Full wwPDB X-ray Structure Validation Report ⓘ

Nov 7, 2023 – 09:42 AM EST

PDB ID	:	7UN2
Title	:	Crystal structure of a lectin from Canavalia maritima seed (ConM) complexed with Indole-3-butyric acid
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Deposited on	:	2022-04-08
Resolution	:	1.80 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:

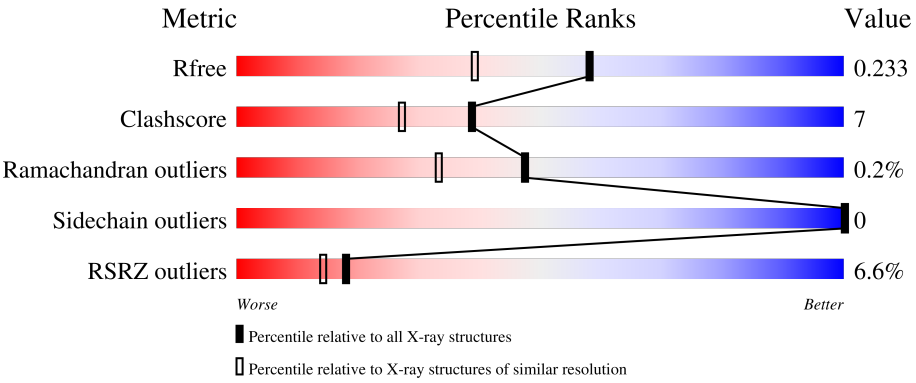
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 <=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	237	6% 87% 11%
1	B	237	7% 89% 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	DBB	B	303	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 3990 atoms, of which 39 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 ConM.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	232	Total	C	H	N	O	S	0	0	0
			1775	1113	14	294	353	1			
1	B	237	Total	C	H	N	O	S	0	0	0
			1826	1135	25	302	363	1			

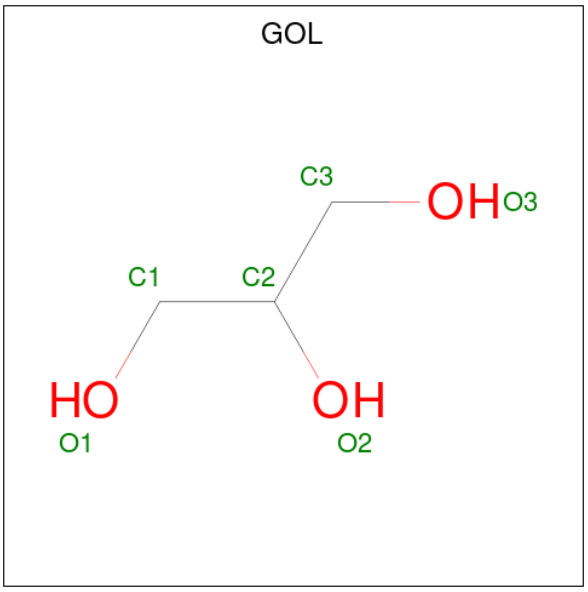
- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		
2	B	1	Total	Ca	0	0
			1	1		

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

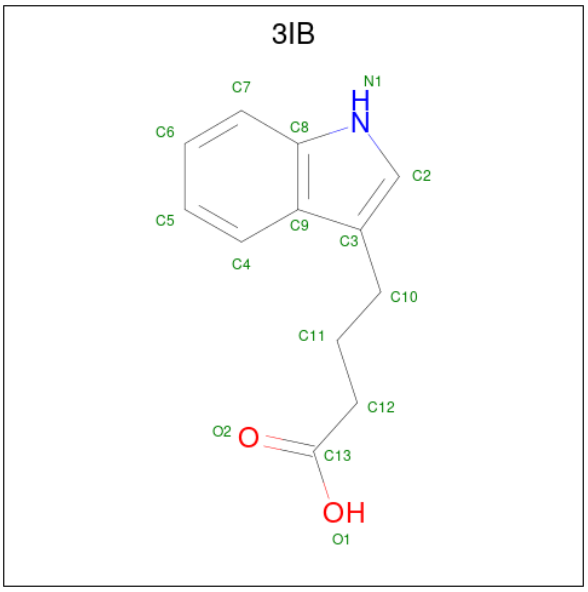
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mn	0	0
			1	1		
3	B	1	Total	Mn	0	0
			1	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is 3-INDOLEBUTYRIC ACID (three-letter code: 3IB) (formula: $C_{12}H_{13}NO_2$) (labeled as "Ligand of Interest" by depositor).

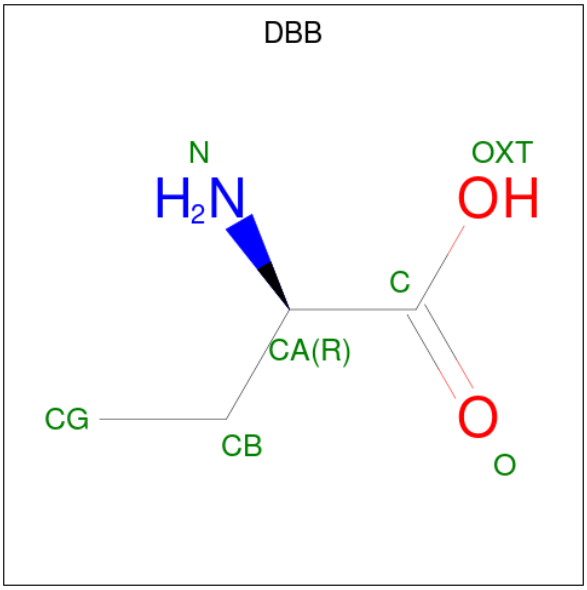


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 15 12 1 2	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Cl 1 1	0	0
6	B	1	Total Cl 1 1	0	0

- Molecule 7 is D-ALPHA-AMINOBUTYRIC ACID (three-letter code: DBB) (formula: $C_4H_9NO_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C N O 7 4 1 2	0	0

- Molecule 8 is water.

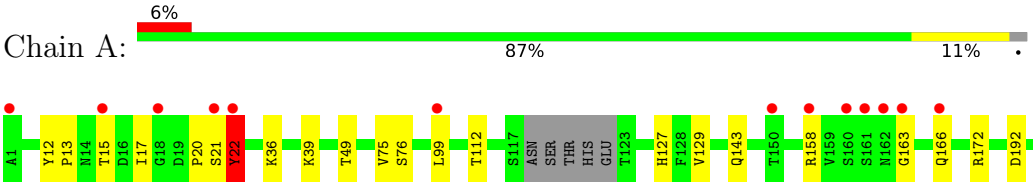
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	146	Total O 146 146	0	0
8	B	203	Total O 203 203	0	0

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.

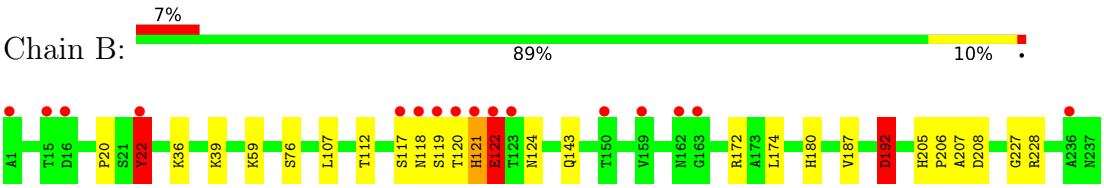
- Molecule 1: ConM

Chain A:



- Molecule 1: ConM

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α, β, γ	67.99Å 71.84Å 98.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.99 – 1.80 33.99 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (33.99-1.80) 99.7 (33.99-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.89 (at 1.81Å)	Xtriage
Refinement program	PHENIX 1.12	Depositor
R, R_{free}	0.203 , 0.233 0.203 , 0.233	Depositor DCC
R_{free} test set	2221 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å^2)	20.1	Xtriage
Anisotropy	0.875	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 51.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3990	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 70.59 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.0405e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CA, CL, 3IB, DBB, MN

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	0.49	2/1800 (0.1%)	1.54	5/2450 (0.2%)
1	B	0.57	4/1842 (0.2%)	1.74	9/2509 (0.4%)
All	All	0.53	6/3642 (0.2%)	1.65	14/4959 (0.3%)

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
1	B	0	4
All	All	0	5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	22	TYR	CG-CD2	9.96	1.52	1.39
1	B	22	TYR	CG-CD2	7.98	1.49	1.39
1	B	22	TYR	CE1-CZ	-7.88	1.28	1.38
1	B	122	GLU	CA-CB	-6.99	1.38	1.53
1	B	22	TYR	CD1-CE1	-5.96	1.30	1.39
1	A	22	TYR	CE1-CZ	-5.57	1.31	1.38

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	22	TYR	CB-CG-CD2	-58.19	86.08	121.00
1	B	22	TYR	CB-CG-CD2	-55.38	87.77	121.00
1	A	22	TYR	CB-CG-CD1	33.07	140.84	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	22	TYR	CB-CG-CD1	31.76	140.06	121.00
1	B	122	GLU	OE1-CD-OE2	-24.29	94.15	123.30
1	B	192	ASP	CB-CG-OD2	-22.67	97.90	118.30
1	B	22	TYR	CD1-CG-CD2	-19.80	96.12	117.90
1	B	122	GLU	CG-CD-OE1	18.07	154.43	118.30
1	A	22	TYR	CD1-CG-CD2	-16.98	99.22	117.90
1	B	122	GLU	CG-CD-OE2	-16.43	85.44	118.30
1	B	192	ASP	CB-CG-OD1	11.01	128.21	118.30
1	B	22	TYR	CG-CD1-CE1	9.21	128.67	121.30
1	A	22	TYR	CG-CD1-CE1	6.70	126.66	121.30
1	A	22	TYR	CG-CD2-CE2	5.45	125.66	121.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	22	TYR	Sidechain
1	B	121	HIS	Peptide
1	B	122	GLU	Sidechain
1	B	192	ASP	Sidechain
1	B	22	TYR	Sidechain

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	1761	14	1716	23	0
1	B	1801	25	1748	30	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
5	A	15	0	12	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	7	0	8	4	0
8	A	146	0	0	1	0
8	B	203	0	0	3	0
All	All	3951	39	3500	53	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 7.

All (53) 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:17:ILE:HD13	1:A:228:ARG:HD2	1.48	0.95
1:B:207:ALA:HB1	1:B:208:ASP:OD1	1.67	0.93
1:A:20:PRO:HB2	1:A:22:TYR:CD1	2.09	0.87
1:B:20:PRO:HB2	1:B:22:TYR:CD1	2.12	0.83
1:A:207:ALA:HB1	1:A:208:ASP:OD1	1.78	0.83
1:B:20:PRO:HB2	1:B:22:TYR:CE1	2.14	0.82
1:B:208:ASP:OD2	1:B:227:GLY:HA2	1.79	0.81
1:A:20:PRO:HB2	1:A:22:TYR:CE1	2.16	0.81
1:B:112:THR:HB	1:B:192:ASP:OD1	1.83	0.77
1:A:208:ASP:OD2	1:A:227:GLY:HA2	1.84	0.77
1:A:158:ARG:HD2	1:A:166:GLN:HG3	1.73	0.70
1:B:180:HIS:HB3	7:B:303:DBB:HA	1.73	0.70
1:A:99:LEU:O	1:A:99:LEU:HD23	1.94	0.68
1:B:180:HIS:O	7:B:303:DBB:HG2	1.94	0.67
1:A:20:PRO:HB2	1:A:22:TYR:HD1	1.59	0.67
1:A:17:ILE:CD1	1:A:228:ARG:HD2	2.24	0.67
1:B:20:PRO:HB2	1:B:22:TYR:HD1	1.59	0.64
1:B:118:ASN:OD1	1:B:119:SER:N	2.32	0.61
1:A:112:THR:HB	1:A:192:ASP:OD1	2.01	0.60
1:A:172:ARG:NH2	8:A:401:HOH:O	2.25	0.57
1:A:20:PRO:CB	1:A:22:TYR:CE1	2.89	0.55
1:B:117:SER:HA	1:B:187:VAL:HG12	1.89	0.55
1:B:118:ASN:ND2	1:B:122:GLU:OE1	2.40	0.55
1:A:36:LYS:HG3	1:A:75:VAL:CG2	2.37	0.54
1:B:20:PRO:CB	1:B:22:TYR:CE1	2.89	0.54
1:B:180:HIS:CB	7:B:303:DBB:HA	2.38	0.54
1:B:228:ARG:HG2	8:B:498:HOH:O	2.08	0.52
1:A:143:GLN:OE1	1:A:172:ARG:HD2	2.11	0.51
1:B:143:GLN:OE1	1:B:172:ARG:HD2	2.11	0.51
1:B:121:HIS:N	1:B:121:HIS:CD2	2.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:LYS:HG3	1:A:75:VAL:HG23	1.95	0.49
1:B:205:HIS:ND1	1:B:206:PRO:O	2.44	0.48
1:B:118:ASN:OD1	1:B:122:GLU:OE1	2.32	0.48
1:B:124:ASN:HB3	7:B:303:DBB:O	2.13	0.48
1:A:49:THR:HG21	5:A:304:3IB:H4	1.96	0.48
1:A:20:PRO:CB	1:A:22:TYR:CD1	2.92	0.48
1:B:117:SER:HB3	1:B:118:ASN:H	1.56	0.47
1:B:36:LYS:HG2	1:B:76:SER:O	2.16	0.46
1:B:59:LYS:HE2	8:B:469:HOH:O	2.18	0.44
1:A:36:LYS:HG2	1:A:76:SER:O	2.17	0.44
1:B:120:THR:OG1	1:B:121:HIS:N	2.51	0.43
1:B:117:SER:CA	1:B:187:VAL:HG12	2.49	0.43
1:A:158:ARG:HB3	1:A:166:GLN:HB2	2.01	0.43
1:B:119:SER:HB2	8:B:555:HOH:O	2.20	0.42
1:B:174:LEU:HD12	1:B:174:LEU:N	2.35	0.42
1:B:22:TYR:CD2	1:B:39:LYS:HG3	2.55	0.41
1:A:12:TYR:HA	1:A:13:PRO:HD3	1.90	0.41
1:A:15:THR:CG2	1:A:21:SER:HA	2.51	0.41
1:A:127:HIS:NE2	1:A:129:VAL:HG23	2.36	0.41
1:B:118:ASN:CG	1:B:122:GLU:OE1	2.60	0.40
1:B:107:LEU:HD12	1:B:107:LEU:N	2.37	0.40
1:A:22:TYR:CE2	1:A:39:LYS:HD3	2.56	0.40
1:B:120:THR:OG1	1:B:121:HIS:CD2	2.75	0.40

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 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	228/237 (96%)	221 (97%)	6 (3%)	1 (0%)	34 21
1	B	235/237 (99%)	226 (96%)	9 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	463/474 (98%)	447 (96%)	15 (3%)	1 (0%)	47 33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	163	GLY

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 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	197/202 (98%)	197 (100%)	0	100 100
1	B	202/202 (100%)	202 (100%)	0	100 100
All	All	399/404 (99%)	399 (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. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	121	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 for Mogul analysis.

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	B	304	-	5,5,5	1.09	0	5,5,5	0.97	0
7	DBB	B	303	-	5,6,6	0.99	0	4,7,7	0.79	0
4	GOL	A	303	-	5,5,5	1.00	0	5,5,5	1.09	0
5	3IB	A	304	-	15,16,16	0.92	0	16,21,21	1.48	2 (12%)

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	B	304	-	-	0/4/4/4	-
7	DBB	B	303	-	-	4/6/6/6	-
4	GOL	A	303	-	-	0/4/4/4	-
5	3IB	A	304	-	-	5/6/6/6	0/2/2/2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	304	3IB	C10-C3-C2	-3.53	119.75	127.19
5	A	304	3IB	C11-C10-C3	-2.07	108.11	114.15

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	304	3IB	C11-C10-C3-C9
5	A	304	3IB	C3-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
7	B	303	DBB	OXT-C-CA-N
7	B	303	DBB	O-C-CA-N
7	B	303	DBB	O-C-CA-CB
7	B	303	DBB	OXT-C-CA-CB
5	A	304	3IB	C11-C10-C3-C2
5	A	304	3IB	C11-C12-C13-O1
5	A	304	3IB	C11-C12-C13-O2

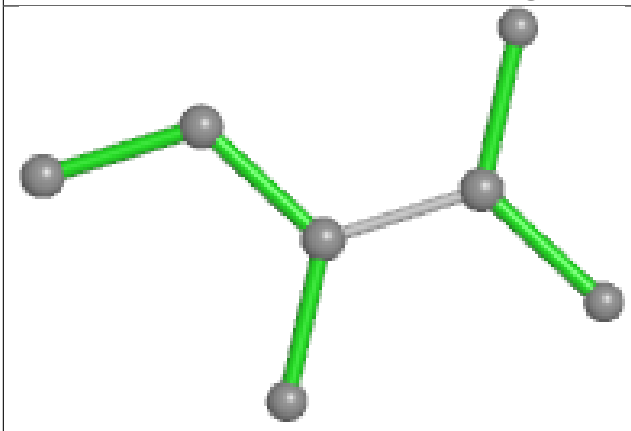
There are no ring outliers.

2 monomers are involved in 5 short contacts:

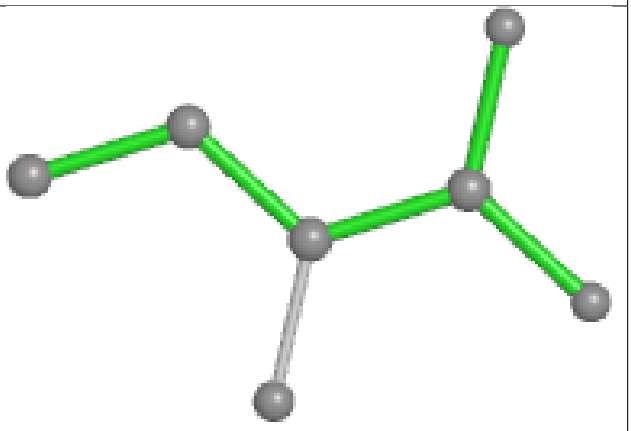
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	303	DBB	4	0
5	A	304	3IB	1	0

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 then 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.

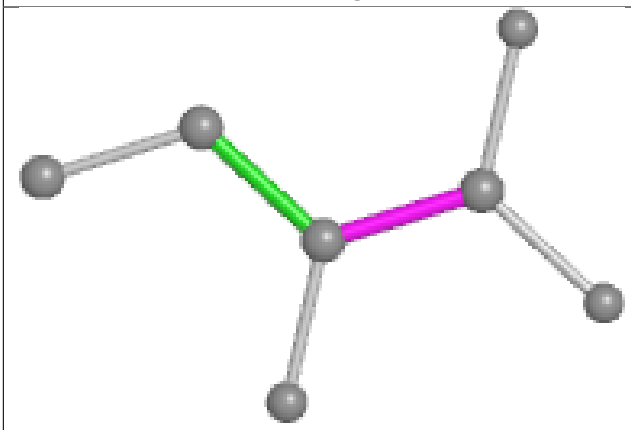
Ligand DBB B 303



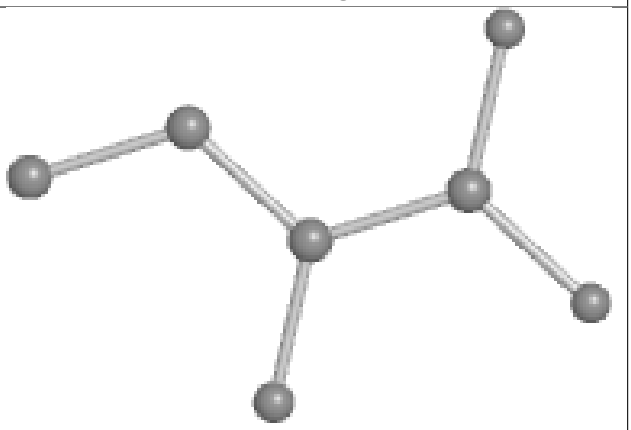
Bond lengths



Bond angles

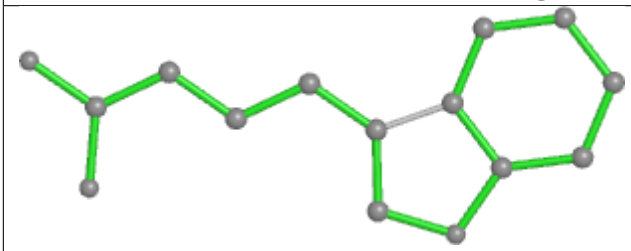


Torsions

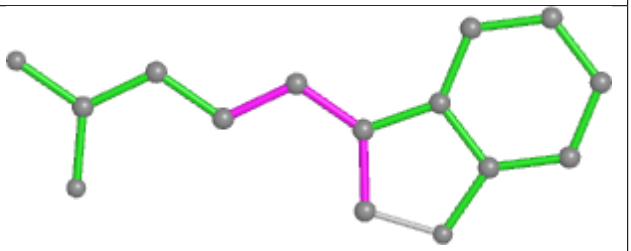


Rings

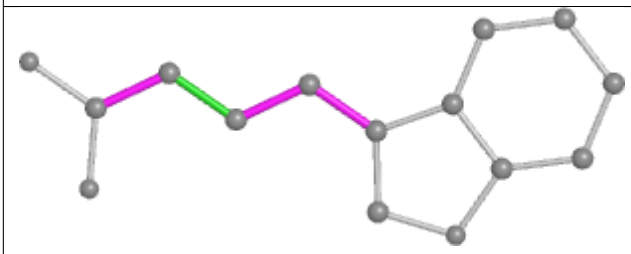
Ligand 3IB A 304



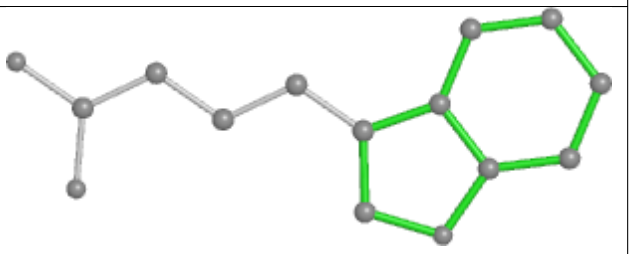
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

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, 95^{th} 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	232/237 (97%)	0.34	15 (6%)	18	15	15, 26, 45, 69	0
1	B	237/237 (100%)	0.23	16 (6%)	17	13	14, 22, 38, 63	0
All	All	469/474 (98%)	0.28	31 (6%)	18	14	14, 24, 44, 69	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	121	HIS	4.9
1	B	119	SER	4.6
1	B	162	ASN	4.5
1	A	163	GLY	4.4
1	B	163	GLY	4.1
1	A	161	SER	4.1
1	B	118	ASN	3.8
1	B	122	GLU	3.8
1	A	162	ASN	3.4
1	A	15	THR	3.1
1	B	120	THR	3.1
1	A	1	ALA	3.0
1	B	1	ALA	2.9
1	A	150	THR	2.6
1	B	117	SER	2.6
1	A	160	SER	2.5
1	B	16	ASP	2.5
1	B	15	THR	2.4
1	A	21	SER	2.3
1	A	22	TYR	2.3
1	A	205	HIS	2.3
1	A	166	GLN	2.3
1	B	150	THR	2.2
1	B	22	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	123	THR	2.2
1	A	237	ASN	2.1
1	B	236	ALA	2.1
1	A	99	LEU	2.1
1	A	18	GLY	2.1
1	A	158	ARG	2.0
1	B	159	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

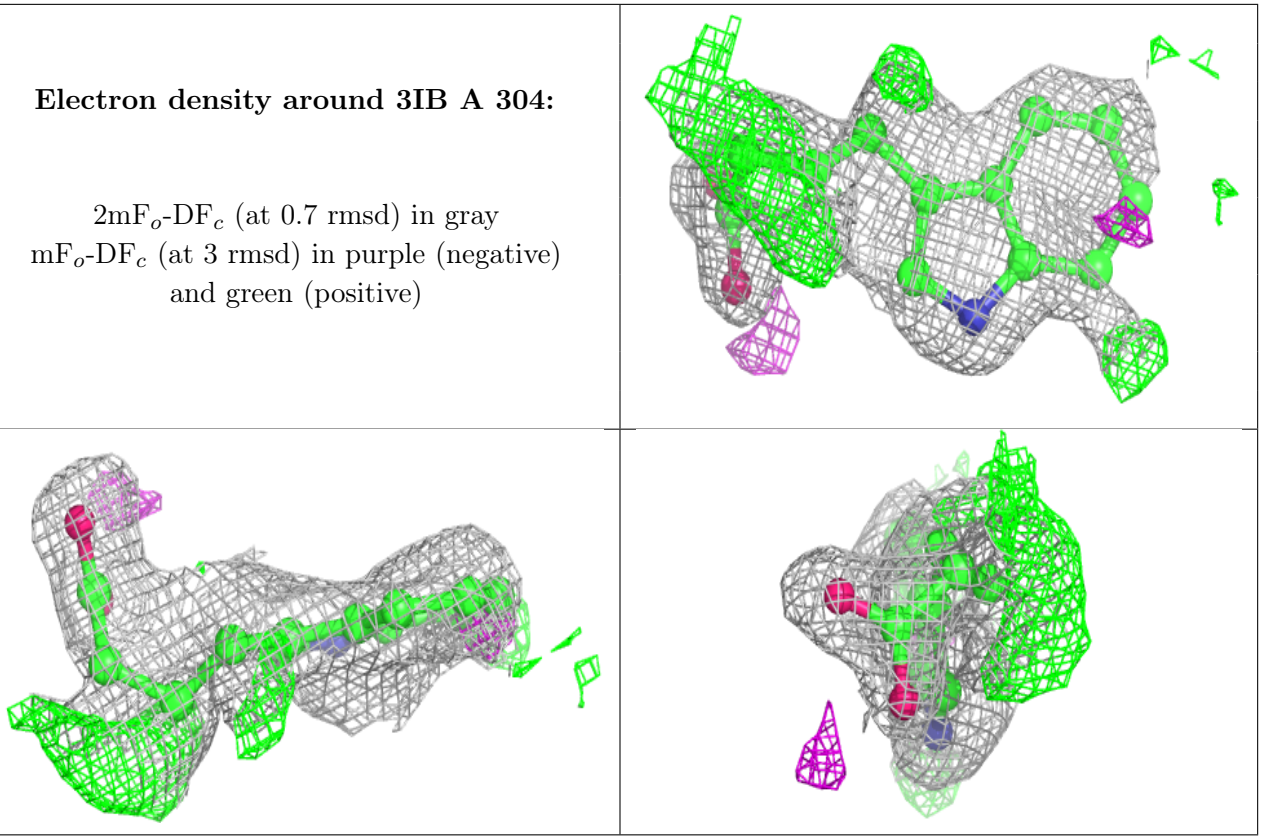
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
5	3IB	A	304	15/15	0.65	0.23	37,44,50,50	0
7	DBB	B	303	7/7	0.68	0.24	14,24,39,42	0
6	CL	A	305	1/1	0.78	0.09	60,60,60,60	0
6	CL	B	305	1/1	0.90	0.07	45,45,45,45	0
3	MN	A	302	1/1	0.90	0.07	36,36,36,36	0
4	GOL	A	303	6/6	0.93	0.10	29,32,34,39	0
2	CA	A	301	1/1	0.94	0.07	30,30,30,30	0
4	GOL	B	304	6/6	0.97	0.08	20,25,27,30	0
2	CA	B	301	1/1	0.98	0.07	20,20,20,20	0
3	MN	B	302	1/1	0.99	0.03	24,24,24,24	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.

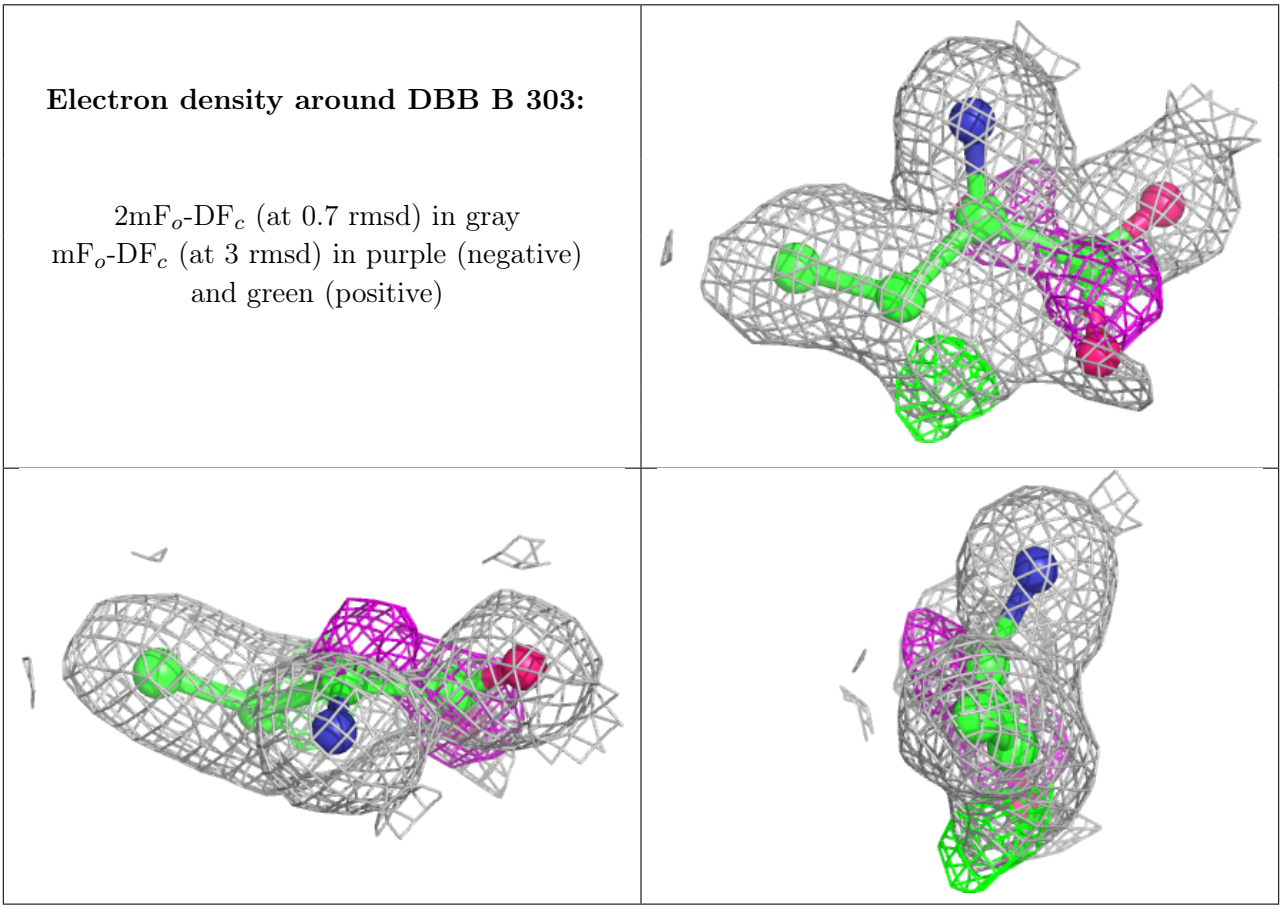
Electron density around 3IB A 304:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around DBB B 303:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.