



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 09:16 pm BST

PDB ID : 3B7Z
Title : Crystal Structure of Yeast Sec14 Homolog Sfh1 in Complex with Phosphatidylcholine or Phosphatidylinositol
Authors : Ortlund, E.A.; Schaaf, G.; Redinbo, M.R.; Bankaitis, V.
Deposited on : 2007-10-31
Resolution : 2.03 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 following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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) : 2.11

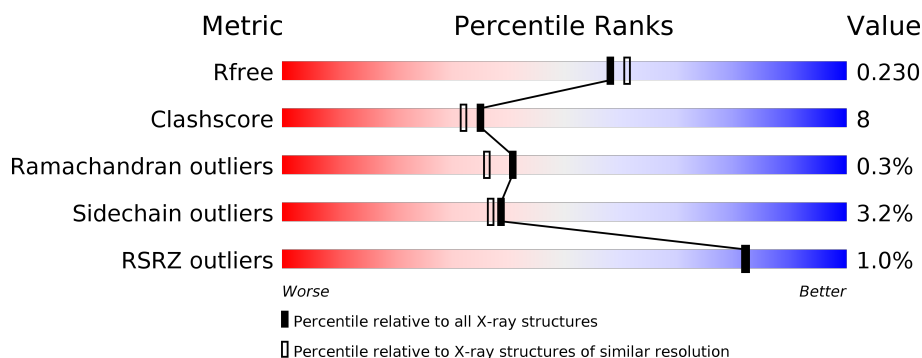
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.03 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	10434 (2.04-2.00)
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (2.04-2.00)

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 on 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	320	<div> <div></div> <div>78%</div> <div>18%</div> <div></div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2829 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.

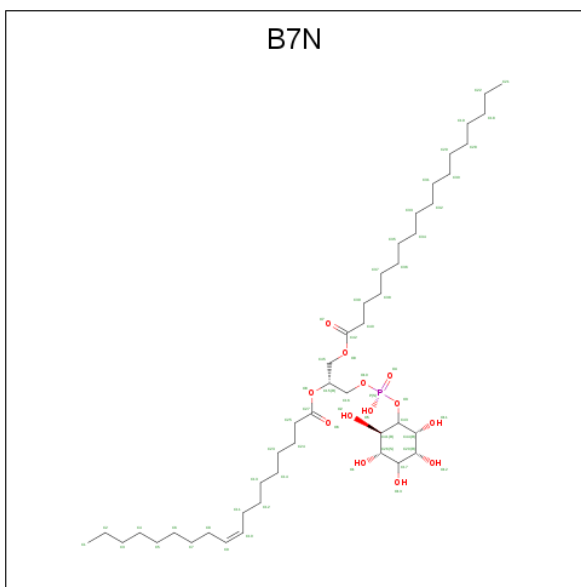
- Molecule 1 is a protein called Uncharacterized protein YKL091C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	307	2518	1626	414	468	10	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

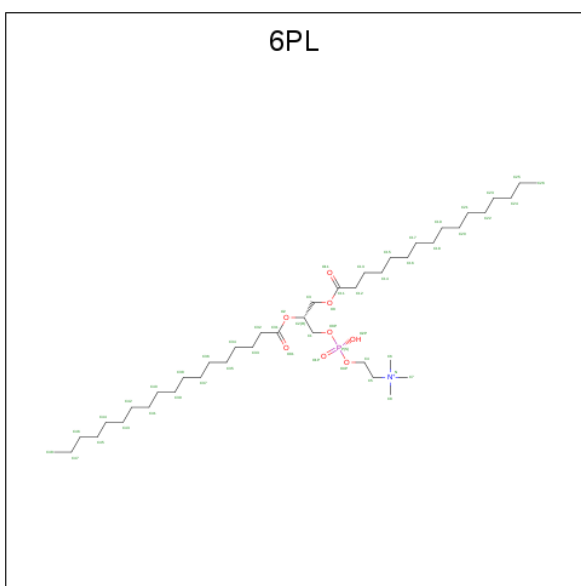
Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MET	-	EXPRESSION TAG	UNP P33324
A	-8	GLY	-	EXPRESSION TAG	UNP P33324
A	-7	HIS	-	EXPRESSION TAG	UNP P33324
A	-6	HIS	-	EXPRESSION TAG	UNP P33324
A	-5	HIS	-	EXPRESSION TAG	UNP P33324
A	-4	HIS	-	EXPRESSION TAG	UNP P33324
A	-3	HIS	-	EXPRESSION TAG	UNP P33324
A	-2	HIS	-	EXPRESSION TAG	UNP P33324
A	-1	HIS	-	EXPRESSION TAG	UNP P33324
A	0	HIS	-	EXPRESSION TAG	UNP P33324

- Molecule 2 is (1R)-2-[[[(S)-hydroxy{[(1S,2R,3R,4S,5S,6R)-2,3,4,5,6-pentahydroxycyclohexyl]oxy}phosphoryl]oxy}-1-[(octadecanoyloxy)methyl]ethyl (9Z)-octadec-9-enoate (three-letter code: B7N) (formula: C₄₅H₈₅O₁₃P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	1
			59	45	13	1		

- Molecule 3 is (4S,7R)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY) METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSAN-1-AMINIUM 4-OXIDE (three-letter code: 6PL) (formula: $C_{42}H_{85}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	1
			45	35	1	8	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	207	Total 207	O 207	0	0

i

- Molecule 1: Uncharacterized protein YKL091C



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	49.35Å 72.93Å 97.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.56 – 2.03 40.56 – 2.02	Depositor EDS
% Data completeness (in resolution range)	92.5 (40.56-2.03) 92.3 (40.56-2.02)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.84 (at 2.03Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.201 , 0.238 0.193 , 0.230	Depositor DCC
R_{free} test set	1560 reflections (6.88%)	wwPDB-VP
Wilson B-factor (Å ²)	26.2	Xtriage
Anisotropy	0.573	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2829	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.74% 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: 6PL, B7N

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	0.32	0/2581	0.57	0/3489

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	2518	0	2504	43	0
2	A	59	0	84	5	0
3	A	45	0	67	7	0
4	A	207	0	0	4	0
All	All	2829	0	2655	43	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 8.

All (43) 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:151:LYS:HE3	4:A:438:HOH:O	1.97	0.64
1:A:162:PRO:O	1:A:166:ARG:HG3	1.99	0.61
1:A:108:MET:HG3	4:A:512:HOH:O	2.00	0.61
1:A:211:MET:HE3	2:A:311[A]:B7N:H45A	1.83	0.60
1:A:19:PRO:HA	1:A:24:ASN:O	2.01	0.60
1:A:89:GLU:HG3	4:A:342:HOH:O	2.01	0.60
1:A:128:LEU:HD22	1:A:181:LEU:CD2	2.32	0.60
1:A:22:PRO:HG3	1:A:55:LEU:HD12	1.86	0.57
1:A:276:ASN:HD22	1:A:276:ASN:N	2.03	0.56
1:A:99:ASP:O	1:A:103:ILE:HG12	2.09	0.53
1:A:225:THR:HA	1:A:228:LYS:NZ	2.24	0.52
1:A:225:THR:HA	1:A:228:LYS:HZ3	1.76	0.50
1:A:123:LEU:HG	1:A:125:PHE:CE1	2.47	0.49
1:A:103:ILE:HD11	1:A:303:PHE:O	2.13	0.49
1:A:231:LYS:N	1:A:232:PRO:CD	2.77	0.48
1:A:113:TYR:OH	3:A:312[B]:6PL:H63	2.13	0.48
1:A:310:SER:HB3	4:A:454:HOH:O	2.14	0.47
1:A:26:THR:OG1	1:A:29:GLN:HG3	2.14	0.47
1:A:161:VAL:HB	1:A:162:PRO:HD3	1.97	0.47
1:A:188:ASN:HB3	2:A:311[A]:B7N:H21B	1.97	0.45
1:A:196:ILE:HD11	3:A:312[B]:6PL:H202	1.97	0.45
1:A:265:LYS:HE3	1:A:266:TYR:CZ	2.51	0.45
1:A:231:LYS:HE3	1:A:239:VAL:HG11	1.98	0.45
1:A:211:MET:CE	2:A:311[A]:B7N:H45A	2.46	0.45
1:A:124:TYR:CE2	1:A:126:GLU:HG3	2.53	0.44
1:A:5:ILE:HD12	1:A:296:GLU:HB3	1.99	0.44
1:A:189:ALA:HA	3:A:312[B]:6PL:H211	2.00	0.43
1:A:151:LYS:HZ1	1:A:302:ILE:HD12	1.82	0.43
1:A:110:PRO:O	1:A:126:GLU:HA	2.19	0.42
1:A:35:GLN:O	1:A:39:ILE:HG13	2.19	0.42
1:A:122:PRO:HG3	1:A:164:CYS:SG	2.59	0.42
1:A:228:LYS:O	1:A:232:PRO:HD3	2.19	0.42
1:A:229:MET:C	1:A:232:PRO:HD2	2.40	0.41
1:A:211:MET:HE3	2:A:311[A]:B7N:C45	2.48	0.41
1:A:152:GLU:HG3	3:A:312[B]:6PL:H61	2.03	0.41
1:A:203:SER:HB2	2:A:311[A]:B7N:O9	2.20	0.41
1:A:129:GLY:HA3	1:A:182:LYS:O	2.20	0.41
1:A:128:LEU:HD22	1:A:181:LEU:HD22	2.02	0.41
1:A:151:LYS:NZ	1:A:302:ILE:HD12	2.36	0.40
1:A:124:TYR:CD2	3:A:312[B]:6PL:H42	2.56	0.40
1:A:12:ILE:HG13	1:A:12:ILE:O	2.20	0.40
1:A:128:LEU:HD23	3:A:312[B]:6PL:H222	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:ILE:HD13	3:A:312[B]:6PL:H181	2.03	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	305/320 (95%)	297 (97%)	7 (2%)	1 (0%)	41 36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	275	PRO

5.3.2 Protein sidechains [i](#)

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	277/290 (96%)	268 (97%)	9 (3%)	39 37

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	LEU
1	A	42	GLU

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Mol	Chain	Res	Type
1	A	77	ARG
1	A	179	LEU
1	A	186	LEU
1	A	193	LEU
1	A	226	MET
1	A	273	HIS
1	A	276	ASN

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

Mol	Chain	Res	Type
1	A	93	ASN
1	A	191	HIS
1	A	276	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

2 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	B7N	A	311[A]	-	59,59,59	0.74	0	69,71,71	0.83	2 (2%)
3	6PL	A	312[B]	-	44,44,51	0.64	0	50,52,59	1.05	4 (8%)

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	B7N	A	311[A]	-	-	24/54/78/78	0/1/1/1
3	6PL	A	312[B]	-	-	29/48/48/55	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	312[B]	6PL	O2-C31-C32	3.86	119.82	111.50
2	A	311[A]	B7N	O8-C27-C25	3.42	118.87	111.50
3	A	312[B]	6PL	C2-O2-C31	-2.58	111.44	117.79
3	A	312[B]	6PL	C1-C2-C3	-2.53	105.81	111.79
2	A	311[A]	B7N	O9-C42-C40	2.31	119.17	111.91
3	A	312[B]	6PL	O3-C11-C12	2.13	118.60	111.91

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	312[B]	6PL	O2-C2-C3-O3
2	A	311[A]	B7N	O7-C42-O9-C45
2	A	311[A]	B7N	C40-C42-O9-C45
3	A	312[B]	6PL	C31-C32-C33-C34
3	A	312[B]	6PL	C32-C31-O2-C2
3	A	312[B]	6PL	C20-C21-C22-C23
3	A	312[B]	6PL	O31-C31-O2-C2
3	A	312[B]	6PL	C34-C35-C36-C37
3	A	312[B]	6PL	C35-C36-C37-C38
3	A	312[B]	6PL	C37-C38-C39-C40
3	A	312[B]	6PL	C32-C33-C34-C35
2	A	311[A]	B7N	C10-C11-C12-C13
2	A	311[A]	B7N	C29-C30-C31-C32

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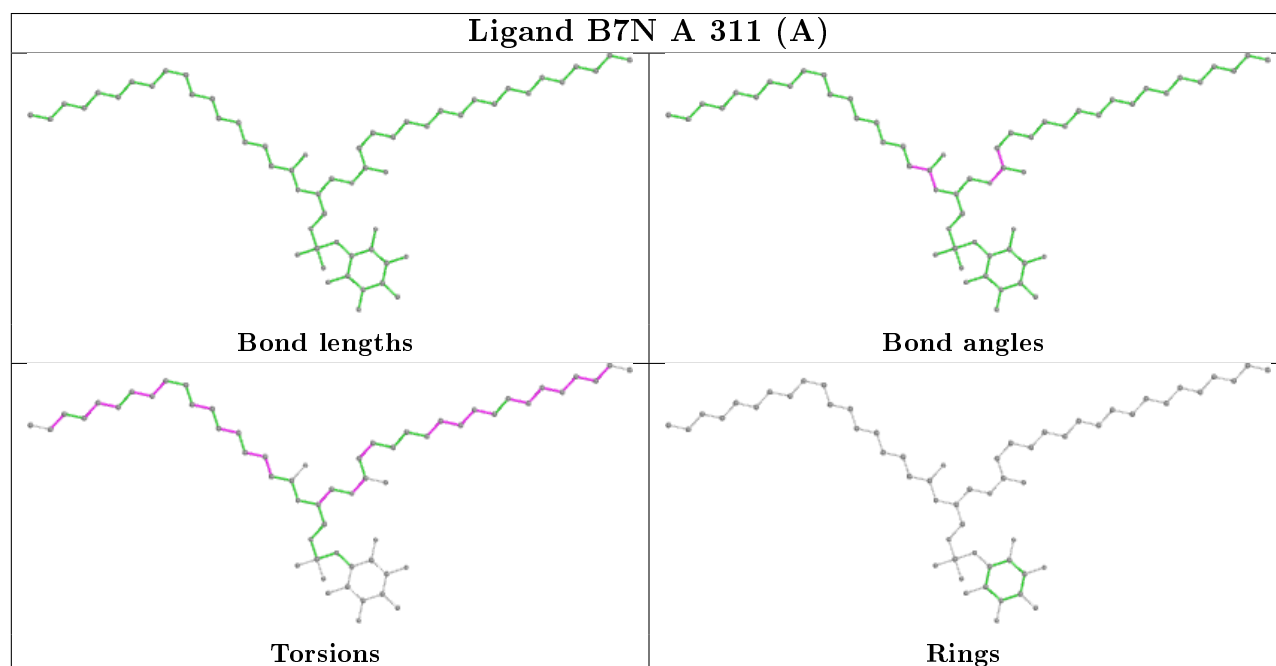
Mol	Chain	Res	Type	Atoms
3	A	312[B]	6PL	C14-C15-C16-C17
3	A	312[B]	6PL	C33-C34-C35-C36
2	A	311[A]	B7N	C28-C29-C30-C31
3	A	312[B]	6PL	C16-C17-C18-C19
2	A	311[A]	B7N	C6-C7-C8-C9
3	A	312[B]	6PL	C22-C23-C24-C25
3	A	312[B]	6PL	C17-C18-C19-C20
2	A	311[A]	B7N	C38-C39-C40-C42
2	A	311[A]	B7N	C23-C24-C25-C27
3	A	312[B]	6PL	O3P-C1-C2-O2
2	A	311[A]	B7N	C14-C23-C24-C25
3	A	312[B]	6PL	C19-C20-C21-C22
2	A	311[A]	B7N	C33-C34-C35-C36
3	A	312[B]	6PL	C36-C37-C38-C39
3	A	312[B]	6PL	C12-C13-C14-C15
2	A	311[A]	B7N	C32-C33-C34-C35
2	A	311[A]	B7N	C3-C4-C5-C6
3	A	312[B]	6PL	C18-C19-C20-C21
2	A	311[A]	B7N	C19-C28-C29-C30
2	A	311[A]	B7N	C16-C15-C45-O9
2	A	311[A]	B7N	C34-C35-C36-C37
2	A	311[A]	B7N	C31-C32-C33-C34
2	A	311[A]	B7N	C4-C5-C6-C7
3	A	312[B]	6PL	O3P-C1-C2-C3
3	A	312[B]	6PL	C1-C2-C3-O3
2	A	311[A]	B7N	C19-C18-C22-C21
2	A	311[A]	B7N	O8-C15-C45-O9
2	A	311[A]	B7N	C18-C19-C28-C29
3	A	312[B]	6PL	C11-C12-C13-C14
3	A	312[B]	6PL	C38-C39-C40-C41
2	A	311[A]	B7N	C22-C18-C19-C28
3	A	312[B]	6PL	O11-C11-O3-C3
2	A	311[A]	B7N	C1-C2-C3-C4
3	A	312[B]	6PL	C12-C11-O3-C3
3	A	312[B]	6PL	C4-O4P-P-O3P
2	A	311[A]	B7N	C12-C13-C14-C23
3	A	312[B]	6PL	O2-C31-C32-C33
2	A	311[A]	B7N	C7-C8-C9-C10
3	A	312[B]	6PL	O31-C31-C32-C33
3	A	312[B]	6PL	C5-C4-O4P-P

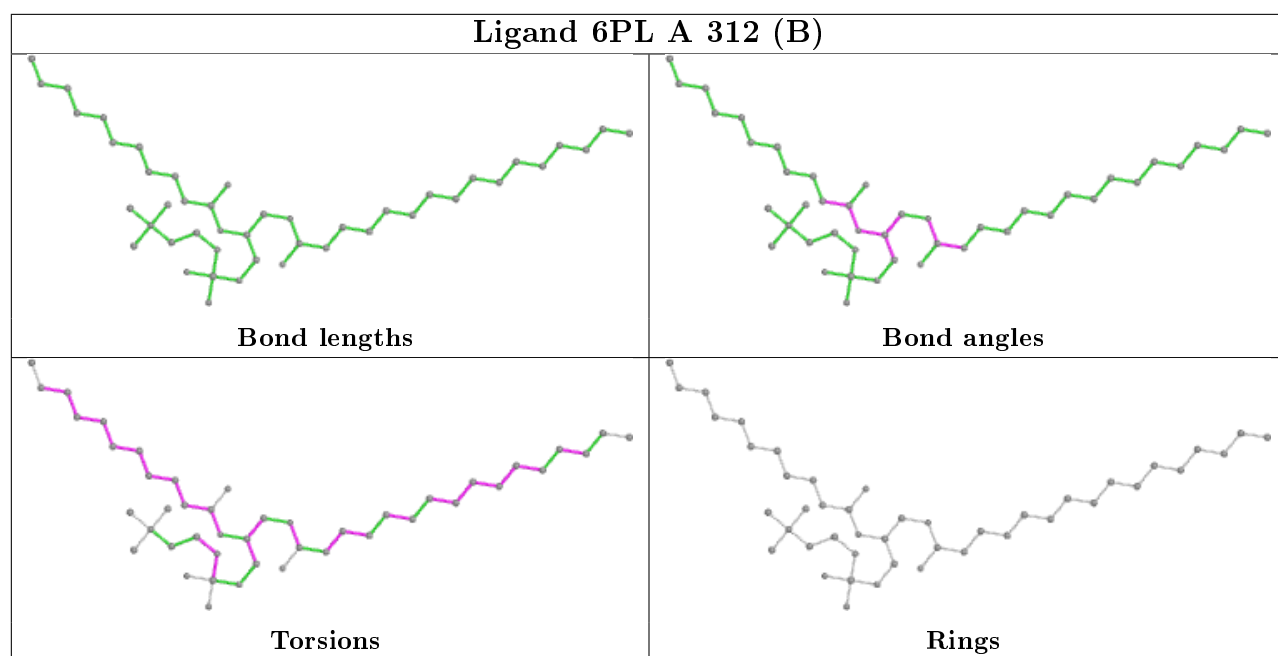
There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	311[A]	B7N	5	0
3	A	312[B]	6PL	7	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	307/320 (95%)	-0.34	3 (0%) 82 82	20, 29, 43, 55	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	275	PRO	3.1
1	A	310	SER	2.9
1	A	276	ASN	2.4

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 [i](#)

There are no carbohydrates 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.

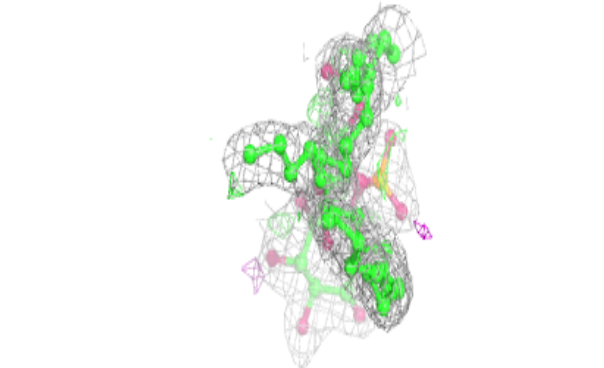
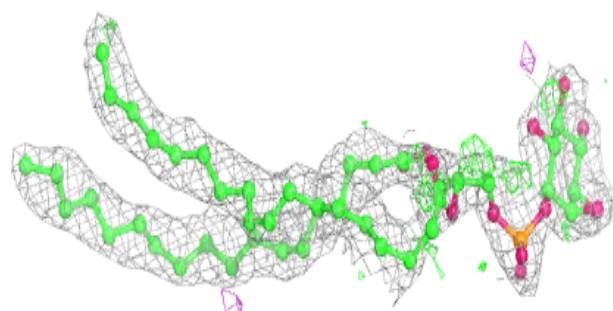
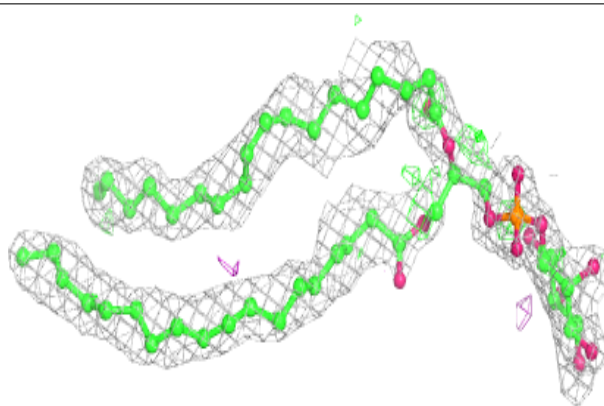
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	B7N	A	311[A]	59/59	0.88	0.17	25,34,41,42	59
3	6PL	A	312[B]	45/52	0.90	0.16	15,28,36,36	45

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.

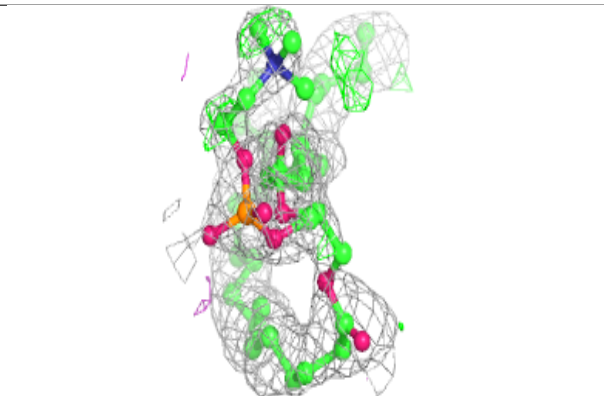
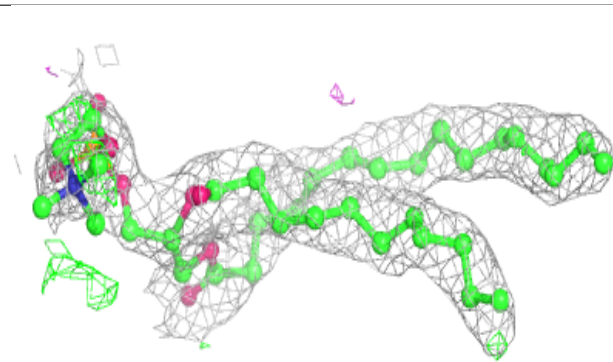
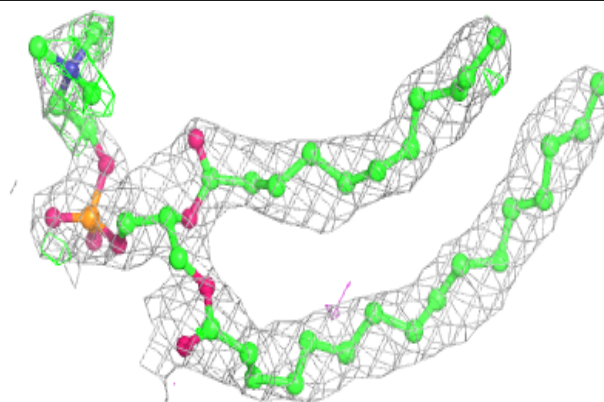
Electron density around B7N A 311 (A):

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



Electron density around 6PL A 312 (B):

$2mF_o-DF_c$ (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.