



Full wwPDB X-ray Structure Validation Report ⓘ

May 5, 2026 – 12:09 PM EDT

PDB ID : 9O6H / pdb_00009o6h
Title : The Structure of PRMT4 in complex with SGC8172
Authors : Bush, M.; Noinaj, N.; Huang, R.; Deng, Y.
Deposited on : 2025-04-13
Resolution : 1.97 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

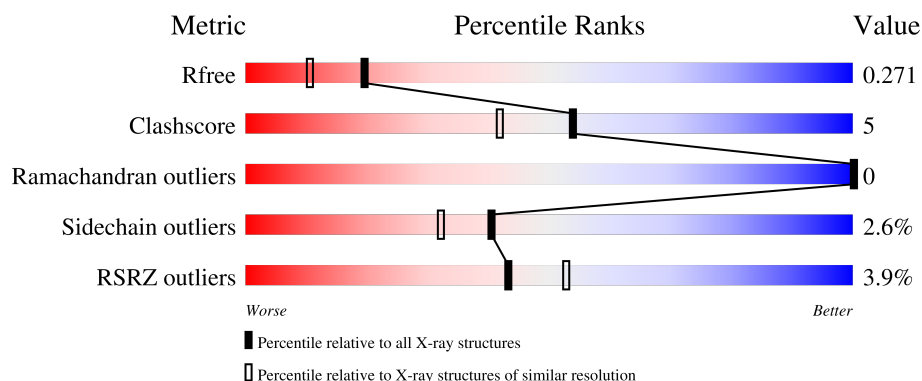
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	331	 4% 87% 12%
1	B	331	 3% 87% 13%
1	C	331	 6% 83% 15%
1	D	331	 2% 84% 15%

2 Entry composition [i](#)

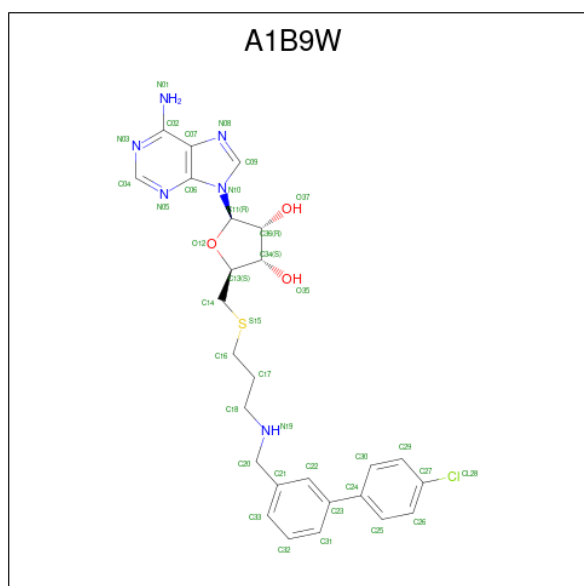
There are 3 unique types of molecules in this entry. The entry contains 11424 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Histone-arginine methyltransferase CARM1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	5	0
			2688	1741	446	485	16			
1	B	331	Total	C	N	O	S	0	7	0
			2703	1750	448	489	16			
1	C	331	Total	C	N	O	S	8	6	0
			2694	1745	447	486	16			
1	D	331	Total	C	N	O	S	0	6	0
			2694	1745	447	486	16			

- Molecule 2 is 5'-S-(3-{[(4'-chloro[1,1'-biphenyl]-3-yl)methyl]amino}propyl)-5'-thioadenosine (CCD ID: A1B9W) (formula: C₂₆H₂₉ClN₆O₃S) (labeled as "Ligand of Interest" by depositor).



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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	B	1	Total 37	C 26	Cl 1	N 6	O 3	S 1	0	0
2	C	1	Total 37	C 26	Cl 1	N 6	O 3	S 1	0	0
2	D	1	Total 37	C 26	Cl 1	N 6	O 3	S 1	0	0

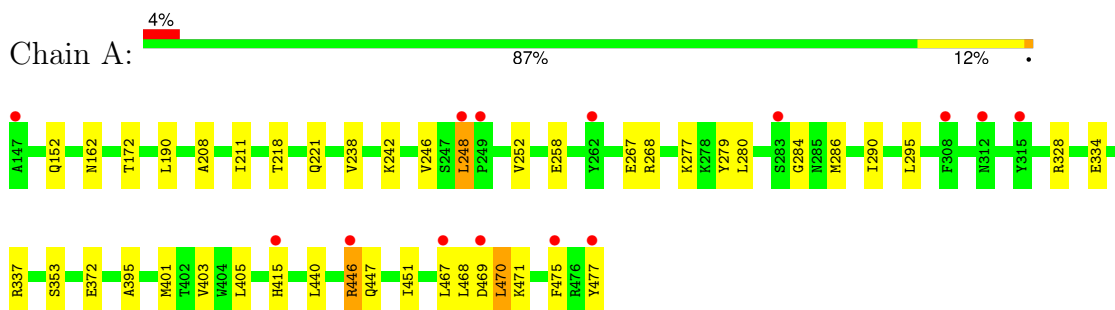
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	107	Total 107	O 107	0	0
3	B	152	Total 152	O 152	0	0
3	C	77	Total 77	O 77	0	0
3	D	161	Total 161	O 161	0	0

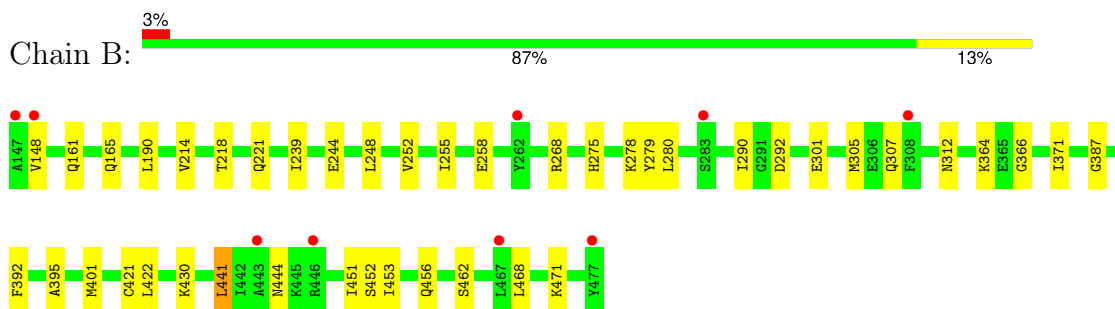
3 Residue-property plots [i](#)

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.

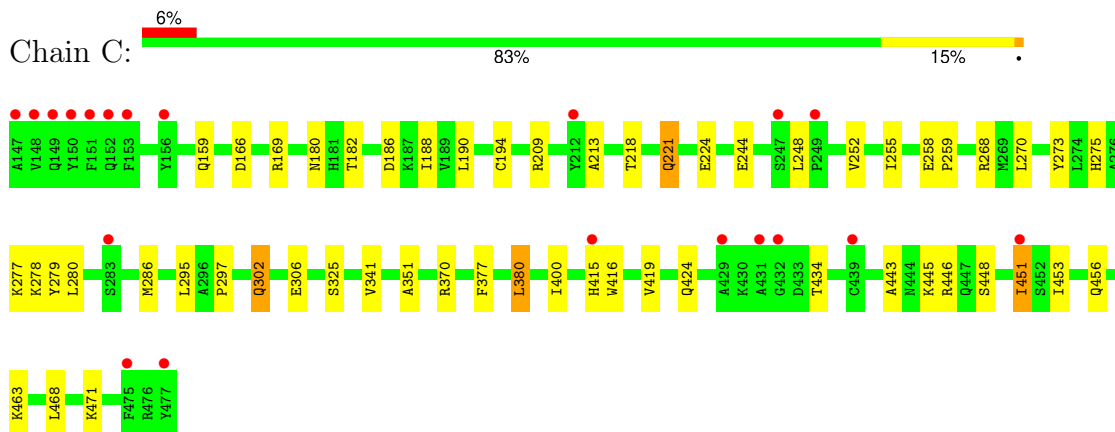
- Molecule 1: Histone-arginine methyltransferase CARM1



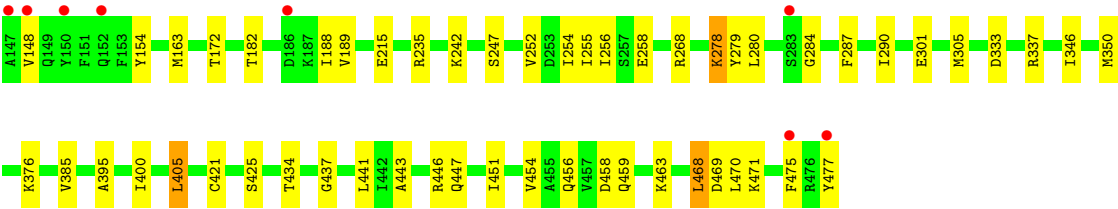
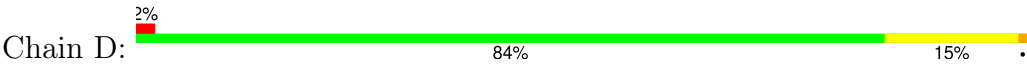
- Molecule 1: Histone-arginine methyltransferase CARM1



- Molecule 1: Histone-arginine methyltransferase CARM1



- Molecule 1: Histone-arginine methyltransferase CARM1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	74.67Å 98.98Å 206.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	89.28 – 1.97 89.28 – 1.97	Depositor EDS
% Data completeness (in resolution range)	98.6 (89.28-1.97) 98.7 (89.28-1.97)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.98 (at 1.97Å)	Xtriage
Refinement program	PHENIX (???)	Depositor
R, R_{free}	0.232 , 0.269 0.234 , 0.271	Depositor DCC
R_{free} test set	2000 reflections (1.83%)	wwPDB-VP
Wilson B-factor (Å ²)	30.3	Xtriage
Anisotropy	0.132	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 35.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11424	wwPDB-VP
Average B, all atoms (Å ²)	34.0	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 29.34 % 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 1.5769e-03. 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: A1B9W

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	0.15	0/2765	0.37	0/3746
1	B	0.16	0/2783	0.40	0/3770
1	C	0.13	0/2774	0.36	0/3758
1	D	0.16	0/2774	0.38	0/3758
All	All	0.15	0/11096	0.38	0/15032

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	2688	0	2640	25	1
1	B	2703	0	2653	21	0
1	C	2694	0	2648	28	1
1	D	2694	0	2648	32	0
2	A	37	0	0	0	0
2	B	37	0	0	0	0
2	C	37	0	0	0	0
2	D	37	0	0	2	0
3	A	107	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	152	0	0	0	0
3	C	77	0	0	1	0
3	D	161	0	0	2	0
All	All	11424	0	10589	106	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (106) 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:B:451:ILE:HB	1:B:468:LEU:HB3	1.64	0.78
1:D:434:THR:HG22	1:D:459:GLN:HE22	1.49	0.78
1:A:446:ARG:HD2	1:A:471:LYS:HB2	1.66	0.78
1:D:154:TYR:HE1	1:D:163:MET:HE1	1.49	0.75
1:D:451:ILE:HB	1:D:468:LEU:HB2	1.68	0.74
1:A:451:ILE:HB	1:A:468:LEU:HB2	1.73	0.70
1:B:190:LEU:HD13	1:B:248:LEU:HD21	1.73	0.70
1:A:268:ARG:HD3	1:A:447:GLN:HA	1.75	0.69
1:A:372:GLU:HG3	1:A:440:LEU:HD13	1.75	0.69
1:C:190:LEU:HD13	1:C:248:LEU:HD21	1.77	0.67
1:A:446:ARG:HH11	1:A:471:LYS:HB2	1.64	0.62
1:D:301:GLU:HG3	1:D:305:MET:HE2	1.82	0.61
1:D:172:THR:HG21	1:D:405:LEU:HB2	1.83	0.59
1:B:290:ILE:HG13	1:B:395:ALA:HB3	1.84	0.59
1:C:255:ILE:HG13	1:C:280:LEU:HD13	1.86	0.58
1:C:180:ASN:HA	1:C:400:ILE:HD12	1.85	0.57
1:D:437:GLY:HA3	1:D:454:VAL:O	2.05	0.57
1:D:154:TYR:CE1	1:D:163:MET:HE1	2.36	0.56
1:D:434:THR:HG23	1:D:458:ASP:HB2	1.88	0.56
1:A:172:THR:HG21	1:A:405:LEU:HB2	1.87	0.55
1:D:268:ARG:HD3	1:D:447:GLN:HA	1.87	0.55
1:C:259:PRO:HG2	1:C:270:LEU:HD23	1.89	0.54
1:A:190:LEU:HB2	1:A:252:VAL:HG11	1.89	0.54
1:B:441:LEU:HD22	1:B:451:ILE:HG13	1.91	0.52
1:D:446:ARG:HB2	1:D:471:LYS:HD2	1.91	0.52
1:C:244:GLU:HG3	1:C:275:HIS:CD2	2.44	0.52
1:D:475:PHE:HB3	1:D:477:TYR:CE2	2.45	0.52
1:B:218:THR:O	1:B:221[B]:GLN:HG2	2.10	0.51
1:D:446:ARG:HH11	1:D:471:LYS:HE3	1.74	0.51
1:C:182:THR:HG23	1:C:400:ILE:HD11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:376:LYS:NZ	3:D:609:HOH:O	2.43	0.51
1:C:218:THR:O	1:C:221[B]:GLN:HG2	2.11	0.51
1:D:290:ILE:HG12	1:D:395:ALA:HB3	1.93	0.51
1:A:277:LYS:HD3	1:A:286:MET:SD	2.51	0.51
1:A:218:THR:O	1:A:221:GLN:HG2	2.12	0.50
1:D:189:VAL:HG13	1:D:254:ILE:HG23	1.93	0.50
1:B:255:ILE:HG13	1:B:280:LEU:HD13	1.92	0.50
1:C:451:ILE:HG23	1:C:468:LEU:HB2	1.94	0.49
1:D:434:THR:HG22	1:D:459:GLN:NE2	2.23	0.48
1:D:469:ASP:OD2	1:D:471:LYS:HE2	2.14	0.48
1:B:364:LYS:HD3	1:B:366:GLY:H	1.79	0.47
1:D:215:GLU:OE2	2:D:501:A1B9W:O37	2.31	0.47
1:A:162:ASN:ND2	3:A:614:HOH:O	2.44	0.47
1:C:188:ILE:HB	1:C:252:VAL:HA	1.96	0.47
1:A:401:MET:HE2	1:A:403:VAL:HG22	1.96	0.47
1:A:248:LEU:HB2	1:A:279:TYR:CE1	2.50	0.47
1:A:295:LEU:O	1:A:353:SER:HA	2.14	0.46
1:D:268:ARG:CZ	1:D:443:ALA:HB1	2.45	0.46
1:C:341:VAL:HG22	1:C:419:VAL:HG22	1.96	0.46
1:A:451:ILE:HD11	1:A:470:LEU:HG	1.98	0.46
1:A:290:ILE:HG12	1:A:395:ALA:HB3	1.97	0.46
1:C:268:ARG:CZ	1:C:443:ALA:HB1	2.44	0.46
1:D:235:ARG:NH2	3:D:617:HOH:O	2.49	0.46
1:A:280:LEU:HD11	1:A:284:GLY:HA3	1.98	0.46
1:A:469:ASP:OD2	1:A:471:LYS:HG2	2.16	0.46
1:C:273:TYR:CZ	1:C:286:MET:HE2	2.52	0.45
1:D:256:ILE:HG22	1:D:287:PHE:HB2	1.98	0.45
1:D:441:LEU:HD22	1:D:451:ILE:HG13	1.98	0.45
1:C:186:ASP:HA	1:C:209:ARG:HB2	1.98	0.45
1:D:255:ILE:HG13	1:D:280:LEU:HD13	1.97	0.45
1:C:448:SER:HB2	1:C:471:LYS:HD3	1.99	0.45
1:C:277:LYS:HD3	1:C:286:MET:SD	2.57	0.45
1:C:446:ARG:O	1:C:471:LYS:HE3	2.17	0.45
1:C:278:LYS:HE3	1:C:279:TYR:CZ	2.52	0.44
1:B:214:VAL:HA	1:B:239:ILE:O	2.17	0.44
1:C:451:ILE:HD11	1:C:453:ILE:HD11	2.00	0.44
1:C:351:ALA:HA	1:C:380:LEU:HD22	1.99	0.44
1:A:334:GLU:HA	1:A:337[B]:ARG:NH1	2.32	0.44
1:D:182:THR:HG23	1:D:400:ILE:HD11	2.00	0.44
1:B:268:ARG:NH1	1:B:444:ASN:O	2.51	0.43
1:C:194:CYS:SG	1:C:213:ALA:HB1	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:ARG:HG3	1:C:416:TRP:HH2	1.82	0.43
1:C:377:PHE:O	1:C:434:THR:HA	2.19	0.43
1:D:280:LEU:HG	1:D:284:GLY:HA3	2.01	0.43
1:D:456:GLN:HB3	1:D:463:LYS:HG3	1.99	0.43
1:D:188:ILE:HB	1:D:252:VAL:HA	1.98	0.43
1:C:166:ASP:OD2	1:C:415[A]:HIS:ND1	2.48	0.43
1:A:208:ALA:HB3	1:A:211:ILE:HD11	2.01	0.42
1:B:292:ASP:O	1:B:392:PHE:HA	2.19	0.42
1:B:456:GLN:HA	1:B:462:SER:O	2.19	0.42
1:B:301:GLU:O	1:B:305:MET:HG2	2.19	0.42
1:B:244:GLU:HG3	1:B:275:HIS:CD2	2.55	0.42
1:B:278:LYS:HE3	1:B:279:TYR:CZ	2.55	0.42
1:B:387:GLY:HA3	1:B:421:CYS:O	2.20	0.42
1:C:325:SER:O	3:C:601:HOH:O	2.22	0.42
1:A:328:ARG:NH1	3:A:607:HOH:O	2.34	0.41
1:D:350[A]:MET:SD	1:D:385:VAL:HG22	2.60	0.41
1:B:371:ILE:HB	1:B:441:LEU:HB2	2.03	0.41
1:D:242:LYS:HA	2:D:501:A1B9W:N03	2.35	0.41
1:C:297:PRO:HD3	1:C:377:PHE:CD1	2.56	0.41
1:B:161:GLN:O	1:B:165:GLN:HG3	2.21	0.41
1:B:190:LEU:HB2	1:B:252:VAL:HG11	2.02	0.41
1:C:456:GLN:OE1	1:C:463:LYS:HE3	2.21	0.41
1:D:278:LYS:HD2	1:D:279:TYR:CZ	2.56	0.41
1:A:475:PHE:HB3	1:A:477:TYR:CZ	2.56	0.41
1:B:307:GLN:HG3	1:B:422:LEU:HD12	2.03	0.41
1:B:421:CYS:SG	1:B:453:ILE:HD12	2.61	0.41
1:A:267:GLU:HB2	3:A:619:HOH:O	2.21	0.40
1:A:242:LYS:O	1:A:246:VAL:HG13	2.21	0.40
1:D:333:ASP:O	1:D:337[B]:ARG:HG3	2.22	0.40
1:A:337[B]:ARG:HG2	1:A:467:LEU:O	2.21	0.40
1:C:302:GLN:O	1:C:306:GLU:HG3	2.22	0.40
1:D:421:CYS:SG	1:D:468:LEU:HG	2.62	0.40
1:A:415[A]:HIS:H	1:A:415[A]:HIS:HD1	1.67	0.40
1:B:401:MET:HE2	1:B:401:MET:HB3	1.95	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:VAL:O	1:C:370[B]:ARG:NH1[4_555]	2.14	0.06

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	334/331 (101%)	328 (98%)	6 (2%)	0	100	100
1	B	336/331 (102%)	324 (96%)	12 (4%)	0	100	100
1	C	335/331 (101%)	327 (98%)	8 (2%)	0	100	100
1	D	335/331 (101%)	327 (98%)	8 (2%)	0	100	100
All	All	1340/1324 (101%)	1306 (98%)	34 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	290/287 (101%)	285 (98%)	5 (2%)	53	48
1	B	292/287 (102%)	285 (98%)	7 (2%)	43	35
1	C	291/287 (101%)	281 (97%)	10 (3%)	32	22
1	D	291/287 (101%)	282 (97%)	9 (3%)	35	26
All	All	1164/1148 (101%)	1133 (97%)	31 (3%)	40	31

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	152	GLN
1	A	248	LEU

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Mol	Chain	Res	Type
1	A	258	GLU
1	A	446	ARG
1	A	470	LEU
1	B	148	VAL
1	B	258	GLU
1	B	312	ASN
1	B	430	LYS
1	B	441	LEU
1	B	452	SER
1	B	471	LYS
1	C	159	GLN
1	C	221[A]	GLN
1	C	221[B]	GLN
1	C	258	GLU
1	C	295	LEU
1	C	302	GLN
1	C	380	LEU
1	C	424	GLN
1	C	445	LYS
1	C	451	ILE
1	D	148	VAL
1	D	247	SER
1	D	258	GLU
1	D	278	LYS
1	D	346	ILE
1	D	405	LEU
1	D	425	SER
1	D	468	LEU
1	D	470	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	359	ASN
1	B	369	HIS

5.3.3 RNA ⓘ

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	A1B9W	B	501	-	41,41,41	1.46	6 (14%)	56,57,57	1.55	13 (23%)
2	A1B9W	A	501	-	41,41,41	1.52	8 (19%)	56,57,57	1.48	14 (25%)
2	A1B9W	C	501	-	41,41,41	1.45	6 (14%)	56,57,57	1.41	12 (21%)
2	A1B9W	D	501	-	41,41,41	1.54	8 (19%)	56,57,57	1.58	14 (25%)

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	A1B9W	B	501	-	-	5/18/34/34	0/5/5/5
2	A1B9W	A	501	-	-	4/18/34/34	0/5/5/5
2	A1B9W	C	501	-	-	10/18/34/34	0/5/5/5
2	A1B9W	D	501	-	-	4/18/34/34	0/5/5/5

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	A1B9W	C09-N10	3.34	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	A1B9W	C09-N10	2.99	1.42	1.37
2	A	501	A1B9W	C23-C24	2.99	1.56	1.49
2	B	501	A1B9W	C23-C24	2.89	1.55	1.49
2	D	501	A1B9W	C23-C24	2.88	1.55	1.49
2	D	501	A1B9W	C09-N10	2.86	1.42	1.37
2	A	501	A1B9W	C09-N10	2.73	1.42	1.37
2	D	501	A1B9W	C22-C21	2.61	1.43	1.39
2	C	501	A1B9W	C23-C24	2.50	1.55	1.49
2	B	501	A1B9W	C22-C21	2.49	1.43	1.39
2	D	501	A1B9W	C11-N10	2.48	1.53	1.46
2	A	501	A1B9W	C22-C21	2.41	1.43	1.39
2	D	501	A1B9W	C09-N08	2.39	1.36	1.31
2	B	501	A1B9W	C09-N08	2.32	1.36	1.31
2	A	501	A1B9W	C11-N10	2.29	1.52	1.46
2	C	501	A1B9W	C11-N10	2.28	1.52	1.46
2	D	501	A1B9W	C22-C23	2.21	1.43	1.39
2	B	501	A1B9W	C11-N10	2.20	1.52	1.46
2	A	501	A1B9W	C09-N08	2.19	1.35	1.31
2	D	501	A1B9W	C07-C06	2.17	1.43	1.39
2	C	501	A1B9W	C22-C21	2.17	1.43	1.39
2	C	501	A1B9W	C09-N08	2.17	1.35	1.31
2	C	501	A1B9W	C07-C06	2.11	1.42	1.39
2	B	501	A1B9W	C22-C23	2.09	1.43	1.39
2	A	501	A1B9W	C20-C21	2.08	1.56	1.51
2	A	501	A1B9W	C22-C23	2.05	1.43	1.39
2	A	501	A1B9W	C30-C29	2.04	1.42	1.38
2	D	501	A1B9W	C27-CL28	2.00	1.79	1.74

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	A1B9W	C14-S15-C16	4.05	114.30	102.26
2	D	501	A1B9W	C22-C23-C24	3.65	126.96	120.84
2	B	501	A1B9W	C31-C23-C22	-3.62	113.25	118.23
2	D	501	A1B9W	C31-C23-C22	-3.60	113.27	118.23
2	B	501	A1B9W	C14-S15-C16	3.60	112.94	102.26
2	A	501	A1B9W	C31-C23-C22	-3.34	113.63	118.23
2	C	501	A1B9W	C14-S15-C16	3.31	112.09	102.26
2	C	501	A1B9W	C31-C23-C22	-3.27	113.72	118.23
2	B	501	A1B9W	C07-C06-N10	3.22	109.32	105.81
2	B	501	A1B9W	C22-C23-C24	3.19	126.18	120.84
2	A	501	A1B9W	C14-S15-C16	3.15	111.63	102.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	A1B9W	C23-C22-C21	3.14	125.38	121.20
2	A	501	A1B9W	C26-C25-C24	3.10	125.10	121.12
2	D	501	A1B9W	C07-C06-N10	3.00	109.08	105.81
2	B	501	A1B9W	C32-C31-C23	2.97	123.92	120.54
2	D	501	A1B9W	C23-C22-C21	2.91	125.09	121.20
2	B	501	A1B9W	C26-C25-C24	2.85	124.78	121.12
2	C	501	A1B9W	C23-C22-C21	2.83	124.97	121.20
2	C	501	A1B9W	C22-C23-C24	2.83	125.57	120.84
2	B	501	A1B9W	C06-C07-N08	-2.80	107.38	110.58
2	D	501	A1B9W	C06-C07-N08	-2.77	107.41	110.58
2	A	501	A1B9W	C07-C06-N10	2.76	108.82	105.81
2	A	501	A1B9W	C30-C24-C25	-2.74	112.78	117.68
2	D	501	A1B9W	C26-C25-C24	2.73	124.63	121.12
2	B	501	A1B9W	C30-C24-C25	-2.72	112.81	117.68
2	B	501	A1B9W	C23-C22-C21	2.70	124.81	121.20
2	C	501	A1B9W	C07-C06-N10	2.70	108.76	105.81
2	D	501	A1B9W	C30-C24-C25	-2.65	112.93	117.68
2	A	501	A1B9W	C06-C07-N08	-2.64	107.56	110.58
2	C	501	A1B9W	C26-C25-C24	2.58	124.44	121.12
2	D	501	A1B9W	C32-C31-C23	2.57	123.46	120.54
2	C	501	A1B9W	C30-C24-C25	-2.50	113.20	117.68
2	D	501	A1B9W	C29-C30-C24	2.50	124.33	121.12
2	B	501	A1B9W	C29-C30-C24	2.47	124.30	121.12
2	C	501	A1B9W	C29-C30-C24	2.45	124.27	121.12
2	A	501	A1B9W	C14-C13-C34	-2.42	109.01	115.06
2	A	501	A1B9W	C07-C06-N05	-2.35	123.49	126.72
2	C	501	A1B9W	C06-C07-N08	-2.34	107.91	110.58
2	A	501	A1B9W	C22-C23-C24	2.34	124.76	120.84
2	D	501	A1B9W	C07-C06-N05	-2.34	123.50	126.72
2	C	501	A1B9W	C32-C31-C23	2.29	123.14	120.54
2	C	501	A1B9W	C14-C13-C34	-2.23	109.47	115.06
2	A	501	A1B9W	C29-C30-C24	2.23	123.99	121.12
2	B	501	A1B9W	C14-C13-C34	-2.21	109.54	115.06
2	B	501	A1B9W	C07-C06-N05	-2.15	123.75	126.72
2	A	501	A1B9W	C32-C31-C23	2.15	122.98	120.54
2	C	501	A1B9W	C07-C06-N05	-2.14	123.77	126.72
2	A	501	A1B9W	C07-N08-C09	2.11	106.77	103.45
2	B	501	A1B9W	C07-N08-C09	2.11	106.76	103.45
2	D	501	A1B9W	O12-C11-C36	-2.08	102.16	106.62
2	D	501	A1B9W	C07-N08-C09	2.07	106.70	103.45
2	D	501	A1B9W	C14-C13-C34	-2.02	110.00	115.06
2	A	501	A1B9W	C30-C24-C23	2.02	124.74	121.25

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	A1B9W	C34-C13-C14-S15
2	B	501	A1B9W	O12-C13-C14-S15
2	C	501	A1B9W	C34-C13-C14-S15
2	C	501	A1B9W	O12-C13-C14-S15
2	D	501	A1B9W	C34-C13-C14-S15
2	D	501	A1B9W	O12-C13-C14-S15
2	D	501	A1B9W	C17-C16-S15-C14
2	C	501	A1B9W	C17-C16-S15-C14
2	C	501	A1B9W	C16-C17-C18-N19
2	D	501	A1B9W	C16-C17-C18-N19
2	C	501	A1B9W	C22-C23-C24-C25
2	C	501	A1B9W	C31-C23-C24-C30
2	C	501	A1B9W	C31-C23-C24-C25
2	C	501	A1B9W	C22-C23-C24-C30
2	A	501	A1B9W	C16-C17-C18-N19
2	A	501	A1B9W	C34-C13-C14-S15
2	A	501	A1B9W	O12-C13-C14-S15
2	A	501	A1B9W	C21-C20-N19-C18
2	C	501	A1B9W	C21-C20-N19-C18
2	B	501	A1B9W	C22-C23-C24-C25
2	B	501	A1B9W	C31-C23-C24-C30
2	B	501	A1B9W	C31-C23-C24-C25
2	C	501	A1B9W	C36-C11-N10-C09

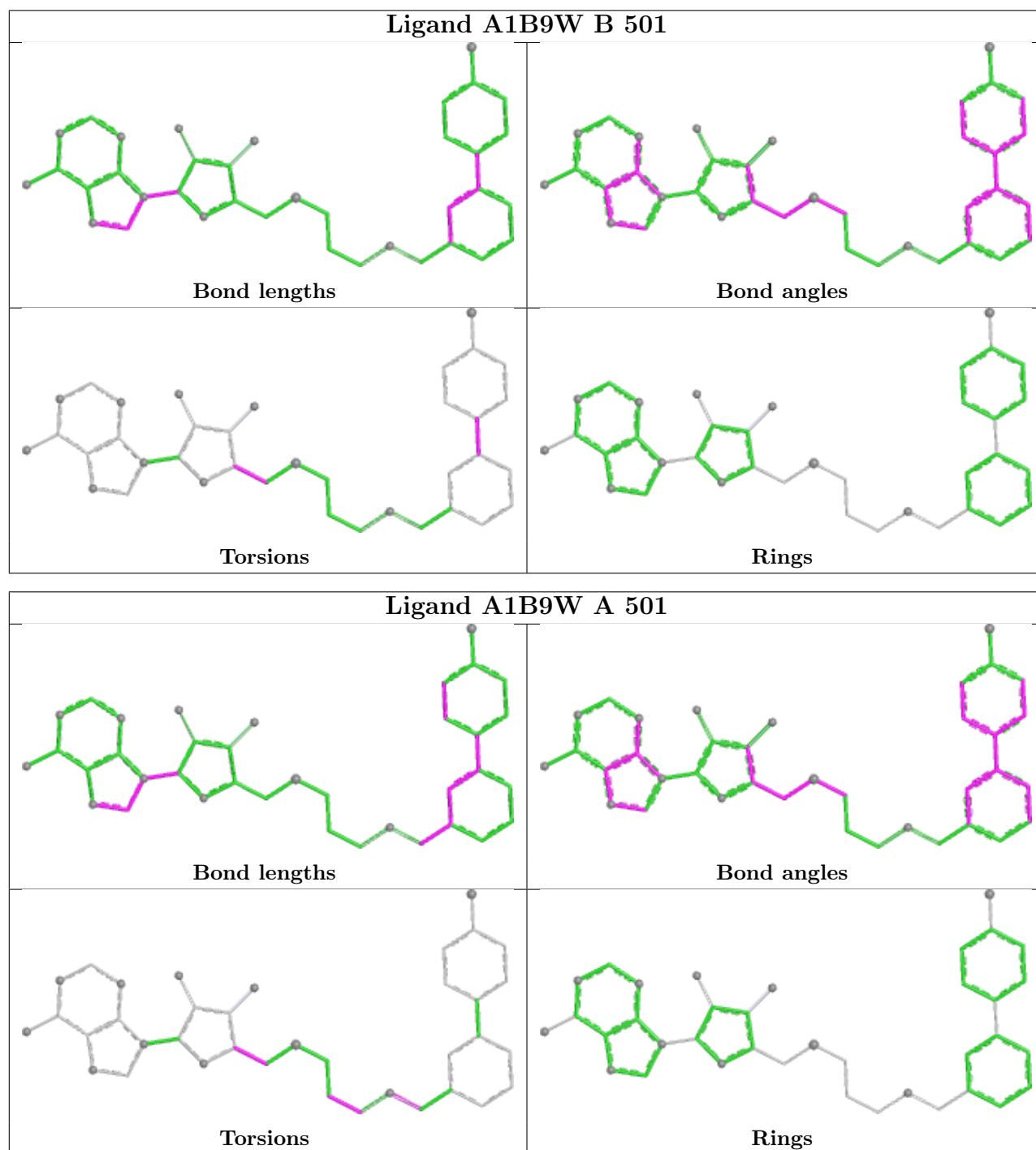
There are no ring outliers.

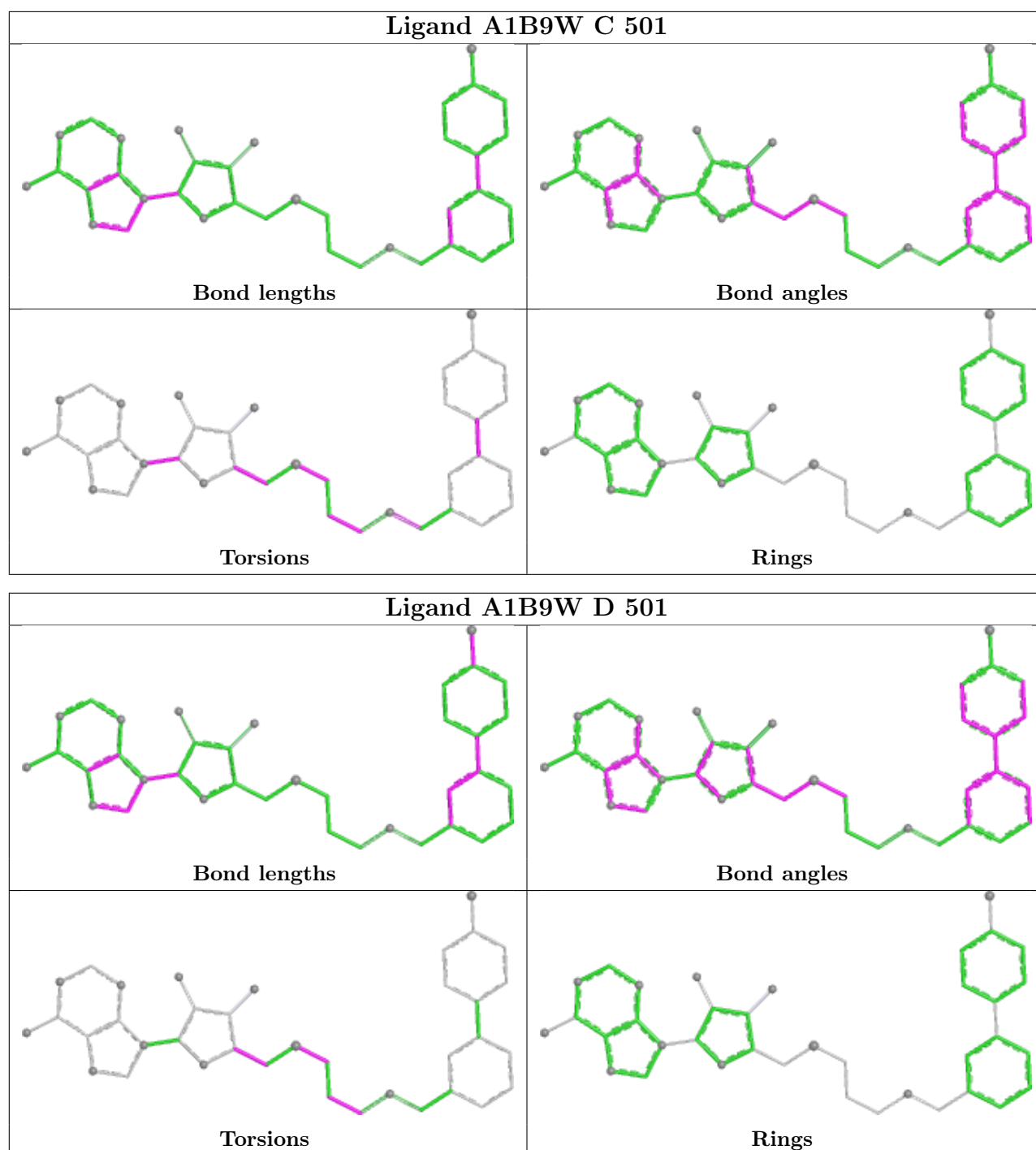
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	A1B9W	2	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	331/331 (100%)	0.57	14 (4%) 40 50	18, 36, 50, 64	5 (1%)
1	B	331/331 (100%)	0.25	9 (2%) 56 66	11, 30, 46, 66	7 (2%)
1	C	331/331 (100%)	0.72	20 (6%) 27 36	16, 39, 53, 85	6 (1%)
1	D	331/331 (100%)	0.23	8 (2%) 59 69	11, 27, 43, 62	6 (1%)
All	All	1324/1324 (100%)	0.44	51 (3%) 43 53	11, 34, 49, 85	24 (1%)

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	148	VAL	6.1
1	D	477	TYR	5.7
1	C	477	TYR	4.3
1	D	148	VAL	3.9
1	C	147	ALA	3.8
1	A	477	TYR	3.6
1	D	152	GLN	3.5
1	B	147	ALA	3.4
1	C	475	PHE	3.4
1	A	315	TYR	3.3
1	C	152	GLN	3.3
1	C	415[A]	HIS	3.2
1	A	283	SER	3.2
1	B	477	TYR	3.1
1	C	439[A]	CYS	3.0
1	C	150	TYR	3.0
1	C	283	SER	2.9
1	C	212	TYR	2.8
1	D	147	ALA	2.8
1	D	475	PHE	2.8
1	A	475	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	151	PHE	2.7
1	C	149	GLN	2.7
1	D	186	ASP	2.7
1	A	308	PHE	2.6
1	C	451	ILE	2.6
1	D	150	TYR	2.6
1	A	147	ALA	2.5
1	D	283	SER	2.5
1	B	308	PHE	2.5
1	C	153	PHE	2.5
1	B	262	TYR	2.4
1	B	283	SER	2.4
1	A	415[A]	HIS	2.4
1	A	467	LEU	2.4
1	A	446	ARG	2.3
1	A	469	ASP	2.3
1	A	249	PRO	2.3
1	C	249	PRO	2.3
1	C	431	ALA	2.3
1	C	247	SER	2.3
1	B	443	ALA	2.2
1	C	429	ALA	2.2
1	A	262	TYR	2.2
1	C	156	TYR	2.1
1	A	312	ASN	2.1
1	C	432	GLY	2.1
1	A	248	LEU	2.1
1	B	467	LEU	2.1
1	B	446	ARG	2.1
1	B	148	VAL	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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

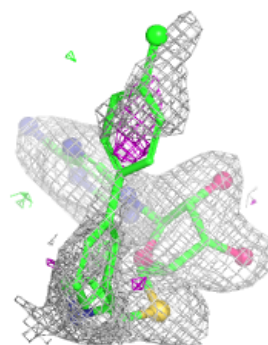
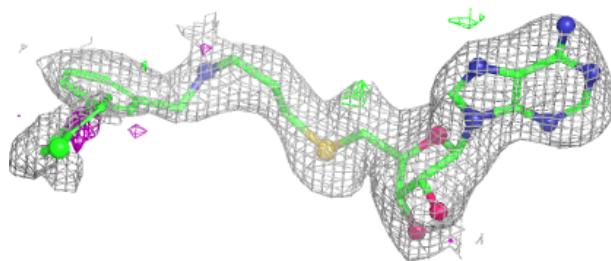
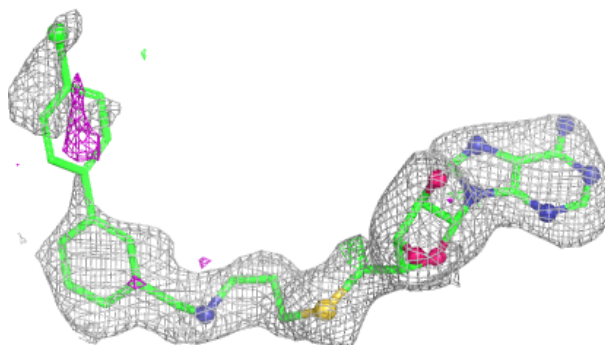
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	A1B9W	C	501	37/37	0.79	0.15	46,52,69,97	0
2	A1B9W	B	501	37/37	0.85	0.14	27,34,67,91	0
2	A1B9W	A	501	37/37	0.88	0.14	26,42,72,118	0
2	A1B9W	D	501	37/37	0.88	0.13	23,37,67,91	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.

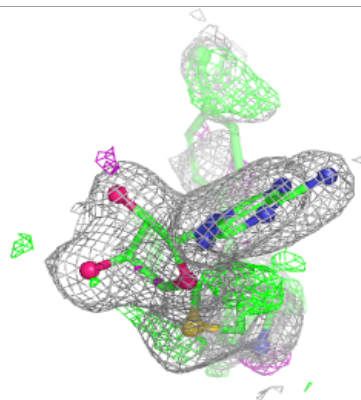
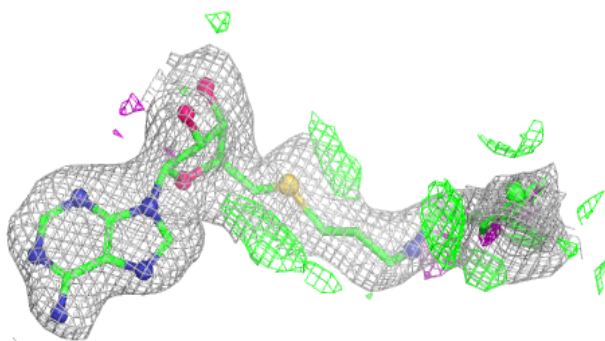
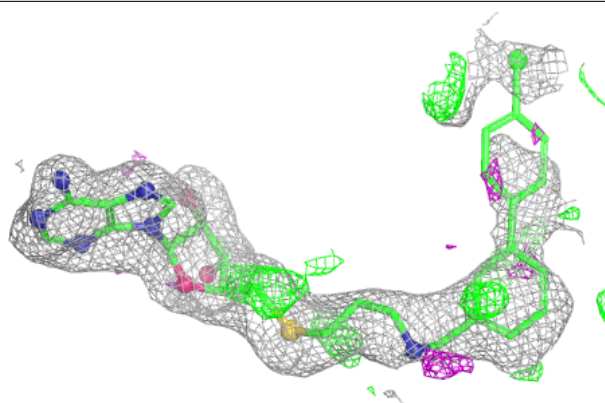
Electron density around A1B9W C 501:

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

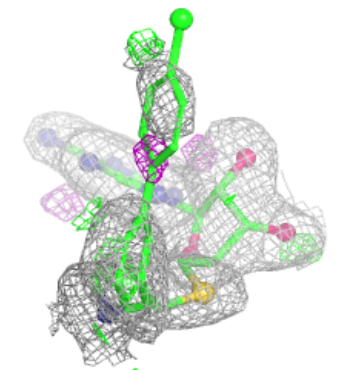
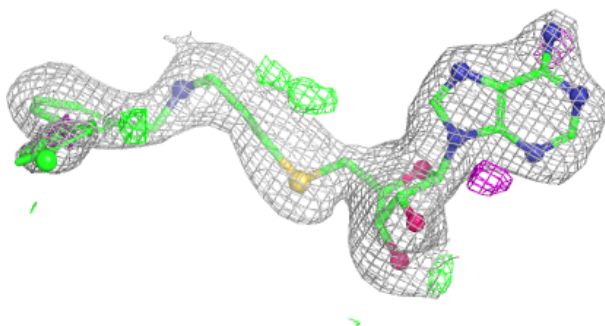
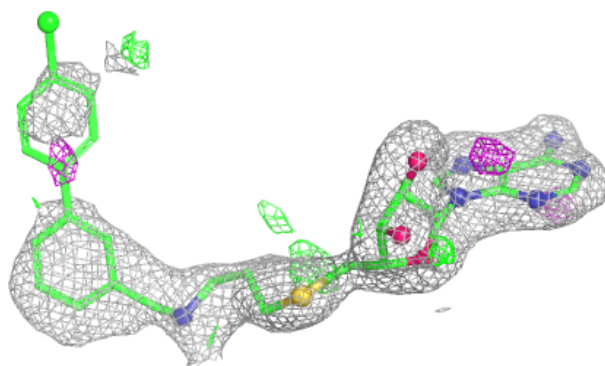


Electron density around A1B9W B 501:

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

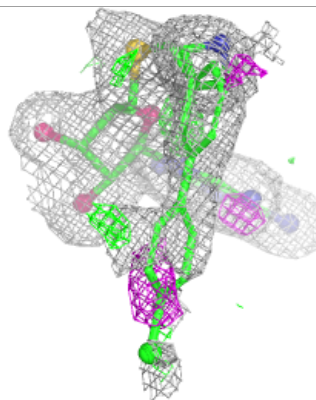
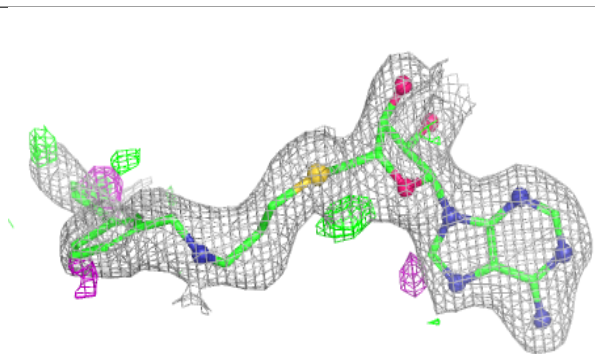
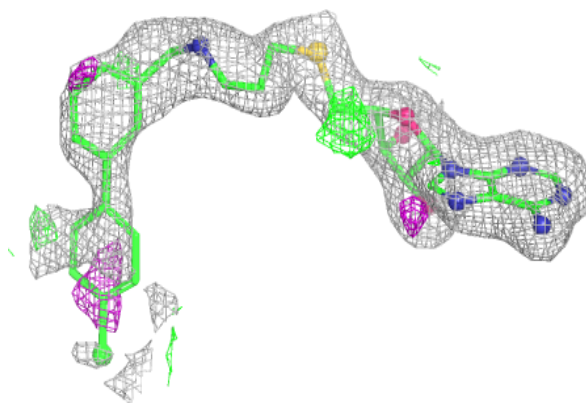
**Electron density around A1B9W A 501:**

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



Electron density around A1B9W D 501:

$2mF_o-DF_c$ (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.