



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:26 PM UTC

PDB ID : 1F4X / pdb_00001f4x
Title : CRYSTAL STRUCTURE OF AN ANTI-CARBOHYDRATE ANTIBODY
DIRECTED AGAINST VIBRIO CHOLERAЕ O1 IN COMPLEX WITH
ANTIGEN
Authors : Alzari, P.M.; Souchon, H.
Deposited on : 2000-06-10
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

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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

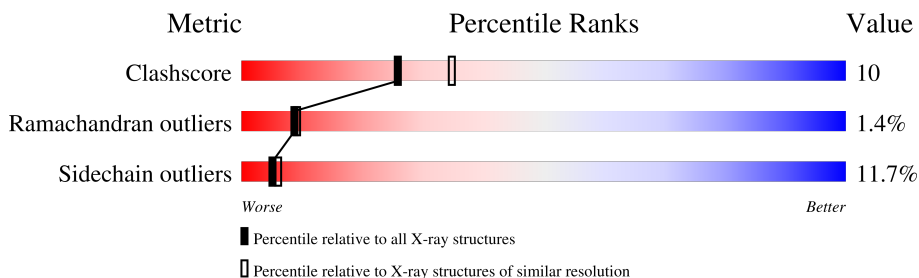
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	210	
2	H	216	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3231 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.

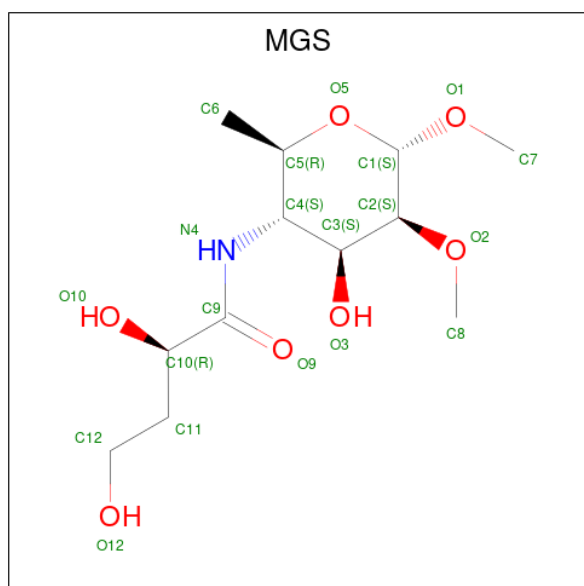
- Molecule 1 is a protein called ANTIBODY S-20-4, FAB FRAGMENT, LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	210	Total	C	N	O	S	0	0	0
			1556	977	254	319	6			

- Molecule 2 is a protein called ANTIBODY S-20-4, FAB FRAGMENT, HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	216	Total	C	N	O	S	0	0	0
			1598	1011	257	322	8			

- Molecule 3 is methyl 4,6-dideoxy-4-{[(2R)-2,4-dihydroxybutanoyl]amino}-2-O-methyl-alpha-D-mannopyranoside (CCD ID: MGS) (formula: C₁₂H₂₃NO₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	H	1	Total	C	N	O	0	0
			20	12	1	7		

- Molecule 4 is water.

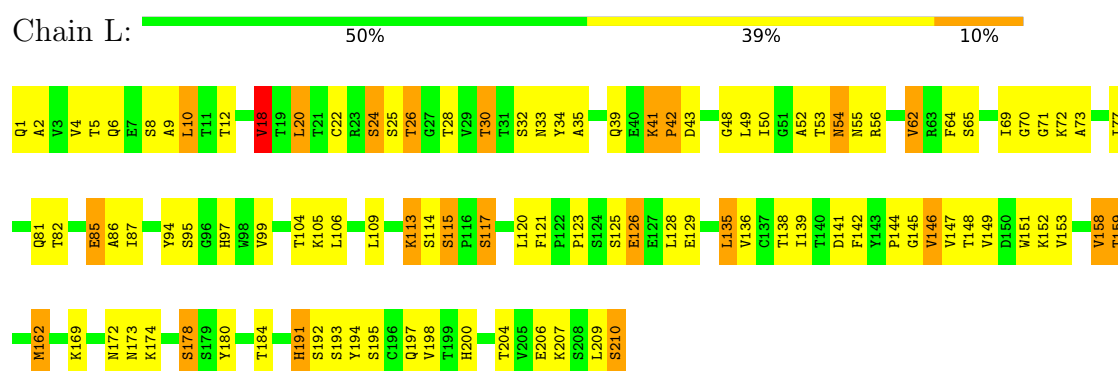
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	33	Total 33	O 33	0	0
4	H	24	Total 24	O 24	0	0

3 Residue-property plots

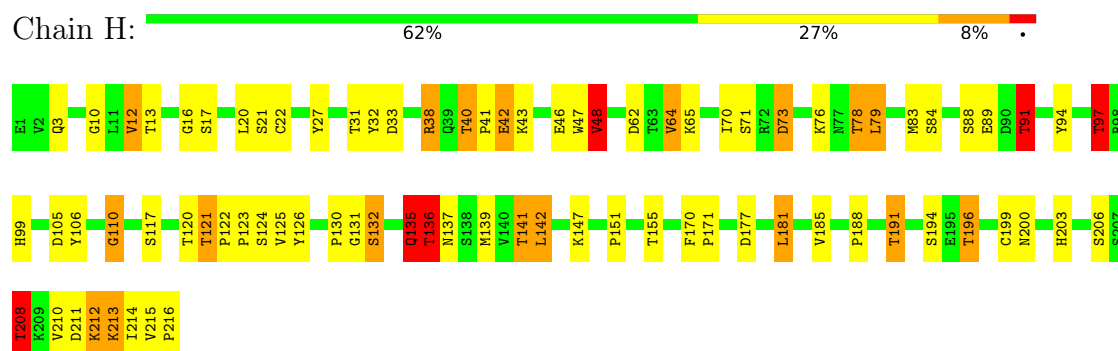
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: ANTIBODY S-20-4, FAB FRAGMENT, LIGHT CHAIN



• Molecule 2: ANTIBODY S-20-4, FAB FRAGMENT, HEAVY CHAIN



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, α , β , γ	45.57Å 113.09Å 46.24Å 90.00° 100.57° 90.00°	Depositor
Resolution (Å)	10.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.30)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.185 , 0.250	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3231	wwPDB-VP
Average B, all atoms (Å ²)	41.0	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: MGS

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	1.02	0/1592	2.23	77/2180 (3.5%)
2	H	1.08	1/1641 (0.1%)	2.24	69/2252 (3.1%)
All	All	1.05	1/3233 (0.0%)	2.24	146/4432 (3.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	216	PRO	N-CD	6.29	1.56	1.47

All (146) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	56	ARG	CD-NE-CZ	10.72	139.41	124.40
2	H	137	ASN	CA-C-O	9.92	129.44	119.91
1	L	18	VAL	CB-CA-C	-9.87	95.61	110.82
2	H	177	ASP	CA-CB-CG	-8.75	103.85	112.60
1	L	178	SER	CA-C-O	-8.73	111.24	121.11
1	L	129	GLU	CA-CB-CG	8.44	130.98	114.10
2	H	48	VAL	N-CA-CB	-8.29	97.56	111.23
2	H	208	THR	N-CA-CB	-8.27	96.94	111.08
2	H	32	TYR	CA-C-O	8.12	130.86	121.28
1	L	25	SER	CA-C-O	8.11	129.37	119.31
2	H	97	THR	CA-CB-OG1	7.69	121.14	109.60
2	H	73	ASP	CA-CB-CG	-7.68	104.92	112.60
2	H	47	TRP	O-C-N	-7.58	114.07	123.01
2	H	79	LEU	O-C-N	-7.56	114.34	123.19
1	L	178	SER	CA-CB-OG	-7.52	96.05	111.10
2	H	21	SER	CA-C-O	-7.49	112.64	121.11
1	L	50	ILE	CA-C-O	-7.47	112.31	120.67
2	H	147	LYS	CA-C-O	7.45	129.57	121.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	25	SER	CA-C-N	7.29	130.78	120.28
1	L	25	SER	C-N-CA	7.29	130.78	120.28
1	L	6	GLN	OE1-CD-NE2	-7.20	115.40	122.60
2	H	147	LYS	N-CA-C	7.14	121.31	109.95
1	L	4	VAL	CA-C-N	-7.14	111.49	122.62
1	L	4	VAL	C-N-CA	-7.14	111.49	122.62
2	H	211	ASP	CA-CB-CG	-7.09	105.51	112.60
2	H	97	THR	CB-CA-C	-7.05	93.90	109.56
1	L	48	GLY	CA-C-O	-7.00	114.39	120.98
1	L	81	GLN	CA-C-N	6.96	129.91	120.38
1	L	81	GLN	C-N-CA	6.96	129.91	120.38
2	H	21	SER	CA-CB-OG	-6.91	97.28	111.10
1	L	128	LEU	CA-C-O	6.84	127.80	120.55
1	L	204	THR	CA-C-N	-6.79	114.21	122.90
1	L	204	THR	C-N-CA	-6.79	114.21	122.90
1	L	200	HIS	CA-CB-CG	6.78	120.58	113.80
1	L	191	HIS	CA-CB-CG	-6.76	107.04	113.80
2	H	38	ARG	CD-NE-CZ	-6.75	114.95	124.40
2	H	124	SER	N-CA-CB	6.73	121.61	110.63
2	H	215	VAL	CA-C-O	6.64	128.85	119.95
2	H	137	ASN	N-CA-C	6.61	118.61	109.29
2	H	199	CYS	N-CA-CB	6.60	121.41	110.52
1	L	62	VAL	O-C-N	-6.59	115.21	121.87
2	H	21	SER	O-C-N	6.59	131.75	123.19
1	L	193	SER	CB-CA-C	-6.56	96.84	109.37
1	L	115	SER	CA-CB-OG	-6.54	98.03	111.10
2	H	191	THR	CB-CA-C	-6.52	98.76	110.70
2	H	62	ASP	CA-C-O	-6.48	112.77	120.10
2	H	71	SER	CA-CB-OG	-6.41	98.28	111.10
2	H	21	SER	CA-C-N	-6.39	113.78	122.86
2	H	21	SER	C-N-CA	-6.39	113.78	122.86
1	L	126	GLU	CA-CB-CG	-6.38	101.35	114.10
2	H	170	PHE	CA-CB-CG	-6.37	107.43	113.80
1	L	172	ASN	CA-C-N	6.35	134.91	124.31
1	L	172	ASN	C-N-CA	6.35	134.91	124.31
2	H	212	LYS	CA-C-N	6.34	130.57	121.50
2	H	212	LYS	C-N-CA	6.34	130.57	121.50
1	L	146	VAL	O-C-N	-6.33	116.36	123.20
2	H	141	THR	CB-CA-C	6.33	120.19	109.75
2	H	126	TYR	O-C-N	6.28	127.66	121.57
1	L	126	GLU	CA-C-O	-6.27	112.76	119.97
2	H	97	THR	N-CA-CB	6.25	123.16	111.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	39	GLN	CB-CG-CD	-6.14	102.16	112.60
1	L	174	LYS	N-CA-C	-6.13	102.62	110.53
1	L	33	ASN	N-CA-C	-6.13	105.84	113.38
2	H	124	SER	N-CA-C	-6.08	100.38	110.17
1	L	138	THR	O-C-N	6.08	130.46	123.29
1	L	158	VAL	CA-C-O	-6.08	113.30	121.02
2	H	141	THR	CA-CB-OG1	6.08	118.71	109.60
2	H	210	VAL	CA-C-O	-6.06	113.94	120.36
2	H	141	THR	O-C-N	-6.01	116.48	123.27
2	H	155	THR	CA-CB-OG1	-6.00	100.60	109.60
1	L	147	VAL	N-CA-CB	5.98	121.27	112.35
2	H	185	VAL	CA-C-O	5.93	127.25	120.90
1	L	55	ASN	OD1-CG-ND2	-5.92	116.68	122.60
2	H	110	GLY	CA-C-O	-5.92	117.50	122.29
1	L	85	GLU	CB-CA-C	5.91	119.13	110.26
2	H	46	GLU	CA-C-O	-5.91	113.75	120.32
1	L	62	VAL	N-CA-CB	-5.88	100.59	110.65
2	H	125	VAL	CA-C-O	5.87	126.50	120.39
1	L	4	VAL	CA-C-O	-5.80	114.33	120.48
2	H	40	THR	CA-CB-OG1	-5.75	100.97	109.60
2	H	32	TYR	N-CA-C	5.72	119.38	110.17
1	L	72	LYS	CB-CG-CD	5.70	124.40	111.30
2	H	64	VAL	N-CA-C	-5.69	107.73	113.20
1	L	198	VAL	CA-C-O	5.68	126.30	120.39
2	H	84	SER	CA-CB-OG	-5.67	99.77	111.10
1	L	56	ARG	NE-CZ-NH2	-5.65	114.11	119.20
1	L	24	SER	CA-C-O	-5.65	114.61	121.28
1	L	184	THR	N-CA-C	-5.64	101.09	110.17
1	L	41	LYS	CA-C-N	5.62	125.94	119.93
1	L	41	LYS	C-N-CA	5.62	125.94	119.93
2	H	212	LYS	O-C-N	-5.60	116.77	123.27
2	H	196	THR	O-C-N	-5.56	116.45	123.01
1	L	129	GLU	N-CA-CB	-5.53	101.40	110.14
2	H	16	GLY	CA-C-N	5.50	131.21	122.62
2	H	16	GLY	C-N-CA	5.50	131.21	122.62
1	L	147	VAL	CB-CA-C	-5.45	101.96	110.52
2	H	89	GLU	O-C-N	-5.45	114.47	122.43
2	H	12	VAL	CB-CA-C	-5.43	102.78	110.82
1	L	65	SER	CA-C-N	-5.43	118.44	122.18
1	L	65	SER	C-N-CA	-5.43	118.44	122.18
1	L	56	ARG	O-C-N	-5.42	116.61	123.01
2	H	91	THR	CB-CA-C	5.41	118.37	110.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	113	LYS	CB-CA-C	5.39	118.67	109.72
2	H	194	SER	CB-CA-C	-5.39	102.42	110.88
1	L	65	SER	CA-CB-OG	-5.38	100.34	111.10
2	H	65	LYS	N-CA-CB	5.37	117.94	109.83
1	L	125	SER	CB-CA-C	-5.37	101.56	110.68
1	L	99	VAL	N-CA-CB	5.36	119.11	111.82
1	L	77	ILE	CA-C-O	-5.32	114.63	120.48
1	L	81	GLN	O-C-N	-5.32	116.24	123.10
1	L	86	ALA	CA-C-O	-5.31	112.92	120.51
2	H	105	ASP	CB-CG-OD1	5.31	130.60	118.40
2	H	147	LYS	O-C-N	-5.30	116.48	123.16
1	L	197	GLN	OE1-CD-NE2	5.28	127.88	122.60
2	H	212	LYS	CA-C-O	5.25	125.92	120.30
1	L	128	LEU	O-C-N	-5.25	116.56	122.12
1	L	159	THR	N-CA-CB	-5.25	102.98	110.80
2	H	200	ASN	CA-CB-CG	-5.23	107.37	112.60
1	L	64	PHE	CA-C-O	-5.21	114.93	120.92
1	L	8	SER	CA-C-O	5.21	125.94	120.42
2	H	137	ASN	CB-CA-C	-5.21	107.89	114.40
1	L	141	ASP	CA-CB-CG	-5.19	107.41	112.60
1	L	73	ALA	O-C-N	-5.17	117.27	123.06
2	H	38	ARG	NE-CZ-NH1	5.17	126.67	121.50
2	H	21	SER	CB-CA-C	-5.14	99.20	109.33
2	H	120	THR	CA-CB-OG1	-5.14	101.89	109.60
1	L	42	PRO	N-CA-CB	5.12	107.80	103.19
2	H	139	MET	CA-CB-CG	5.12	124.34	114.10
1	L	121	PHE	N-CA-C	5.11	117.36	110.31
2	H	31	THR	N-CA-CB	-5.10	102.37	110.28
1	L	136	VAL	CA-C-N	5.09	130.50	123.07
1	L	136	VAL	C-N-CA	5.09	130.50	123.07
2	H	27	TYR	CA-C-O	-5.08	115.99	121.38
1	L	8	SER	O-C-N	-5.07	116.37	122.15
2	H	171	PRO	O-C-N	-5.07	116.73	123.01
1	L	22	CYS	N-CA-CB	-5.06	102.52	110.77
1	L	54	ASN	CA-C-O	-5.06	114.25	119.51
1	L	117	SER	O-C-N	-5.06	117.45	123.22
1	L	8	SER	CA-CB-OG	-5.05	101.00	111.10
1	L	114	SER	CA-C-N	5.04	128.34	120.68
1	L	114	SER	C-N-CA	5.04	128.34	120.68
1	L	97	HIS	CA-C-O	-5.03	115.38	120.71
2	H	10	GLY	CA-C-O	-5.03	117.07	121.04
2	H	117	SER	CA-C-O	-5.03	113.47	119.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	151	TRP	O-C-N	5.01	129.71	123.19
2	H	123	PRO	CA-C-O	-5.00	115.97	122.13

There are no chirality outliers.

There are no planarity outliers.

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	1556	0	1490	30	0
2	H	1598	0	1517	29	0
3	H	20	0	23	1	0
4	H	24	0	0	0	0
4	L	33	0	0	0	0
All	All	3231	0	3030	59	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 (59) 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)
2:H:196:THR:HG23	2:H:213:LYS:HD3	1.47	0.96
2:H:88:SER:O	2:H:91:THR:HG23	1.84	0.78
1:L:87:ILE:HD12	1:L:105:LYS:HG2	1.69	0.74
2:H:122:PRO:HB3	2:H:208:THR:HG21	1.69	0.74
2:H:40:THR:HB	2:H:41:PRO:HD2	1.71	0.72
1:L:30:THR:HG22	1:L:32:SER:H	1.54	0.71
1:L:1:GLN:HG2	1:L:2:ALA:H	1.60	0.67
1:L:30:THR:CG2	1:L:32:SER:H	2.09	0.66
2:H:203:HIS:HB3	2:H:208:THR:HG22	1.78	0.66
1:L:169:LYS:HE3	1:L:173:ASN:OD1	1.96	0.66
1:L:20:LEU:HD13	1:L:104:THR:HG21	1.81	0.62
2:H:130:PRO:HD3	2:H:142:LEU:CD1	2.29	0.62
2:H:135:GLN:O	2:H:136:THR:C	2.40	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:130:PRO:HD3	2:H:142:LEU:HD12	1.82	0.62
1:L:191:HIS:HB2	1:L:194:TYR:OH	2.04	0.58
1:L:113:LYS:HG2	1:L:144:PRO:HD3	1.85	0.56
2:H:12:VAL:HG12	2:H:13:THR:H	1.71	0.56
1:L:120:LEU:CD2	1:L:209:LEU:HG	2.36	0.55
1:L:169:LYS:HZ1	1:L:173:ASN:HB3	1.72	0.55
1:L:169:LYS:NZ	1:L:173:ASN:HB3	2.22	0.54
2:H:76:LYS:HB2	2:H:78:THR:HG23	1.88	0.54
1:L:24:SER:OG	1:L:26:THR:HB	2.09	0.52
2:H:131:GLY:O	2:H:132:SER:HB2	2.09	0.52
2:H:12:VAL:HG12	2:H:13:THR:N	2.25	0.51
2:H:203:HIS:HD2	2:H:206:SER:OG	1.93	0.51
1:L:120:LEU:HD23	1:L:209:LEU:HG	1.94	0.50
2:H:181:LEU:C	2:H:181:LEU:HD23	2.37	0.50
2:H:76:LYS:O	2:H:78:THR:HG22	2.13	0.49
1:L:162:MET:HE2	1:L:162:MET:H	1.77	0.49
1:L:153:VAL:HG23	1:L:158:VAL:CG2	2.43	0.49
2:H:42:GLU:O	2:H:43:LYS:HB2	2.13	0.48
1:L:12:THR:HG21	1:L:18:VAL:HG22	1.96	0.48
1:L:192:SER:O	1:L:210:SER:HA	2.15	0.47
1:L:41:LYS:HB3	1:L:42:PRO:CD	2.45	0.46
2:H:70:ILE:HD11	2:H:79:LEU:HD11	1.98	0.45
2:H:188:PRO:HD2	2:H:191:THR:OG1	2.16	0.45
1:L:139:ILE:HG22	1:L:142:PHE:CD1	2.52	0.45
2:H:38:ARG:HD3	2:H:48:VAL:HG21	2.00	0.43
1:L:139:ILE:HG22	1:L:142:PHE:CE1	2.54	0.43
2:H:94:TYR:O	2:H:110:GLY:HA2	2.17	0.43
2:H:97:THR:HG22	2:H:106:TYR:O	2.19	0.43
1:L:85:GLU:HA	1:L:106:LEU:O	2.19	0.43
2:H:121:THR:HA	2:H:122:PRO:HD3	1.86	0.43
1:L:28:THR:HG23	1:L:71:GLY:HA2	2.00	0.43
1:L:52:ALA:O	1:L:53:THR:HB	2.19	0.43
2:H:142:LEU:HG	2:H:214:ILE:HG21	2.00	0.43
1:L:94:TYR:O	1:L:95:SER:C	2.61	0.43
2:H:151:PRO:O	2:H:203:HIS:HE1	2.02	0.43
2:H:73:ASP:OD1	2:H:73:ASP:C	2.61	0.42
1:L:34:TYR:O	1:L:35:ALA:C	2.61	0.42
2:H:40:THR:HB	2:H:41:PRO:CD	2.45	0.42
1:L:69:ILE:O	1:L:70:GLY:C	2.60	0.42
1:L:123:PRO:HD3	1:L:135:LEU:HD22	2.00	0.42
1:L:9:ALA:O	1:L:10:LEU:HD13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:126:GLU:OE1	2:H:212:LYS:NZ	2.42	0.41
1:L:162:MET:HA	1:L:180:TYR:O	2.20	0.41
3:H:301:MGS:HC73	3:H:301:MGS:HC5	2.02	0.41
2:H:20:LEU:HG	2:H:83:MET:HE2	2.02	0.41
2:H:33:ASP:HB2	2:H:99:HIS:HB2	2.02	0.41

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	208/210 (99%)	198 (95%)	7 (3%)	3 (1%)	9	9
2	H	214/216 (99%)	203 (95%)	8 (4%)	3 (1%)	9	9
All	All	422/426 (99%)	401 (95%)	15 (4%)	6 (1%)	9	9

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	135	GLN
1	L	43	ASP
2	H	132	SER
1	L	109	LEU
2	H	136	THR
1	L	145	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	L	172/177 (97%)	148 (86%)	24 (14%)	3	3
2	H	178/186 (96%)	161 (90%)	17 (10%)	8	10
All	All	350/363 (96%)	309 (88%)	41 (12%)	5	6

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	5	THR
1	L	10	LEU
1	L	18	VAL
1	L	20	LEU
1	L	26	THR
1	L	30	THR
1	L	49	LEU
1	L	54	ASN
1	L	62	VAL
1	L	82	THR
1	L	115	SER
1	L	117	SER
1	L	135	LEU
1	L	146	VAL
1	L	148	THR
1	L	149	VAL
1	L	152	LYS
1	L	159	THR
1	L	162	MET
1	L	178	SER
1	L	195	SER
1	L	206	GLU
1	L	207	LYS
1	L	210	SER
2	H	3	GLN
2	H	17	SER
2	H	22	CYS
2	H	42	GLU
2	H	48	VAL
2	H	64	VAL
2	H	78	THR
2	H	91	THR
2	H	97	THR

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Mol	Chain	Res	Type
2	H	121	THR
2	H	135	GLN
2	H	136	THR
2	H	141	THR
2	H	142	LEU
2	H	181	LEU
2	H	208	THR
2	H	213	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	131	ASN
1	L	191	HIS
2	H	175	GLN
2	H	203	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	MGS	H	301	-	20,20,20	1.04	1 (5%)	23,27,27	3.30	7 (30%)

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	MGS	H	301	-	-	7/15/35/35	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	301	MGS	C4-N4	3.17	1.50	1.45

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	301	MGS	O9-C9-C10	-9.53	106.52	120.61
3	H	301	MGS	C4-N4-C9	-8.52	110.23	123.20
3	H	301	MGS	O10-C10-C11	4.35	120.68	109.14
3	H	301	MGS	O9-C9-N4	-4.31	115.24	122.96
3	H	301	MGS	O12-C12-C11	-3.78	98.95	111.34
3	H	301	MGS	C8-O2-C2	-2.80	107.30	114.47
3	H	301	MGS	C1-O5-C5	-2.39	109.56	113.63

There are no chirality outliers.

All (7) torsion outliers are listed below:

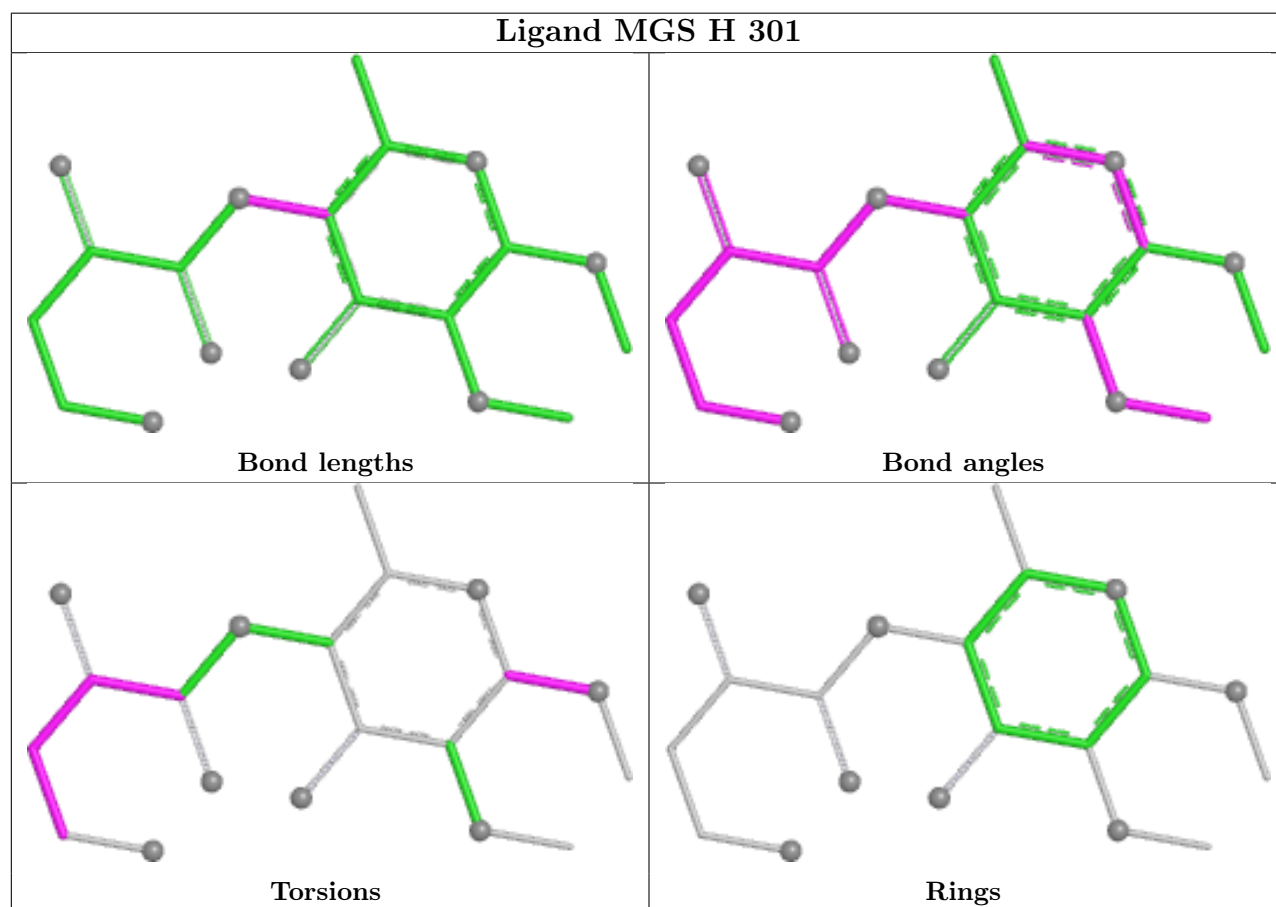
Mol	Chain	Res	Type	Atoms
3	H	301	MGS	O5-C1-O1-C7
3	H	301	MGS	C11-C10-C9-N4
3	H	301	MGS	O10-C10-C9-N4
3	H	301	MGS	C11-C10-C9-O9
3	H	301	MGS	C10-C11-C12-O12
3	H	301	MGS	O10-C10-C11-C12
3	H	301	MGS	O10-C10-C9-O9

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	301	MGS	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 ⓘ

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.