



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:07 AM UTC

PDB ID : 8STT / pdb_00008stt
Title : Crystal Structure of HIV-1 Reverse Transcriptase (Y181C, V106A) variant in Complex with 8-(2-(2-(2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)ethoxy)phenoxy)indolizine-2-carbonitrile (JLJ555), a non-nucleoside inhibitor
Authors : Hollander, K.; Jorgensen, W.L.; Anderson, K.S.
Deposited on : 2023-05-11
Resolution : 2.62 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

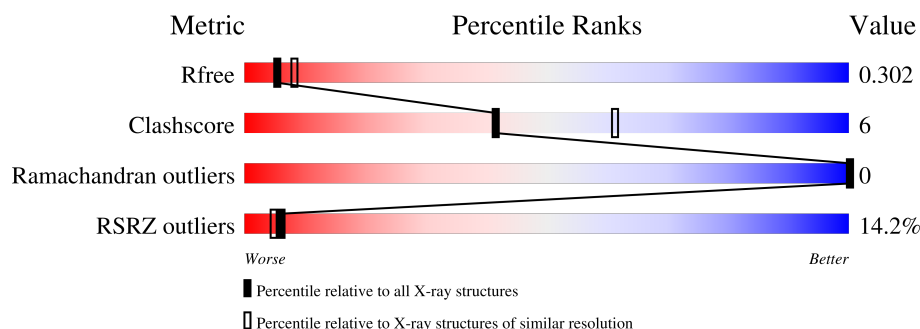
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.62 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	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)

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	558	
1	C	558	
2	B	428	
2	D	428	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14881 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	547	Total	C	N	O	S	0	1	0
			4184	2692	686	799	7			
1	C	544	Total	C	N	O	S	0	3	0
			4225	2706	704	808	7			

There are 14 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	106	ALA	VAL	engineered mutation	UNP P03366
A	172	ALA	LYS	engineered mutation	UNP P03366
A	173	ALA	LYS	engineered mutation	UNP P03366
A	181	CYS	TYR	engineered mutation	UNP P03366
A	280	SER	CYS	engineered mutation	UNP P03366
C	-1	MET	-	expression tag	UNP P03366
C	0	VAL	-	expression tag	UNP P03366
C	106	ALA	VAL	engineered mutation	UNP P03366
C	172	ALA	LYS	engineered mutation	UNP P03366
C	173	ALA	LYS	engineered mutation	UNP P03366
C	181	CYS	TYR	engineered mutation	UNP P03366
C	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	405	Total	C	N	O	S	23	2	0
			3270	2123	532	609	6			
2	D	401	Total	C	N	O	S	14	1	0
			3078	1989	508	577	4			

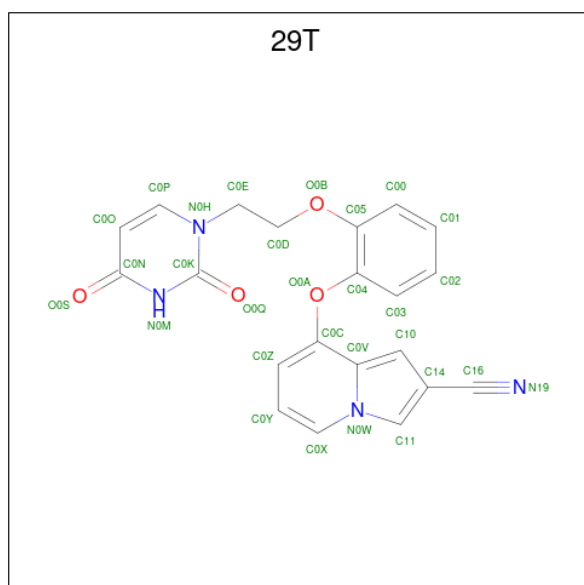
There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0

- Molecule 4 is 8-{2-[2-(2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)ethoxy]phenoxy}indolizine-2-carbonitrile (CCD ID: 29T) (formula: C₂₁H₁₆N₄O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 29	C 21	N 4	O 4	0	0
4	C	1	Total 29	C 21	N 4	O 4	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	26	Total O 26 26	0	0

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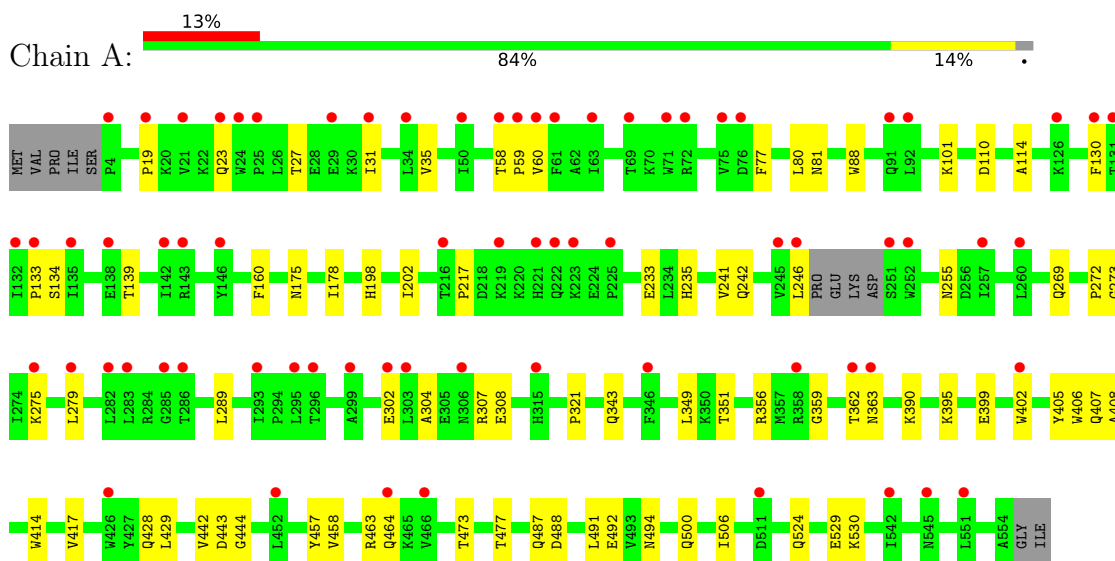
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	27	Total 27	O 27	0	0
5	C	10	Total 10	O 10	0	0
5	D	1	Total 1	O 1	0	0

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

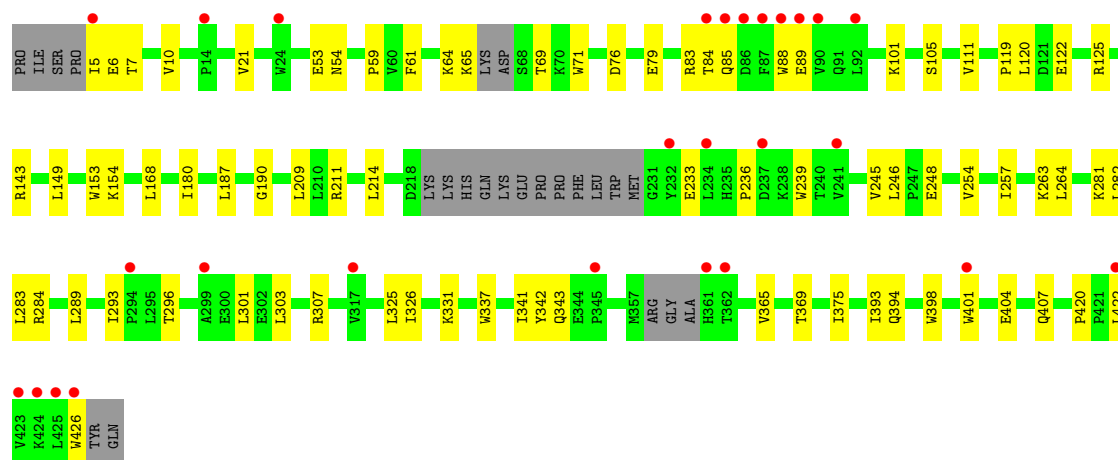


- Molecule 1: Reverse transcriptase/ribonuclease H



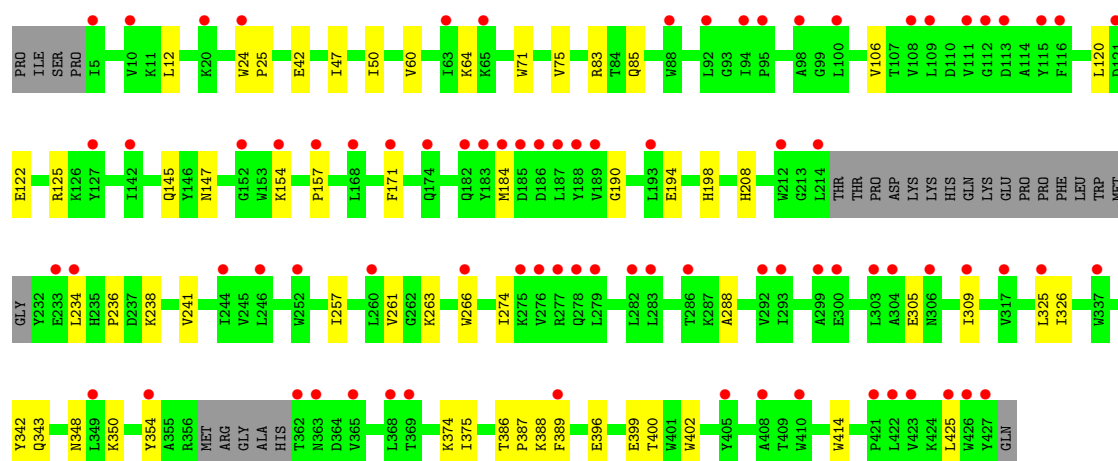
• Molecule 2: p51 RT

Chain B: 



• Molecule 2: p51 RT

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	111.69Å 73.01Å 170.47Å 90.00° 97.60° 90.00°	Depositor
Resolution (Å)	54.79 – 2.62 54.79 – 2.62	Depositor EDS
% Data completeness (in resolution range)	99.1 (54.79-2.62) 99.0 (54.79-2.62)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.263 , 0.291 0.277 , 0.302	Depositor DCC
R_{free} test set	4013 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	77.9	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 56.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	14881	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 3.07% 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: 29T, MG

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	0.22	0/4296	0.39	0/5880
1	C	0.21	0/4328	0.36	0/5894
2	B	0.26	0/3366	0.42	0/4592
2	D	0.18	0/3169	0.33	0/4343
All	All	0.22	0/15159	0.37	0/20709

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 [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	4184	0	3930	51	0
1	C	4225	0	4032	47	0
2	B	3270	0	3199	53	0
2	D	3078	0	2821	42	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	29	0	16	0	0
4	C	29	0	16	1	0
5	A	26	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	27	0	0	3	0
5	C	10	0	0	0	0
5	D	1	0	0	0	0
All	All	14881	0	14014	184	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 (184) 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:C:328:GLU:HG2	1:C:390:LYS:HB2	1.76	0.68
1:C:132:ILE:HB	1:C:142:ILE:HD12	1.76	0.67
2:B:85:GLN:HG3	2:B:154:LYS:HB3	1.77	0.66
1:C:460:ASN:HD22	2:D:288:ALA:HB2	1.63	0.64
2:B:84:THR:HG21	2:B:153:TRP:HZ2	1.64	0.63
1:A:175:ASN:HB3	1:A:178:ILE:HD13	1.80	0.63
1:C:90:VAL:HG21	1:C:157:PRO:HB2	1.83	0.60
2:D:157:PRO:HG2	2:D:184:MET:HA	1.83	0.60
1:C:441:TYR:CD2	1:C:544:GLY:HA3	2.36	0.60
2:B:85:GLN:O	2:B:89:GLU:N	2.34	0.60
1:A:58:THR:HG22	1:A:59:PRO:HD2	1.83	0.60
2:B:64:LYS:HD2	2:B:69:THR:O	2.01	0.60
2:D:348:ASN:N	2:D:348:ASN:OD1	2.34	0.60
1:A:356:ARG:NH1	1:A:359:GLY:O	2.34	0.59
2:B:10:VAL:HA	2:B:88:TRP:CH2	2.37	0.59
1:C:253:THR:HG23	1:C:256:ASP:H	1.67	0.59
2:D:194:GLU:O	2:D:198:HIS:N	2.32	0.59
1:A:402:TRP:C	1:A:402:TRP:CD1	2.81	0.58
1:A:390:LYS:HB3	1:A:417:VAL:HG21	1.86	0.57
2:B:7:THR:HG22	2:B:119:PRO:HG2	1.87	0.57
1:C:444:GLY:HA2	1:C:552:VAL:HG21	1.86	0.56
1:C:331:LYS:NZ	1:C:333:GLY:O	2.38	0.56
2:B:257:ILE:HB	2:B:283:LEU:HD21	1.87	0.56
1:C:89:GLU:HG2	1:C:92:LEU:HG	1.87	0.56
2:B:254:VAL:HG13	2:B:283:LEU:HD22	1.87	0.56
1:A:255:ASN:HB2	1:A:289:LEU:HB3	1.89	0.56
2:B:65:LYS:HA	2:B:407:GLN:OE1	2.06	0.55
1:A:23:GLN:HE22	1:A:133:PRO:HD3	1.70	0.55
1:C:445:ALA:HB3	1:C:553:SER:HB3	1.89	0.55
2:B:64:LYS:HD3	2:B:71:TRP:CE2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:171:PHE:HB2	2:D:208:HIS:HD1	1.72	0.53
1:A:31:ILE:HG12	1:A:133:PRO:HG2	1.89	0.53
1:A:399:GLU:HA	1:A:402:TRP:CE3	2.44	0.53
1:A:241:VAL:HG12	1:A:242:GLN:O	2.09	0.53
1:C:343:GLN:HG3	1:C:349:LEU:HD21	1.91	0.52
1:A:442:VAL:HG12	1:A:457:TYR:HB3	1.91	0.52
2:B:369:THR:HG22	2:B:398:TRP:CH2	2.45	0.52
2:D:325:LEU:HD23	2:D:343:GLN:HG3	1.90	0.52
1:C:503:LEU:HD22	1:C:535:TRP:HB2	1.90	0.52
2:D:12:LEU:HD22	2:D:83:ARG:HB2	1.92	0.52
2:D:125:ARG:HD3	2:D:147:ASN:HA	1.91	0.52
1:A:101:LYS:HE3	1:A:321:PRO:HG3	1.90	0.51
2:D:60:VAL:HG12	2:D:75:VAL:HG22	1.92	0.51
2:B:54:ASN:O	2:B:143:ARG:NH2	2.44	0.51
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.93	0.51
2:B:111:VAL:HG11	2:B:187:LEU:HD22	1.92	0.50
1:C:46:LYS:HD2	1:C:116:PHE:HB3	1.94	0.50
1:C:58:THR:HG22	1:C:59:PRO:HD2	1.93	0.50
1:A:110:ASP:O	1:A:217:PRO:HD3	2.12	0.49
2:D:375:ILE:HB	2:D:389:PHE:HZ	1.76	0.49
2:D:24[B]:TRP:HZ3	2:D:402:TRP:HE1	1.60	0.49
1:A:443:ASP:OD1	1:A:444:GLY:N	2.46	0.49
2:B:5:ILE:HD12	2:B:6:GLU:HG3	1.95	0.49
2:B:233:GLU:HG3	5:B:527:HOH:O	2.12	0.49
1:C:453:GLY:HA3	1:C:469:LEU:HB2	1.94	0.49
1:A:457:TYR:HE1	1:A:463:ARG:HG2	1.78	0.49
2:B:245:VAL:O	2:B:263:LYS:NZ	2.38	0.49
1:A:500:GLN:HG3	2:B:422:LEU:HD13	1.94	0.48
2:B:426:TRP:NE1	5:B:506:HOH:O	2.46	0.48
2:D:388:LYS:O	2:D:414:TRP:HA	2.14	0.48
1:C:114:ALA:HB1	1:C:160:PHE:CE1	2.48	0.47
1:A:492:GLU:HG2	1:A:530:LYS:HB2	1.95	0.47
1:C:180:ILE:HG23	1:C:189:VAL:HG22	1.95	0.47
1:A:491:LEU:HD13	1:A:529:GLU:OE2	2.14	0.47
1:A:31:ILE:O	1:A:35:VAL:HG23	2.15	0.47
2:B:187:LEU:HD12	2:B:187:LEU:HA	1.72	0.47
2:B:365:VAL:O	2:B:369:THR:HG23	2.15	0.47
1:A:405:TYR:CE2	1:A:407:GLN:HB2	2.50	0.47
1:C:167:ILE:O	1:C:170:PRO:HD2	2.15	0.47
1:C:458:VAL:HG23	1:C:548:VAL:HG13	1.96	0.47
1:A:390:LYS:HB3	1:A:417:VAL:CG2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:120:LEU:HD13	2:B:149:LEU:HD23	1.97	0.47
2:D:64:LYS:HE2	2:D:71:TRP:CZ2	2.50	0.47
2:D:387:PRO:HD2	2:D:389:PHE:HE2	1.80	0.46
2:B:79:GLU:OE1	2:B:83:ARG:NH1	2.48	0.46
2:B:211:ARG:HB3	1:C:212:TRP:CZ2	2.51	0.46
2:B:331:LYS:HB2	2:B:337:TRP:CZ3	2.51	0.46
1:A:428:GLN:HE21	1:A:428:GLN:HA	1.80	0.46
2:B:303:LEU:O	2:B:307:ARG:HG3	2.15	0.46
2:B:325:LEU:HD23	2:B:343:GLN:HG3	1.97	0.46
2:D:50:ILE:HG21	2:D:145:GLN:HB3	1.96	0.46
2:D:238:LYS:HA	2:D:238:LYS:HD2	1.59	0.46
2:D:396:GLU:OE1	2:D:396:GLU:N	2.45	0.46
2:B:84:THR:HG21	2:B:153:TRP:CZ2	2.48	0.46
1:C:203:GLU:OE2	1:C:206:ARG:NH1	2.47	0.46
1:A:494:ASN:HB3	2:B:289:LEU:HD12	1.98	0.46
2:B:246:LEU:HD11	2:B:264:LEU:HD21	1.97	0.46
1:C:9:PRO:HA	1:C:121:ASP:OD2	2.15	0.46
2:D:171:PHE:HB2	2:D:208:HIS:ND1	2.31	0.46
2:B:61:PHE:HE1	2:B:76:ASP:HB2	1.81	0.45
2:B:394:GLN:NE2	5:B:507:HOH:O	2.49	0.45
1:A:60:VAL:CG2	1:A:130:PHE:HB2	2.46	0.45
1:A:473:THR:O	1:A:477:THR:HG23	2.16	0.45
2:D:305:GLU:O	2:D:309:ILE:HG12	2.16	0.45
1:A:134:SER:HB2	1:A:139:THR:HB	1.97	0.45
1:C:465:LYS:HE3	1:C:488:ASP:OD2	2.17	0.45
1:A:114:ALA:HB1	1:A:160:PHE:CE1	2.51	0.45
1:A:27:THR:O	1:A:31:ILE:HG13	2.17	0.45
1:A:273:GLY:O	1:A:275:LYS:NZ	2.44	0.45
1:A:487:GLN:HG2	1:A:524:GLN:NE2	2.32	0.45
2:D:396:GLU:O	2:D:400:THR:OG1	2.30	0.45
1:C:164:MET:HE2	1:C:164:MET:HB2	1.86	0.44
1:C:296:THR:O	1:C:300:GLU:HG2	2.17	0.44
2:D:266:TRP:CG	2:D:425:LEU:HD13	2.52	0.44
2:D:24[A]:TRP:CD2	2:D:25:PRO:HD2	2.52	0.44
1:C:12:LEU:HD22	1:C:83:ARG:HB3	1.99	0.44
2:D:326:ILE:HG22	2:D:388:LYS:HB3	2.00	0.44
1:C:171:PHE:CZ	1:C:205:LEU:HB2	2.52	0.44
2:B:168:LEU:HD13	2:B:180:ILE:HG21	1.99	0.44
2:D:274:ILE:HD12	2:D:274:ILE:HA	1.90	0.44
1:A:272:PRO:HA	1:A:351:THR:HG21	1.98	0.44
1:A:406:TRP:CD1	2:B:420:PRO:HB3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:LEU:HD11	1:A:506:ILE:HG22	2.00	0.43
1:C:320:ASP:OD2	1:C:323:LYS:NZ	2.51	0.43
2:D:326:ILE:HG12	2:D:342:TYR:O	2.18	0.43
1:A:23:GLN:NE2	1:A:60:VAL:HB	2.33	0.43
1:A:60:VAL:HG22	1:A:130:PHE:HB2	1.99	0.43
2:B:209:LEU:HB3	2:B:214:LEU:HB2	2.00	0.43
1:C:59:PRO:O	1:C:75:VAL:HG13	2.17	0.43
2:B:101:LYS:O	2:B:236:PRO:HB2	2.18	0.43
1:C:325:LEU:HD21	1:C:383:TRP:CE3	2.54	0.43
2:D:120:LEU:HD23	2:D:125:ARG:HG2	1.99	0.43
1:C:82:LYS:HB2	1:C:82:LYS:HE3	1.81	0.43
2:B:248:GLU:HB2	2:B:307:ARG:HH22	1.84	0.43
1:A:233:GLU:HB3	1:A:235:HIS:CE1	2.54	0.43
2:B:281:LYS:HA	2:B:284:ARG:HG3	2.01	0.43
2:B:341:ILE:HD11	2:B:375:ILE:HG23	2.01	0.43
1:C:473:THR:O	1:C:477:THR:HG23	2.18	0.43
2:B:64:LYS:HG3	2:B:71:TRP:HA	2.01	0.43
1:A:279:LEU:HG	1:A:302:GLU:OE1	2.19	0.42
1:A:395:LYS:NZ	1:A:414:TRP:O	2.43	0.42
2:D:234:LEU:O	2:D:236:PRO:HD3	2.19	0.42
1:C:221:HIS:CD2	1:C:221:HIS:H	2.35	0.42
2:D:24[A]:TRP:CG	2:D:25:PRO:HD2	2.53	0.42
1:A:88:TRP:CE2	2:B:143:ARG:HD3	2.53	0.42
1:A:408:ALA:O	2:B:393:ILE:HG13	2.19	0.42
2:B:248:GLU:HB2	2:B:307:ARG:NH2	2.35	0.42
1:A:198:HIS:NE2	1:A:202:ILE:HD11	2.35	0.42
1:A:343:GLN:HG3	1:A:349:LEU:HD11	2.01	0.42
2:D:354:TYR:HB2	2:D:374:LYS:HE3	2.00	0.42
1:C:229:TRP:CD2	4:C:602:29T:H2	2.55	0.42
1:C:239:TRP:NE1	1:C:316:GLY:HA3	2.34	0.42
2:B:282:LEU:HD12	2:B:293:ILE:CG2	2.49	0.42
1:C:471:ASN:O	1:C:471:ASN:ND2	2.52	0.42
2:B:401:TRP:HD1	2:B:404[A]:GLU:HG3	1.84	0.42
2:D:122:GLU:HA	2:D:125:ARG:NE	2.35	0.42
2:D:375:ILE:HB	2:D:389:PHE:CZ	2.54	0.42
2:B:122:GLU:HA	2:B:125:ARG:HG3	2.02	0.42
2:B:326:ILE:HG12	2:B:342:TYR:CE2	2.55	0.42
1:C:90:VAL:HG13	1:C:161:GLN:HG3	2.02	0.42
1:C:165:THR:O	1:C:169:GLU:HG3	2.20	0.42
1:C:5:ILE:HD13	1:C:5:ILE:HA	1.95	0.42
1:C:238:LYS:HE3	1:C:238:LYS:HB2	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:GLN:O	1:A:351:THR:N	2.48	0.41
1:A:304:ALA:O	1:A:308[A]:GLU:HG2	2.20	0.41
2:D:241:VAL:HG12	2:D:350:LYS:HG2	2.01	0.41
1:A:19:PRO:HG3	1:A:80:LEU:HB2	2.00	0.41
1:C:478:GLU:O	1:C:482:ILE:HG12	2.19	0.41
2:D:12:LEU:HD23	2:D:12:LEU:HA	1.90	0.41
1:C:261:VAL:HG13	1:C:276:VAL:HB	2.01	0.41
1:C:122:GLU:HA	1:C:125:ARG:HD2	2.03	0.41
2:D:106:VAL:HA	2:D:190:GLY:HA2	2.03	0.41
1:A:246:LEU:CB	1:A:307:ARG:HE	2.34	0.41
1:C:58:THR:N	1:C:129:ALA:O	2.54	0.41
1:C:350:LYS:HE3	1:C:378:GLU:OE2	2.20	0.41
2:D:85:GLN:NE2	2:D:154:LYS:HB2	2.36	0.41
1:A:457:TYR:OH	1:A:488:ASP:OD2	2.31	0.41
2:D:386:THR:HA	2:D:387:PRO:HD3	1.86	0.41
2:B:53:GLU:OE1	2:B:53:GLU:N	2.45	0.41
2:B:301:LEU:HD22	2:B:301:LEU:HA	1.95	0.41
1:A:362:THR:HG22	1:A:363:ASN:H	1.86	0.40
2:B:105:SER:O	2:B:190:GLY:HA2	2.21	0.40
1:C:198:HIS:O	1:C:202:ILE:HG12	2.21	0.40
2:D:257:ILE:O	2:D:261:VAL:HG23	2.21	0.40
1:C:460:ASN:ND2	2:D:288:ALA:HB2	2.33	0.40
2:D:24[B]:TRP:CH2	2:D:399:GLU:HG2	2.56	0.40
2:D:263:LYS:HG2	2:D:425:LEU:CD2	2.50	0.40
1:A:77:PHE:O	1:A:81:ASN:N	2.40	0.40
1:A:458:VAL:HG22	1:A:464:GLN:HG2	2.03	0.40
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.56	0.40
1:A:406:TRP:CG	2:B:420:PRO:HB3	2.57	0.40
2:B:282:LEU:HD11	2:B:296:THR:HG23	2.02	0.40
2:D:42:GLU:HA	2:D:47:ILE:O	2.21	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	544/558 (98%)	533 (98%)	11 (2%)	0	100	100
1	C	535/558 (96%)	525 (98%)	10 (2%)	0	100	100
2	B	399/428 (93%)	392 (98%)	7 (2%)	0	100	100
2	D	396/428 (92%)	387 (98%)	9 (2%)	0	100	100
All	All	1874/1972 (95%)	1837 (98%)	37 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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
4	29T	C	602	-	32,32,32	0.62	0	38,44,44	0.80	1 (2%)
4	29T	A	602	-	32,32,32	0.45	0	38,44,44	0.75	1 (2%)

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
4	29T	C	602	-	-	1/10/12/12	0/4/4/4
4	29T	A	602	-	-	0/10/12/12	0/4/4/4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	C	602	29T	C14-C16-N19	-3.58	173.46	178.10
4	A	602	29T	C14-C16-N19	-2.62	174.70	178.10

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	602	29T	C05-C04-O0A-C0C

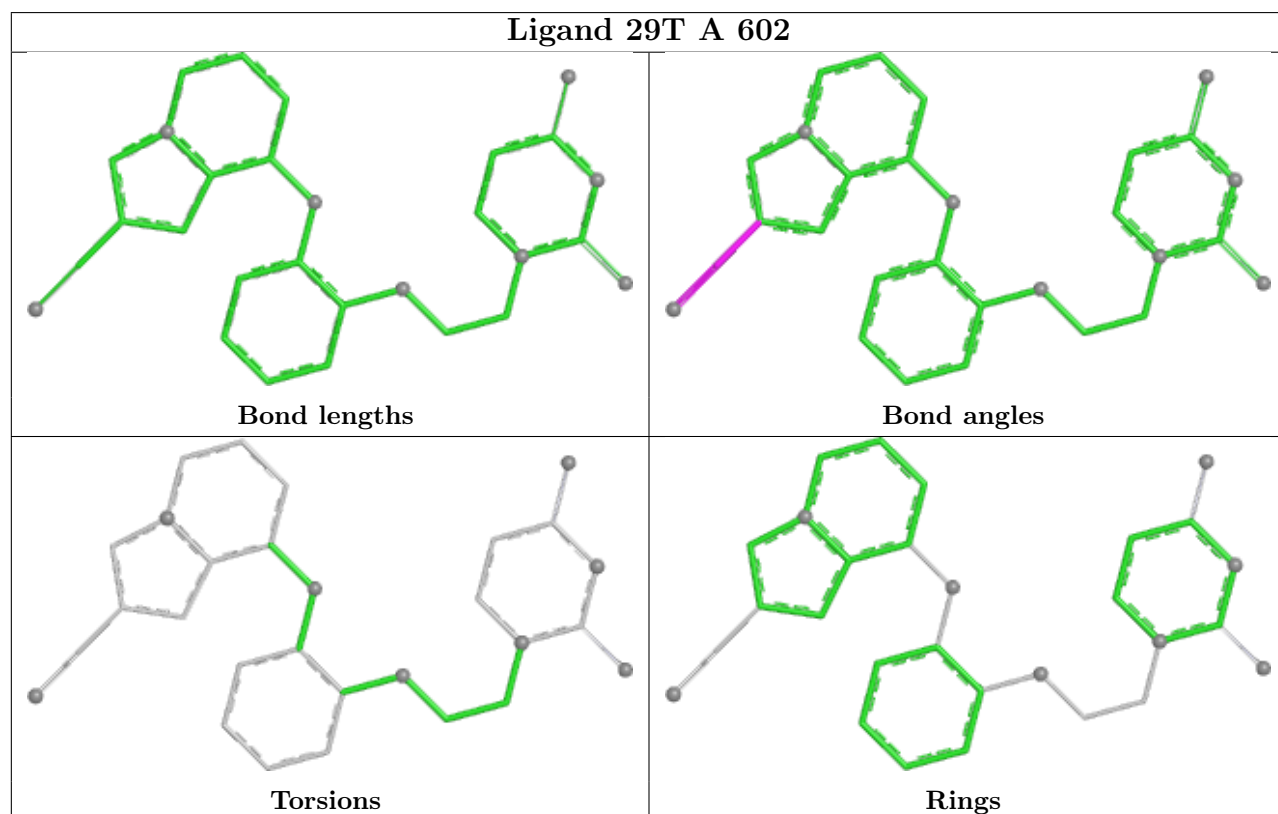
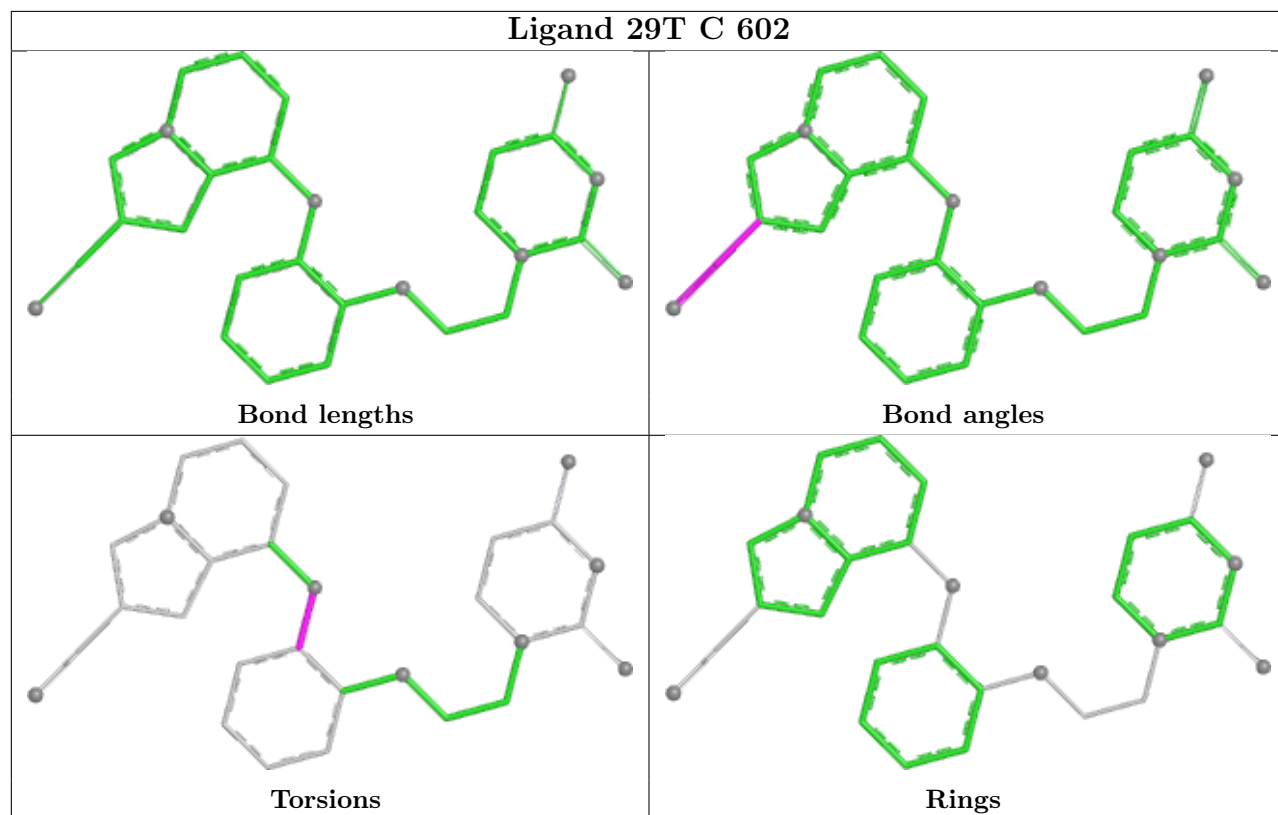
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	602	29T	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	547/558 (98%)	0.84	71 (12%) 7 6	39, 76, 139, 160	1 (0%)
1	C	544/558 (97%)	1.24	89 (16%) 4 3	53, 100, 134, 159	3 (0%)
2	B	405/428 (94%)	0.63	27 (6%) 24 19	36, 69, 105, 134	9 (2%)
2	D	401/428 (93%)	1.43	82 (20%) 3 2	57, 114, 141, 155	6 (1%)
All	All	1897/1972 (96%)	1.04	269 (14%) 6 5	36, 91, 137, 160	19 (1%)

All (269) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	24[A]	TRP	6.8
1	C	130	PHE	6.5
2	D	427	TYR	6.1
1	A	225	PRO	5.7
1	A	282	LEU	5.7
2	B	362	THR	5.5
2	D	184	MET	5.4
1	C	61	PHE	5.3
1	C	276	VAL	5.1
1	A	146	TYR	5.0
2	D	109	LEU	4.3
2	D	115	TYR	4.3
1	C	225	PRO	4.1
2	D	185	ASP	4.1
2	D	111	VAL	4.1
2	B	232	TYR	4.0
2	D	425	LEU	3.9
1	C	252	TRP	3.8
2	D	246	LEU	3.8
2	B	425	LEU	3.7
1	C	21	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	132	ILE	3.7
1	A	142	ILE	3.7
1	C	5	ILE	3.7
1	A	251	SER	3.7
2	D	279	LEU	3.7
1	C	554	ALA	3.7
1	C	398	TRP	3.6
2	D	244	ILE	3.6
1	A	246	LEU	3.6
1	A	223	LYS	3.6
2	D	362	THR	3.5
2	B	88	TRP	3.5
2	D	276	VAL	3.5
1	C	359	GLY	3.5
1	A	252	TRP	3.5
2	D	95	PRO	3.5
2	D	283	LEU	3.5
2	D	116	PHE	3.5
2	D	212	TRP	3.5
2	D	363	ASN	3.4
2	D	303	LEU	3.4
1	A	346	PHE	3.4
2	B	426	TRP	3.4
1	C	128	THR	3.4
2	D	426	TRP	3.4
2	B	84	THR	3.4
1	C	409	THR	3.3
2	D	286	THR	3.3
1	A	275	LYS	3.3
2	D	94	ILE	3.3
2	B	24	TRP	3.3
1	C	50	ILE	3.3
1	C	292	VAL	3.3
1	A	130	PHE	3.3
1	A	63	ILE	3.3
1	A	279	LEU	3.2
2	D	154	LYS	3.2
1	C	332[A]	GLN	3.2
1	C	244	ILE	3.2
2	D	282	LEU	3.2
2	B	345	PRO	3.2
1	A	464	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	132	ILE	3.2
2	B	85	GLN	3.2
1	A	75	VAL	3.2
2	B	87	PHE	3.2
2	D	354	TYR	3.2
2	B	92	LEU	3.1
1	A	299	ALA	3.1
1	A	76	ASP	3.1
1	C	119	PRO	3.1
2	D	252	TRP	3.1
1	A	4	PRO	3.1
2	D	152	GLY	3.1
1	A	286	THR	3.0
2	D	369	THR	3.0
1	A	60	VAL	3.0
1	C	221	HIS	3.0
1	C	54	ASN	3.0
2	D	405	TYR	3.0
2	D	389	PHE	3.0
1	A	69	THR	3.0
1	A	295	LEU	3.0
2	D	188	TYR	3.0
2	D	317	VAL	3.0
1	C	441	TYR	2.9
2	B	86	ASP	2.9
1	C	63	ILE	2.9
1	C	246	LEU	2.9
2	D	300	GLU	2.9
2	D	277	ARG	2.9
2	B	5	ILE	2.9
1	C	118	VAL	2.9
2	B	317	VAL	2.9
2	B	361	HIS	2.9
2	D	186	ASP	2.9
1	A	551	LEU	2.9
1	C	34	LEU	2.9
1	C	59	PRO	2.8
1	C	131	THR	2.8
1	A	91	GLN	2.8
1	A	24	TRP	2.8
1	A	511	ASP	2.8
1	A	303	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	295	LEU	2.8
1	C	245	VAL	2.8
2	D	10	VAL	2.8
2	D	423	VAL	2.8
1	C	297	GLU	2.8
1	A	245	VAL	2.8
2	D	410	TRP	2.8
1	A	293	ILE	2.7
1	C	414	TRP	2.7
2	D	266	TRP	2.7
1	C	555	GLY	2.7
1	C	150	PRO	2.7
2	D	182	GLN	2.7
2	D	422	LEU	2.7
1	C	88	TRP	2.7
1	C	299	ALA	2.7
1	C	511	ASP	2.7
2	D	189	VAL	2.7
2	D	292	VAL	2.7
1	A	257	ILE	2.7
1	C	3	SER	2.7
2	D	88	TRP	2.7
1	A	61	PHE	2.7
2	B	90	VAL	2.7
1	C	177	ASP	2.7
2	D	100	LEU	2.7
1	A	260	LEU	2.6
1	C	260	LEU	2.6
1	A	34	LEU	2.6
1	C	120	LEU	2.6
2	D	325	LEU	2.6
1	A	363	ASN	2.6
1	A	92	LEU	2.6
1	C	92	LEU	2.6
2	D	304	ALA	2.6
1	A	23	GLN	2.6
1	A	452	LEU	2.6
1	C	282	LEU	2.6
1	C	15	GLY	2.6
2	D	112	GLY	2.6
1	C	142	ILE	2.5
1	C	425	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	448	ARG	2.5
2	D	421	PRO	2.5
1	C	296	THR	2.5
1	A	71	TRP	2.5
1	A	542	ILE	2.5
1	C	74	LEU	2.5
2	D	349	LEU	2.5
2	B	423	VAL	2.5
1	C	355	ALA	2.5
1	A	545	ASN	2.5
1	C	397	THR	2.5
1	C	110[A]	ASP	2.5
1	C	219	LYS	2.5
1	C	402	TRP	2.5
1	A	133	PRO	2.5
1	C	161	GLN	2.5
2	D	299	ALA	2.5
2	B	237	ASP	2.5
2	D	121	ASP	2.5
1	A	221	HIS	2.5
2	D	127	TYR	2.5
2	D	183	TYR	2.5
2	D	278	GLN	2.5
2	D	142	ILE	2.4
1	C	360	ALA	2.4
1	C	471	ASN	2.4
1	A	362	THR	2.4
2	B	422	LEU	2.4
1	A	306	ASN	2.4
2	D	65	LYS	2.4
1	C	152	GLY	2.4
2	B	241	VAL	2.4
1	C	146	TYR	2.4
2	D	171	PHE	2.4
1	C	283	LEU	2.4
1	A	58	THR	2.4
2	D	113	ASP	2.4
1	C	71	TRP	2.4
1	C	401	TRP	2.4
1	C	64	LYS	2.4
2	D	168	LEU	2.3
1	C	411	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	324	ASP	2.3
2	B	14	PRO	2.3
1	C	23	GLN	2.3
1	C	151	GLN	2.3
1	C	466	VAL	2.3
1	A	126	LYS	2.3
2	D	275	LYS	2.3
1	C	4	PRO	2.3
2	D	337	TRP	2.3
1	C	31	ILE	2.3
1	C	293	ILE	2.3
2	B	424	LYS	2.3
2	B	294	PRO	2.3
2	B	401	TRP	2.3
2	D	187	LEU	2.3
1	A	135	ILE	2.3
1	A	302	GLU	2.3
2	D	306	ASN	2.3
1	C	227	PHE	2.3
1	A	31	ILE	2.2
1	A	25	PRO	2.2
1	A	21	VAL	2.2
2	B	234	LEU	2.2
2	D	214	LEU	2.2
1	A	315	HIS	2.2
1	C	495	ILE	2.2
1	A	131	THR	2.2
1	C	358	ARG	2.2
1	C	542	ILE	2.2
2	D	5	ILE	2.2
2	B	89	GLU	2.2
1	C	306	ASN	2.2
2	D	260	LEU	2.2
1	C	435	VAL	2.2
1	A	50	ILE	2.2
1	C	87	PHE	2.2
2	D	98	ALA	2.2
2	D	233	GLU	2.2
1	A	222	GLN	2.2
2	D	20	LYS	2.2
1	C	458	VAL	2.2
1	A	426	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	72	ARG	2.1
2	D	157	PRO	2.1
1	C	20	LYS	2.1
1	C	16	MET	2.1
2	B	299	ALA	2.1
1	A	402	TRP	2.1
1	C	89	GLU	2.1
1	C	351	THR	2.1
1	A	466	VAL	2.1
2	D	293	ILE	2.1
2	D	365	VAL	2.1
1	C	124	PHE	2.1
1	A	29	GLU	2.1
1	A	143	ARG	2.1
1	C	72	ARG	2.1
1	A	219	LYS	2.1
2	D	174	GLN	2.1
2	D	234	LEU	2.1
1	A	285	GLY	2.1
2	D	408	ALA	2.1
1	C	58	THR	2.1
1	A	19	PRO	2.1
2	D	193	LEU	2.1
1	C	37	ILE	2.1
2	D	108	VAL	2.1
1	A	138	GLU	2.0
1	A	283	LEU	2.0
2	D	63	ILE	2.0
2	D	309	ILE	2.0
1	C	144	TYR	2.0
1	C	317	VAL	2.0
1	A	358	ARG	2.0
1	A	59	PRO	2.0
1	A	216	THR	2.0
1	A	296	THR	2.0
1	C	226	PRO	2.0
2	D	92	LEU	2.0
2	D	368	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

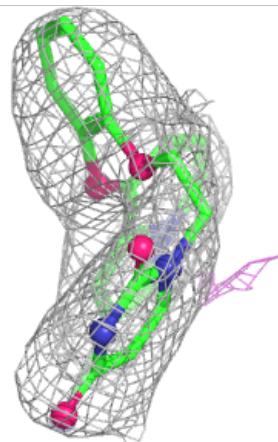
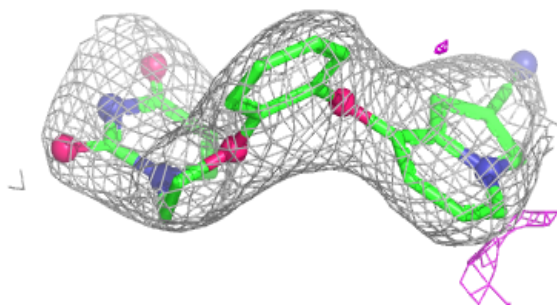
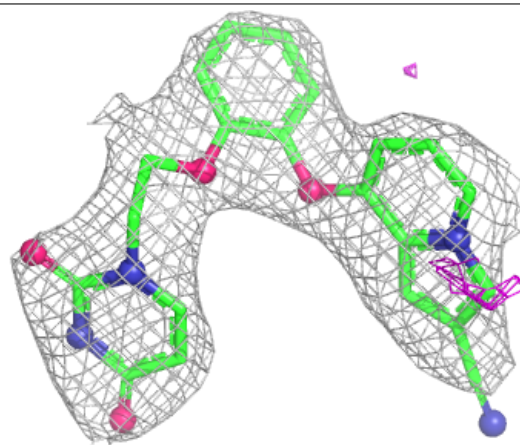
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	A	601	1/1	0.80	0.17	85,85,85,85	0
3	MG	C	601	1/1	0.80	0.20	86,86,86,86	0
4	29T	C	602	29/29	0.92	0.14	75,82,95,98	0
4	29T	A	602	29/29	0.95	0.11	48,58,66,69	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.

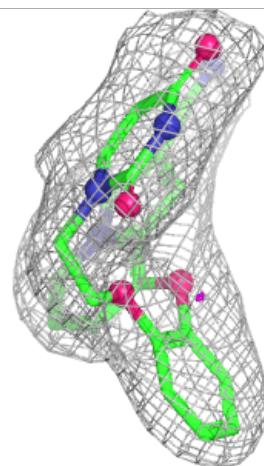
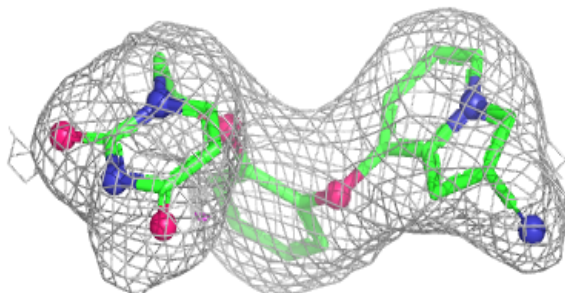
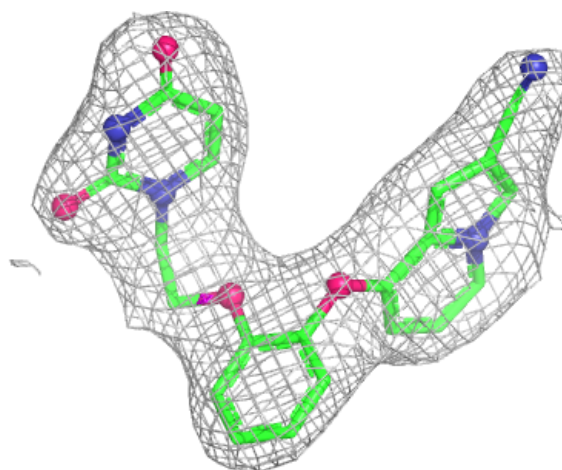
Electron density around 29T C 602:

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 29T 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.