



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 08:10 AM UTC

PDB ID : 5W14 / pdb_00005w14
Title : ADC-7 in complex with boronic acid transition state inhibitor S03043
Authors : Smolen, K.A.; Powers, R.A.; Wallar, B.J.
Deposited on : 2017-06-01
Resolution : 1.88 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

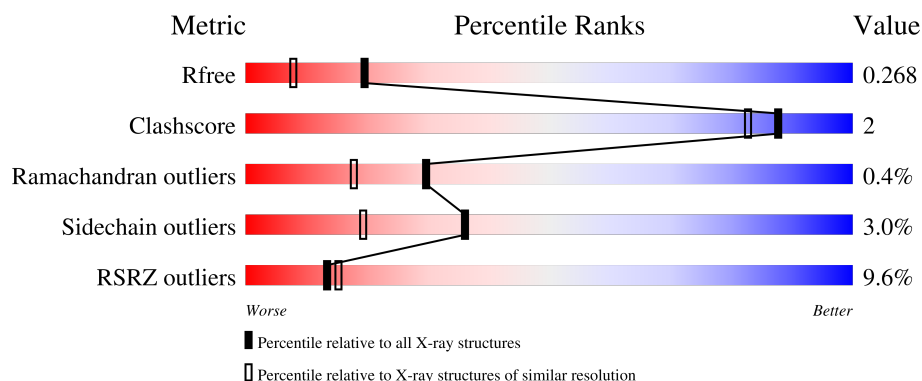
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.88 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	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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	361	12% 86% 11% ..
1	B	361	% 91% 7% ..
1	C	361	11% 89% 9% ..
1	D	361	14% 89% 9% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11693 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.

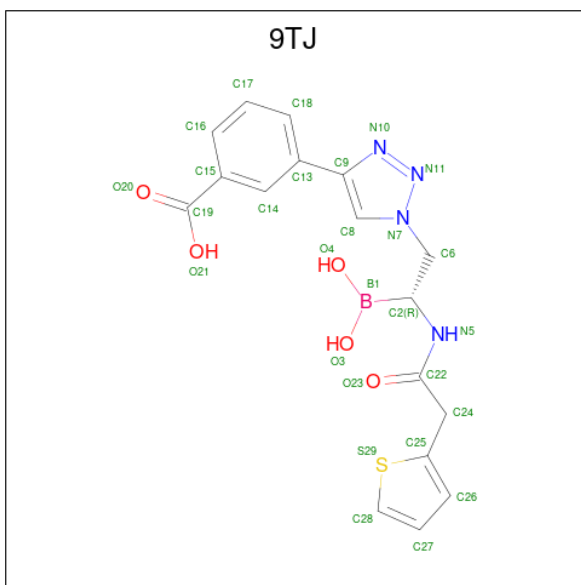
- Molecule 1 is a protein called Beta-lactamase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	356	Total	C	N	O	S	0	1	0
			2738	1761	452	516	9			
1	B	359	Total	C	N	O	S	0	0	0
			2829	1816	468	536	9			
1	C	357	Total	C	N	O	S	0	0	0
			2744	1765	455	515	9			
1	D	352	Total	C	N	O	S	0	0	0
			2672	1721	443	499	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP Q6DRA1
B	-1	MET	-	initiating methionine	UNP Q6DRA1
C	-1	MET	-	initiating methionine	UNP Q6DRA1
D	-1	MET	-	initiating methionine	UNP Q6DRA1

- Molecule 2 is 3-{1-[(2R)-2-borono-2-[[[(thiophen-2-yl)acetyl]amino]ethyl]-1H-1,2,3-triazol-4-yl]benzoic acid (CCD ID: 9TJ) (formula: C₁₇H₁₇BN₄O₅S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 28	B 1	C 17	N 4	O 5	S 1	0	0
2	B	1	Total 28	B 1	C 17	N 4	O 5	S 1	0	0
2	C	1	Total 28	B 1	C 17	N 4	O 5	S 1	0	0
2	D	1	Total 28	B 1	C 17	N 4	O 5	S 1	0	0

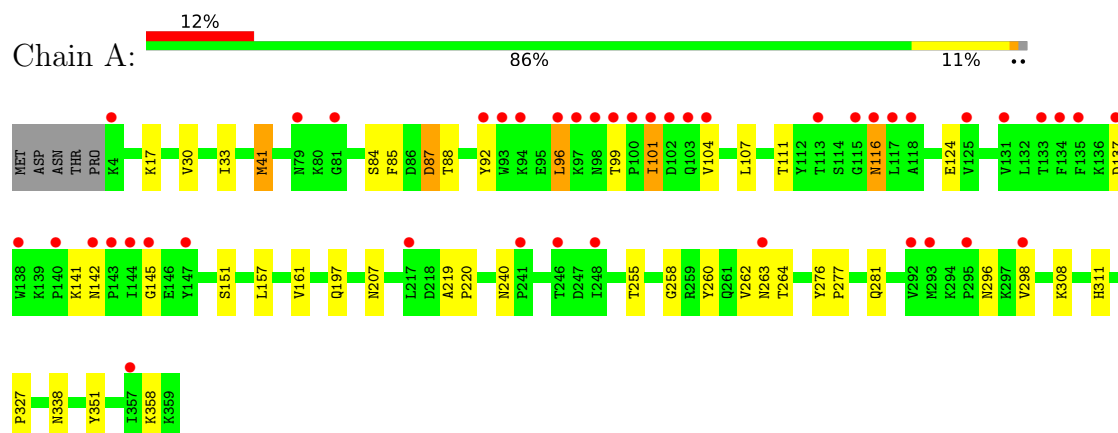
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	125	Total	O	0	4
			129	129		
3	B	257	Total	O	0	5
			262	262		
3	C	129	Total	O	0	0
			129	129		
3	D	78	Total	O	0	0
			78	78		

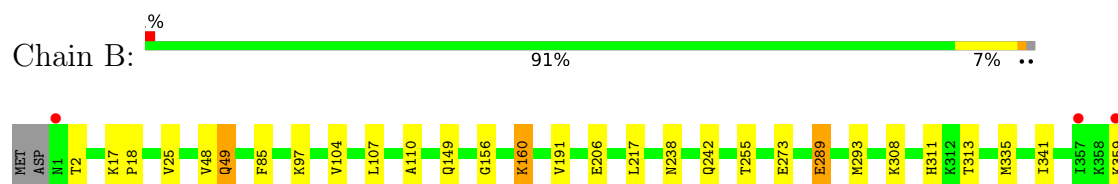
3 Residue-property plots [i](#)

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.

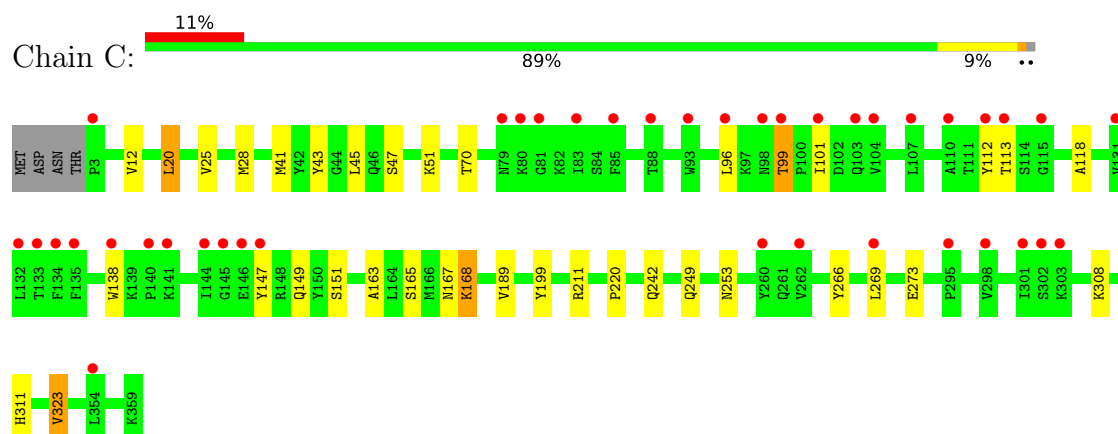
• Molecule 1: Beta-lactamase



• Molecule 1: Beta-lactamase

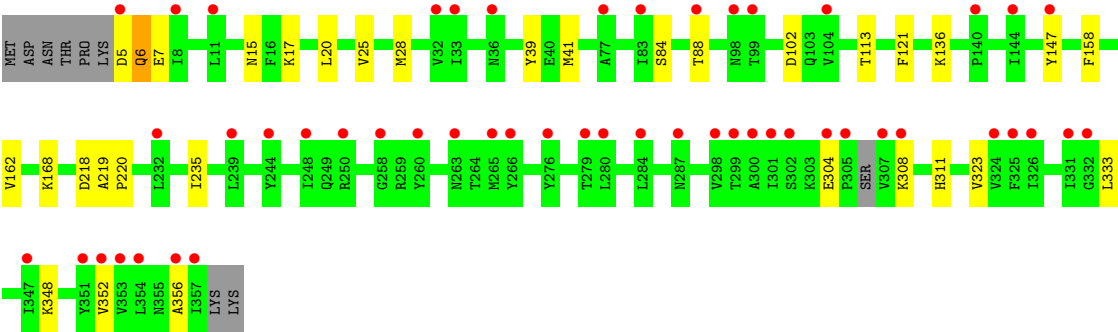


• Molecule 1: Beta-lactamase



• Molecule 1: Beta-lactamase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	89.01Å 81.30Å 106.44Å 90.00° 112.70° 90.00°	Depositor
Resolution (Å)	50.00 – 1.88 50.00 – 1.88	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.00-1.88) 99.7 (50.00-1.88)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 1.88Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.202 , 0.256 (Not available) , 0.268	Depositor DCC
R_{free} test set	5673 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	26.8	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.016 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11693	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.40 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.1905e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: 9TJ

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	1.30	7/2805 (0.2%)	1.20	9/3823 (0.2%)
1	B	1.34	7/2897 (0.2%)	1.17	9/3936 (0.2%)
1	C	1.17	3/2812 (0.1%)	1.08	9/3837 (0.2%)
1	D	1.10	1/2738 (0.0%)	1.13	10/3736 (0.3%)
All	All	1.23	18/11252 (0.2%)	1.15	37/15332 (0.2%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	25	VAL	N-CA	7.41	1.51	1.46
1	B	110	ALA	N-CA	6.91	1.54	1.46
1	D	308	LYS	CA-C	6.38	1.60	1.52
1	A	255	THR	CA-C	-5.82	1.44	1.52
1	B	104	VAL	C-O	-5.67	1.17	1.24
1	B	242	GLN	N-CA	5.66	1.53	1.46
1	A	262	VAL	CA-C	-5.57	1.46	1.52
1	A	104	VAL	N-CA	5.53	1.52	1.46
1	C	47	SER	N-CA	5.38	1.52	1.46
1	C	253	ASN	N-CA	5.20	1.52	1.46
1	A	30	VAL	CA-CB	-5.16	1.48	1.54
1	B	255	THR	N-CA	5.10	1.52	1.46
1	B	335	MET	N-CA	5.08	1.52	1.46
1	C	189	VAL	C-O	5.06	1.29	1.24
1	A	240	ASN	N-CA	5.04	1.52	1.46
1	B	313	THR	C-O	5.04	1.30	1.23
1	A	17	LYS	CA-C	5.01	1.59	1.52
1	A	258	GLY	N-CA	5.00	1.50	1.45

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	49	GLN	CB-CA-C	-7.57	98.70	110.81
1	D	17	LYS	CA-C-N	-7.14	112.35	119.56
1	D	17	LYS	C-N-CA	-7.14	112.35	119.56
1	A	145	GLY	N-CA-C	-6.82	106.05	114.92
1	A	151	SER	N-CA-C	6.36	119.07	108.13
1	A	351	TYR	N-CA-C	6.33	118.74	111.02
1	A	116	ASN	N-CA-C	6.21	118.96	107.60
1	D	121	PHE	CA-C-N	-6.16	113.44	119.78
1	D	121	PHE	C-N-CA	-6.16	113.44	119.78
1	D	6	GLN	N-CA-C	6.08	123.75	110.80
1	A	298	VAL	N-CA-C	6.00	117.42	108.23
1	B	238	ASN	N-CA-C	5.92	118.68	111.82
1	D	25	VAL	CA-C-N	-5.90	112.42	118.85
1	D	25	VAL	C-N-CA	-5.90	112.42	118.85
1	D	168	LYS	CA-C-N	-5.85	113.66	119.92
1	D	168	LYS	C-N-CA	-5.85	113.66	119.92
1	B	191	VAL	N-CA-C	-5.74	103.69	108.63
1	C	45	LEU	CA-C-N	5.67	128.34	120.29
1	C	45	LEU	C-N-CA	5.67	128.34	120.29
1	A	33	ILE	CB-CA-C	5.62	118.95	110.63
1	C	25	VAL	CA-C-N	-5.60	112.74	118.85
1	C	25	VAL	C-N-CA	-5.60	112.74	118.85
1	A	281	GLN	N-CA-C	5.59	117.38	111.28
1	C	323	VAL	N-CA-CB	-5.57	102.30	111.44
1	C	168	LYS	CA-C-N	-5.48	114.05	119.92
1	C	168	LYS	C-N-CA	-5.48	114.05	119.92
1	C	99	THR	CA-C-N	5.47	125.30	119.28
1	C	99	THR	C-N-CA	5.47	125.30	119.28
1	D	218	ASP	N-CA-C	5.42	117.19	111.28
1	A	240	ASN	CB-CA-C	-5.39	103.98	111.41
1	A	264	THR	N-CA-C	5.37	119.31	112.87
1	B	2	THR	CA-C-N	-5.34	114.26	119.76
1	B	2	THR	C-N-CA	-5.34	114.26	119.76
1	B	48	VAL	CA-C-N	5.14	127.48	120.54
1	B	48	VAL	C-N-CA	5.14	127.48	120.54
1	B	341	ILE	CA-C-N	-5.00	114.80	119.90
1	B	341	ILE	C-N-CA	-5.00	114.80	119.90

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	2738	0	2635	13	0
1	B	2829	0	2799	6	0
1	C	2744	0	2633	13	0
1	D	2672	0	2542	12	0
2	A	28	0	0	0	0
2	B	28	0	0	0	0
2	C	28	0	0	0	0
2	D	28	0	0	0	0
3	A	129	0	0	0	0
3	B	262	0	0	1	0
3	C	129	0	0	0	0
3	D	78	0	0	0	0
All	All	11693	0	10609	44	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 2.

All (44) 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:D:235:ILE:HD11	1:D:323:VAL:HG13	1.47	0.96
1:A:87:ASP:OD2	1:A:92:TYR:OH	2.01	0.77
1:C:113:THR:HA	1:C:147:TYR:O	1.88	0.72
1:D:235:ILE:HD11	1:D:323:VAL:CG1	2.23	0.69
1:D:20:LEU:HD11	1:D:28:MET:HE2	1.75	0.68
1:A:96:LEU:HD11	1:A:101:ILE:HG22	1.76	0.66
1:D:5:ASP:CB	1:D:39:TYR:CE1	2.82	0.62
1:A:111:THR:O	1:A:260:TYR:OH	2.17	0.61
1:B:289:GLU:OE1	1:B:293:MET:HG3	2.02	0.60
1:C:118:ALA:O	1:C:151:SER:OG	2.19	0.60
1:D:5:ASP:O	1:D:7:GLU:N	2.36	0.58
1:D:88:THR:CB	1:D:102:ASP:O	2.52	0.58
1:A:96:LEU:HD12	1:A:96:LEU:O	2.07	0.53
1:C:112:TYR:HB3	1:C:149:GLN:O	2.10	0.51
1:C:163:ALA:HB1	1:C:168:LYS:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:PHE:HB3	1:A:107:LEU:HB2	1.94	0.49
1:B:85:PHE:HB3	1:B:107:LEU:HB2	1.94	0.49
1:A:84:SER:O	1:A:87:ASP:HB2	2.13	0.48
1:D:20:LEU:CD1	1:D:28:MET:HE2	2.43	0.48
1:B:17:LYS:N	1:B:18:PRO:CD	2.78	0.47
1:B:273:GLU:OE2	1:B:308:LYS:HG2	2.16	0.46
1:A:276:TYR:CD1	1:A:277:PRO:HA	2.50	0.46
1:A:96:LEU:CD1	1:A:99:THR:CB	2.94	0.45
1:C:199:TYR:CZ	1:C:211:ARG:HD3	2.52	0.45
1:A:116:ASN:HB2	1:A:141:LYS:HB3	1.99	0.45
1:C:70:THR:OG1	1:C:220:PRO:O	2.17	0.44
1:B:156:GLY:C	1:B:217:LEU:HD13	2.43	0.44
1:C:20:LEU:HD21	1:C:28:MET:HE2	1.99	0.44
1:C:242:GLN:HA	1:C:249:GLN:OE1	2.17	0.44
1:C:12:VAL:HG21	1:C:41:MET:HE3	2.00	0.44
1:D:113:THR:HA	1:D:147:TYR:O	2.18	0.43
1:A:96:LEU:HD13	1:A:99:THR:CB	2.49	0.43
1:C:96:LEU:O	1:C:99:THR:OG1	2.23	0.43
1:C:266:TYR:HB2	1:C:273:GLU:HB3	2.00	0.42
1:D:333:LEU:C	1:D:333:LEU:HD23	2.45	0.42
1:A:157:LEU:O	1:A:161:VAL:HG23	2.20	0.42
1:C:28:MET:HE3	1:C:43:TYR:CD2	2.55	0.42
1:D:158:PHE:O	1:D:162:VAL:HG23	2.20	0.41
1:A:219:ALA:HB3	1:A:220:PRO:HD3	2.03	0.41
1:A:41:MET:HE3	1:A:41:MET:HB2	1.97	0.41
1:D:219:ALA:HB3	1:D:220:PRO:HD3	2.02	0.41
1:C:101:ILE:HA	1:C:138:TRP:CZ3	2.56	0.40
1:B:160:LYS:HE3	3:B:646:HOH:O	2.20	0.40
1:D:15:ASN:OD1	1:D:352:VAL:HG23	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	355/361 (98%)	333 (94%)	19 (5%)	3 (1%)	16	5
1	B	357/361 (99%)	349 (98%)	8 (2%)	0	100	100
1	C	355/361 (98%)	343 (97%)	12 (3%)	0	100	100
1	D	348/361 (96%)	331 (95%)	14 (4%)	3 (1%)	14	4
All	All	1415/1444 (98%)	1356 (96%)	53 (4%)	6 (0%)	30	18

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	6	GLN
1	A	358	LYS
1	A	87	ASP
1	A	207	ASN
1	D	304	GLU
1	D	356	ALA

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	287/319 (90%)	273 (95%)	14 (5%)	22	7
1	B	309/319 (97%)	301 (97%)	8 (3%)	40	24
1	C	286/319 (90%)	278 (97%)	8 (3%)	38	22
1	D	273/319 (86%)	268 (98%)	5 (2%)	51	38
All	All	1155/1276 (90%)	1120 (97%)	35 (3%)	36	19

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	MET
1	A	88	THR
1	A	96	LEU
1	A	101	ILE
1	A	124	GLU

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Mol	Chain	Res	Type
1	A	137	ASP
1	A	142	ASN
1	A	197	GLN
1	A	263	ASN
1	A	296	ASN
1	A	308	LYS
1	A	311	HIS
1	A	327	PRO
1	A	338	ASN
1	B	49	GLN
1	B	97	LYS
1	B	149	GLN
1	B	160	LYS
1	B	206	GLU
1	B	289	GLU
1	B	311	HIS
1	B	359	LYS
1	C	20	LEU
1	C	51	LYS
1	C	165	SER
1	C	167	ASN
1	C	269	LEU
1	C	308	LYS
1	C	311	HIS
1	C	323	VAL
1	D	41	MET
1	D	84	SER
1	D	136	LYS
1	D	311	HIS
1	D	348	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	108	GLN
1	A	130	GLN
1	A	142	ASN
1	A	195	GLN
1	A	198	ASN
1	A	205	GLN
1	A	240	ASN

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Mol	Chain	Res	Type
1	A	287	ASN
1	A	296	ASN
1	A	330	ASN
1	A	338	ASN
1	A	343	ASN
1	B	205	GLN
1	C	36	ASN
1	C	149	GLN
1	C	195	GLN
1	C	198	ASN
1	C	240	ASN
1	C	290	GLN
1	D	195	GLN
1	D	198	ASN
1	D	290	GLN
1	D	296	ASN

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](#)

4 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	9TJ	A	401	1	27,30,30	1.42	3 (11%)	34,41,41	1.70	9 (26%)
2	9TJ	D	401	1	27,30,30	1.59	3 (11%)	34,41,41	1.70	10 (29%)
2	9TJ	B	401	1	27,30,30	1.85	6 (22%)	34,41,41	1.87	11 (32%)
2	9TJ	C	401	1	27,30,30	1.54	2 (7%)	34,41,41	1.30	5 (14%)

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	9TJ	A	401	1	-	0/18/24/24	0/3/3/3
2	9TJ	D	401	1	-	4/18/24/24	0/3/3/3
2	9TJ	B	401	1	-	4/18/24/24	0/3/3/3
2	9TJ	C	401	1	-	2/18/24/24	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	9TJ	N10-N11	6.24	1.42	1.32
2	D	401	9TJ	N10-N11	4.64	1.39	1.32
2	C	401	9TJ	N10-N11	4.53	1.39	1.32
2	A	401	9TJ	N10-N11	4.49	1.39	1.32
2	D	401	9TJ	N7-N11	4.06	1.41	1.34
2	B	401	9TJ	N7-N11	4.02	1.41	1.34
2	C	401	9TJ	N7-N11	3.89	1.41	1.34
2	B	401	9TJ	C8-C9	2.95	1.42	1.37
2	B	401	9TJ	C14-C15	2.25	1.42	1.39
2	A	401	9TJ	C15-C19	2.24	1.54	1.49
2	A	401	9TJ	C17-C16	2.13	1.42	1.38
2	B	401	9TJ	C15-C19	2.08	1.53	1.49
2	D	401	9TJ	C24-C22	2.07	1.54	1.51
2	B	401	9TJ	C16-C15	2.05	1.42	1.39

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	9TJ	O21-C19-C15	4.34	125.98	114.84
2	A	401	9TJ	C24-C25-S29	-3.94	113.77	122.11
2	B	401	9TJ	C24-C25-S29	-3.79	114.09	122.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	9TJ	C24-C25-S29	-3.54	114.61	122.11
2	A	401	9TJ	C6-N7-N11	-3.49	113.53	120.28
2	D	401	9TJ	C13-C9-C8	-3.41	124.44	129.65
2	A	401	9TJ	O21-C19-C15	3.37	123.49	114.84
2	B	401	9TJ	C24-C25-C26	3.24	136.02	126.56
2	D	401	9TJ	C24-C25-S29	-3.22	115.30	122.11
2	B	401	9TJ	C6-N7-N11	-3.19	114.12	120.28
2	B	401	9TJ	N7-N11-N10	-3.11	104.23	107.02
2	B	401	9TJ	C17-C18-C13	-2.94	117.48	120.36
2	B	401	9TJ	O21-C19-O20	-2.87	117.19	123.35
2	D	401	9TJ	C6-N7-N11	-2.84	114.79	120.28
2	D	401	9TJ	C18-C13-C9	2.83	124.04	120.87
2	A	401	9TJ	C6-N7-C8	2.83	135.23	129.27
2	D	401	9TJ	C14-C13-C9	-2.79	115.70	120.43
2	D	401	9TJ	C6-N7-C8	2.71	134.97	129.27
2	A	401	9TJ	O21-C19-O20	-2.65	117.65	123.35
2	D	401	9TJ	C24-C25-C26	2.52	133.93	126.56
2	A	401	9TJ	C24-C25-C26	2.48	133.79	126.56
2	C	401	9TJ	C24-C25-C26	2.46	133.76	126.56
2	A	401	9TJ	C17-C18-C13	-2.45	117.96	120.36
2	D	401	9TJ	C8-C9-N10	2.40	110.16	107.85
2	B	401	9TJ	C6-N7-C8	2.39	134.30	129.27
2	C	401	9TJ	C6-N7-C8	2.35	134.23	129.27
2	A	401	9TJ	N7-N11-N10	-2.35	104.91	107.02
2	B	401	9TJ	C18-C13-C9	-2.31	118.28	120.87
2	D	401	9TJ	C17-C18-C13	-2.28	118.12	120.36
2	B	401	9TJ	O23-C22-C24	-2.19	117.94	121.40
2	B	401	9TJ	C18-C13-C14	2.16	121.75	119.25
2	C	401	9TJ	C9-C8-N7	2.15	107.01	105.28
2	A	401	9TJ	C18-C13-C9	-2.11	118.51	120.87
2	D	401	9TJ	C13-C9-N10	2.07	125.37	122.05
2	C	401	9TJ	C6-N7-N11	-2.02	116.38	120.28

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	401	9TJ	C18-C13-C9-N10
2	D	401	9TJ	C14-C13-C9-N10
2	D	401	9TJ	C14-C13-C9-C8
2	D	401	9TJ	C18-C13-C9-C8
2	B	401	9TJ	C18-C13-C9-C8

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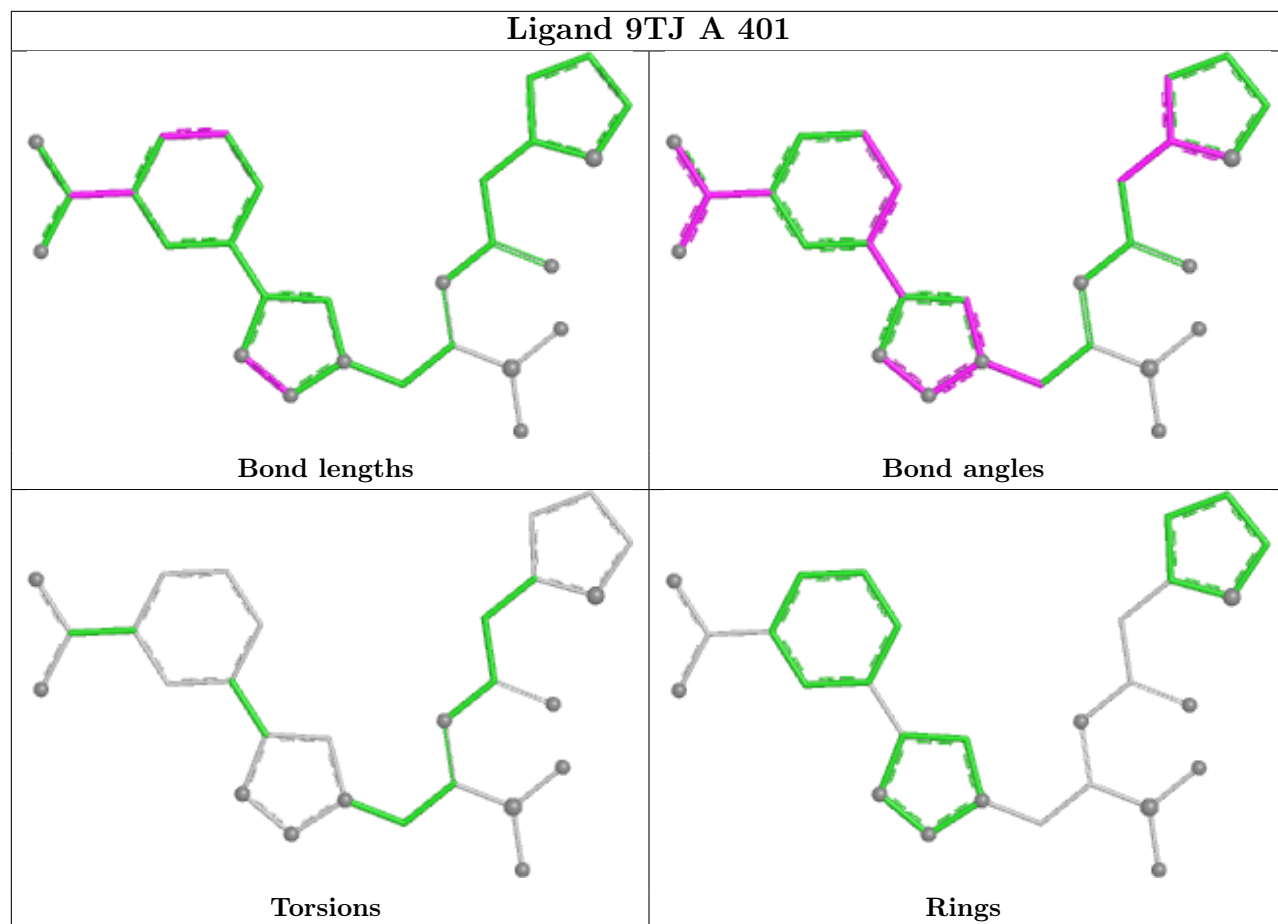
Mol	Chain	Res	Type	Atoms
2	B	401	9TJ	C14-C13-C9-C8
2	C	401	9TJ	C6-C2-N5-C22
2	B	401	9TJ	C18-C13-C9-N10
2	B	401	9TJ	C14-C13-C9-N10
2	C	401	9TJ	C18-C13-C9-N10

There are no ring outliers.

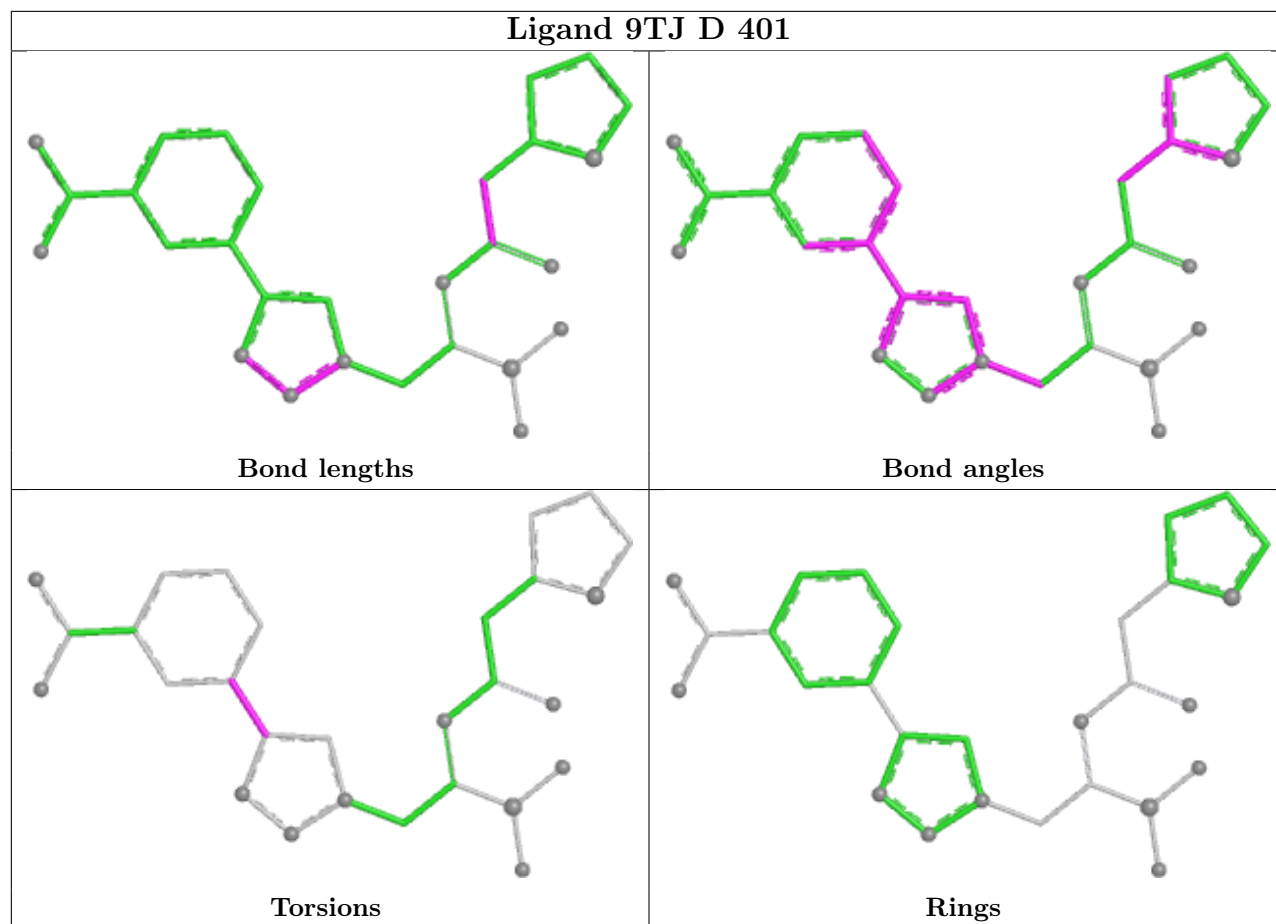
No monomer is involved in short contacts.

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.

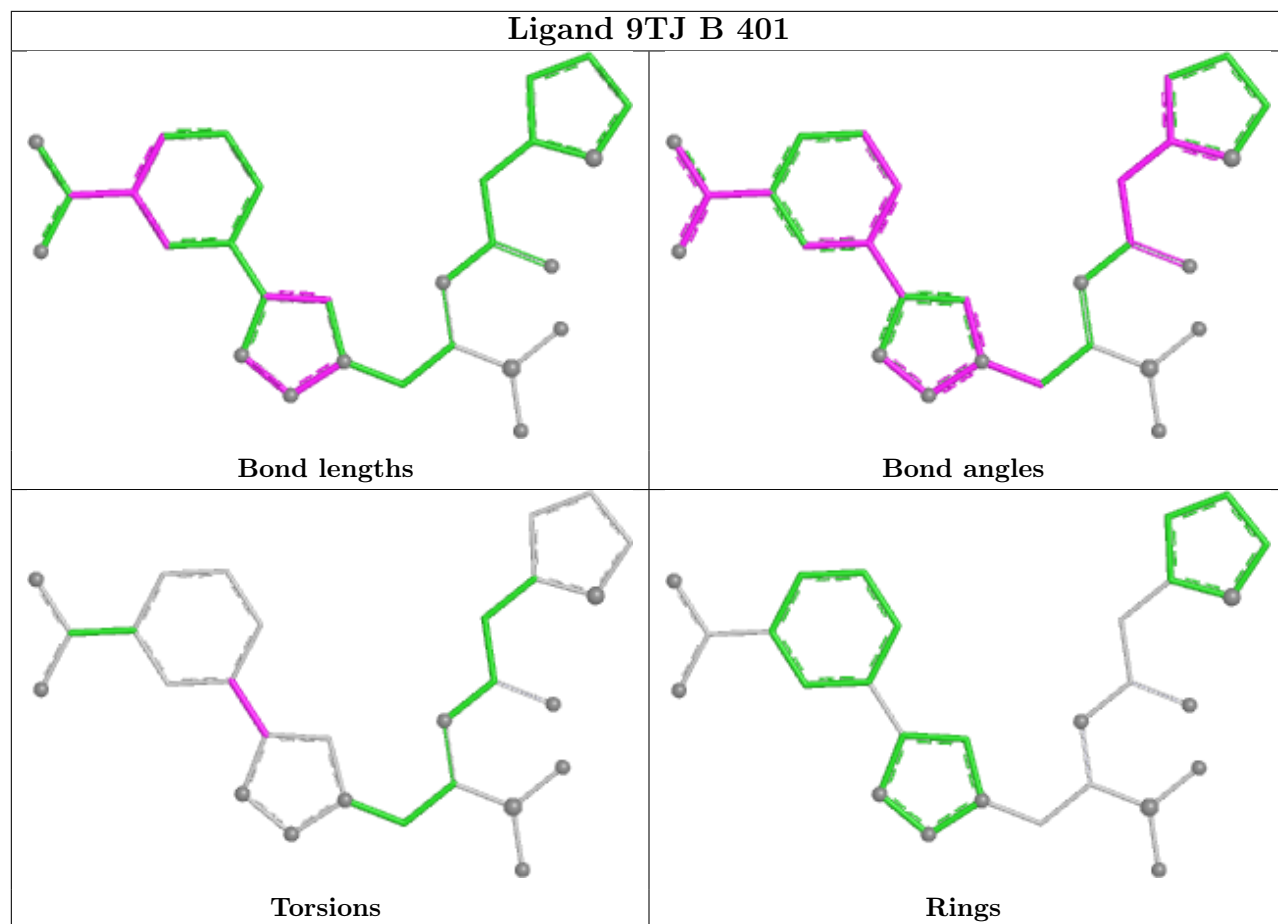
Ligand 9TJ A 401

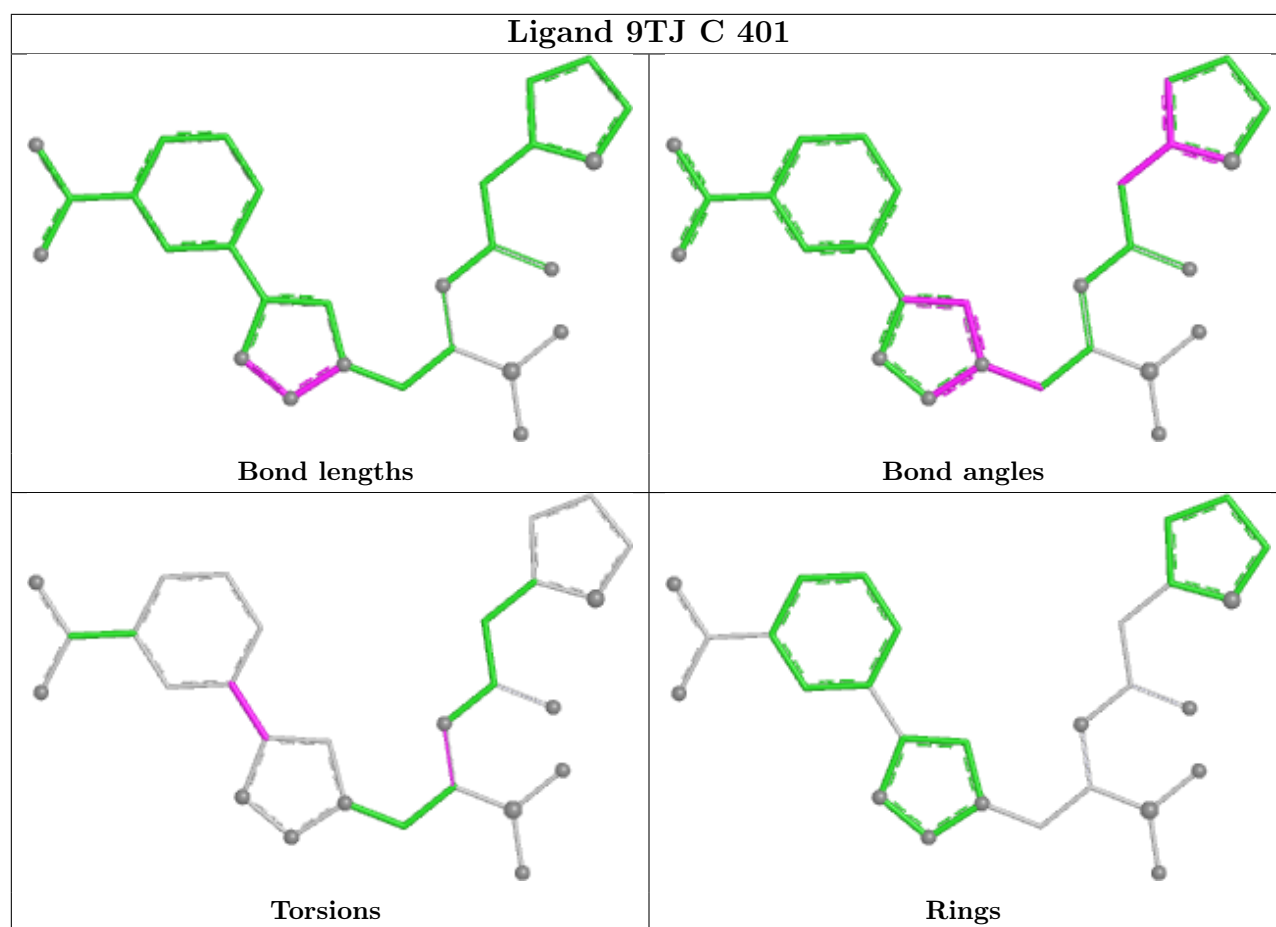


Ligand 9TJ D 401



Ligand 9TJ B 401





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	356/361 (98%)	0.74	43 (12%) 8 9	13, 34, 58, 80	1 (0%)
1	B	359/361 (99%)	-0.14	3 (0%) 82 86	17, 25, 40, 66	0
1	C	357/361 (98%)	0.78	40 (11%) 10 12	20, 39, 63, 74	0
1	D	352/361 (97%)	1.05	51 (14%) 6 6	21, 44, 60, 84	0
All	All	1424/1444 (98%)	0.60	137 (9%) 13 15	13, 35, 59, 84	1 (0%)

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	356	ALA	5.8
1	A	138	TRP	5.2
1	D	352	VAL	5.2
1	A	131	VAL	4.4
1	D	307	VAL	4.1
1	A	135	PHE	4.1
1	C	144	ILE	4.0
1	A	134	PHE	4.0
1	D	301	ILE	4.0
1	A	96	LEU	3.7
1	D	266	TYR	3.7
1	A	92	TYR	3.7
1	A	144	ILE	3.6
1	A	101	ILE	3.6
1	A	117	LEU	3.6
1	A	93	TRP	3.5
1	A	104	VAL	3.5
1	C	132	LEU	3.5
1	A	143	PRO	3.5
1	C	3	PRO	3.5
1	A	115	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	141	LYS	3.5
1	C	145	GLY	3.3
1	D	331	ILE	3.3
1	A	133	THR	3.3
1	D	357	ILE	3.3
1	C	138	TRP	3.3
1	D	284	LEU	3.2
1	A	99	THR	3.2
1	A	147	TYR	3.2
1	C	101	ILE	3.1
1	D	276	TYR	3.1
1	C	140	PRO	3.1
1	D	83	ILE	3.0
1	D	11	LEU	3.0
1	D	351	TYR	3.0
1	A	298	VAL	3.0
1	C	298	VAL	3.0
1	C	302	SER	3.0
1	D	88	THR	3.0
1	D	305	PRO	3.0
1	A	357	ILE	2.9
1	D	326	ILE	2.9
1	C	85	PHE	2.9
1	D	332	GLY	2.9
1	C	107	LEU	2.8
1	A	246	THR	2.8
1	A	140	PRO	2.8
1	C	79	ASN	2.8
1	D	258	GLY	2.7
1	C	147	TYR	2.7
1	C	88	THR	2.7
1	D	280	LEU	2.7
1	D	324	VAL	2.7
1	A	102	ASP	2.6
1	C	295	PRO	2.6
1	D	36	ASN	2.6
1	D	353	VAL	2.6
1	D	244	TYR	2.6
1	D	260	TYR	2.6
1	C	133	THR	2.6
1	D	287	ASN	2.6
1	A	100	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	354	LEU	2.6
1	A	125	VAL	2.6
1	C	146	GLU	2.6
1	D	32	VAL	2.6
1	D	298	VAL	2.6
1	A	79	ASN	2.6
1	A	263	ASN	2.6
1	D	98	ASN	2.6
1	C	104	VAL	2.6
1	D	325	PHE	2.5
1	A	145	GLY	2.5
1	D	302	SER	2.5
1	C	134	PHE	2.5
1	A	81	GLY	2.5
1	A	142	ASN	2.5
1	B	1	ASN	2.5
1	C	110	ALA	2.5
1	C	98	ASN	2.4
1	A	113	THR	2.4
1	C	131	VAL	2.4
1	A	103	GLN	2.4
1	D	300	ALA	2.4
1	A	295	PRO	2.4
1	D	263	ASN	2.4
1	C	81	GLY	2.4
1	A	97	LYS	2.4
1	D	33	ILE	2.3
1	A	94	LYS	2.3
1	D	239	LEU	2.3
1	C	113	THR	2.3
1	A	293	MET	2.3
1	D	8	ILE	2.3
1	C	135	PHE	2.3
1	D	140	PRO	2.3
1	B	357	ILE	2.3
1	C	99	THR	2.3
1	D	265	MET	2.3
1	D	347	ILE	2.2
1	C	262	VAL	2.2
1	D	308	LYS	2.2
1	D	5	ASP	2.2
1	C	93	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	144	ILE	2.2
1	A	292	VAL	2.2
1	C	260	TYR	2.2
1	C	83	ILE	2.2
1	A	98	ASN	2.2
1	D	99	THR	2.2
1	D	299	THR	2.2
1	A	241	PRO	2.2
1	A	118	ALA	2.2
1	D	77	ALA	2.2
1	D	147	TYR	2.1
1	A	137	ASP	2.1
1	D	104	VAL	2.1
1	C	80	LYS	2.1
1	A	248	ILE	2.1
1	C	301	ILE	2.1
1	A	4	LYS	2.1
1	A	116	ASN	2.1
1	C	269	LEU	2.1
1	C	354	LEU	2.1
1	C	103	GLN	2.1
1	D	279	THR	2.1
1	D	304	GLU	2.1
1	D	232	LEU	2.1
1	C	303	LYS	2.0
1	D	248	ILE	2.0
1	A	217	LEU	2.0
1	C	96	LEU	2.0
1	B	359	LYS	2.0
1	C	115	GLY	2.0
1	C	112	TYR	2.0
1	D	250	ARG	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](#)

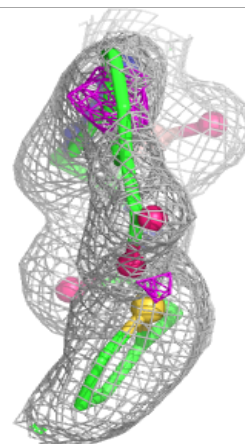
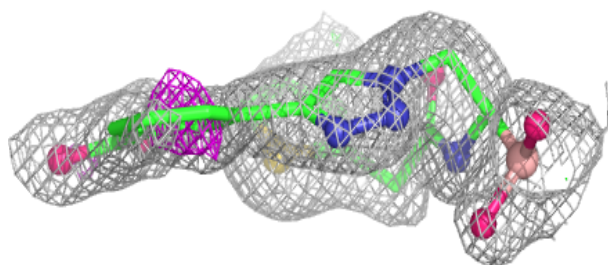
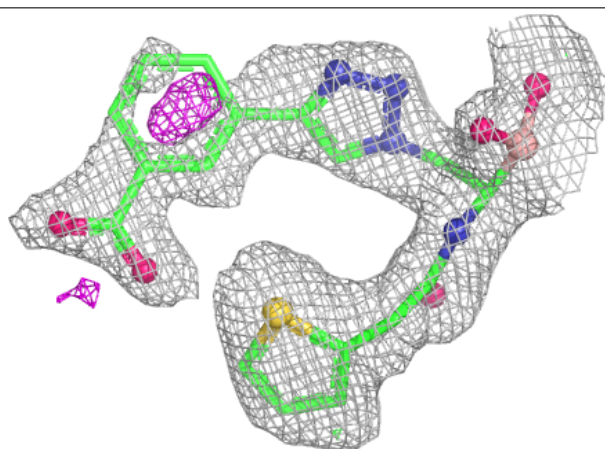
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	9TJ	C	401	28/28	0.87	0.12	38,48,59,60	0
2	9TJ	D	401	28/28	0.87	0.12	34,53,66,68	0
2	9TJ	A	401	28/28	0.91	0.10	31,45,56,59	0
2	9TJ	B	401	28/28	0.91	0.11	23,36,43,46	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.

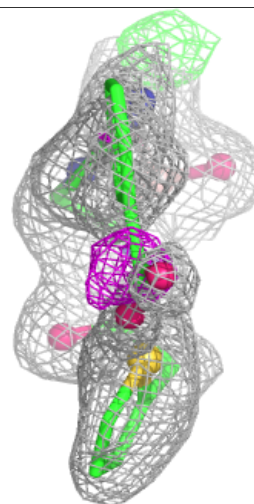
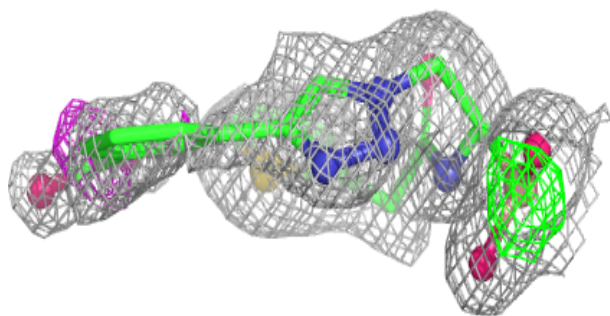
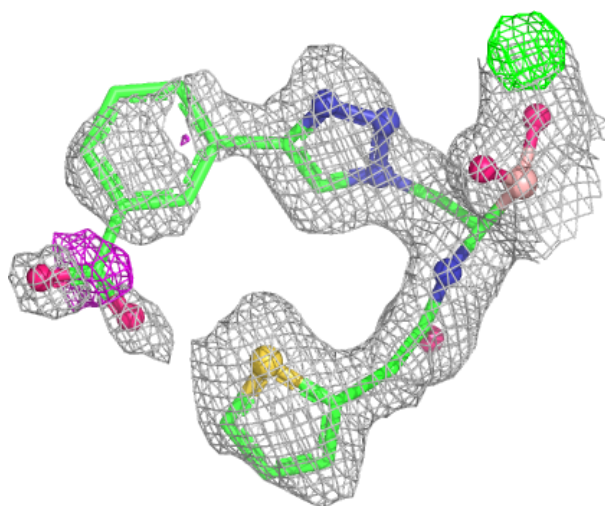
Electron density around 9TJ C 401:

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



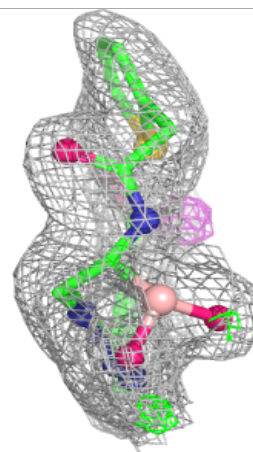
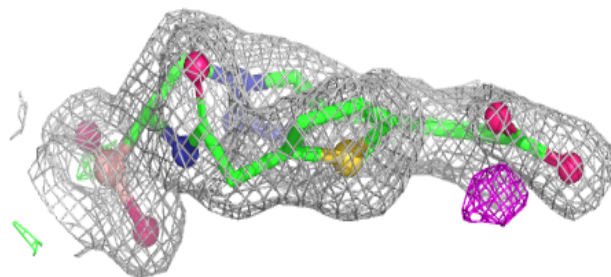
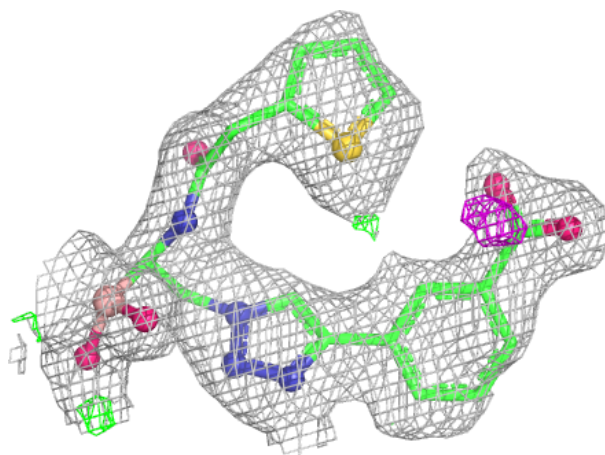
Electron density around 9TJ D 401:

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



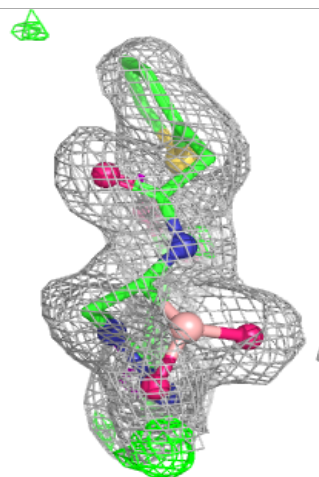
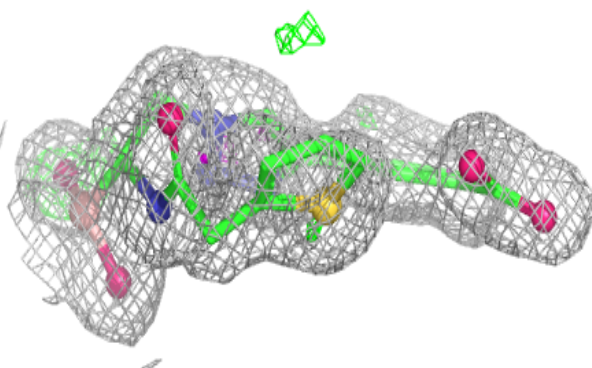
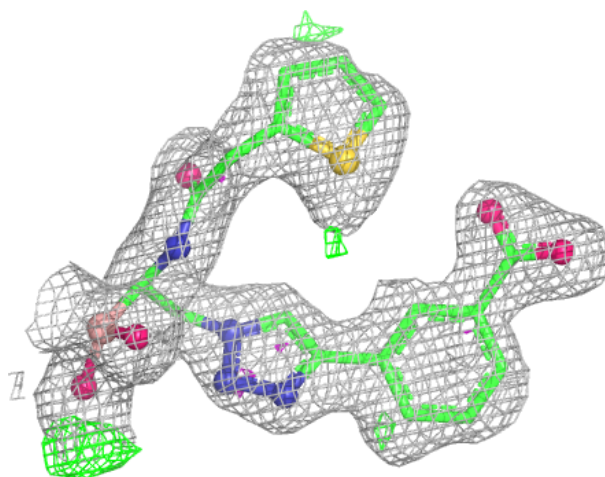
Electron density around 9TJ A 401:

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



Electron density around 9TJ B 401:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.