



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:10 PM UTC

PDB ID : 7SLR / pdb_00007slr
Title : HIV Reverse Transcriptase with compound Pyr01
Authors : Klein, D.J.; Zebisch, M.; Gu, M.
Deposited on : 2021-10-24
Resolution : 2.18 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

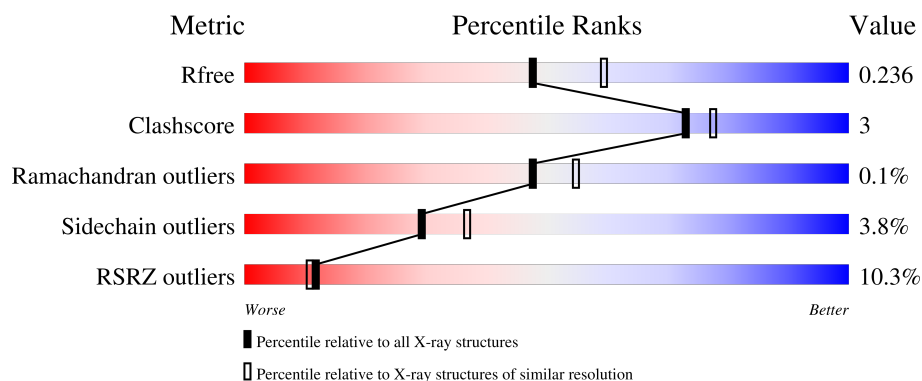
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.18 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	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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	561	4% 86% 10% .
1	B	561	13% 64% 8% . 28%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8087 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.

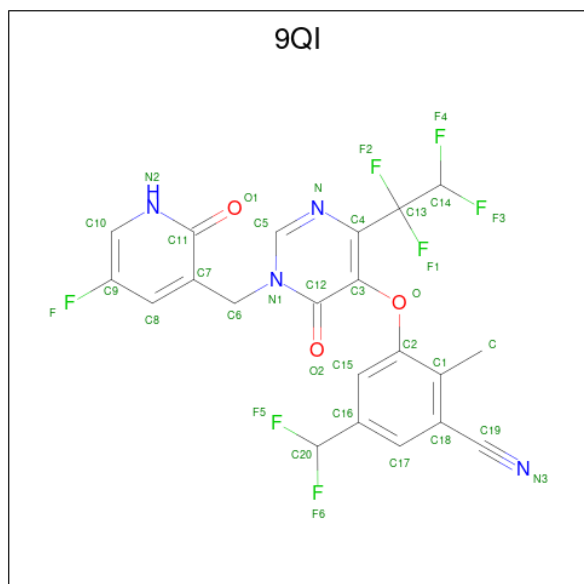
- Molecule 1 is a protein called Reverse transcriptase/ribonuclease H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	539	Total	C	N	O	S	0	4	0
			4438	2875	737	816	10			
1	B	404	Total	C	N	O	S	0	2	0
			3358	2189	554	609	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P04585
B	0	MET	-	initiating methionine	UNP P04585

- Molecule 2 is 5-(difluoromethyl)-3-({1-[(5-fluoro-2-oxo-1,2-dihydropyridin-3-yl)methyl]-6-oxo-4-(1,1,2,2-tetrafluoroethyl)-1,6-dihydropyrimidin-5-yl}oxy)-2-methylbenzonitrile (CCD ID: 9QI) (formula: C₂₁H₁₃F₇N₄O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			35	21	7	4	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	142	Total	O	0	0
			142	142		
3	B	114	Total	O	0	0
			114	114		

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	117.43Å 154.24Å 155.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	93.43 – 2.18 93.43 – 2.18	Depositor EDS
% Data completeness (in resolution range)	78.7 (93.43-2.18) 78.7 (93.43-2.18)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 2.18Å)	Xtriage
Refinement program	BUSTER 2.11.7 (18-SEP-2020)	Depositor
R, R_{free}	0.200 , 0.232 (Not available) , 0.236	Depositor DCC
R_{free} test set	2853 reflections (3.87%)	wwPDB-VP
Wilson B-factor (Å ²)	54.0	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8087	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% 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: 9QI

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	0.75	0/4562	1.03	7/6200 (0.1%)
1	B	0.73	0/3459	1.04	2/4701 (0.0%)
All	All	0.74	0/8021	1.03	9/10901 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	116	PHE	CA-CB-CG	7.85	121.65	113.80
1	A	132	ILE	N-CA-C	-6.08	101.62	107.76
1	A	349	LEU	N-CA-C	-5.88	104.22	111.40
1	A	460	ASN	CA-C-N	5.85	132.96	122.38
1	A	460	ASN	C-N-CA	5.85	132.96	122.38
1	B	93	GLY	N-CA-C	5.34	117.61	111.36
1	A	52	PRO	CA-C-N	5.25	127.62	120.54
1	A	52	PRO	C-N-CA	5.25	127.62	120.54
1	A	493	VAL	N-CA-C	5.04	115.53	108.17

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	4438	0	4487	30	0
1	B	3358	0	3392	33	0
2	A	35	0	0	0	0
3	A	142	0	0	0	0
3	B	114	0	0	0	0
All	All	8087	0	7879	50	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 3.

All (50) 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:255:ASN:HB2	1:A:289:LEU:HG	1.41	1.01
1:A:373:GLN:NE2	1:B:400:THR:OG1	2.30	0.65
1:B:115:TYR:HB3	1:B:149:LEU:HB2	1.80	0.64
1:A:60:VAL:HG12	1:A:75:VAL:HG22	1.80	0.64
1:A:535:TRP:CD2	1:B:422:LEU:HD13	2.33	0.64
1:A:406:TRP:CH2	1:B:418:ASN:HA	2.34	0.62
1:A:535:TRP:CG	1:B:422:LEU:HD11	2.35	0.60
1:A:285:GLY:HA3	1:A:287:LYS:NZ	2.18	0.59
1:A:61[B]:PHE:HE1	1:A:76:ASP:HB2	1.68	0.59
1:B:252:TRP:NE1	1:B:295:LEU:HD11	2.20	0.56
1:B:209:LEU:HD22	1:B:214:LEU:HD22	1.88	0.54
1:B:252:TRP:CD1	1:B:295:LEU:HD11	2.43	0.54
1:B:365:VAL:O	1:B:369:THR:HG23	2.08	0.54
1:A:441:TYR:CD1	1:B:286:THR:HG23	2.43	0.53
1:A:535:TRP:CG	1:B:422:LEU:CD1	2.92	0.52
1:A:503:LEU:HD22	1:A:535:TRP:HB2	1.92	0.52
1:A:167:ILE:O	1:A:170:PRO:HD2	2.08	0.52
1:A:79:GLU:HG3	1:A:83:ARG:HE	1.75	0.52
1:A:244:ILE:HD13	1:A:267:ALA:HB2	1.94	0.50
1:B:79:GLU:HG3	1:B:83:ARG:NE	2.27	0.49
1:B:60:VAL:HG23	1:B:75:VAL:HG22	1.94	0.49
1:A:405:TYR:CE2	1:A:407:GLN:HB3	2.48	0.48
1:B:24[B]:TRP:H	1:B:24[B]:TRP:CD1	2.31	0.48
1:A:407:GLN:HG3	1:B:393:ILE:HA	1.95	0.48
1:A:328:GLU:HG2	1:A:390:LYS:HB2	1.95	0.47
1:A:503:LEU:HD23	1:B:421:PRO:HB2	1.96	0.47
1:B:61:PHE:CD1	1:B:403:THR:HG21	2.50	0.47
1:B:79:GLU:HG3	1:B:83:ARG:HE	1.80	0.46
1:A:500:GLN:HG2	1:B:422:LEU:CD1	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:GLY:HA3	1:B:356:ARG:HG2	1.96	0.46
1:A:254:VAL:HG21	1:A:287:LYS:HB2	1.97	0.45
1:A:535:TRP:CD2	1:B:422:LEU:CD1	2.99	0.45
1:B:209:LEU:HB3	1:B:214:LEU:HB2	1.97	0.45
1:A:345:PRO:HA	1:A:346:PHE:HA	1.62	0.44
1:B:85:GLN:O	1:B:89:GLU:HB3	2.16	0.44
1:A:500:GLN:HG2	1:B:422:LEU:HD12	1.99	0.44
1:A:230[B]:MET:HE2	1:A:230[B]:MET:HB3	1.90	0.44
1:A:365:VAL:HG11	1:A:401:TRP:CG	2.52	0.44
1:A:458:VAL:HG12	1:B:286:THR:HG21	2.00	0.44
1:A:285:GLY:HA3	1:A:287:LYS:HZ3	1.82	0.44
1:B:346:PHE:N	1:B:346:PHE:CD1	2.85	0.42
1:B:255:ASN:O	1:B:259:LYS:HG3	2.20	0.42
1:A:297:GLU:O	1:A:301:LEU:HG	2.20	0.41
1:B:65:LYS:HG2	1:B:72:ARG:HD2	2.01	0.41
1:A:16:MET:HE2	1:A:83:ARG:HG2	2.02	0.41
1:B:24[B]:TRP:H	1:B:24[B]:TRP:HD1	1.69	0.41
1:B:279:LEU:HA	1:B:282:LEU:HD12	2.01	0.41
1:B:340:GLN:HG3	1:B:351:THR:HG22	2.01	0.41
1:A:535:TRP:CE3	1:B:422:LEU:HD22	2.56	0.41

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	541/561 (96%)	528 (98%)	13 (2%)	0	100	100
1	B	400/561 (71%)	390 (98%)	9 (2%)	1 (0%)	36	39
All	All	941/1122 (84%)	918 (98%)	22 (2%)	1 (0%)	48	55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	232	TYR

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	430/501 (86%)	412 (96%)	18 (4%)	26	32
1	B	370/501 (74%)	357 (96%)	13 (4%)	32	40
All	All	800/1002 (80%)	769 (96%)	31 (4%)	29	36

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	GLU
1	A	63	ILE
1	A	65	LYS
1	A	66	LYS
1	A	70	LYS
1	A	82	LYS
1	A	102	LYS
1	A	122	GLU
1	A	126	LYS
1	A	245	VAL
1	A	312	GLU
1	A	388	LYS
1	A	396	GLU
1	A	434	ILE
1	A	448	ARG
1	A	461	ARG
1	A	467	VAL
1	A	470	THR
1	B	22	LYS
1	B	24[A]	TRP
1	B	24[B]	TRP
1	B	58	THR
1	B	68	SER

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Mol	Chain	Res	Type
1	B	116	PHE
1	B	122	GLU
1	B	161	GLN
1	B	249	LYS
1	B	276	VAL
1	B	280	CYS
1	B	336	GLN
1	B	403	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	222	GLN
1	A	336	GLN
1	A	474	ASN
1	A	475	GLN
1	A	500	GLN
1	A	507	GLN
1	A	520	GLN
1	B	147	ASN
1	B	255	ASN
1	B	258	GLN
1	B	278	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
2	9QI	A	4000	-	35,37,37	0.57	2 (5%)	39,55,55	0.59	1 (2%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	9QI	A	4000	-	-	4/24/26/26	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4000	9QI	C13-C14	2.11	1.58	1.51
2	A	4000	9QI	C13-C4	2.01	1.54	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4000	9QI	C13-C4-N	2.15	115.69	111.84

There are no chirality outliers.

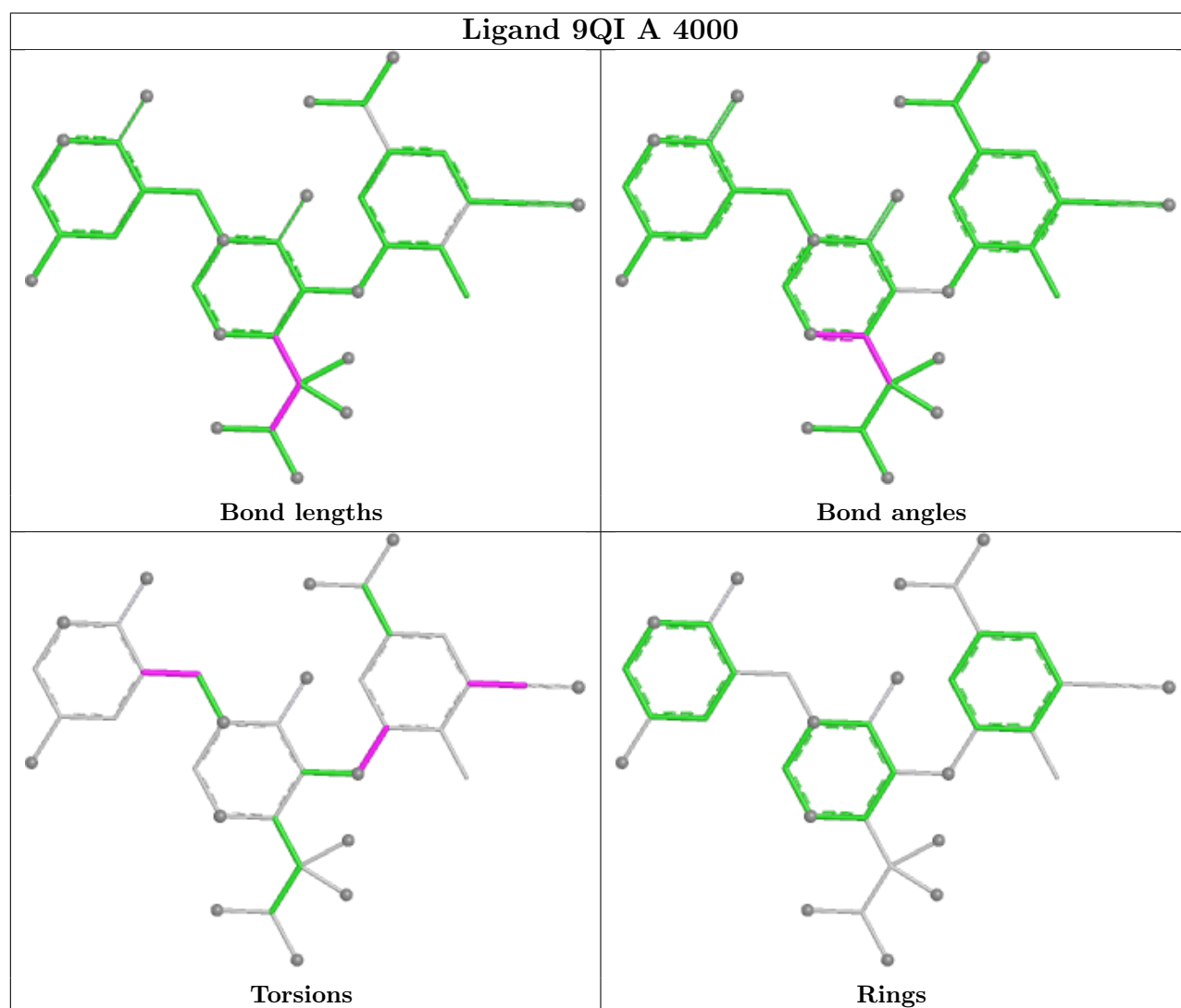
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	4000	9QI	C15-C2-O-C3
2	A	4000	9QI	N1-C6-C7-C8
2	A	4000	9QI	C1-C2-O-C3
2	A	4000	9QI	C1-C18-C19-N3

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	539/561 (96%)	0.43	25 (4%) 37 36	26, 59, 79, 100	4 (0%)
1	B	404/561 (72%)	0.83	72 (17%) 4 3	30, 59, 104, 123	2 (0%)
All	All	943/1122 (84%)	0.61	97 (10%) 12 11	26, 59, 96, 123	6 (0%)

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	266	TRP	6.8
1	B	426	TRP	6.3
1	A	61[A]	PHE	6.0
1	B	241	VAL	5.9
1	B	422	LEU	5.9
1	B	346	PHE	5.4
1	B	421	PRO	5.2
1	B	270	ILE	5.1
1	B	232	TYR	5.0
1	B	216	THR	4.5
1	A	286	THR	4.3
1	B	423	VAL	4.2
1	B	425	LEU	4.1
1	B	231	GLY	4.0
1	B	24[A]	TRP	3.9
1	A	91[A]	GLN	3.8
1	B	282	LEU	3.7
1	A	289	LEU	3.7
1	B	279	LEU	3.7
1	B	272	PRO	3.7
1	B	66	LYS	3.6
1	A	88	TRP	3.6
1	A	52	PRO	3.4
1	B	303	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	214	LEU	3.2
1	B	65	LYS	3.2
1	A	2	ILE	3.1
1	B	243	PRO	3.1
1	B	117	SER	3.1
1	B	276	VAL	3.0
1	B	310	LEU	3.0
1	B	271	TYR	3.0
1	B	247	PRO	3.0
1	B	244	ILE	2.9
1	B	265	ASN	2.9
1	B	275	LYS	2.9
1	B	283	LEU	2.9
1	B	215	THR	2.9
1	B	301	LEU	2.8
1	B	267	ALA	2.8
1	A	406	TRP	2.8
1	A	315[A]	HIS	2.7
1	B	252	TRP	2.7
1	B	295	LEU	2.7
1	B	362	THR	2.7
1	B	299	ALA	2.6
1	B	240	THR	2.6
1	B	424	LYS	2.6
1	B	292	VAL	2.6
1	B	262	GLY	2.5
1	A	92	LEU	2.5
1	A	452	LEU	2.5
1	B	264	LEU	2.5
1	B	116	PHE	2.5
1	A	24	TRP	2.5
1	B	212	TRP	2.5
1	A	359	GLY	2.5
1	B	277	ARG	2.5
1	A	0	MET	2.4
1	B	289	LEU	2.4
1	A	535	TRP	2.4
1	B	10	VAL	2.4
1	A	537	PRO	2.4
1	B	263	LYS	2.4
1	B	260	LEU	2.4
1	B	213	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	237	ASP	2.4
1	A	87	PHE	2.4
1	B	293	ILE	2.4
1	B	419	THR	2.4
1	B	427	TYR	2.3
1	A	116	PHE	2.3
1	B	13	LYS	2.3
1	B	8	VAL	2.3
1	B	269	GLN	2.3
1	B	251	SER	2.3
1	B	14	PRO	2.3
1	B	345	PRO	2.3
1	A	288	ALA	2.3
1	A	434	ILE	2.2
1	B	313	PRO	2.2
1	A	493	VAL	2.2
1	B	356	ARG	2.2
1	B	296	THR	2.2
1	B	288	ALA	2.1
1	B	68	SER	2.1
1	B	87	PHE	2.1
1	A	360	ALA	2.1
1	B	311	LYS	2.1
1	B	16	MET	2.1
1	B	72	ARG	2.1
1	A	66	LYS	2.1
1	B	287	LYS	2.1
1	B	15	GLY	2.1
1	A	536	VAL	2.1
1	A	230[A]	MET	2.0
1	B	69	THR	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 ⓘ

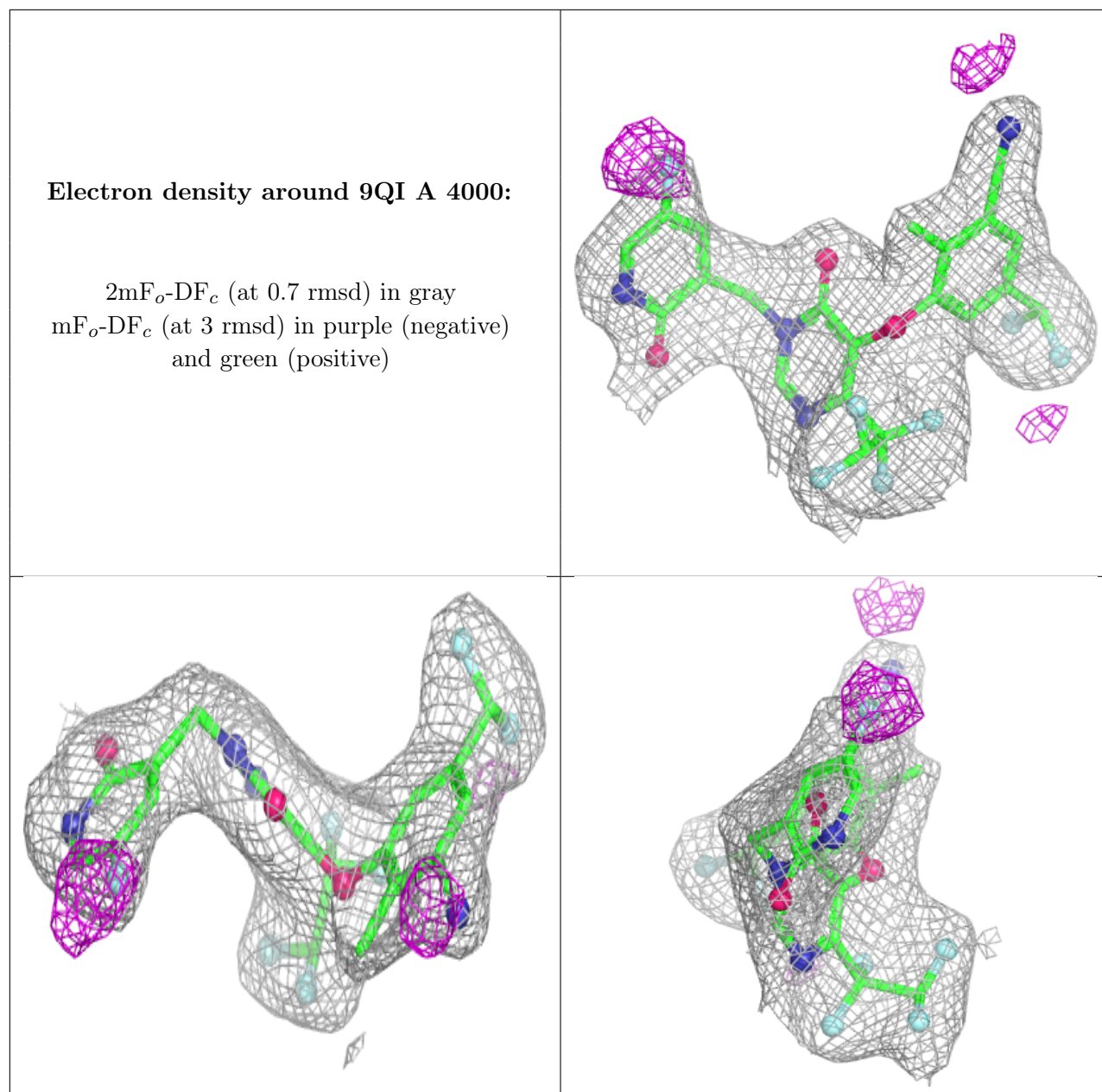
There are no oligosaccharides in this entry.

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
2	9QI	A	4000	35/35	0.96	0.07	48,50,54,56	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 ⓘ

There are no such residues in this entry.