



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:53 PM UTC

PDB ID : 8U6A / pdb_00008u6a
Title : Crystal Structure of HIV-1 Reverse Transcriptase in Complex with (JLJ729),
a non-nucleoside inhibitor
Authors : Hollander, K.; Carter, Z.; Jorgensen, W.L.; Anderson, K.S.
Deposited on : 2023-09-13
Resolution : 2.37 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

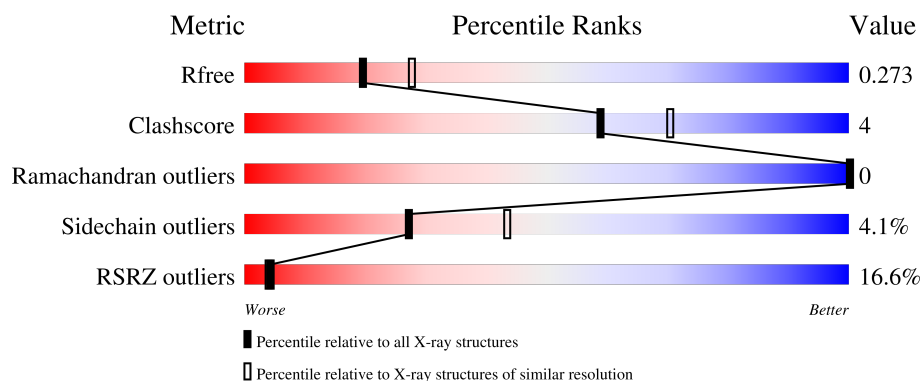
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.37 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	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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	18% 85% 13% .
2	B	428	14% 81% 12% 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7419 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	549	Total	C	N	O	S	0	0	0
			4157	2679	699	772	7			

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

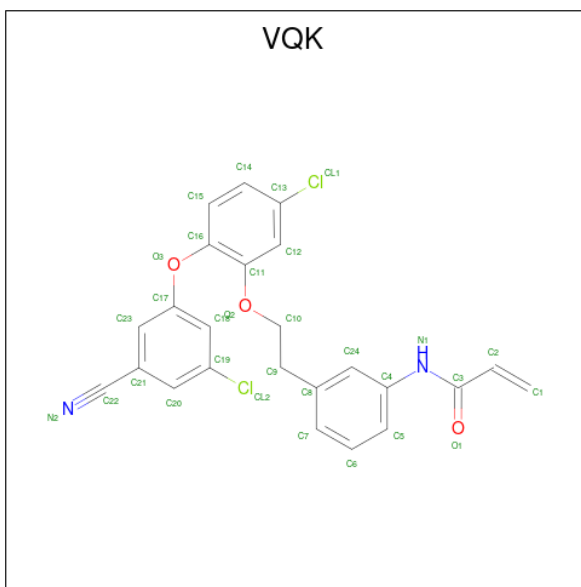
- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	399	Total	C	N	O	S	0	0	0
			3145	2039	518	582	6			

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 N-(3-{2-[5-chloro-2-(3-chloro-5-cyanophenoxy)phenoxy]ethyl}phenyl)prop-2-enamide (CCD ID: VQK) (formula: C₂₄H₁₈Cl₂N₂O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	1
			62	48	4	4	6		

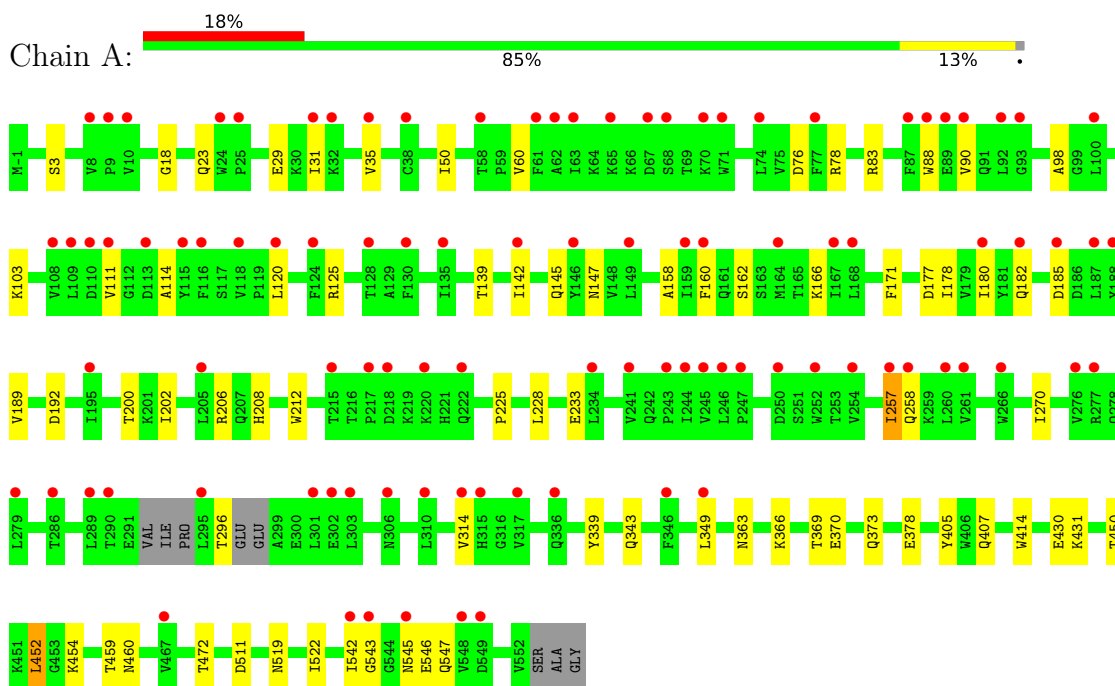
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	39	Total	O	0	0
			39	39		
4	B	16	Total	O	0	0
			16	16		

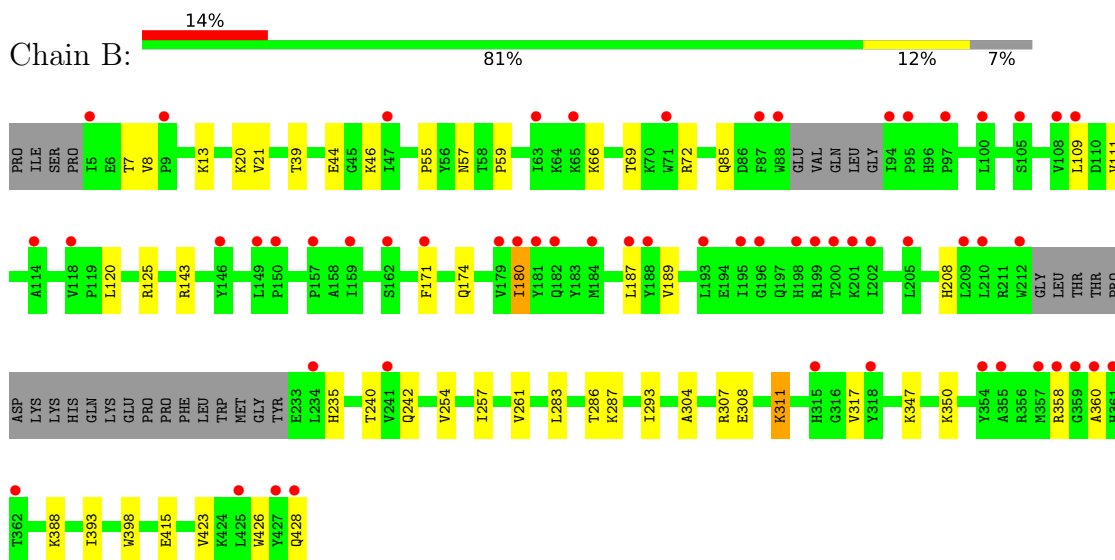
3 Residue-property plots

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: 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	162.90Å 73.81Å 108.45Å 90.00° 100.16° 90.00°	Depositor
Resolution (Å)	106.75 – 2.37 106.75 – 2.37	Depositor EDS
% Data completeness (in resolution range)	98.7 (106.75-2.37) 98.7 (106.75-2.37)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 2.37Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.245 , 0.271 0.252 , 0.273	Depositor DCC
R_{free} test set	2003 reflections (3.87%)	wwPDB-VP
Wilson B-factor (Å ²)	72.9	Xtriage
Anisotropy	0.257	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 53.0	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	0.94	EDS
Total number of atoms	7419	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.48% 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: VQK

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	0.25	0/4268	0.43	0/5843
2	B	0.25	0/3233	0.42	0/4413
All	All	0.25	0/7501	0.42	0/10256

There are no bond length outliers.

There are no bond angle outliers.

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	4157	0	3862	40	0
2	B	3145	0	3022	27	0
3	A	62	0	0	1	0
4	A	39	0	0	4	0
4	B	16	0	0	0	0
All	All	7419	0	6884	63	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 (63) 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:414:TRP:NE1	4:A:706:HOH:O	2.33	0.60
2:B:358:ARG:O	2:B:360:ALA:N	2.35	0.58
1:A:543:GLY:HA3	2:B:283:LEU:O	2.10	0.52
2:B:20:LYS:HE2	2:B:55:PRO:HB2	1.91	0.52
1:A:343:GLN:HG3	1:A:349:LEU:HD11	1.92	0.51
2:B:13:LYS:HG3	2:B:85:GLN:HA	1.93	0.50
2:B:317:VAL:HG22	2:B:347:LYS:HG3	1.92	0.50
1:A:545:ASN:OD1	4:A:701:HOH:O	2.20	0.50
1:A:50:ILE:HG21	1:A:145:GLN:HB3	1.92	0.50
1:A:454:LYS:NZ	4:A:709:HOH:O	2.45	0.49
1:A:208:HIS:CE1	1:A:212:TRP:HZ3	2.30	0.49
1:A:228:LEU:HD22	1:A:233:GLU:HG2	1.95	0.49
1:A:114:ALA:HB1	1:A:160:PHE:CE1	2.47	0.49
2:B:423:VAL:HG12	2:B:426:TRP:CZ3	2.48	0.48
1:A:519:ASN:HA	1:A:522:ILE:HD12	1.94	0.48
2:B:254:VAL:HG22	2:B:293:ILE:HD11	1.95	0.48
2:B:307:ARG:O	2:B:311:LYS:HG3	2.14	0.48
2:B:111:VAL:HG11	2:B:187:LEU:HD22	1.95	0.48
2:B:423:VAL:HG12	2:B:426:TRP:CE3	2.50	0.47
1:A:88:TRP:CD1	2:B:143:ARG:HD2	2.50	0.47
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.96	0.47
2:B:423:VAL:HA	2:B:426:TRP:CE3	2.49	0.47
1:A:202:ILE:O	1:A:206:ARG:HG3	2.15	0.47
1:A:430:GLU:O	4:A:702:HOH:O	2.20	0.46
2:B:240:THR:O	2:B:350:LYS:HD2	2.16	0.46
2:B:393:ILE:HD13	2:B:398:TRP:HB2	1.97	0.46
1:A:180:ILE:HG12	1:A:189:VAL:HG13	1.97	0.46
1:A:257:ILE:HG13	1:A:258:GLN:N	2.30	0.46
1:A:76:ASP:OD1	1:A:78:ARG:HG3	2.16	0.46
1:A:120:LEU:HD23	1:A:125:ARG:HG2	1.98	0.45
2:B:308:GLU:HG2	2:B:311:LYS:NZ	2.32	0.45
1:A:111:VAL:HG12	1:A:185:ASP:O	2.17	0.45
1:A:31:ILE:O	1:A:35:VAL:HG23	2.17	0.45
1:A:171:PHE:HB2	1:A:208:HIS:CD2	2.52	0.45
1:A:18:GLY:H	1:A:83:ARG:NH1	2.14	0.45
1:A:125:ARG:HD3	1:A:147:ASN:HA	1.98	0.45
1:A:363:ASN:HA	1:A:511:ASP:OD1	2.18	0.44
2:B:44:GLU:OE1	2:B:46:LYS:NZ	2.43	0.44
1:A:90:VAL:HG11	1:A:158:ALA:HA	1.99	0.44
1:A:98:ALA:HB1	1:A:349:LEU:HB3	2.00	0.44
1:A:88:TRP:NE1	2:B:143:ARG:HD2	2.31	0.44
2:B:21:VAL:O	2:B:57:ASN:ND2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:187:LEU:HD12	2:B:187:LEU:HA	1.78	0.44
1:A:111:VAL:HG13	1:A:114:ALA:HB2	1.99	0.43
1:A:405:TYR:CE2	1:A:407:GLN:HB2	2.53	0.43
2:B:257:ILE:O	2:B:261:VAL:HG23	2.19	0.43
1:A:460:ASN:HA	2:B:286:THR:O	2.18	0.43
2:B:120:LEU:HD23	2:B:125:ARG:HG2	2.00	0.43
1:A:225:PRO:HG3	3:A:601[B]:VQK:O1	2.19	0.43
1:A:366:LYS:O	1:A:370:GLU:HG3	2.19	0.43
1:A:369:THR:O	1:A:373:GLN:HG2	2.19	0.43
1:A:450:THR:HB	1:A:452:LEU:HD12	2.01	0.42
1:A:270:ILE:HG13	1:A:314:VAL:HG12	2.01	0.42
1:A:3:SER:HB2	1:A:212:TRP:CD1	2.54	0.42
2:B:171:PHE:HB2	2:B:208:HIS:CD2	2.55	0.42
1:A:103:LYS:HA	1:A:192:ASP:OD1	2.20	0.42
2:B:180:ILE:HG13	2:B:189:VAL:HG12	2.01	0.41
2:B:304:ALA:O	2:B:308:GLU:HG3	2.20	0.41
1:A:206:ARG:HB3	1:A:206:ARG:CZ	2.51	0.41
1:A:339:TYR:OH	1:A:378:GLU:OE1	2.33	0.41
1:A:23:GLN:HE22	1:A:60:VAL:H	1.69	0.40
1:A:162:SER:O	1:A:166:LYS:HG3	2.21	0.40
2:B:388:LYS:HE3	2:B:415:GLU:CD	2.46	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	543/557 (98%)	531 (98%)	12 (2%)	0	100	100
2	B	393/428 (92%)	387 (98%)	6 (2%)	0	100	100
All	All	936/985 (95%)	918 (98%)	18 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	402/495 (81%)	386 (96%)	16 (4%)	28	44
2	B	326/390 (84%)	312 (96%)	14 (4%)	26	41
All	All	728/885 (82%)	698 (96%)	30 (4%)	27	43

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	GLU
1	A	139	THR
1	A	142	ILE
1	A	177	ASP
1	A	178	ILE
1	A	182	GLN
1	A	200	THR
1	A	257	ILE
1	A	296	THR
1	A	431	LYS
1	A	452	LEU
1	A	459	THR
1	A	472	THR
1	A	542	ILE
1	A	546	GLU
1	A	547	GLN
2	B	7	THR
2	B	8	VAL
2	B	39	THR
2	B	66	LYS
2	B	69	THR
2	B	72	ARG
2	B	109	LEU
2	B	174	GLN
2	B	180	ILE

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Mol	Chain	Res	Type
2	B	235	HIS
2	B	242	GLN
2	B	287	LYS
2	B	311	LYS
2	B	428	GLN

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	182	GLN
1	A	208	HIS
1	A	221	HIS
1	A	336	GLN
1	A	520	GLN
1	A	524	GLN
2	B	137	ASN
2	B	182	GLN
2	B	208	HIS
2	B	255	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 [i](#)

2 ligands are 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	VQK	A	601[B]	-	33,33,33	0.31	0	44,44,44	1.20	2 (4%)
3	VQK	A	601[A]	-	33,33,33	0.26	0	44,44,44	0.64	0

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	VQK	A	601[B]	-	-	3/18/18/18	0/3/3/3
3	VQK	A	601[A]	-	-	3/18/18/18	0/3/3/3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601[B]	VQK	C2-C3-N1	6.40	118.18	113.84
3	A	601[B]	VQK	O1-C3-C2	-2.18	119.44	122.70

There are no chirality outliers.

All (6) torsion outliers are listed below:

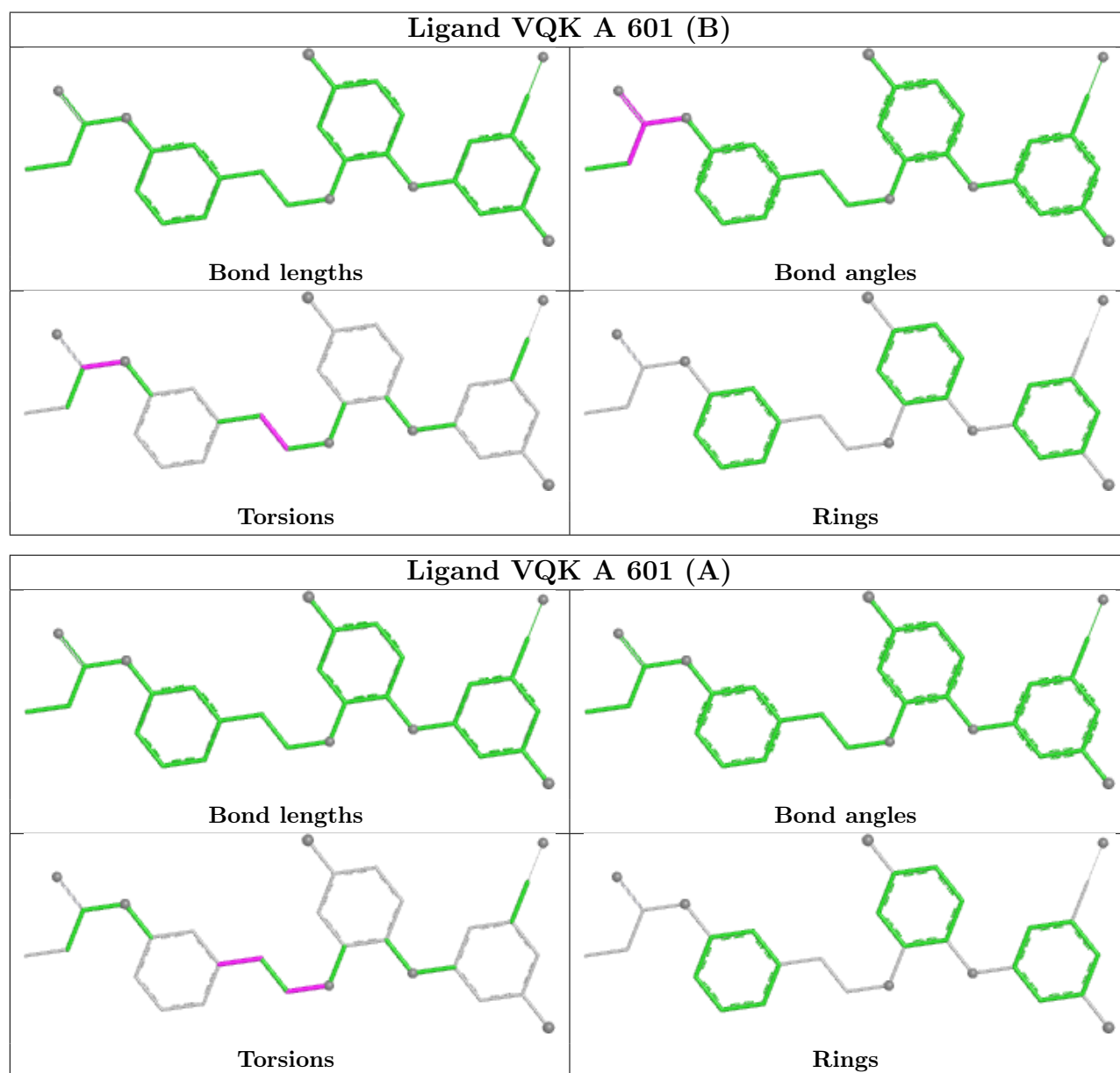
Mol	Chain	Res	Type	Atoms
3	A	601[B]	VQK	C2-C3-N1-C4
3	A	601[B]	VQK	O1-C3-N1-C4
3	A	601[A]	VQK	C9-C10-O2-C11
3	A	601[B]	VQK	O2-C10-C9-C8
3	A	601[A]	VQK	C7-C8-C9-C10
3	A	601[A]	VQK	C24-C8-C9-C10

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601[B]	VQK	1	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	549/557 (98%)	1.08	99 (18%) 3 3	50, 102, 143, 162	0
2	B	399/428 (93%)	1.01	58 (14%) 6 5	53, 85, 129, 140	0
All	All	948/985 (96%)	1.05	157 (16%) 4 4	50, 93, 137, 162	0

All (157) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	24	TRP	5.4
2	B	88	TRP	5.0
1	A	113	ASP	4.4
1	A	279	LEU	4.2
1	A	168	LEU	4.0
2	B	362	THR	3.8
2	B	234	LEU	3.7
1	A	124	PHE	3.6
2	B	357	MET	3.6
1	A	92	LEU	3.6
2	B	159	ILE	3.6
1	A	116	PHE	3.5
2	B	182	GLN	3.5
2	B	360	ALA	3.5
2	B	195	ILE	3.5
1	A	130	PHE	3.5
1	A	215	THR	3.5
1	A	164	MET	3.4
1	A	205	LEU	3.4
1	A	260	LEU	3.3
2	B	149	LEU	3.3
1	A	90	VAL	3.2
1	A	146	TYR	3.2
1	A	289	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	150	PRO	3.2
1	A	244	ILE	3.2
1	A	38	CYS	3.1
2	B	198	HIS	3.1
2	B	428	GLN	3.1
2	B	5	ILE	3.1
1	A	110	ASP	3.1
2	B	241	VAL	3.1
2	B	65	LYS	3.1
1	A	222	GLN	3.1
1	A	188	TYR	3.0
2	B	354	TYR	3.0
1	A	252	TRP	3.0
2	B	361	HIS	3.0
2	B	427	TYR	3.0
1	A	246	LEU	3.0
2	B	108	VAL	3.0
2	B	196	GLY	2.9
2	B	105	SER	2.9
1	A	65	LYS	2.9
1	A	234	LEU	2.9
1	A	266	TRP	2.9
2	B	193	LEU	2.9
1	A	549	ASP	2.9
2	B	95	PRO	2.8
2	B	181	TYR	2.8
1	A	108	VAL	2.8
1	A	245	VAL	2.8
1	A	276	VAL	2.8
1	A	290	THR	2.8
2	B	180	ILE	2.8
2	B	318	TYR	2.8
1	A	346	PHE	2.8
1	A	314	VAL	2.8
1	A	167	ILE	2.7
1	A	111	VAL	2.7
1	A	67	ASP	2.7
2	B	100	LEU	2.7
2	B	355	ALA	2.7
1	A	9	PRO	2.7
1	A	68	SER	2.7
1	A	303	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	209	LEU	2.7
1	A	61	PHE	2.7
1	A	118	VAL	2.7
1	A	74	LEU	2.7
1	A	77	PHE	2.6
1	A	8	VAL	2.6
2	B	200	THR	2.6
1	A	277	ARG	2.6
2	B	358	ARG	2.6
1	A	317	VAL	2.6
2	B	210	LEU	2.6
1	A	115	TYR	2.6
2	B	162	SER	2.6
1	A	120	LEU	2.5
1	A	187	LEU	2.5
1	A	306	ASN	2.5
2	B	184	MET	2.5
1	A	315	HIS	2.5
1	A	135	ILE	2.5
1	A	195	ILE	2.5
1	A	548	VAL	2.5
2	B	188	TYR	2.5
2	B	9	PRO	2.5
2	B	425	LEU	2.4
1	A	247	PRO	2.4
1	A	58	THR	2.4
1	A	35	VAL	2.4
2	B	94	ILE	2.4
2	B	109	LEU	2.4
2	B	187	LEU	2.4
2	B	199	ARG	2.4
1	A	149	LEU	2.4
1	A	258	GLN	2.4
1	A	286	THR	2.4
1	A	63	ILE	2.4
1	A	218	ASP	2.3
1	A	62	ALA	2.3
1	A	128	THR	2.3
2	B	71	TRP	2.3
2	B	63	ILE	2.3
1	A	160	PHE	2.3
2	B	118	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	545	ASN	2.3
2	B	179	VAL	2.3
1	A	88	TRP	2.3
1	A	89	GLU	2.3
1	A	32	LYS	2.3
1	A	70	LYS	2.3
1	A	220	LYS	2.3
1	A	109	LEU	2.2
1	A	543	GLY	2.2
1	A	302	GLU	2.2
1	A	87	PHE	2.2
1	A	159	ILE	2.2
1	A	100	LEU	2.2
1	A	241	VAL	2.2
1	A	254	VAL	2.2
1	A	185	ASP	2.2
1	A	217	PRO	2.2
1	A	261	VAL	2.2
1	A	467	VAL	2.2
2	B	87	PHE	2.2
1	A	25	PRO	2.2
2	B	157	PRO	2.2
1	A	93	GLY	2.2
1	A	257	ILE	2.1
1	A	301	LEU	2.1
2	B	202	ILE	2.1
1	A	10	VAL	2.1
2	B	315	HIS	2.1
2	B	114	ALA	2.1
2	B	146	TYR	2.1
2	B	47	ILE	2.1
1	A	182	GLN	2.1
1	A	180	ILE	2.1
1	A	295	LEU	2.1
1	A	310	LEU	2.1
2	B	205	LEU	2.1
2	B	359	GLY	2.1
1	A	71	TRP	2.1
1	A	336	GLN	2.0
1	A	349	LEU	2.0
1	A	542	ILE	2.0
1	A	243	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	171	PHE	2.0
2	B	201	LYS	2.0
2	B	212	TRP	2.0
1	A	250	ASP	2.0
1	A	31	ILE	2.0
1	A	142	ILE	2.0
2	B	97	PRO	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](#)

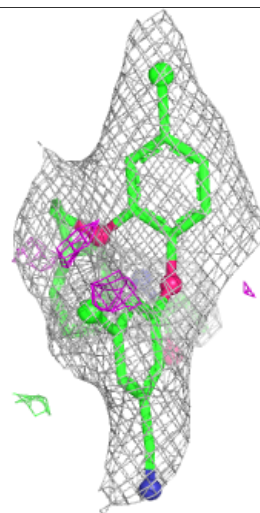
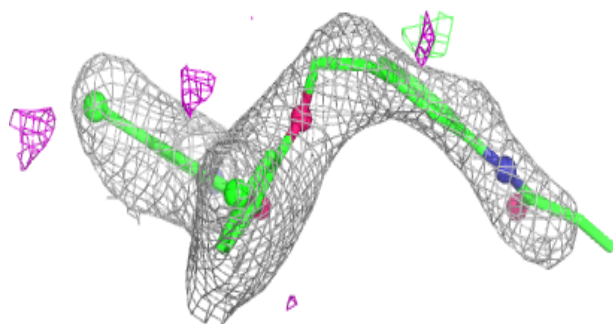
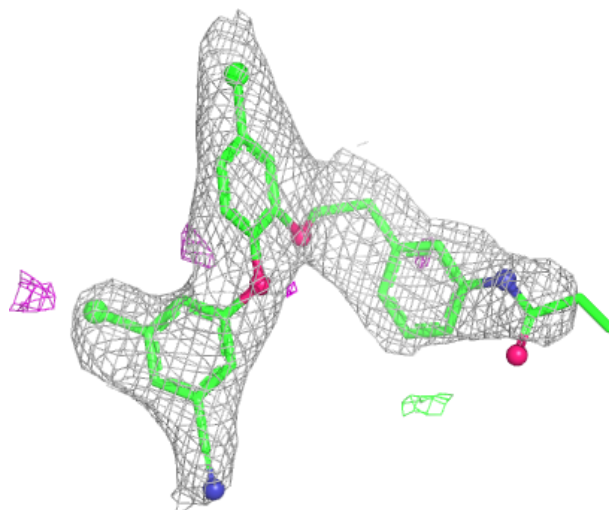
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	VQK	A	601[A]	31/31	0.82	0.18	101,105,114,121	31
3	VQK	A	601[B]	31/31	0.82	0.18	101,105,113,121	31

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.

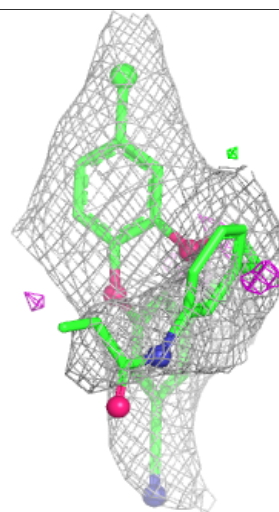
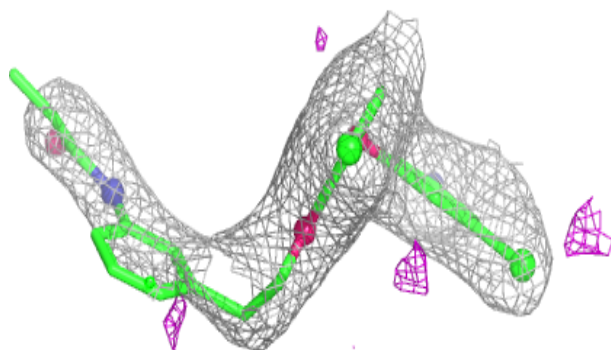
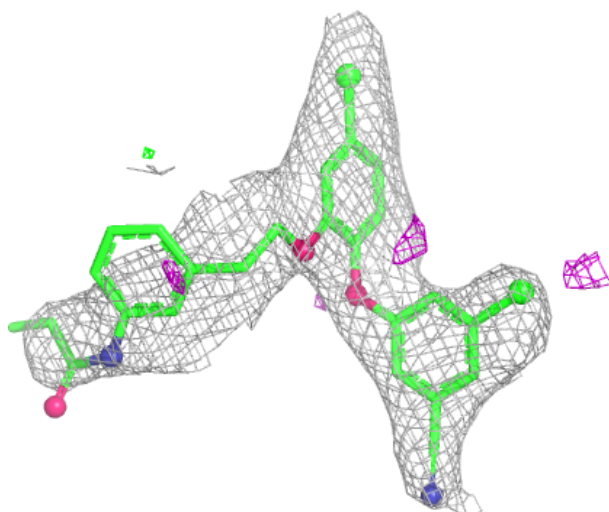
Electron density around VQK A 601 (A):

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around VQK A 601 (B):

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.