



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:52 AM UTC

PDB ID : 4ICL / pdb_00004icl
Title : HIV-1 reverse transcriptase with bound fragment at the incoming dNTP binding site
Authors : Bauman, J.D.; Patel, D.; Arnold, E.
Deposited on : 2012-12-10
Resolution : 1.80 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

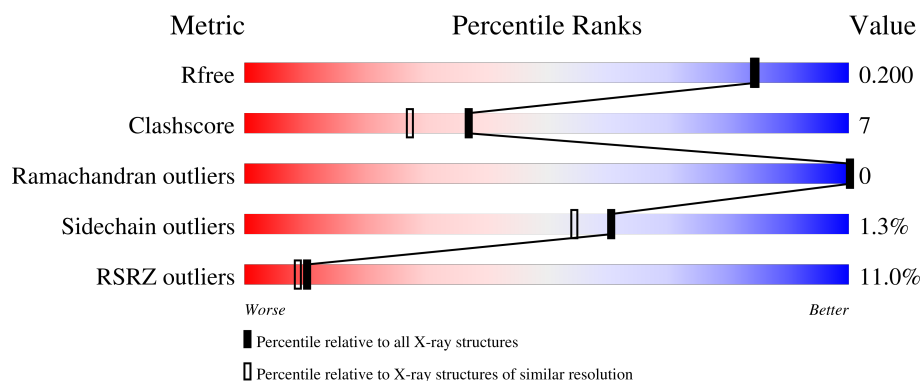
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	557	8% 91% 9%
2	B	429	15% 82% 13% ...

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	-
5	DMS	A	604	-	-	X	-
5	DMS	B	502	-	-	X	-
5	DMS	B	505	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 17737 atoms, of which 9009 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
1	A	556	Total	C	H	N	O	S	0	3	0
			9127	2932	4596	753	838	8			

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

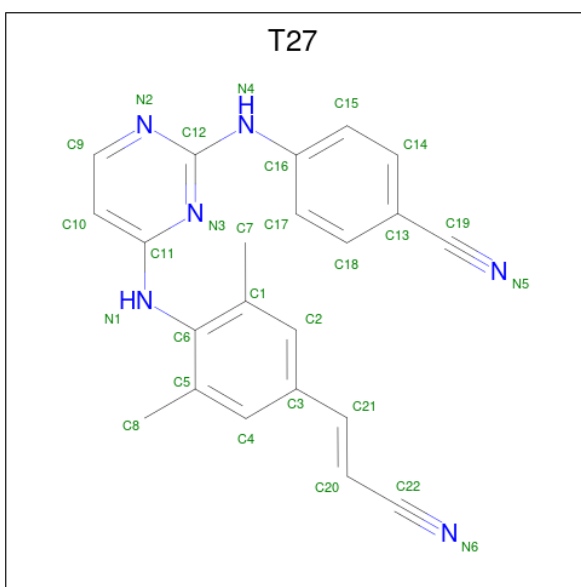
- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	412	Total	C	H	N	O	S	0	2	0
			6874	2228	3455	565	619	7			

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}benzonitrile (CCD ID: T27) (formula: C₂₂H₁₈N₆).

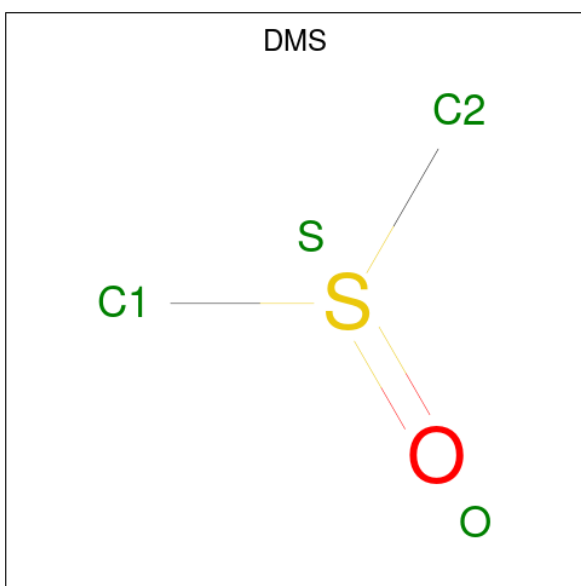


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	N	0	0
			46	22	18	6		

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

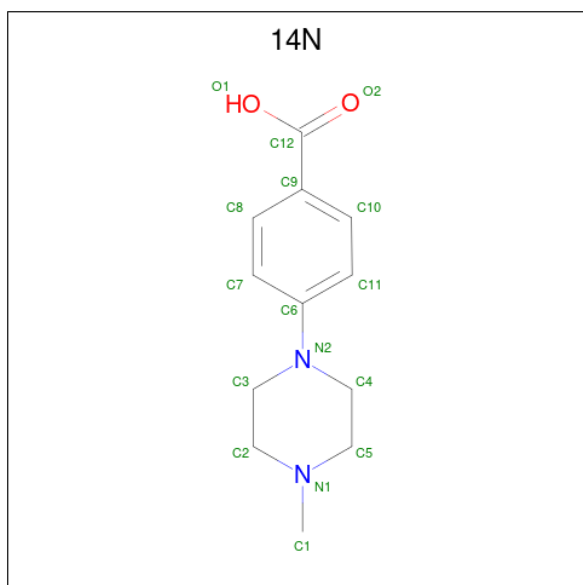
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		

- Molecule 5 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



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	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 4-(4-methylpiperazin-1-yl)benzoic acid (CCD ID: 14N) (formula: C₁₂H₁₆N₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			16	12	2	2		

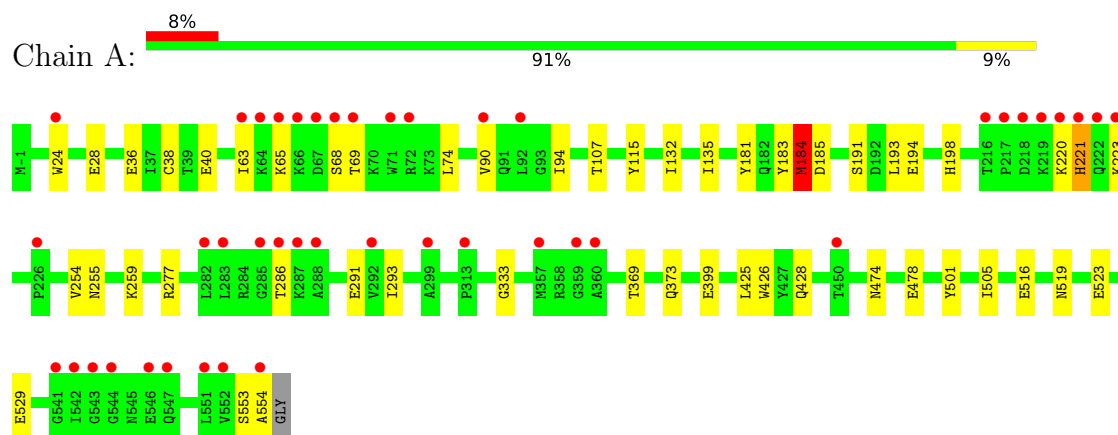
- Molecule 7 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	429	Total	H	O	0	0
			1013	584	429		
7	B	260	Total	H	O	0	0
			616	356	260		

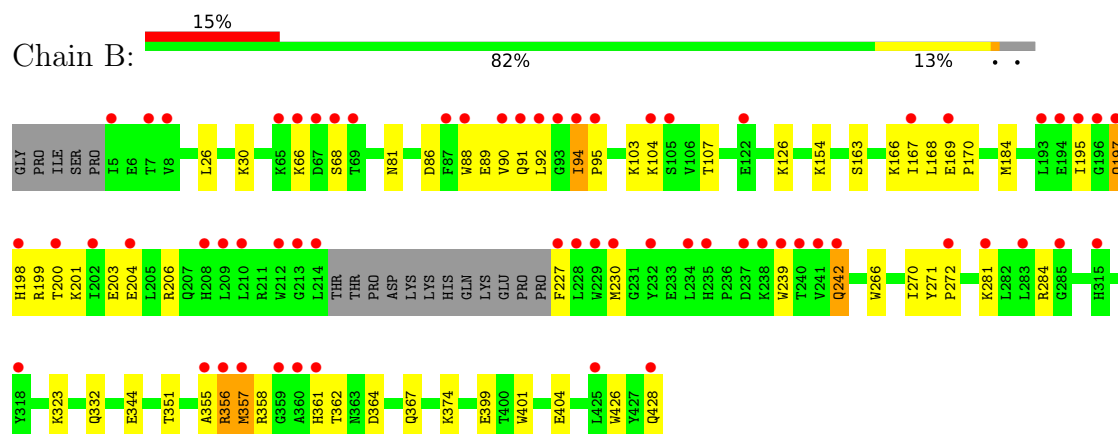
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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, α , β , γ	163.05Å 72.65Å 109.48Å 90.00° 100.85° 90.00°	Depositor
Resolution (Å)	38.00 – 1.80 38.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.4 (38.00-1.80) 90.6 (38.00-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 1.79Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.179 , 0.199 0.180 , 0.200	Depositor DCC
R_{free} test set	2349 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	30.2	Xtriage
Anisotropy	0.191	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 48.4	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	0.96	EDS
Total number of atoms	17737	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% 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: DMS, T27, 14N, MG

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	0.76	0/4661	0.87	4/6334 (0.1%)
2	B	0.74	0/3525	0.91	4/4787 (0.1%)
All	All	0.75	0/8186	0.89	8/11121 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	364	ASP	CB-CA-C	-6.54	99.94	110.79
1	A	24	TRP	CA-C-N	-6.41	113.38	119.85
1	A	24	TRP	C-N-CA	-6.41	113.38	119.85
1	A	184	MET	CB-CA-C	-5.97	109.70	116.63
1	A	90	VAL	N-CA-C	5.92	118.49	111.09
2	B	401	TRP	N-CA-C	5.27	120.71	113.97
2	B	168	LEU	N-CA-C	5.21	119.64	113.28
2	B	270	ILE	N-CA-C	-5.17	107.37	111.81

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	4531	4596	4575	47	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3419	3455	3437	61	2
3	A	28	18	18	1	0
4	A	1	0	0	0	0
5	A	16	0	24	13	0
5	B	28	0	42	17	0
6	A	16	0	15	5	0
7	A	429	584	0	9	0
7	B	260	356	0	9	0
All	All	8728	9009	8111	115	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 7.

All (115) 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	1.09	1.18
2:B:399:GLU:HB3	5:B:505:DMS:H13	1.18	1.12
2:B:26:LEU:H	5:B:503:DMS:H11	1.13	1.06
5:B:502:DMS:H23	7:B:642:HOH:O	1.55	1.06
2:B:399:GLU:HB3	5:B:505:DMS:C1	1.90	1.01
2:B:399:GLU:O	5:B:505:DMS:H12	1.71	0.90
1:A:428:GLN:H	5:A:604:DMS:C2	1.89	0.86
1:A:428:GLN:N	5:A:604:DMS:H23	1.92	0.85
5:B:506:DMS:H22	7:B:773:HOH:O	1.79	0.83
2:B:426:TRP:O	5:B:507:DMS:H12	1.82	0.80
1:A:426:TRP:H	5:A:603:DMS:H23	1.47	0.78
2:B:227:PHE:N	7:B:764:HOH:O	2.17	0.78
1:A:220:LYS:NZ	7:A:1022:HOH:O	2.16	0.77
2:B:26:LEU:N	5:B:503:DMS:H11	1.97	0.76
2:B:166:LYS:O	2:B:169:GLU:OE1	2.04	0.75
2:B:361:HIS:O	7:B:841:HOH:O	2.04	0.74
1:A:255:ASN:OD1	1:A:259:LYS:NZ	2.21	0.72
5:B:505:DMS:H11	7:B:697:HOH:O	1.91	0.70
1:A:107:THR:OG1	1:A:198:HIS:HE1	1.75	0.70
1:A:69:THR:O	1:A:69:THR:HG22	1.92	0.69
2:B:357:MET:HE1	2:B:374:LYS:HD3	1.74	0.68
2:B:169:GLU:CD	2:B:170:PRO:HD3	2.18	0.68
1:A:193:LEU:O	7:A:1031:HOH:O	2.12	0.68
2:B:332:GLN:OE1	2:B:428:GLN:HG2	1.96	0.66
1:A:426:TRP:H	5:A:603:DMS:C2	2.11	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:ASN:HB2	5:A:606:DMS:H12	1.78	0.64
1:A:254:VAL:HG23	1:A:293:ILE:HD11	1.81	0.62
2:B:362:THR:HA	7:B:841:HOH:O	1.99	0.62
1:A:516:GLU:CD	1:A:516:GLU:H	2.08	0.61
1:A:474:ASN:H	5:A:606:DMS:H23	1.66	0.61
1:A:286:THR:HG21	1:A:291:GLU:OE1	2.00	0.61
2:B:66:LYS:HE2	2:B:358:ARG:HD2	1.84	0.60
2:B:195:ILE:HD11	2:B:199:ARG:CZ	2.31	0.60
2:B:197:GLN:O	2:B:201:LYS:HG2	2.02	0.60
1:A:553:SER:O	1:A:554:ALA:CB	2.50	0.59
1:A:293:ILE:HD12	1:A:293:ILE:N	2.18	0.58
2:B:68:SER:HB2	2:B:230:MET:CE	2.34	0.57
2:B:227:PHE:HD1	2:B:230:MET:HE3	1.69	0.57
1:A:553:SER:O	1:A:554:ALA:HB2	2.03	0.57
2:B:26:LEU:O	5:B:503:DMS:H21	2.05	0.57
2:B:356:ARG:H	2:B:356:ARG:CD	2.17	0.57
1:A:69:THR:O	1:A:69:THR:CG2	2.53	0.56
1:A:63:ILE:HG13	1:A:63:ILE:O	2.06	0.56
2:B:126:LYS:NZ	5:B:502:DMS:H21	2.20	0.56
2:B:68:SER:HB2	2:B:230:MET:HE1	1.88	0.56
2:B:169:GLU:N	2:B:170:PRO:HD2	2.21	0.56
1:A:185:ASP:OD2	6:A:607:14N:H10	2.08	0.54
3:A:601:T27:N3	3:A:601:T27:H17	2.23	0.54
1:A:474:ASN:HD22	5:A:606:DMS:H12	1.73	0.54
1:A:478:GLU:HG2	7:A:905:HOH:O	2.09	0.52
2:B:169:GLU:OE1	2:B:170:PRO:HD3	2.10	0.52
2:B:81:ASN:O	2:B:154:LYS:HE2	2.09	0.52
2:B:94:ILE:O	2:B:95:PRO:C	2.51	0.51
2:B:88:TRP:HA	2:B:91:GLN:O	2.10	0.51
2:B:356:ARG:HD3	2:B:374:LYS:NZ	2.26	0.50
1:A:373[A]:GLN:NE2	7:A:939:HOH:O	2.14	0.50
1:A:516:GLU:CD	1:A:516:GLU:N	2.70	0.50
5:A:603:DMS:H22	7:A:885:HOH:O	2.11	0.50
1:A:425:LEU:HA	5:A:603:DMS:H23	1.94	0.50
2:B:30:LYS:NZ	2:B:404:GLU:OE2	2.37	0.50
2:B:356:ARG:H	2:B:356:ARG:HD2	1.77	0.50
2:B:323:LYS:NZ	2:B:344:GLU:OE2	2.45	0.49
2:B:195:ILE:HD11	2:B:199:ARG:NH2	2.27	0.49
2:B:357:MET:HB3	2:B:367:GLN:HG2	1.94	0.49
2:B:184:MET:HE3	7:B:690:HOH:O	2.12	0.49
1:A:65:LYS:O	1:A:68:SER:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:355:ALA:H	2:B:356:ARG:HE	1.61	0.48
1:A:40:GLU:HG2	7:A:1115:HOH:O	2.12	0.48
2:B:86:ASP:HB3	2:B:88:TRP:CZ2	2.50	0.47
2:B:68:SER:CB	2:B:230:MET:HE1	2.44	0.47
2:B:89:GLU:HG3	2:B:90:VAL:HG23	1.97	0.47
5:B:506:DMS:C2	7:B:773:HOH:O	2.49	0.47
2:B:107:THR:OG1	2:B:198:HIS:CE1	2.67	0.47
1:A:181:TYR:CE2	1:A:183:TYR:HB2	2.50	0.46
2:B:169:GLU:HG2	2:B:170:PRO:N	2.29	0.46
1:A:428:GLN:N	5:A:604:DMS:C2	2.64	0.46
2:B:126:LYS:HZ3	5:B:502:DMS:H21	1.79	0.46
1:A:185:ASP:OD2	6:A:607:14N:H4	2.16	0.46
1:A:254:VAL:CG2	1:A:293:ILE:HD11	2.46	0.45
2:B:399:GLU:C	5:B:505:DMS:H12	2.40	0.45
1:A:333:GLY:HA2	5:A:605:DMS:H23	1.96	0.45
2:B:163:SER:O	2:B:167:ILE:HG13	2.16	0.45
1:A:519:ASN:O	1:A:523:GLU:HG2	2.16	0.45
2:B:356:ARG:H	2:B:356:ARG:NE	2.15	0.45
1:A:369:THR:O	1:A:373[B]:GLN:HG2	2.16	0.45
1:A:28:GLU:HG3	1:A:135:ILE:HD12	1.99	0.44
2:B:356:ARG:NH1	7:B:850:HOH:O	2.40	0.44
1:A:36:GLU:HG3	7:A:995:HOH:O	2.18	0.44
2:B:89:GLU:HG3	2:B:90:VAL:N	2.33	0.44
2:B:201:LYS:O	2:B:204:GLU:HB2	2.18	0.43
1:A:277:ARG:HD3	7:A:1011:HOH:O	2.17	0.43
1:A:501:TYR:CZ	1:A:505:ILE:HD11	2.53	0.43
2:B:86:ASP:HB3	2:B:88:TRP:CE2	2.54	0.43
2:B:239:TRP:CD1	5:B:504:DMS:H22	2.54	0.43
2:B:271:TYR:HA	2:B:272:PRO:HD3	1.85	0.43
2:B:107:THR:OG1	2:B:198:HIS:HE1	2.01	0.42
2:B:203:GLU:OE1	2:B:206:ARG:HD2	2.19	0.42
6:A:607:14N:H1	7:A:1058:HOH:O	2.19	0.42
1:A:221:HIS:HD2	1:A:223:LYS:HB2	1.84	0.42
2:B:169:GLU:N	2:B:170:PRO:CD	2.82	0.42
2:B:242:GLN:HB2	2:B:351:THR:OG1	2.20	0.42
2:B:227:PHE:HD1	2:B:230:MET:CE	2.31	0.42
1:A:74:LEU:C	1:A:74:LEU:HD23	2.45	0.41
1:A:426:TRP:N	5:A:603:DMS:H23	2.24	0.41
2:B:126:LYS:HD3	5:B:502:DMS:C2	2.50	0.41
1:A:184:MET:HA	1:A:184:MET:HE2	2.03	0.41
1:A:191:SER:OG	1:A:198:HIS:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ASP:CG	6:A:607:14N:H4	2.45	0.41
2:B:126:LYS:HD3	5:B:502:DMS:H22	2.02	0.41
2:B:281:LYS:O	2:B:284:ARG:HG3	2.21	0.41
2:B:266:TRP:CG	2:B:426:TRP:CD1	3.09	0.40
2:B:200:THR:O	2:B:204:GLU:HG3	2.21	0.40
1:A:38:CYS:SG	1:A:132:ILE:HD11	2.61	0.40
1:A:115:TYR:CE2	6:A:607:14N:H17	2.56	0.40
2:B:103:LYS:HA	2:B:103:LYS:HD3	1.85	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)
1:A:529:GLU:OE2	2:B:104:LYS:HZ1[4_545]	1.40	0.20
1:A:529:GLU:OE2	2:B:104:LYS:NZ[4_545]	2.11	0.09

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	557/557 (100%)	545 (98%)	12 (2%)	0	100	100
2	B	410/429 (96%)	398 (97%)	12 (3%)	0	100	100
All	All	967/986 (98%)	943 (98%)	24 (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	498/495 (101%)	493 (99%)	5 (1%)	68	64
2	B	376/390 (96%)	370 (98%)	6 (2%)	55	47
All	All	874/885 (99%)	863 (99%)	11 (1%)	61	54

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

Mol	Chain	Res	Type
1	A	94	ILE
1	A	184	MET
1	A	194	GLU
1	A	221	HIS
1	A	399	GLU
2	B	92	LEU
2	B	94	ILE
2	B	197	GLN
2	B	242	GLN
2	B	356	ARG
2	B	357	MET

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	198	HIS
1	A	221	HIS
1	A	487	GLN
2	B	197	GLN
2	B	198	HIS
2	B	235	HIS
2	B	269	GLN
2	B	278	GLN
2	B	407	GLN

5.3.3 RNA ⓘ

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](#)

Of 14 ligands modelled in this entry, 1 is monoatomic - leaving 13 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	2.69	1 (33%)	3,3,3	0.51	0
5	DMS	B	502	-	3,3,3	2.79	1 (33%)	3,3,3	0.87	0
6	14N	A	607	-	17,17,17	3.45	4 (23%)	23,23,23	2.15	6 (26%)
5	DMS	B	505	-	3,3,3	2.34	1 (33%)	3,3,3	1.32	1 (33%)
5	DMS	B	504	-	3,3,3	2.70	1 (33%)	3,3,3	0.56	0
5	DMS	B	503	-	3,3,3	2.78	1 (33%)	3,3,3	1.65	1 (33%)
5	DMS	B	501	-	3,3,3	2.75	1 (33%)	3,3,3	0.82	0
5	DMS	B	506	-	3,3,3	2.72	1 (33%)	3,3,3	0.60	0
5	DMS	A	604	-	3,3,3	2.91	1 (33%)	3,3,3	0.62	0
5	DMS	B	507	-	3,3,3	2.57	1 (33%)	3,3,3	0.80	0
5	DMS	A	606	-	3,3,3	2.86	1 (33%)	3,3,3	0.80	0
5	DMS	A	605	-	3,3,3	2.70	1 (33%)	3,3,3	1.06	0
3	T27	A	601	-	30,30,30	1.08	1 (3%)	37,40,40	1.49	7 (18%)

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
6	14N	A	607	-	-	4/8/18/18	0/2/2/2
3	T27	A	601	-	-	0/13/14/14	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	607	14N	C10-C9	9.12	1.53	1.39
6	A	607	14N	C8-C7	8.04	1.51	1.38
6	A	607	14N	C11-C6	5.93	1.50	1.39
5	A	604	DMS	O-S	4.91	1.82	1.50
5	A	606	DMS	O-S	4.79	1.81	1.50
5	B	502	DMS	O-S	4.76	1.81	1.50
5	B	503	DMS	O-S	4.61	1.80	1.50
5	B	501	DMS	O-S	4.60	1.80	1.50
5	B	506	DMS	O-S	4.58	1.80	1.50
5	A	603	DMS	O-S	4.57	1.80	1.50
5	A	605	DMS	O-S	4.53	1.80	1.50
5	B	504	DMS	O-S	4.52	1.80	1.50
5	B	507	DMS	O-S	4.30	1.78	1.50
5	B	505	DMS	O-S	3.82	1.75	1.50
3	A	601	T27	C12-N4	3.02	1.42	1.36
6	A	607	14N	C6-N2	2.64	1.46	1.38

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	607	14N	C1-N1-C2	6.33	122.69	110.63
3	A	601	T27	C10-C9-N2	-4.10	118.95	123.97
6	A	607	14N	C1-N1-C5	3.80	117.88	110.63
6	A	607	14N	C4-N2-C3	3.53	119.51	111.57
3	A	601	T27	C9-N2-C12	3.52	118.37	115.42
6	A	607	14N	C2-C3-N2	-3.03	104.42	110.78
3	A	601	T27	C2-C1-C6	2.36	120.96	118.25
3	A	601	T27	C7-C1-C6	-2.35	118.56	121.42
3	A	601	T27	C4-C3-C21	-2.33	113.64	120.61
3	A	601	T27	C15-C16-N4	-2.33	112.74	120.61
6	A	607	14N	C7-C6-N2	-2.22	118.31	121.39
5	B	505	DMS	O-S-C1	2.20	117.51	106.49
6	A	607	14N	C4-N2-C6	2.16	124.01	118.11
5	B	503	DMS	O-S-C2	2.09	116.96	106.49
3	A	601	T27	C10-C11-N3	-2.08	119.67	123.15

There are no chirality outliers.

All (4) torsion outliers are listed below:

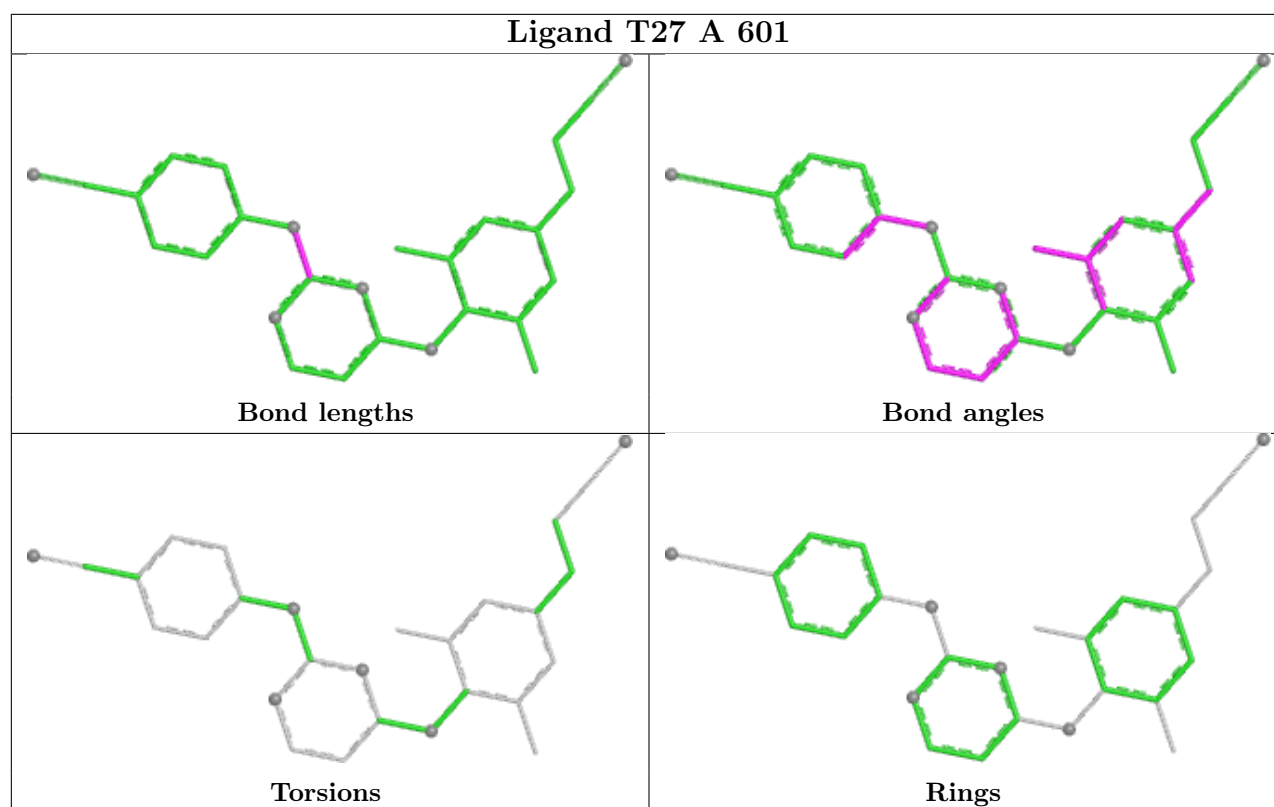
Mol	Chain	Res	Type	Atoms
6	A	607	14N	O2-C12-C9-C10
6	A	607	14N	O2-C12-C9-C8
6	A	607	14N	O1-C12-C9-C10
6	A	607	14N	O1-C12-C9-C8

There are no ring outliers.

12 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	603	DMS	5	0
5	B	502	DMS	5	0
6	A	607	14N	5	0
5	B	505	DMS	5	0
5	B	504	DMS	1	0
5	B	503	DMS	3	0
5	B	506	DMS	2	0
5	A	604	DMS	4	0
5	B	507	DMS	1	0
5	A	606	DMS	3	0
5	A	605	DMS	1	0
3	A	601	T27	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	556/557 (99%)	0.22	43 (7%) 19 17	15, 41, 91, 165	2 (0%)
2	B	412/429 (96%)	0.61	63 (15%) 5 4	15, 46, 116, 170	1 (0%)
All	All	968/986 (98%)	0.38	106 (10%) 10 9	15, 43, 108, 170	3 (0%)

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	92	LEU	7.3
2	B	95	PRO	7.3
2	B	94	ILE	6.7
2	B	240	THR	5.7
2	B	90	VAL	5.6
2	B	283	LEU	5.6
1	A	554	ALA	5.5
2	B	241	VAL	4.8
2	B	5	ILE	4.8
2	B	88	TRP	4.7
2	B	212	TRP	4.7
1	A	357	MET	4.6
2	B	93	GLY	4.4
2	B	214	LEU	4.4
2	B	229	TRP	4.3
1	A	90	VAL	4.3
1	A	221	HIS	4.1
2	B	359	GLY	4.1
2	B	195	ILE	4.0
2	B	202	ILE	4.0
1	A	68	SER	4.0
2	B	66	LYS	3.9
1	A	69	THR	3.9
2	B	360	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	544	GLY	3.8
2	B	315	HIS	3.7
1	A	220	LYS	3.7
2	B	200	THR	3.7
1	A	92	LEU	3.6
1	A	63	ILE	3.5
2	B	198	HIS	3.4
1	A	217	PRO	3.4
1	A	288	ALA	3.4
1	A	286	THR	3.4
2	B	361	HIS	3.3
2	B	272	PRO	3.3
2	B	210	LEU	3.2
2	B	213	GLY	3.2
2	B	356	ARG	3.2
2	B	69	THR	3.2
2	B	234	LEU	3.2
2	B	196	GLY	3.2
1	A	24	TRP	3.2
2	B	357	MET	3.2
1	A	543	GLY	3.2
2	B	87	PHE	3.1
2	B	239	TRP	3.1
2	B	193	LEU	3.1
2	B	228	LEU	3.1
2	B	209	LEU	3.0
1	A	285	GLY	3.0
2	B	68	SER	2.9
2	B	235	HIS	2.9
2	B	425	LEU	2.9
1	A	282	LEU	2.8
1	A	222	GLN	2.8
2	B	91	GLN	2.8
2	B	105	SER	2.8
1	A	66	LYS	2.8
2	B	237	ASP	2.8
2	B	167	ILE	2.7
2	B	242	GLN	2.7
2	B	355	ALA	2.7
1	A	64	LYS	2.7
1	A	292	VAL	2.7
1	A	218	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	285	GLY	2.6
1	A	71	TRP	2.6
1	A	360	ALA	2.6
2	B	232	TYR	2.6
1	A	450	THR	2.6
2	B	104	LYS	2.6
2	B	238	LYS	2.5
1	A	542	ILE	2.5
2	B	65	LYS	2.4
2	B	7	THR	2.4
1	A	299	ALA	2.4
1	A	546	GLU	2.4
1	A	359	GLY	2.4
1	A	67	ASP	2.4
1	A	72	ARG	2.4
2	B	122	GLU	2.3
2	B	169	GLU	2.3
2	B	318	TYR	2.3
1	A	283	LEU	2.3
2	B	208	HIS	2.3
1	A	223	LYS	2.3
2	B	281	LYS	2.3
1	A	216	THR	2.3
1	A	219	LYS	2.3
1	A	313	PRO	2.2
1	A	552	VAL	2.2
1	A	65	LYS	2.2
2	B	428	GLN	2.2
1	A	287	LYS	2.2
2	B	227	PHE	2.2
2	B	197	GLN	2.2
2	B	67	ASP	2.2
1	A	541	GLY	2.1
1	A	551	LEU	2.1
2	B	204	GLU	2.1
2	B	194	GLU	2.1
1	A	226	PRO	2.1
1	A	547	GLN	2.0
2	B	230	MET	2.0
2	B	8	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

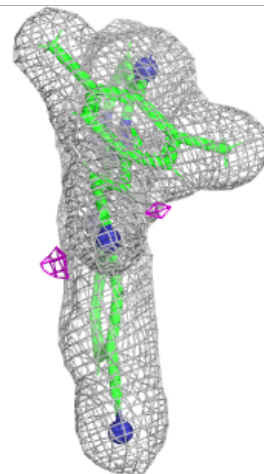
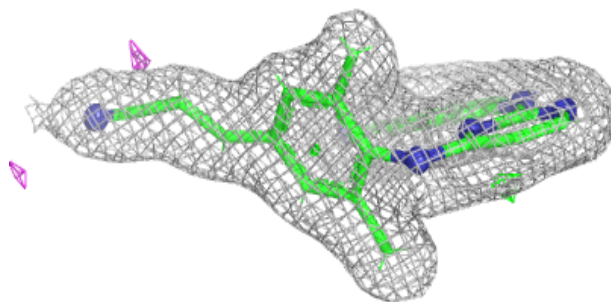
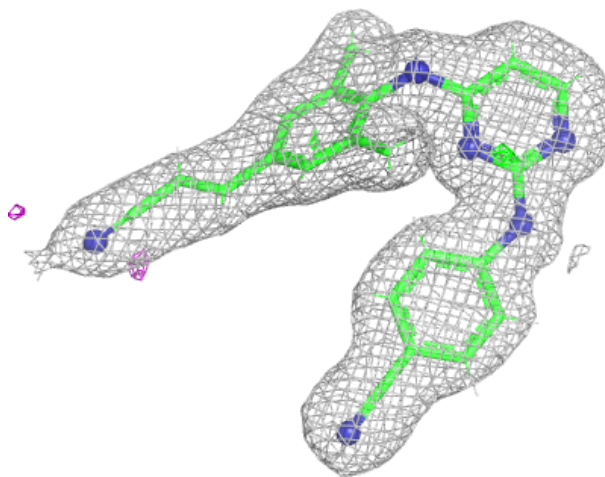
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MG	A	602	1/1	0.63	0.23	65,65,65,65	0
5	DMS	B	504	4/4	0.80	0.21	50,76,81,132	0
5	DMS	A	606	4/4	0.85	0.23	45,56,81,86	0
5	DMS	B	507	4/4	0.88	0.21	29,30,83,117	0
5	DMS	B	501	4/4	0.89	0.21	43,52,52,117	0
5	DMS	A	605	4/4	0.90	0.15	45,53,66,70	0
5	DMS	B	506	4/4	0.92	0.22	57,76,96,106	0
5	DMS	B	503	4/4	0.93	0.21	20,27,56,147	0
6	14N	A	607	16/16	0.93	0.11	34,39,56,56	0
5	DMS	A	603	4/4	0.95	0.22	22,51,73,163	0
5	DMS	B	505	4/4	0.96	0.16	32,35,43,146	0
3	T27	A	601	28/28	0.96	0.07	25,30,41,41	0
5	DMS	A	604	4/4	0.97	0.08	34,40,44,48	0
5	DMS	B	502	4/4	0.98	0.09	31,36,41,49	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 T27 A 601:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.