



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 09:57 PM UTC

PDB ID : 4C1I / pdb_00004c1i
Title : Selective Inhibitors of PDE2, PDE9, and PDE10: Modulators of Activity of the Central Nervous System
Authors : Jorgensen, M.; Kehler, J.; Langgard, M.; Svenstrup, N.; Tagmose, L.
Deposited on : 2013-08-12
Resolution : 2.40 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

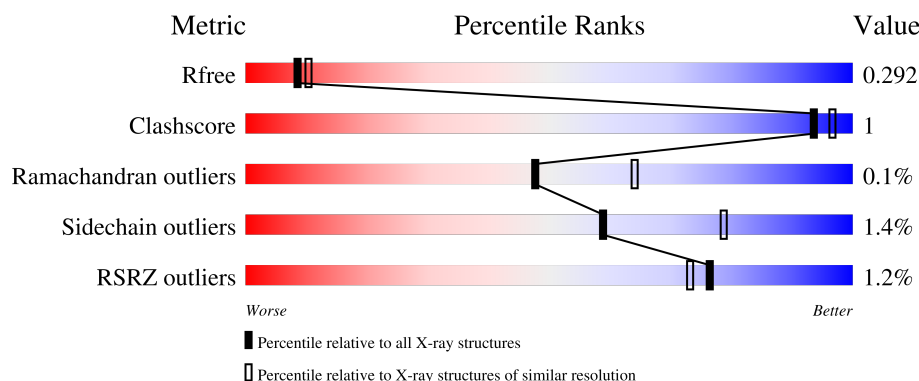
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	353	88% 8%
1	B	353	85% 6% 9%
1	C	353	86% 5% 10%
1	D	353	87% 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EH9	A	1906	X	-	-	-
2	EH9	B	1900	X	-	-	-
2	EH9	C	1900	X	-	-	-
2	EH9	D	1900	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10670 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 CGMP-DEPENDENT 3', 5'-CYCLIC PHOSPHODIESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	325	Total	C	N	O	S	0	0	0
			2625	1673	451	476	25			
1	B	320	Total	C	N	O	S	0	0	0
			2581	1646	437	473	25			
1	C	319	Total	C	N	O	S	0	0	0
			2577	1641	440	472	24			
1	D	319	Total	C	N	O	S	0	0	0
			2551	1626	434	466	25			

There are 36 discrepancies between the modelled and reference sequences:

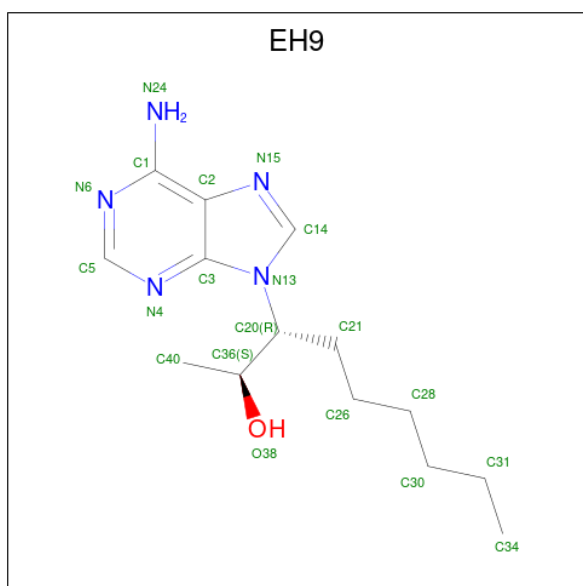
Chain	Residue	Modelled	Actual	Comment	Reference
A	576	MET	-	expression tag	UNP O00408
A	577	GLY	-	expression tag	UNP O00408
A	922	ARG	-	expression tag	UNP O00408
A	923	HIS	-	expression tag	UNP O00408
A	924	HIS	-	expression tag	UNP O00408
A	925	HIS	-	expression tag	UNP O00408
A	926	HIS	-	expression tag	UNP O00408
A	927	HIS	-	expression tag	UNP O00408
A	928	HIS	-	expression tag	UNP O00408
B	576	MET	-	expression tag	UNP O00408
B	577	GLY	-	expression tag	UNP O00408
B	922	ARG	-	expression tag	UNP O00408
B	923	HIS	-	expression tag	UNP O00408
B	924	HIS	-	expression tag	UNP O00408
B	925	HIS	-	expression tag	UNP O00408
B	926	HIS	-	expression tag	UNP O00408
B	927	HIS	-	expression tag	UNP O00408
B	928	HIS	-	expression tag	UNP O00408
C	576	MET	-	expression tag	UNP O00408
C	577	GLY	-	expression tag	UNP O00408
C	922	ARG	-	expression tag	UNP O00408

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Chain	Residue	Modelled	Actual	Comment	Reference
C	923	HIS	-	expression tag	UNP O00408
C	924	HIS	-	expression tag	UNP O00408
C	925	HIS	-	expression tag	UNP O00408
C	926	HIS	-	expression tag	UNP O00408
C	927	HIS	-	expression tag	UNP O00408
C	928	HIS	-	expression tag	UNP O00408
D	576	MET	-	expression tag	UNP O00408
D	577	GLY	-	expression tag	UNP O00408
D	922	ARG	-	expression tag	UNP O00408
D	923	HIS	-	expression tag	UNP O00408
D	924	HIS	-	expression tag	UNP O00408
D	925	HIS	-	expression tag	UNP O00408
D	926	HIS	-	expression tag	UNP O00408
D	927	HIS	-	expression tag	UNP O00408
D	928	HIS	-	expression tag	UNP O00408

- Molecule 2 is (2S,3R)-3-(6-amino-9H-purin-9-yl)nonan-2-ol (CCD ID: EH9) (formula: C₁₄H₂₃N₅O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			20	14	5	1		
2	B	1	Total	C	N	O	0	0
			20	14	5	1		
2	C	1	Total	C	N	O	0	0
			20	14	5	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total	C	N	O	0	0
			20	14	5	1		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

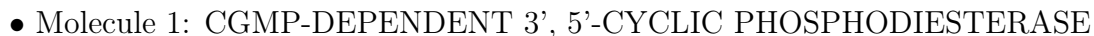
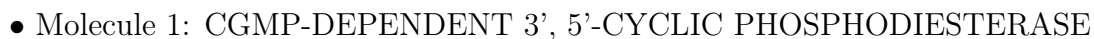
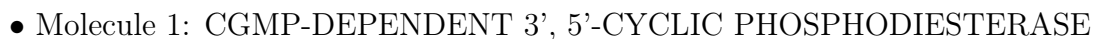
- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	68	Total	O	0	0
			68	68		
5	B	59	Total	O	0	0
			59	59		
5	C	74	Total	O	0	0
			74	74		
5	D	47	Total	O	0	0
			47	47		

- Molecule 1: CGMP-DEPENDENT 3', 5'-CYCLIC PHOSPHODIESTERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	47.05Å 81.81Å 93.34Å 110.16° 95.66° 93.21°	Depositor
Resolution (Å)	18.47 – 2.40 18.47 – 2.40	Depositor EDS
% Data completeness (in resolution range)	94.0 (18.47-2.40) 94.0 (18.47-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.225 , 0.287 0.232 , 0.292	Depositor DCC
R_{free} test set	2434 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	29.0	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 36.6	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	10670	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.37% 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: MG, ZN, EH9

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	0.46	0/2689	0.73	2/3636 (0.1%)
1	B	0.45	0/2644	0.72	0/3577
1	C	0.44	0/2640	0.71	0/3573
1	D	0.44	0/2613	0.71	0/3538
All	All	0.45	0/10586	0.72	2/14324 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	652	ASP	CA-C-N	-5.17	115.05	120.38
1	A	652	ASP	C-N-CA	-5.17	115.05	120.38

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	2625	0	2531	4	0
1	B	2581	0	2481	9	0
1	C	2577	0	2472	7	0
1	D	2551	0	2437	5	0
2	A	20	0	23	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	20	0	23	2	0
2	C	20	0	23	2	0
2	D	20	0	23	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	68	0	0	0	0
5	B	59	0	0	0	0
5	C	74	0	0	1	0
5	D	47	0	0	0	0
All	All	10670	0	10013	29	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 1.

All (29) 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:C:848:MET:HE3	5:C:2062:HOH:O	1.95	0.67
1:D:744:ASN:ND2	1:D:747:ASP:OD1	2.35	0.60
1:B:596:ILE:HG12	1:B:617:MET:HE1	1.87	0.57
1:C:833:GLN:NE2	1:C:848:MET:HE1	2.20	0.56
1:A:875:GLN:HE21	1:A:882:ALA:HA	1.74	0.53
2:B:1900:EH9:H402	2:B:1900:EH9:C14	2.40	0.51
1:B:582:TYR:CE1	1:B:641:ARG:HG3	2.46	0.50
2:C:1900:EH9:H402	2:C:1900:EH9:C14	2.42	0.49
1:B:590:ILE:HG21	1:B:624:GLN:CB	2.43	0.49
1:C:768:THR:CG2	1:C:804:MET:HE2	2.44	0.48
1:C:863:MET:HA	1:C:867:ALA:HB3	1.96	0.46
1:A:645:MET:HG3	1:A:743:CYS:SG	2.56	0.45
1:B:603:PHE:CD1	1:B:884:LEU:HD21	2.52	0.45
1:C:868:MET:HE3	1:C:889:ALA:HB2	1.98	0.45
1:B:582:TYR:HA	1:B:644:LEU:HD11	1.99	0.44
1:B:827:TYR:CE2	1:B:855:ILE:HG23	2.53	0.44
1:C:656:HIS:ND1	1:C:829:GLU:OE1	2.49	0.44
1:B:590:ILE:HG23	1:B:621:SER:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:619:ILE:HA	1:D:622:MET:HE3	2.01	0.42
2:B:1900:EH9:C14	2:B:1900:EH9:C40	2.97	0.42
2:C:1900:EH9:C14	2:C:1900:EH9:C40	2.98	0.42
1:B:645:MET:HG3	1:B:743:CYS:SG	2.60	0.41
1:A:634:ILE:HG21	1:A:639:LEU:HD13	2.02	0.41
1:A:805:THR:HG23	1:A:870:ILE:HD13	2.02	0.41
1:D:664:VAL:HG13	1:D:807:CYS:HB3	2.02	0.41
1:B:599:ASN:ND2	1:B:604:THR:OG1	2.54	0.41
1:D:767:ALA:HA	1:D:772:HIS:CD2	2.56	0.41
1:D:782:LYS:O	1:D:786:VAL:HG22	2.21	0.40
1:C:692:SER:O	1:C:696:HIS:HB3	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	323/353 (92%)	316 (98%)	7 (2%)	0	100	100
1	B	318/353 (90%)	311 (98%)	6 (2%)	1 (0%)	36	50
1	C	317/353 (90%)	313 (99%)	4 (1%)	0	100	100
1	D	317/353 (90%)	310 (98%)	7 (2%)	0	100	100
All	All	1275/1412 (90%)	1250 (98%)	24 (2%)	1 (0%)	48	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	747	ASP

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	282/319 (88%)	274 (97%)	8 (3%)	38	60
1	B	278/319 (87%)	275 (99%)	3 (1%)	65	82
1	C	277/319 (87%)	273 (99%)	4 (1%)	59	79
1	D	272/319 (85%)	271 (100%)	1 (0%)	84	92
All	All	1109/1276 (87%)	1093 (99%)	16 (1%)	59	79

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	588	ASP
1	A	758	LEU
1	A	794	GLN
1	A	797	ARG
1	A	805	THR
1	A	828	LYS
1	A	899	SER
1	A	901	LYS
1	B	584	LYS
1	B	683	ASP
1	B	887	ARG
1	C	806	SER
1	C	820	ARG
1	C	824	GLU
1	C	843	ARG
1	D	847	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	599	ASN
1	A	708	GLN
1	A	772	HIS

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Mol	Chain	Res	Type
1	A	781	GLN
1	A	794	GLN
1	A	875	GLN
1	A	894	HIS
1	B	599	ASN
1	B	700	HIS
1	B	708	GLN
1	B	741	HIS
1	C	666	HIS
1	C	772	HIS
1	C	795	HIS
1	C	894	HIS
1	D	587	HIS
1	D	674	ASN
1	D	772	HIS
1	D	795	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

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	EH9	C	1900	-	20,21,21	1.12	3 (15%)	24,28,28	2.33	8 (33%)
2	EH9	A	1906	-	20,21,21	1.10	3 (15%)	24,28,28	2.35	8 (33%)
2	EH9	B	1900	-	20,21,21	1.01	3 (15%)	24,28,28	2.45	8 (33%)
2	EH9	D	1900	-	20,21,21	1.17	3 (15%)	24,28,28	2.27	8 (33%)

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	EH9	C	1900	-	1/1/2/2	4/14/14/14	0/2/2/2
2	EH9	A	1906	-	1/1/2/2	6/14/14/14	0/2/2/2
2	EH9	B	1900	-	1/1/2/2	5/14/14/14	0/2/2/2
2	EH9	D	1900	-	1/1/2/2	7/14/14/14	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1900	EH9	C2-N15	-3.26	1.33	1.39
2	A	1906	EH9	C2-N15	-2.97	1.33	1.39
2	C	1900	EH9	C2-N15	-2.97	1.33	1.39
2	B	1900	EH9	C2-N15	-2.72	1.34	1.39
2	D	1900	EH9	C3-N13	-2.47	1.32	1.37
2	D	1900	EH9	C14-N13	-2.41	1.33	1.37
2	B	1900	EH9	C3-N13	-2.36	1.32	1.37
2	C	1900	EH9	C3-N13	-2.32	1.32	1.37
2	A	1906	EH9	C3-N13	-2.28	1.32	1.37
2	B	1900	EH9	C14-N13	-2.24	1.33	1.37
2	A	1906	EH9	C14-N13	-2.17	1.33	1.37
2	C	1900	EH9	C14-N13	-2.10	1.34	1.37

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1906	EH9	C2-C3-N4	-5.20	119.55	126.72
2	C	1900	EH9	C2-C3-N4	-4.97	119.88	126.72
2	B	1900	EH9	C2-C3-N4	-4.89	119.98	126.72
2	D	1900	EH9	C2-C3-N4	-4.76	120.17	126.72
2	A	1906	EH9	N6-C5-N4	-4.69	121.47	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1900	EH9	N6-C5-N4	-4.60	121.62	128.58
2	D	1900	EH9	N6-C5-N4	-4.57	121.66	128.58
2	B	1900	EH9	N13-C14-N15	-4.54	107.50	113.94
2	B	1900	EH9	N6-C5-N4	-4.52	121.74	128.58
2	B	1900	EH9	C3-N13-C14	4.39	110.35	105.74
2	C	1900	EH9	N13-C14-N15	-4.16	108.03	113.94
2	A	1906	EH9	N13-C14-N15	-4.09	108.13	113.94
2	B	1900	EH9	N4-C3-N13	4.08	134.11	127.17
2	D	1900	EH9	N13-C14-N15	-3.92	108.38	113.94
2	D	1900	EH9	N4-C3-N13	3.87	133.75	127.17
2	A	1906	EH9	N4-C3-N13	3.87	133.75	127.17
2	C	1900	EH9	N4-C3-N13	3.79	133.61	127.17
2	D	1900	EH9	C3-N13-C14	3.68	109.60	105.74
2	A	1906	EH9	C5-N4-C3	3.62	120.67	111.83
2	C	1900	EH9	C3-N13-C14	3.57	109.49	105.74
2	C	1900	EH9	C5-N4-C3	3.50	120.38	111.83
2	B	1900	EH9	C5-N4-C3	3.49	120.36	111.83
2	A	1906	EH9	C3-N13-C14	3.44	109.35	105.74
2	B	1900	EH9	C2-N15-C14	3.36	108.73	103.45
2	D	1900	EH9	C5-N4-C3	3.32	119.93	111.83
2	C	1900	EH9	C2-N15-C14	3.16	108.41	103.45
2	A	1906	EH9	C2-N15-C14	3.03	108.22	103.45
2	D	1900	EH9	C2-N15-C14	2.81	107.87	103.45
2	B	1900	EH9	C3-C2-N15	-2.69	107.51	110.58
2	C	1900	EH9	C3-C2-N15	-2.64	107.56	110.58
2	A	1906	EH9	C3-C2-N15	-2.61	107.60	110.58
2	D	1900	EH9	C3-C2-N15	-2.19	108.07	110.58

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1906	EH9	C36
2	B	1900	EH9	C36
2	C	1900	EH9	C36
2	D	1900	EH9	C36

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1906	EH9	N13-C20-C36-O38
2	A	1906	EH9	N13-C20-C36-C40
2	A	1906	EH9	C21-C20-C36-O38

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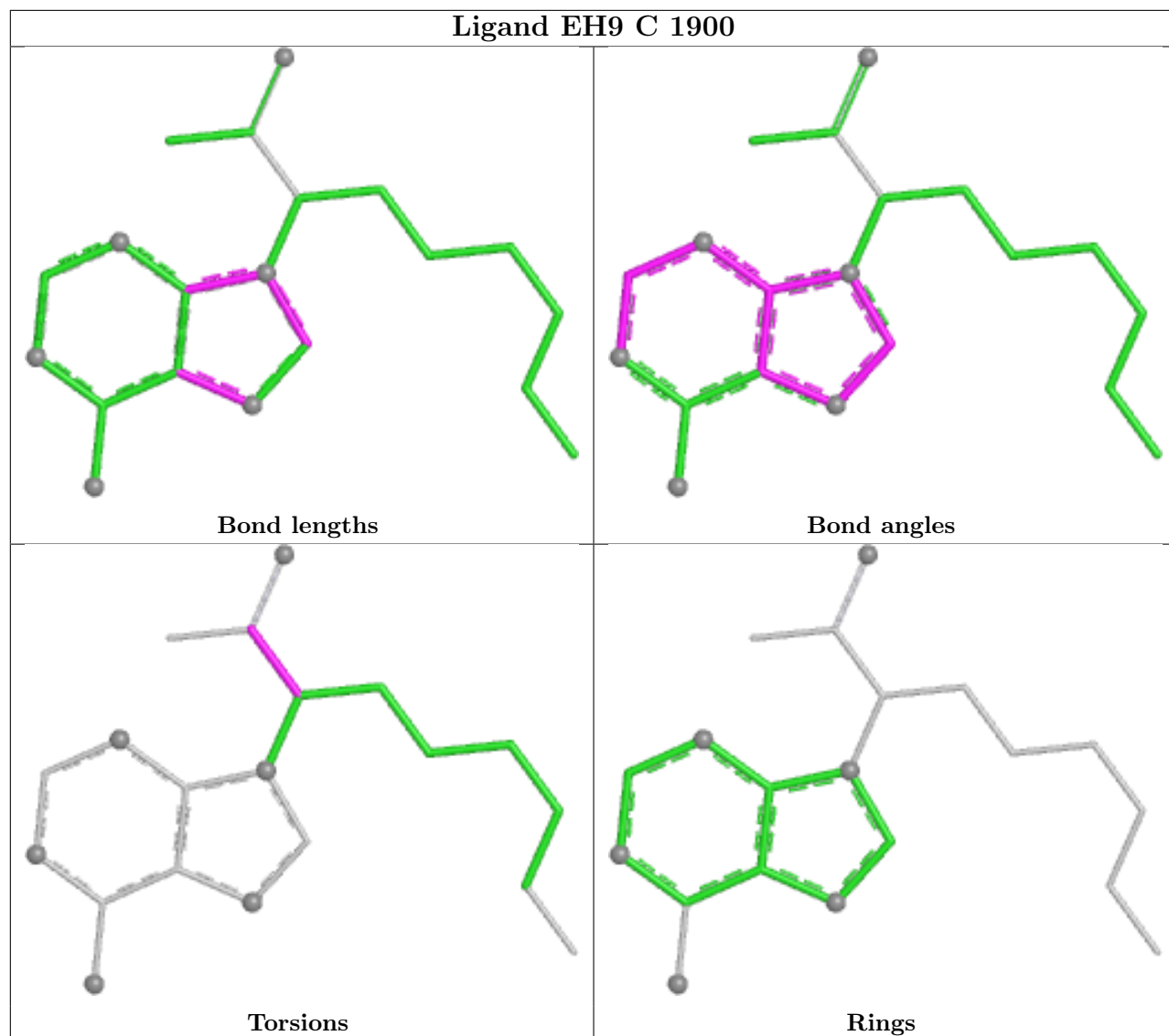
Mol	Chain	Res	Type	Atoms
2	A	1906	EH9	C21-C20-C36-C40
2	B	1900	EH9	N13-C20-C36-O38
2	B	1900	EH9	N13-C20-C36-C40
2	B	1900	EH9	C21-C20-C36-O38
2	B	1900	EH9	C21-C20-C36-C40
2	C	1900	EH9	N13-C20-C36-O38
2	C	1900	EH9	N13-C20-C36-C40
2	C	1900	EH9	C21-C20-C36-O38
2	C	1900	EH9	C21-C20-C36-C40
2	D	1900	EH9	C36-C20-C21-C26
2	D	1900	EH9	N13-C20-C36-O38
2	D	1900	EH9	N13-C20-C36-C40
2	D	1900	EH9	C21-C20-C36-O38
2	D	1900	EH9	C21-C20-C36-C40
2	D	1900	EH9	N13-C20-C21-C26
2	D	1900	EH9	C21-C26-C28-C30
2	A	1906	EH9	C21-C26-C28-C30
2	B	1900	EH9	C21-C26-C28-C30
2	A	1906	EH9	N13-C20-C21-C26

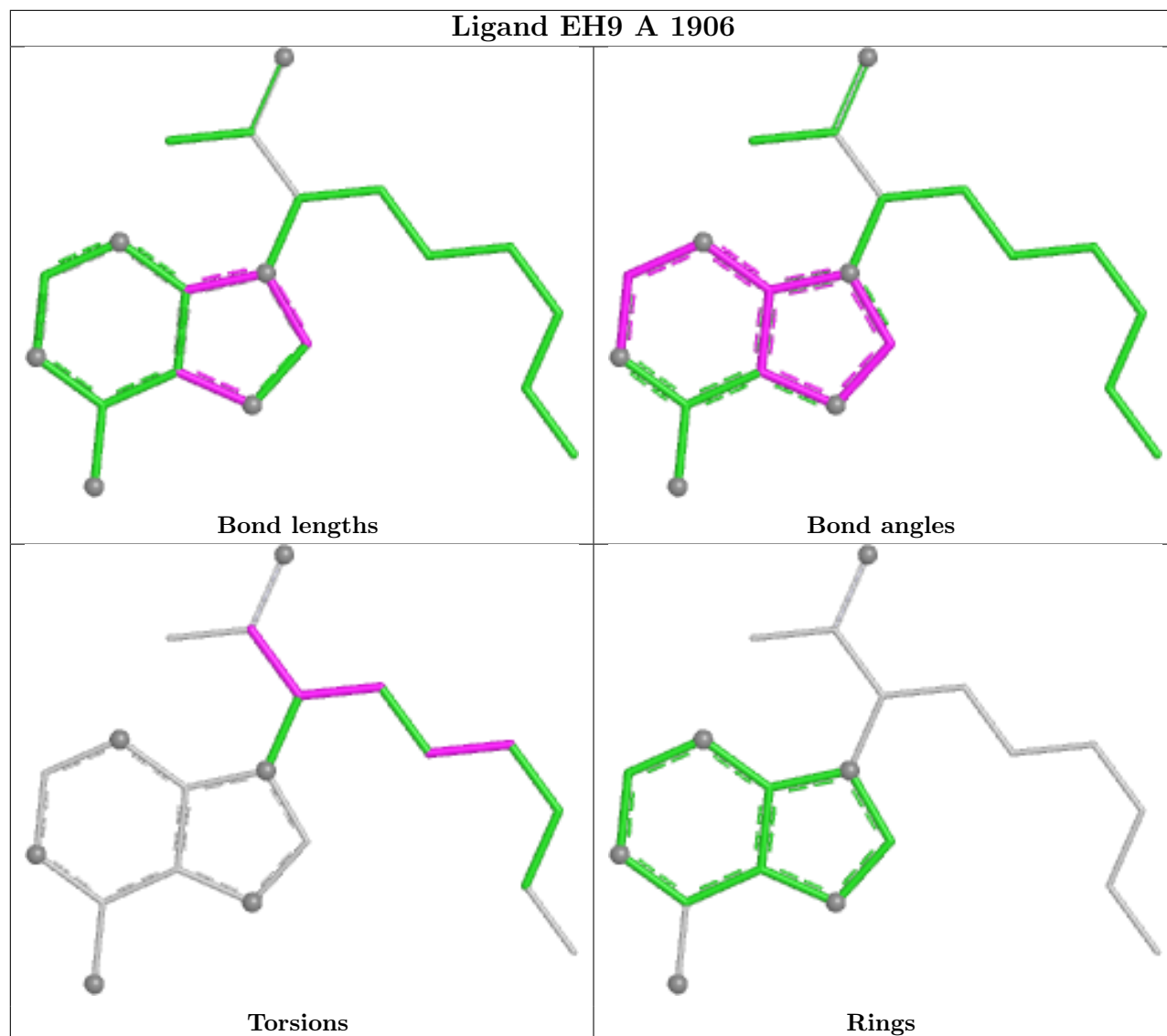
There are no ring outliers.

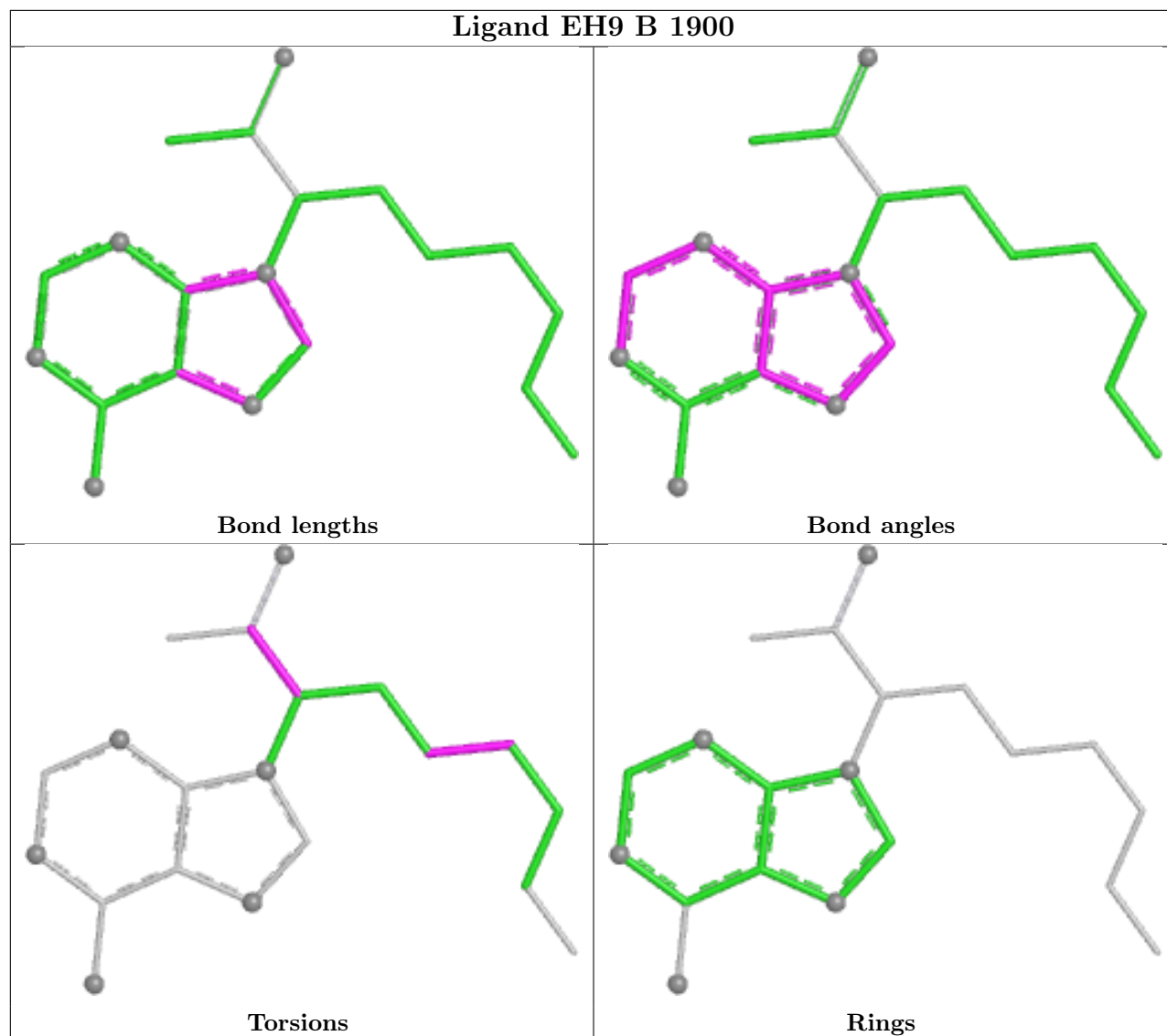
2 monomers are involved in 4 short contacts:

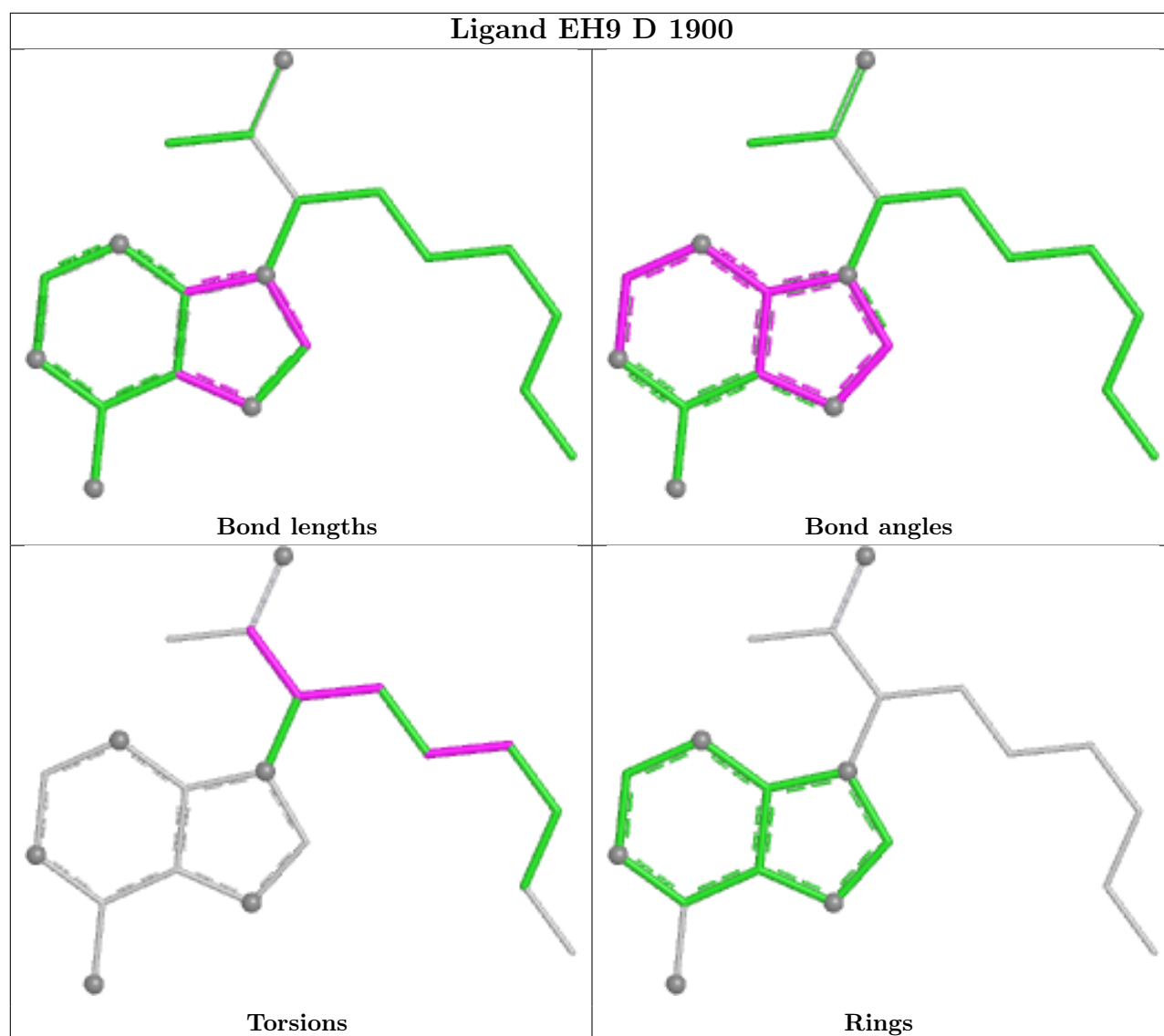
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1900	EH9	2	0
2	B	1900	EH9	2	0

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	325/353 (92%)	0.07	3 (0%) 81 78	14, 26, 42, 79	0
1	B	320/353 (90%)	0.17	2 (0%) 85 83	16, 28, 45, 60	0
1	C	319/353 (90%)	0.15	3 (0%) 81 78	16, 28, 46, 64	0
1	D	319/353 (90%)	0.38	7 (2%) 62 58	19, 34, 57, 81	0
All	All	1283/1412 (90%)	0.19	15 (1%) 76 73	14, 29, 50, 81	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	899	SER	4.4
1	D	582	TYR	3.9
1	C	581	GLU	3.2
1	A	582	TYR	3.1
1	D	583	THR	2.9
1	D	786	VAL	2.9
1	A	583	THR	2.7
1	A	587	HIS	2.6
1	D	584	LYS	2.6
1	C	582	TYR	2.5
1	C	587	HIS	2.3
1	D	834	GLY	2.3
1	D	893	GLU	2.2
1	B	887	ARG	2.2
1	B	588	ASP	2.1

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

There are no oligosaccharides in this entry.

6.4 Ligands

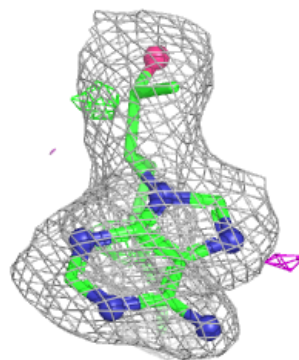
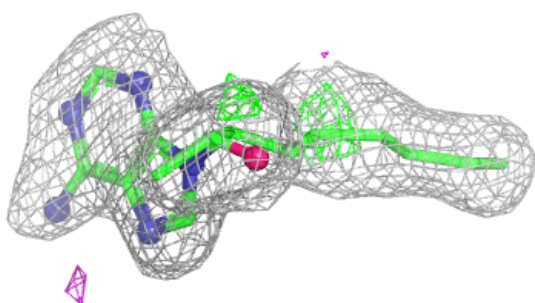
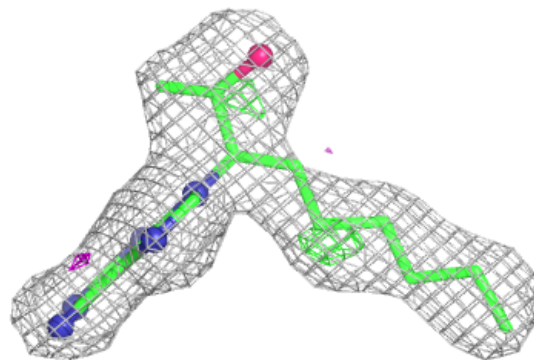
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	EH9	B	1900	20/20	0.83	0.12	25,26,26,27	0
2	EH9	D	1900	20/20	0.88	0.11	28,29,30,31	0
4	MG	A	1908	1/1	0.89	0.06	16,16,16,16	0
2	EH9	A	1906	20/20	0.91	0.09	23,24,26,26	0
2	EH9	C	1900	20/20	0.91	0.10	30,32,34,34	0
4	MG	C	1902	1/1	0.92	0.04	20,20,20,20	0
4	MG	D	1902	1/1	0.96	0.04	19,19,19,19	0
3	ZN	B	1901	1/1	0.98	0.04	20,20,20,20	0
4	MG	B	1902	1/1	0.98	0.04	16,16,16,16	0
3	ZN	A	1907	1/1	0.99	0.03	18,18,18,18	0
3	ZN	D	1901	1/1	0.99	0.03	26,26,26,26	0
3	ZN	C	1901	1/1	1.00	0.02	21,21,21,21	0

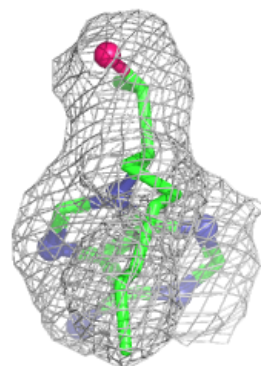
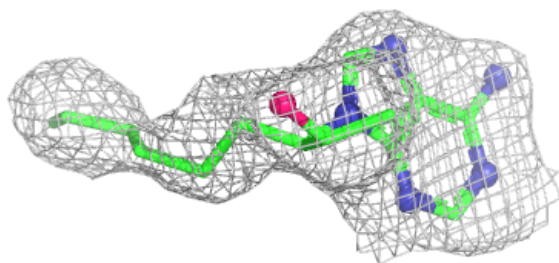
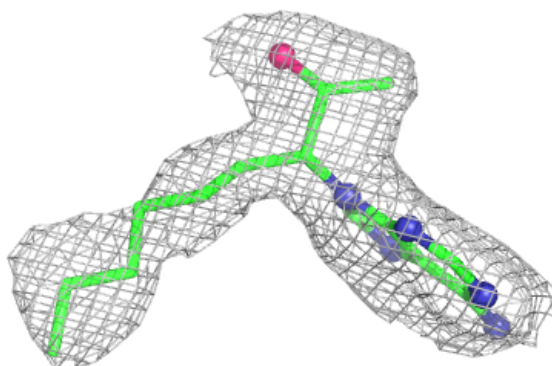
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around EH9 B 1900:

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

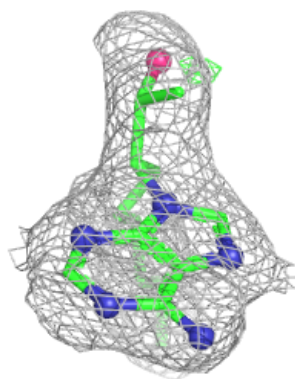
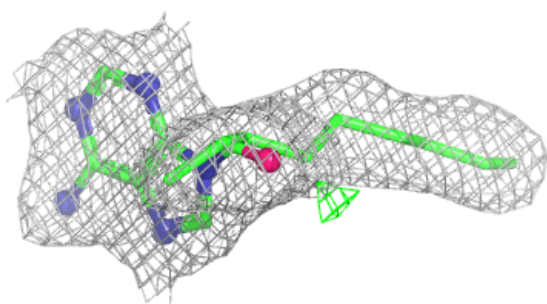
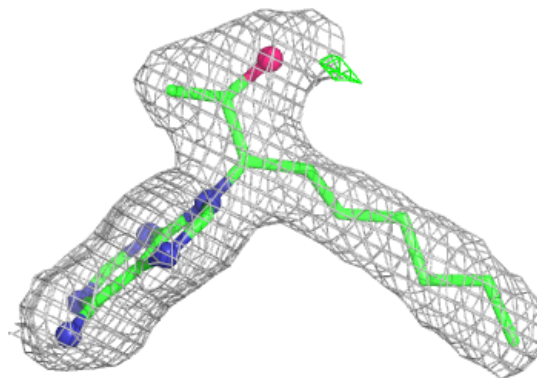
**Electron density around EH9 D 1900:**

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

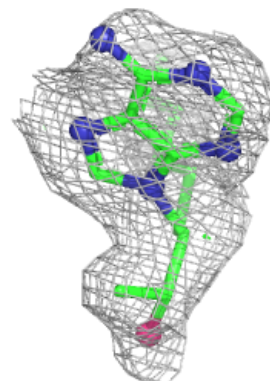
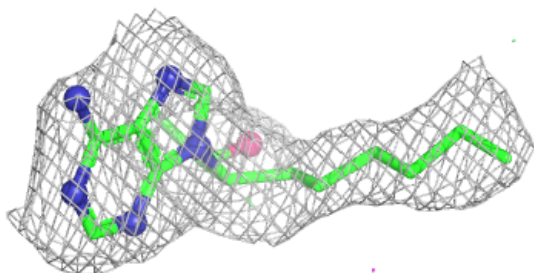
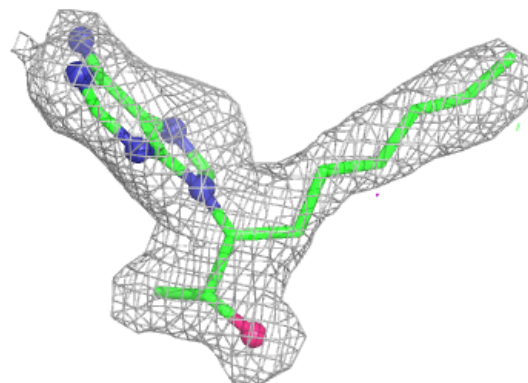


Electron density around EH9 A 1906:

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

**Electron density around EH9 C 1900:**

$2mF_o-DF_c$ (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.