



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2026 – 11:31 am BST

PDB ID : 8RPN / pdb_00008rpn
Title : hJAK3 in complex with LAW931 inhibitor
Authors : Lozoya, E.; Bach, J.; Lammens, A.
Deposited on : 2024-01-16
Resolution : 2.72 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 : 1.8.4, CSD as541be (2020)
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 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

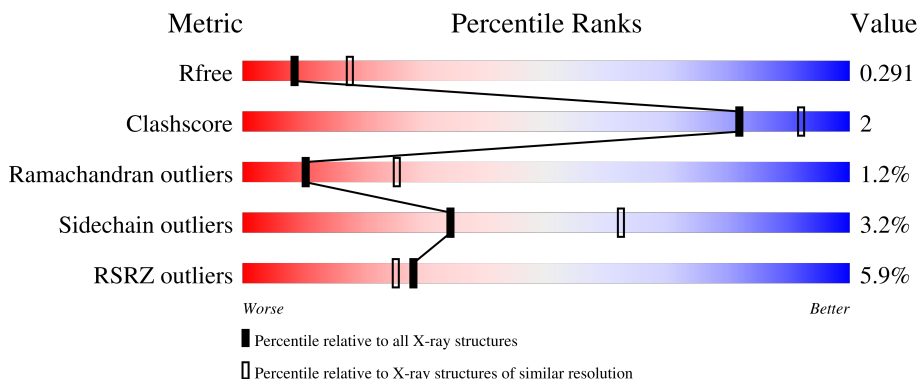
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.72 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	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
Sidechain outliers	187428	4585 (2.74-2.70)
RSRZ outliers	180081	4348 (2.74-2.70)

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	298	4% 79% 7% 13%
1	B	298	6% 79% 8% 12%
1	C	298	5% 75% 11% 13%
1	D	298	5% 79% 8% 13%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8515 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.

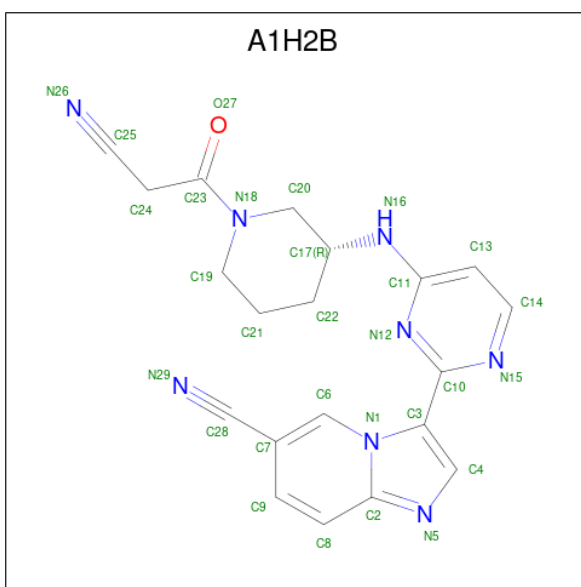
- Molecule 1 is a protein called Tyrosine-protein kinase JAK3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	P	S	0	0	0
			2086	1334	359	377	2	14			
1	B	262	Total	C	N	O	P	S	0	0	0
			2108	1345	364	383	2	14			
1	C	260	Total	C	N	O	P	S	0	0	0
			2094	1335	362	382	2	13			
1	D	260	Total	C	N	O	P	S	0	0	0
			2098	1340	362	380	2	14			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	814	PRO	-	expression tag	UNP P52333
A	815	THR	-	expression tag	UNP P52333
A	1048	SER	CYS	engineered mutation	UNP P52333
B	814	PRO	-	expression tag	UNP P52333
B	815	THR	-	expression tag	UNP P52333
B	1048	SER	CYS	engineered mutation	UNP P52333
C	814	PRO	-	expression tag	UNP P52333
C	815	THR	-	expression tag	UNP P52333
C	1048	SER	CYS	engineered mutation	UNP P52333
D	814	PRO	-	expression tag	UNP P52333
D	815	THR	-	expression tag	UNP P52333
D	1048	SER	CYS	engineered mutation	UNP P52333

- Molecule 2 is 3-[4-[(3 {R})-1-(2-cyanoethanoyl)piperidin-3-yl]amino]pyrimidin-2-yl]imidazo [1,2-a]pyridine-6-carbonitrile (CCD ID: A1H2B) (formula: C₂₀H₁₈N₈O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			29	20	8	1		
2	B	1	Total	C	N	O	0	0
			29	20	8	1		
2	C	1	Total	C	N	O	0	0
			29	20	8	1		
2	D	1	Total	C	N	O	0	0
			29	20	8	1		

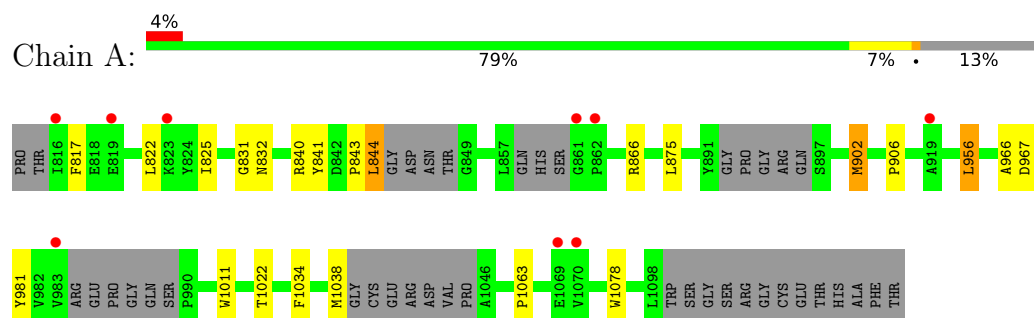
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	O	0	0
			4	4		
3	B	1	Total	O	0	0
			1	1		
3	C	4	Total	O	0	0
			4	4		
3	D	4	Total	O	0	0
			4	4		

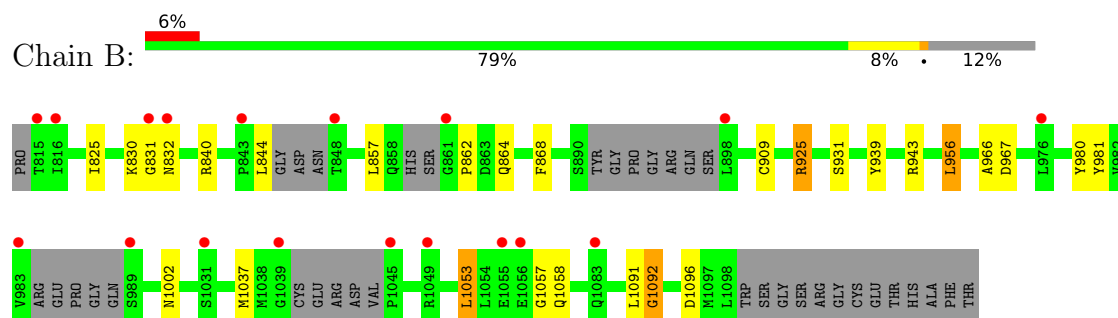
3 Residue-property plots [i](#)

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.

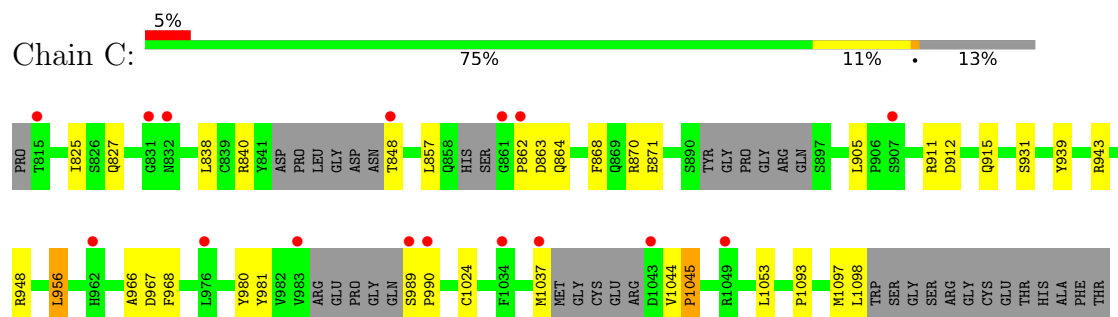
• Molecule 1: Tyrosine-protein kinase JAK3



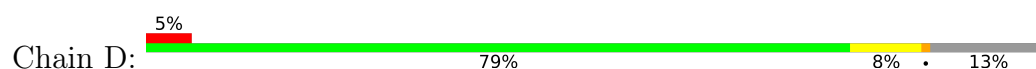
• Molecule 1: Tyrosine-protein kinase JAK3

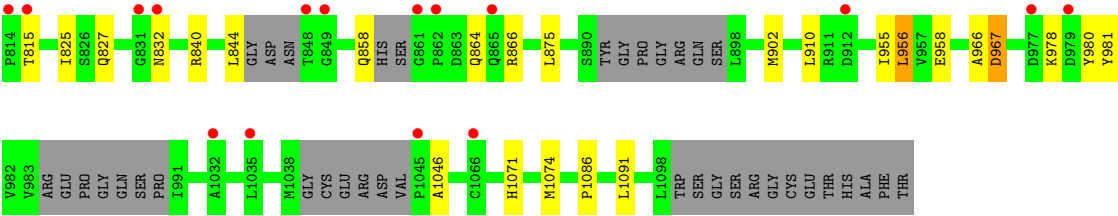


• Molecule 1: Tyrosine-protein kinase JAK3



• Molecule 1: Tyrosine-protein kinase JAK3





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	57.09Å 69.10Å 93.29Å 86.31° 83.62° 81.58°	Depositor
Resolution (Å)	46.73 – 2.72 46.73 – 2.72	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.73-2.72) 95.3 (46.73-2.72)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.247 , 0.287 0.250 , 0.291	Depositor DCC
R_{free} test set	1075 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å ²)	44.3	Xtriage
Anisotropy	0.562	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 33.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	8515	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.49% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PTR, A1H2B

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	0.47	0/2096	0.73	0/2822
1	B	0.46	0/2118	0.72	0/2853
1	C	0.50	0/2103	0.73	0/2834
1	D	0.47	0/2108	0.72	0/2839
All	All	0.48	0/8425	0.73	0/11348

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	2086	0	2076	12	0
1	B	2108	0	2099	10	0
1	C	2094	0	2083	13	0
1	D	2098	0	2093	8	0
2	A	29	0	0	1	0
2	B	29	0	0	0	0
2	C	29	0	0	0	0
2	D	29	0	0	0	0
3	A	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	4	0	0	0	0
3	D	4	0	0	1	0
All	All	8515	0	8351	42	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 (42) 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:956:LEU:HD22	1:B:966:ALA:HB2	1.81	0.63
1:B:825:ILE:HD11	1:B:840:ARG:HB2	1.88	0.54
1:C:956:LEU:HD22	1:C:966:ALA:HB2	1.89	0.54
1:B:939:TYR:O	1:B:943:ARG:HG2	2.10	0.52
1:C:1093:PRO:O	1:C:1097:MET:HG2	2.10	0.51
1:B:1002:ASN:N	1:B:1002:ASN:HD22	2.09	0.50
1:D:956:LEU:HD22	1:D:966:ALA:HB2	1.94	0.49
1:A:817:PHE:HB3	1:A:822:LEU:HD11	1.95	0.48
1:D:1071:HIS:HA	1:D:1074:MET:HE3	1.95	0.48
1:A:956:LEU:HD22	1:A:966:ALA:HB2	1.96	0.47
1:D:910:LEU:HD22	1:D:955:ILE:HG21	1.95	0.47
1:C:857:LEU:HD21	1:C:868:PHE:HB2	1.96	0.46
1:C:825:ILE:HD11	1:C:840:ARG:HB2	1.97	0.46
1:B:931:SER:OG	1:B:1096:ASP:OD1	2.34	0.46
1:B:1037:MET:HE2	1:B:1053:LEU:HD21	1.98	0.45
1:A:1022:THR:HG22	1:A:1063:PRO:HB3	1.98	0.44
1:B:925:ARG:HA	1:B:925:ARG:HE	1.82	0.44
1:A:831:GLY:HA3	2:A:1201:A1H2B:C24	2.48	0.44
1:D:825:ILE:HD11	1:D:840:ARG:HB2	1.99	0.44
1:D:875:LEU:HD22	1:D:902:MET:HE3	1.98	0.44
1:A:875:LEU:HD22	1:A:902:MET:HE3	2.00	0.44
1:B:857:LEU:HD21	1:B:868:PHE:HB2	1.99	0.44
1:A:825:ILE:HD11	1:A:840:ARG:HB2	2.00	0.43
1:D:858:GLN:C	3:D:1302:HOH:O	2.61	0.43
1:C:989:SER:N	1:C:990:PRO:CD	2.82	0.42
1:C:1037:MET:HE2	1:C:1053:LEU:HD21	2.01	0.42
1:A:956:LEU:CD2	1:A:966:ALA:HB2	2.50	0.42
1:A:906:PRO:HB2	1:C:838:LEU:HD21	2.01	0.42
1:A:822:LEU:HD12	1:A:841:TYR:HD1	1.84	0.42
1:A:1034:PHE:O	1:A:1038:MET:HE3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:832:ASN:ND2	1:D:967:ASP:OD1	2.53	0.42
1:C:912:ASP:HA	1:C:915:GLN:HE21	1.85	0.42
1:C:871:GLU:HG3	1:C:968:PHE:HB2	2.01	0.41
1:B:1091:LEU:O	1:B:1092:GLY:C	2.64	0.41
1:C:905:LEU:HD22	1:C:956:LEU:HB3	2.02	0.41
1:C:911:ARG:HA	1:C:1024:CYS:SG	2.61	0.41
1:A:1011:TRP:CE3	1:A:1078:TRP:HA	2.55	0.41
1:A:843:PRO:C	1:A:844:LEU:HD23	2.46	0.40
1:C:1044:VAL:O	1:C:1045:PRO:C	2.63	0.40
1:D:1086:PRO:HG2	1:D:1091:LEU:HD21	2.03	0.40
1:C:939:TYR:O	1:C:943:ARG:HG2	2.21	0.40
1:B:1053:LEU:O	1:B:1057:GLY:O	2.40	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	244/298 (82%)	233 (96%)	10 (4%)	1 (0%)	30	52
1	B	248/298 (83%)	235 (95%)	8 (3%)	5 (2%)	6	14
1	C	246/298 (83%)	234 (95%)	9 (4%)	3 (1%)	10	25
1	D	246/298 (83%)	232 (94%)	11 (4%)	3 (1%)	10	25
All	All	984/1192 (83%)	934 (95%)	38 (4%)	12 (1%)	10	25

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	815	THR
1	D	1046	ALA
1	B	831	GLY

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Mol	Chain	Res	Type
1	C	967	ASP
1	A	967	ASP
1	D	967	ASP
1	B	967	ASP
1	B	1058	GLN
1	C	862	PRO
1	B	862	PRO
1	B	1092	GLY
1	C	1045	PRO

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	225/257 (88%)	220 (98%)	5 (2%)	45	72
1	B	228/257 (89%)	220 (96%)	8 (4%)	32	59
1	C	227/257 (88%)	218 (96%)	9 (4%)	28	55
1	D	227/257 (88%)	220 (97%)	7 (3%)	35	63
All	All	907/1028 (88%)	878 (97%)	29 (3%)	34	62

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	832	ASN
1	A	844	LEU
1	A	866	ARG
1	A	902	MET
1	A	956	LEU
1	B	830	LYS
1	B	832	ASN
1	B	844	LEU
1	B	864	GLN
1	B	909	CYS
1	B	925	ARG
1	B	956	LEU

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Mol	Chain	Res	Type
1	B	1053	LEU
1	C	827	GLN
1	C	848	THR
1	C	863	ASP
1	C	864	GLN
1	C	870	ARG
1	C	931	SER
1	C	948	ARG
1	C	956	LEU
1	C	1098	LEU
1	D	827	GLN
1	D	844	LEU
1	D	864	GLN
1	D	866	ARG
1	D	956	LEU
1	D	958	GLU
1	D	978	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	827	GLN
1	A	856	GLN
1	A	865	GLN
1	A	869	GLN
1	A	915	GLN
1	B	821	HIS
1	B	827	GLN
1	B	864	GLN
1	B	869	GLN
1	B	879	HIS
1	B	1002	ASN
1	C	827	GLN
1	C	856	GLN
1	C	864	GLN
1	C	869	GLN
1	C	873	GLN
1	C	915	GLN
1	D	858	GLN
1	D	864	GLN
1	D	869	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues 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
1	PTR	D	981	1	15,16,17	2.03	1 (6%)	19,22,24	0.43	0
1	PTR	D	980	1	15,16,17	2.01	1 (6%)	19,22,24	0.65	1 (5%)
1	PTR	B	981	1	15,16,17	2.03	2 (13%)	19,22,24	0.58	0
1	PTR	B	980	1	15,16,17	1.93	2 (13%)	19,22,24	0.60	0
1	PTR	A	981	1	15,16,17	1.99	1 (6%)	19,22,24	0.57	0
1	PTR	C	980	1	15,16,17	2.03	1 (6%)	19,22,24	0.48	0
1	PTR	A	980	1	15,16,17	1.94	2 (13%)	19,22,24	0.62	0
1	PTR	C	981	1	15,16,17	1.92	1 (6%)	19,22,24	0.67	0

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
1	PTR	D	981	1	-	0/10/11/13	0/1/1/1
1	PTR	D	980	1	-	0/10/11/13	0/1/1/1
1	PTR	B	981	1	-	0/10/11/13	0/1/1/1
1	PTR	B	980	1	-	0/10/11/13	0/1/1/1
1	PTR	A	981	1	-	0/10/11/13	0/1/1/1
1	PTR	C	980	1	-	0/10/11/13	0/1/1/1
1	PTR	A	980	1	-	0/10/11/13	0/1/1/1
1	PTR	C	981	1	-	0/10/11/13	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	980	PTR	OH-CZ	-7.41	1.23	1.40
1	D	981	PTR	OH-CZ	-7.39	1.23	1.40
1	C	980	PTR	OH-CZ	-7.33	1.24	1.40
1	B	981	PTR	OH-CZ	-7.13	1.24	1.40
1	A	981	PTR	OH-CZ	-7.12	1.24	1.40
1	B	980	PTR	OH-CZ	-7.04	1.24	1.40
1	A	980	PTR	OH-CZ	-7.04	1.24	1.40
1	C	981	PTR	OH-CZ	-7.03	1.24	1.40
1	A	980	PTR	P-OH	2.26	1.62	1.59
1	B	981	PTR	P-OH	2.13	1.62	1.59
1	B	980	PTR	P-OH	2.02	1.62	1.59

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	980	PTR	O2P-P-OH	2.40	112.75	105.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	A1H2B	C	1201	-	30,32,32	1.77	5 (16%)	31,44,44	2.39	11 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	A1H2B	B	1201	-	30,32,32	1.93	8 (26%)	31,44,44	2.23	12 (38%)
2	A1H2B	A	1201	-	30,32,32	1.85	7 (23%)	31,44,44	2.31	11 (35%)
2	A1H2B	D	1201	-	30,32,32	1.88	8 (26%)	31,44,44	2.17	13 (41%)

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	A1H2B	C	1201	-	-	0/12/27/27	0/4/4/4
2	A1H2B	B	1201	-	-	0/12/27/27	0/4/4/4
2	A1H2B	A	1201	-	-	0/12/27/27	0/4/4/4
2	A1H2B	D	1201	-	-	0/12/27/27	0/4/4/4

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1201	A1H2B	C3-N1	-5.01	1.34	1.39
2	A	1201	A1H2B	C2-N1	-4.76	1.33	1.39
2	D	1201	A1H2B	C3-N1	-4.74	1.34	1.39
2	B	1201	A1H2B	C2-N1	-4.60	1.33	1.39
2	D	1201	A1H2B	C2-N1	-4.52	1.33	1.39
2	C	1201	A1H2B	C3-N1	-4.48	1.34	1.39
2	A	1201	A1H2B	C3-N1	-4.43	1.34	1.39
2	C	1201	A1H2B	C2-N1	-4.38	1.33	1.39
2	D	1201	A1H2B	C10-N12	3.95	1.38	1.34
2	B	1201	A1H2B	C10-N12	3.92	1.38	1.34
2	A	1201	A1H2B	C10-N12	3.80	1.38	1.34
2	C	1201	A1H2B	C10-N12	3.23	1.37	1.34
2	A	1201	A1H2B	C10-N15	2.64	1.39	1.33
2	D	1201	A1H2B	C10-N15	2.50	1.38	1.33
2	C	1201	A1H2B	C10-N15	2.43	1.38	1.33
2	D	1201	A1H2B	C14-N15	2.37	1.39	1.34
2	B	1201	A1H2B	C14-N15	2.36	1.39	1.34
2	D	1201	A1H2B	C8-C2	-2.29	1.37	1.41
2	B	1201	A1H2B	C11-N12	2.26	1.38	1.34
2	D	1201	A1H2B	C23-N18	2.23	1.39	1.35
2	B	1201	A1H2B	C23-N18	2.21	1.39	1.35
2	A	1201	A1H2B	C9-C7	-2.18	1.39	1.44
2	A	1201	A1H2B	C14-N15	2.17	1.39	1.34
2	B	1201	A1H2B	C10-N15	2.14	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	A1H2B	C23-N18	2.12	1.39	1.35
2	D	1201	A1H2B	C9-C7	-2.12	1.39	1.44
2	C	1201	A1H2B	C9-C7	-2.01	1.39	1.44
2	B	1201	A1H2B	C9-C7	-2.01	1.39	1.44

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1201	A1H2B	N15-C10-N12	-6.14	119.10	125.27
2	C	1201	A1H2B	N15-C10-N12	-6.11	119.13	125.27
2	A	1201	A1H2B	N15-C10-N12	-5.96	119.29	125.27
2	D	1201	A1H2B	N15-C10-N12	-5.74	119.51	125.27
2	C	1201	A1H2B	C4-N5-C2	5.51	107.67	105.11
2	A	1201	A1H2B	C14-C13-C11	4.63	119.79	116.76
2	C	1201	A1H2B	C3-C4-N5	-4.44	106.64	111.99
2	A	1201	A1H2B	C3-C4-N5	-4.15	106.99	111.99
2	A	1201	A1H2B	C4-N5-C2	4.13	107.03	105.11
2	B	1201	A1H2B	C3-C4-N5	-4.00	107.17	111.99
2	B	1201	A1H2B	C4-N5-C2	3.98	106.96	105.11
2	D	1201	A1H2B	C14-C13-C11	3.98	119.36	116.76
2	D	1201	A1H2B	C3-C4-N5	-3.83	107.38	111.99
2	C	1201	A1H2B	C14-N15-C10	3.78	119.79	115.51
2	B	1201	A1H2B	C14-N15-C10	3.68	119.67	115.51
2	C	1201	A1H2B	C14-C13-C11	3.56	119.09	116.76
2	D	1201	A1H2B	C4-N5-C2	3.53	106.75	105.11
2	A	1201	A1H2B	C14-N15-C10	3.51	119.48	115.51
2	A	1201	A1H2B	C11-N12-C10	3.31	121.52	116.00
2	D	1201	A1H2B	C14-N15-C10	3.29	119.23	115.51
2	B	1201	A1H2B	C11-N12-C10	3.26	121.43	116.00
2	C	1201	A1H2B	C11-N12-C10	3.26	121.43	116.00
2	D	1201	A1H2B	C11-N12-C10	3.24	121.40	116.00
2	B	1201	A1H2B	C14-C13-C11	3.08	118.78	116.76
2	A	1201	A1H2B	C13-C14-N15	-2.85	120.42	123.96
2	B	1201	A1H2B	C7-C28-N29	-2.84	174.09	178.01
2	A	1201	A1H2B	C24-C25-N26	-2.83	169.76	177.86
2	C	1201	A1H2B	C24-C25-N26	-2.83	169.79	177.86
2	C	1201	A1H2B	C13-C14-N15	-2.59	120.73	123.96
2	D	1201	A1H2B	C13-C14-N15	-2.50	120.85	123.96
2	C	1201	A1H2B	C8-C2-N1	2.43	120.91	118.41
2	D	1201	A1H2B	C8-C2-N1	2.39	120.87	118.41
2	C	1201	A1H2B	C4-C3-N1	2.39	108.59	104.52
2	A	1201	A1H2B	C8-C2-N1	2.37	120.85	118.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1201	A1H2B	C7-C6-N1	-2.30	118.54	121.74
2	B	1201	A1H2B	C20-C17-N16	2.30	112.65	109.71
2	D	1201	A1H2B	C7-C6-N1	-2.29	118.56	121.74
2	B	1201	A1H2B	C13-C14-N15	-2.26	121.15	123.96
2	A	1201	A1H2B	C4-C3-N1	2.21	108.29	104.52
2	D	1201	A1H2B	C7-C28-N29	-2.17	175.02	178.01
2	A	1201	A1H2B	C13-C11-N12	-2.16	119.51	123.16
2	B	1201	A1H2B	C8-C2-N1	2.15	120.62	118.41
2	D	1201	A1H2B	C24-C25-N26	-2.12	171.80	177.86
2	B	1201	A1H2B	C7-C6-N1	-2.11	118.81	121.74
2	B	1201	A1H2B	C4-C3-N1	2.11	108.12	104.52
2	D	1201	A1H2B	C4-C3-N1	2.10	108.11	104.52
2	D	1201	A1H2B	C13-C11-N12	-2.08	119.66	123.16

There are no chirality outliers.

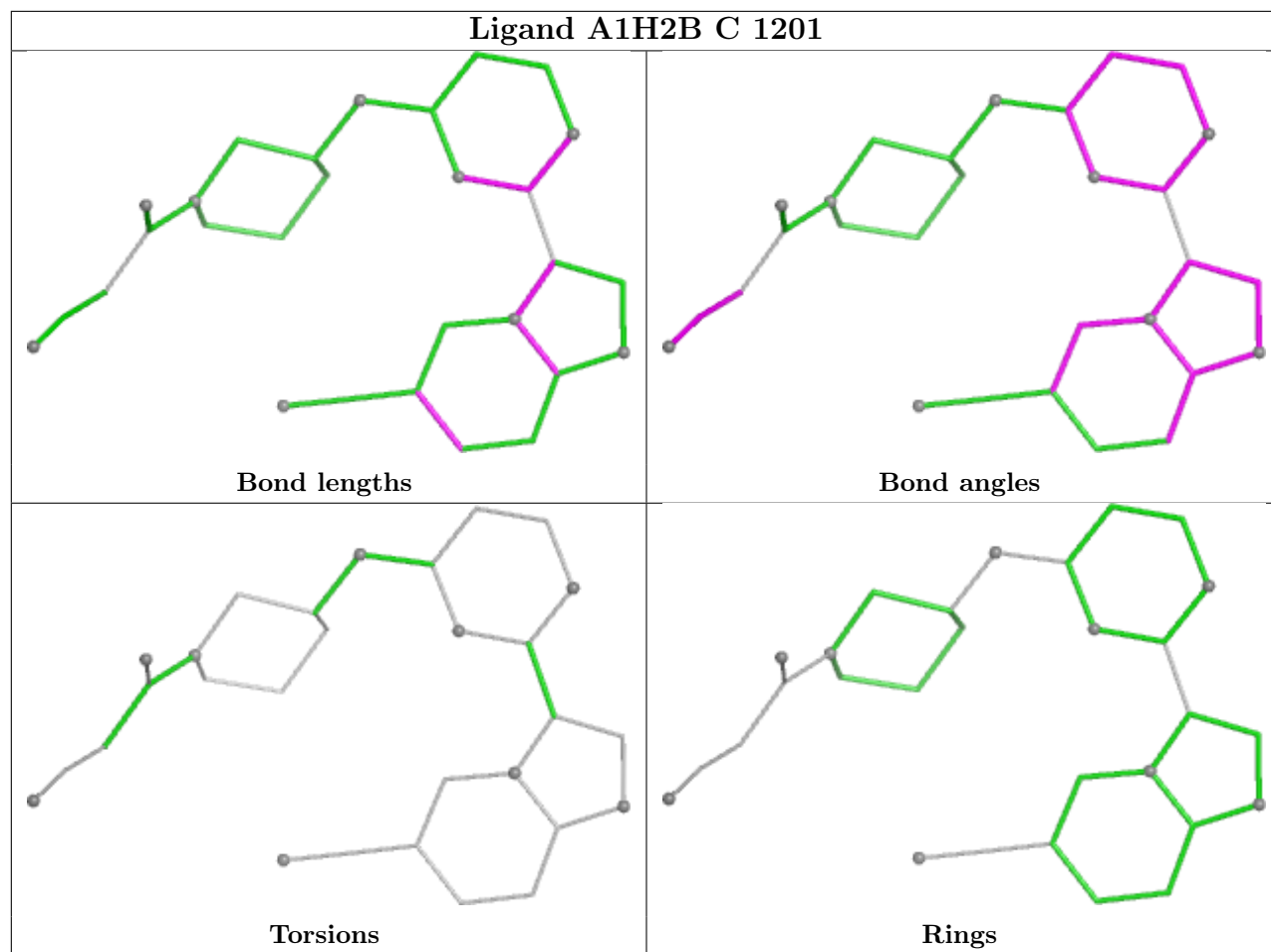
There are no torsion outliers.

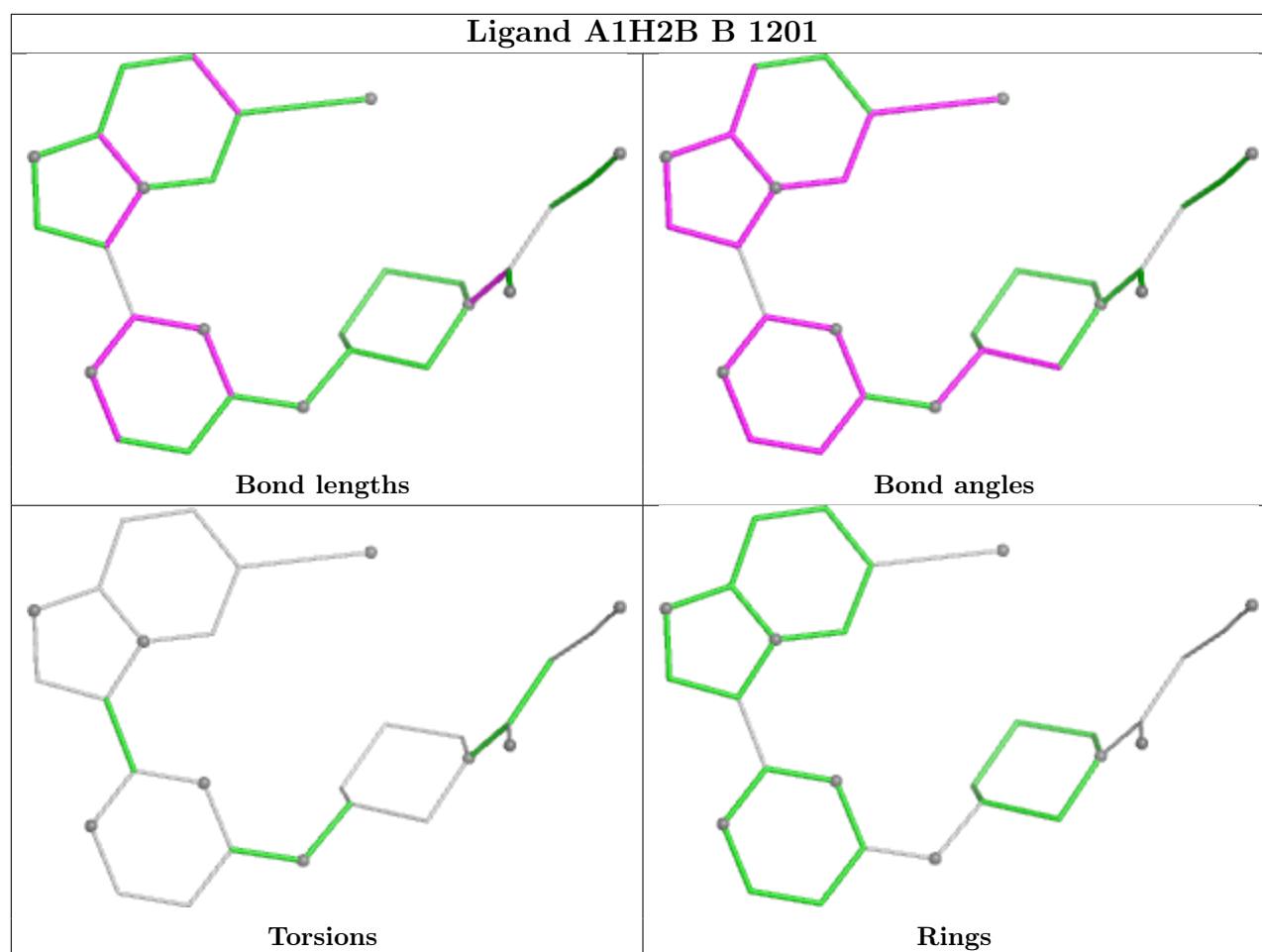
There are no ring outliers.

1 monomer is involved in 1 short contact:

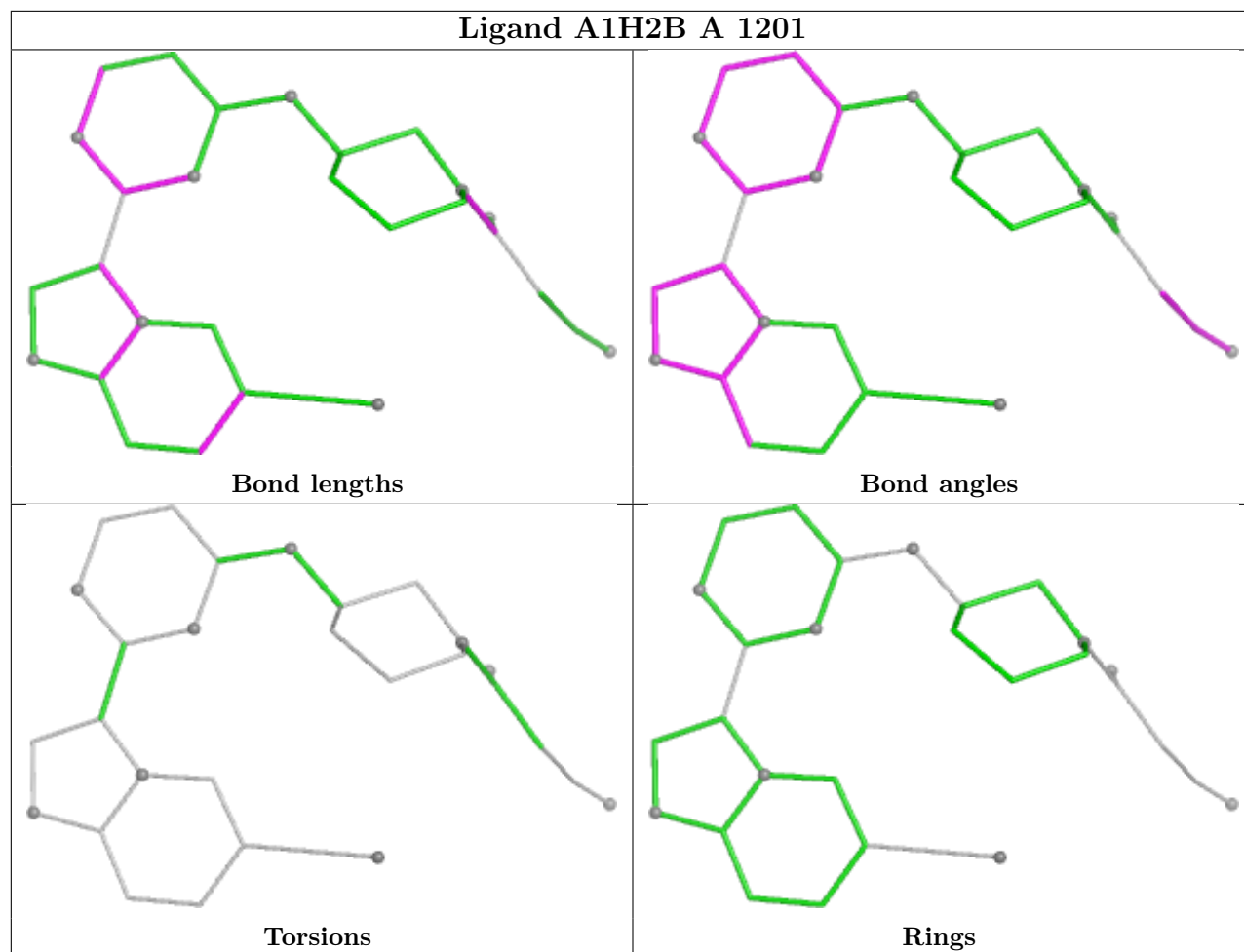
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1201	A1H2B	1	0

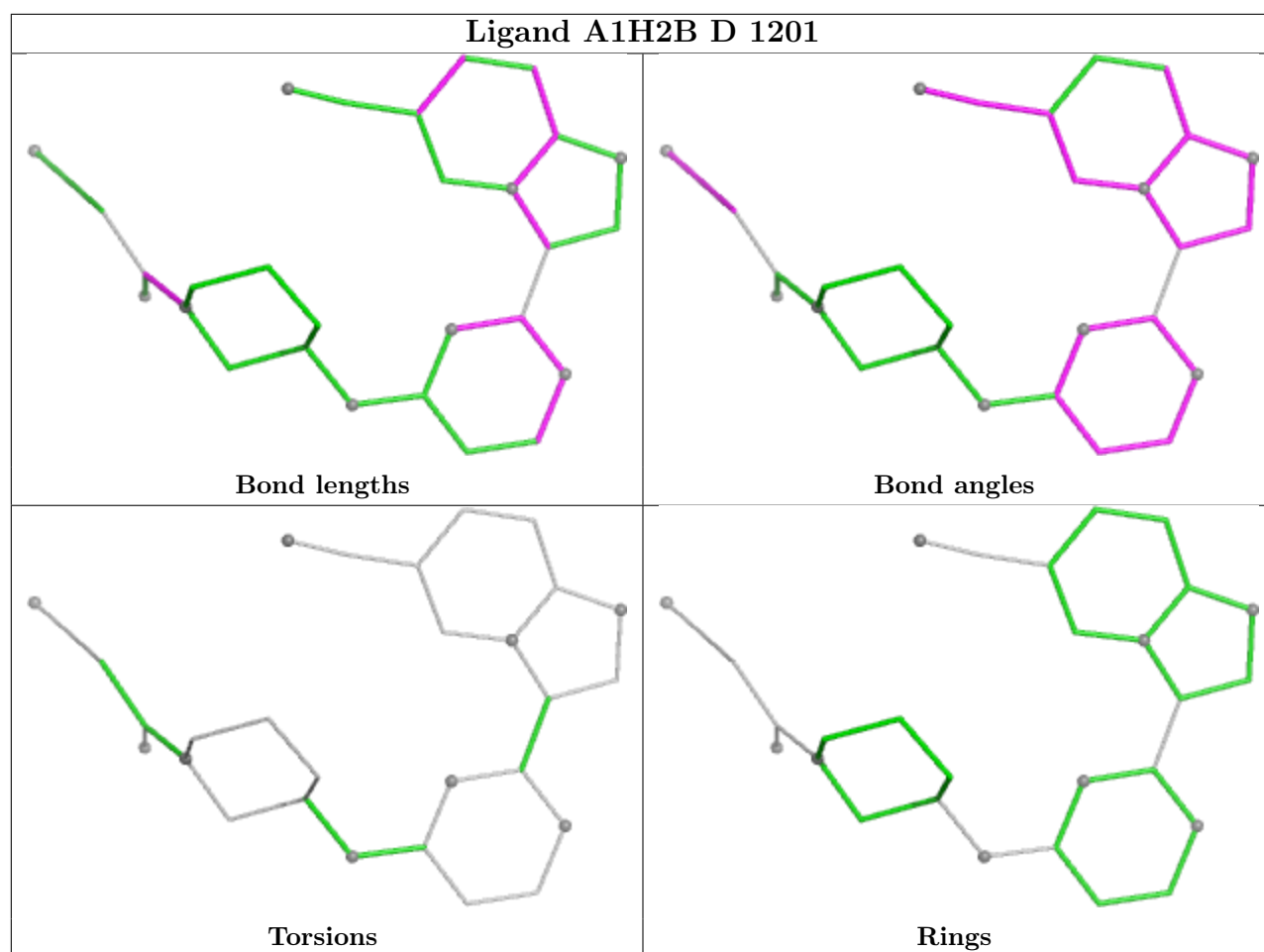
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





Ligand A1H2B A 1201





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	256/298 (85%)	0.65	11 (4%)	40 36	24, 47, 66, 76	2 (0%)
1	B	260/298 (87%)	0.72	18 (6%)	23 20	24, 47, 66, 76	1 (0%)
1	C	258/298 (86%)	0.71	16 (6%)	26 23	24, 47, 66, 74	1 (0%)
1	D	258/298 (86%)	0.78	16 (6%)	26 23	24, 47, 66, 76	0
All	All	1032/1192 (86%)	0.72	61 (5%)	28 25	24, 47, 66, 76	4 (0%)

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	861	GLY	4.6
1	C	1049	ARG	4.3
1	D	848	THR	4.3
1	D	861	GLY	4.0
1	C	989	SER	3.7
1	D	815	THR	3.6
1	D	831	GLY	3.6
1	C	848	THR	3.5
1	A	861	GLY	3.4
1	A	983	VAL	3.3
1	B	976	LEU	3.3
1	D	814	PRO	3.3
1	B	831	GLY	3.2
1	B	983	VAL	3.2
1	C	983	VAL	3.1
1	D	832	ASN	3.0
1	C	1043	ASP	2.9
1	B	861	GLY	2.9
1	B	815	THR	2.9
1	D	1045	PRO	2.8
1	B	816	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	862	PRO	2.8
1	B	989	SER	2.7
1	B	1056	GLU	2.7
1	B	1045	PRO	2.7
1	D	1032	ALA	2.7
1	C	976	LEU	2.7
1	C	862	PRO	2.7
1	B	848	THR	2.6
1	A	1069	GLU	2.6
1	C	832	ASN	2.5
1	A	816	ILE	2.5
1	A	919	ALA	2.4
1	A	976	LEU	2.4
1	A	823	LYS	2.3
1	B	1031	SER	2.3
1	D	979	ASP	2.3
1	A	819	GLU	2.3
1	B	1049	ARG	2.3
1	C	907	SER	2.3
1	C	990	PRO	2.3
1	A	862	PRO	2.2
1	B	843	PRO	2.2
1	D	865	GLN	2.2
1	A	977	ASP	2.2
1	C	962	HIS	2.2
1	C	831	GLY	2.2
1	D	1066	CYS	2.1
1	B	832	ASN	2.1
1	B	898	LEU	2.1
1	D	1035	LEU	2.1
1	B	1039	GLY	2.1
1	D	849	GLY	2.1
1	C	815	THR	2.1
1	D	912	ASP	2.1
1	D	977	ASP	2.0
1	B	1055	GLU	2.0
1	A	1070	VAL	2.0
1	C	1034	PHE	2.0
1	C	1037	MET	2.0
1	B	1083	GLN	2.0

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

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
1	PTR	A	980	16/17	0.83	0.14	57,60,66,69	0
1	PTR	C	980	16/17	0.85	0.12	57,60,67,67	0
1	PTR	D	981	16/17	0.87	0.14	56,57,63,64	0
1	PTR	D	980	16/17	0.88	0.12	57,59,67,68	0
1	PTR	B	980	16/17	0.89	0.13	57,60,66,68	0
1	PTR	C	981	16/17	0.89	0.13	56,58,63,63	0
1	PTR	A	981	16/17	0.91	0.10	57,57,63,64	0
1	PTR	B	981	16/17	0.91	0.13	56,57,63,64	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

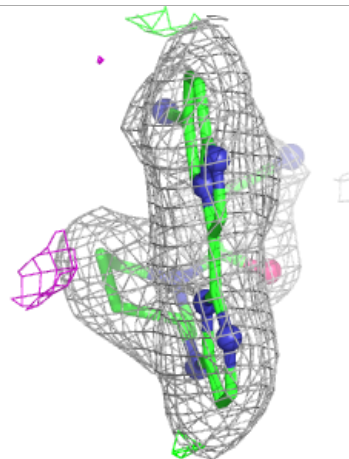
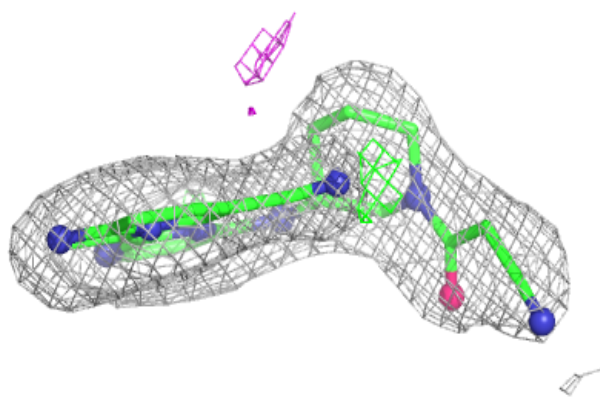
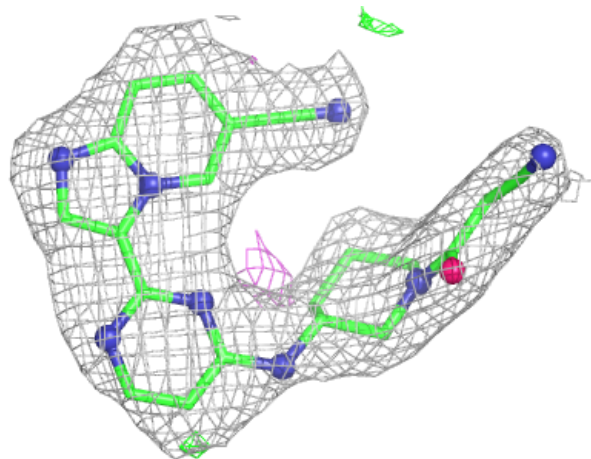
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	A1H2B	B	1201	29/29	0.90	0.12	29,34,36,44	0
2	A1H2B	A	1201	29/29	0.91	0.10	20,28,31,31	0
2	A1H2B	D	1201	29/29	0.92	0.10	32,38,39,40	0
2	A1H2B	C	1201	29/29	0.94	0.08	26,29,33,44	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.

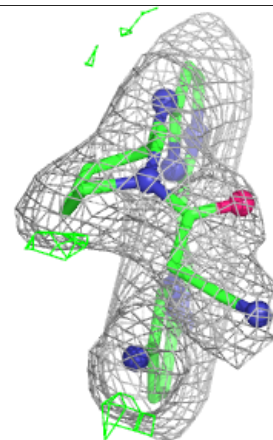
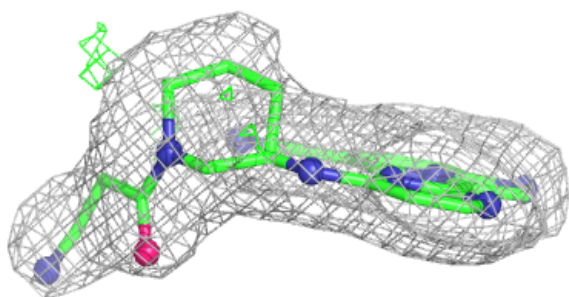
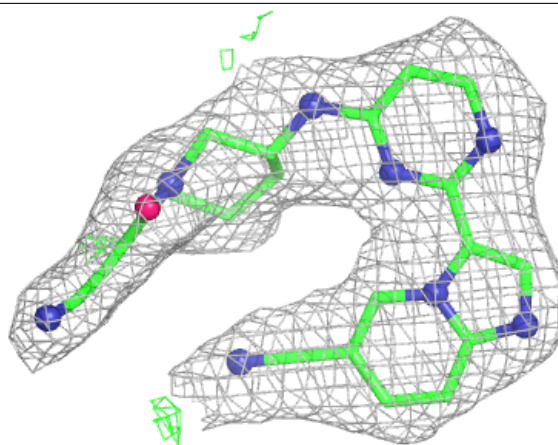
Electron density around A1H2B B 1201:

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



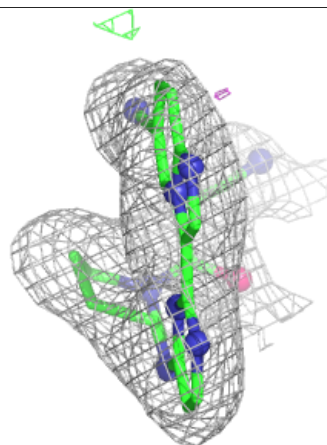
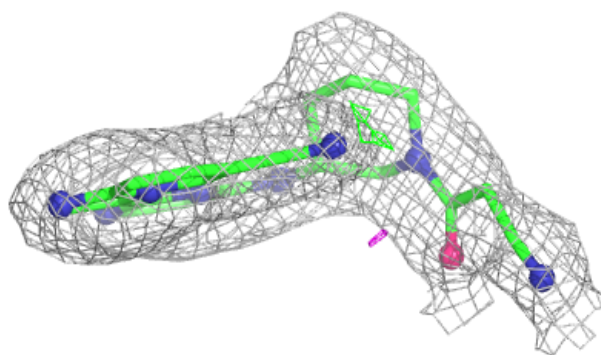
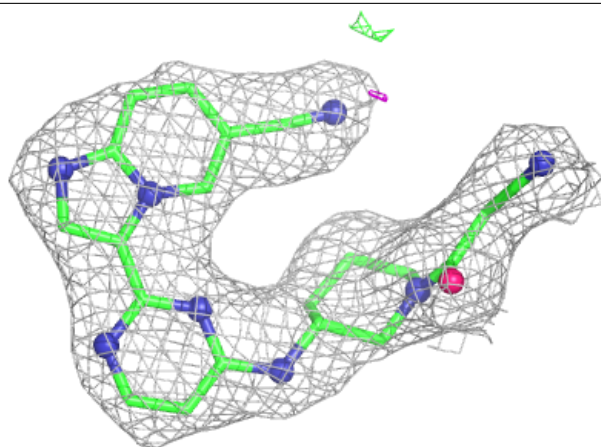
Electron density around A1H2B A 1201:

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

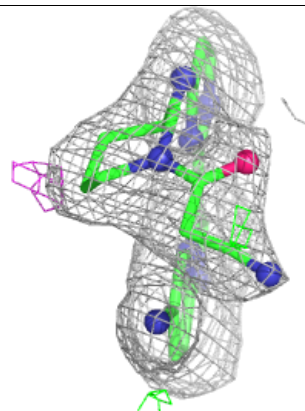
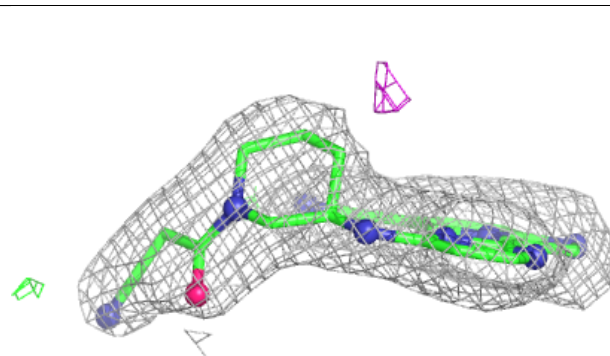
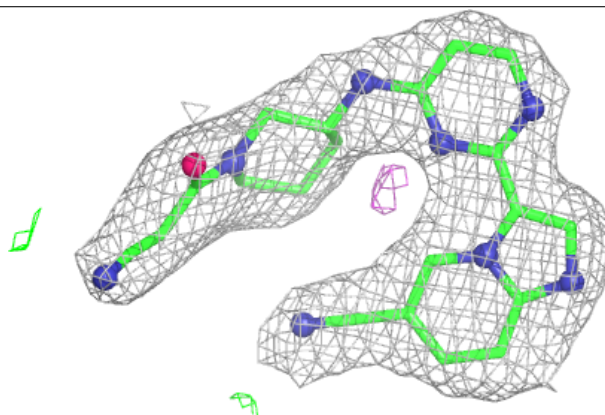


Electron density around A1H2B D 1201:

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

**Electron density around A1H2B C 1201:**

$2mF_o-DF_c$ (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.