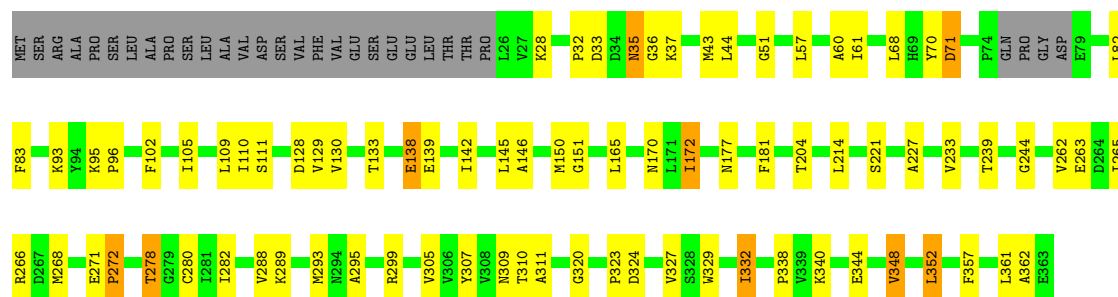


- Molecule 1: Deoxyhypusine synthase related protein, putative



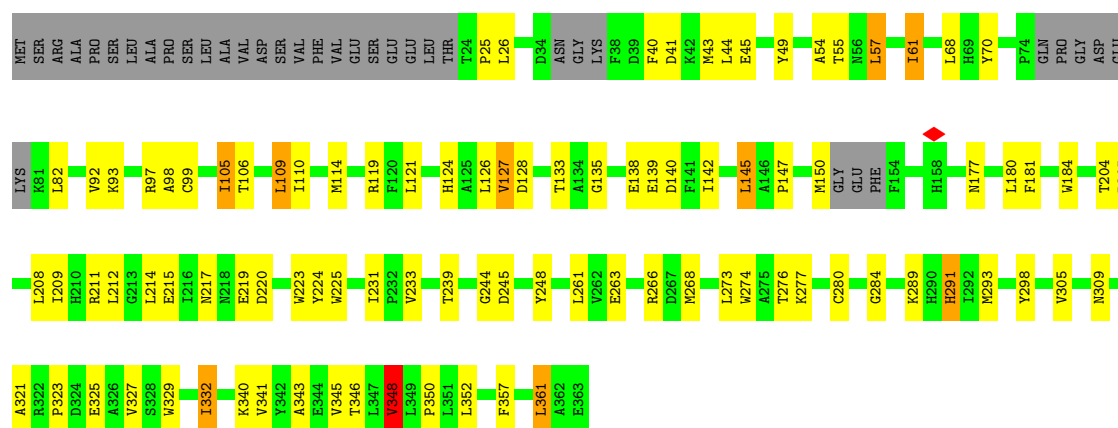
- Molecule 1: Deoxyhypusine synthase related protein, putative





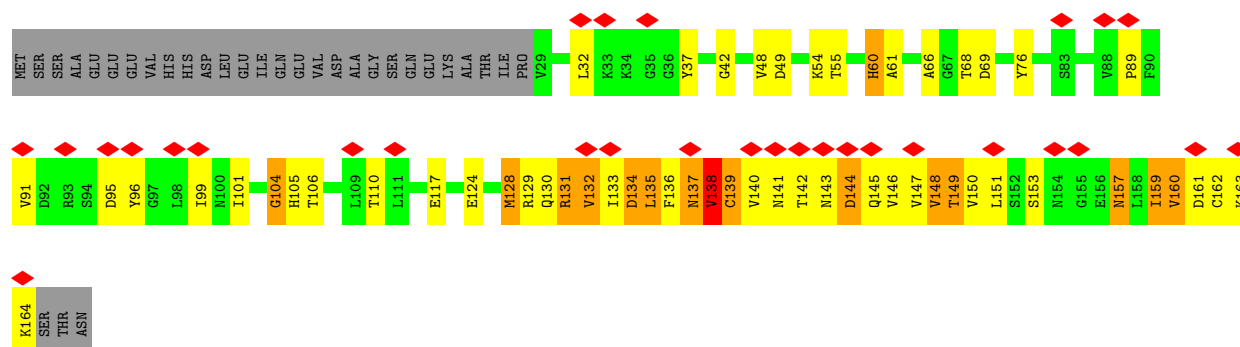
- Molecule 1: Deoxyhypusine synthase related protein, putative

Chain D: 64% 24% 10%



- Molecule 2: Eukaryotic translation initiation factor 5A

Chain E: 18% 47% 25% 9% 19%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	422161	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.183	Depositor
Minimum map value	-0.797	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.0754	Depositor
Map size (Å)	297.6512, 297.6512, 297.6512	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84560007, 0.84560007, 0.84560007	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAD, SPD

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	0.92	0/2683	1.28	2/3636 (0.1%)
1	B	0.92	1/2681 (0.0%)	1.27	6/3633 (0.2%)
1	C	0.91	0/2692	1.27	4/3646 (0.1%)
1	D	0.91	0/2641	1.31	5/3579 (0.1%)
2	E	2.21	28/1070 (2.6%)	2.57	71/1448 (4.9%)
All	All	1.10	29/11767 (0.2%)	1.45	88/15942 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	E	0	6

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	159	ILE	C-N	-26.25	1.01	1.34
2	E	143	ASN	C-N	-21.87	1.02	1.33
2	E	146	VAL	C-N	-20.90	1.02	1.33
2	E	37	TYR	C-O	19.29	1.48	1.23
2	E	134	ASP	C-N	-18.33	1.05	1.33
2	E	130	GLN	C-N	-15.54	1.12	1.33
2	E	133	ILE	C-O	11.52	1.36	1.24
2	E	130	GLN	N-CA	11.18	1.59	1.46
2	E	148	VAL	C-N	-10.84	1.19	1.33
2	E	37	TYR	CA-C	10.25	1.66	1.52
2	E	164	LYS	C-O	9.38	1.42	1.23
2	E	161	ASP	C-N	-8.18	1.23	1.33
2	E	134	ASP	N-CA	7.43	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	131	ARG	CA-C	7.39	1.63	1.52
2	E	129	ARG	C-O	7.33	1.32	1.24
2	E	132	VAL	C-N	-7.22	1.25	1.33
2	E	136	PHE	C-O	7.15	1.33	1.24
2	E	42	GLY	C-O	7.15	1.34	1.24
2	E	133	ILE	CA-C	7.03	1.61	1.52
2	E	99	ILE	C-O	6.65	1.30	1.23
2	E	140	VAL	C-O	6.31	1.31	1.24
2	E	132	VAL	N-CA	6.30	1.55	1.46
2	E	42	GLY	N-CA	6.28	1.53	1.45
2	E	145	GLN	C-O	-6.17	1.16	1.23
2	E	128	MET	C-N	-5.51	1.27	1.33
2	E	131	ARG	C-O	5.40	1.30	1.24
2	E	42	GLY	CA-C	5.30	1.59	1.51
2	E	130	GLN	C-O	5.24	1.30	1.24
1	B	95	LYS	N-CA	5.13	1.49	1.46

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	104	GLY	CA-C-N	22.85	162.29	121.85
2	E	104	GLY	C-N-CA	22.85	162.29	121.85
2	E	143	ASN	CA-C-N	20.18	150.36	121.50
2	E	143	ASN	C-N-CA	20.18	150.36	121.50
2	E	143	ASN	O-C-N	-17.86	95.95	122.39
2	E	37	TYR	CA-C-O	-17.45	100.37	121.66
2	E	146	VAL	O-C-N	-14.89	105.97	122.95
2	E	140	VAL	O-C-N	14.89	137.17	121.83
2	E	136	PHE	O-C-N	14.08	141.19	122.33
2	E	130	GLN	O-C-N	-13.51	107.80	122.12
2	E	163	LYS	O-C-N	12.41	137.17	123.52
2	E	133	ILE	CA-C-O	-11.97	108.48	121.29
2	E	37	TYR	O-C-N	11.00	135.46	123.03
2	E	142	THR	O-C-N	10.96	138.62	122.94
2	E	133	ILE	O-C-N	10.70	132.96	121.94
2	E	131	ARG	CA-C-O	-10.69	106.55	119.49
2	E	134	ASP	O-C-N	-10.57	109.85	122.22
2	E	128	MET	O-C-N	10.12	134.06	122.22
2	E	146	VAL	CA-C-N	9.60	135.03	122.93
2	E	146	VAL	C-N-CA	9.60	135.03	122.93
2	E	42	GLY	CA-C-O	-9.51	108.46	119.01
2	E	160	VAL	O-C-N	-9.23	112.97	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	141	ASN	O-C-N	9.12	133.28	122.34
2	E	145	GLN	O-C-N	-9.11	112.74	123.03
2	E	140	VAL	CA-C-O	-9.04	111.27	120.85
2	E	164	LYS	CA-C-O	-8.82	105.80	120.80
2	E	129	ARG	O-C-N	8.64	131.08	122.09
2	E	129	ARG	CA-C-O	-8.63	111.67	120.90
2	E	136	PHE	CA-C-N	-8.58	105.92	120.58
2	E	136	PHE	C-N-CA	-8.58	105.92	120.58
2	E	142	THR	CA-C-N	-8.55	104.85	121.94
2	E	142	THR	C-N-CA	-8.55	104.85	121.94
2	E	128	MET	CA-C-N	-8.47	109.11	120.54
2	E	128	MET	C-N-CA	-8.47	109.11	120.54
2	E	145	GLN	CA-C-N	8.46	133.28	122.37
2	E	145	GLN	C-N-CA	8.46	133.28	122.37
2	E	138	VAL	O-C-N	-8.37	112.11	122.57
1	D	98	ALA	N-CA-C	-7.88	104.15	113.21
2	E	140	VAL	CA-C-N	-7.58	110.52	122.65
2	E	140	VAL	C-N-CA	-7.58	110.52	122.65
2	E	137	ASN	CA-C-N	-7.39	108.67	121.97
2	E	137	ASN	C-N-CA	-7.39	108.67	121.97
2	E	161	ASP	CA-C-N	-7.37	110.27	122.21
2	E	161	ASP	C-N-CA	-7.37	110.27	122.21
2	E	130	GLN	CA-C-O	7.29	128.28	120.55
2	E	144	ASP	O-C-N	-7.22	114.59	123.04
2	E	132	VAL	O-C-N	7.06	134.76	121.84
2	E	48	VAL	N-CA-C	-6.99	106.49	113.20
2	E	149	THR	CA-C-O	-6.91	112.85	120.38
2	E	161	ASP	O-C-N	6.83	131.13	123.48
2	E	132	VAL	CA-C-N	-6.82	112.17	120.70
2	E	132	VAL	C-N-CA	-6.82	112.17	120.70
2	E	163	LYS	CA-C-N	-6.80	109.47	121.70
2	E	163	LYS	C-N-CA	-6.80	109.47	121.70
1	B	147	PRO	N-CA-C	6.62	120.99	111.13
2	E	136	PHE	CA-C-O	-6.61	111.99	119.79
2	E	162	CYS	O-C-N	6.55	131.10	123.17
1	B	54	ALA	N-CA-C	-6.41	104.29	111.28
1	D	348	VAL	N-CA-C	6.33	117.11	110.72
1	D	61	ILE	N-CA-C	-6.29	104.20	110.62
2	E	130	GLN	CA-C-N	6.20	130.52	120.60
2	E	130	GLN	C-N-CA	6.20	130.52	120.60
1	D	276	THR	N-CA-C	-6.13	105.45	113.12
1	C	307	TYR	CB-CA-C	-6.12	100.14	110.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	37	TYR	N-CA-C	6.12	119.90	110.42
1	C	51	GLY	CA-C-O	-6.10	117.70	122.52
1	A	51	GLY	CA-C-O	-6.07	117.72	122.52
1	B	130	VAL	CA-CB-CG1	5.93	120.48	110.40
1	C	272	PRO	CB-CA-C	-5.68	103.78	111.85
1	D	147	PRO	N-CA-C	5.66	120.37	111.38
2	E	131	ARG	N-CA-C	-5.65	105.48	112.38
2	E	160	VAL	CA-C-N	5.52	132.23	121.63
2	E	160	VAL	C-N-CA	5.52	132.23	121.63
2	E	42	GLY	O-C-N	5.48	128.97	122.50
2	E	139	CYS	O-C-N	5.45	128.63	122.20
2	E	160	VAL	CA-C-O	-5.38	113.50	119.20
1	C	35	ASN	N-CA-C	-5.38	106.91	112.93
2	E	131	ARG	O-C-N	5.30	129.28	122.39
1	B	51	GLY	CA-C-O	-5.27	118.02	122.29
1	B	114	MET	N-CA-C	-5.21	106.87	113.18
2	E	147	VAL	O-C-N	5.20	128.80	123.03
2	E	130	GLN	CB-CA-C	-5.20	102.16	110.79
1	B	276	THR	N-CA-C	-5.18	105.54	111.14
2	E	135	LEU	CA-C-N	5.09	129.33	120.68
2	E	135	LEU	C-N-CA	5.09	129.33	120.68
2	E	139	CYS	CA-C-N	-5.04	113.26	120.42
2	E	139	CYS	C-N-CA	-5.04	113.26	120.42
1	A	274	TRP	N-CA-C	5.01	116.82	111.36

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	104	GLY	Peptide
2	E	131	ARG	Mainchain
2	E	134	ASP	Mainchain
2	E	135	LEU	Mainchain
2	E	138	VAL	Mainchain
2	E	144	ASP	Mainchain

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	2620	0	2575	55	0
1	B	2618	0	2571	67	0
1	C	2629	0	2583	46	0
1	D	2580	0	2536	63	0
2	E	1055	0	1052	22	0
3	A	44	0	26	0	0
3	B	44	0	26	1	0
3	C	44	0	26	0	0
3	D	44	0	26	0	0
4	A	10	0	19	1	0
4	C	10	0	19	0	0
4	D	10	0	19	0	0
All	All	11708	0	11478	228	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 10.

All (228) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:VAL:HG11	1:B:223:TRP:CZ3	1.69	1.26
1:A:362:ALA:HB2	1:C:36:GLY:HA3	1.46	0.94
1:B:130:VAL:CG1	1:B:223:TRP:CZ3	2.52	0.92
1:B:175:ASN:ND2	2:E:55:THR:HG21	1.88	0.89
1:B:130:VAL:HG11	1:B:223:TRP:HZ3	1.38	0.86
1:B:175:ASN:HD21	2:E:55:THR:CG2	1.95	0.79
2:E:49:ASP:HB3	2:E:66:ALA:HB3	1.63	0.78
1:A:142:ILE:HB	1:A:177:ASN:HD21	1.49	0.76
1:B:130:VAL:HG12	1:B:233:VAL:HG13	1.70	0.74
2:E:150:VAL:HG12	2:E:157:ASN:HB2	1.71	0.73
1:D:121:LEU:HD23	1:D:126:LEU:HB2	1.72	0.71
2:E:149:THR:O	2:E:159:ILE:HA	1.91	0.70
1:D:273:LEU:HD21	1:D:298:TYR:HB3	1.73	0.70
1:C:204:THR:HG21	1:C:263:GLU:HB3	1.75	0.68
1:B:293:MET:HB3	1:B:331:ALA:HB1	1.74	0.68
1:A:142:ILE:HG22	1:A:181:PHE:HB2	1.73	0.68
1:B:239:THR:HA	1:B:244:GLY:HA3	1.77	0.67
1:B:150:MET:SD	1:D:25:PRO:HB2	2.34	0.67
1:B:142:ILE:HG22	1:B:181:PHE:HB2	1.75	0.67
1:B:93:LYS:HE3	1:B:361:LEU:HG	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:PHE:HZ	1:B:275:ALA:HA	1.60	0.65
1:B:83:PHE:CZ	1:B:275:ALA:HA	2.32	0.65
1:C:142:ILE:HG22	1:C:181:PHE:HB2	1.79	0.63
1:D:341:VAL:HG11	1:D:348:VAL:HG21	1.81	0.63
1:C:214:LEU:HD13	1:C:227:ALA:HB1	1.81	0.63
1:D:142:ILE:HG22	1:D:181:PHE:HB2	1.81	0.63
1:A:109:LEU:HD21	1:A:345:VAL:HG11	1.79	0.63
1:C:142:ILE:HB	1:C:177:ASN:HD21	1.63	0.62
1:C:282:ILE:HD13	1:C:289:LYS:HA	1.80	0.62
1:D:239:THR:HA	1:D:244:GLY:HA3	1.80	0.62
1:D:114:MET:HE1	1:D:350:PRO:HG3	1.80	0.62
1:D:219:GLU:HB3	1:D:225:TRP:HE1	1.65	0.62
1:A:105:ILE:HD12	1:A:110:ILE:HD11	1.81	0.61
1:A:362:ALA:HB2	1:C:36:GLY:CA	2.27	0.61
1:B:27:VAL:HG22	1:D:150:MET:HG3	1.83	0.60
1:B:150:MET:HE1	1:D:49:TYR:HD1	1.67	0.60
1:A:27:VAL:HG22	1:C:150:MET:HG3	1.82	0.60
1:A:166:ASN:HD21	4:A:402:SPD:H71	1.66	0.59
1:A:36:GLY:HA3	1:C:362:ALA:HB2	1.83	0.59
1:B:175:ASN:ND2	2:E:55:THR:CG2	2.54	0.59
1:A:115:ARG:HD2	1:A:143:LYS:HE2	1.84	0.59
1:D:121:LEU:HD22	1:D:127:VAL:HG13	1.84	0.58
1:B:179:CYS:HB2	2:E:60:HIS:ND1	2.18	0.58
1:B:282:ILE:HD13	1:B:289:LYS:HA	1.86	0.58
1:D:268:MET:HG2	1:D:291:HIS:CD2	2.40	0.56
1:D:280:CYS:HB2	1:D:305:VAL:HG23	1.88	0.56
1:D:184:TRP:HH2	1:D:212:LEU:HB3	1.69	0.56
2:E:91:VAL:HG22	2:E:153:SER:HB2	1.86	0.56
1:C:68:LEU:HD11	1:C:357:PHE:CD1	2.41	0.56
1:C:61:ILE:HG13	1:C:352:LEU:HD12	1.88	0.56
1:A:353:VAL:HG11	1:C:32:PRO:HG2	1.86	0.55
1:B:142:ILE:HD13	1:B:177:ASN:HB3	1.87	0.55
1:A:117:TYR:HB3	1:A:353:VAL:HG21	1.89	0.55
1:B:40:PHE:HE2	1:D:44:LEU:HD13	1.71	0.55
1:B:130:VAL:HG21	1:B:223:TRP:HZ3	1.71	0.55
1:A:309:ASN:OD1	1:A:340:LYS:HE3	2.07	0.54
1:D:321:ALA:HB1	1:D:325:GLU:HB3	1.89	0.54
1:B:158:HIS:O	1:B:162:LYS:HG2	2.07	0.54
1:B:346:THR:HG23	1:D:54:ALA:HB2	1.88	0.54
1:B:175:ASN:HD21	2:E:55:THR:HG23	1.72	0.54
1:B:346:THR:CG2	1:D:54:ALA:H	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:LEU:HB3	1:A:85:LEU:HD21	1.89	0.54
1:A:293:MET:HB3	1:A:331:ALA:HB1	1.90	0.54
2:E:96:TYR:HD2	2:E:110:THR:HA	1.73	0.53
1:C:271:GLU:HB3	1:C:272:PRO:HD3	1.90	0.53
1:D:105:ILE:HG22	1:D:109:LEU:HD22	1.90	0.53
1:B:130:VAL:CG1	1:B:223:TRP:HZ3	2.05	0.53
1:C:239:THR:O	1:C:244:GLY:HA3	2.09	0.53
1:A:239:THR:O	1:A:244:GLY:HA3	2.08	0.52
1:B:95:LYS:HE3	1:B:361:LEU:HA	1.90	0.52
1:B:130:VAL:CG1	1:B:223:TRP:CH2	2.92	0.52
1:A:139:GLU:O	1:A:142:ILE:HG13	2.10	0.52
2:E:95:ASP:HA	2:E:148:VAL:O	2.10	0.52
1:B:204:THR:HG21	1:B:263:GLU:HB3	1.92	0.52
1:C:142:ILE:HD13	1:C:177:ASN:OD1	2.10	0.52
1:A:329:TRP:HB3	1:B:166:ASN:HD22	1.73	0.52
1:B:150:MET:HE1	1:D:49:TYR:CD1	2.45	0.52
1:B:184:TRP:HH2	1:B:212:LEU:HB3	1.74	0.51
1:B:82:LEU:HD23	1:B:97:ARG:HD2	1.92	0.51
1:A:213:GLY:O	1:A:216:ILE:HG22	2.11	0.51
1:B:152:GLU:HG2	1:B:153:PHE:H	1.74	0.51
1:C:151:GLY:O	1:C:170:ASN:HB2	2.10	0.51
2:E:105:HIS:HB2	2:E:117:GLU:O	2.11	0.51
1:D:204:THR:HG21	1:D:263:GLU:HB3	1.93	0.51
1:A:270:ASN:HA	1:A:273:LEU:HD12	1.92	0.51
1:B:67:MET:HE2	1:B:304:PHE:HB2	1.93	0.50
1:D:145:LEU:HB3	1:D:180:LEU:HD23	1.93	0.50
1:B:323:PRO:HB3	1:B:338:PRO:HB2	1.92	0.50
1:B:323:PRO:HB3	1:B:338:PRO:CB	2.41	0.50
1:A:138:GLU:HG3	1:A:242:SER:HB3	1.94	0.50
1:B:263:GLU:HA	1:B:266:ARG:HD3	1.93	0.49
1:C:133:THR:HG23	1:C:288:VAL:HG13	1.94	0.49
1:B:152:GLU:HG2	1:B:153:PHE:N	2.26	0.49
1:C:293:MET:HE2	1:C:332:ILE:HG12	1.94	0.49
1:B:346:THR:HG23	1:D:54:ALA:CB	2.43	0.49
1:C:139:GLU:HA	1:C:142:ILE:HG13	1.95	0.49
1:C:293:MET:CE	1:C:332:ILE:HG12	2.43	0.49
1:A:142:ILE:HB	1:A:177:ASN:ND2	2.22	0.49
1:C:139:GLU:O	1:C:142:ILE:HG13	2.13	0.49
1:D:109:LEU:HD21	1:D:345:VAL:HG11	1.94	0.49
1:A:261:LEU:HD11	1:B:261:LEU:HD21	1.94	0.49
1:A:121:LEU:HD21	1:A:357:PHE:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:184:TRP:CH2	1:D:212:LEU:HB3	2.48	0.48
1:D:97:ARG:C	1:D:99:CYS:H	2.19	0.48
1:D:289:LYS:O	1:D:293:MET:HG2	2.14	0.48
2:E:128:MET:HE3	2:E:160:VAL:O	2.13	0.48
1:A:139:GLU:HA	1:A:142:ILE:HG13	1.95	0.48
1:A:278:THR:HG23	1:A:299:ARG:HH21	1.79	0.48
1:A:167:ARG:HH21	1:B:325:GLU:HB2	1.78	0.48
1:D:70:TYR:CE2	1:D:277:LYS:HG3	2.49	0.48
1:D:97:ARG:NH1	1:D:99:CYS:O	2.46	0.48
1:D:239:THR:HA	1:D:244:GLY:CA	2.44	0.47
1:D:61:ILE:HG13	1:D:352:LEU:HD12	1.95	0.47
1:A:121:LEU:HD22	1:A:127:VAL:HG13	1.96	0.47
1:B:224:TYR:O	1:B:228:LYS:HG2	2.15	0.47
1:C:57:LEU:HD23	1:C:348:VAL:HG13	1.95	0.47
1:D:211:ARG:O	1:D:215:GLU:HG2	2.15	0.47
2:E:105:HIS:HD2	2:E:117:GLU:HB3	1.78	0.47
1:B:138:GLU:HG3	1:B:242:SER:HB3	1.96	0.47
1:B:308:VAL:HB	1:B:345:VAL:HG22	1.96	0.47
1:B:289:LYS:O	1:B:293:MET:HG2	2.15	0.47
1:A:184:TRP:O	1:A:187:PRO:HD2	2.15	0.46
1:B:323:PRO:CB	1:B:338:PRO:HB2	2.46	0.46
1:B:105:ILE:HD12	1:B:110:ILE:HD11	1.97	0.46
1:D:142:ILE:HB	1:D:177:ASN:HD21	1.80	0.46
1:A:122:VAL:HG11	1:A:222:VAL:HG13	1.96	0.46
1:A:248:TYR:CE2	1:B:266:ARG:HA	2.50	0.46
1:B:52:PHE:HB2	1:D:346:THR:HG21	1.98	0.46
1:A:97:ARG:HH21	1:A:126:LEU:HA	1.80	0.46
1:A:97:ARG:NH2	1:A:125:ALA:O	2.48	0.46
1:C:165:LEU:HB3	1:C:172:ILE:CG2	2.45	0.46
1:C:70:TYR:O	1:C:71:ASP:C	2.59	0.45
1:C:129:VAL:HG21	1:C:271:GLU:HG2	1.98	0.45
1:D:135:GLY:O	1:D:139:GLU:HB2	2.17	0.45
1:D:204:THR:CG2	1:D:263:GLU:HB3	2.46	0.45
2:E:137:ASN:O	2:E:138:VAL:C	2.55	0.45
1:A:226:ALA:HB1	1:A:231:ILE:HB	1.99	0.45
1:C:266:ARG:HA	1:D:248:TYR:CD2	2.52	0.45
1:D:305:VAL:HB	1:D:332:ILE:HD11	1.97	0.45
1:C:311:ALA:HB3	1:C:320:GLY:HA2	1.99	0.45
1:D:119:ARG:NE	1:D:220:ASP:O	2.49	0.45
1:B:155:HIS:O	1:B:156:ASP:C	2.60	0.45
1:B:182:GLU:O	1:B:186:MET:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:110:ILE:HG22	1:D:139:GLU:HB3	1.99	0.45
1:C:268:MET:HE3	1:C:295:ALA:HB2	1.99	0.44
1:D:92:VAL:HG21	1:D:225:TRP:CH2	2.52	0.44
2:E:69:ASP:HB2	2:E:76:TYR:HE1	1.82	0.44
1:A:130:VAL:HG23	1:A:233:VAL:HG13	2.00	0.44
1:B:176:LYS:H	1:B:176:LYS:HG3	1.53	0.44
1:D:93:LYS:HE3	1:D:361:LEU:HG	2.00	0.44
1:D:128:ASP:O	1:D:231:ILE:HG23	2.18	0.44
1:D:217:ASN:HA	1:D:224:TYR:CE1	2.52	0.44
1:B:186:MET:HE1	1:B:250:HIS:HB2	1.99	0.44
1:D:139:GLU:HA	1:D:142:ILE:HG13	1.98	0.44
1:A:134:ALA:HB3	1:A:240:ASP:O	2.17	0.44
1:A:305:VAL:HG11	1:A:332:ILE:HD13	1.98	0.44
1:A:143:LYS:HE3	1:A:143:LYS:HB3	1.86	0.44
1:C:102:PHE:HE1	1:C:278:THR:HG22	1.83	0.44
1:A:205:PRO:O	1:A:209:ILE:HG13	2.18	0.43
1:B:61:ILE:HG13	1:B:352:LEU:HD12	2.01	0.43
1:B:309:ASN:HA	3:B:401:NAD:N3A	2.33	0.43
1:C:33:ASP:HB2	1:C:37:LYS:H	1.82	0.43
1:A:293:MET:CE	1:A:332:ILE:HG12	2.47	0.43
1:C:83:PHE:HB3	1:C:128:ASP:OD2	2.17	0.43
1:D:124:HIS:CD2	1:D:361:LEU:HD21	2.54	0.43
1:C:95:LYS:HA	1:C:96:PRO:HD3	1.91	0.43
1:D:121:LEU:HB3	1:D:127:VAL:HG22	2.00	0.43
1:B:102:PHE:HE1	1:B:278:THR:HG22	1.84	0.43
1:C:43:MET:HE3	1:C:43:MET:HB3	1.84	0.43
1:C:146:ALA:HB3	1:C:177:ASN:HD22	1.82	0.43
1:C:28:LYS:HA	1:C:28:LYS:HD2	1.81	0.43
1:C:323:PRO:O	1:C:327:VAL:HG23	2.18	0.43
1:C:139:GLU:HA	1:C:142:ILE:CG1	2.49	0.43
1:C:262:VAL:O	1:C:265:ILE:HG22	2.19	0.42
1:D:121:LEU:HD21	1:D:357:PHE:CZ	2.53	0.42
1:A:121:LEU:HD21	1:A:357:PHE:CZ	2.53	0.42
1:D:57:LEU:HD23	1:D:348:VAL:HG13	2.01	0.42
1:C:93:LYS:HE3	1:C:361:LEU:HG	2.00	0.42
1:B:44:LEU:HD22	1:D:40:PHE:HE2	1.85	0.42
2:E:101:ILE:HA	2:E:106:THR:HG22	2.00	0.42
1:A:129:VAL:HG21	1:A:271:GLU:HG2	2.02	0.42
1:A:140:ASP:HB3	1:A:223:TRP:CD1	2.55	0.42
1:B:226:ALA:HB1	1:B:231:ILE:HB	2.01	0.42
1:C:138:GLU:O	1:C:142:ILE:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:92:VAL:HG21	1:D:225:TRP:HH2	1.84	0.42
1:D:323:PRO:O	1:D:327:VAL:HG23	2.20	0.41
1:A:82:LEU:HD12	1:A:82:LEU:HA	1.81	0.41
1:A:188:ILE:HG12	1:A:215:GLU:HG3	2.01	0.41
1:A:282:ILE:HD13	1:A:289:LYS:HA	2.02	0.41
1:A:280:CYS:HB2	1:A:305:VAL:HG23	2.01	0.41
1:A:265:ILE:HD12	1:A:265:ILE:HA	1.95	0.41
1:D:106:THR:HG23	1:D:284:GLY:HA3	2.02	0.41
1:B:39:ASP:HB3	1:B:42:LYS:HB2	2.01	0.41
1:B:160:LEU:HD13	1:B:167:ARG:HB2	2.02	0.41
1:B:177:ASN:N	1:B:177:ASN:HD22	2.18	0.41
1:B:293:MET:HE2	1:B:332:ILE:HG12	2.02	0.41
1:C:204:THR:CG2	1:C:263:GLU:HB3	2.46	0.41
1:C:280:CYS:O	1:C:305:VAL:HA	2.20	0.41
2:E:32:LEU:HD23	2:E:32:LEU:HA	1.74	0.41
1:A:131:VAL:HG12	1:A:288:VAL:HG12	2.02	0.41
1:B:307:TYR:OH	1:B:332:ILE:HD11	2.21	0.41
1:C:323:PRO:HB3	1:C:338:PRO:HB2	2.01	0.41
1:C:309:ASN:OD1	1:C:340:LYS:HE3	2.20	0.41
1:D:106:THR:CG2	1:D:284:GLY:HA3	2.49	0.41
1:D:341:VAL:O	1:D:343:ALA:N	2.53	0.41
1:A:82:LEU:HG	1:A:96:PRO:HB3	2.03	0.41
1:B:335:GLU:H	1:B:335:GLU:HG2	1.52	0.41
1:A:57:LEU:HD23	1:A:348:VAL:HG13	2.01	0.41
1:A:61:ILE:HG13	1:A:352:LEU:HD12	2.03	0.41
1:D:68:LEU:HD11	1:D:357:PHE:CD1	2.55	0.41
1:D:205:PRO:O	1:D:209:ILE:HG13	2.21	0.41
1:D:261:LEU:HD23	1:D:261:LEU:HA	1.95	0.41
1:D:263:GLU:HA	1:D:266:ARG:HD3	2.02	0.41
1:A:97:ARG:NH2	1:A:126:LEU:HA	2.36	0.41
1:D:139:GLU:HA	1:D:142:ILE:CG1	2.50	0.40
1:A:112:SER:C	1:A:114:MET:H	2.30	0.40
1:A:204:THR:HG23	1:A:207:LYS:HE2	2.02	0.40
1:C:151:GLY:N	1:C:170:ASN:O	2.55	0.40
1:D:309:ASN:OD1	1:D:340:LYS:HE3	2.21	0.40
1:B:337:LYS:HD3	1:B:337:LYS:HA	1.91	0.40
1:C:60:ALA:CB	1:C:352:LEU:HD11	2.51	0.40
2:E:128:MET:O	2:E:132:VAL:HG23	2.21	0.40
2:E:137:ASN:C	2:E:139:CYS:N	2.77	0.40
1:B:289:LYS:HE2	1:B:307:TYR:CE1	2.56	0.40
1:D:140:ASP:HB3	1:D:223:TRP:CD1	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:208:LEU:O	1:D:212:LEU:HG	2.20	0.40
2:E:54:LYS:O	2:E:61:ALA:HB2	2.22	0.40
2:E:150:VAL:HG22	2:E:159:ILE:HG12	2.04	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	327/364 (90%)	321 (98%)	6 (2%)	0	100	100
1	B	329/364 (90%)	318 (97%)	11 (3%)	0	100	100
1	C	330/364 (91%)	320 (97%)	10 (3%)	0	100	100
1	D	320/364 (88%)	311 (97%)	9 (3%)	0	100	100
2	E	134/167 (80%)	120 (90%)	13 (10%)	1 (1%)	18	51
All	All	1440/1623 (89%)	1390 (96%)	49 (3%)	1 (0%)	49	79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	89	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	283/309 (92%)	266 (94%)	17 (6%)	17	48
1	B	282/309 (91%)	261 (93%)	21 (7%)	13	40
1	C	283/309 (92%)	260 (92%)	23 (8%)	11	36
1	D	279/309 (90%)	257 (92%)	22 (8%)	11	37
2	E	120/147 (82%)	115 (96%)	5 (4%)	26	59
All	All	1247/1383 (90%)	1159 (93%)	88 (7%)	15	42

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	THR
1	A	31	VAL
1	A	44	LEU
1	A	57	LEU
1	A	82	LEU
1	A	105	ILE
1	A	109	LEU
1	A	128	ASP
1	A	145	LEU
1	A	155	HIS
1	A	221	SER
1	A	239	THR
1	A	264	ASP
1	A	291	HIS
1	A	327	VAL
1	A	332	ILE
1	A	344	GLU
1	B	46	GLN
1	B	47	MET
1	B	55	THR
1	B	57	LEU
1	B	61	ILE
1	B	64	ILE
1	B	72	TYR
1	B	105	ILE
1	B	121	LEU
1	B	126	LEU
1	B	130	VAL
1	B	133	THR
1	B	138	GLU
1	B	145	LEU

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Mol	Chain	Res	Type
1	B	166	ASN
1	B	221	SER
1	B	291	HIS
1	B	329	TRP
1	B	335	GLU
1	B	344	GLU
1	B	346	THR
1	C	35	ASN
1	C	44	LEU
1	C	71	ASP
1	C	82	LEU
1	C	105	ILE
1	C	109	LEU
1	C	110	ILE
1	C	111	SER
1	C	130	VAL
1	C	138	GLU
1	C	145	LEU
1	C	172	ILE
1	C	221	SER
1	C	233	VAL
1	C	278	THR
1	C	299	ARG
1	C	310	THR
1	C	324	ASP
1	C	329	TRP
1	C	332	ILE
1	C	344	GLU
1	C	348	VAL
1	C	352	LEU
1	D	26	LEU
1	D	41	ASP
1	D	43	MET
1	D	45	GLU
1	D	55	THR
1	D	57	LEU
1	D	82	LEU
1	D	105	ILE
1	D	109	LEU
1	D	127	VAL
1	D	133	THR
1	D	138	GLU

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Mol	Chain	Res	Type
1	D	145	LEU
1	D	214	LEU
1	D	233	VAL
1	D	245	ASP
1	D	274	TRP
1	D	291	HIS
1	D	329	TRP
1	D	332	ILE
1	D	348	VAL
1	D	361	LEU
2	E	60	HIS
2	E	68	THR
2	E	124	GLU
2	E	151	LEU
2	E	157	ASN

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

Mol	Chain	Res	Type
1	A	46	GLN
1	A	166	ASN
1	A	177	ASN
1	A	296	ASN
1	B	46	GLN
1	B	166	ASN
1	B	175	ASN
1	B	177	ASN
1	B	269	ASN
1	C	46	GLN
1	C	108	ASN
1	C	124	HIS
1	C	155	HIS
1	C	177	ASN
1	C	196	GLN
1	C	250	HIS
1	D	46	GLN
1	D	69	HIS
1	D	108	ASN
1	D	124	HIS
1	D	250	HIS
1	D	300	ASN
2	E	58	HIS

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Mol	Chain	Res	Type
2	E	84	HIS
2	E	105	HIS
2	E	157	ASN

5.3.3 RNA [i](#)

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](#)

7 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAD	B	401	-	46,48,48	0.51	0	64,73,73	0.61	2 (3%)
4	SPD	C	402	-	9,9,9	0.15	0	8,8,8	0.17	0
3	NAD	D	402	-	46,48,48	0.53	0	64,73,73	0.57	1 (1%)
4	SPD	D	401	-	9,9,9	0.16	0	8,8,8	0.22	0
3	NAD	C	401	-	46,48,48	0.52	0	64,73,73	0.56	1 (1%)
4	SPD	A	402	-	9,9,9	0.15	0	8,8,8	0.17	0
3	NAD	A	401	-	46,48,48	0.57	1 (2%)	64,73,73	0.53	1 (1%)

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
3	NAD	B	401	-	-	6/30/62/62	0/5/5/5
4	SPD	C	402	-	-	0/7/7/7	-
3	NAD	D	402	-	-	7/30/62/62	0/5/5/5
4	SPD	D	401	-	-	0/7/7/7	-
3	NAD	C	401	-	-	0/30/62/62	0/5/5/5
4	SPD	A	402	-	-	0/7/7/7	-
3	NAD	A	401	-	-	1/30/62/62	0/5/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	NAD	C2N-N1N	2.38	1.37	1.35

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	402	NAD	C6N-N1N-C2N	-2.57	119.69	121.88
3	A	401	NAD	C6N-N1N-C2N	-2.52	119.73	121.88
3	C	401	NAD	C6N-N1N-C2N	-2.43	119.81	121.88
3	B	401	NAD	C6N-N1N-C2N	-2.22	119.99	121.88
3	B	401	NAD	C2B-C3B-C4B	-2.01	98.73	102.61

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	NAD	PA-O3-PN-O5D
3	B	401	NAD	C5B-O5B-PA-O1A
3	B	401	NAD	C5B-O5B-PA-O2A
3	B	401	NAD	C5B-O5B-PA-O3
3	B	401	NAD	PA-O3-PN-O5D
3	B	401	NAD	O4D-C4D-C5D-O5D
3	D	402	NAD	C5B-O5B-PA-O1A
3	D	402	NAD	C5B-O5B-PA-O2A
3	D	402	NAD	C5B-O5B-PA-O3
3	D	402	NAD	PA-O3-PN-O5D
3	D	402	NAD	C5D-O5D-PN-O3
3	D	402	NAD	C5D-O5D-PN-O1N
3	B	401	NAD	C3D-C4D-C5D-O5D

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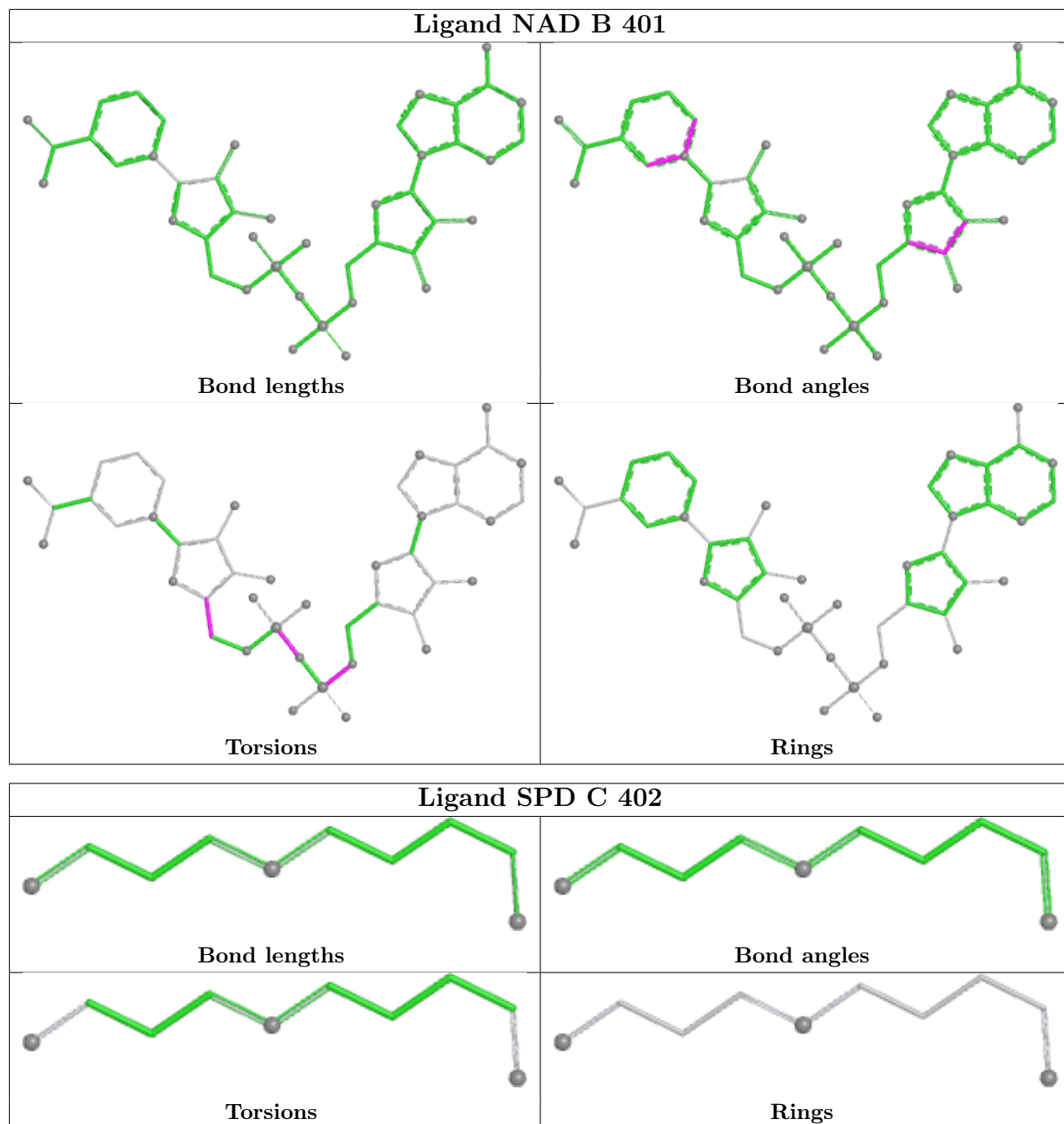
Mol	Chain	Res	Type	Atoms
3	D	402	NAD	C5D-O5D-PN-O2N

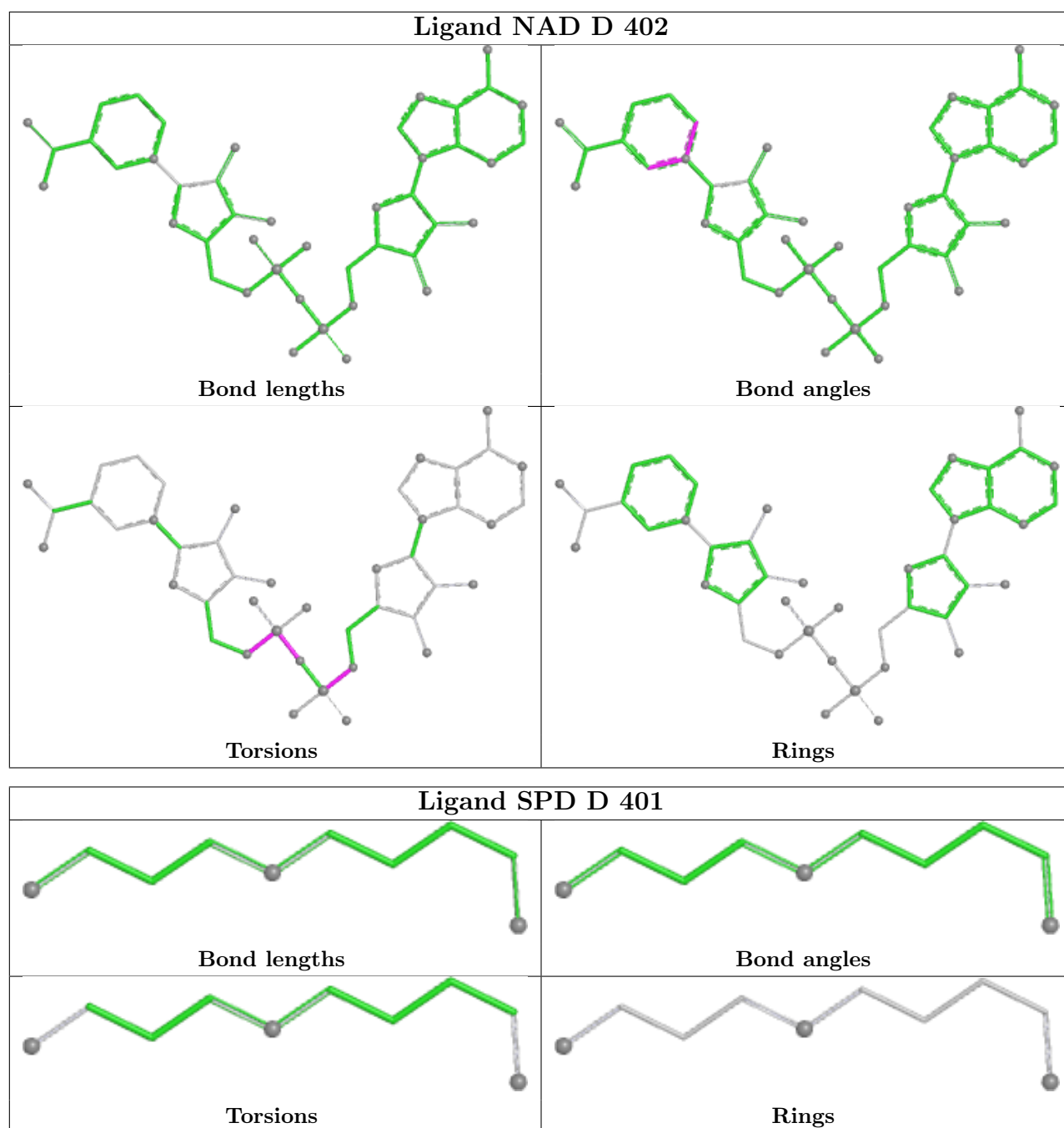
There are no ring outliers.

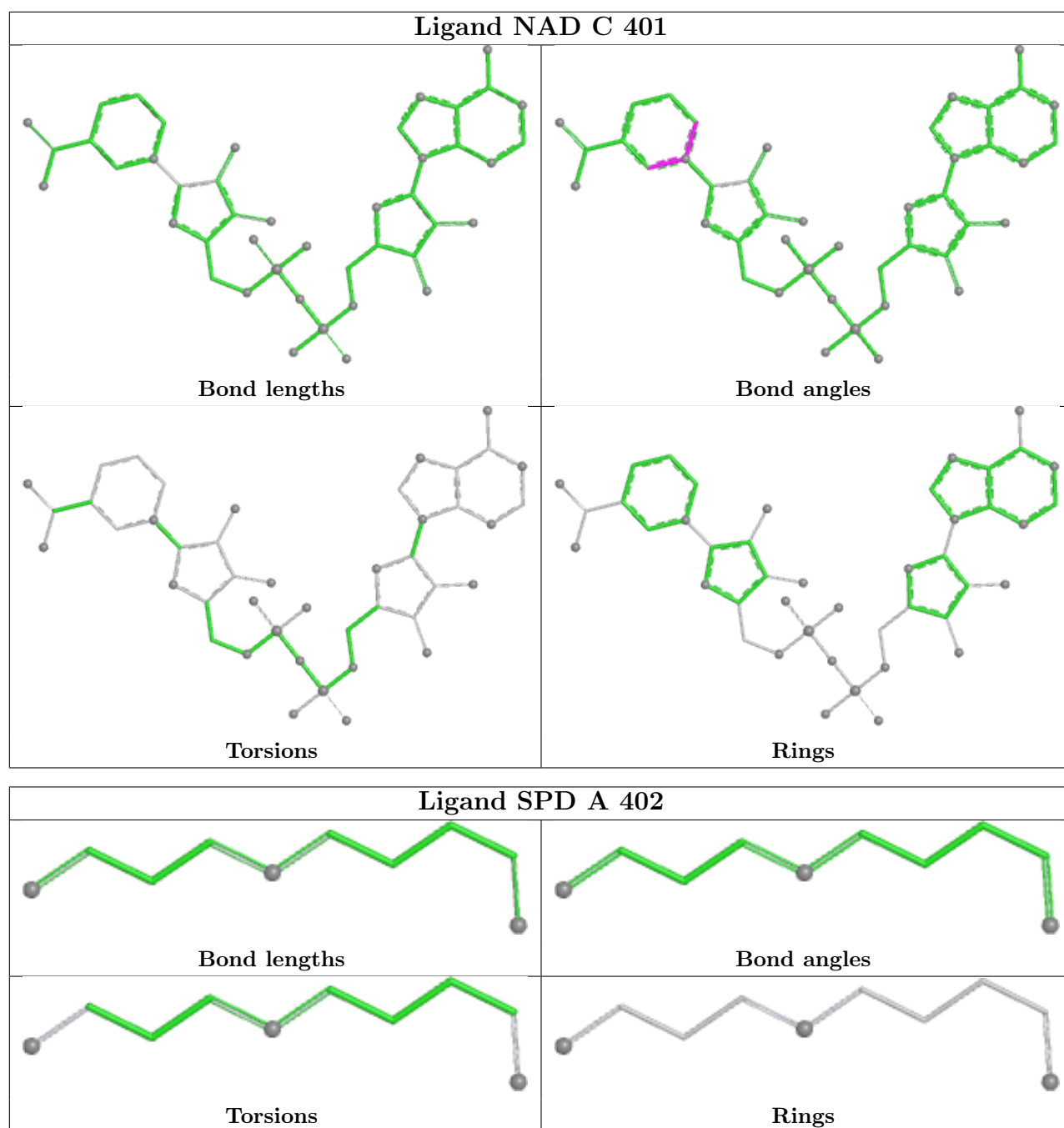
2 monomers are involved in 2 short contacts:

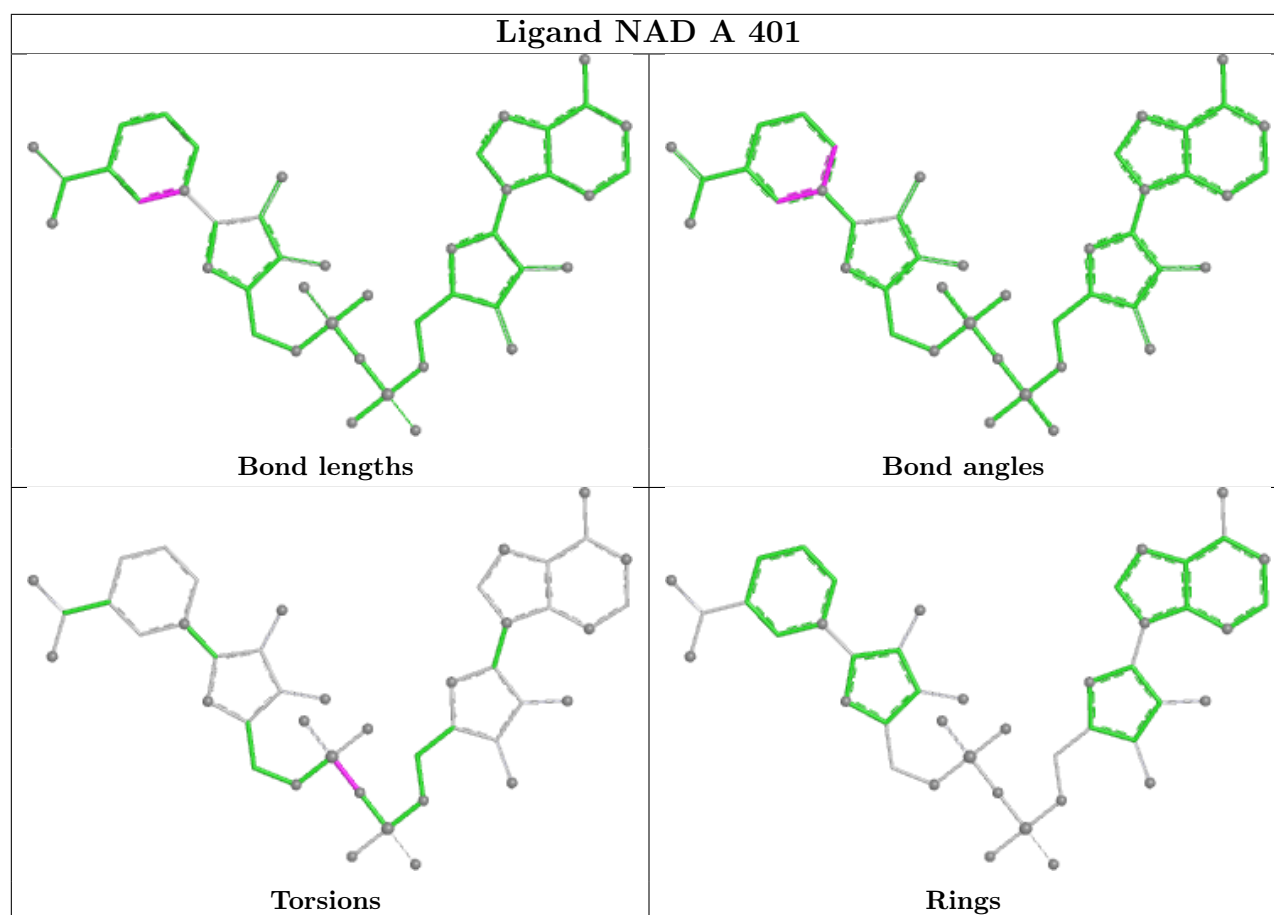
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	401	NAD	1	0
4	A	402	SPD	1	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	E	6

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	148:VAL	C	149:THR	N	1.19
1	E	130:GLN	C	131:ARG	N	1.13
1	E	134:ASP	C	135:LEU	N	1.05
1	E	143:ASN	C	144:ASP	N	1.02
1	E	146:VAL	C	147:VAL	N	1.02
1	E	159:ILE	C	160:VAL	N	1.01

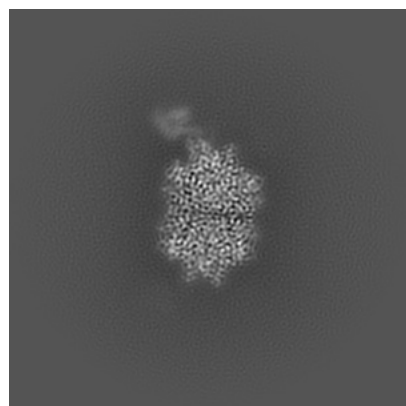
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18784. These allow visual inspection of the internal detail of the map and identification of artifacts.

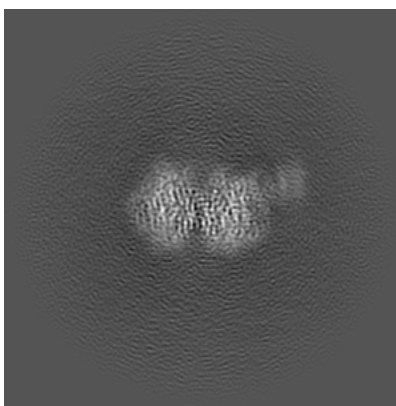
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

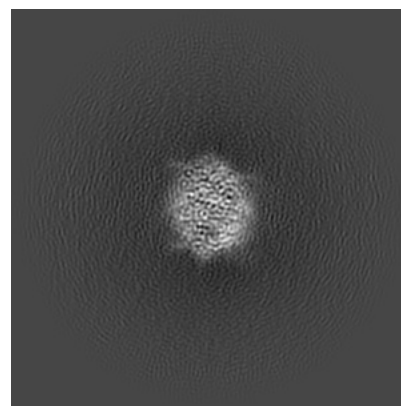
6.1.1 Primary map



X

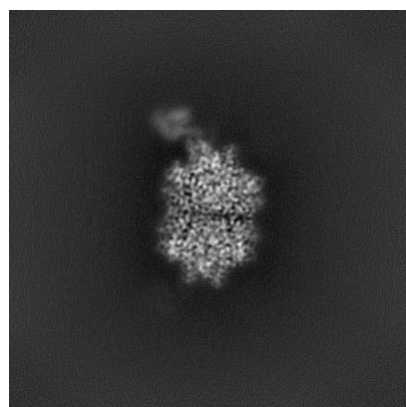


Y

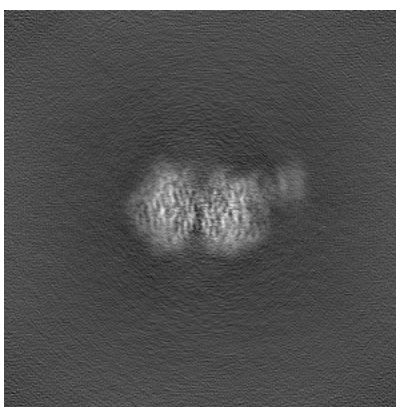


Z

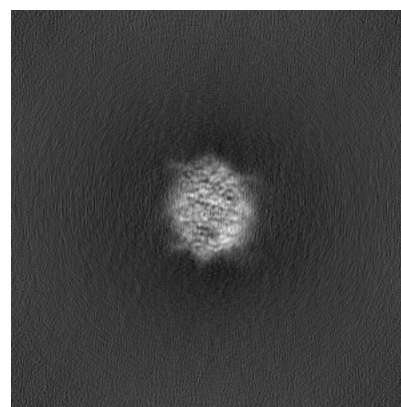
6.1.2 Raw map



X



Y

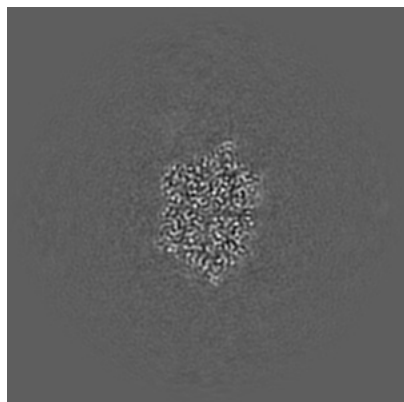


Z

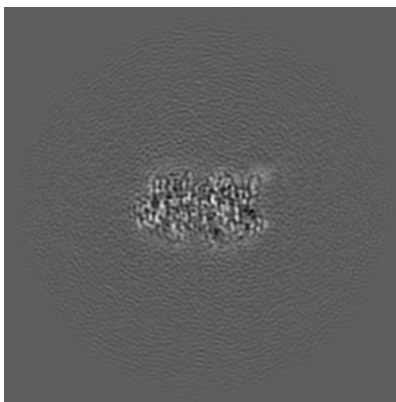
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

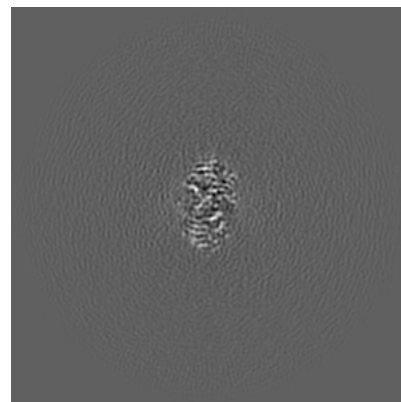
6.2.1 Primary map



X Index: 176

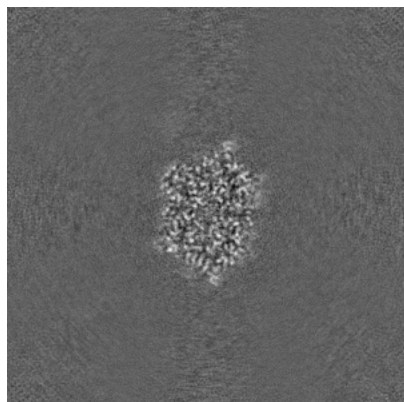


Y Index: 176

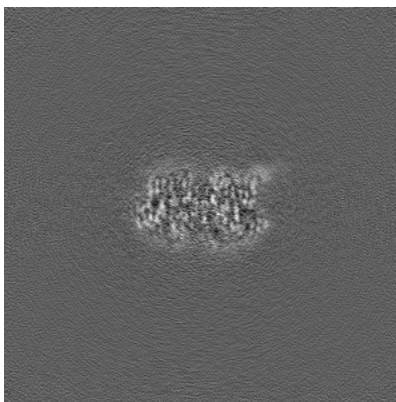


Z Index: 176

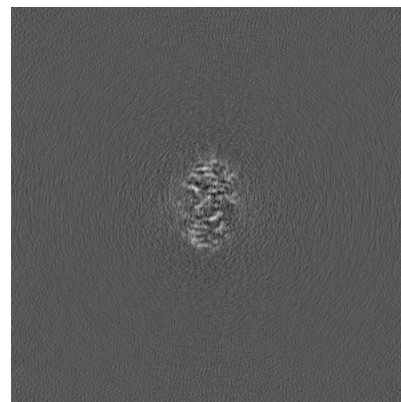
6.2.2 Raw map



X Index: 176



Y Index: 176

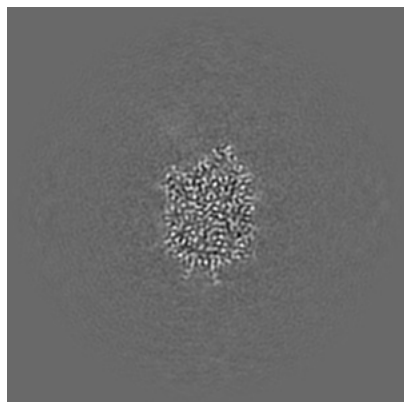


Z Index: 176

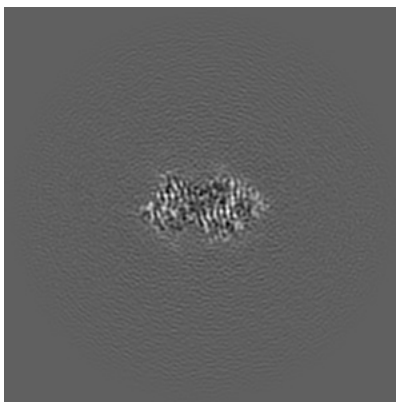
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

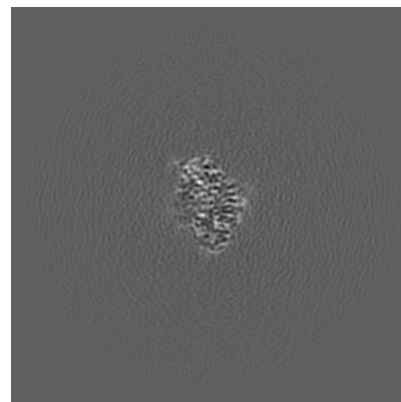
6.3.1 Primary map



X Index: 180

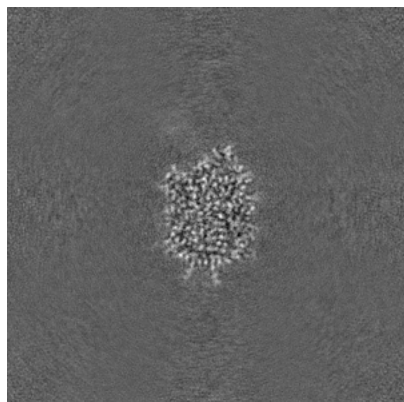


Y Index: 192

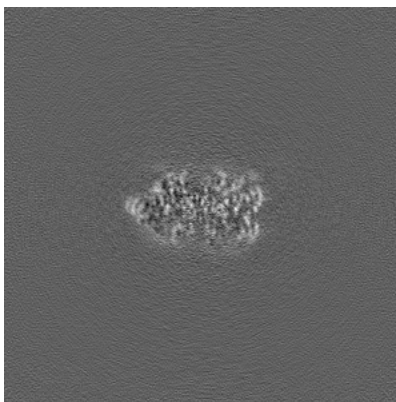


Z Index: 192

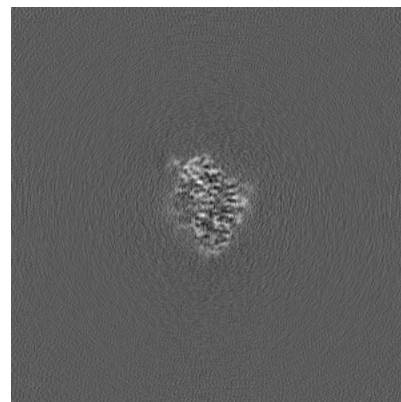
6.3.2 Raw map



X Index: 180



Y Index: 183

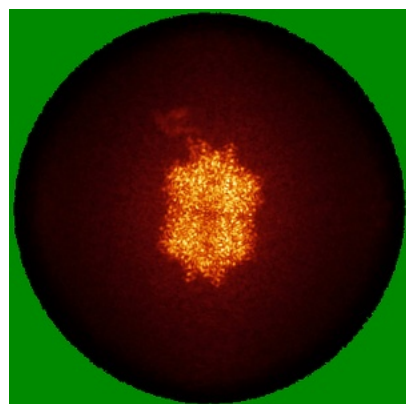


Z Index: 192

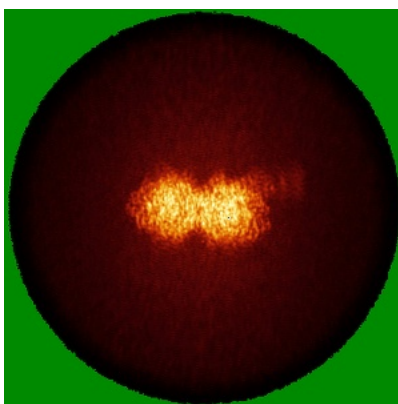
The images above show the largest variance slices of the map in three orthogonal directions.

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

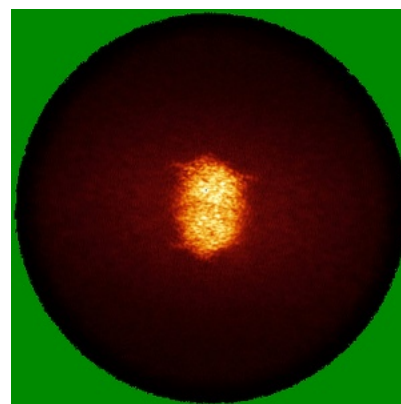
6.4.1 Primary map



X

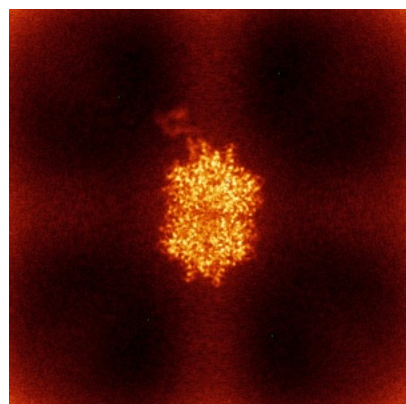


Y

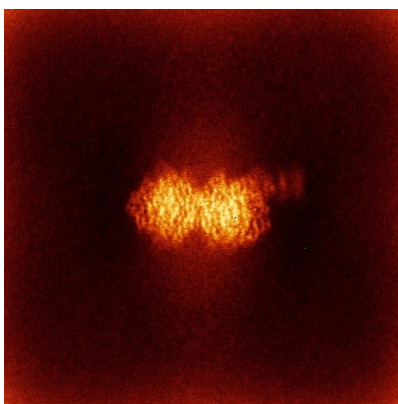


Z

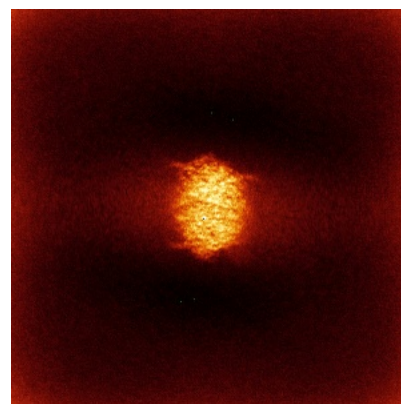
6.4.2 Raw map



X



Y

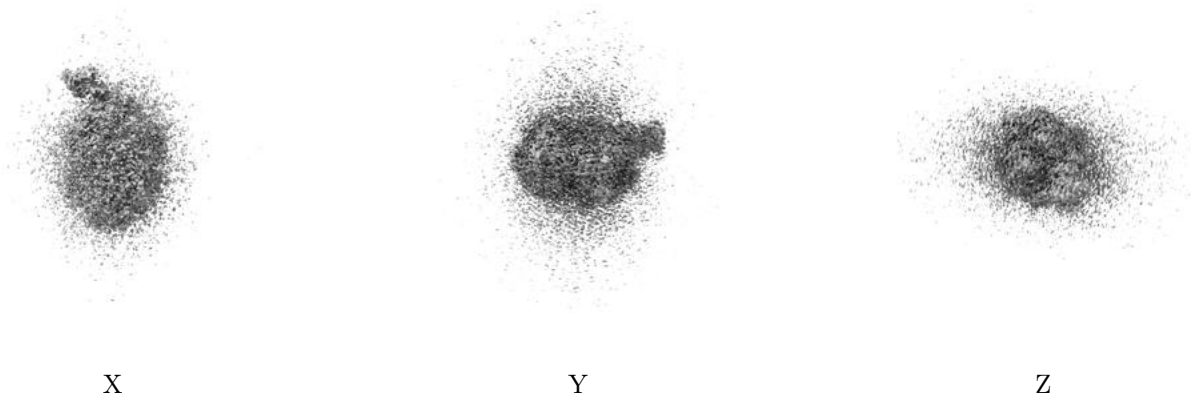


Z

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.

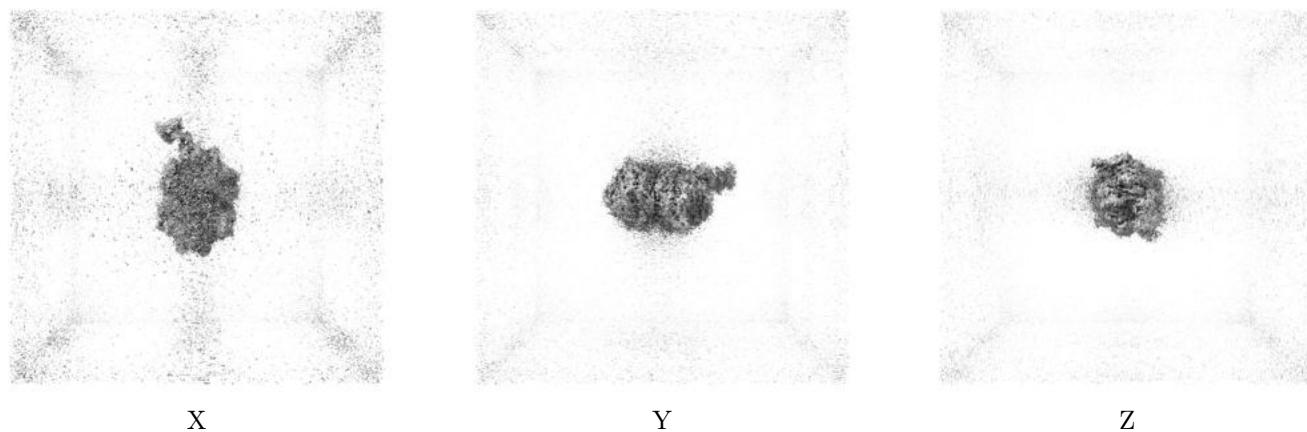
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0754. 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.

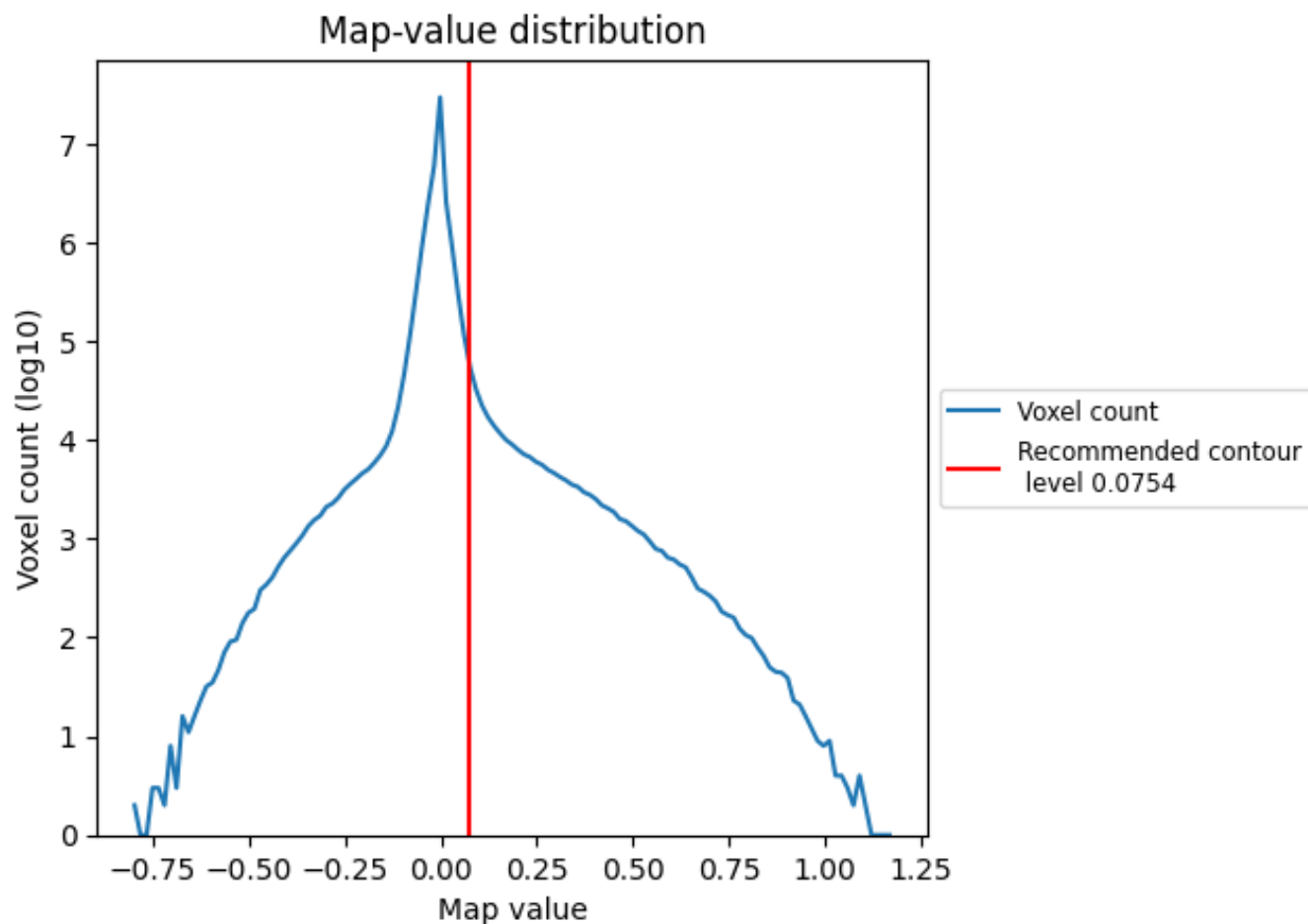
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

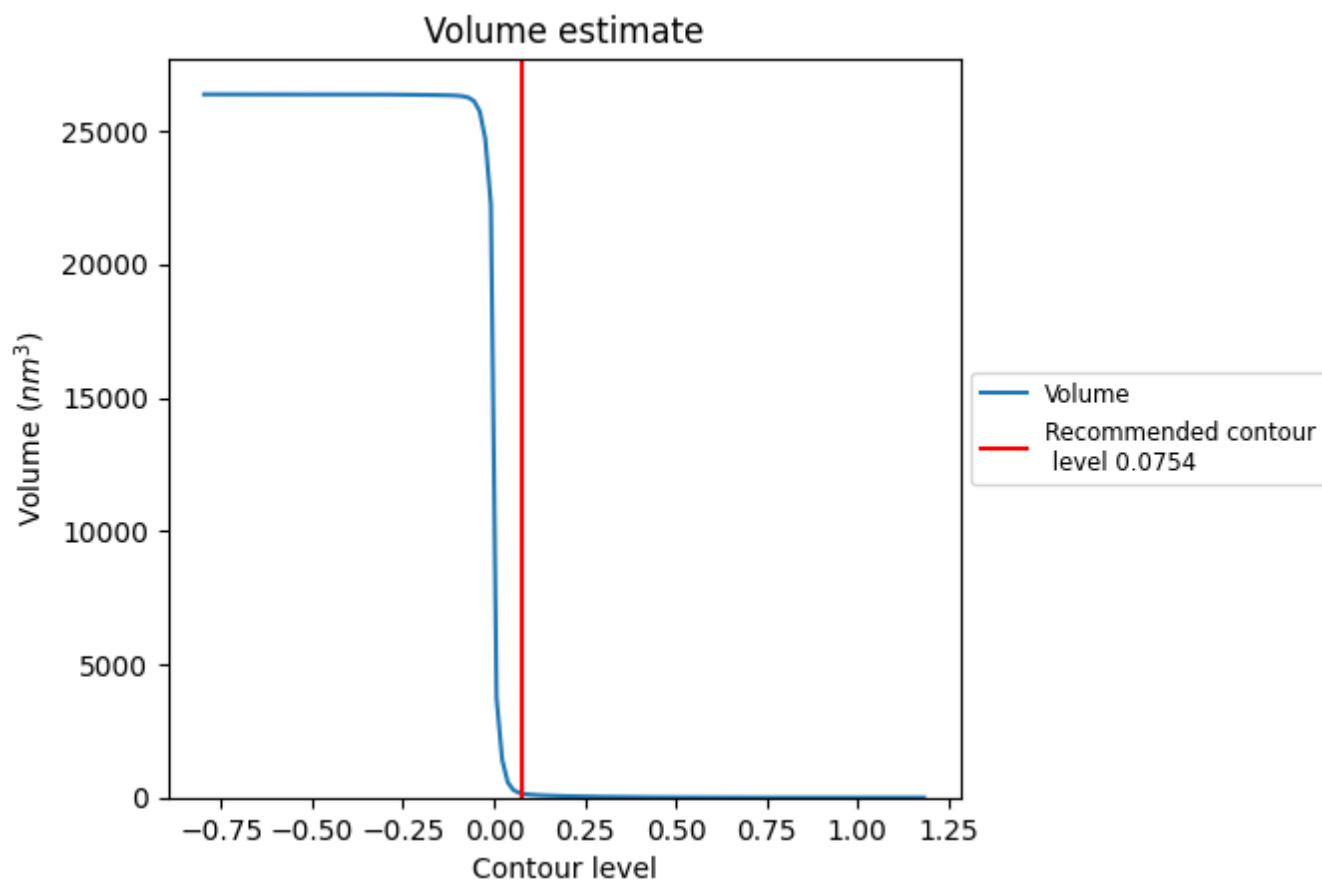
This section contains the results of statistical analysis of the map.

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.

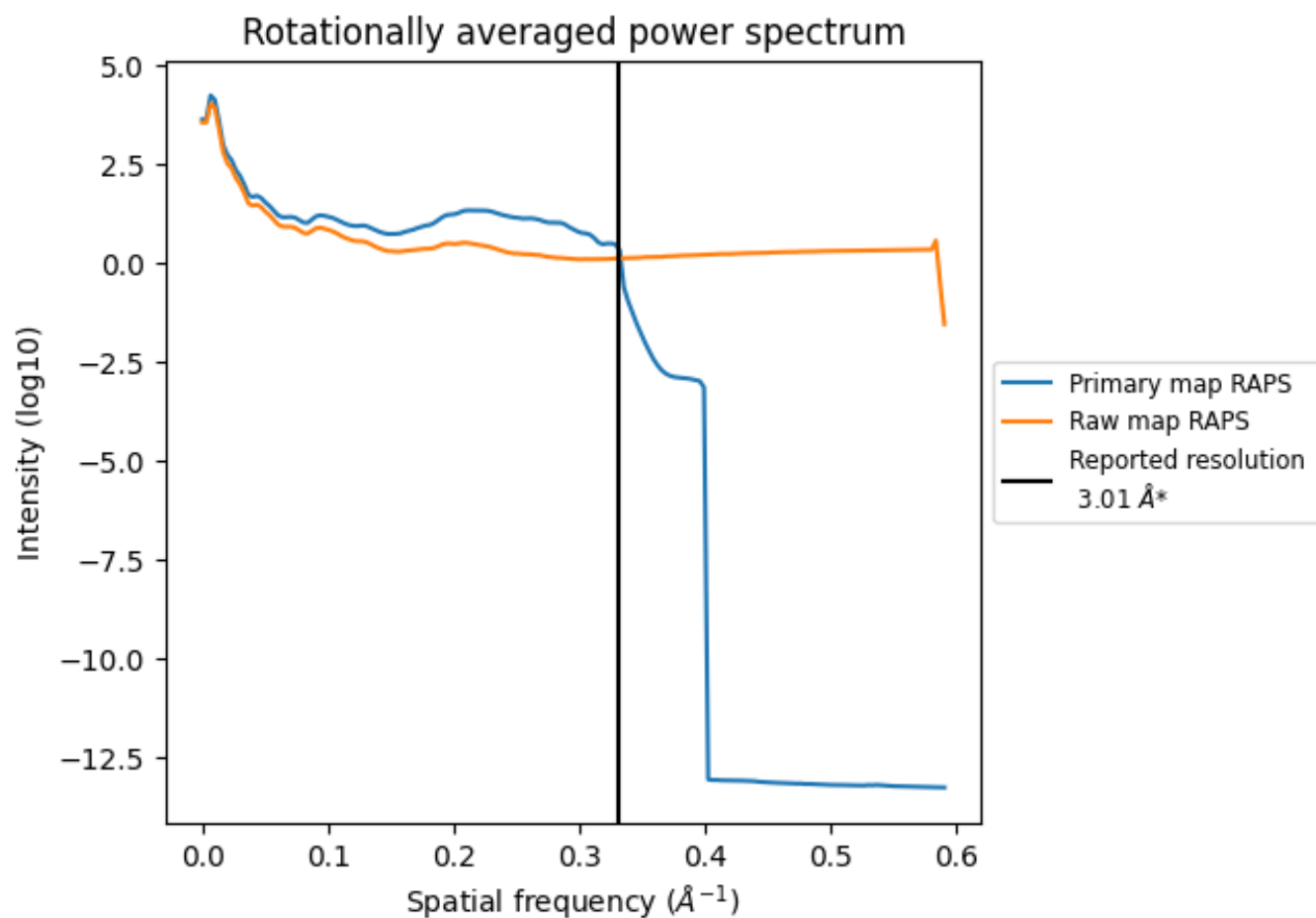
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 161 nm^3 ; this corresponds to an approximate mass of 146 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 ⓘ

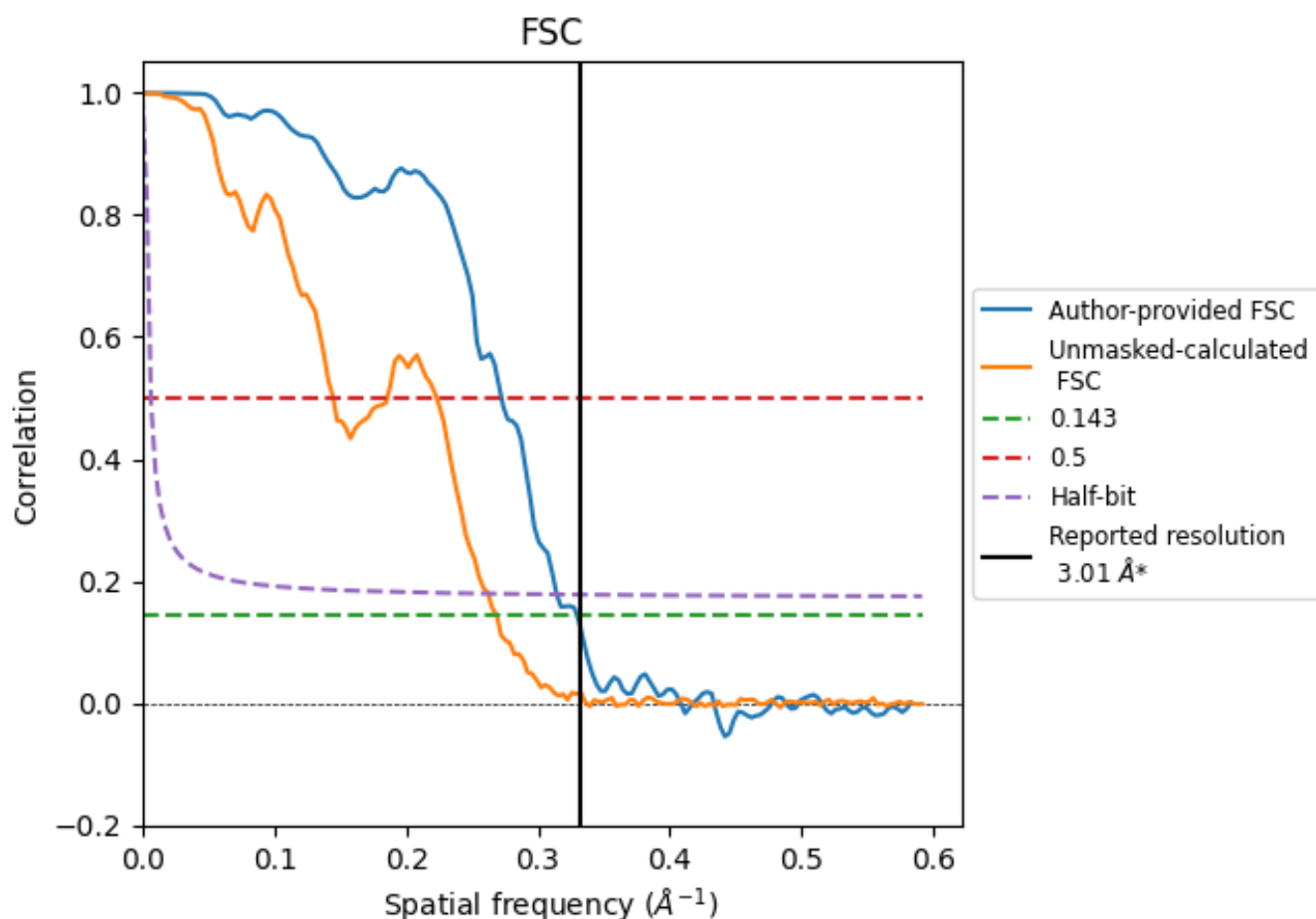


*Reported resolution corresponds to spatial frequency of 0.332 Å⁻¹

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 0.332 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

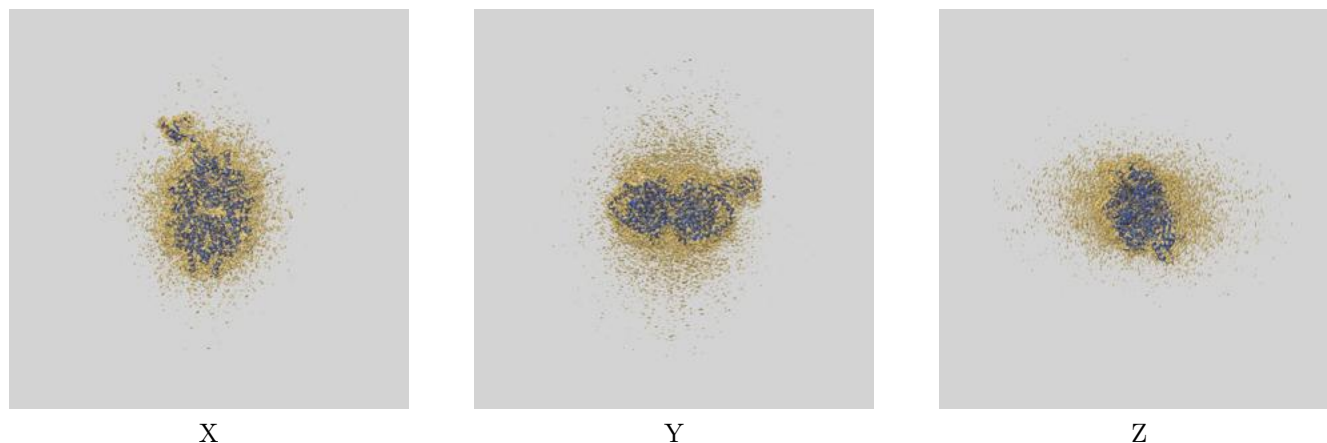
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.01	-	-
Author-provided FSC curve	3.03	3.67	3.18
Unmasked-calculated*	3.72	6.91	3.81

*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 3.72 differs from the reported value 3.01 by more than 10 %

9 Map-model fit [i](#)

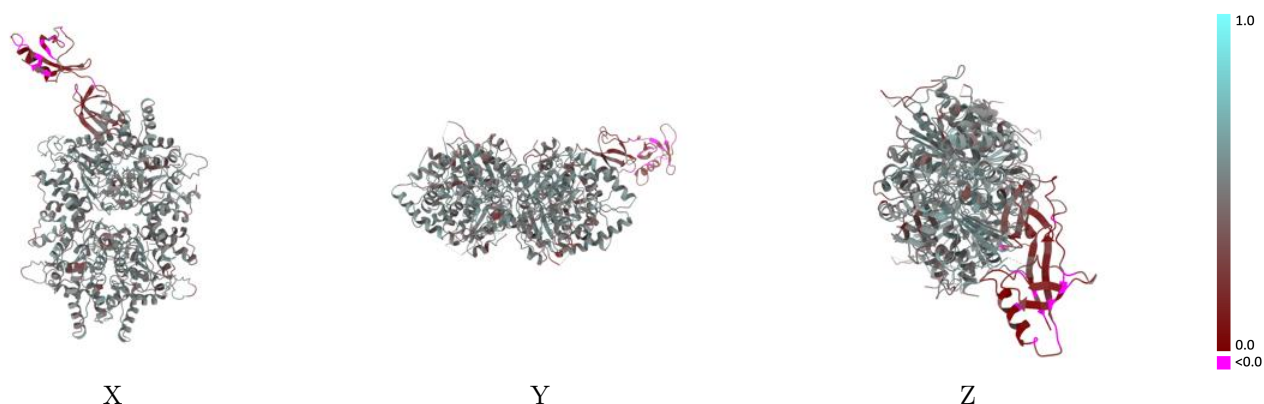
This section contains information regarding the fit between EMDB map EMD-18784 and PDB model 8QZX. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



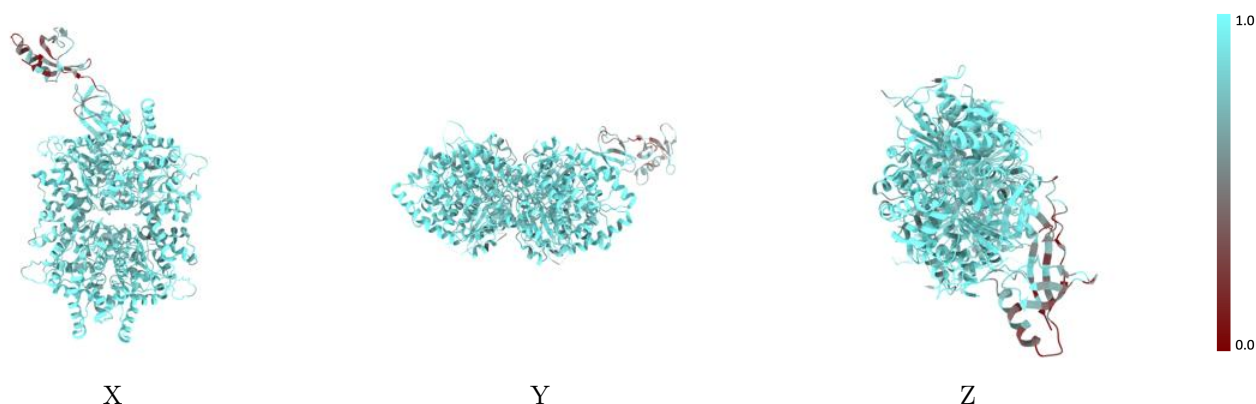
The images above show the 3D surface view of the map at the recommended contour level 0.0754 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



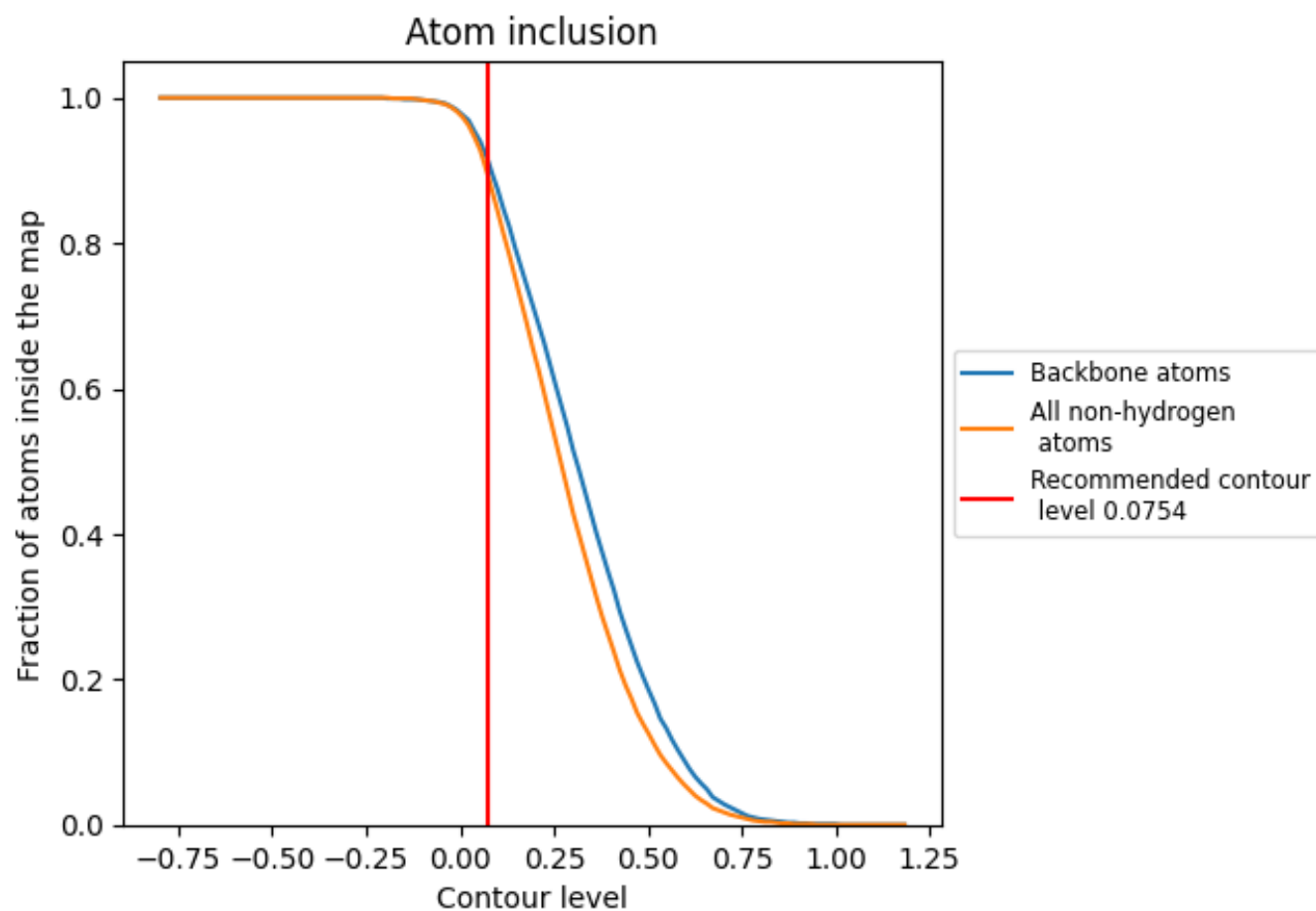
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0754).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 89% 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 (0.0754) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8910	0.4650
A	0.9270	0.5020
B	0.9140	0.4840
C	0.9130	0.4840
D	0.9190	0.4940
E	0.6190	0.1980

