



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:20 PM UTC

PDB ID : 8DXH / pdb_00008dxh
Title : HIV-1 reverse transcriptase/rilpivirine with bound fragment 5-fluoroquinazolin-4-ol at W266 site
Authors : Chopra, A.; Ruiz, F.X.; Bauman, J.D.; Arnold, E.
Deposited on : 2022-08-02
Resolution : 1.80 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

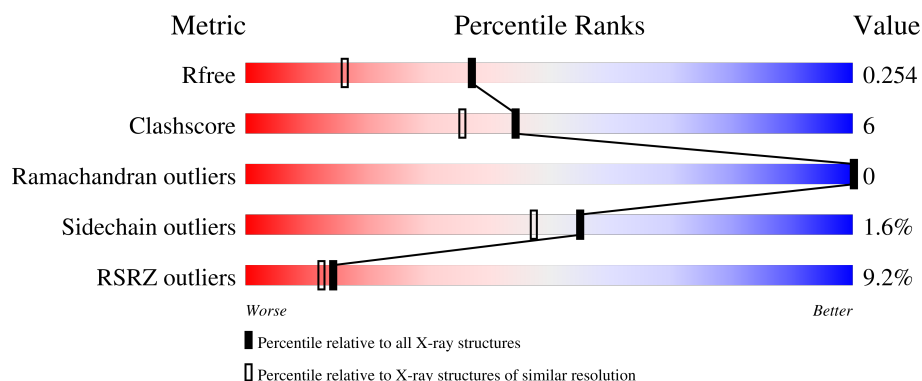
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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% 89% 11%
2	B	428	11% 85% 11% ...

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	JBQ	A	601	X	-	-	-
5	DMS	A	604	-	-	X	-
5	DMS	A	606	-	-	X	-
5	DMS	B	503	-	-	X	-
5	DMS	B	504	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 8803 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	556	Total	C	N	O	S	0	3	0
			4536	2936	755	837	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

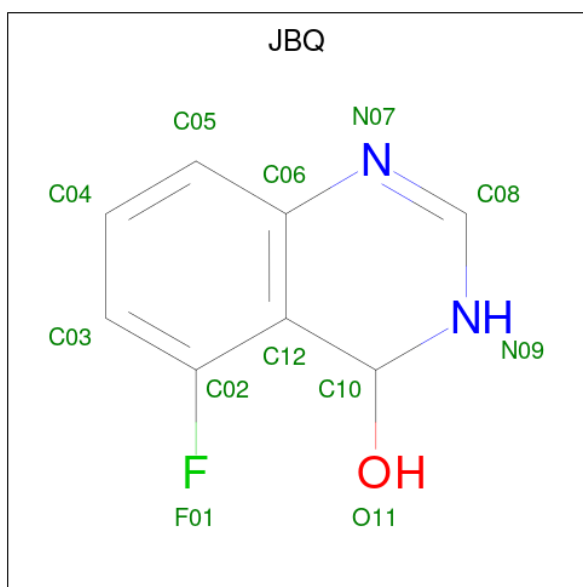
- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	415	Total	C	N	O	S	0	4	0
			3455	2254	570	624	7			

There is a discrepancy between the modelled and reference sequences:

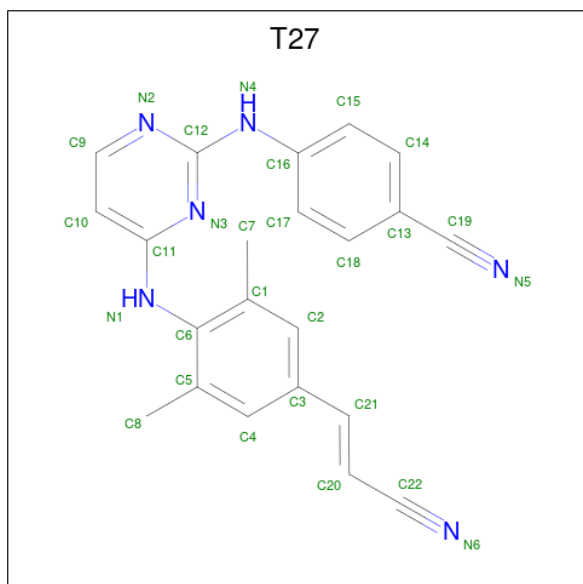
Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 3 is 5-fluoranyl-3,4-dihydroquinazolin-4-ol (CCD ID: JBQ) (formula: C₈H₇FN₂O) (labeled as "Ligand of Interest" by depositor).



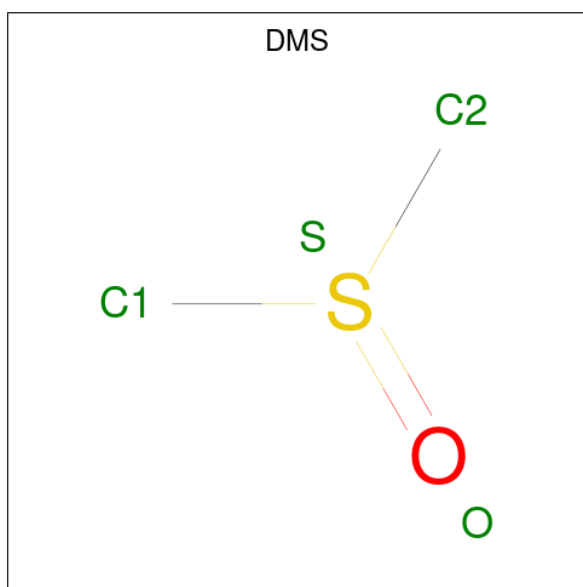
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			12	8	1	2	1		

- Molecule 4 is 4-{[4-({4-[(E)-2-cyanoethenyl]-2,6-dimethylphenyl}amino)pyrimidin-2-yl]amino}benzonitrile (CCD ID: T27) (formula: C₂₂H₁₈N₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			28	22	6		

- Molecule 5 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).

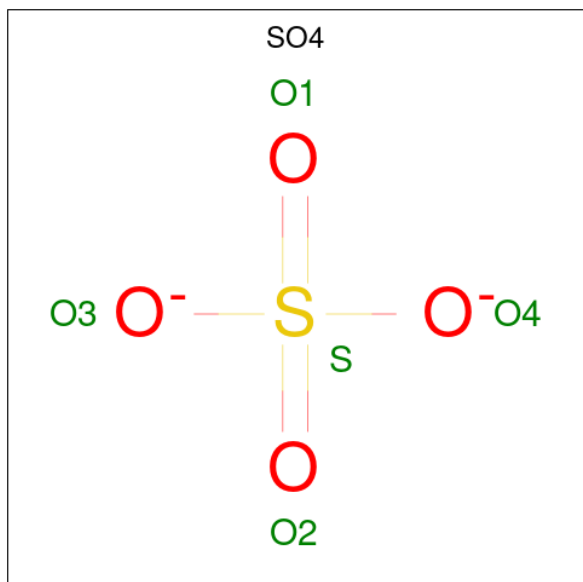


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Mg	0	0
			1	1		

- Molecule 8 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	S	0	0
			5	4	1		
8	B	1	Total	O	S	0	0
			5	4	1		

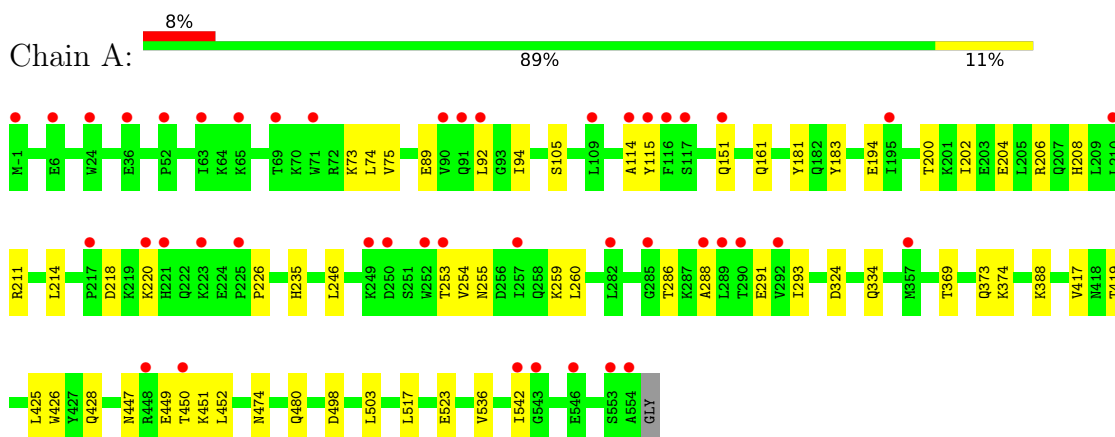
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	415	Total	O	0	0
			415	415		
9	B	290	Total	O	0	0
			290	290		

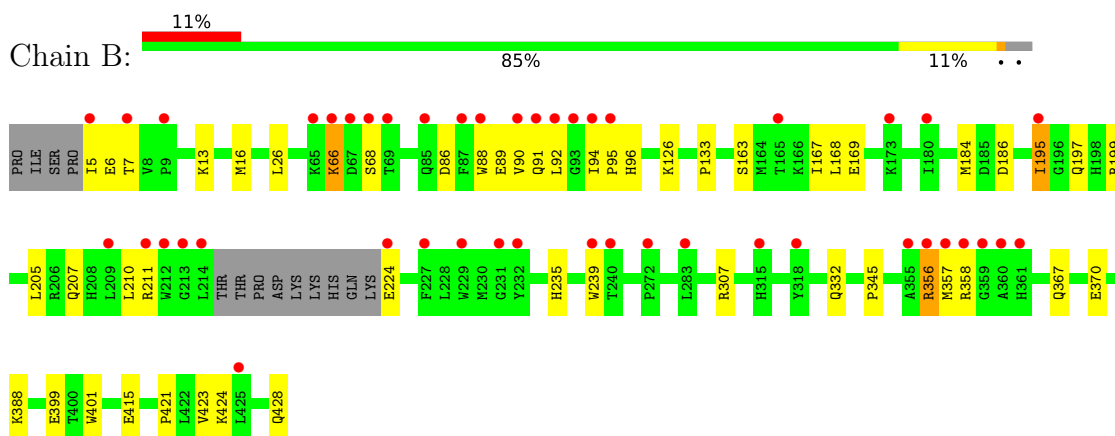
3 Residue-property plots [i](#)

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: 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	162.00Å 72.76Å 109.39Å 90.00° 100.59° 90.00°	Depositor
Resolution (Å)	40.25 – 1.80 40.25 – 1.80	Depositor EDS
% Data completeness (in resolution range)	96.6 (40.25-1.80) 92.2 (40.25-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 1.79Å)	Xtriage
Refinement program	PHENIX dev_3051	Depositor
R, R_{free}	0.190 , 0.213 (Not available) , 0.254	Depositor DCC
R_{free} test set	2000 reflections (1.72%)	wwPDB-VP
Wilson B-factor (Å ²)	28.1	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.8	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	0.96	EDS
Total number of atoms	8803	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.09% 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: T27, SO4, MG, JBQ, DMS, EDO

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	0.68	0/4663	0.75	0/6337
2	B	0.69	0/3565	0.76	1/4844 (0.0%)
All	All	0.69	0/8228	0.76	1/11181 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	186	ASP	CA-CB-CG	5.03	117.63	112.60

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	4536	0	4601	52	0
2	B	3455	0	3485	42	0
3	A	12	0	0	0	0
4	A	28	0	18	1	0
5	A	20	0	30	14	0
5	B	28	0	42	12	0
6	A	4	0	6	0	0
6	B	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	1	0	0	0	0
8	A	5	0	0	0	0
8	B	5	0	0	0	0
9	A	415	0	0	9	0
9	B	290	0	0	12	0
All	All	8803	0	8188	98	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 (98) 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:26:LEU:H	5:B:503:DMS:H11	1.18	1.05
5:B:502:DMS:H23	9:B:737:HOH:O	1.57	1.02
1:A:428:GLN:H	5:A:605:DMS:H23	1.31	0.92
1:A:480[B]:GLN:HG3	1:A:517:LEU:HD21	1.60	0.81
5:A:606:DMS:H21	9:A:828:HOH:O	1.81	0.80
2:B:239:TRP:HE1	5:B:504:DMS:H23	1.47	0.80
1:A:426:TRP:H	5:A:604:DMS:H23	1.48	0.79
1:A:373:GLN:HE21	1:A:373:GLN:HA	1.50	0.76
1:A:151:GLN:H	5:A:606:DMS:H23	1.50	0.75
2:B:224:GLU:N	9:B:601:HOH:O	2.21	0.73
1:A:428:GLN:N	5:A:605:DMS:H23	2.04	0.73
2:B:92:LEU:HD23	2:B:92:LEU:O	1.89	0.73
2:B:26:LEU:O	5:B:503:DMS:H21	1.90	0.72
2:B:95:PRO:HA	9:B:603:HOH:O	1.89	0.72
1:A:450:THR:HG23	1:A:452:LEU:H	1.55	0.71
1:A:417:VAL:HG22	1:A:419:THR:HG23	1.73	0.71
2:B:358:ARG:NH2	2:B:370[B]:GLU:OE1	2.25	0.70
1:A:373:GLN:HA	1:A:373:GLN:NE2	2.07	0.68
1:A:373:GLN:HE22	2:B:401:TRP:HE1	1.39	0.67
1:A:426:TRP:H	5:A:604:DMS:C2	2.06	0.67
1:A:480[A]:GLN:NE2	9:A:706:HOH:O	2.28	0.66
2:B:26:LEU:N	5:B:503:DMS:H11	2.03	0.66
1:A:254:VAL:HG23	1:A:293:ILE:HD11	1.77	0.66
2:B:424:LYS:HD2	9:B:712:HOH:O	1.95	0.65
1:A:151:GLN:H	5:A:606:DMS:C2	2.10	0.64
1:A:161:GLN:HG2	9:A:811:HOH:O	1.97	0.64
2:B:235:HIS:H	5:B:504:DMS:H21	1.63	0.63
2:B:239:TRP:HE1	5:B:504:DMS:C2	2.10	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:THR:O	1:A:451:LYS:HG2	2.00	0.62
1:A:369:THR:O	1:A:373:GLN:HG2	2.02	0.59
5:B:501:DMS:H11	9:B:835:HOH:O	2.02	0.58
1:A:253:THR:HG22	1:A:255:ASN:H	1.68	0.58
1:A:286:THR:HG21	1:A:291:GLU:OE1	2.05	0.57
2:B:388:LYS:HE3	2:B:415:GLU:OE1	2.04	0.57
1:A:324:ASP:OD2	1:A:388:LYS:NZ	2.35	0.57
2:B:424:LYS:CD	9:B:712:HOH:O	2.52	0.56
5:A:604:DMS:H22	9:A:862:HOH:O	2.05	0.56
1:A:254:VAL:CG2	1:A:293:ILE:HD11	2.36	0.55
1:A:447:ASN:HB3	1:A:450:THR:HG22	1.88	0.55
1:A:474:ASN:H	5:A:607:DMS:H23	1.72	0.55
4:A:602:T27:N3	4:A:602:T27:H17	2.22	0.54
1:A:114:ALA:HA	1:A:214:LEU:HD22	1.89	0.54
1:A:151:GLN:HG2	5:A:606:DMS:H23	1.90	0.54
2:B:332:GLN:OE1	2:B:428:GLN:HG2	2.10	0.52
2:B:307:ARG:NH2	9:B:607:HOH:O	2.32	0.51
2:B:89:GLU:HG3	2:B:90:VAL:HG23	1.92	0.51
1:A:451:LYS:HG3	9:A:819:HOH:O	2.11	0.50
1:A:73:LYS:NZ	5:A:606:DMS:O	2.44	0.50
1:A:426:TRP:HB2	5:A:604:DMS:H21	1.94	0.49
1:A:480[B]:GLN:NE2	9:A:714:HOH:O	2.38	0.49
2:B:235:HIS:H	5:B:504:DMS:C2	2.25	0.49
2:B:86:ASP:HB3	2:B:88:TRP:CE2	2.48	0.48
2:B:399:GLU:HB3	5:B:505:DMS:H12	1.95	0.48
1:A:293:ILE:HD12	1:A:293:ILE:N	2.29	0.48
2:B:5:ILE:HD12	2:B:6:GLU:N	2.28	0.48
2:B:86:ASP:HB3	2:B:88:TRP:CZ2	2.49	0.48
1:A:74:LEU:C	1:A:74:LEU:HD23	2.39	0.47
2:B:163:SER:O	2:B:167:ILE:HG13	2.15	0.47
2:B:195:ILE:HD11	2:B:199:ARG:CZ	2.45	0.46
2:B:126:LYS:HD2	5:B:502:DMS:H22	1.96	0.46
2:B:5:ILE:HD12	2:B:5:ILE:C	2.40	0.46
1:A:428:GLN:HG2	9:A:1055:HOH:O	2.16	0.46
2:B:207:GLN:O	2:B:211:ARG:HG3	2.15	0.46
2:B:356:ARG:H	2:B:356:ARG:CD	2.28	0.46
1:A:200:THR:O	1:A:204:GLU:HG3	2.16	0.46
1:A:425:LEU:HA	5:A:604:DMS:H23	1.98	0.46
2:B:7:THR:HA	9:B:628:HOH:O	2.15	0.45
1:A:324:ASP:CG	1:A:388:LYS:NZ	2.75	0.45
2:B:96:HIS:N	9:B:603:HOH:O	2.27	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:LYS:HE2	1:A:75:VAL:HG23	1.99	0.44
1:A:447:ASN:HB3	1:A:450:THR:CG2	2.47	0.44
1:A:334:GLN:NE2	9:A:709:HOH:O	2.34	0.44
2:B:168:LEU:HD22	2:B:205:LEU:HD11	2.00	0.44
1:A:114:ALA:O	1:A:115:TYR:C	2.59	0.44
1:A:373:GLN:NE2	1:A:373:GLN:CA	2.73	0.44
2:B:421:PRO:HB2	2:B:423[A]:VAL:HG12	2.00	0.44
2:B:184:MET:HE3	9:B:651:HOH:O	2.18	0.44
1:A:259:LYS:HE3	9:A:975:HOH:O	2.17	0.44
1:A:181:TYR:CE2	1:A:183:TYR:HB2	2.53	0.43
2:B:94:ILE:HD11	9:B:731:HOH:O	2.18	0.43
1:A:246:LEU:HD22	1:A:260:LEU:HD12	2.00	0.43
2:B:345:PRO:HG3	9:B:860:HOH:O	2.18	0.43
1:A:474:ASN:HD22	5:A:607:DMS:H12	1.84	0.43
2:B:357:MET:HB3	2:B:367:GLN:HG2	1.99	0.43
1:A:218:ASP:O	1:A:220:LYS:HD2	2.19	0.42
1:A:286:THR:HG22	1:A:288:ALA:H	1.84	0.42
2:B:66:LYS:HA	2:B:66:LYS:HD2	1.78	0.42
2:B:88:TRP:HA	2:B:91:GLN:O	2.19	0.42
1:A:89:GLU:HB2	1:A:92:LEU:HD13	2.02	0.42
2:B:195:ILE:HD11	2:B:199:ARG:NH2	2.34	0.42
2:B:13:LYS:O	2:B:16:MET:HB3	2.20	0.42
2:B:133:PRO:CG	5:B:503:DMS:H12	2.49	0.41
1:A:226:PRO:HB3	1:A:235:HIS:CE1	2.55	0.41
1:A:498:ASP:OD1	1:A:498:ASP:C	2.64	0.41
1:A:208:HIS:HA	1:A:211[B]:ARG:HD3	2.03	0.41
2:B:94:ILE:O	2:B:95:PRO:C	2.64	0.41
1:A:536:VAL:HB	1:A:542:ILE:HD13	2.03	0.40
1:A:202:ILE:O	1:A:206:ARG:HG3	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	557/557 (100%)	546 (98%)	11 (2%)	0	100	100
2	B	415/428 (97%)	400 (96%)	15 (4%)	0	100	100
All	All	972/985 (99%)	946 (97%)	26 (3%)	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	498/495 (101%)	491 (99%)	7 (1%)	59	52
2	B	380/390 (97%)	373 (98%)	7 (2%)	51	43
All	All	878/885 (99%)	864 (98%)	14 (2%)	55	47

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	ILE
1	A	105	SER
1	A	194	GLU
1	A	374	LYS
1	A	449	GLU
1	A	503	LEU
1	A	523	GLU
2	B	66	LYS
2	B	68	SER
2	B	169	GLU
2	B	195	ILE
2	B	197	GLN
2	B	210	LEU
2	B	356	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	ASN
1	A	197	GLN
1	A	258	GLN
1	A	373	GLN
1	A	428	GLN
1	A	520	GLN
2	B	85	GLN
2	B	336	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](#)

Of 19 ligands modelled in this entry, 1 is monoatomic - leaving 18 for Mogul analysis.

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
5	DMS	B	502	-	3,3,3	2.79	1 (33%)	3,3,3	0.65	0
3	JBQ	A	601	-	12,13,13	2.61	4 (33%)	14,18,18	1.84	2 (14%)
5	DMS	B	507	-	3,3,3	2.43	1 (33%)	3,3,3	0.89	0
4	T27	A	602	-	30,30,30	1.42	5 (16%)	37,40,40	1.99	13 (35%)
5	DMS	B	506	-	3,3,3	2.47	1 (33%)	3,3,3	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	B	501	-	3,3,3	2.88	1 (33%)	3,3,3	0.99	0
5	DMS	A	605	-	3,3,3	2.94	1 (33%)	3,3,3	0.87	0
5	DMS	B	504	-	3,3,3	2.66	1 (33%)	3,3,3	0.98	0
5	DMS	A	607	-	3,3,3	2.83	1 (33%)	3,3,3	0.87	0
8	SO4	A	610	-	4,4,4	0.44	0	6,6,6	0.10	0
6	EDO	B	508	-	3,3,3	0.34	0	2,2,2	0.40	0
6	EDO	A	608	-	3,3,3	0.71	0	2,2,2	0.89	0
5	DMS	A	603	-	3,3,3	2.74	1 (33%)	3,3,3	0.76	0
5	DMS	B	503	-	3,3,3	2.99	1 (33%)	3,3,3	1.65	1 (33%)
5	DMS	B	505	-	3,3,3	2.25	1 (33%)	3,3,3	1.85	1 (33%)
5	DMS	A	604	-	3,3,3	2.82	1 (33%)	3,3,3	0.50	0
8	SO4	B	509	-	4,4,4	0.45	0	6,6,6	0.07	0
5	DMS	A	606	-	3,3,3	2.70	1 (33%)	3,3,3	0.73	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
6	EDO	B	508	-	-	0/1/1/1	-
6	EDO	A	608	-	-	0/1/1/1	-
3	JBQ	A	601	-	1/1/1/3	-	0/2/2/2
4	T27	A	602	-	-	0/13/14/14	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	JBQ	C12-C10	-7.08	1.42	1.50
5	A	605	DMS	O-S	4.99	1.83	1.50
5	B	503	DMS	O-S	4.94	1.82	1.50
5	B	501	DMS	O-S	4.86	1.82	1.50
5	B	502	DMS	O-S	4.75	1.81	1.50
5	A	604	DMS	O-S	4.73	1.81	1.50
5	A	607	DMS	O-S	4.65	1.80	1.50
5	A	606	DMS	O-S	4.62	1.80	1.50
5	A	603	DMS	O-S	4.61	1.80	1.50
5	B	504	DMS	O-S	4.52	1.80	1.50
5	B	506	DMS	O-S	4.15	1.77	1.50
5	B	507	DMS	O-S	4.00	1.76	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	JBQ	C10-N09	-3.60	1.34	1.45
5	B	505	DMS	O-S	3.51	1.73	1.50
4	A	602	T27	C12-N4	3.33	1.43	1.36
4	A	602	T27	C17-C16	-2.72	1.34	1.39
4	A	602	T27	C4-C3	-2.66	1.35	1.39
4	A	602	T27	C22-N6	2.54	1.20	1.14
3	A	601	JBQ	O11-C10	-2.29	1.31	1.40
4	A	602	T27	C14-C13	-2.17	1.35	1.39
3	A	601	JBQ	C12-C02	2.11	1.41	1.39

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	602	T27	C10-C9-N2	-5.58	117.13	123.97
3	A	601	JBQ	C02-C12-C10	4.67	128.13	120.31
4	A	602	T27	C20-C22-N6	-4.50	160.56	176.36
3	A	601	JBQ	O11-C10-C12	3.80	119.16	111.28
4	A	602	T27	C9-N2-C12	3.44	118.29	115.42
4	A	602	T27	C7-C1-C6	-3.39	117.30	121.42
5	B	505	DMS	O-S-C1	3.11	122.07	106.49
4	A	602	T27	C2-C1-C6	2.99	121.68	118.25
4	A	602	T27	C2-C3-C21	2.77	128.90	120.61
4	A	602	T27	C10-C11-N3	-2.69	118.65	123.15
5	B	503	DMS	C2-S-C1	2.59	111.69	98.42
4	A	602	T27	C5-C6-C1	-2.45	118.07	121.55
4	A	602	T27	C1-C6-N1	2.33	123.42	119.38
4	A	602	T27	C15-C16-N4	-2.23	113.04	120.61
4	A	602	T27	C17-C16-N4	2.21	128.09	120.61
4	A	602	T27	C4-C3-C21	-2.16	114.15	120.61
4	A	602	T27	C6-N1-C11	-2.10	120.33	124.11

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	601	JBQ	C10

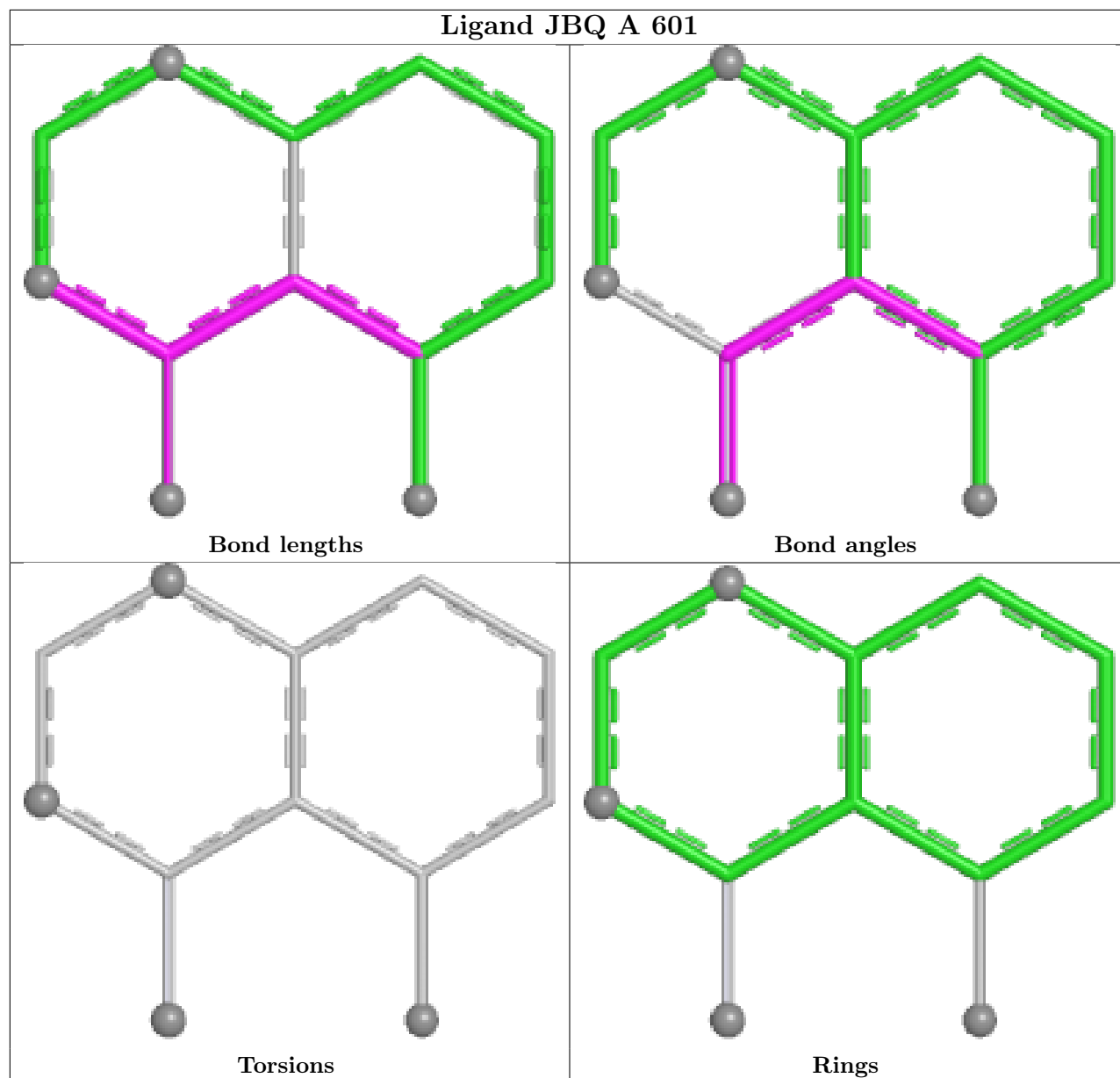
There are no torsion outliers.

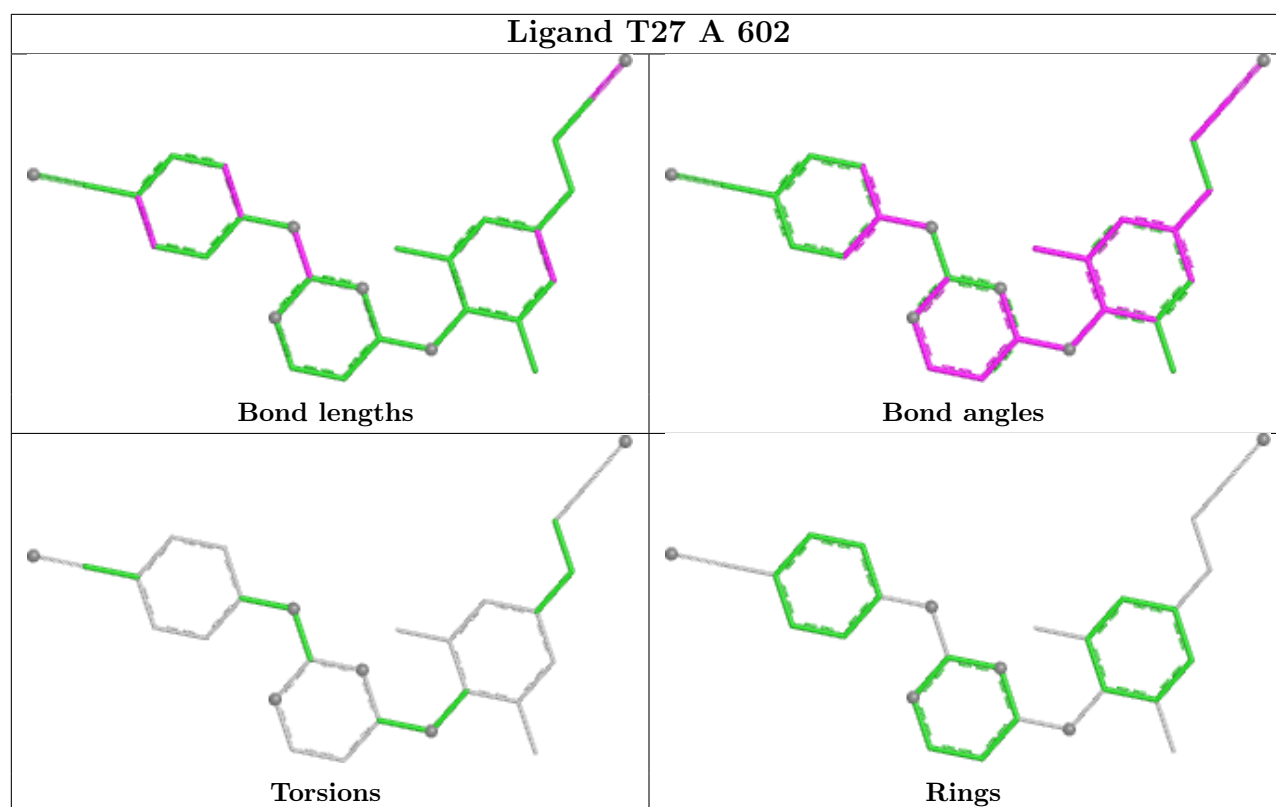
There are no ring outliers.

10 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	502	DMS	2	0
4	A	602	T27	1	0
5	B	501	DMS	1	0
5	A	605	DMS	2	0
5	B	504	DMS	4	0
5	A	607	DMS	2	0
5	B	503	DMS	4	0
5	B	505	DMS	1	0
5	A	604	DMS	5	0
5	A	606	DMS	5	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	556/557 (99%)	0.39	44 (7%) 18 16	16, 34, 80, 156	3 (0%)
2	B	415/428 (96%)	0.54	45 (10%) 11 9	12, 36, 85, 144	4 (0%)
All	All	971/985 (98%)	0.46	89 (9%) 14 12	12, 35, 85, 156	7 (0%)

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	92	LEU	6.9
2	B	5	ILE	6.6
1	A	116	PHE	6.4
2	B	214	LEU	6.0
1	A	554	ALA	5.4
2	B	94	ILE	5.3
2	B	90	VAL	4.8
1	A	92	LEU	4.8
2	B	69	THR	4.6
2	B	95	PRO	4.6
1	A	24	TRP	4.4
2	B	356	ARG	4.2
2	B	357	MET	4.1
1	A	114	ALA	4.0
2	B	88	TRP	4.0
2	B	93	GLY	3.9
1	A	115	TYR	3.9
1	A	543	GLY	3.8
2	B	272	PRO	3.8
1	A	65	LYS	3.8
1	A	223	LYS	3.5
2	B	66	LYS	3.3
1	A	117	SER	3.3
2	B	212	TRP	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	69	THR	3.3
1	A	553	SER	3.3
1	A	221	HIS	3.2
2	B	68	SER	3.2
1	A	90	VAL	3.2
2	B	227	PHE	3.2
2	B	283	LEU	3.1
2	B	65	LYS	3.1
2	B	355	ALA	3.1
1	A	292	VAL	3.1
1	A	109	LEU	3.0
2	B	209	LEU	3.0
2	B	67	ASP	3.0
2	B	232	TYR	3.0
1	A	220	LYS	3.0
2	B	240	THR	3.0
2	B	315[A]	HIS	2.9
1	A	450	THR	2.9
2	B	361	HIS	2.9
2	B	425	LEU	2.9
2	B	359	GLY	2.9
2	B	213	GLY	2.9
2	B	195	ILE	2.8
2	B	165	THR	2.8
1	A	546	GLU	2.8
1	A	288	ALA	2.8
1	A	285	GLY	2.8
1	A	250	ASP	2.8
2	B	229	TRP	2.7
1	A	289	LEU	2.6
1	A	-1	MET	2.6
1	A	6	GLU	2.5
1	A	71	TRP	2.5
1	A	195	ILE	2.5
1	A	52	PRO	2.4
1	A	282	LEU	2.4
2	B	231	GLY	2.4
1	A	253	THR	2.4
2	B	360	ALA	2.4
1	A	542	ILE	2.3
2	B	180	ILE	2.3
1	A	36	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	257	ILE	2.3
2	B	211	ARG	2.3
1	A	290	THR	2.3
2	B	7	THR	2.3
1	A	91[A]	GLN	2.3
2	B	239	TRP	2.2
2	B	9	PRO	2.2
2	B	87	PHE	2.2
2	B	91	GLN	2.2
1	A	225	PRO	2.2
2	B	85	GLN	2.2
1	A	210	LEU	2.2
1	A	252	TRP	2.2
1	A	217	PRO	2.2
1	A	357	MET	2.1
2	B	318	TYR	2.1
1	A	249	LYS	2.1
2	B	173	LYS	2.1
1	A	151	GLN	2.1
1	A	448	ARG	2.1
2	B	358	ARG	2.1
2	B	224	GLU	2.0
1	A	63	ILE	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.

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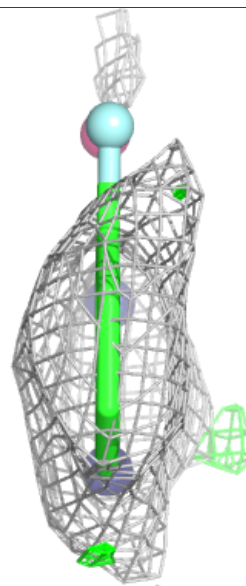
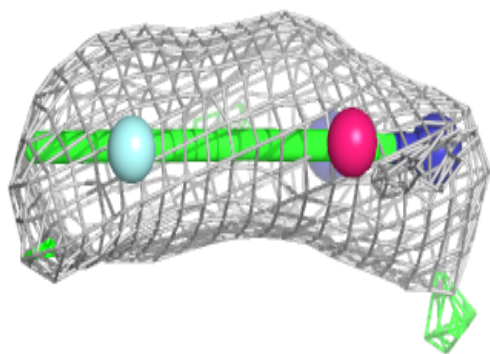
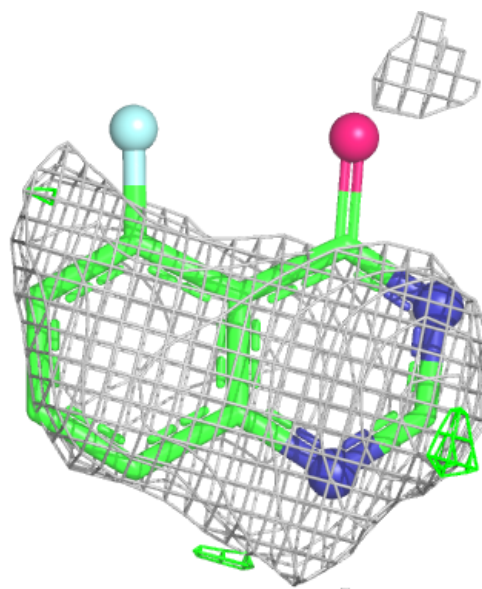
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	SO4	A	610	5/5	0.73	0.11	69,73,76,88	0
5	DMS	A	606	4/4	0.74	0.24	40,57,63,65	0
6	EDO	A	608	4/4	0.77	0.23	40,41,49,50	0
8	SO4	B	509	5/5	0.79	0.13	52,54,58,71	0
5	DMS	A	607	4/4	0.81	0.19	37,48,48,62	0
5	DMS	A	603	4/4	0.82	0.22	49,56,56,58	0
3	JBQ	A	601	12/12	0.83	0.18	40,44,50,51	12
5	DMS	B	503	4/4	0.83	0.21	21,28,42,50	0
5	DMS	B	504	4/4	0.83	0.16	47,51,60,67	0
5	DMS	A	604	4/4	0.88	0.16	25,32,43,44	0
7	MG	A	609	1/1	0.88	0.10	50,50,50,50	0
5	DMS	B	506	4/4	0.91	0.15	40,45,51,51	0
5	DMS	B	507	4/4	0.91	0.15	29,43,45,49	0
6	EDO	B	508	4/4	0.92	0.13	32,35,39,40	0
5	DMS	B	505	4/4	0.95	0.13	30,34,39,50	0
5	DMS	B	501	4/4	0.95	0.13	37,38,40,43	0
4	T27	A	602	28/28	0.96	0.07	24,26,34,38	0
5	DMS	A	605	4/4	0.98	0.10	27,30,34,37	0
5	DMS	B	502	4/4	0.98	0.09	34,38,39,40	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.

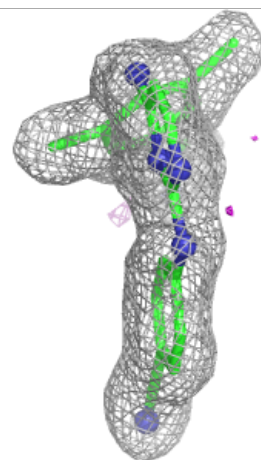
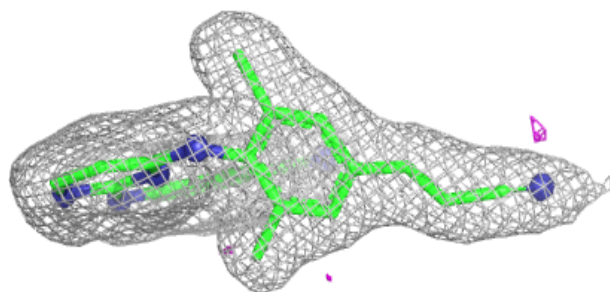
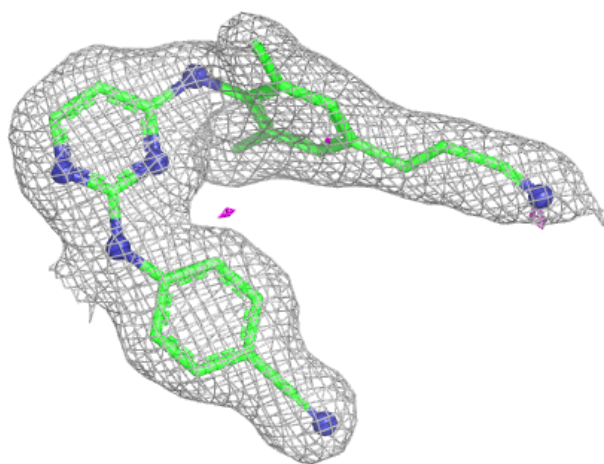
Electron density around JBQ A 601:

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



Electron density around T27 A 602:

$2mF_o-DF_c$ (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.