



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:10 PM UTC

PDB ID : 7SO1 / pdb_00007so1
Title : Crystal Structure of HIV-1 Reverse Transcriptase in Complex with (E)-4-((4-((4-(2-cyanovinyl)-2,6-dimethylphenyl)amino)-6-(3-morpholinopropoxy)-1,3,5-triazin-2-yl)amino)benzonitrile (JLJ564)
Authors : Frey, K.M.; Anderson, K.S.
Deposited on : 2021-10-28
Resolution : 2.73 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

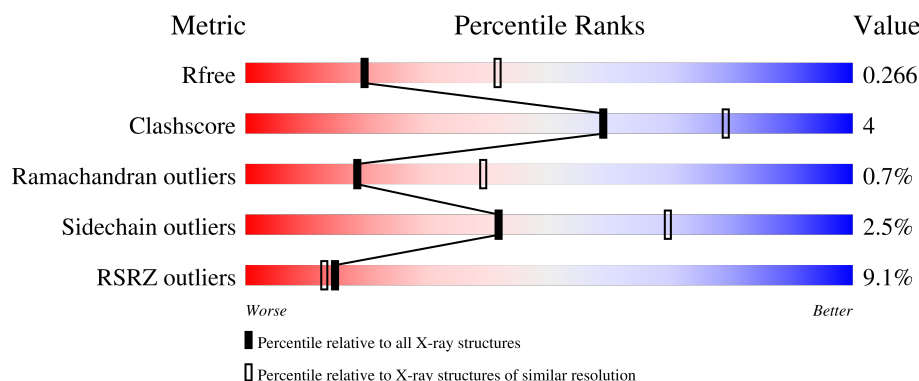
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.73 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	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
Sidechain outliers	187428	4585 (2.74-2.70)
RSRZ outliers	180081	4348 (2.74-2.70)

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% 84% 14% ..
2	B	428	9% 82% 14% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7866 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 p66.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	549	4415	2859	726	823	7	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

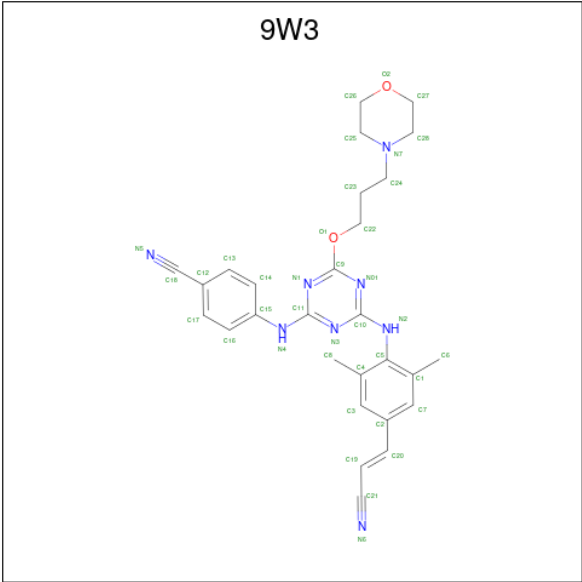
- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	412	3413	2225	564	617	7	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	conflict	UNP P03366

- Molecule 3 is 4-[(4-{4-[(E)-2-cyanoethenyl]-2,6-dimethylanilino}-6-[3-(morpholin-4-yl)propoxy]-1,3,5-triazin-2-yl)amino]benzonitrile (CCD ID: 9W3) (formula: C₂₈H₃₀N₈O₂) (labeled as "Ligand of Interest" by depositor).

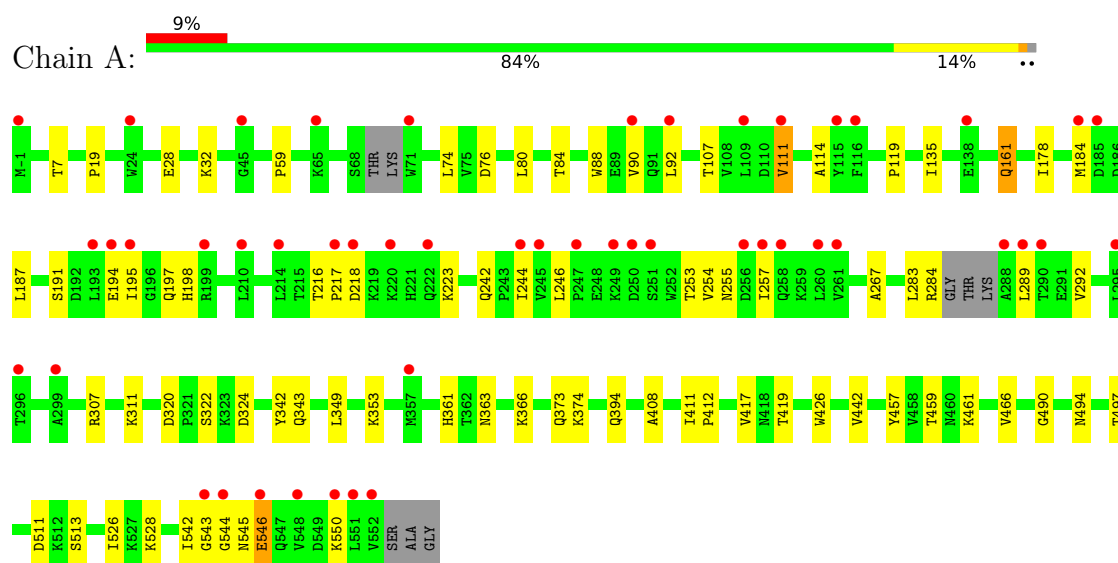


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			38	28	8	2		

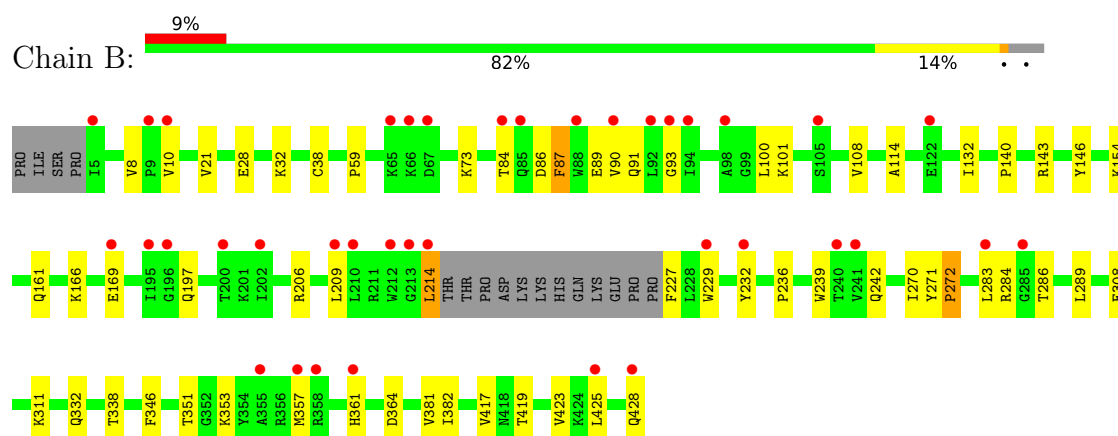
3 Residue-property plots [i](#)

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 p66



- 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	162.03Å 73.40Å 108.53Å 90.00° 100.38° 90.00°	Depositor
Resolution (Å)	38.04 – 2.73 38.04 – 2.73	Depositor EDS
% Data completeness (in resolution range)	98.2 (38.04-2.73) 98.1 (38.04-2.73)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.15 (at 2.72Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.217 , 0.264 0.220 , 0.266	Depositor DCC
R_{free} test set	1655 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	59.9	Xtriage
Anisotropy	0.409	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 35.7	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	0.92	EDS
Total number of atoms	7866	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.56% 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: 9W3

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	0/4531	0.70	2/6174 (0.0%)
2	B	0.29	0/3511	0.67	0/4768
All	All	0.29	0/8042	0.69	2/10942 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	242	GLN	CA-C-N	5.42	126.62	119.84
1	A	242	GLN	C-N-CA	5.42	126.62	119.84

There are no chirality outliers.

There are no planarity outliers.

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	4415	0	4387	43	1
2	B	3413	0	3443	33	1
3	A	38	0	0	0	0
All	All	7866	0	7830	69	1

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 4.

All (69) 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:91:GLN:HG3	2:B:93:GLY:H	1.46	0.77
1:A:544:GLY:HA2	2:B:286:THR:HG22	1.68	0.74
1:A:28:GLU:HG3	1:A:135:ILE:HD12	1.73	0.69
1:A:543:GLY:HA3	2:B:284:ARG:HA	1.75	0.68
1:A:59:PRO:HG2	1:A:76:ASP:HB3	1.77	0.66
2:B:114:ALA:HB2	2:B:214:LEU:HD13	1.80	0.62
1:A:320:ASP:OD2	1:A:322:SER:OG	2.21	0.58
1:A:255:ASN:HB2	1:A:289:LEU:HB3	1.87	0.56
2:B:308:GLU:HA	2:B:311:LYS:HE2	1.89	0.53
2:B:353:LYS:HE3	2:B:428:GLN:HE22	1.73	0.53
1:A:353:LYS:O	1:A:374:LYS:NZ	2.40	0.53
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.89	0.53
1:A:88:TRP:CD1	2:B:143:ARG:HD2	2.43	0.53
1:A:178:ILE:HG22	1:A:191:SER:HB3	1.92	0.52
2:B:89:GLU:HB2	2:B:91:GLN:HG2	1.92	0.51
2:B:91:GLN:OE1	2:B:161:GLN:NE2	2.34	0.51
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.91	0.50
2:B:89:GLU:N	2:B:89:GLU:OE1	2.44	0.50
1:A:111:VAL:HG12	1:A:114:ALA:HB3	1.92	0.49
1:A:191:SER:OG	1:A:198:HIS:ND1	2.45	0.48
1:A:363:ASN:ND2	1:A:366:LYS:HE3	2.29	0.48
2:B:270:ILE:HG12	2:B:346:PHE:HB3	1.95	0.48
2:B:206:ARG:NH1	2:B:229:TRP:O	2.47	0.48
1:A:257:ILE:HB	1:A:283:LEU:HD21	1.97	0.47
2:B:28:GLU:HG2	2:B:32:LYS:HE2	1.96	0.47
1:A:194:GLU:HB3	1:A:197:GLN:HE21	1.80	0.47
1:A:244:ILE:HG13	1:A:267:ALA:HB2	1.98	0.46
1:A:253:THR:HG22	1:A:292:VAL:HG22	1.97	0.46
1:A:19:PRO:HD3	1:A:80:LEU:HD13	1.97	0.46
1:A:494:ASN:HB3	2:B:289:LEU:HD12	1.99	0.45
1:A:343:GLN:HG3	1:A:349:LEU:HD11	1.98	0.45
2:B:101:LYS:HD3	2:B:382:ILE:HG23	1.99	0.45
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.53	0.44
1:A:80:LEU:O	1:A:84:THR:OG1	2.29	0.44
1:A:417:VAL:HG22	1:A:419:THR:HG23	1.99	0.44
1:A:466:VAL:HG22	1:A:550:LYS:NZ	2.32	0.44
2:B:332:GLN:HG3	2:B:338:THR:HG23	2.00	0.44
1:A:90:VAL:HG21	2:B:140:PRO:HB3	1.99	0.44
2:B:209:LEU:HD22	2:B:214:LEU:HD21	2.00	0.44
2:B:10:VAL:HG13	2:B:87:PHE:HE1	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:LEU:HD12	1:A:307:ARG:HG2	1.99	0.43
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.57	0.43
2:B:84:THR:HG23	2:B:154:LYS:HE2	2.00	0.43
1:A:361:HIS:ND1	1:A:513:SER:OG	2.50	0.43
1:A:363:ASN:HA	1:A:511:ASP:OD1	2.18	0.43
2:B:73:LYS:NZ	2:B:146:TYR:OH	2.36	0.43
1:A:90:VAL:HG11	1:A:161:GLN:HG2	2.01	0.43
1:A:216:THR:C	1:A:218:ASP:H	2.27	0.43
2:B:242:GLN:HB2	2:B:351:THR:OG1	2.19	0.42
1:A:253:THR:HA	1:A:292:VAL:HA	2.01	0.42
1:A:111:VAL:HG21	1:A:187:LEU:HG	2.01	0.42
1:A:28:GLU:HG2	1:A:32:LYS:HE3	2.00	0.42
1:A:254:VAL:HB	1:A:289:LEU:HA	2.02	0.42
2:B:271:TYR:HA	2:B:272:PRO:HD3	1.92	0.42
1:A:426:TRP:HB3	1:A:526:ILE:HG12	2.01	0.41
1:A:7:THR:HG22	1:A:119:PRO:HG2	2.03	0.41
1:A:342:TYR:HA	1:A:349:LEU:HD13	2.01	0.41
1:A:490:GLY:O	1:A:528:LYS:NZ	2.41	0.41
2:B:100:LEU:HG	2:B:381:VAL:HG13	2.01	0.41
1:A:542:ILE:HG12	2:B:283:LEU:HD12	2.03	0.41
1:A:461:LYS:HE2	1:A:461:LYS:HB3	1.91	0.41
2:B:357:MET:SD	2:B:361:HIS:HB2	2.60	0.41
1:A:311:LYS:HE2	1:A:311:LYS:HB3	1.94	0.41
2:B:166:LYS:HA	2:B:169:GLU:HG2	2.03	0.41
1:A:544:GLY:O	1:A:546:GLU:N	2.53	0.40
2:B:10:VAL:HG22	2:B:87:PHE:HZ	1.86	0.40
1:A:442:VAL:HG12	1:A:457:TYR:HB3	2.03	0.40
2:B:108:VAL:HB	2:B:232:TYR:HB3	2.02	0.40
1:A:411:ILE:HG22	1:A:412:PRO:O	2.21	0.40

All (1) 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:28:GLU:OE2	2:B:419:THR:OG1[4_748]	2.15	0.05

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	543/557 (98%)	522 (96%)	17 (3%)	4 (1%)	18	39
2	B	408/428 (95%)	386 (95%)	19 (5%)	3 (1%)	18	39
All	All	951/985 (96%)	908 (96%)	36 (4%)	7 (1%)	18	39

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	184	MET
1	A	545	ASN
2	B	86	ASP
2	B	272	PRO
1	A	92	LEU
1	A	217	PRO
2	B	423	VAL

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	477/495 (96%)	464 (97%)	13 (3%)	39	68
2	B	374/390 (96%)	366 (98%)	8 (2%)	47	73
All	All	851/885 (96%)	830 (98%)	21 (2%)	42	69

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	LEU
1	A	107	THR
1	A	111	VAL
1	A	161	GLN
1	A	195	ILE
1	A	223	LYS
1	A	284	ARG
1	A	324	ASP
1	A	373	GLN
1	A	394	GLN
1	A	459	THR
1	A	497	THR
1	A	546	GLU
2	B	8	VAL
2	B	87	PHE
2	B	90	VAL
2	B	197	GLN
2	B	214	LEU
2	B	227	PHE
2	B	417	VAL
2	B	425	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	161	GLN
1	A	174	GLN
1	A	197	GLN
1	A	235	HIS
1	A	475	GLN
1	A	524	GLN
1	A	547	GLN
2	B	235	HIS
2	B	330	GLN
2	B	334	GLN
2	B	340	GLN
2	B	418	ASN
2	B	428	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](#)

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	9W3	A	601	-	41,41,41	4.05	8 (19%)	53,54,54	2.44	10 (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	9W3	A	601	-	-	5/20/29/29	0/4/4/4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	9W3	O1-C9	24.14	1.63	1.34
3	A	601	9W3	C5-C4	4.53	1.46	1.40
3	A	601	9W3	C7-C1	3.30	1.44	1.39
3	A	601	9W3	C16-C15	2.87	1.44	1.39
3	A	601	9W3	C17-C16	2.52	1.42	1.38
3	A	601	9W3	C14-C15	2.38	1.43	1.39
3	A	601	9W3	C5-C1	2.36	1.43	1.40
3	A	601	9W3	C10-N2	2.25	1.41	1.36

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	9W3	C9-N01-C10	9.05	120.24	112.86
3	A	601	9W3	C9-N1-C11	8.70	119.96	112.86
3	A	601	9W3	C11-N3-C10	4.52	121.96	113.85
3	A	601	9W3	N3-C10-N01	-4.47	118.93	126.26
3	A	601	9W3	N01-C9-N1	-4.39	119.67	127.65
3	A	601	9W3	C22-O1-C9	4.37	124.18	117.80
3	A	601	9W3	N3-C11-N1	-4.28	119.24	126.26
3	A	601	9W3	C8-C4-C5	2.53	124.51	121.42
3	A	601	9W3	C8-C4-C3	-2.29	115.55	119.57
3	A	601	9W3	C4-C5-C1	-2.23	118.38	121.55

There are no chirality outliers.

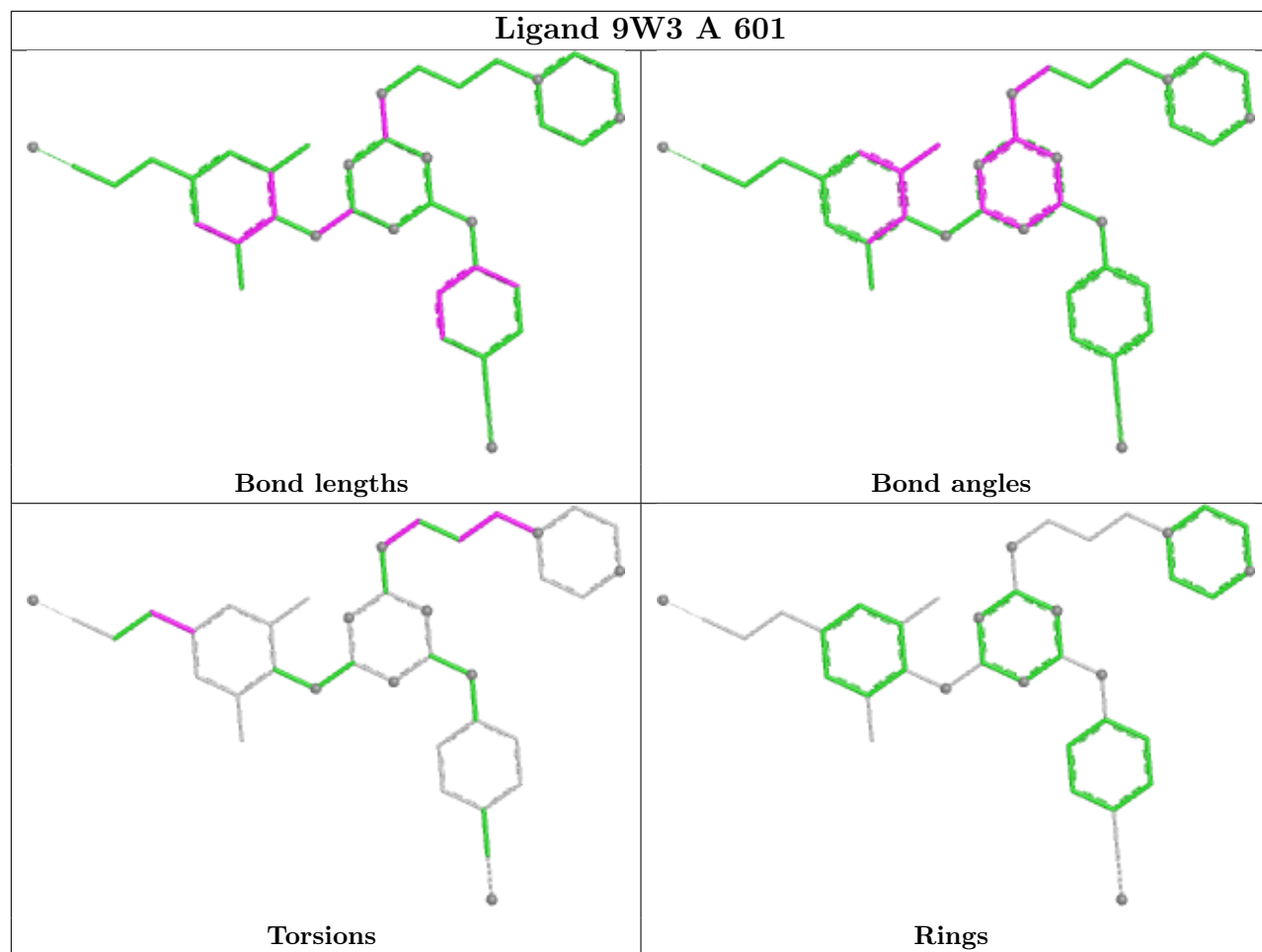
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	9W3	C23-C24-N7-C25
3	A	601	9W3	C23-C22-O1-C9
3	A	601	9W3	C22-C23-C24-N7
3	A	601	9W3	C7-C2-C20-C19
3	A	601	9W3	C3-C2-C20-C19

There are no ring outliers.

No monomer is involved in short contacts.

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	549/557 (98%)	0.60	49 (8%) 15 13	33, 69, 116, 135	0
2	B	412/428 (96%)	0.58	38 (9%) 14 13	38, 64, 122, 142	0
All	All	961/985 (97%)	0.60	87 (9%) 15 13	33, 67, 118, 142	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	240	THR	7.2
2	B	93	GLY	5.5
2	B	92	LEU	5.5
2	B	357	MET	5.0
1	A	288	ALA	4.9
1	A	290	THR	4.4
1	A	548	VAL	4.4
1	A	260	LEU	4.4
2	B	214	LEU	4.3
2	B	241	VAL	4.2
2	B	94	ILE	4.1
2	B	425	LEU	4.0
2	B	202	ILE	4.0
1	A	551	LEU	3.9
2	B	90	VAL	3.9
1	A	65	LYS	3.6
1	A	289	LEU	3.5
1	A	544	GLY	3.5
2	B	88	TRP	3.4
1	A	217	PRO	3.4
1	A	295	LEU	3.4
2	B	428	GLN	3.4
1	A	109	LEU	3.3
2	B	195	ILE	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	210	LEU	3.2
1	A	220	LYS	3.2
1	A	24	TRP	3.1
1	A	195	ILE	3.1
1	A	90	VAL	3.1
2	B	85	GLN	3.1
1	A	543	GLY	3.0
2	B	355	ALA	3.0
1	A	546	GLU	2.9
2	B	196	GLY	2.9
1	A	194	GLU	2.9
1	A	245	VAL	2.9
1	A	199	ARG	2.8
1	A	115	TYR	2.8
1	A	222	GLN	2.8
1	A	296	THR	2.8
2	B	361	HIS	2.8
2	B	122	GLU	2.8
1	A	-1	MET	2.8
1	A	251	SER	2.7
1	A	111	VAL	2.7
2	B	200	THR	2.7
1	A	257	ILE	2.7
1	A	550	LYS	2.7
1	A	116	PHE	2.6
1	A	214	LEU	2.6
1	A	247	PRO	2.6
1	A	552	VAL	2.6
2	B	10	VAL	2.6
1	A	261	VAL	2.5
2	B	212	TRP	2.5
2	B	213	GLY	2.5
2	B	285	GLY	2.5
1	A	71	TRP	2.5
2	B	232	TYR	2.5
2	B	66	LYS	2.5
1	A	299	ALA	2.5
1	A	92	LEU	2.4
2	B	84	THR	2.4
2	B	229	TRP	2.4
2	B	9	PRO	2.3
2	B	283	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	65	LYS	2.3
1	A	45	GLY	2.3
2	B	358	ARG	2.3
1	A	258	GLN	2.2
1	A	357	MET	2.2
1	A	244	ILE	2.2
2	B	98	ALA	2.2
1	A	185	ASP	2.2
1	A	210	LEU	2.2
1	A	184	MET	2.2
1	A	218	ASP	2.2
1	A	256	ASP	2.2
2	B	67	ASP	2.1
2	B	105	SER	2.1
1	A	249	LYS	2.1
2	B	5	ILE	2.1
1	A	193	LEU	2.0
1	A	138	GLU	2.0
1	A	250	ASP	2.0
2	B	169	GLU	2.0
2	B	209	LEU	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](#)

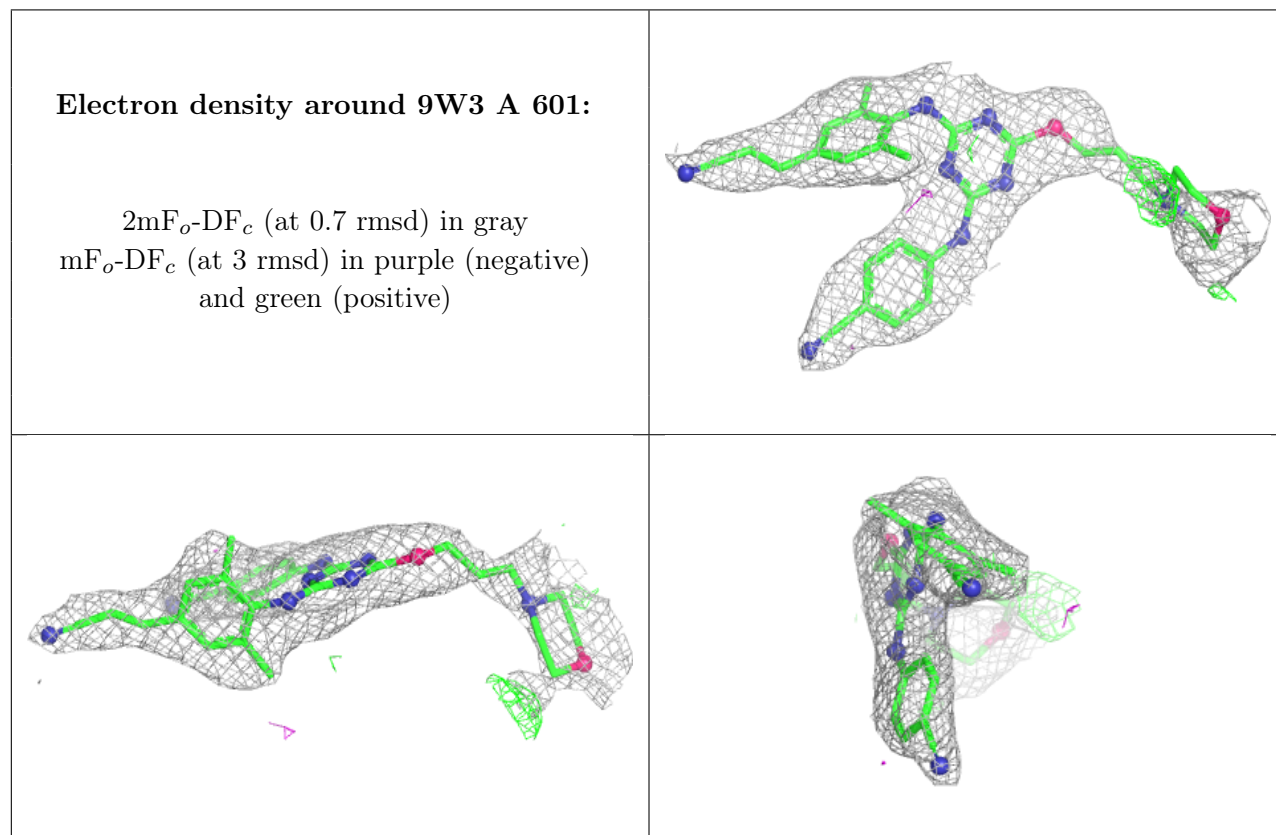
There are no oligosaccharides in this entry.

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, 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	9W3	A	601	38/38	0.89	0.12	54,62,94,95	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.