



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2026 – 02:02 AM EDT

PDB ID : 9OBD / pdb_00009obd
Title : Crystal structure of human Argonaute2 in complex with a fully modified siRNA with a 5'-phenylpropargyl phosphate
Authors : Gebert, L.F.R.; MacRae, I.J.
Deposited on : 2025-04-22
Resolution : 2.02 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

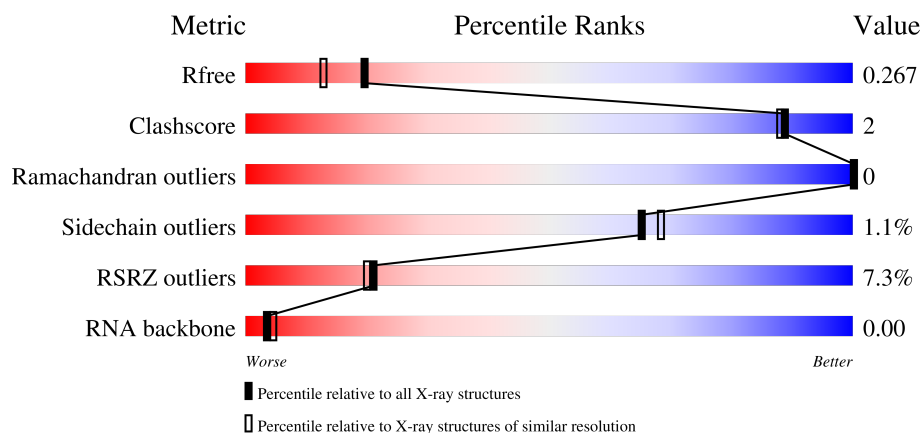
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.02 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	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (2.04-2.00)
RNA backbone	3983	1000 (2.38-1.66)

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	859	
2	B	21	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7120 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 Protein argonaute-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	810	Total	C	N	O	S	0	0	0
			6506	4139	1171	1155	41			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	387	ASP	SER	conflict	UNP Q9UKV8
A	824	ALA	SER	conflict	UNP Q9UKV8
A	828	ASP	SER	conflict	UNP Q9UKV8
A	831	ASP	SER	conflict	UNP Q9UKV8
A	834	ALA	SER	conflict	UNP Q9UKV8

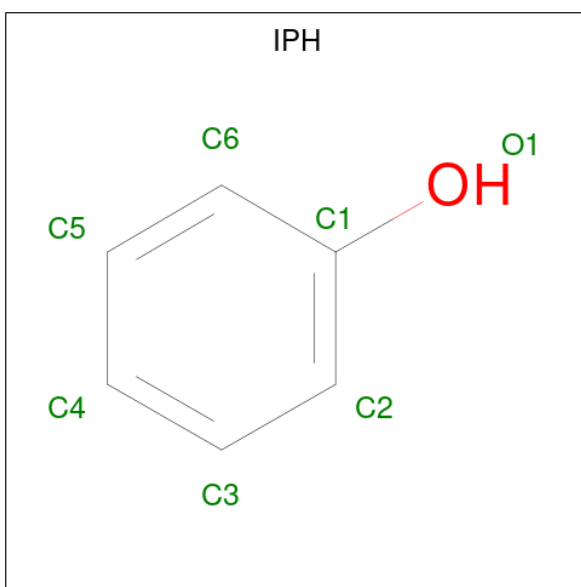
- Molecule 2 is a RNA chain called fully modified siRNA with a 5' phenylpropargyl phosphate.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	12	Total	C	F	N	O	P	S	0	0
			274	129	7	45	77	12	4		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

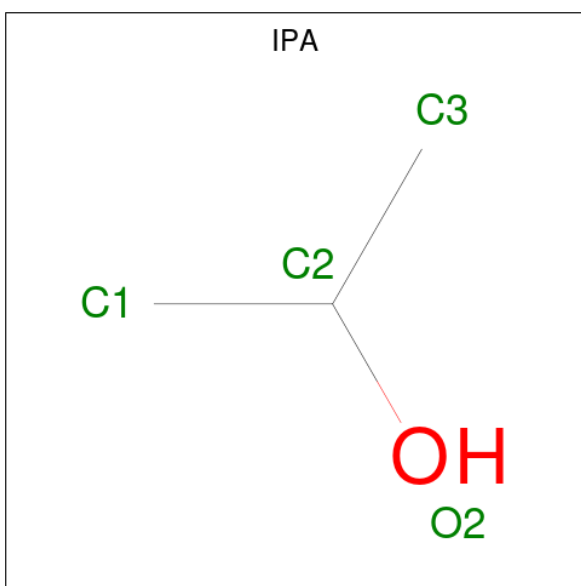
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is PHENOL (CCD ID: IPH) (formula: C₆H₆O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	6	1		
4	A	1	Total	C	O	0	0
			7	6	1		
4	A	1	Total	C	O	0	0
			7	6	1		

- Molecule 5 is ISOPROPYL ALCOHOL (CCD ID: IPA) (formula: C_3H_8O) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	287	Total	O	0	0
			287	287		
6	B	23	Total	O	0	0
			23	23		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.91Å 108.93Å 67.93Å 90.00° 107.80° 90.00°	Depositor
Resolution (Å)	64.68 – 2.02 64.68 – 2.02	Depositor EDS
% Data completeness (in resolution range)	98.7 (64.68-2.02) 98.7 (64.68-2.02)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 2.02Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.232 , 0.267 0.232 , 0.267	Depositor DCC
R_{free} test set	2809 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	35.7	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 36.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7120	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1CAL, GF2, UFT, A1CAK, F2T, OKT, RFJ, IPH, OMG, MG, IPA, AF2

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	0.11	0/6658	0.28	0/9008

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

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	6506	0	6567	23	0
2	B	274	0	75	6	0
3	A	1	0	0	0	0
4	A	21	0	18	1	0
5	A	8	0	14	2	0
6	A	287	0	0	0	0
6	B	23	0	0	0	0
All	All	7120	0	6674	26	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 (26) 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)
2:B:901:A1CAL:CB'	2:B:905:RFJ:S	2.75	0.74
1:A:62:LYS:NZ	1:A:64:GLU:OE2	2.34	0.57
1:A:618:MET:HE3	1:A:626:CYS:HB2	1.84	0.56
1:A:562:ASN:OD1	2:B:902:A1CAK:N2	2.40	0.55
1:A:709:LYS:NZ	5:A:907:IPA:H33	2.22	0.55
1:A:104:MET:HE3	1:A:105:PRO:HD2	1.88	0.55
1:A:605:ASP:OD1	1:A:606:GLY:N	2.44	0.51
1:A:111:ASP:N	1:A:111:ASP:OD1	2.44	0.50
1:A:524:GLY:O	2:B:901:A1CAL:N3	2.45	0.49
1:A:92:PRO:HB3	1:A:102:THR:HG22	1.95	0.48
1:A:184:ALA:O	1:A:186:GLU:HG3	2.14	0.48
2:B:907:GF2:O5'	2:B:907:GF2:H8	2.13	0.47
1:A:364:MET:HG3	2:B:909:OMG:HM23	1.97	0.47
1:A:47:MET:HE2	1:A:49:ILE:HD11	1.98	0.46
1:A:266:LYS:HE3	1:A:280:ARG:NH2	2.30	0.46
1:A:60:ASP:HB3	1:A:131:SER:HB2	1.98	0.45
1:A:381:LYS:HG2	1:A:384:ARG:HH22	1.82	0.44
1:A:737:ASP:HA	1:A:741:THR:HG21	1.98	0.44
1:A:709:LYS:HZ1	5:A:907:IPA:H33	1.83	0.43
1:A:590:PRO:HA	4:A:904:IPH:C1	2.49	0.43
1:A:42:ALA:C	1:A:44:PHE:H	2.27	0.42
1:A:167:ARG:HB2	1:A:181:PHE:HZ	1.86	0.41
1:A:428:ALA:HB2	1:A:440:LYS:HE2	2.03	0.41
1:A:533:LYS:HA	1:A:533:LYS:HD3	1.73	0.41
1:A:260:LYS:O	1:A:354:LYS:HE2	2.21	0.40
2:B:906:AF2:H8	2:B:906:AF2:O5'	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	798/859 (93%)	778 (98%)	20 (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	720/750 (96%)	712 (99%)	8 (1%)	65 68

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	LYS
1	A	111	ASP
1	A	127	ILE
1	A	186	GLU
1	A	241	LYS
1	A	269	ILE
1	A	607	LYS
1	A	853	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	461	GLN
1	A	558	GLN
1	A	681	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	0/21	-	-

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

12 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
2	GF2	B	907	2	22,25,26	3.72	14 (63%)	32,37,40	2.23	11 (34%)
2	UFT	B	908	2	18,21,22	4.19	14 (77%)	25,30,33	2.27	5 (20%)
2	F2T	B	923	2	18,21,22	4.67	15 (83%)	25,30,33	2.14	8 (32%)
2	AF2	B	912	2	21,24,25	3.39	9 (42%)	30,35,38	2.69	15 (50%)
2	OMG	B	911	2	23,26,27	0.48	0	32,38,41	0.67	0
2	A1CAL	B	901	2	32,33,33	3.92	14 (43%)	43,46,46	1.41	6 (13%)
2	RFJ	B	905	2	23,26,27	3.19	13 (56%)	32,38,41	2.09	11 (34%)
2	OMG	B	909	2	23,26,27	1.39	3 (13%)	32,38,41	1.18	3 (9%)
2	AF2	B	906	2	21,24,25	3.39	9 (42%)	30,35,38	2.59	12 (40%)
2	OKT	B	922	2	19,22,23	4.14	14 (73%)	25,31,34	1.94	6 (24%)
2	UFT	B	910	2	18,21,22	4.17	13 (72%)	25,30,33	1.93	5 (20%)
2	A1CAK	B	902	2	22,25,26	3.58	12 (54%)	32,37,40	2.27	11 (34%)

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	GF2	B	907	2	-	0/7/25/26	0/3/3/3
2	UFT	B	908	2	-	0/7/25/26	0/2/2/2
2	F2T	B	923	2	-	0/7/25/26	0/2/2/2
2	AF2	B	912	2	-	1/7/25/26	0/3/3/3
2	OMG	B	911	2	-	3/9/27/28	0/3/3/3
2	A1CAL	B	901	2	-	6/19/36/36	0/3/3/3
2	RFJ	B	905	2	-	1/9/27/28	0/3/3/3
2	OMG	B	909	2	-	1/9/27/28	0/3/3/3
2	AF2	B	906	2	-	0/7/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OKT	B	922	2	-	2/9/27/28	0/2/2/2
2	UFT	B	910	2	-	0/7/25/26	0/2/2/2
2	A1CAK	B	902	2	-	0/7/25/26	0/3/3/3

All (130) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	A1CAL	C3'-C4'	-10.76	1.25	1.53
2	B	902	A1CAK	C3'-C4'	-9.41	1.29	1.53
2	B	907	GF2	C3'-C4'	-9.05	1.30	1.53
2	B	908	UFT	O4'-C4'	-8.25	1.26	1.45
2	B	923	F2T	C2-N1	8.15	1.51	1.38
2	B	912	AF2	C3'-C4'	-7.99	1.32	1.53
2	B	910	UFT	O4'-C4'	-7.98	1.27	1.45
2	B	901	A1CAL	C2'-C1'	-7.97	1.33	1.53
2	B	906	AF2	C3'-C4'	-7.93	1.32	1.53
2	B	922	OKT	O4'-C4'	-7.88	1.27	1.45
2	B	905	RFJ	C2'-C1'	-7.83	1.33	1.53
2	B	923	F2T	C2-N3	7.69	1.51	1.38
2	B	901	A1CAL	O4'-C4'	7.48	1.61	1.45
2	B	912	AF2	C6-N6	7.27	1.52	1.34
2	B	901	A1CAL	C2-N3	7.19	1.50	1.38
2	B	910	UFT	C2-N1	7.04	1.49	1.38
2	B	906	AF2	C6-N6	6.95	1.52	1.34
2	B	922	OKT	C2-N3	6.89	1.50	1.38
2	B	901	A1CAL	C2-N1	6.87	1.49	1.38
2	B	912	AF2	O4'-C4'	6.87	1.60	1.45
2	B	902	A1CAK	F-C2'	-6.87	1.26	1.40
2	B	908	UFT	C2-N1	6.80	1.49	1.38
2	B	923	F2T	C6-C5	6.63	1.50	1.35
2	B	906	AF2	O4'-C4'	6.63	1.59	1.45
2	B	922	OKT	C2-N1	6.49	1.48	1.38
2	B	907	GF2	C4-N3	6.46	1.49	1.34
2	B	923	F2T	O4'-C4'	-6.30	1.31	1.45
2	B	905	RFJ	C4-N3	6.29	1.48	1.34
2	B	901	A1CAL	C3'-C2'	6.12	1.66	1.53
2	B	907	GF2	F-C2'	-6.11	1.28	1.40
2	B	910	UFT	C2-N3	6.04	1.48	1.38
2	B	908	UFT	C2-N3	6.00	1.48	1.38
2	B	923	F2T	C2'-C1'	5.94	1.60	1.53
2	B	922	OKT	C6-C5	5.43	1.47	1.35
2	B	902	A1CAK	C4-N3	5.43	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	906	AF2	O4'-C1'	-5.42	1.29	1.42
2	B	905	RFJ	C2-N3	5.41	1.46	1.33
2	B	910	UFT	C6-C5	5.29	1.47	1.35
2	B	908	UFT	C6-C5	5.28	1.47	1.35
2	B	923	F2T	C1'-N1	-5.28	1.32	1.47
2	B	907	GF2	C2-N3	5.27	1.46	1.33
2	B	907	GF2	O4'-C1'	-5.26	1.29	1.42
2	B	901	A1CAL	O2-C2	-5.18	1.13	1.23
2	B	912	AF2	O4'-C1'	-5.13	1.30	1.42
2	B	908	UFT	C1'-N1	-5.09	1.33	1.47
2	B	922	OKT	C3'-C4'	4.89	1.65	1.53
2	B	923	F2T	C3'-C4'	4.83	1.65	1.53
2	B	910	UFT	C1'-N1	-4.80	1.33	1.47
2	B	910	UFT	F2'-C2'	4.72	1.49	1.40
2	B	922	OKT	C1'-N1	-4.66	1.34	1.47
2	B	922	OKT	O4'-C1'	4.64	1.52	1.42
2	B	908	UFT	F2'-C2'	4.60	1.49	1.40
2	B	907	GF2	C2-N2	4.59	1.44	1.34
2	B	902	A1CAK	C2-N3	4.38	1.43	1.33
2	B	901	A1CAL	C6-C5	4.35	1.45	1.35
2	B	922	OKT	C4-N3	4.24	1.45	1.38
2	B	902	A1CAK	C5-N7	-4.22	1.30	1.39
2	B	923	F2T	O2-C2	-4.11	1.15	1.23
2	B	910	UFT	C3'-C4'	4.09	1.63	1.53
2	B	908	UFT	C3'-C4'	4.07	1.63	1.53
2	B	923	F2T	C4-N3	4.03	1.45	1.38
2	B	922	OKT	O01-C2'	4.02	1.52	1.42
2	B	909	OMG	O5'-C5'	-3.99	1.32	1.44
2	B	910	UFT	O4'-C1'	3.97	1.51	1.42
2	B	905	RFJ	C2-N2	3.89	1.43	1.34
2	B	902	A1CAK	C2-N2	3.85	1.43	1.34
2	B	908	UFT	O4-C4	-3.73	1.17	1.24
2	B	902	A1CAK	O6-C6	-3.72	1.16	1.23
2	B	908	UFT	O4'-C1'	3.66	1.50	1.42
2	B	923	F2T	O4'-C1'	3.65	1.50	1.42
2	B	905	RFJ	O3'-C3'	-3.58	1.34	1.43
2	B	901	A1CAL	CE'-CD'	3.53	1.52	1.44
2	B	908	UFT	C4-N3	3.50	1.44	1.38
2	B	910	UFT	C4-N3	3.48	1.44	1.38
2	B	923	F2T	F2'-C2'	3.44	1.47	1.40
2	B	910	UFT	O4-C4	-3.43	1.17	1.24
2	B	901	A1CAL	O4-C4	-3.38	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	923	F2T	O4-C4	-3.37	1.17	1.24
2	B	901	A1CAL	O4'-C1'	3.35	1.49	1.42
2	B	907	GF2	C5-N7	-3.34	1.32	1.39
2	B	905	RFJ	C5-N7	-3.32	1.32	1.39
2	B	902	A1CAK	C4-N9	-3.20	1.29	1.38
2	B	923	F2T	C5-C4	3.19	1.50	1.43
2	B	905	RFJ	O2'-C2'	3.14	1.50	1.42
2	B	922	OKT	C6-N1	3.13	1.45	1.38
2	B	910	UFT	O3'-C3'	3.11	1.50	1.43
2	B	906	AF2	C5-N7	-3.11	1.33	1.39
2	B	905	RFJ	C2-N1	3.10	1.45	1.37
2	B	908	UFT	O3'-C3'	3.09	1.50	1.43
2	B	906	AF2	F-C2'	-3.08	1.34	1.40
2	B	905	RFJ	C5-C6	2.97	1.55	1.44
2	B	908	UFT	O2-C2	-2.96	1.17	1.23
2	B	912	AF2	O3'-C3'	2.93	1.50	1.43
2	B	907	GF2	O6-C6	-2.90	1.18	1.23
2	B	923	F2T	C6-N1	2.84	1.44	1.38
2	B	906	AF2	O3'-C3'	2.84	1.50	1.43
2	B	910	UFT	O2-C2	-2.79	1.18	1.23
2	B	922	OKT	O4-C4	-2.77	1.19	1.24
2	B	912	AF2	C5-N7	-2.73	1.34	1.39
2	B	907	GF2	C2-N1	2.72	1.44	1.37
2	B	907	GF2	C2'-C3'	2.72	1.56	1.52
2	B	922	OKT	O2-C2	-2.68	1.18	1.23
2	B	912	AF2	C1'-N9	2.67	1.53	1.46
2	B	901	A1CAL	C4-N3	2.66	1.43	1.38
2	B	912	AF2	F-C2'	-2.63	1.35	1.40
2	B	901	A1CAL	C6-N1	2.63	1.44	1.38
2	B	902	A1CAK	C2'-C3'	2.55	1.56	1.52
2	B	906	AF2	C5-C4	-2.54	1.34	1.39
2	B	905	RFJ	O6-C6	-2.53	1.18	1.23
2	B	922	OKT	C5-C4	2.51	1.49	1.43
2	B	909	OMG	C2-N2	2.49	1.40	1.34
2	B	907	GF2	C2'-C1'	2.46	1.56	1.53
2	B	907	GF2	O3'-C3'	2.42	1.48	1.43
2	B	905	RFJ	C1'-N9	-2.40	1.40	1.47
2	B	907	GF2	C5-C6	2.33	1.53	1.44
2	B	907	GF2	C4-N9	-2.32	1.32	1.38
2	B	906	AF2	C1'-N9	2.32	1.52	1.46
2	B	901	A1CAL	CB'-CC'	2.32	1.54	1.46
2	B	905	RFJ	C4-N9	-2.30	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	902	A1CAK	O3'-C3'	2.30	1.48	1.43
2	B	910	UFT	C6-N1	2.29	1.43	1.38
2	B	902	A1CAK	O5'-C5'	-2.25	1.37	1.44
2	B	922	OKT	O3'-C3'	2.25	1.48	1.43
2	B	905	RFJ	O5'-C5'	-2.24	1.37	1.44
2	B	909	OMG	O4'-C4'	-2.19	1.40	1.45
2	B	902	A1CAK	O4'-C4'	2.17	1.49	1.45
2	B	912	AF2	C2-N3	2.17	1.37	1.33
2	B	908	UFT	C6-N1	2.15	1.43	1.38
2	B	908	UFT	C2'-C1'	2.09	1.55	1.53
2	B	923	F2T	O3'-C3'	2.04	1.48	1.43

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	908	UFT	C4-N3-C2	-6.07	119.08	126.61
2	B	906	AF2	C5-C4-N3	-5.98	118.48	126.72
2	B	912	AF2	C5-C4-N3	-5.76	118.78	126.72
2	B	906	AF2	N3-C2-N1	-5.67	120.00	128.58
2	B	912	AF2	N3-C2-N1	-5.61	120.09	128.58
2	B	910	UFT	C4-N3-C2	-5.60	119.66	126.61
2	B	922	OKT	C4-N3-C2	-5.59	119.67	126.61
2	B	908	UFT	C2'-C1'-N1	-5.48	105.84	114.27
2	B	923	F2T	C4-N3-C2	-5.43	119.87	126.61
2	B	906	AF2	C1'-N9-C8	5.30	138.85	127.09
2	B	912	AF2	C1'-N9-C8	5.22	138.69	127.09
2	B	905	RFJ	C5-C4-N3	-5.15	120.19	128.39
2	B	907	GF2	C5-C4-N3	-5.12	120.25	128.39
2	B	902	A1CAK	C5-C4-N3	-5.08	120.31	128.39
2	B	923	F2T	C2'-C1'-N1	-4.97	106.62	114.27
2	B	905	RFJ	C2-N3-C4	4.49	120.04	112.30
2	B	907	GF2	C1'-N9-C4	-4.41	113.46	126.49
2	B	908	UFT	C5-C4-N3	4.30	120.83	114.80
2	B	902	A1CAK	C2-N3-C4	4.26	119.64	112.30
2	B	907	GF2	C2-N3-C4	4.22	119.57	112.30
2	B	906	AF2	C4-N9-C1'	-4.17	116.89	126.63
2	B	912	AF2	C4-N9-C1'	-4.13	116.98	126.63
2	B	906	AF2	C2-N3-C4	4.11	121.87	111.83
2	B	906	AF2	N6-C6-N1	-4.10	109.25	118.38
2	B	902	A1CAK	C1'-N9-C4	-4.03	114.58	126.49
2	B	912	AF2	N6-C6-N1	-3.96	109.56	118.38
2	B	901	A1CAL	C5-C4-N3	3.95	120.33	114.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	912	AF2	C2-N3-C4	3.91	121.38	111.83
2	B	906	AF2	C5-C4-N9	3.91	110.07	105.81
2	B	901	A1CAL	C4-N3-C2	-3.90	121.77	126.61
2	B	922	OKT	N3-C2-N1	3.88	119.95	114.89
2	B	910	UFT	C5-C4-N3	3.84	120.17	114.80
2	B	922	OKT	C5-C4-N3	3.82	120.15	114.80
2	B	923	F2T	N3-C2-N1	3.80	119.84	114.89
2	B	910	UFT	N3-C2-N1	3.80	119.83	114.89
2	B	908	UFT	N3-C2-N1	3.79	119.82	114.89
2	B	907	GF2	C1'-N9-C8	3.74	137.35	126.73
2	B	923	F2T	C5-C4-N3	3.74	120.03	114.80
2	B	912	AF2	C5-C4-N9	3.73	109.87	105.81
2	B	902	A1CAK	O4'-C1'-C2'	-3.62	102.01	105.84
2	B	912	AF2	C2'-C3'-C4'	3.47	107.01	102.43
2	B	902	A1CAK	N9-C4-N3	3.43	132.81	125.95
2	B	905	RFJ	C3'-C2'-C1'	3.39	109.31	102.81
2	B	902	A1CAK	N9-C8-N7	-3.39	107.12	113.40
2	B	907	GF2	N9-C4-N3	3.35	132.65	125.95
2	B	907	GF2	N9-C8-N7	-3.35	107.19	113.40
2	B	908	UFT	O4-C4-C5	-3.31	119.45	125.16
2	B	902	A1CAK	C1'-N9-C8	3.30	136.12	126.73
2	B	901	A1CAL	O1-CB'-CC'	-3.30	101.59	109.29
2	B	905	RFJ	C2-N1-C6	-3.23	119.24	125.11
2	B	902	A1CAK	C3'-C2'-C1'	-3.21	99.37	103.10
2	B	907	GF2	C2-N1-C6	-3.20	119.30	125.11
2	B	905	RFJ	N9-C8-N7	-3.07	107.71	113.40
2	B	922	OKT	O4-C4-C5	-3.02	119.96	125.16
2	B	902	A1CAK	C2-N1-C6	-3.00	119.66	125.11
2	B	923	F2T	O4-C4-C5	-2.97	120.03	125.16
2	B	910	UFT	C2'-C1'-N1	-2.89	109.83	114.27
2	B	910	UFT	O4-C4-C5	-2.84	120.26	125.16
2	B	905	RFJ	N9-C4-N3	2.82	131.59	125.95
2	B	902	A1CAK	O6-C6-C5	-2.78	119.18	126.53
2	B	905	RFJ	C5-C6-N1	2.73	120.21	113.25
2	B	907	GF2	O4'-C4'-C3'	2.72	110.55	105.15
2	B	907	GF2	C5-C6-N1	2.64	119.97	113.25
2	B	905	RFJ	O4'-C1'-C2'	2.63	111.12	106.59
2	B	905	RFJ	C2'-C1'-N9	-2.61	109.28	114.24
2	B	909	OMG	N1-C2-N3	2.59	128.05	123.32
2	B	922	OKT	O4'-C4'-C3'	2.57	110.26	105.15
2	B	907	GF2	O6-C6-C5	-2.54	119.82	126.53
2	B	912	AF2	C3'-C2'-C1'	2.54	106.05	103.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	906	AF2	N3-C4-N9	2.52	131.45	127.17
2	B	902	A1CAK	C5-C6-N1	2.50	119.61	113.25
2	B	901	A1CAL	C4'-O4'-C1'	-2.49	103.97	109.47
2	B	906	AF2	C5-C6-N1	2.49	123.83	117.51
2	B	912	AF2	N3-C4-N9	2.46	131.35	127.17
2	B	901	A1CAL	O4-C4-C5	-2.40	121.02	125.16
2	B	922	OKT	O2-C2-N1	-2.37	119.71	122.80
2	B	901	A1CAL	O4'-C4'-C5'	-2.34	101.84	109.33
2	B	923	F2T	O2-C2-N1	-2.29	119.82	122.80
2	B	923	F2T	C2'-C3'-C4'	-2.28	99.43	102.43
2	B	912	AF2	C5-C6-N1	2.26	123.24	117.51
2	B	907	GF2	C8-N7-C5	2.23	108.23	104.26
2	B	912	AF2	C4-C5-N7	-2.23	108.03	110.58
2	B	905	RFJ	O6-C6-C5	-2.20	120.72	126.53
2	B	905	RFJ	C8-N7-C5	2.16	108.10	104.26
2	B	909	OMG	O6-C6-C5	2.15	132.21	126.53
2	B	906	AF2	C4-C5-N7	-2.15	108.13	110.58
2	B	906	AF2	N9-C8-N7	-2.13	110.92	113.94
2	B	912	AF2	C5-N7-C8	2.12	106.78	103.45
2	B	912	AF2	N9-C8-N7	-2.08	110.98	113.94
2	B	909	OMG	C3'-C2'-C1'	-2.05	98.89	102.81
2	B	906	AF2	C5-N7-C8	2.03	106.64	103.45
2	B	923	F2T	C3'-C2'-C1'	-2.01	100.77	103.10
2	B	912	AF2	C2'-C1'-N9	-2.01	110.33	113.92

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	901	A1CAL	C3'-C4'-C5'-O5'
2	B	901	A1CAL	O4'-C4'-C5'-O5'
2	B	901	A1CAL	CB'-O1-P-O5'
2	B	901	A1CAL	CB'-O1-P-OP2
2	B	901	A1CAL	CB'-O1-P-OP1
2	B	905	RFJ	C1'-C2'-O2'-C
2	B	911	OMG	C1'-C2'-O2'-CM2
2	B	922	OKT	C3'-C4'-C5'-O5'
2	B	911	OMG	O4'-C4'-C5'-O5'
2	B	911	OMG	C3'-C4'-C5'-O5'
2	B	922	OKT	O4'-C4'-C5'-O5'
2	B	909	OMG	O4'-C4'-C5'-O5'
2	B	901	A1CAL	O1-CB'-CC'-CD'

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Mol	Chain	Res	Type	Atoms
2	B	912	AF2	C2'-C1'-N9-C8

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	907	GF2	1	0
2	B	901	A1CAL	2	0
2	B	905	RFJ	1	0
2	B	909	OMG	1	0
2	B	906	AF2	1	0
2	B	902	A1CAK	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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	$\# Z > 2$
4	IPH	A	903	-	7,7,7	0.57	0	8,8,8	0.29	0
5	IPA	A	907	-	3,3,3	0.59	0	3,3,3	1.33	0
4	IPH	A	905	-	7,7,7	0.58	0	8,8,8	0.30	0
4	IPH	A	904	-	7,7,7	0.61	0	8,8,8	0.32	0
5	IPA	A	906	-	3,3,3	0.59	0	3,3,3	1.34	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
4	IPH	A	905	-	-	-	0/1/1/1
4	IPH	A	903	-	-	-	0/1/1/1
4	IPH	A	904	-	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

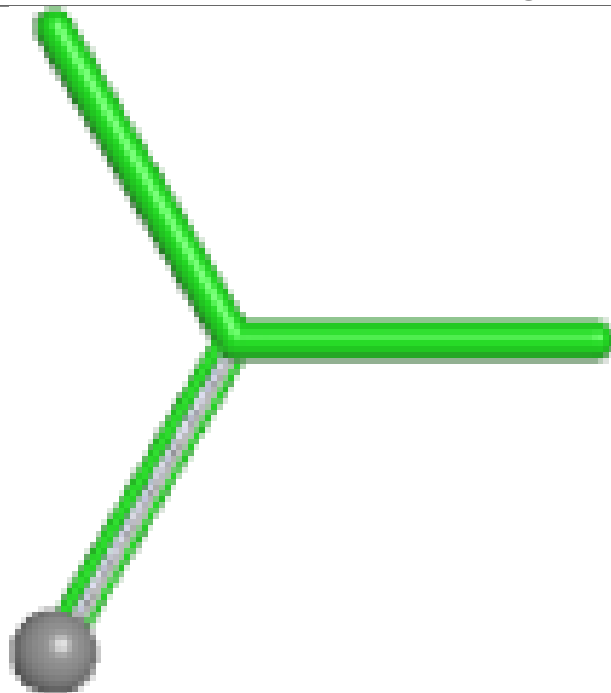
There are no ring outliers.

2 monomers are involved in 3 short contacts:

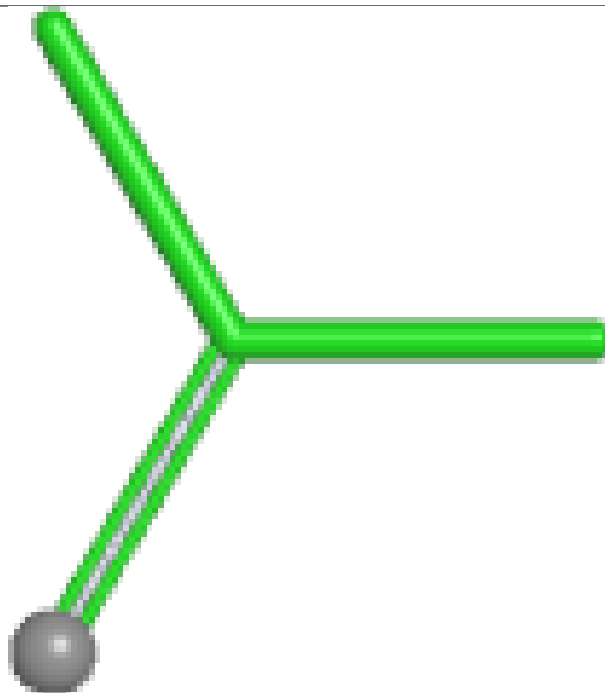
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	907	IPA	2	0
4	A	904	IPH	1	0

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.

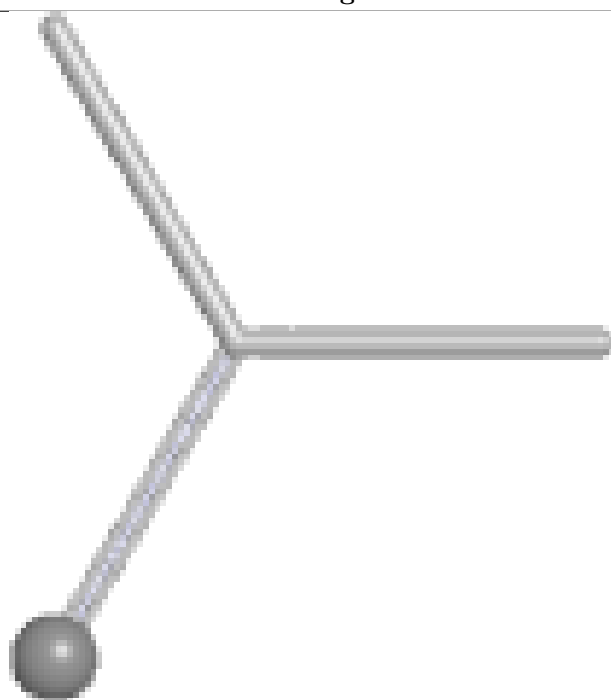
Ligand IPA A 907



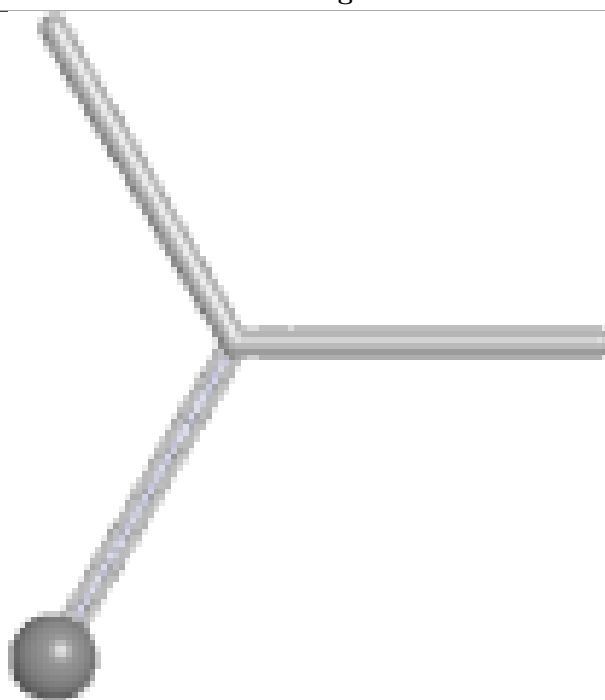
Bond lengths



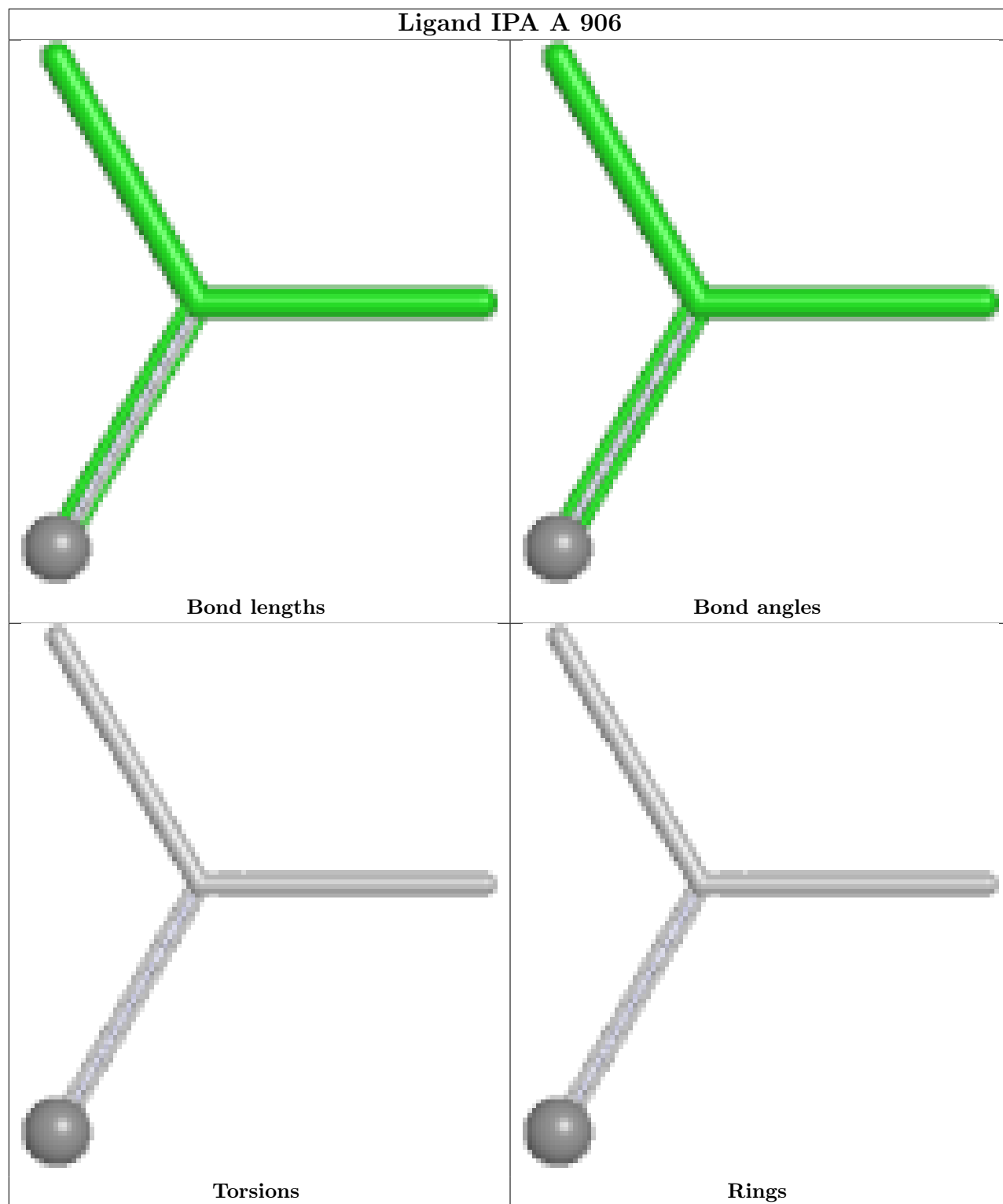
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	810/859 (94%)	0.62	59 (7%) 21 20	22, 43, 71, 87	0
2	B	0/21	-	-	-	-
All	All	810/880 (92%)	0.62	59 (7%) 21 20	22, 43, 71, 87	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	369	ALA	4.4
1	A	185	SER	4.2
1	A	602	PRO	4.0
1	A	127	ILE	3.9
1	A	54	ILE	3.7
1	A	272	CYS	3.4
1	A	98	LYS	3.4
1	A	22	ALA	3.2
1	A	134	TRP	3.2
1	A	156	PHE	3.0
1	A	820	LYS	3.0
1	A	120	PRO	3.0
1	A	336	HIS	3.0
1	A	104	MET	2.9
1	A	275	MET	2.9
1	A	189	SER	2.9
1	A	63	PRO	2.7
1	A	253	SER	2.7
1	A	86	ILE	2.7
1	A	137	CYS	2.6
1	A	490	CYS	2.6
1	A	151	LEU	2.6
1	A	128	PHE	2.5
1	A	491	PHE	2.5
1	A	132	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	240	PHE	2.5
1	A	117	VAL	2.4
1	A	368	THR	2.4
1	A	481	ALA	2.4
1	A	52	ILE	2.4
1	A	243	ILE	2.4
1	A	853	LEU	2.4
1	A	149	GLY	2.4
1	A	424	ASN	2.3
1	A	465	VAL	2.3
1	A	69	ARG	2.3
1	A	84	THR	2.2
1	A	504	MET	2.2
1	A	513	ALA	2.2
1	A	61	ILE	2.2
1	A	352	CYS	2.2
1	A	77	HIS	2.2
1	A	249	PRO	2.2
1	A	304	VAL	2.2
1	A	184	ALA	2.2
1	A	523	PRO	2.1
1	A	487	GLY	2.1
1	A	554	ARG	2.1
1	A	154	VAL	2.1
1	A	452	ALA	2.1
1	A	333	GLU	2.1
1	A	492	CYS	2.1
1	A	130	VAL	2.1
1	A	561	SER	2.1
1	A	119	LEU	2.0
1	A	113	VAL	2.0
1	A	59	LEU	2.0
1	A	250	LEU	2.0
1	A	81	HIS	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($\text{\AA}^2$)	Q<0.9
2	AF2	B	912	22/23	0.73	0.18	49,75,79,81	0
2	OKT	B	922	21/22	0.73	0.15	48,59,70,83	0
2	OMG	B	911	24/25	0.87	0.15	38,66,80,84	0
2	OMG	B	909	24/25	0.92	0.08	39,43,49,53	0
2	A1CAL	B	901	31/31	0.92	0.10	43,46,54,57	0
2	UFT	B	910	20/21	0.94	0.08	36,41,48,55	0
2	A1CAK	B	902	23/24	0.94	0.07	36,40,42,49	0
2	F2T	B	923	20/21	0.94	0.08	35,41,47,52	0
2	RFJ	B	905	24/25	0.95	0.08	31,38,42,45	0
2	AF2	B	906	22/23	0.96	0.07	24,32,42,43	0
2	GF2	B	907	23/24	0.96	0.07	22,32,43,46	0
2	UFT	B	908	20/21	0.96	0.07	25,34,45,52	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

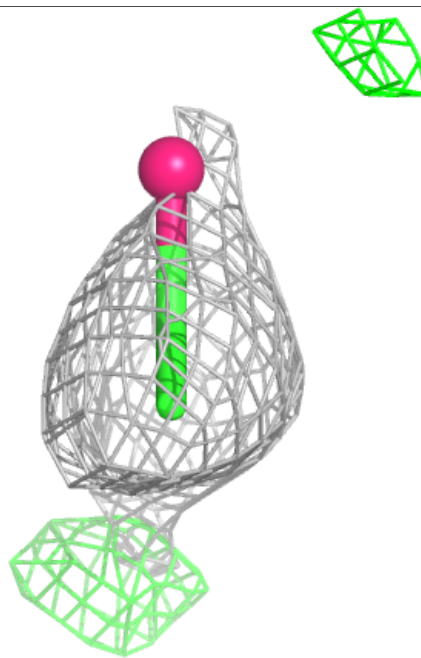
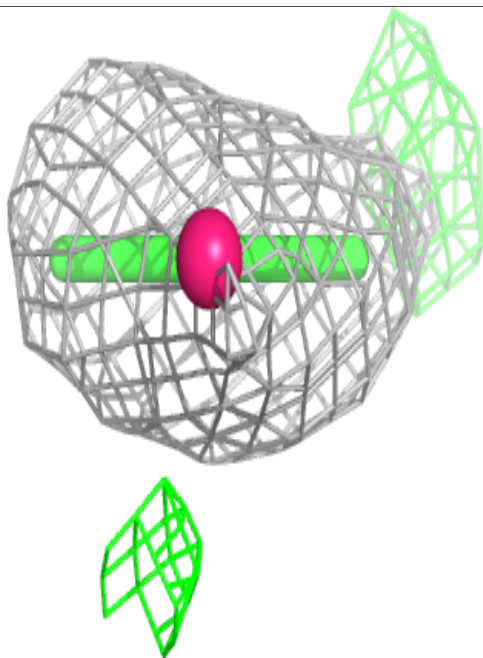
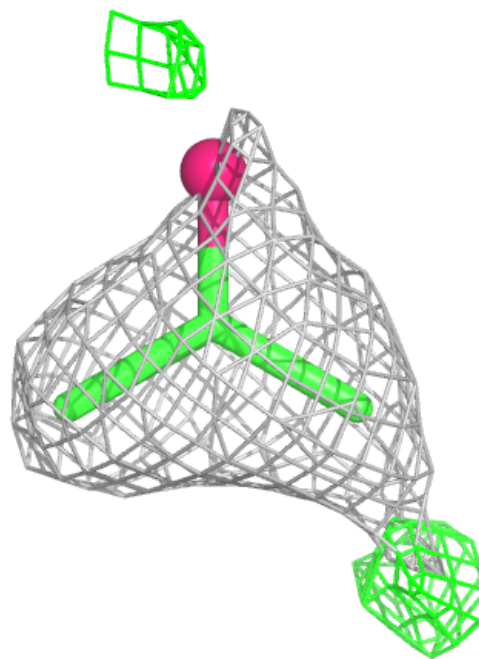
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	IPH	A	905	7/7	0.53	0.22	42,50,53,57	0
4	IPH	A	904	7/7	0.55	0.21	35,39,45,51	0
5	IPA	A	906	4/4	0.69	0.24	43,48,50,59	0
5	IPA	A	907	4/4	0.73	0.22	41,47,48,55	0
4	IPH	A	903	7/7	0.83	0.14	34,40,41,44	0
3	MG	A	902	1/1	0.92	0.07	39,39,39,39	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.

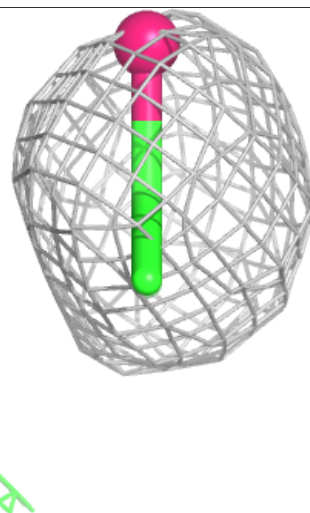
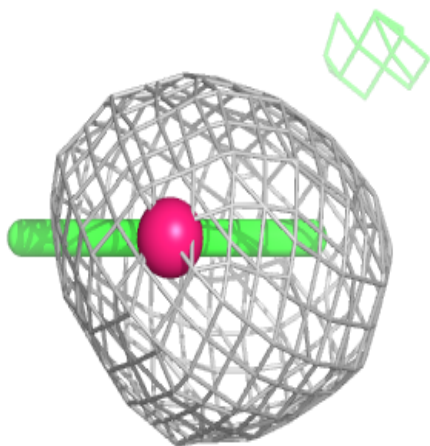
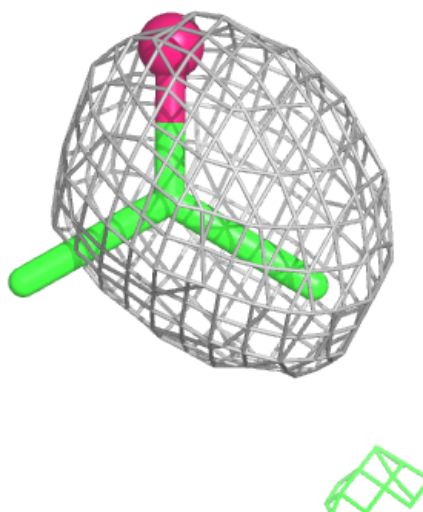
Electron density around IPA A 906:

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



Electron density around IPA A 907:

$2mF_o-DF_c$ (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.