



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:34 PM UTC

PDB ID : 1IBG / pdb_00001ibg
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

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

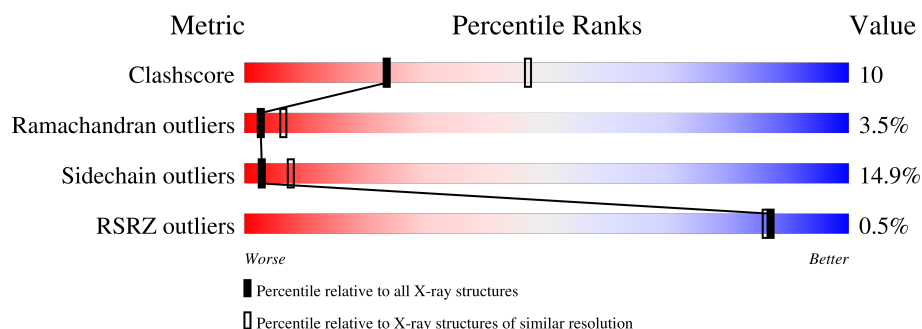
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 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	L	217	
2	H	217	

2 Entry composition

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
1	L	217	Total	C	N	O	S	13	0	0
			1677	1046	285	340	6			

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

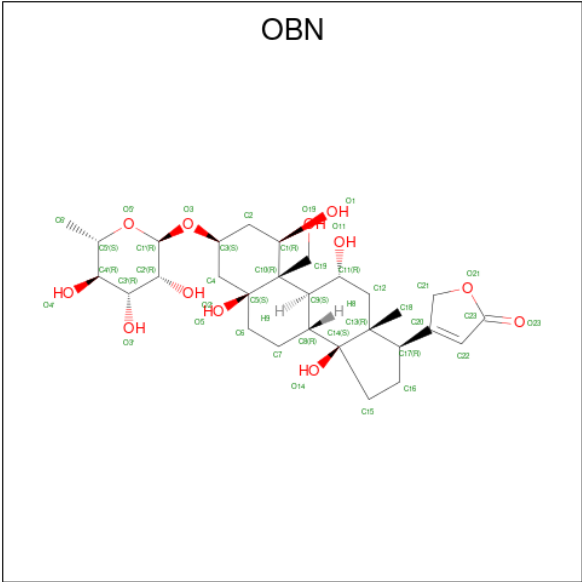
- Molecule 2 is a protein called IGG2B-KAPPA 40-50 FAB (HEAVY CHAIN).

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

- Molecule 3 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

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

- Molecule 4 is OUABAIN (CCD ID: OBN) (formula: C₂₉H₄₄O₁₂).



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		

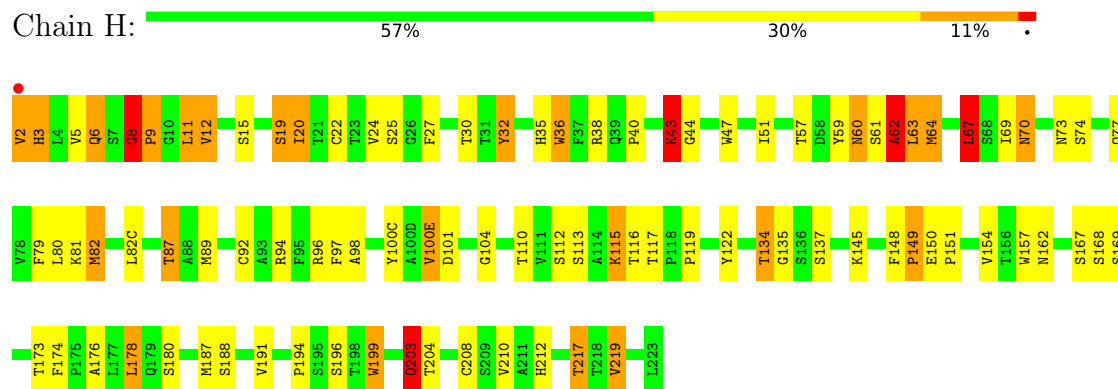
3 Residue-property plots

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: 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, α , β , γ	93.66Å 84.77Å 70.08Å 90.00° 127.95° 90.00°	Depositor
Resolution (Å)	10.00 – 2.70 10.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.70) 83.2 (10.00-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.65 (at 2.42Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.209 , (Not available) 0.214 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	43.6	Xtriage
Anisotropy	0.426	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 61.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3348	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage'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.*

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

5.1 Standard geometry

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	1.03	2/1717 (0.1%)	2.00	66/2334 (2.8%)
2	H	1.05	2/1675 (0.1%)	1.96	44/2293 (1.9%)
All	All	1.04	4/3392 (0.1%)	1.98	110/4627 (2.4%)

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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	153	SER	CA-CB	6.99	1.61	1.52
2	H	20	ILE	CA-CB	5.53	1.60	1.54
2	H	191	VAL	CA-CB	5.37	1.62	1.54
1	L	115	VAL	CA-CB	5.28	1.61	1.54

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	101	ASP	CA-CB-CG	11.21	123.81	112.60
2	H	70	ASN	CA-CB-CG	10.40	123.00	112.60
1	L	137	ASN	CA-CB-CG	8.82	121.42	112.60
1	L	202	THR	N-CA-C	-8.77	100.90	111.69
2	H	60	ASN	OD1-CG-ND2	-8.50	114.10	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	210	ASN	CA-CB-CG	8.22	120.82	112.60
1	L	167	ASP	CA-CB-CG	8.14	120.75	112.60
2	H	101	ASP	N-CA-C	8.04	123.22	113.41
1	L	154	GLU	N-CA-C	-7.97	96.23	109.46
2	H	62	ALA	N-CA-C	-7.90	93.97	110.80
1	L	81	GLU	CA-CB-CG	7.78	129.66	114.10
1	L	71	PHE	CA-CB-CG	-7.69	106.11	113.80
1	L	199	LYS	N-CA-C	7.59	126.96	110.80
1	L	100	ALA	N-CA-C	7.56	122.08	113.01
1	L	185	GLU	CA-CB-CG	7.53	129.16	114.10
1	L	184	ASP	CA-CB-CG	7.46	120.06	112.60
1	L	66	GLY	N-CA-C	7.44	119.74	111.85
2	H	98	ALA	N-CA-C	-7.40	104.10	113.43
2	H	60	ASN	CB-CG-ND2	7.35	127.42	116.40
1	L	145	ASN	CA-CB-CG	-7.09	105.51	112.60
2	H	67	LEU	N-CA-C	7.02	119.85	109.24
2	H	100(E)	VAL	N-CA-C	-6.89	95.22	106.32
2	H	9	PRO	O-C-N	6.66	131.63	122.64
2	H	174	PHE	CA-CB-CG	-6.61	107.19	113.80
2	H	32	TYR	O-C-N	6.58	131.30	123.27
1	L	93	GLU	CA-CB-CG	6.56	127.22	114.10
1	L	6	GLN	CG-CD-NE2	6.55	126.22	116.40
2	H	87	THR	N-CA-C	-6.54	99.97	109.59
1	L	150	ILE	N-CA-CB	-6.51	103.69	111.90
1	L	194	CYS	N-CA-C	-6.50	96.45	108.02
1	L	95	PRO	O-C-N	6.48	133.42	121.10
2	H	176	ALA	N-CA-C	6.46	120.81	109.96
1	L	175	MET	O-C-N	6.42	130.72	123.27
2	H	89	MET	N-CA-C	-6.41	100.08	110.20
1	L	42	GLN	CA-C-O	-6.38	115.40	121.08
1	L	195	GLU	CA-CB-CG	6.37	126.84	114.10
2	H	20	ILE	N-CA-C	-6.34	99.30	108.17
1	L	108	ARG	N-CA-CB	-6.30	101.28	111.24
2	H	9	PRO	N-CA-CB	-6.27	96.67	103.25
1	L	105	GLU	N-CA-C	-6.23	98.23	108.76
2	H	81	LYS	CA-CB-CG	-6.21	101.67	114.10
1	L	210	ASN	OD1-CG-ND2	-6.17	116.43	122.60
2	H	115	LYS	CB-CG-CD	6.12	125.39	111.30
2	H	51	ILE	CA-CB-CG1	-6.11	100.01	110.40
1	L	91	SER	CA-CB-OG	6.10	123.30	111.10
2	H	3	HIS	CA-C-O	-6.10	114.09	120.92
1	L	150	ILE	CA-C-O	6.06	127.15	120.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	212	ASN	N-CA-C	6.05	119.30	107.57
1	L	137	ASN	N-CA-C	6.02	119.28	109.59
1	L	105	GLU	CA-CB-CG	5.99	126.09	114.10
1	L	97	THR	O-C-N	5.99	130.19	123.19
2	H	40	PRO	N-CA-C	-5.97	103.42	110.70
2	H	148	PHE	O-C-N	-5.93	117.70	121.85
1	L	210	ASN	CB-CG-ND2	5.83	125.15	116.40
2	H	174	PHE	CA-C-O	-5.83	114.97	119.46
2	H	63	LEU	O-C-N	5.81	128.28	122.12
1	L	205	ILE	N-CA-C	-5.80	101.55	109.55
2	H	217	THR	N-CA-C	-5.77	100.30	109.59
1	L	129	GLY	CA-C-O	-5.77	115.14	121.77
2	H	167	SER	N-CA-C	-5.74	98.39	109.24
2	H	73	ASN	CA-CB-CG	5.71	118.31	112.60
2	H	178	LEU	N-CA-C	-5.70	101.21	109.59
2	H	162	ASN	OD1-CG-ND2	-5.69	116.91	122.60
2	H	162	ASN	CB-CG-ND2	5.68	124.92	116.40
2	H	73	ASN	OD1-CG-ND2	-5.66	116.94	122.60
1	L	108	ARG	CA-CB-CG	5.59	125.28	114.10
1	L	9	ALA	N-CA-C	-5.54	105.25	112.23
2	H	82	MET	CA-CB-CG	-5.53	103.03	114.10
1	L	212	ASN	CA-C-N	5.50	130.66	122.74
1	L	212	ASN	C-N-CA	5.50	130.66	122.74
2	H	134	THR	N-CA-C	-5.50	101.51	109.59
1	L	212	ASN	O-C-N	5.49	129.33	122.63
2	H	208	CYS	N-CA-C	-5.47	100.96	109.72
1	L	99	GLY	N-CA-C	-5.45	103.19	112.51
1	L	62	PHE	CA-CB-CG	-5.43	108.37	113.80
1	L	182	THR	N-CA-C	-5.43	103.22	110.55
1	L	116	SER	CA-C-O	-5.40	114.44	120.66
1	L	213	GLU	CA-C-N	5.39	131.41	121.70
1	L	213	GLU	C-N-CA	5.39	131.41	121.70
1	L	4	LEU	CA-C-O	5.39	126.52	120.70
1	L	138	ASN	CA-CB-CG	5.37	117.97	112.60
1	L	132	VAL	N-CA-C	-5.37	100.66	108.17
1	L	75	ILE	N-CA-C	-5.36	99.83	107.77
1	L	209	PHE	CA-CB-CG	5.35	119.15	113.80
1	L	39	LYS	CA-CB-CG	5.33	124.75	114.10
1	L	150	ILE	CB-CA-C	5.31	117.90	110.99
1	L	156	GLN	OE1-CD-NE2	-5.28	117.32	122.60
1	L	149	LYS	N-CA-C	-5.25	100.35	108.90
1	L	124	GLN	O-C-N	5.22	128.10	122.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	117	THR	CB-CA-C	5.19	117.07	110.16
2	H	36	TRP	N-CA-C	-5.19	100.94	109.40
2	H	81	LYS	CB-CG-CD	5.19	123.24	111.30
1	L	93	GLU	N-CA-C	-5.19	101.03	108.60
1	L	2	ILE	CA-C-O	-5.17	112.01	120.80
1	L	17	GLN	CG-CD-NE2	5.15	124.12	116.40
1	L	78	VAL	N-CA-C	-5.14	102.05	108.84
1	L	207	LYS	N-CA-C	-5.14	101.38	109.50
2	H	203	GLN	OE1-CD-NE2	-5.13	117.47	122.60
1	L	210	ASN	CA-C-O	-5.11	114.70	120.32
2	H	145	LYS	N-CA-C	5.10	117.39	108.76
2	H	2	VAL	CA-C-O	-5.09	112.14	120.80
1	L	171	SER	N-CA-CB	-5.09	101.93	110.22
2	H	43	LYS	CA-CB-CG	5.07	124.25	114.10
1	L	137	ASN	CA-C-N	5.06	131.21	121.54
1	L	137	ASN	C-N-CA	5.06	131.21	121.54
1	L	70	ASP	CA-CB-CG	5.05	117.65	112.60
1	L	64	GLY	CA-C-O	-5.05	115.99	120.94
1	L	58	VAL	N-CA-C	-5.04	104.30	108.63
2	H	157	TRP	CA-C-N	5.04	129.97	122.82
2	H	157	TRP	C-N-CA	5.04	129.97	122.82

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 ⓘ

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	38	0
3	L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	41	0	44	1	0
5	L	1	0	0	0	0
All	All	3348	0	3221	65	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 (65) 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:HB2	2:H:43:LYS:HZ2	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
2:H:63:LEU:HD23	2:H:82:MET:HE1	1.88	0.54
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
1:L:14:SER:O	1:L:17:GLN:HB2	2.07	0.53
2:H:35:HIS:HD2	2:H:47:TRP:HE1	1.56	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
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
1:L:150:ILE:HG21	1:L:156:GLN:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:38:ARG:NH2	2:H:63:LEU:HD21	2.30	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
1:L:90:HIS:HD2	1:L:92:ARG:HB3	1.80	0.45
2:H:12:VAL:HG21	2:H:82(C):LEU:HD12	1.99	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:H41	4:H:1:OBN:H71	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:136:LEU:HG	1:L:175:MET:HE2	2.01	0.42
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:187:MET:HE2	2:H:187:MET:HB2	1.89	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
2:H:11:LEU:HD21	2:H:112:SER:OG	2.22	0.40
1:L:34:HIS:O	1:L:88:CYS:HA	2.21	0.40
2:H:96:ARG:O	2:H:100(C):TYR:HA	2.20	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%)	4	9
2	H	215/217 (99%)	180 (84%)	26 (12%)	9 (4%)	2	4
All	All	430/434 (99%)	372 (86%)	43 (10%)	15 (4%)	3	6

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
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%)	162 (85%)	28 (15%)	3	8
2	H	186/186 (100%)	158 (85%)	28 (15%)	3	7
All	All	376/376 (100%)	320 (85%)	56 (15%)	3	8

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	3	VAL
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	40	PRO
1	L	52	SER
1	L	54	LEU
1	L	65	SER
1	L	77	PRO
1	L	80	GLU
1	L	81	GLU
1	L	82	ASP
1	L	89	GLN
1	L	90	HIS
1	L	92	ARG
1	L	106	LEU
1	L	108	ARG
1	L	164	THR
1	L	170	ASP
1	L	180	THR
1	L	184	ASP
1	L	191	SER
1	L	201	SER
1	L	202	THR
1	L	210	ASN
2	H	3	HIS
2	H	5	VAL
2	H	6	GLN
2	H	11	LEU
2	H	12	VAL
2	H	19	SER
2	H	30	THR

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Mol	Chain	Res	Type
2	H	43	LYS
2	H	57	THR
2	H	60	ASN
2	H	67	LEU
2	H	74	SER
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	168	SER
2	H	169	SER
2	H	173	THR
2	H	178	LEU
2	H	180	SER
2	H	188	SER
2	H	194	PRO
2	H	203	GLN
2	H	219	VAL

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

Mol	Chain	Res	Type
1	L	89	GLN
1	L	90	HIS
1	L	198	HIS
2	H	16	GLN
2	H	35	HIS
2	H	39	GLN
2	H	83	GLN
2	H	179	GLN
2	H	203	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	1.08	2 (4%)	69,76,76	1.60	18 (26%)

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	-	-	2/11/116/116	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	2.60	1.56	1.53
4	H	1	OBN	O3-C3	-2.57	1.41	1.44

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1	OBN	C5-C4-C3	3.92	118.70	113.95
4	H	1	OBN	C1'-O5'-C5'	3.67	119.89	113.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1	OBN	O5-C5-C10	3.39	114.83	109.60
4	H	1	OBN	C6-C5-C10	-3.18	107.43	111.16
4	H	1	OBN	C19-C10-C5	-3.08	105.19	109.46
4	H	1	OBN	C6-C7-C8	-2.77	108.42	113.14
4	H	1	OBN	O5'-C1'-C2'	-2.73	104.75	110.37
4	H	1	OBN	C15-C14-C13	-2.46	101.54	103.37
4	H	1	OBN	C7-C6-C5	-2.39	109.91	112.72
4	H	1	OBN	C14-C13-C17	2.37	106.17	103.61
4	H	1	OBN	C13-C14-C8	2.36	116.70	113.84
4	H	1	OBN	C4-C5-C10	-2.25	108.88	111.63
4	H	1	OBN	C10-C9-C11	2.23	118.55	115.19
4	H	1	OBN	O5'-C5'-C4'	2.17	113.45	109.55
4	H	1	OBN	C13-C17-C20	2.12	118.75	115.79
4	H	1	OBN	C18-C13-C12	-2.11	108.16	111.08
4	H	1	OBN	C6'-C5'-C4'	-2.09	109.26	113.08
4	H	1	OBN	O4'-C4'-C3'	-2.02	105.63	110.38

There are no chirality outliers.

All (2) torsion outliers are listed below:

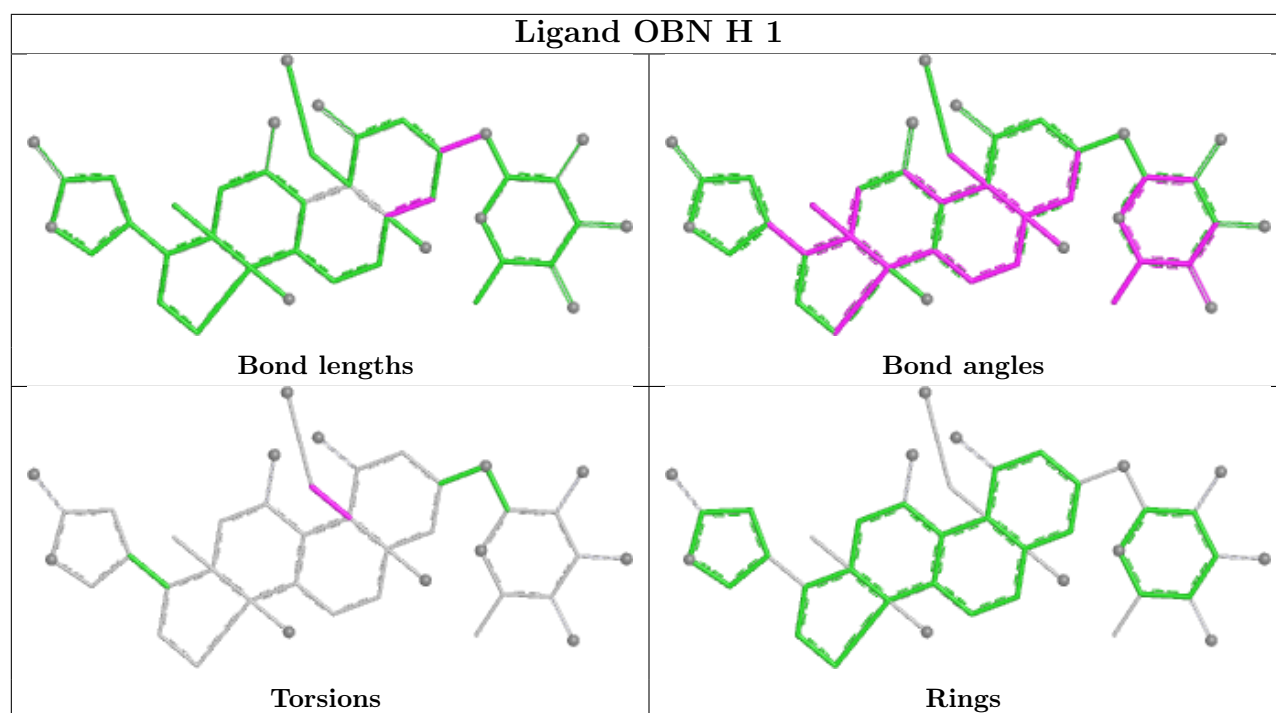
Mol	Chain	Res	Type	Atoms
4	H	1	OBN	C9-C10-C19-O19
4	H	1	OBN	C1-C10-C19-O19

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, 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	L	216/217 (99%)	-0.48	1 (0%) 87 86	7, 33, 56, 91	1 (0%)
2	H	204/217 (94%)	-0.48	1 (0%) 87 86	8, 28, 51, 67	0
All	All	420/434 (96%)	-0.48	2 (0%) 87 86	7, 30, 55, 91	1 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	2	VAL	2.4
1	L	153	SER	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](#)

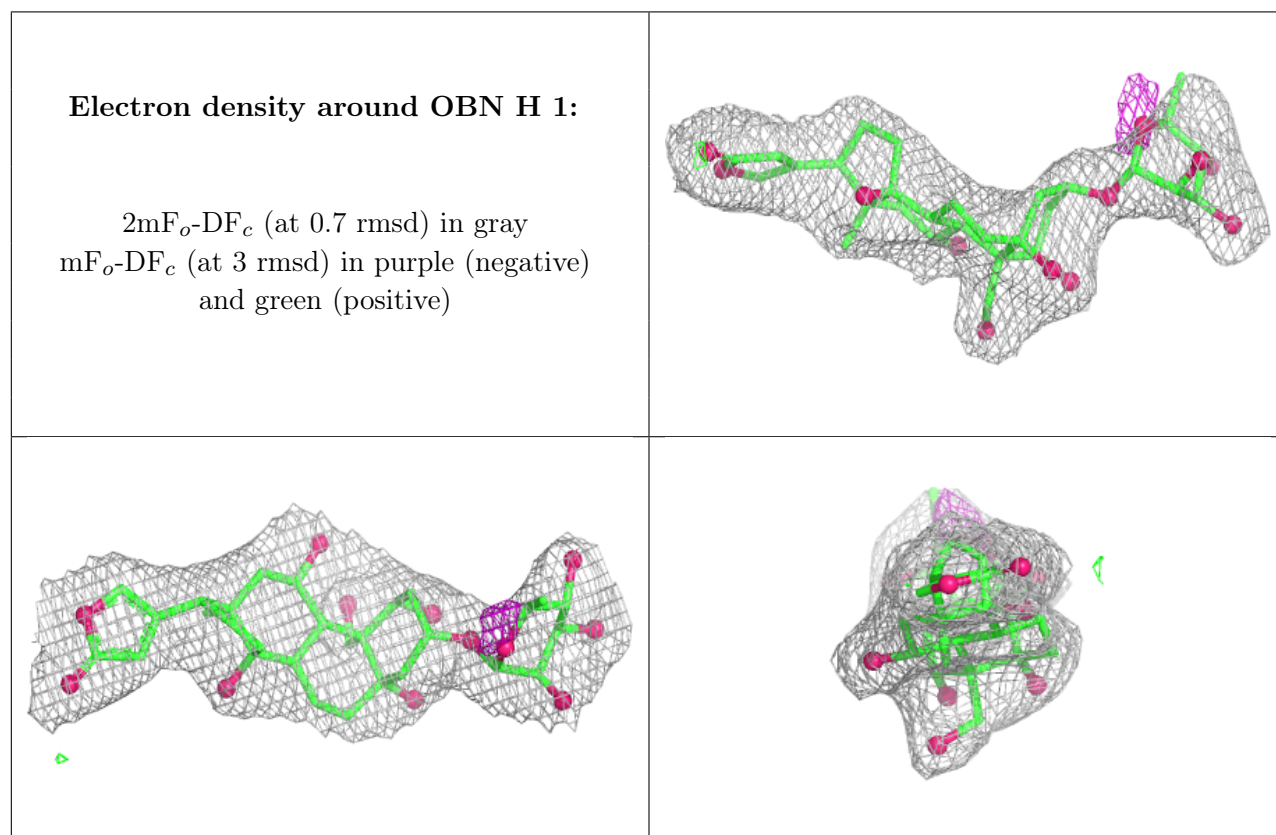
There are no oligosaccharides in this entry.

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	OBN	H	1	41/41	0.90	0.07	21,30,59,61	0
3	CU	L	1	1/1	0.95	0.04	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.