



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:44 AM UTC

PDB ID : 8U6N / pdb_00008u6n
Title : Crystal Structure of HIV-1 Reverse Transcriptase in Complex with 3-(2-((6-cyanonaphthalen-1-yl)oxy)phenoxy)-N,N-dimethylpropanamide (JLJ752), a non-nucleoside inhibitor
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Deposited on : 2023-09-13
Resolution : 2.74 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

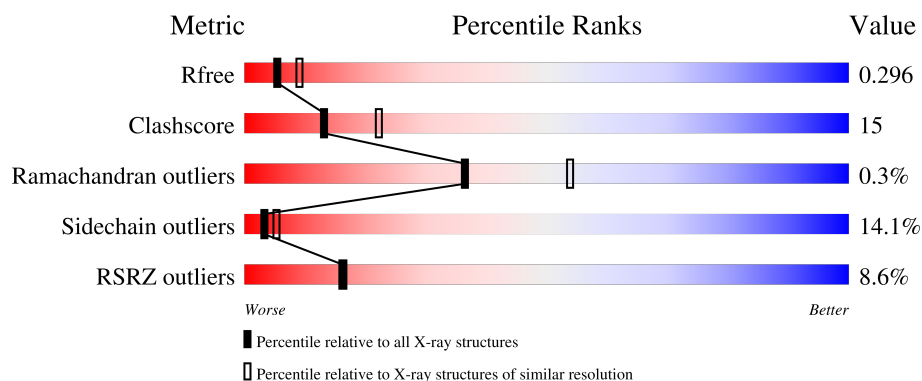
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.74 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	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
Sidechain outliers	187428	1831 (2.76-2.72)
RSRZ outliers	180081	1819 (2.76-2.72)

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	539	8% 62% 30% . .
2	B	428	9% 66% 24% . 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6757 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	521	Total	C	N	O	S	0	0	0
			3724	2390	636	691	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

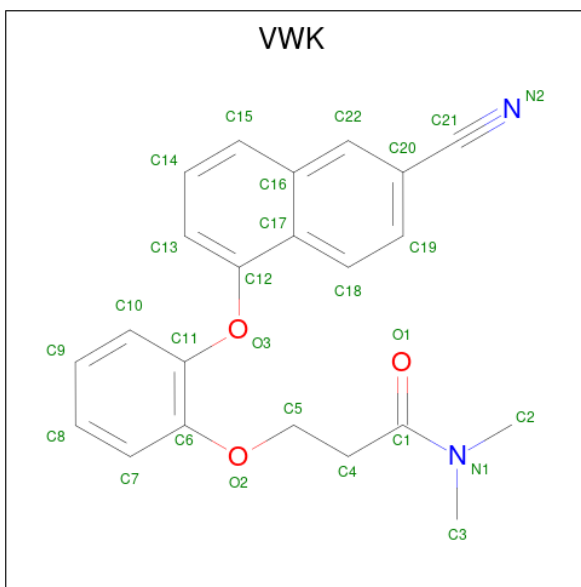
- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	401	Total	C	N	O	S	0	0	0
			2998	1940	494	559	5			

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 3-{2-[(6-cyanonaphthalen-1-yl)oxy]phenoxy}-N,N-dimethylpropanamide (CCD ID: VWK) (formula: C₂₂H₂₀N₂O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			27	22	2	3		

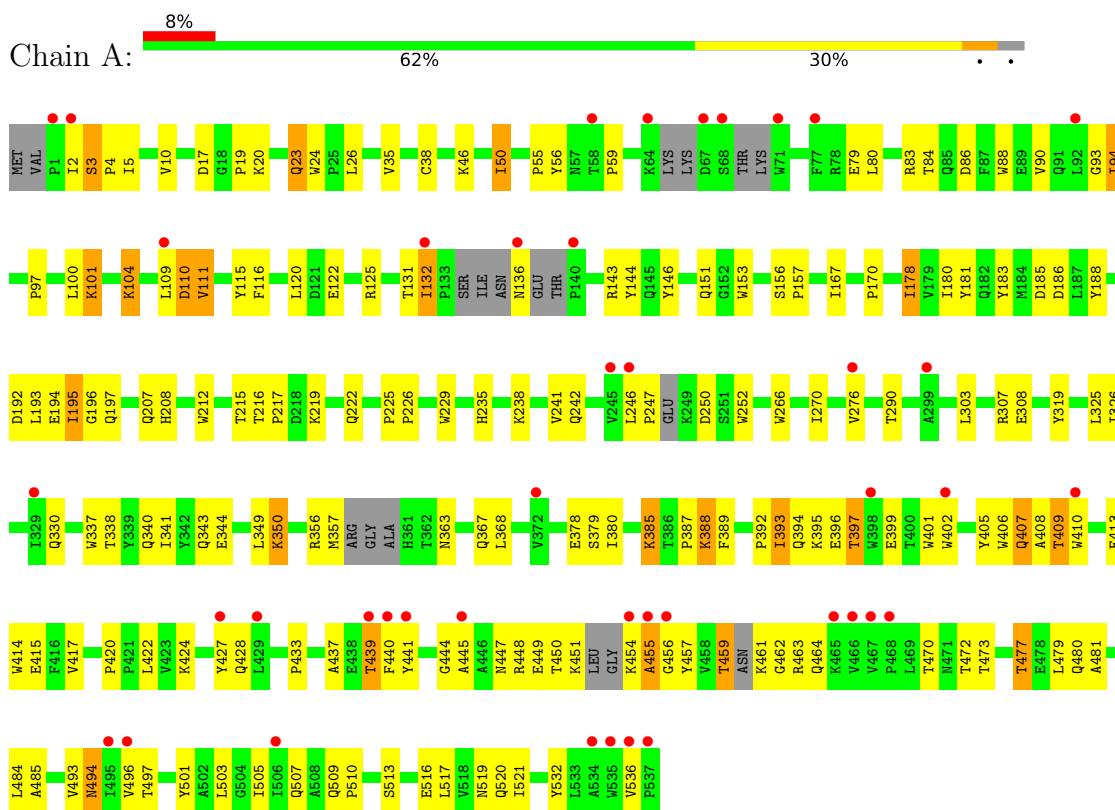
- Molecule 4 is water.

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

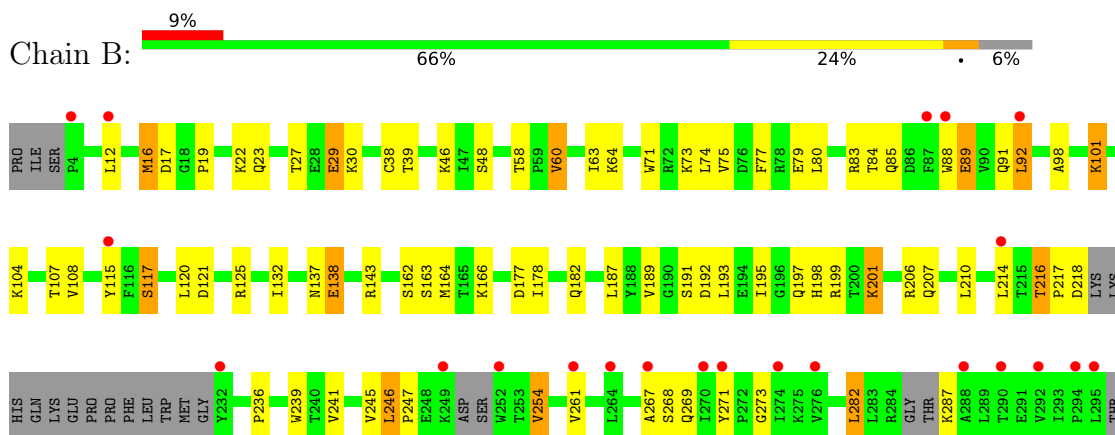
3 Residue-property plots [i](#)

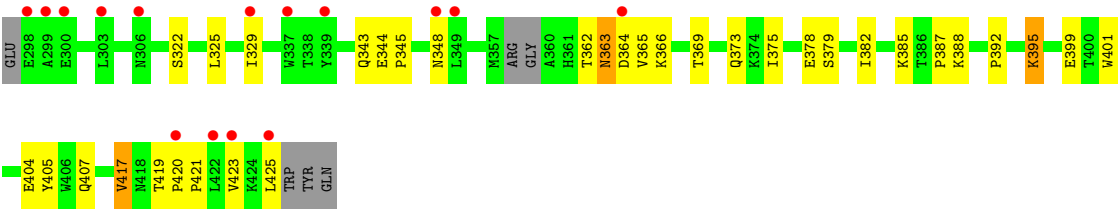
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 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	209.57Å 65.65Å 100.57Å 90.00° 114.67° 90.00°	Depositor
Resolution (Å)	36.45 – 2.74 36.45 – 2.74	Depositor EDS
% Data completeness (in resolution range)	99.7 (36.45-2.74) 99.7 (36.45-2.74)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 2.72Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.253 , 0.291 0.266 , 0.296	Depositor DCC
R_{free} test set	1655 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	90.0	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 78.9	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	0.93	EDS
Total number of atoms	6757	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: VWK

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	0.53	0/3822	0.71	1/5252 (0.0%)
2	B	0.52	0/3079	0.72	0/4225
All	All	0.52	0/6901	0.71	1/9477 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	448	ARG	N-CA-C	-5.04	106.83	112.87

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3724	0	3214	130	0
2	B	2998	0	2732	70	0
3	A	27	0	0	1	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
All	All	6757	0	5946	189	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 15.

All (189) 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:84:THR:HG21	1:A:153:TRP:HE1	1.45	0.81
1:A:122:GLU:HA	1:A:125:ARG:HD2	1.62	0.80
2:B:401:TRP:HE3	2:B:404:GLU:HG3	1.47	0.78
1:A:5:ILE:CD1	1:A:167:ILE:HD11	2.15	0.77
1:A:459:THR:C	2:B:287:LYS:HA	2.12	0.73
1:A:303:LEU:HD21	1:A:307:ARG:HH21	1.53	0.73
2:B:329:ILE:HD11	2:B:375:ILE:HD13	1.72	0.71
1:A:5:ILE:HD11	1:A:167:ILE:HD11	1.72	0.70
2:B:163:SER:HA	2:B:166:LYS:HE2	1.71	0.70
1:A:104:LYS:HB2	1:A:192:ASP:HA	1.72	0.70
1:A:380:ILE:HD13	2:B:27:THR:HG22	1.73	0.70
1:A:109:LEU:HD22	1:A:216:THR:HB	1.73	0.70
2:B:120:LEU:HD23	2:B:125:ARG:HG2	1.73	0.69
1:A:406:TRP:CD2	2:B:420:PRO:HG3	2.29	0.68
2:B:79:GLU:OE2	2:B:83:ARG:NH1	2.27	0.67
1:A:88:TRP:NE1	2:B:143:ARG:HD2	2.11	0.66
1:A:241:VAL:HG12	1:A:242:GLN:O	1.96	0.66
2:B:369:THR:HG21	2:B:405:TYR:HB2	1.79	0.64
1:A:459:THR:O	2:B:287:LYS:HA	1.99	0.63
1:A:437:ALA:CB	1:A:493:VAL:HA	2.30	0.62
2:B:329:ILE:HD11	2:B:375:ILE:CD1	2.30	0.62
1:A:80:LEU:O	1:A:84:THR:HG23	2.00	0.61
1:A:408:ALA:HA	2:B:364:ASP:OD2	2.00	0.61
1:A:363:ASN:HD21	1:A:401:TRP:HE1	1.48	0.61
1:A:17:ASP:O	1:A:83:ARG:HD3	2.00	0.60
2:B:29:GLU:HG2	2:B:30:LYS:N	2.15	0.60
2:B:63:ILE:HD13	2:B:74:LEU:HD22	1.83	0.60
2:B:85:GLN:HG2	2:B:89:GLU:HB3	1.83	0.60
2:B:392:PRO:HA	2:B:417:VAL:HG22	1.83	0.59
1:A:19:PRO:HG3	1:A:80:LEU:HB2	1.83	0.59
1:A:84:THR:HG21	1:A:153:TRP:NE1	2.18	0.58
1:A:451:LYS:CB	1:A:470:THR:HA	2.34	0.58
2:B:16:MET:HE2	2:B:83:ARG:HG2	1.86	0.58
1:A:401:TRP:HZ3	1:A:409:THR:HG21	1.69	0.58
1:A:101:LYS:NZ	1:A:101:LYS:HB2	2.18	0.57
2:B:423:VAL:HG23	2:B:425:LEU:H	1.68	0.57
1:A:450:THR:O	1:A:451:LYS:C	2.47	0.57
2:B:193:LEU:HD23	2:B:197:GLN:HB3	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:GLY:HA2	1:A:464:GLN:CB	2.35	0.56
1:A:393:ILE:HD11	1:A:397:THR:HB	1.86	0.56
2:B:91:GLN:HG2	2:B:92:LEU:HG	1.87	0.56
1:A:23:GLN:HE21	1:A:59:PRO:HB3	1.70	0.56
2:B:164:MET:HE1	2:B:214:LEU:HD11	1.88	0.56
1:A:93:GLY:O	1:A:94:ILE:HD12	2.06	0.56
1:A:356:ARG:HG2	1:A:367:GLN:HE21	1.71	0.56
2:B:363:ASN:ND2	2:B:366:LYS:H	2.04	0.55
1:A:94:ILE:HD11	1:A:183:TYR:CZ	2.42	0.55
1:A:516:GLU:HA	1:A:519:ASN:HD22	1.72	0.55
2:B:85:GLN:HA	2:B:88:TRP:HB3	1.88	0.55
1:A:241:VAL:HG13	1:A:266:TRP:HE1	1.71	0.55
1:A:5:ILE:HG13	1:A:212:TRP:CE3	2.42	0.54
2:B:325:LEU:HD23	2:B:343:GLN:HG2	1.87	0.54
2:B:239:TRP:CH2	2:B:378:GLU:HG2	2.43	0.54
1:A:5:ILE:CG1	1:A:167:ILE:HD11	2.38	0.54
1:A:406:TRP:CE2	2:B:420:PRO:HG3	2.43	0.54
1:A:5:ILE:HG12	1:A:167:ILE:HD11	1.89	0.53
1:A:23:GLN:HG2	1:A:59:PRO:HA	1.91	0.53
1:A:343:GLN:HG3	1:A:349:LEU:HD11	1.92	0.52
1:A:517:LEU:O	1:A:521:ILE:HG13	2.10	0.52
2:B:85:GLN:NE2	2:B:89:GLU:HG2	2.23	0.52
1:A:178:ILE:HD11	1:A:180:ILE:HD11	1.91	0.52
1:A:440:PHE:HA	1:A:457:TYR:HB2	1.92	0.51
1:A:447:ASN:C	1:A:449:GLU:N	2.68	0.51
1:A:90:VAL:HG21	1:A:157:PRO:HB2	1.92	0.51
2:B:419:THR:O	2:B:421:PRO:HD3	2.10	0.51
1:A:325:LEU:HB2	1:A:385:LYS:HD3	1.93	0.50
1:A:19:PRO:O	1:A:56:TYR:HB3	2.12	0.50
2:B:191:SER:HG	2:B:198:HIS:HD1	1.52	0.50
2:B:401:TRP:CE3	2:B:404:GLU:HG3	2.38	0.50
1:A:337:TRP:CZ3	1:A:368:LEU:HD13	2.47	0.50
1:A:241:VAL:HG13	1:A:266:TRP:NE1	2.27	0.49
1:A:94:ILE:HD11	1:A:183:TYR:CE1	2.47	0.49
1:A:480:GLN:O	1:A:484:LEU:N	2.44	0.49
1:A:447:ASN:C	1:A:449:GLU:H	2.19	0.49
2:B:115:TYR:C	2:B:117:SER:H	2.21	0.49
2:B:379:SER:OG	2:B:387:PRO:HD3	2.11	0.49
1:A:88:TRP:CD1	2:B:143:ARG:HD2	2.46	0.49
2:B:369:THR:HG22	2:B:373:GLN:NE2	2.27	0.49
1:A:10:VAL:HG21	1:A:153:TRP:HH2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:THR:HG21	1:A:424:LYS:HA	1.95	0.49
2:B:12:LEU:CD2	2:B:84:THR:HG22	2.43	0.49
2:B:107:THR:HG22	2:B:108:VAL:H	1.78	0.49
2:B:182:GLN:HG3	2:B:187:LEU:HD12	1.95	0.49
1:A:4:PRO:HG2	1:A:212:TRP:CE3	2.47	0.48
2:B:254:VAL:HG22	2:B:282:LEU:HD21	1.94	0.48
1:A:167:ILE:HG23	1:A:212:TRP:CD1	2.48	0.48
1:A:229:TRP:HB2	3:A:601:VWK:N2	2.28	0.48
1:A:392:PRO:HA	1:A:417:VAL:O	2.13	0.48
2:B:84:THR:OG1	2:B:85:GLN:N	2.47	0.48
1:A:379:SER:CB	1:A:387:PRO:HD3	2.44	0.48
1:A:319:TYR:OH	1:A:385:LYS:HD2	2.14	0.48
1:A:479:LEU:HD22	1:A:501:TYR:HE1	1.79	0.48
1:A:428:GLN:HA	1:A:509:GLN:HE22	1.79	0.48
1:A:125:ARG:HG2	1:A:146:TYR:O	2.14	0.47
1:A:406:TRP:CG	2:B:420:PRO:HG3	2.49	0.47
2:B:12:LEU:HD23	2:B:84:THR:HG22	1.94	0.47
1:A:481:ALA:O	1:A:485:ALA:N	2.47	0.47
2:B:395:LYS:O	2:B:399:GLU:HG3	2.14	0.47
1:A:444:GLY:HA3	1:A:477:THR:HB	1.96	0.47
2:B:344:GLU:OE1	2:B:345:PRO:HD2	2.15	0.47
1:A:439:THR:OG1	1:A:440:PHE:N	2.48	0.47
2:B:98:ALA:O	2:B:101:LYS:HD3	2.15	0.47
1:A:454:LYS:O	1:A:455:ALA:HB3	2.16	0.46
2:B:191:SER:OG	2:B:198:HIS:ND1	2.28	0.46
2:B:206:ARG:O	2:B:210:LEU:HG	2.14	0.46
1:A:94:ILE:HD11	1:A:183:TYR:OH	2.15	0.46
1:A:303:LEU:HG	1:A:307:ARG:HE	1.79	0.46
2:B:363:ASN:HD21	2:B:365:VAL:HB	1.80	0.46
1:A:186:ASP:HB3	1:A:188:TYR:CE1	2.50	0.46
1:A:437:ALA:HB1	1:A:493:VAL:HA	1.97	0.46
1:A:394:GLN:HA	1:A:414:TRP:HH2	1.80	0.46
1:A:104:LYS:NZ	1:A:194:GLU:HA	2.29	0.46
1:A:225:PRO:HA	1:A:226:PRO:C	2.41	0.46
2:B:85:GLN:O	2:B:89:GLU:HG3	2.15	0.46
1:A:50:ILE:O	1:A:143:ARG:HB2	2.16	0.46
2:B:246:LEU:HD12	2:B:247:PRO:HD2	1.98	0.45
1:A:111:VAL:HG13	1:A:185:ASP:O	2.15	0.45
1:A:507:GLN:C	1:A:509:GLN:H	2.24	0.45
1:A:516:GLU:HA	1:A:519:ASN:ND2	2.31	0.45
2:B:104:LYS:HG3	2:B:192:ASP:HA	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:363:ASN:CG	2:B:365:VAL:H	2.24	0.45
1:A:459:THR:HG23	1:A:462:GLY:H	1.81	0.45
1:A:46:LYS:HD2	1:A:116:PHE:HB3	1.98	0.45
1:A:247:PRO:HG2	1:A:252:TRP:CH2	2.52	0.45
1:A:503:LEU:O	1:A:507:GLN:HB2	2.16	0.45
1:A:2:ILE:O	1:A:3:SER:CB	2.65	0.45
1:A:235:HIS:HB2	1:A:238:LYS:O	2.17	0.44
1:A:387:PRO:HG2	1:A:389:PHE:CZ	2.52	0.44
2:B:19:PRO:HG3	2:B:80:LEU:HB2	1.98	0.44
1:A:219:LYS:HA	1:A:222:GLN:HG2	1.99	0.44
1:A:444:GLY:CA	1:A:477:THR:HB	2.47	0.44
1:A:97:PRO:HA	1:A:100:LEU:HG	1.98	0.44
2:B:101:LYS:HG2	2:B:382:ILE:HA	1.98	0.44
2:B:88:TRP:CE2	2:B:92:LEU:HD11	2.52	0.44
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.53	0.44
1:A:507:GLN:C	1:A:509:GLN:N	2.76	0.44
2:B:195:ILE:HG22	2:B:199:ARG:HE	1.82	0.44
1:A:55:PRO:HG2	1:A:143:ARG:NH1	2.32	0.44
2:B:64:LYS:HE2	2:B:71:TRP:CZ2	2.53	0.44
2:B:405:TYR:O	2:B:407:GLN:HG3	2.18	0.43
1:A:399:GLU:HA	1:A:402:TRP:NE1	2.33	0.43
1:A:110:ASP:O	1:A:217:PRO:HD3	2.18	0.43
1:A:395:LYS:O	1:A:396:GLU:C	2.61	0.43
1:A:270:ILE:HD12	1:A:270:ILE:HA	1.79	0.43
1:A:56:TYR:CD1	1:A:56:TYR:N	2.87	0.43
1:A:459:THR:HG23	1:A:461:LYS:N	2.34	0.43
1:A:516:GLU:O	1:A:520:GLN:N	2.47	0.43
2:B:75:VAL:HG11	2:B:77:PHE:CZ	2.54	0.42
1:A:505:ILE:O	1:A:510:PRO:HD3	2.20	0.42
1:A:195:ILE:HD12	1:A:196:GLY:H	1.83	0.42
1:A:408:ALA:HB1	2:B:364:ASP:HB3	2.02	0.42
2:B:269:GLN:C	2:B:271:TYR:H	2.27	0.42
1:A:79:GLU:HG3	1:A:83:ARG:HE	1.85	0.42
1:A:440:PHE:O	1:A:441:TYR:C	2.63	0.42
1:A:80:LEU:HG	1:A:84:THR:CG2	2.50	0.42
1:A:115:TYR:CD2	1:A:156:SER:HB3	2.54	0.42
1:A:131:THR:HG23	1:A:143:ARG:HD2	2.02	0.42
1:A:325:LEU:HD22	1:A:385:LYS:HD3	2.02	0.42
2:B:267:ALA:C	2:B:269:GLN:N	2.76	0.42
1:A:433:PRO:HD3	1:A:532:TYR:CZ	2.55	0.42
1:A:444:GLY:O	1:A:445:ALA:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:VAL:HG23	1:A:132:ILE:HD11	2.02	0.42
1:A:405:TYR:CE2	1:A:407:GLN:HB3	2.55	0.42
1:A:437:ALA:HB3	1:A:494:ASN:OD1	2.19	0.42
1:A:38:CYS:HB3	1:A:144:TYR:CE2	2.55	0.41
1:A:401:TRP:CE3	1:A:402:TRP:HB3	2.55	0.41
1:A:325:LEU:O	1:A:388:LYS:HD3	2.21	0.41
1:A:420:PRO:HA	1:A:422:LEU:N	2.34	0.41
1:A:193:LEU:HD13	1:A:197:GLN:NE2	2.36	0.41
1:A:379:SER:HB3	1:A:385:LYS:O	2.21	0.41
1:A:109:LEU:HD23	1:A:217:PRO:HG2	2.03	0.41
2:B:17:ASP:C	2:B:83:ARG:HH21	2.28	0.41
1:A:5:ILE:HD11	1:A:167:ILE:CD1	2.44	0.41
1:A:24:TRP:O	1:A:26:LEU:N	2.53	0.41
1:A:427:TYR:OH	1:A:509:GLN:HA	2.21	0.41
2:B:162:SER:O	2:B:166:LYS:HG3	2.21	0.41
1:A:170:PRO:HB2	1:A:208:HIS:HE1	1.86	0.41
1:A:477:THR:O	1:A:481:ALA:N	2.46	0.41
1:A:501:TYR:CD1	1:A:501:TYR:C	2.99	0.41
1:A:181:TYR:HE1	2:B:138:GLU:CD	2.29	0.41
1:A:394:GLN:O	1:A:395:LYS:C	2.64	0.41
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.61	0.41
1:A:387:PRO:HG2	1:A:389:PHE:CE1	2.56	0.40
2:B:178:ILE:HD11	2:B:201:LYS:HG2	2.03	0.40
1:A:350:LYS:NZ	1:A:378:GLU:OE2	2.37	0.40
2:B:216:THR:HB	2:B:217:PRO:HD2	2.02	0.40
1:A:457:TYR:CZ	1:A:463:ARG:O	2.74	0.40
1:A:461:LYS:O	1:A:463:ARG:N	2.54	0.40
2:B:23:GLN:OE1	2:B:60:VAL:HG13	2.21	0.40

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	504/539 (94%)	454 (90%)	48 (10%)	2 (0%)	30	47
2	B	389/428 (91%)	354 (91%)	34 (9%)	1 (0%)	36	54
All	All	893/967 (92%)	808 (90%)	82 (9%)	3 (0%)	36	54

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	455	ALA
1	A	3	SER
2	B	273	GLY

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	321/483 (66%)	272 (85%)	49 (15%)	3	3
2	B	287/390 (74%)	250 (87%)	37 (13%)	4	7
All	All	608/873 (70%)	522 (86%)	86 (14%)	3	5

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LYS
1	A	23	GLN
1	A	50	ILE
1	A	86	ASP
1	A	94	ILE
1	A	101	LYS
1	A	104	LYS
1	A	110	ASP
1	A	111	VAL
1	A	120	LEU
1	A	132	ILE
1	A	136	ASN
1	A	151	GLN

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Mol	Chain	Res	Type
1	A	178	ILE
1	A	195	ILE
1	A	207	GLN
1	A	215	THR
1	A	246	LEU
1	A	250	ASP
1	A	276	VAL
1	A	290	THR
1	A	308	GLU
1	A	326	ILE
1	A	330	GLN
1	A	338	THR
1	A	340	GLN
1	A	341	ILE
1	A	344	GLU
1	A	350	LYS
1	A	357	MET
1	A	385	LYS
1	A	388	LYS
1	A	393	ILE
1	A	397	THR
1	A	407	GLN
1	A	409	THR
1	A	410	TRP
1	A	413	GLU
1	A	415	GLU
1	A	439	THR
1	A	459	THR
1	A	472	THR
1	A	473	THR
1	A	477	THR
1	A	494	ASN
1	A	496	VAL
1	A	497	THR
1	A	513	SER
1	A	536	VAL
2	B	16	MET
2	B	22	LYS
2	B	29	GLU
2	B	39	THR
2	B	46	LYS
2	B	48	SER

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Mol	Chain	Res	Type
2	B	58	THR
2	B	60	VAL
2	B	73	LYS
2	B	89	GLU
2	B	92	LEU
2	B	101	LYS
2	B	117	SER
2	B	121	ASP
2	B	137	ASN
2	B	138	GLU
2	B	177	ASP
2	B	189	VAL
2	B	201	LYS
2	B	207	GLN
2	B	216	THR
2	B	218	ASP
2	B	241	VAL
2	B	245	VAL
2	B	246	LEU
2	B	254	VAL
2	B	261	VAL
2	B	268	SER
2	B	282	LEU
2	B	322	SER
2	B	348	ASN
2	B	362	THR
2	B	363	ASN
2	B	385	LYS
2	B	388	LYS
2	B	395	LYS
2	B	417	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	161	GLN
1	A	315	HIS
1	A	330	GLN
1	A	509	GLN
2	B	137	ASN
2	B	207	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	VWK	A	601	-	29,29,29	2.21	3 (10%)	38,39,39	1.18	4 (10%)

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	VWK	A	601	-	-	4/16/16/16	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	VWK	C1-N1	10.10	1.46	1.34
3	A	601	VWK	C20-C21	2.98	1.50	1.44
3	A	601	VWK	C22-C16	-2.19	1.37	1.42

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	VWK	C4-C1-N1	2.49	121.63	118.03
3	A	601	VWK	C18-C17-C16	2.47	121.11	117.92
3	A	601	VWK	C12-O3-C11	-2.09	113.34	119.10
3	A	601	VWK	C22-C20-C21	-2.07	117.91	119.66

There are no chirality outliers.

All (4) torsion outliers are listed below:

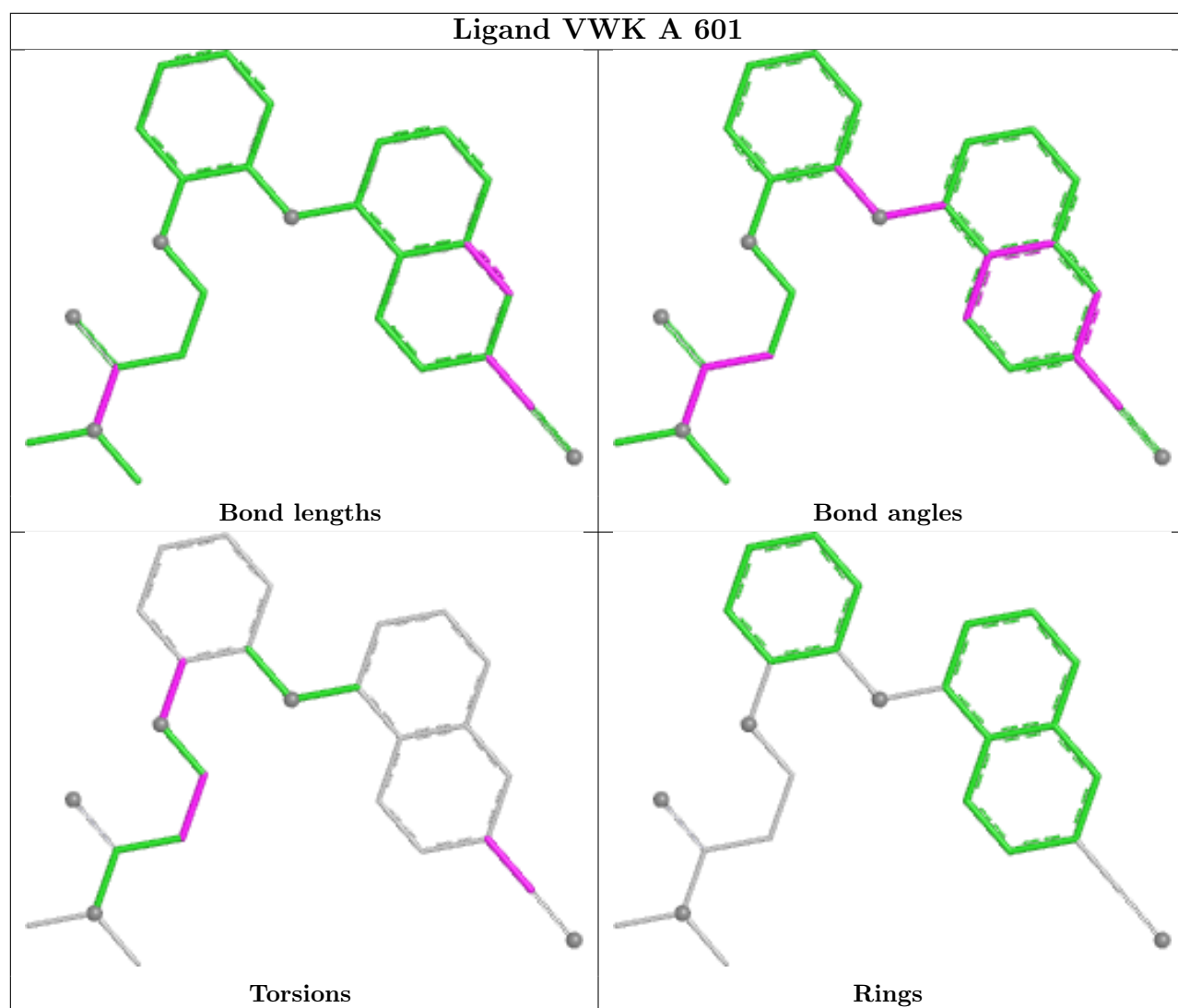
Mol	Chain	Res	Type	Atoms
3	A	601	VWK	C11-C6-O2-C5
3	A	601	VWK	C7-C6-O2-C5
3	A	601	VWK	C1-C4-C5-O2
3	A	601	VWK	C22-C20-C21-N2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	VWK	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	521/539 (96%)	0.62	42 (8%)	18 18	30, 107, 158, 450	1 (0%)
2	B	401/428 (93%)	0.59	37 (9%)	14 14	54, 90, 186, 491	0
All	All	922/967 (95%)	0.60	79 (8%)	16 16	30, 100, 166, 491	1 (0%)

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	299	ALA	7.1
1	A	455	ALA	6.3
1	A	454	LYS	5.8
1	A	456	GLY	5.7
2	B	267	ALA	5.6
2	B	300	GLU	4.7
2	B	276	VAL	4.7
2	B	425	LEU	4.7
2	B	295	LEU	4.7
2	B	364	ASP	4.5
2	B	252	TRP	4.5
2	B	298	GLU	4.4
1	A	68	SER	4.2
1	A	506	ILE	4.1
2	B	329	ILE	4.0
1	A	2	ILE	4.0
2	B	270	ILE	3.9
2	B	261	VAL	3.8
2	B	423	VAL	3.8
2	B	249	LYS	3.8
1	A	109	LEU	3.8
1	A	71	TRP	3.6
1	A	537	PRO	3.5
2	B	88	TRP	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	1	PRO	3.5
2	B	337	TRP	3.4
1	A	534	ALA	3.4
1	A	140	PRO	3.4
1	A	276	VAL	3.2
1	A	67	ASP	3.1
2	B	303	LEU	3.0
1	A	410	TRP	3.0
2	B	12	LEU	2.8
1	A	496	VAL	2.8
1	A	536	VAL	2.8
2	B	292	VAL	2.7
1	A	429	LEU	2.7
1	A	136	ASN	2.7
2	B	4	PRO	2.7
1	A	468	PRO	2.7
1	A	246	LEU	2.6
1	A	441	TYR	2.6
1	A	58	THR	2.6
2	B	339	TYR	2.5
1	A	440	PHE	2.5
2	B	115	TYR	2.5
2	B	274	ILE	2.5
2	B	271	TYR	2.5
2	B	348	ASN	2.4
2	B	294	PRO	2.4
2	B	420	PRO	2.4
1	A	427	TYR	2.4
1	A	466	VAL	2.4
2	B	290	THR	2.4
1	A	495	ILE	2.4
2	B	92	LEU	2.4
1	A	92	LEU	2.3
1	A	132	ILE	2.3
1	A	245	VAL	2.3
1	A	372	VAL	2.3
1	A	445	ALA	2.3
2	B	264	LEU	2.3
2	B	306	ASN	2.3
1	A	329	ILE	2.2
1	A	398	TRP	2.2
2	B	422	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	535	TRP	2.2
2	B	87	PHE	2.2
1	A	299	ALA	2.1
1	A	77	PHE	2.1
1	A	465	LYS	2.1
1	A	439	THR	2.1
1	A	402	TRP	2.1
2	B	214	LEU	2.1
2	B	232	TYR	2.1
1	A	467	VAL	2.1
2	B	288	ALA	2.0
1	A	64	LYS	2.0
2	B	349	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](#)

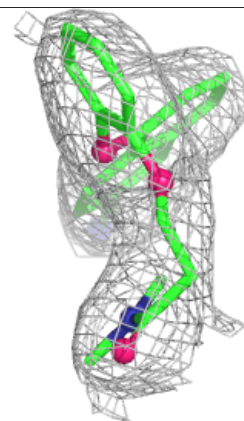
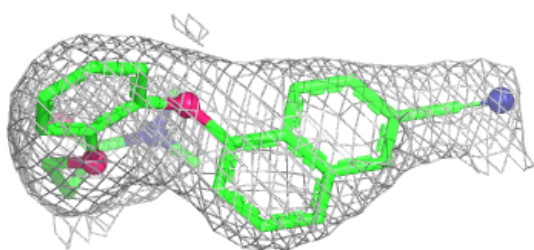
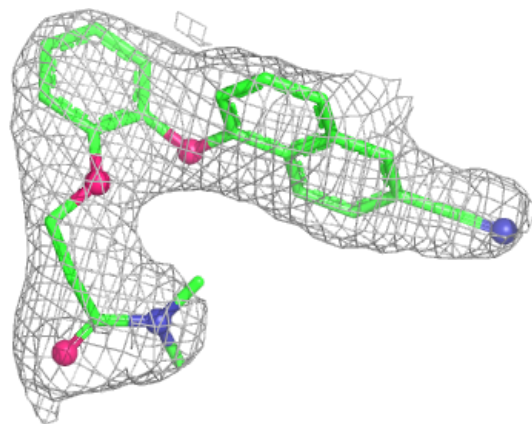
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	VWK	A	601	27/27	0.96	0.08	63,70,74,75	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.

Electron density around VWK A 601:

$2mF_o - DF_c$ (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.