



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:42 PM UTC

PDB ID : 4IG3 / pdb_00004ig3
Title : HIV-1 reverse transcriptase with bound fragment near Knuckles site
Authors : Bauman, J.D.; Patel, D.; Arnold, E.
Deposited on : 2012-12-15
Resolution : 1.95 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

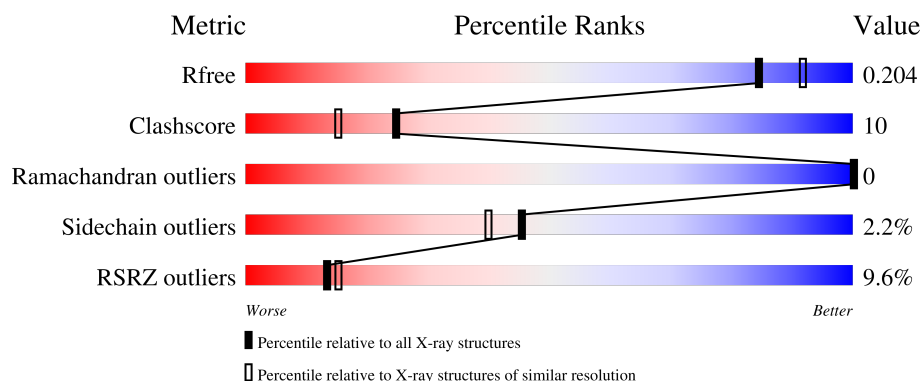
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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% 86% 13% .
2	B	429	12% 80% 16% ..

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
4	DMS	A	602	-	-	X	-
4	DMS	A	605	-	-	X	-
4	DMS	A	607	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9006 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	1	0
			4521	2926	751	836	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

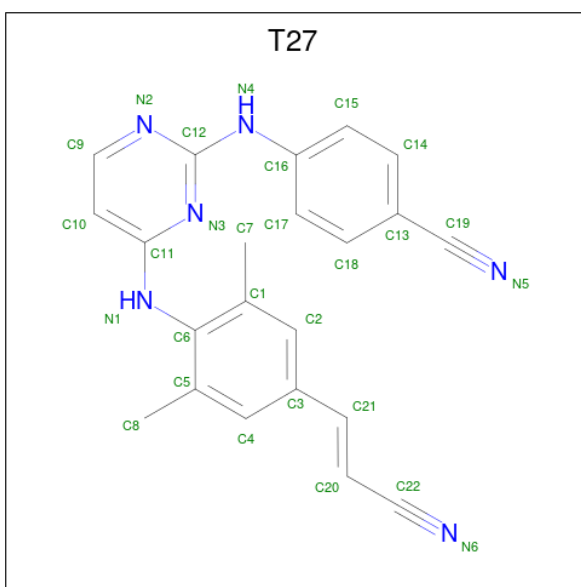
- Molecule 2 is a protein called P51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	416	Total	C	N	O	S	0	3	0
			3458	2254	571	626	7			

There are 2 discrepancies between the modelled and reference sequences:

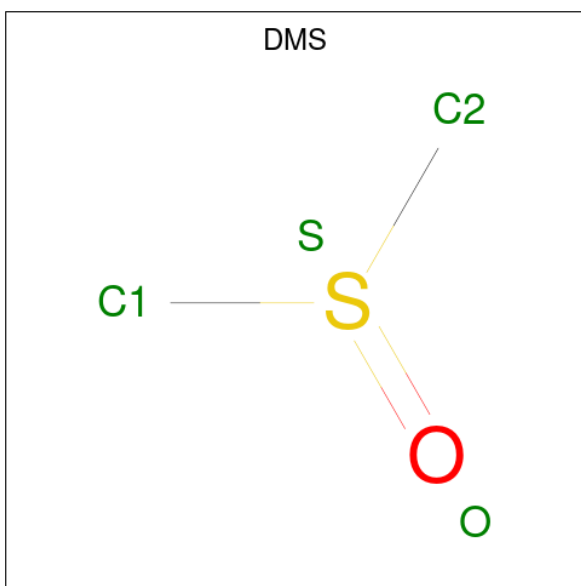
Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	expression tag	UNP P03366
B	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 3 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
3	A	1	Total	C	N	0	0
			28	22	6		

- Molecule 4 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



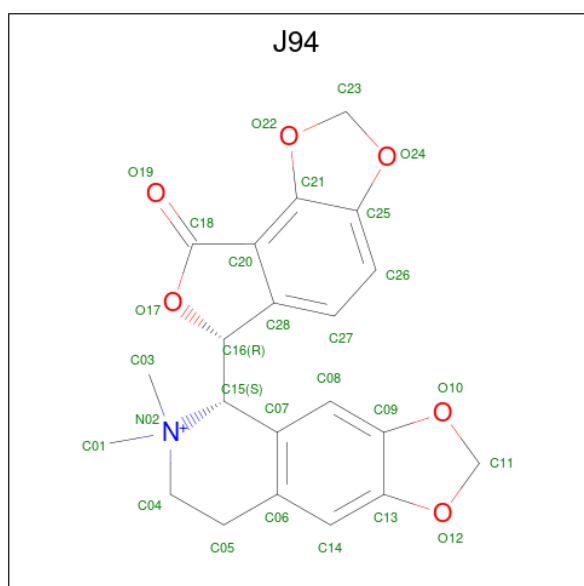
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		

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

- Molecule 5 is (5S)-6,6-dimethyl-5-[(6R)-8-oxo-6,8-dihydrofuro[3,4-e][1,3]benzodioxol-6-yl]-5,6,7,8-tetrahydro[1,3]dioxolo[4,5-g]isoquinolin-6-ium (CCD ID: J94) (formula: C₂₁H₂₀NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			28	21	1	6		

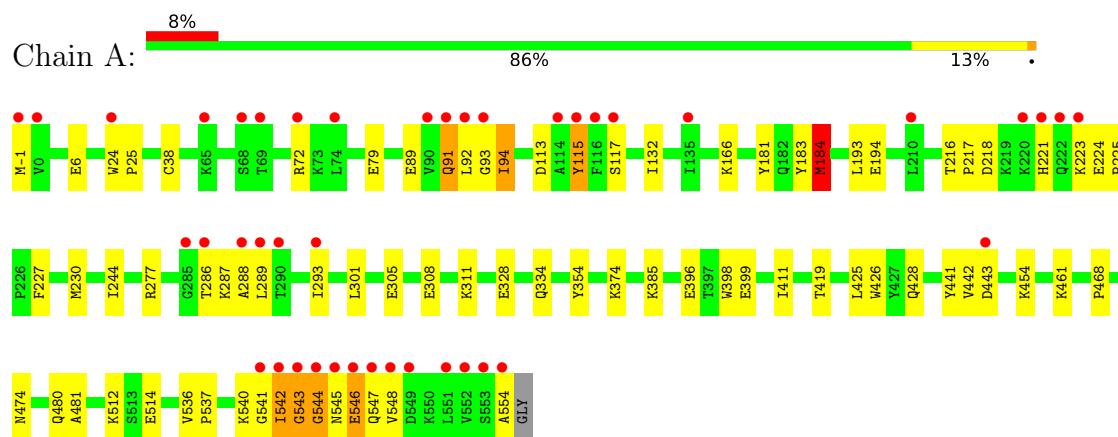
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	569	Total	O	0	0
			569	569		
6	B	342	Total	O	0	0
			342	342		

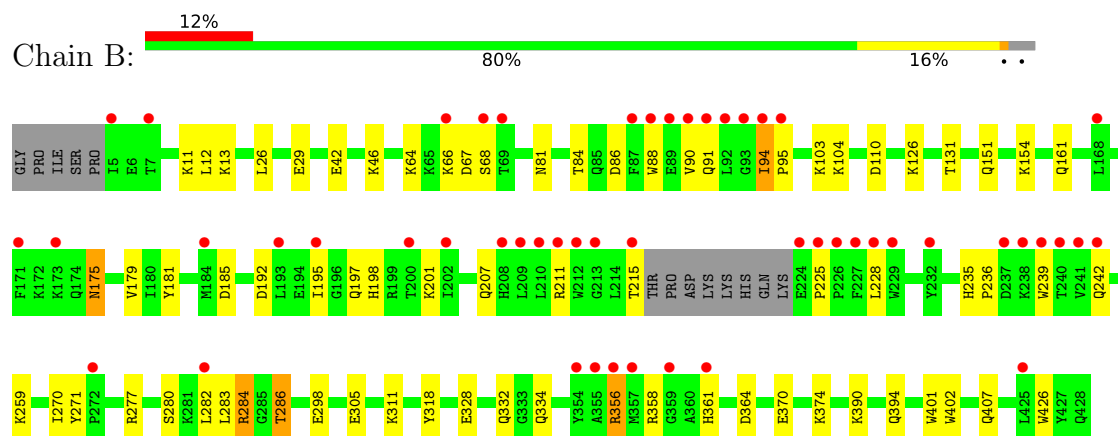
3 Residue-property plots [i](#)

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	161.76Å 73.07Å 109.03Å 90.00° 100.03° 90.00°	Depositor
Resolution (Å)	33.21 – 1.95 33.21 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.1 (33.21-1.95) 92.7 (33.21-1.95)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 1.89Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1233)	Depositor
R, R_{free}	0.178 , 0.203 0.180 , 0.204	Depositor DCC
R_{free} test set	1926 reflections (1.94%)	wwPDB-VP
Wilson B-factor (Å ²)	26.5	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 57.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9006	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% 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: DMS, T27, J94

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	0.58	0/4643	0.92	10/6311 (0.2%)
2	B	0.59	0/3565	0.98	14/4844 (0.3%)
All	All	0.58	0/8208	0.95	24/11155 (0.2%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	271	TYR	CA-C-N	9.02	128.62	119.24
2	B	271	TYR	C-N-CA	9.02	128.62	119.24
2	B	284	ARG	CA-C-N	-7.29	114.53	122.55
2	B	284	ARG	C-N-CA	-7.29	114.53	122.55
1	A	541	GLY	N-CA-C	-7.21	105.27	115.43
1	A	544	GLY	N-CA-C	-7.17	96.19	113.18
2	B	175	ASN	CA-C-N	6.59	126.21	119.56
2	B	175	ASN	C-N-CA	6.59	126.21	119.56
2	B	131	THR	CA-C-N	-6.53	118.16	122.60
2	B	131	THR	C-N-CA	-6.53	118.16	122.60
2	B	364	ASP	CB-CA-C	-6.34	100.27	110.79
1	A	184	MET	CB-CA-C	-6.24	109.40	116.63
1	A	543	GLY	N-CA-C	6.04	118.97	112.33
1	A	287	LYS	N-CA-C	5.82	119.50	111.71
1	A	542	ILE	CA-C-N	5.36	126.28	120.44
1	A	542	ILE	C-N-CA	5.36	126.28	120.44
2	B	286	THR	CB-CA-C	-5.35	104.19	111.95
1	A	115	TYR	N-CA-C	5.28	117.72	111.33
2	B	270	ILE	N-CA-C	-5.25	107.30	111.81
1	A	24	TRP	CA-C-N	-5.18	114.62	119.85
1	A	24	TRP	C-N-CA	-5.18	114.62	119.85
2	B	90	VAL	N-CA-C	5.17	115.39	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	361	HIS	N-CA-C	5.15	117.63	111.71
2	B	401	TRP	N-CA-C	5.15	120.56	113.97

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	4521	0	4576	92	0
2	B	3458	0	3483	77	0
3	A	28	0	18	1	0
4	A	28	0	42	18	0
4	B	32	0	48	15	0
5	A	28	0	20	2	0
6	A	569	0	0	41	1
6	B	342	0	0	18	1
All	All	9006	0	8187	160	1

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 10.

All (160) 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:244:ILE:H	4:A:607:DMS:H21	1.19	1.03
2:B:26:LEU:H	4:B:503:DMS:H11	1.15	1.03
1:A:428:GLN:H	4:A:603:DMS:H23	1.31	0.93
2:B:68:SER:O	6:B:893:HOH:O	1.85	0.91
1:A:334:GLN:H	4:A:605:DMS:H11	1.33	0.91
2:B:318:TYR:HB3	4:B:507:DMS:H13	1.55	0.85
1:A:480:GLN:NE2	6:A:1257:HOH:O	2.11	0.84
2:B:334:GLN:OE1	6:B:882:HOH:O	1.96	0.83
2:B:94:ILE:O	6:B:894:HOH:O	1.97	0.83
1:A:328:GLU:OE2	6:A:1127:HOH:O	1.97	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:402:TRP:HE1	4:B:506:DMS:H22	1.45	0.80
1:A:72:ARG:NH2	6:A:1227:HOH:O	2.15	0.80
2:B:91:GLN:HE22	2:B:94:ILE:HG23	1.45	0.80
1:A:468:PRO:O	6:A:993:HOH:O	2.00	0.78
1:A:426:TRP:H	4:A:602:DMS:C2	1.97	0.78
2:B:235:HIS:H	4:B:504:DMS:H21	1.49	0.77
1:A:244:ILE:N	4:A:607:DMS:H21	1.97	0.76
1:A:224:GLU:OE1	6:A:890:HOH:O	2.05	0.75
1:A:547:GLN:NE2	6:A:1035:HOH:O	2.18	0.75
1:A:308:GLU:OE1	6:A:1155:HOH:O	2.05	0.75
2:B:390:LYS:NZ	6:B:858:HOH:O	2.18	0.74
1:A:426:TRP:H	4:A:602:DMS:H23	1.53	0.74
1:A:89:GLU:OE1	6:A:1225:HOH:O	2.06	0.74
2:B:26:LEU:N	4:B:503:DMS:H11	1.99	0.73
1:A:546:GLU:OE2	2:B:284:ARG:HG2	1.89	0.72
2:B:402:TRP:HE1	4:B:506:DMS:C2	2.02	0.71
1:A:512:LYS:NZ	4:A:605:DMS:S	2.63	0.71
2:B:358:ARG:NH1	2:B:370[B]:GLU:OE2	2.24	0.70
4:B:507:DMS:S	6:B:922:HOH:O	2.50	0.69
2:B:11:LYS:HD2	2:B:12:LEU:H	1.58	0.69
1:A:461:LYS:NZ	6:A:1040:HOH:O	2.26	0.69
1:A:334:GLN:H	4:A:605:DMS:C1	2.06	0.68
4:A:607:DMS:H22	6:A:913:HOH:O	1.94	0.68
2:B:42:GLU:OE1	6:B:854:HOH:O	2.10	0.68
2:B:29:GLU:OE2	6:B:855:HOH:O	2.12	0.67
1:A:546:GLU:O	6:A:1163:HOH:O	2.13	0.67
1:A:543:GLY:HA3	2:B:284:ARG:C	2.19	0.67
1:A:288:ALA:N	6:A:1252:HOH:O	2.07	0.67
2:B:426:TRP:O	4:B:505:DMS:H12	1.93	0.66
1:A:514:GLU:OE1	6:A:992:HOH:O	2.13	0.66
1:A:428:GLN:N	4:A:603:DMS:H23	2.06	0.66
2:B:311:LYS:NZ	6:B:900:HOH:O	2.24	0.66
1:A:543:GLY:N	2:B:283:LEU:O	2.29	0.65
1:A:425:LEU:HA	4:A:602:DMS:H23	1.79	0.65
2:B:26:LEU:O	4:B:503:DMS:H21	1.97	0.65
4:A:602:DMS:H22	6:A:956:HOH:O	1.98	0.64
1:A:443:ASP:OD1	6:A:780:HOH:O	2.15	0.64
2:B:207:GLN:O	2:B:211:ARG:HG3	1.98	0.64
1:A:79:GLU:OE1	6:A:1247:HOH:O	2.15	0.63
1:A:443:ASP:HB2	1:A:548:VAL:HG23	1.81	0.62
1:A:115:TYR:OH	6:A:1112:HOH:O	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:64:LYS:O	2:B:407:GLN:NE2	2.25	0.61
2:B:225:PRO:HG3	2:B:228:LEU:HD22	1.82	0.60
2:B:305:GLU:OE1	6:B:744:HOH:O	2.17	0.59
1:A:72:ARG:NH2	6:A:1048:HOH:O	2.04	0.59
1:A:72:ARG:NH1	6:A:1065:HOH:O	2.13	0.58
1:A:536:VAL:HB	1:A:542:ILE:HD13	1.85	0.58
2:B:181:TYR:OH	6:B:904:HOH:O	2.16	0.58
1:A:115:TYR:CE1	6:A:1112:HOH:O	2.52	0.57
1:A:540:LYS:O	2:B:280:SER:HB3	2.04	0.57
2:B:94:ILE:HB	6:B:894:HOH:O	2.05	0.57
2:B:370[B]:GLU:OE2	6:B:815:HOH:O	2.17	0.57
1:A:543:GLY:HA3	2:B:284:ARG:HA	1.88	0.56
1:A:244:ILE:H	4:A:607:DMS:C2	2.07	0.56
1:A:91:GLN:NE2	6:A:1225:HOH:O	2.37	0.56
1:A:426:TRP:H	4:A:602:DMS:H21	1.70	0.55
2:B:104:LYS:HE3	2:B:192:ASP:HB3	1.89	0.54
1:A:543:GLY:HA3	2:B:284:ARG:O	2.07	0.54
1:A:545:ASN:HB2	6:A:1147:HOH:O	2.08	0.54
1:A:286:THR:HG22	6:A:1252:HOH:O	2.07	0.54
2:B:81:ASN:O	2:B:154:LYS:HE2	2.08	0.54
2:B:225:PRO:HB2	2:B:228:LEU:HD13	1.90	0.53
2:B:370[B]:GLU:CD	6:B:815:HOH:O	2.50	0.53
1:A:542:ILE:HB	6:A:754:HOH:O	2.09	0.52
1:A:542:ILE:HG12	2:B:283:LEU:HD12	1.91	0.52
1:A:419:THR:HB	6:A:943:HOH:O	2.10	0.52
2:B:239:TRP:HE1	4:B:504:DMS:H23	1.75	0.51
1:A:115:TYR:CZ	6:A:1112:HOH:O	2.63	0.51
1:A:223:LYS:NZ	6:A:1000:HOH:O	2.44	0.51
1:A:441:TYR:O	1:A:548:VAL:HG11	2.11	0.51
1:A:396:GLU:HG3	6:A:964:HOH:O	2.11	0.50
1:A:545:ASN:CB	6:A:1147:HOH:O	2.59	0.50
1:A:72:ARG:NH1	6:A:1205:HOH:O	2.44	0.50
1:A:545:ASN:ND2	6:A:1147:HOH:O	1.97	0.50
1:A:543:GLY:HA3	2:B:284:ARG:CA	2.41	0.50
1:A:543:GLY:CA	2:B:284:ARG:HA	2.43	0.48
1:A:193:LEU:O	6:A:911:HOH:O	2.20	0.48
1:A:542:ILE:HG23	2:B:283:LEU:HB3	1.95	0.48
2:B:402:TRP:NE1	4:B:506:DMS:H22	2.21	0.48
2:B:197:GLN:O	2:B:201:LYS:HG2	2.13	0.48
1:A:224:GLU:HG3	1:A:225:PRO:HD2	1.95	0.48
2:B:298:GLU:OE1	2:B:298:GLU:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:GLY:H	2:B:283:LEU:C	2.21	0.48
2:B:94:ILE:HG23	2:B:161:GLN:HE22	1.79	0.47
1:A:474:ASN:H	4:A:606:DMS:C2	2.27	0.47
2:B:86:ASP:HB3	2:B:88:TRP:CE2	2.49	0.47
1:A:25:PRO:HA	6:A:1157:HOH:O	2.15	0.47
1:A:543:GLY:CA	2:B:283:LEU:O	2.63	0.47
1:A:544:GLY:HA2	2:B:286:THR:HG22	1.97	0.47
6:A:1104:HOH:O	2:B:394:GLN:HG3	2.15	0.47
1:A:544:GLY:O	1:A:548:VAL:HG22	2.15	0.47
1:A:537:PRO:O	1:A:542:ILE:HD12	2.16	0.46
3:A:601:T27:H15	3:A:601:T27:N3	2.31	0.46
2:B:277:ARG:NH1	6:B:878:HOH:O	2.14	0.46
1:A:334:GLN:N	4:A:605:DMS:H11	2.14	0.46
1:A:223:LYS:HG2	1:A:227:PHE:HE1	1.80	0.46
1:A:426:TRP:N	4:A:602:DMS:H23	2.27	0.46
2:B:11:LYS:HD2	2:B:12:LEU:N	2.30	0.46
2:B:66:LYS:O	2:B:67:ASP:HB2	2.16	0.46
2:B:126:LYS:HD2	4:B:502:DMS:H22	1.97	0.45
1:A:181:TYR:CE2	1:A:183:TYR:HB2	2.51	0.45
2:B:86:ASP:HB3	2:B:88:TRP:CZ2	2.52	0.45
1:A:25:PRO:O	6:A:1204:HOH:O	2.20	0.45
2:B:225:PRO:CG	2:B:228:LEU:HD22	2.47	0.45
1:A:293:ILE:O	6:A:1160:HOH:O	2.21	0.45
1:A:543:GLY:C	1:A:545:ASN:N	2.72	0.45
2:B:356:ARG:H	2:B:356:ARG:CD	2.30	0.45
2:B:110:ASP:O	2:B:228:LEU:HD12	2.17	0.45
2:B:370[B]:GLU:OE2	2:B:374:LYS:HE2	2.18	0.44
1:A:398:TRP:CZ2	1:A:411:ILE:HG12	2.52	0.44
1:A:6:GLU:OE2	5:A:609:J94:H14	2.17	0.44
2:B:103:LYS:NZ	6:B:912:HOH:O	2.07	0.44
1:A:184:MET:HA	1:A:184:MET:HE2	2.00	0.44
1:A:543:GLY:O	1:A:545:ASN:N	2.49	0.44
1:A:385:LYS:HD2	6:A:1183:HOH:O	2.17	0.43
1:A:542:ILE:O	1:A:545:ASN:HB3	2.19	0.43
5:A:609:J94:H14	5:A:609:J94:H4	1.81	0.43
2:B:13:LYS:HE3	2:B:84:THR:O	2.18	0.43
2:B:94:ILE:O	2:B:95:PRO:C	2.60	0.43
1:A:277:ARG:NH2	4:A:608:DMS:O	2.50	0.43
2:B:11:LYS:CD	2:B:12:LEU:H	2.29	0.43
2:B:103:LYS:HE3	2:B:179:VAL:CG2	2.49	0.43
2:B:318:TYR:HB3	4:B:507:DMS:C1	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:LYS:NZ	6:A:825:HOH:O	2.50	0.43
1:A:94:ILE:HG21	1:A:230:MET:HE2	2.01	0.42
2:B:66:LYS:HZ1	2:B:358:ARG:NH1	2.17	0.42
2:B:175:ASN:C	6:B:924:HOH:O	2.62	0.42
2:B:195:ILE:HA	2:B:198:HIS:HB3	2.02	0.42
2:B:236:PRO:HA	2:B:239:TRP:CG	2.55	0.42
1:A:354:TYR:HD1	1:A:374:LYS:HD2	1.84	0.42
1:A:442:VAL:HB	1:A:481:ALA:HB1	2.01	0.42
1:A:92:LEU:HD12	1:A:93:GLY:N	2.34	0.42
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.55	0.42
2:B:46:LYS:NZ	6:B:685:HOH:O	2.36	0.42
1:A:540:LYS:O	2:B:280:SER:CB	2.68	0.41
1:A:288:ALA:HB3	6:A:1252:HOH:O	2.19	0.41
1:A:454:LYS:NZ	1:A:554:ALA:HB3	2.34	0.41
2:B:235:HIS:N	4:B:504:DMS:H21	2.26	0.41
1:A:547:GLN:CD	6:A:1035:HOH:O	2.61	0.41
2:B:151:GLN:HB3	2:B:185:ASP:OD2	2.20	0.41
2:B:328:GLU:OE1	6:B:771:HOH:O	2.22	0.41
1:A:301:LEU:O	1:A:305:GLU:HG3	2.21	0.41
1:A:38:CYS:SG	1:A:132:ILE:HD11	2.61	0.41
1:A:166:LYS:HD2	1:A:166:LYS:HA	1.88	0.41
2:B:358:ARG:NH1	2:B:370[B]:GLU:CD	2.79	0.41
1:A:545:ASN:HA	1:A:548:VAL:HG22	2.02	0.40
2:B:358:ARG:NH2	2:B:370[B]:GLU:OE1	2.53	0.40
1:A:328:GLU:CG	6:A:1127:HOH:O	2.70	0.40
2:B:332:GLN:C	4:B:508:DMS:H22	2.47	0.40
1:A:216:THR:HA	1:A:217:PRO:HD3	1.90	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1056:HOH:O	6:B:858:HOH:O[4_546]	1.77	0.43

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	555/557 (100%)	542 (98%)	13 (2%)	0	100	100
2	B	415/429 (97%)	401 (97%)	14 (3%)	0	100	100
All	All	970/986 (98%)	943 (97%)	27 (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	496/495 (100%)	483 (97%)	13 (3%)	40	33
2	B	380/390 (97%)	374 (98%)	6 (2%)	55	52
All	All	876/885 (99%)	857 (98%)	19 (2%)	45	40

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	MET
1	A	91	GLN
1	A	94	ILE
1	A	113	ASP
1	A	117	SER
1	A	184	MET
1	A	194	GLU
1	A	218	ASP
1	A	221	HIS
1	A	289	LEU
1	A	311	LYS
1	A	399	GLU
1	A	546	GLU
2	B	94	ILE

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Mol	Chain	Res	Type
2	B	215	THR
2	B	242	GLN
2	B	259	LYS
2	B	282	LEU
2	B	356	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	278	GLN
2	B	91	GLN
2	B	161	GLN
2	B	265	ASN
2	B	269	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](#)

17 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
4	DMS	A	608	-	3,3,3	0.66	0	3,3,3	0.85	0
4	DMS	B	507	-	3,3,3	0.59	0	3,3,3	0.88	0
4	DMS	B	503	-	3,3,3	0.77	0	3,3,3	1.17	0
4	DMS	A	606	-	3,3,3	0.72	0	3,3,3	0.87	0
4	DMS	B	508	-	3,3,3	0.62	0	3,3,3	0.78	0
4	DMS	B	505	-	3,3,3	0.90	0	3,3,3	1.35	1 (33%)
5	J94	A	609	-	33,33,33	2.32	14 (42%)	49,52,52	1.42	5 (10%)
4	DMS	B	502	-	3,3,3	0.53	0	3,3,3	0.51	0
4	DMS	A	607	-	3,3,3	0.57	0	3,3,3	0.50	0
4	DMS	A	602	-	3,3,3	0.48	0	3,3,3	0.51	0
4	DMS	B	501	-	3,3,3	0.64	0	3,3,3	0.44	0
4	DMS	B	504	-	3,3,3	0.67	0	3,3,3	0.59	0
4	DMS	B	506	-	3,3,3	0.60	0	3,3,3	0.86	0
4	DMS	A	603	-	3,3,3	0.57	0	3,3,3	0.73	0
4	DMS	A	604	-	3,3,3	0.65	0	3,3,3	0.91	0
3	T27	A	601	-	30,30,30	1.24	4 (13%)	37,40,40	1.80	6 (16%)
4	DMS	A	605	-	3,3,3	0.54	0	3,3,3	0.52	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
5	J94	A	609	-	-	0/4/44/44	0/6/6/6
3	T27	A	601	-	-	0/13/14/14	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	609	J94	C15-C16	-5.00	1.46	1.54
5	A	609	J94	C20-C28	-4.63	1.34	1.39
5	A	609	J94	C27-C28	4.04	1.44	1.39
5	A	609	J94	O17-C16	-3.75	1.41	1.46
5	A	609	J94	C05-C06	-3.67	1.45	1.51
3	A	601	T27	C12-N4	3.66	1.44	1.36
5	A	609	J94	C14-C13	3.60	1.45	1.38
3	A	601	T27	C11-N1	3.11	1.44	1.38
5	A	609	J94	C08-C07	3.11	1.44	1.39
5	A	609	J94	O17-C18	3.00	1.40	1.36
5	A	609	J94	C06-C07	-2.69	1.35	1.40
5	A	609	J94	C03-N02	-2.32	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	609	J94	C14-C06	2.29	1.43	1.39
3	A	601	T27	C13-C19	2.15	1.49	1.44
5	A	609	J94	C07-C15	2.13	1.55	1.52
5	A	609	J94	O22-C21	2.12	1.40	1.38
5	A	609	J94	C20-C21	2.10	1.45	1.40
3	A	601	T27	C2-C1	-2.08	1.36	1.39

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	T27	C9-N2-C12	5.85	120.31	115.42
3	A	601	T27	C10-C9-N2	-4.97	117.89	123.97
5	A	609	J94	O17-C18-O19	4.02	124.65	121.18
5	A	609	J94	O17-C16-C15	3.64	113.26	108.62
5	A	609	J94	O22-C21-C20	3.46	132.20	128.33
3	A	601	T27	N2-C12-N3	-3.11	123.41	126.42
3	A	601	T27	C6-N1-C11	-2.74	119.17	124.11
5	A	609	J94	O12-C13-C14	2.49	131.17	127.86
3	A	601	T27	C10-C11-N3	-2.39	119.14	123.15
3	A	601	T27	C4-C5-C6	2.29	120.87	118.25
5	A	609	J94	O24-C25-C26	2.11	131.78	127.72
4	B	505	DMS	C2-S-C1	2.09	109.11	98.42

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	608	DMS	1	0
4	B	507	DMS	3	0
4	B	503	DMS	3	0
4	A	606	DMS	1	0
4	B	508	DMS	1	0
4	B	505	DMS	1	0
5	A	609	J94	2	0
4	B	502	DMS	1	0
4	A	607	DMS	4	0
4	A	602	DMS	6	0
4	B	504	DMS	3	0
4	B	506	DMS	3	0

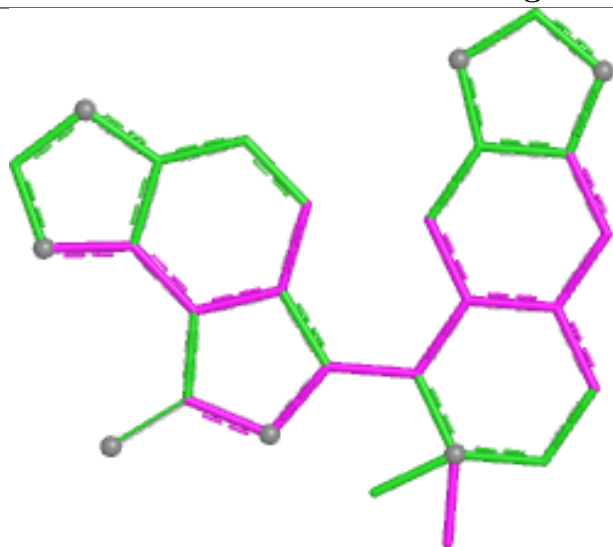
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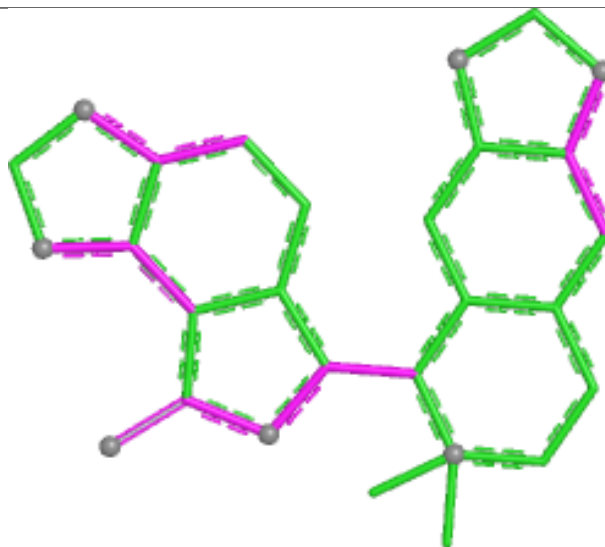
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	603	DMS	2	0
3	A	601	T27	1	0
4	A	605	DMS	4	0

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.

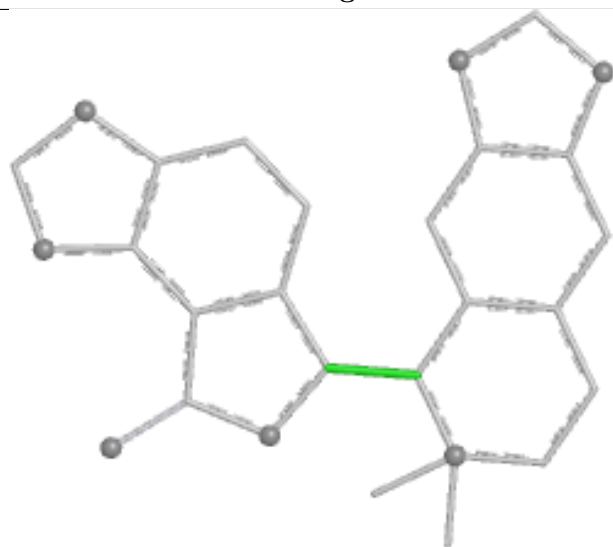
Ligand J94 A 609



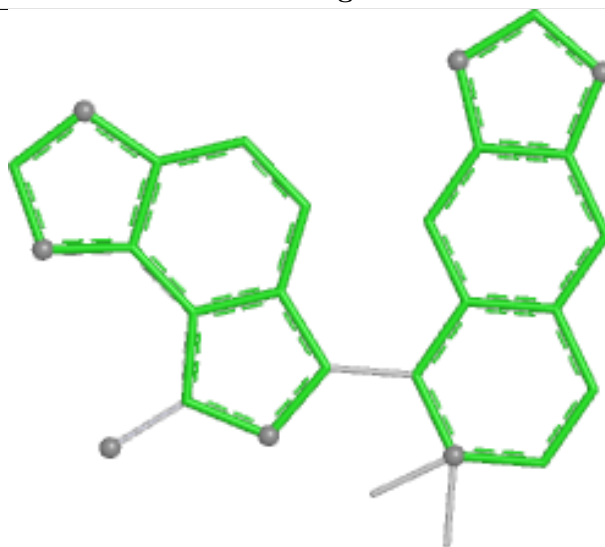
Bond lengths



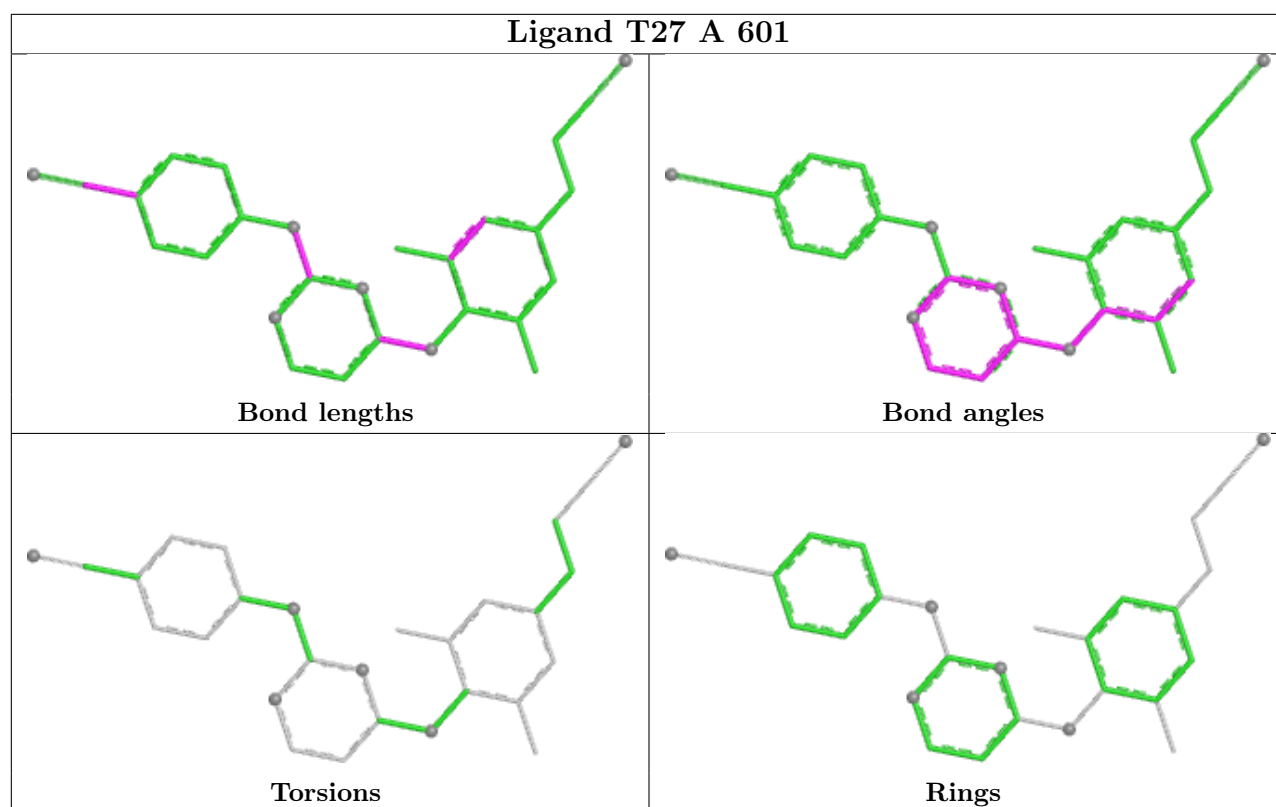
Bond angles



Torsions



Rings



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%)	0.19	42 (7%) 20 22	13, 33, 83, 121	1 (0%)
2	B	416/429 (96%)	0.42	51 (12%) 8 9	12, 36, 96, 142	3 (0%)
All	All	972/986 (98%)	0.29	93 (9%) 13 15	12, 34, 90, 142	4 (0%)

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	92	LEU	7.6
1	A	116	PHE	7.3
2	B	90	VAL	7.1
1	A	542	ILE	7.0
2	B	95	PRO	6.3
1	A	92	LEU	5.9
1	A	543	GLY	5.7
1	A	115	TYR	5.2
1	A	90	VAL	5.1
1	A	548	VAL	5.0
2	B	228	LEU	4.6
2	B	357	MET	4.5
2	B	93	GLY	4.5
2	B	88	TRP	4.3
2	B	242	GLN	4.3
1	A	541	GLY	4.2
1	A	551	LEU	4.2
2	B	94	ILE	4.1
1	A	554	ALA	4.1
1	A	289	LEU	4.1
2	B	240	THR	4.0
1	A	552	VAL	3.9
1	A	24	TRP	3.9
1	A	545	ASN	3.8

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Mol	Chain	Res	Type	RSRZ
2	B	69	THR	3.8
2	B	5	ILE	3.7
1	A	546	GLU	3.7
1	A	547	GLN	3.6
2	B	87	PHE	3.6
1	A	553	SER	3.5
1	A	544	GLY	3.4
2	B	209	LEU	3.3
2	B	229	TRP	3.3
2	B	239	TRP	3.2
2	B	232	TYR	3.2
1	A	117	SER	3.1
2	B	195	ILE	3.1
1	A	-1	MET	3.1
1	A	114	ALA	3.1
1	A	221	HIS	3.1
1	A	288	ALA	3.1
2	B	212	TRP	3.0
1	A	210	LEU	3.0
2	B	208	HIS	3.0
1	A	93	GLY	3.0
2	B	355	ALA	3.0
1	A	286	THR	2.9
2	B	210	LEU	2.9
2	B	193	LEU	2.9
2	B	241	VAL	2.9
1	A	549	ASP	2.8
2	B	215	THR	2.8
2	B	168	LEU	2.7
2	B	7	THR	2.6
2	B	200	THR	2.6
2	B	272	PRO	2.6
2	B	184	MET	2.6
1	A	220	LYS	2.6
1	A	0	VAL	2.6
1	A	223	LYS	2.5
2	B	213	GLY	2.5
2	B	91	GLN	2.5
1	A	68	SER	2.5
2	B	225	PRO	2.5
2	B	227	PHE	2.5
1	A	290	THR	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	211	ARG	2.4
2	B	361	HIS	2.4
1	A	293	ILE	2.4
2	B	68	SER	2.4
2	B	173	LYS	2.4
2	B	202	ILE	2.3
2	B	354	TYR	2.3
2	B	226	PRO	2.3
2	B	238	LYS	2.3
2	B	356	ARG	2.2
1	A	69	THR	2.2
1	A	74	LEU	2.2
2	B	89	GLU	2.2
2	B	224	GLU	2.2
1	A	65	LYS	2.2
2	B	282	LEU	2.2
2	B	171	PHE	2.1
2	B	425	LEU	2.1
1	A	135	ILE	2.1
1	A	222	GLN	2.1
2	B	66	LYS	2.1
1	A	443	ASP	2.1
2	B	237	ASP	2.1
1	A	72	ARG	2.1
2	B	359	GLY	2.0
1	A	91	GLN	2.0
1	A	285	GLY	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,

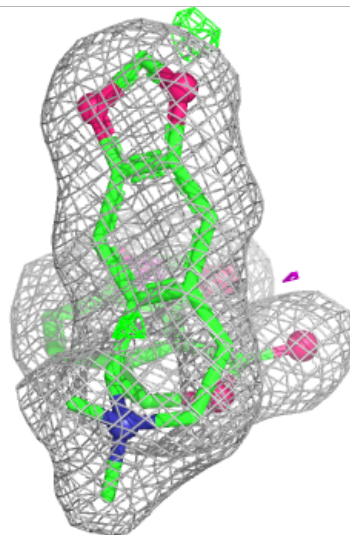
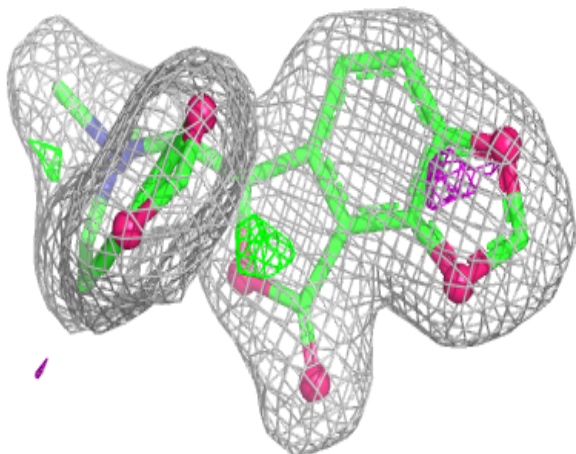
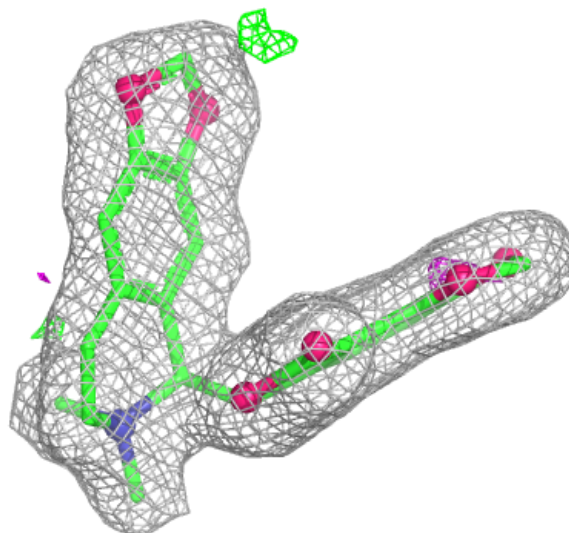
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	DMS	A	606	4/4	0.68	0.21	53,56,64,80	0
4	DMS	B	504	4/4	0.71	0.17	37,61,187,187	0
4	DMS	B	508	4/4	0.82	0.21	39,63,77,78	0
4	DMS	B	505	4/4	0.84	0.21	22,29,61,61	0
4	DMS	A	608	4/4	0.84	0.16	57,71,75,81	0
4	DMS	B	507	4/4	0.85	0.20	62,68,71,95	0
4	DMS	B	503	4/4	0.87	0.22	16,21,56,75	0
4	DMS	A	605	4/4	0.88	0.14	27,48,57,76	0
4	DMS	A	604	4/4	0.91	0.17	46,58,60,77	0
4	DMS	A	607	4/4	0.91	0.13	33,48,63,71	0
4	DMS	A	602	4/4	0.93	0.13	15,31,39,52	0
5	J94	A	609	28/28	0.94	0.07	22,30,36,38	0
3	T27	A	601	28/28	0.95	0.07	16,22,25,30	0
4	DMS	B	502	4/4	0.97	0.08	27,29,38,44	0
4	DMS	B	501	4/4	0.97	0.09	36,39,43,48	0
4	DMS	B	506	4/4	0.97	0.09	21,35,44,45	0
4	DMS	A	603	4/4	0.98	0.07	25,30,32,38	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.

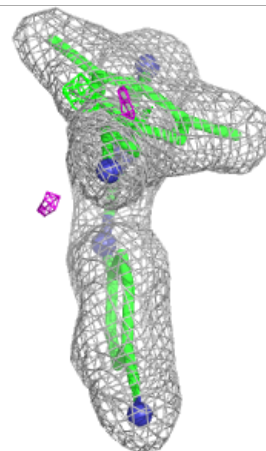
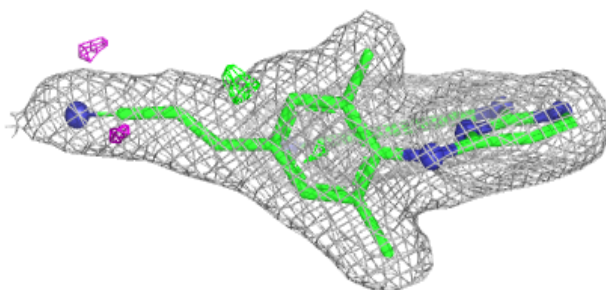
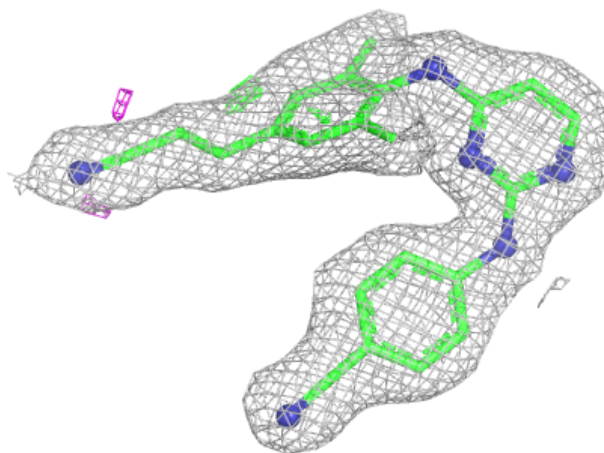
Electron density around J94 A 609:

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 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.