



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 09:31 AM BST

PDB ID : 4OVW  
Title : ENDOGLUCANASE I COMPLEXED WITH EPOXYBUTYL CELLULOSE  
Authors : Davies, G.J.; Schulein, M.  
Deposited on : 1997-10-06  
Resolution : 2.30 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

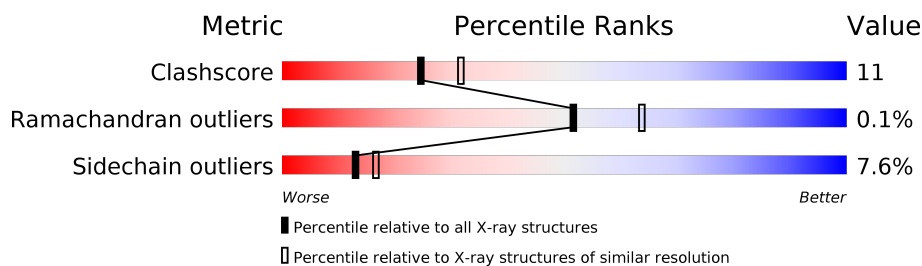
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	411	
1	B	411	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6833 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 ENDOGLUCANASE I.

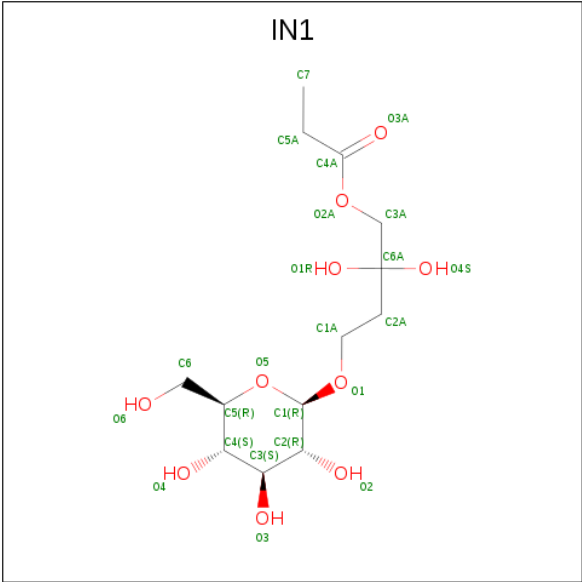
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	400	Total	C	N	O	S	0	0	0
			3030	1875	536	590	29			
1	B	400	Total	C	N	O	S	0	0	0
			3030	1875	536	590	29			

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 3 is 4-(beta-D-glucopyranosyloxy)-2,2-dihydroxybutyl propanoate (three-letter code: IN1) (formula:  $C_{13}H_{24}O_{10}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			23	13	10		
3	B	1	Total	C	O	0	0
			23	13	10		

- Molecule 4 is water.

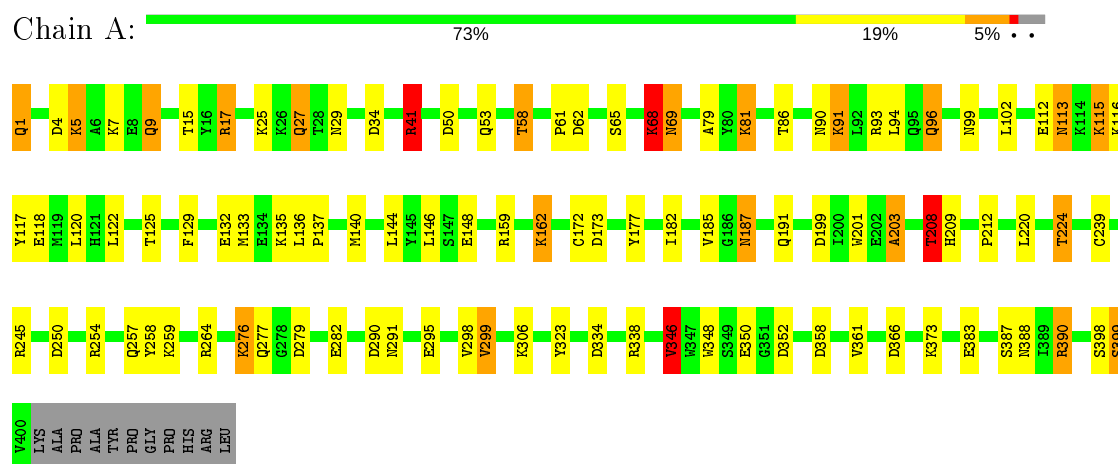
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	356	Total	O	0	0
			356	356		
4	B	343	Total	O	0	0
			343	343		

### 3 Residue-property plots

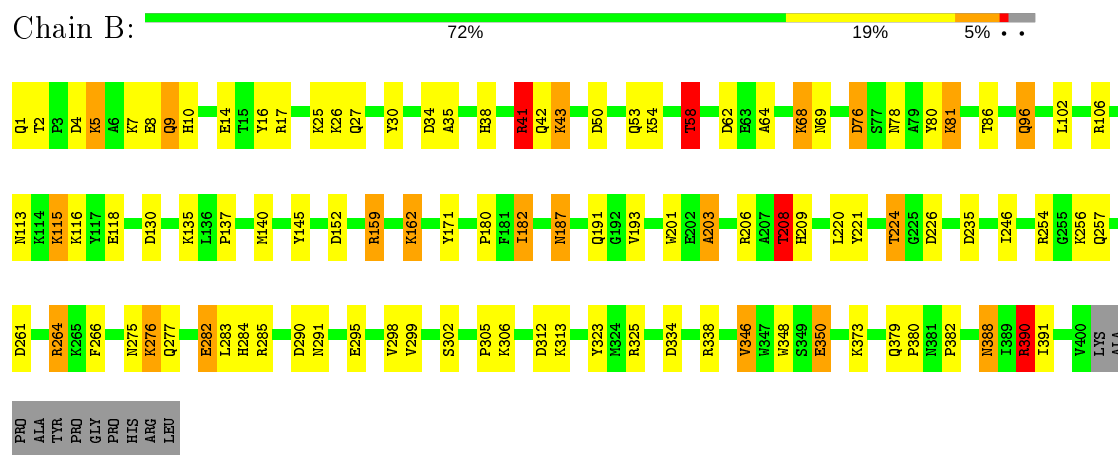
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

#### • Molecule 1: ENDOGLUCANASE I



#### • Molecule 1: ENDOGLUCANASE I



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.94Å 82.62Å 73.16Å 90.00° 94.16° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.30)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.180 , 0.270	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6833	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PCA, NAG, IN1

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	0.80	0/3084	1.81	66/4166 (1.6%)
1	B	0.81	0/3084	1.91	63/4166 (1.5%)
All	All	0.80	0/6168	1.86	129/8332 (1.5%)

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	1

There are no bond length outliers.

All (129) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	264	ARG	CD-NE-CZ	29.86	165.41	123.60
1	A	159	ARG	CD-NE-CZ	25.28	158.99	123.60
1	B	264	ARG	NE-CZ-NH2	22.69	131.64	120.30
1	B	159	ARG	NE-CZ-NH1	18.61	129.61	120.30
1	B	390	ARG	CD-NE-CZ	13.34	142.28	123.60
1	B	17	ARG	NE-CZ-NH1	13.27	126.93	120.30
1	B	264	ARG	NE-CZ-NH1	-12.87	113.87	120.30
1	A	159	ARG	NE-CZ-NH1	-12.68	113.96	120.30
1	B	338	ARG	NE-CZ-NH1	12.52	126.56	120.30
1	A	159	ARG	NE-CZ-NH2	12.13	126.37	120.30
1	B	159	ARG	CD-NE-CZ	11.73	140.02	123.60
1	A	17	ARG	NE-CZ-NH1	11.47	126.04	120.30
1	B	323	TYR	CB-CG-CD1	11.27	127.76	121.00
1	A	93	ARG	NE-CZ-NH2	11.13	125.87	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	338	ARG	NE-CZ-NH1	-10.52	115.04	120.30
1	A	34	ASP	CB-CG-OD1	10.45	127.71	118.30
1	A	62	ASP	CB-CG-OD1	10.26	127.53	118.30
1	A	390	ARG	CD-NE-CZ	9.95	137.53	123.60
1	A	352	ASP	CB-CG-OD1	9.87	127.18	118.30
1	B	34	ASP	CB-CG-OD1	9.82	127.14	118.30
1	B	9	GLN	CG-CD-OE1	9.79	141.18	121.60
1	B	390	ARG	NE-CZ-NH1	9.77	125.19	120.30
1	A	245	ARG	NE-CZ-NH2	-9.24	115.68	120.30
1	A	62	ASP	CB-CG-OD2	-9.01	110.19	118.30
1	A	1	PCA	O-C-N	-8.99	108.31	122.70
1	A	358	ASP	CB-CG-OD1	8.80	126.22	118.30
1	A	250	ASP	CB-CG-OD1	8.69	126.12	118.30
1	A	264	ARG	CD-NE-CZ	8.64	135.69	123.60
1	B	76	ASP	CB-CG-OD2	-8.56	110.60	118.30
1	A	390	ARG	NE-CZ-NH2	-8.45	116.08	120.30
1	B	206	ARG	NE-CZ-NH2	8.25	124.43	120.30
1	A	93	ARG	CD-NE-CZ	8.22	135.11	123.60
1	B	254	ARG	NE-CZ-NH1	-8.20	116.20	120.30
1	B	1	PCA	C-N-CA	8.10	141.94	121.70
1	B	261	ASP	CB-CG-OD1	7.98	125.48	118.30
1	A	118	GLU	OE1-CD-OE2	-7.94	113.77	123.30
1	A	117	TYR	CB-CG-CD1	7.87	125.72	121.00
1	A	17	ARG	NE-CZ-NH2	-7.86	116.37	120.30
1	A	17	ARG	CD-NE-CZ	7.83	134.57	123.60
1	B	30	TYR	CB-CG-CD1	7.79	125.67	121.00
1	A	258	TYR	CB-CG-CD2	7.64	125.58	121.00
1	A	68	LYS	CB-CG-CD	7.54	131.21	111.60
1	B	285	ARG	NE-CZ-NH1	7.41	124.00	120.30
1	A	132	GLU	OE1-CD-OE2	-7.37	114.45	123.30
1	A	117	TYR	CB-CG-CD2	-7.34	116.59	121.00
1	B	346	VAL	CB-CA-C	-7.30	97.53	111.40
1	B	346	VAL	CG1-CB-CG2	7.29	122.57	110.90
1	B	266	PHE	CB-CG-CD1	7.25	125.88	120.80
1	A	208	THR	CA-CB-CG2	-7.17	102.37	112.40
1	B	235	ASP	CB-CG-OD1	7.15	124.74	118.30
1	A	177	TYR	CB-CG-CD2	-7.11	116.74	121.00
1	A	323	TYR	CB-CG-CD1	-7.06	116.76	121.00
1	B	130	ASP	CB-CG-OD1	7.06	124.66	118.30
1	B	312	ASP	CB-CG-OD1	7.06	124.65	118.30
1	B	9	GLN	OE1-CD-NE2	-7.03	105.74	121.90
1	A	245	ARG	NE-CZ-NH1	7.01	123.81	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	346	VAL	CB-CA-C	-6.87	98.34	111.40
1	B	145	TYR	CB-CG-CD2	6.85	125.11	121.00
1	B	41	ARG	N-CA-CB	-6.84	98.28	110.60
1	A	338	ARG	NE-CZ-NH2	6.79	123.70	120.30
1	B	224	THR	CA-CB-CG2	-6.79	102.89	112.40
1	B	1	PCA	O-C-N	-6.78	111.85	122.70
1	B	58	THR	CA-CB-CG2	6.73	121.82	112.40
1	A	68	LYS	CG-CD-CE	6.72	132.07	111.90
1	B	53	GLN	CA-CB-CG	6.69	128.12	113.40
1	B	17	ARG	NE-CZ-NH2	-6.65	116.98	120.30
1	B	159	ARG	NH1-CZ-NH2	-6.65	112.09	119.40
1	A	27	GLN	N-CA-CB	6.61	122.49	110.60
1	A	390	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	B	206	ARG	CD-NE-CZ	6.54	132.76	123.60
1	B	106	ARG	NE-CZ-NH2	6.44	123.52	120.30
1	A	50	ASP	CB-CG-OD1	6.41	124.07	118.30
1	B	206	ARG	NE-CZ-NH1	-6.40	117.10	120.30
1	A	282	GLU	OE1-CD-OE2	-6.36	115.67	123.30
1	A	366	ASP	CB-CG-OD1	6.25	123.92	118.30
1	A	9	GLN	CG-CD-OE1	6.23	134.06	121.60
1	B	41	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	A	279	ASP	CB-CG-OD2	6.17	123.85	118.30
1	A	199	ASP	CB-CG-OD1	6.14	123.83	118.30
1	A	41	ARG	CB-CA-C	-6.10	98.21	110.40
1	A	282	GLU	CG-CD-OE1	6.06	130.42	118.30
1	A	113	ASN	CB-CG-OD1	-6.04	109.53	121.60
1	B	226	ASP	CB-CG-OD1	6.02	123.72	118.30
1	B	203	ALA	N-CA-CB	-6.02	101.67	110.10
1	A	172	CYS	CA-CB-SG	5.98	124.77	114.00
1	B	43	LYS	O-C-N	-5.97	113.14	122.70
1	A	173	ASP	N-CA-CB	5.96	121.34	110.60
1	B	334	ASP	CB-CG-OD1	5.88	123.60	118.30
1	A	148	GLU	OE1-CD-OE2	-5.85	116.28	123.30
1	B	282	GLU	CB-CG-CD	5.85	130.00	114.20
1	A	53	GLN	CA-CB-CG	5.85	126.26	113.40
1	A	346	VAL	CA-CB-CG2	5.84	119.66	110.90
1	B	17	ARG	CD-NE-CZ	5.83	131.76	123.60
1	B	209	HIS	CA-CB-CG	5.79	123.44	113.60
1	A	299	VAL	CA-CB-CG1	5.75	119.52	110.90
1	B	261	ASP	CB-CG-OD2	-5.64	113.22	118.30
1	B	118	GLU	OE1-CD-OE2	-5.60	116.58	123.30
1	A	41	ARG	O-C-N	5.58	131.63	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	ALA	CB-CA-C	-5.56	101.75	110.10
1	B	159	ARG	CA-CB-CG	5.54	125.59	113.40
1	A	1	PCA	C-N-CA	5.54	135.55	121.70
1	A	258	TYR	CB-CG-CD1	-5.54	117.68	121.00
1	A	79	ALA	CB-CA-C	5.49	118.33	110.10
1	B	382	PRO	N-CA-CB	5.45	109.83	103.30
1	A	254	ARG	CD-NE-CZ	5.43	131.20	123.60
1	B	235	ASP	OD1-CG-OD2	-5.40	113.05	123.30
1	B	62	ASP	CB-CG-OD1	5.35	123.12	118.30
1	B	325	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	B	302	SER	CB-CA-C	-5.27	100.09	110.10
1	B	50	ASP	CB-CG-OD2	-5.25	113.58	118.30
1	B	152	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	282	GLU	CB-CA-C	5.22	120.83	110.40
1	B	106	ARG	NE-CZ-NH1	-5.21	117.69	120.30
1	B	171	TYR	CB-CG-CD2	-5.21	117.88	121.00
1	A	224	THR	CA-CB-CG2	-5.19	105.13	112.40
1	A	69	ASN	N-CA-CB	-5.19	101.26	110.60
1	B	80	TYR	CB-CG-CD2	5.17	124.10	121.00
1	B	180	PRO	N-CA-CB	5.15	109.48	103.30
1	A	208	THR	OG1-CB-CG2	5.14	121.83	110.00
1	B	338	ARG	CD-NE-CZ	5.13	130.78	123.60
1	A	323	TYR	CB-CG-CD2	5.12	124.07	121.00
1	A	334	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	358	ASP	OD1-CG-OD2	-5.10	113.61	123.30
1	A	361	VAL	CA-CB-CG2	5.09	118.54	110.90
1	B	50	ASP	CB-CG-OD1	5.05	122.85	118.30
1	A	93	ARG	NH1-CZ-NH2	-5.02	113.88	119.40
1	B	208	THR	CB-CA-C	-5.02	98.04	111.60
1	B	208	THR	CA-CB-OG1	5.01	119.53	109.00
1	A	113	ASN	CB-CG-ND2	5.00	128.71	116.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	PCA	Mainchain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3030	0	2915	56	0
1	B	3030	0	2915	75	0
2	A	14	0	12	0	0
2	B	14	0	13	1	0
3	A	23	0	4	0	0
3	B	23	0	4	0	0
4	A	356	0	0	19	0
4	B	343	0	0	26	0
All	All	6833	0	5863	131	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 11.

All (131) 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:B:182:ILE:HD11	1:B:220:LEU:HD21	1.50	0.91
1:B:5:LYS:H	1:B:5:LYS:HZ2	1.19	0.90
1:A:203:ALA:HB2	1:A:208:THR:HG23	1.57	0.85
1:B:113:ASN:HD22	1:B:115:LYS:H	1.27	0.83
1:B:350:GLU:HG3	4:B:975:HOH:O	1.80	0.80
1:A:201:TRP:CZ3	1:A:208:THR:HG21	2.19	0.78
1:A:7:LYS:HD2	1:A:9:GLN:HE21	1.49	0.78
1:A:257:GLN:HB3	4:A:989:HOH:O	1.85	0.76
1:A:350:GLU:HG3	4:A:1084:HOH:O	1.86	0.76
1:B:2:THR:HA	4:B:1058:HOH:O	1.87	0.74
1:B:81:LYS:HG2	4:B:1059:HOH:O	1.86	0.73
1:A:120:LEU:HD12	1:A:146:LEU:HD21	1.69	0.73
1:A:81:LYS:HD3	1:A:86:THR:HG22	1.70	0.73
1:A:4:ASP:HB2	1:A:5:LYS:HE3	1.71	0.72
1:B:201:TRP:CZ3	1:B:208:THR:HG21	2.25	0.71
1:B:182:ILE:HD11	1:B:220:LEU:CD2	2.21	0.71
1:B:182:ILE:HD13	4:B:955:HOH:O	1.92	0.69
1:B:81:LYS:HD3	1:B:86:THR:HG22	1.74	0.69
1:B:4:ASP:HB2	1:B:5:LYS:NZ	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:ILE:CD1	4:B:955:HOH:O	2.41	0.69
1:B:5:LYS:H	1:B:5:LYS:NZ	1.91	0.69
1:B:295:GLU:HG3	4:B:817:HOH:O	1.92	0.68
1:A:113:ASN:HD22	1:A:115:LYS:H	1.40	0.67
1:B:5:LYS:N	1:B:5:LYS:HZ2	1.92	0.66
1:B:388:ASN:HD21	1:B:390:ARG:HH11	1.42	0.66
1:B:162:LYS:HD3	4:B:1087:HOH:O	1.95	0.66
1:B:257:GLN:HB3	4:B:1072:HOH:O	1.96	0.66
1:A:7:LYS:HD2	1:A:9:GLN:NE2	2.10	0.65
1:A:398:SER:O	1:A:399:SER:HB3	1.96	0.65
1:B:162:LYS:HB2	4:B:1058:HOH:O	1.95	0.65
1:B:187:ASN:HD21	1:B:191:GLN:H	1.46	0.64
1:A:99:ASN:HB3	4:A:956:HOH:O	1.98	0.63
1:B:26:LYS:HE2	4:B:1022:HOH:O	1.97	0.63
1:A:68:LYS:HD2	4:A:991:HOH:O	2.00	0.62
1:A:135:LYS:HE2	1:A:383:GLU:HG2	1.82	0.62
1:B:391:ILE:HG22	4:B:1112:HOH:O	2.00	0.62
1:B:298:VAL:HG12	1:B:299:VAL:O	2.00	0.61
1:B:78:ASN:HB3	4:B:1099:HOH:O	1.99	0.61
1:A:187:ASN:HD21	1:A:191:GLN:H	1.49	0.60
1:B:4:ASP:HB2	1:B:5:LYS:CE	2.32	0.59
1:A:298:VAL:HG12	1:A:299:VAL:O	2.03	0.58
1:A:295:GLU:HG3	4:A:932:HOH:O	2.02	0.58
1:A:220:LEU:C	1:A:220:LEU:HD23	2.24	0.58
1:A:96:GLN:HA	1:A:96:GLN:HE21	1.69	0.58
1:B:4:ASP:HB2	1:B:5:LYS:HE3	1.85	0.57
1:B:182:ILE:HD12	1:B:193:VAL:HG13	1.86	0.57
1:A:58:THR:HG22	4:A:959:HOH:O	2.05	0.56
1:B:182:ILE:HG12	4:B:955:HOH:O	2.05	0.56
1:A:41:ARG:NH1	4:A:945:HOH:O	2.39	0.56
1:B:8:GLU:HG2	1:B:10:HIS:CE1	2.40	0.56
1:A:116:LYS:NZ	4:A:1142:HOH:O	2.32	0.55
1:A:137:PRO:HD2	1:A:140:MET:HG3	1.90	0.54
1:A:81:LYS:HD3	1:A:86:THR:CG2	2.37	0.54
1:B:182:ILE:CG1	4:B:955:HOH:O	2.56	0.54
1:B:290:ASP:O	1:B:291:ASN:HB2	2.07	0.53
1:B:182:ILE:CD1	1:B:220:LEU:HD21	2.30	0.53
1:A:290:ASP:O	1:A:291:ASN:HB2	2.09	0.53
1:B:305:PRO:HG3	1:B:313:LYS:HD3	1.91	0.53
1:B:162:LYS:HG3	4:B:1058:HOH:O	2.09	0.52
1:B:203:ALA:HB2	1:B:208:THR:HG23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:ARG:NH1	1:B:290:ASP:OD1	2.39	0.52
1:B:276:LYS:NZ	1:B:276:LYS:H	2.08	0.52
1:A:277:GLN:HG3	4:A:826:HOH:O	2.10	0.51
1:B:7:LYS:HG3	1:B:9:GLN:HE21	1.76	0.51
1:B:64:ALA:O	1:B:68:LYS:HD3	2.10	0.51
1:A:201:TRP:CH2	1:A:208:THR:HG21	2.46	0.50
1:A:15:THR:OG1	1:A:29:ASN:ND2	2.44	0.50
1:A:7:LYS:HE3	4:A:912:HOH:O	2.12	0.50
1:A:135:LYS:HE2	1:A:383:GLU:CG	2.41	0.50
1:B:54:LYS:HE3	4:B:1031:HOH:O	2.12	0.50
1:B:81:LYS:HD3	1:B:86:THR:CG2	2.42	0.50
1:B:113:ASN:ND2	1:B:115:LYS:H	2.05	0.49
1:A:5:LYS:HD3	4:A:1085:HOH:O	2.12	0.49
1:A:61:PRO:HD2	1:A:65:SER:HB2	1.95	0.49
1:A:162:LYS:HE2	4:A:1011:HOH:O	2.12	0.49
1:B:81:LYS:CD	1:B:86:THR:HG22	2.42	0.49
1:B:282:GLU:HG3	1:B:284:HIS:CE1	2.48	0.48
1:B:16:TYR:HB2	1:B:390:ARG:HB3	1.96	0.48
1:B:41:ARG:NH2	4:B:956:HOH:O	2.45	0.48
1:A:133:MET:CE	1:A:136:LEU:HD12	2.43	0.48
1:B:182:ILE:CD1	1:B:193:VAL:HG13	2.43	0.48
1:A:276:LYS:N	1:A:276:LYS:HD3	2.29	0.48
1:A:112:GLU:HG2	4:A:1054:HOH:O	2.14	0.47
1:B:5:LYS:H	1:B:5:LYS:CE	2.27	0.46
1:B:283:LEU:HD12	1:B:283:LEU:N	2.30	0.46
1:B:291:ASN:HB3	4:B:915:HOH:O	2.14	0.46
1:A:201:TRP:CE3	1:A:208:THR:HG21	2.50	0.46
1:A:350:GLU:OE2	4:A:1084:HOH:O	2.21	0.46
1:A:182:ILE:O	1:A:185:VAL:HG22	2.16	0.45
1:B:282:GLU:HG3	1:B:284:HIS:HE1	1.81	0.45
1:A:4:ASP:HB2	1:A:5:LYS:CE	2.43	0.45
1:A:69:ASN:ND2	4:A:999:HOH:O	2.49	0.45
1:B:277:GLN:HB3	4:B:973:HOH:O	2.16	0.45
1:B:5:LYS:CD	1:B:5:LYS:H	2.30	0.44
1:B:96:GLN:HA	1:B:96:GLN:HE21	1.81	0.44
1:A:90:ASN:OD1	1:A:387:SER:HB2	2.17	0.44
1:B:137:PRO:HD2	1:B:140:MET:HG3	2.00	0.44
1:A:129:PHE:CE2	1:A:144:LEU:HD13	2.52	0.44
1:B:276:LYS:HD3	1:B:276:LYS:N	2.33	0.44
1:A:5:LYS:H	1:A:5:LYS:CD	2.30	0.44
1:B:58:THR:HG22	4:B:1101:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:ARG:NH2	4:A:880:HOH:O	2.51	0.43
1:A:91:LYS:HE3	4:A:985:HOH:O	2.18	0.43
1:B:9:GLN:NE2	1:B:76:ASP:HB2	2.34	0.43
1:A:129:PHE:CD2	1:A:144:LEU:HD13	2.54	0.43
1:B:42:GLN:NE2	4:B:904:HOH:O	2.48	0.43
1:A:212:PRO:HD2	1:A:239:CYS:O	2.18	0.43
1:B:14:GLU:HB3	1:B:26:LYS:HD2	2.00	0.43
1:B:35:ALA:O	1:B:38:HIS:HB2	2.19	0.43
1:B:116:LYS:HE3	4:B:1094:HOH:O	2.18	0.42
1:B:182:ILE:HD12	1:B:193:VAL:CG1	2.47	0.42
1:A:81:LYS:CD	1:A:86:THR:HG22	2.47	0.42
1:A:208:THR:HG22	1:A:209:HIS:H	1.83	0.42
1:B:78:ASN:CB	4:B:1099:HOH:O	2.61	0.42
1:B:246:ILE:H	1:B:246:ILE:HG13	1.75	0.42
1:B:379:GLN:HA	1:B:380:PRO:HD2	1.93	0.42
1:A:257:GLN:OE1	4:A:1034:HOH:O	2.21	0.42
1:B:220:LEU:C	1:B:220:LEU:HD23	2.40	0.42
1:B:284:HIS:HD2	4:B:1131:HOH:O	2.02	0.41
1:B:275:ASN:C	1:B:275:ASN:OD1	2.59	0.41
1:A:203:ALA:CB	1:A:208:THR:HG23	2.39	0.41
1:A:259:LYS:HD2	4:A:858:HOH:O	2.20	0.41
1:B:313:LYS:HB2	4:B:1048:HOH:O	2.21	0.41
1:A:122:LEU:HA	1:A:125:THR:OG1	2.20	0.41
1:B:220:LEU:HD23	1:B:221:TYR:N	2.35	0.41
1:B:69:ASN:ND2	4:B:893:HOH:O	2.49	0.41
1:A:94:LEU:HB3	1:A:346:VAL:HG22	2.03	0.41
1:B:58:THR:HG23	2:B:800:NAG:H5	2.03	0.41
1:B:137:PRO:HD2	1:B:140:MET:CG	2.51	0.40
1:A:17:ARG:HD3	1:A:17:ARG:HA	1.83	0.40
1:B:305:PRO:HG3	1:B:313:LYS:CD	2.50	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 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	398/411 (97%)	381 (96%)	16 (4%)	1 (0%)	41	50
1	B	398/411 (97%)	385 (97%)	13 (3%)	0	100	100
All	All	796/822 (97%)	766 (96%)	29 (4%)	1 (0%)	51	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	399	SER

### 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	324/333 (97%)	302 (93%)	22 (7%)	16	21
1	B	324/333 (97%)	297 (92%)	27 (8%)	11	14
All	All	648/666 (97%)	599 (92%)	49 (8%)	13	16

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	25	LYS
1	A	27	GLN
1	A	41	ARG
1	A	58	THR
1	A	68	LYS
1	A	81	LYS
1	A	91	LYS
1	A	96	GLN
1	A	102	LEU
1	A	115	LYS
1	A	162	LYS

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Mol	Chain	Res	Type
1	A	187	ASN
1	A	208	THR
1	A	224	THR
1	A	276	LYS
1	A	306	LYS
1	A	346	VAL
1	A	348	TRP
1	A	373	LYS
1	A	388	ASN
1	A	390	ARG
1	B	5	LYS
1	B	25	LYS
1	B	27	GLN
1	B	41	ARG
1	B	43	LYS
1	B	58	THR
1	B	68	LYS
1	B	81	LYS
1	B	96	GLN
1	B	102	LEU
1	B	115	LYS
1	B	135	LYS
1	B	159	ARG
1	B	162	LYS
1	B	182	ILE
1	B	187	ASN
1	B	208	THR
1	B	224	THR
1	B	256	LYS
1	B	276	LYS
1	B	306	LYS
1	B	346	VAL
1	B	348	TRP
1	B	350	GLU
1	B	373	LYS
1	B	388	ASN
1	B	390	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN

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Mol	Chain	Res	Type
1	A	53	GLN
1	A	69	ASN
1	A	95	GLN
1	A	96	GLN
1	A	113	ASN
1	A	187	ASN
1	A	284	HIS
1	A	331	GLN
1	A	388	ASN
1	B	9	GLN
1	B	27	GLN
1	B	29	ASN
1	B	42	GLN
1	B	69	ASN
1	B	96	GLN
1	B	113	ASN
1	B	121	HIS
1	B	175	GLN
1	B	187	ASN
1	B	284	HIS
1	B	331	GLN
1	B	388	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	PCA	A	1	1	7,8,9	1.40	2 (28%)	9,10,12	2.01	4 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	PCA	B	1	1	7,8,9	1.48	2 (28%)	9,10,12	1.36	1 (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
1	PCA	A	1	1	-	0/0/11/13	0/1/1/1
1	PCA	B	1	1	-	0/0/11/13	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	PCA	CG-CD	2.51	1.57	1.50
1	A	1	PCA	O-C	2.31	1.29	1.19
1	B	1	PCA	CG-CD	2.22	1.56	1.50
1	B	1	PCA	O-C	2.17	1.28	1.19

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	PCA	OE-CD-CG	-3.50	120.66	126.76
1	A	1	PCA	CB-CG-CD	-2.82	99.86	104.40
1	A	1	PCA	CA-N-CD	-2.45	105.20	113.58
1	A	1	PCA	CG-CD-N	2.11	113.85	108.39
1	B	1	PCA	OE-CD-CG	-2.08	123.14	126.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

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
3	IN1	B	801	1	23,23,23	1.16	3 (13%)	28,32,32	1.58	3 (10%)
3	IN1	A	801	1	23,23,23	1.37	4 (17%)	28,32,32	1.96	5 (17%)
2	NAG	B	800	1	14,14,15	1.48	1 (7%)	17,19,21	1.74	4 (23%)
2	NAG	A	800	1	14,14,15	1.39	1 (7%)	17,19,21	2.42	7 (41%)

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	IN1	B	801	1	-	6/17/37/37	0/1/1/1
3	IN1	A	801	1	-	7/17/37/37	0/1/1/1
2	NAG	B	800	1	-	0/6/23/26	0/1/1/1
2	NAG	A	800	1	-	0/6/23/26	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	800	NAG	O7-C7	-4.15	1.13	1.23
2	A	800	NAG	O7-C7	-3.70	1.14	1.23
3	B	801	IN1	O5-C1	3.15	1.49	1.41
3	B	801	IN1	O2A-C4A	3.10	1.42	1.33
3	A	801	IN1	O1-C1	2.96	1.45	1.40
3	A	801	IN1	O2A-C4A	2.56	1.40	1.33
3	A	801	IN1	O2A-C3A	-2.50	1.40	1.45
3	A	801	IN1	C2A-C6A	2.35	1.56	1.52
3	B	801	IN1	O1-C1	2.11	1.43	1.40

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	IN1	C1A-O1-C1	-6.09	103.74	113.84
3	B	801	IN1	C1A-O1-C1	-5.67	104.44	113.84
3	A	801	IN1	C3A-O2A-C4A	5.22	125.93	116.88
2	A	800	NAG	O3-C3-C2	5.07	119.95	109.47
2	A	800	NAG	O6-C6-C5	5.04	128.59	111.29
2	A	800	NAG	O3-C3-C4	-3.57	102.11	110.35
2	B	800	NAG	C8-C7-N2	-3.28	110.55	116.10
2	B	800	NAG	O5-C1-C2	-3.21	106.22	111.29
2	A	800	NAG	C2-N2-C7	-2.77	118.96	122.90
2	A	800	NAG	C8-C7-N2	-2.53	111.81	116.10
3	A	801	IN1	O6-C6-C5	-2.47	102.82	111.29
3	B	801	IN1	O2A-C4A-C5A	-2.46	104.92	111.38
2	B	800	NAG	C4-C3-C2	-2.42	107.47	111.02
2	A	800	NAG	O5-C1-C2	-2.29	107.67	111.29
3	A	801	IN1	O5-C1-O1	-2.29	104.55	109.97
3	B	801	IN1	O1-C1A-C2A	2.19	113.33	108.81
2	A	800	NAG	O7-C7-C8	2.09	125.95	122.06
3	A	801	IN1	O2-C2-C3	2.00	114.98	110.35
2	B	800	NAG	C2-N2-C7	-2.00	120.05	122.90

There are no chirality outliers.

All (13) torsion outliers are listed below:

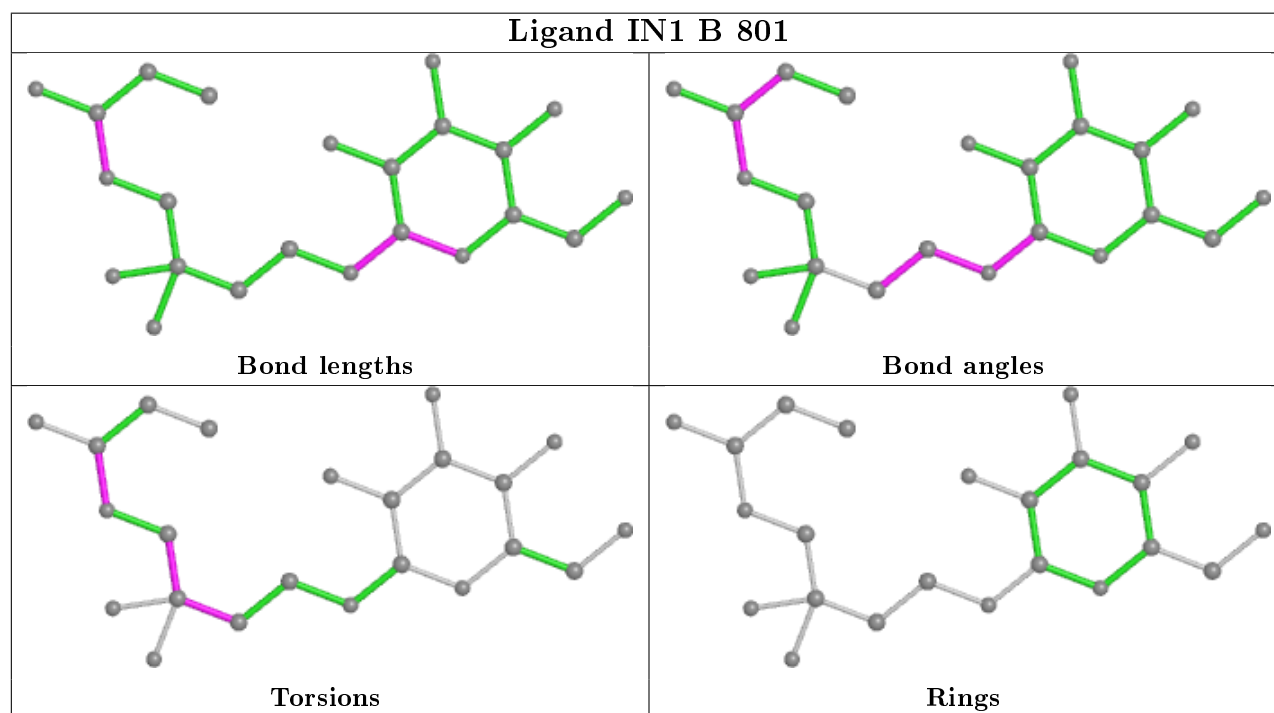
Mol	Chain	Res	Type	Atoms
3	B	801	IN1	C1A-C2A-C6A-C3A
3	B	801	IN1	C1A-C2A-C6A-O4S
3	B	801	IN1	O2A-C3A-C6A-C2A
3	A	801	IN1	C1A-C2A-C6A-C3A
3	A	801	IN1	C1A-C2A-C6A-O4S
3	A	801	IN1	O2A-C3A-C6A-C2A
3	A	801	IN1	O2A-C3A-C6A-O4S
3	B	801	IN1	C1A-C2A-C6A-O1R
3	A	801	IN1	C1A-C2A-C6A-O1R
3	B	801	IN1	C5A-C4A-O2A-C3A
3	B	801	IN1	O2A-C3A-C6A-O4S
3	A	801	IN1	O2A-C3A-C6A-O1R
3	A	801	IN1	C5A-C4A-O2A-C3A

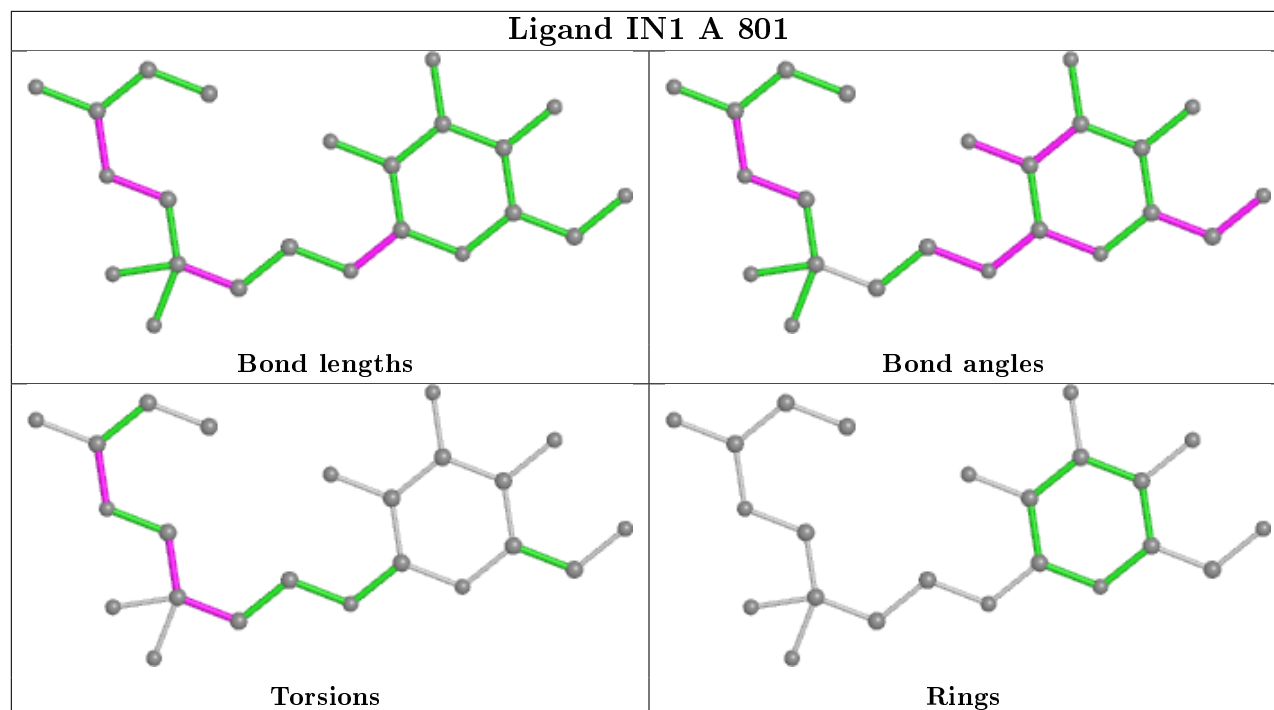
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	800	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 [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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.