



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:07 PM UTC

PDB ID : 4I2P / pdb_00004i2p
Title : Crystal structure of HIV-1 reverse transcriptase in complex with rilpivirine (TMC278) based analogue
Authors : Patel, D.; Bauman, J.D.; Das, K.; Arnold, E.
Deposited on : 2012-11-22
Resolution : 2.30 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

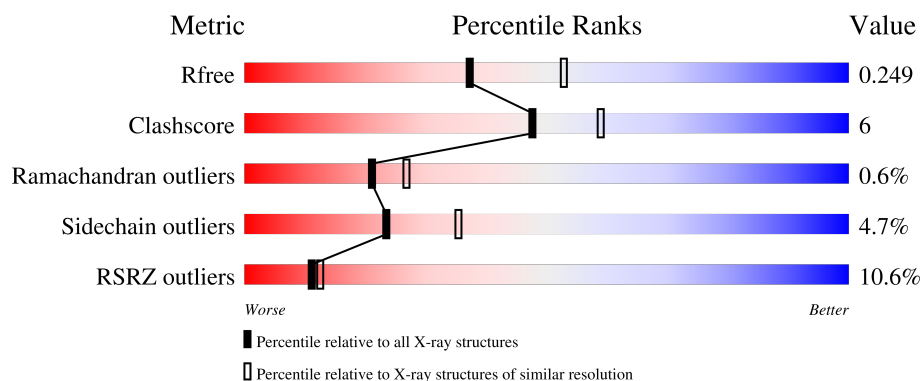
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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% 84% 14% ..
2	B	428	13% 78% 17% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8249 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 Gag-Pol polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	554	Total	C	N	O	S	0	0	0
			4505	2917	748	832	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

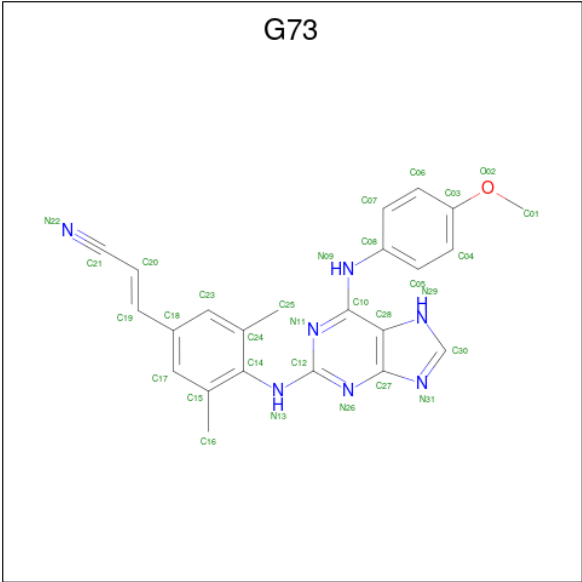
- Molecule 2 is a protein called Gag-Pol polyprotein.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 3 is (2E)-3-[4-({6-[(4-methoxyphenyl)amino]-7H-purin-2-yl}amino)-3,5-dimethylphenyl]prop-2-enenitrile (CCD ID: G73) (formula: C₂₃H₂₁N₇O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			31	23	7	1		

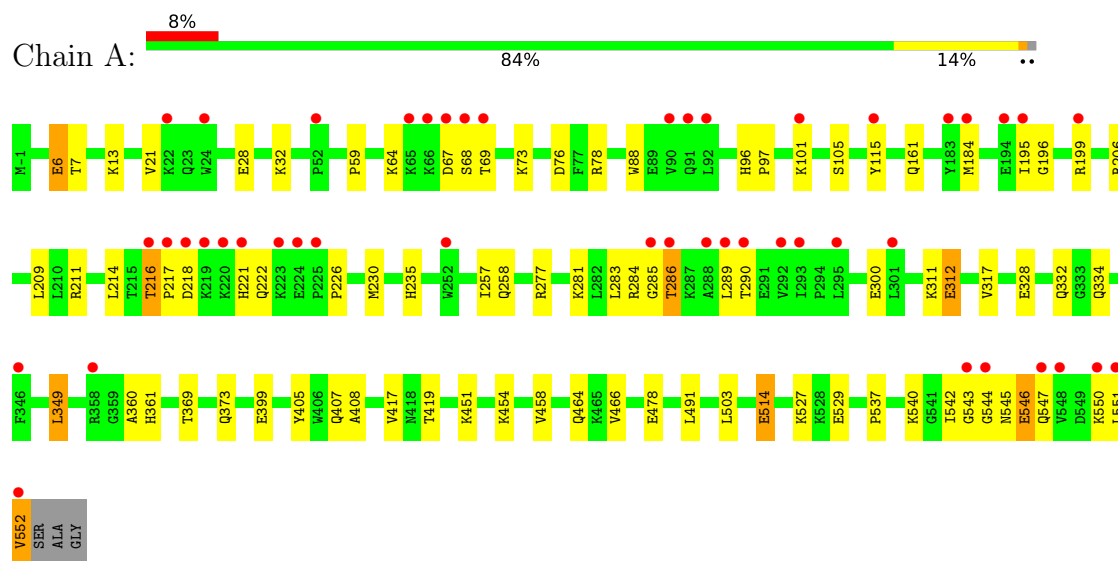
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	178	Total	O	0	0
			178	178		
4	B	122	Total	O	0	0
			122	122		

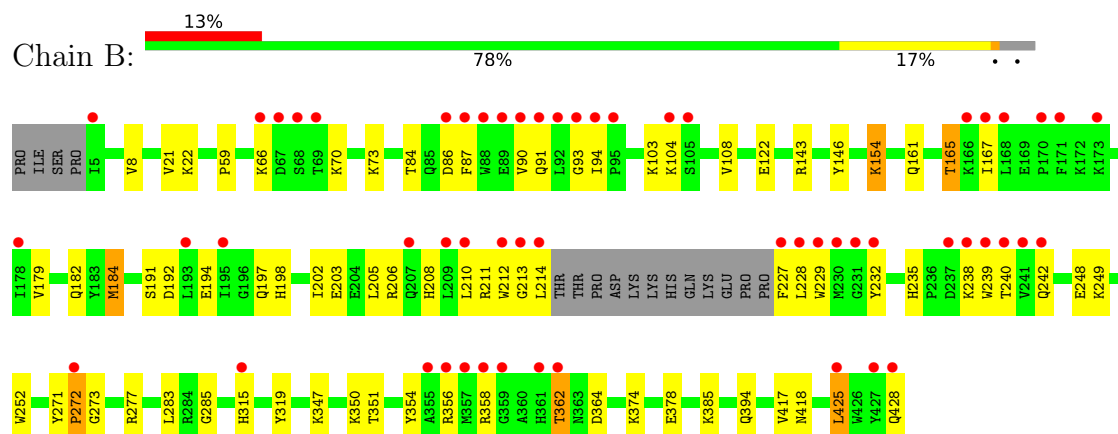
3 Residue-property plots [i](#)

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: Gag-Pol polyprotein



• Molecule 2: Gag-Pol polyprotein



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	162.65Å 72.99Å 109.60Å 90.00° 100.59° 90.00°	Depositor
Resolution (Å)	41.29 – 2.30 41.29 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.8 (41.29-2.30) 98.8 (41.29-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.216 , 0.260 0.216 , 0.249	Depositor DCC
R_{free} test set	2000 reflections (2.30%)	wwPDB-VP
Wilson B-factor (Å ²)	36.0	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 35.8	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	0.94	EDS
Total number of atoms	8249	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 4.82% 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: G73

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	0.34	0/4623	0.74	2/6284 (0.0%)
2	B	0.34	0/3511	0.76	4/4768 (0.1%)
All	All	0.34	0/8134	0.75	6/11052 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	216	THR	CA-C-N	8.17	130.06	119.84
1	A	216	THR	C-N-CA	8.17	130.06	119.84
2	B	235	HIS	CA-C-N	6.12	125.61	119.24
2	B	235	HIS	C-N-CA	6.12	125.61	119.24
2	B	184	MET	CB-CA-C	-5.96	109.68	116.54
2	B	285	GLY	N-CA-C	-5.21	106.02	112.33

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	4505	0	4562	47	0
2	B	3413	0	3443	47	0
3	A	31	0	21	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	178	0	0	9	0
4	B	122	0	0	10	0
All	All	8249	0	8026	90	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 6.

All (90) 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:182:GLN:O	4:B:617:HOH:O	1.91	0.89
1:A:101:LYS:HE2	3:A:601:G73:H23	1.59	0.82
2:B:347:LYS:O	4:B:525:HOH:O	1.98	0.81
1:A:328:GLU:OE2	4:A:864:HOH:O	2.01	0.79
2:B:154:LYS:HA	2:B:184:MET:HE1	1.67	0.75
2:B:428:GLN:OXT	4:B:557:HOH:O	2.06	0.71
2:B:358:ARG:HH12	2:B:374:LYS:HD2	1.56	0.69
2:B:91:GLN:HG3	2:B:93:GLY:H	1.58	0.68
1:A:332:GLN:OE1	4:A:833:HOH:O	2.11	0.67
2:B:206:ARG:NH1	2:B:229:TRP:O	2.29	0.66
2:B:425:LEU:O	4:B:557:HOH:O	2.14	0.65
2:B:194:GLU:HB3	2:B:197:GLN:HG2	1.80	0.64
2:B:240:THR:O	2:B:350:LYS:NZ	2.31	0.64
2:B:143:ARG:HD3	4:B:527:HOH:O	1.99	0.63
2:B:73:LYS:NZ	2:B:146:TYR:OH	2.32	0.62
2:B:202:ILE:HG22	2:B:206:ARG:HE	1.64	0.62
1:A:216:THR:O	1:A:218:ASP:N	2.32	0.61
1:A:6:GLU:H	1:A:6:GLU:CD	2.07	0.61
2:B:239:TRP:O	4:B:520:HOH:O	2.17	0.60
2:B:108:VAL:HB	2:B:232:TYR:HB3	1.83	0.59
1:A:311:LYS:HE3	1:A:312:GLU:HG2	1.85	0.59
1:A:527:LYS:NZ	4:A:808:HOH:O	2.36	0.59
1:A:257:ILE:HB	1:A:283:LEU:HD21	1.86	0.58
1:A:360:ALA:HA	1:A:514:GLU:HG3	1.86	0.57
1:A:218:ASP:OD1	4:A:843:HOH:O	2.18	0.56
3:A:601:G73:H5	3:A:601:G73:N11	2.22	0.55
1:A:206:ARG:CZ	1:A:218:ASP:HB2	2.37	0.54
1:A:88:TRP:CD1	2:B:143:ARG:HD2	2.43	0.54
1:A:88:TRP:NE1	2:B:143:ARG:HD2	2.22	0.54
1:A:101:LYS:H	3:A:601:G73:H22	1.55	0.54
2:B:425:LEU:HD13	2:B:428:GLN:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:103:LYS:HE3	2:B:179:VAL:HG23	1.91	0.53
2:B:161:GLN:O	2:B:165:THR:OG1	2.26	0.53
1:A:454:LYS:HZ1	1:A:552:VAL:HB	1.74	0.52
2:B:273:GLY:N	4:B:543:HOH:O	2.36	0.51
1:A:478:GLU:HG2	4:A:853:HOH:O	2.08	0.51
2:B:122:GLU:O	4:B:512:HOH:O	2.19	0.51
1:A:454:LYS:NZ	1:A:552:VAL:HB	2.26	0.51
1:A:405:TYR:CE2	1:A:407:GLN:HB2	2.47	0.50
2:B:198:HIS:O	2:B:202:ILE:HG12	2.11	0.50
1:A:28:GLU:HG2	1:A:32:LYS:HE3	1.93	0.50
1:A:277:ARG:HD2	1:A:334:GLN:HB3	1.93	0.50
1:A:491:LEU:HB3	1:A:529:GLU:HG2	1.95	0.49
1:A:76:ASP:OD1	1:A:78:ARG:HG3	2.12	0.49
2:B:70:LYS:O	4:B:536:HOH:O	2.20	0.49
2:B:208:HIS:O	2:B:212:TRP:HD1	1.95	0.49
1:A:258:GLN:HG2	1:A:283:LEU:HD13	1.93	0.49
1:A:543:GLY:N	2:B:283:LEU:O	2.46	0.48
2:B:191:SER:OG	2:B:198:HIS:ND1	2.39	0.48
1:A:317:VAL:HG23	1:A:349:LEU:HD12	1.94	0.48
1:A:451:LYS:NZ	4:A:876:HOH:O	2.46	0.48
1:A:458:VAL:HG12	1:A:464:GLN:HG2	1.94	0.48
2:B:239:TRP:N	4:B:520:HOH:O	2.46	0.48
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.95	0.48
1:A:544:GLY:O	1:A:546:GLU:N	2.48	0.47
1:A:369:THR:O	1:A:373:GLN:HG2	2.14	0.47
1:A:115:TYR:O	4:A:803:HOH:O	2.20	0.47
1:A:466:VAL:HG22	1:A:550:LYS:NZ	2.29	0.47
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.99	0.45
1:A:546:GLU:HA	4:A:750:HOH:O	2.17	0.45
1:A:21:VAL:HB	1:A:59:PRO:HD3	1.99	0.45
1:A:547:GLN:O	1:A:551:LEU:N	2.47	0.44
1:A:542:ILE:HG23	2:B:283:LEU:HD13	1.99	0.44
2:B:203:GLU:C	2:B:205:LEU:H	2.24	0.44
2:B:211:ARG:C	2:B:213:GLY:H	2.25	0.44
2:B:242:GLN:HB2	2:B:351:THR:OG1	2.17	0.44
1:A:196:GLY:HA2	1:A:199:ARG:HH21	1.83	0.44
1:A:68:SER:OG	1:A:69:THR:N	2.51	0.44
2:B:104:LYS:HB2	2:B:192:ASP:HA	2.00	0.44
2:B:208:HIS:O	2:B:208:HIS:ND1	2.51	0.43
1:A:466:VAL:HG22	1:A:550:LYS:HZ3	1.83	0.43
2:B:91:GLN:HB2	2:B:94:ILE:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:537:PRO:HB2	1:A:540:LYS:HG3	2.01	0.43
1:A:226:PRO:HB3	1:A:235:HIS:CE1	2.54	0.43
1:A:417:VAL:HG22	1:A:419:THR:HG23	2.01	0.43
1:A:281:LYS:HA	1:A:284:ARG:HG3	2.01	0.42
1:A:64:LYS:HD2	1:A:68:SER:O	2.19	0.42
2:B:249:LYS:HB2	2:B:252:TRP:CE2	2.55	0.42
2:B:315:HIS:O	2:B:347:LYS:NZ	2.42	0.42
2:B:277:ARG:HD3	2:B:277:ARG:HA	1.81	0.42
2:B:84:THR:O	2:B:154:LYS:NZ	2.50	0.41
2:B:271:TYR:HA	2:B:272:PRO:HD3	1.92	0.41
1:A:13:LYS:NZ	4:A:820:HOH:O	2.54	0.41
2:B:394:GLN:OE1	2:B:418:ASN:ND2	2.51	0.41
2:B:167:ILE:HG23	2:B:212:TRP:CG	2.56	0.41
2:B:354:TYR:OH	2:B:378:GLU:OE2	2.35	0.41
1:A:96:HIS:HA	1:A:97:PRO:HD3	1.96	0.40
2:B:362:THR:O	2:B:362:THR:OG1	2.38	0.40
1:A:209:LEU:HB3	1:A:214:LEU:HB2	2.03	0.40
2:B:319:TYR:OH	2:B:385:LYS:HE2	2.22	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	552/557 (99%)	529 (96%)	19 (3%)	4 (1%)	18	23
2	B	408/428 (95%)	388 (95%)	18 (4%)	2 (0%)	24	31
All	All	960/985 (98%)	917 (96%)	37 (4%)	6 (1%)	21	27

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	217	PRO
1	A	545	ASN
1	A	285	GLY
2	B	272	PRO
1	A	286	THR
2	B	86	ASP

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	494/495 (100%)	470 (95%)	24 (5%)	22	34
2	B	374/390 (96%)	357 (96%)	17 (4%)	24	37
All	All	868/885 (98%)	827 (95%)	41 (5%)	23	35

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLU
1	A	7	THR
1	A	67	ASP
1	A	73	LYS
1	A	105	SER
1	A	161	GLN
1	A	184	MET
1	A	195	ILE
1	A	211	ARG
1	A	221	HIS
1	A	222	GLN
1	A	230	MET
1	A	286	THR
1	A	289	LEU
1	A	290	THR
1	A	300	GLU
1	A	312	GLU
1	A	349	LEU

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Mol	Chain	Res	Type
1	A	361	HIS
1	A	399	GLU
1	A	503	LEU
1	A	514	GLU
1	A	546	GLU
1	A	552	VAL
2	B	8	VAL
2	B	22	LYS
2	B	66	LYS
2	B	87	PHE
2	B	90	VAL
2	B	154	LYS
2	B	165	THR
2	B	210	LEU
2	B	214	LEU
2	B	227	PHE
2	B	228	LEU
2	B	238	LYS
2	B	248	GLU
2	B	356	ARG
2	B	362	THR
2	B	417	VAL
2	B	425	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	161	GLN
1	A	197	GLN
1	A	418	ASN
1	A	480	GLN
1	A	487	GLN
1	A	539	HIS
1	A	545	ASN
2	B	147	ASN
2	B	207	GLN
2	B	278	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	G73	A	601	-	34,34,34	1.38	3 (8%)	44,47,47	2.67	11 (25%)

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	G73	A	601	-	-	4/13/14/14	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	G73	C10-N09	4.27	1.44	1.36
3	A	601	G73	C12-N13	3.96	1.44	1.36
3	A	601	G73	C27-N26	3.64	1.39	1.34

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	G73	N26-C27-N31	10.63	134.24	125.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	G73	C27-N31-C30	7.69	108.73	103.84
3	A	601	G73	C28-C27-N26	-5.98	118.95	124.22
3	A	601	G73	C28-C27-N31	-4.59	106.81	110.46
3	A	601	G73	N26-C12-N11	-3.59	120.38	126.26
3	A	601	G73	N29-C30-N31	-3.52	108.50	113.87
3	A	601	G73	C14-N13-C12	-3.29	117.94	123.38
3	A	601	G73	C27-C28-N29	3.00	107.29	105.28
3	A	601	G73	C28-N29-C30	2.86	108.66	106.27
3	A	601	G73	C12-N11-C10	2.43	122.33	116.36
3	A	601	G73	C18-C19-C20	-2.24	113.61	125.50

There are no chirality outliers.

All (4) torsion outliers are listed below:

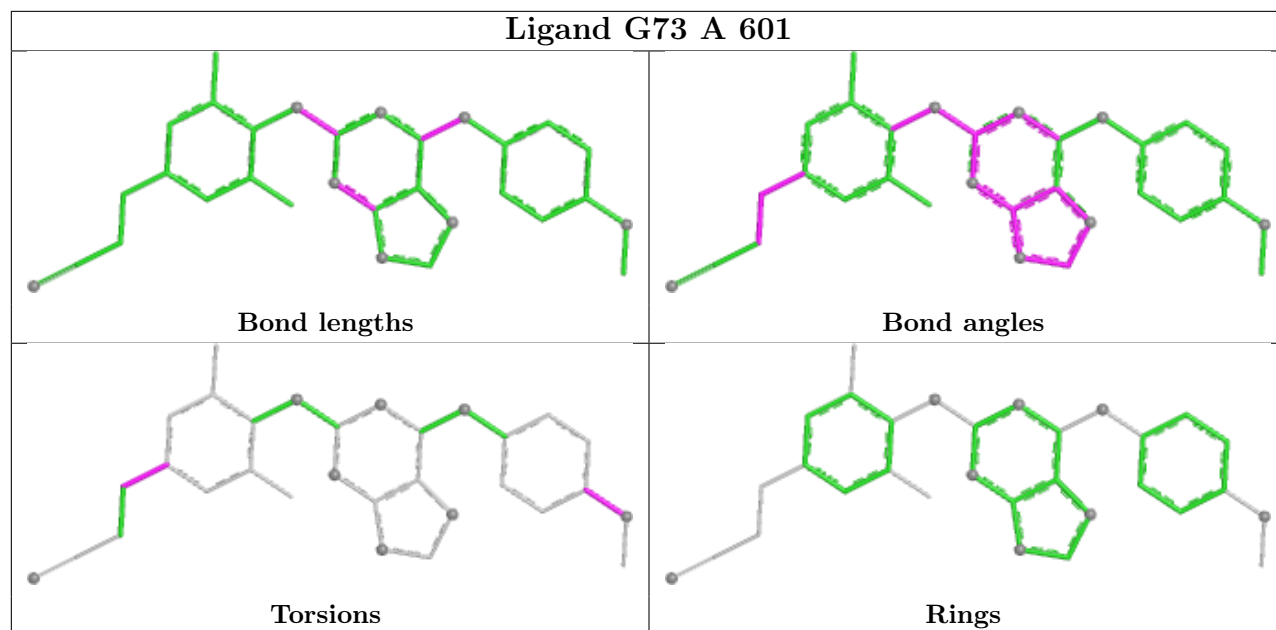
Mol	Chain	Res	Type	Atoms
3	A	601	G73	C23-C18-C19-C20
3	A	601	G73	C17-C18-C19-C20
3	A	601	G73	C04-C03-O02-C01
3	A	601	G73	C06-C03-O02-C01

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	G73	3	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	554/557 (99%)	0.47	46 (8%) 17 19	25, 46, 86, 129	0
2	B	412/428 (96%)	0.71	56 (13%) 7 7	26, 47, 95, 125	0
All	All	966/985 (98%)	0.57	102 (10%) 11 12	25, 47, 92, 129	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	92	LEU	7.1
2	B	90	VAL	6.7
2	B	88	TRP	6.2
1	A	551	LEU	6.1
2	B	240	THR	6.0
2	B	227	PHE	5.8
2	B	93	GLY	5.6
2	B	229	TRP	5.6
2	B	241	VAL	5.2
2	B	228	LEU	5.2
1	A	544	GLY	5.2
2	B	214	LEU	5.0
2	B	94	ILE	4.8
1	A	552	VAL	4.7
2	B	357	MET	4.7
2	B	5	ILE	4.4
2	B	95	PRO	4.2
1	A	221	HIS	4.1
1	A	225	PRO	4.1
2	B	361	HIS	4.0
2	B	87	PHE	4.0
1	A	543	GLY	3.8
2	B	425	LEU	3.7
2	B	66	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
2	B	230	MET	3.6
1	A	220	LYS	3.5
1	A	90	VAL	3.5
1	A	218	ASP	3.4
2	B	232	TYR	3.4
1	A	92	LEU	3.4
2	B	358	ARG	3.4
2	B	212	TRP	3.3
1	A	289	LEU	3.3
2	B	171	PHE	3.3
1	A	91	GLN	3.3
2	B	355	ALA	3.2
2	B	428	GLN	3.2
2	B	91	GLN	3.2
1	A	65	LYS	3.2
2	B	170	PRO	3.1
2	B	210	LEU	3.1
2	B	231	GLY	3.1
1	A	548	VAL	3.1
1	A	547	GLN	3.0
1	A	24	TRP	3.0
1	A	194	GLU	3.0
1	A	217	PRO	3.0
1	A	550	LYS	2.9
2	B	239	TRP	2.9
2	B	167	ILE	2.8
1	A	219	LYS	2.8
1	A	183	TYR	2.8
1	A	67	ASP	2.7
2	B	68	SER	2.7
1	A	184	MET	2.7
1	A	195	ILE	2.7
2	B	356	ARG	2.7
2	B	67	ASP	2.6
2	B	168	LEU	2.6
2	B	89	GLU	2.6
2	B	359	GLY	2.6
1	A	216	THR	2.5
2	B	315	HIS	2.5
1	A	252	TRP	2.5
2	B	193	LEU	2.5
2	B	86	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	213	GLY	2.5
2	B	105	SER	2.4
1	A	288	ALA	2.4
1	A	358	ARG	2.4
2	B	362	THR	2.4
2	B	195	ILE	2.4
2	B	209	LEU	2.4
2	B	69	THR	2.4
2	B	166	LYS	2.4
1	A	292	VAL	2.4
1	A	286	THR	2.4
1	A	22	LYS	2.3
1	A	66	LYS	2.3
2	B	173	LYS	2.3
1	A	69	THR	2.3
2	B	238	LYS	2.3
2	B	427	TYR	2.3
1	A	223	LYS	2.3
1	A	285	GLY	2.2
1	A	301	LEU	2.2
2	B	272	PRO	2.2
1	A	290	THR	2.2
1	A	199	ARG	2.1
1	A	295	LEU	2.1
1	A	346	PHE	2.1
1	A	101	LYS	2.1
1	A	52	PRO	2.1
1	A	68	SER	2.1
1	A	224	GLU	2.1
1	A	293	ILE	2.1
2	B	242	GLN	2.1
1	A	115	TYR	2.1
2	B	207	GLN	2.0
2	B	237	ASP	2.0
2	B	178	ILE	2.0
2	B	104	LYS	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 [i](#)

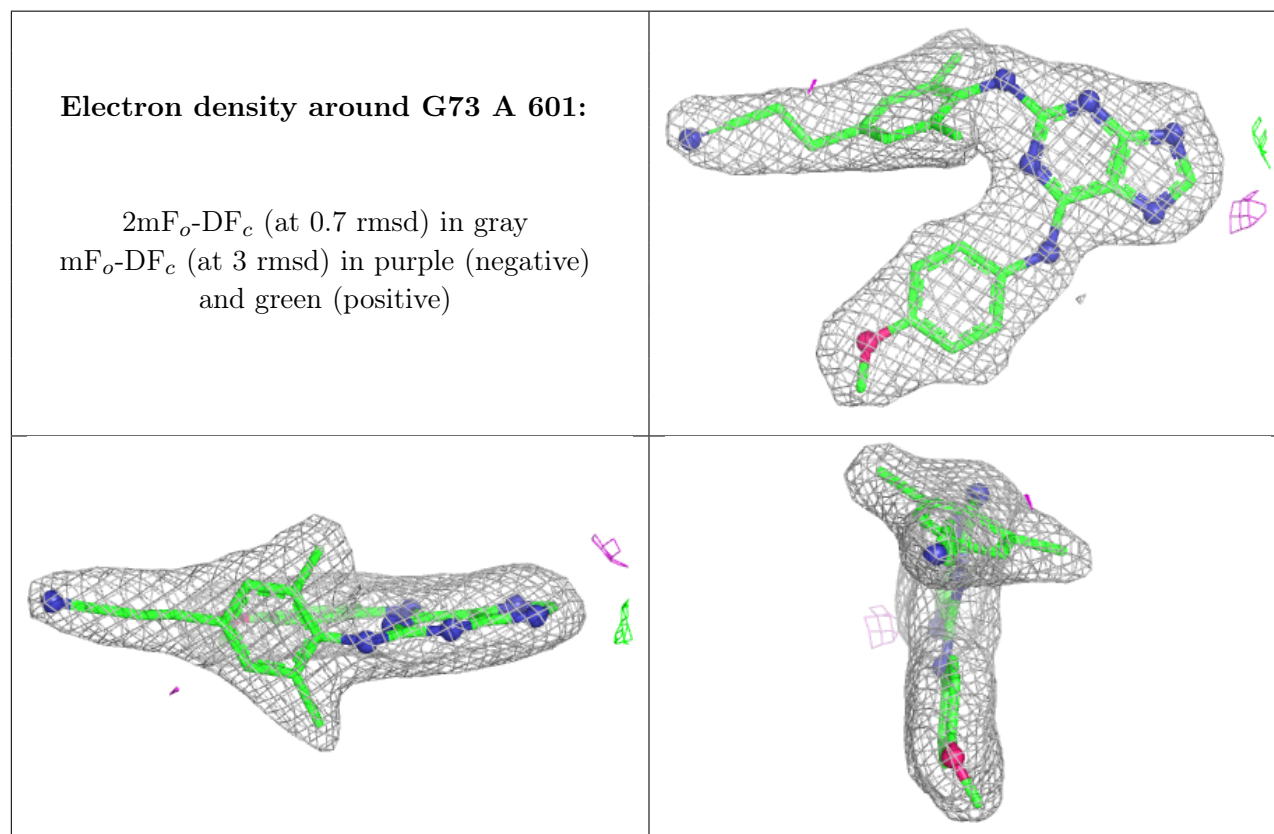
There are no oligosaccharides in this entry.

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(Å ²)	Q<0.9
3	G73	A	601	31/31	0.95	0.08	31,38,49,52	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.