



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:00 AM UTC

PDB ID : 4IFY / pdb\_00004ify  
Title : HIV-1 reverse transcriptase with bound fragment at the Knuckles site  
Authors : Bauman, J.D.; Patel, D.; Arnold, E.  
Deposited on : 2012-12-15  
Resolution : 2.10 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](mailto: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)  
Xtrriage (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

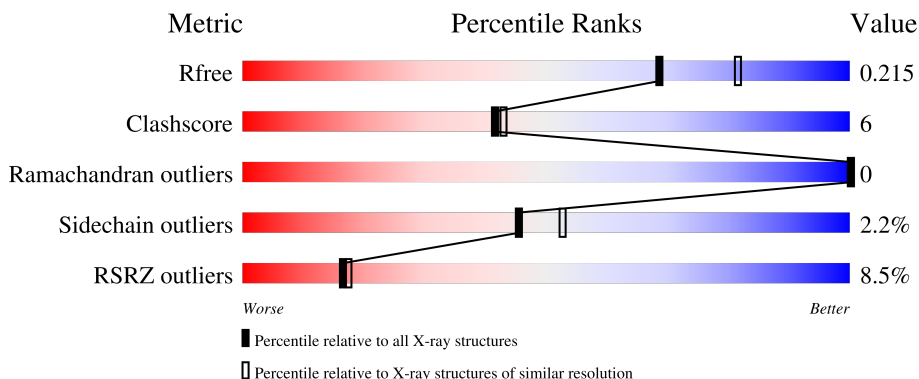
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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  $\geq 3$ , 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	557	 6% 87% 12%
2	B	429	 11% 81% 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
5	DMS	A	603	-	-	X	-

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 8703 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 REVERSE TRANSCRIPTASE/RIBONUCLEASE H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	556	4516	2923	750	835	8	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP P03366
A	0	VAL	-	expression tag	UNP P03366
A	172	ALA	LYS	engineered mutation	UNP P03366
A	173	ALA	LYS	engineered mutation	UNP P03366
A	280	SER	CYS	engineered mutation	UNP P03366

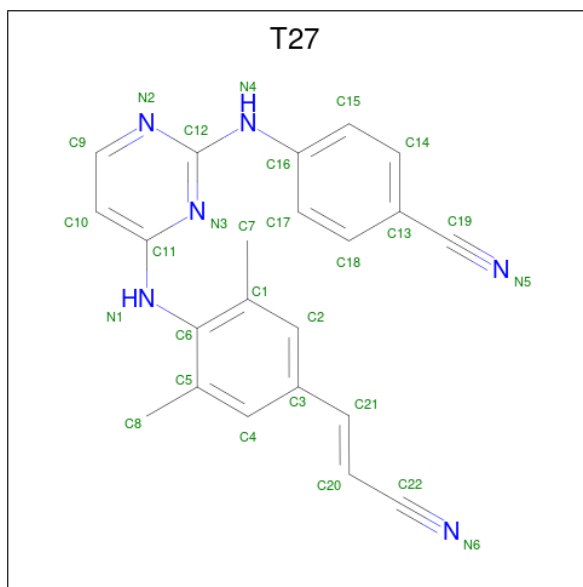
- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	412	3419	2228	565	619	7	0	1	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	expression tag	UNP P03366
B	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 3 is 4-{{4-({4-[(E)-2-cyanoethenyl]-2,6-dimethylphenyl}amino)pyrimidin-2-yl}amino}benzotrile (CCD ID: T27) (formula: C<sub>22</sub>H<sub>18</sub>N<sub>6</sub>).

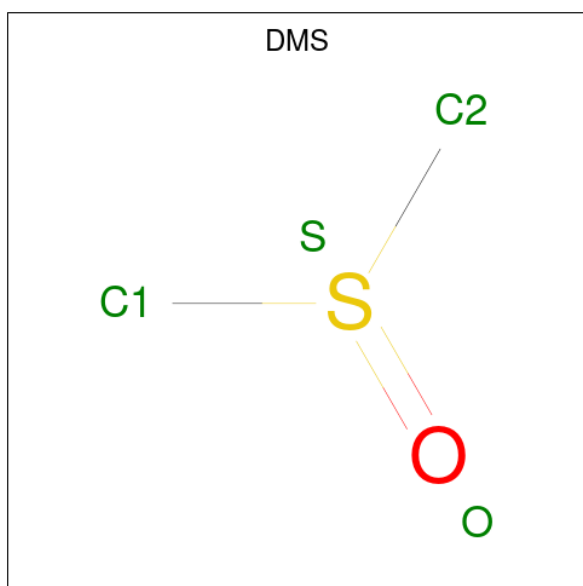


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N 28 22 6	0	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

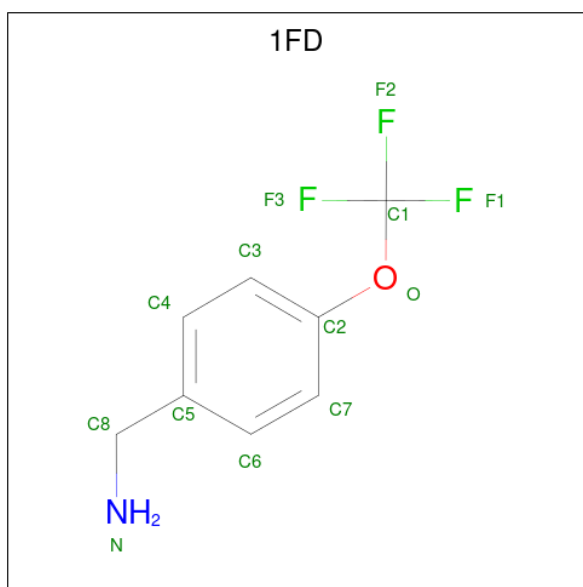
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0

- Molecule 5 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C<sub>2</sub>H<sub>6</sub>OS).



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

- Molecule 6 is 1-[4-(trifluoromethoxy)phenyl]methanamine (CCD ID: 1FD) (formula: C<sub>8</sub>H<sub>8</sub>F<sub>3</sub>NO).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
6	A	1	13	8	3	1	1	0	0

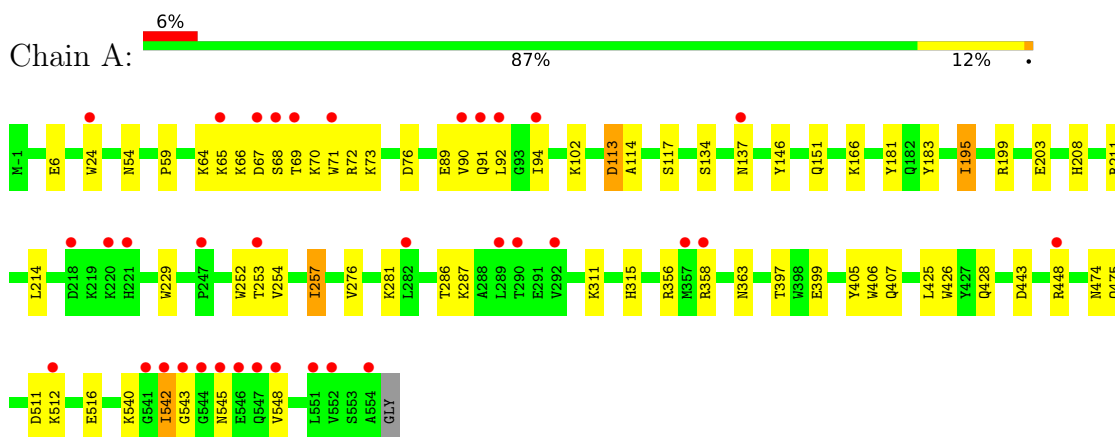
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	419	Total	O	0	0
			419	419		
7	B	243	Total	O	0	0
			243	243		

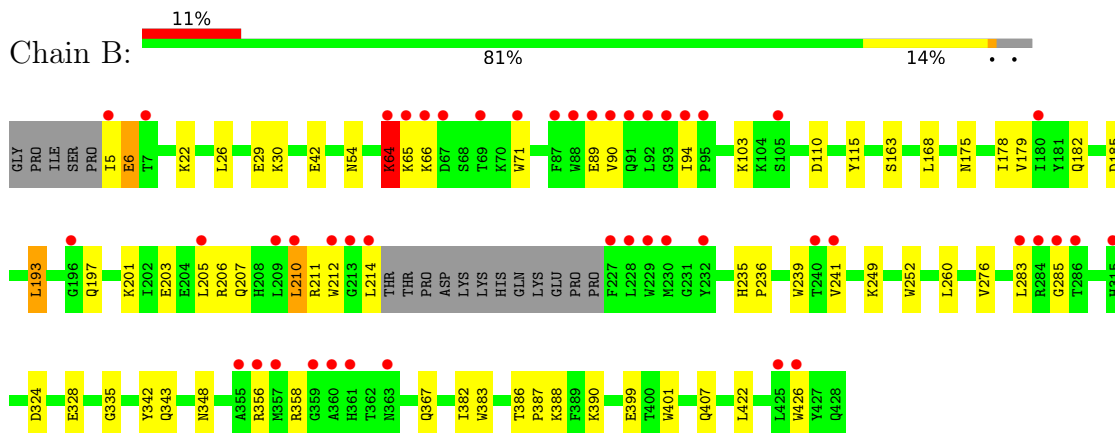
### 3 Residue-property plots [i](#)

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: REVERSE TRANSCRIPTASE/RIBONUCLEASE H



- Molecule 2: p51 RT



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	161.95Å 73.05Å 108.75Å 90.00° 100.47° 90.00°	Depositor
Resolution (Å)	31.31 – 2.10 31.31 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (31.31-2.10) 93.1 (31.31-2.10)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.11 (at 2.01Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: dev_1233)	Depositor
R, $R_{free}$	0.186 , 0.213 0.188 , 0.215	Depositor DCC
$R_{free}$ test set	1643 reflections (1.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.5	Xtrriage
Anisotropy	0.215	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 56.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8703	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.90% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MG, DMS, T27, 1FD

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	0.51	0/4634	0.80	3/6299 (0.0%)
2	B	0.51	0/3517	0.88	9/4776 (0.2%)
All	All	0.51	0/8151	0.84	12/11075 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	54	ASN	CA-C-N	10.22	129.96	119.64
2	B	54	ASN	C-N-CA	10.22	129.96	119.64
2	B	401	TRP	N-CA-C	9.28	124.92	113.50
2	B	285	GLY	N-CA-C	-8.00	99.03	110.46
1	A	276	VAL	N-CA-C	7.25	119.86	112.90
2	B	64	LYS	CB-CA-C	-6.52	100.16	110.79
1	A	54	ASN	CA-C-N	6.44	127.00	120.04
1	A	54	ASN	C-N-CA	6.44	127.00	120.04
2	B	6	GLU	N-CA-C	5.77	118.24	111.02
2	B	382	ILE	N-CA-C	5.26	115.36	110.42
2	B	276	VAL	N-CA-C	5.15	117.92	112.83
2	B	383	TRP	N-CA-C	5.07	119.61	113.38

There are no chirality outliers.

There are no planarity outliers.

### 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	4516	0	4572	59	0
2	B	3419	0	3447	42	0
3	A	28	0	18	1	0
4	A	1	0	0	0	0
5	A	32	0	48	13	0
5	B	32	0	48	11	0
6	A	13	0	8	0	0
7	A	419	0	0	7	2
7	B	243	0	0	11	1
All	All	8703	0	8141	104	2

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 (104) 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:428:GLN:H	5:A:604:DMS:H23	1.21	1.04
2:B:26:LEU:H	5:B:503:DMS:H11	1.21	1.03
2:B:178:ILE:HD11	2:B:201:LYS:HD3	1.52	0.92
1:A:65:LYS:HG3	1:A:72:ARG:HH12	1.43	0.81
2:B:185:ASP:OD1	7:B:791:HOH:O	2.03	0.74
2:B:42:GLU:OE1	7:B:778:HOH:O	2.05	0.74
1:A:114:ALA:HB2	1:A:214:LEU:HD13	1.71	0.73
1:A:166:LYS:NZ	7:A:875:HOH:O	2.18	0.72
1:A:426:TRP:H	5:A:603:DMS:H23	1.55	0.71
1:A:203:GLU:OE1	7:A:1039:HOH:O	2.10	0.70
1:A:428:GLN:N	5:A:604:DMS:H23	2.04	0.67
2:B:64:LYS:O	2:B:407:GLN:NE2	2.30	0.64
1:A:542:ILE:HG13	1:A:545:ASN:HB3	1.80	0.64
2:B:175:ASN:OD1	2:B:201:LYS:NZ	2.30	0.64
1:A:426:TRP:H	5:A:603:DMS:C2	2.10	0.64
2:B:239:TRP:HE1	5:B:504:DMS:H23	1.62	0.63
2:B:207:GLN:HA	2:B:210:LEU:HG	1.79	0.63
2:B:235:HIS:H	5:B:504:DMS:H21	1.66	0.60
2:B:26:LEU:N	5:B:503:DMS:H11	2.05	0.60
1:A:428:GLN:H	5:A:604:DMS:C2	2.07	0.58
2:B:168:LEU:HD22	2:B:205:LEU:HD11	1.85	0.58
5:B:502:DMS:H23	7:B:742:HOH:O	2.05	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:ARG:NE	7:A:975:HOH:O	2.15	0.57
2:B:163:SER:OG	7:B:829:HOH:O	2.17	0.57
1:A:195:ILE:HG13	1:A:199:ARG:NH1	2.20	0.55
5:B:507:DMS:H13	7:B:781:HOH:O	2.06	0.55
2:B:22:LYS:HG3	7:B:822:HOH:O	2.07	0.55
1:A:94:ILE:HD11	1:A:229:TRP:CZ2	2.42	0.55
1:A:113:ASP:O	1:A:117:SER:OG	2.19	0.55
1:A:181:TYR:CE2	1:A:183:TYR:HB2	2.42	0.54
3:A:601:T27:H15	3:A:601:T27:N3	2.23	0.53
1:A:73:LYS:NZ	1:A:146:TYR:OH	2.42	0.53
5:A:603:DMS:H22	7:A:916:HOH:O	2.08	0.53
2:B:65:LYS:NZ	2:B:110:ASP:OD2	2.42	0.52
1:A:195:ILE:HG13	1:A:199:ARG:HH12	1.73	0.52
1:A:64:LYS:HD3	1:A:71:TRP:CH2	2.44	0.52
2:B:399:GLU:HB3	5:B:505:DMS:H12	1.91	0.52
1:A:69:THR:HG23	1:A:70:LYS:HE3	1.93	0.51
1:A:448:ARG:HG2	5:A:606:DMS:H21	1.94	0.50
2:B:115:TYR:OH	2:B:182:GLN:NE2	2.44	0.50
2:B:26:LEU:O	5:B:503:DMS:H21	2.13	0.49
2:B:203:GLU:OE2	2:B:207:GLN:NE2	2.38	0.48
1:A:363:ASN:HA	1:A:511:ASP:OD1	2.14	0.48
1:A:425:LEU:HA	5:A:603:DMS:H23	1.96	0.47
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.50	0.47
1:A:315:HIS:HB2	5:A:608:DMS:O	2.15	0.47
1:A:474:ASN:HD22	5:A:606:DMS:H12	1.80	0.47
1:A:287:LYS:HD3	1:A:287:LYS:HA	1.75	0.47
2:B:426:TRP:O	5:B:507:DMS:H12	2.14	0.46
1:A:358:ARG:HA	1:A:358:ARG:HD3	1.57	0.46
1:A:6:GLU:OE2	1:A:166:LYS:NZ	2.49	0.46
2:B:29:GLU:OE2	7:B:743:HOH:O	2.20	0.46
1:A:356:ARG:HE	1:A:358:ARG:HH12	1.63	0.46
1:A:474:ASN:H	5:A:606:DMS:H23	1.81	0.46
2:B:178:ILE:CD1	2:B:201:LYS:HD3	2.36	0.46
2:B:212:TRP:HE3	2:B:214:LEU:HD23	1.81	0.46
2:B:388:LYS:NZ	7:B:810:HOH:O	2.47	0.45
1:A:542:ILE:HG13	1:A:542:ILE:O	2.16	0.45
1:A:66:LYS:O	1:A:67:ASP:HB2	2.16	0.45
1:A:64:LYS:HD2	1:A:64:LYS:HA	1.70	0.45
2:B:193:LEU:HD13	2:B:197:GLN:HG2	1.98	0.45
1:A:540:LYS:HD3	1:A:540:LYS:HA	1.78	0.45
1:A:134:SER:OG	1:A:137:ASN:HA	2.17	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:TRP:HB3	1:A:257:ILE:HD11	1.99	0.44
1:A:253:THR:HG22	1:A:254:VAL:N	2.33	0.44
1:A:542:ILE:HB	2:B:283:LEU:HD13	1.99	0.44
2:B:252:TRP:CZ3	2:B:260:LEU:HD22	2.53	0.44
1:A:59:PRO:HG2	1:A:76:ASP:HB3	2.00	0.43
1:A:65:LYS:HG3	1:A:72:ARG:NH1	2.21	0.43
1:A:70:LYS:HA	1:A:70:LYS:HD3	1.84	0.43
1:A:151:GLN:HA	5:A:607:DMS:H22	2.00	0.43
1:A:443:ASP:HB2	1:A:548:VAL:HG13	2.01	0.43
2:B:30:LYS:HG2	2:B:71:TRP:CZ3	2.53	0.43
1:A:65:LYS:HZ2	1:A:68:SER:HB3	1.83	0.43
1:A:252:TRP:HB3	1:A:257:ILE:CD1	2.48	0.43
2:B:386:THR:HA	2:B:387:PRO:HD3	1.91	0.43
2:B:249:LYS:HE3	7:B:831:HOH:O	2.17	0.43
1:A:397:THR:HG23	1:A:425:LEU:HG	2.01	0.43
2:B:239:TRP:HE1	5:B:504:DMS:C2	2.30	0.43
1:A:89:GLU:OE1	1:A:91:GLN:NE2	2.50	0.42
1:A:475:GLN:NE2	7:A:892:HOH:O	2.12	0.42
1:A:516:GLU:CD	1:A:516:GLU:H	2.27	0.42
1:A:405:TYR:CE2	1:A:407:GLN:HB2	2.54	0.42
2:B:5:ILE:C	2:B:6:GLU:HG2	2.44	0.42
1:A:281:LYS:NZ	5:A:610:DMS:H13	2.35	0.42
2:B:210:LEU:HD12	2:B:211:ARG:HG3	2.01	0.42
1:A:208:HIS:O	1:A:211:ARG:HG3	2.20	0.42
2:B:66:LYS:HE3	2:B:66:LYS:HB3	1.92	0.42
2:B:193:LEU:HD11	2:B:201:LYS:HD2	2.02	0.42
1:A:406:TRP:CE2	1:A:407:GLN:HG3	2.54	0.42
2:B:203:GLU:OE1	2:B:206:ARG:HD2	2.20	0.42
2:B:324:ASP:O	2:B:343:GLN:HG2	2.20	0.41
5:B:507:DMS:C1	7:B:781:HOH:O	2.68	0.41
2:B:335:GLY:HA2	2:B:367:GLN:OE1	2.21	0.41
1:A:24:TRP:H	1:A:24:TRP:CD1	2.39	0.41
1:A:286:THR:HG22	1:A:287:LYS:N	2.35	0.41
1:A:89:GLU:HA	7:A:854:HOH:O	2.20	0.41
1:A:166:LYS:HE3	1:A:166:LYS:HB2	1.80	0.41
1:A:543:GLY:HA3	2:B:283:LEU:O	2.21	0.41
2:B:328:GLU:HG2	2:B:390:LYS:HD3	2.03	0.41
1:A:90:VAL:HG13	7:B:770:HOH:O	2.21	0.40
1:A:211:ARG:HD2	7:A:990:HOH:O	2.20	0.40
2:B:342:TYR:HB3	2:B:348:ASN:HD22	1.86	0.40
2:B:356:ARG:HH22	2:B:358:ARG:HD2	1.86	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1094:HOH:O	7:A:1107:HOH:O[4_556]	1.99	0.21
7:A:928:HOH:O	7:B:748:HOH:O[4_545]	2.18	0.02

## 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	554/557 (100%)	546 (99%)	8 (1%)	0	100	100
2	B	409/429 (95%)	401 (98%)	8 (2%)	0	100	100
All	All	963/986 (98%)	947 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	495/495 (100%)	486 (98%)	9 (2%)	51	60
2	B	375/390 (96%)	365 (97%)	10 (3%)	39	45
All	All	870/885 (98%)	851 (98%)	19 (2%)	45	53

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	LEU
1	A	102	LYS
1	A	113	ASP
1	A	195	ILE
1	A	257	ILE
1	A	311	LYS
1	A	399	GLU
1	A	512	LYS
1	A	542	ILE
2	B	64	LYS
2	B	89	GLU
2	B	90	VAL
2	B	94	ILE
2	B	103	LYS
2	B	179	VAL
2	B	193	LEU
2	B	210	LEU
2	B	241	VAL
2	B	422	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	ASN
1	A	334	GLN
1	A	487	GLN
2	B	182	GLN
2	B	265	ASN
2	B	348	ASN

### 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

Of 19 ligands modelled in this entry, 1 is monoatomic - leaving 18 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	DMS	A	603	-	3,3,3	0.39	0	3,3,3	0.52	0
5	DMS	B	502	-	3,3,3	0.54	0	3,3,3	0.45	0
5	DMS	A	609	-	3,3,3	0.64	0	3,3,3	0.73	0
5	DMS	A	604	-	3,3,3	0.52	0	3,3,3	0.69	0
5	DMS	B	506	-	3,3,3	0.68	0	3,3,3	0.70	0
5	DMS	A	605	-	3,3,3	0.66	0	3,3,3	0.49	0
5	DMS	A	610	-	3,3,3	0.68	0	3,3,3	0.45	0
5	DMS	B	507	-	3,3,3	0.64	0	3,3,3	0.61	0
5	DMS	A	608	-	3,3,3	0.64	0	3,3,3	0.77	0
5	DMS	B	501	-	3,3,3	0.68	0	3,3,3	0.45	0
5	DMS	B	505	-	3,3,3	0.72	0	3,3,3	0.98	0
6	1FD	A	611	-	13,13,13	0.49	0	18,18,18	0.61	0
5	DMS	A	606	-	3,3,3	0.69	0	3,3,3	0.59	0
5	DMS	A	607	-	3,3,3	0.66	0	3,3,3	0.63	0
5	DMS	B	508	-	3,3,3	0.68	0	3,3,3	0.71	0
3	T27	A	601	-	30,30,30	1.19	3 (10%)	37,40,40	1.82	4 (10%)
5	DMS	B	503	-	3,3,3	0.65	0	3,3,3	0.73	0
5	DMS	B	504	-	3,3,3	0.63	0	3,3,3	0.47	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
3	T27	A	601	-	-	0/13/14/14	0/3/3/3
6	1FD	A	611	-	-	3/7/7/7	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	T27	C12-N4	3.33	1.43	1.36
3	A	601	T27	C11-N1	3.20	1.44	1.38
3	A	601	T27	C13-C19	2.49	1.49	1.44

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	T27	C9-N2-C12	6.55	120.90	115.42
3	A	601	T27	C10-C9-N2	-5.04	117.80	123.97
3	A	601	T27	N2-C12-N3	-3.76	122.78	126.42
3	A	601	T27	C10-C11-N3	-2.52	118.93	123.15

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	611	1FD	F1-C1-O-C2
6	A	611	1FD	F2-C1-O-C2
6	A	611	1FD	F3-C1-O-C2

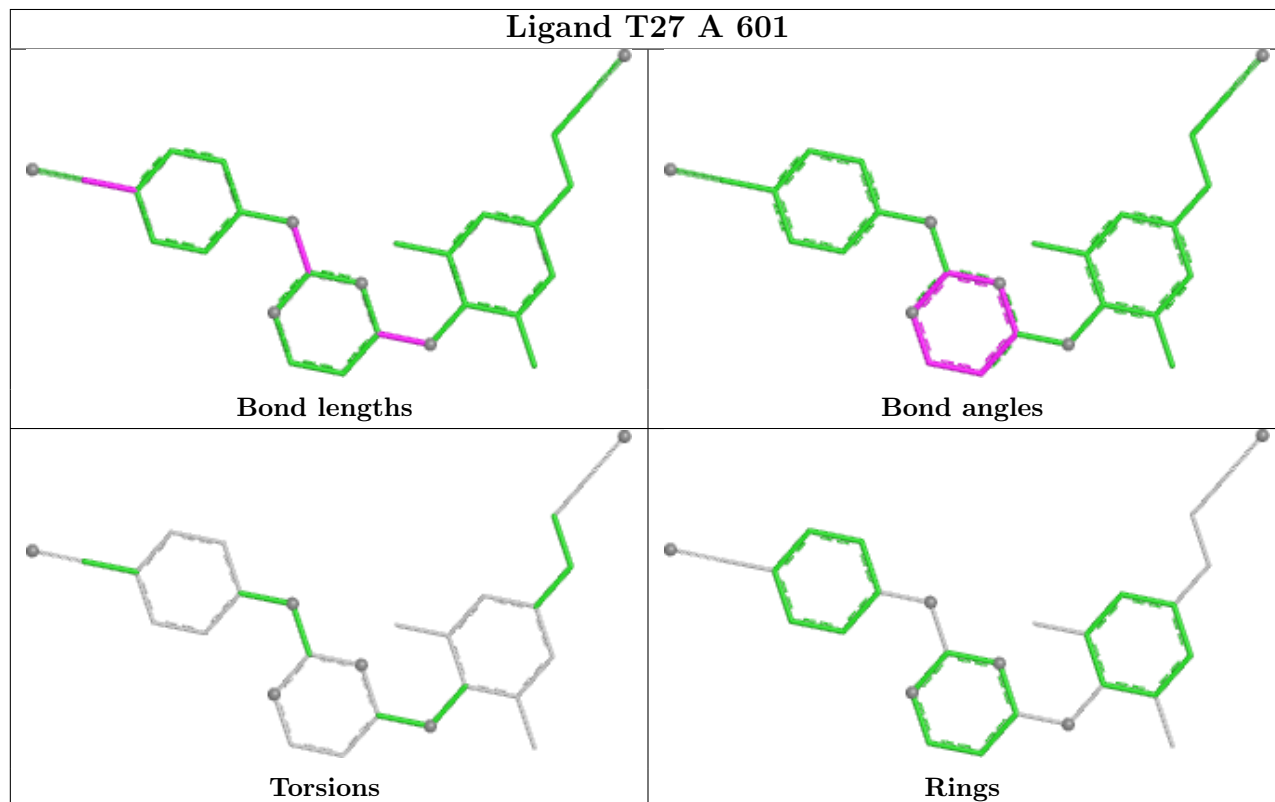
There are no ring outliers.

12 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	603	DMS	4	0
5	B	502	DMS	1	0
5	A	604	DMS	3	0
5	A	610	DMS	1	0
5	B	507	DMS	3	0
5	A	608	DMS	1	0
5	B	505	DMS	1	0
5	A	606	DMS	3	0
5	A	607	DMS	1	0
3	A	601	T27	1	0
5	B	503	DMS	3	0
5	B	504	DMS	3	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	556/557 (99%)	0.07	35 (6%) 26 27	17, 36, 87, 129	0
2	B	412/429 (96%)	0.40	47 (11%) 10 10	15, 42, 101, 145	1 (0%)
All	All	968/986 (98%)	0.21	82 (8%) 16 17	15, 39, 96, 145	1 (0%)

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	214	LEU	6.3
2	B	94	ILE	5.7
2	B	90	VAL	5.6
2	B	213	GLY	5.5
2	B	92	LEU	5.2
1	A	92	LEU	5.0
1	A	554	ALA	4.9
2	B	228	LEU	4.7
2	B	359	GLY	4.7
1	A	552	VAL	4.7
2	B	355	ALA	4.4
2	B	88	TRP	4.3
1	A	24	TRP	4.1
2	B	5	ILE	4.1
2	B	360	ALA	4.0
2	B	93	GLY	4.0
2	B	64	LYS	4.0
2	B	241	VAL	3.9
1	A	546	GLU	3.9
1	A	289	LEU	3.5
1	A	548	VAL	3.5
1	A	543	GLY	3.5
1	A	544	GLY	3.5
2	B	356	ARG	3.3

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	B	69	THR	3.2
2	B	71	TRP	3.2
2	B	95	PRO	3.2
1	A	292	VAL	3.1
2	B	357	MET	3.1
2	B	67	ASP	3.1
2	B	209	LEU	3.1
1	A	90	VAL	3.0
1	A	221	HIS	3.0
1	A	551	LEU	2.9
1	A	65	LYS	2.9
2	B	180	ILE	2.9
2	B	87	PHE	2.9
1	A	91	GLN	2.9
2	B	91	GLN	2.9
1	A	253	THR	2.8
2	B	229	TRP	2.8
1	A	94	ILE	2.7
1	A	69	THR	2.7
2	B	286	THR	2.7
1	A	71	TRP	2.7
1	A	358	ARG	2.7
2	B	315	HIS	2.6
2	B	361	HIS	2.6
1	A	541	GLY	2.6
1	A	220	LYS	2.6
1	A	67	ASP	2.6
2	B	210	LEU	2.6
2	B	285	GLY	2.6
1	A	545	ASN	2.6
1	A	68	SER	2.6
2	B	232	TYR	2.5
1	A	137	ASN	2.5
2	B	212	TRP	2.5
2	B	65	LYS	2.4
2	B	205	LEU	2.4
2	B	425	LEU	2.4
1	A	282	LEU	2.4
1	A	547	GLN	2.4
2	B	227	PHE	2.3
2	B	230	MET	2.3
1	A	542	ILE	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	218	ASP	2.3
2	B	284	ARG	2.3
2	B	66	LYS	2.3
2	B	240	THR	2.2
2	B	196	GLY	2.2
1	A	290	THR	2.2
1	A	357	MET	2.2
1	A	247	PRO	2.1
2	B	105	SER	2.1
1	A	448	ARG	2.1
2	B	89	GLU	2.1
2	B	363	ASN	2.1
2	B	283	LEU	2.0
2	B	7	THR	2.0
1	A	512	LYS	2.0
2	B	426	TRP	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, 95<sup>th</sup> 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.

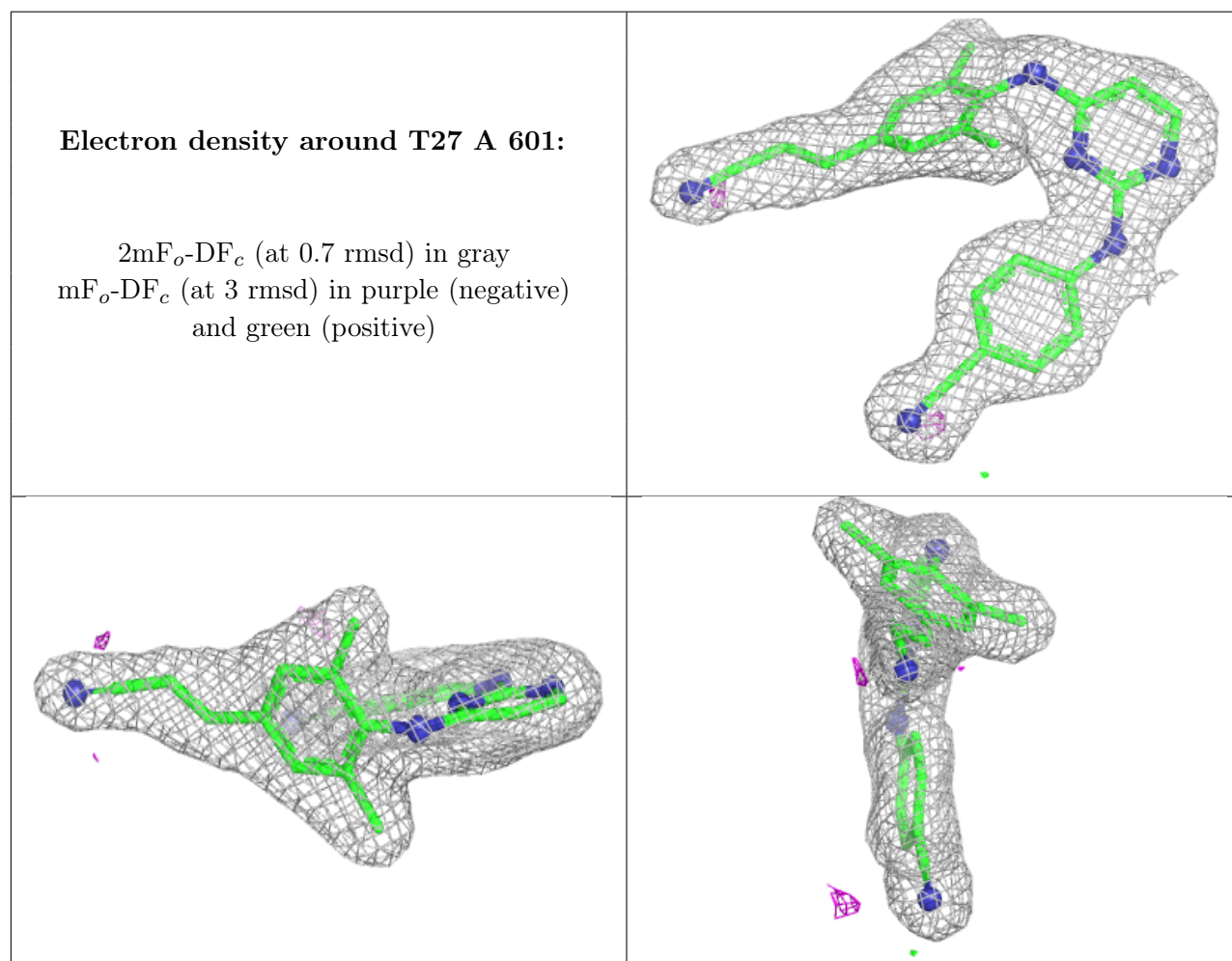
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	DMS	B	504	4/4	0.64	0.24	40,92,100,102	0
5	DMS	A	606	4/4	0.70	0.26	71,91,94,95	0
4	MG	A	602	1/1	0.77	0.16	54,54,54,54	0
6	1FD	A	611	13/13	0.83	0.17	70,77,80,80	0
5	DMS	A	608	4/4	0.84	0.19	63,69,81,81	0
5	DMS	A	605	4/4	0.88	0.15	43,49,54,59	0
5	DMS	B	506	4/4	0.88	0.22	50,72,75,96	0

*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	DMS	A	609	4/4	0.88	0.16	47,62,75,77	0
5	DMS	B	508	4/4	0.90	0.14	48,56,76,77	0
5	DMS	A	607	4/4	0.90	0.14	44,70,72,74	0
5	DMS	A	610	4/4	0.91	0.14	52,54,68,71	0
5	DMS	B	507	4/4	0.91	0.14	38,48,54,79	0
5	DMS	B	503	4/4	0.93	0.12	19,19,71,71	0
5	DMS	A	603	4/4	0.93	0.16	11,45,55,61	0
5	DMS	B	501	4/4	0.94	0.11	37,37,51,55	0
5	DMS	B	502	4/4	0.95	0.10	23,28,46,50	0
3	T27	A	601	28/28	0.96	0.06	19,26,30,33	0
5	DMS	A	604	4/4	0.97	0.08	18,34,34,41	0
5	DMS	B	505	4/4	0.98	0.09	33,37,42,92	0

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.