



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:58 PM UTC

PDB ID : 5W12 / pdb_00005w12
Title : ADC-7 in complex with boronic acid transition state inhibitor EC04
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

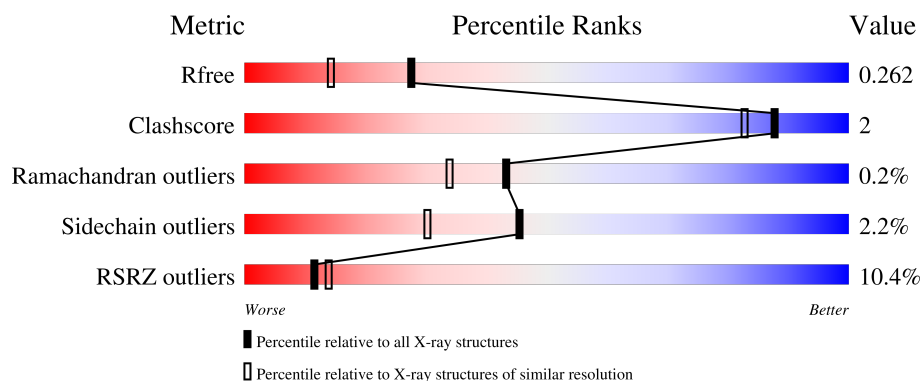
1 Overall quality at a glance

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	11% 89% 8% .
1	B	361	93% 6% .
1	C	361	14% 86% 12% .
1	D	361	16% 90% 8% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11794 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.

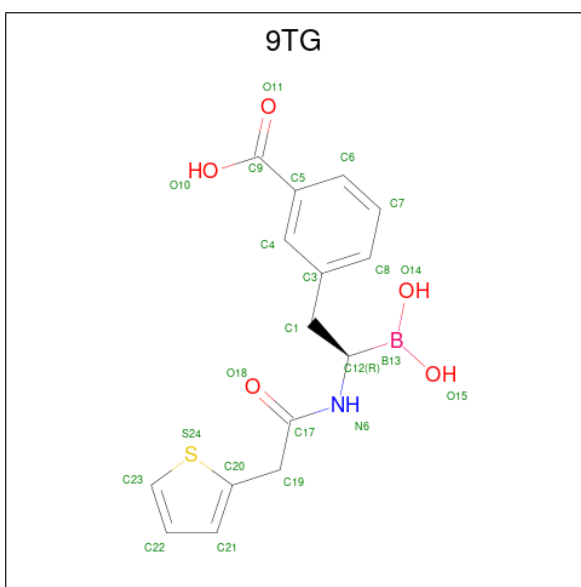
- Molecule 1 is a protein called Beta-lactamase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	353	Total	C	N	O	S	0	0	0
			2748	1769	453	517	9			
1	B	358	Total	C	N	O	S	0	2	0
			2843	1825	472	537	9			
1	C	357	Total	C	N	O	S	0	0	0
			2805	1805	467	524	9			
1	D	355	Total	C	N	O	S	0	1	0
			2776	1785	462	520	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-[(2R)-2-borono-2-[(thiophen-2-yl)acetyl]amino}ethyl]benzoic acid (CCD ID: 9TG) (formula: C₁₅H₁₆BNO₅S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 23	B 1	C 15	N 1	O 5	S 1	0	0
2	B	1	Total 28	B 1	C 19	N 1	O 5	S 2	0	1
2	C	1	Total 23	B 1	C 15	N 1	O 5	S 1	0	0
2	D	1	Total 23	B 1	C 15	N 1	O 5	S 1	0	0

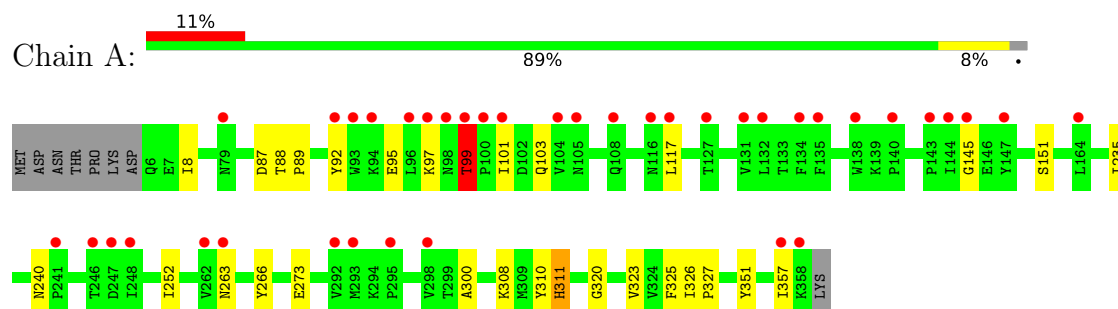
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	116	Total	O	0	0
			116	116		
3	B	239	Total	O	0	7
			246	246		
3	C	93	Total	O	0	2
			95	95		
3	D	68	Total	O	0	0
			68	68		

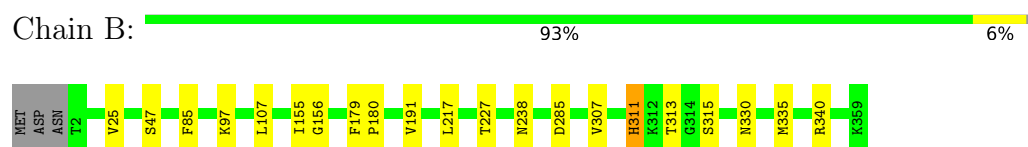
3 Residue-property plots [i](#)

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.

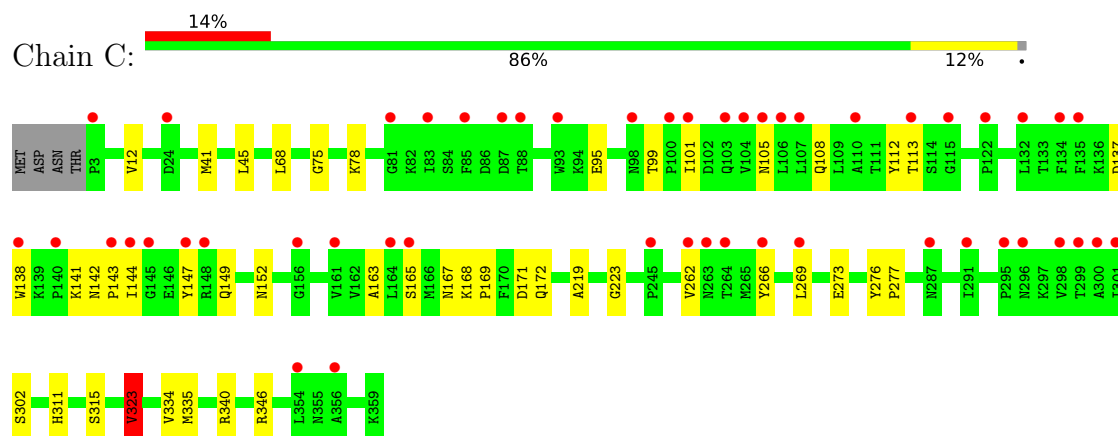
• Molecule 1: Beta-lactamase



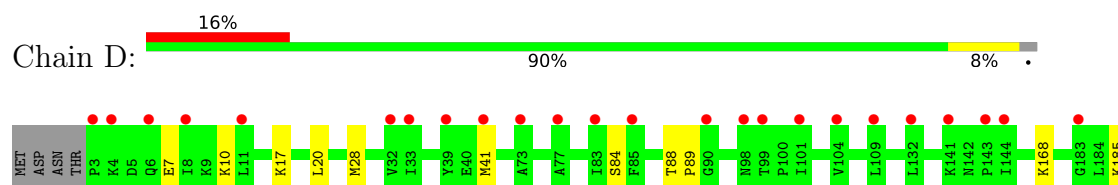
• Molecule 1: Beta-lactamase

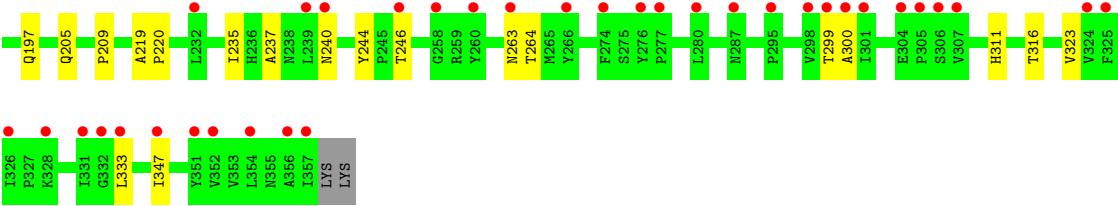


• Molecule 1: Beta-lactamase



• 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	89.53Å 81.30Å 106.69Å 90.00° 112.89° 90.00°	Depositor
Resolution (Å)	98.28 – 1.88 98.28 – 1.88	Depositor EDS
% Data completeness (in resolution range)	99.0 (98.28-1.88) 99.0 (98.28-1.88)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 1.88Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.201 , 0.255 0.209 , 0.262	Depositor DCC
R_{free} test set	5668 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	28.8	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11794	wwPDB-VP
Average B, all atoms (Å ²)	40.0	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 36.20 % 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 5.1847e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: 9TG

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	1.26	3/2815 (0.1%)	1.21	13/3831 (0.3%)
1	B	1.27	8/2911 (0.3%)	1.12	4/3953 (0.1%)
1	C	1.11	1/2873 (0.0%)	1.07	5/3901 (0.1%)
1	D	1.06	0/2844	1.10	8/3869 (0.2%)
All	All	1.18	12/11443 (0.1%)	1.13	30/15554 (0.2%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	335	MET	N-CA	7.99	1.55	1.46
1	A	240	ASN	N-CA	6.71	1.53	1.46
1	A	320	GLY	CA-C	5.74	1.56	1.52
1	B	47	SER	C-O	5.51	1.30	1.23
1	B	307	VAL	N-CA	5.42	1.52	1.46
1	B	313	THR	C-O	5.42	1.30	1.23
1	B	227	THR	C-O	5.33	1.30	1.23
1	B	227	THR	CA-C	-5.27	1.46	1.52
1	B	285	ASP	C-O	-5.20	1.17	1.24
1	B	25	VAL	N-CA	5.19	1.50	1.46
1	A	300	ALA	CA-C	-5.07	1.46	1.52
1	C	152	ASN	C-O	-5.02	1.19	1.24

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	151	SER	N-CA-C	7.55	121.12	108.13
1	A	99	THR	N-CA-C	-7.45	100.37	110.36
1	D	316	THR	N-CA-C	-6.70	100.04	109.69
1	D	17	LYS	CA-C-N	-6.65	112.95	119.87
1	D	17	LYS	C-N-CA	-6.65	112.95	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	240	ASN	N-CA-C	6.62	119.16	109.30
1	A	252	ILE	N-CA-C	6.34	116.51	110.42
1	A	357	ILE	CB-CA-C	6.25	120.22	113.22
1	A	145	GLY	N-CA-C	-6.13	106.05	114.64
1	D	168	LYS	CA-C-N	-5.86	113.65	119.92
1	D	168	LYS	C-N-CA	-5.86	113.65	119.92
1	A	240	ASN	CA-C-N	-5.77	113.74	119.56
1	A	240	ASN	C-N-CA	-5.77	113.74	119.56
1	C	45	LEU	CA-C-N	5.61	128.25	120.29
1	C	45	LEU	C-N-CA	5.61	128.25	120.29
1	B	238	ASN	N-CA-C	5.57	117.43	111.36
1	B	191	VAL	N-CA-C	-5.45	103.94	108.63
1	A	351	TYR	N-CA-C	5.39	116.83	111.07
1	C	323	VAL	N-CA-CB	-5.36	102.67	111.45
1	A	240	ASN	CB-CA-C	-5.32	104.07	111.41
1	C	68	LEU	N-CA-C	5.22	117.05	111.36
1	D	41	MET	N-CA-C	5.16	117.31	108.90
1	D	347	ILE	N-CA-C	5.16	115.88	110.62
1	C	75	GLY	N-CA-C	5.09	120.51	113.99
1	B	155	ILE	CA-C-N	5.06	125.60	119.98
1	B	155	ILE	C-N-CA	5.06	125.60	119.98
1	A	103	GLN	N-CA-C	5.03	119.39	113.16
1	A	326	ILE	CA-C-N	5.03	126.12	119.84
1	A	326	ILE	C-N-CA	5.03	126.12	119.84
1	D	209	PRO	N-CA-C	5.00	119.04	111.19

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	2748	0	2693	12	0
1	B	2843	0	2824	5	0
1	C	2805	0	2788	17	0
1	D	2776	0	2728	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	23	0	0	0	0
2	B	28	0	0	0	0
2	C	23	0	0	0	0
2	D	23	0	0	0	0
3	A	116	0	0	1	0
3	B	246	0	0	0	0
3	C	95	0	0	0	0
3	D	68	0	0	0	0
All	All	11794	0	11033	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:A:235:ILE:HD11	1:A:323:VAL:CG1	2.00	0.90
1:B:315:SER:HB3	1:B:340:ARG:HD3	1.61	0.83
1:D:20:LEU:HD11	1:D:28:MET:HE2	1.62	0.82
1:D:235:ILE:HD11	1:D:323:VAL:HG13	1.66	0.77
1:A:235:ILE:HD11	1:A:323:VAL:HG13	1.70	0.71
1:C:113:THR:HA	1:C:147:TYR:O	1.91	0.71
1:A:99:THR:CG2	1:A:101:ILE:HG22	2.23	0.67
1:C:163:ALA:HB1	1:C:168:LYS:O	1.95	0.66
1:A:87:ASP:OD2	1:A:92:TYR:OH	2.16	0.63
1:D:20:LEU:CD1	1:D:28:MET:HE2	2.27	0.63
1:C:105:ASN:ND2	1:C:108:GLN:CD	2.59	0.61
1:A:235:ILE:HD11	1:A:323:VAL:HG11	1.84	0.60
1:D:7:GLU:O	1:D:10:LYS:CB	2.54	0.56
1:A:99:THR:HG22	1:A:101:ILE:HG22	1.88	0.54
1:A:263:ASN:ND2	3:A:504:HOH:O	2.36	0.52
1:C:12:VAL:HG21	1:C:41:MET:HE3	1.94	0.49
1:C:323:VAL:HG22	1:C:334:VAL:HG22	1.95	0.48
1:C:105:ASN:HD21	1:C:108:GLN:CD	2.22	0.48
1:D:88:THR:HB	1:D:89:PRO:HD2	1.96	0.47
1:C:112:TYR:HB3	1:C:149:GLN:O	2.15	0.47
1:C:276:TYR:HA	1:C:277:PRO:C	2.39	0.47
1:C:141:LYS:O	1:C:142:ASN:C	2.58	0.47
1:C:169:PRO:HB2	1:C:171:ASP:OD1	2.16	0.46
1:D:263:ASN:CG	1:D:264:THR:H	2.23	0.46
1:A:311:HIS:CD2	1:A:311:HIS:C	2.93	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:ILE:HA	1:C:138:TRP:CZ3	2.52	0.45
1:A:266:TYR:HB2	1:A:273:GLU:HB3	1.99	0.44
1:D:333:LEU:C	1:D:333:LEU:HD23	2.43	0.44
1:C:335:MET:HE1	1:C:346:ARG:HG2	2.00	0.43
1:A:117:LEU:HD23	1:A:117:LEU:HA	1.93	0.42
1:B:85:PHE:HB3	1:B:107:LEU:HB2	2.01	0.42
1:C:276:TYR:CD1	1:C:277:PRO:HA	2.55	0.42
1:B:311:HIS:CD2	1:B:311:HIS:C	2.98	0.41
1:B:156:GLY:C	1:B:217:LEU:HD13	2.46	0.41
1:B:179:PHE:HB2	1:B:180:PRO:HD3	2.01	0.41
1:A:88:THR:HB	1:A:89:PRO:HD2	2.03	0.41
1:D:299:THR:HG22	1:D:300:ALA:O	2.20	0.41
1:C:266:TYR:HB2	1:C:273:GLU:HB3	2.01	0.41
1:C:219:ALA:HA	1:C:223:GLY:HA3	2.03	0.41
1:A:310:TYR:HB2	1:A:325:PHE:CE1	2.56	0.40
1:C:315:SER:HB3	1:C:340:ARG:HD3	2.03	0.40
1:D:219:ALA:N	1:D:220:PRO:HD2	2.37	0.40
1:D:237:ALA:HA	1:D:244:TYR:CE1	2.56	0.40
1:C:142:ASN:O	1:C:143:PRO:C	2.64	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	351/361 (97%)	329 (94%)	20 (6%)	2 (1%)	21	10
1	B	358/361 (99%)	351 (98%)	7 (2%)	0	100	100
1	C	355/361 (98%)	337 (95%)	17 (5%)	1 (0%)	36	26
1	D	354/361 (98%)	342 (97%)	12 (3%)	0	100	100
All	All	1418/1444 (98%)	1359 (96%)	56 (4%)	3 (0%)	43	34

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	97	LYS
1	A	95	GLU
1	C	302	SER

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	295/319 (92%)	290 (98%)	5 (2%)	53	40
1	B	312/319 (98%)	309 (99%)	3 (1%)	68	60
1	C	305/319 (96%)	293 (96%)	12 (4%)	28	12
1	D	299/319 (94%)	292 (98%)	7 (2%)	44	29
All	All	1211/1276 (95%)	1184 (98%)	27 (2%)	45	30

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ILE
1	A	99	THR
1	A	308	LYS
1	A	311	HIS
1	A	327	PRO
1	B	97	LYS
1	B	311	HIS
1	B	330	ASN
1	C	78	LYS
1	C	95	GLU
1	C	99	THR
1	C	137	ASP
1	C	144	ILE
1	C	165	SER
1	C	167	ASN
1	C	172	GLN
1	C	262	VAL

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Mol	Chain	Res	Type
1	C	269	LEU
1	C	311	HIS
1	C	323	VAL
1	D	84	SER
1	D	185	LYS
1	D	197	GLN
1	D	205	GLN
1	D	240	ASN
1	D	246	THR
1	D	311	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	197	GLN
1	A	287	ASN
1	A	343	ASN
1	B	14	GLN
1	B	186	HIS
1	B	198	ASN
1	B	238	ASN
1	C	149	GLN
1	C	186	HIS
1	C	240	ASN
1	C	281	GLN
1	C	290	GLN
1	D	36	ASN
1	D	195	GLN
1	D	197	GLN
1	D	198	ASN
1	D	205	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 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	9TG	D	401	1	20,24,24	1.10	2 (10%)	26,32,32	0.92	1 (3%)
2	9TG	C	401	1	20,24,24	0.92	0	26,32,32	1.06	1 (3%)
2	9TG	B	401[B]	-	20,24,24	1.09	1 (5%)	26,32,32	1.57	7 (26%)
2	9TG	A	401	1	20,24,24	1.05	0	26,32,32	1.39	6 (23%)
2	9TG	B	401[A]	-	20,24,24	1.09	1 (5%)	26,32,32	1.46	6 (23%)

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	9TG	D	401	1	-	5/15/20/20	0/2/2/2
2	9TG	C	401	1	-	1/15/20/20	0/2/2/2
2	9TG	B	401[B]	-	-	1/15/20/20	0/2/2/2
2	9TG	A	401	1	-	4/15/20/20	0/2/2/2
2	9TG	B	401[A]	-	-	1/15/20/20	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	9TG	C19-C17	2.63	1.55	1.51
2	B	401[A]	9TG	O10-C9	-2.24	1.23	1.30
2	B	401[B]	9TG	O10-C9	-2.24	1.23	1.30
2	D	401	9TG	C19-C20	2.19	1.54	1.50

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401[A]	9TG	O18-C17-C19	-3.69	115.58	121.40
2	B	401[B]	9TG	O18-C17-C19	-3.69	115.58	121.40
2	A	401	9TG	C19-C20-S24	-3.26	115.20	122.11
2	A	401	9TG	O18-C17-C19	-2.97	116.72	121.40
2	B	401[B]	9TG	C19-C20-S24	-2.88	116.02	122.11
2	B	401[A]	9TG	O10-C9-O11	-2.85	117.22	123.35
2	B	401[B]	9TG	O10-C9-O11	-2.85	117.22	123.35
2	B	401[A]	9TG	O10-C9-C5	2.70	121.77	114.84
2	B	401[B]	9TG	O10-C9-C5	2.70	121.77	114.84
2	B	401[A]	9TG	C19-C17-N6	2.65	120.84	116.31
2	B	401[B]	9TG	C19-C17-N6	2.65	120.84	116.31
2	B	401[B]	9TG	C19-C20-C21	2.60	134.16	126.56
2	A	401	9TG	O10-C9-O11	-2.51	117.96	123.35
2	D	401	9TG	C19-C20-C21	2.51	133.88	126.56
2	C	401	9TG	O18-C17-C19	-2.49	117.48	121.40
2	A	401	9TG	C19-C17-N6	2.41	120.43	116.31
2	A	401	9TG	C19-C20-C21	2.37	133.49	126.56
2	B	401[A]	9TG	C19-C20-C21	2.34	133.40	126.56
2	B	401[A]	9TG	C19-C20-S24	-2.23	117.39	122.11
2	B	401[B]	9TG	C17-C19-C20	-2.02	106.23	111.92
2	A	401	9TG	C17-C19-C20	-2.01	106.27	111.92

There are no chirality outliers.

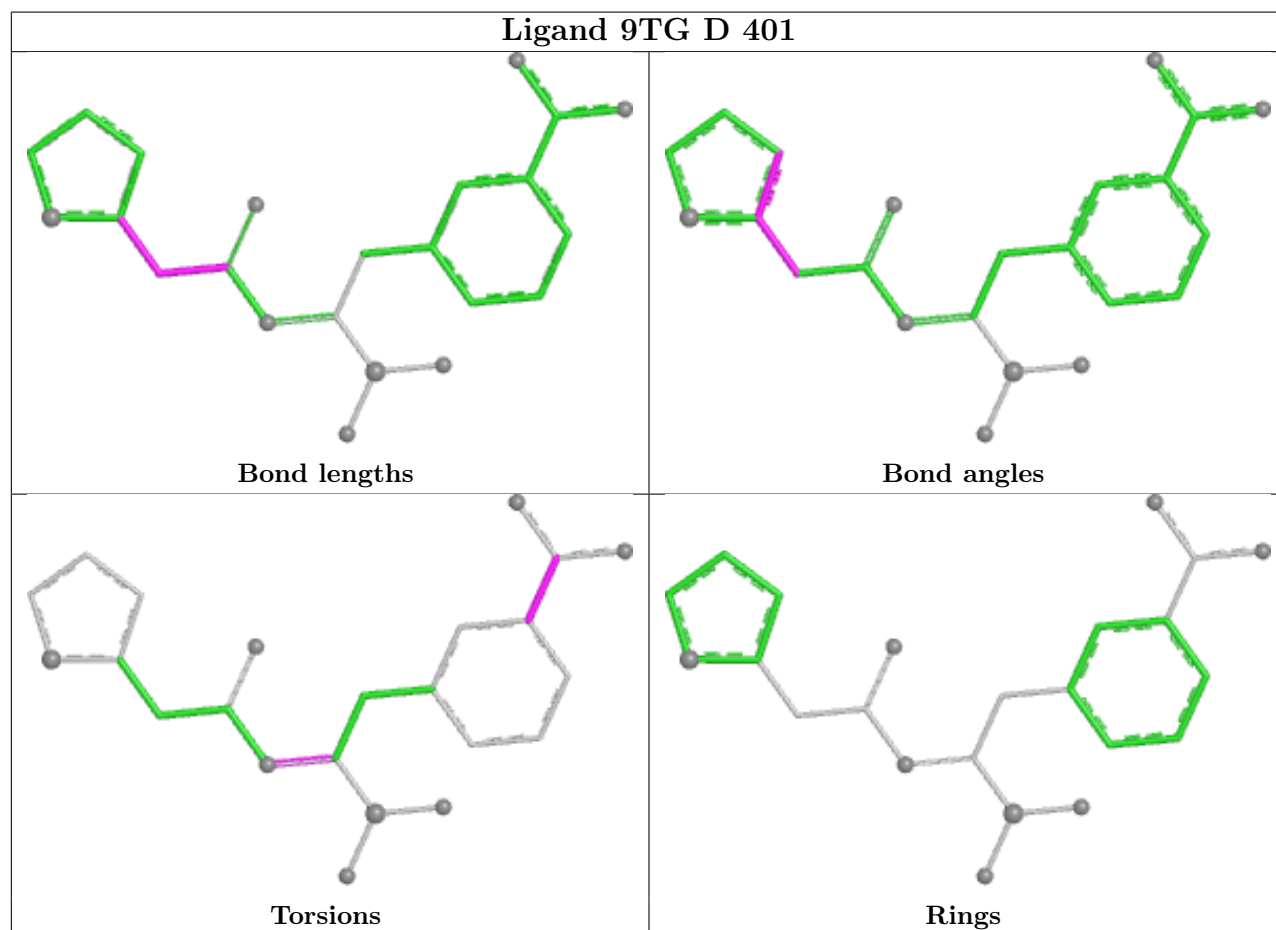
All (12) torsion outliers are listed below:

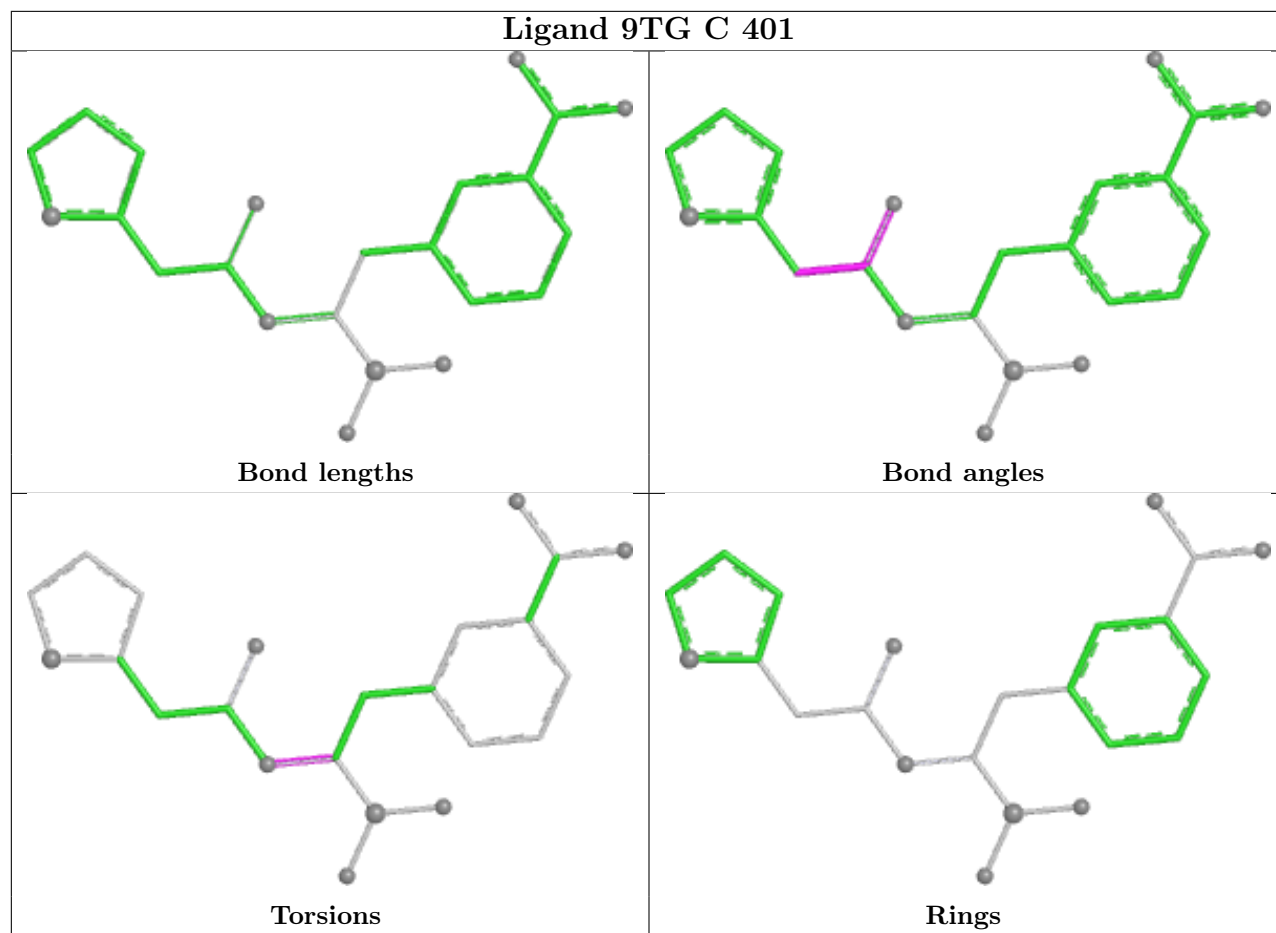
Mol	Chain	Res	Type	Atoms
2	D	401	9TG	C4-C5-C9-O11
2	D	401	9TG	C6-C5-C9-O11
2	D	401	9TG	C4-C5-C9-O10
2	D	401	9TG	C6-C5-C9-O10
2	C	401	9TG	C1-C12-N6-C17
2	D	401	9TG	C1-C12-N6-C17
2	B	401[A]	9TG	C1-C12-N6-C17
2	B	401[B]	9TG	C1-C12-N6-C17
2	A	401	9TG	O18-C17-C19-C20
2	A	401	9TG	C4-C5-C9-O10
2	A	401	9TG	N6-C17-C19-C20
2	A	401	9TG	C1-C12-N6-C17

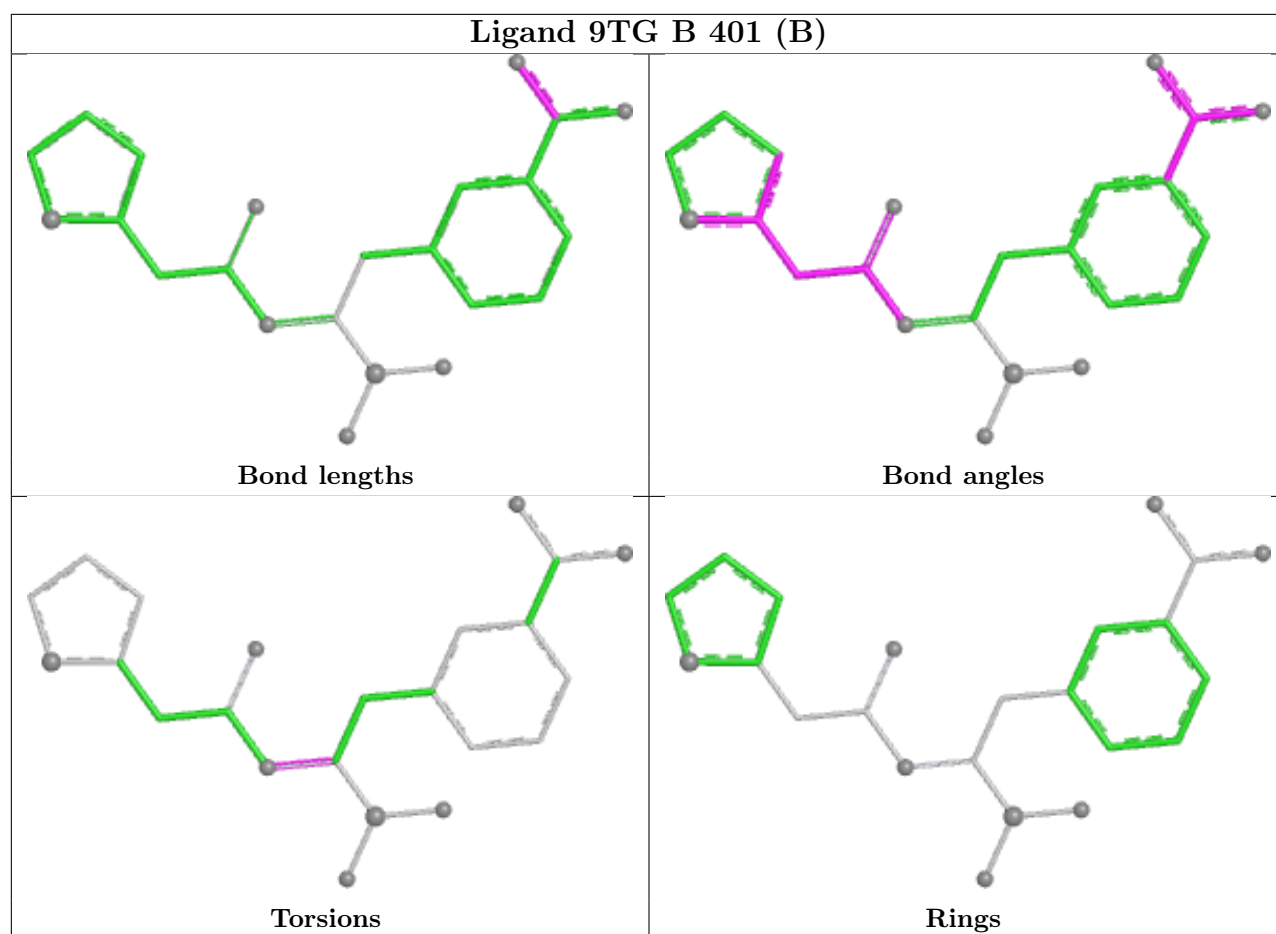
There are no ring outliers.

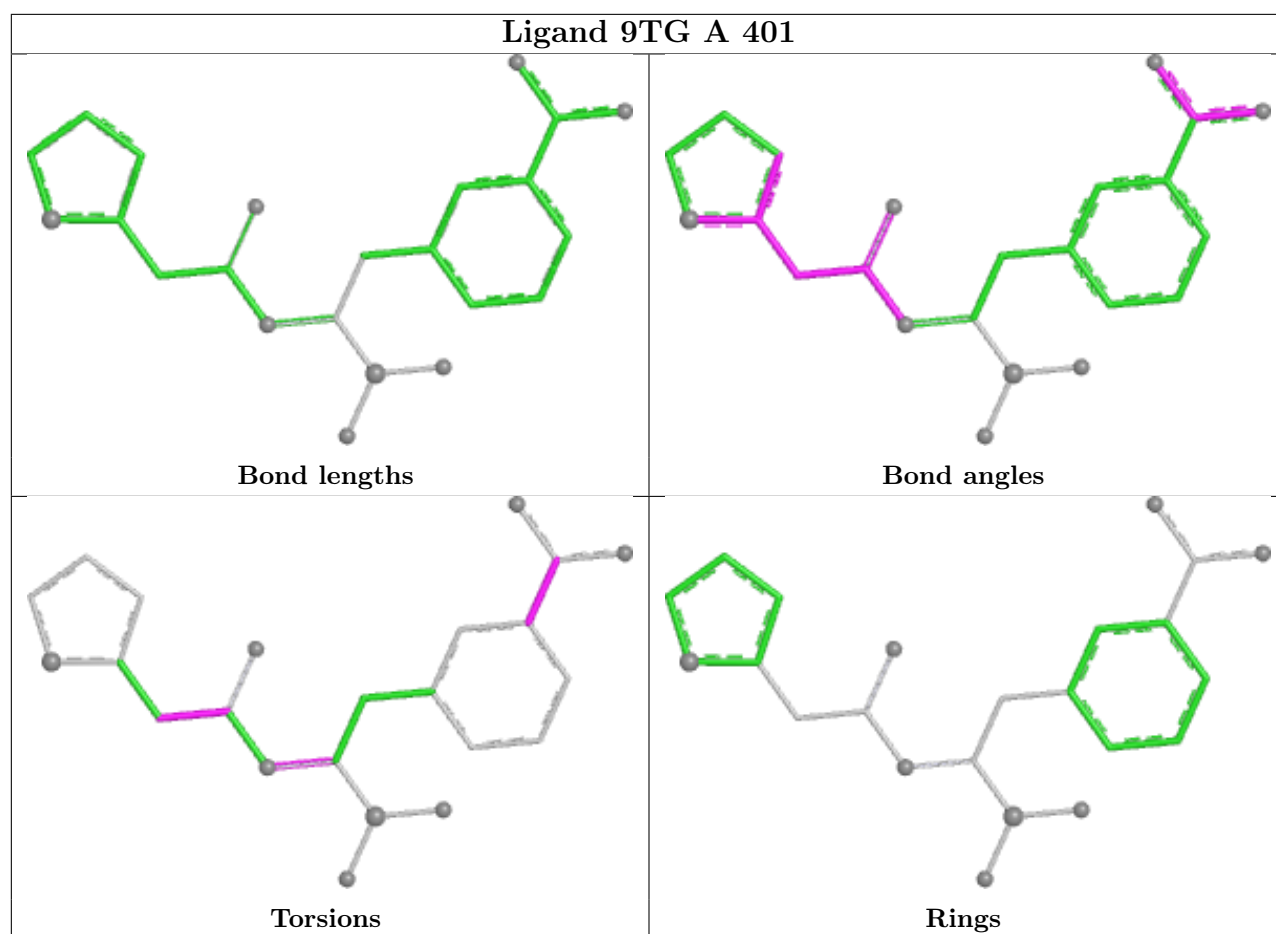
No monomer is involved in short contacts.

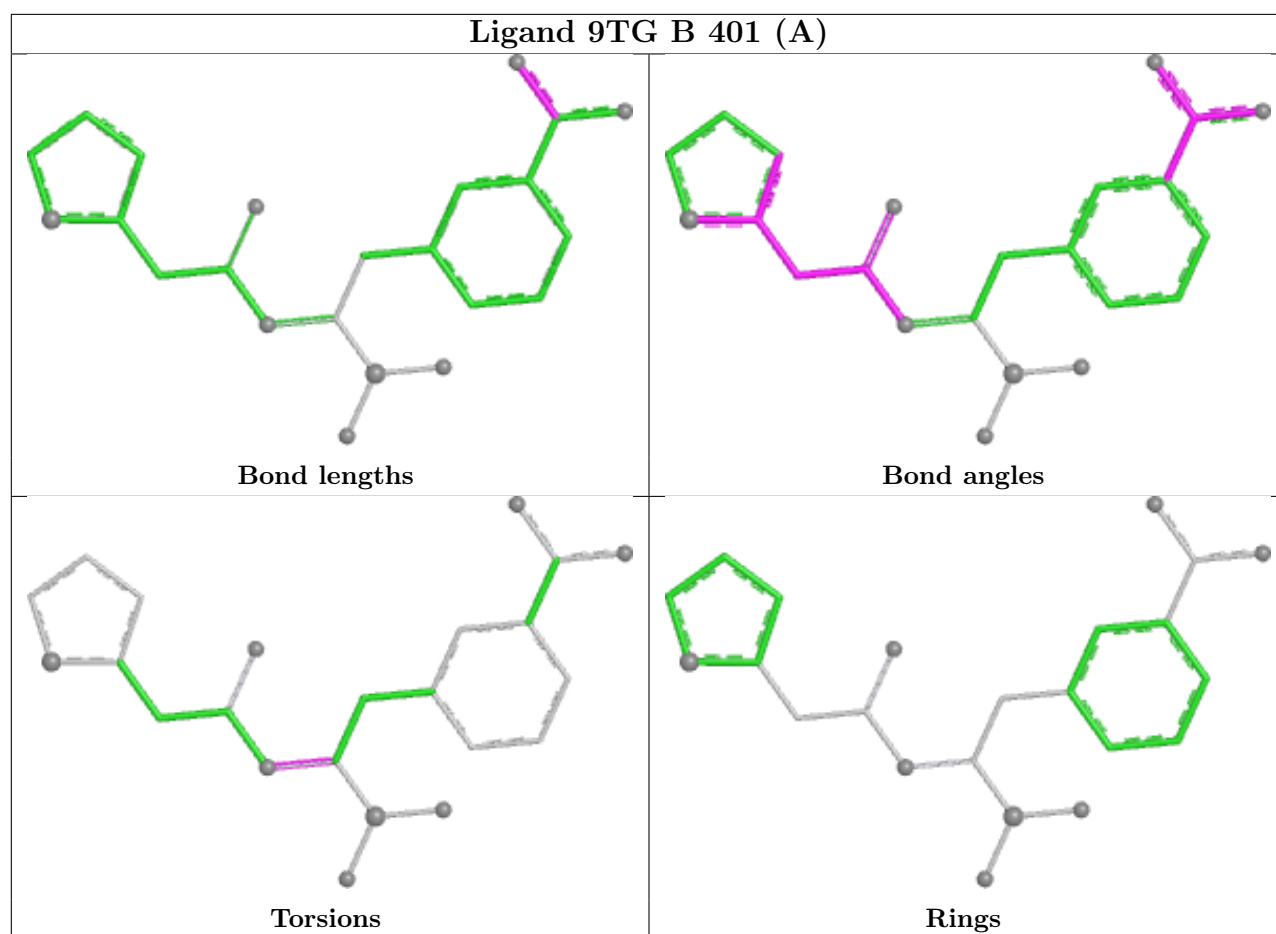
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.











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	353/361 (97%)	0.70	39 (11%) 10 12	21, 36, 63, 74	0
1	B	358/361 (99%)	-0.12	0 100 100	11, 27, 42, 60	2 (0%)
1	C	357/361 (98%)	0.94	50 (14%) 6 6	22, 43, 71, 85	0
1	D	355/361 (98%)	1.15	59 (16%) 4 5	15, 48, 71, 93	1 (0%)
All	All	1423/1444 (98%)	0.67	148 (10%) 11 14	11, 38, 66, 93	3 (0%)

All (148) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	101	ILE	6.0
1	A	138	TRP	5.1
1	C	298	VAL	4.5
1	A	135	PHE	4.4
1	D	357	ILE	4.3
1	A	101	ILE	4.0
1	A	96	LEU	4.0
1	D	3	PRO	4.0
1	C	144	ILE	4.0
1	A	143	PRO	3.9
1	C	104	VAL	3.9
1	C	132	LEU	3.9
1	D	298	VAL	3.8
1	A	263	ASN	3.8
1	D	98	ASN	3.7
1	D	352	VAL	3.6
1	A	132	LEU	3.6
1	A	117	LEU	3.6
1	D	301	ILE	3.5
1	D	331	ILE	3.5
1	D	32	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	98	ASN	3.4
1	A	93	TRP	3.4
1	C	135	PHE	3.4
1	D	104	VAL	3.4
1	A	94	LYS	3.4
1	A	131	VAL	3.4
1	D	300	ALA	3.3
1	C	107	LEU	3.3
1	A	99	THR	3.3
1	A	358	LYS	3.3
1	D	326	ILE	3.3
1	D	4	LYS	3.3
1	D	246	THR	3.3
1	C	300	ALA	3.2
1	A	100	PRO	3.2
1	D	351	TYR	3.2
1	D	356	ALA	3.2
1	C	164	LEU	3.2
1	C	147	TYR	3.1
1	D	324	VAL	3.1
1	A	357	ILE	3.1
1	C	81	GLY	3.1
1	A	298	VAL	3.1
1	C	85	PHE	3.1
1	D	33	ILE	3.0
1	D	325	PHE	3.0
1	D	39	TYR	3.0
1	A	140	PRO	3.0
1	C	145	GLY	3.0
1	D	306	SER	2.9
1	C	93	TRP	2.9
1	A	144	ILE	2.9
1	D	276	TYR	2.9
1	C	295	PRO	2.9
1	A	134	PHE	2.9
1	D	304	GLU	2.9
1	D	307	VAL	2.9
1	D	274	PHE	2.8
1	C	138	TRP	2.8
1	D	83	ILE	2.8
1	D	354	LEU	2.8
1	C	3	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	354	LEU	2.8
1	A	104	VAL	2.8
1	C	262	VAL	2.8
1	D	266	TYR	2.8
1	A	97	LYS	2.8
1	C	269	LEU	2.8
1	A	79	ASN	2.7
1	D	101	ILE	2.7
1	C	143	PRO	2.7
1	D	295	PRO	2.7
1	D	8	ILE	2.7
1	D	347	ILE	2.7
1	A	295	PRO	2.7
1	C	301	ILE	2.7
1	D	258	GLY	2.6
1	D	332	GLY	2.6
1	D	73	ALA	2.6
1	C	287	ASN	2.6
1	C	106	LEU	2.6
1	D	280	LEU	2.6
1	C	103	GLN	2.6
1	C	296	ASN	2.6
1	A	246	THR	2.6
1	D	99	THR	2.6
1	C	83	ILE	2.5
1	A	127	THR	2.5
1	C	115	GLY	2.5
1	C	299	THR	2.5
1	D	299	THR	2.5
1	A	293	MET	2.5
1	C	140	PRO	2.5
1	C	110	ALA	2.4
1	C	105	ASN	2.4
1	D	11	LEU	2.4
1	D	287	ASN	2.3
1	C	161	VAL	2.3
1	A	92	TYR	2.3
1	C	113	THR	2.3
1	D	144	ILE	2.3
1	D	232	LEU	2.3
1	A	147	TYR	2.3
1	C	148	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	247	ASP	2.3
1	A	292	VAL	2.3
1	A	98	ASN	2.3
1	C	245	PRO	2.2
1	D	85	PHE	2.2
1	D	263	ASN	2.2
1	D	141	LYS	2.2
1	D	239	LEU	2.2
1	C	100	PRO	2.2
1	C	264	THR	2.2
1	C	122	PRO	2.2
1	D	277	PRO	2.2
1	D	77	ALA	2.2
1	C	291	ILE	2.2
1	D	90	GLY	2.2
1	A	116	ASN	2.1
1	A	164	LEU	2.1
1	D	41	MET	2.1
1	D	240	ASN	2.1
1	C	266	TYR	2.1
1	C	88	THR	2.1
1	C	165	SER	2.1
1	A	262	VAL	2.1
1	D	183	GLY	2.1
1	D	143	PRO	2.1
1	A	105	ASN	2.1
1	D	6	GLN	2.1
1	C	87	ASP	2.1
1	A	108	GLN	2.1
1	D	305	PRO	2.1
1	D	109	LEU	2.1
1	D	333	LEU	2.1
1	C	356	ALA	2.1
1	D	328	LYS	2.0
1	C	156	GLY	2.0
1	A	241	PRO	2.0
1	D	132	LEU	2.0
1	C	24	ASP	2.0
1	A	248	ILE	2.0
1	C	134	PHE	2.0
1	A	145	GLY	2.0
1	C	263	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	260	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](#)

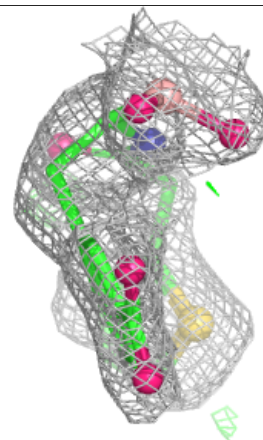
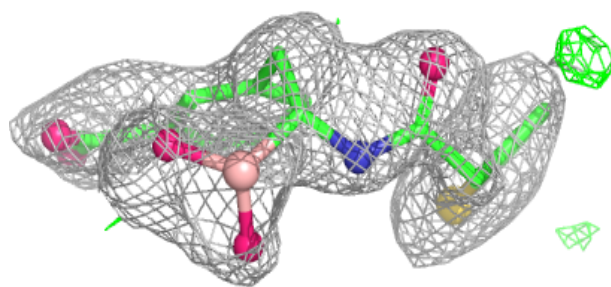
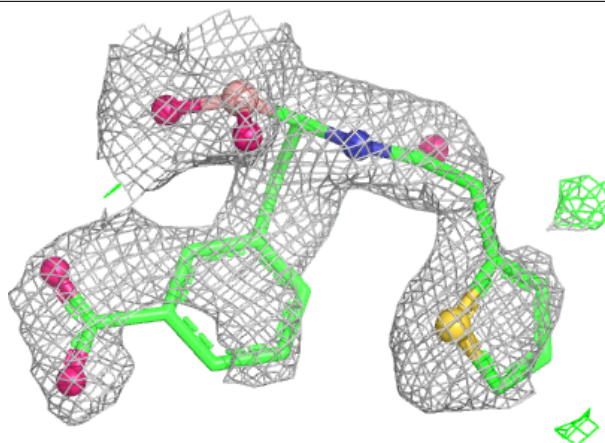
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	9TG	C	401	23/23	0.79	0.15	47,68,84,87	0
2	9TG	D	401	23/23	0.81	0.15	40,63,75,82	0
2	9TG	A	401	23/23	0.87	0.12	38,52,63,65	0
2	9TG	B	401[A]	23/23	0.88	0.12	29,44,55,58	5
2	9TG	B	401[B]	23/23	0.88	0.12	29,45,55,58	5

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.

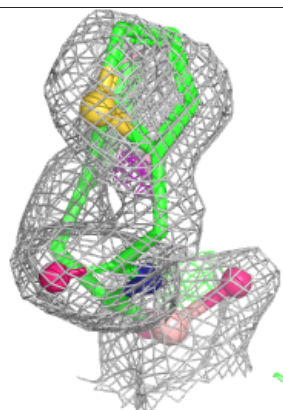
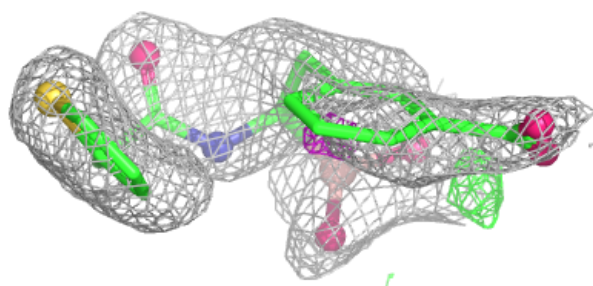
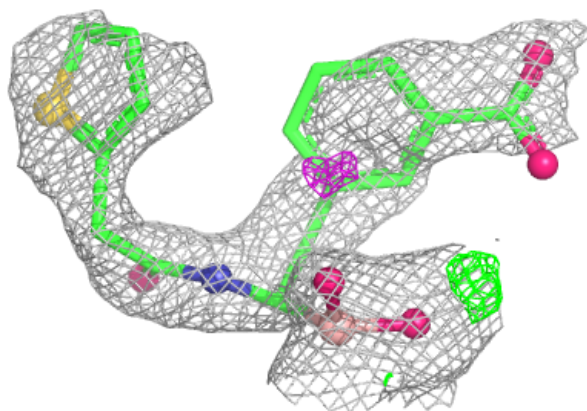
Electron density around 9TG C 401:

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



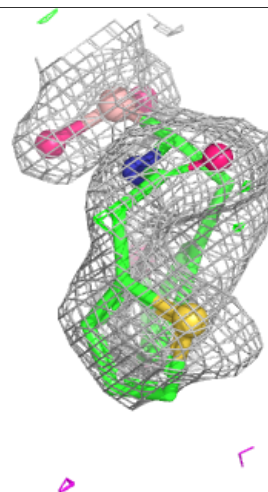
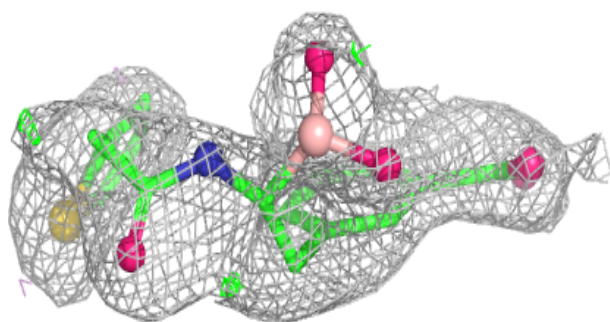
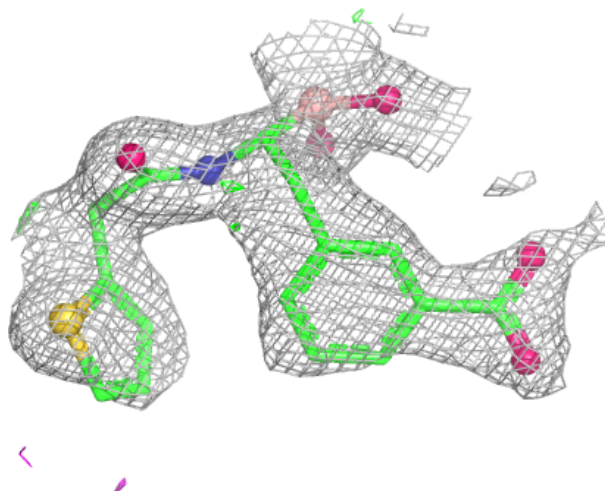
Electron density around 9TG D 401:

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



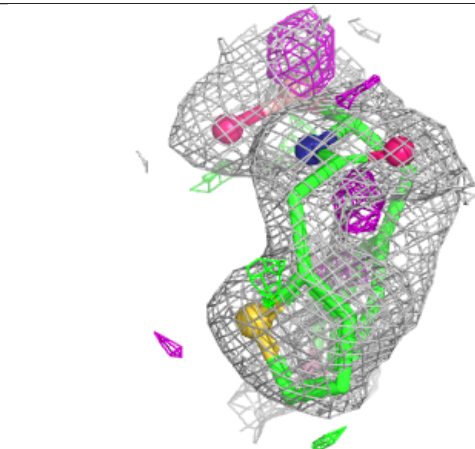
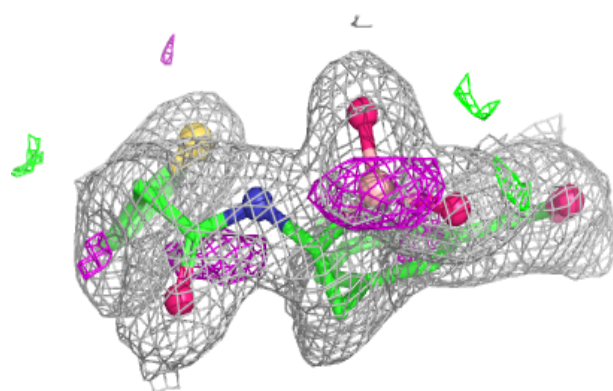
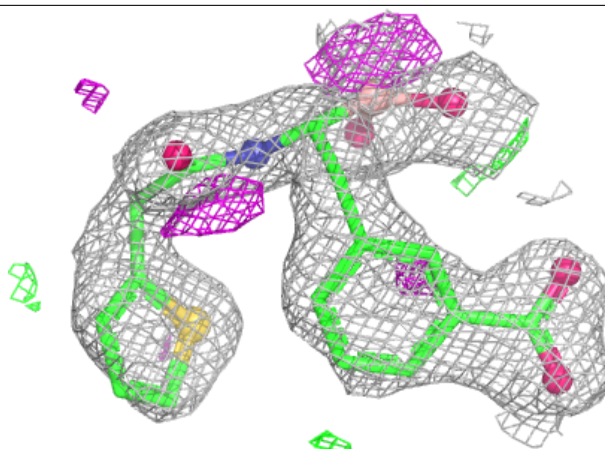
Electron density around 9TG A 401:

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



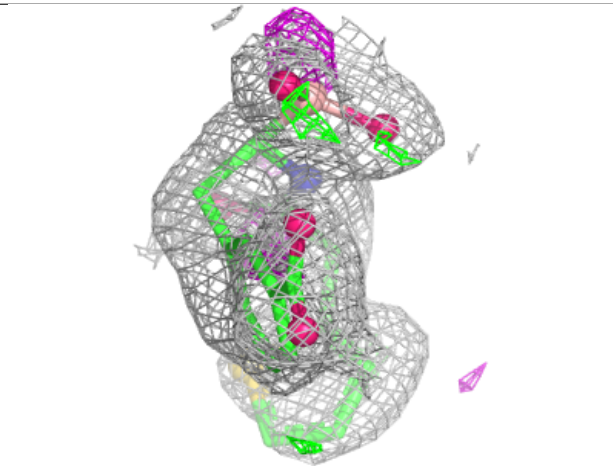
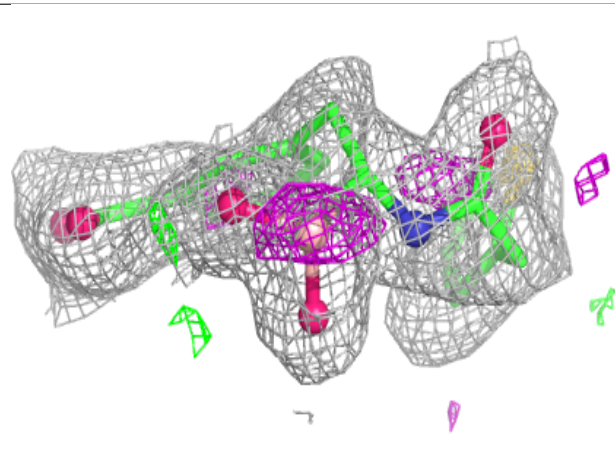
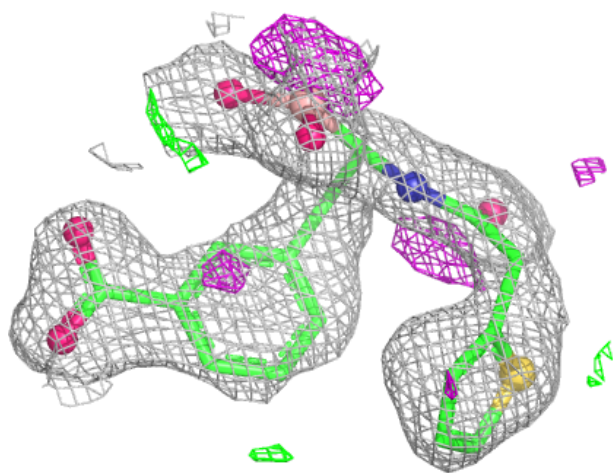
Electron density around 9TG B 401 (A):

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



Electron density around 9TG B 401 (B):

$2mF_o-DF_c$ (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.