



wwPDB EM Validation Summary Report ⓘ

Jul 15, 2025 – 08:14 PM JST

PDB ID : 8ZKU / pdb_00008zku
EMDB ID : EMD-60209
Title : Structure of Polycystin-1/Polycystin-2 complex with GOF mutations
Authors : Chen, M.Y.; Su, Q.; Shi, Y.G.
Deposited on : 2024-05-17
Resolution : 3.34 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 : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

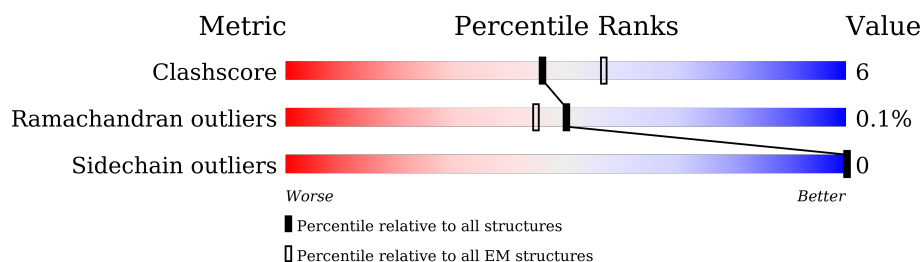
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.34 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	1261	
2	B	1007	
2	C	1007	
2	D	1007	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16174 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 Polycystin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	748	Total	C	N	O	S	0	0
			5555	3581	1016	940	18		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3043	MET	-	initiating methionine	UNP P98161
A	3044	ASP	-	expression tag	UNP P98161
A	3045	TYR	-	expression tag	UNP P98161
A	3046	LYS	-	expression tag	UNP P98161
A	3047	ASP	-	expression tag	UNP P98161
A	3048	ASP	-	expression tag	UNP P98161
A	3049	ASP	-	expression tag	UNP P98161
A	3050	ASP	-	expression tag	UNP P98161
A	3051	LYS	-	expression tag	UNP P98161

- Molecule 2 is a protein called Polycystin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	476	Total	C	N	O	S	0	0
			3932	2597	621	693	21		
2	C	468	Total	C	N	O	S	0	0
			3860	2550	608	682	20		
2	D	479	Total	C	N	O	S	0	0
			2743	1702	501	532	8		

There are 117 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-38	MET	-	initiating methionine	UNP Q13563
B	-37	GLY	-	expression tag	UNP Q13563
B	-36	ALA	-	expression tag	UNP Q13563
B	-35	SER	-	expression tag	UNP Q13563

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-34	SER	-	expression tag	UNP Q13563
B	-33	ALA	-	expression tag	UNP Q13563
B	-32	TRP	-	expression tag	UNP Q13563
B	-31	SER	-	expression tag	UNP Q13563
B	-30	HIS	-	expression tag	UNP Q13563
B	-29	PRO	-	expression tag	UNP Q13563
B	-28	GLN	-	expression tag	UNP Q13563
B	-27	PHE	-	expression tag	UNP Q13563
B	-26	GLU	-	expression tag	UNP Q13563
B	-25	LYS	-	expression tag	UNP Q13563
B	-24	GLY	-	expression tag	UNP Q13563
B	-23	GLY	-	expression tag	UNP Q13563
B	-22	GLY	-	expression tag	UNP Q13563
B	-21	SER	-	expression tag	UNP Q13563
B	-20	GLY	-	expression tag	UNP Q13563
B	-19	GLY	-	expression tag	UNP Q13563
B	-18	GLY	-	expression tag	UNP Q13563
B	-17	SER	-	expression tag	UNP Q13563
B	-16	GLY	-	expression tag	UNP Q13563
B	-15	GLY	-	expression tag	UNP Q13563
B	-14	SER	-	expression tag	UNP Q13563
B	-13	ALA	-	expression tag	UNP Q13563
B	-12	TRP	-	expression tag	UNP Q13563
B	-11	SER	-	expression tag	UNP Q13563
B	-10	HIS	-	expression tag	UNP Q13563
B	-9	PRO	-	expression tag	UNP Q13563
B	-8	GLN	-	expression tag	UNP Q13563
B	-7	PHE	-	expression tag	UNP Q13563
B	-6	GLU	-	expression tag	UNP Q13563
B	-5	LYS	-	expression tag	UNP Q13563
B	-4	GLY	-	expression tag	UNP Q13563
B	-3	SER	-	linker	UNP Q13563
B	-2	ALA	-	linker	UNP Q13563
B	-1	ALA	-	linker	UNP Q13563
B	0	ALA	-	linker	UNP Q13563
C	-38	MET	-	initiating methionine	UNP Q13563
C	-37	GLY	-	expression tag	UNP Q13563
C	-36	ALA	-	expression tag	UNP Q13563
C	-35	SER	-	expression tag	UNP Q13563
C	-34	SER	-	expression tag	UNP Q13563
C	-33	ALA	-	expression tag	UNP Q13563
C	-32	TRP	-	expression tag	UNP Q13563

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-31	SER	-	expression tag	UNP Q13563
C	-30	HIS	-	expression tag	UNP Q13563
C	-29	PRO	-	expression tag	UNP Q13563
C	-28	GLN	-	expression tag	UNP Q13563
C	-27	PHE	-	expression tag	UNP Q13563
C	-26	GLU	-	expression tag	UNP Q13563
C	-25	LYS	-	expression tag	UNP Q13563
C	-24	GLY	-	expression tag	UNP Q13563
C	-23	GLY	-	expression tag	UNP Q13563
C	-22	GLY	-	expression tag	UNP Q13563
C	-21	SER	-	expression tag	UNP Q13563
C	-20	GLY	-	expression tag	UNP Q13563
C	-19	GLY	-	expression tag	UNP Q13563
C	-18	GLY	-	expression tag	UNP Q13563
C	-17	SER	-	expression tag	UNP Q13563
C	-16	GLY	-	expression tag	UNP Q13563
C	-15	GLY	-	expression tag	UNP Q13563
C	-14	SER	-	expression tag	UNP Q13563
C	-13	ALA	-	expression tag	UNP Q13563
C	-12	TRP	-	expression tag	UNP Q13563
C	-11	SER	-	expression tag	UNP Q13563
C	-10	HIS	-	expression tag	UNP Q13563
C	-9	PRO	-	expression tag	UNP Q13563
C	-8	GLN	-	expression tag	UNP Q13563
C	-7	PHE	-	expression tag	UNP Q13563
C	-6	GLU	-	expression tag	UNP Q13563
C	-5	LYS	-	expression tag	UNP Q13563
C	-4	GLY	-	expression tag	UNP Q13563
C	-3	SER	-	linker	UNP Q13563
C	-2	ALA	-	linker	UNP Q13563
C	-1	ALA	-	linker	UNP Q13563
C	0	ALA	-	linker	UNP Q13563
D	-38	MET	-	initiating methionine	UNP Q13563
D	-37	GLY	-	expression tag	UNP Q13563
D	-36	ALA	-	expression tag	UNP Q13563
D	-35	SER	-	expression tag	UNP Q13563
D	-34	SER	-	expression tag	UNP Q13563
D	-33	ALA	-	expression tag	UNP Q13563
D	-32	TRP	-	expression tag	UNP Q13563
D	-31	SER	-	expression tag	UNP Q13563
D	-30	HIS	-	expression tag	UNP Q13563
D	-29	PRO	-	expression tag	UNP Q13563

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-28	GLN	-	expression tag	UNP Q13563
D	-27	PHE	-	expression tag	UNP Q13563
D	-26	GLU	-	expression tag	UNP Q13563
D	-25	LYS	-	expression tag	UNP Q13563
D	-24	GLY	-	expression tag	UNP Q13563
D	-23	GLY	-	expression tag	UNP Q13563
D	-22	GLY	-	expression tag	UNP Q13563
D	-21	SER	-	expression tag	UNP Q13563
D	-20	GLY	-	expression tag	UNP Q13563
D	-19	GLY	-	expression tag	UNP Q13563
D	-18	GLY	-	expression tag	UNP Q13563
D	-17	SER	-	expression tag	UNP Q13563
D	-16	GLY	-	expression tag	UNP Q13563
D	-15	GLY	-	expression tag	UNP Q13563
D	-14	SER	-	expression tag	UNP Q13563
D	-13	ALA	-	expression tag	UNP Q13563
D	-12	TRP	-	expression tag	UNP Q13563
D	-11	SER	-	expression tag	UNP Q13563
D	-10	HIS	-	expression tag	UNP Q13563
D	-9	PRO	-	expression tag	UNP Q13563
D	-8	GLN	-	expression tag	UNP Q13563
D	-7	PHE	-	expression tag	UNP Q13563
D	-6	GLU	-	expression tag	UNP Q13563
D	-5	LYS	-	expression tag	UNP Q13563
D	-4	GLY	-	expression tag	UNP Q13563
D	-3	SER	-	linker	UNP Q13563
D	-2	ALA	-	linker	UNP Q13563
D	-1	ALA	-	linker	UNP Q13563
D	0	ALA	-	linker	UNP Q13563

- Molecule 3 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
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	

[illegible]

ARG	PRO	GLY	VAL	SER	THR	GLN	GLY	GLY	THR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GL
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	----

● Molecule 2: Polycystin-2

Chain D:

45%

52%

MET	GLY	ALA	SER	ALA	TRP	SER	HIS	PRO	PHE	GLU	LYS	GLY	GLY	SER	GLY	GLY	ALA	GLN	PHE	GLU	GLY	GLY	GLY	GLY	GLY	ALA	ALA	ALA	SER	ARG	VAL	GLN	PRO	GLY	ASP	GLY	ALA	ARG	PRO	PRO	PRO	PRO	PRO		
ARG	ALA	PRO	ASP	PRO	GLY	ARG	LEU	MET	CYS	ALA	VAL	ALA	ALA	SER	GLY	LEU	ALA	ALA	GLY	GLY	CYS	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ASP	PRO	GLN	ILE	GLY	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	
CYS	SER	ARG	GLN	ALA	TRP	SER	ARG	ASP	PRO	GLY	PHE	GLU	ALA	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	LEU	
GLY	GLY	TYR	HIS	GLY	ALA	GLY	HIS	PRO	ARG	ARG	ARG	ARG	ARG	ARG	GLY	GLN	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	TRP
GLY	THR	ARG	LEU	MET	GLU	SER	SER	THR	ASN	ARG	GLY	LYS	L217	L217	F310	TYR	ASN	L314	Q585	L586	T589	R592	C593	D596	L597	F600	M603	F619	V623	D624	D625	E631	N645	F646	G657	V665	F669	F670	N674	M675	F676				
K688	E697	M698	GLU	LEU	SER	ASP	LEU	ILE	ARG	GLY	TYR	HIS	ALA	VAL	VAL	LYS	LEU	GLN	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	
ILE	GLU	ALA	ILE	PHE	THR	LYS	TYR	ASP	GLN	ASP	GLY	GLN	GLU	GLU	THR	GLY	HIS	GLN	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	
ASP	ASP	GLU	ASP	SER	GLY	HIS	GLY	SER	ARG	GLY	VAL	SER	GLY	SER	SER	GLY	VAL	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	LYS	
LEU	LYS	ARG	ARG	VAL	LEU	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	

LEU	ASN	GLY	GLN	PRO	ARG	PRO	ARG	SER	SER	ARG	PRO	SER	SER	SER	GLN	SER	THR	GLU	GLY	MET	GLU	GLY	GLY	ALA	GLY	GLY	ASN	GLY	SER	SER	SER	ASN	VAL	HIS	VAL
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	196662	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	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	0.16	0/5688	0.37	0/7754
2	B	0.19	0/4036	0.34	0/5473
2	C	0.18	0/3962	0.34	0/5375
2	D	0.14	0/2764	0.31	0/3810
All	All	0.17	0/16450	0.34	0/22412

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	5555	0	5368	76	0
2	B	3932	0	3886	45	0
2	C	3860	0	3814	59	0
2	D	2743	0	1705	17	0
3	B	42	0	39	0	0
3	C	42	0	39	1	0
All	All	16174	0	14851	185	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 6.

The worst 5 of 185 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:331:CYS:SG	2:B:344:CYS:SG	1.17	1.12
2:B:331:CYS:SG	2:B:344:CYS:CB	2.46	1.02
2:C:581:ARG:NH2	2:C:695:LYS:HE2	2.05	0.72
1:A:3854:LEU:HG	1:A:3855:THR:H	1.55	0.71
1:A:3621:ARG:NH1	1:A:3623:HIS:O	2.23	0.70

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	736/1261 (58%)	658 (89%)	77 (10%)	1 (0%)	48	76
2	B	472/1007 (47%)	444 (94%)	27 (6%)	1 (0%)	44	72
2	C	464/1007 (46%)	437 (94%)	27 (6%)	0	100	100
2	D	475/1007 (47%)	444 (94%)	31 (6%)	0	100	100
All	All	2147/4282 (50%)	1983 (92%)	162 (8%)	2 (0%)	50	76

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3855	THR
2	B	624	ASP

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	516/1041 (50%)	516 (100%)	0	100	100
2	B	429/860 (50%)	429 (100%)	0	100	100
2	C	421/860 (49%)	421 (100%)	0	100	100
2	D	101/860 (12%)	101 (100%)	0	100	100
All	All	1467/3621 (40%)	1467 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	555	GLN
2	C	674	ASN
2	B	498	HIS
2	C	313	ASN
2	C	412	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](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	C	1003	2	14,14,15	0.25	0	17,19,21	0.51	0
3	NAG	B	1002	2	14,14,15	0.74	1 (7%)	17,19,21	0.84	0
3	NAG	C	1002	2	14,14,15	0.21	0	17,19,21	0.42	0
3	NAG	B	1003	2	14,14,15	0.24	0	17,19,21	0.49	0
3	NAG	B	1001	2	14,14,15	0.28	0	17,19,21	0.53	0
3	NAG	C	1001	2	14,14,15	0.85	1 (7%)	17,19,21	1.75	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	1003	2	-	2/6/23/26	0/1/1/1
3	NAG	B	1002	2	-	2/6/23/26	0/1/1/1
3	NAG	C	1002	2	-	2/6/23/26	0/1/1/1
3	NAG	B	1003	2	-	0/6/23/26	0/1/1/1
3	NAG	B	1001	2	-	0/6/23/26	0/1/1/1
3	NAG	C	1001	2	-	4/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1001	NAG	O5-C1	2.82	1.48	1.43
3	B	1002	NAG	O5-C1	-2.39	1.39	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1001	NAG	C1-O5-C5	5.01	118.98	112.19
3	C	1001	NAG	C2-N2-C7	4.35	129.10	122.90

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1003	NAG	O5-C5-C6-O6
3	C	1003	NAG	C4-C5-C6-O6
3	C	1002	NAG	O5-C5-C6-O6
3	C	1002	NAG	C4-C5-C6-O6
3	C	1001	NAG	C8-C7-N2-C2

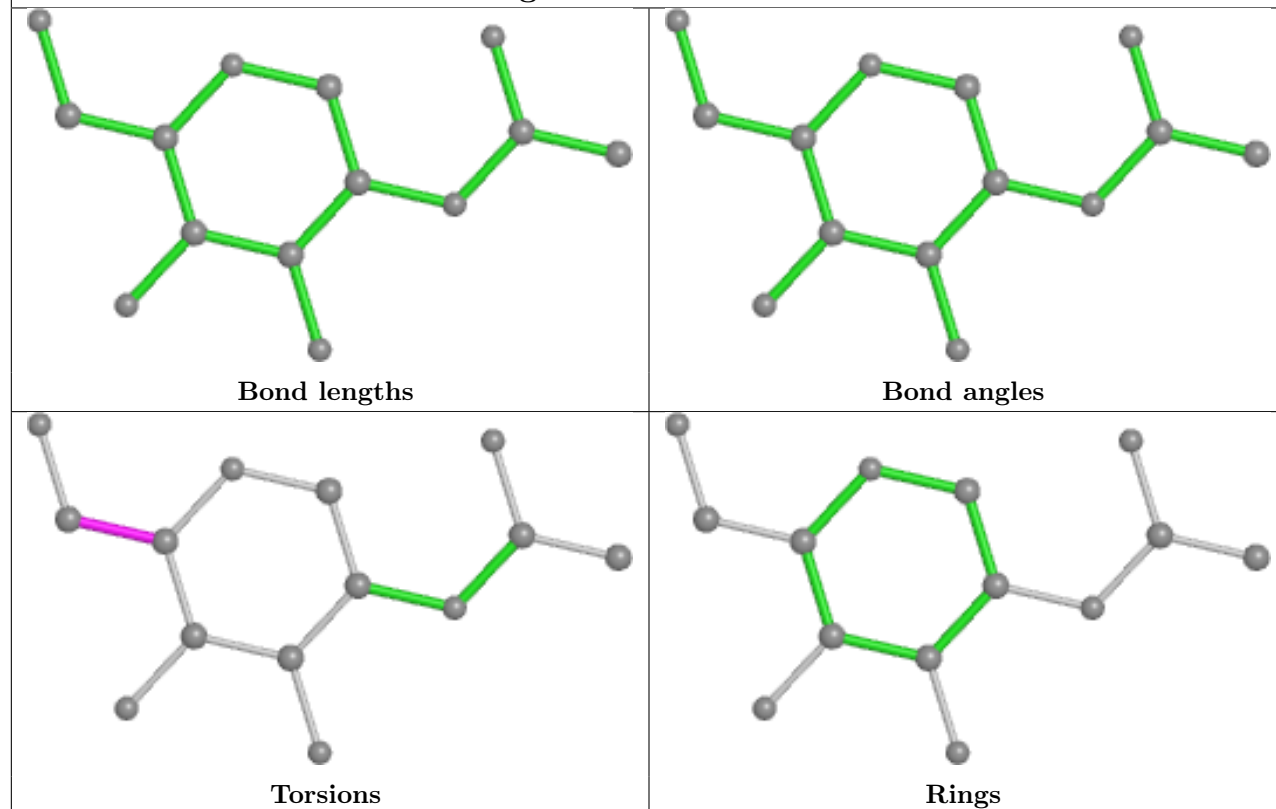
There are no ring outliers.

1 monomer is involved in 1 short contact:

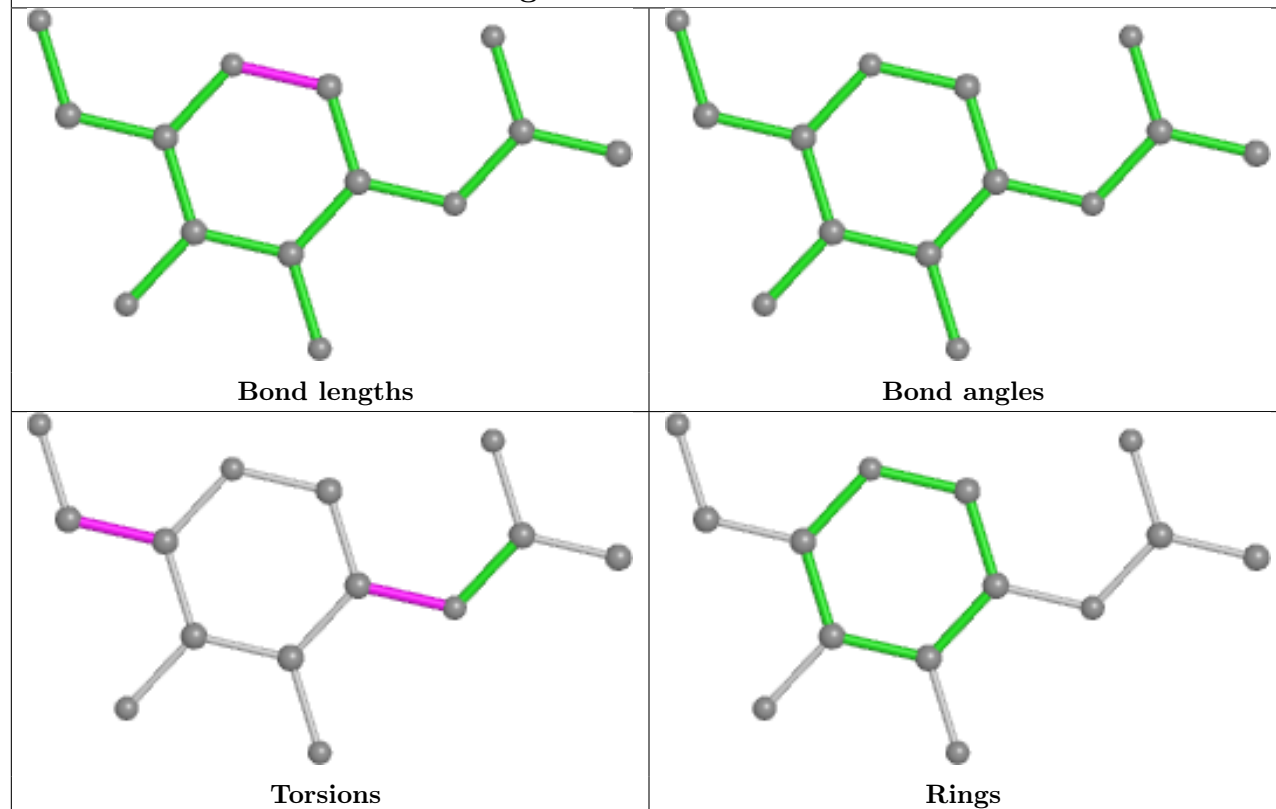
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1001	NAG	1	0

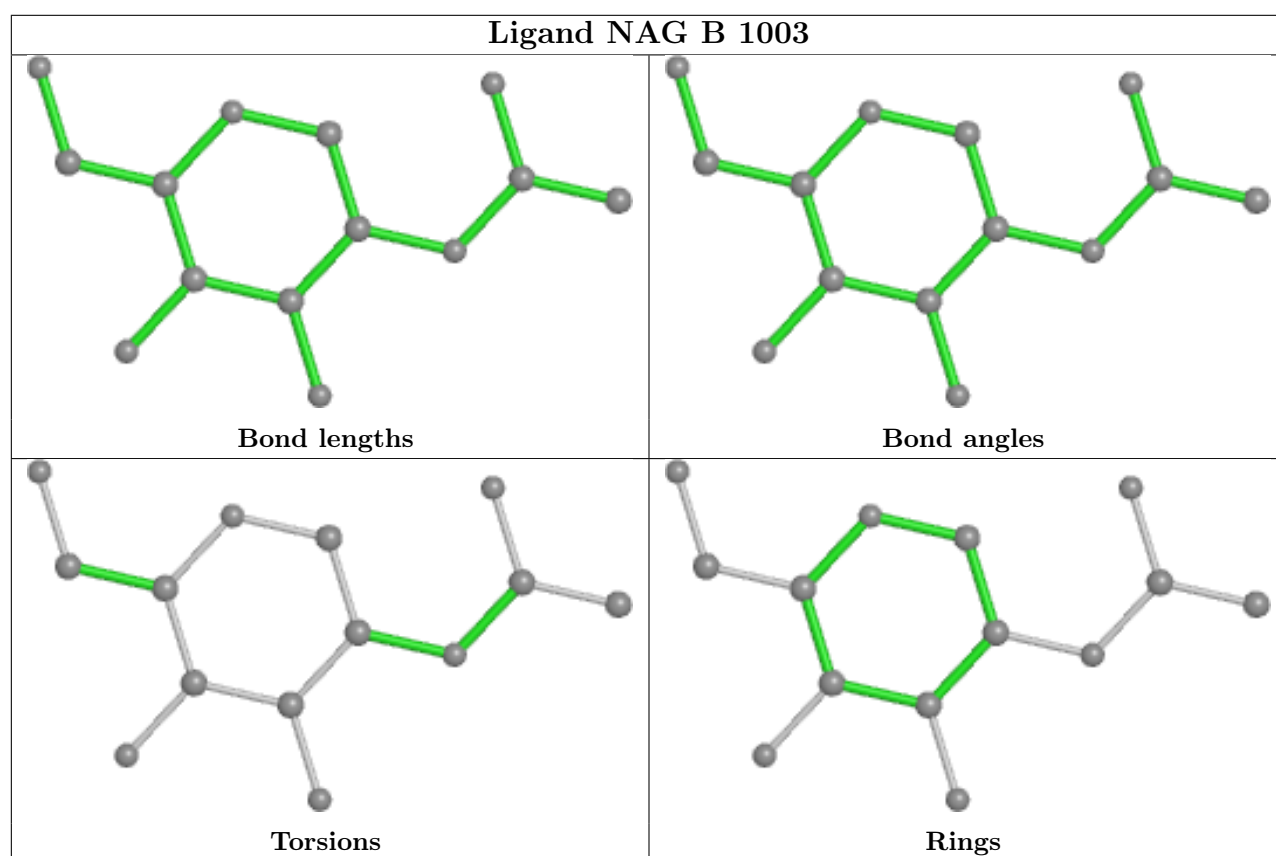
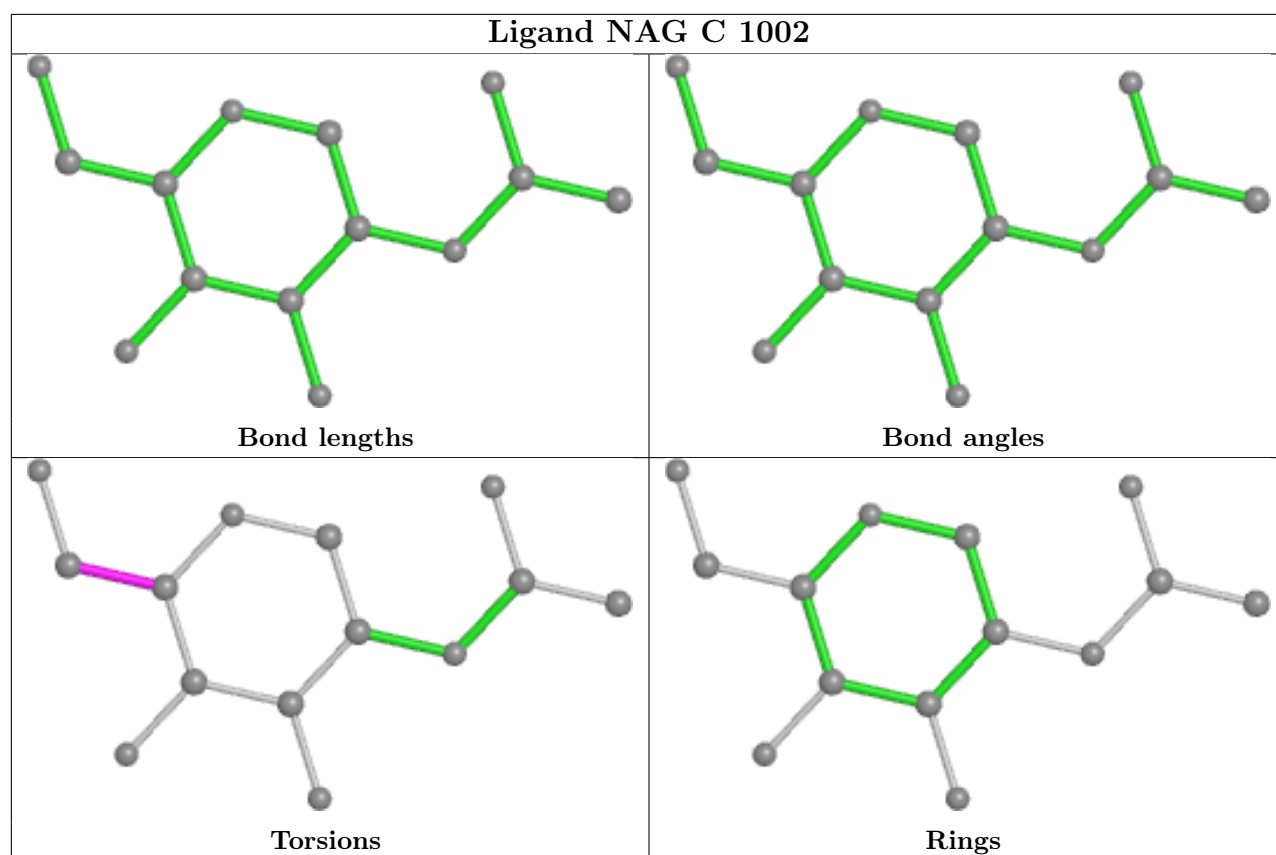
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

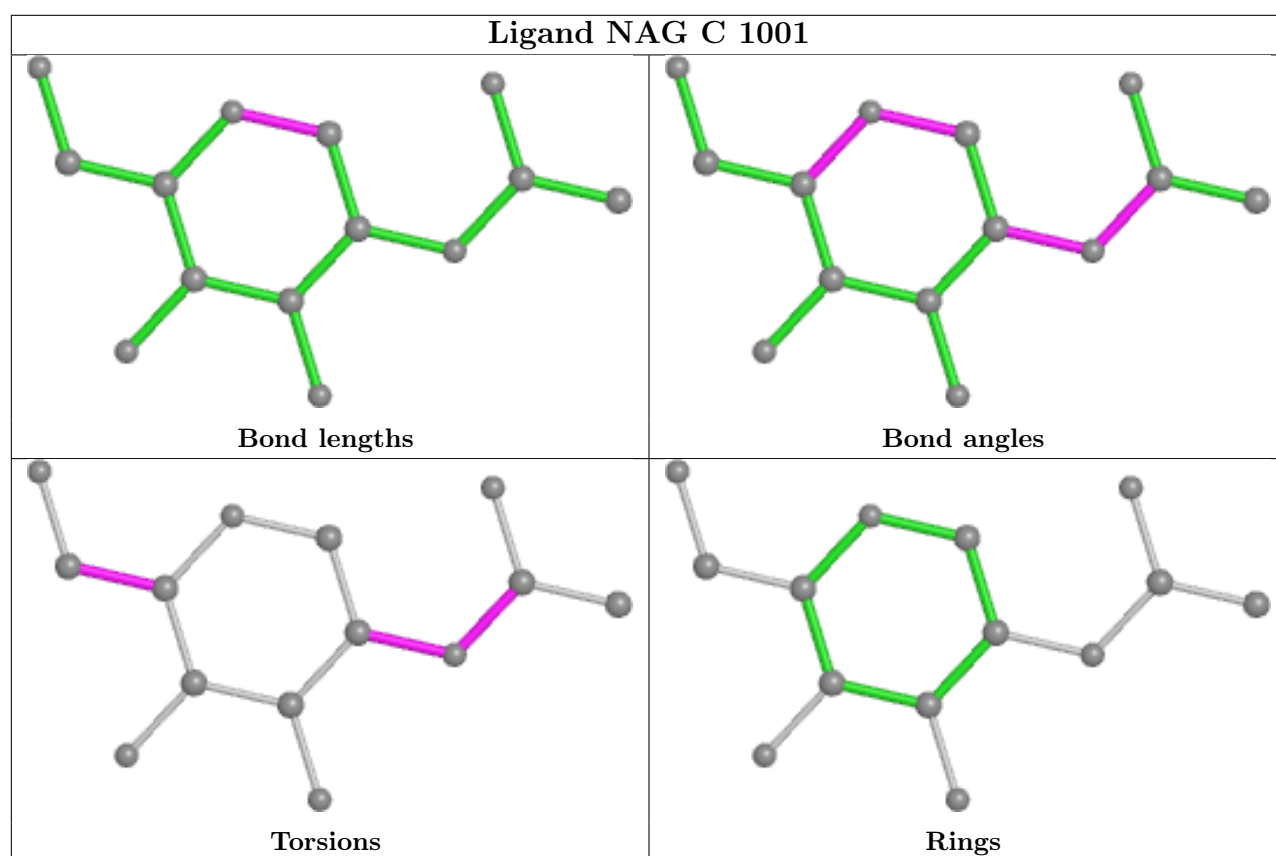
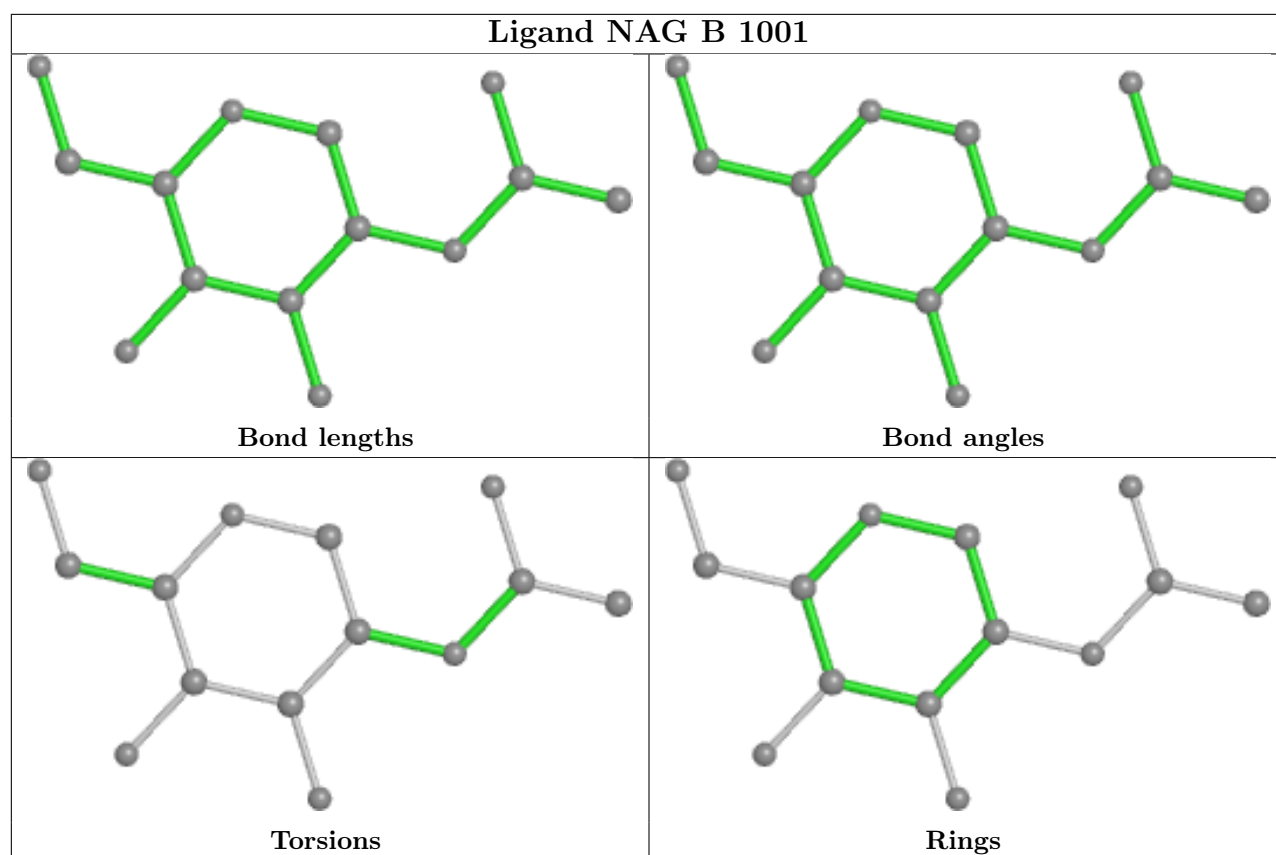
Ligand NAG C 1003



Ligand NAG B 1002







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.