



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 09:43 AM UTC

PDB ID : 9B2M / pdb_00009b2m
EMDB ID : EMD-44112
Title : Hemagglutinin H1 New Caledonia 1999 in complex with monoclonal antibody Fab 43_S0008
Authors : Torrents de la Pena, A.; de Paiva Froes Rocha, R.; Ward, A.B.; Ataca, S.; Kanekiyo, M.
Deposited on : 2024-03-15
Resolution : 3.09 Å (reported)
Based on initial model : 4m4y

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:

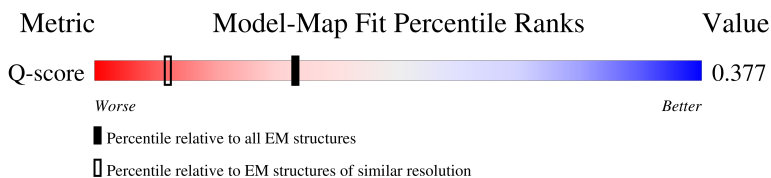
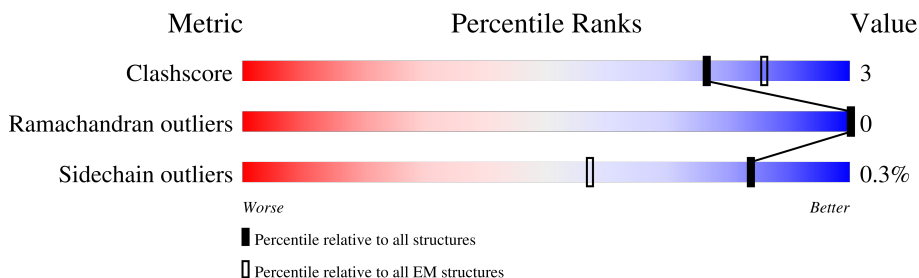
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.09 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	14003 (2.59 - 3.59)

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	339	
1	C	339	
1	G	339	

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Mol	Chain	Length	Quality of chain
2	B	226	
2	D	226	
2	I	226	
3	E	233	
3	H	233	
3	J	233	
4	F	220	
4	K	220	
4	L	220	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 17412 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 Hemagglutinin HA1 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	321	Total	C	N	O	S	0	0
			2522	1597	435	479	11		
1	A	321	Total	C	N	O	S	0	0
			2522	1597	435	479	11		
1	G	321	Total	C	N	O	S	0	0
			2522	1597	435	479	11		

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	168	Total	C	N	O	S	0	0
			1362	852	234	269	7		
2	B	168	Total	C	N	O	S	0	0
			1362	852	234	269	7		
2	I	168	Total	C	N	O	S	0	0
			1362	852	234	269	7		

- Molecule 3 is a protein called Heavy chain monoclonal antibody Fab 3_S0008.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	127	Total	C	N	O	S	0	0
			986	632	165	184	5		
3	E	127	Total	C	N	O	S	0	0
			986	632	165	184	5		
3	J	127	Total	C	N	O	S	0	0
			986	632	165	184	5		

- Molecule 4 is a protein called Light chain monoclonal antibody Fab 3_S0008.

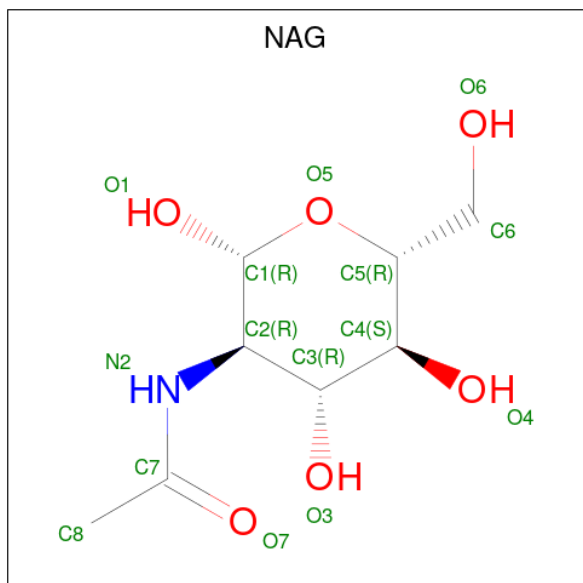
Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	113	Total	C	N	O	S	0	0
			864	548	146	168	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	113	Total	C	N	O	S	0	0
			864	548	146	168	2		
4	K	113	Total	C	N	O	S	0	0
			864	548	146	168	2		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



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

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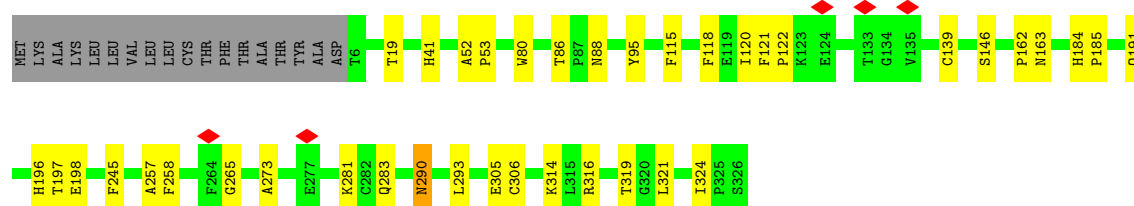
Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	G	1	Total	C	N	O	0
			14	8	1	5	
5	G	1	Total	C	N	O	0
			14	8	1	5	
5	G	1	Total	C	N	O	0
			14	8	1	5	
5	G	1	Total	C	N	O	0
			14	8	1	5	

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.

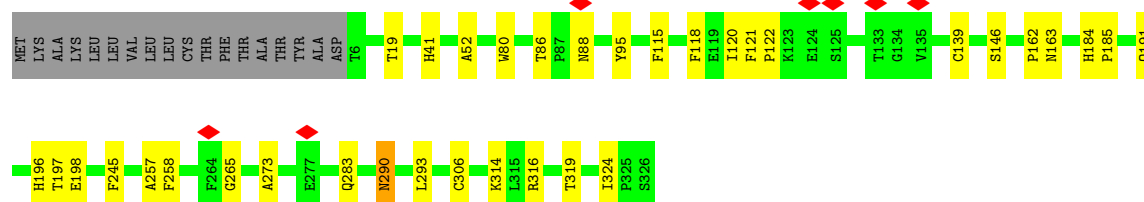
- Molecule 1: Hemagglutinin HA1 chain

Chain C: 



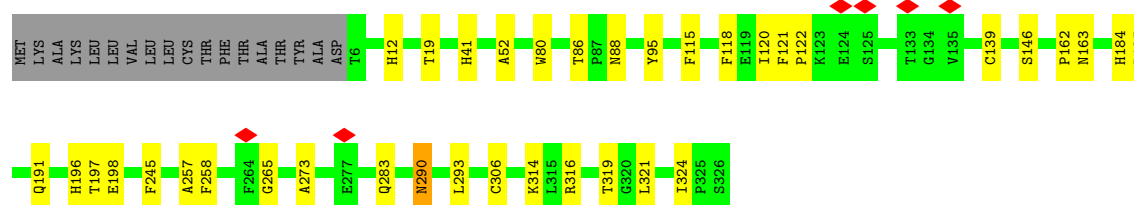
- Molecule 1: Hemagglutinin HA1 chain

Chain A: 



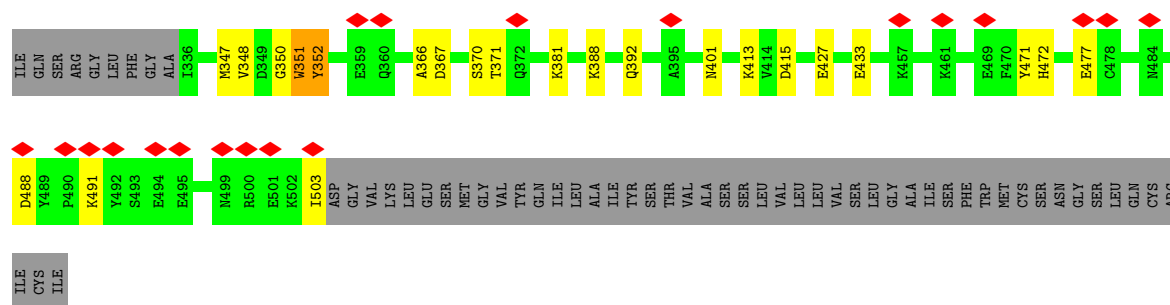
- Molecule 1: Hemagglutinin HA1 chain

Chain G: 

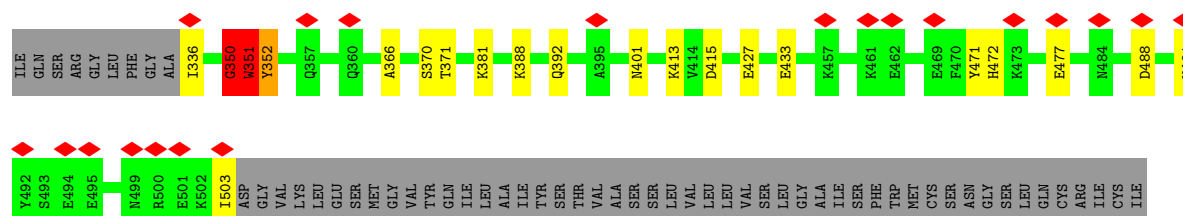


- Molecule 2: Hemagglutinin HA2 chain

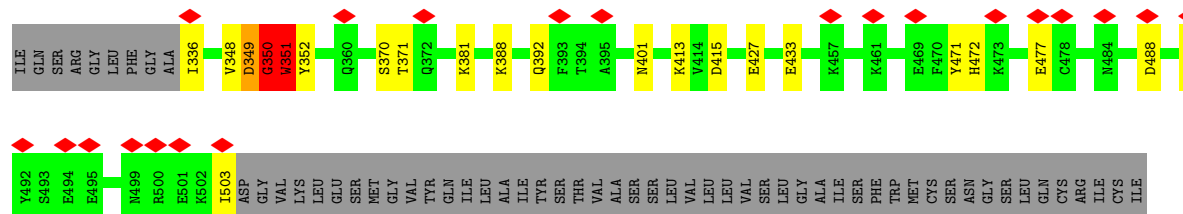
Chain D: 



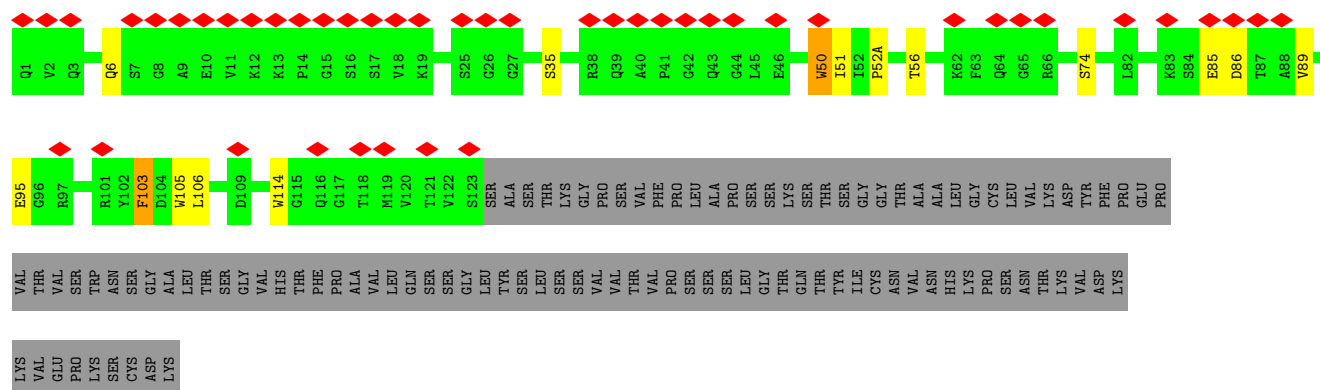
• Molecule 2: Hemagglutinin HA2 chain



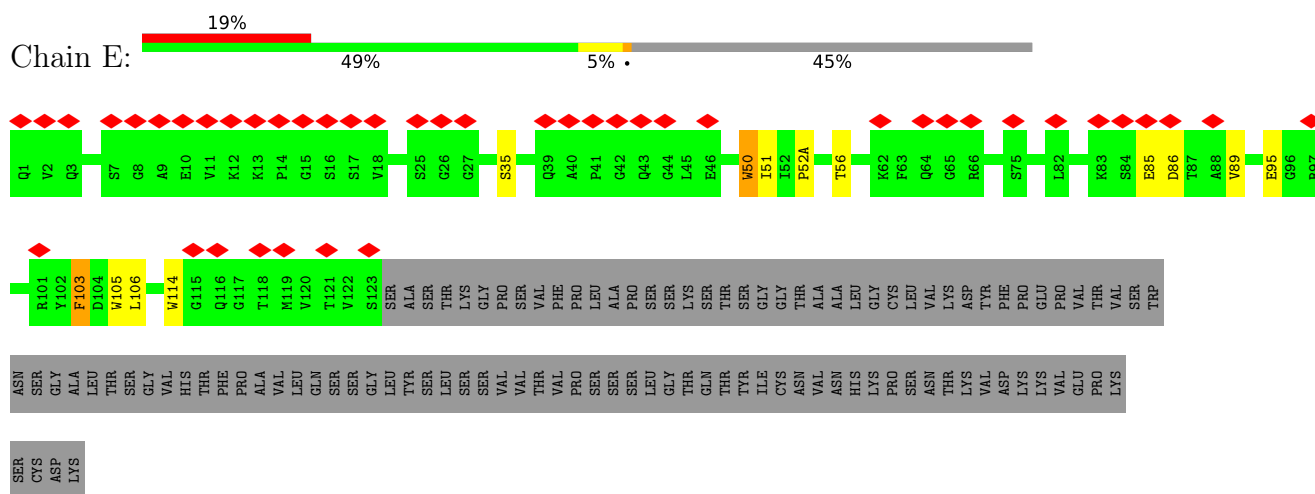
• Molecule 2: Hemagglutinin HA2 chain



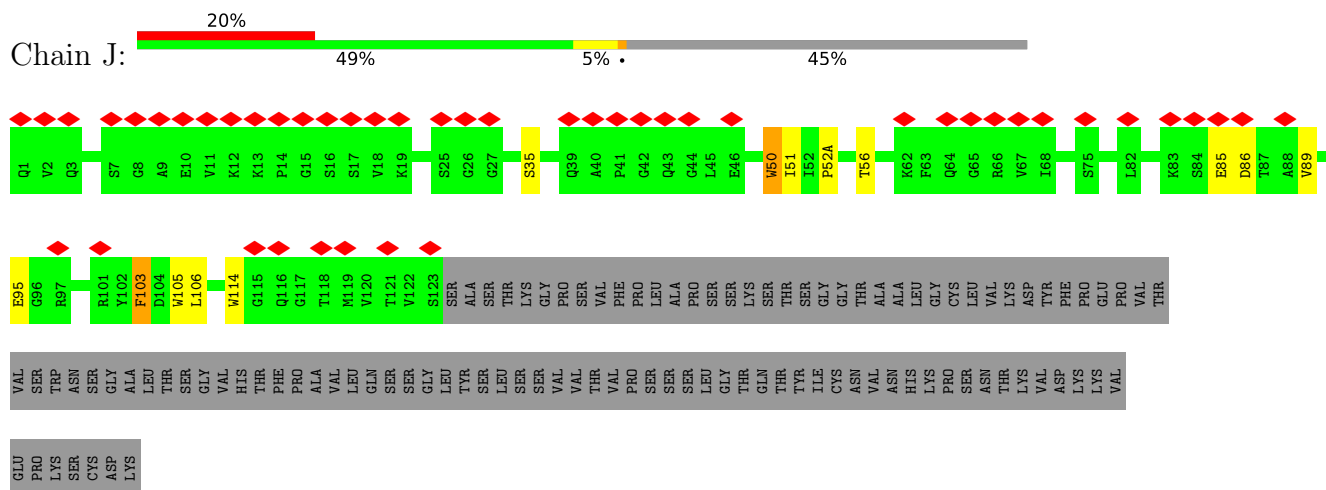
• Molecule 3: Heavy chain monoclonal antibody Fab 3_S0008



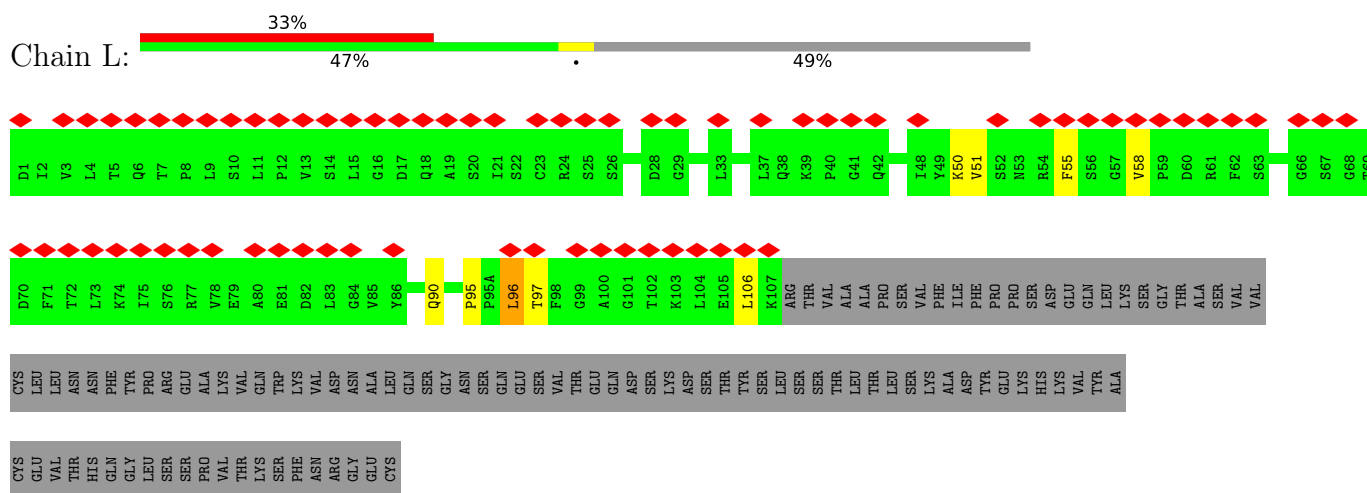
• Molecule 3: Heavy chain monoclonal antibody Fab 3_S0008



• Molecule 3: Heavy chain monoclonal antibody Fab 3_S0008

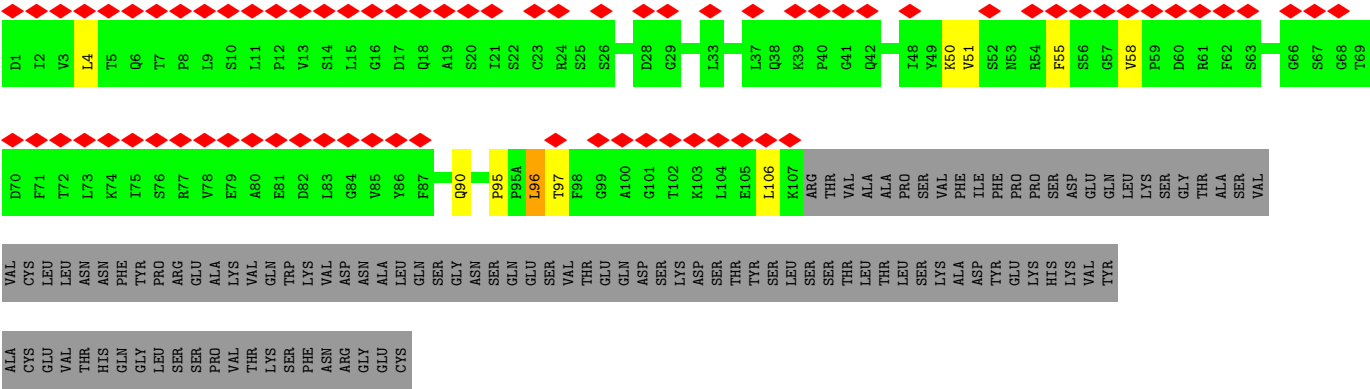


• Molecule 4: Light chain monoclonal antibody Fab 3_S0008

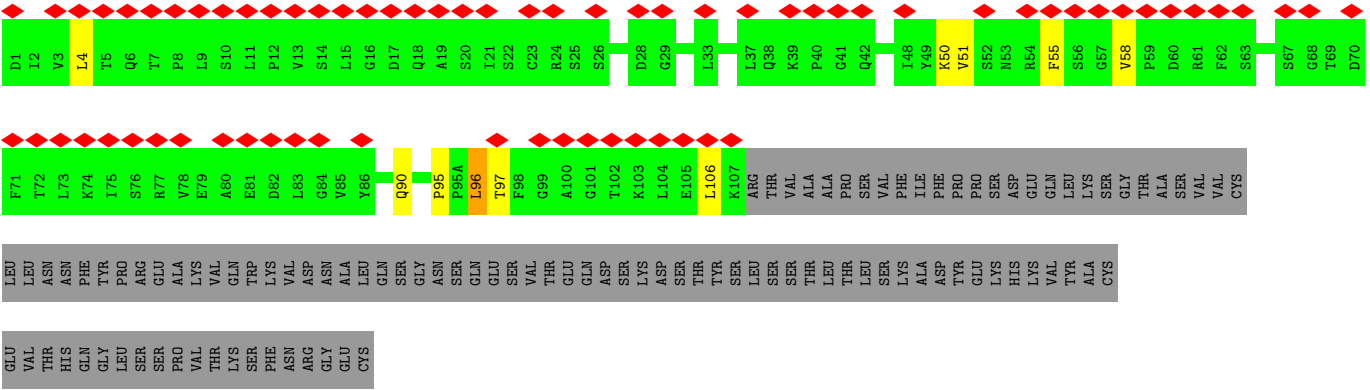


• Molecule 4: Light chain monoclonal antibody Fab 3_S0008





● Molecule 4: Light chain monoclonal antibody Fab 3_S0008



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	190711	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.247	Depositor
Minimum map value	-1.824	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.038	Depositor
Recommended contour level	0.25	Depositor
Map size ($\text{\AA}$)	334.4, 334.4, 334.4	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.045, 1.045, 1.045	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.27	7/2590 (0.3%)	1.42	40/3530 (1.1%)
1	C	1.28	8/2590 (0.3%)	1.42	40/3530 (1.1%)
1	G	1.28	7/2590 (0.3%)	1.42	40/3530 (1.1%)
2	B	1.22	6/1388 (0.4%)	1.20	7/1865 (0.4%)
2	D	1.18	4/1388 (0.3%)	1.25	8/1865 (0.4%)
2	I	1.20	5/1388 (0.4%)	1.28	9/1865 (0.5%)
3	E	1.06	1/1010 (0.1%)	1.34	8/1370 (0.6%)
3	H	1.06	1/1010 (0.1%)	1.34	8/1370 (0.6%)
3	J	1.06	1/1010 (0.1%)	1.34	8/1370 (0.6%)
4	F	1.01	0/884	1.31	8/1200 (0.7%)
4	K	1.01	0/884	1.31	8/1200 (0.7%)
4	L	1.01	0/884	1.31	8/1200 (0.7%)
All	All	1.18	40/17616 (0.2%)	1.35	192/23895 (0.8%)

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	B	0	1
2	I	0	1
All	All	0	2

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	350	GLY	C-O	8.81	1.35	1.23
1	C	245	PHE	CB-CG	-8.22	1.31	1.50
1	G	245	PHE	CB-CG	-8.20	1.31	1.50
1	A	245	PHE	CB-CG	-8.19	1.31	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	41	HIS	CB-CG	-7.53	1.39	1.50
1	G	41	HIS	CB-CG	-7.51	1.39	1.50
1	A	41	HIS	CB-CG	-7.50	1.39	1.50
2	I	336	ILE	CB-CG1	6.99	1.67	1.53
2	B	336	ILE	CB-CG1	6.95	1.67	1.53
3	H	114	TRP	NE1-CE2	-6.52	1.30	1.37
3	E	114	TRP	NE1-CE2	-6.51	1.30	1.37
3	J	114	TRP	NE1-CE2	-6.45	1.30	1.37
2	I	472	HIS	CB-CG	6.42	1.59	1.50
2	B	472	HIS	CB-CG	6.42	1.59	1.50
2	D	472	HIS	CB-CG	6.41	1.59	1.50
2	B	503	ILE	CB-CG1	6.39	1.66	1.53
2	I	503	ILE	CB-CG1	6.38	1.66	1.53
2	D	503	ILE	CB-CG1	6.37	1.66	1.53
2	I	352	TYR	CB-CG	-6.13	1.38	1.51
2	D	352	TYR	CB-CG	-6.11	1.38	1.51
2	B	352	TYR	CB-CG	-6.08	1.38	1.51
1	C	80	TRP	NE1-CE2	-5.67	1.31	1.37
1	G	80	TRP	NE1-CE2	-5.62	1.31	1.37
2	D	471	TYR	CB-CG	-5.61	1.39	1.51
2	I	471	TYR	CB-CG	-5.59	1.39	1.51
1	C	118	PHE	CB-CG	-5.59	1.37	1.50
1	A	118	PHE	CB-CG	-5.59	1.37	1.50
2	B	471	TYR	CB-CG	-5.58	1.39	1.51
1	A	80	TRP	NE1-CE2	-5.58	1.31	1.37
1	G	118	PHE	CB-CG	-5.58	1.37	1.50
1	G	283	GLN	CG-CD	-5.47	1.38	1.52
1	C	283	GLN	CG-CD	-5.45	1.38	1.52
1	G	118	PHE	CA-C	-5.45	1.46	1.52
1	A	283	GLN	CG-CD	-5.44	1.38	1.52
1	A	118	PHE	CA-C	-5.43	1.46	1.52
1	C	118	PHE	CA-C	-5.43	1.46	1.52
1	A	80	TRP	CE2-CZ2	-5.19	1.28	1.39
1	G	80	TRP	CE2-CZ2	-5.18	1.28	1.39
1	C	80	TRP	CE2-CZ2	-5.17	1.29	1.39
1	C	53	PRO	CA-C	-5.08	1.47	1.52

All (192) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	351	TRP	N-CA-C	-17.53	89.87	113.18
2	D	351	TRP	N-CA-C	-13.01	97.18	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	350	GLY	O-C-N	-11.70	114.38	123.27
2	B	351	TRP	N-CA-C	-9.22	91.16	110.80
1	A	319	THR	N-CA-C	-8.60	103.38	114.04
1	G	319	THR	N-CA-C	-8.60	103.38	114.04
1	C	319	THR	N-CA-C	-8.58	103.40	114.04
1	C	258	PHE	N-CA-C	7.52	120.89	109.23
1	G	258	PHE	N-CA-C	7.51	120.88	109.23
1	A	258	PHE	N-CA-C	7.50	120.86	109.23
1	C	306	CYS	CA-C-N	7.48	127.92	120.52
1	C	306	CYS	C-N-CA	7.48	127.92	120.52
1	A	306	CYS	CA-C-N	7.40	127.85	120.52
1	A	306	CYS	C-N-CA	7.40	127.85	120.52
1	G	306	CYS	CA-C-N	7.38	127.83	120.52
1	G	306	CYS	C-N-CA	7.38	127.83	120.52
1	G	185	PRO	CA-C-N	7.30	126.93	119.56
1	G	185	PRO	C-N-CA	7.30	126.93	119.56
2	D	351	TRP	CA-C-N	-7.25	111.31	122.62
2	D	351	TRP	C-N-CA	-7.25	111.31	122.62
1	A	185	PRO	CA-C-N	7.24	126.87	119.56
1	A	185	PRO	C-N-CA	7.24	126.87	119.56
3	J	89	VAL	N-CA-C	7.20	118.85	108.48
3	H	89	VAL	N-CA-C	7.20	118.84	108.48
1	C	185	PRO	CA-C-N	7.19	126.82	119.56
1	C	185	PRO	C-N-CA	7.19	126.82	119.56
4	K	95	PRO	N-CA-C	-7.17	101.95	110.70
4	L	95	PRO	N-CA-C	-7.17	101.95	110.70
1	G	257	ALA	N-CA-C	-7.17	101.07	110.53
1	A	257	ALA	N-CA-C	-7.16	101.08	110.53
3	E	89	VAL	N-CA-C	7.16	118.79	108.48
4	F	95	PRO	N-CA-C	-7.16	101.96	110.70
1	C	257	ALA	N-CA-C	-7.14	101.11	110.53
1	A	52	ALA	CA-C-N	6.76	127.22	120.52
1	A	52	ALA	C-N-CA	6.76	127.22	120.52
1	C	52	ALA	CA-C-N	6.75	127.20	120.52
1	C	52	ALA	C-N-CA	6.75	127.20	120.52
1	G	52	ALA	CA-C-N	6.75	127.20	120.52
1	G	52	ALA	C-N-CA	6.75	127.20	120.52
1	A	324	ILE	CA-C-O	-6.67	116.34	120.88
1	C	324	ILE	CA-C-O	-6.63	116.37	120.88
1	G	324	ILE	CA-C-O	-6.62	116.38	120.88
2	D	348	VAL	N-CA-C	-6.56	106.85	113.47
4	F	97	THR	N-CA-C	-6.51	100.80	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	97	THR	N-CA-C	-6.47	100.85	110.23
4	K	97	THR	N-CA-C	-6.46	100.87	110.23
1	G	324	ILE	CA-C-N	6.38	126.35	119.78
1	G	324	ILE	C-N-CA	6.38	126.35	119.78
1	C	115	PHE	CA-CB-CG	6.36	120.16	113.80
1	C	293	LEU	CA-C-N	6.33	126.82	119.47
1	C	293	LEU	C-N-CA	6.33	126.82	119.47
1	A	293	LEU	CA-C-N	6.33	126.82	119.47
1	A	293	LEU	C-N-CA	6.33	126.82	119.47
1	A	115	PHE	CA-CB-CG	6.32	120.12	113.80
1	G	115	PHE	CA-CB-CG	6.32	120.12	113.80
1	A	324	ILE	CA-C-N	6.31	126.28	119.78
1	A	324	ILE	C-N-CA	6.31	126.28	119.78
3	E	56	THR	CA-C-N	6.31	126.27	120.03
3	E	56	THR	C-N-CA	6.31	126.27	120.03
1	G	293	LEU	CA-C-N	6.29	126.77	119.47
1	G	293	LEU	C-N-CA	6.29	126.77	119.47
1	C	324	ILE	CA-C-N	6.28	126.25	119.78
1	C	324	ILE	C-N-CA	6.28	126.25	119.78
3	J	51	ILE	N-CA-C	6.27	117.51	108.48
3	H	56	THR	CA-C-N	6.27	126.24	120.03
3	H	56	THR	C-N-CA	6.27	126.24	120.03
3	H	51	ILE	N-CA-C	6.25	117.48	108.48
3	J	56	THR	CA-C-N	6.25	126.22	120.03
3	J	56	THR	C-N-CA	6.25	126.22	120.03
3	E	51	ILE	N-CA-C	6.23	117.45	108.48
1	G	306	CYS	N-CA-C	6.20	118.45	110.39
1	C	306	CYS	N-CA-C	6.18	118.42	110.39
1	A	306	CYS	N-CA-C	6.17	118.42	110.39
1	A	245	PHE	CA-CB-CG	6.15	119.95	113.80
1	C	245	PHE	CA-CB-CG	6.13	119.93	113.80
1	A	257	ALA	CA-C-N	-6.13	112.18	122.29
1	A	257	ALA	C-N-CA	-6.13	112.18	122.29
1	G	245	PHE	CA-CB-CG	6.12	119.92	113.80
1	G	257	ALA	CA-C-N	-6.10	112.22	122.29
1	G	257	ALA	C-N-CA	-6.10	112.22	122.29
1	C	257	ALA	CA-C-N	-6.09	112.23	122.29
1	C	257	ALA	C-N-CA	-6.09	112.23	122.29
3	H	106	LEU	N-CA-C	-6.09	102.09	109.83
3	J	106	LEU	N-CA-C	-6.09	102.10	109.83
3	E	106	LEU	N-CA-C	-6.07	102.12	109.83
1	G	122	PRO	N-CA-C	6.02	122.55	114.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	273	ALA	CA-C-N	6.01	125.98	120.03
1	C	273	ALA	C-N-CA	6.01	125.98	120.03
1	G	273	ALA	CA-C-N	6.00	125.97	120.03
1	G	273	ALA	C-N-CA	6.00	125.97	120.03
1	C	122	PRO	N-CA-C	5.99	122.51	114.18
1	A	122	PRO	N-CA-C	5.99	122.50	114.18
2	I	351	TRP	CA-C-N	-5.98	112.42	122.29
2	I	351	TRP	C-N-CA	-5.98	112.42	122.29
4	L	58	VAL	CA-C-N	5.96	126.30	119.92
4	L	58	VAL	C-N-CA	5.96	126.30	119.92
1	A	273	ALA	CA-C-N	5.95	125.92	120.03
1	A	273	ALA	C-N-CA	5.95	125.92	120.03
1	G	245	PHE	N-CA-CB	-5.94	101.38	110.65
4	K	58	VAL	CA-C-N	5.93	126.27	119.92
4	K	58	VAL	C-N-CA	5.93	126.27	119.92
1	C	245	PHE	N-CA-CB	-5.92	101.42	110.65
4	F	58	VAL	CA-C-N	5.92	126.25	119.92
4	F	58	VAL	C-N-CA	5.92	126.25	119.92
1	A	245	PHE	N-CA-CB	-5.92	101.42	110.65
1	C	139	CYS	N-CA-C	-5.86	103.40	110.44
1	G	139	CYS	N-CA-C	-5.86	103.41	110.44
1	A	139	CYS	N-CA-C	-5.83	103.45	110.44
2	B	351	TRP	N-CA-CB	5.78	120.26	110.49
1	C	95	TYR	CA-C-N	5.77	125.72	119.78
1	C	95	TYR	C-N-CA	5.77	125.72	119.78
1	A	184	HIS	CA-C-N	5.77	126.32	120.38
1	A	184	HIS	C-N-CA	5.77	126.32	120.38
1	C	184	HIS	CA-C-N	5.76	126.31	120.38
1	C	184	HIS	C-N-CA	5.76	126.31	120.38
1	G	290	ASN	CA-CB-CG	5.75	118.35	112.60
1	C	290	ASN	CA-CB-CG	5.75	118.35	112.60
1	G	184	HIS	CA-C-N	5.74	126.30	120.38
1	G	184	HIS	C-N-CA	5.74	126.30	120.38
1	G	120	ILE	N-CA-C	-5.74	106.09	111.48
1	A	290	ASN	CA-CB-CG	5.72	118.33	112.60
1	A	95	TYR	CA-C-N	5.72	125.67	119.78
1	A	95	TYR	C-N-CA	5.72	125.67	119.78
1	G	95	TYR	CA-C-N	5.72	125.67	119.78
1	G	95	TYR	C-N-CA	5.72	125.67	119.78
1	C	120	ILE	N-CA-C	-5.71	106.11	111.48
1	A	120	ILE	N-CA-C	-5.71	106.12	111.48
1	A	121	PHE	CA-C-N	5.63	125.32	119.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	121	PHE	C-N-CA	5.63	125.32	119.64
1	A	191	GLN	N-CA-C	-5.63	104.63	112.45
1	C	191	GLN	N-CA-C	-5.61	104.66	112.45
1	G	191	GLN	N-CA-C	-5.60	104.66	112.45
1	C	121	PHE	CA-C-N	5.59	125.29	119.64
1	C	121	PHE	C-N-CA	5.59	125.29	119.64
1	C	196	HIS	N-CA-C	-5.57	102.24	110.48
1	A	196	HIS	N-CA-C	-5.55	102.26	110.48
1	G	196	HIS	N-CA-C	-5.55	102.27	110.48
1	G	121	PHE	CA-C-N	5.54	125.24	119.64
1	G	121	PHE	C-N-CA	5.54	125.24	119.64
3	J	103	PHE	CA-CB-CG	5.54	119.34	113.80
3	H	103	PHE	CA-CB-CG	5.52	119.32	113.80
3	E	103	PHE	CA-CB-CG	5.52	119.32	113.80
1	C	265	GLY	N-CA-C	-5.51	108.14	114.69
1	G	265	GLY	N-CA-C	-5.50	108.15	114.69
1	A	265	GLY	N-CA-C	-5.48	108.17	114.69
1	C	88	ASN	CA-C-N	5.44	125.39	119.78
1	C	88	ASN	C-N-CA	5.44	125.39	119.78
1	G	88	ASN	CA-C-N	5.44	125.39	119.78
1	G	88	ASN	C-N-CA	5.44	125.39	119.78
2	B	401	ASN	CA-CB-CG	5.44	118.04	112.60
1	A	88	ASN	CA-C-N	5.42	125.36	119.78
1	A	88	ASN	C-N-CA	5.42	125.36	119.78
2	D	401	ASN	CA-CB-CG	5.41	118.01	112.60
2	B	350	GLY	CA-C-O	-5.40	113.96	122.27
2	I	401	ASN	CA-CB-CG	5.38	117.98	112.60
2	I	392	GLN	N-CA-C	5.35	117.89	109.39
2	B	392	GLN	N-CA-C	5.35	117.89	109.39
2	I	349	ASP	CA-C-O	-5.33	116.24	122.37
2	D	392	GLN	N-CA-C	5.33	117.86	109.39
1	C	146	SER	N-CA-C	5.31	115.25	108.24
1	G	146	SER	N-CA-C	5.31	115.25	108.24
1	A	146	SER	N-CA-C	5.30	115.24	108.24
4	F	96	LEU	CB-CA-C	-5.26	100.98	109.72
4	L	96	LEU	CB-CA-C	-5.26	100.99	109.72
4	K	96	LEU	CB-CA-C	-5.25	101.01	109.72
1	G	86	THR	CA-C-N	5.20	125.50	119.47
1	G	86	THR	C-N-CA	5.20	125.50	119.47
3	E	52(A)	PRO	N-CA-C	5.20	121.34	113.81
3	J	52(A)	PRO	N-CA-C	5.19	121.34	113.81
3	H	52(A)	PRO	N-CA-C	5.18	121.31	113.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	86	THR	CA-C-N	5.16	125.45	119.47
1	C	86	THR	C-N-CA	5.16	125.45	119.47
1	A	86	THR	CA-C-N	5.13	125.42	119.47
1	A	86	THR	C-N-CA	5.13	125.42	119.47
3	H	50	TRP	N-CA-C	5.13	116.77	108.26
2	D	477	GLU	CA-C-N	5.11	127.08	120.44
2	D	477	GLU	C-N-CA	5.11	127.08	120.44
2	I	477	GLU	CA-C-N	5.11	127.08	120.44
2	I	477	GLU	C-N-CA	5.11	127.08	120.44
3	J	50	TRP	N-CA-C	5.11	116.74	108.26
2	B	477	GLU	CA-C-N	5.10	127.07	120.44
2	B	477	GLU	C-N-CA	5.10	127.07	120.44
3	E	50	TRP	N-CA-C	5.09	116.72	108.26
4	F	55	PHE	CA-CB-CG	5.06	118.86	113.80
4	K	55	PHE	CA-CB-CG	5.05	118.85	113.80
4	L	55	PHE	CA-CB-CG	5.05	118.85	113.80
4	L	106	LEU	CA-C-N	5.04	130.78	121.70
4	L	106	LEU	C-N-CA	5.04	130.78	121.70
4	F	106	LEU	CA-C-N	5.04	130.76	121.70
4	F	106	LEU	C-N-CA	5.04	130.76	121.70
4	K	106	LEU	CA-C-N	5.03	130.76	121.70
4	K	106	LEU	C-N-CA	5.03	130.76	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	350	GLY	Mainchain
2	I	350	GLY	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	2522	0	2435	8	0
1	C	2522	0	2436	15	0
1	G	2522	0	2435	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1362	0	1295	18	0
2	D	1362	0	1295	18	0
2	I	1362	0	1295	18	0
3	E	986	0	972	15	0
3	H	986	0	970	13	0
3	J	986	0	972	11	0
4	F	864	0	859	3	0
4	K	864	0	859	3	0
4	L	864	0	859	2	0
5	A	70	0	65	0	0
5	C	70	0	65	0	0
5	G	70	0	65	0	0
All	All	17412	0	16877	102	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 3.

All (102) 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)
2:D:371:THR:OG1	3:H:105:TRP:CH2	2.12	1.02
2:I:371:THR:OG1	3:J:105:TRP:CH2	2.11	1.01
2:B:371:THR:OG1	3:E:105:TRP:CH2	2.11	1.01
1:C:281:LYS:HB3	1:C:305:GLU:CG	1.96	0.94
2:D:351:TRP:H	3:H:103:PHE:HZ	1.02	0.94
2:B:350:GLY:O	3:E:103:PHE:CE1	2.26	0.88
2:B:350:GLY:O	3:E:103:PHE:HE1	1.56	0.88
2:D:351:TRP:N	3:H:103:PHE:HZ	1.74	0.86
1:C:281:LYS:HB3	1:C:305:GLU:HG2	1.63	0.81
1:G:314:LYS:HE3	1:G:316:ARG:HE	1.47	0.80
1:C:314:LYS:HE3	1:C:316:ARG:HE	1.47	0.80
1:A:314:LYS:HE3	1:A:316:ARG:HE	1.47	0.79
3:J:35:SER:HB3	3:J:50:TRP:HE3	1.48	0.79
3:E:35:SER:HB3	3:E:50:TRP:HE3	1.47	0.79
3:H:35:SER:HB3	3:H:50:TRP:HE3	1.47	0.79
1:C:281:LYS:HB3	1:C:305:GLU:OE2	1.82	0.78
1:G:12:HIS:HD2	2:I:350:GLY:O	1.67	0.77
2:B:370:SER:HB3	3:E:103:PHE:HE2	1.55	0.72
1:C:281:LYS:HB3	1:C:305:GLU:CD	2.15	0.71
2:D:370:SER:HB3	3:H:103:PHE:HE2	1.55	0.71
3:E:35:SER:HB3	3:E:50:TRP:CE3	2.26	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:12:HIS:CD2	2:I:350:GLY:O	2.44	0.71
3:J:35:SER:HB3	3:J:50:TRP:CE3	2.26	0.70
3:H:35:SER:HB3	3:H:50:TRP:CE3	2.26	0.70
2:D:350:GLY:HA3	2:D:366:ALA:HB2	1.74	0.68
2:I:349:ASP:O	2:I:349:ASP:OD1	2.15	0.65
2:I:370:SER:HB2	3:J:103:PHE:HE2	1.62	0.65
2:B:350:GLY:C	3:E:103:PHE:CZ	2.77	0.63
2:D:350:GLY:CA	2:D:366:ALA:HB2	2.31	0.61
1:A:19:THR:O	1:A:314:LYS:NZ	2.23	0.61
2:I:351:TRP:N	3:J:103:PHE:HZ	1.98	0.61
1:A:314:LYS:CE	1:A:316:ARG:HE	2.14	0.61
2:D:350:GLY:HA2	3:H:103:PHE:CZ	2.36	0.60
1:G:314:LYS:CE	1:G:316:ARG:HE	2.14	0.60
1:C:314:LYS:CE	1:C:316:ARG:HE	2.14	0.59
1:C:19:THR:O	1:C:314:LYS:NZ	2.23	0.59
2:B:427:GLU:OE1	2:I:388:LYS:NZ	2.36	0.59
2:D:427:GLU:OE1	2:B:388:LYS:NZ	2.36	0.59
2:D:351:TRP:N	3:H:103:PHE:CZ	2.61	0.58
2:B:350:GLY:HA2	2:B:366:ALA:HB2	1.83	0.58
2:D:388:LYS:NZ	2:I:427:GLU:OE1	2.36	0.58
2:I:350:GLY:C	3:J:103:PHE:CZ	2.83	0.57
1:G:19:THR:O	1:G:314:LYS:NZ	2.23	0.57
1:G:314:LYS:HE2	1:G:316:ARG:CB	2.35	0.57
1:C:314:LYS:HE2	1:C:316:ARG:CB	2.35	0.56
2:B:351:TRP:N	3:E:103:PHE:HZ	2.02	0.56
3:H:6:GLN:N	3:H:6:GLN:OE1	2.38	0.56
1:A:314:LYS:HE2	1:A:316:ARG:CB	2.35	0.56
2:D:381:LYS:NZ	2:D:433:GLU:OE1	2.39	0.55
2:I:381:LYS:NZ	2:I:433:GLU:OE1	2.39	0.55
2:B:413:LYS:NZ	2:I:415:ASP:OD1	2.35	0.55
3:H:50:TRP:HH2	3:H:95:GLU:CG	2.08	0.55
2:B:350:GLY:O	3:E:103:PHE:CZ	2.59	0.55
2:D:347:MET:HE3	2:D:350:GLY:O	2.07	0.55
3:E:50:TRP:HH2	3:E:95:GLU:CG	2.08	0.55
2:B:381:LYS:NZ	2:B:433:GLU:OE1	2.39	0.54
1:C:314:LYS:HE2	1:C:316:ARG:HB3	1.91	0.53
1:G:314:LYS:HE2	1:G:316:ARG:HB3	1.91	0.53
2:I:350:GLY:C	3:J:103:PHE:HZ	2.17	0.52
1:A:314:LYS:HE2	1:A:316:ARG:HB3	1.91	0.51
2:D:413:LYS:NZ	2:B:415:ASP:OD1	2.35	0.51
2:B:488:ASP:OD2	2:B:491:LYS:NZ	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:488:ASP:OD2	2:I:491:LYS:NZ	2.42	0.50
1:G:12:HIS:HD2	2:I:350:GLY:C	2.19	0.49
4:L:90:GLN:H	4:L:96:LEU:HB2	1.78	0.49
3:J:50:TRP:HH2	3:J:95:GLU:CG	2.09	0.49
4:K:90:GLN:H	4:K:96:LEU:HB2	1.78	0.49
2:I:349:ASP:O	2:I:349:ASP:CG	2.56	0.48
2:D:488:ASP:OD2	2:D:491:LYS:NZ	2.42	0.48
4:F:90:GLN:H	4:F:96:LEU:HB2	1.77	0.48
1:G:197:THR:OG1	1:G:198:GLU:N	2.47	0.47
1:C:197:THR:OG1	1:C:198:GLU:N	2.47	0.47
3:H:105:TRP:CD1	3:H:105:TRP:H	2.32	0.47
3:E:105:TRP:CD1	3:E:105:TRP:H	2.32	0.47
1:C:321:LEU:HD11	2:D:351:TRP:HA	1.95	0.47
2:D:415:ASP:OD1	2:I:413:LYS:NZ	2.35	0.47
3:J:105:TRP:H	3:J:105:TRP:CD1	2.32	0.47
1:A:197:THR:OG1	1:A:198:GLU:N	2.47	0.46
3:J:85:GLU:O	3:J:86:ASP:C	2.60	0.45
2:B:350:GLY:C	3:E:103:PHE:CE1	2.94	0.45
4:L:50:LYS:O	4:L:51:VAL:C	2.60	0.45
1:C:305:GLU:O	1:C:305:GLU:HG3	2.16	0.44
1:C:162:PRO:O	1:C:163:ASN:C	2.59	0.44
1:A:162:PRO:O	1:A:163:ASN:C	2.59	0.44
2:B:351:TRP:N	3:E:103:PHE:CZ	2.84	0.44
1:G:162:PRO:O	1:G:163:ASN:C	2.59	0.44
2:B:352:TYR:N	2:B:370:SER:OG	2.49	0.44
2:B:350:GLY:C	3:E:103:PHE:HZ	2.22	0.43
4:K:50:LYS:O	4:K:51:VAL:C	2.60	0.43
3:H:85:GLU:O	3:H:86:ASP:C	2.59	0.43
1:A:314:LYS:HE2	1:A:316:ARG:HB2	2.01	0.42
1:C:290:ASN:HB2	3:H:74:SER:HB2	2.01	0.42
1:G:321:LEU:HD11	2:I:351:TRP:HA	2.01	0.42
3:E:85:GLU:O	3:E:86:ASP:C	2.59	0.42
4:F:50:LYS:O	4:F:51:VAL:C	2.60	0.42
1:C:314:LYS:HE2	1:C:316:ARG:HB2	2.01	0.42
2:I:351:TRP:N	3:J:103:PHE:CZ	2.84	0.42
4:K:4:LEU:HB3	4:K:96:LEU:HD21	2.02	0.41
2:D:352:TYR:N	2:D:370:SER:OG	2.49	0.41
1:G:314:LYS:HE2	1:G:316:ARG:HB2	2.01	0.41
4:F:4:LEU:HB3	4:F:96:LEU:HD21	2.02	0.41
2:D:367:ASP:OD1	2:D:367:ASP:C	2.63	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	319/339 (94%)	315 (99%)	4 (1%)	0	100	100
1	C	319/339 (94%)	315 (99%)	4 (1%)	0	100	100
1	G	319/339 (94%)	315 (99%)	4 (1%)	0	100	100
2	B	166/226 (74%)	162 (98%)	4 (2%)	0	100	100
2	D	166/226 (74%)	163 (98%)	3 (2%)	0	100	100
2	I	166/226 (74%)	163 (98%)	3 (2%)	0	100	100
3	E	125/233 (54%)	118 (94%)	7 (6%)	0	100	100
3	H	125/233 (54%)	118 (94%)	7 (6%)	0	100	100
3	J	125/233 (54%)	118 (94%)	7 (6%)	0	100	100
4	F	111/220 (50%)	110 (99%)	1 (1%)	0	100	100
4	K	111/220 (50%)	110 (99%)	1 (1%)	0	100	100
4	L	111/220 (50%)	110 (99%)	1 (1%)	0	100	100
All	All	2163/3054 (71%)	2117 (98%)	46 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	282/297 (95%)	281 (100%)	1 (0%)	84	86
1	C	282/297 (95%)	282 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	282/297 (95%)	281 (100%)	1 (0%)	84	86
2	B	147/195 (75%)	146 (99%)	1 (1%)	76	82
2	D	147/195 (75%)	147 (100%)	0	100	100
2	I	147/195 (75%)	145 (99%)	2 (1%)	59	76
3	E	104/196 (53%)	104 (100%)	0	100	100
3	H	104/196 (53%)	104 (100%)	0	100	100
3	J	104/196 (53%)	104 (100%)	0	100	100
4	F	100/196 (51%)	100 (100%)	0	100	100
4	K	100/196 (51%)	100 (100%)	0	100	100
4	L	100/196 (51%)	100 (100%)	0	100	100
All	All	1899/2652 (72%)	1894 (100%)	5 (0%)	84	87

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	290	ASN
2	B	351	TRP
1	G	290	ASN
2	I	348	VAL
2	I	351	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
3	H	61	GLN
3	E	61	GLN
1	G	12	HIS
1	G	191	GLN
1	G	250	ASN
3	J	61	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

15 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	$\# Z > 2$
5	NAG	G	404	1	14,14,15	2.23	7 (50%)	17,19,21	1.14	2 (11%)
5	NAG	C	404	-	14,14,15	2.24	7 (50%)	17,19,21	1.15	2 (11%)
5	NAG	A	403	1	14,14,15	2.23	6 (42%)	17,19,21	1.33	3 (17%)
5	NAG	C	402	1	14,14,15	2.10	6 (42%)	17,19,21	1.15	3 (17%)
5	NAG	A	402	1	14,14,15	2.11	5 (35%)	17,19,21	1.15	3 (17%)
5	NAG	C	403	1	14,14,15	2.22	5 (35%)	17,19,21	1.34	3 (17%)
5	NAG	G	401	1	14,14,15	2.26	5 (35%)	17,19,21	0.95	0
5	NAG	G	405	1	14,14,15	2.24	5 (35%)	17,19,21	1.00	1 (5%)
5	NAG	C	405	1	14,14,15	2.24	5 (35%)	17,19,21	1.00	1 (5%)
5	NAG	A	405	1	14,14,15	2.22	5 (35%)	17,19,21	1.00	1 (5%)
5	NAG	G	402	1	14,14,15	2.12	6 (42%)	17,19,21	1.14	2 (11%)
5	NAG	G	403	1	14,14,15	2.23	5 (35%)	17,19,21	1.33	3 (17%)
5	NAG	C	401	1	14,14,15	2.24	5 (35%)	17,19,21	0.94	0
5	NAG	A	401	1	14,14,15	2.24	5 (35%)	17,19,21	0.95	0
5	NAG	A	404	1	14,14,15	2.24	7 (50%)	17,19,21	1.14	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	G	404	1	-	0/6/23/26	0/1/1/1
5	NAG	C	404	-	-	0/6/23/26	0/1/1/1
5	NAG	A	403	1	-	0/6/23/26	0/1/1/1
5	NAG	C	402	1	-	2/6/23/26	0/1/1/1
5	NAG	A	402	1	-	2/6/23/26	0/1/1/1
5	NAG	C	403	1	-	0/6/23/26	0/1/1/1
5	NAG	G	401	1	-	0/6/23/26	0/1/1/1
5	NAG	G	405	1	-	0/6/23/26	0/1/1/1
5	NAG	C	405	1	-	0/6/23/26	0/1/1/1
5	NAG	A	405	1	-	0/6/23/26	0/1/1/1
5	NAG	G	402	1	-	2/6/23/26	0/1/1/1
5	NAG	G	403	1	-	0/6/23/26	0/1/1/1
5	NAG	C	401	1	-	0/6/23/26	0/1/1/1
5	NAG	A	401	1	-	0/6/23/26	0/1/1/1
5	NAG	A	404	1	-	0/6/23/26	0/1/1/1

All (84) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	403	NAG	C1-C2	6.00	1.60	1.52
5	G	405	NAG	C1-C2	6.00	1.60	1.52
5	A	403	NAG	C1-C2	5.99	1.60	1.52
5	C	405	NAG	C1-C2	5.97	1.60	1.52
5	C	403	NAG	C1-C2	5.93	1.60	1.52
5	A	405	NAG	C1-C2	5.92	1.60	1.52
5	G	401	NAG	C1-C2	5.86	1.60	1.52
5	A	401	NAG	C1-C2	5.85	1.60	1.52
5	C	401	NAG	C1-C2	5.84	1.60	1.52
5	A	402	NAG	C1-C2	5.68	1.60	1.52
5	G	402	NAG	C1-C2	5.67	1.60	1.52
5	C	402	NAG	C1-C2	5.57	1.59	1.52
5	A	404	NAG	C1-C2	5.47	1.59	1.52
5	G	404	NAG	C1-C2	5.45	1.59	1.52
5	C	404	NAG	C1-C2	5.42	1.59	1.52
5	C	404	NAG	O5-C5	3.42	1.50	1.43
5	A	404	NAG	O5-C5	3.41	1.50	1.43
5	G	404	NAG	O5-C5	3.40	1.50	1.43
5	G	401	NAG	O5-C5	3.38	1.50	1.43
5	C	401	NAG	O5-C5	3.33	1.49	1.43
5	A	401	NAG	O5-C5	3.30	1.49	1.43
5	C	405	NAG	O5-C5	3.07	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	405	NAG	O5-C5	3.04	1.49	1.43
5	G	405	NAG	O5-C5	3.02	1.49	1.43
5	A	402	NAG	O5-C5	2.81	1.48	1.43
5	C	402	NAG	O5-C5	2.79	1.48	1.43
5	G	402	NAG	O5-C5	2.77	1.48	1.43
5	G	404	NAG	O5-C1	2.76	1.48	1.43
5	G	403	NAG	O5-C5	2.76	1.48	1.43
5	A	404	NAG	O5-C1	2.75	1.48	1.43
5	C	404	NAG	O5-C1	2.74	1.48	1.43
5	A	403	NAG	O5-C5	2.72	1.48	1.43
5	C	403	NAG	O5-C5	2.71	1.48	1.43
5	G	401	NAG	O5-C1	2.70	1.48	1.43
5	C	403	NAG	C3-C2	2.70	1.58	1.52
5	C	401	NAG	O5-C1	2.69	1.48	1.43
5	A	401	NAG	O5-C1	2.69	1.48	1.43
5	G	403	NAG	C3-C2	2.64	1.58	1.52
5	A	403	NAG	C3-C2	2.64	1.58	1.52
5	C	403	NAG	O5-C1	2.54	1.48	1.43
5	G	405	NAG	O5-C1	2.52	1.47	1.43
5	A	405	NAG	O5-C1	2.51	1.47	1.43
5	A	403	NAG	O5-C1	2.50	1.47	1.43
5	C	405	NAG	O5-C1	2.49	1.47	1.43
5	G	403	NAG	O5-C1	2.46	1.47	1.43
5	A	401	NAG	C3-C2	2.42	1.57	1.52
5	G	401	NAG	C3-C2	2.41	1.57	1.52
5	C	401	NAG	C3-C2	2.38	1.57	1.52
5	C	405	NAG	C3-C2	2.32	1.57	1.52
5	C	404	NAG	C3-C2	2.31	1.57	1.52
5	A	404	NAG	C3-C2	2.31	1.57	1.52
5	G	405	NAG	C3-C2	2.31	1.57	1.52
5	A	405	NAG	C3-C2	2.29	1.57	1.52
5	G	404	NAG	C3-C2	2.28	1.57	1.52
5	C	404	NAG	C2-N2	2.28	1.50	1.46
5	G	402	NAG	O5-C1	2.28	1.47	1.43
5	G	404	NAG	C2-N2	2.27	1.50	1.46
5	A	402	NAG	O5-C1	2.25	1.47	1.43
5	C	402	NAG	O5-C1	2.24	1.47	1.43
5	C	404	NAG	C4-C5	2.22	1.57	1.53
5	A	404	NAG	C2-N2	2.21	1.49	1.46
5	C	402	NAG	C3-C2	2.19	1.57	1.52
5	G	404	NAG	C4-C5	2.18	1.57	1.53
5	G	405	NAG	C4-C5	2.17	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	404	NAG	C4-C5	2.16	1.57	1.53
5	C	405	NAG	C4-C5	2.16	1.57	1.53
5	G	402	NAG	C3-C2	2.15	1.57	1.52
5	A	402	NAG	C3-C2	2.14	1.57	1.52
5	A	405	NAG	C4-C5	2.14	1.57	1.53
5	G	401	NAG	C4-C5	2.13	1.57	1.53
5	A	401	NAG	C4-C5	2.10	1.57	1.53
5	C	401	NAG	C4-C5	2.10	1.57	1.53
5	C	402	NAG	C4-C5	2.10	1.57	1.53
5	G	402	NAG	C4-C5	2.08	1.57	1.53
5	A	404	NAG	C4-C3	2.07	1.57	1.52
5	G	404	NAG	C4-C3	2.07	1.57	1.52
5	C	403	NAG	C2-N2	2.07	1.49	1.46
5	G	403	NAG	C2-N2	2.06	1.49	1.46
5	A	402	NAG	C4-C5	2.06	1.57	1.53
5	C	404	NAG	C4-C3	2.05	1.57	1.52
5	A	403	NAG	C2-N2	2.05	1.49	1.46
5	C	402	NAG	C2-N2	2.04	1.49	1.46
5	G	402	NAG	C2-N2	2.02	1.49	1.46
5	A	403	NAG	C4-C5	2.01	1.57	1.53

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	403	NAG	C8-C7-N2	3.18	121.39	116.12
5	A	403	NAG	C8-C7-N2	3.17	121.37	116.12
5	G	403	NAG	C8-C7-N2	3.15	121.34	116.12
5	C	403	NAG	O7-C7-C8	-2.91	116.88	122.05
5	A	403	NAG	O7-C7-C8	-2.89	116.90	122.05
5	G	403	NAG	O7-C7-C8	-2.88	116.93	122.05
5	C	404	NAG	C8-C7-N2	2.77	120.71	116.12
5	A	404	NAG	C8-C7-N2	2.77	120.71	116.12
5	G	404	NAG	C8-C7-N2	2.77	120.71	116.12
5	G	403	NAG	C1-O5-C5	2.45	115.47	112.19
5	C	403	NAG	C1-O5-C5	2.44	115.45	112.19
5	A	403	NAG	C1-O5-C5	2.40	115.41	112.19
5	A	402	NAG	C8-C7-N2	2.32	119.97	116.12
5	C	402	NAG	C8-C7-N2	2.32	119.96	116.12
5	G	402	NAG	C8-C7-N2	2.29	119.91	116.12
5	C	402	NAG	C1-O5-C5	2.26	115.22	112.19
5	A	402	NAG	C1-O5-C5	2.26	115.22	112.19
5	G	402	NAG	C1-O5-C5	2.26	115.21	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	402	NAG	O7-C7-C8	-2.02	118.46	122.05
5	C	405	NAG	C8-C7-N2	2.01	119.46	116.12
5	G	405	NAG	C8-C7-N2	2.01	119.45	116.12
5	G	404	NAG	O7-C7-C8	-2.01	118.48	122.05
5	A	402	NAG	O7-C7-C8	-2.01	118.48	122.05
5	A	405	NAG	C8-C7-N2	2.01	119.44	116.12
5	C	404	NAG	O7-C7-C8	-2.00	118.48	122.05

There are no chirality outliers.

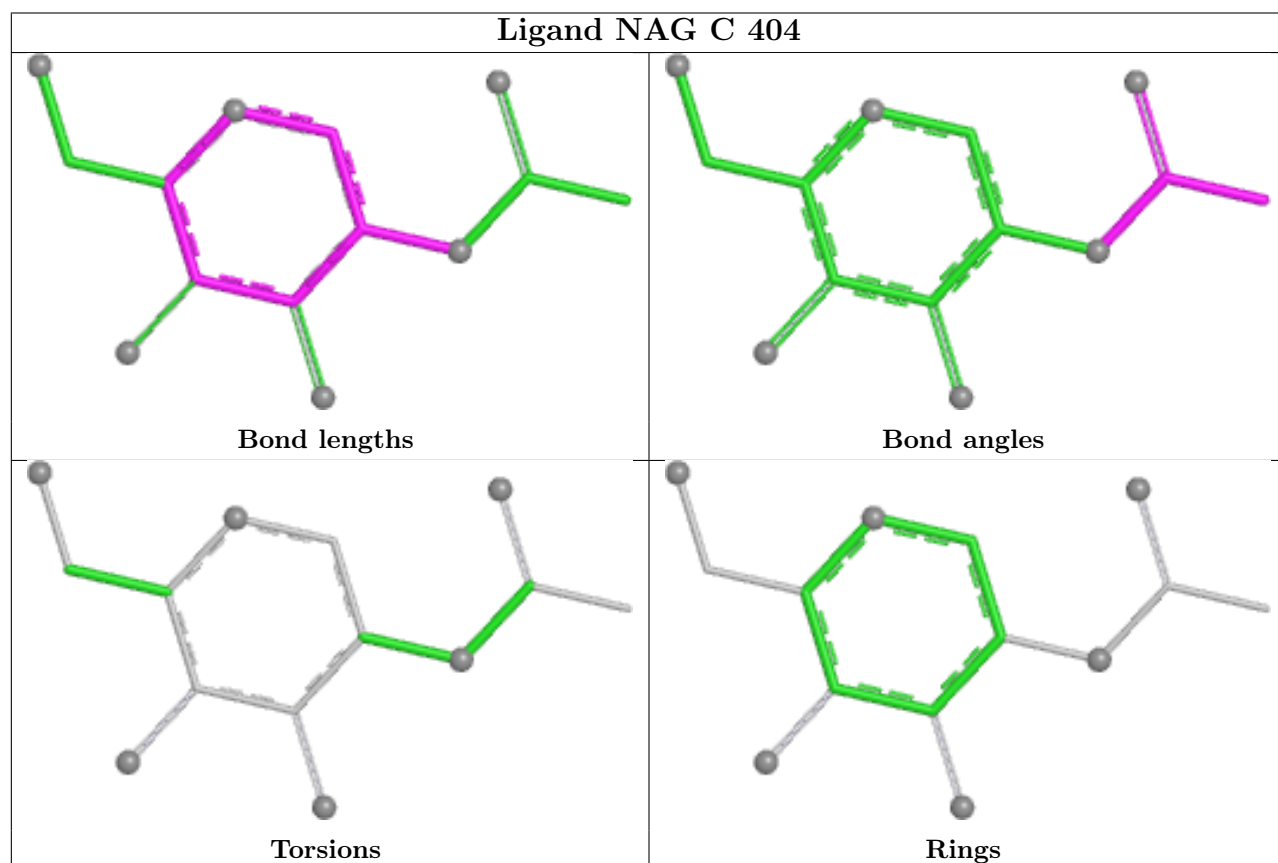
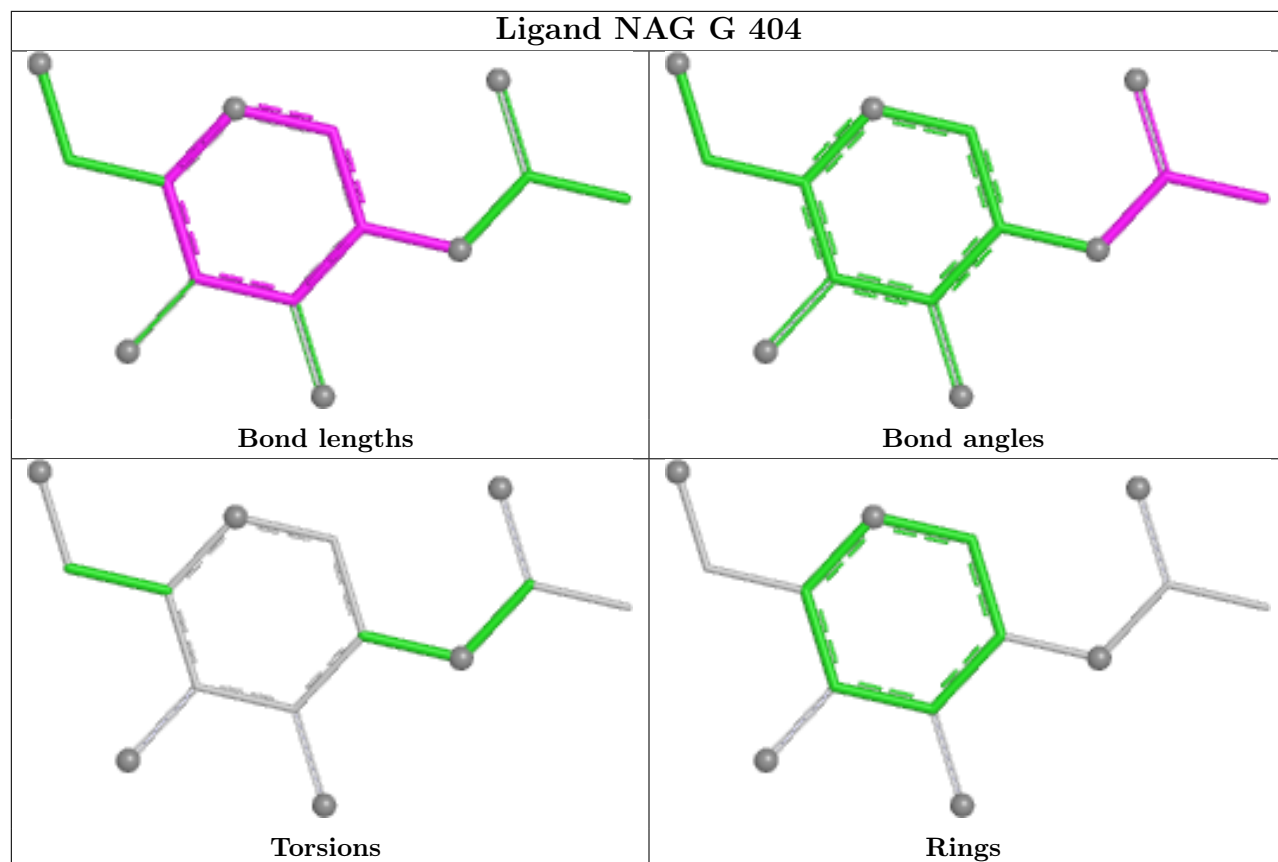
All (6) torsion outliers are listed below:

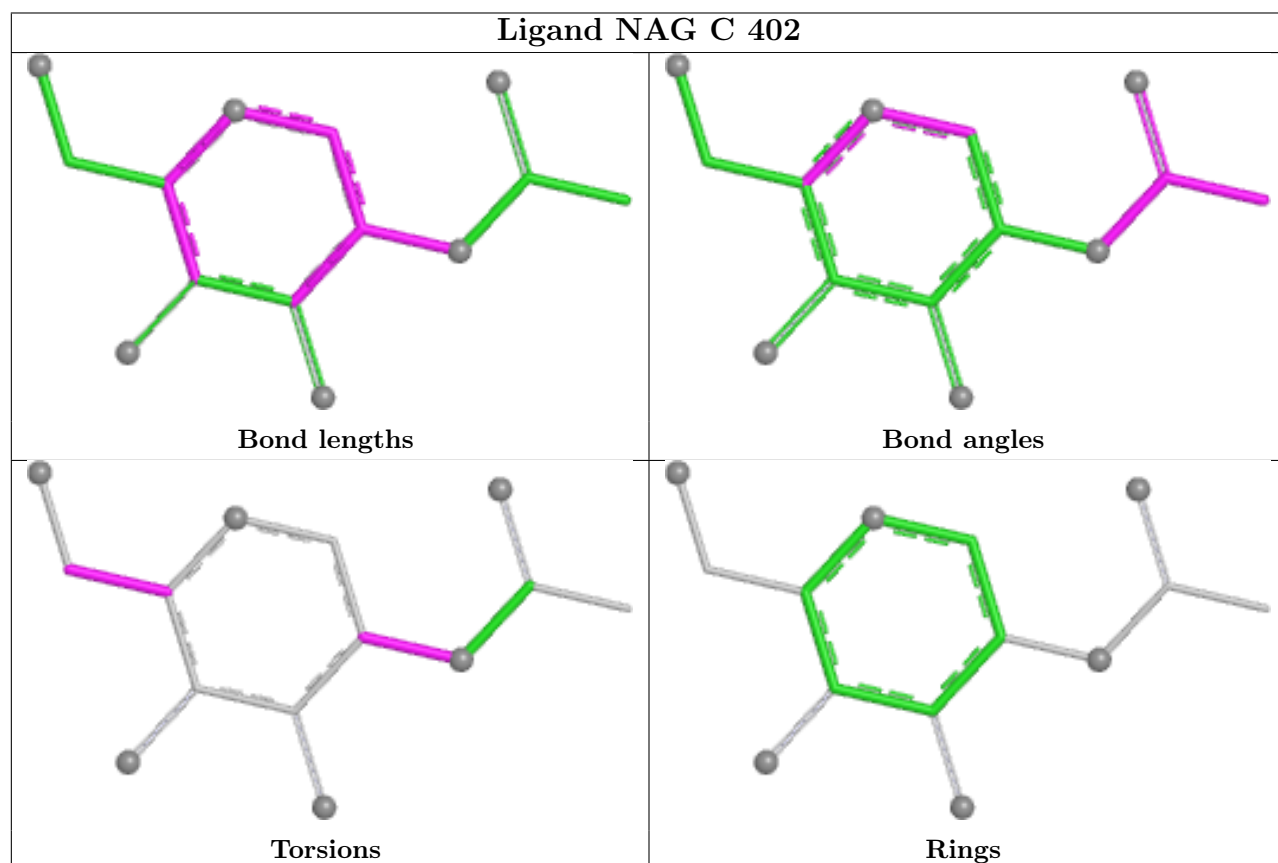
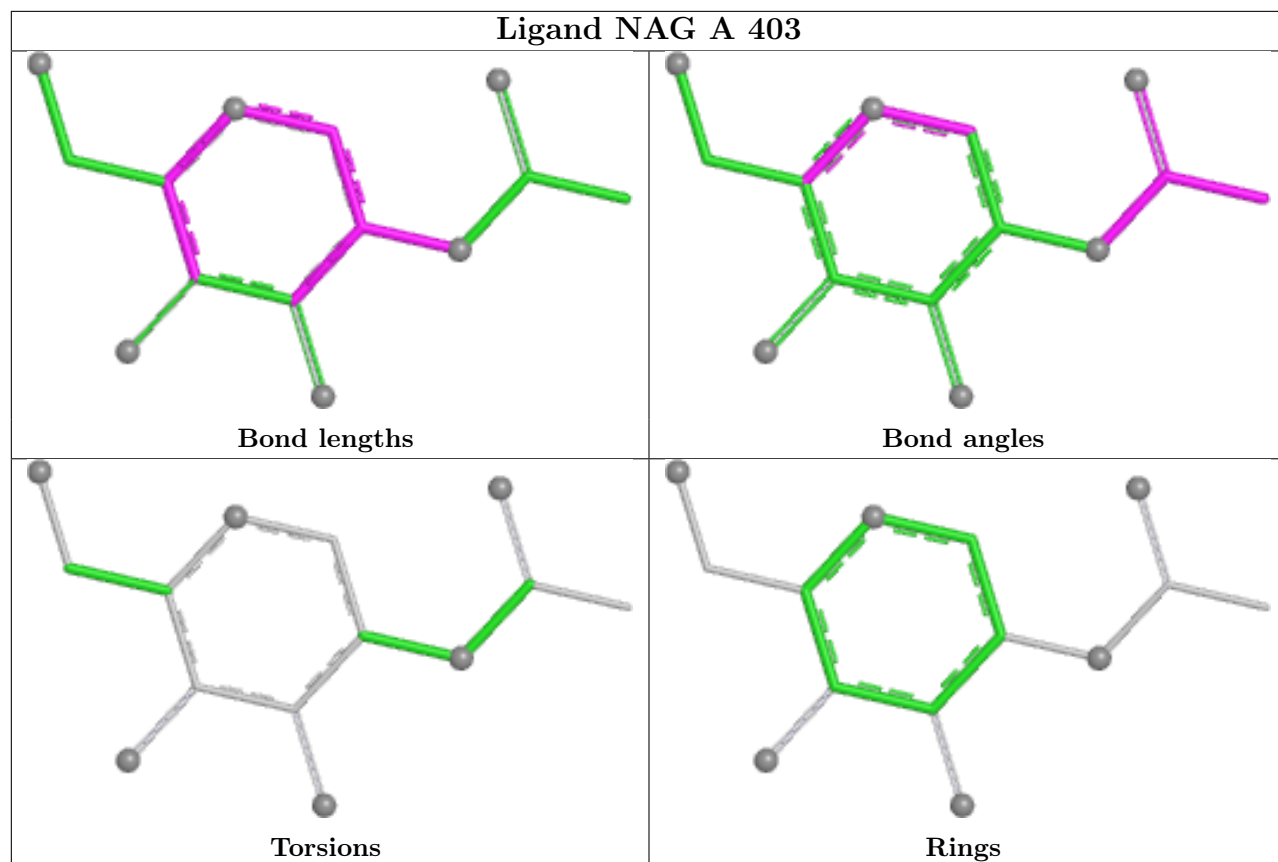
Mol	Chain	Res	Type	Atoms
5	C	402	NAG	O5-C5-C6-O6
5	A	402	NAG	O5-C5-C6-O6
5	G	402	NAG	O5-C5-C6-O6
5	C	402	NAG	C1-C2-N2-C7
5	A	402	NAG	C1-C2-N2-C7
5	G	402	NAG	C1-C2-N2-C7

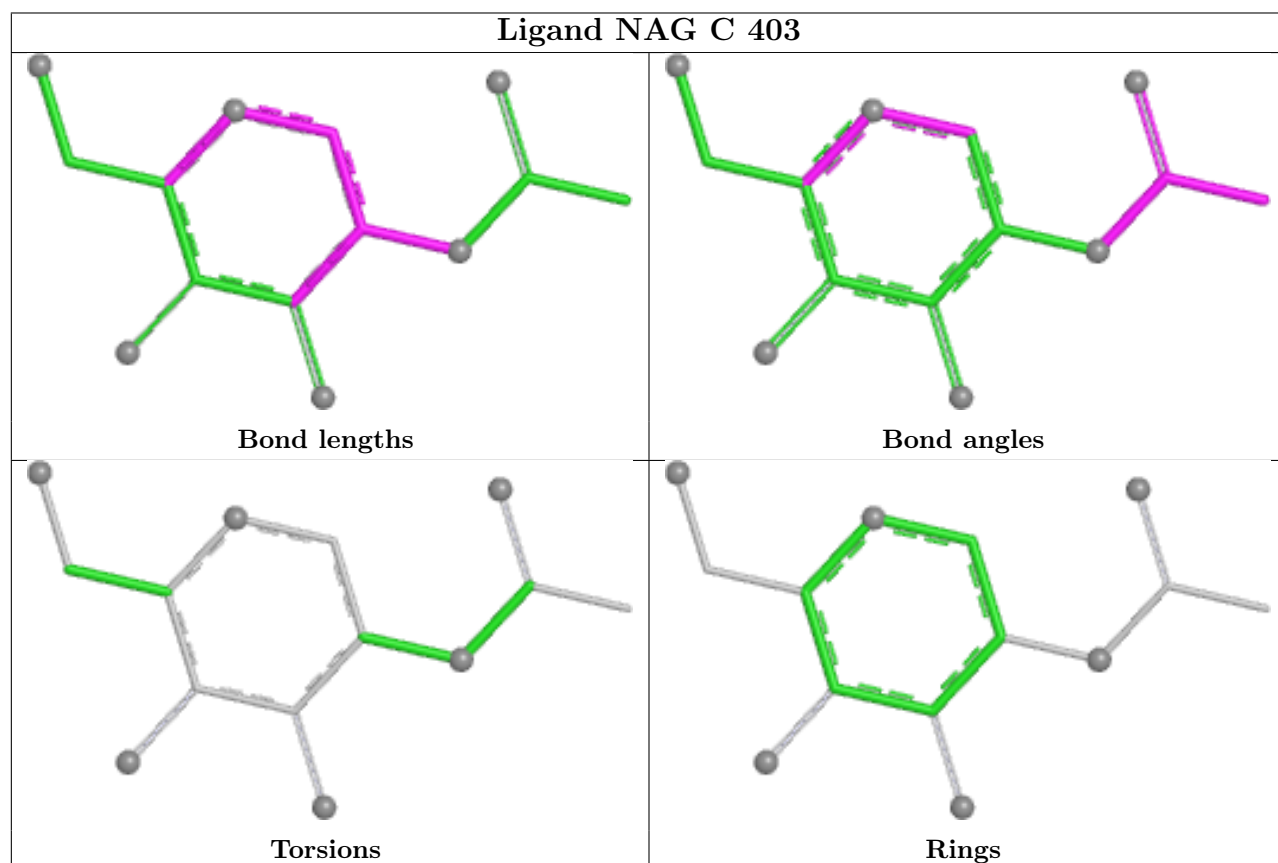
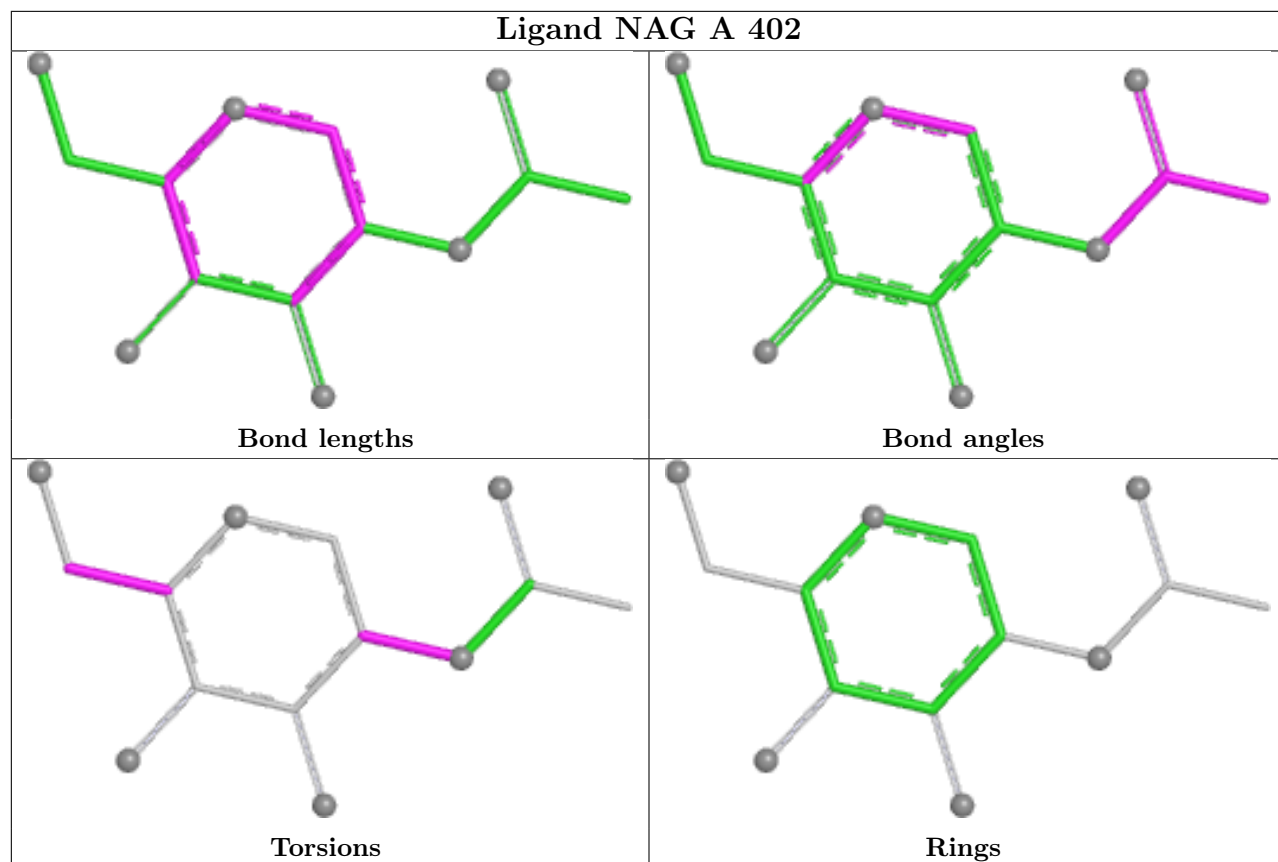
There are no ring outliers.

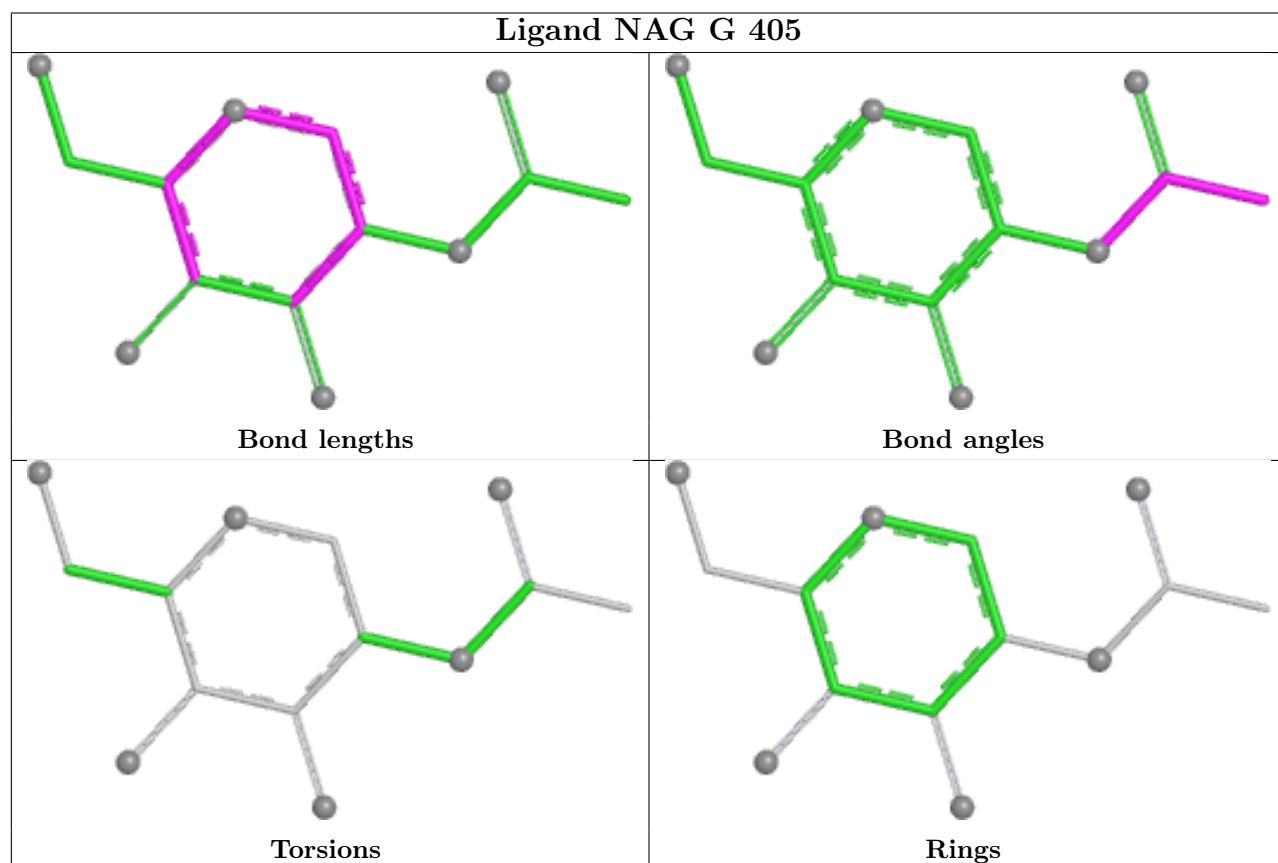
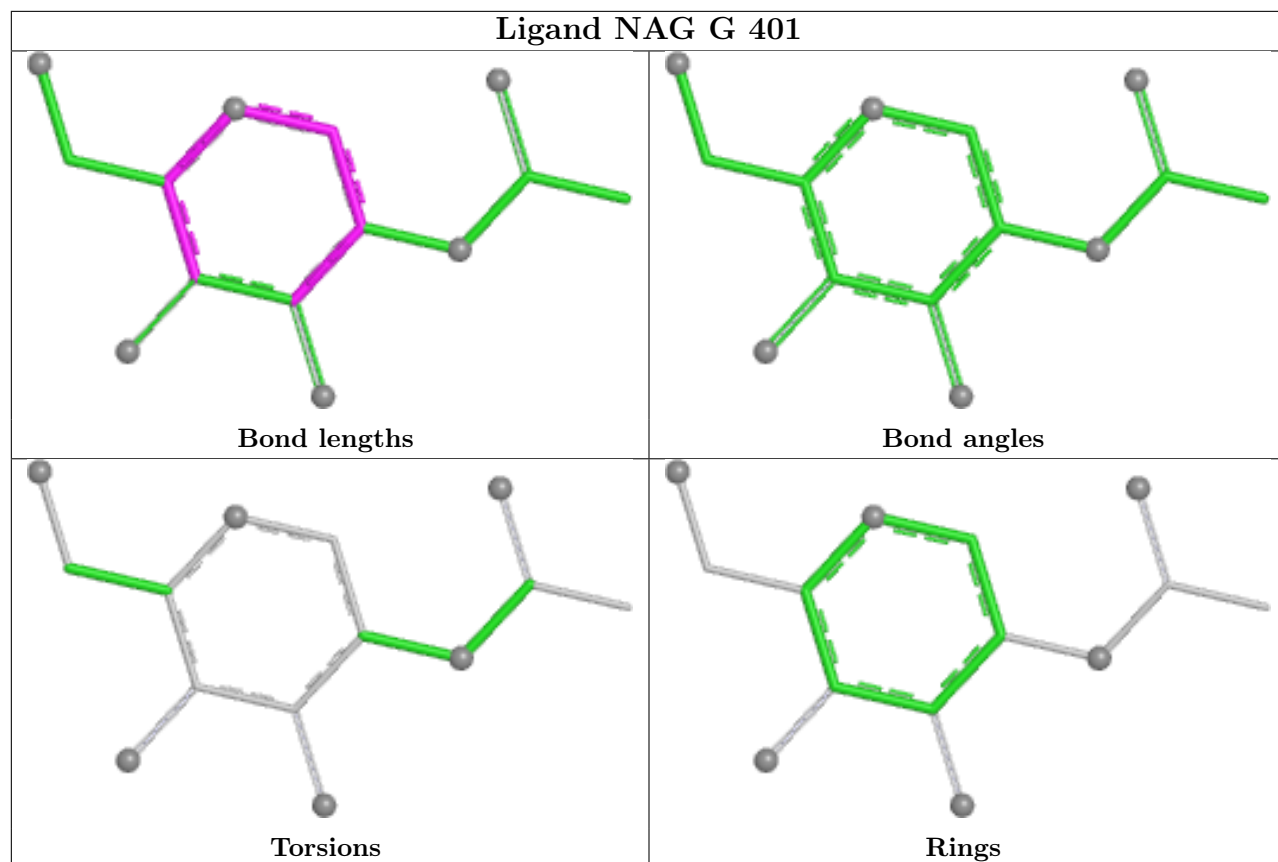
No monomer is involved in short contacts.

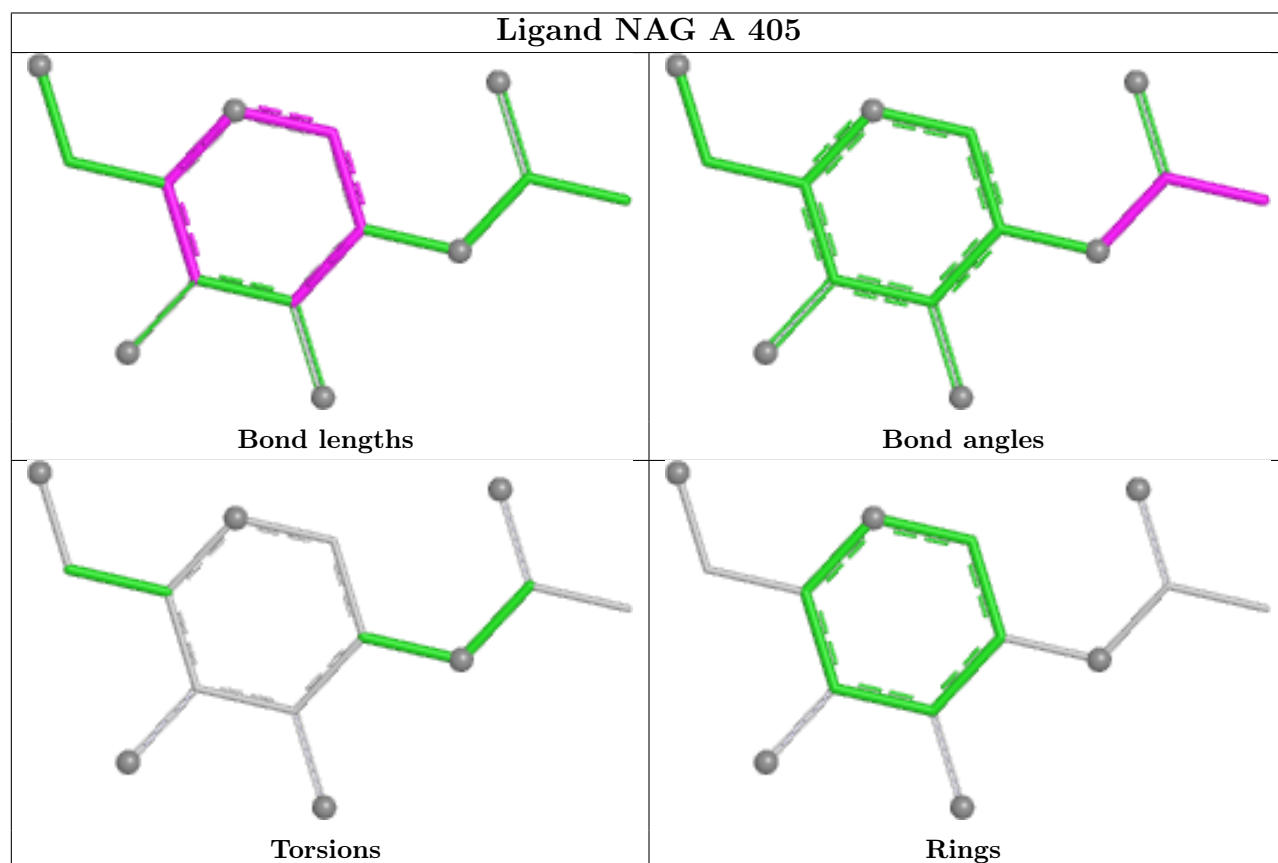
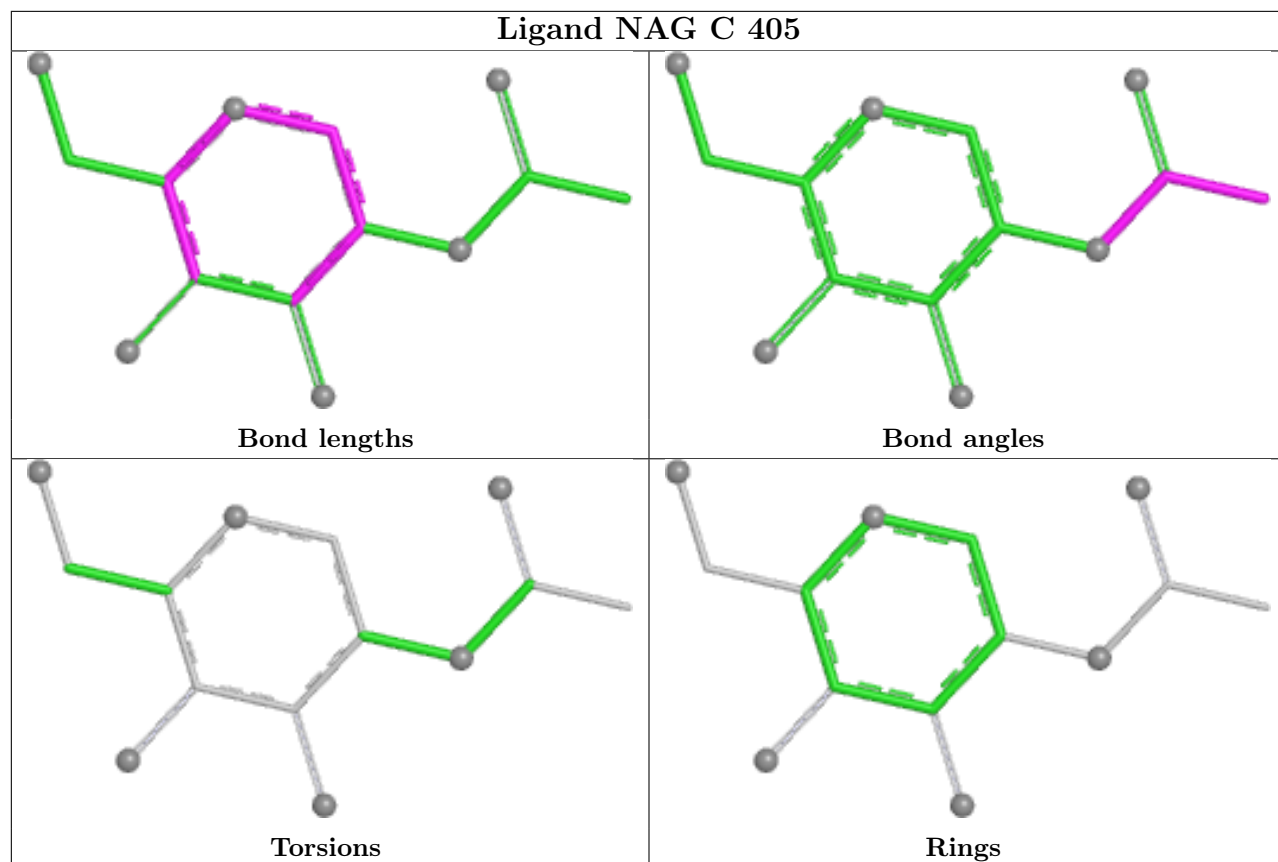
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

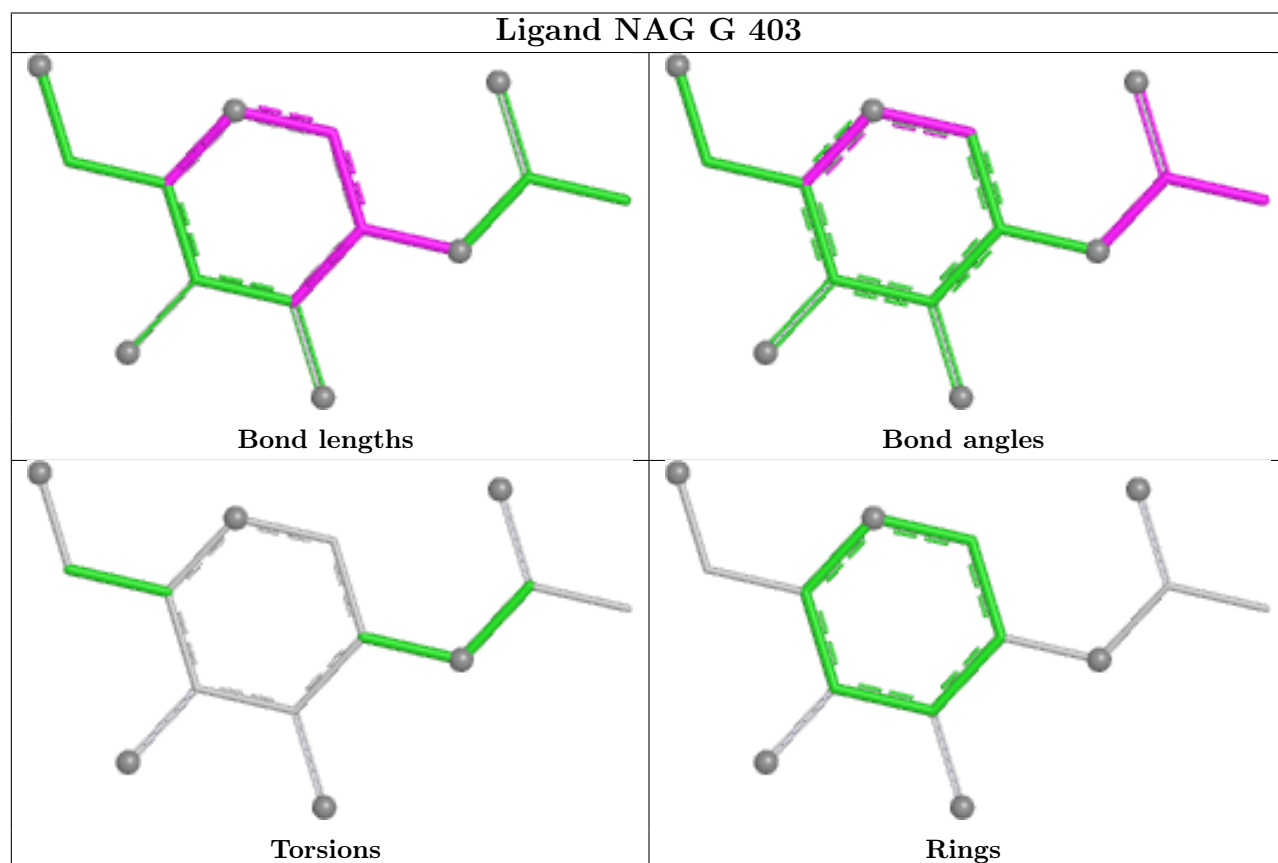
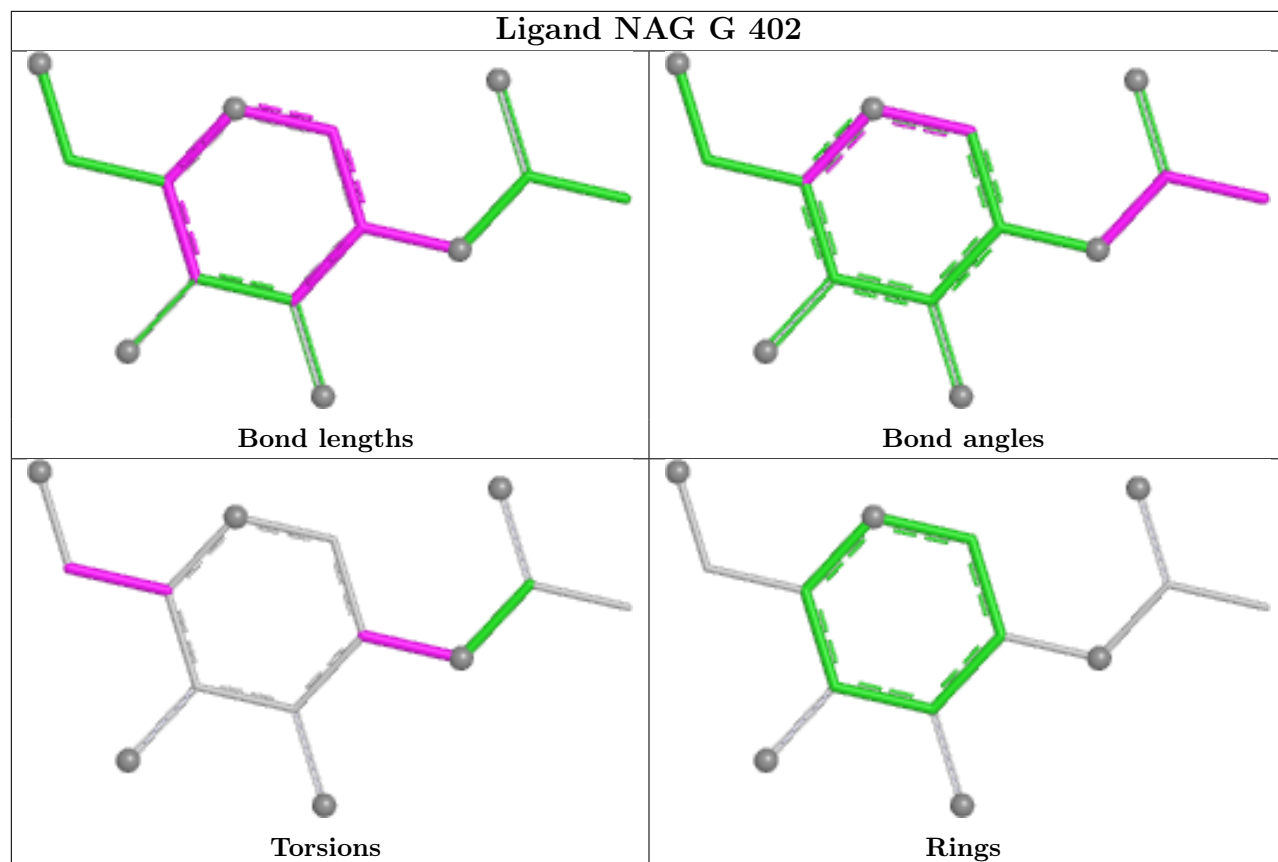


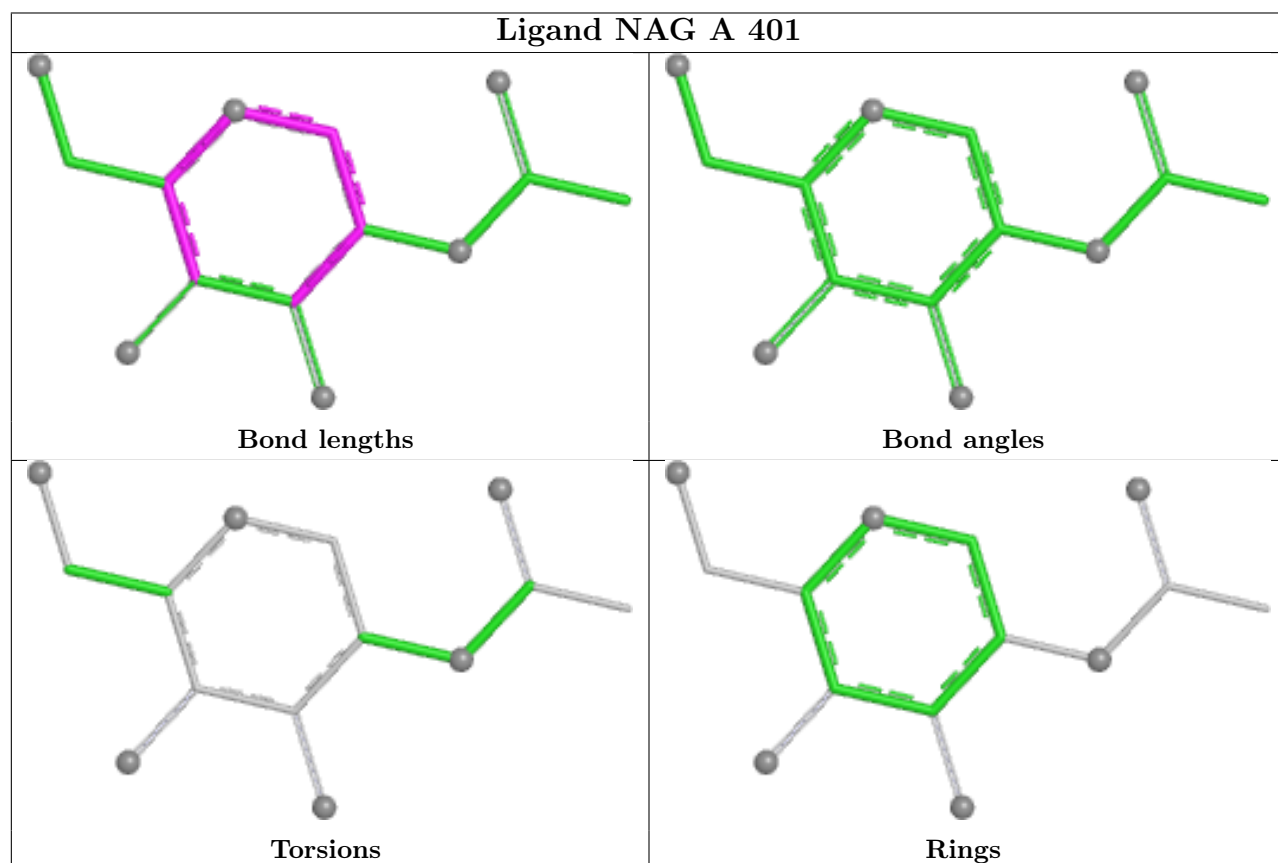
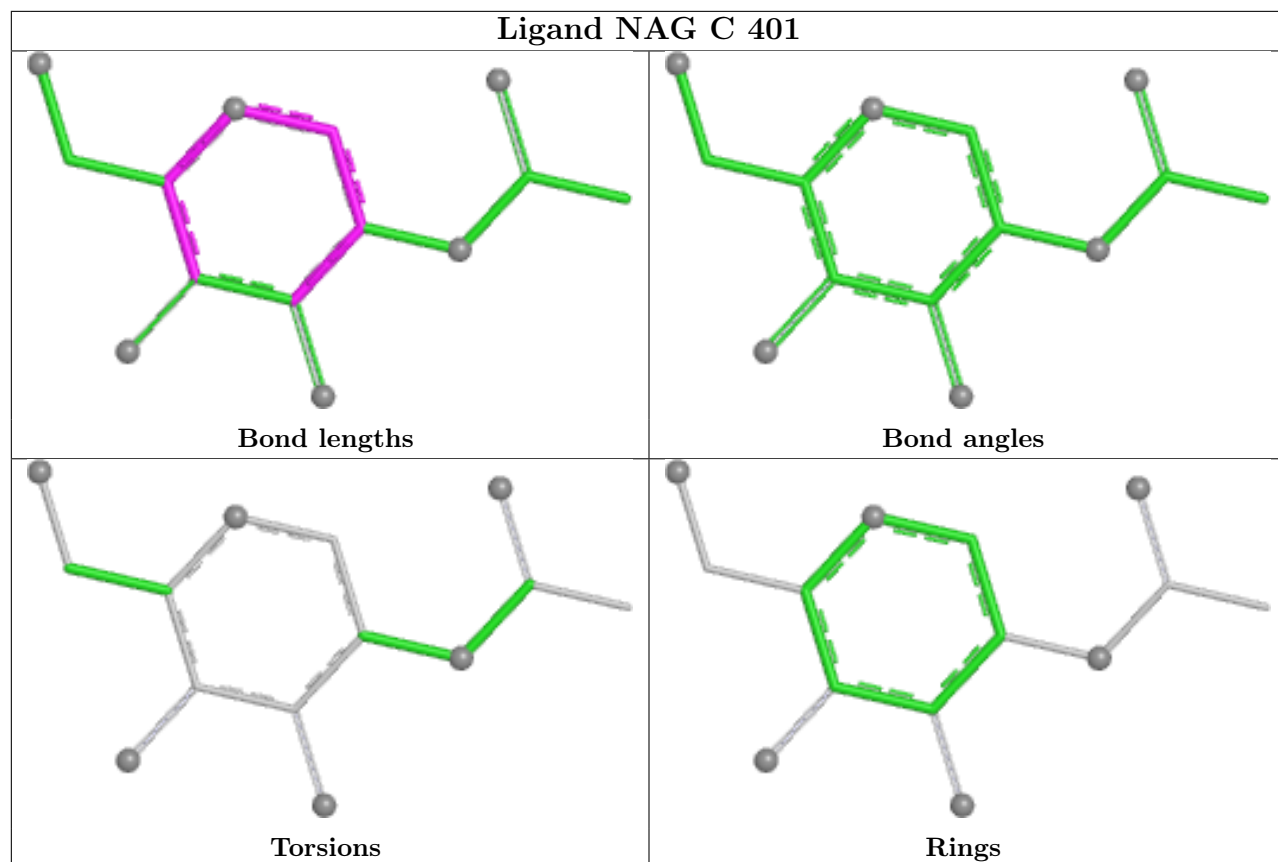


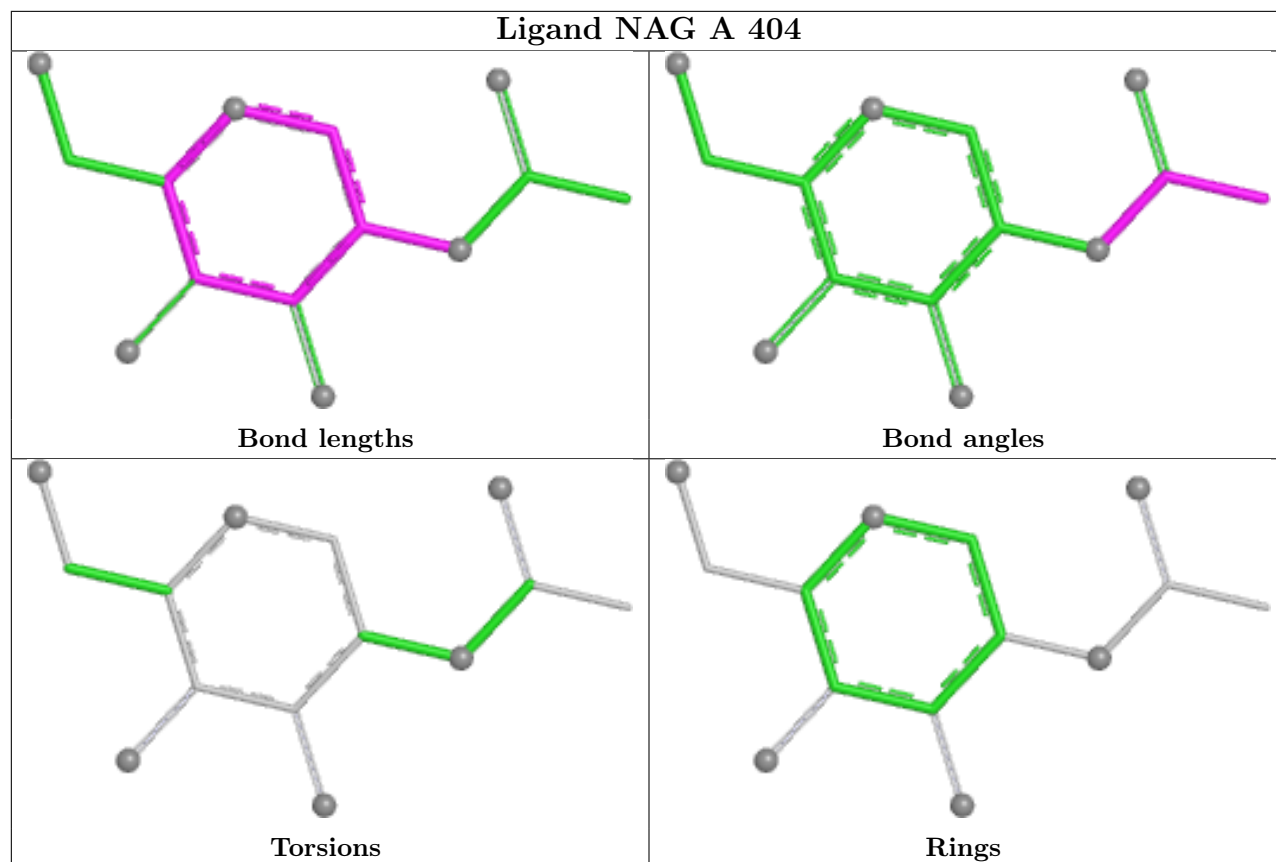












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

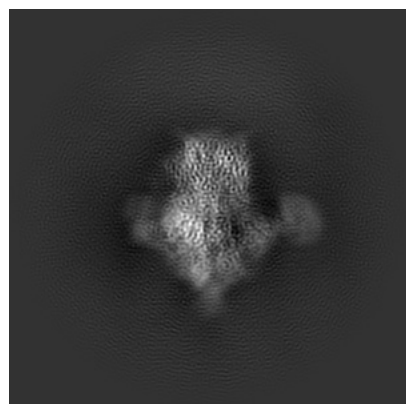
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44112. These allow visual inspection of the internal detail of the map and identification of artifacts.

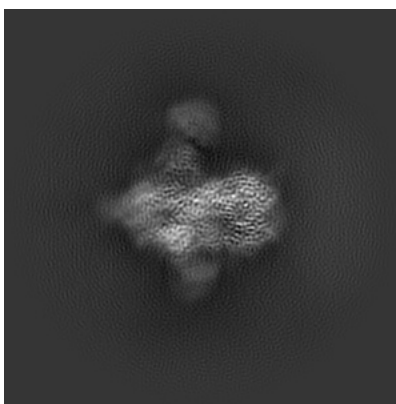
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

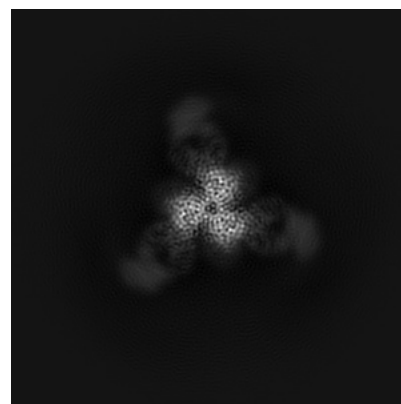
6.1.1 Primary map



X

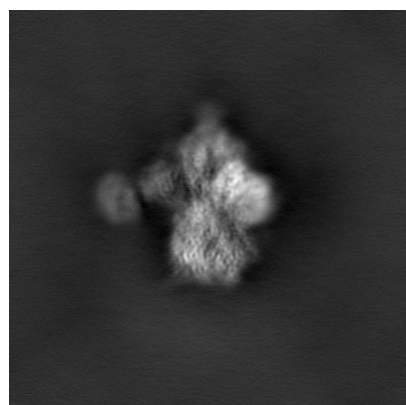


Y

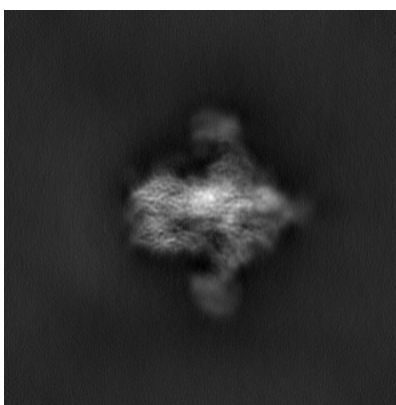


Z

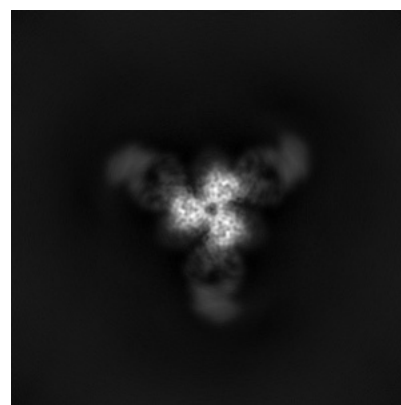
6.1.2 Raw map



X



Y

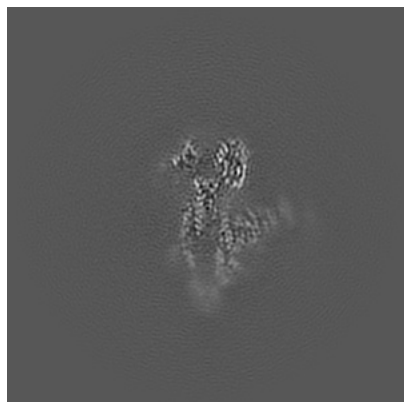


Z

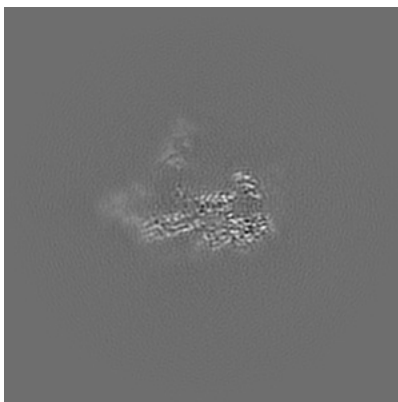
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

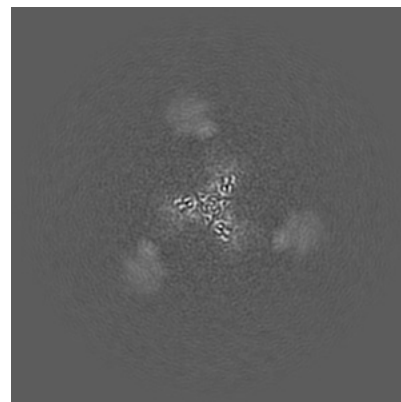
6.2.1 Primary map



X Index: 160

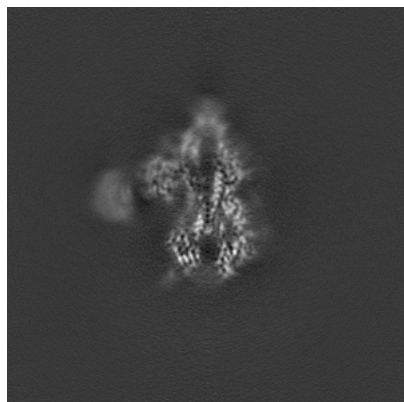


Y Index: 160

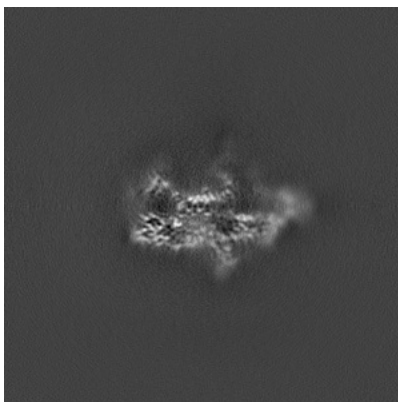


Z Index: 160

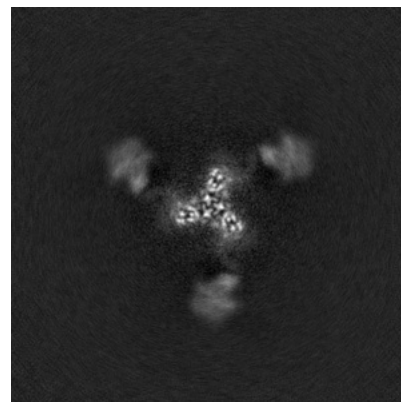
6.2.2 Raw map



X Index: 160



Y Index: 160

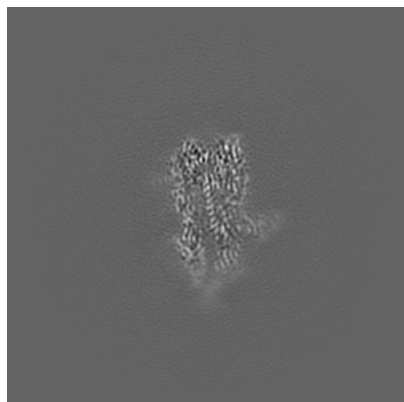


Z Index: 160

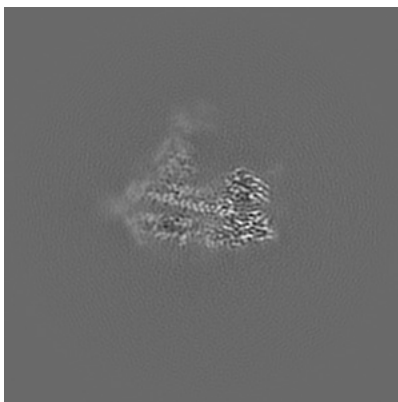
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

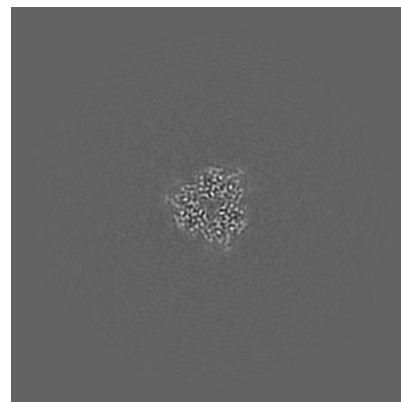
6.3.1 Primary map



X Index: 168

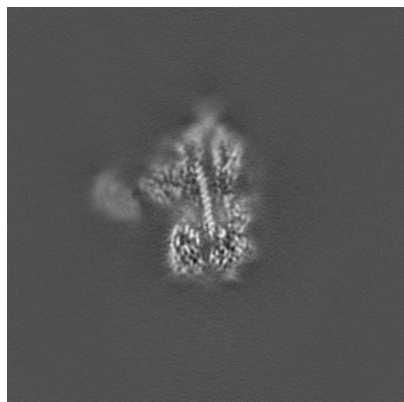


Y Index: 154

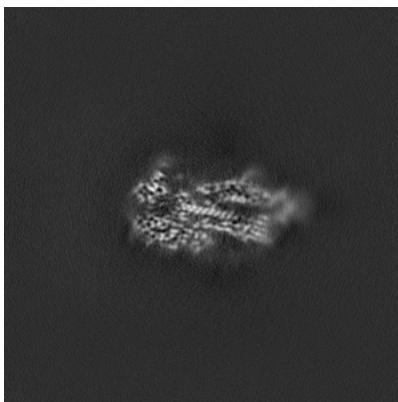


Z Index: 197

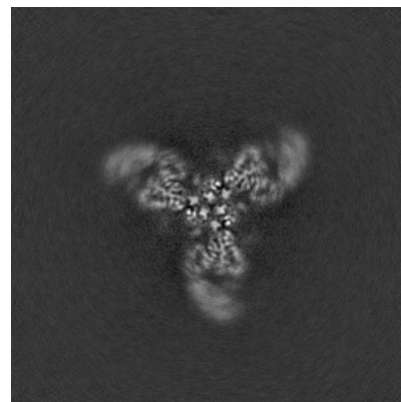
6.3.2 Raw map



X Index: 167



Y Index: 154

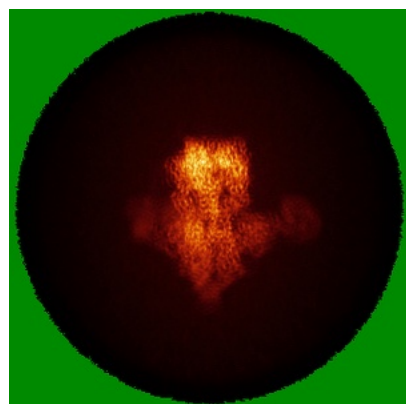


Z Index: 175

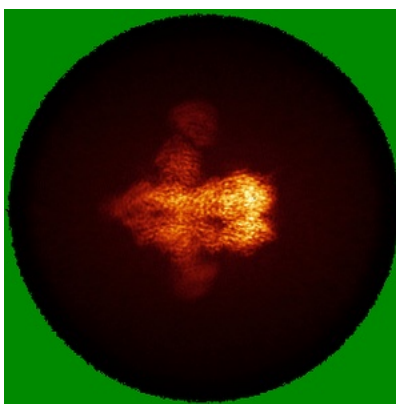
The images above show the largest variance slices of the map in three orthogonal directions.

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

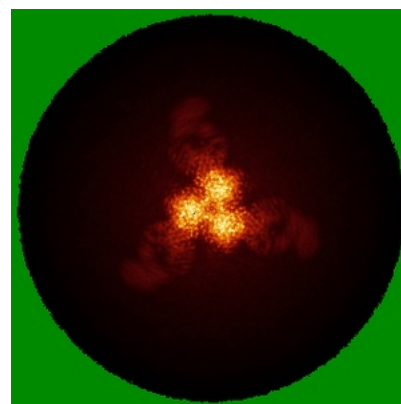
6.4.1 Primary map



X

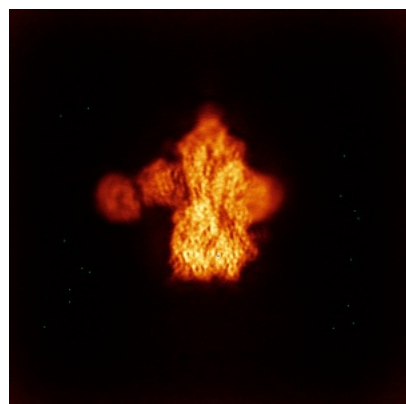


Y

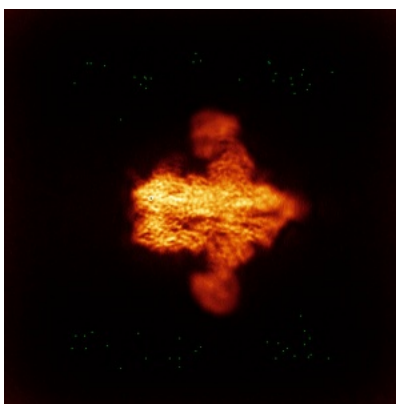


Z

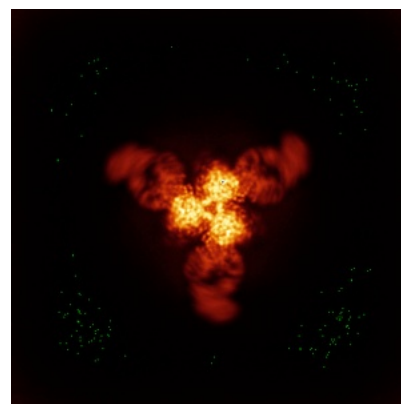
6.4.2 Raw map



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.

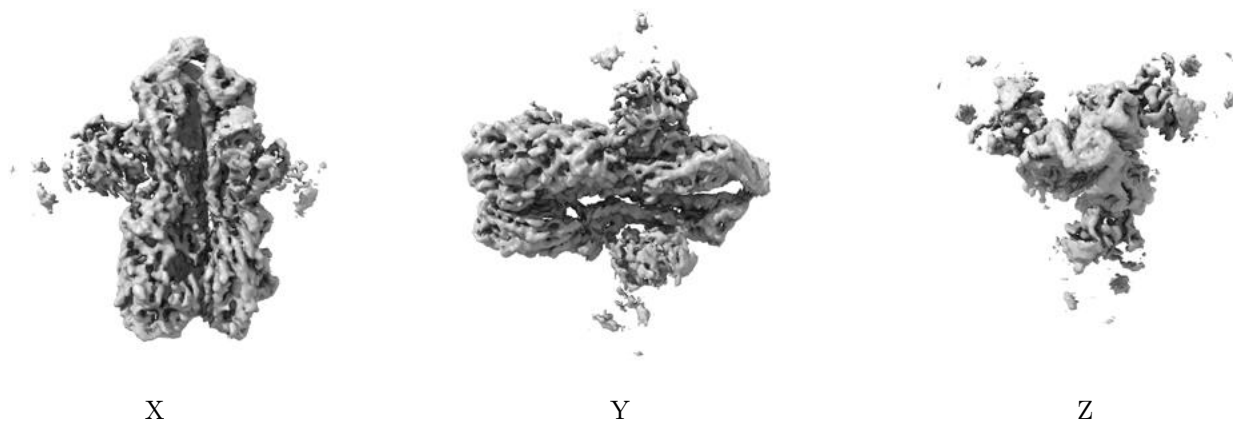
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.25. 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.

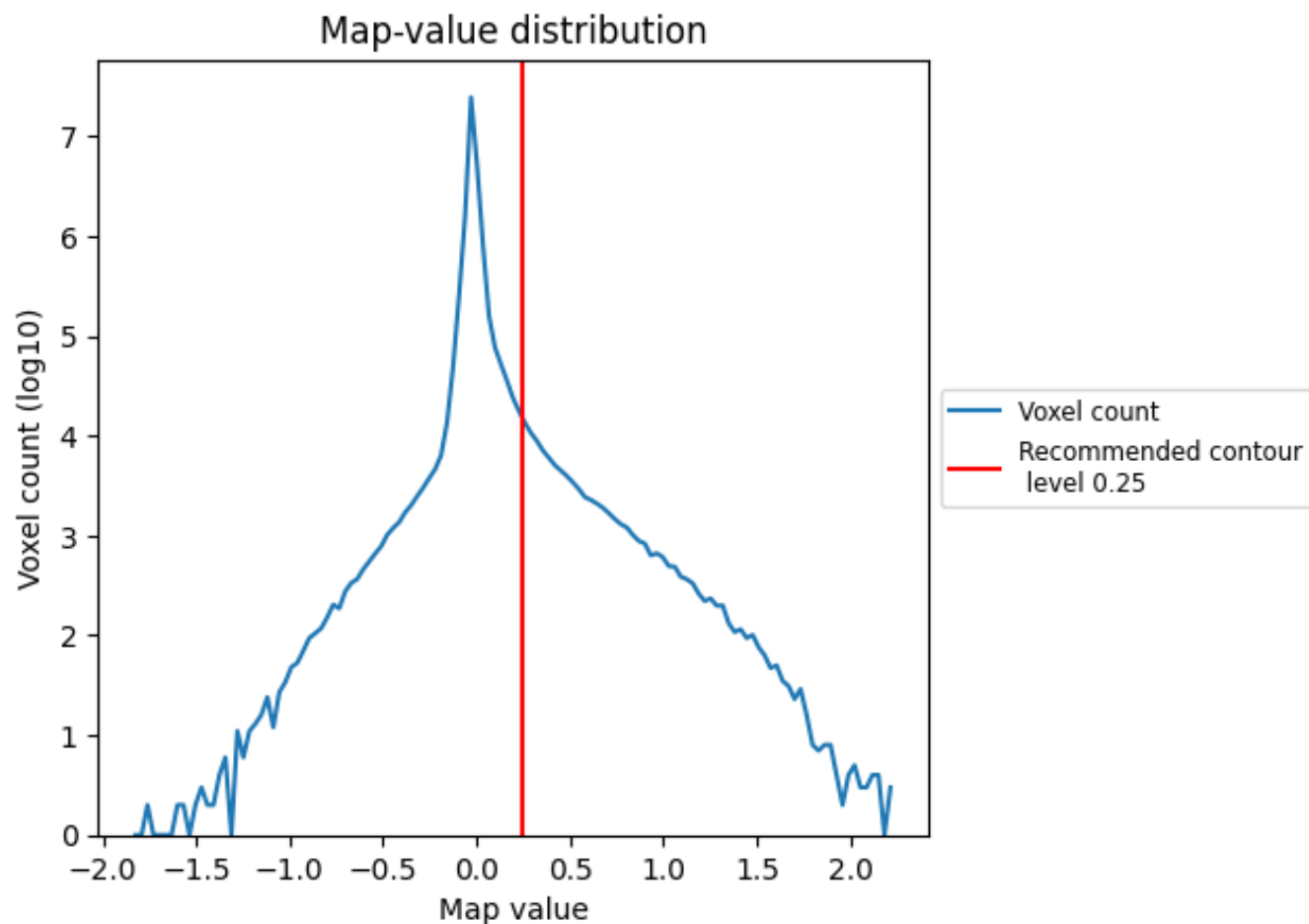
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

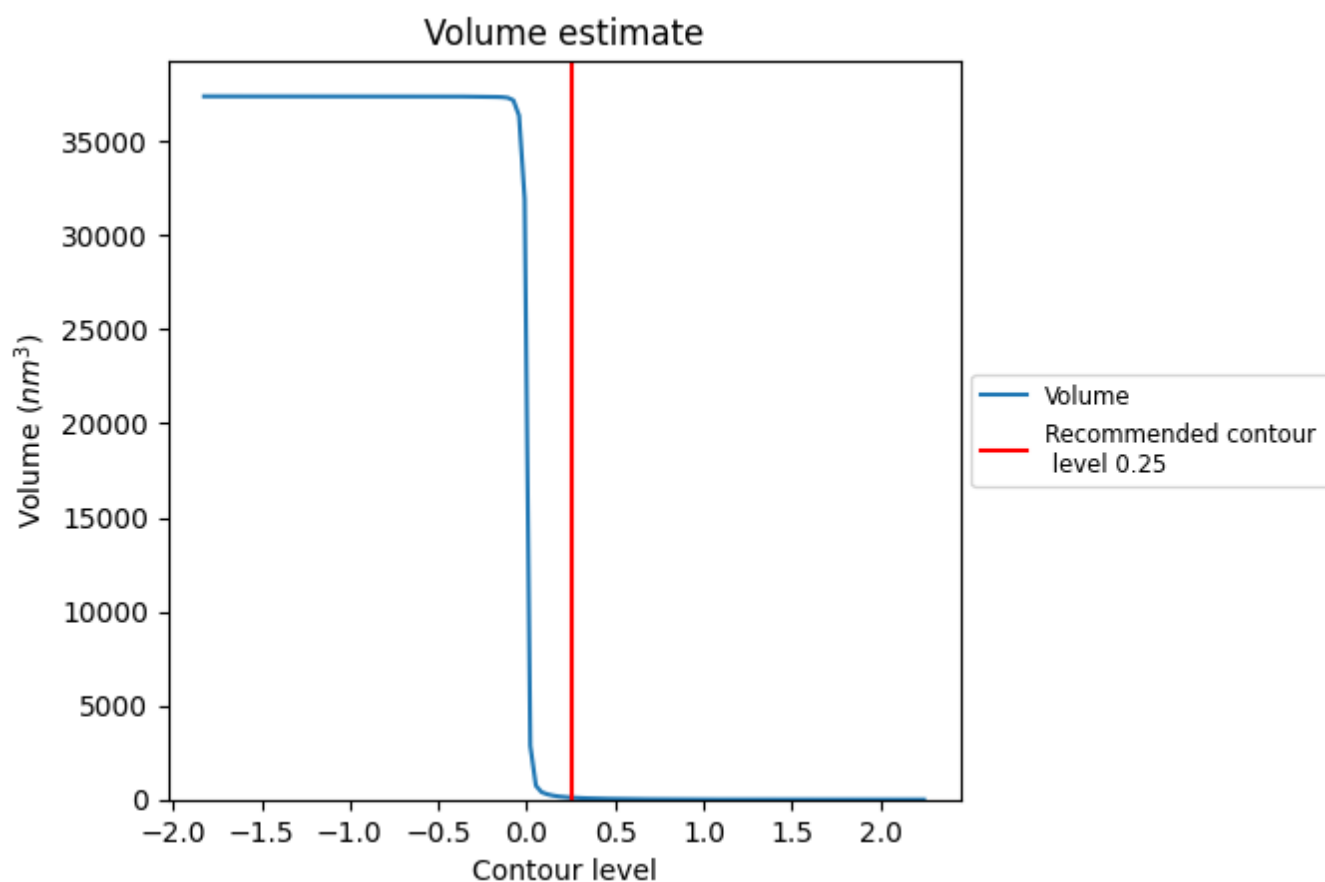
This section contains the results of statistical analysis of the map.

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.

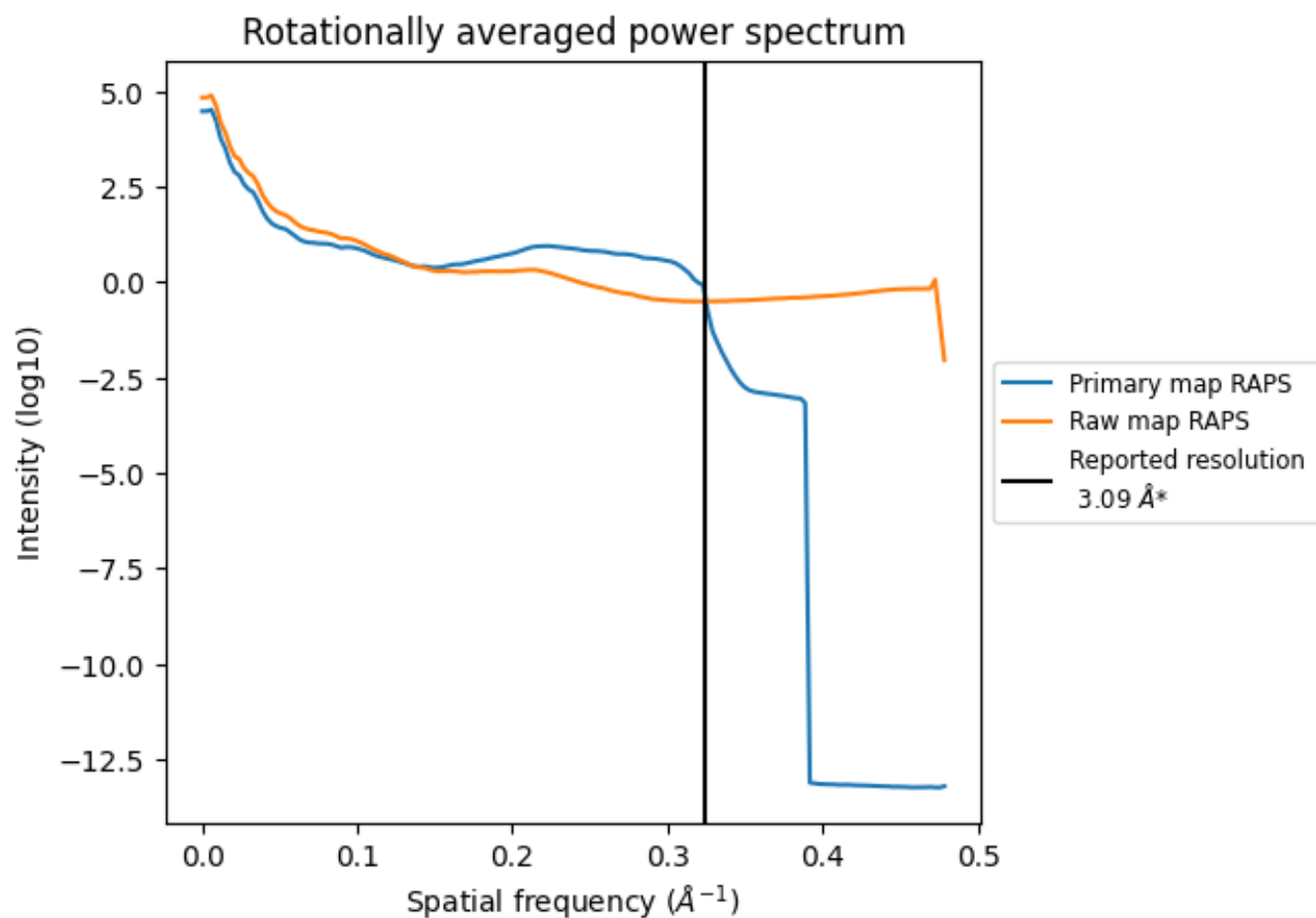
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 107 nm³; this corresponds to an approximate mass of 97 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 ⓘ

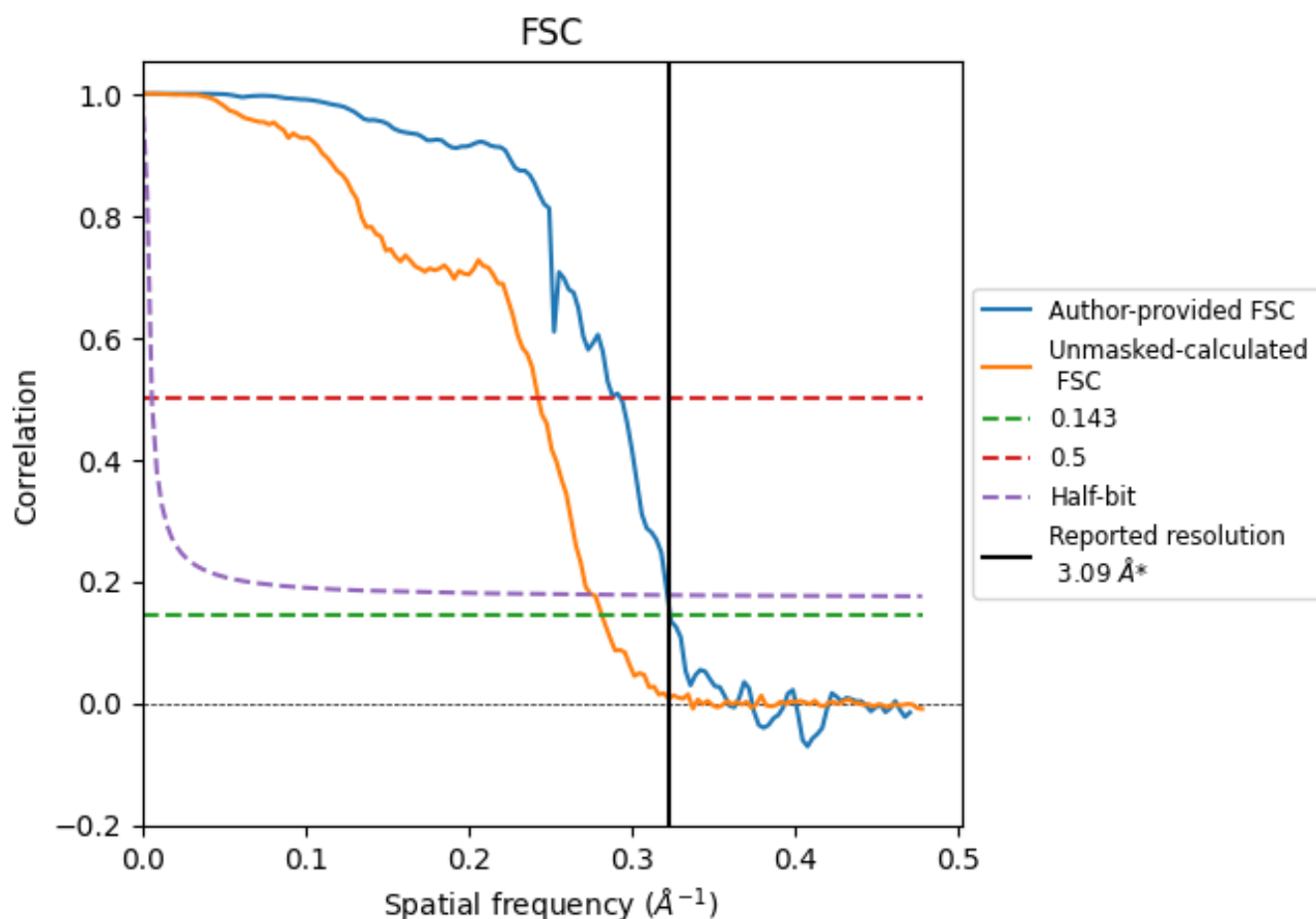


*Reported resolution corresponds to spatial frequency of 0.324 Å⁻¹

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 0.324 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.09	-	-
Author-provided FSC curve	3.09	3.41	3.10
Unmasked-calculated*	3.54	4.11	3.62

*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 3.54 differs from the reported value 3.09 by more than 10 %

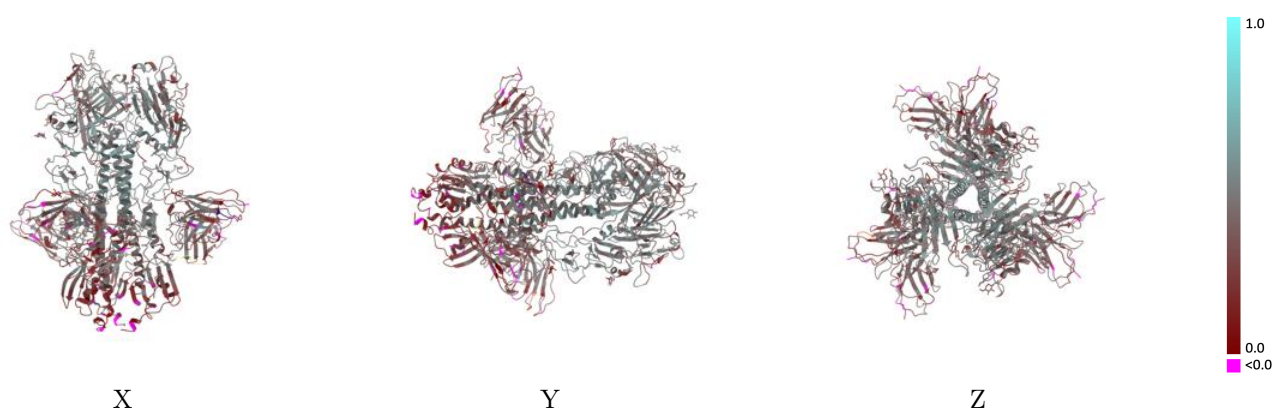
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-44112 and PDB model 9B2M. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)

This section was not generated.

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

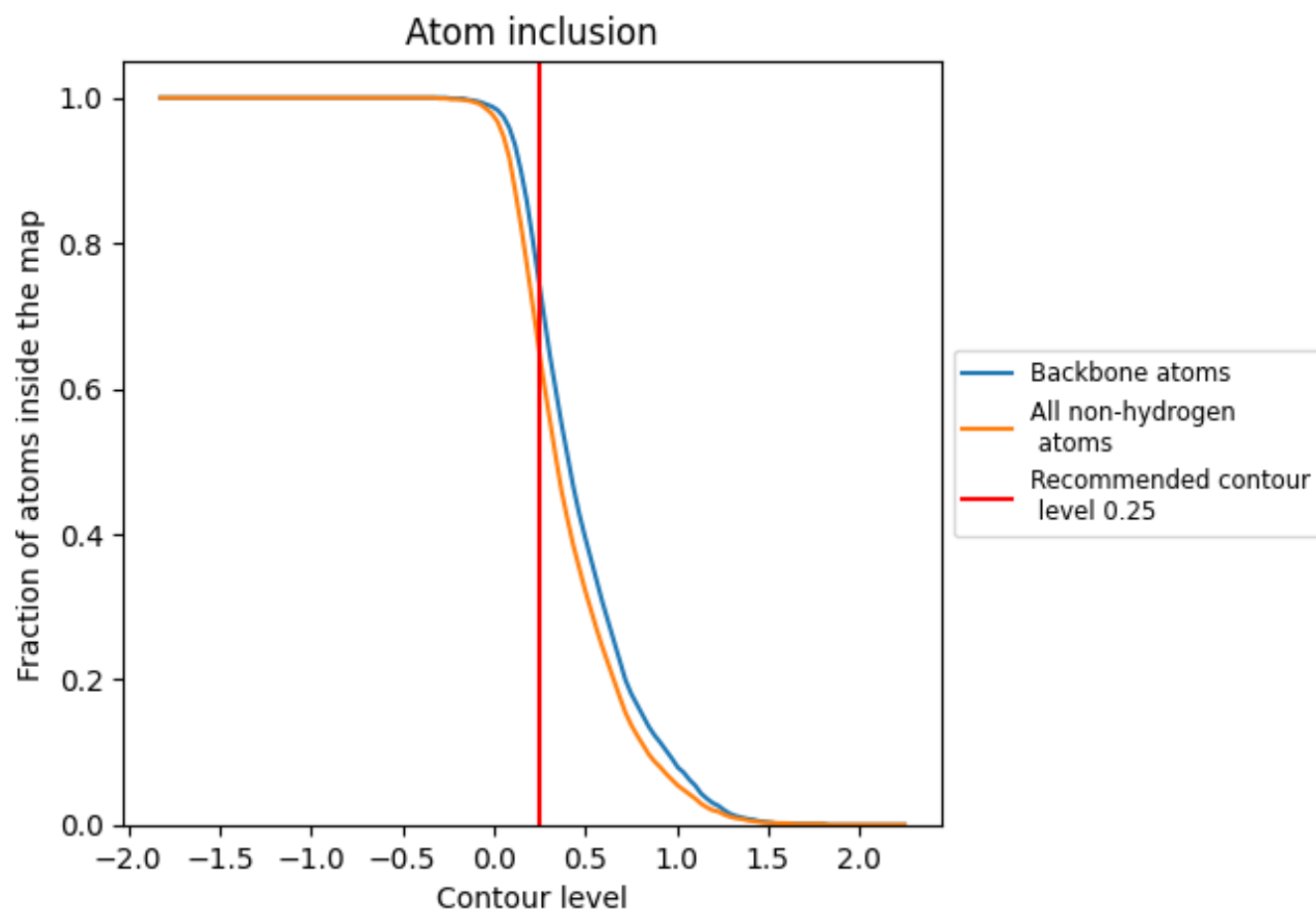


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 65% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6480	0.3770
A	0.7810	0.4350
B	0.7020	0.3590
C	0.7890	0.4370
D	0.7070	0.3670
E	0.5000	0.3310
F	0.3030	0.2780
G	0.7900	0.4330
H	0.4970	0.3440
I	0.6970	0.3540
J	0.5000	0.3270
K	0.3200	0.2790
L	0.3270	0.2890

1.0

0.0

<0.0