



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:25 AM UTC

PDB ID : 7O9Z / pdb_00007o9z
Title : Crystal structure of Human Menin in complex with BD-08
Authors : Groves, M.R.; Gao, K.
Deposited on : 2021-04-18
Resolution : 1.98 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

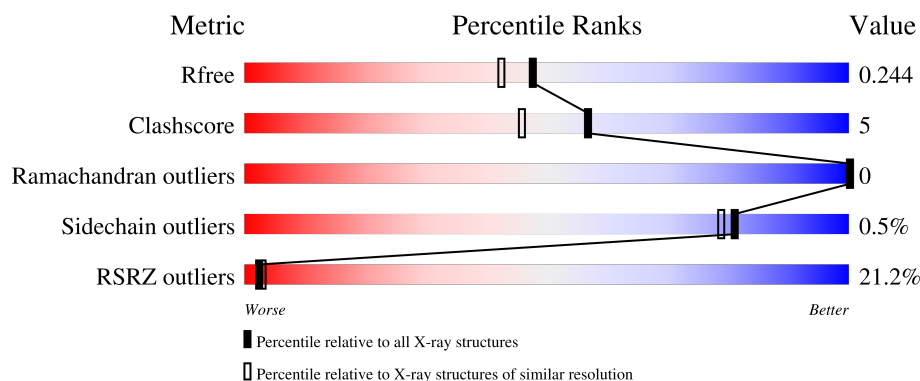
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	494	20% 84% 10% 6%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3875 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Menin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	462	3640	2328	623	674	15	0	1	0

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ALA	-	expression tag	UNP A0A024R5E3
A	?	-	ILE	deletion	UNP A0A024R5E3
A	?	-	PRO	deletion	UNP A0A024R5E3
A	?	-	THR	deletion	UNP A0A024R5E3
A	?	-	ASN	deletion	UNP A0A024R5E3
A	?	-	VAL	deletion	UNP A0A024R5E3
A	?	-	PRO	deletion	UNP A0A024R5E3
A	?	-	GLU	deletion	UNP A0A024R5E3
A	?	-	LEU	deletion	UNP A0A024R5E3
A	?	-	THR	deletion	UNP A0A024R5E3
A	?	-	PHE	deletion	UNP A0A024R5E3
A	?	-	GLN	deletion	UNP A0A024R5E3
A	?	-	PRO	deletion	UNP A0A024R5E3
A	?	-	SER	deletion	UNP A0A024R5E3
A	?	-	PRO	deletion	UNP A0A024R5E3
A	?	-	ALA	deletion	UNP A0A024R5E3
A	?	-	PRO	deletion	UNP A0A024R5E3
A	?	-	ASP	deletion	UNP A0A024R5E3
A	?	-	PRO	deletion	UNP A0A024R5E3
A	?	-	PRO	deletion	UNP A0A024R5E3
A	?	-	GLY	deletion	UNP A0A024R5E3
A	?	-	GLU	deletion	UNP A0A024R5E3
A	?	-	GLU	deletion	UNP A0A024R5E3
A	?	-	ARG	deletion	UNP A0A024R5E3
A	?	-	PRO	deletion	UNP A0A024R5E3
A	?	-	GLY	deletion	UNP A0A024R5E3
A	?	-	GLU	deletion	UNP A0A024R5E3

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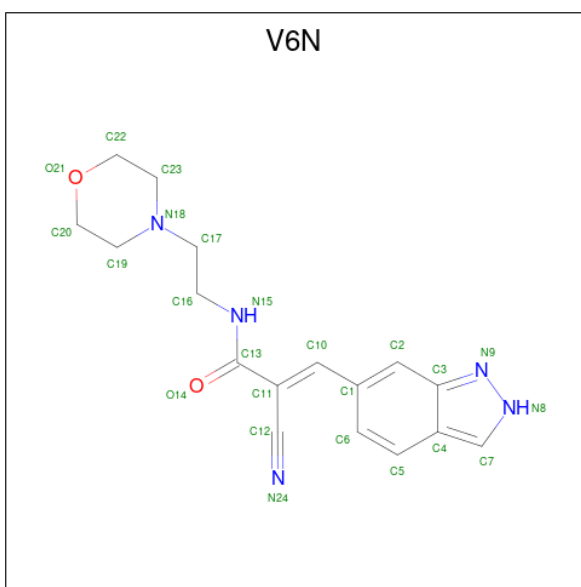
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLN	deletion	UNP A0A024R5E3
A	?	-	SER	deletion	UNP A0A024R5E3
A	?	-	GLN	deletion	UNP A0A024R5E3
A	?	-	GLY	deletion	UNP A0A024R5E3
A	?	-	THR	deletion	UNP A0A024R5E3
A	?	-	ARG	deletion	UNP A0A024R5E3
A	?	-	GLU	deletion	UNP A0A024R5E3
A	?	-	ALA	deletion	UNP A0A024R5E3
A	?	-	GLU	deletion	UNP A0A024R5E3
A	?	-	ALA	deletion	UNP A0A024R5E3
A	?	-	ALA	deletion	UNP A0A024R5E3
A	?	-	GLU	deletion	UNP A0A024R5E3
A	?	-	ALA	deletion	UNP A0A024R5E3
A	?	-	GLU	deletion	UNP A0A024R5E3
A	?	-	GLU	deletion	UNP A0A024R5E3
A	?	-	PRO	deletion	UNP A0A024R5E3
A	?	-	TRP	deletion	UNP A0A024R5E3
A	?	-	GLY	deletion	UNP A0A024R5E3
A	?	-	GLU	deletion	UNP A0A024R5E3
A	?	-	GLU	deletion	UNP A0A024R5E3
A	?	-	ALA	deletion	UNP A0A024R5E3
A	?	-	ARG	deletion	UNP A0A024R5E3
A	?	-	GLU	deletion	UNP A0A024R5E3
A	?	-	GLY	deletion	UNP A0A024R5E3
A	?	-	ARG	deletion	UNP A0A024R5E3
A	?	-	ARG	deletion	UNP A0A024R5E3
A	?	-	ARG	deletion	UNP A0A024R5E3
A	?	-	GLY	deletion	UNP A0A024R5E3
A	?	-	PRO	deletion	UNP A0A024R5E3
A	?	-	ARG	deletion	UNP A0A024R5E3
A	?	-	ARG	deletion	UNP A0A024R5E3
A	?	-	GLU	deletion	UNP A0A024R5E3
A	?	-	SER	deletion	UNP A0A024R5E3
A	?	-	LYS	deletion	UNP A0A024R5E3
A	?	-	PRO	deletion	UNP A0A024R5E3
A	?	-	GLU	deletion	UNP A0A024R5E3
A	?	-	GLU	deletion	UNP A0A024R5E3
A	?	-	PRO	deletion	UNP A0A024R5E3
A	?	-	PRO	deletion	UNP A0A024R5E3
A	?	-	PRO	deletion	UNP A0A024R5E3
A	?	-	PRO	deletion	UNP A0A024R5E3
A	?	-	LYS	deletion	UNP A0A024R5E3

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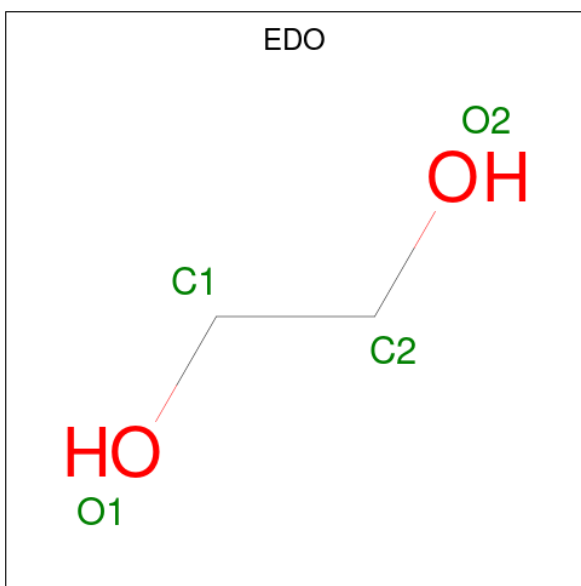
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LYS	deletion	UNP A0A024R5E3
A	?	-	PRO	deletion	UNP A0A024R5E3
A	?	-	ALA	deletion	UNP A0A024R5E3
A	?	-	LEU	deletion	UNP A0A024R5E3
A	?	-	ASP	deletion	UNP A0A024R5E3
A	?	-	LYS	deletion	UNP A0A024R5E3
A	?	-	GLY	deletion	UNP A0A024R5E3
A	?	-	LEU	deletion	UNP A0A024R5E3
A	?	-	GLY	deletion	UNP A0A024R5E3
A	?	-	THR	deletion	UNP A0A024R5E3
A	?	-	GLY	deletion	UNP A0A024R5E3
A	?	-	GLN	deletion	UNP A0A024R5E3
A	461	THR	ALA	conflict	UNP A0A024R5E3
A	523	ALA	SER	conflict	UNP A0A024R5E3
A	525	THR	PRO	conflict	UNP A0A024R5E3
A	526	ALA	PRO	conflict	UNP A0A024R5E3
A	?	-	LYS	deletion	UNP A0A024R5E3
A	?	-	PRO	deletion	UNP A0A024R5E3
A	?	-	PRO	deletion	UNP A0A024R5E3
A	?	-	GLY	deletion	UNP A0A024R5E3
A	?	-	THR	deletion	UNP A0A024R5E3
A	?	-	VAL	deletion	UNP A0A024R5E3
A	?	-	ALA	deletion	UNP A0A024R5E3
A	?	-	GLY	deletion	UNP A0A024R5E3
A	?	-	THR	deletion	UNP A0A024R5E3
A	?	-	ALA	deletion	UNP A0A024R5E3
A	?	-	ARG	deletion	UNP A0A024R5E3

- Molecule 2 is ({E})-2-cyano-3-(2 {H}-indazol-6-yl)- {N}-(2-morpholin-4-ylethyl)prop-2-enamide (CCD ID: V6N) (formula: C₁₇H₁₉N₅O₂) (labeled as "Ligand of Interest" by depositor).



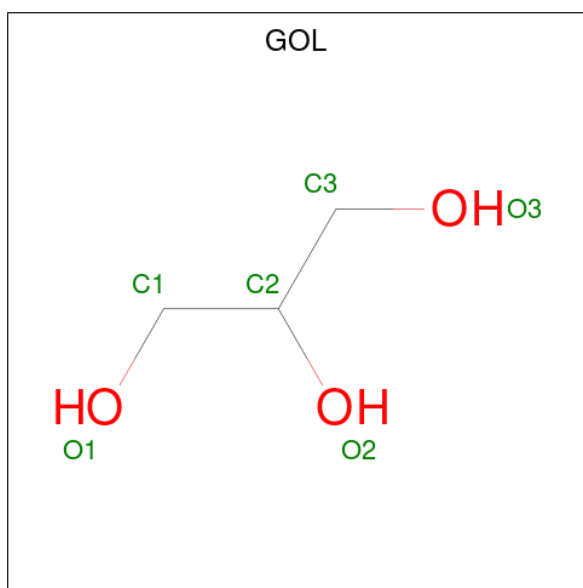
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			24	17	5	2		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

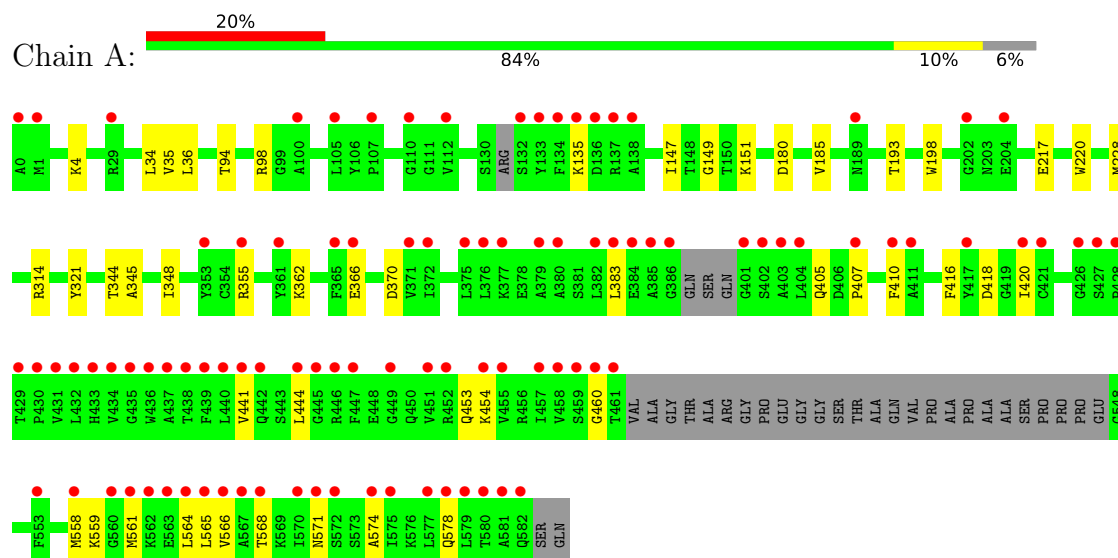
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	187	Total	O	0	0
			187	187		

3 Residue-property plots [i](#)

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 electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: Menin



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α , β , γ	107.19Å 107.19Å 107.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.03 – 1.98 48.03 – 1.98	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.03-1.98) 99.9 (48.03-1.98)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.70 (at 1.98Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.211 , 0.243 0.215 , 0.244	Depositor DCC
R_{free} test set	2392 reflections (5.40%)	wwPDB-VP
Wilson B-factor (Å ²)	35.2	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for -h,l,k 0.004 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3875	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: GOL, EDO, V6N

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	0.48	3/3722 (0.1%)	0.59	0/5043

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	34	LEU	C-O	-5.68	1.17	1.24
1	A	36	LEU	C-O	-5.30	1.18	1.24
1	A	35	VAL	C-O	-5.09	1.18	1.24

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	3640	0	3604	33	0
2	A	24	0	0	0	0
3	A	12	0	18	1	0
4	A	12	0	16	0	0
5	A	187	0	0	3	0
All	All	3875	0	3638	34	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 (34) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:GLN:HA	1:A:566:VAL:CG1	2.22	0.69
1:A:564:LEU:HD12	1:A:564:LEU:N	2.13	0.64
1:A:564:LEU:H	1:A:564:LEU:CD1	2.13	0.61
1:A:441:VAL:HA	1:A:444:LEU:HD12	1.85	0.59
1:A:460:GLY:H	1:A:559:LYS:HE2	1.66	0.59
1:A:418:ASP:HA	1:A:558:MET:HG3	1.85	0.58
1:A:566:VAL:HG12	1:A:566:VAL:O	2.03	0.58
1:A:564:LEU:HD12	1:A:564:LEU:H	1.69	0.57
1:A:410:PHE:HE1	1:A:444:LEU:HD23	1.68	0.57
1:A:453:GLN:HA	1:A:566:VAL:HG13	1.87	0.56
1:A:383:LEU:HD21	1:A:405:GLN:OE1	2.07	0.54
1:A:345:ALA:HA	1:A:348:ILE:HG22	1.89	0.53
1:A:416:PHE:CZ	1:A:420:ILE:HD11	2.43	0.53
1:A:564:LEU:N	1:A:564:LEU:CD1	2.72	0.53
1:A:217:GLU:OE1	1:A:355:ARG:NH2	2.43	0.52
1:A:185:VAL:HG12	1:A:193:THR:HG22	1.90	0.52
1:A:321:TYR:HB2	1:A:344:THR:HG22	1.94	0.49
1:A:561:MET:HE2	1:A:578:GLN:HB3	1.95	0.49
1:A:314:ARG:HD3	5:A:733:HOH:O	2.13	0.49
1:A:561:MET:HA	1:A:564:LEU:HD13	1.95	0.48
1:A:453:GLN:HG2	1:A:566:VAL:HG12	1.96	0.47
1:A:94:THR:O	1:A:98:ARG:HG3	2.17	0.45
1:A:180:ASP:HB2	1:A:220:TRP:CH2	2.53	0.44
1:A:147:ILE:HD13	1:A:147:ILE:HA	1.89	0.44
1:A:228:MET:HE2	1:A:228:MET:HB3	1.87	0.44
1:A:135:LYS:HB3	1:A:198:TRP:CZ2	2.52	0.43
3:A:606:EDO:H22	5:A:813:HOH:O	2.17	0.43
1:A:407:PRO:HG3	1:A:454:LYS:HD2	1.99	0.42
1:A:149:GLY:O	1:A:151:LYS:HG3	2.20	0.42
1:A:4:LYS:HD3	5:A:715:HOH:O	2.20	0.42
1:A:362:LYS:O	1:A:366:GLU:HG2	2.19	0.42
1:A:410:PHE:CE1	1:A:444:LEU:HD23	2.53	0.41
1:A:366:GLU:O	1:A:370[A]:ASP:HB3	2.20	0.41
1:A:571:ASN:HB3	1:A:574:ALA:HB3	2.03	0.41

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 X-ray entries followed by that with respect to entries of similar resolution.

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	455/494 (92%)	439 (96%)	16 (4%)	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 X-ray entries followed by that with respect to entries of similar resolution.

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	384/408 (94%)	382 (100%)	2 (0%)	81	79

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

Mol	Chain	Res	Type
1	A	565	LEU
1	A	568	THR

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	174	HIS
1	A	303	HIS
1	A	333	ASN
1	A	442	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
4	GOL	A	603	-	5,5,5	0.26	0	5,5,5	0.63	0
3	EDO	A	602	-	3,3,3	0.52	0	2,2,2	0.24	0
3	EDO	A	606	-	3,3,3	0.56	0	2,2,2	0.53	0
2	V6N	A	601	-	24,26,26	1.08	1 (4%)	27,34,34	1.41	3 (11%)
3	EDO	A	605	-	3,3,3	0.58	0	2,2,2	0.46	0
4	GOL	A	604	-	5,5,5	0.28	0	5,5,5	0.84	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	GOL	A	603	-	-	2/4/4/4	-
3	EDO	A	602	-	-	1/1/1/1	-
3	EDO	A	606	-	-	0/1/1/1	-
2	V6N	A	601	-	-	2/15/24/24	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	605	-	-	0/1/1/1	-
4	GOL	A	604	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	V6N	C11-C13	-4.20	1.42	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	V6N	C7-N8-N9	-3.89	106.63	112.59
2	A	601	V6N	C3-N9-N8	2.92	111.47	105.24
2	A	601	V6N	C11-C13-N15	2.21	119.06	116.86

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	V6N	C11-C13-N15-C16
4	A	603	GOL	O1-C1-C2-C3
2	A	601	V6N	O14-C13-N15-C16
4	A	604	GOL	O1-C1-C2-C3
4	A	603	GOL	O1-C1-C2-O2
4	A	604	GOL	O1-C1-C2-O2
3	A	602	EDO	O1-C1-C2-O2

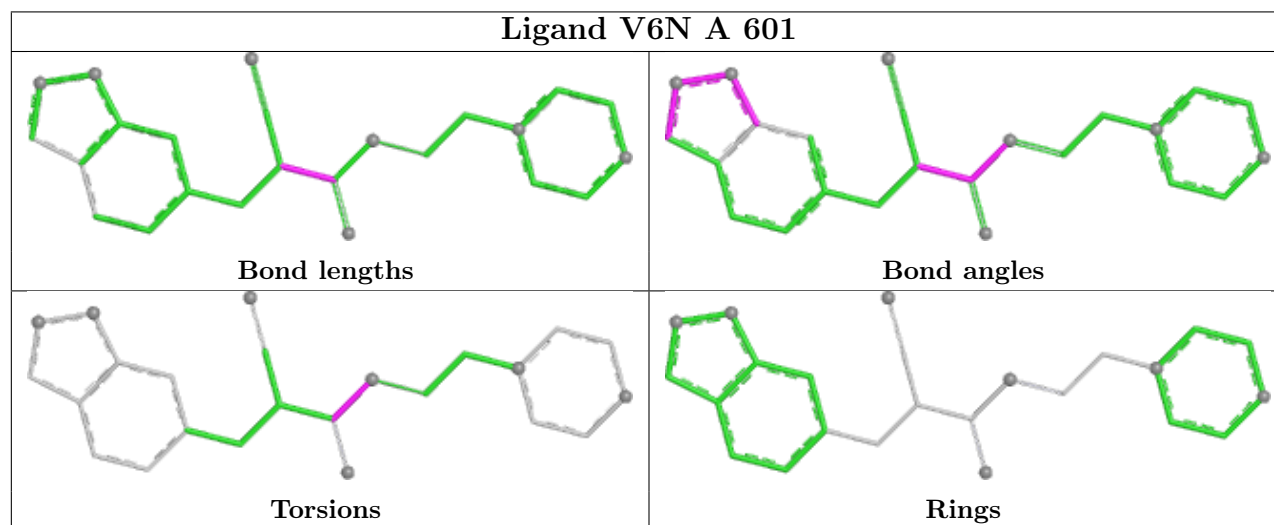
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	606	EDO	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	462/494 (93%)	0.98	98 (21%) 2 3	21, 41, 82, 94	1 (0%)

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	429	THR	6.4
1	A	577	LEU	5.8
1	A	134	PHE	5.6
1	A	430	PRO	5.6
1	A	575	ILE	5.5
1	A	574	ALA	5.4
1	A	431	VAL	5.0
1	A	386	GLY	5.0
1	A	434	VAL	5.0
1	A	570	ILE	5.0
1	A	437	ALA	4.9
1	A	455	VAL	4.9
1	A	438	THR	4.7
1	A	136	ASP	4.5
1	A	566	VAL	4.3
1	A	581	ALA	4.3
1	A	439	PHE	4.2
1	A	564	LEU	4.2
1	A	565	LEU	4.1
1	A	440	LEU	4.1
1	A	383	LEU	3.9
1	A	441	VAL	3.9
1	A	135	LYS	3.9
1	A	133	TYR	3.9
1	A	444	LEU	3.9
1	A	432	LEU	3.8
1	A	355	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	457	ILE	3.7
1	A	401	GLY	3.7
1	A	567	ALA	3.6
1	A	426	GLY	3.6
1	A	447	PHE	3.5
1	A	458	VAL	3.5
1	A	404	LEU	3.5
1	A	579	LEU	3.4
1	A	353	TYR	3.4
1	A	410	PHE	3.4
1	A	436	TRP	3.3
1	A	427	SER	3.3
1	A	568	THR	3.2
1	A	454	LYS	3.2
1	A	562	LYS	3.1
1	A	403	ALA	3.0
1	A	417	TYR	3.0
1	A	461	THR	3.0
1	A	452	ARG	3.0
1	A	572	SER	2.9
1	A	365	PHE	2.9
1	A	376	LEU	2.9
1	A	553	PHE	2.9
1	A	375	LEU	2.9
1	A	451	VAL	2.9
1	A	132	SER	2.8
1	A	449	GLY	2.8
1	A	428	PRO	2.8
1	A	445	GLY	2.8
1	A	105	LEU	2.8
1	A	382	LEU	2.8
1	A	371	VAL	2.8
1	A	460	GLY	2.8
1	A	435	GLY	2.7
1	A	372	ILE	2.7
1	A	100	ALA	2.7
1	A	582	GLN	2.7
1	A	361	TYR	2.6
1	A	578	GLN	2.6
1	A	563	GLU	2.6
1	A	420	ILE	2.6
1	A	385	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	1	MET	2.6
1	A	560	GLY	2.6
1	A	138	ALA	2.5
1	A	107	PRO	2.5
1	A	558	MET	2.5
1	A	379	ALA	2.4
1	A	446	ARG	2.4
1	A	580	THR	2.3
1	A	402	SER	2.3
1	A	411	ALA	2.3
1	A	137	ARG	2.2
1	A	0	ALA	2.2
1	A	380	ALA	2.2
1	A	433	HIS	2.2
1	A	29	ARG	2.2
1	A	561	MET	2.2
1	A	112	VAL	2.2
1	A	204	GLU	2.2
1	A	384	GLU	2.2
1	A	421	CYS	2.2
1	A	202	GLY	2.2
1	A	366	GLU	2.2
1	A	110	GLY	2.1
1	A	189	ASN	2.1
1	A	459	SER	2.1
1	A	442	GLN	2.1
1	A	407	PRO	2.1
1	A	377	LYS	2.0
1	A	571	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

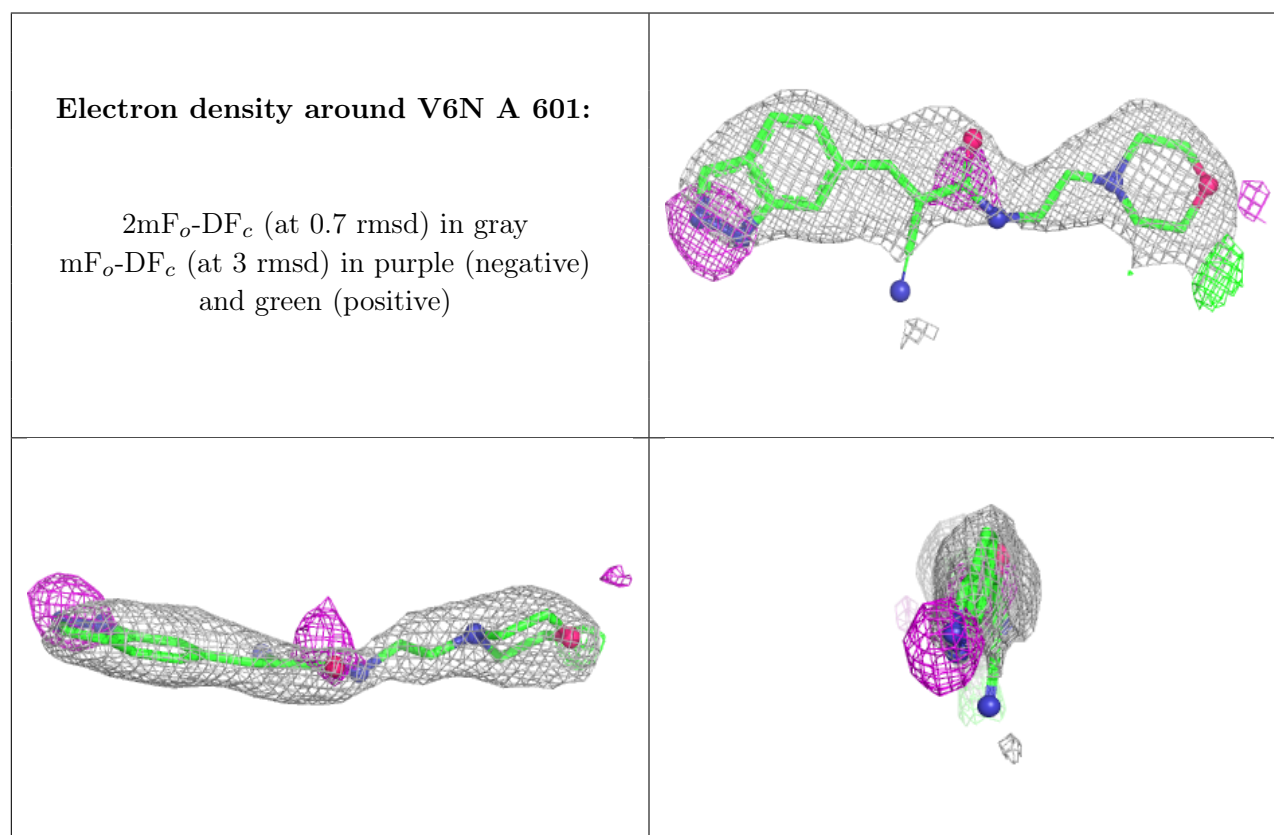
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	A	604	6/6	0.72	0.19	52,58,61,65	0
2	V6N	A	601	24/24	0.73	0.18	44,54,61,63	0
4	GOL	A	603	6/6	0.75	0.16	60,64,69,73	0
3	EDO	A	605	4/4	0.84	0.13	46,51,53,57	0
3	EDO	A	606	4/4	0.88	0.16	45,49,53,54	0
3	EDO	A	602	4/4	0.89	0.14	39,51,56,60	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.