



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:22 AM UTC

PDB ID : 3T1A / pdb_00003t1a
Title : Crystal Structure of HIV-1 Reverse Transcriptase (K103N mutant) in Complex with Inhibitor M05
Authors : Yan, Y.; Reid, J.
Deposited on : 2011-07-21
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

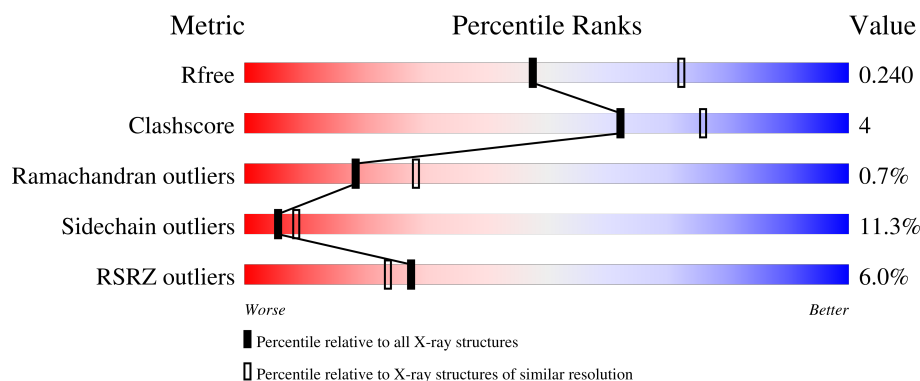
1 Overall quality at a glance

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	563	5% 79% 17% ...
1	B	563	6% 55% 13% .. 29%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8113 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.

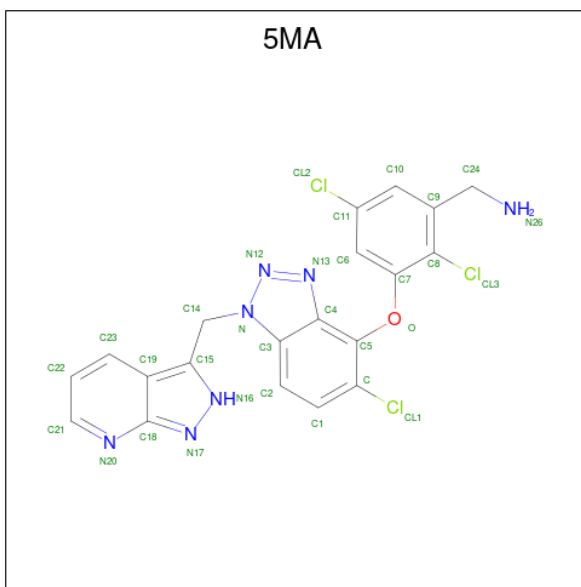
- Molecule 1 is a protein called Reverse Transcriptase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	554	Total	C	N	O	S	0	0	0
			4503	2911	751	833	8			
1	B	400	Total	C	N	O	S	0	0	0
			3311	2155	548	602	6			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	expression tag	UNP P04585
A	-1	ASN	-	expression tag	UNP P04585
A	0	SER	-	expression tag	UNP P04585
A	103	ASN	LYS	engineered mutation	UNP P04585
B	-2	MET	-	expression tag	UNP P04585
B	-1	ASN	-	expression tag	UNP P04585
B	0	SER	-	expression tag	UNP P04585
B	103	ASN	LYS	engineered mutation	UNP P04585

- Molecule 2 is 1-(2,5-dichloro-3-{[5-chloro-1-(2H-pyrazolo[3,4-b]pyridin-3-ylmethyl)-1H-benzotriazol-4-yl]oxy}phenyl)methanamine (CCD ID: 5MA) (formula: C₂₀H₁₄Cl₃N₇O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			31	20	3	7	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	159	Total	O	0	0
			159	159		
3	B	109	Total	O	0	0
			109	109		

GLU
LEU
VAL
ASN
GLN
ILE
ILE
GLU
GLN
LEU
ILE
LYS
LYS
GLU
LYS
VAL
TYR
LEU
ALA
TRP
VAL
PRO
ALA
HIS
LYS
GLY
ILE
GLY
GLY
ASN
GLU
GLN
VAL
ASP
LYS
LEU
VAL
SER
ALA
GLY
ILE
ARG
LYS
VAL
LEU

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	118.33Å 154.23Å 155.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.14 – 2.40 35.14 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.8 (35.14-2.40) 96.8 (35.14-2.40)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 2.39Å)	Xtriage
Refinement program	BUSTER 2.9.7	Depositor
R, R_{free}	0.205 , 0.250 (Not available) , 0.240	Depositor DCC
R_{free} test set	2753 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	46.7	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8113	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% 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: 5MA

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	0.84	1/4619 (0.0%)	1.33	23/6279 (0.4%)
1	B	0.84	1/3404 (0.0%)	1.33	20/4627 (0.4%)
All	All	0.84	2/8023 (0.0%)	1.33	43/10906 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	184	MET	SD-CE	-5.22	1.66	1.79
1	B	347	LYS	CA-C	5.13	1.59	1.52

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	345	PRO	CA-C-N	8.72	140.34	124.82
1	A	345	PRO	C-N-CA	8.72	140.34	124.82
1	B	111	VAL	N-CA-CB	-7.71	102.14	112.16
1	A	470	THR	N-CA-C	7.05	121.90	111.96
1	A	349	LEU	N-CA-C	-6.87	103.02	111.40
1	B	401	TRP	N-CA-C	6.73	121.62	113.41
1	B	8	VAL	N-CA-CB	6.55	117.23	110.23
1	A	496	VAL	N-CA-CB	6.50	120.09	111.90
1	B	233	GLU	N-CA-C	6.40	119.32	107.99
1	B	271	TYR	N-CA-C	6.24	117.92	109.24
1	A	132	ILE	N-CA-C	-6.08	101.62	107.76
1	B	116	PHE	CA-CB-CG	5.84	119.64	113.80
1	A	409	THR	CB-CA-C	5.81	120.85	109.35
1	A	398	TRP	CA-C-N	5.77	128.01	120.28
1	A	398	TRP	C-N-CA	5.77	128.01	120.28
1	B	214	LEU	N-CA-C	5.76	118.41	110.35
1	A	3	SER	N-CA-C	5.70	116.58	109.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	153	TRP	CA-C-N	5.66	129.30	120.82
1	A	153	TRP	C-N-CA	5.66	129.30	120.82
1	A	139	THR	N-CA-C	5.64	117.79	110.40
1	A	38	CYS	N-CA-C	5.62	117.41	111.28
1	A	333	GLY	CA-C-N	5.45	131.94	121.54
1	A	333	GLY	C-N-CA	5.45	131.94	121.54
1	B	249	LYS	CA-C-N	5.39	127.96	120.63
1	B	249	LYS	C-N-CA	5.39	127.96	120.63
1	A	491	LEU	N-CA-C	5.30	122.08	110.80
1	B	121	ASP	CA-C-N	5.28	127.61	120.38
1	B	121	ASP	C-N-CA	5.28	127.61	120.38
1	B	414	TRP	CA-C-N	5.27	130.86	122.59
1	B	414	TRP	C-N-CA	5.27	130.86	122.59
1	A	21	VAL	CB-CA-C	5.25	118.17	110.98
1	A	106	VAL	N-CA-CB	5.25	119.18	111.52
1	B	391	LEU	N-CA-C	5.24	116.52	109.24
1	B	195	ILE	N-CA-C	5.24	116.59	110.62
1	B	256	ASP	CA-CB-CG	5.17	117.77	112.60
1	B	293	ILE	CB-CA-C	5.17	117.13	111.18
1	A	297	GLU	CA-C-N	5.14	127.17	120.28
1	A	297	GLU	C-N-CA	5.14	127.17	120.28
1	B	194	GLU	N-CA-C	-5.12	103.39	110.35
1	B	253	THR	CB-CA-C	5.09	118.74	109.83
1	B	416	PHE	CA-CB-CG	-5.05	108.75	113.80
1	A	503	LEU	CA-C-N	5.04	125.68	119.99
1	A	503	LEU	C-N-CA	5.04	125.68	119.99

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	4503	0	4540	32	0
1	B	3311	0	3326	33	0
2	A	31	0	14	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	159	0	0	3	0
3	B	109	0	0	1	0
All	All	8113	0	7880	64	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 4.

All (64) 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:330:GLN:HE22	1:A:340:GLN:HE22	1.28	0.77
1:B:317:VAL:HG13	1:B:347:LYS:HG2	1.74	0.67
1:B:337:TRP:HE1	1:B:367:GLN:HE21	1.45	0.64
1:B:373:GLN:O	1:B:377:THR:HG23	1.98	0.64
1:A:195:ILE:HD12	1:A:199:ARG:HE	1.63	0.63
1:A:103:ASN:H	2:A:561:5MA:HN16	1.47	0.63
1:A:244:ILE:HD13	1:A:267:ALA:HB2	1.83	0.60
1:A:328:GLU:HG2	1:A:390:LYS:HB2	1.84	0.60
1:B:214:LEU:HD23	1:B:214:LEU:H	1.68	0.59
1:B:394:GLN:HB3	1:B:397:THR:HG23	1.84	0.58
1:B:275:LYS:H	1:B:306:ASN:HD21	1.50	0.57
1:A:175:ASN:HD21	1:A:201:LYS:NZ	2.06	0.53
1:A:59:PRO:HG2	1:A:76:ASP:HB3	1.89	0.53
1:A:406:TRP:CH2	1:B:418:ASN:HA	2.44	0.53
1:A:318:TYR:CZ	2:A:561:5MA:H14A	2.45	0.52
1:A:60:VAL:HG12	1:A:75:VAL:HG22	1.91	0.51
1:B:335:GLY:HA3	1:B:356:ARG:HG2	1.92	0.51
1:B:180:ILE:HG12	1:B:189:VAL:HG13	1.91	0.51
1:A:399:GLU:HA	1:A:402:TRP:CE3	2.46	0.50
1:A:193:LEU:HB3	1:A:197:GLN:HG3	1.94	0.49
1:B:317:VAL:CG1	1:B:347:LYS:HG2	2.43	0.49
1:A:7:THR:HG21	3:A:597:HOH:O	2.12	0.49
1:B:344:GLU:H	1:B:347:LYS:HD3	1.78	0.48
1:B:115:TYR:HB3	1:B:149:LEU:HB2	1.95	0.48
1:B:163:SER:HA	1:B:166:LYS:HE3	1.95	0.48
1:A:395:LYS:NZ	1:A:416:PHE:H	2.12	0.47
1:A:94:ILE:HD13	1:A:230:MET:HE2	1.95	0.47
1:B:287:LYS:HE3	1:B:293:ILE:HG21	1.97	0.47
1:B:343:GLN:H	1:B:347:LYS:HE2	1.80	0.46
1:B:345:PRO:O	1:B:346:PHE:HB2	2.15	0.46
1:B:244:ILE:HB	1:B:310:LEU:HG	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:GLN:NE2	1:B:407:GLN:H	2.13	0.46
1:A:296:THR:HG21	3:A:566:HOH:O	2.16	0.45
1:B:373:GLN:HE22	1:B:407:GLN:H	1.65	0.45
1:B:57:ASN:OD1	1:B:143:ARG:NH1	2.50	0.44
1:B:253:THR:HG22	1:B:256:ASP:H	1.82	0.44
1:B:269:GLN:HB3	1:B:346:PHE:CE1	2.53	0.44
1:A:194:GLU:H	1:A:194:GLU:CD	2.24	0.44
1:A:365:VAL:O	1:A:369:THR:HG23	2.17	0.44
1:B:266:TRP:HZ2	1:B:427:TYR:CZ	2.35	0.43
1:A:57:ASN:HD22	1:A:143:ARG:NH1	2.15	0.43
1:B:377:THR:HG22	1:B:410:TRP:HZ2	1.82	0.43
1:A:175:ASN:HB3	1:A:178:ILE:HD12	2.01	0.43
1:B:325:LEU:HD12	1:B:385:LYS:HG3	2.00	0.43
1:A:246:LEU:O	1:A:307:ARG:NH2	2.52	0.43
1:B:282:LEU:HB3	1:B:293:ILE:HD11	2.00	0.43
1:A:5:ILE:HG22	1:A:212:TRP:CE3	2.54	0.42
1:B:116:PHE:C	1:B:116:PHE:HD1	2.27	0.42
1:B:111:VAL:HG21	1:B:187:LEU:HD22	2.00	0.42
1:A:181:TYR:HB2	1:A:188:TYR:HB2	2.01	0.42
1:B:116:PHE:C	1:B:116:PHE:CD1	2.98	0.42
1:A:57:ASN:HD22	1:A:143:ARG:HH12	1.66	0.42
1:A:288:ALA:O	1:A:291:GLU:HB3	2.20	0.42
1:B:401:TRP:HE3	1:B:404:GLU:HG3	1.85	0.41
1:B:58:THR:HG23	1:B:76:ASP:O	2.20	0.41
1:A:296:THR:HG23	1:A:299:ALA:H	1.85	0.41
1:A:63:ILE:HG13	1:A:72:ARG:HG3	2.03	0.41
1:B:79:GLU:HG3	1:B:83:ARG:HE	1.86	0.41
1:A:21:VAL:HG22	1:A:59:PRO:HD3	2.02	0.41
1:A:402:TRP:CD1	1:A:402:TRP:C	2.99	0.41
1:B:172:ARG:HD2	3:B:616:HOH:O	2.20	0.41
1:A:255:ASN:HB2	1:A:289:LEU:HD23	2.02	0.40
1:A:369:THR:HG22	1:A:411:ILE:HD11	2.03	0.40
1:A:395:LYS:HE3	3:A:574:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	550/563 (98%)	525 (96%)	20 (4%)	5 (1%)	14	22
1	B	392/563 (70%)	379 (97%)	11 (3%)	2 (0%)	24	37
All	All	942/1126 (84%)	904 (96%)	31 (3%)	7 (1%)	18	28

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	334	GLN
1	B	347	LYS
1	A	543	GLY
1	A	491	LEU
1	B	346	PHE
1	A	195	ILE
1	A	219	LYS

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	492/503 (98%)	439 (89%)	53 (11%)	6	9
1	B	364/503 (72%)	320 (88%)	44 (12%)	5	7
All	All	856/1006 (85%)	759 (89%)	97 (11%)	5	8

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	6	GLU
1	A	7	THR
1	A	21	VAL
1	A	26	LEU
1	A	63	ILE
1	A	64	LYS
1	A	69	THR
1	A	70	LYS
1	A	94	ILE
1	A	104	LYS
1	A	106	VAL
1	A	118	VAL
1	A	126	LYS
1	A	138	GLU
1	A	161	GLN
1	A	166	LYS
1	A	173	LYS
1	A	194	GLU
1	A	195	ILE
1	A	205	LEU
1	A	215	THR
1	A	220	LYS
1	A	228	LEU
1	A	248	GLU
1	A	260	LEU
1	A	276	VAL
1	A	279	LEU
1	A	287	LYS
1	A	289	LEU
1	A	297	GLU
1	A	303	LEU
1	A	311	LYS
1	A	357	MET
1	A	368	LEU
1	A	373	GLN
1	A	402	TRP
1	A	422	LEU
1	A	425	LEU
1	A	428	GLN
1	A	449	GLU
1	A	459	THR
1	A	463	ARG

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Mol	Chain	Res	Type
1	A	466	VAL
1	A	479	LEU
1	A	491	LEU
1	A	493	VAL
1	A	496	VAL
1	A	500	GLN
1	A	503	LEU
1	A	528	LYS
1	A	547	GLN
1	A	548	VAL
1	B	6	GLU
1	B	8	VAL
1	B	11	LYS
1	B	12	LEU
1	B	17	ASP
1	B	26	LEU
1	B	42	GLU
1	B	58	THR
1	B	64	LYS
1	B	80	LEU
1	B	90	VAL
1	B	91	GLN
1	B	111	VAL
1	B	116	PHE
1	B	120	LEU
1	B	138	GLU
1	B	173	LYS
1	B	187	LEU
1	B	205	LEU
1	B	209	LEU
1	B	214	LEU
1	B	248	GLU
1	B	250	ASP
1	B	253	THR
1	B	260	LEU
1	B	265	ASN
1	B	270	ILE
1	B	279	LEU
1	B	286	THR
1	B	293	ILE
1	B	295	LEU
1	B	297	GLU

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Mol	Chain	Res	Type
1	B	300	GLU
1	B	301	LEU
1	B	310	LEU
1	B	347	LYS
1	B	349	LEU
1	B	362	THR
1	B	377	THR
1	B	394	GLN
1	B	397	THR
1	B	403	THR
1	B	422	LEU
1	B	425	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	91	GLN
1	A	103	ASN
1	A	136	ASN
1	A	175	ASN
1	A	198	HIS
1	A	258	GLN
1	A	278	GLN
1	A	330	GLN
1	A	332	GLN
1	A	500	GLN
1	A	512	GLN
1	B	96	HIS
1	B	103	ASN
1	B	147	ASN
1	B	151	GLN
1	B	161	GLN
1	B	175	ASN
1	B	182	GLN
1	B	208	HIS
1	B	255	ASN
1	B	306	ASN
1	B	332	GLN
1	B	336	GLN
1	B	367	GLN
1	B	373	GLN

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Mol	Chain	Res	Type
1	B	428	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	5MA	A	561	-	32,35,35	1.66	7 (21%)	36,51,51	1.95	10 (27%)

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	5MA	A	561	-	-	3/10/10/10	0/5/5/5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	561	5MA	N13-N12	3.77	1.36	1.30
2	A	561	5MA	C14-C15	3.68	1.55	1.50
2	A	561	5MA	C21-N20	2.62	1.40	1.34
2	A	561	5MA	C22-C23	2.54	1.43	1.38
2	A	561	5MA	C5-C	-2.47	1.36	1.41
2	A	561	5MA	C5-C4	2.31	1.47	1.42
2	A	561	5MA	C11-CL2	-2.14	1.69	1.74

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	561	5MA	C18-N17-N16	5.84	113.99	103.03
2	A	561	5MA	O-C5-C	-4.58	115.20	120.51
2	A	561	5MA	C15-N16-N17	-3.67	105.90	112.64
2	A	561	5MA	N-N12-N13	-3.59	105.33	108.82
2	A	561	5MA	C10-C11-C6	2.64	124.84	121.64
2	A	561	5MA	C21-N20-C18	-2.61	113.52	116.64
2	A	561	5MA	O-C7-C8	2.28	120.05	116.72
2	A	561	5MA	C6-C11-CL2	-2.26	116.34	119.17
2	A	561	5MA	C11-C10-C9	-2.16	117.13	119.96
2	A	561	5MA	C23-C22-C21	-2.05	115.95	118.92

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	561	5MA	N26-C24-C9-C8
2	A	561	5MA	N-C14-C15-C19
2	A	561	5MA	C8-C7-O-C5

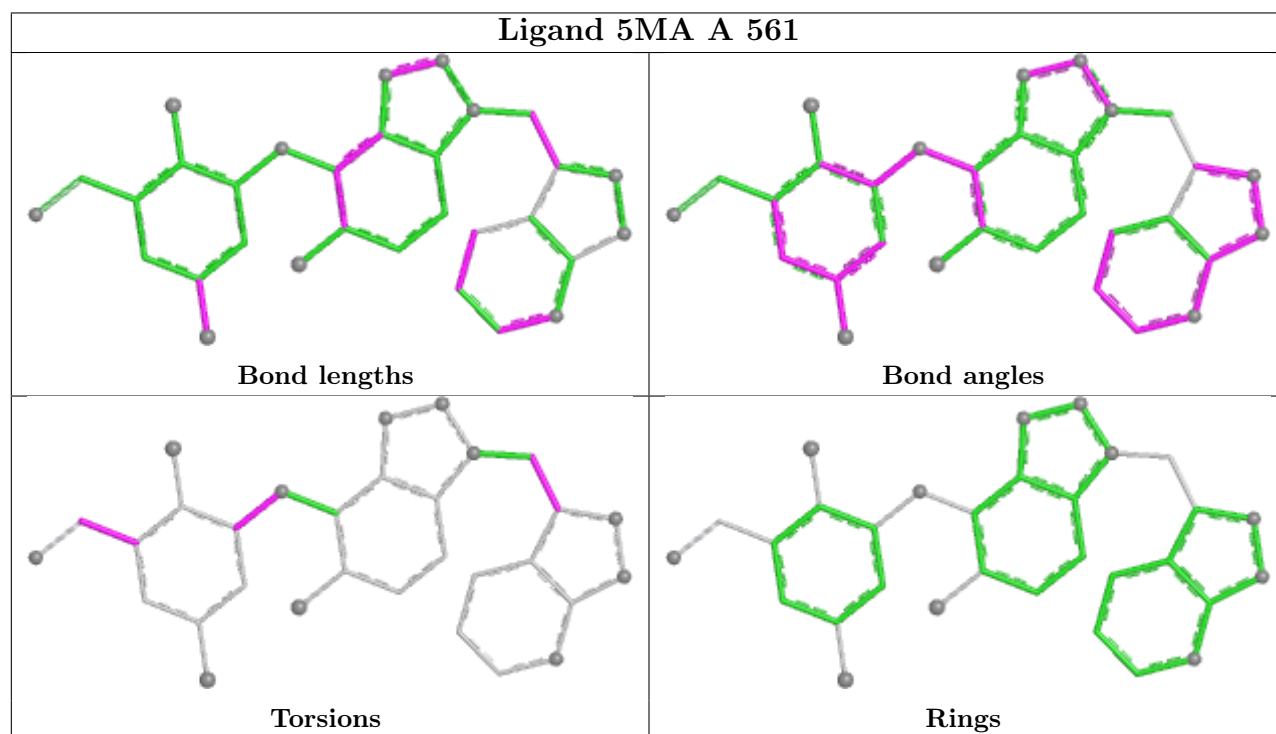
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	561	5MA	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	554/563 (98%)	0.27	26 (4%)	36 32	27, 50, 76, 99	0
1	B	400/563 (71%)	0.38	31 (7%)	19 15	28, 49, 86, 107	0
All	All	954/1126 (84%)	0.32	57 (5%)	27 24	27, 50, 82, 107	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	215	THR	4.4
1	B	347	LYS	4.2
1	B	24	TRP	4.0
1	B	346	PHE	3.8
1	B	266	TRP	3.6
1	A	356	ARG	3.5
1	B	240	THR	3.4
1	B	422	LEU	3.3
1	A	174	GLN	3.2
1	A	92	LEU	3.2
1	B	361	HIS	3.2
1	A	557	ARG	3.1
1	B	294	PRO	3.1
1	A	402	TRP	3.1
1	B	69	THR	3.0
1	A	195	ILE	3.0
1	B	270	ILE	2.9
1	B	293	ILE	2.9
1	B	232	TYR	2.9
1	A	406	TRP	2.8
1	A	410	TRP	2.7
1	A	69	THR	2.7
1	A	173	LYS	2.7
1	B	14	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	543	GLY	2.7
1	A	5	ILE	2.7
1	A	22	LYS	2.7
1	B	428	GLN	2.7
1	B	362	THR	2.6
1	A	288	ALA	2.6
1	A	287	LYS	2.5
1	B	16	MET	2.5
1	A	24	TRP	2.4
1	A	311	LYS	2.4
1	B	212	TRP	2.4
1	B	301	LEU	2.3
1	B	336	GLN	2.3
1	B	292	VAL	2.3
1	A	286	THR	2.3
1	A	0	SER	2.3
1	B	296	THR	2.3
1	B	308	GLU	2.2
1	B	278	GLN	2.2
1	B	22	LYS	2.2
1	A	357	MET	2.1
1	A	52	PRO	2.1
1	A	210	LEU	2.1
1	B	213	GLY	2.1
1	A	359	GLY	2.1
1	B	283	LEU	2.1
1	B	356	ARG	2.1
1	A	136	ASN	2.1
1	A	64	LYS	2.1
1	A	193	LEU	2.0
1	B	295	LEU	2.0
1	B	426	TRP	2.0
1	B	252	TRP	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 ⓘ

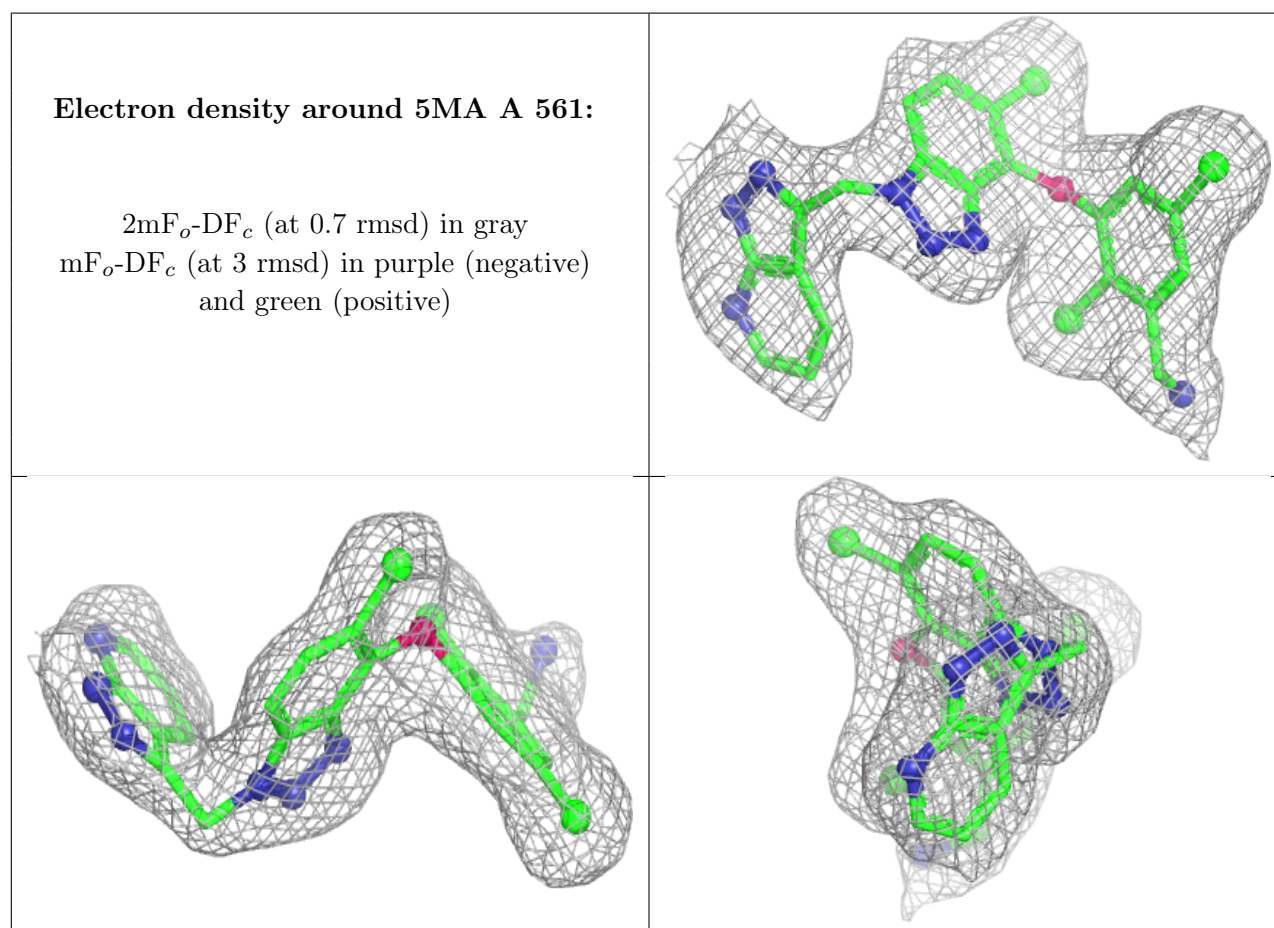
There are no oligosaccharides in this entry.

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(Å ²)	Q<0.9
2	5MA	A	561	31/31	0.97	0.06	30,41,47,47	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.