



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 09:10 AM EDT

PDB ID : 4HY1 / pdb_00004hy1
Title : Pyrrolopyrimidine inhibitors of dna gyrase b and topoisomerase iv, part i: structure guided discovery and optimization of dual targeting agents with potent, broad-spectrum enzymatic activity.
Authors : Bensen, D.C.; Creighton, C.J.; Kwan, B.; Tari, L.W.
Deposited on : 2012-11-12
Resolution : 1.90 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

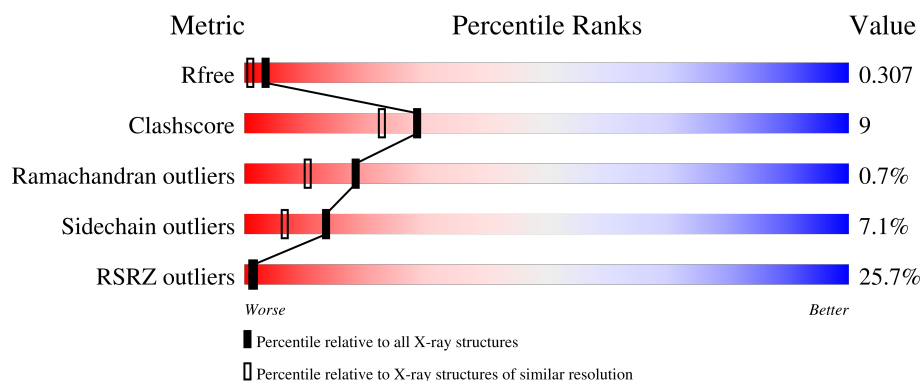
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	390	
1	B	390	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5292 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.

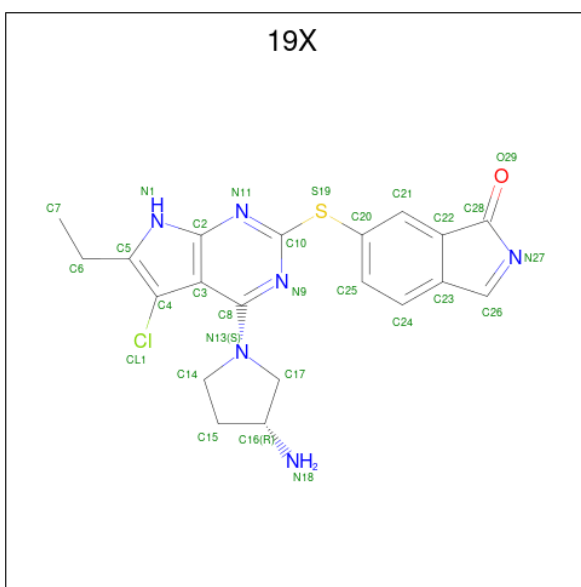
- Molecule 1 is a protein called Topoisomerase IV, subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	360	Total	C	N	O	S	0	3	0
			2855	1822	477	548	8			
1	B	228	Total	C	N	O	S	0	0	0
			1806	1156	302	343	5			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	258	PRO	LEU	SEE REMARK 999	UNP Q2A1P5
A	383	LEU	-	expression tag	UNP Q2A1P5
A	384	GLU	-	expression tag	UNP Q2A1P5
A	385	HIS	-	expression tag	UNP Q2A1P5
A	386	HIS	-	expression tag	UNP Q2A1P5
A	387	HIS	-	expression tag	UNP Q2A1P5
A	388	HIS	-	expression tag	UNP Q2A1P5
A	389	HIS	-	expression tag	UNP Q2A1P5
A	390	HIS	-	expression tag	UNP Q2A1P5
B	258	PRO	LEU	SEE REMARK 999	UNP Q2A1P5
B	383	LEU	-	expression tag	UNP Q2A1P5
B	384	GLU	-	expression tag	UNP Q2A1P5
B	385	HIS	-	expression tag	UNP Q2A1P5
B	386	HIS	-	expression tag	UNP Q2A1P5
B	387	HIS	-	expression tag	UNP Q2A1P5
B	388	HIS	-	expression tag	UNP Q2A1P5
B	389	HIS	-	expression tag	UNP Q2A1P5
B	390	HIS	-	expression tag	UNP Q2A1P5

- Molecule 2 is 6-({4-[(3R)-3-aminopyrrolidin-1-yl]-5-chloro-6-ethyl-7H-pyrrolo[2,3-d]pyrimidin-2-yl}sulfanyl)-1H-isoindol-1-one (CCD ID: 19X) (formula: C₂₀H₁₉ClN₆OS).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	S	0	0
			29	20	1	6	1	1		
2	B	1	Total	C	Cl	N	O	S	0	0
			29	20	1	6	1	1		

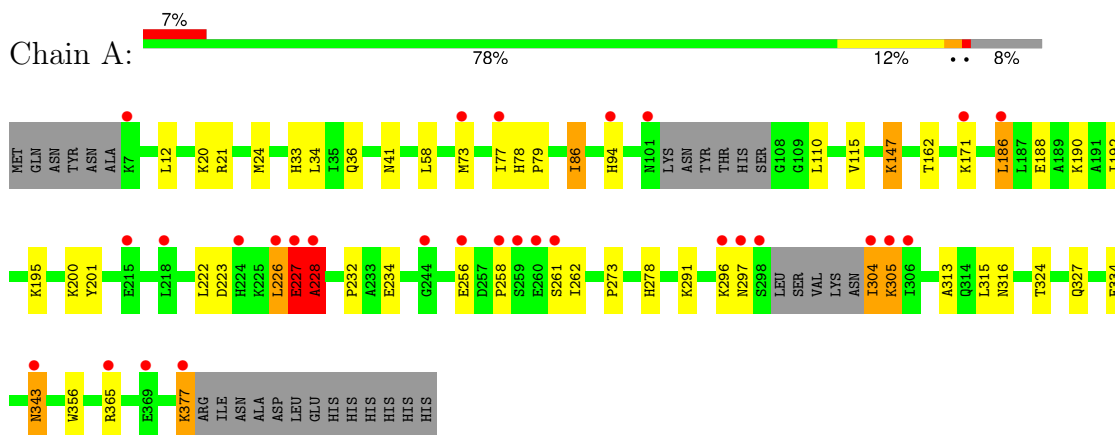
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	401	Total	O	0	0
			401	401		
3	B	172	Total	O	0	0
			172	172		

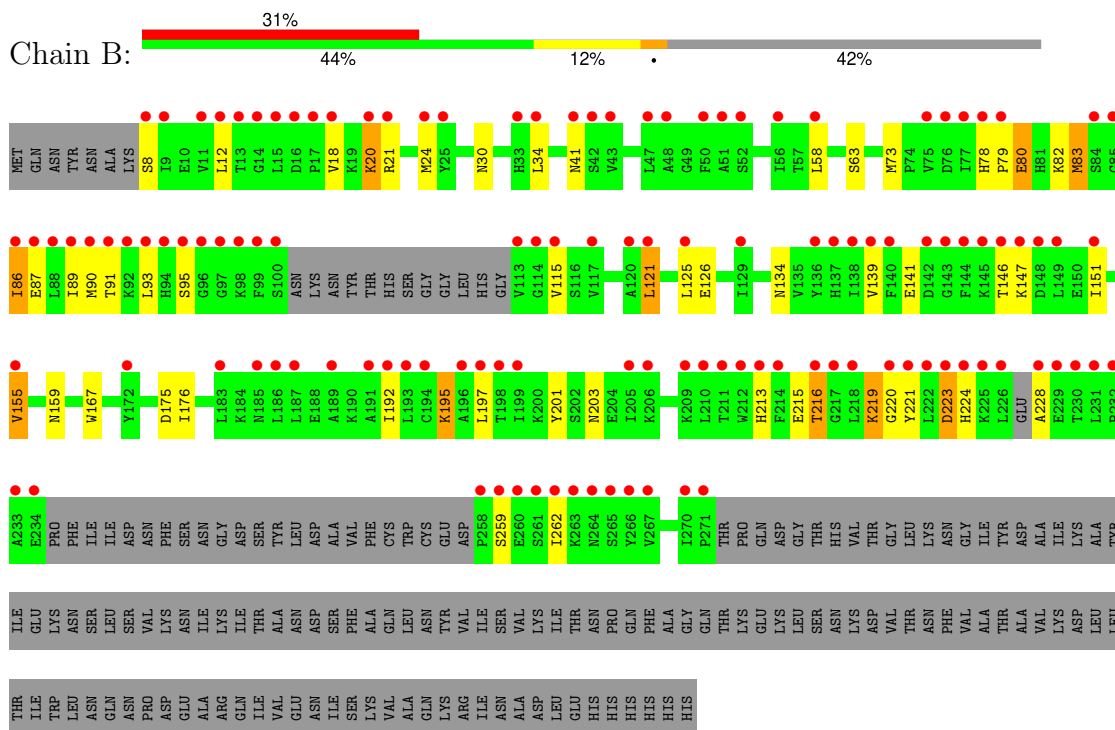
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Topoisomerase IV, subunit B



• Molecule 1: Topoisomerase IV, subunit B



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	44.16Å 130.28Å 80.27Å 90.00° 98.12° 90.00°	Depositor
Resolution (Å)	38.96 – 1.90 38.96 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (38.96-1.90) 99.3 (38.96-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.241 , 0.299 0.252 , 0.307	Depositor DCC
R_{free} test set	3546 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	30.7	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5292	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.20% 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: 19X

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	1.01	2/2916 (0.1%)	1.04	8/3939 (0.2%)
1	B	0.86	0/1837	0.90	0/2473
All	All	0.95	2/4753 (0.0%)	0.99	8/6412 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	33	HIS	CE1-NE2	6.56	1.39	1.32
1	A	192	ILE	N-CA	5.24	1.52	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	227	GLU	CA-C-N	6.18	132.82	121.70
1	A	227	GLU	C-N-CA	6.18	132.82	121.70
1	A	324	THR	N-CA-C	5.56	118.53	111.69
1	A	228	ALA	N-CA-C	5.43	126.20	111.00
1	A	313	ALA	N-CA-C	5.31	117.07	111.28
1	A	201	TYR	CA-CB-CG	5.21	123.27	113.90
1	A	188	GLU	N-CA-C	-5.11	105.79	111.36
1	A	297	ASN	N-CA-C	5.07	120.31	113.72

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	2855	0	2883	49	0
1	B	1806	0	1839	33	0
2	A	29	0	19	2	0
2	B	29	0	19	3	0
3	A	401	0	0	12	0
3	B	172	0	0	4	0
All	All	5292	0	4760	83	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 9.

All (83) 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:365:ARG:HD3	3:A:1823:HOH:O	1.56	1.03
1:A:343:ASN:HD22	1:A:343:ASN:H	1.05	0.98
1:A:227:GLU:HA	1:A:228:ALA:O	1.69	0.92
1:A:73:MET:HE1	1:A:86:ILE:HD12	1.54	0.89
1:A:73:MET:CE	1:A:86:ILE:HD12	2.04	0.87
1:A:256:GLU:O	1:A:258:PRO:HD3	1.77	0.84
1:A:73:MET:CE	1:A:86:ILE:CD1	2.58	0.81
1:A:343:ASN:H	1:A:343:ASN:ND2	1.69	0.76
1:B:21:ARG:HG2	1:B:21:ARG:HH11	1.52	0.74
1:A:73:MET:HE2	1:A:86:ILE:CD1	2.17	0.74
1:B:155:VAL:HG13	1:B:159:ASN:HB3	1.70	0.72
1:A:21:ARG:HB3	1:A:24[B]:MET:HG3	1.71	0.71
1:A:186:LEU:HD12	3:A:1574:HOH:O	1.92	0.69
1:A:262:ILE:H	1:A:316:ASN:HD22	1.41	0.68
1:A:73:MET:HE2	1:A:86:ILE:HD13	1.79	0.64
1:A:200:LYS:HE2	3:A:1677:HOH:O	1.96	0.64
1:A:343:ASN:HD22	1:A:343:ASN:N	1.86	0.63
1:A:73:MET:HG2	2:A:1401:19X:C8	2.29	0.62
1:B:213:HIS:HE1	1:B:215:GLU:OE1	1.83	0.62
1:A:36[B]:GLN:NE2	1:A:190:LYS:HZ3	1.97	0.61
1:B:78:HIS:HD2	3:B:1634:HOH:O	1.83	0.61
1:A:73:MET:CE	1:A:86:ILE:HD13	2.33	0.59
1:A:195:LYS:HE2	3:A:1709:HOH:O	2.02	0.59
1:A:262:ILE:H	1:A:316:ASN:ND2	2.01	0.58
1:A:73:MET:HE2	1:A:86:ILE:HD12	1.82	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36[B]:GLN:HE21	1:A:190:LYS:NZ	2.02	0.57
1:A:73:MET:HE1	1:A:86:ILE:CD1	2.28	0.56
1:A:226:LEU:O	1:A:227:GLU:C	2.48	0.56
1:A:261:SER:HA	1:A:316:ASN:HD21	1.71	0.55
1:B:216:THR:HB	1:B:219:LYS:HB3	1.87	0.55
1:B:79:PRO:O	1:B:80:GLU:HB2	2.06	0.55
1:A:304:ILE:N	3:A:1663:HOH:O	2.41	0.54
1:A:36[B]:GLN:NE2	1:A:190:LYS:NZ	2.56	0.54
2:B:1401:19X:H6	2:B:1401:19X:CL1	2.45	0.54
1:B:18:VAL:HG12	1:B:121:LEU:CD1	2.39	0.53
1:A:327:GLN:HG2	3:A:1653:HOH:O	2.08	0.53
1:A:377:LYS:HG3	3:A:1833:HOH:O	2.09	0.52
1:A:41:ASN:ND2	1:A:115:VAL:HG13	2.25	0.52
1:A:256:GLU:C	1:A:258:PRO:HD3	2.34	0.52
1:B:18:VAL:HG12	1:B:121:LEU:HD13	1.92	0.52
1:A:273:PRO:HD2	1:A:334:GLU:HB3	1.90	0.51
1:B:21:ARG:HB3	1:B:24:MET:HG2	1.93	0.51
1:B:91:THR:O	1:B:91:THR:HG22	2.12	0.50
1:A:20:LYS:NZ	3:A:1730:HOH:O	2.38	0.49
1:B:90:MET:HE2	1:B:115:VAL:HG23	1.94	0.49
1:A:36[A]:GLN:HG2	1:A:186:LEU:HD22	1.94	0.49
1:B:63:SER:HB3	1:B:167:TRP:CD1	2.48	0.49
1:A:115:VAL:HG11	2:A:1401:19X:CL1	2.50	0.48
1:A:227:GLU:HA	1:A:228:ALA:C	2.38	0.47
1:A:77:ILE:HD11	3:A:1609:HOH:O	2.13	0.47
1:B:83:MET:HE2	1:B:87:GLU:HG2	1.98	0.46
1:B:89:ILE:HD13	2:B:1401:19X:H14	1.98	0.46
1:B:195:LYS:HD3	1:B:195:LYS:H	1.81	0.46
1:B:220:GLY:HA2	1:B:223:ASP:OD1	2.16	0.45
1:B:82:LYS:HG2	3:B:1522:HOH:O	2.16	0.45
1:B:141:GLU:HB2	1:B:146:THR:HG21	1.99	0.44
1:B:79:PRO:O	1:B:80:GLU:CB	2.66	0.44
1:B:221:TYR:N	3:B:1571:HOH:O	2.51	0.44
1:A:78:HIS:HA	1:A:79:PRO:HD3	1.87	0.44
1:A:147[A]:LYS:HE3	1:A:147[A]:LYS:HB2	1.47	0.43
1:A:261:SER:HA	1:A:316:ASN:ND2	2.34	0.43
1:A:73:MET:HG3	1:A:162:THR:HG21	2.01	0.43
1:B:201:TYR:CZ	1:B:203:ASN:HB2	2.53	0.43
1:B:125:LEU:C	1:B:125:LEU:HD23	2.44	0.43
1:B:73:MET:SD	1:B:86:ILE:HD12	2.58	0.43
1:A:256:GLU:HG2	3:A:1691:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:ASN:HB3	3:A:1600:HOH:O	2.19	0.43
1:B:21:ARG:HG2	1:B:21:ARG:NH1	2.24	0.43
1:A:147[B]:LYS:HB3	1:A:147[B]:LYS:HE3	1.55	0.42
1:B:134:ASN:HB3	1:B:151:ILE:HG23	2.01	0.42
1:A:232:PRO:HB3	1:A:356:TRP:CZ2	2.55	0.42
1:B:30:ASN:HA	1:B:175:ASP:O	2.20	0.42
1:B:18:VAL:HG23	1:B:93:LEU:HD11	2.00	0.42
1:B:126:GLU:HG2	1:B:139:VAL:HG22	2.01	0.42
1:A:12:LEU:HD21	1:A:94:HIS:CD2	2.55	0.42
1:B:228:ALA:HB3	3:B:1563:HOH:O	2.20	0.41
1:B:197:LEU:O	1:B:213:HIS:HD2	2.03	0.41
1:A:200:LYS:CE	3:A:1677:HOH:O	2.64	0.41
1:A:305:LYS:HD3	1:A:305:LYS:O	2.21	0.41
1:B:20:LYS:HG2	1:B:21:ARG:HG3	2.02	0.40
1:B:41:ASN:HB3	2:B:1401:19X:CL1	2.58	0.40
1:B:139:VAL:HB	1:B:147:LYS:HB3	2.04	0.40
1:A:223:ASP:O	1:A:227:GLU:HG2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	357/390 (92%)	344 (96%)	11 (3%)	2 (1%)	21	13
1	B	220/390 (56%)	207 (94%)	11 (5%)	2 (1%)	14	6
All	All	577/780 (74%)	551 (96%)	22 (4%)	4 (1%)	18	10

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	228	ALA

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Mol	Chain	Res	Type
1	B	80	GLU
1	B	259	SER
1	A	227	GLU

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	319/344 (93%)	299 (94%)	20 (6%)	16	8
1	B	202/344 (59%)	184 (91%)	18 (9%)	9	4
All	All	521/688 (76%)	483 (93%)	38 (7%)	13	6

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LEU
1	A	58	LEU
1	A	86	ILE
1	A	110	LEU
1	A	147[A]	LYS
1	A	147[B]	LYS
1	A	171	LYS
1	A	186	LEU
1	A	222	LEU
1	A	226	LEU
1	A	227	GLU
1	A	234	GLU
1	A	278	HIS
1	A	291	LYS
1	A	296	LYS
1	A	304	ILE
1	A	305	LYS
1	A	315	LEU
1	A	343	ASN
1	A	377	LYS

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Mol	Chain	Res	Type
1	B	8	SER
1	B	12	LEU
1	B	20	LYS
1	B	34	LEU
1	B	58	LEU
1	B	83	MET
1	B	86	ILE
1	B	95	SER
1	B	121	LEU
1	B	155	VAL
1	B	176	ILE
1	B	192	ILE
1	B	195	LYS
1	B	216	THR
1	B	219	LYS
1	B	223	ASP
1	B	224	HIS
1	B	262	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	HIS
1	A	94	HIS
1	A	134	ASN
1	A	137	HIS
1	A	154	ASN
1	A	224	HIS
1	A	316	ASN
1	A	343	ASN
1	B	36	GLN
1	B	78	HIS
1	B	81	HIS
1	B	134	ASN
1	B	154	ASN
1	B	213	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	19X	A	1401	-	33,33,33	3.23	12 (36%)	36,49,49	3.19	20 (55%)
2	19X	B	1401	-	33,33,33	3.47	11 (33%)	36,49,49	3.12	19 (52%)

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
2	19X	A	1401	-	-	2/10/28/28	0/5/5/5
2	19X	B	1401	-	-	1/10/28/28	0/5/5/5

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1401	19X	C4-C5	13.08	1.47	1.35
2	A	1401	19X	C4-C5	12.25	1.46	1.35
2	B	1401	19X	C3-C8	6.73	1.51	1.41
2	B	1401	19X	C3-C2	6.15	1.49	1.41
2	A	1401	19X	C3-C2	5.64	1.48	1.41
2	B	1401	19X	C10-S19	-5.28	1.68	1.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1401	19X	C26-N27	5.25	1.49	1.33
2	A	1401	19X	C3-C8	5.23	1.49	1.41
2	B	1401	19X	C26-N27	5.21	1.49	1.33
2	A	1401	19X	C20-S19	-4.02	1.70	1.77
2	B	1401	19X	C22-C23	4.00	1.47	1.41
2	B	1401	19X	C20-S19	-3.90	1.70	1.77
2	A	1401	19X	C23-C26	3.90	1.46	1.42
2	A	1401	19X	C22-C23	3.86	1.47	1.41
2	B	1401	19X	C23-C26	3.83	1.46	1.42
2	A	1401	19X	O29-C28	3.74	1.29	1.23
2	A	1401	19X	C10-S19	-3.69	1.70	1.76
2	B	1401	19X	O29-C28	3.22	1.29	1.23
2	B	1401	19X	C4-CL1	3.01	1.80	1.74
2	A	1401	19X	C5-N1	-2.93	1.33	1.38
2	A	1401	19X	C4-CL1	2.46	1.79	1.74
2	B	1401	19X	C6-C5	2.09	1.53	1.50
2	A	1401	19X	C6-C5	2.02	1.52	1.50

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1401	19X	C21-C22-C28	6.61	135.94	128.88
2	A	1401	19X	C3-C2-N11	-6.42	116.44	126.54
2	B	1401	19X	C3-C2-N11	-6.34	116.57	126.54
2	A	1401	19X	C6-C5-N1	6.25	130.41	121.45
2	B	1401	19X	C10-S19-C20	5.73	113.14	102.76
2	A	1401	19X	C8-C3-C2	5.67	120.25	115.61
2	A	1401	19X	C21-C22-C28	5.53	134.79	128.88
2	B	1401	19X	C6-C5-N1	5.17	128.86	121.45
2	A	1401	19X	C3-C8-N9	-5.13	115.07	123.53
2	B	1401	19X	C8-C3-C2	4.98	119.68	115.61
2	B	1401	19X	C3-C8-N9	-4.97	115.34	123.53
2	A	1401	19X	C23-C26-N27	-4.65	103.78	112.12
2	B	1401	19X	C23-C26-N27	-4.52	104.01	112.12
2	A	1401	19X	C10-S19-C20	4.51	110.92	102.76
2	A	1401	19X	C22-C23-C26	3.87	112.55	107.41
2	A	1401	19X	C22-C21-C20	-3.86	115.84	120.74
2	A	1401	19X	C10-N9-C8	3.79	122.21	112.29
2	B	1401	19X	C22-C23-C26	3.73	112.36	107.41
2	B	1401	19X	C10-N9-C8	3.72	122.03	112.29
2	B	1401	19X	C22-C21-C20	-3.70	116.05	120.74
2	B	1401	19X	C3-C2-N1	3.69	112.42	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1401	19X	C21-C22-C23	3.63	124.00	120.20
2	A	1401	19X	C5-C4-CL1	-3.56	120.17	127.66
2	B	1401	19X	C25-C24-C23	-3.55	116.95	121.74
2	A	1401	19X	C25-C24-C23	-3.55	116.95	121.74
2	A	1401	19X	C3-C2-N1	3.49	112.24	109.24
2	B	1401	19X	C24-C23-C26	-3.37	128.06	135.71
2	B	1401	19X	C3-C8-N13	3.15	127.67	122.08
2	A	1401	19X	C3-C8-N13	3.11	127.61	122.08
2	A	1401	19X	C24-C23-C26	-3.10	128.66	135.71
2	A	1401	19X	O29-C28-C22	-2.71	118.99	122.62
2	A	1401	19X	N1-C2-N11	2.70	131.32	125.30
2	B	1401	19X	C21-C22-C23	2.69	123.01	120.20
2	B	1401	19X	C22-C28-N27	2.62	114.26	109.58
2	A	1401	19X	C22-C28-N27	2.60	114.22	109.58
2	B	1401	19X	N1-C2-N11	2.56	131.01	125.30
2	A	1401	19X	C24-C25-C20	2.41	123.26	120.48
2	B	1401	19X	C10-N11-C2	2.39	122.08	117.54
2	B	1401	19X	C5-C4-CL1	-2.37	122.68	127.66

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1401	19X	C25-C20-S19-C10
2	A	1401	19X	C21-C20-S19-C10
2	B	1401	19X	C25-C20-S19-C10

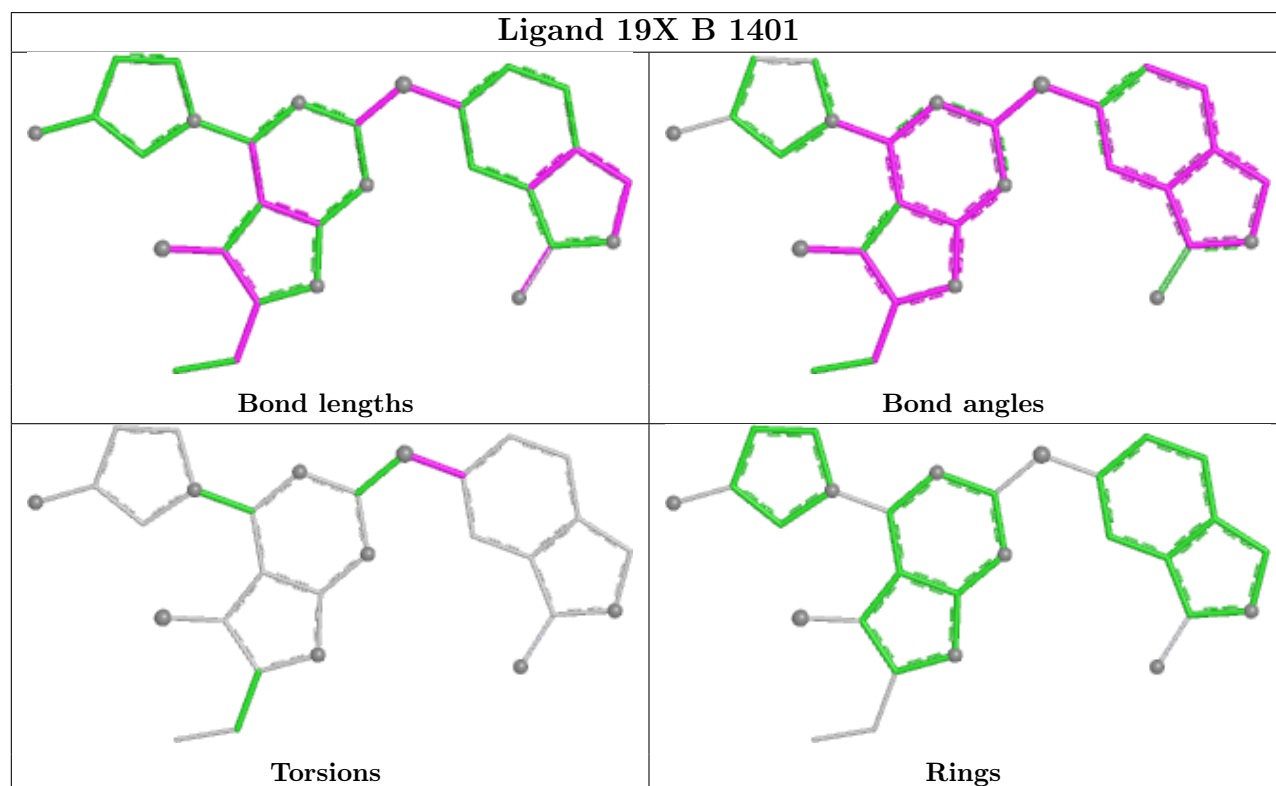
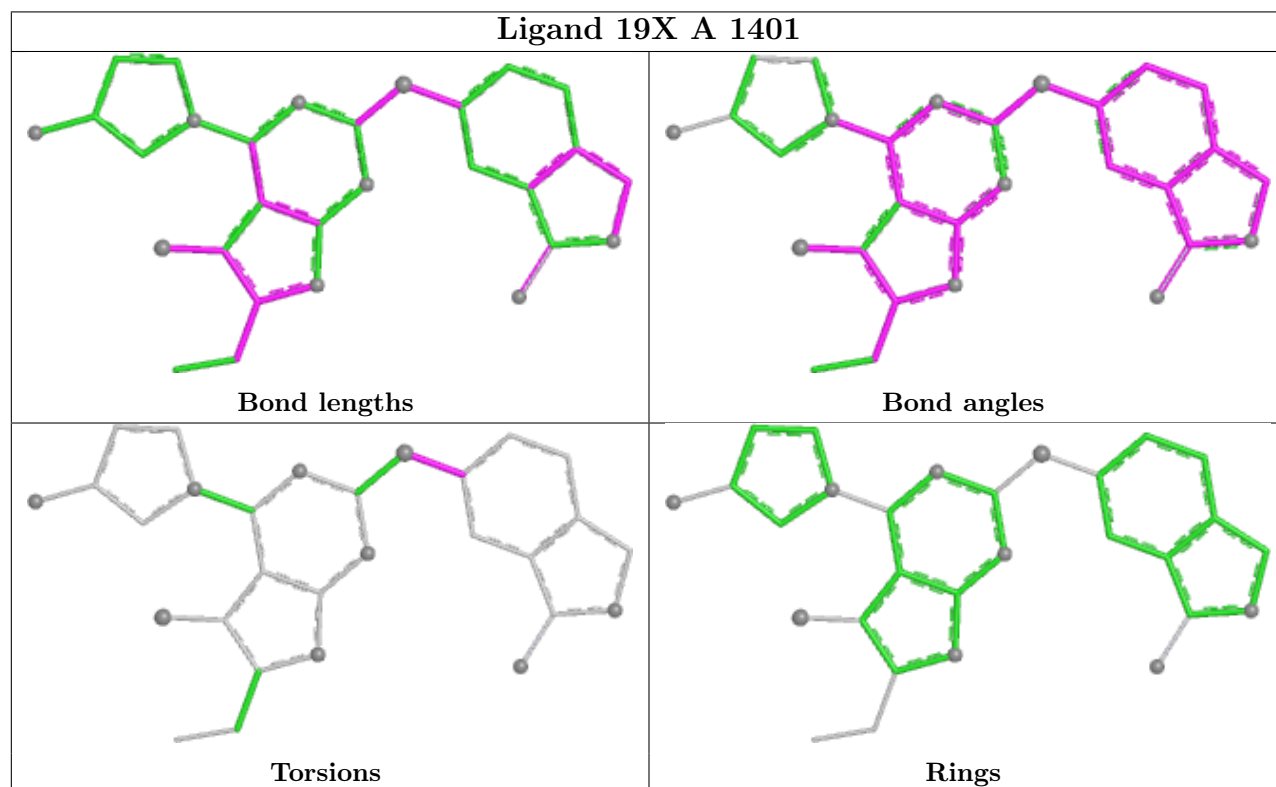
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1401	19X	2	0
2	B	1401	19X	3	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	360/390 (92%)	0.76	29 (8%) 18 19	18, 33, 55, 77	3 (0%)
1	B	228/390 (58%)	2.31	122 (53%) 0 0	30, 51, 83, 113	0
All	All	588/780 (75%)	1.36	151 (25%) 1 1	18, 38, 73, 113	3 (0%)

All (151) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	267	VAL	6.9
1	B	224	HIS	5.8
1	B	93	LEU	5.4
1	B	218	LEU	5.1
1	B	113	VAL	5.1
1	B	233	ALA	5.0
1	B	221	TYR	4.9
1	B	24	MET	4.9
1	B	77	ILE	4.8
1	B	258	PRO	4.8
1	B	144	PHE	4.7
1	B	99	PHE	4.7
1	B	222	LEU	4.7
1	B	94	HIS	4.5
1	B	25	TYR	4.5
1	B	196	ALA	4.3
1	B	96	GLY	4.3
1	B	220	GLY	4.2
1	B	214	PHE	4.1
1	B	15	LEU	4.1
1	B	228	ALA	4.1
1	B	12	LEU	4.1
1	B	13	THR	4.0
1	B	260	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	100	SER	4.0
1	B	217	GLY	4.0
1	B	231	LEU	4.0
1	B	98	LYS	3.9
1	B	18	VAL	3.9
1	B	226	LEU	3.9
1	B	192	ILE	3.9
1	B	11	VAL	3.8
1	B	186	LEU	3.7
1	B	262	ILE	3.7
1	A	227	GLU	3.7
1	B	230	THR	3.7
1	B	146	THR	3.7
1	A	258	PRO	3.6
1	B	9	ILE	3.5
1	B	140	PHE	3.5
1	B	47	LEU	3.5
1	B	265	SER	3.5
1	A	304	ILE	3.5
1	B	205	ILE	3.5
1	B	86	ILE	3.4
1	B	85	GLY	3.4
1	B	193	LEU	3.4
1	B	225	LYS	3.4
1	A	228	ALA	3.4
1	B	91	THR	3.4
1	A	377	LYS	3.3
1	B	194	CYS	3.3
1	B	232	PRO	3.3
1	B	84	SER	3.3
1	B	88	LEU	3.2
1	B	136	TYR	3.2
1	B	78	HIS	3.1
1	B	48	ALA	3.1
1	B	199	ILE	3.1
1	B	234	GLU	3.1
1	B	271	PRO	3.1
1	B	89	ILE	3.0
1	B	115	VAL	3.0
1	B	198	THR	3.0
1	B	114	GLY	3.0
1	B	50	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	197	LEU	2.9
1	B	87	GLU	2.9
1	B	79	PRO	2.9
1	B	143	GLY	2.9
1	B	145	LYS	2.8
1	B	56	ILE	2.8
1	B	138	ILE	2.8
1	A	256	GLU	2.8
1	B	139	VAL	2.8
1	A	298	SER	2.8
1	B	191	ALA	2.8
1	B	155	VAL	2.8
1	B	76	ASP	2.7
1	A	365	ARG	2.7
1	B	189	ALA	2.7
1	B	261	SER	2.7
1	B	211	THR	2.7
1	B	52	SER	2.7
1	B	209	LYS	2.7
1	B	117	VAL	2.7
1	A	261	SER	2.6
1	B	185	ASN	2.6
1	B	97	GLY	2.6
1	A	343	ASN	2.6
1	B	172	TYR	2.6
1	B	210	LEU	2.6
1	A	297	ASN	2.6
1	B	259	SER	2.6
1	B	34	LEU	2.5
1	B	58	LEU	2.5
1	B	187	LEU	2.5
1	B	212	TRP	2.5
1	A	260	GLU	2.5
1	A	171	LYS	2.5
1	B	20	LYS	2.5
1	B	121	LEU	2.5
1	B	75	VAL	2.5
1	B	223	ASP	2.5
1	B	14	GLY	2.5
1	A	306	ILE	2.5
1	B	147	LYS	2.5
1	B	149	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	213	HIS	2.4
1	B	206	LYS	2.4
1	B	92	LYS	2.4
1	B	33	HIS	2.4
1	B	8	SER	2.4
1	B	183	LEU	2.4
1	B	216	THR	2.4
1	A	94	HIS	2.4
1	B	263	LYS	2.4
1	B	41	ASN	2.3
1	A	305	LYS	2.3
1	B	43	VAL	2.3
1	B	148	ASP	2.3
1	B	125	LEU	2.3
1	B	95	SER	2.3
1	B	270	ILE	2.3
1	A	259	SER	2.3
1	B	42	SER	2.3
1	B	21	ARG	2.2
1	A	215	GLU	2.2
1	B	264	ASN	2.2
1	B	229	GLU	2.2
1	A	244	GLY	2.2
1	B	151	ILE	2.2
1	A	101	ASN	2.2
1	A	218	LEU	2.2
1	B	120	ALA	2.2
1	A	73	MET	2.2
1	A	186	LEU	2.2
1	B	17	PRO	2.2
1	B	129	ILE	2.1
1	B	16	ASP	2.1
1	B	90	MET	2.1
1	B	137	HIS	2.1
1	A	224	HIS	2.1
1	A	226	LEU	2.1
1	B	51	ALA	2.1
1	A	369	GLU	2.1
1	A	7	LYS	2.0
1	A	77	ILE	2.0
1	A	296	LYS	2.0
1	B	142	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	266	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

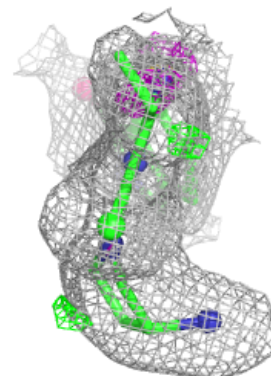
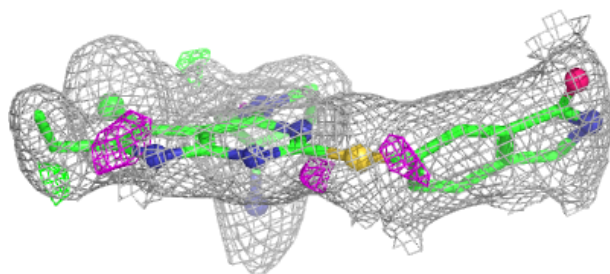
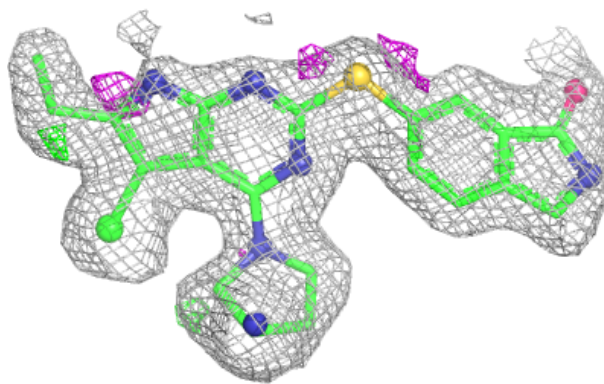
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	19X	B	1401	29/29	0.85	0.15	39,54,64,68	0
2	19X	A	1401	29/29	0.95	0.09	22,29,46,47	0

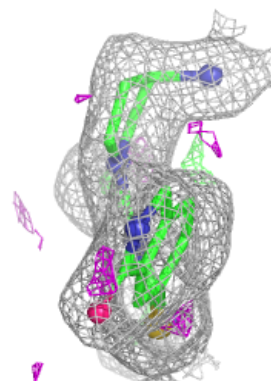
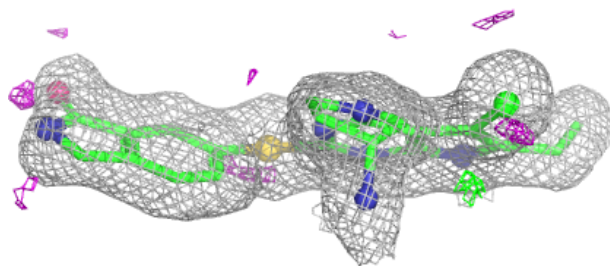
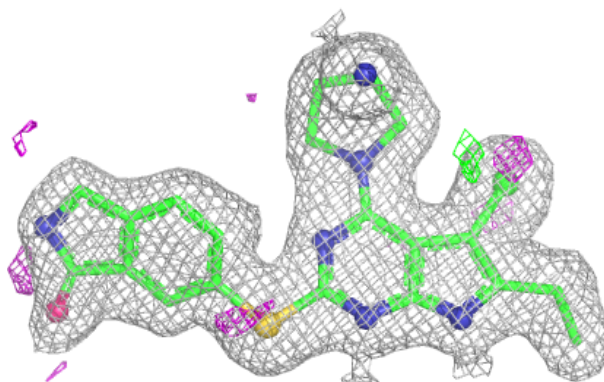
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 19X B 1401:

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

**Electron density around 19X A 1401:**

$2mF_o-DF_c$ (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.