



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 21, 2026 – 04:08 PM EDT

PDB ID : 7TAZ / pdb_00007taz
Title : Crystal structure of HIV-1 reverse transcriptase (RT) in complex with VM-1500A, a non-nucleoside RT inhibitor
Authors : Snyder, A.A.; Risener, C.J.; Kirby, K.A.; Sarafianos, S.G.
Deposited on : 2021-12-21
Resolution : 2.40 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

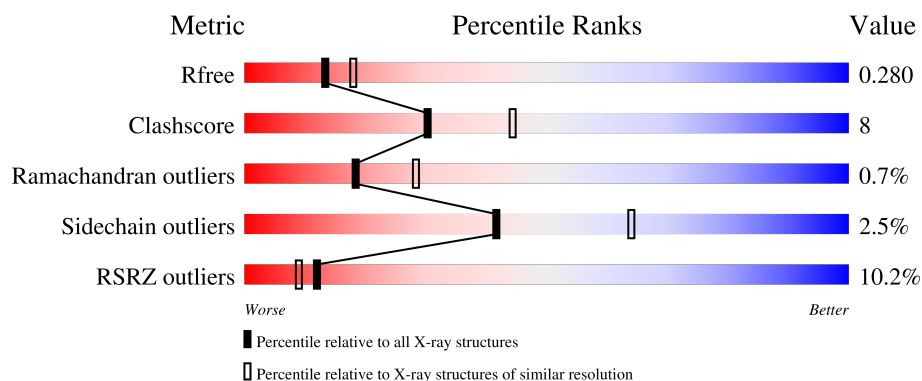
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	9% 78% 16% • 5%
2	B	429	10% 77% 16% • 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15605 atoms, of which 7801 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	530	Total	C	H	N	O	S	0	2	0
			8727	2813	4393	719	794	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

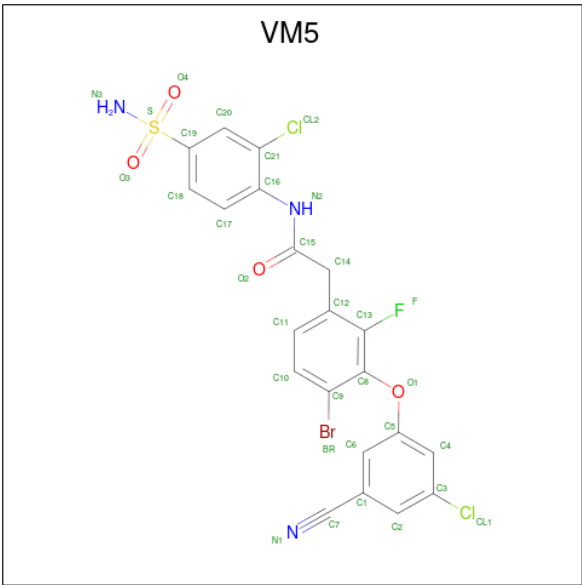
- Molecule 2 is a protein called Reverse transcriptase p51.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	404	Total	C	H	N	O	S	0	3	0
			6748	2186	3395	554	606	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 2-[4-bromo-3-(3-chloro-5-cyanophenoxy)-2-fluorophenyl]-N-(2-chloro-4-sulfamoylphenyl)acetamide (CCD ID: VM5) (formula: C₂₁H₁₃BrCl₂FN₃O₄S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms									ZeroOcc	AltConf
			Total	Br	C	Cl	F	H	N	O	S		
3	A	1	46	1	21	2	1	13	3	4	1	0	0

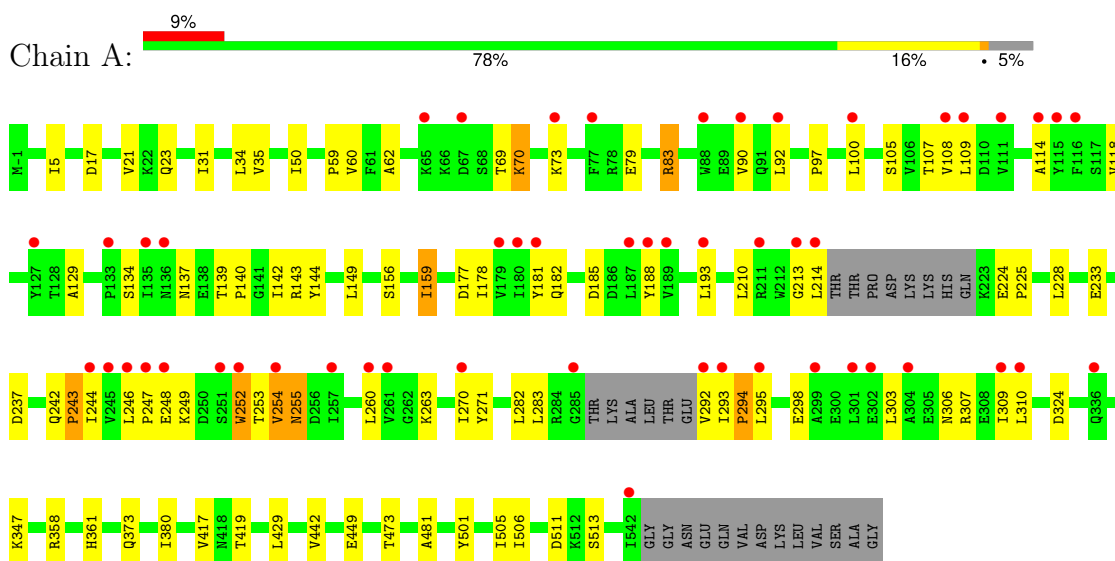
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	53	Total	O	0	0
			53	53		
4	B	31	Total	O	0	0
			31	31		

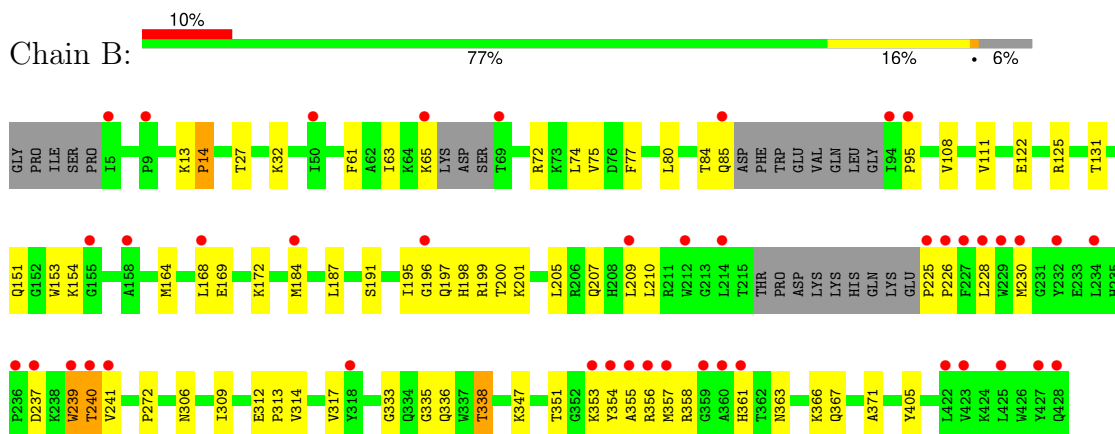
3 Residue-property plots

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: Reverse transcriptase p51



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 73.87Å 108.64Å 90.00° 99.96° 90.00°	Depositor
Resolution (Å)	31.38 – 2.40 31.38 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (31.38-2.40) 99.9 (31.38-2.40)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.60 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.247 , 0.279 0.249 , 0.280	Depositor DCC
R_{free} test set	2478 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	66.5	Xtriage
Anisotropy	0.339	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15605	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.24% 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: VM5

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	0.29	0/4455	0.48	3/6053 (0.0%)
2	B	0.24	0/3459	0.54	7/4696 (0.1%)
All	All	0.27	0/7914	0.51	10/10749 (0.1%)

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
2	B	0	2

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	237	ASP	N-CA-C	15.52	134.07	109.39
1	A	255	ASN	N-CA-C	-11.07	99.50	113.23
2	B	237	ASP	CB-CA-C	-9.03	97.47	112.00
2	B	240	THR	N-CA-C	-8.84	100.92	112.68
1	A	254	VAL	CB-CA-C	-8.30	101.11	112.24
1	A	254	VAL	N-CA-C	7.83	119.54	111.00
2	B	239	TRP	CB-CA-C	6.69	122.99	110.95
2	B	333	GLY	CA-C-O	-6.02	118.08	122.23
2	B	237	ASP	CA-C-N	5.43	128.90	122.44
2	B	237	ASP	C-N-CA	5.43	128.90	122.44

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	356	ARG	Sidechain
2	B	358	ARG	Sidechain

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	4334	4393	4390	68	0
2	B	3353	3395	3381	63	0
3	A	33	13	0	2	0
4	A	53	0	0	0	0
4	B	31	0	0	0	0
All	All	7804	7801	7771	130	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 8.

All (130) 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)
2:B:357:MET:HE2	2:B:367:GLN:NE2	1.27	1.49
2:B:357:MET:SD	2:B:361:HIS:HB2	1.81	1.21
2:B:357:MET:CE	2:B:367:GLN:NE2	2.12	1.13
1:A:282:LEU:HD23	1:A:293:ILE:HG22	1.18	1.06
2:B:357:MET:SD	2:B:361:HIS:CB	2.49	1.00
1:A:282:LEU:HD23	1:A:293:ILE:CG2	1.89	1.00
2:B:357:MET:HE2	2:B:367:GLN:HE22	1.32	0.95
1:A:294:PRO:O	1:A:295:LEU:HD12	1.69	0.92
2:B:363:ASN:HD22	2:B:366:LYS:HB2	1.34	0.91
2:B:65:LYS:HD3	2:B:230:MET:SD	2.13	0.89
1:A:225:PRO:HG2	3:A:601:VM5:O4	1.73	0.88
2:B:357:MET:HE2	2:B:367:GLN:CD	2.01	0.86
2:B:357:MET:CE	2:B:367:GLN:HE22	1.85	0.86
2:B:363:ASN:ND2	2:B:366:LYS:HB2	1.93	0.83
2:B:357:MET:HE1	2:B:361:HIS:ND1	1.93	0.82
2:B:357:MET:SD	2:B:361:HIS:CA	2.70	0.79
1:A:294:PRO:C	1:A:295:LEU:HD12	2.08	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:357:MET:HE1	2:B:361:HIS:CG	2.19	0.76
2:B:84:THR:HG21	2:B:153:TRP:HE1	1.51	0.74
1:A:253:THR:HB	1:A:292:VAL:HG22	1.72	0.70
2:B:80:LEU:O	2:B:84:THR:HG23	1.92	0.69
2:B:335:GLY:CA	2:B:357:MET:HE3	2.23	0.69
1:A:248:GLU:O	1:A:249:LYS:HG3	1.95	0.67
1:A:17:ASP:O	1:A:83:ARG:NE	2.29	0.66
1:A:282:LEU:O	1:A:293:ILE:HD13	1.96	0.65
1:A:449:GLU:OE1	1:A:449:GLU:N	2.31	0.64
1:A:247:PRO:HG2	1:A:260:LEU:HD21	1.80	0.63
1:A:134:SER:HB2	1:A:139:THR:HG22	1.80	0.63
1:A:282:LEU:HB3	1:A:293:ILE:HG21	1.79	0.62
1:A:31:ILE:O	1:A:35:VAL:HG23	2.00	0.62
2:B:357:MET:CE	2:B:367:GLN:CD	2.68	0.62
2:B:335:GLY:HA2	2:B:357:MET:HE3	1.83	0.61
1:A:149:LEU:HD23	1:A:156:SER:HA	1.83	0.60
2:B:335:GLY:HA3	2:B:357:MET:HE3	1.84	0.59
2:B:225:PRO:HG3	2:B:228:LEU:HD23	1.83	0.59
1:A:246:LEU:HG	1:A:310:LEU:HD12	1.82	0.59
2:B:196:GLY:O	2:B:200:THR:HG23	2.03	0.59
1:A:134:SER:CB	1:A:139:THR:HG22	2.33	0.58
1:A:114:ALA:HB2	1:A:214:LEU:HD11	1.86	0.58
2:B:164:MET:HA	2:B:164:MET:HE3	1.85	0.58
1:A:246:LEU:HD12	1:A:307:ARG:HA	1.84	0.57
2:B:357:MET:CE	2:B:361:HIS:HA	2.35	0.57
2:B:207:GLN:HA	2:B:210:LEU:HD12	1.88	0.56
2:B:357:MET:SD	2:B:361:HIS:HA	2.45	0.56
2:B:317:VAL:HG22	2:B:347:LYS:HD3	1.88	0.56
2:B:195:ILE:HD11	2:B:199:ARG:NH2	2.20	0.56
1:A:97:PRO:HA	1:A:100:LEU:HD12	1.86	0.55
1:A:134:SER:CB	1:A:139:THR:CG2	2.84	0.55
2:B:197:GLN:O	2:B:200:THR:OG1	2.17	0.55
2:B:336:GLN:HE21	2:B:355:ALA:HB2	1.71	0.55
1:A:248:GLU:O	1:A:249:LYS:CG	2.56	0.54
2:B:336:GLN:HA	2:B:355:ALA:HA	1.90	0.54
2:B:336:GLN:HE21	2:B:355:ALA:CB	2.21	0.54
2:B:75:VAL:HG11	2:B:77:PHE:CZ	2.43	0.54
1:A:361:HIS:ND1	1:A:513:SER:OG	2.37	0.53
1:A:417:VAL:HG22	1:A:419:THR:HG23	1.91	0.53
2:B:354:TYR:CD2	2:B:371:ALA:HB2	2.43	0.53
2:B:357:MET:HE1	2:B:367:GLN:HE22	1.71	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:SER:HB2	1:A:139:THR:CG2	2.39	0.52
1:A:252:TRP:N	1:A:252:TRP:CD1	2.79	0.51
1:A:380:ILE:HD12	2:B:27:THR:HG22	1.94	0.50
1:A:34:LEU:HD21	1:A:62:ALA:HB2	1.93	0.50
2:B:306:ASN:HA	2:B:309:ILE:HD12	1.92	0.50
1:A:283:LEU:O	1:A:283:LEU:HG	2.12	0.50
2:B:111:VAL:HG11	2:B:187:LEU:HD12	1.93	0.49
2:B:84:THR:O	2:B:85:GLN:C	2.55	0.49
2:B:357:MET:SD	2:B:361:HIS:N	2.86	0.48
2:B:13:LYS:HB3	2:B:14:PRO:HD2	1.95	0.48
2:B:314:VAL:HB	2:B:317:VAL:HG21	1.94	0.48
2:B:240:THR:HG23	2:B:241:VAL:N	2.29	0.48
1:A:303:LEU:O	1:A:303:LEU:HD13	2.13	0.48
2:B:13:LYS:O	2:B:14:PRO:C	2.56	0.48
2:B:74:LEU:HD23	2:B:75:VAL:N	2.29	0.48
1:A:50:ILE:HG13	1:A:143:ARG:HB3	1.96	0.47
2:B:63:ILE:HD13	2:B:74:LEU:HD12	1.96	0.47
2:B:363:ASN:ND2	2:B:405:TYR:CZ	2.80	0.47
1:A:79:GLU:O	1:A:83:ARG:HG3	2.14	0.46
1:A:242:GLN:O	1:A:243:PRO:C	2.59	0.46
2:B:164:MET:HE2	2:B:168:LEU:HG	1.97	0.46
2:B:338:THR:HG23	2:B:353:LYS:CD	2.45	0.46
1:A:34:LEU:HD22	1:A:73:LYS:HE2	1.96	0.46
1:A:139:THR:OG1	1:A:140:PRO:HD2	2.16	0.46
1:A:107:THR:HG22	1:A:109:LEU:CD1	2.45	0.46
2:B:197:GLN:O	2:B:201:LYS:HG2	2.16	0.46
2:B:72:ARG:NH2	2:B:151:GLN:OE1	2.49	0.45
1:A:114:ALA:HB2	1:A:214:LEU:CD1	2.47	0.45
1:A:248:GLU:HA	1:A:307:ARG:HH22	1.82	0.45
1:A:210:LEU:O	1:A:210:LEU:HD13	2.16	0.45
1:A:213:GLY:O	1:A:214:LEU:HD22	2.16	0.45
2:B:239:TRP:HA	2:B:239:TRP:CE3	2.52	0.45
1:A:69:THR:OG1	1:A:70:LYS:NZ	2.50	0.44
2:B:122:GLU:OE2	2:B:125:ARG:NH2	2.50	0.44
2:B:354:TYR:O	2:B:354:TYR:CG	2.71	0.44
1:A:108:VAL:HG13	1:A:188:TYR:CD1	2.53	0.44
2:B:191:SER:OG	2:B:198:HIS:ND1	2.47	0.44
1:A:254:VAL:HG23	1:A:292:VAL:CA	2.48	0.44
1:A:271:TYR:HB3	1:A:309:ILE:CG2	2.48	0.44
1:A:129:ALA:HA	1:A:144:TYR:O	2.18	0.44
1:A:501:TYR:CZ	1:A:505:ILE:HD11	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:TYR:CD2	3:A:601:VM5:BR	3.27	0.43
1:A:142:ILE:HD12	1:A:142:ILE:N	2.33	0.43
1:A:303:LEU:O	1:A:307:ARG:HG2	2.19	0.43
1:A:21:VAL:HB	1:A:59:PRO:HD3	2.00	0.43
1:A:246:LEU:HD11	1:A:306:ASN:HB3	2.00	0.43
2:B:195:ILE:HD11	2:B:199:ARG:HH21	1.82	0.43
1:A:5:ILE:HG21	1:A:118:VAL:HG13	2.01	0.42
1:A:92:LEU:HD23	1:A:92:LEU:N	2.35	0.42
1:A:244:ILE:HG23	1:A:263:LYS:HE2	2.02	0.42
1:A:429:LEU:HD11	1:A:506:ILE:CG2	2.49	0.42
1:A:34:LEU:HD22	1:A:73:LYS:CE	2.49	0.42
2:B:241:VAL:HG13	2:B:351:THR:CG2	2.48	0.42
1:A:23:GLN:OE1	1:A:60:VAL:HG12	2.20	0.42
1:A:149:LEU:HD21	1:A:159:ILE:HB	2.01	0.42
1:A:228:LEU:HD22	1:A:233:GLU:HG2	2.02	0.42
1:A:442:VAL:HB	1:A:481:ALA:HB1	2.02	0.42
2:B:32:LYS:HA	2:B:32:LYS:HE2	2.02	0.42
1:A:358:ARG:NE	1:A:358:ARG:HA	2.35	0.41
1:A:224:GLU:HG2	1:A:225:PRO:HD2	2.02	0.41
2:B:61:PHE:CZ	2:B:74:LEU:HD13	2.54	0.41
2:B:154:LYS:HA	2:B:184:MET:HE1	2.02	0.41
1:A:177:ASP:OD1	1:A:193:LEU:HD11	2.20	0.41
1:A:282:LEU:HD23	1:A:293:ILE:HG21	1.93	0.41
1:A:511:ASP:OD1	1:A:511:ASP:C	2.63	0.41
2:B:169:GLU:HA	2:B:172:LYS:HD2	2.02	0.41
2:B:312:GLU:HB3	2:B:313:PRO:HD2	2.02	0.41
2:B:168:LEU:HD21	2:B:209:LEU:HD21	2.02	0.41
1:A:271:TYR:HB3	1:A:309:ILE:HG22	2.03	0.41
1:A:248:GLU:C	1:A:249:LYS:HG3	2.44	0.41
2:B:164:MET:HE2	2:B:168:LEU:CG	2.51	0.41
1:A:237:ASP:OD1	1:A:237:ASP:N	2.51	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	526/557 (94%)	502 (95%)	22 (4%)	2 (0%)	30	43
2	B	399/429 (93%)	372 (93%)	23 (6%)	4 (1%)	12	20
All	All	925/986 (94%)	874 (94%)	45 (5%)	6 (1%)	18	32

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	294	PRO
2	B	14	PRO
2	B	272	PRO
1	A	243	PRO
2	B	226	PRO
2	B	95	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	475/495 (96%)	457 (96%)	18 (4%)	29	49
2	B	370/390 (95%)	366 (99%)	4 (1%)	65	82
All	All	845/885 (96%)	823 (97%)	22 (3%)	42	63

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	LYS
1	A	83	ARG
1	A	90	VAL
1	A	105	SER
1	A	137	ASN
1	A	159	ILE
1	A	178	ILE

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Mol	Chain	Res	Type
1	A	182	GLN
1	A	185	ASP
1	A	252	TRP
1	A	255	ASN
1	A	270	ILE
1	A	298	GLU
1	A	324	ASP
1	A	347	LYS
1	A	373[A]	GLN
1	A	373[B]	GLN
1	A	473	THR
2	B	108	VAL
2	B	131	THR
2	B	205	LEU
2	B	338	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	GLN
1	A	182	GLN
1	A	336	GLN
2	B	85	GLN
2	B	137	ASN
2	B	255	ASN
2	B	336	GLN
2	B	363	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

1 ligand is 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
3	VM5	A	601	-	35,35,35	1.66	5 (14%)	50,51,51	2.47	9 (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
3	VM5	A	601	-	-	2/20/20/20	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	VM5	S-N3	5.16	1.70	1.60
3	A	601	VM5	C15-N2	4.33	1.44	1.35
3	A	601	VM5	C1-C7	3.79	1.52	1.44
3	A	601	VM5	O2-C15	-2.42	1.18	1.23
3	A	601	VM5	C19-S	2.31	1.80	1.77

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	VM5	O4-S-O3	-11.16	101.63	118.80
3	A	601	VM5	C12-C14-C15	-8.23	97.59	113.56
3	A	601	VM5	C11-C12-C13	4.95	120.10	116.46
3	A	601	VM5	O4-S-C19	3.92	111.78	107.35
3	A	601	VM5	O4-S-N3	3.54	112.45	107.35
3	A	601	VM5	C20-C21-C16	-3.09	119.31	121.77
3	A	601	VM5	O3-S-N3	2.77	111.35	107.35
3	A	601	VM5	O1-C8-C9	-2.59	116.93	120.61
3	A	601	VM5	C17-C16-C21	2.33	121.00	117.89

There are no chirality outliers.

All (2) torsion outliers are listed below:

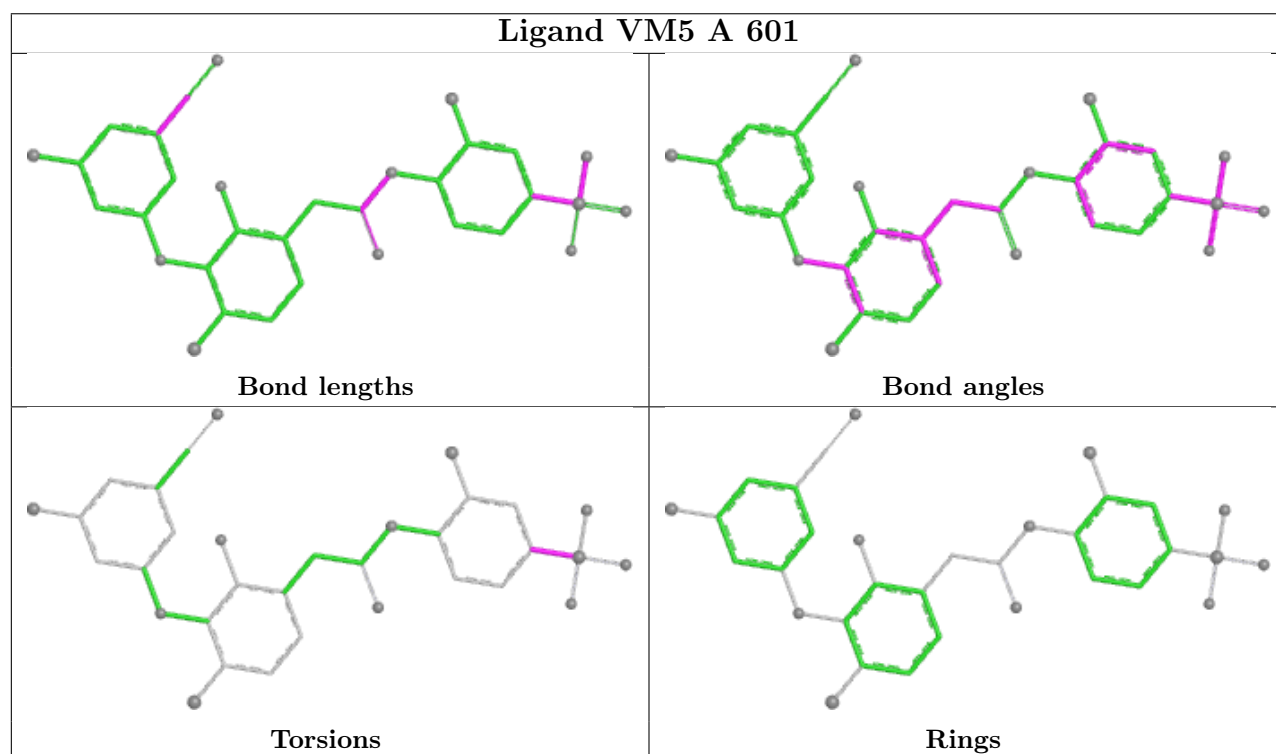
Mol	Chain	Res	Type	Atoms
3	A	601	VM5	C20-C19-S-O3
3	A	601	VM5	C18-C19-S-O3

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	VM5	2	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	530/557 (95%)	0.68	52 (9%) 13 10	39, 103, 178, 217	2 (0%)
2	B	404/429 (94%)	0.64	43 (10%) 11 8	40, 90, 174, 221	2 (0%)
All	All	934/986 (94%)	0.66	95 (10%) 12 9	39, 96, 176, 221	4 (0%)

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	247	PRO	6.1
2	B	94	ILE	5.8
2	B	354	TYR	5.0
1	A	260	LEU	4.6
1	A	90	VAL	4.4
2	B	360	ALA	4.3
1	A	116	PHE	4.2
2	B	227	PHE	4.1
2	B	239	TRP	4.1
1	A	92	LEU	4.1
2	B	423	VAL	4.0
1	A	246	LEU	3.9
2	B	356	ARG	3.9
2	B	228	LEU	3.8
2	B	353	LYS	3.7
2	B	232	TYR	3.6
1	A	114	ALA	3.6
2	B	234	LEU	3.6
2	B	427	TYR	3.5
2	B	236	PRO	3.4
2	B	214	LEU	3.3
1	A	115	TYR	3.3
2	B	240	THR	3.3
1	A	135	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	270	ILE	3.3
1	A	189	VAL	3.2
1	A	261	VAL	3.2
2	B	225	PRO	3.1
1	A	310	LEU	3.1
2	B	212	TRP	3.1
2	B	318	TYR	3.1
2	B	422	LEU	3.0
1	A	252	TRP	3.0
1	A	257	ILE	3.0
1	A	111	VAL	2.9
1	A	254	VAL	2.9
2	B	65	LYS	2.9
1	A	214	LEU	2.9
2	B	5	ILE	2.9
1	A	251	SER	2.8
1	A	108	VAL	2.8
1	A	73	LYS	2.8
2	B	361	HIS	2.7
1	A	295	LEU	2.7
1	A	293	ILE	2.6
1	A	244	ILE	2.6
1	A	181	TYR	2.6
1	A	309	ILE	2.6
1	A	245	VAL	2.6
1	A	133	PRO	2.6
2	B	425	LEU	2.6
2	B	355	ALA	2.6
1	A	188	TYR	2.6
2	B	359	GLY	2.5
2	B	209	LEU	2.5
2	B	428	GLN	2.5
1	A	100	LEU	2.5
2	B	226	PRO	2.5
1	A	301	LEU	2.5
2	B	230	MET	2.5
2	B	237	ASP	2.4
2	B	85	GLN	2.4
2	B	69	THR	2.4
1	A	187	LEU	2.4
2	B	229	TRP	2.4
1	A	77	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	357	MET	2.4
2	B	9	PRO	2.3
1	A	213	GLY	2.3
1	A	88	TRP	2.3
1	A	136	ASN	2.3
2	B	184	MET	2.3
1	A	304	ALA	2.3
1	A	336	GLN	2.3
2	B	196	GLY	2.3
1	A	180	ILE	2.3
2	B	95	PRO	2.2
1	A	302	GLU	2.2
2	B	241	VAL	2.2
2	B	158	ALA	2.2
1	A	193	LEU	2.2
1	A	65	LYS	2.2
1	A	292	VAL	2.1
1	A	179	VAL	2.1
2	B	50	ILE	2.1
1	A	67	ASP	2.1
1	A	109	LEU	2.1
2	B	155	GLY	2.1
1	A	127	TYR	2.1
2	B	168	LEU	2.1
1	A	285	GLY	2.1
1	A	542	ILE	2.1
1	A	299	ALA	2.0
1	A	248	GLU	2.0
1	A	211[A]	ARG	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 ⓘ

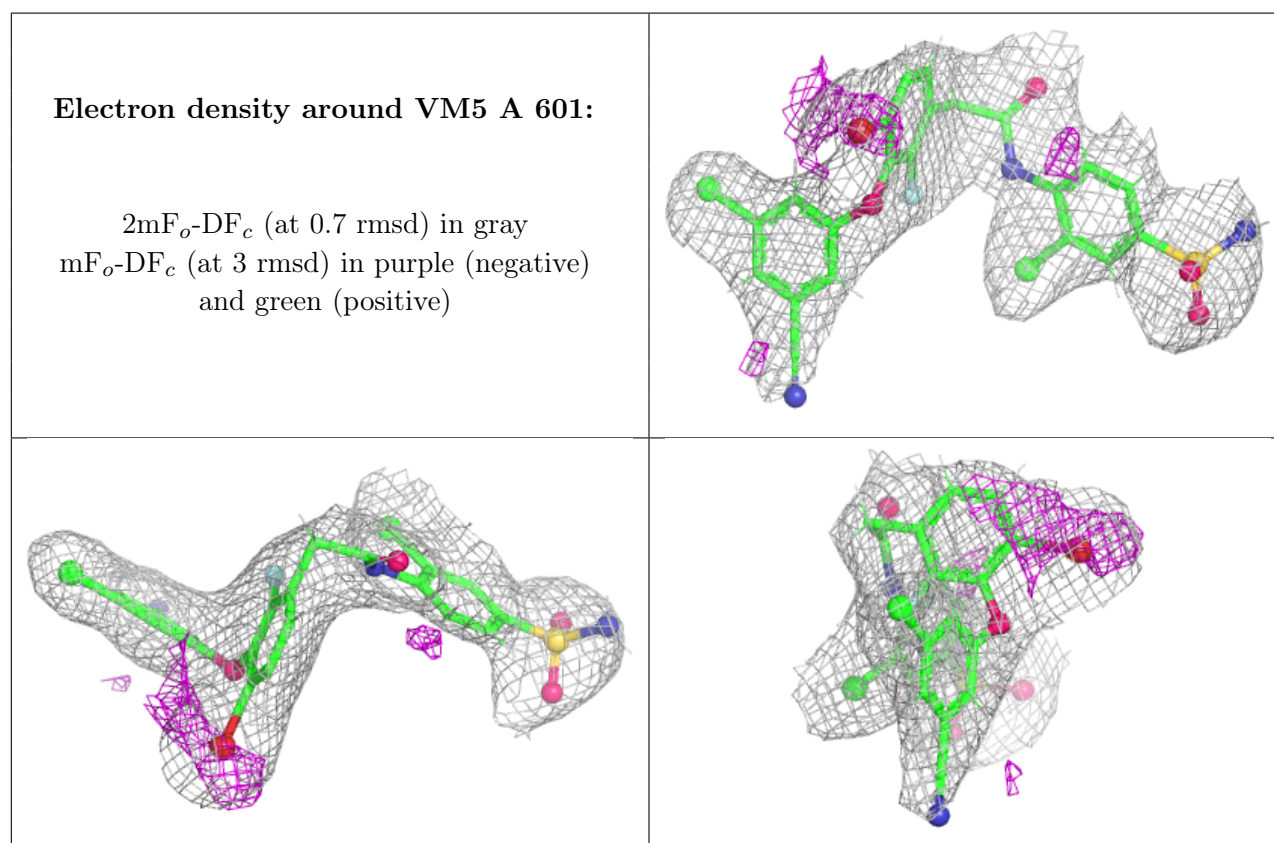
There are no oligosaccharides in this entry.

6.4 Ligands [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($\text{\AA}^2$)	Q<0.9
3	VM5	A	601	33/33	0.93	0.11	81,88,114,123	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.