



Full wwPDB EM Validation Report ⓘ

Mar 19, 2026 – 08:54 PM UTC

PDB ID : 7XRP / pdb_00007xrp
EMDB ID : EMD-33416
Title : Cryo-EM structure of SARS-CoV-2 spike protein in complex with nanobody C5G2 (localized refinement)
Authors : Liu, L.; Sun, H.; Jiang, Y.; Liu, X.; Zhao, D.; Zheng, Q.; Li, S.; Xia, N.
Deposited on : 2022-05-11
Resolution : 3.88 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

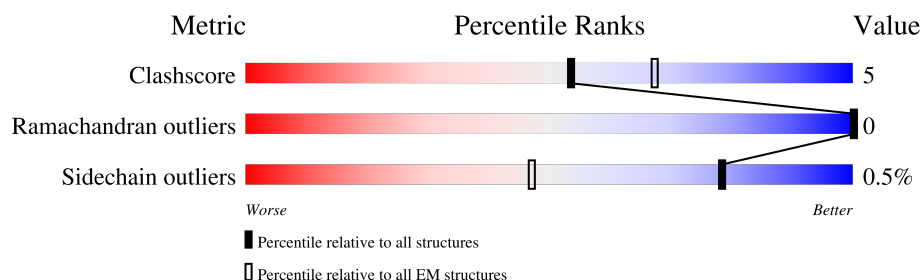
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.88 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	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	283	 63% 10% • 26%
2	B	125	 82% 18% •
3	F	192	 81% 12% • 5%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4129 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 Spike protein S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	209	Total	C	N	O	S	0	0
			1684	1102	269	309	4		

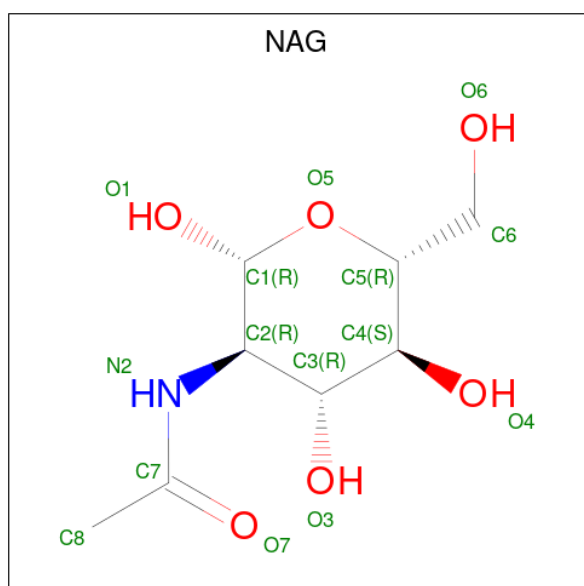
- Molecule 2 is a protein called C5G2 nanobody.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	124	Total	C	N	O	S	0	0
			935	588	160	184	3		

- Molecule 3 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	182	Total	C	N	O	S	0	0
			1454	933	241	273	7		

- 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	A	1	Total	C	N	O	0
			14	8	1	5	
4	F	1	Total	C	N	O	0
			14	8	1	5	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	120400	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60.0	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	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	0.37	1/1726 (0.1%)	0.70	5/2347 (0.2%)
2	B	0.19	0/954	0.46	0/1291
3	F	0.69	5/1495 (0.3%)	0.86	6/2032 (0.3%)
All	All	0.48	6/4175 (0.1%)	0.72	11/5670 (0.2%)

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
3	F	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	352	ALA	CA-C	-8.26	1.44	1.53
3	F	349	SER	CA-C	-7.39	1.43	1.53
3	F	346	ARG	CA-C	-6.18	1.45	1.52
3	F	347	PHE	CA-C	-5.99	1.45	1.52
3	F	348	ALA	CA-C	-5.21	1.46	1.53
1	A	216	LEU	CA-C	-5.08	1.48	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	214	ARG	N-CA-C	-16.02	84.30	109.76
3	F	350	VAL	N-CA-C	7.68	118.46	110.62
1	A	122	ASN	N-CA-C	7.00	118.92	111.28
3	F	473	TYR	N-CA-C	6.69	121.61	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	130	VAL	N-CA-C	-6.10	107.19	113.10
3	F	410	ILE	N-CA-C	-5.80	107.09	112.83
3	F	432	CYS	N-CA-C	5.69	119.57	107.67
3	F	429	PHE	N-CA-C	5.64	120.66	113.55
3	F	425	LEU	N-CA-C	-5.31	101.35	109.64
1	A	216	LEU	N-CA-C	-5.21	97.23	107.91
1	A	213	VAL	N-CA-C	5.18	120.11	109.34

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	F	336	CYS	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	1684	0	1645	18	0
2	B	935	0	893	17	0
3	F	1454	0	1373	10	0
4	A	42	0	39	1	0
4	F	14	0	13	0	0
All	All	4129	0	3963	42	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (42) 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:18:LEU:H	2:B:83:MET:HB2	1.71	0.56
2:B:18:LEU:HB2	2:B:83:MET:HG3	1.93	0.51
3:F:364:ASP:O	3:F:388:ASN:ND2	2.43	0.51
1:A:106:PHE:O	1:A:117:LEU:N	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:PHE:HB2	1:A:117:LEU:HB3	1.95	0.49
2:B:36:TRP:HB2	2:B:49:ALA:HB3	1.95	0.49
2:B:67:ARG:HE	2:B:85:SER:HG	1.59	0.49
1:A:290:ASP:O	1:A:297:SER:OG	2.28	0.49
2:B:19:ARG:NE	2:B:82:GLN:OE1	2.44	0.49
2:B:67:ARG:NH2	2:B:85:SER:O	2.46	0.49
3:F:478:THR:HG22	3:F:480:CYS:H	1.78	0.48
1:A:274:THR:HG23	1:A:291:CYS:HB2	1.95	0.47
1:A:201:PHE:HB3	1:A:229:LEU:HB2	1.97	0.47
2:B:103:SER:O	2:B:103:SER:OG	2.29	0.46
1:A:39:PRO:HG3	1:A:51:THR:HG21	1.97	0.46
1:A:123:ALA:HB2	4:A:403:NAG:HN2	1.80	0.46
3:F:425:LEU:HD23	3:F:425:LEU:HA	1.57	0.46
1:A:28:TYR:HE1	1:A:63:THR:HG22	1.81	0.45
1:A:167:THR:HG22	2:B:104:ARG:HB3	1.98	0.45
1:A:206:LYS:HA	1:A:206:LYS:HD2	1.74	0.45
3:F:422:ASN:HD22	3:F:422:ASN:N	2.15	0.45
2:B:20:LEU:HB2	2:B:81:LEU:HB3	1.98	0.45
1:A:213:VAL:HG13	1:A:213:VAL:O	2.17	0.44
2:B:67:ARG:NE	2:B:85:SER:HG	2.15	0.44
3:F:401:VAL:HG12	3:F:509:ARG:HG2	2.01	0.43
1:A:37:TYR:OH	1:A:54:LEU:O	2.33	0.43
2:B:39:GLN:OE1	2:B:45:ARG:NE	2.45	0.43
1:A:232:GLY:O	2:B:106:ASN:ND2	2.52	0.43
3:F:383:SER:OG	3:F:385:THR:O	2.28	0.43
3:F:430:THR:HG22	3:F:430:THR:O	2.19	0.42
1:A:103:GLY:O	1:A:241:LEU:N	2.52	0.42
1:A:51:THR:O	1:A:274:THR:OG1	2.26	0.42
2:B:110:ILE:HD11	3:F:356:LYS:HB2	2.02	0.42
1:A:193:VAL:HB	1:A:204:TYR:HD2	1.85	0.41
3:F:410:ILE:O	3:F:425:LEU:HD12	2.20	0.41
1:A:130:VAL:O	1:A:130:VAL:HG12	2.20	0.41
2:B:67:ARG:NE	2:B:85:SER:OG	2.52	0.41
1:A:105:ILE:N	1:A:239:GLN:O	2.49	0.40
2:B:88:PRO:HG3	2:B:124:SER:HA	2.04	0.40
3:F:393:THR:OG1	3:F:517:LEU:O	2.40	0.40
2:B:38:ARG:HH22	2:B:63:SER:HB3	1.87	0.40
2:B:91:THR:HG22	2:B:123:VAL:H	1.86	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	197/283 (70%)	176 (89%)	21 (11%)	0	100	100
2	B	122/125 (98%)	116 (95%)	6 (5%)	0	100	100
3	F	180/192 (94%)	165 (92%)	15 (8%)	0	100	100
All	All	499/600 (83%)	457 (92%)	42 (8%)	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	189/253 (75%)	188 (100%)	1 (0%)	81	81
2	B	96/97 (99%)	96 (100%)	0	100	100
3	F	158/167 (95%)	157 (99%)	1 (1%)	78	80
All	All	443/517 (86%)	441 (100%)	2 (0%)	78	81

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	121	ASN
3	F	395	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	271	GLN
2	B	106	ASN
3	F	394	ASN
3	F	481	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	F	601	3	14,14,15	0.31	0	17,19,21	0.72	0
4	NAG	A	401	1	14,14,15	0.27	0	17,19,21	0.99	1 (5%)
4	NAG	A	403	1	14,14,15	0.28	0	17,19,21	0.60	0
4	NAG	A	402	1	14,14,15	0.30	0	17,19,21	0.57	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	F	601	3	-	2/6/23/26	0/1/1/1
4	NAG	A	401	1	-	3/6/23/26	0/1/1/1
4	NAG	A	403	1	-	2/6/23/26	0/1/1/1
4	NAG	A	402	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	401	NAG	C2-N2-C7	2.63	126.42	122.90

There are no chirality outliers.

All (7) torsion outliers are listed below:

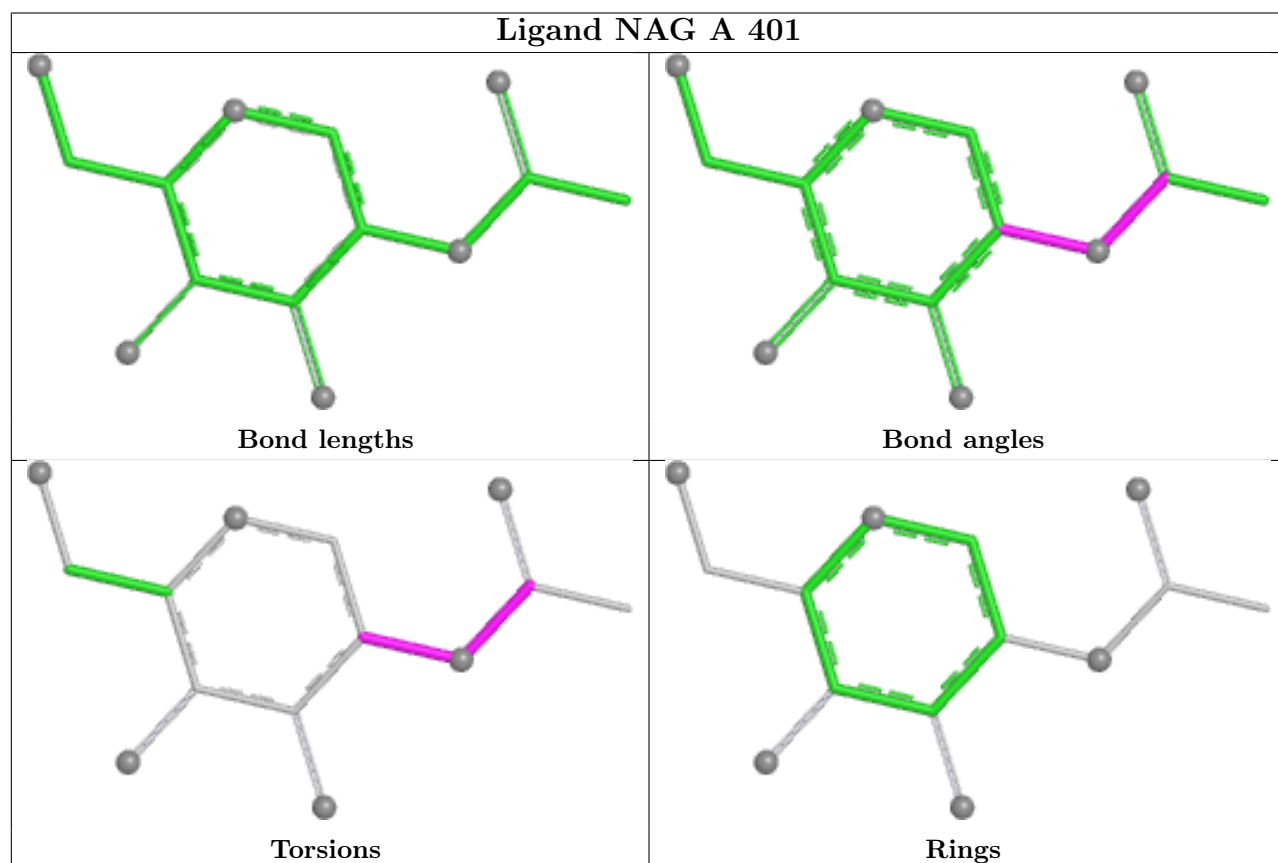
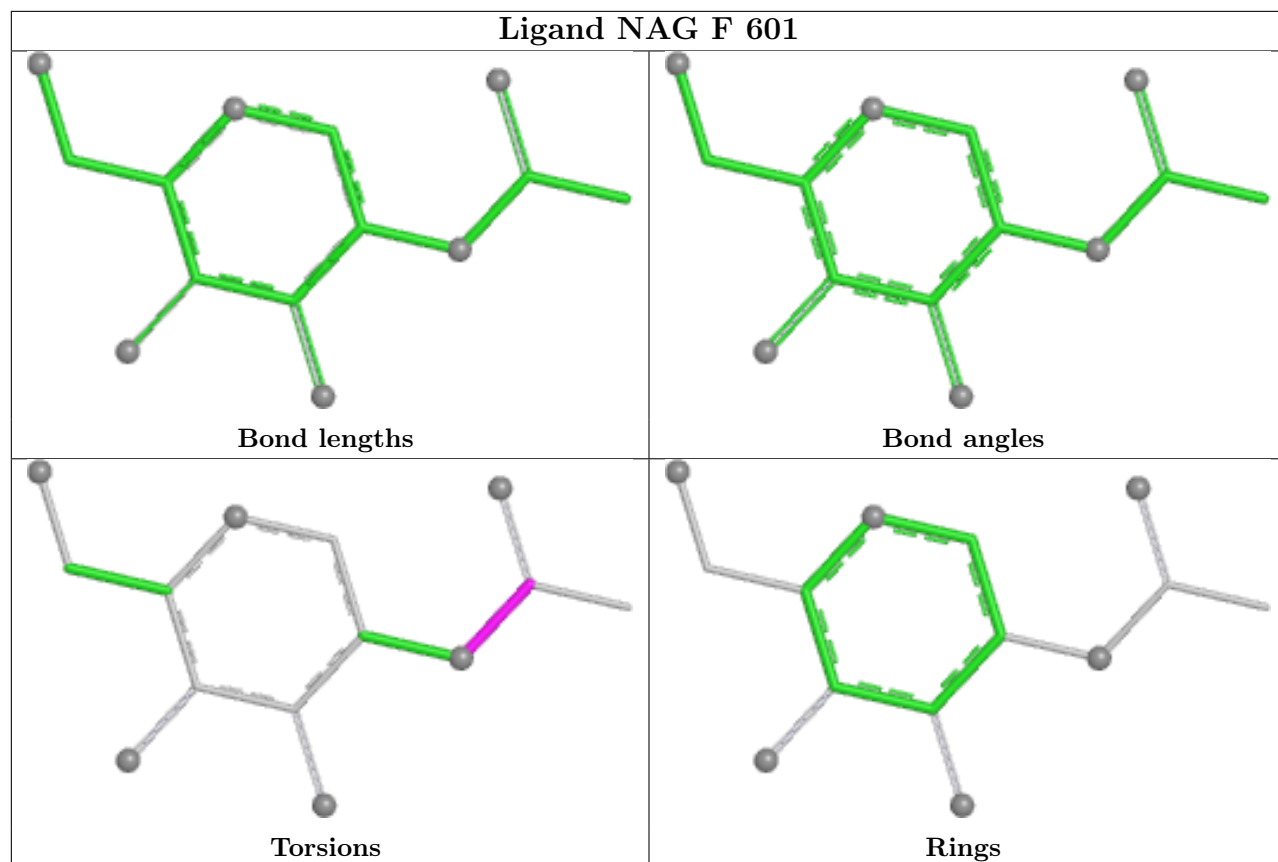
Mol	Chain	Res	Type	Atoms
4	A	401	NAG	C1-C2-N2-C7
4	A	401	NAG	C8-C7-N2-C2
4	A	401	NAG	O7-C7-N2-C2
4	A	403	NAG	C8-C7-N2-C2
4	A	403	NAG	O7-C7-N2-C2
4	F	601	NAG	C8-C7-N2-C2
4	F	601	NAG	O7-C7-N2-C2

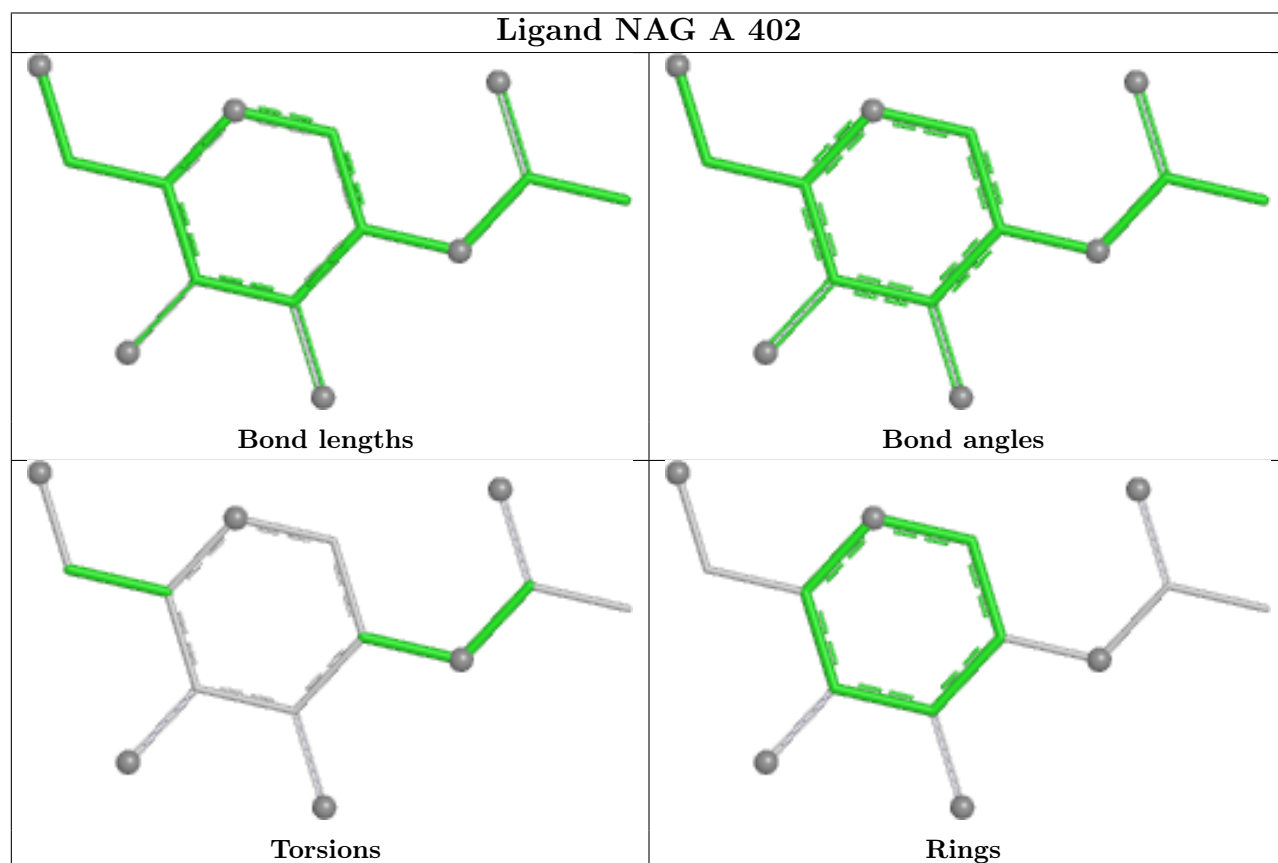
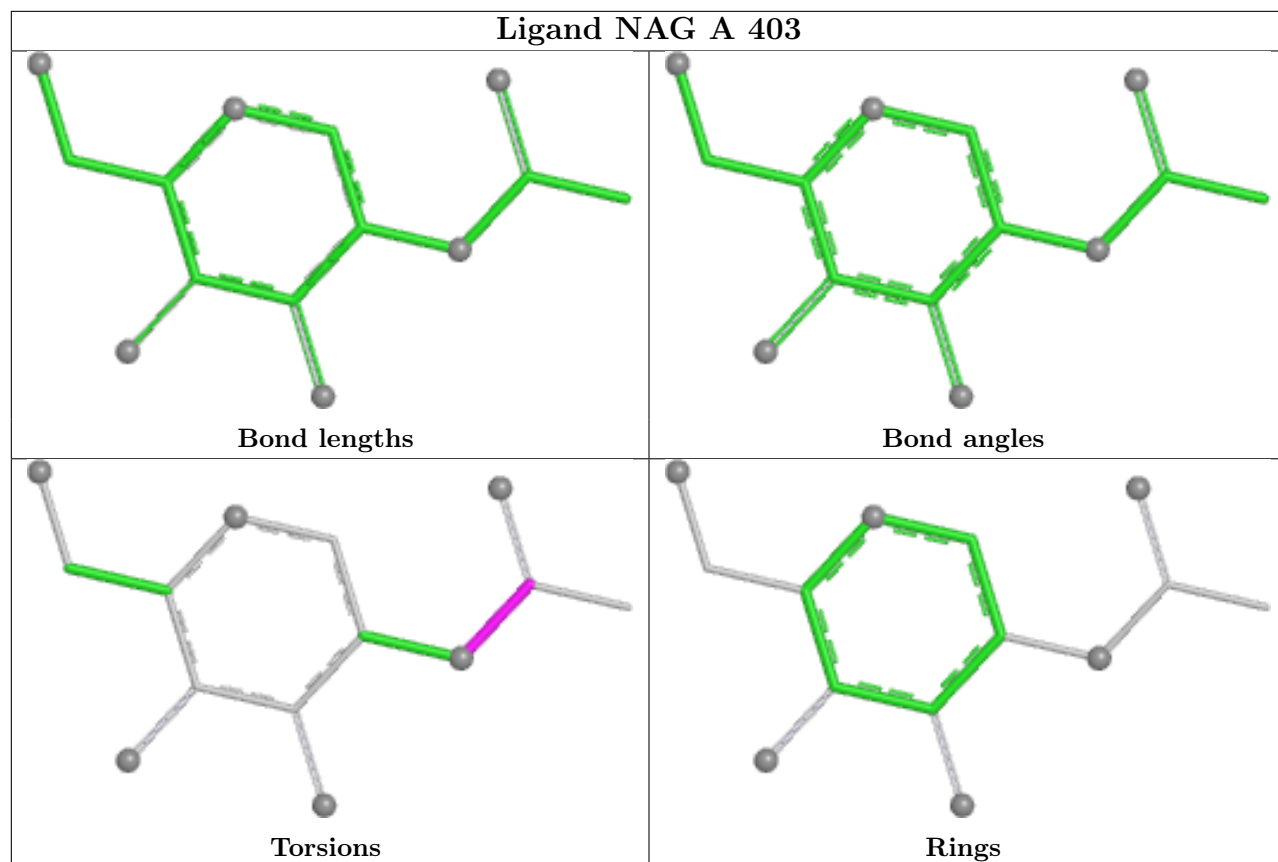
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	403	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

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-33416. 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

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.