



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 03:29 PM UTC

PDB ID : 6W65 / pdb_00006w65
Title : Human PARP16 in complex with RBN010860
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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 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

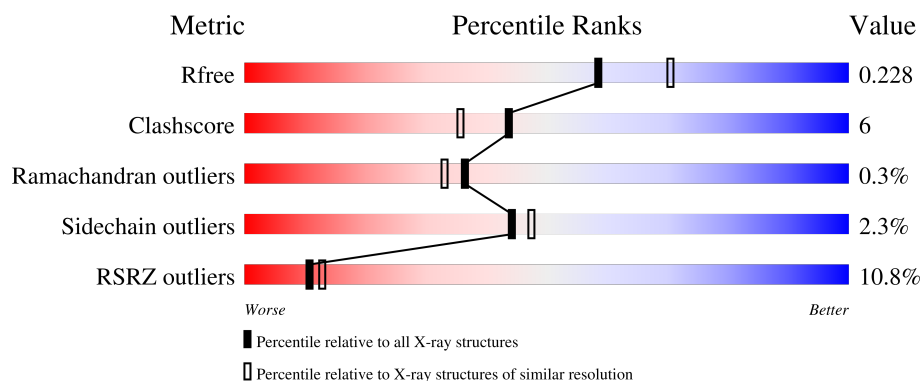
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.13 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}	180053	3689 (2.16-2.12)
Clashscore	190562	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)
RSRZ outliers	180081	3691 (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 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	277	9% 77% 10% 12%
1	B	277	10% 74% 10% 16%
1	C	277	8% 76% 9% 14%

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	-
4	GOL	B	307	-	-	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.

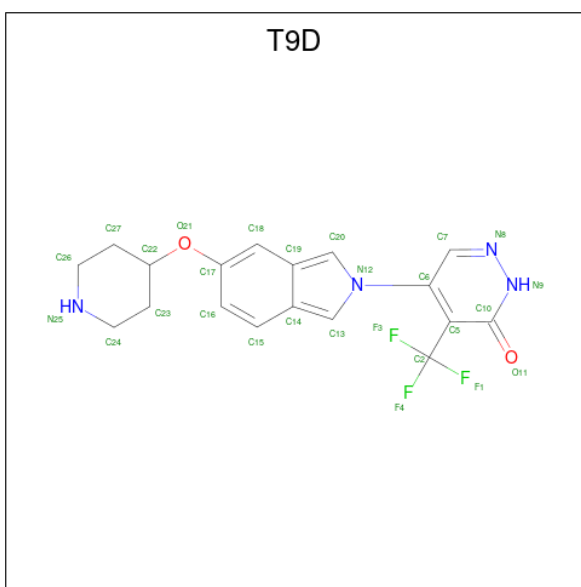
- Molecule 1 is a protein called Protein mono-ADP-ribosyltransferase PARP16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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:

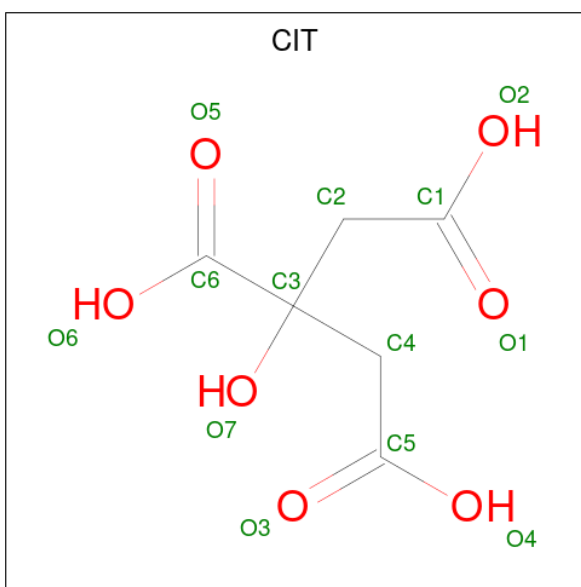
Chain	Residue	Modelled	Actual	Comment	Reference
A	3	SER	-	expression tag	UNP Q8N5Y8
A	4	MET	-	expression tag	UNP Q8N5Y8
B	3	SER	-	expression tag	UNP Q8N5Y8
B	4	MET	-	expression tag	UNP Q8N5Y8
C	3	SER	-	expression tag	UNP Q8N5Y8
C	4	MET	-	expression tag	UNP Q8N5Y8

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



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 (CCD ID: CIT) (formula: $C_6H_8O_7$).



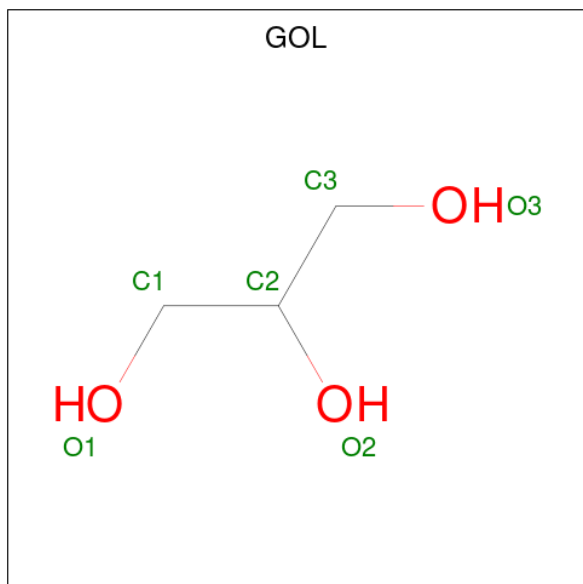
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		

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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



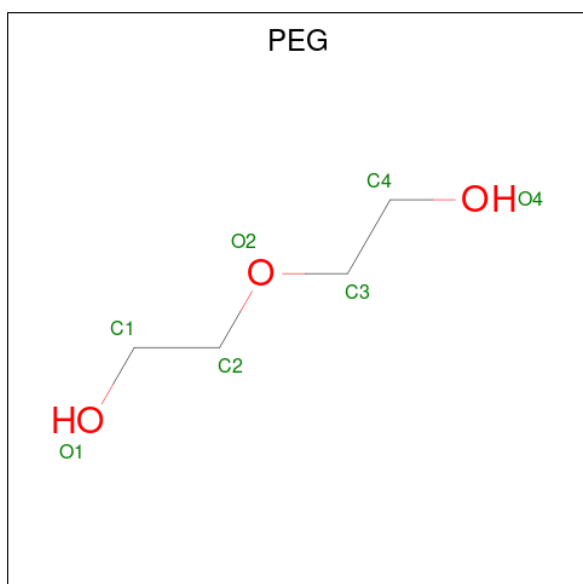
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total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

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: 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		

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 37.78 – 2.13	Depositor EDS
% Data completeness (in resolution range)	99.9 (37.78-2.13) 99.9 (37.78-2.13)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 2.14Å)	Xtriage
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 (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	46.0	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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

5.1 Standard geometry

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

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	1.04	0/2005	1.30	0/2719
1	B	1.04	0/1927	1.30	0/2611
1	C	1.04	0/1938	1.32	3/2623 (0.1%)
All	All	1.04	0/5870	1.31	3/7953 (0.0%)

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

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

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	259	ASN	CA-C-N	7.25	130.97	120.38
1	C	259	ASN	C-N-CA	7.25	130.97	120.38
1	C	178	GLY	CA-C-O	-6.05	117.95	122.37

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 ⓘ

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	36	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	1	0
3	B	13	0	5	1	0
4	A	24	0	32	1	0
4	B	30	0	40	15	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	71	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 (71) 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:77:ASP:C	4:B:303:GOL:H31	2.12	0.74
1:B:80:LYS:N	4:B:307:GOL:H2	2.06	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:252:PRO:CD	1:B:192[B]:ILE:HG23	2.24	0.68
1:A:202:HIS:ND1	5:A:307:EDO:O1	2.25	0.66
1:C:116:HIS:HE1	7:C:465:HOH:O	1.78	0.65
3:B:302:CIT:O2	3:B:302:CIT:O7	2.14	0.64
1:B:77:ASP:CA	4:B:303:GOL:C3	2.66	0.63
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:6:TRP:CH2	1:A:80:LYS:HG2	2.39	0.57
1:A:75:SER:CB	1:A:79:HIS:ND1	2.66	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:56:GLU:H	1:B:56:GLU:CD	2.16	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: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:98:HIS:HA	6:C:303:PEG:C4	2.45	0.47
1:C:152:HIS:HB2	1:C:183:LEU:HD23	1.97	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:4:MET:HG3	1:B:8:ALA:HB3	2.00	0.43
1:B:80:LYS:H	4:B:307:GOL:H2	1.83	0.43
1:B:266:LYS:HD2	1:B:266:LYS:HA	1.87	0.43
3:A:302:CIT:O1	3:A:302:CIT:O7	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:78:ASN:C	4:B:307:GOL:H11	2.44	0.43
1:C:223:VAL:HB	1:C:257:VAL:HG22	2.00	0.43
1:B:77:ASP:C	4:B:303:GOL:C3	2.88	0.42
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
1:A:61:ASP:OD2	1:A:81:ARG:HD3	2.20	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:17[B]:MET:HE3	1:B:17[B]:MET:HB2	1.87	0.40
1:B:201[B]:GLN:HG3	1:B:202:HIS:CD2	2.56	0.40
1:C:266:LYS:HD2	1:C:266:LYS:HA	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 ⓘ

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	243/277 (88%)	234 (96%)	7 (3%)	2 (1%)	16	9
1	B	232/277 (84%)	230 (99%)	2 (1%)	0	100	100
1	C	231/277 (83%)	227 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	706/831 (85%)	691 (98%)	13 (2%)	2 (0%)	36	33

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	170	HIS
1	A	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	209/235 (89%)	203 (97%)	6 (3%)	37	38
1	B	201/235 (86%)	197 (98%)	4 (2%)	48	53
1	C	202/235 (86%)	198 (98%)	4 (2%)	48	53
All	All	612/705 (87%)	598 (98%)	14 (2%)	44	47

All (14) 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	A	274	LYS
1	B	49	ARG
1	B	56	GLU
1	B	74	SER
1	B	274	LYS
1	C	74	SER
1	C	221	PRO
1	C	223	VAL
1	C	263	LEU

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

Mol	Chain	Res	Type
1	A	158	ASN
1	A	168	HIS
1	A	201	GLN
1	B	73	GLN
1	B	78	ASN
1	B	196	HIS
1	C	73	GLN
1	C	164	HIS
1	C	196	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](#)

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	-	25,30,30	2.14	3 (12%)	31,44,44	2.30	11 (35%)
2	T9D	C	301	-	25,30,30	2.21	4 (16%)	31,44,44	2.39	9 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	T9D	A	301	-	25,30,30	2.25	5 (20%)	31,44,44	2.18	10 (32%)
4	GOL	B	305	-	5,5,5	0.19	0	5,5,5	0.28	0
4	GOL	B	306	-	5,5,5	0.14	0	5,5,5	0.32	0
3	CIT	A	302	-	12,12,12	1.08	0	17,17,17	1.30	1 (5%)
4	GOL	A	306	-	5,5,5	0.12	0	5,5,5	0.31	0
5	EDO	B	309	-	3,3,3	0.54	0	2,2,2	0.39	0
4	GOL	B	307	-	5,5,5	0.27	0	5,5,5	0.77	0
3	CIT	B	302	-	12,12,12	1.22	0	17,17,17	1.31	3 (17%)
6	PEG	B	308	-	6,6,6	0.47	0	5,5,5	0.30	0
4	GOL	A	303	-	5,5,5	0.32	0	5,5,5	0.69	0
4	GOL	A	305	-	5,5,5	0.17	0	5,5,5	0.47	0
4	GOL	B	304	-	5,5,5	0.09	0	5,5,5	0.45	0
5	EDO	B	310	-	3,3,3	0.48	0	2,2,2	0.34	0
5	EDO	C	304	-	3,3,3	0.10	0	2,2,2	0.14	0
6	PEG	C	303	-	6,6,6	0.25	0	5,5,5	0.20	0
4	GOL	C	302	-	5,5,5	0.22	0	5,5,5	0.42	0
4	GOL	B	303	-	5,5,5	0.36	0	5,5,5	0.98	0
5	EDO	A	307	-	3,3,3	0.46	0	2,2,2	0.48	0
4	GOL	A	304	-	5,5,5	0.18	0	5,5,5	0.49	0

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	-	-	6/12/22/22	0/4/4/4
2	T9D	C	301	-	-	4/12/22/22	0/4/4/4
2	T9D	A	301	-	-	4/12/22/22	0/4/4/4
4	GOL	B	305	-	-	0/4/4/4	-
4	GOL	B	306	-	-	2/4/4/4	-
3	CIT	A	302	-	-	6/16/16/16	-
4	GOL	A	306	-	-	2/4/4/4	-
5	EDO	B	309	-	-	1/1/1/1	-
4	GOL	B	307	-	-	2/4/4/4	-
3	CIT	B	302	-	-	11/16/16/16	-
6	PEG	B	308	-	-	1/4/4/4	-
4	GOL	A	303	-	-	0/4/4/4	-
4	GOL	A	305	-	-	2/4/4/4	-
4	GOL	B	304	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	B	310	-	-	1/1/1/1	-
5	EDO	C	304	-	-	1/1/1/1	-
6	PEG	C	303	-	-	4/4/4/4	-
4	GOL	C	302	-	-	2/4/4/4	-
4	GOL	B	303	-	-	0/4/4/4	-
5	EDO	A	307	-	-	1/1/1/1	-
4	GOL	A	304	-	-	4/4/4/4	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	T9D	C13-N12	7.89	1.50	1.38
2	C	301	T9D	C13-N12	7.13	1.49	1.38
2	B	301	T9D	C13-N12	6.84	1.48	1.38
2	B	301	T9D	C20-N12	6.50	1.48	1.38
2	C	301	T9D	C20-N12	5.89	1.47	1.38
2	A	301	T9D	C20-N12	5.45	1.46	1.38
2	A	301	T9D	C6-N12	-3.27	1.37	1.42
2	C	301	T9D	N9-N8	2.71	1.42	1.36
2	C	301	T9D	C6-N12	-2.69	1.38	1.42
2	A	301	T9D	C2-C5	2.49	1.56	1.50
2	B	301	T9D	C7-N8	-2.28	1.27	1.30
2	A	301	T9D	C7-N8	-2.18	1.28	1.30

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	T9D	O11-C10-N9	-7.87	110.93	120.68
2	B	301	T9D	F4-C2-C5	-6.57	98.83	112.83
2	A	301	T9D	C17-O21-C22	6.33	130.62	119.18
2	B	301	T9D	C13-N12-C20	-5.12	103.39	108.92
2	C	301	T9D	F3-C2-C5	-4.96	102.26	112.83
2	C	301	T9D	C13-N12-C20	-4.42	104.16	108.92
2	A	301	T9D	C14-C19-C18	-4.36	118.75	124.45
2	B	301	T9D	O11-C10-C5	-3.82	120.46	124.72
2	A	301	T9D	O11-C10-C5	-3.73	120.56	124.72
2	C	301	T9D	C2-C5-C6	3.70	128.61	117.58
2	B	301	T9D	C2-C5-C6	3.66	128.50	117.58
2	A	301	T9D	F4-C2-C5	-3.58	105.21	112.83
2	A	301	T9D	C2-C5-C6	3.40	127.71	117.58
3	A	302	CIT	O5-C6-C3	-3.29	115.71	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	T9D	C14-C19-C18	-3.18	120.29	124.45
2	C	301	T9D	C10-N9-N8	-3.06	120.42	126.84
2	B	301	T9D	O11-C10-N9	-3.02	116.94	120.68
2	B	301	T9D	F1-C2-C5	3.00	119.22	112.83
2	A	301	T9D	C13-N12-C20	-2.89	105.80	108.92
3	B	302	CIT	O5-C6-C3	-2.72	116.83	122.09
2	C	301	T9D	C16-C17-C18	-2.65	116.94	120.50
2	B	301	T9D	C10-N9-N8	-2.60	121.38	126.84
2	C	301	T9D	C7-N8-N9	2.50	118.74	116.53
2	B	301	T9D	C17-O21-C22	2.49	123.68	119.18
2	A	301	T9D	O11-C10-N9	-2.46	117.63	120.68
2	A	301	T9D	F1-C2-C5	2.42	117.99	112.83
2	C	301	T9D	C13-N12-C6	2.32	129.33	125.81
3	B	302	CIT	O3-C5-C4	-2.29	116.47	122.95
2	B	301	T9D	C27-C22-C23	-2.29	107.01	111.67
2	A	301	T9D	C13-N12-C6	-2.26	122.39	125.81
3	B	302	CIT	O6-C6-C3	2.25	117.45	113.14
2	A	301	T9D	C20-N12-C6	2.24	129.20	125.81
2	C	301	T9D	C27-C22-C23	-2.10	107.39	111.67
2	B	301	T9D	C7-N8-N9	2.10	118.38	116.53

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	T9D	C5-C6-N12-C13
2	A	301	T9D	C5-C6-N12-C20
2	B	301	T9D	C5-C6-N12-C13
2	B	301	T9D	C5-C6-N12-C20
2	C	301	T9D	C5-C6-N12-C13
2	C	301	T9D	C5-C6-N12-C20
3	A	302	CIT	C1-C2-C3-C4
3	A	302	CIT	C1-C2-C3-C6
3	B	302	CIT	C1-C2-C3-O7
3	B	302	CIT	C1-C2-C3-C6
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
4	A	305	GOL	C1-C2-C3-O3
4	A	306	GOL	O1-C1-C2-C3
4	B	304	GOL	O1-C1-C2-C3

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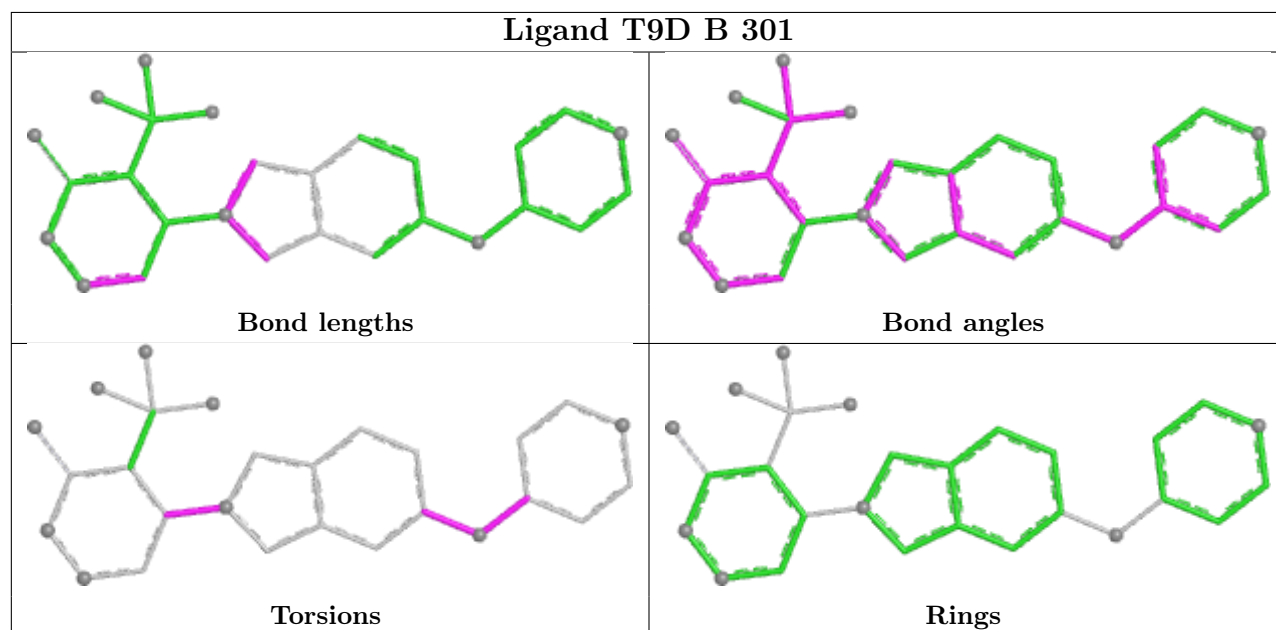
Mol	Chain	Res	Type	Atoms
4	B	307	GOL	C1-C2-C3-O3
4	B	307	GOL	O2-C2-C3-O3
4	C	302	GOL	C1-C2-C3-O3
4	C	302	GOL	O2-C2-C3-O3
3	B	302	CIT	C1-C2-C3-C4
3	B	302	CIT	C2-C3-C4-C5
4	A	305	GOL	O2-C2-C3-O3
4	B	304	GOL	O1-C1-C2-O2
6	B	308	PEG	O2-C3-C4-O4
2	B	301	T9D	C16-C17-O21-C22
6	C	303	PEG	O1-C1-C2-O2
3	A	302	CIT	O7-C3-C4-C5
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
3	A	302	CIT	C6-C3-C4-C5
5	A	307	EDO	O1-C1-C2-O2
5	B	310	EDO	O1-C1-C2-O2
2	B	301	T9D	C18-C17-O21-C22
2	B	301	T9D	C27-C22-O21-C17
3	A	302	CIT	C1-C2-C3-O7
5	C	304	EDO	O1-C1-C2-O2
4	A	306	GOL	O1-C1-C2-O2
3	A	302	CIT	C2-C3-C4-C5
2	A	301	T9D	C16-C17-O21-C22
2	B	301	T9D	C23-C22-O21-C17
2	A	301	T9D	C18-C17-O21-C22
3	B	302	CIT	C3-C4-C5-O4
3	B	302	CIT	C3-C4-C5-O3
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
3	B	302	CIT	C2-C3-C6-O6
3	B	302	CIT	O1-C1-C2-C3
3	B	302	CIT	O2-C1-C2-C3

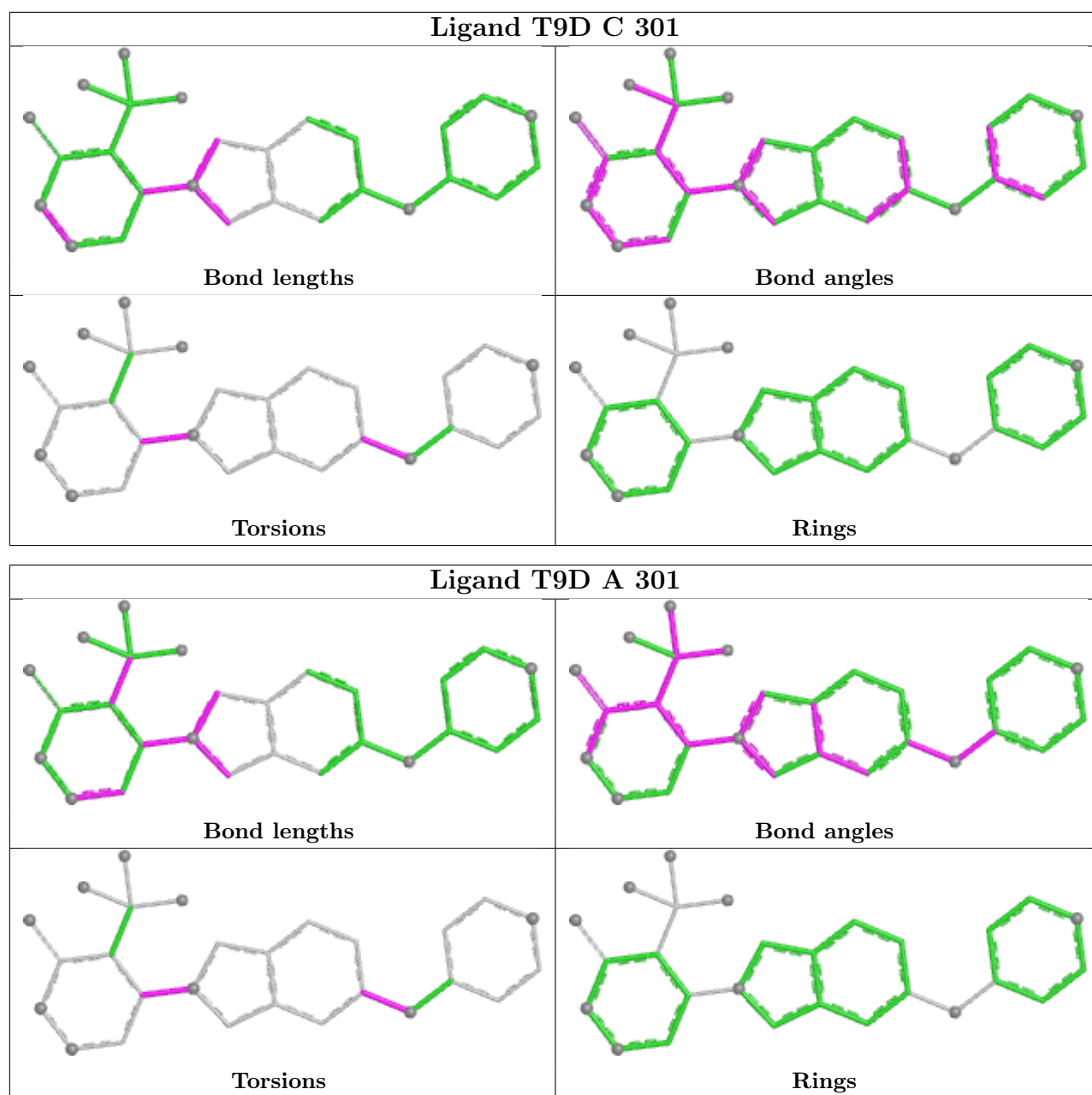
There are no ring outliers.

10 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	T9D	1	0
3	A	302	CIT	1	0
4	B	307	GOL	4	0
3	B	302	CIT	1	0
4	B	304	GOL	1	0
5	B	310	EDO	1	0
6	C	303	PEG	5	0
4	B	303	GOL	10	0
5	A	307	EDO	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%)	0.41	26 (10%)	11 13	22, 46, 104, 131	4 (1%)
1	B	234/277 (84%)	0.60	28 (11%)	9 10	19, 51, 122, 146	4 (1%)
1	C	237/277 (85%)	0.69	23 (9%)	13 15	25, 56, 103, 130	2 (0%)
All	All	714/831 (85%)	0.56	77 (10%)	11 13	19, 52, 110, 146	10 (1%)

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	177	PHE	6.8
1	A	76	GLY	5.9
1	C	252	PRO	5.4
1	A	171	LEU	5.0
1	C	176	LEU	4.8
1	C	274	LYS	4.5
1	A	252	PRO	4.5
1	B	169	CYS	4.3
1	C	169	CYS	4.2
1	B	102	LYS	4.2
1	A	103	ALA	4.1
1	B	168	HIS	4.0
1	B	220	HIS	3.9
1	A	74	SER	3.8
1	A	6	TRP	3.8
1	B	134	ALA	3.7
1	B	252	PRO	3.6
1	A	177	PHE	3.6
1	C	6	TRP	3.5
1	A	274	LYS	3.5
1	A	220	HIS	3.4
1	B	49	ARG	3.4
1	B	274	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	251	PRO	3.3
1	A	253	LYS	3.3
1	B	250	ILE	3.3
1	C	80	LYS	3.3
1	B	139	TYR	3.2
1	A	250	ILE	3.2
1	C	79	HIS	3.2
1	A	102	LYS	3.1
1	C	102	LYS	3.1
1	B	103	ALA	3.0
1	A	176	LEU	3.0
1	C	111	LEU	3.0
1	B	254	TYR	3.0
1	B	133	PRO	3.0
1	C	75	SER	2.9
1	C	103	ALA	2.9
1	B	253	LYS	2.9
1	A	173	LYS	2.9
1	B	52	CYS	2.8
1	C	32	GLN	2.8
1	B	51	ASP	2.8
1	B	76	GLY	2.8
1	B	262	LEU	2.7
1	B	255	PHE	2.7
1	A	254	TYR	2.7
1	B	218	ILE	2.7
1	B	50	GLY	2.7
1	C	201[A]	GLN	2.6
1	A	174	THR	2.6
1	B	136	ALA	2.6
1	C	253	LYS	2.5
1	C	258	THR	2.5
1	C	149	TYR	2.5
1	A	75	SER	2.5
1	B	75	SER	2.5
1	B	138	PHE	2.4
1	C	145	ARG	2.3
1	B	179	GLU	2.3
1	A	78	ASN	2.2
1	B	145	ARG	2.2
1	B	137	LYS	2.2
1	A	101	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	48	ALA	2.2
1	A	79	HIS	2.2
1	C	3	SER	2.2
1	A	77	ASP	2.2
1	C	34	TYR	2.1
1	A	113	GLY	2.1
1	B	217	VAL	2.1
1	C	64	LYS	2.1
1	C	254	TYR	2.1
1	A	73	GLN	2.1
1	A	80	LYS	2.1
1	A	108	ILE	2.1

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

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

6.3 Carbohydrates [i](#)

There are no 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	GOL	A	304	6/6	0.67	0.19	53,59,69,78	0
5	EDO	A	307	4/4	0.74	0.23	60,73,74,78	0
5	EDO	B	309	4/4	0.77	0.19	59,69,71,76	0
4	GOL	B	303	6/6	0.79	0.17	53,67,73,75	0
3	CIT	B	302	13/13	0.83	0.13	67,91,99,100	0
4	GOL	A	305	6/6	0.85	0.17	73,84,90,91	0
4	GOL	C	302	6/6	0.85	0.17	70,72,78,82	0
4	GOL	B	307	6/6	0.86	0.14	42,54,63,67	6
6	PEG	B	308	7/7	0.86	0.22	71,80,82,83	0
3	CIT	A	302	13/13	0.88	0.12	53,66,89,98	0
5	EDO	B	310	4/4	0.89	0.15	57,58,59,74	0

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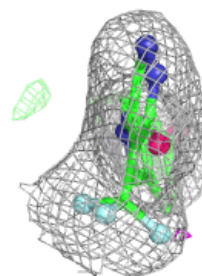
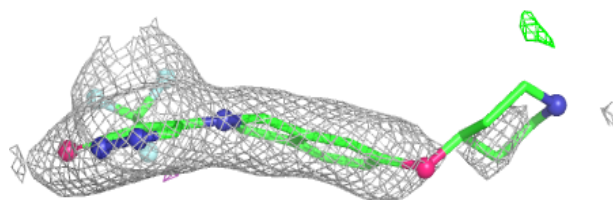
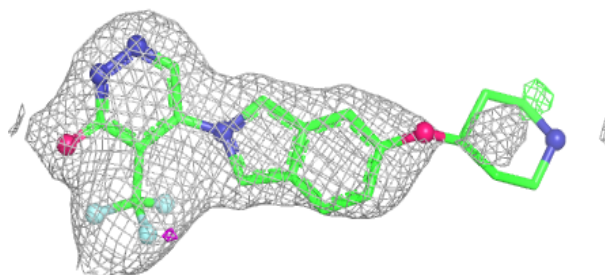
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	A	306	6/6	0.90	0.15	82,95,96,97	0
4	GOL	B	304	6/6	0.90	0.16	39,59,65,70	0
6	PEG	C	303	7/7	0.90	0.14	68,69,81,83	0
2	T9D	B	301	27/27	0.91	0.14	45,76,139,141	0
2	T9D	C	301	27/27	0.91	0.13	46,70,106,111	0
4	GOL	A	303	6/6	0.91	0.14	59,67,70,71	0
4	GOL	B	305	6/6	0.92	0.13	58,61,63,67	0
4	GOL	B	306	6/6	0.93	0.10	73,85,85,87	0
5	EDO	C	304	4/4	0.93	0.15	88,90,90,94	0
2	T9D	A	301	27/27	0.95	0.10	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.

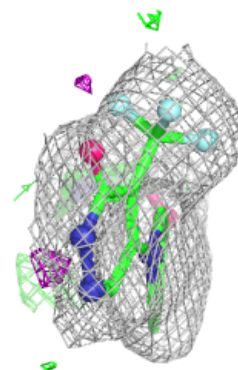
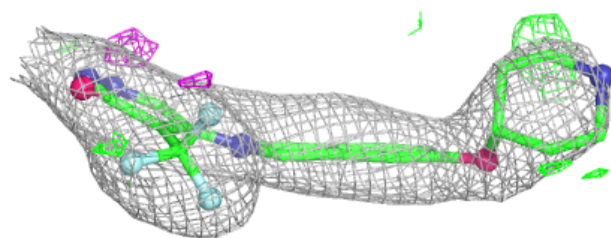
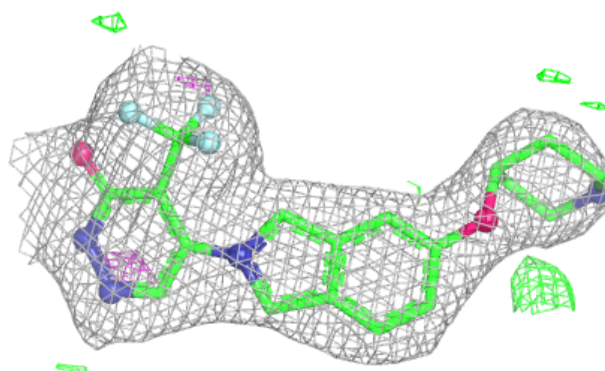
Electron density around T9D B 301:

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mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

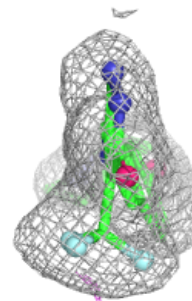
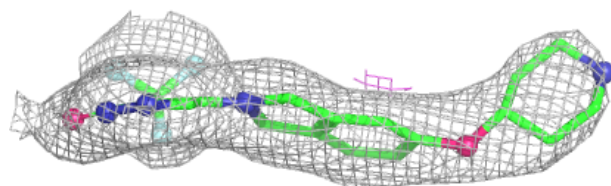
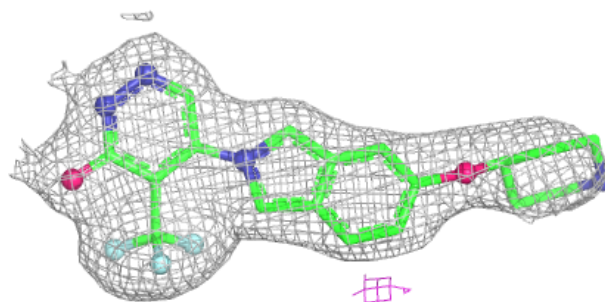


Electron density around T9D C 301:

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

**Electron density around T9D 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.