



wwPDB EM Validation Summary Report ⓘ

Apr 14, 2025 – 12:32 PM JST

PDB ID : 8Z7N / pdb_00008z7n
EMDB ID : EMD-39820
Title : Structure of HIV-1 CH119 SOSIP.664 trimer in complex with CD4 molecules
Authors : Li, D.; Wang, T.
Deposited on : 2024-04-20
Resolution : 3.58 Å(reported)

This is a wwPDB EM Validation Summary 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.dev117
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

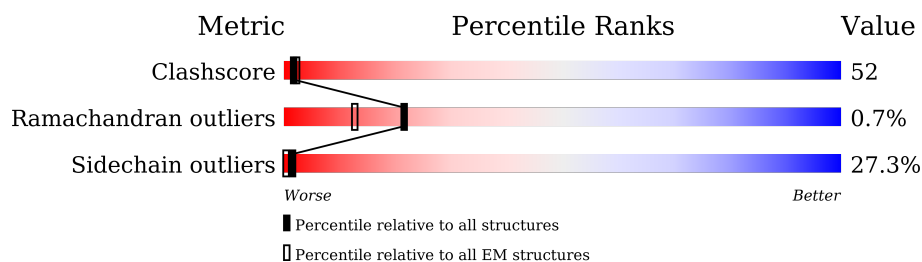
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.58 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	518	
1	D	518	
1	G	518	
2	B	164	
2	E	164	
2	H	164	
3	C	401	
3	F	401	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	I	401	<div><div><div></div><div></div><div></div><div></div><div></div></div><div><div>5%</div><div>11%</div><div>27%</div><div>6%</div><div>56%</div></div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16641 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 Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	386	Total	C	N	O	S	0	0
			3019	1895	525	574	25		
1	D	386	Total	C	N	O	S	0	0
			3019	1895	525	574	25		
1	G	386	Total	C	N	O	S	0	0
			3019	1895	525	574	25		

There are 123 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A1EAH4
A	2	ASP	-	expression tag	UNP A1EAH4
A	3	ALA	-	expression tag	UNP A1EAH4
A	4	MET	-	expression tag	UNP A1EAH4
A	5	LYS	-	expression tag	UNP A1EAH4
A	6	ARG	-	expression tag	UNP A1EAH4
A	7	GLY	-	expression tag	UNP A1EAH4
A	8	LEU	-	expression tag	UNP A1EAH4
A	9	CYS	-	expression tag	UNP A1EAH4
A	10	CYS	-	expression tag	UNP A1EAH4
A	11	VAL	-	expression tag	UNP A1EAH4
A	12	LEU	-	expression tag	UNP A1EAH4
A	13	LEU	-	expression tag	UNP A1EAH4
A	14	LEU	-	expression tag	UNP A1EAH4
A	15	CYS	-	expression tag	UNP A1EAH4
A	16	GLY	-	expression tag	UNP A1EAH4
A	17	ALA	-	expression tag	UNP A1EAH4
A	18	VAL	-	expression tag	UNP A1EAH4
A	19	PHE	-	expression tag	UNP A1EAH4
A	20	VAL	-	expression tag	UNP A1EAH4
A	21	SER	-	expression tag	UNP A1EAH4
A	22	PRO	-	expression tag	UNP A1EAH4
A	23	SER	-	expression tag	UNP A1EAH4
A	24	GLN	-	expression tag	UNP A1EAH4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	GLU	-	expression tag	UNP A1EAH4
A	26	ILE	-	expression tag	UNP A1EAH4
A	27	HIS	-	expression tag	UNP A1EAH4
A	28	ALA	-	expression tag	UNP A1EAH4
A	29	ARG	-	expression tag	UNP A1EAH4
A	30	PHE	-	expression tag	UNP A1EAH4
A	31	ARG	-	expression tag	UNP A1EAH4
A	32	ARG	-	expression tag	UNP A1EAH4
A	33	GLY	-	expression tag	UNP A1EAH4
A	34	ALA	-	expression tag	UNP A1EAH4
A	35	ARG	-	expression tag	UNP A1EAH4
A	507	CYS	ALA	engineered mutation	UNP A1EAH4
A	515	ARG	-	expression tag	UNP A1EAH4
A	516	ARG	-	expression tag	UNP A1EAH4
A	517	ARG	-	expression tag	UNP A1EAH4
A	518	ARG	-	expression tag	UNP A1EAH4
A	519	ARG	-	expression tag	UNP A1EAH4
D	1	MET	-	initiating methionine	UNP A1EAH4
D	2	ASP	-	expression tag	UNP A1EAH4
D	3	ALA	-	expression tag	UNP A1EAH4
D	4	MET	-	expression tag	UNP A1EAH4
D	5	LYS	-	expression tag	UNP A1EAH4
D	6	ARG	-	expression tag	UNP A1EAH4
D	7	GLY	-	expression tag	UNP A1EAH4
D	8	LEU	-	expression tag	UNP A1EAH4
D	9	CYS	-	expression tag	UNP A1EAH4
D	10	CYS	-	expression tag	UNP A1EAH4
D	11	VAL	-	expression tag	UNP A1EAH4
D	12	LEU	-	expression tag	UNP A1EAH4
D	13	LEU	-	expression tag	UNP A1EAH4
D	14	LEU	-	expression tag	UNP A1EAH4
D	15	CYS	-	expression tag	UNP A1EAH4
D	16	GLY	-	expression tag	UNP A1EAH4
D	17	ALA	-	expression tag	UNP A1EAH4
D	18	VAL	-	expression tag	UNP A1EAH4
D	19	PHE	-	expression tag	UNP A1EAH4
D	20	VAL	-	expression tag	UNP A1EAH4
D	21	SER	-	expression tag	UNP A1EAH4
D	22	PRO	-	expression tag	UNP A1EAH4
D	23	SER	-	expression tag	UNP A1EAH4
D	24	GLN	-	expression tag	UNP A1EAH4
D	25	GLU	-	expression tag	UNP A1EAH4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	26	ILE	-	expression tag	UNP A1EAH4
D	27	HIS	-	expression tag	UNP A1EAH4
D	28	ALA	-	expression tag	UNP A1EAH4
D	29	ARG	-	expression tag	UNP A1EAH4
D	30	PHE	-	expression tag	UNP A1EAH4
D	31	ARG	-	expression tag	UNP A1EAH4
D	32	ARG	-	expression tag	UNP A1EAH4
D	33	GLY	-	expression tag	UNP A1EAH4
D	34	ALA	-	expression tag	UNP A1EAH4
D	35	ARG	-	expression tag	UNP A1EAH4
D	507	CYS	ALA	engineered mutation	UNP A1EAH4
D	515	ARG	-	expression tag	UNP A1EAH4
D	516	ARG	-	expression tag	UNP A1EAH4
D	517	ARG	-	expression tag	UNP A1EAH4
D	518	ARG	-	expression tag	UNP A1EAH4
D	519	ARG	-	expression tag	UNP A1EAH4
G	1	MET	-	initiating methionine	UNP A1EAH4
G	2	ASP	-	expression tag	UNP A1EAH4
G	3	ALA	-	expression tag	UNP A1EAH4
G	4	MET	-	expression tag	UNP A1EAH4
G	5	LYS	-	expression tag	UNP A1EAH4
G	6	ARG	-	expression tag	UNP A1EAH4
G	7	GLY	-	expression tag	UNP A1EAH4
G	8	LEU	-	expression tag	UNP A1EAH4
G	9	CYS	-	expression tag	UNP A1EAH4
G	10	CYS	-	expression tag	UNP A1EAH4
G	11	VAL	-	expression tag	UNP A1EAH4
G	12	LEU	-	expression tag	UNP A1EAH4
G	13	LEU	-	expression tag	UNP A1EAH4
G	14	LEU	-	expression tag	UNP A1EAH4
G	15	CYS	-	expression tag	UNP A1EAH4
G	16	GLY	-	expression tag	UNP A1EAH4
G	17	ALA	-	expression tag	UNP A1EAH4
G	18	VAL	-	expression tag	UNP A1EAH4
G	19	PHE	-	expression tag	UNP A1EAH4
G	20	VAL	-	expression tag	UNP A1EAH4
G	21	SER	-	expression tag	UNP A1EAH4
G	22	PRO	-	expression tag	UNP A1EAH4
G	23	SER	-	expression tag	UNP A1EAH4
G	24	GLN	-	expression tag	UNP A1EAH4
G	25	GLU	-	expression tag	UNP A1EAH4
G	26	ILE	-	expression tag	UNP A1EAH4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	27	HIS	-	expression tag	UNP A1EAH4
G	28	ALA	-	expression tag	UNP A1EAH4
G	29	ARG	-	expression tag	UNP A1EAH4
G	30	PHE	-	expression tag	UNP A1EAH4
G	31	ARG	-	expression tag	UNP A1EAH4
G	32	ARG	-	expression tag	UNP A1EAH4
G	33	GLY	-	expression tag	UNP A1EAH4
G	34	ALA	-	expression tag	UNP A1EAH4
G	35	ARG	-	expression tag	UNP A1EAH4
G	507	CYS	ALA	engineered mutation	UNP A1EAH4
G	515	ARG	-	expression tag	UNP A1EAH4
G	516	ARG	-	expression tag	UNP A1EAH4
G	517	ARG	-	expression tag	UNP A1EAH4
G	518	ARG	-	expression tag	UNP A1EAH4
G	519	ARG	-	expression tag	UNP A1EAH4

- Molecule 2 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	135	Total	C	N	O	S	0	0
			1070	680	181	202	7		
2	E	135	Total	C	N	O	S	0	0
			1070	680	181	202	7		
2	H	135	Total	C	N	O	S	0	0
			1070	680	181	202	7		

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	566	PRO	ILE	engineered mutation	UNP A1EAH4
B	612	CYS	THR	engineered mutation	UNP A1EAH4
B	672	GLY	-	expression tag	UNP A1EAH4
B	673	GLY	-	expression tag	UNP A1EAH4
B	674	GLY	-	expression tag	UNP A1EAH4
B	675	GLY	-	expression tag	UNP A1EAH4
B	676	GLY	-	expression tag	UNP A1EAH4
B	677	HIS	-	expression tag	UNP A1EAH4
B	678	HIS	-	expression tag	UNP A1EAH4
B	679	HIS	-	expression tag	UNP A1EAH4
B	680	HIS	-	expression tag	UNP A1EAH4
B	681	HIS	-	expression tag	UNP A1EAH4
B	682	HIS	-	expression tag	UNP A1EAH4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	566	PRO	ILE	engineered mutation	UNP A1EAH4
E	612	CYS	THR	engineered mutation	UNP A1EAH4
E	672	GLY	-	expression tag	UNP A1EAH4
E	673	GLY	-	expression tag	UNP A1EAH4
E	674	GLY	-	expression tag	UNP A1EAH4
E	675	GLY	-	expression tag	UNP A1EAH4
E	676	GLY	-	expression tag	UNP A1EAH4
E	677	HIS	-	expression tag	UNP A1EAH4
E	678	HIS	-	expression tag	UNP A1EAH4
E	679	HIS	-	expression tag	UNP A1EAH4
E	680	HIS	-	expression tag	UNP A1EAH4
E	681	HIS	-	expression tag	UNP A1EAH4
E	682	HIS	-	expression tag	UNP A1EAH4
H	566	PRO	ILE	engineered mutation	UNP A1EAH4
H	612	CYS	THR	engineered mutation	UNP A1EAH4
H	672	GLY	-	expression tag	UNP A1EAH4
H	673	GLY	-	expression tag	UNP A1EAH4
H	674	GLY	-	expression tag	UNP A1EAH4
H	675	GLY	-	expression tag	UNP A1EAH4
H	676	GLY	-	expression tag	UNP A1EAH4
H	677	HIS	-	expression tag	UNP A1EAH4
H	678	HIS	-	expression tag	UNP A1EAH4
H	679	HIS	-	expression tag	UNP A1EAH4
H	680	HIS	-	expression tag	UNP A1EAH4
H	681	HIS	-	expression tag	UNP A1EAH4
H	682	HIS	-	expression tag	UNP A1EAH4

- Molecule 3 is a protein called T-cell surface glycoprotein CD4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	177	Total	C	N	O	S	0	0
			1374	858	241	271	4		
3	F	177	Total	C	N	O	S	0	0
			1374	858	241	271	4		
3	I	177	Total	C	N	O	S	0	0
			1374	858	241	271	4		

There are 27 discrepancies between the modelled and reference sequences:

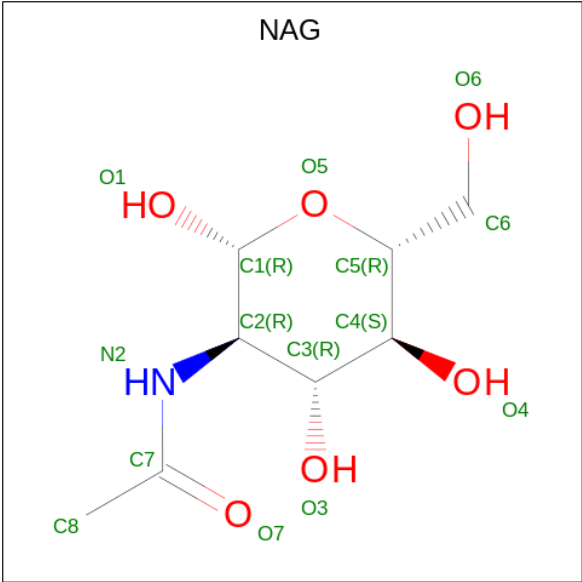
Chain	Residue	Modelled	Actual	Comment	Reference
C	370	GLY	-	expression tag	UNP P01730
C	371	SER	-	expression tag	UNP P01730

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	372	GLY	-	expression tag	UNP P01730
C	373	HIS	-	expression tag	UNP P01730
C	374	HIS	-	expression tag	UNP P01730
C	375	HIS	-	expression tag	UNP P01730
C	376	HIS	-	expression tag	UNP P01730
C	377	HIS	-	expression tag	UNP P01730
C	378	HIS	-	expression tag	UNP P01730
F	370	GLY	-	expression tag	UNP P01730
F	371	SER	-	expression tag	UNP P01730
F	372	GLY	-	expression tag	UNP P01730
F	373	HIS	-	expression tag	UNP P01730
F	374	HIS	-	expression tag	UNP P01730
F	375	HIS	-	expression tag	UNP P01730
F	376	HIS	-	expression tag	UNP P01730
F	377	HIS	-	expression tag	UNP P01730
F	378	HIS	-	expression tag	UNP P01730
I	370	GLY	-	expression tag	UNP P01730
I	371	SER	-	expression tag	UNP P01730
I	372	GLY	-	expression tag	UNP P01730
I	373	HIS	-	expression tag	UNP P01730
I	374	HIS	-	expression tag	UNP P01730
I	375	HIS	-	expression tag	UNP P01730
I	376	HIS	-	expression tag	UNP P01730
I	377	HIS	-	expression tag	UNP P01730
I	378	HIS	-	expression tag	UNP P01730

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).

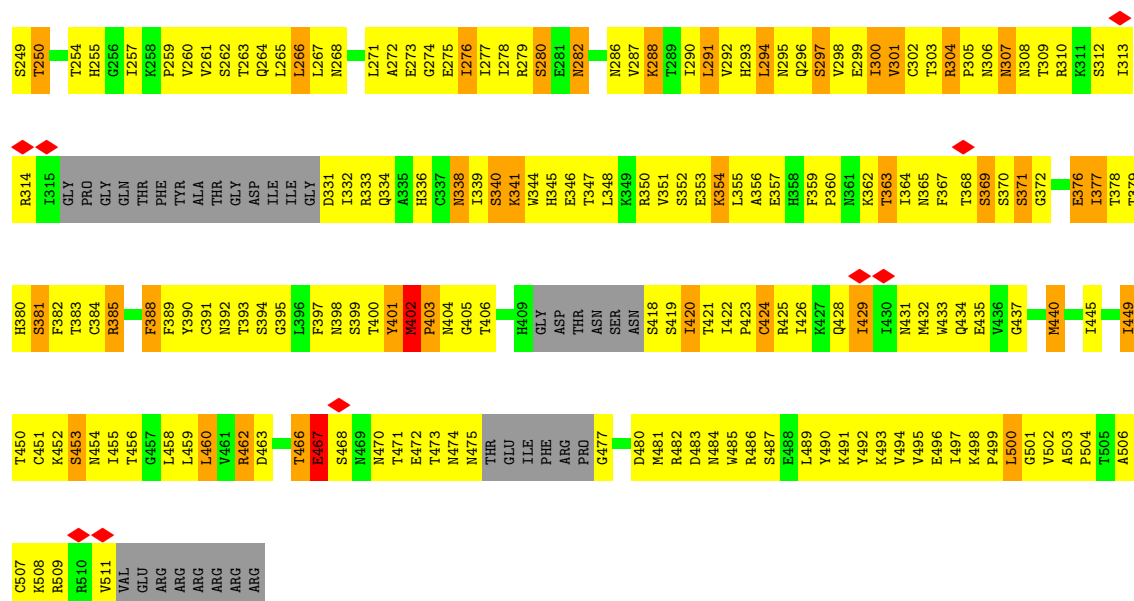


Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	D	1	Total	C	N	O	0
			14	8	1	5	
4	D	1	Total	C	N	O	0
			14	8	1	5	
4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

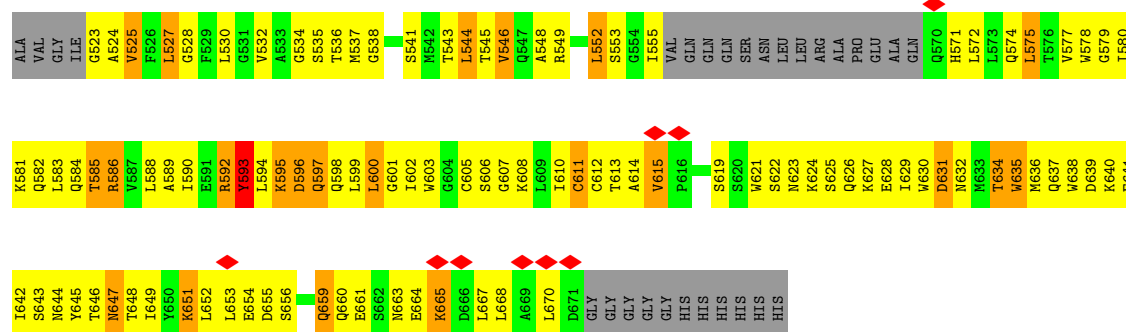
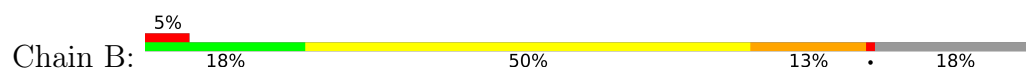
Continued on next page...

Continued from previous page...

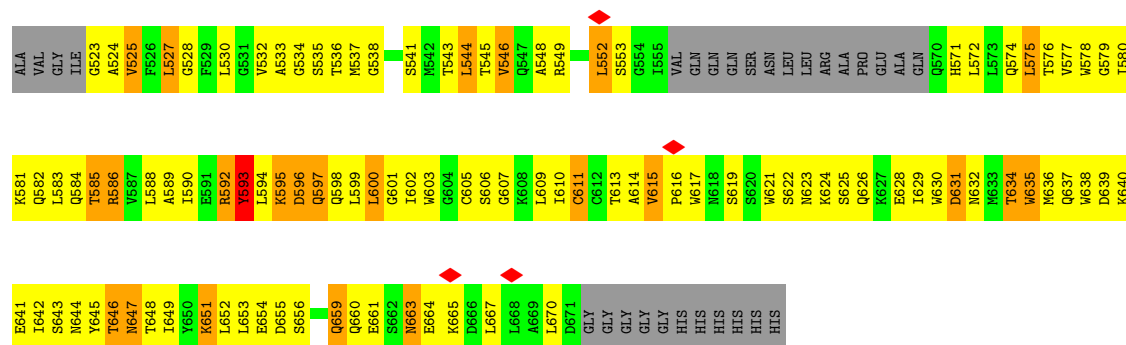
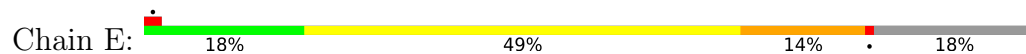
Mol	Chain	Residues	Atoms				AltConf
4	H	1	Total	C	N	O	0
			14	8	1	5	
4	H	1	Total	C	N	O	0
			14	8	1	5	
4	H	1	Total	C	N	O	0
			14	8	1	5	
4	H	1	Total	C	N	O	0
			14	8	1	5	



- Molecule 2: Envelope glycoprotein gp160



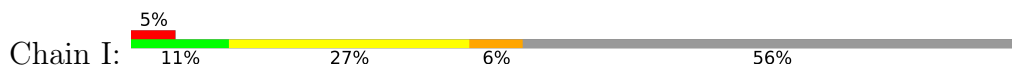
- Molecule 2: Envelope glycoprotein gp160



- Molecule 2: Envelope glycoprotein gp160

[illegible]

- Molecule 3: T-cell surface glycoprotein CD4



NET	ASN	ARG	GLY	VAL	PRO	PHE	ARG	HIS	LEU	LEU	LEU	VAL	LEU	LEU	GLN	ALA	LEU	ALA	ALA	ALA	THR	GLN	GLY	K3	K4	K5	V5	V6	L7	G8	K9	K10	G11	D12	T13	V14	E15	L16	L17	T18	C19	T19	A20	S21	K22	K23	K24	S25	I26	Q27	F28	H29	W30	K31	K31	N32	S33	S33	N34	Q35	N35	N36	I36	K37	K37
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	----	----	----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

I38
L39
G40
N41
Q42
G43
S44
F45
L46
T47
K48
G49
P50
S51
K52
L53
N54
D55
R56
M61
S62
L63
W64
D65
Q66
G67
N68
F69
P70
L71
L76
K77
I78
E79
D80
S81
D82
T83
Y84
I85
C86
E87
V88
E89
Q90
Q91
K92
E93
E94
V95
Q96
L97
L98
V99
G101
L102

A104	A105	A106	D107	H108	H109	L110	L111	G112	G113	G114	S115	L116	T117	L118	T119	L120	E121	S122	P123	P124	P128	S129	V130	Q131	S132	R133	S134	P135	R136	G137	K138	M139	L140	Q141	K144	T145	L146	S147	V148	S149	Q150	L151	S152	L153	M159	T160	T162	V163	L164	Q165	M166	Q167	K168	K169
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

E171	F172	K173	I174	D175	I176	V177	V178	L179	ALA	PHE	GLN	LYS	ALA	SER	SER	ILE	VAL	TYR	LYS	LYS	GLY	GLU	GLN	GLU	VAL	GLY	PHE	SER	SER	PRO	PHE	PHE	LEU	LEU	THR	GLY	SER	SER	GLY	GLY	LEU	TRP	GLN	ALA	ALA	GLY	ARG	ALA	SER	SER	SER	LYS	SER	TRP	ILE
------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

PHE.	ASP	LEU	LYS	ASN	GLY	VAL	SER	LYS	ARG	THR	GLN	ASP	PRO	LYS	LEU	GLN	MET	GLY	LYS	LYS	PRO	LEU	HIS	THR	LEU	PRO	GLN	ALA	ALA	PRO	GLN	TYR	ALA	ALA	SER	SER	GLY	ASN	LEU	THR	LYS	GLY	LYS	HIS	GLN	GLU	VAL	ASN
------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

LEU	VAL	VAL	VAL	ARG	ALA	THR	GLN	LEU	GLN	LYS	ASN	LEU	THR	CYS	GLU	TRP	GLY	PRO	THR	SER	SER	LYS	LEU	MET	LEU	SER	LYS	LEU	GLU	ASN	LYS	GLU	ALA	LYS	VAL	SER	LYS	ARG	GLU	LYS	ALA	VAL	VAL	LEU	ASN	PRO	GLU	ALA	GLY	MET	TRP	GLN	CYS	LEU	LEU	LEU	SER
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

ASP
SER
GLY
GLN
VAL
LEU
LEU
GLU
SER
ASN
ILE
LYS
VAL
LEU
PRO
THR
TRP
SER
THR
THR
GLY
SER
GLY
HIS
HIS
HIS
HIS
HIS

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	1045667	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 ($e^-/\text{\AA}^2$)	50.8	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.521	Depositor
Minimum map value	-1.179	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.049	Depositor
Map size (\AA)	415.0, 415.0, 415.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.83, 0.83, 0.83	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.53	0/3082	0.74	3/4192 (0.1%)
1	D	0.53	0/3082	0.74	3/4192 (0.1%)
1	G	0.53	0/3082	0.74	3/4192 (0.1%)
2	B	0.51	1/1089 (0.1%)	0.74	2/1474 (0.1%)
2	E	0.51	1/1089 (0.1%)	0.74	2/1474 (0.1%)
2	H	0.51	1/1089 (0.1%)	0.74	2/1474 (0.1%)
3	C	0.39	0/1393	0.65	0/1878
3	F	0.39	0/1393	0.65	0/1878
3	I	0.39	0/1393	0.65	0/1878
All	All	0.49	3/16692 (0.0%)	0.72	15/22632 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	D	0	3
1	G	0	3
2	B	0	2
2	E	0	2
2	H	0	2
3	C	0	1
3	F	0	1
3	I	0	1
All	All	0	18

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	593	TYR	CD1-CE1	-5.74	1.30	1.39
2	B	593	TYR	CD1-CE1	-5.73	1.30	1.39
2	H	593	TYR	CD1-CE1	-5.66	1.30	1.39

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	552	LEU	CA-CB-CG	7.21	131.88	115.30
2	E	552	LEU	CA-CB-CG	7.20	131.86	115.30
2	B	552	LEU	CA-CB-CG	7.19	131.84	115.30
1	A	402	MET	N-CA-C	-6.41	93.70	111.00
1	D	402	MET	N-CA-C	-6.40	93.71	111.00

There are no chirality outliers.

5 of 18 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	401	TYR	Peptide
1	A	402	MET	Peptide
1	A	82	PRO	Peptide
2	B	611	CYS	Peptide
2	B	634	THR	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3019	0	2956	333	0
1	D	3019	0	2957	423	0
1	G	3019	0	2956	339	0
2	B	1070	0	1059	135	0
2	E	1070	0	1060	196	0
2	H	1070	0	1059	138	0
3	C	1374	0	1396	107	0
3	F	1374	0	1396	144	0
3	I	1374	0	1396	108	0
4	A	28	0	26	2	0
4	B	56	0	52	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	28	0	26	1	0
4	E	56	0	52	1	0
4	G	28	0	26	0	0
4	H	56	0	52	1	0
All	All	16641	0	16469	1718	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 52.

The worst 5 of 1718 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:B:593:TYR:O	2:B:597:GLN:HB3	1.34	1.25
2:H:593:TYR:O	2:H:597:GLN:HB3	1.34	1.20
2:E:593:TYR:O	2:E:597:GLN:HB3	1.34	1.20
1:D:90:LEU:HB2	2:E:532:VAL:HG23	1.27	1.14
1:D:49:PRO:O	2:E:635:TRP:HB2	1.53	1.09

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	374/518 (72%)	280 (75%)	90 (24%)	4 (1%)	12	45
1	D	374/518 (72%)	279 (75%)	91 (24%)	4 (1%)	12	45
1	G	374/518 (72%)	279 (75%)	91 (24%)	4 (1%)	12	45
2	B	131/164 (80%)	101 (77%)	29 (22%)	1 (1%)	16	51
2	E	131/164 (80%)	101 (77%)	29 (22%)	1 (1%)	16	51
2	H	131/164 (80%)	101 (77%)	29 (22%)	1 (1%)	16	51

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	175/401 (44%)	141 (81%)	34 (19%)	0	100	100
3	F	175/401 (44%)	141 (81%)	34 (19%)	0	100	100
3	I	175/401 (44%)	141 (81%)	34 (19%)	0	100	100
All	All	2040/3249 (63%)	1564 (77%)	461 (23%)	15 (1%)	21	53

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	282	ASN
1	A	305	PRO
1	A	307	ASN
1	D	282	ASN
1	D	305	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	347/462 (75%)	254 (73%)	93 (27%)	0	3
1	D	347/462 (75%)	254 (73%)	93 (27%)	0	3
1	G	347/462 (75%)	254 (73%)	93 (27%)	0	3
2	B	117/137 (85%)	87 (74%)	30 (26%)	0	3
2	E	117/137 (85%)	87 (74%)	30 (26%)	0	3
2	H	117/137 (85%)	87 (74%)	30 (26%)	0	3
3	C	160/355 (45%)	113 (71%)	47 (29%)	0	2
3	F	160/355 (45%)	113 (71%)	47 (29%)	0	2
3	I	160/355 (45%)	112 (70%)	48 (30%)	0	2
All	All	1872/2862 (65%)	1361 (73%)	511 (27%)	1	2

5 of 511 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	352	SER
2	H	596	ASP
2	E	660	GLN
2	H	575	LEU
3	I	34	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	658	ASN
3	I	66	GLN
1	G	109	GLN
2	H	637	GLN
3	F	131	GLN

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](#)

18 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
4	NAG	E	704	2	14,14,15	0.55	0	17,19,21	0.44	0
4	NAG	B	702	2	14,14,15	0.26	0	17,19,21	0.41	0
4	NAG	A	601	1	14,14,15	0.48	0	17,19,21	0.45	0
4	NAG	E	702	2	14,14,15	0.38	0	17,19,21	0.42	0
4	NAG	H	702	2	14,14,15	0.56	0	17,19,21	0.45	0
4	NAG	A	602	1	14,14,15	0.69	1 (7%)	17,19,21	0.38	0
4	NAG	D	602	1	14,14,15	0.36	0	17,19,21	0.73	1 (5%)
4	NAG	G	601	1	14,14,15	0.20	0	17,19,21	0.44	0
4	NAG	G	602	1	14,14,15	0.39	0	17,19,21	0.43	0
4	NAG	H	703	2	14,14,15	0.37	0	17,19,21	0.50	0
4	NAG	H	701	2	14,14,15	0.23	0	17,19,21	0.47	0
4	NAG	D	601	1	14,14,15	0.48	0	17,19,21	0.49	0
4	NAG	E	703	2	14,14,15	0.16	0	17,19,21	0.55	0
4	NAG	B	703	2	14,14,15	0.20	0	17,19,21	0.56	0
4	NAG	B	701	2	14,14,15	0.19	0	17,19,21	0.59	1 (5%)
4	NAG	H	704	2	14,14,15	0.40	0	17,19,21	0.47	0
4	NAG	E	701	2	14,14,15	0.43	0	17,19,21	0.52	0
4	NAG	B	704	2	14,14,15	0.45	0	17,19,21	0.42	0

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
4	NAG	E	704	2	-	4/6/23/26	0/1/1/1
4	NAG	B	702	2	-	1/6/23/26	0/1/1/1
4	NAG	A	601	1	-	3/6/23/26	0/1/1/1
4	NAG	E	702	2	-	1/6/23/26	0/1/1/1
4	NAG	H	702	2	-	1/6/23/26	0/1/1/1
4	NAG	A	602	1	-	0/6/23/26	0/1/1/1
4	NAG	D	602	1	-	1/6/23/26	0/1/1/1
4	NAG	G	601	1	-	2/6/23/26	0/1/1/1
4	NAG	G	602	1	-	2/6/23/26	0/1/1/1
4	NAG	H	703	2	-	4/6/23/26	0/1/1/1
4	NAG	H	701	2	-	2/6/23/26	0/1/1/1
4	NAG	D	601	1	-	3/6/23/26	0/1/1/1
4	NAG	E	703	2	-	2/6/23/26	0/1/1/1
4	NAG	B	703	2	-	2/6/23/26	0/1/1/1
4	NAG	B	701	2	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	H	704	2	-	3/6/23/26	0/1/1/1
4	NAG	E	701	2	-	2/6/23/26	0/1/1/1
4	NAG	B	704	2	-	3/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	602	NAG	O5-C1	-2.27	1.40	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	602	NAG	C1-O5-C5	2.52	115.60	112.19
4	B	701	NAG	C1-O5-C5	2.02	114.93	112.19

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	701	NAG	O5-C5-C6-O6
4	B	701	NAG	O5-C5-C6-O6
4	G	601	NAG	O5-C5-C6-O6
4	H	703	NAG	O5-C5-C6-O6
4	B	701	NAG	C4-C5-C6-O6

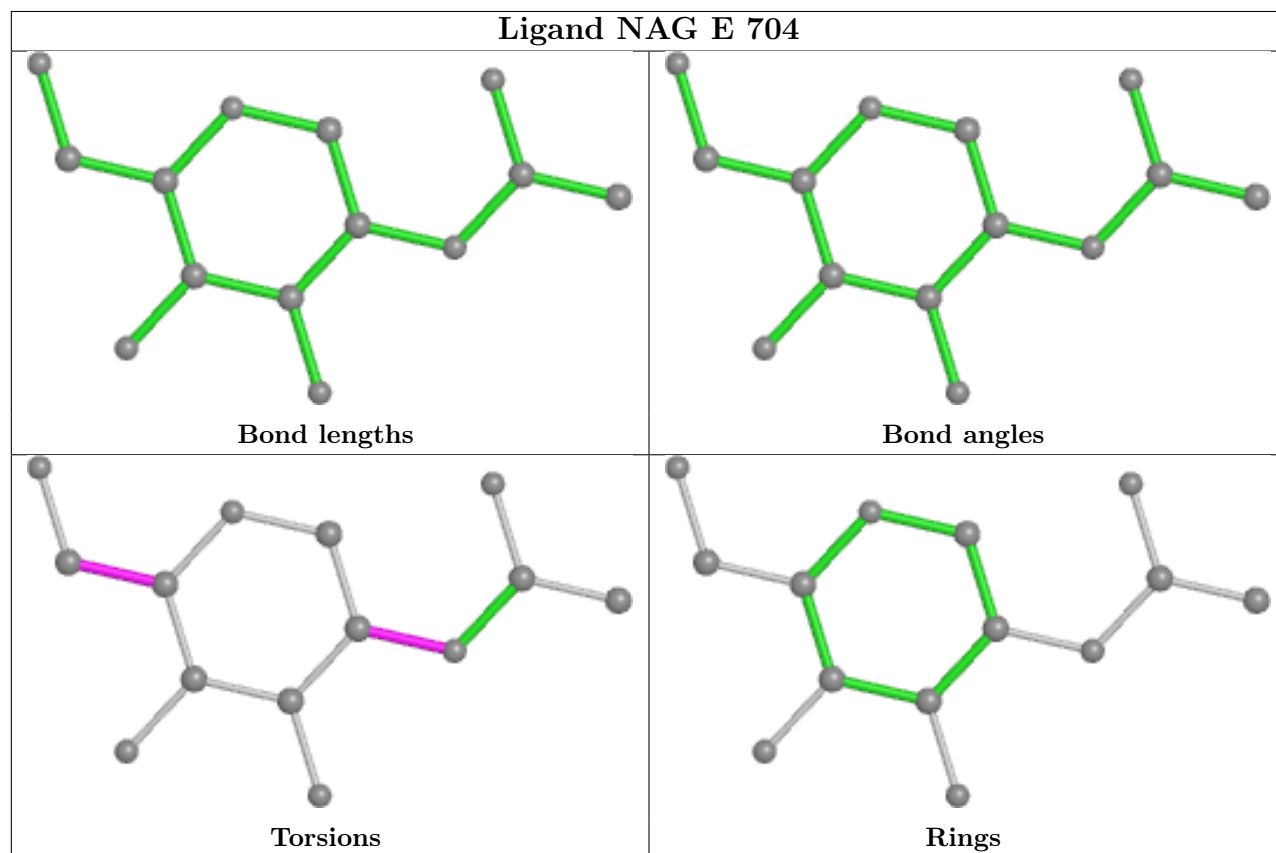
There are no ring outliers.

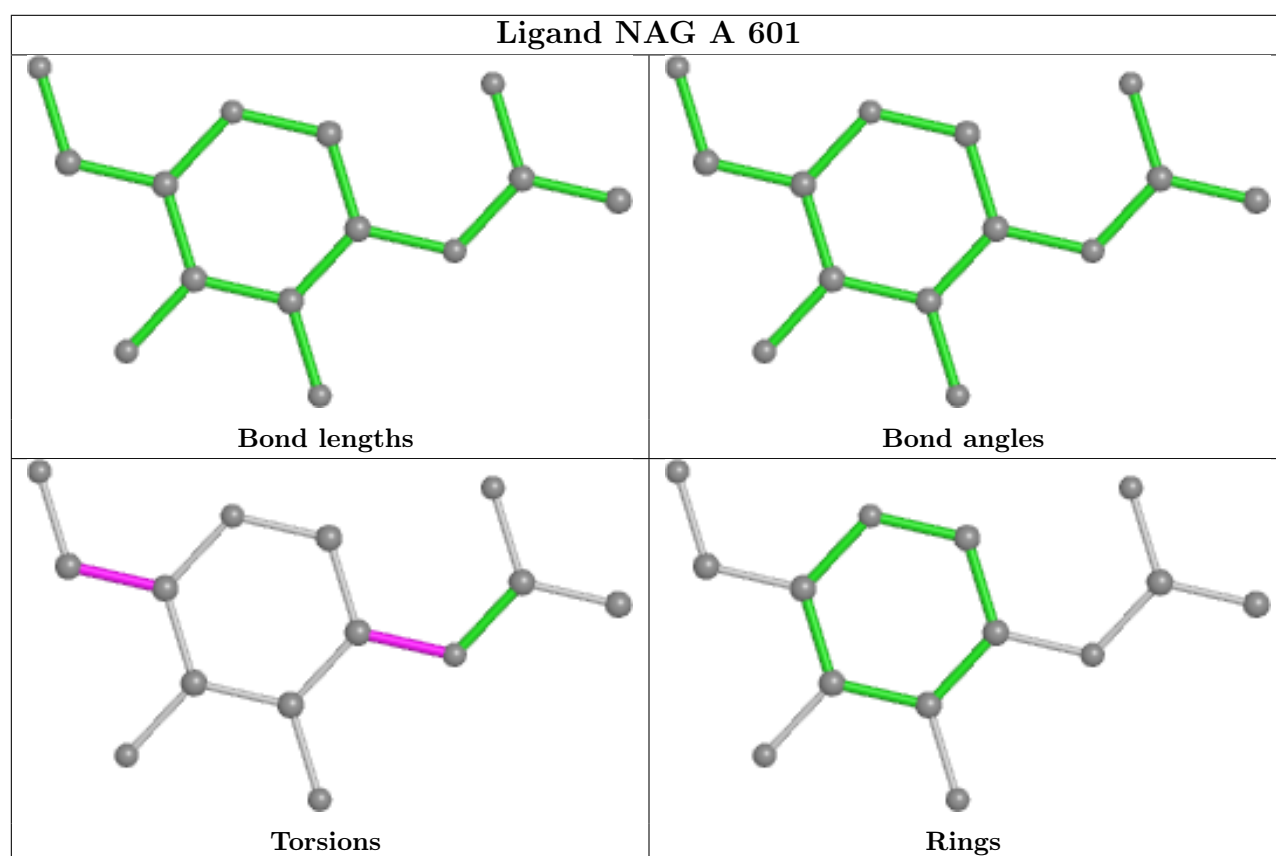
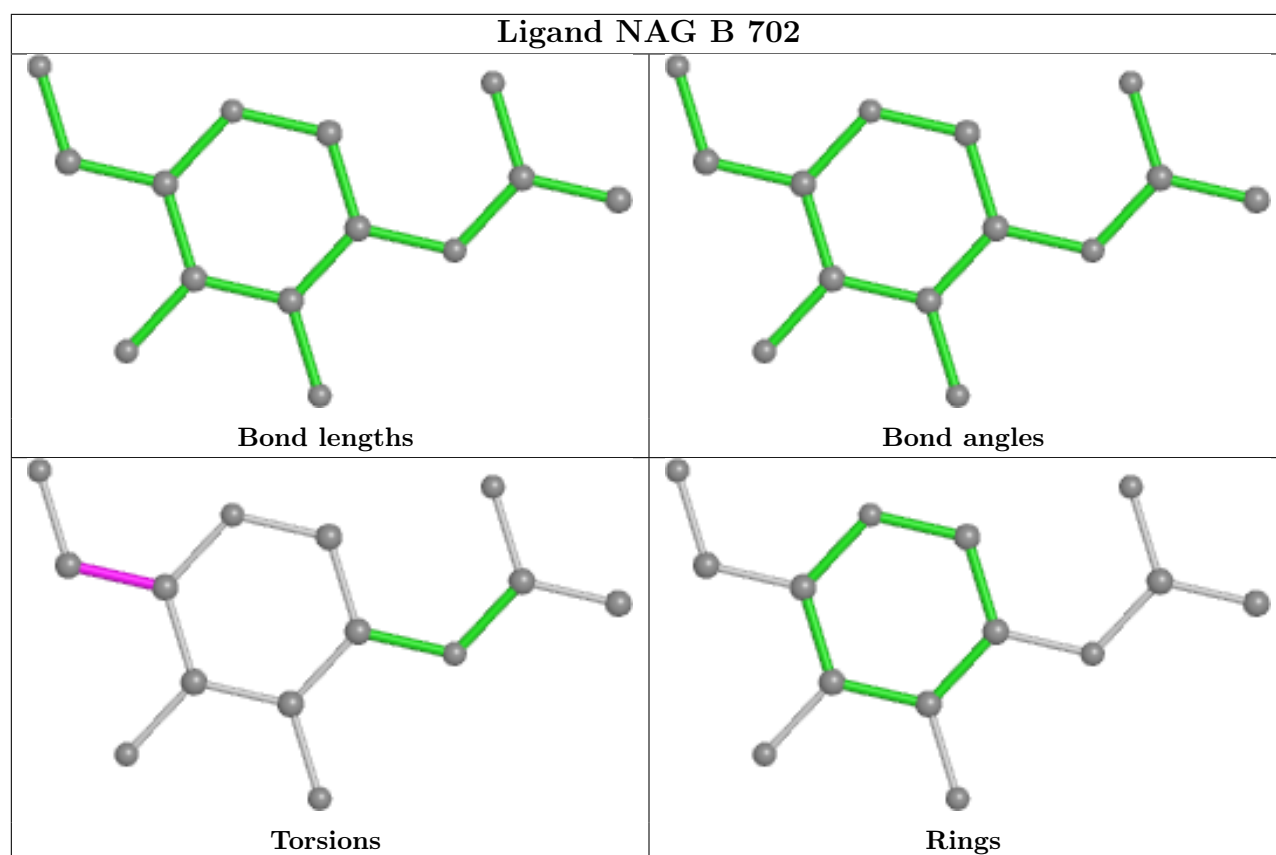
5 monomers are involved in 6 short contacts:

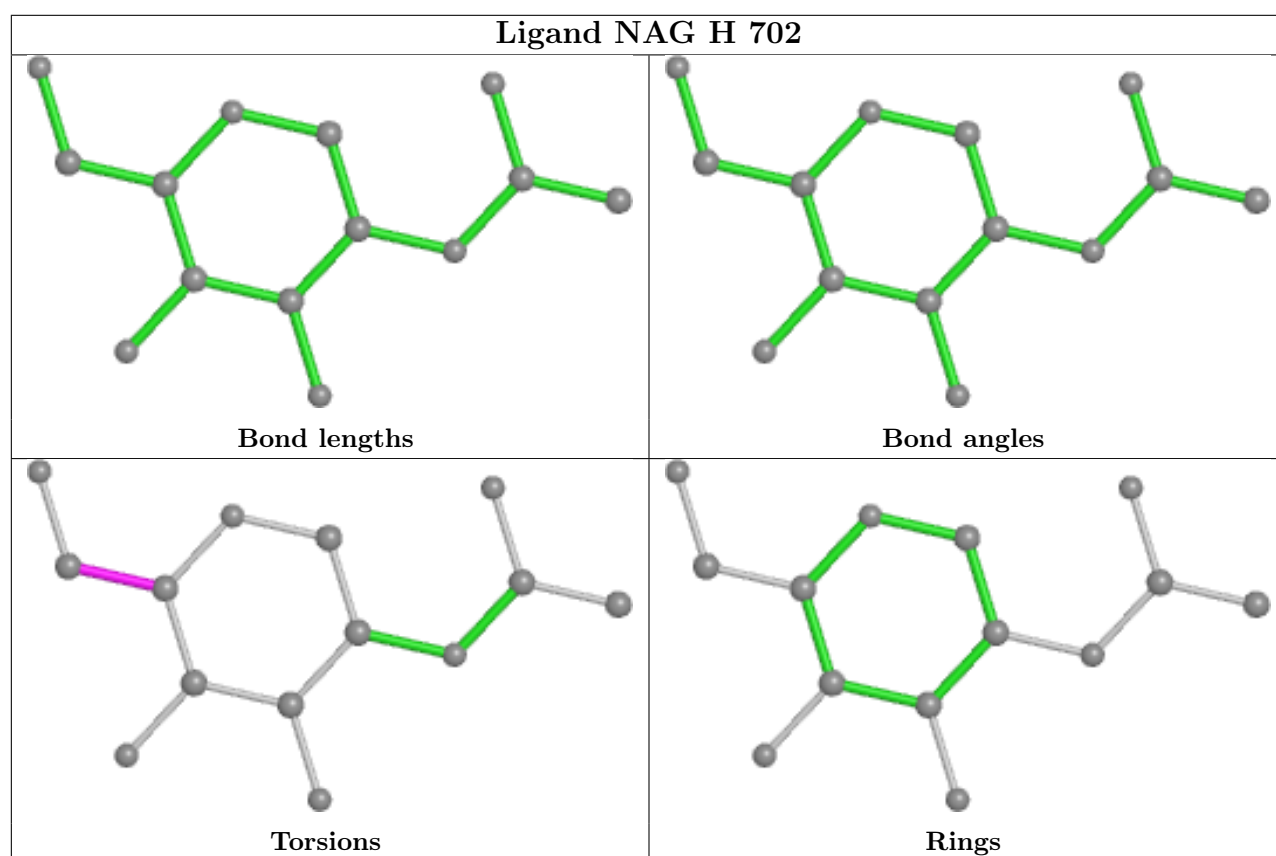
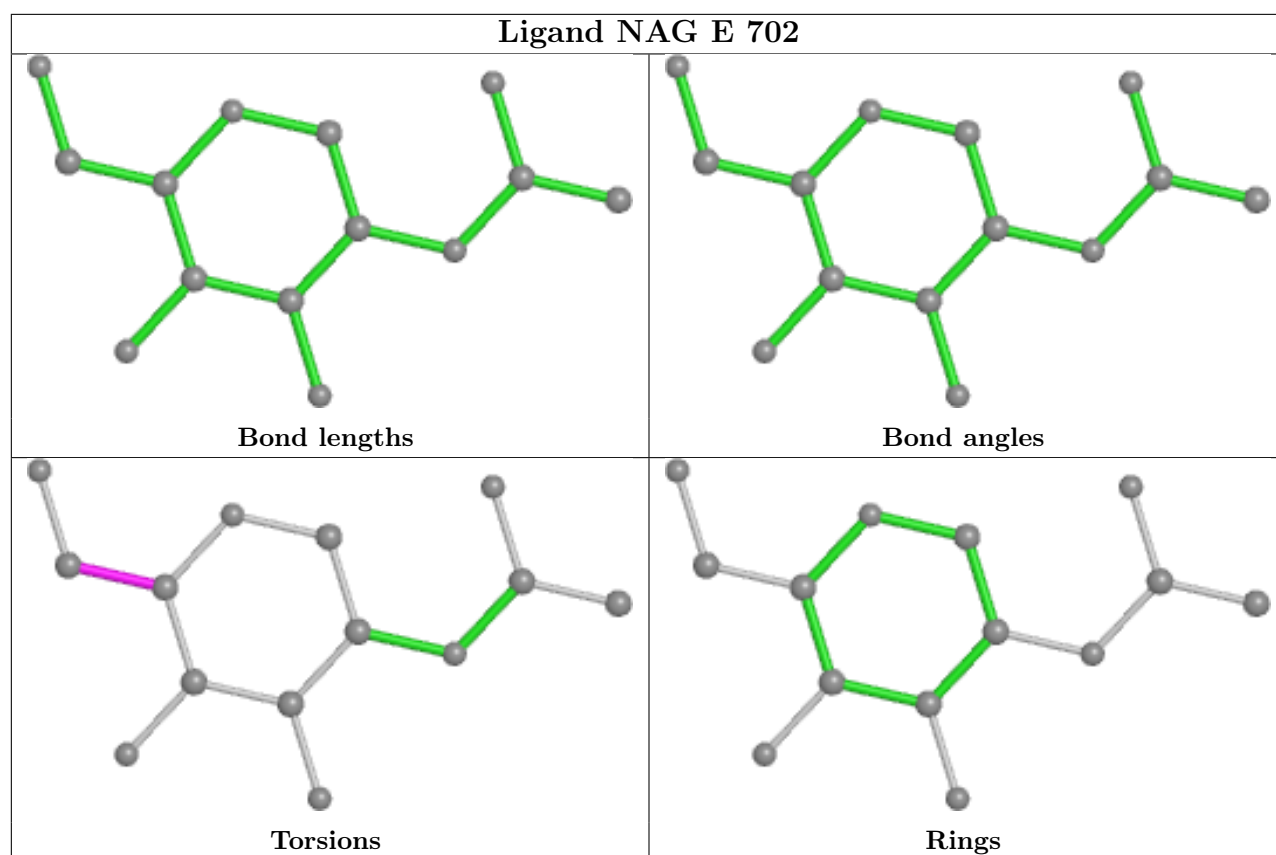
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	704	NAG	1	0
4	A	601	NAG	2	0
4	D	601	NAG	1	0
4	B	703	NAG	1	0
4	H	704	NAG	1	0

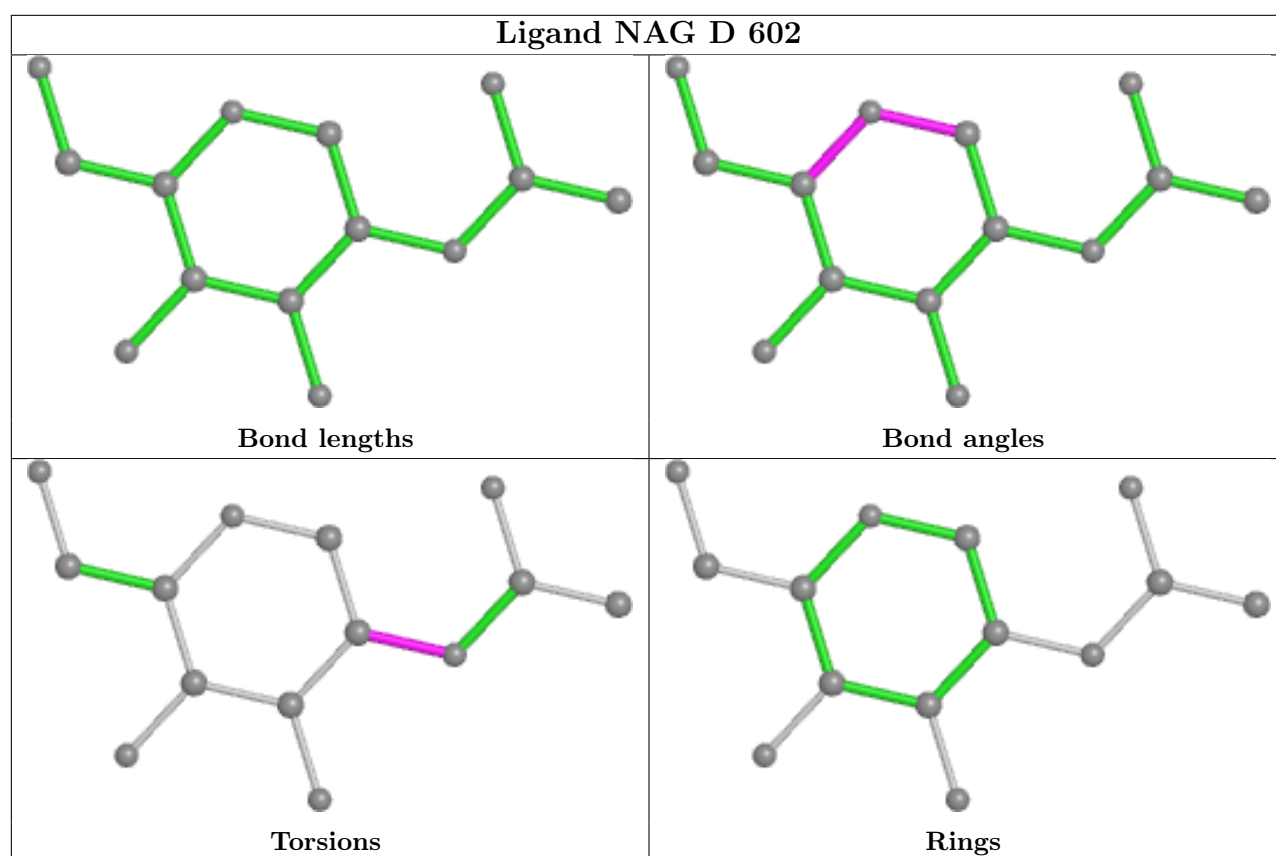
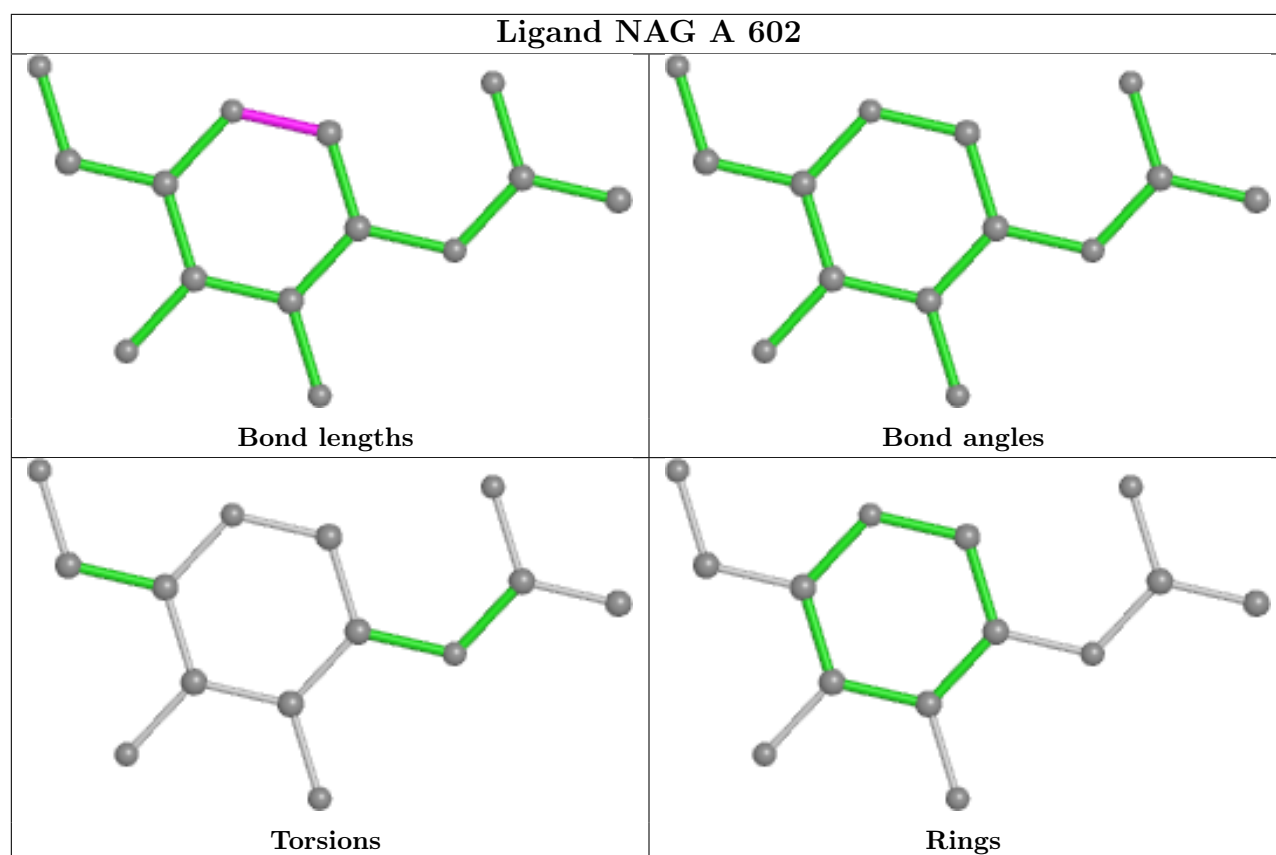
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

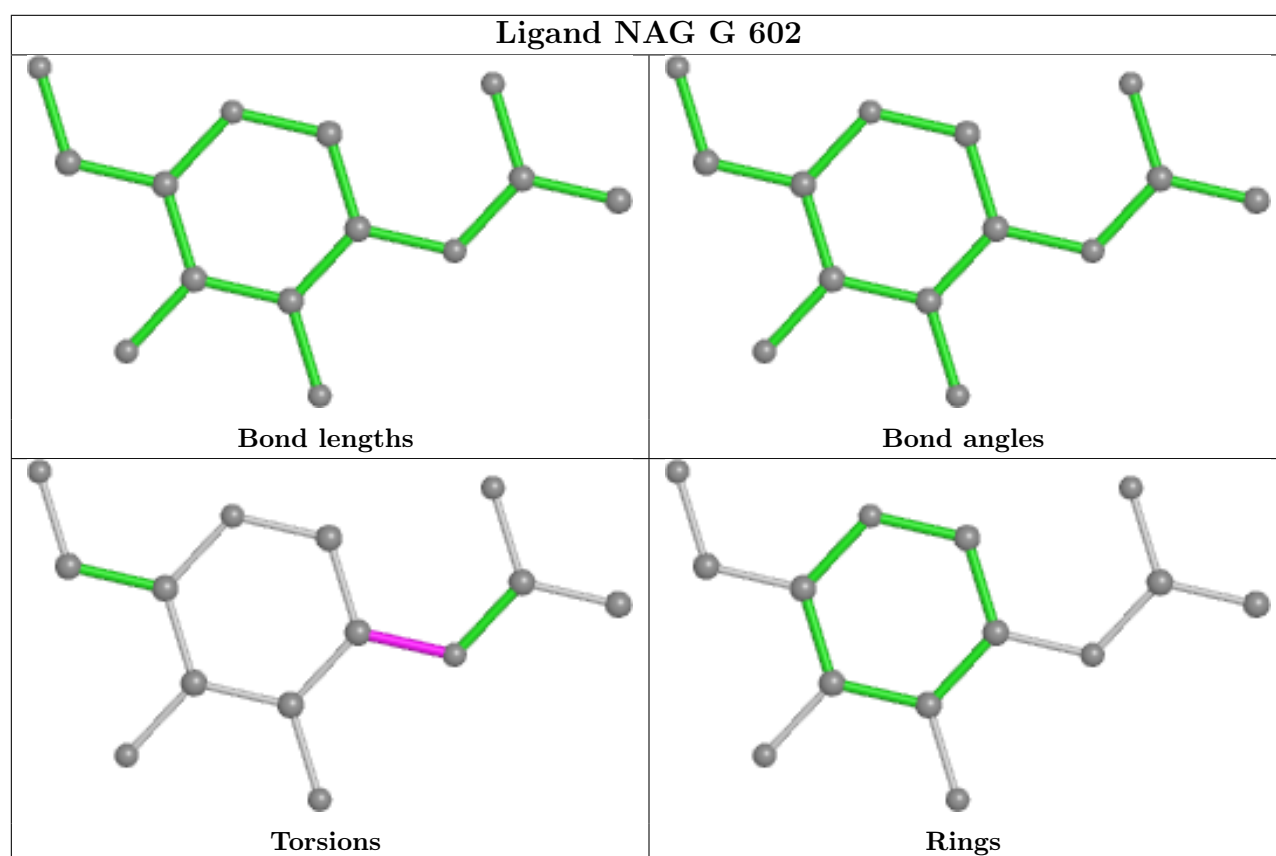
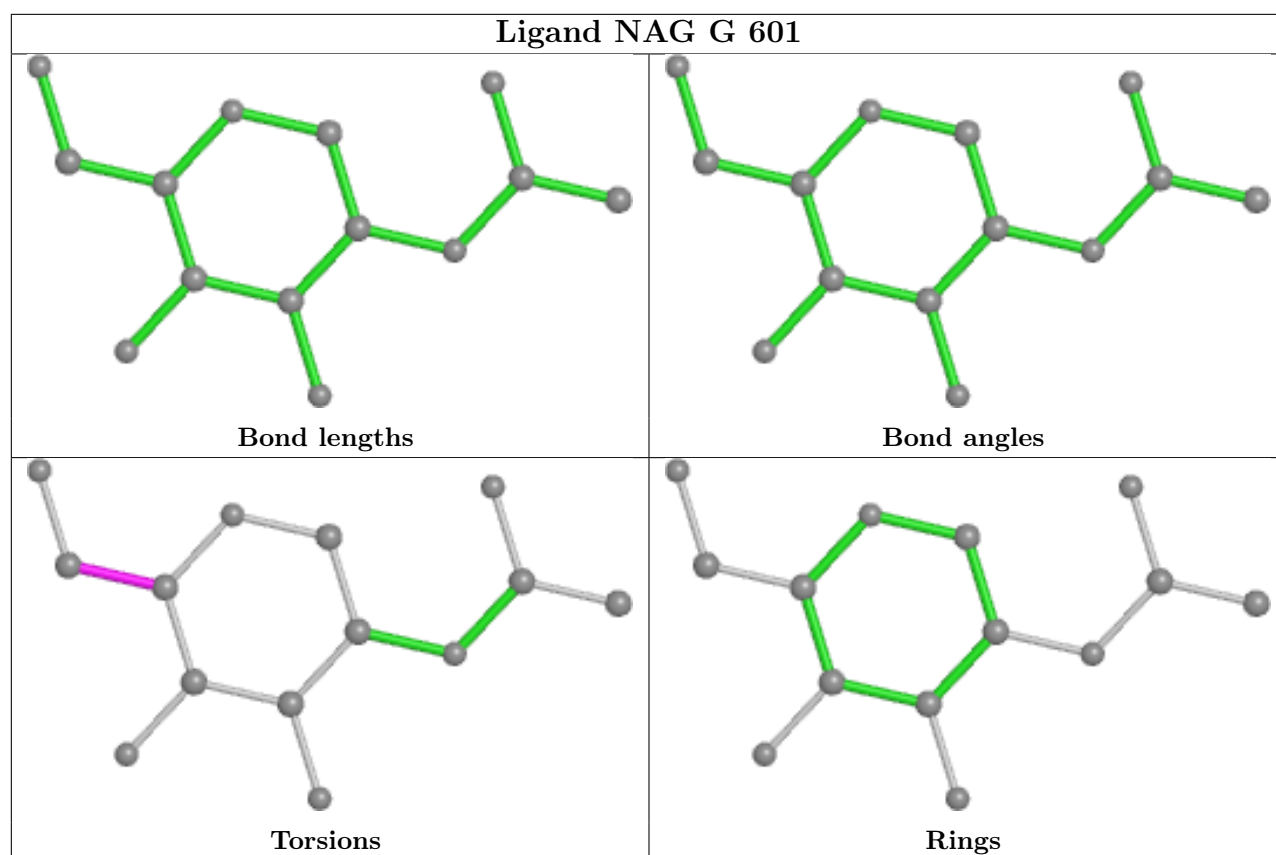
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

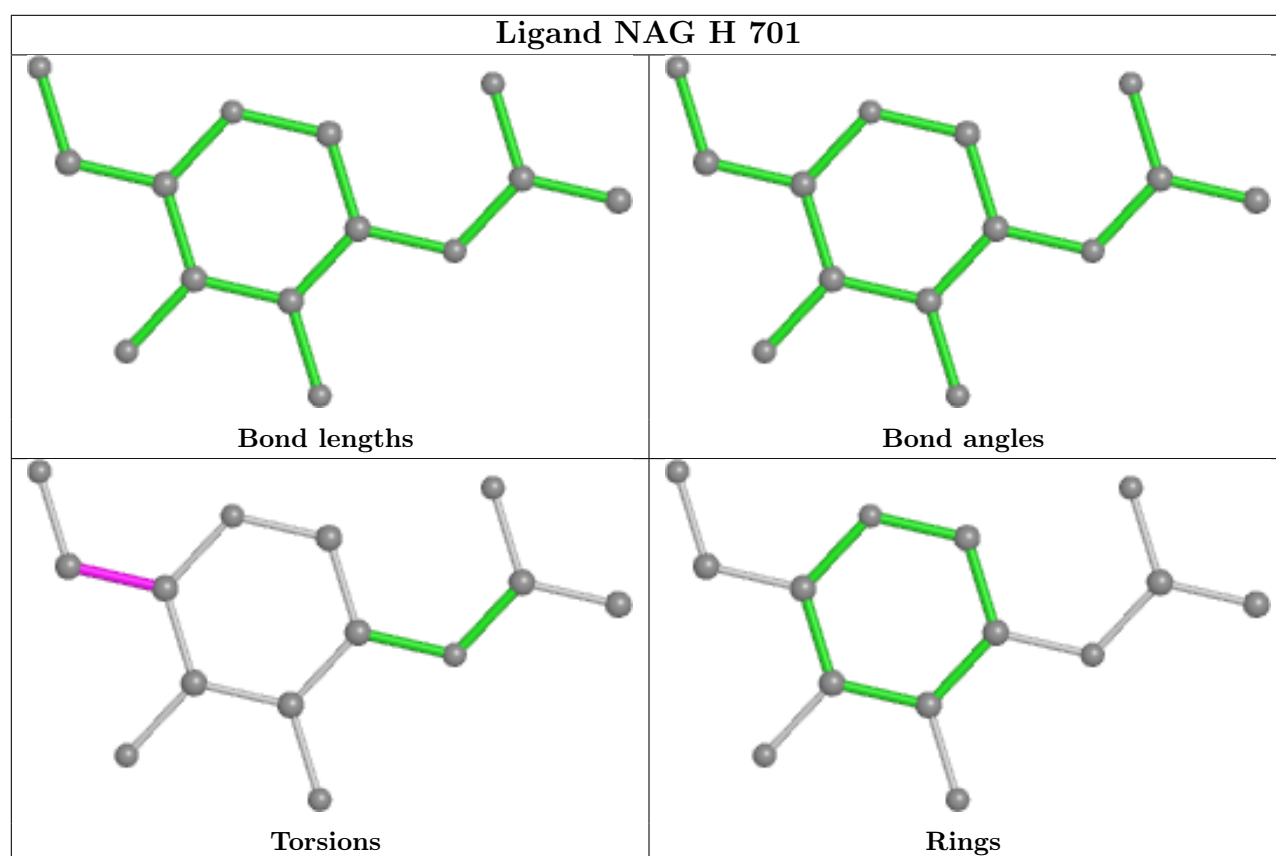
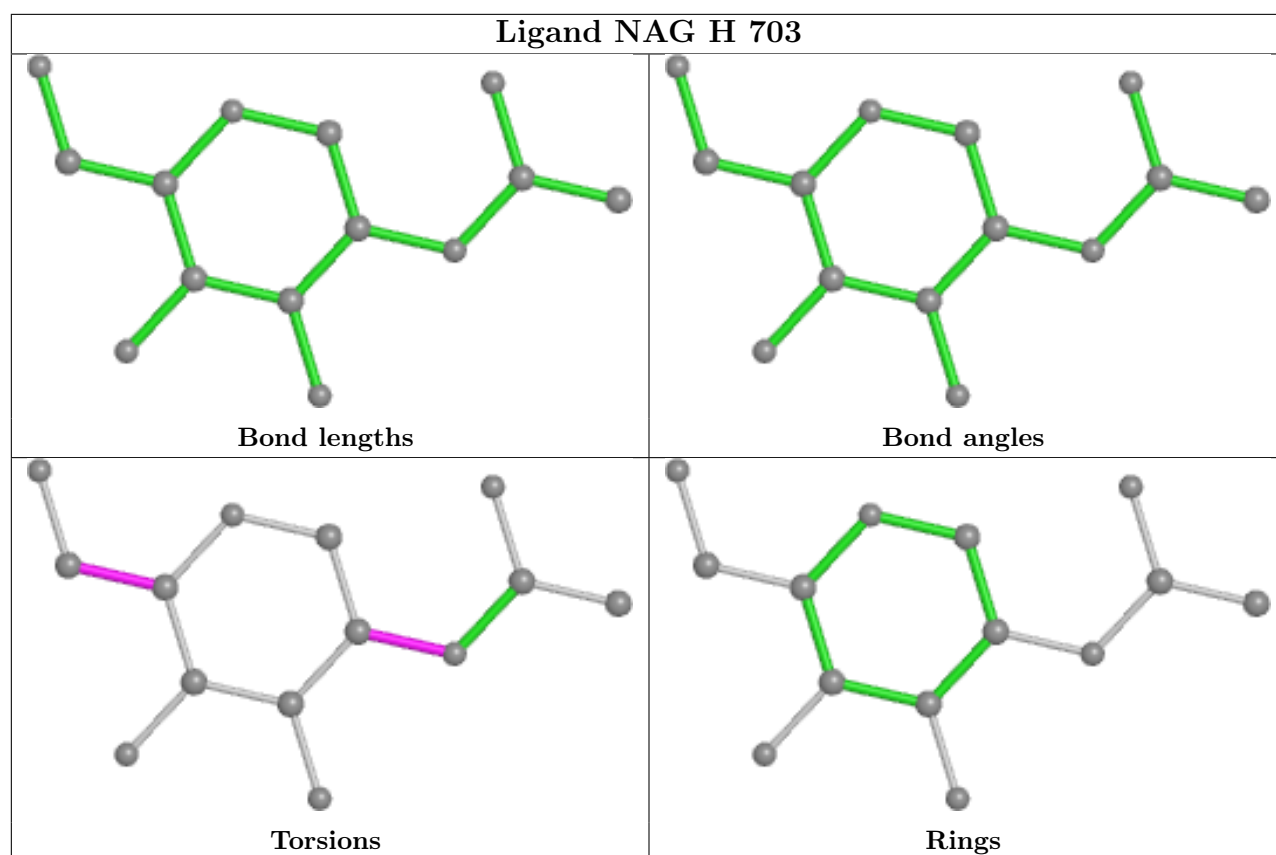


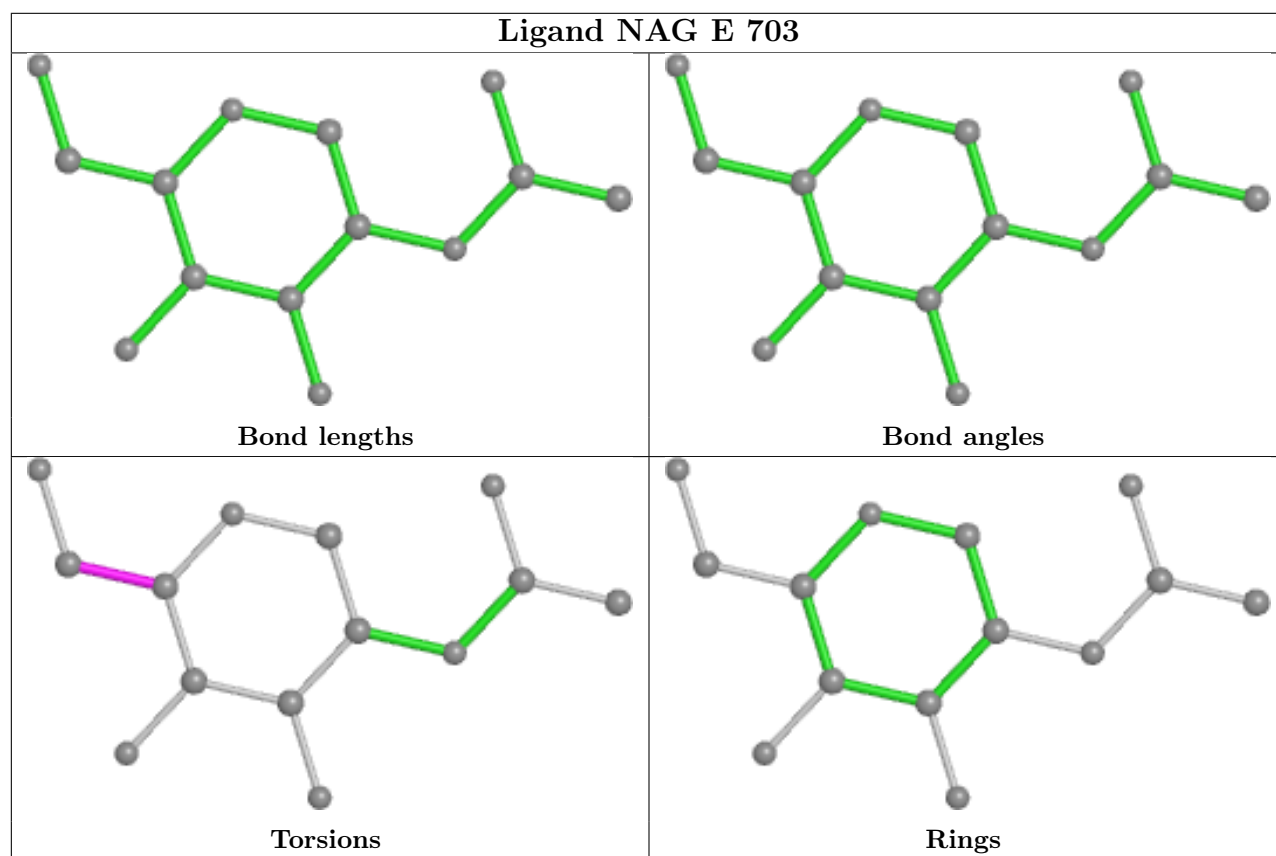
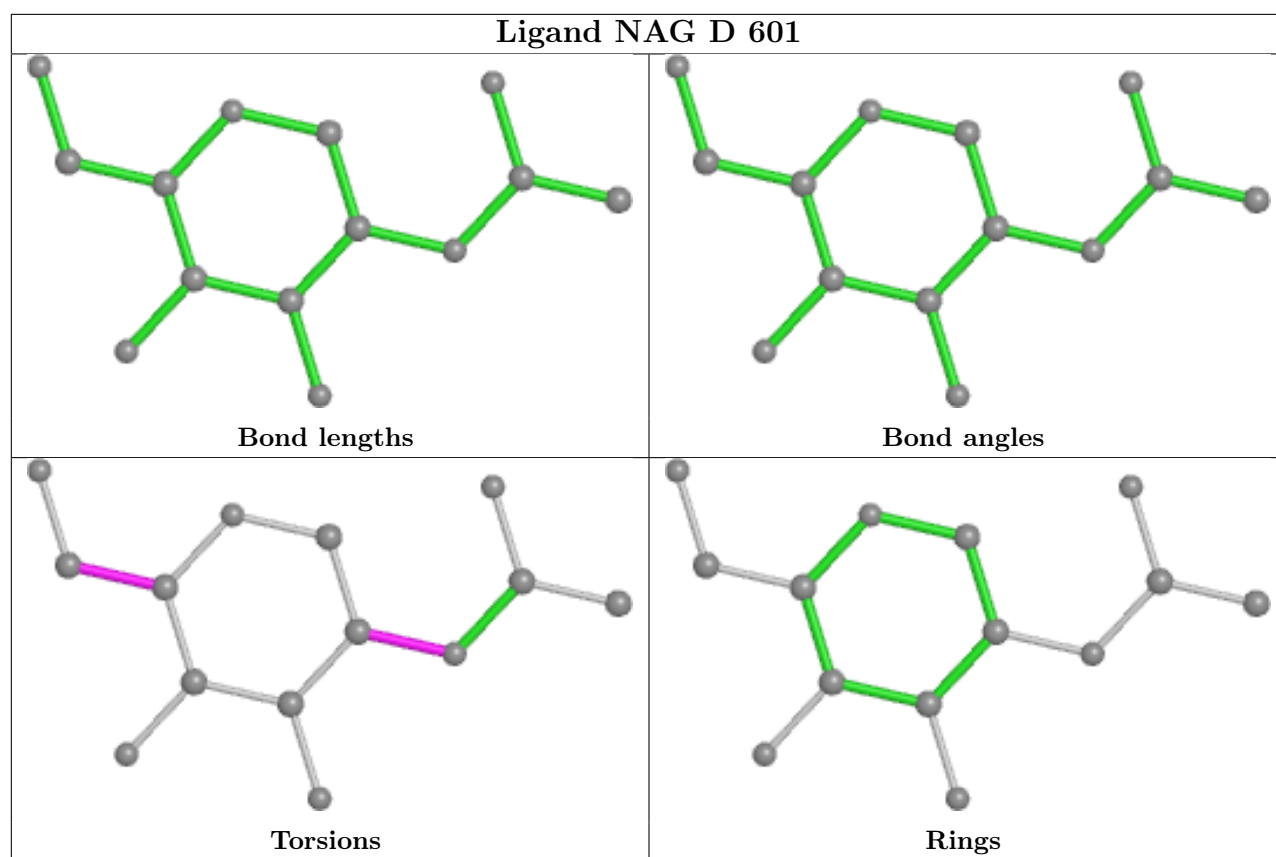


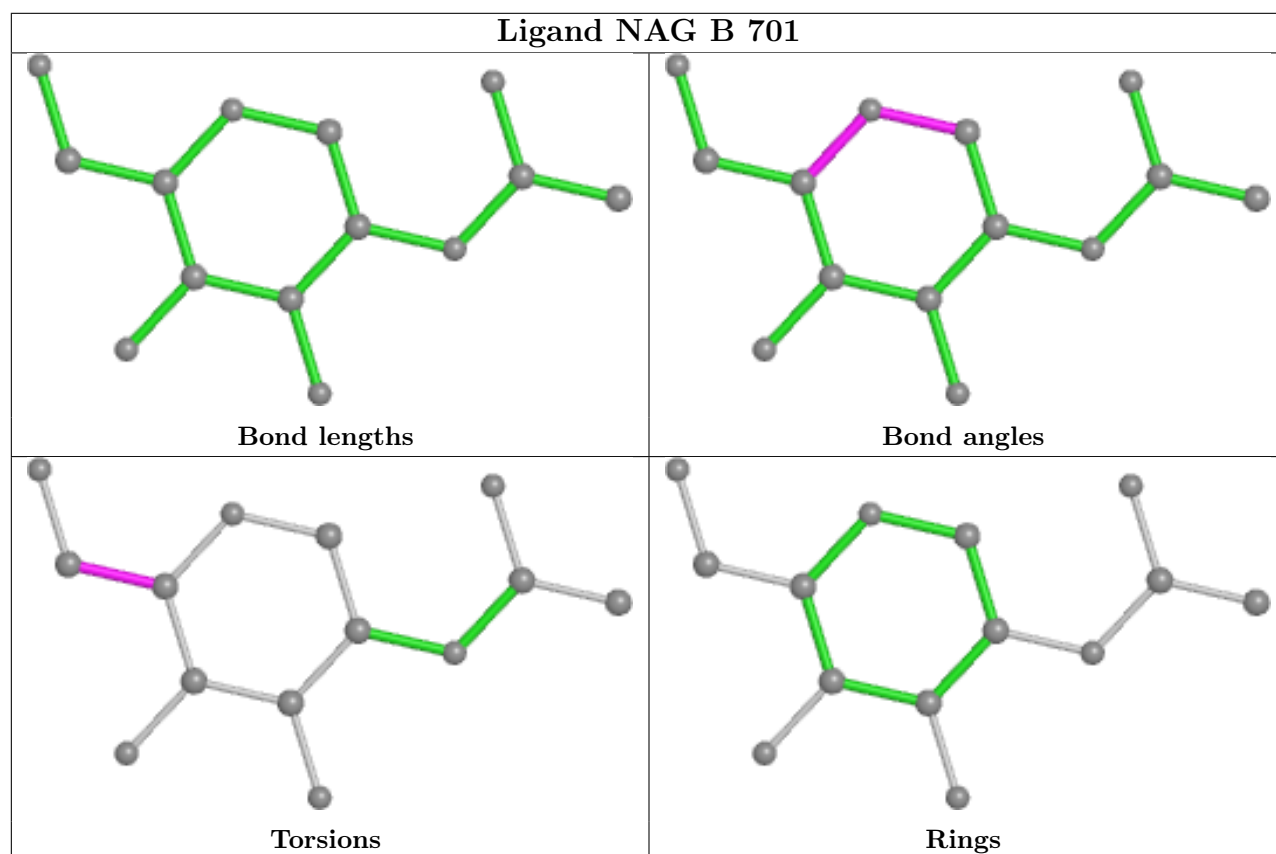
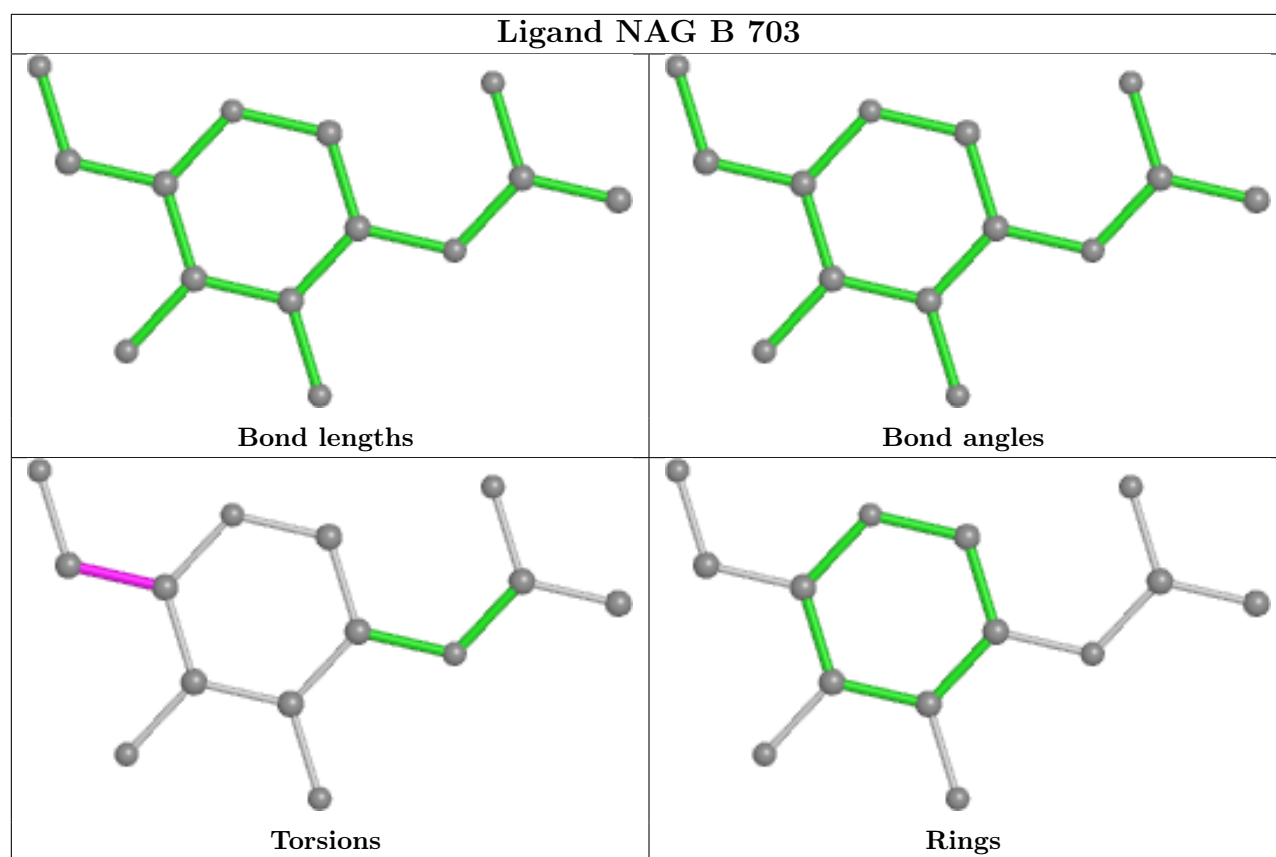


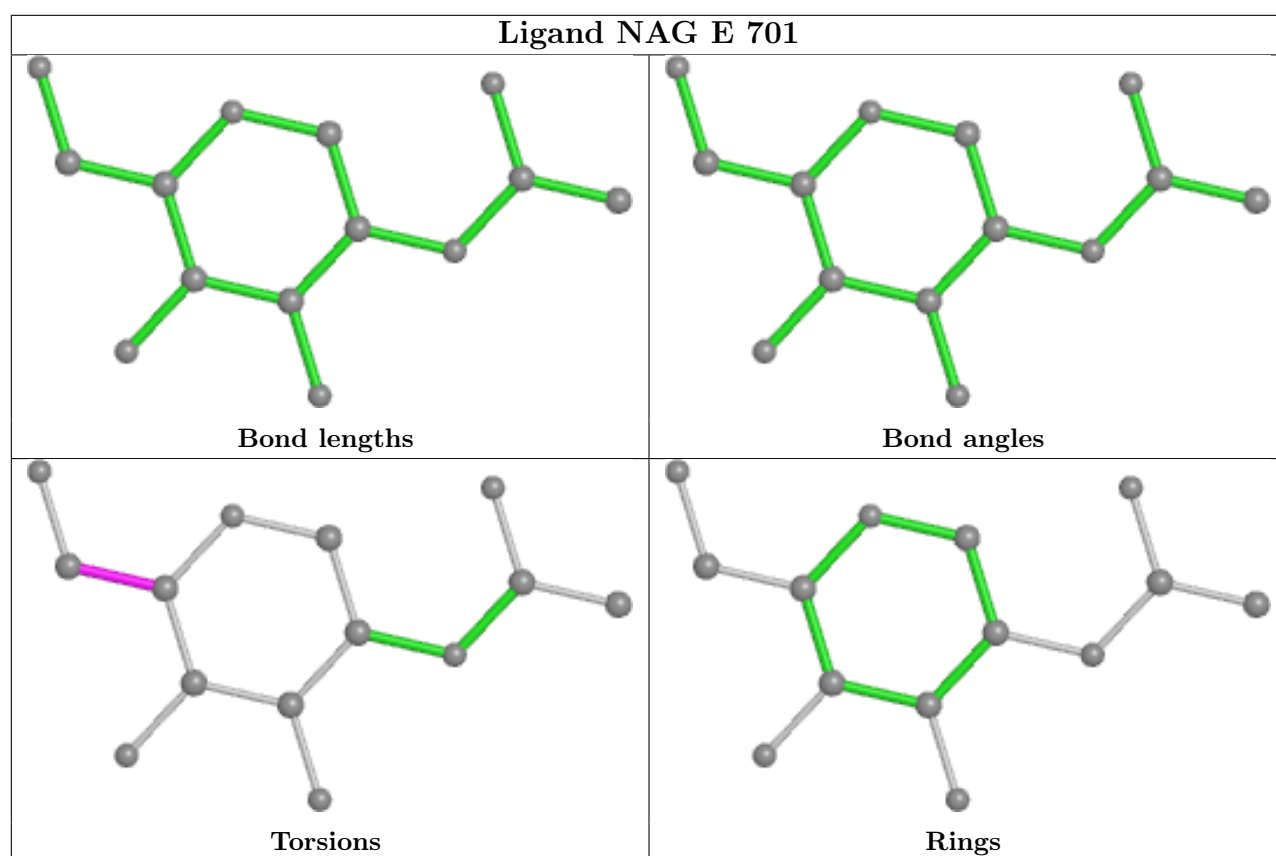
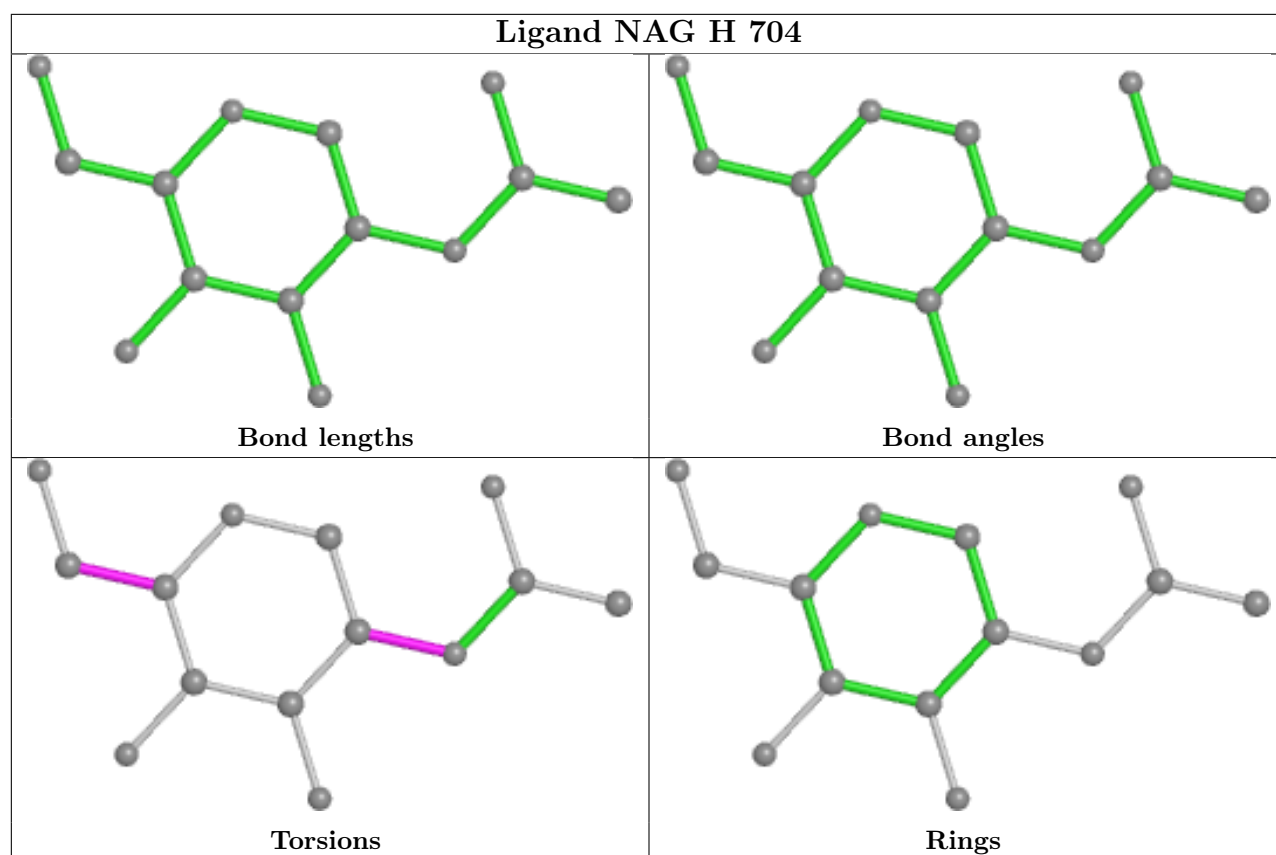


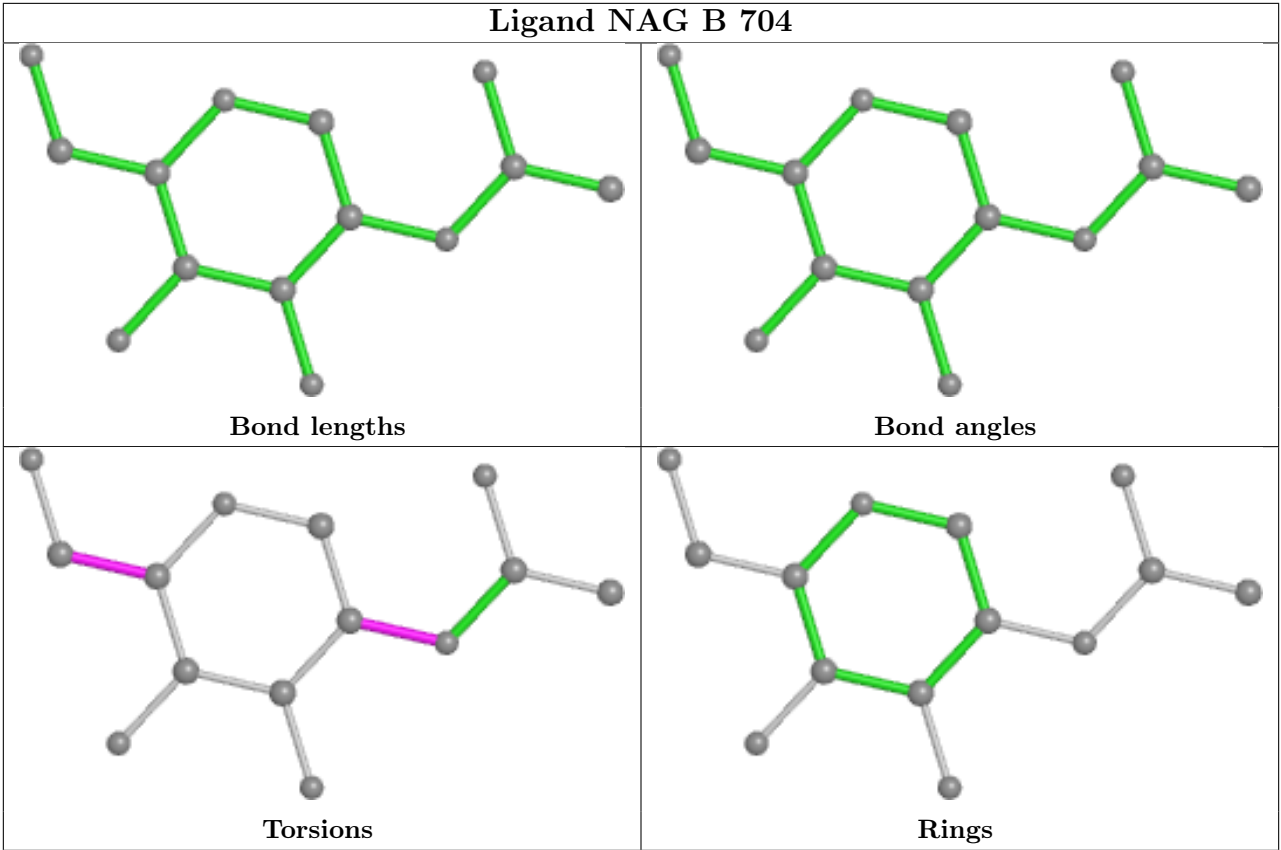












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
1	D	1
1	G	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	341:LYS	C	344:TRP	N	6.12
1	D	341:LYS	C	344:TRP	N	6.12
1	G	341:LYS	C	344:TRP	N	6.12

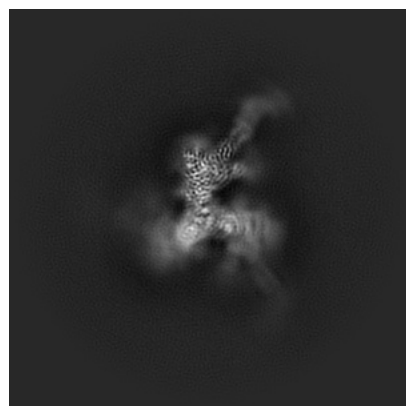
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39820. These allow visual inspection of the internal detail of the map and identification of artifacts.

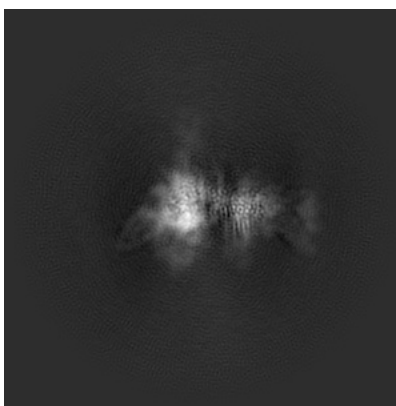
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

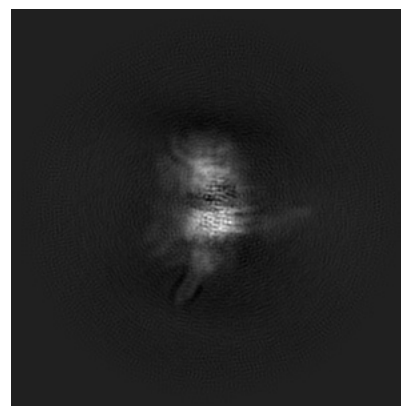
6.1.1 Primary map



X

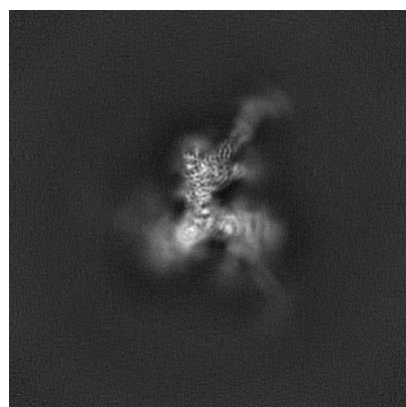


Y

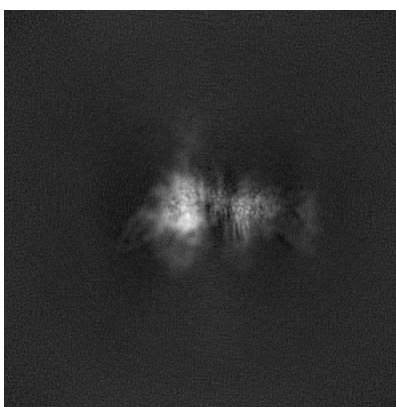


Z

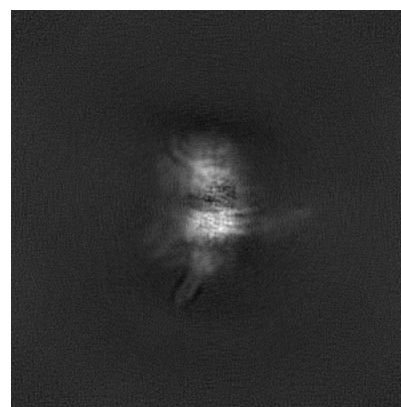
6.1.2 Raw map



X



Y

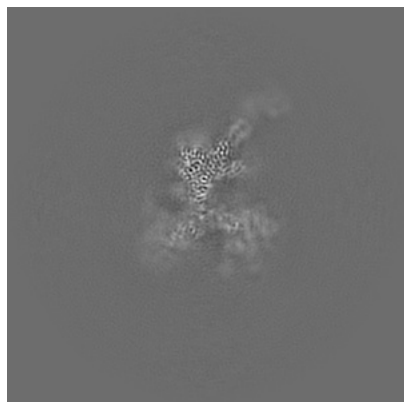


Z

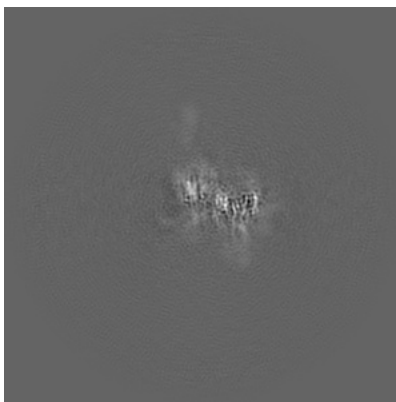
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

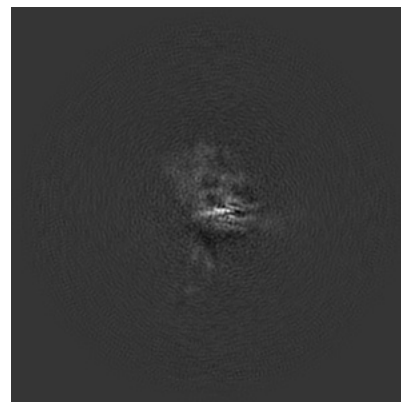
6.2.1 Primary map



X Index: 250

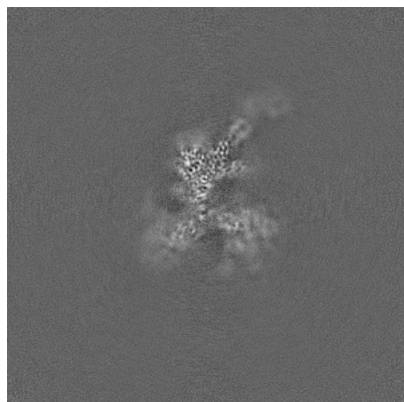


Y Index: 250



Z Index: 250

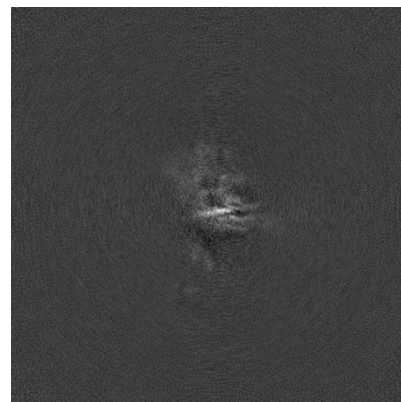
6.2.2 Raw map



X Index: 250



Y Index: 250

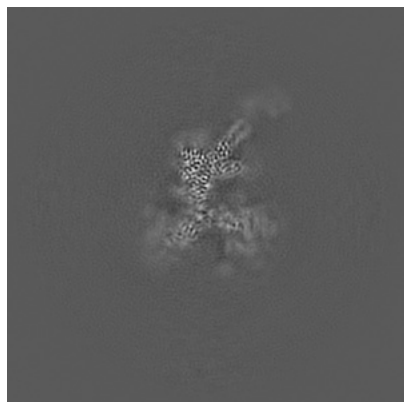


Z Index: 250

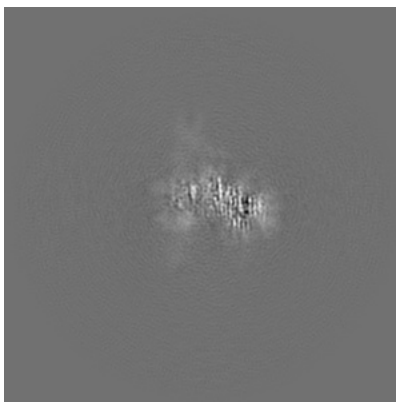
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

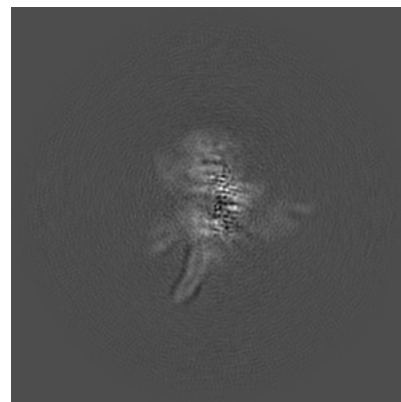
6.3.1 Primary map



X Index: 252

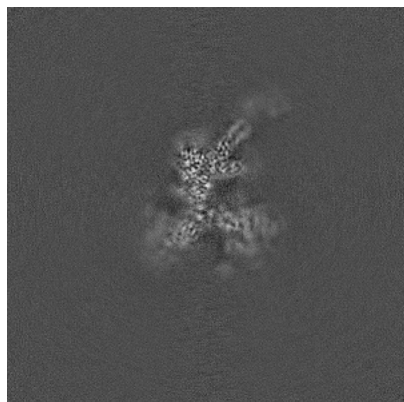


Y Index: 234

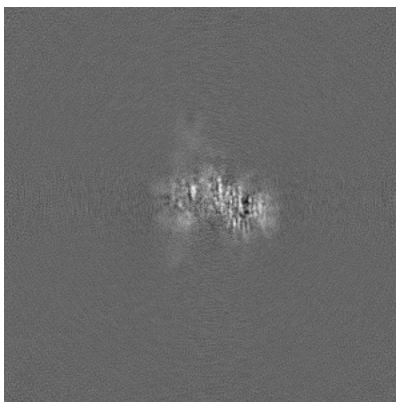


Z Index: 229

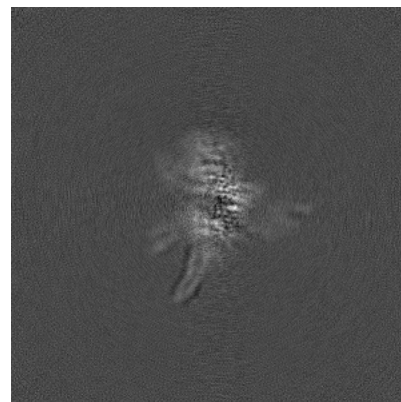
6.3.2 Raw map



X Index: 252



Y Index: 234

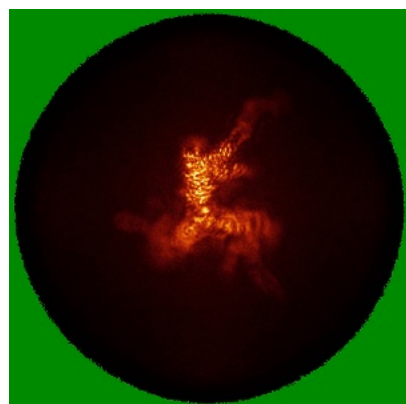


Z Index: 229

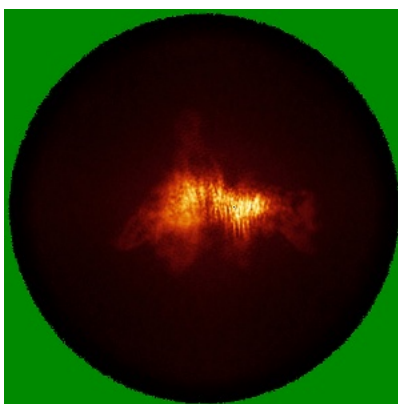
The images above show the largest variance slices of the map in three orthogonal directions.

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

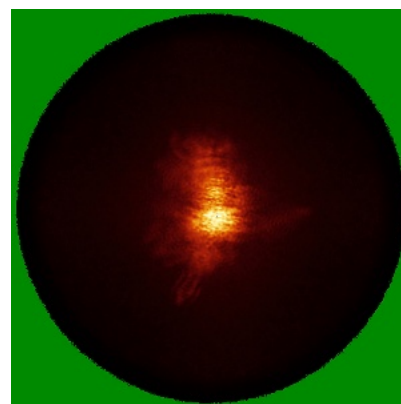
6.4.1 Primary map



X



Y

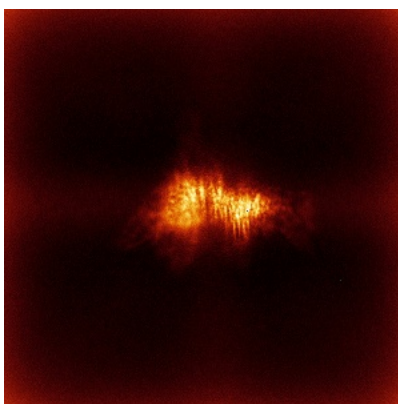


Z

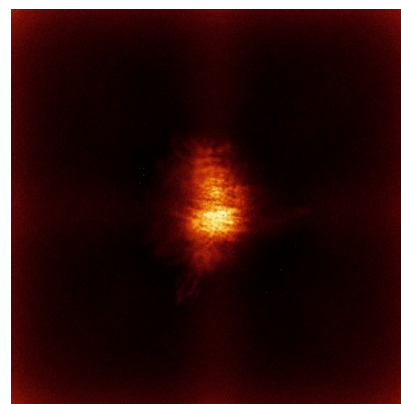
6.4.2 Raw map



X



Y

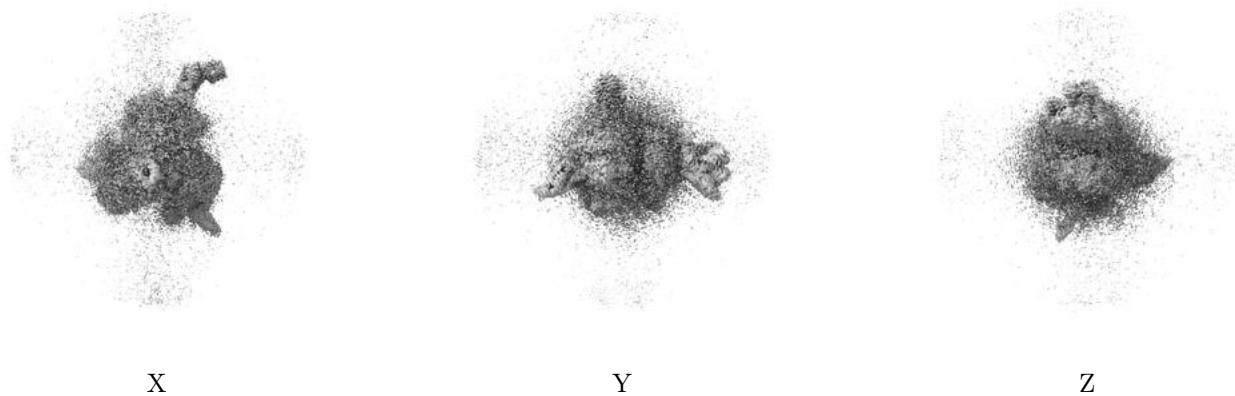


Z

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.

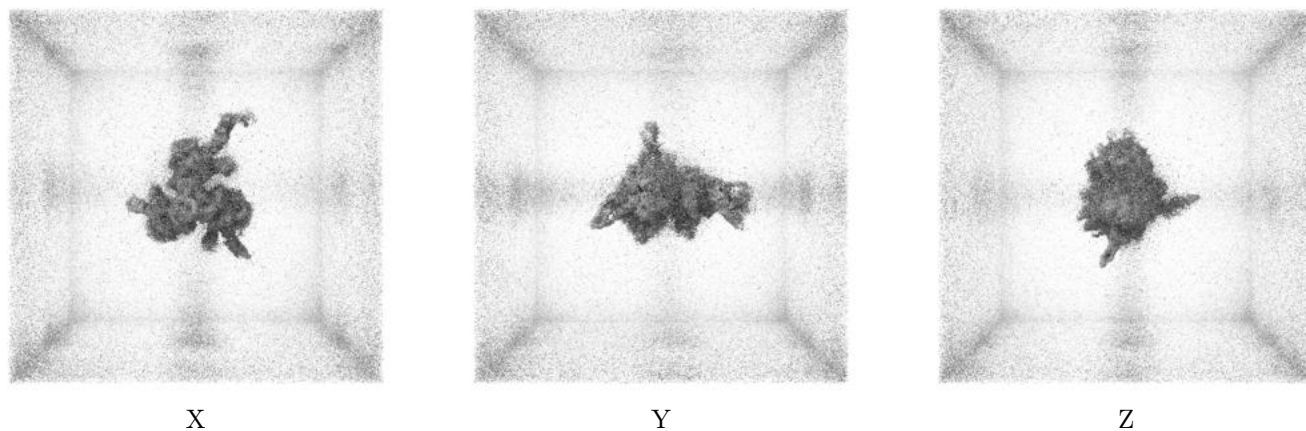
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.049. 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.

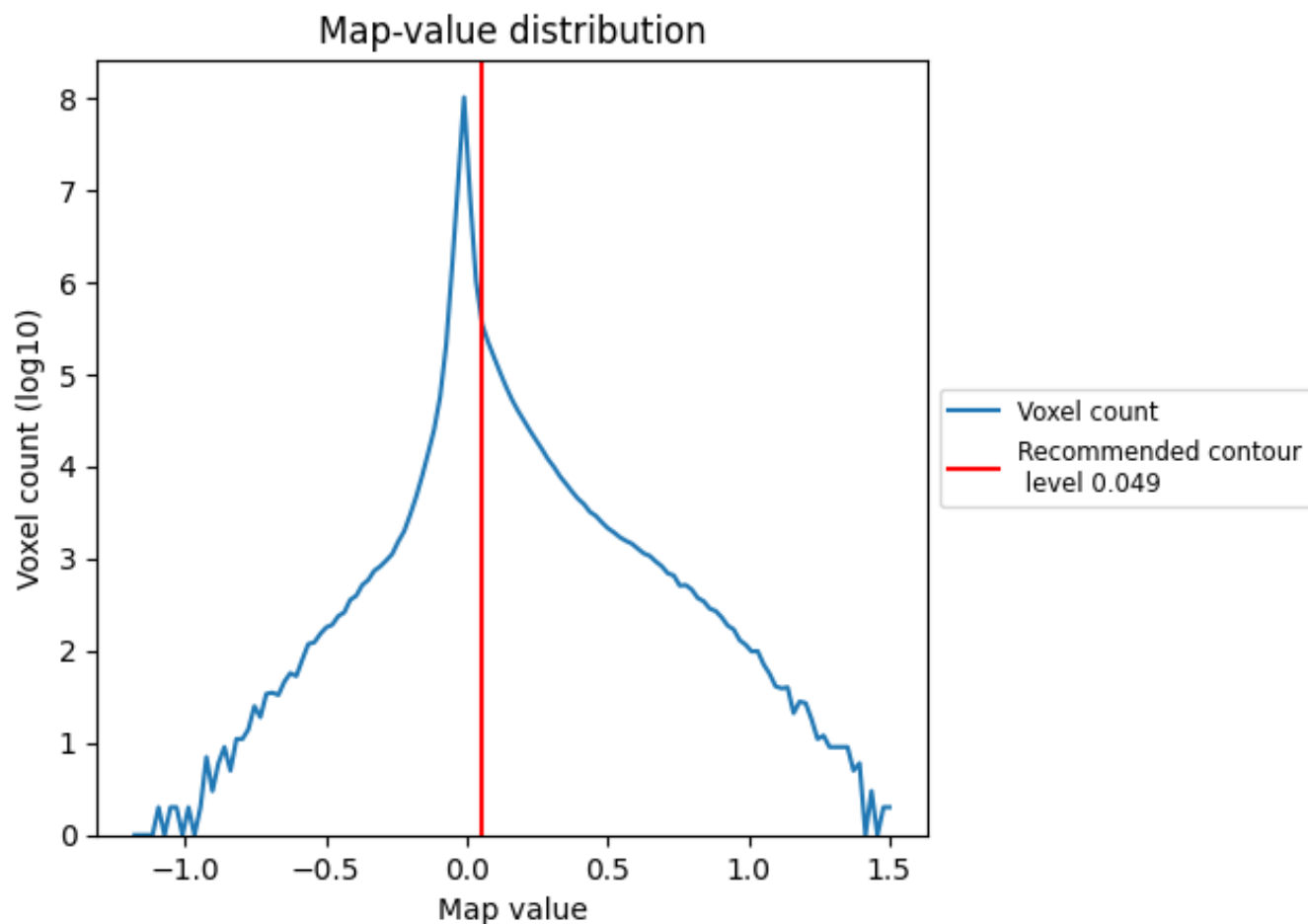
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

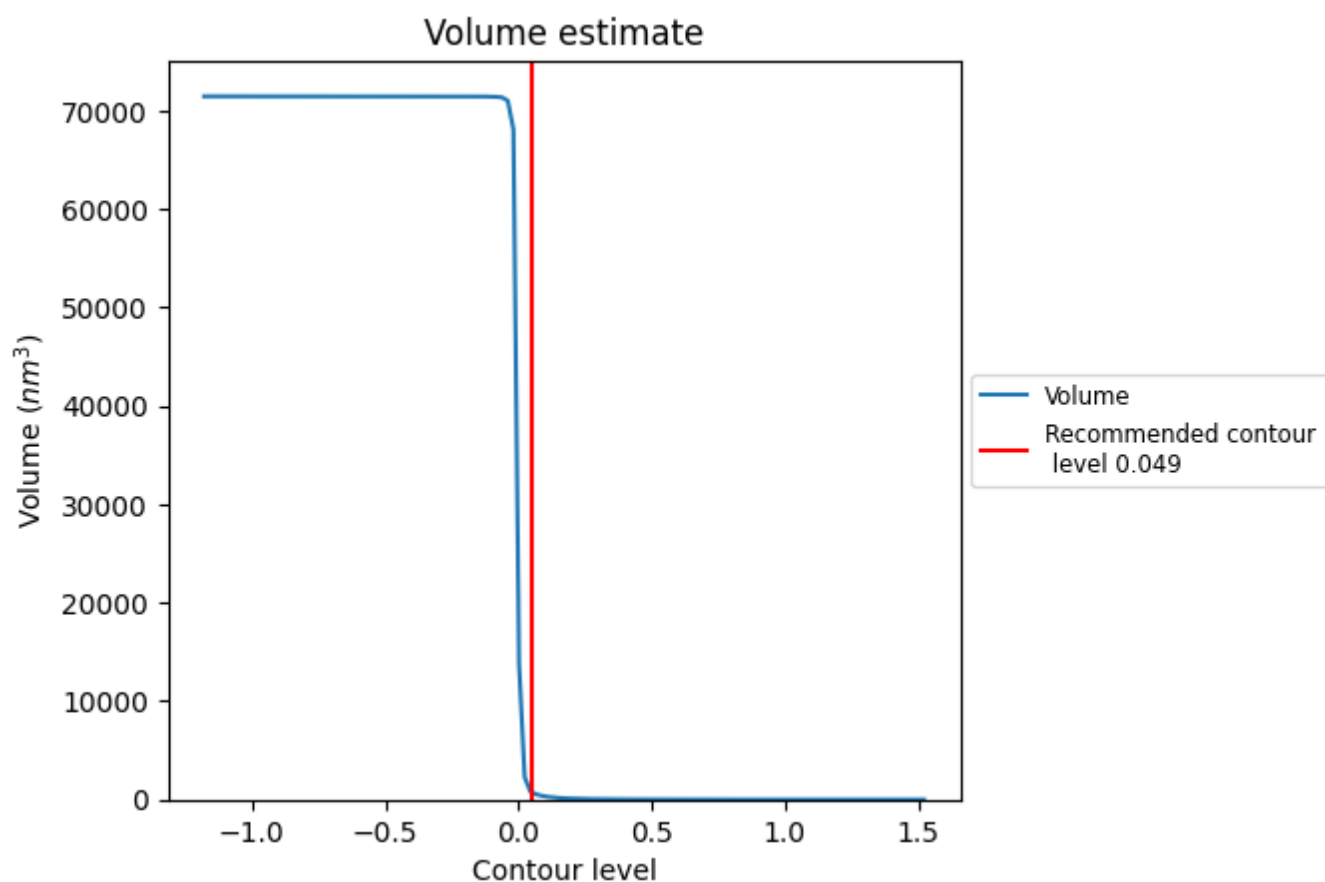
This section contains the results of statistical analysis of the map.

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.

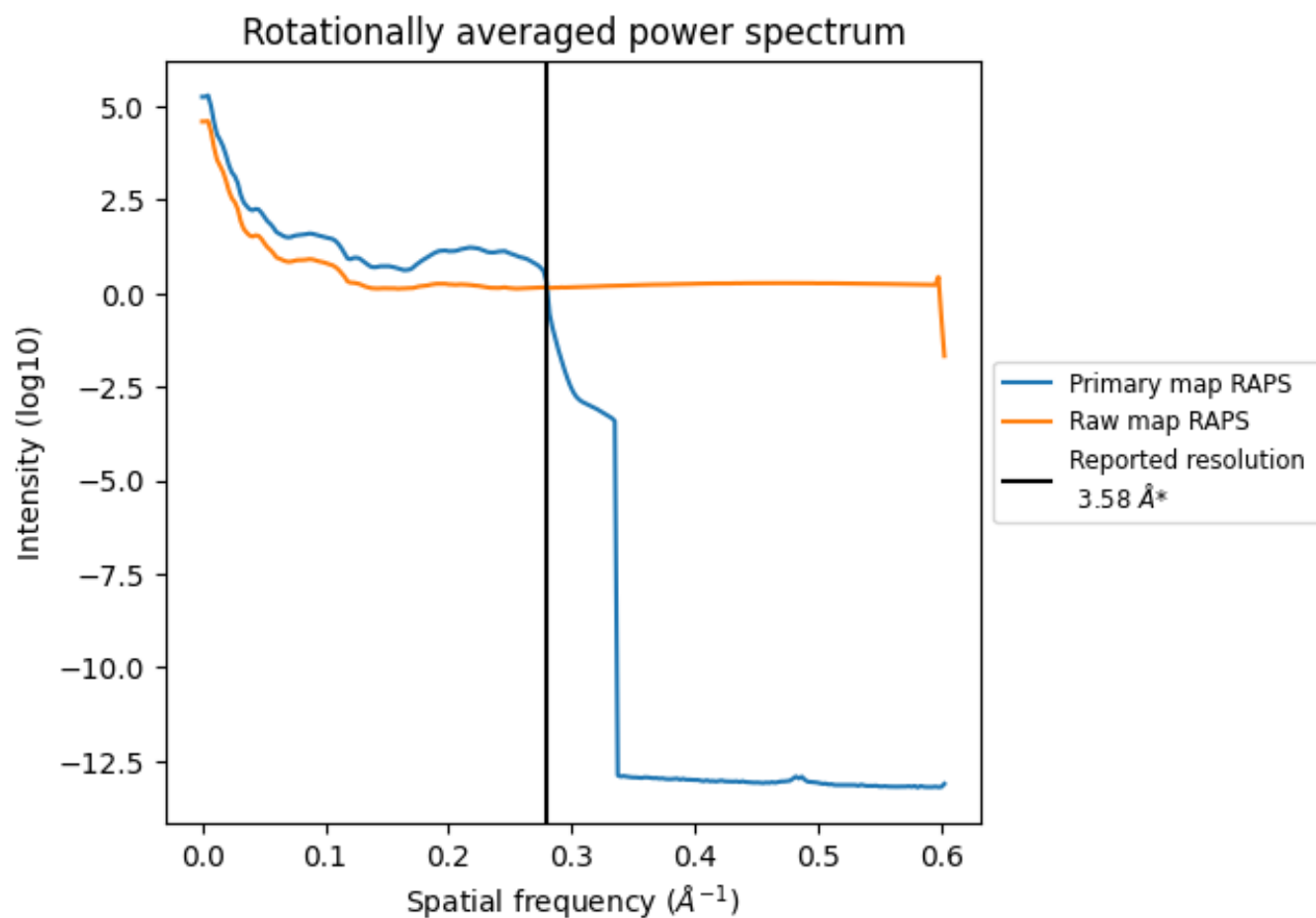
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 757 nm³; this corresponds to an approximate mass of 684 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 ⓘ

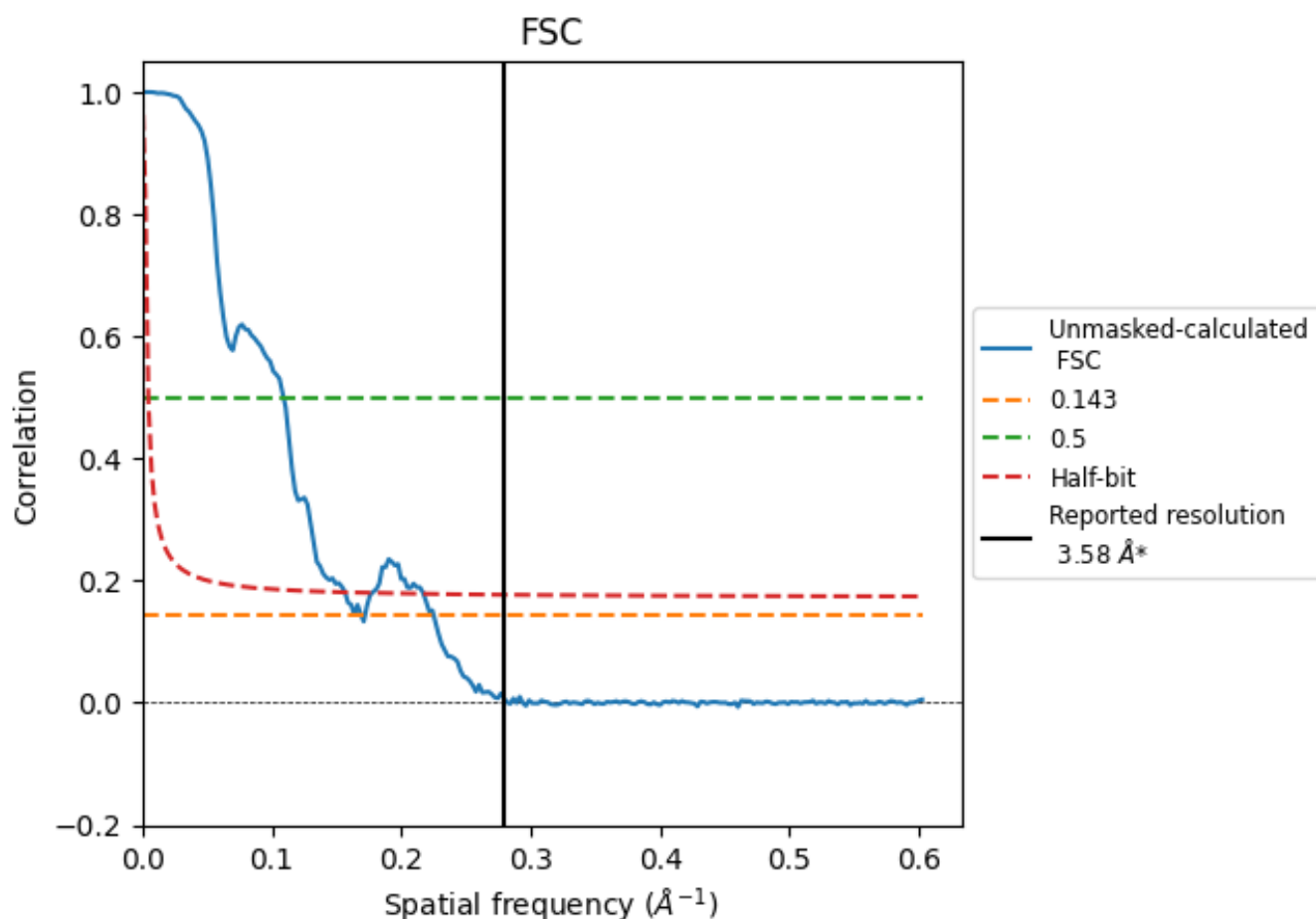


*Reported resolution corresponds to spatial frequency of 0.279 \AA^{-1}

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 0.279 Å⁻¹

8.2 Resolution estimates [i](#)

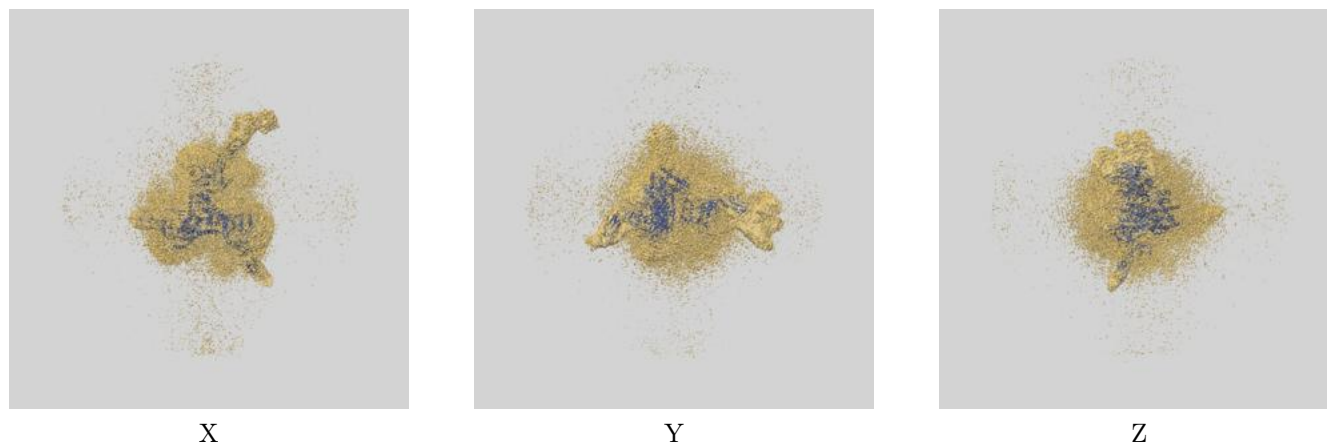
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.58	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	5.91	9.16	6.38

*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 5.91 differs from the reported value 3.58 by more than 10 %

9 Map-model fit [i](#)

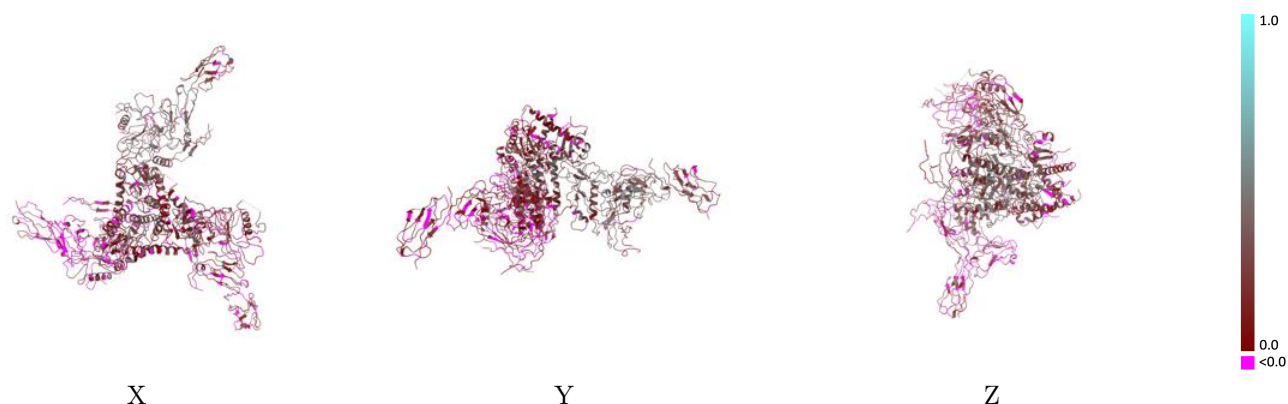
This section contains information regarding the fit between EMDB map EMD-39820 and PDB model 8Z7N. Per-residue inclusion information can be found in [section 3](#) on [page 12](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.049 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](#)



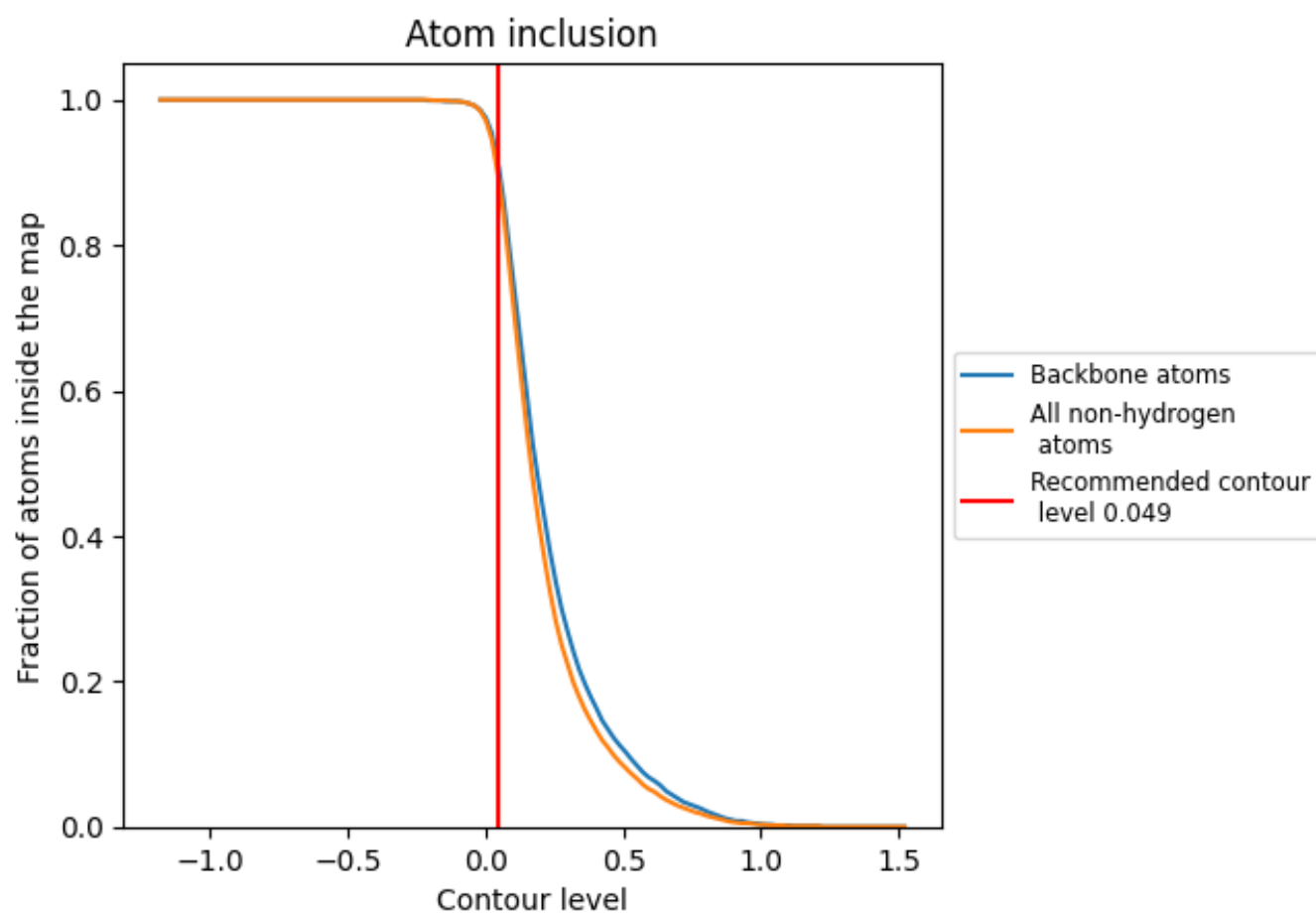
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.049).

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 (0.049) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.8890</div>	<div><div></div>0.1820</div>
A	<div><div></div>0.9330</div>	<div><div></div>0.3200</div>
B	<div><div></div>0.8530</div>	<div><div></div>0.2260</div>
C	<div><div></div>0.9460</div>	<div><div></div>0.3170</div>
D	<div><div></div>0.8590</div>	<div><div></div>0.1230</div>
E	<div><div></div>0.8860</div>	<div><div></div>0.1930</div>
F	<div><div></div>0.8150</div>	<div><div></div>0.0190</div>
G	<div><div></div>0.9240</div>	<div><div></div>0.1320</div>
H	<div><div></div>0.9080</div>	<div><div></div>0.1840</div>
I	<div><div></div>0.8190</div>	<div><div></div>0.0950</div>

1.0

0.0

<0.0