WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 18, 2024 – 10:16 PM EST

PDB ID	:	4HNW
Title	:	The NatA Acetyltransferase Complex Bound To Inositol Hexakisphosphate
Authors	:	Neubauer, J.L.; Immormino, R.M.; Dollins, D.E.; Endo-Streeter, S.T.; Pemble IV, C.W.; York, J.D.
Deposited on	:	2012-10-21
Resolution	:	2.80 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.80 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.
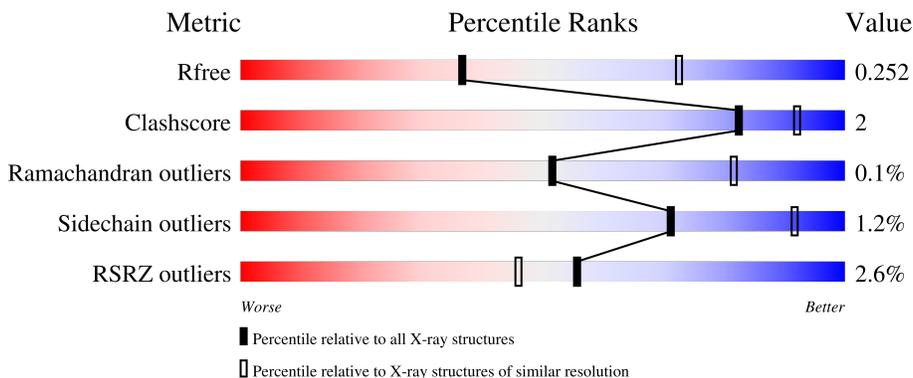
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 <=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	863	3% 85% 6% 9%
2	B	248	71% 5% 24%

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 14257 atoms, of which 6749 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 N-terminal acetyltransferase A complex subunit NAT1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	782	Total 11159	C 3749	H 5289	N 986	O 1114	S 21	3	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	855	TYR	-	expression tag	UNP P12945
A	856	PRO	-	expression tag	UNP P12945
A	857	TYR	-	expression tag	UNP P12945
A	858	ASP	-	expression tag	UNP P12945
A	859	VAL	-	expression tag	UNP P12945
A	860	PRO	-	expression tag	UNP P12945
A	861	ASP	-	expression tag	UNP P12945
A	862	TYR	-	expression tag	UNP P12945
A	863	ALA	-	expression tag	UNP P12945

- Molecule 2 is a protein called N-terminal acetyltransferase A complex catalytic subunit ARD1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	189	Total 2816	C 921	H 1364	N 246	O 274	S 11	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	239	GLU	-	expression tag	UNP P07347
B	240	GLN	-	expression tag	UNP P07347
B	241	LYS	-	expression tag	UNP P07347
B	242	LEU	-	expression tag	UNP P07347
B	243	ILE	-	expression tag	UNP P07347
B	244	SER	-	expression tag	UNP P07347

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Chain	Residue	Modelled	Actual	Comment	Reference
B	245	GLU	-	expression tag	UNP P07347
B	246	GLU	-	expression tag	UNP P07347
B	247	ASP	-	expression tag	UNP P07347
B	248	LEU	-	expression tag	UNP P07347

- Molecule 3 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$).
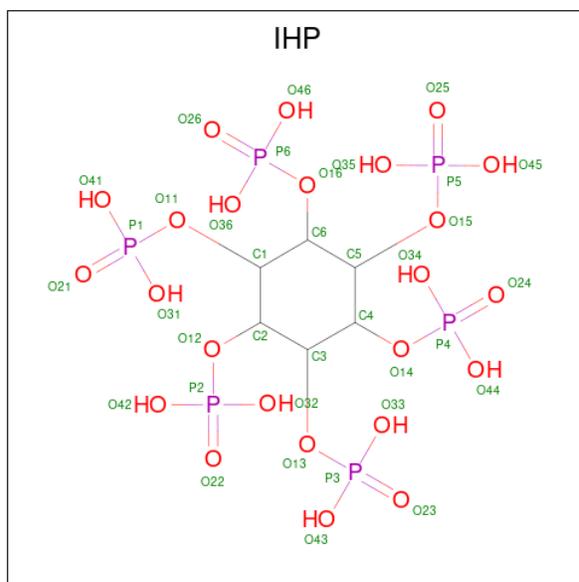
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	O	P		
3	A	1	42	6	6	24	6	0	0

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).

PG4
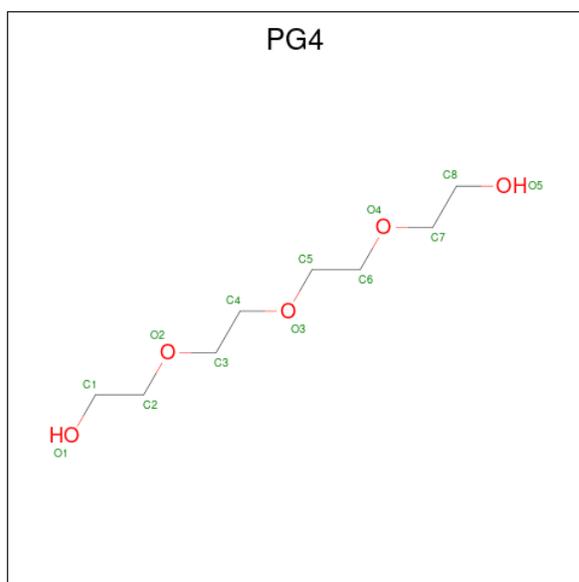
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 31	C 8	H 18	O 5	0	0
4	A	1	Total 31	C 8	H 18	O 5	0	0
4	A	1	Total 31	C 8	H 18	O 5	0	0
4	A	1	Total 31	C 8	H 18	O 5	0	0
4	A	1	Total 31	C 8	H 18	O 5	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	61	Total 61	O 61	0	0
5	B	24	Total 24	O 24	0	0

3 Residue-property plots ⓘ

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: N-terminal acetyltransferase A complex subunit NAT1

Chain A:
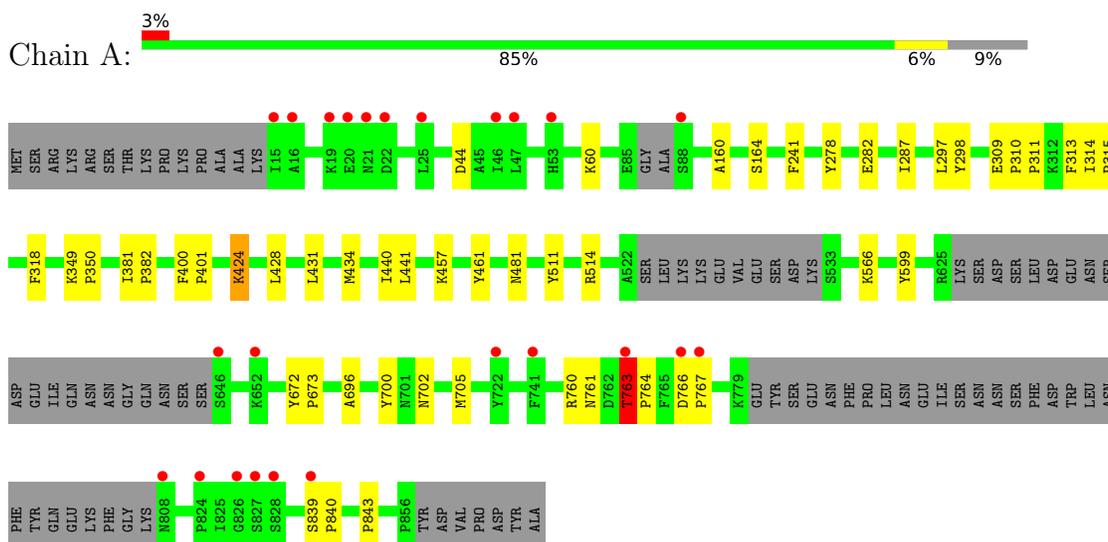
• Molecule 2: N-terminal acetyltransferase A complex catalytic subunit ARD1

Chain B:
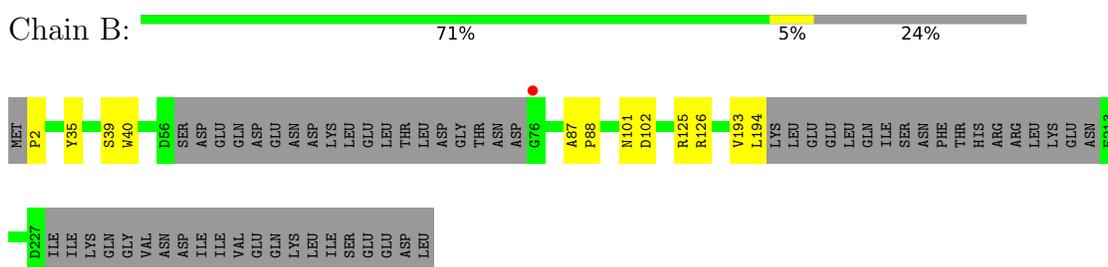
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	135.66Å 135.66Å 175.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.49 – 2.80 43.05 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (41.49-2.80) 99.7 (43.05-2.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.10 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928), CNS	Depositor
R, R_{free}	0.229 , 0.251 0.227 , 0.252	Depositor DCC
R_{free} test set	2351 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	61.5	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 58.0	EDS
L-test for twinning [2]	$< |L| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	14257	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: PG4, IHP

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	0.22	0/5993	0.36	0/8153
2	B	0.22	0/1480	0.39	0/2014
All	All	0.22	0/7473	0.36	0/10167

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	5870	5289	5278	29	0
2	B	1452	1364	1358	7	0
3	A	36	6	5	1	0
4	A	65	90	90	0	0
5	A	61	0	0	1	0
5	B	24	0	0	1	0
All	All	7508	6749	6731	35	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 (35) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:LYS:NZ	3:A:901:IHP:O36	2.27	0.68
1:A:763:THR:HB	1:A:764:PRO:CD	2.25	0.67
1:A:381:ILE:HB	1:A:382:PRO:HD3	1.81	0.63
1:A:766:ASP:CB	1:A:767:PRO:HD3	2.31	0.59
1:A:44:ASP:OD1	1:A:60:LYS:NZ	2.34	0.59
1:A:160:ALA:O	1:A:164:SER:OG	2.15	0.58
1:A:349:LYS:N	1:A:350:PRO:HD2	2.22	0.54
1:A:763:THR:HB	1:A:764:PRO:HD3	1.89	0.54
2:B:101:ASN:O	5:B:319:HOH:O	2.19	0.53
1:A:441:LEU:HD12	1:A:461:TYR:CG	2.44	0.53
1:A:282:GLU:OE1	1:A:298:TYR:OH	2.22	0.49
1:A:313:PHE:CZ	2:B:2:PRO:HD3	2.48	0.49
1:A:760:ARG:HA	1:A:761:ASN:HA	1.67	0.47
1:A:424:LYS:HG2	1:A:440:ILE:HD13	1.97	0.47
1:A:599:TYR:CD2	1:A:702:ASN:HB3	2.50	0.46
1:A:315:PRO:HA	1:A:318:PHE:CE2	2.50	0.46
2:B:39:SER:HB2	2:B:40:TRP:CE3	2.51	0.45
2:B:125:ARG:HG3	2:B:126:ARG:HG3	1.98	0.44
1:A:278:TYR:CE2	1:A:310:PRO:HG2	2.51	0.44
1:A:696:ALA:HA	1:A:700:TYR:HB3	1.98	0.44
1:A:428:LEU:HD12	1:A:440:ILE:HD12	2.00	0.44
1:A:310:PRO:HB2	1:A:311:PRO:HD3	2.00	0.43
1:A:431:LEU:HA	1:A:843:PRO:HG2	1.99	0.43
1:A:314:ILE:N	1:A:315:PRO:CD	2.82	0.43
1:A:672:TYR:HB3	1:A:673:PRO:HD2	2.01	0.42
1:A:400:PHE:N	1:A:401:PRO:CD	2.82	0.42
2:B:35:TYR:OH	2:B:102:ASP:OD1	2.31	0.42
1:A:309:GLU:HB2	1:A:310:PRO:HD3	2.01	0.42
1:A:566:LYS:HD2	5:A:1027:HOH:O	2.19	0.41
1:A:839:SER:CB	1:A:840:PRO:HD3	2.51	0.41
1:A:766:ASP:CB	1:A:767:PRO:CD	2.97	0.41
2:B:193:VAL:O	2:B:194:LEU:HD12	2.21	0.41
1:A:309:GLU:N	1:A:310:PRO:CD	2.84	0.40
1:A:287:ILE:HD11	1:A:297:LEU:HD22	2.04	0.40
2:B:87:ALA:HB1	2:B:88:PRO:HD2	2.03	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	772/863 (90%)	738 (96%)	33 (4%)	1 (0%)	51	81
2	B	183/248 (74%)	181 (99%)	2 (1%)	0	100	100
All	All	955/1111 (86%)	919 (96%)	35 (4%)	1 (0%)	51	81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	763	THR

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	542/767 (71%)	534 (98%)	8 (2%)	65	89
2	B	146/226 (65%)	146 (100%)	0	100	100
All	All	688/993 (69%)	680 (99%)	8 (1%)	71	92

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

Mol	Chain	Res	Type
1	A	241	PHE
1	A	424	LYS
1	A	434	MET
1	A	481	ASN
1	A	511	TYR

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Mol	Chain	Res	Type
1	A	514	ARG
1	A	705	MET
1	A	763	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	209	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

6 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	$\#|Z| > 2$
3	IHP	A	901	-	36,36,36	1.12	0	54,60,60	1.12	3 (5%)
4	PG4	A	903	-	12,12,12	0.66	0	11,11,11	0.63	0
4	PG4	A	905	-	12,12,12	0.65	0	11,11,11	0.68	0
4	PG4	A	902	-	12,12,12	0.64	0	11,11,11	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$\|Z\|$ > 2	Counts	RMSZ	#$\|Z\|$ > 2
4	PG4	A	906	-	12,12,12	0.65	0	11,11,11	0.88	0
4	PG4	A	904	-	12,12,12	0.67	0	11,11,11	0.79	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
3	IHP	A	901	-	-	2/30/54/54	0/1/1/1
4	PG4	A	903	-	-	3/10/10/10	-
4	PG4	A	905	-	-	1/10/10/10	-
4	PG4	A	902	-	-	2/10/10/10	-
4	PG4	A	906	-	-	3/10/10/10	-
4	PG4	A	904	-	-	5/10/10/10	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	901	IHP	C5-C4-C3	5.33	122.09	110.41
3	A	901	IHP	O14-C4-C3	3.96	118.02	108.69
3	A	901	IHP	O14-C4-C5	3.65	117.29	108.69

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	901	IHP	C4-O14-P4-O24
4	A	902	PG4	C4-C3-O2-C2
4	A	906	PG4	C8-C7-O4-C6
4	A	906	PG4	O3-C5-C6-O4
4	A	904	PG4	O3-C5-C6-O4
4	A	903	PG4	O3-C5-C6-O4
3	A	901	IHP	C4-O14-P4-O34
4	A	905	PG4	C4-C3-O2-C2
4	A	906	PG4	O1-C1-C2-O2
4	A	903	PG4	C3-C4-O3-C5
4	A	904	PG4	O4-C7-C8-O5
4	A	904	PG4	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	A	903	PG4	C8-C7-O4-C6
4	A	902	PG4	O2-C3-C4-O3
4	A	904	PG4	C3-C4-O3-C5
4	A	904	PG4	O2-C3-C4-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	901	IHP	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 then 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 IHP A 901

Bond lengths

Bond angles

Torsions

Rings
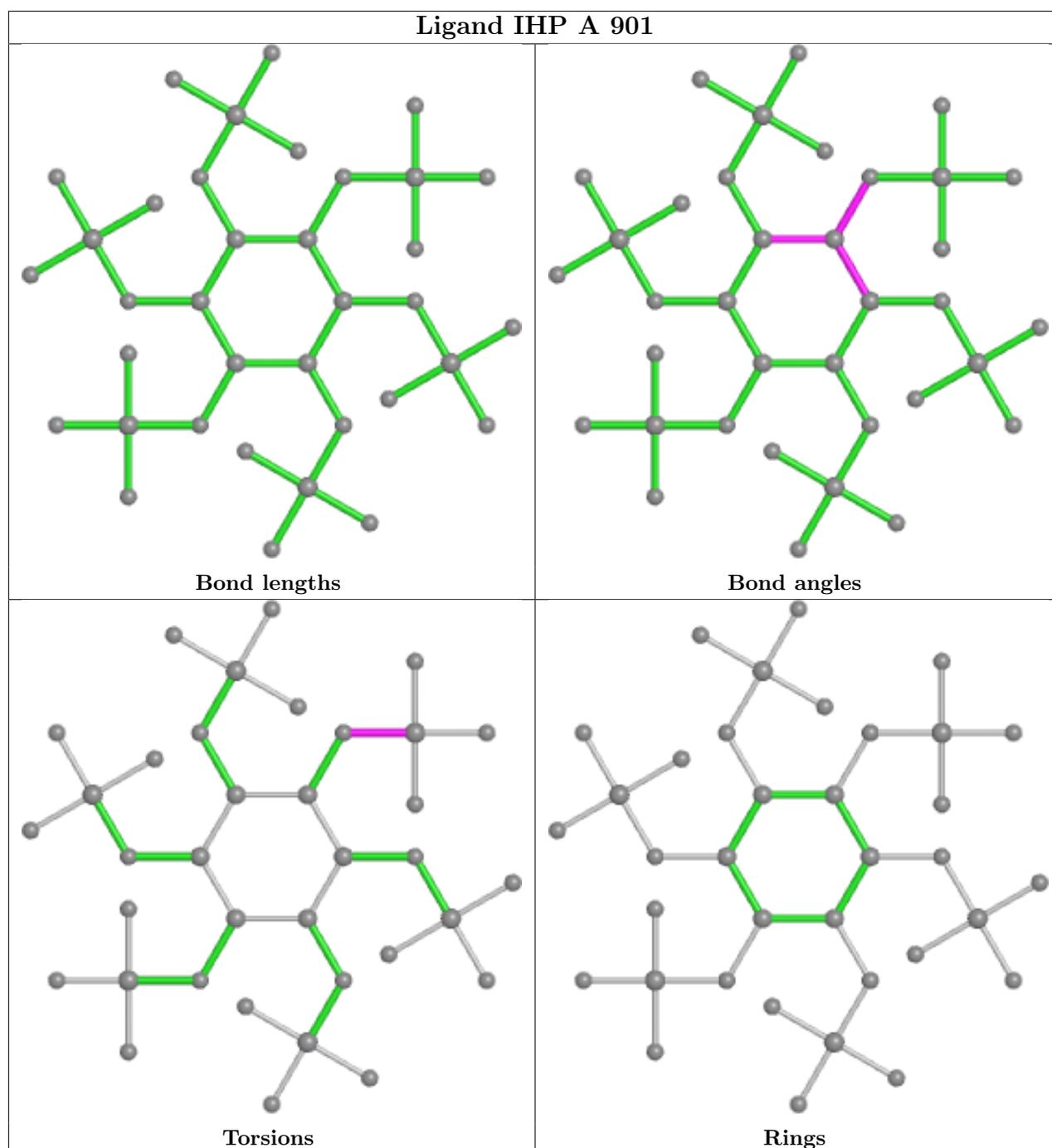
5.7 Other polymers ⓘ

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(Å²)	Q<0.9
1	A	782/863 (90%)	0.07	24 (3%)	49	39	37, 60, 113, 159	0
2	B	189/248 (76%)	0.07	1 (0%)	91	88	37, 54, 114, 142	0
All	All	971/1111 (87%)	0.07	25 (2%)	56	46	37, 59, 114, 159	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	646	SER	7.5
1	A	763	THR	3.8
1	A	767	PRO	3.7
1	A	824	PRO	3.6
1	A	16	ALA	3.5
1	A	828	SER	3.2
1	A	21	ASN	3.2
1	A	827	SER	3.1
1	A	808	ASN	3.1
1	A	25	LEU	2.9
1	A	88	SER	2.9
2	B	76	GLY	2.9
1	A	22	ASP	2.8
1	A	53	HIS	2.8
1	A	741	PHE	2.5
1	A	47	LEU	2.5
1	A	826	GLY	2.5
1	A	20	GLU	2.4
1	A	46	ILE	2.4
1	A	722	TYR	2.3
1	A	15	ILE	2.2
1	A	766	ASP	2.2
1	A	839	SER	2.2
1	A	652	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	19	LYS	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 ⓘ
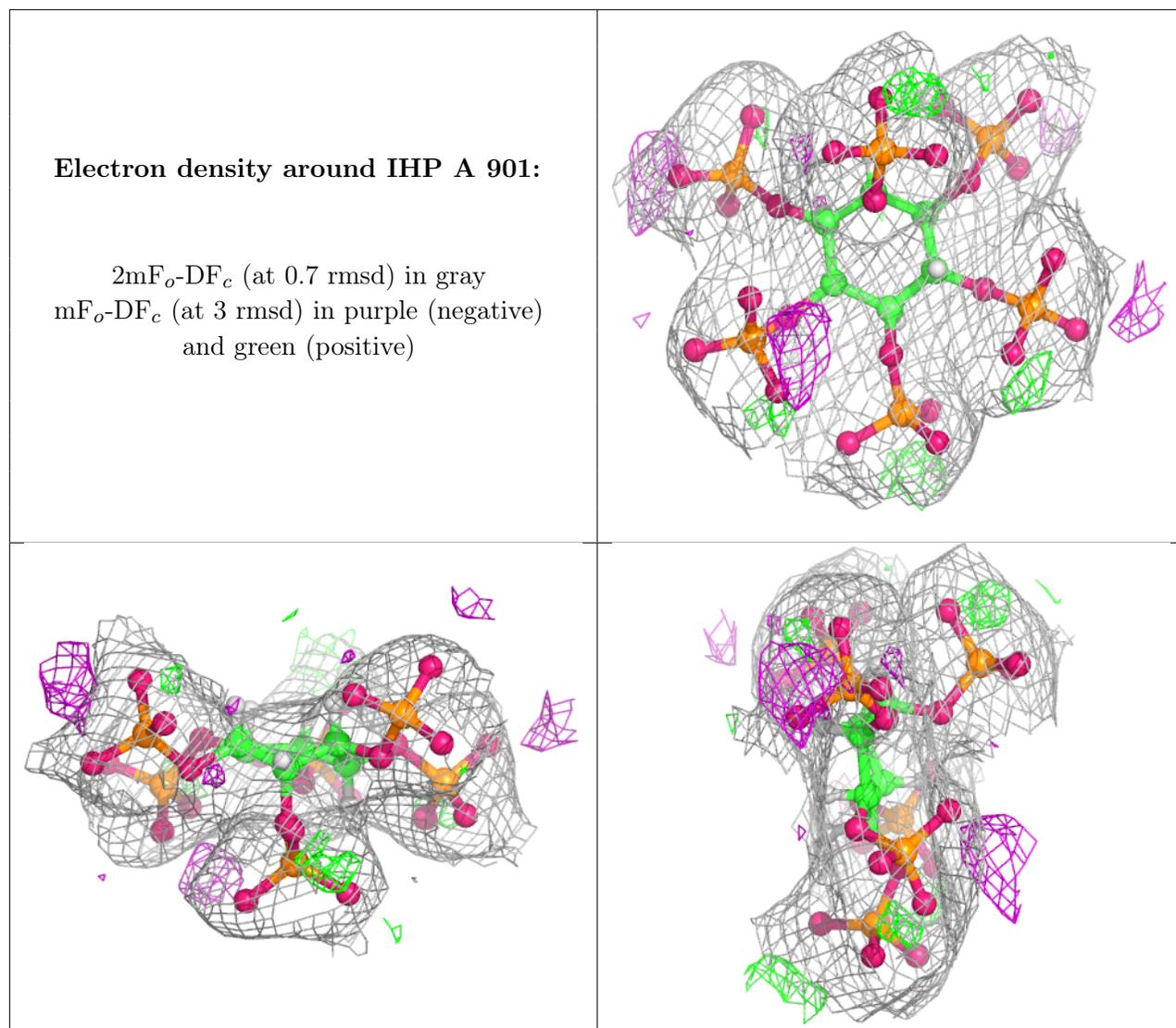
There are no monosaccharides in this entry.

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
4	PG4	A	902	13/13	0.80	0.22	72,88,94,94	0
4	PG4	A	905	13/13	0.82	0.23	64,78,95,96	0
4	PG4	A	903	13/13	0.85	0.27	81,98,101,101	0
4	PG4	A	904	13/13	0.86	0.19	78,93,95,96	0
4	PG4	A	906	13/13	0.86	0.21	64,76,85,85	0
3	IHP	A	901	36/36	0.95	0.28	45,52,68,68	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 IHP A 901:

$2mF_o$-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 ⓘ

There are no such residues in this entry.