



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 28, 2020 – 06:15 PM EDT

PDB ID : 6W65
Title : Human PARP16 in complex with RBN010860
Authors : Swinger, K.K.; Wigle, T.J.; Kuntz, K.W.
Deposited on : 2020-03-16
Resolution : 2.13 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 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 : 2.14.6
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) : 2.14.6

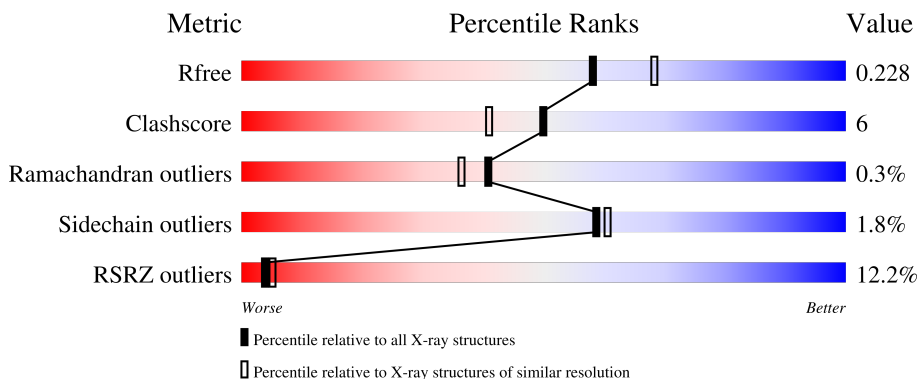
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.13 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2523 (2.16-2.12)
Clashscore	141614	2653 (2.16-2.12)
Ramachandran outliers	138981	2618 (2.16-2.12)
Sidechain outliers	138945	2617 (2.16-2.12)
RSRZ outliers	127900	2485 (2.16-2.12)

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 ≥ 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	277	
1	B	277	
1	C	277	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	B	303	-	-	X	-
6	PEG	C	303	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6183 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.

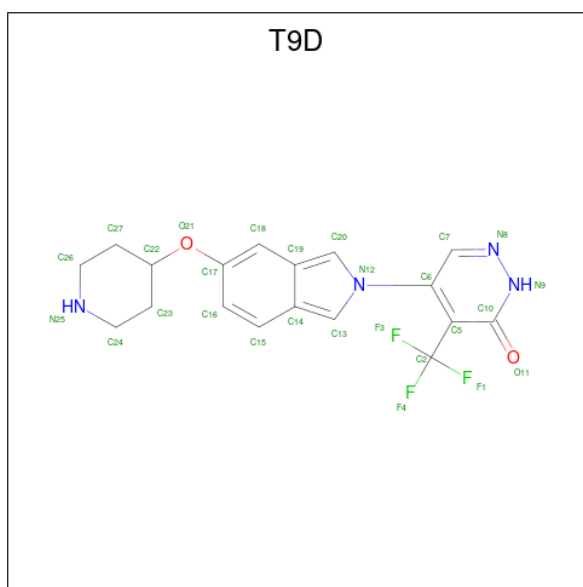
- Molecule 1 is a protein called Protein mono-ADP-ribosyltransferase PARP16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	243	Total	C	N	O	S	0	4	0
			1946	1256	334	349	7			
1	B	234	Total	C	N	O	S	0	4	0
			1872	1205	320	339	8			
1	C	237	Total	C	N	O	S	0	2	0
			1889	1218	323	340	8			

There are 6 discrepancies between the modelled and reference sequences:

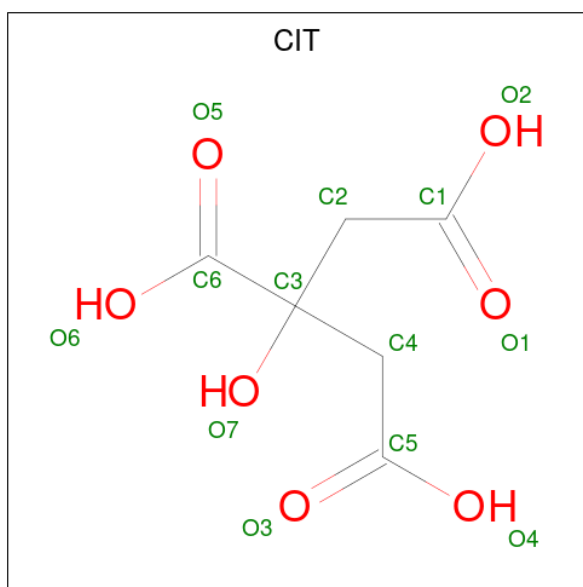
Chain	Residue	Modelled	Actual	Comment	Reference
A	3	SER	-	expression tag	UNP Q8N5Y8
A	4	MET	-	expression tag	UNP Q8N5Y8
B	3	SER	-	expression tag	UNP Q8N5Y8
B	4	MET	-	expression tag	UNP Q8N5Y8
C	3	SER	-	expression tag	UNP Q8N5Y8
C	4	MET	-	expression tag	UNP Q8N5Y8

- Molecule 2 is 5-{5-[(piperidin-4-yl)oxy]-2H-isoindol-2-yl}-4-(trifluoromethyl)pyridazin-3(2H)-one (three-letter code: T9D) (formula: C₁₈H₁₇F₃N₄O₂) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	A	1	Total	C	F	N	O	0	0
			27	18	3	4	2		
2	B	1	Total	C	F	N	O	0	0
			27	18	3	4	2		
2	C	1	Total	C	F	N	O	0	0
			27	18	3	4	2		

- Molecule 3 is CITRIC ACID (three-letter code: CIT) (formula: C₆H₈O₇).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
3	A	1	Total	C	O	0	0
			13	6	7		

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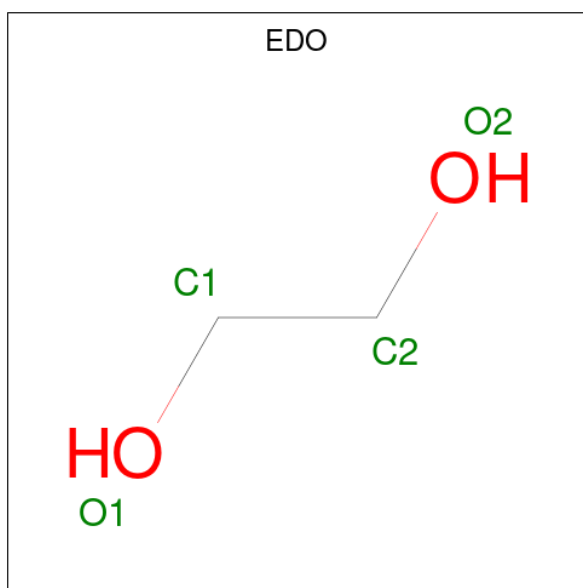
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	B	1	13	6	7	0	0

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



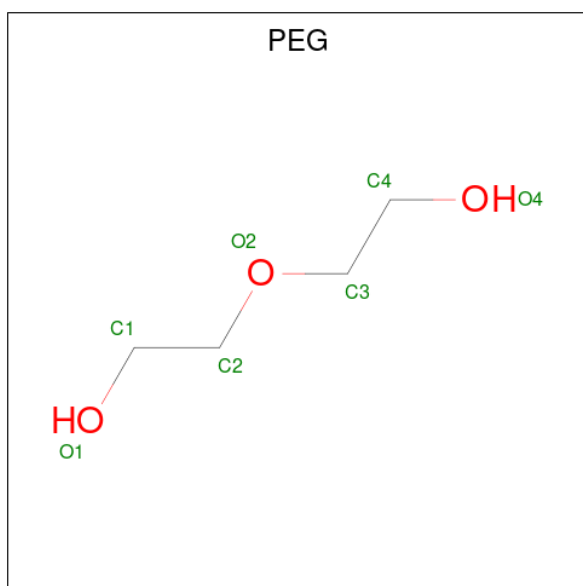
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	6	3	3	0	0
4	A	1	6	3	3	0	0
4	A	1	6	3	3	0	0
4	A	1	6	3	3	0	0
4	B	1	6	3	3	0	0
4	B	1	6	3	3	0	0
4	B	1	6	3	3	0	0
4	B	1	6	3	3	0	0
4	B	1	6	3	3	0	0
4	C	1	6	3	3	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			7	4	3		
6	C	1	Total	C	O	0	0
			7	4	3		

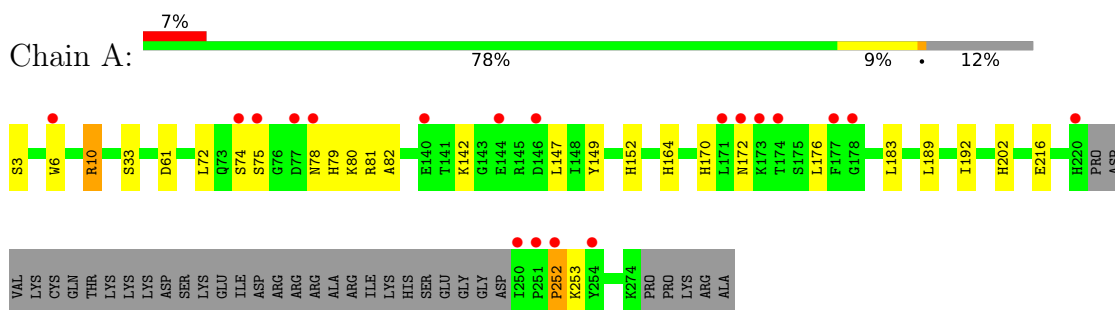
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	124	Total	O	0	0
			124	124		
7	B	80	Total	O	0	0
			80	80		
7	C	75	Total	O	0	0
			75	75		

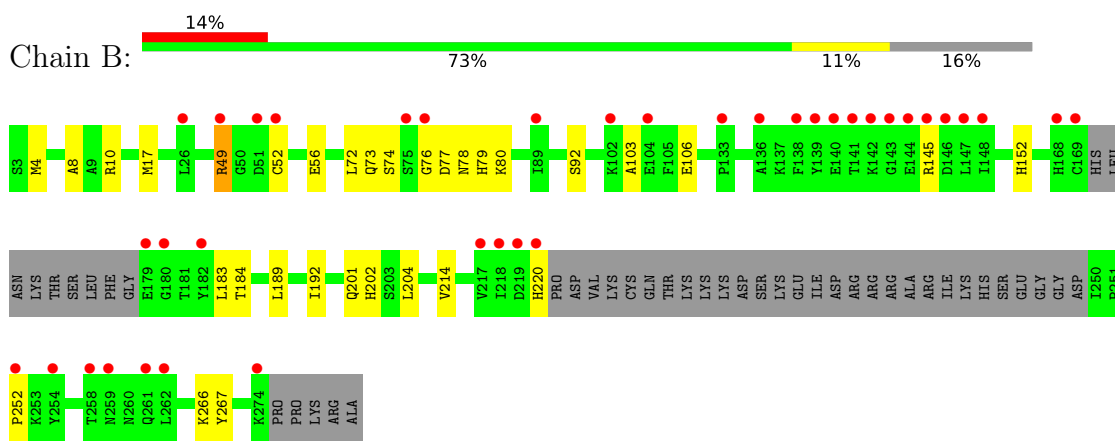
3 Residue-property plots [i](#)

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.

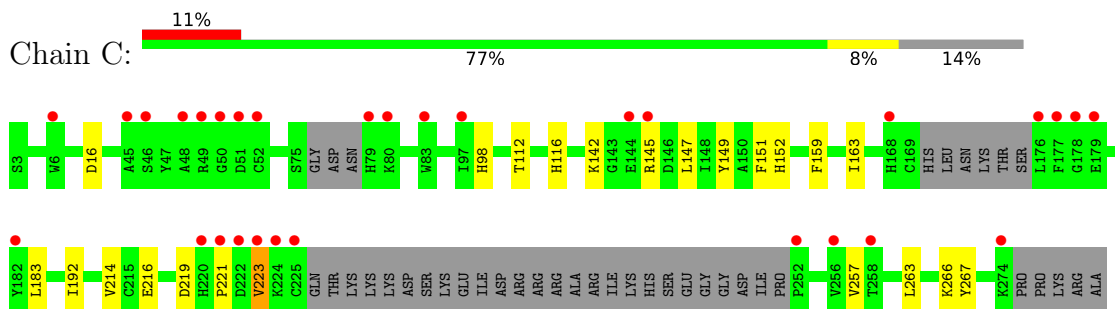
- Molecule 1: Protein mono-ADP-ribosyltransferase PARP16



- Molecule 1: Protein mono-ADP-ribosyltransferase PARP16



- Molecule 1: Protein mono-ADP-ribosyltransferase PARP16



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	147.12Å 147.12Å 99.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.78 – 2.13 37.75 – 2.13	Depositor EDS
% Data completeness (in resolution range)	99.9 (37.78-2.13) 99.9 (37.75-2.13)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 2.14Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.190 , 0.225 0.197 , 0.228	Depositor DCC
R_{free} test set	3047 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	46.0	Xtrriage
Anisotropy	0.026	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 44.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6183	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: T9D, GOL, PEG, EDO, CIT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.71	0/2005	0.83	0/2719
1	B	0.70	0/1927	0.83	0/2611
1	C	0.71	0/1938	0.83	0/2623
All	All	0.71	0/5870	0.83	0/7953

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	74	SER	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1946	0	1930	21	0
1	B	1872	0	1850	34	0
1	C	1889	0	1866	17	0
2	A	27	0	0	0	0
2	B	27	0	0	1	0
2	C	27	0	0	0	0
3	A	13	0	5	0	0
3	B	13	0	5	1	0
4	A	24	0	32	1	0
4	B	30	0	40	13	0
4	C	6	0	8	0	0
5	A	4	0	6	1	0
5	B	8	0	12	1	0
5	C	4	0	6	0	0
6	B	7	0	10	0	0
6	C	7	0	10	5	0
7	A	124	0	0	1	0
7	B	80	0	0	1	0
7	C	75	0	0	2	0
All	All	6183	0	5780	68	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 6.

All (68) 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:B:77:ASP:HA	4:B:303:GOL:C3	1.82	1.08
1:B:77:ASP:HA	4:B:303:GOL:H31	1.48	0.93
1:A:33:SER:HA	4:A:304:GOL:H32	1.54	0.86
1:C:98:HIS:ND1	6:C:303:PEG:H42	1.94	0.83
1:B:77:ASP:HA	4:B:303:GOL:H32	1.58	0.83
1:B:77:ASP:CA	4:B:303:GOL:H31	2.10	0.80
1:B:80:LYS:N	4:B:307:GOL:H2	2.06	0.71
1:A:75:SER:HB3	1:A:79:HIS:ND1	2.07	0.69
1:A:252:PRO:HD2	1:B:192[B]:ILE:HG23	1.73	0.69
1:B:77:ASP:C	4:B:303:GOL:H31	2.12	0.69
1:A:252:PRO:CD	1:B:192[B]:ILE:HG23	2.24	0.68
1:C:116:HIS:HE1	7:C:465:HOH:O	1.78	0.65
1:A:202:HIS:ND1	5:A:307:EDO:O1	2.25	0.64
3:B:302:CIT:O7	3:B:302:CIT:O2	2.14	0.64
1:B:77:ASP:CA	4:B:303:GOL:C3	2.66	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192[A]:ILE:HG23	1:B:252:PRO:HD2	1.79	0.63
1:A:189:LEU:O	1:A:192[B]:ILE:HG12	2.00	0.62
1:B:189:LEU:O	1:B:192[A]:ILE:HG12	2.00	0.61
1:B:49:ARG:O	1:B:49:ARG:HG3	2.03	0.59
1:B:78:ASN:O	4:B:307:GOL:H11	2.04	0.58
1:B:92:SER:N	4:B:304:GOL:H12	2.18	0.58
1:A:75:SER:CB	1:A:79:HIS:ND1	2.66	0.57
1:A:6:TRP:CH2	1:A:80:LYS:HG2	2.39	0.57
1:C:192:ILE:HD11	7:C:442:HOH:O	2.04	0.57
1:C:16:ASP:OD2	6:C:303:PEG:H41	2.05	0.56
1:B:76:GLY:O	4:B:303:GOL:H2	2.05	0.56
1:C:98:HIS:ND1	6:C:303:PEG:C4	2.67	0.56
1:A:6:TRP:HH2	1:A:80:LYS:HG2	1.72	0.54
1:A:192[A]:ILE:HG23	1:B:252:PRO:CD	2.37	0.54
1:B:78:ASN:N	4:B:303:GOL:H31	2.25	0.52
1:C:145:ARG:HG2	1:C:219:ASP:O	2.10	0.52
1:C:257:VAL:HG11	1:C:263:LEU:HD23	1.93	0.51
1:B:103:ALA:O	1:B:106:GLU:HG2	2.11	0.50
1:B:56:GLU:H	1:B:56:GLU:CD	2.16	0.49
1:C:112:THR:HG21	1:C:151:PHE:CZ	2.47	0.49
1:A:10:ARG:NH2	1:A:75:SER:O	2.33	0.48
1:C:152:HIS:HB2	1:C:183:LEU:HD23	1.97	0.47
1:C:98:HIS:HA	6:C:303:PEG:C4	2.45	0.47
1:B:10:ARG:HH21	5:B:310:EDO:H21	1.81	0.46
1:C:159:PHE:O	1:C:163[B]:ILE:HG23	2.16	0.46
1:B:214:VAL:HB	1:B:267:TYR:HB2	1.98	0.45
1:C:142:LYS:HE2	1:C:147:LEU:HG	1.99	0.45
1:A:252:PRO:HD3	1:B:192[B]:ILE:HG23	1.97	0.45
1:A:149:TYR:CE2	1:A:216:GLU:HG3	2.53	0.44
1:B:4:MET:CG	1:B:8:ALA:HB3	2.48	0.44
1:B:266:LYS:HD2	1:B:266:LYS:HA	1.87	0.43
1:B:80:LYS:H	4:B:307:GOL:H2	1.83	0.43
1:B:4:MET:HG3	1:B:8:ALA:HB3	2.00	0.43
1:A:152:HIS:HB2	1:A:183:LEU:HD23	2.00	0.43
1:B:152:HIS:HB2	1:B:183:LEU:HD23	2.00	0.43
1:C:98:HIS:HA	6:C:303:PEG:H42	2.01	0.43
1:C:223:VAL:HB	1:C:257:VAL:HG22	2.00	0.43
1:A:142:LYS:HE2	1:A:147:LEU:HG	2.01	0.42
1:A:164:HIS:HD2	7:A:412:HOH:O	2.01	0.42
1:A:10:ARG:NH2	1:A:72:LEU:O	2.53	0.42
1:A:79:HIS:HB3	1:A:82:ALA:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:ASP:OD2	1:A:81:ARG:HD3	2.20	0.42
1:B:17[B]:MET:HE1	1:B:72:LEU:HD22	2.02	0.42
1:B:17[B]:MET:HG2	1:B:204:LEU:CD1	2.50	0.42
1:C:214:VAL:HB	1:C:267:TYR:HB2	2.02	0.41
1:B:184:THR:HG22	2:B:301:T9D:F3	2.10	0.41
1:C:149:TYR:CE2	1:C:216:GLU:HG2	2.55	0.41
1:B:79:HIS:HD2	7:B:429:HOH:O	2.03	0.41
1:B:77:ASP:CA	4:B:303:GOL:H32	2.39	0.41
1:B:201[B]:GLN:HG3	1:B:202:HIS:CD2	2.56	0.40
1:C:266:LYS:HA	1:C:266:LYS:HD2	1.88	0.40
1:A:176:LEU:HD12	1:A:176:LEU:HA	1.95	0.40
1:B:145:ARG:NH1	1:B:220:HIS:ND1	2.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	243/277 (88%)	234 (96%)	7 (3%)	2 (1%)	19	11
1	B	232/277 (84%)	230 (99%)	2 (1%)	0	100	100
1	C	231/277 (83%)	227 (98%)	4 (2%)	0	100	100
All	All	706/831 (85%)	691 (98%)	13 (2%)	2 (0%)	41	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	170	HIS
1	A	252	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	A	209/235 (89%)	204 (98%)	5 (2%)	49	49
1	B	201/235 (86%)	197 (98%)	4 (2%)	55	57
1	C	202/235 (86%)	200 (99%)	2 (1%)	76	79
All	All	612/705 (87%)	601 (98%)	11 (2%)	59	60

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	10	ARG
1	A	78	ASN
1	A	172	ASN
1	A	253	LYS
1	B	49	ARG
1	B	52	CYS
1	B	73	GLN
1	B	74	SER
1	C	221	PRO
1	C	223	VAL

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

Mol	Chain	Res	Type
1	B	73	GLN
1	B	196	HIS
1	C	73	GLN
1	C	164	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

21 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	T9D	B	301	-	30,30,30	3.33	8 (26%)	30,44,44	1.86	6 (20%)
2	T9D	A	301	-	30,30,30	3.54	9 (30%)	30,44,44	1.92	7 (23%)
4	GOL	B	303	-	5,5,5	0.35	0	5,5,5	0.94	0
6	PEG	C	303	-	6,6,6	0.25	0	5,5,5	0.20	0
5	EDO	A	307	-	3,3,3	0.47	0	2,2,2	0.57	0
4	GOL	B	307	-	5,5,5	0.27	0	5,5,5	0.74	0
6	PEG	B	308	-	6,6,6	0.47	0	5,5,5	0.30	0
4	GOL	B	305	-	5,5,5	0.18	0	5,5,5	0.27	0
4	GOL	B	304	-	5,5,5	0.09	0	5,5,5	0.44	0
3	CIT	A	302	-	3,12,12	0.47	0	3,17,17	0.60	0
4	GOL	A	306	-	5,5,5	0.12	0	5,5,5	0.32	0
5	EDO	C	304	-	3,3,3	0.11	0	2,2,2	0.22	0
4	GOL	C	302	-	5,5,5	0.22	0	5,5,5	0.42	0
5	EDO	B	309	-	3,3,3	0.54	0	2,2,2	0.46	0
5	EDO	B	310	-	3,3,3	0.47	0	2,2,2	0.40	0
4	GOL	A	305	-	5,5,5	0.16	0	5,5,5	0.46	0
3	CIT	B	302	-	3,12,12	0.34	0	3,17,17	1.57	1 (33%)
4	GOL	A	304	-	5,5,5	0.17	0	5,5,5	0.47	0
4	GOL	B	306	-	5,5,5	0.14	0	5,5,5	0.33	0
4	GOL	A	303	-	5,5,5	0.31	0	5,5,5	0.68	0
2	T9D	C	301	-	30,30,30	3.61	10 (33%)	30,44,44	1.83	6 (20%)

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	T9D	B	301	-	-	6/14/22/22	0/4/4/4
2	T9D	A	301	-	-	4/14/22/22	0/4/4/4
4	GOL	B	303	-	-	0/4/4/4	-
6	PEG	C	303	-	-	4/4/4/4	-
5	EDO	A	307	-	-	1/1/1/1	-
4	GOL	B	307	-	-	2/4/4/4	-
6	PEG	B	308	-	-	1/4/4/4	-
4	GOL	B	305	-	-	0/4/4/4	-
4	GOL	B	304	-	-	2/4/4/4	-
3	CIT	A	302	-	-	6/6/16/16	-
4	GOL	A	306	-	-	2/4/4/4	-
5	EDO	C	304	-	-	1/1/1/1	-
4	GOL	C	302	-	-	3/4/4/4	-
5	EDO	B	309	-	-	1/1/1/1	-
5	EDO	B	310	-	-	1/1/1/1	-
4	GOL	A	305	-	-	2/4/4/4	-
3	CIT	B	302	-	-	6/6/16/16	-
4	GOL	A	304	-	-	4/4/4/4	-
4	GOL	B	306	-	-	2/4/4/4	-
4	GOL	A	303	-	-	0/4/4/4	-
2	T9D	C	301	-	-	4/14/22/22	0/4/4/4

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	T9D	C19-C14	-10.56	1.38	1.49
2	A	301	T9D	C13-N12	9.70	1.50	1.39
2	A	301	T9D	C19-C14	-9.52	1.39	1.49
2	B	301	T9D	C19-C14	-9.29	1.39	1.49
2	C	301	T9D	C13-N12	8.68	1.49	1.39
2	B	301	T9D	C13-N12	8.30	1.48	1.39
2	B	301	T9D	C20-N12	7.85	1.48	1.39
2	C	301	T9D	C20-N12	7.04	1.47	1.39
2	A	301	T9D	C6-N12	-6.90	1.37	1.45
2	A	301	T9D	C20-N12	6.46	1.46	1.39
2	A	301	T9D	C20-C19	6.10	1.53	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	T9D	C6-N12	-6.10	1.38	1.45
2	C	301	T9D	N8-N9	5.70	1.42	1.35
2	B	301	T9D	C13-C14	5.67	1.52	1.40
2	C	301	T9D	C13-C14	5.50	1.52	1.40
2	B	301	T9D	C20-C19	5.33	1.52	1.40
2	A	301	T9D	C13-C14	4.30	1.49	1.40
2	B	301	T9D	C6-N12	-4.29	1.40	1.45
2	A	301	T9D	N8-N9	4.27	1.40	1.35
2	C	301	T9D	C20-C19	4.12	1.49	1.40
2	B	301	T9D	N8-N9	2.75	1.38	1.35
2	A	301	T9D	C7-C6	2.61	1.44	1.39
2	C	301	T9D	C6-C5	2.17	1.43	1.40
2	C	301	T9D	C7-C6	2.16	1.43	1.39
2	C	301	T9D	C18-C19	-2.13	1.37	1.42
2	B	301	T9D	C18-C17	2.12	1.40	1.37
2	A	301	T9D	C2-C5	2.09	1.56	1.51

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	T9D	C17-O21-C22	5.72	130.62	119.13
2	B	301	T9D	F4-C2-C5	-5.70	98.83	112.34
2	B	301	T9D	C5-C6-N12	4.87	127.75	119.93
2	C	301	T9D	C5-C6-N12	4.31	126.85	119.93
2	C	301	T9D	F3-C2-C5	-4.25	102.26	112.34
2	C	301	T9D	C20-C19-C18	-3.48	127.91	134.80
2	A	301	T9D	C5-C6-N12	3.37	125.35	119.93
2	A	301	T9D	F4-C2-C5	-3.01	105.21	112.34
2	B	301	T9D	F1-C2-C5	2.90	119.22	112.34
2	A	301	T9D	C5-C10-N9	-2.89	121.60	124.26
2	C	301	T9D	C16-C17-C18	-2.88	116.94	120.81
2	A	301	T9D	C10-N9-N8	2.70	123.25	118.97
2	C	301	T9D	C20-C19-C14	2.57	110.17	104.73
2	B	301	T9D	C27-C22-C23	-2.45	107.01	111.74
2	A	301	T9D	F1-C2-C5	2.38	117.99	112.34
2	B	301	T9D	C17-O21-C22	2.27	123.68	119.13
2	C	301	T9D	C27-C22-C23	-2.26	107.39	111.74
2	B	301	T9D	C5-C10-N9	-2.24	122.20	124.26
2	A	301	T9D	C20-C19-C14	2.23	109.43	104.73
3	B	302	CIT	C3-C4-C5	2.01	118.20	114.98

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	T9D	C5-C6-N12-C13
2	B	301	T9D	C5-C6-N12-C20
2	A	301	T9D	C5-C6-N12-C13
2	A	301	T9D	C5-C6-N12-C20
4	B	307	GOL	C1-C2-C3-O3
4	B	307	GOL	O2-C2-C3-O3
4	C	302	GOL	C1-C2-C3-O3
4	C	302	GOL	O2-C2-C3-O3
4	B	304	GOL	O1-C1-C2-C3
3	A	302	CIT	C1-C2-C3-C4
3	A	302	CIT	C1-C2-C3-C6
3	A	302	CIT	C6-C3-C4-C5
4	A	306	GOL	O1-C1-C2-C3
4	A	305	GOL	C1-C2-C3-O3
3	B	302	CIT	C1-C2-C3-O7
3	B	302	CIT	C1-C2-C3-C4
3	B	302	CIT	C1-C2-C3-C6
3	B	302	CIT	C2-C3-C4-C5
3	B	302	CIT	O7-C3-C4-C5
3	B	302	CIT	C6-C3-C4-C5
4	A	304	GOL	O1-C1-C2-C3
4	A	304	GOL	C1-C2-C3-O3
2	C	301	T9D	C5-C6-N12-C13
2	C	301	T9D	C5-C6-N12-C20
3	A	302	CIT	O7-C3-C4-C5
2	B	301	T9D	C16-C17-O21-C22
4	B	304	GOL	O1-C1-C2-O2
4	A	305	GOL	O2-C2-C3-O3
6	B	308	PEG	O2-C3-C4-O4
6	C	303	PEG	O1-C1-C2-O2
4	B	306	GOL	C1-C2-C3-O3
4	A	304	GOL	O1-C1-C2-O2
4	A	304	GOL	O2-C2-C3-O3
4	B	306	GOL	O2-C2-C3-O3
2	B	301	T9D	C18-C17-O21-C22
5	A	307	EDO	O1-C1-C2-O2
5	C	304	EDO	O1-C1-C2-O2
5	B	310	EDO	O1-C1-C2-O2
3	A	302	CIT	C1-C2-C3-O7
3	A	302	CIT	C2-C3-C4-C5
2	B	301	T9D	C23-C22-O21-C17
2	B	301	T9D	C27-C22-O21-C17

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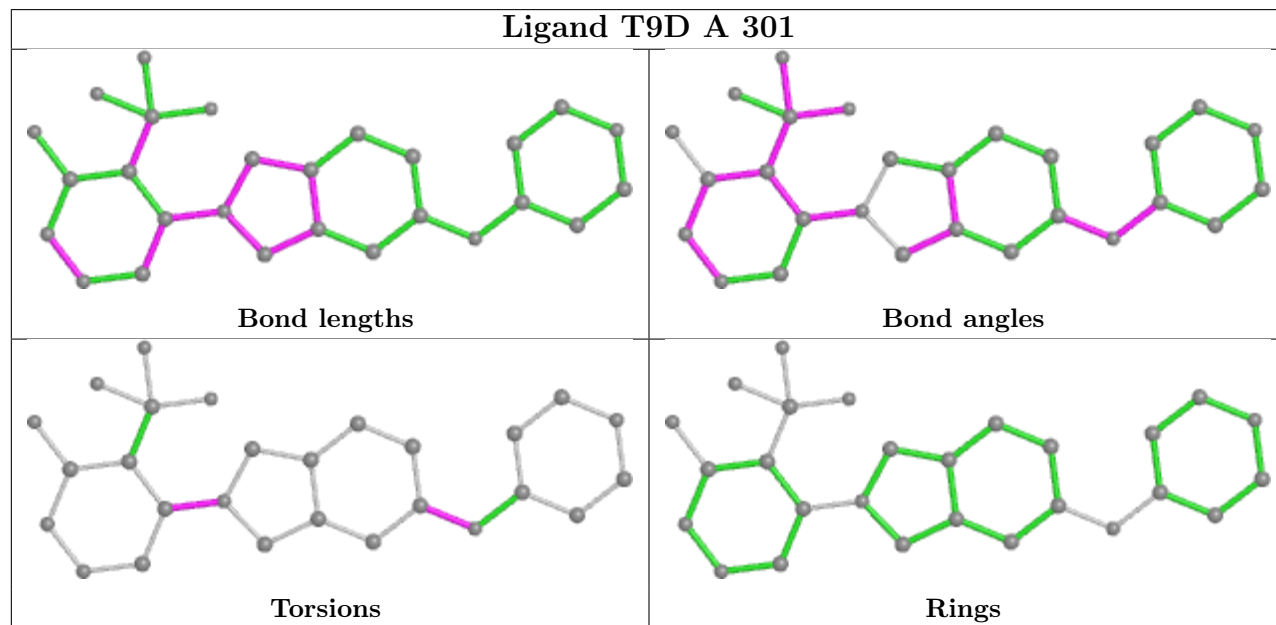
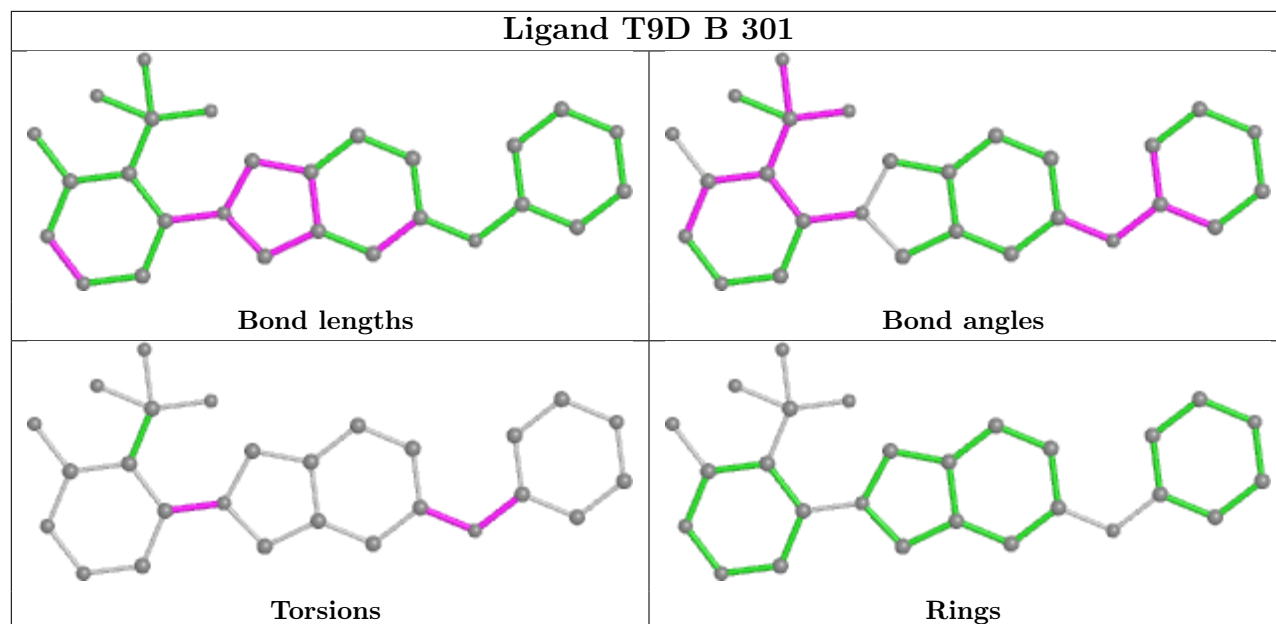
Mol	Chain	Res	Type	Atoms
2	A	301	T9D	C16-C17-O21-C22
4	A	306	GOL	O1-C1-C2-O2
2	A	301	T9D	C18-C17-O21-C22
6	C	303	PEG	C4-C3-O2-C2
6	C	303	PEG	O2-C3-C4-O4
2	C	301	T9D	C16-C17-O21-C22
2	C	301	T9D	C18-C17-O21-C22
5	B	309	EDO	O1-C1-C2-O2
6	C	303	PEG	C1-C2-O2-C3
4	C	302	GOL	O1-C1-C2-C3

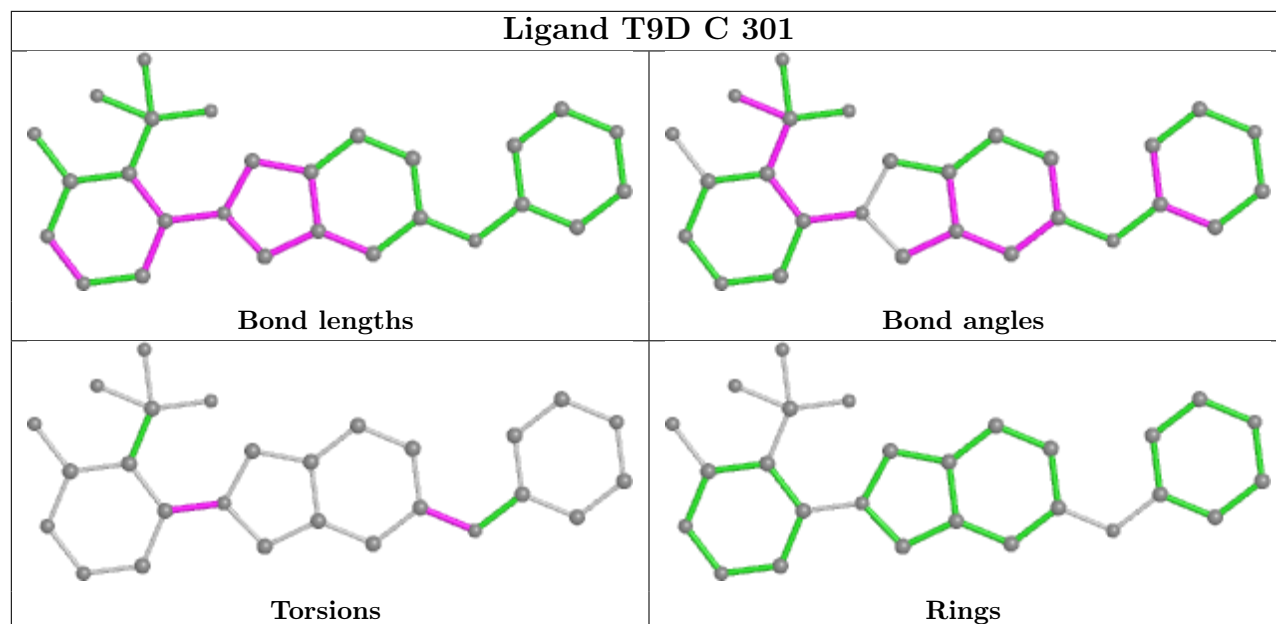
There are no ring outliers.

9 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	T9D	1	0
4	B	303	GOL	9	0
6	C	303	PEG	5	0
5	A	307	EDO	1	0
4	B	307	GOL	3	0
4	B	304	GOL	1	0
5	B	310	EDO	1	0
3	B	302	CIT	1	0
4	A	304	GOL	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

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	243/277 (87%)	0.42	19 (7%) 13 16	29, 46, 104, 131	0
1	B	234/277 (84%)	0.75	38 (16%) 1 2	33, 51, 122, 146	0
1	C	237/277 (85%)	0.53	30 (12%) 3 4	39, 56, 103, 130	0
All	All	714/831 (85%)	0.56	87 (12%) 4 5	29, 52, 110, 146	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	171	LEU	8.2
1	C	177	PHE	7.9
1	B	139	TYR	6.7
1	B	144	GLU	6.6
1	A	173	LYS	6.2
1	B	169	CYS	6.0
1	C	225	CYS	5.2
1	B	143	GLY	5.1
1	A	174	THR	5.0
1	B	218	ILE	4.9
1	A	77	ASP	4.7
1	B	146	ASP	4.6
1	A	220	HIS	4.6
1	A	74	SER	4.4
1	C	223	VAL	4.4
1	B	140	GLU	4.3
1	C	221	PRO	4.3
1	B	51	ASP	4.2
1	A	252	PRO	4.2
1	A	6	TRP	4.2
1	C	176	LEU	4.2
1	B	168	HIS	4.1
1	B	220	HIS	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	261	GLN	4.0
1	C	220	HIS	3.9
1	B	142	LYS	3.9
1	B	262	LEU	3.8
1	B	145	ARG	3.7
1	C	274	LYS	3.4
1	B	76	GLY	3.4
1	C	224	LYS	3.4
1	C	46	SER	3.3
1	C	145	ARG	3.3
1	A	251	PRO	3.3
1	C	6	TRP	3.2
1	B	274	LYS	3.2
1	B	219	ASP	3.2
1	C	179	GLU	3.2
1	B	49	ARG	3.2
1	B	258	THR	3.2
1	C	258	THR	3.2
1	B	254	TYR	3.1
1	B	179	GLU	3.0
1	C	178	GLY	3.0
1	A	177	PHE	3.0
1	A	75	SER	3.0
1	B	141	THR	3.0
1	B	133	PRO	3.0
1	B	75	SER	2.9
1	C	80	LYS	2.9
1	B	147	LEU	2.9
1	B	148	ILE	2.8
1	B	102	LYS	2.8
1	A	78	ASN	2.8
1	B	26	LEU	2.7
1	B	52	CYS	2.7
1	C	144	GLU	2.7
1	B	180	GLY	2.7
1	C	51	ASP	2.6
1	A	254	TYR	2.6
1	A	178	GLY	2.6
1	C	50	GLY	2.6
1	A	172	ASN	2.6
1	C	168	HIS	2.6
1	C	256	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	182	TYR	2.5
1	B	259	ASN	2.4
1	C	222	ASP	2.3
1	B	104	GLU	2.3
1	A	250	ILE	2.3
1	B	252	PRO	2.3
1	C	252	PRO	2.2
1	C	97	ILE	2.2
1	A	146	ASP	2.2
1	A	140	GLU	2.2
1	A	144	GLU	2.2
1	C	79	HIS	2.2
1	B	217	VAL	2.2
1	C	49	ARG	2.2
1	B	138	PHE	2.1
1	B	136	ALA	2.1
1	B	89	ILE	2.1
1	C	52	CYS	2.1
1	B	182	TYR	2.0
1	C	83	TRP	2.0
1	C	48	ALA	2.0
1	C	45	ALA	2.0

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

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

6.3 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

6.4 Ligands [\(i\)](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
5	EDO	A	307	4/4	0.66	0.17	60,73,74,78	0

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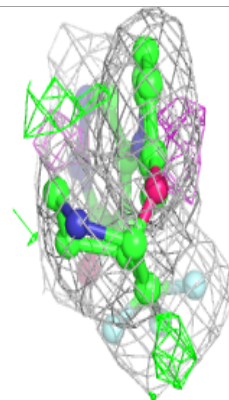
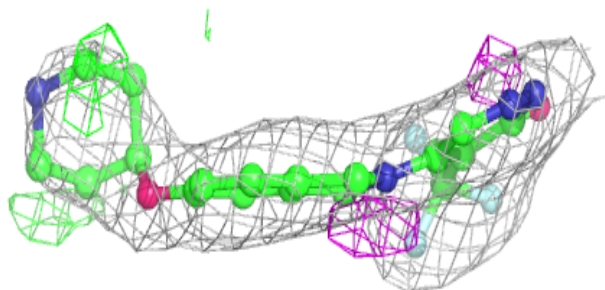
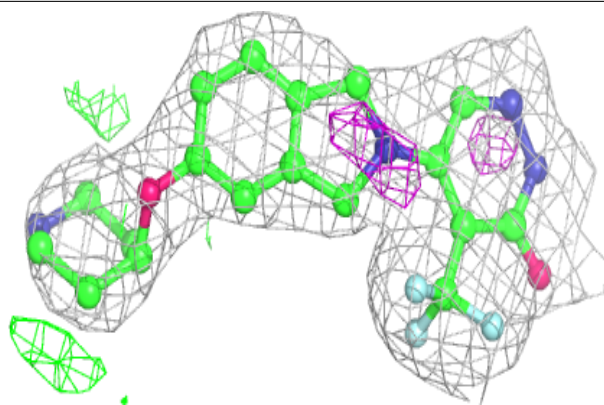
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	PEG	B	308	7/7	0.73	0.16	71,80,82,83	0
5	EDO	B	309	4/4	0.77	0.16	59,69,71,76	0
4	GOL	B	303	6/6	0.77	0.22	53,67,73,75	0
4	GOL	A	304	6/6	0.77	0.23	53,59,69,78	0
3	CIT	B	302	13/13	0.80	0.22	67,91,99,100	0
4	GOL	A	305	6/6	0.81	0.14	73,84,90,91	0
5	EDO	C	304	4/4	0.81	0.16	88,90,90,94	0
4	GOL	C	302	6/6	0.85	0.19	70,72,78,82	0
4	GOL	A	303	6/6	0.86	0.21	59,67,70,71	0
4	GOL	B	306	6/6	0.87	0.09	73,85,85,87	0
4	GOL	B	304	6/6	0.87	0.23	39,59,65,70	0
5	EDO	B	310	4/4	0.89	0.29	57,58,59,74	0
4	GOL	A	306	6/6	0.89	0.15	82,95,96,97	0
6	PEG	C	303	7/7	0.90	0.25	68,69,81,83	0
4	GOL	B	307	6/6	0.91	0.28	42,54,63,67	6
3	CIT	A	302	13/13	0.91	0.12	53,66,89,98	0
2	T9D	C	301	27/27	0.93	0.13	46,70,106,111	0
4	GOL	B	305	6/6	0.94	0.13	58,61,63,67	0
2	T9D	B	301	27/27	0.94	0.17	45,76,139,141	0
2	T9D	A	301	27/27	0.96	0.14	40,52,104,107	0

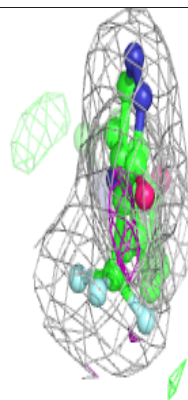
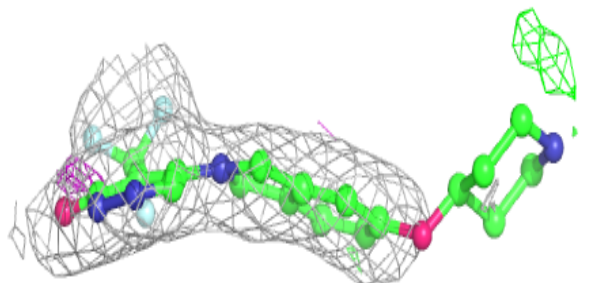
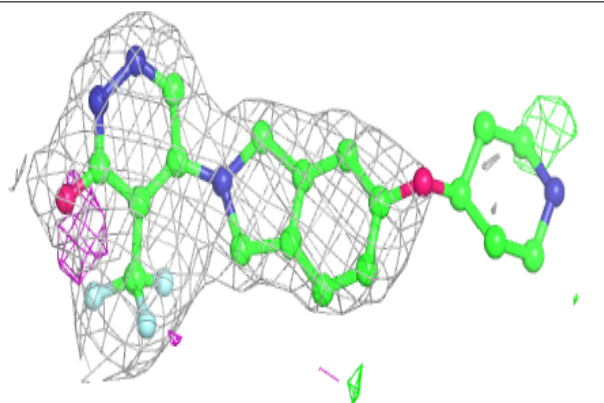
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

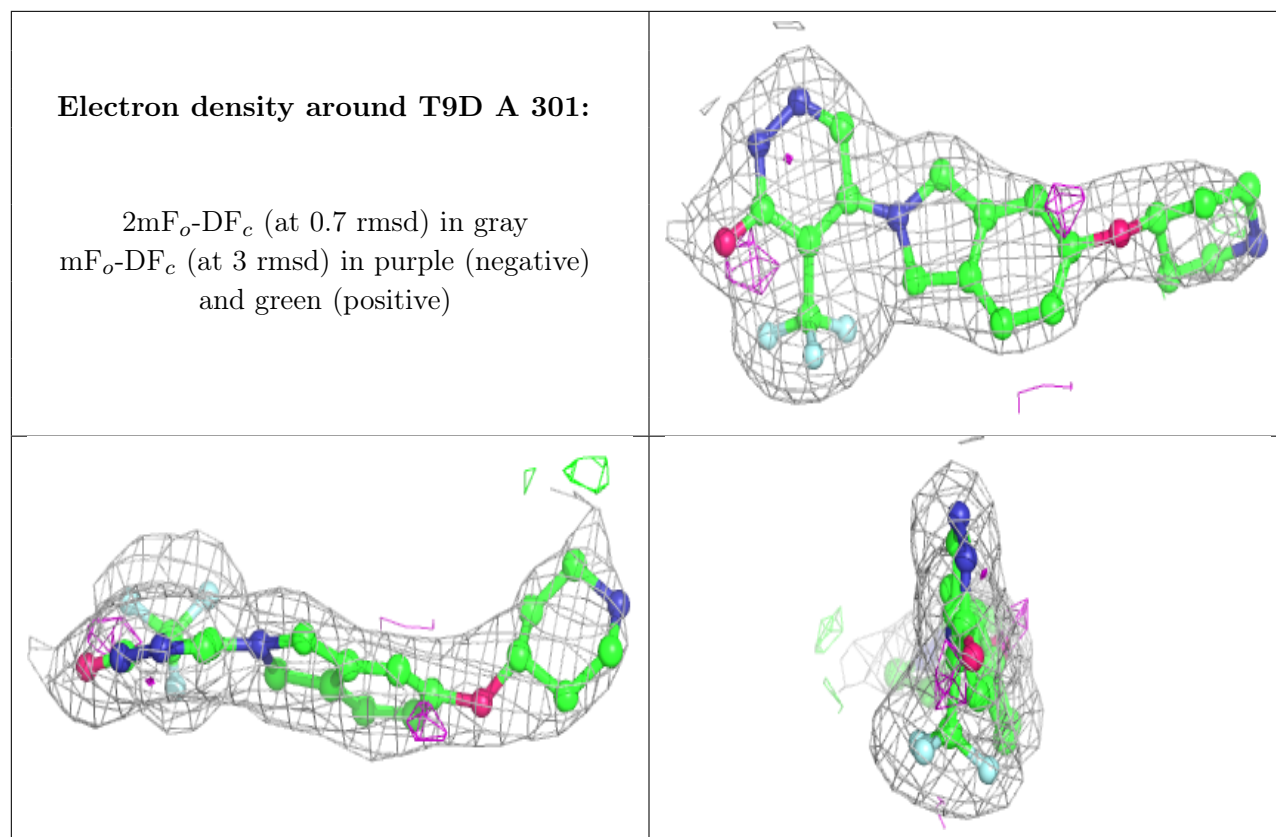
Electron density around T9D C 301:

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

**Electron density around T9D B 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.