



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:26 AM UTC

PDB ID : 6HXR / pdb_00006hxr
Title : Human PARP16 (ARTD15) IN COMPLEX WITH EB-47
Authors : Karlberg, T.; Pinto, A.F.; Thorsell, A.G.; Schuler, H.
Deposited on : 2018-10-18
Resolution : 2.90 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

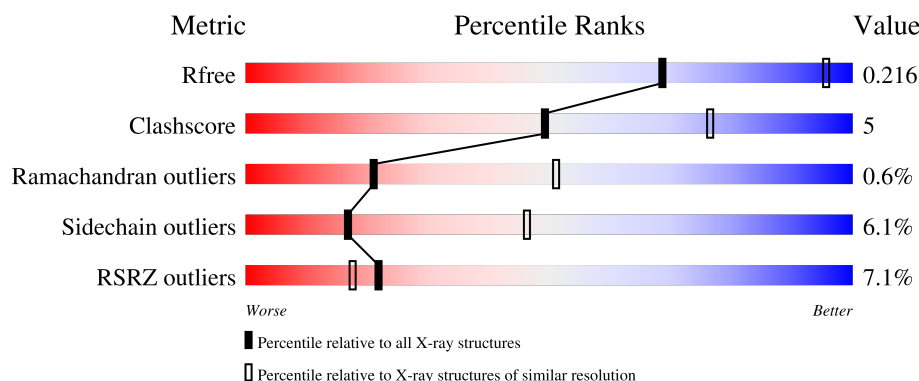
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	A	298	5% 64% 13% • 19%
1	B	298	3% 67% 11% • 20%
1	C	298	8% 62% 13% • 23%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5634 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 Mono [ADP-ribose] polymerase PARP16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	240	Total	C	N	O	S	0	0	0
			1887	1214	325	341	7			
1	B	238	Total	C	N	O	S	0	0	0
			1869	1202	323	337	7			
1	C	228	Total	C	N	O	S	0	0	0
			1800	1159	310	324	7			

There are 69 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	initiating methionine	UNP Q8N5Y8
A	-17	HIS	-	expression tag	UNP Q8N5Y8
A	-16	HIS	-	expression tag	UNP Q8N5Y8
A	-15	HIS	-	expression tag	UNP Q8N5Y8
A	-14	HIS	-	expression tag	UNP Q8N5Y8
A	-13	HIS	-	expression tag	UNP Q8N5Y8
A	-12	HIS	-	expression tag	UNP Q8N5Y8
A	-11	SER	-	expression tag	UNP Q8N5Y8
A	-10	SER	-	expression tag	UNP Q8N5Y8
A	-9	GLY	-	expression tag	UNP Q8N5Y8
A	-8	VAL	-	expression tag	UNP Q8N5Y8
A	-7	ASP	-	expression tag	UNP Q8N5Y8
A	-6	LEU	-	expression tag	UNP Q8N5Y8
A	-5	GLY	-	expression tag	UNP Q8N5Y8
A	-4	THR	-	expression tag	UNP Q8N5Y8
A	-3	GLU	-	expression tag	UNP Q8N5Y8
A	-2	ASN	-	expression tag	UNP Q8N5Y8
A	-1	LEU	-	expression tag	UNP Q8N5Y8
A	0	TYR	-	expression tag	UNP Q8N5Y8
A	1	PHE	-	expression tag	UNP Q8N5Y8
A	2	GLN	-	expression tag	UNP Q8N5Y8
A	3	SER	-	expression tag	UNP Q8N5Y8
A	4	MET	-	expression tag	UNP Q8N5Y8

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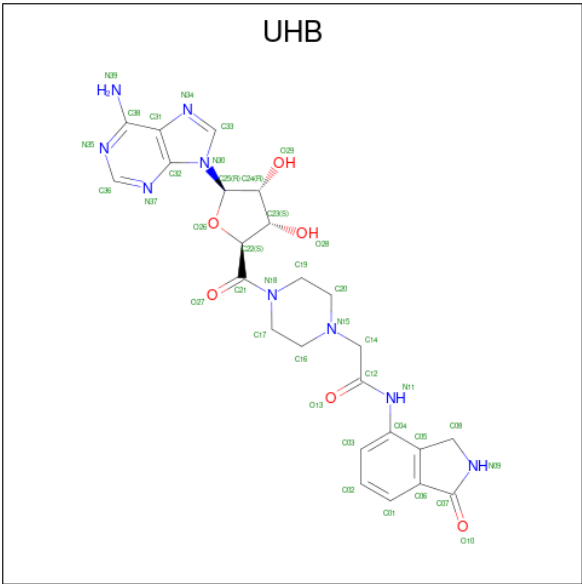
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	MET	-	initiating methionine	UNP Q8N5Y8
B	-17	HIS	-	expression tag	UNP Q8N5Y8
B	-16	HIS	-	expression tag	UNP Q8N5Y8
B	-15	HIS	-	expression tag	UNP Q8N5Y8
B	-14	HIS	-	expression tag	UNP Q8N5Y8
B	-13	HIS	-	expression tag	UNP Q8N5Y8
B	-12	HIS	-	expression tag	UNP Q8N5Y8
B	-11	SER	-	expression tag	UNP Q8N5Y8
B	-10	SER	-	expression tag	UNP Q8N5Y8
B	-9	GLY	-	expression tag	UNP Q8N5Y8
B	-8	VAL	-	expression tag	UNP Q8N5Y8
B	-7	ASP	-	expression tag	UNP Q8N5Y8
B	-6	LEU	-	expression tag	UNP Q8N5Y8
B	-5	GLY	-	expression tag	UNP Q8N5Y8
B	-4	THR	-	expression tag	UNP Q8N5Y8
B	-3	GLU	-	expression tag	UNP Q8N5Y8
B	-2	ASN	-	expression tag	UNP Q8N5Y8
B	-1	LEU	-	expression tag	UNP Q8N5Y8
B	0	TYR	-	expression tag	UNP Q8N5Y8
B	1	PHE	-	expression tag	UNP Q8N5Y8
B	2	GLN	-	expression tag	UNP Q8N5Y8
B	3	SER	-	expression tag	UNP Q8N5Y8
B	4	MET	-	expression tag	UNP Q8N5Y8
C	-18	MET	-	initiating methionine	UNP Q8N5Y8
C	-17	HIS	-	expression tag	UNP Q8N5Y8
C	-16	HIS	-	expression tag	UNP Q8N5Y8
C	-15	HIS	-	expression tag	UNP Q8N5Y8
C	-14	HIS	-	expression tag	UNP Q8N5Y8
C	-13	HIS	-	expression tag	UNP Q8N5Y8
C	-12	HIS	-	expression tag	UNP Q8N5Y8
C	-11	SER	-	expression tag	UNP Q8N5Y8
C	-10	SER	-	expression tag	UNP Q8N5Y8
C	-9	GLY	-	expression tag	UNP Q8N5Y8
C	-8	VAL	-	expression tag	UNP Q8N5Y8
C	-7	ASP	-	expression tag	UNP Q8N5Y8
C	-6	LEU	-	expression tag	UNP Q8N5Y8
C	-5	GLY	-	expression tag	UNP Q8N5Y8
C	-4	THR	-	expression tag	UNP Q8N5Y8
C	-3	GLU	-	expression tag	UNP Q8N5Y8
C	-2	ASN	-	expression tag	UNP Q8N5Y8
C	-1	LEU	-	expression tag	UNP Q8N5Y8
C	0	TYR	-	expression tag	UNP Q8N5Y8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1	PHE	-	expression tag	UNP Q8N5Y8
C	2	GLN	-	expression tag	UNP Q8N5Y8
C	3	SER	-	expression tag	UNP Q8N5Y8
C	4	MET	-	expression tag	UNP Q8N5Y8

- Molecule 2 is 2-[4-[(2S,3S,4R,5R)-5-(6-aminopurin-9-yl)-3,4-bis(oxidanyl)oxolan-2-yl]carbon ylpiperazin-1-yl]-N-(1-oxidanylidene-2,3-dihydroisoindol-4-yl)ethanamide (CCD ID: UHB) (formula: C₂₄H₂₇N₉O₆).

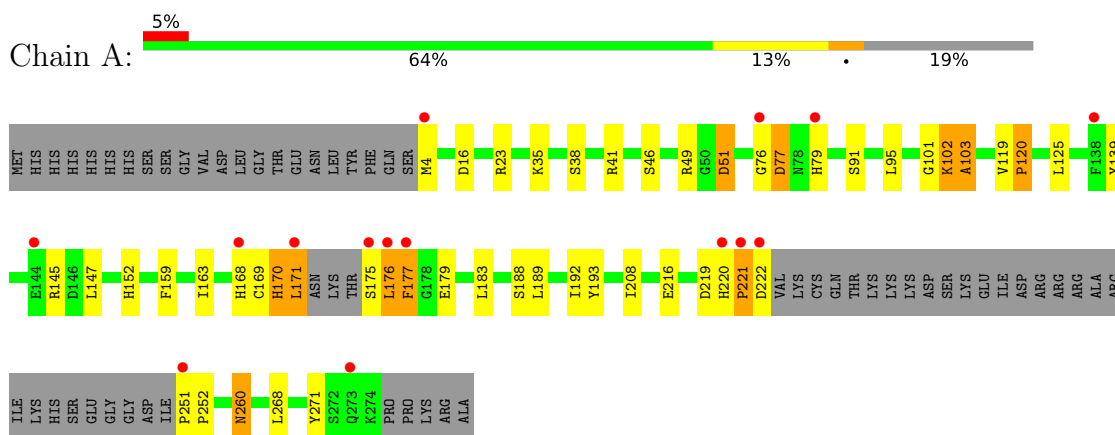


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			39	24	9	6		
2	B	1	Total	C	N	O	0	0
			39	24	9	6		

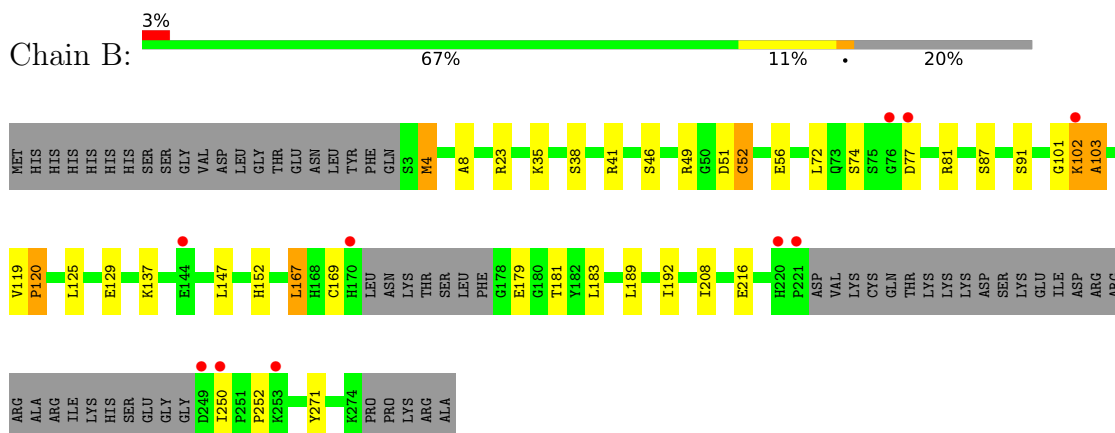
3 Residue-property plots [i](#)

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.

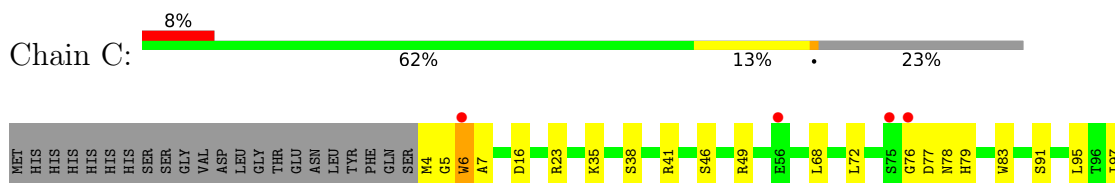
- Molecule 1: Mono [ADP-ribose] polymerase PARP16

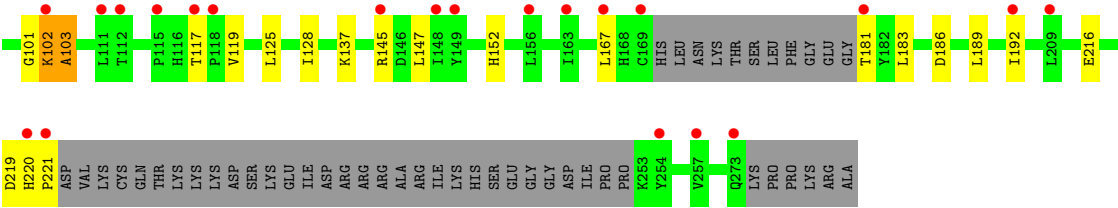


- Molecule 1: Mono [ADP-ribose] polymerase PARP16



- Molecule 1: Mono [ADP-ribose] polymerase PARP16





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	148.06Å 148.06Å 99.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.70 – 2.90 33.70 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (33.70-2.90) 99.9 (33.70-2.90)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.91Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.199 , 0.230 (Not available) , 0.216	Depositor DCC
R_{free} test set	1260 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	71.5	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 65.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5634	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% 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: UHB

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	1.05	3/1937 (0.2%)	1.41	20/2625 (0.8%)
1	B	1.10	2/1920 (0.1%)	1.38	16/2604 (0.6%)
1	C	0.84	0/1848	1.34	13/2506 (0.5%)
All	All	1.01	5/5705 (0.1%)	1.38	49/7735 (0.6%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	119	VAL	C-N	5.90	1.40	1.33
1	B	119	VAL	C-N	5.90	1.40	1.33
1	B	208	ILE	CG1-CD1	-5.56	1.30	1.51
1	A	120	PRO	N-CD	5.13	1.54	1.47
1	A	208	ILE	CG1-CD1	-5.01	1.32	1.51

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	91	SER	N-CA-C	11.14	126.39	113.02
1	A	51	ASP	CA-CB-CG	9.24	121.84	112.60
1	A	252	PRO	N-CA-CB	8.52	110.76	103.35
1	B	167	LEU	CA-C-N	7.66	136.17	121.54
1	B	167	LEU	C-N-CA	7.66	136.17	121.54
1	C	76	GLY	CA-C-N	7.58	135.35	121.70
1	C	76	GLY	C-N-CA	7.58	135.35	121.70
1	A	251	PRO	N-CA-CB	7.14	110.85	103.00
1	B	119	VAL	CA-C-N	-6.86	113.18	120.66
1	B	119	VAL	C-N-CA	-6.86	113.18	120.66
1	B	74	SER	CA-C-N	6.76	133.06	121.29
1	B	74	SER	C-N-CA	6.76	133.06	121.29
1	A	119	VAL	CA-C-N	-6.67	113.39	120.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	119	VAL	C-N-CA	-6.67	113.39	120.66
1	B	91	SER	CA-C-N	6.59	130.06	120.71
1	B	91	SER	C-N-CA	6.59	130.06	120.71
1	A	16	ASP	CA-CB-CG	6.56	119.16	112.60
1	A	77	ASP	N-CA-C	-6.44	103.72	113.89
1	A	222	ASP	CA-CB-CG	6.36	118.96	112.60
1	C	6	TRP	CA-CB-CG	6.30	125.57	113.60
1	A	102	LYS	CA-C-N	6.17	132.07	122.26
1	A	102	LYS	C-N-CA	6.17	132.07	122.26
1	C	103	ALA	N-CA-C	-5.94	105.99	113.72
1	B	91	SER	CB-CA-C	-5.85	99.95	110.37
1	A	49	ARG	CA-CB-CG	-5.76	102.58	114.10
1	B	103	ALA	N-CA-C	-5.75	106.24	113.72
1	B	51	ASP	CA-CB-CG	5.67	118.27	112.60
1	B	102	LYS	CA-C-N	5.67	131.27	122.26
1	B	102	LYS	C-N-CA	5.67	131.27	122.26
1	A	76	GLY	CA-C-N	5.64	130.79	121.99
1	A	76	GLY	C-N-CA	5.64	130.79	121.99
1	A	79	HIS	CA-C-N	5.59	128.08	120.54
1	A	79	HIS	C-N-CA	5.59	128.08	120.54
1	A	103	ALA	N-CA-C	-5.58	106.46	113.72
1	A	260	ASN	CA-CB-CG	5.47	118.07	112.60
1	C	102	LYS	CA-C-N	5.44	130.91	122.26
1	C	102	LYS	C-N-CA	5.44	130.91	122.26
1	C	78	ASN	N-CA-C	-5.40	106.70	113.72
1	C	5	GLY	CA-C-N	5.33	127.87	120.29
1	C	5	GLY	C-N-CA	5.33	127.87	120.29
1	B	119	VAL	O-C-N	5.33	125.05	121.69
1	C	186	ASP	CA-CB-CG	5.31	117.91	112.60
1	B	129	GLU	CB-CG-CD	5.29	121.60	112.60
1	A	119	VAL	O-C-N	5.12	124.91	121.69
1	C	79	HIS	CA-C-N	5.12	127.44	120.54
1	C	79	HIS	C-N-CA	5.12	127.44	120.54
1	C	16	ASP	CA-CB-CG	5.11	117.71	112.60
1	A	159	PHE	CA-CB-CG	-5.09	108.71	113.80
1	A	49	ARG	CB-CG-CD	5.08	122.98	111.30

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	A	1887	0	1845	30	0
1	B	1869	0	1834	13	0
1	C	1800	0	1770	17	0
2	A	39	0	25	2	0
2	B	39	0	26	0	0
All	All	5634	0	5500	60	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 5.

All (60) 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:176:LEU:HD12	1:A:177:PHE:N	1.19	1.48
1:A:176:LEU:CD1	1:A:177:PHE:HB2	1.70	1.21
1:A:176:LEU:CD1	1:A:177:PHE:N	2.11	1.12
1:A:176:LEU:HD12	1:A:177:PHE:CA	1.85	1.05
1:C:95:LEU:HD12	1:C:128:ILE:HG23	1.44	1.00
1:A:176:LEU:CD1	1:A:177:PHE:H	1.75	0.95
1:A:176:LEU:CD1	1:A:177:PHE:CB	2.50	0.90
1:A:176:LEU:HD12	1:A:177:PHE:CB	2.02	0.89
1:A:176:LEU:HD12	1:A:177:PHE:H	1.04	0.87
1:C:95:LEU:HD12	1:C:128:ILE:CG2	2.05	0.86
1:A:4:MET:HB3	1:A:91:SER:OG	1.85	0.77
1:A:176:LEU:HD13	1:A:177:PHE:HB2	1.66	0.76
1:A:170:HIS:CG	1:A:171:LEU:H	2.03	0.75
1:C:4:MET:HB3	1:C:91:SER:OG	1.89	0.72
1:C:117:THR:O	1:C:119:VAL:HG13	1.89	0.71
1:B:81:ARG:HG3	1:B:81:ARG:HH11	1.60	0.67
1:A:176:LEU:HD11	1:A:177:PHE:HB2	1.73	0.66
1:C:68:LEU:O	1:C:72:LEU:HD13	1.96	0.66
1:A:175:SER:O	1:A:176:LEU:HB3	1.96	0.64
1:B:49:ARG:HB2	1:B:52:CYS:SG	2.39	0.61
1:C:95:LEU:CD1	1:C:128:ILE:CG2	2.78	0.61
1:A:169:CYS:SG	1:A:260:ASN:HB3	2.43	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:HIS:HB2	1:B:183:LEU:HD23	1.85	0.58
1:A:152:HIS:HB2	1:A:183:LEU:HD23	1.86	0.57
1:A:176:LEU:CG	1:A:177:PHE:H	2.18	0.56
1:C:152:HIS:HB2	1:C:183:LEU:HD23	1.88	0.55
1:A:168:HIS:CD2	1:A:168:HIS:C	2.85	0.54
1:C:6:TRP:HD1	1:C:83:TRP:CD2	2.28	0.52
1:A:169:CYS:O	1:A:170:HIS:HB3	2.10	0.51
1:A:120:PRO:HG2	1:A:271:TYR:CE2	2.46	0.51
1:C:167:LEU:HD13	1:C:181:THR:HG21	1.93	0.51
1:B:38:SER:HA	1:B:41:ARG:HE	1.77	0.49
1:B:4:MET:HG3	1:B:8:ALA:HB3	1.95	0.48
1:B:167:LEU:HD13	1:B:181:THR:HG21	1.95	0.47
1:A:220:HIS:CE1	1:A:221:PRO:HD2	2.50	0.47
1:C:220:HIS:ND1	1:C:221:PRO:HD2	2.30	0.47
1:B:120:PRO:HG2	1:B:271:TYR:CE2	2.50	0.47
1:C:189:LEU:O	1:C:192:ILE:HG12	2.15	0.46
1:C:38:SER:HA	1:C:41:ARG:HE	1.80	0.46
2:A:301:UHB:O28	2:A:301:UHB:H19	2.16	0.46
1:B:81:ARG:HG3	1:B:81:ARG:NH1	2.30	0.46
1:C:220:HIS:CE1	1:C:221:PRO:HD2	2.51	0.46
1:B:189:LEU:O	1:B:192:ILE:HG12	2.16	0.45
1:A:38:SER:HA	1:A:41:ARG:HE	1.81	0.45
1:A:163:ILE:HD11	1:A:268:LEU:HD11	1.99	0.45
1:B:147:LEU:HD13	1:B:216:GLU:HG2	1.99	0.45
1:A:139:TYR:CD1	1:C:7:ALA:CB	3.00	0.44
1:A:189:LEU:O	1:A:192:ILE:HG12	2.18	0.44
1:A:193:TYR:HA	1:B:250:ILE:HG21	2.00	0.44
1:C:147:LEU:HD13	1:C:216:GLU:HG2	2.00	0.44
1:B:4:MET:HE2	1:B:87:SER:O	2.18	0.43
1:C:101:GLY:C	1:C:103:ALA:H	2.26	0.43
1:A:101:GLY:C	1:A:103:ALA:H	2.26	0.43
1:A:220:HIS:ND1	1:A:221:PRO:HD2	2.33	0.43
1:B:101:GLY:C	1:B:103:ALA:H	2.26	0.43
1:A:170:HIS:CG	1:A:171:LEU:N	2.73	0.42
1:A:145:ARG:HD2	1:A:219:ASP:O	2.20	0.42
2:A:301:UHB:H19	2:A:301:UHB:C23	2.50	0.42
1:C:145:ARG:HD2	1:C:219:ASP:O	2.19	0.41
1:A:147:LEU:HD13	1:A:216:GLU:HG2	2.02	0.41

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	234/298 (78%)	222 (95%)	9 (4%)	3 (1%)	9	32
1	B	232/298 (78%)	222 (96%)	9 (4%)	1 (0%)	30	59
1	C	222/298 (74%)	216 (97%)	6 (3%)	0	100	100
All	All	688/894 (77%)	660 (96%)	24 (4%)	4 (1%)	21	51

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	170	HIS
1	A	176	LEU
1	A	221	PRO
1	B	252	PRO

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	184/254 (72%)	172 (94%)	12 (6%)	15	44
1	B	198/254 (78%)	184 (93%)	14 (7%)	13	40
1	C	191/254 (75%)	182 (95%)	9 (5%)	23	56
All	All	573/762 (75%)	538 (94%)	35 (6%)	17	46

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ARG
1	A	35	LYS
1	A	46	SER
1	A	51	ASP
1	A	77	ASP
1	A	95	LEU
1	A	102	LYS
1	A	125	LEU
1	A	171	LEU
1	A	177	PHE
1	A	179	GLU
1	A	188	SER
1	B	4	MET
1	B	23	ARG
1	B	35	LYS
1	B	46	SER
1	B	52	CYS
1	B	56	GLU
1	B	72	LEU
1	B	77	ASP
1	B	102	LYS
1	B	120	PRO
1	B	125	LEU
1	B	137	LYS
1	B	169	CYS
1	B	179	GLU
1	C	23	ARG
1	C	35	LYS
1	C	46	SER
1	C	49	ARG
1	C	77	ASP
1	C	97	ILE
1	C	102	LYS
1	C	125	LEU
1	C	137	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	158	ASN
1	A	168	HIS
1	A	170	HIS

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Mol	Chain	Res	Type
1	A	201	GLN
1	B	73	GLN
1	B	78	ASN
1	B	158	ASN
1	B	168	HIS
1	C	73	GLN
1	C	158	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	UHB	A	301	-	44,44,44	4.39	22 (50%)	62,65,65	4.01	30 (48%)
2	UHB	B	301	-	44,44,44	4.48	18 (40%)	62,65,65	3.37	30 (48%)

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
2	UHB	A	301	-	-	3/20/55/55	0/6/6/6
2	UHB	B	301	-	-	3/20/55/55	0/6/6/6

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	UHB	C08-C05	-13.96	1.38	1.50
2	B	301	UHB	C08-C05	-13.46	1.38	1.50
2	B	301	UHB	C06-C07	-13.24	1.30	1.48
2	A	301	UHB	C07-N09	-10.37	1.27	1.35
2	B	301	UHB	C36-N35	8.94	1.49	1.33
2	A	301	UHB	C36-N35	8.81	1.49	1.33
2	A	301	UHB	C06-C07	-8.76	1.36	1.48
2	B	301	UHB	C36-N37	8.74	1.49	1.33
2	B	301	UHB	C08-N09	-8.68	1.36	1.45
2	A	301	UHB	C23-C22	-8.29	1.42	1.53
2	A	301	UHB	O28-C23	-8.01	1.23	1.43
2	A	301	UHB	O27-C21	7.37	1.35	1.22
2	B	301	UHB	C07-N09	-7.33	1.29	1.35
2	B	301	UHB	C12-N11	-6.97	1.20	1.35
2	B	301	UHB	C04-N11	-6.37	1.29	1.41
2	B	301	UHB	C21-N18	5.77	1.43	1.35
2	B	301	UHB	O27-C21	5.15	1.31	1.22
2	A	301	UHB	C04-C05	4.76	1.45	1.40
2	A	301	UHB	C01-C06	4.70	1.47	1.39
2	A	301	UHB	C08-N09	-4.43	1.41	1.45
2	A	301	UHB	O26-C25	-4.00	1.32	1.42
2	A	301	UHB	C14-N15	3.70	1.54	1.47
2	A	301	UHB	C31-N34	-3.42	1.32	1.39
2	A	301	UHB	C21-N18	3.15	1.39	1.35
2	B	301	UHB	O13-C12	-3.13	1.17	1.23
2	A	301	UHB	C36-N37	3.12	1.39	1.33
2	B	301	UHB	C22-C21	2.91	1.59	1.53
2	A	301	UHB	C24-C23	-2.85	1.45	1.53
2	B	301	UHB	C01-C06	2.83	1.44	1.39
2	B	301	UHB	C19-N18	2.82	1.52	1.47
2	A	301	UHB	C22-C21	2.82	1.59	1.53
2	A	301	UHB	C32-N30	-2.73	1.32	1.37
2	A	301	UHB	C33-N30	-2.72	1.32	1.37
2	B	301	UHB	C14-N15	-2.48	1.41	1.47
2	A	301	UHB	C12-N11	-2.46	1.30	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	UHB	C24-C25	-2.44	1.45	1.53
2	A	301	UHB	C31-C38	-2.34	1.34	1.41
2	B	301	UHB	C14-C12	-2.28	1.48	1.52
2	B	301	UHB	C02-C01	2.25	1.42	1.38
2	B	301	UHB	C25-N30	2.12	1.52	1.46

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	UHB	N37-C36-N35	-11.45	111.24	128.58
2	B	301	UHB	C06-C07-N09	11.40	112.81	106.33
2	B	301	UHB	N37-C36-N35	-10.69	112.40	128.58
2	A	301	UHB	C06-C07-N09	9.79	111.89	106.33
2	A	301	UHB	C14-N15-C20	9.78	126.36	111.14
2	A	301	UHB	C08-C05-C06	-9.66	102.57	109.72
2	A	301	UHB	C05-C08-N09	9.11	110.61	101.75
2	A	301	UHB	C08-N09-C07	-8.42	106.19	113.86
2	B	301	UHB	C04-N11-C12	8.37	154.68	126.61
2	A	301	UHB	C24-C23-C22	7.72	110.80	101.69
2	A	301	UHB	C08-C05-C04	6.70	136.26	129.47
2	B	301	UHB	C14-N15-C16	-6.14	101.59	111.14
2	B	301	UHB	C20-N15-C16	5.88	121.52	108.84
2	B	301	UHB	C08-N09-C07	-5.62	108.73	113.86
2	A	301	UHB	O26-C22-C23	-5.50	97.54	105.15
2	B	301	UHB	O28-C23-C22	4.88	122.79	111.21
2	B	301	UHB	C06-C05-C04	-4.72	118.77	120.97
2	A	301	UHB	C36-N35-C38	4.62	126.31	118.73
2	B	301	UHB	C36-N37-C32	4.41	122.61	111.83
2	A	301	UHB	O10-C07-N09	-4.38	120.48	125.35
2	A	301	UHB	C05-C04-N11	4.27	128.21	119.53
2	A	301	UHB	C19-C20-N15	4.23	119.18	110.65
2	B	301	UHB	O13-C12-C14	4.15	128.28	121.02
2	B	301	UHB	N30-C33-N34	-4.12	108.10	113.94
2	B	301	UHB	C17-C16-N15	3.98	118.67	110.65
2	B	301	UHB	C32-C31-N34	-3.89	106.14	110.58
2	A	301	UHB	C32-N30-C25	-3.88	117.55	126.63
2	A	301	UHB	C14-N15-C16	-3.81	105.22	111.14
2	A	301	UHB	C20-N15-C16	3.80	117.03	108.84
2	A	301	UHB	C03-C04-C05	-3.70	116.24	120.67
2	A	301	UHB	O29-C24-C25	3.69	122.81	110.10
2	B	301	UHB	C31-C32-N30	3.65	109.79	105.81
2	A	301	UHB	C25-N30-C33	3.50	134.87	127.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	UHB	C14-C12-N11	3.41	120.54	114.23
2	B	301	UHB	C31-C32-N37	-3.39	122.05	126.72
2	B	301	UHB	C31-N34-C33	3.27	108.58	103.45
2	A	301	UHB	O13-C12-C14	-3.23	115.37	121.02
2	A	301	UHB	C36-N37-C32	3.17	119.57	111.83
2	A	301	UHB	N30-C33-N34	-3.14	109.48	113.94
2	A	301	UHB	C17-C16-N15	3.06	116.83	110.65
2	B	301	UHB	C14-C12-N11	-2.82	109.02	114.23
2	A	301	UHB	O26-C25-C24	-2.79	100.65	106.62
2	B	301	UHB	C02-C01-C06	-2.76	114.80	119.80
2	B	301	UHB	O26-C25-N30	2.73	113.34	108.09
2	A	301	UHB	C03-C04-N11	-2.73	115.49	121.82
2	B	301	UHB	C14-N15-C20	2.68	115.31	111.14
2	A	301	UHB	C20-C19-N18	2.58	115.56	110.42
2	B	301	UHB	C08-C05-C04	2.51	132.01	129.47
2	A	301	UHB	C02-C01-C06	-2.43	115.41	119.80
2	B	301	UHB	C03-C02-C01	2.42	123.35	120.24
2	B	301	UHB	O26-C25-C24	-2.28	101.73	106.62
2	A	301	UHB	C03-C02-C01	2.27	123.16	120.24
2	B	301	UHB	O10-C07-N09	-2.22	122.88	125.35
2	B	301	UHB	C19-C20-N15	2.19	115.07	110.65
2	B	301	UHB	C05-C08-N09	2.18	103.88	101.75
2	B	301	UHB	O27-C21-N18	2.18	124.21	121.61
2	B	301	UHB	C20-C19-N18	2.16	114.71	110.42
2	B	301	UHB	C31-C38-N35	2.03	122.67	117.51
2	A	301	UHB	C31-C32-N30	2.03	108.02	105.81
2	B	301	UHB	O28-C23-C24	2.01	118.25	111.82

There are no chirality outliers.

All (6) torsion outliers are listed below:

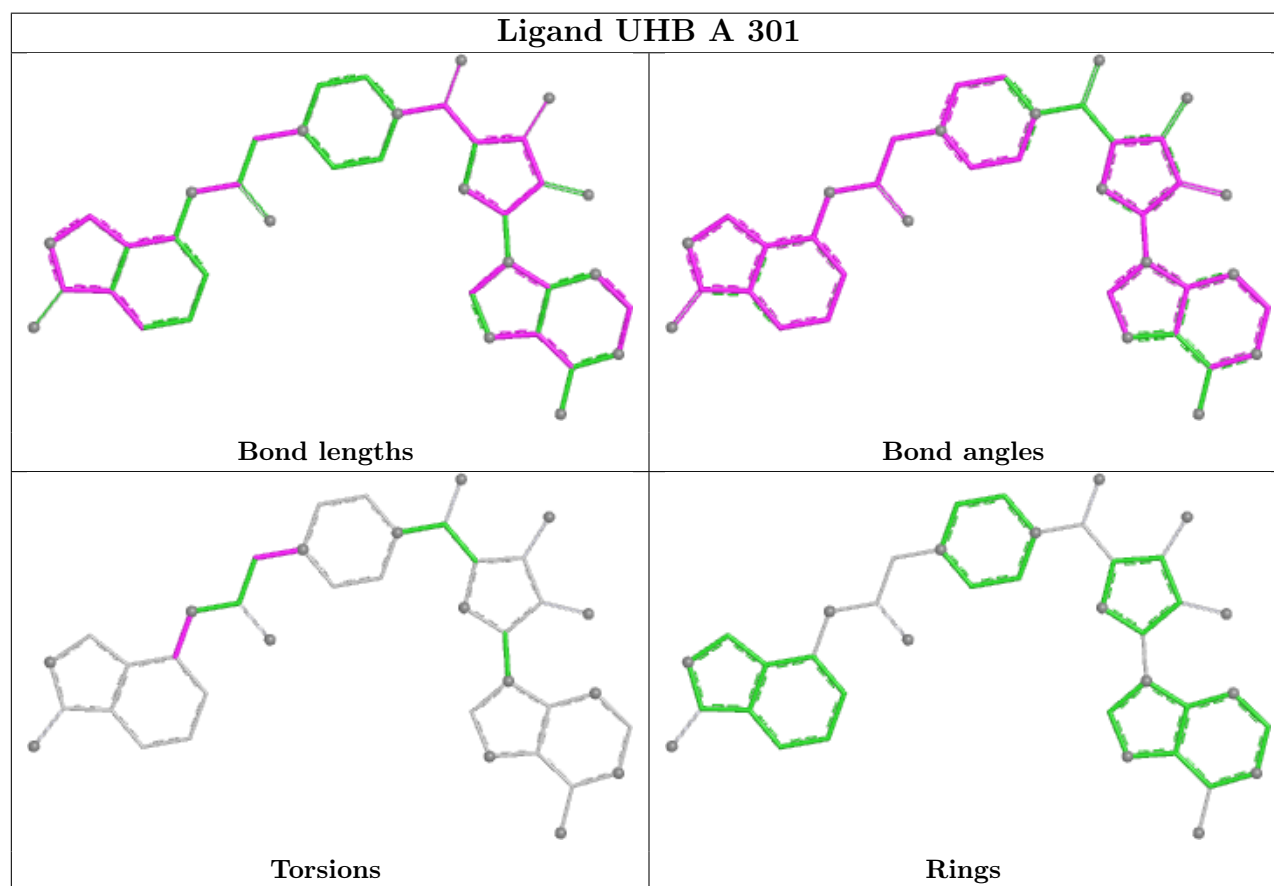
Mol	Chain	Res	Type	Atoms
2	A	301	UHB	C05-C04-N11-C12
2	A	301	UHB	C03-C04-N11-C12
2	A	301	UHB	C12-C14-N15-C20
2	B	301	UHB	C24-C25-N30-C33
2	B	301	UHB	C12-C14-N15-C16
2	B	301	UHB	O26-C25-N30-C33

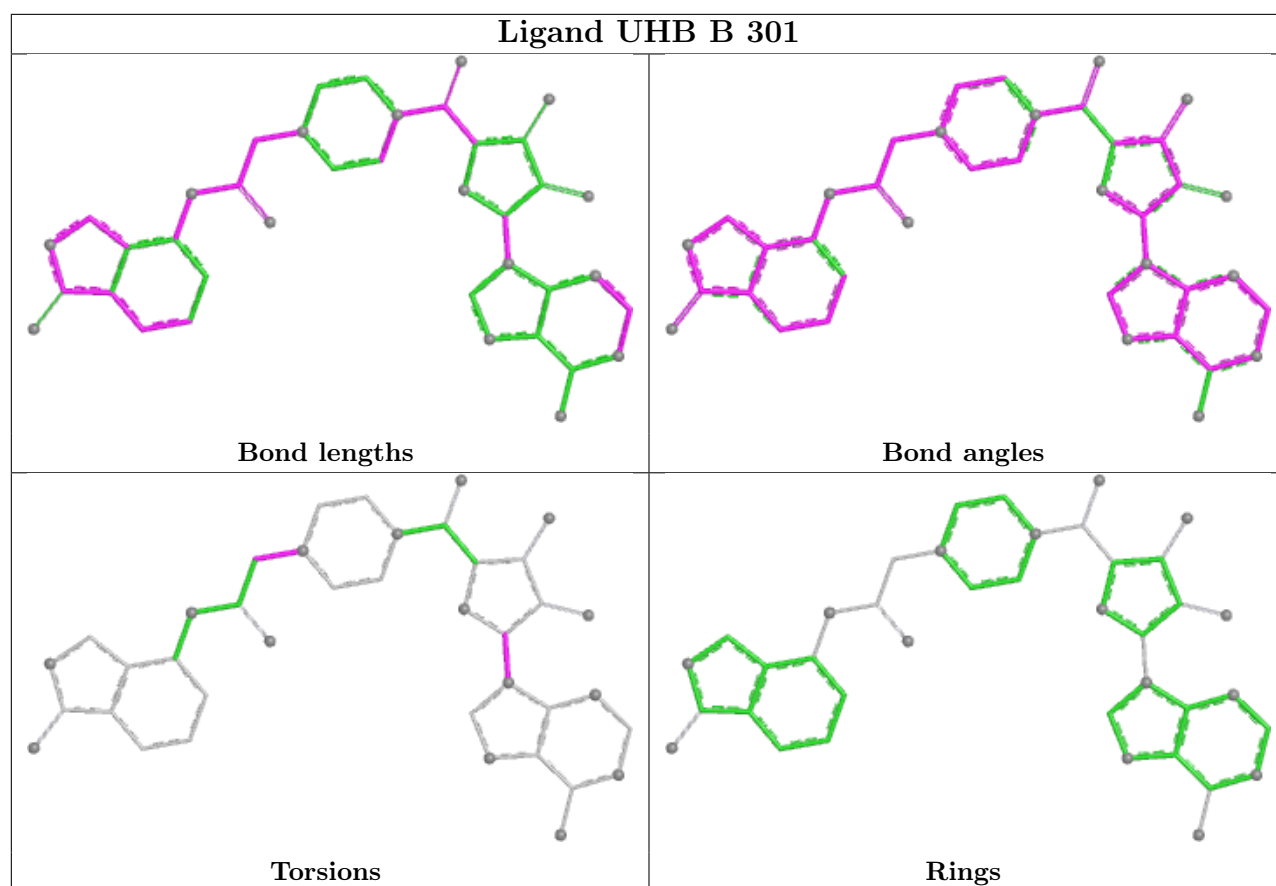
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	UHB	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	A	240/298 (80%)	0.20	15 (6%) 26 20	33, 66, 132, 164	0
1	B	238/298 (79%)	0.15	10 (4%) 40 32	38, 65, 138, 172	0
1	C	228/298 (76%)	1.03	25 (10%) 10 9	78, 126, 176, 198	0
All	All	706/894 (78%)	0.45	50 (7%) 22 17	33, 89, 155, 198	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	220	HIS	6.7
1	C	111	LEU	6.6
1	C	220	HIS	6.5
1	B	220	HIS	6.0
1	C	221	PRO	5.2
1	B	221	PRO	5.0
1	A	175	SER	4.8
1	A	171	LEU	4.2
1	A	251	PRO	4.1
1	C	117	THR	4.1
1	A	221	PRO	3.4
1	C	257	VAL	3.3
1	B	249	ASP	3.2
1	A	176	LEU	3.1
1	A	144	GLU	3.1
1	B	76	GLY	3.0
1	C	6	TRP	3.0
1	C	169	CYS	3.0
1	A	79	HIS	2.9
1	C	148	ILE	2.9
1	C	56	GLU	2.7
1	C	102	LYS	2.7
1	B	253	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	118	PRO	2.6
1	A	138	PHE	2.6
1	A	177	PHE	2.6
1	C	145	ARG	2.5
1	C	254	TYR	2.5
1	C	112	THR	2.5
1	B	77	ASP	2.5
1	C	167	LEU	2.4
1	B	144	GLU	2.4
1	B	170	HIS	2.4
1	B	102	LYS	2.4
1	A	222	ASP	2.4
1	C	75	SER	2.3
1	C	156	LEU	2.3
1	C	163	ILE	2.3
1	C	192	ILE	2.3
1	C	209	LEU	2.2
1	C	273	GLN	2.2
1	C	76	GLY	2.2
1	A	168	HIS	2.2
1	C	181	THR	2.2
1	C	115	PRO	2.2
1	A	4	MET	2.2
1	C	149	TYR	2.1
1	A	273	GLN	2.1
1	A	76	GLY	2.1
1	B	250	ILE	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 oligosaccharides in this entry.

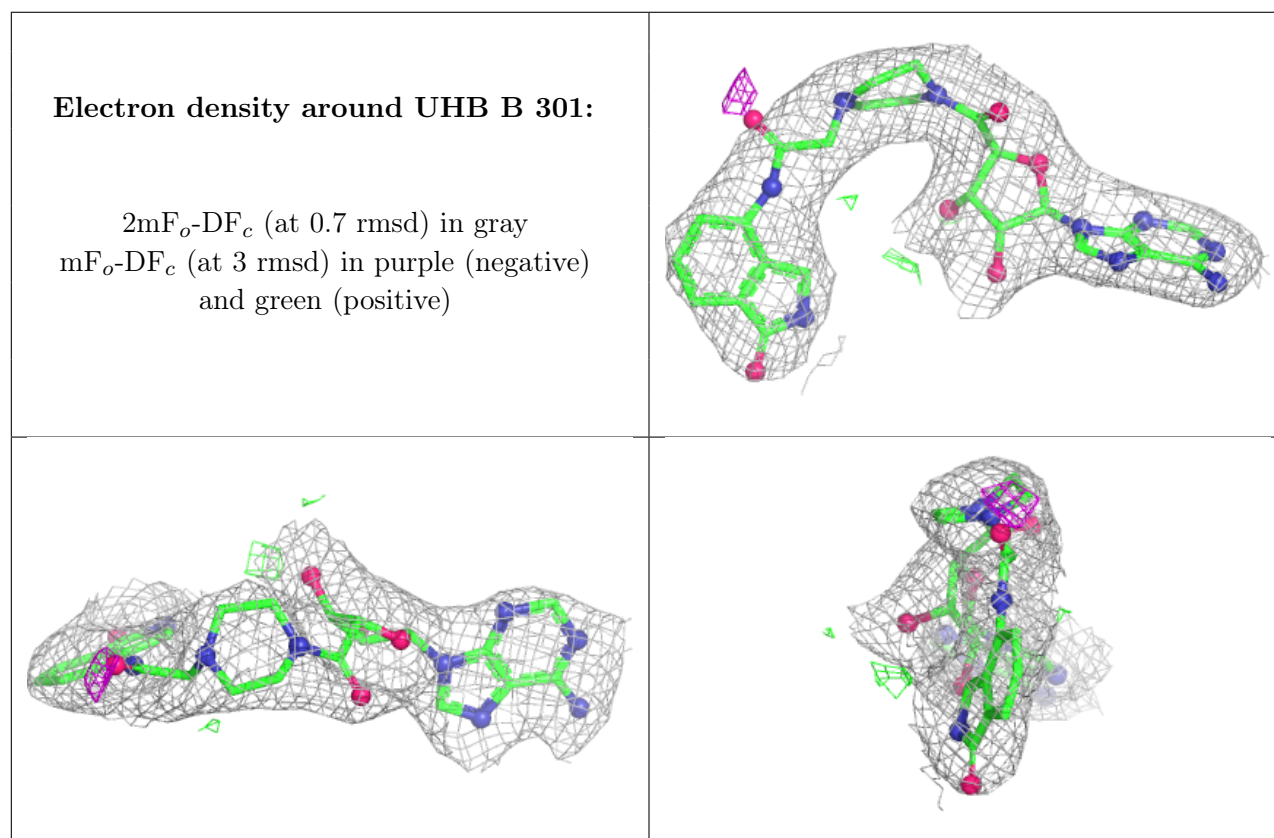
6.4 Ligands [i](#)

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.

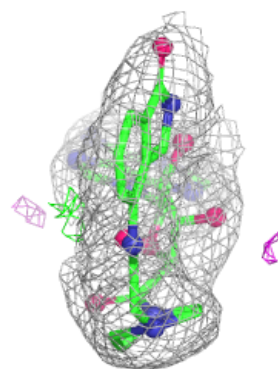
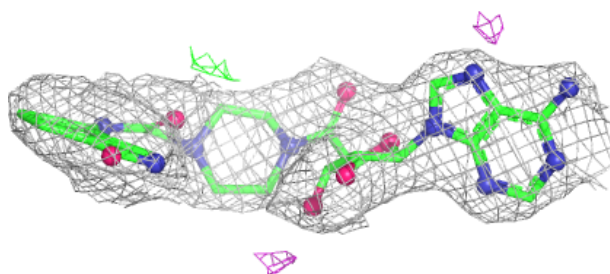
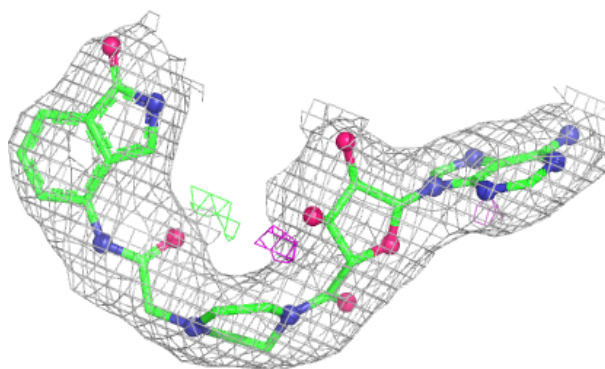
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	UHB	B	301	39/39	0.92	0.09	64,75,88,95	0
2	UHB	A	301	39/39	0.94	0.07	52,62,73,73	0

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 UHB A 301:

$2mF_o-DF_c$ (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.