



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 06:39 am BST

PDB ID : 1IBG  
Title : STRUCTURE AND SPECIFICITY OF THE ANTI-DIGOXIN ANTIBODY  
40-50  
Authors : Jeffrey, P.D.; Sheriff, S.  
Deposited on : 1994-10-25  
Resolution : 2.70 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) : 1.13  
EDS : 2.11  
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) : 2.11

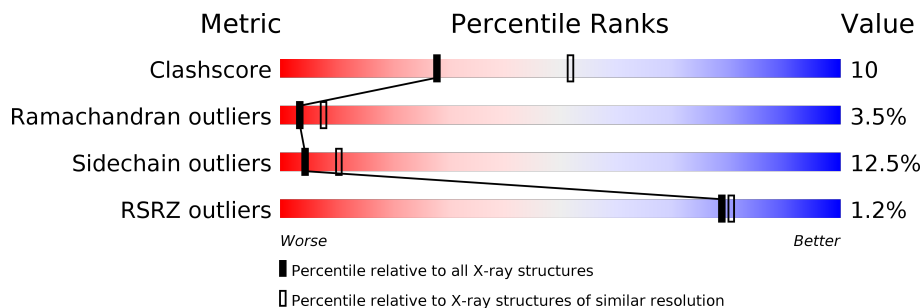
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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  $\leq 5\%$ . 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	L	217	 2% 62% 32% 6%
2	H	217	 64% 27% 7% 2%

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3348 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 IGG2B-KAPPA 40-50 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	217	1677	1046	285	340	6	13	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	27D	THR	ALA	CONFLICT	PIR JC5810
L	31	SER	ILE	CONFLICT	PIR JC5810
L	32	HIS	TYR	CONFLICT	PIR JC5810
L	33	ILE	MET	CONFLICT	PIR JC5810
L	49	TYR	SER	CONFLICT	PIR JC5810
L	53	ILE	ASN	CONFLICT	PIR JC5810
L	83	ALA	VAL	CONFLICT	PIR JC5810
L	94	TYR	LEU	CONFLICT	PIR JC5810
L	103	GLU	LYS	CONFLICT	PIR JC5810

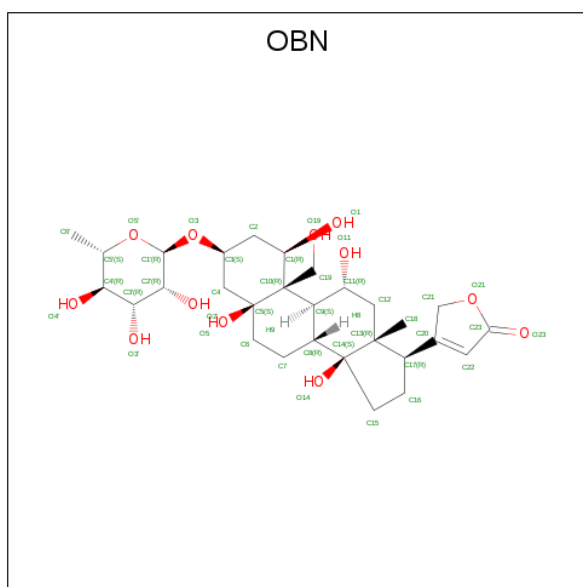
- Molecule 2 is a protein called IGG2B-KAPPA 40-50 FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	217	1628	1033	265	321	9	78	0	0

- Molecule 3 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	1	Total	Cu	0	0
			1	1		

- Molecule 4 is OUABAIN (three-letter code: OBN) (formula: C<sub>29</sub>H<sub>44</sub>O<sub>12</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
4	H	1	Total	C	O	0	0
			41	29	12		

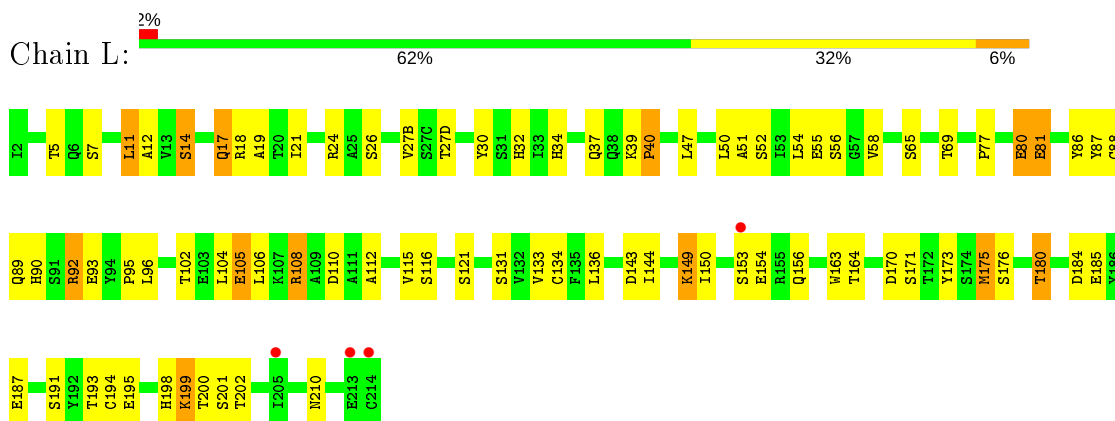
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	L	1	Total	O	0	0
			1	1		

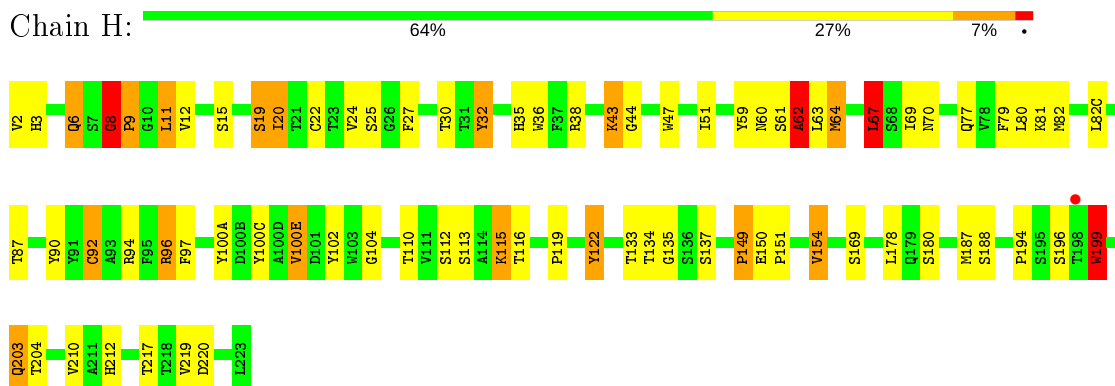
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: IGG2B-KAPPA 40-50 FAB (LIGHT CHAIN)



- Molecule 2: IGG2B-KAPPA 40-50 FAB (HEAVY CHAIN)



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.66Å 84.77Å 70.08Å 90.00° 127.95° 90.00°	Depositor
Resolution (Å)	10.00 – 2.70 46.72 – 2.42	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.70) 73.6 (46.72-2.42)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.65 (at 2.42Å)	Xtrriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.209 , (Not available) 0.205 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.6	Xtrriage
Anisotropy	0.426	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 95.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	3348	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.23% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: OBN, CU

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	L	0.82	1/1717 (0.1%)	1.65	25/2334 (1.1%)
2	H	0.83	0/1675	1.64	22/2293 (1.0%)
All	All	0.83	1/3392 (0.0%)	1.65	47/4627 (1.0%)

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	L	0	1
2	H	0	2
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	153	SER	CA-CB	5.51	1.61	1.52

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	96	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	L	81	GLU	CA-CB-CG	7.39	129.66	113.40
1	L	185	GLU	CA-CB-CG	7.17	129.16	113.40
2	H	67	LEU	CA-CB-CG	6.74	130.81	115.30
1	L	95	PRO	O-C-N	6.70	133.42	122.70
2	H	62	ALA	N-CA-C	-6.31	93.97	111.00
1	L	93	GLU	CA-CB-CG	6.28	127.22	113.40
1	L	195	GLU	CA-CB-CG	6.11	126.84	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	133	VAL	CG1-CB-CG2	-6.11	101.13	110.90
2	H	92	CYS	CA-CB-SG	6.06	124.90	114.00
2	H	82	MET	CA-CB-CG	-6.04	103.03	113.30
1	L	95	PRO	CA-C-N	-6.03	103.94	117.20
2	H	90	TYR	CB-CG-CD2	-5.99	117.41	121.00
2	H	187	MET	CA-CB-CG	5.96	123.43	113.30
1	L	18	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	L	199	LYS	N-CA-C	5.91	126.96	111.00
2	H	9	PRO	CA-C-N	-5.89	104.41	116.20
1	L	87	TYR	CB-CG-CD1	-5.89	117.47	121.00
2	H	100(E)	VAL	N-CA-C	-5.84	95.22	111.00
2	H	20	ILE	CG1-CB-CG2	-5.83	98.57	111.40
1	L	175	MET	CG-SD-CE	-5.80	90.92	100.20
2	H	51	ILE	CA-CB-CG1	-5.78	100.01	111.00
1	L	105	GLU	CA-CB-CG	5.77	126.09	113.40
1	L	171	SER	N-CA-CB	-5.72	101.93	110.50
2	H	133	THR	CA-C-N	-5.70	104.67	117.20
2	H	122	TYR	CB-CG-CD2	-5.68	117.59	121.00
2	H	220	ASP	CB-CG-OD1	5.56	123.31	118.30
2	H	102	TYR	CB-CG-CD1	-5.55	117.67	121.00
1	L	54	LEU	CA-CB-CG	5.52	127.99	115.30
1	L	154	GLU	N-CA-C	-5.47	96.23	111.00
1	L	173	TYR	CB-CG-CD2	-5.46	117.72	121.00
1	L	56	SER	CA-C-N	-5.44	105.32	116.20
1	L	108	ARG	CA-CB-CG	5.40	125.28	113.40
1	L	194	CYS	N-CA-C	-5.39	96.45	111.00
2	H	9	PRO	N-CA-CB	-5.39	96.67	102.60
2	H	81	LYS	CA-CB-CG	-5.33	101.67	113.40
2	H	115	LYS	CB-CG-CD	5.30	125.39	111.60
2	H	100(A)	TYR	CB-CG-CD1	5.27	124.16	121.00
2	H	154	VAL	CG1-CB-CG2	-5.24	102.51	110.90
2	H	32	TYR	CA-C-N	-5.23	105.75	116.20
1	L	110	ASP	CB-CG-OD1	5.19	122.97	118.30
1	L	108	ARG	N-CA-CB	-5.18	101.28	110.60
2	H	100(A)	TYR	CB-CG-CD2	-5.17	117.90	121.00
1	L	96	LEU	CB-CG-CD1	-5.16	102.22	111.00
1	L	30	TYR	CB-CG-CD1	-5.16	117.90	121.00
1	L	39	LYS	CA-CB-CG	5.16	124.75	113.40
1	L	175	MET	O-C-N	5.01	130.72	122.70

There are no chirality outliers.

All (3) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
2	H	199	TRP	Peptide
2	H	8	GLY	Peptide
1	L	86	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	L	1677	0	1607	27	0
2	H	1628	0	1570	36	0
3	L	1	0	0	0	0
4	H	41	0	44	1	0
5	L	1	0	0	0	0
All	All	3348	0	3221	63	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 10.

All (63) 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:L:12:ALA:HA	1:L:105:GLU:O	1.86	0.75
2:H:67:LEU:HD22	2:H:80:LEU:HD11	1.72	0.72
2:H:43:LYS:HZ2	2:H:43:LYS:HB2	1.58	0.68
1:L:112:ALA:HB2	1:L:200:THR:HG21	1.79	0.65
1:L:115:VAL:HG12	1:L:136:LEU:HD22	1.78	0.65
2:H:2:VAL:N	2:H:25:SER:HG	1.95	0.65
2:H:154:VAL:HG22	2:H:210:VAL:HG22	1.80	0.63
2:H:59:TYR:HE1	2:H:69:ILE:HG13	1.63	0.63
2:H:87:THR:HG23	2:H:110:THR:HA	1.82	0.61
2:H:24:VAL:HB	2:H:27:PHE:CZ	2.39	0.58
2:H:63:LEU:HD12	2:H:63:LEU:H	1.68	0.58
1:L:47:LEU:O	1:L:58:VAL:HG21	2.04	0.57
2:H:6:GLN:NE2	2:H:92:CYS:SG	2.78	0.57
2:H:116:THR:HG22	2:H:149:PRO:HD3	1.88	0.55
1:L:21:ILE:HD12	1:L:102:THR:HG21	1.90	0.54
1:L:11:LEU:HD23	1:L:104:LEU:HG	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:35:HIS:HD2	2:H:47:TRP:HE1	1.56	0.53
1:L:14:SER:O	1:L:17:GLN:HB2	2.07	0.53
1:L:149:LYS:HB2	1:L:193:THR:HB	1.90	0.53
1:L:131:SER:OG	1:L:180:THR:HG23	2.08	0.52
1:L:37:GLN:HB2	1:L:47:LEU:HD11	1.91	0.52
2:H:19:SER:HA	2:H:80:LEU:O	2.09	0.51
2:H:61:SER:HA	2:H:64:MET:HB2	1.91	0.51
2:H:70:ASN:OD1	2:H:79:PHE:HD2	1.93	0.51
1:L:136:LEU:HG	1:L:175:MET:HE2	1.92	0.50
2:H:8:GLY:HA3	2:H:20:ILE:HA	1.95	0.49
1:L:11:LEU:HD21	1:L:19:ALA:HB1	1.95	0.48
2:H:43:LYS:NZ	2:H:44:GLY:H	2.11	0.48
2:H:6:GLN:HE22	2:H:104:GLY:HA3	1.78	0.47
1:L:116:SER:O	1:L:134:CYS:HA	2.14	0.47
2:H:38:ARG:NH2	2:H:63:LEU:HD21	2.30	0.47
1:L:150:ILE:HG21	1:L:156:GLN:HG2	1.96	0.47
2:H:22:CYS:O	2:H:77:GLN:HA	2.15	0.46
1:L:55:GLU:O	1:L:58:VAL:HG22	2.16	0.46
2:H:43:LYS:HZ1	2:H:44:GLY:H	1.62	0.46
2:H:97:PHE:HD1	2:H:100(C):TYR:HB3	1.80	0.46
2:H:12:VAL:HG21	2:H:82(C):LEU:HD12	1.99	0.45
1:L:90:HIS:HD2	1:L:92:ARG:HB3	1.80	0.45
2:H:94:ARG:HH21	2:H:96:ARG:HG3	1.81	0.45
1:L:90:HIS:CD2	1:L:92:ARG:HB3	2.52	0.45
2:H:20:ILE:CD1	2:H:80:LEU:HD23	2.47	0.45
1:L:121:SER:OG	2:H:122:TYR:HB3	2.17	0.44
2:H:35:HIS:CE1	2:H:100(E):VAL:HG22	2.53	0.44
4:H:1:OBN:H71	4:H:1:OBN:H41	1.75	0.44
2:H:22:CYS:HB2	2:H:36:TRP:CZ2	2.52	0.44
2:H:203:GLN:HE21	2:H:203:GLN:HA	1.84	0.43
2:H:119:PRO:HD2	2:H:217:THR:HG21	2.01	0.43
1:L:32:HIS:HA	1:L:50:LEU:HD12	2.00	0.43
1:L:143:ASP:O	1:L:198:HIS:HD2	2.02	0.43
1:L:144:ILE:HG22	1:L:163:TRP:CZ2	2.55	0.42
1:L:24:ARG:HA	1:L:69:THR:O	2.18	0.42
2:H:27:PHE:HB2	2:H:32:TYR:CD2	2.55	0.41
2:H:70:ASN:OD1	2:H:79:PHE:CD2	2.73	0.41
1:L:136:LEU:N	1:L:175:MET:O	2.52	0.41
2:H:212:HIS:HB3	2:H:217:THR:HB	2.02	0.41
2:H:217:THR:HG22	2:H:219:VAL:HG12	2.03	0.41
1:L:47:LEU:HA	1:L:58:VAL:HG11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:11:LEU:HD21	2:H:112:SER:OG	2.22	0.40
2:H:96:ARG:O	2:H:100(C):TYR:HA	2.20	0.40
1:L:34:HIS:O	1:L:88:CYS:HA	2.21	0.40
1:L:80:GLU:HA	1:L:106:LEU:HD22	2.04	0.40
2:H:62:ALA:HB3	2:H:63:LEU:H	1.72	0.40
1:L:198:HIS:O	1:L:200:THR:N	2.54	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	L	215/217 (99%)	192 (89%)	17 (8%)	6 (3%)	5	11
2	H	215/217 (99%)	180 (84%)	26 (12%)	9 (4%)	3	5
All	All	430/434 (99%)	372 (86%)	43 (10%)	15 (4%)	3	8

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	199	LYS
2	H	15	SER
2	H	62	ALA
2	H	64	MET
2	H	199	TRP
2	H	135	GLY
2	H	196	SER
1	L	40	PRO
1	L	27(B)	VAL
2	H	8	GLY
1	L	51	ALA
1	L	184	ASP

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Mol	Chain	Res	Type
1	L	187	GLU
2	H	204	THR
2	H	9	PRO

### 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	L	190/190 (100%)	165 (87%)	25 (13%)	<b>4</b> <b>9</b>
2	H	186/186 (100%)	164 (88%)	22 (12%)	<b>5</b> <b>12</b>
All	All	376/376 (100%)	329 (88%)	47 (12%)	<b>4</b> <b>10</b>

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	5	THR
1	L	7	SER
1	L	11	LEU
1	L	14	SER
1	L	17	GLN
1	L	26	SER
1	L	27(D)	THR
1	L	40	PRO
1	L	52	SER
1	L	65	SER
1	L	77	PRO
1	L	80	GLU
1	L	81	GLU
1	L	89	GLN
1	L	92	ARG
1	L	108	ARG
1	L	149	LYS
1	L	164	THR
1	L	170	ASP
1	L	176	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	L	180	THR
1	L	191	SER
1	L	201	SER
1	L	202	THR
1	L	210	ASN
2	H	3	HIS
2	H	6	GLN
2	H	11	LEU
2	H	19	SER
2	H	30	THR
2	H	43	LYS
2	H	60	ASN
2	H	67	LEU
2	H	113	SER
2	H	115	LYS
2	H	134	THR
2	H	137	SER
2	H	149	PRO
2	H	150	GLU
2	H	151	PRO
2	H	169	SER
2	H	178	LEU
2	H	180	SER
2	H	188	SER
2	H	194	PRO
2	H	199	TRP
2	H	203	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	L	89	GLN
1	L	90	HIS
1	L	190	ASN
1	L	210	ASN
2	H	35	HIS
2	H	39	GLN
2	H	60	ASN
2	H	179	GLN
2	H	203	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	OBN	H	1	-	44,46,46	1.07	2 (4%)	66,76,76	1.56	17 (25%)

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	OBN	H	1	-	-	1/11/116/116	0/6/6/6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	1	OBN	C4-C5	2.63	1.56	1.53
4	H	1	OBN	O3-C3	-2.46	1.41	1.44

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1	OBN	C5-C4-C3	4.03	118.70	114.14
4	H	1	OBN	C1'-O5'-C5'	3.62	119.89	113.67
4	H	1	OBN	O5-C5-C10	3.40	114.83	109.54
4	H	1	OBN	C6-C5-C10	-3.11	107.43	111.12
4	H	1	OBN	C6-C7-C8	-2.71	108.42	113.11
4	H	1	OBN	O5'-C1'-C2'	-2.64	104.75	110.35
4	H	1	OBN	C15-C14-C13	-2.35	101.54	103.37
4	H	1	OBN	C7-C6-C5	-2.29	109.91	112.76
4	H	1	OBN	C14-C13-C17	2.28	106.17	103.56
4	H	1	OBN	C10-C9-C11	2.23	118.55	115.19
4	H	1	OBN	C13-C14-C8	2.21	116.70	113.83
4	H	1	OBN	O5'-C5'-C4'	2.19	113.45	109.52
4	H	1	OBN	C18-C13-C12	-2.14	108.16	111.11
4	H	1	OBN	C6'-C5'-C4'	-2.06	109.26	113.07
4	H	1	OBN	O4'-C4'-C3'	-2.04	105.63	110.35
4	H	1	OBN	C4-C5-C10	-2.02	108.88	111.58
4	H	1	OBN	C13-C17-C20	2.01	118.75	115.81

There are no chirality outliers.

All (1) torsion outliers are listed below:

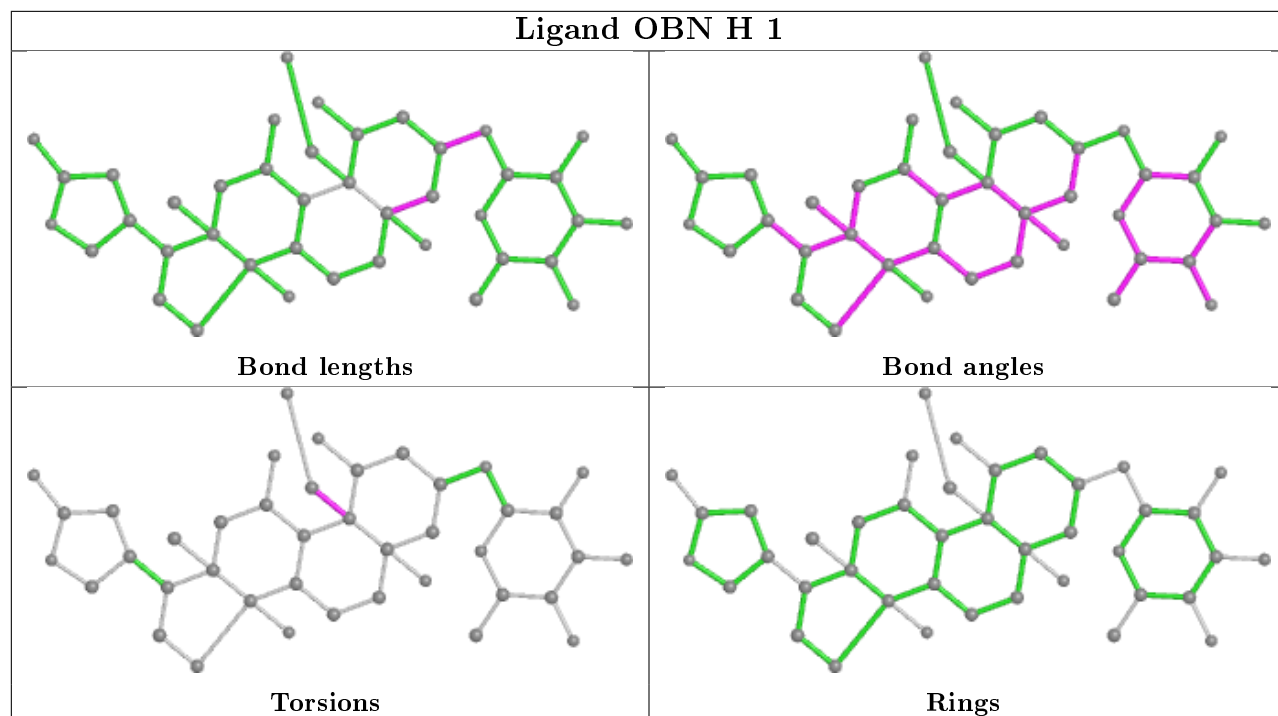
Mol	Chain	Res	Type	Atoms
4	H	1	OBN	C9-C10-C19-O19

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	1	OBN	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	L	216/217 (99%)	-0.34	4 (1%) 66 69	7, 33, 56, 91	1 (0%)
2	H	204/217 (94%)	-0.50	1 (0%) 91 92	8, 28, 51, 67	0
All	All	420/434 (96%)	-0.42	5 (1%) 79 80	7, 30, 55, 91	1 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	213	GLU	8.2
1	L	214	CYS	7.8
2	H	198	THR	4.8
1	L	153	SER	2.3
1	L	205	ILE	2.1

### 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](#)

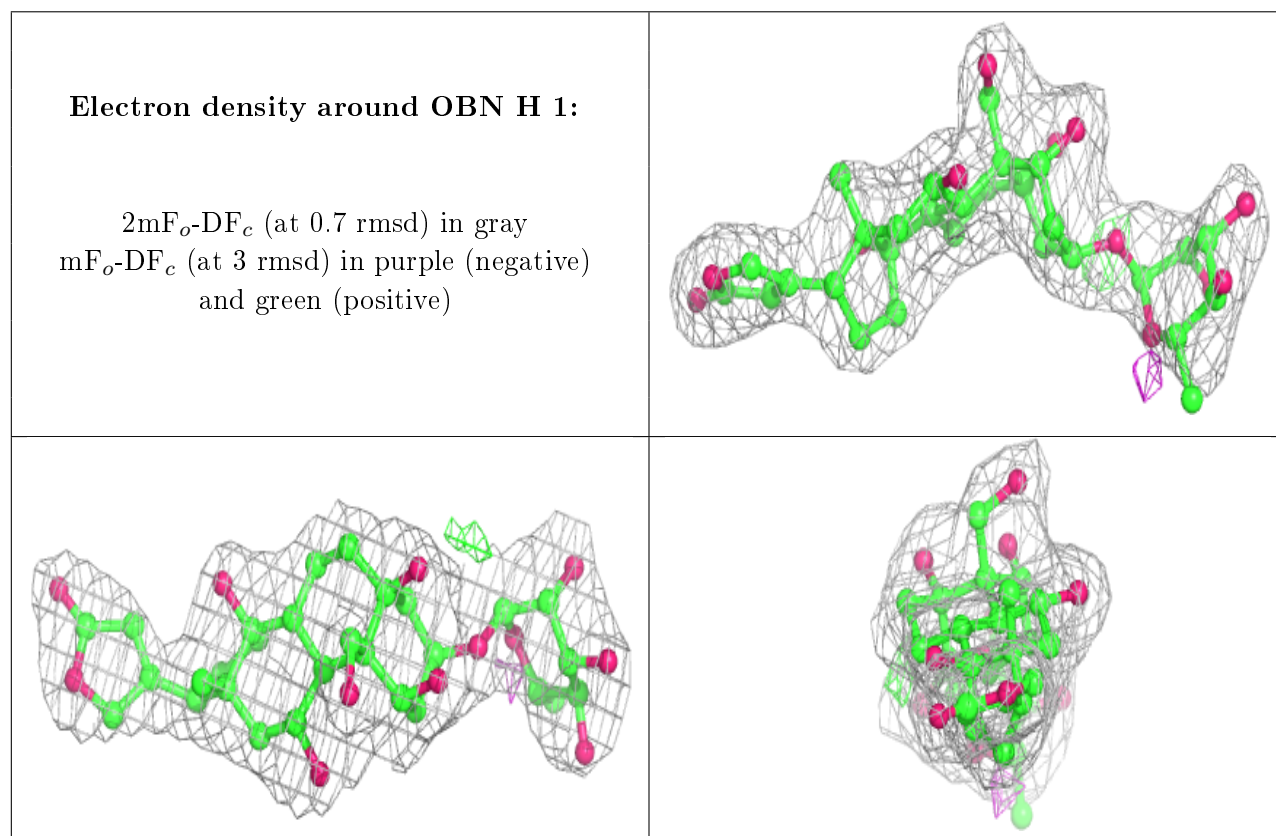
There are no carbohydrates in this entry.

### 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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
4	OBN	H	1	41/41	0.91	0.13	21,30,59,61	0
3	CU	L	1	1/1	0.97	0.15	35,35,35,35	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.