



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 7, 2023 – 05:53 AM EDT

PDB ID : 4F7U  
Title : The 6S snRNP assembly intermediate  
Authors : Grimm, C.; Pelz, J.P.  
Deposited on : 2012-05-16  
Resolution : 1.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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 : 2.35  
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) : 2.35

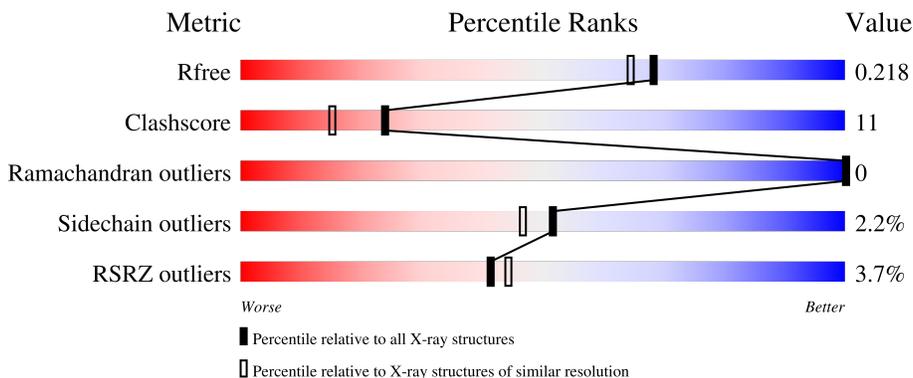
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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  $\geq 3$ , 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	119	 3% 57% 12% 28%
1	C	119	 3% 51% 15% 32%
2	B	118	 3% 48% 19% 30%
2	D	118	 7% 58% 13% 22%
3	E	92	 2% 65% 20% 13%

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Mol	Chain	Length	Quality of chain
3	H	92	 70% 15% 15%
4	F	86	 67% 17% 15%
4	I	86	 66% 17% 14%
5	G	76	 70% 20% 11%
5	J	76	 74% 14% 12%
6	P	129	 3% 77% 13% 10%
6	Q	129	 14% 67% 25% 7%

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 8542 atoms, of which 17 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 Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	82	Total 655	C 418	N 114	O 119	S 4	0	1	0
1	C	81	Total 647	C 412	N 112	O 120	S 3	0	1	0

- Molecule 2 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	80	Total 653	C 410	N 120	O 117	S 6	0	1	0
2	D	85	Total 706	C 441	N 131	O 128	S 6	0	2	0

- Molecule 3 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	78	Total 653	C 417	N 114	O 116	S 6	0	2	0
3	H	78	Total 658	C 419	N 115	O 118	S 6	0	3	0

- Molecule 4 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	F	73	Total 571	C 369	N 94	O 103	S 5	0	0	0
4	I	74	Total 590	C 382	N 96	O 107	S 5	0	2	0

- Molecule 5 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	G	68	Total	C	N	O	S	0	4	0
			551	350	96	99	6			
5	J	67	Total	C	N	O	S	0	1	0
			527	333	93	95	6			

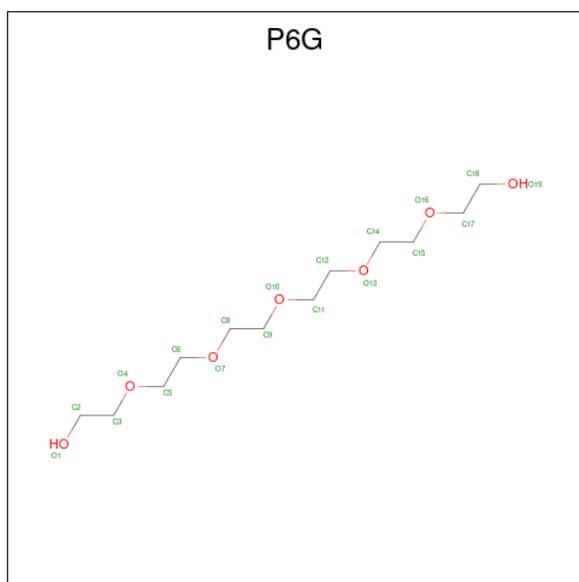
- Molecule 6 is a protein called Methylosome subunit pICln.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	Q	120	Total	C	N	O	S	0	1	0
			948	606	156	177	9			
6	P	116	Total	C	N	O	S	0	9	0
			981	627	161	184	9			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	6006	HIS	ARG	SEE REMARK 999	UNP A1ZAW5
Q	6144	ALA	HIS	engineered mutation	UNP A1ZAW5
Q	6161	HIS	-	expression tag	UNP A1ZAW5
Q	6162	HIS	-	expression tag	UNP A1ZAW5
Q	6163	HIS	-	expression tag	UNP A1ZAW5
Q	6164	HIS	-	expression tag	UNP A1ZAW5
Q	6165	HIS	-	expression tag	UNP A1ZAW5
P	6006	HIS	ARG	SEE REMARK 999	UNP A1ZAW5
P	6144	ALA	HIS	engineered mutation	UNP A1ZAW5
P	6161	HIS	-	expression tag	UNP A1ZAW5
P	6162	HIS	-	expression tag	UNP A1ZAW5
P	6163	HIS	-	expression tag	UNP A1ZAW5
P	6164	HIS	-	expression tag	UNP A1ZAW5
P	6165	HIS	-	expression tag	UNP A1ZAW5

- Molecule 7 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: C<sub>12</sub>H<sub>26</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	H	1	Total	C	H	O	0	0
			30	8	17	5		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	39	Total	O	0	0
			39	39		
8	B	16	Total	O	0	0
			16	16		
8	C	34	Total	O	0	0
			34	34		
8	D	21	Total	O	0	0
			21	21		
8	E	45	Total	O	0	0
			45	45		
8	H	39	Total	O	0	0
			39	39		
8	F	33	Total	O	0	0
			33	33		
8	I	31	Total	O	0	0
			31	31		
8	G	19	Total	O	0	0
			19	19		
8	J	21	Total	O	0	0
			21	21		
8	Q	26	Total	O	0	0
			26	26		

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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
8	P	48	Total	O	0	0
			48	48		



LEU  
ILE  
ALA  
GLY  
LYS

- Molecule 3: Small nuclear ribonucleoprotein E



MET  
ALA  
TYR  
ARG  
GLY  
GLN  
GLY  
GLN  
LYS  
VAL  
GLN  
VAL  
LYS  
V3013  
V3018  
N3019  
L3020  
L3021  
F3022  
R3023  
R3028  
S3029  
R3030  
I3031  
Y3036  
N3040  
E3044  
E3045  
C3046  
E3052  
D3059  
I3077  
L3087  
V3090  
SER  
ASN

- Molecule 3: Small nuclear ribonucleoprotein E



MET  
ALA  
TYR  
ARG  
GLY  
GLN  
GLY  
GLN  
LYS  
VAL  
GLN  
VAL  
LYS  
VAL  
R3014  
V3015  
I3016  
L3020  
R3023  
I3031  
I3032  
Y3033  
R3040  
F3050  
D3059  
I3077  
R3078  
T3085  
L3086  
L3087  
S3091  
ASN

- Molecule 4: Small nuclear ribonucleoprotein F



MET  
SER  
LEU  
P4004  
K4008  
P4009  
K4022  
M4027  
E4028  
L4033  
V4036  
M4042  
Q4043  
L4059  
C4066  
R4073  
G4074  
V4075  
E4076  
GLU  
GLU  
GLU  
GLU  
ASP  
GLY  
GLY  
MET  
MET  
ARG  
GLU

- Molecule 4: Small nuclear ribonucleoprotein F



MET  
SER  
L4003  
N4006  
F4010  
L4011  
K4022  
M4025  
C4026  
M4027  
V4036  
D4037  
E4048  
L4059  
V4062  
R4065  
C4066  
N4067  
V4069  
L4070  
R4073  
E4076  
GLU  
GLU  
GLU  
GLU  
ASP  
GLY  
GLY  
MET  
MET  
ARG  
GLU

- Molecule 5: Small nuclear ribonucleoprotein G



MET  
SER  
LYS  
ALA  
HIS  
PRO  
P5007  
E5008  
L5009  
M5013  
D5014  
K5020  
L5021  
N5022  
H5026  
R5032  
G5033  
F5034  
D5035  
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M5038  
N5039  
I5042  
I5062  
N5065  
E5074  
ARG  
VAL

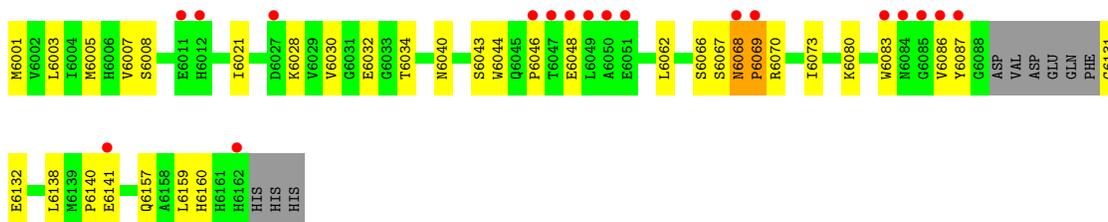
- Molecule 5: Small nuclear ribonucleoprotein G



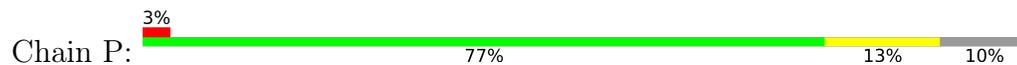
MET  
SER  
LYS  
ALA  
HIS  
PRO  
P5008  
K5011  
K5016  
I5030  
L5031  
R5032  
D5035  
P5036  
S5051  
M5059  
S5066  
L5073  
E5074  
ARG  
VAL

- Molecule 6: Methylosome subunit pICln





- Molecule 6: Methylosome subunit pICln



## 4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	180.72Å 65.30Å 99.35Å 90.00° 92.47° 90.00°	Depositor
Resolution (Å)	49.63 – 1.90 49.63 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.1 (49.63-1.90) 96.1 (49.63-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.69 (at 1.90Å)	Xtrriage
Refinement program	PHENIX phenix.refine: 1.7.1_743	Depositor
R, $R_{free}$	0.181 , 0.221 0.177 , 0.218	Depositor DCC
$R_{free}$ test set	4426 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.9	Xtrriage
Anisotropy	0.420	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 53.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	8542	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: P6G

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	0.64	0/666	0.76	0/899
1	C	0.64	0/658	0.71	0/890
2	B	0.63	0/663	0.74	0/890
2	D	0.62	0/719	0.71	1/963 (0.1%)
3	E	0.79	0/667	0.83	0/896
3	H	0.74	0/675	0.82	0/906
4	F	0.83	1/583 (0.2%)	0.79	0/787
4	I	0.73	0/608	0.74	0/822
5	G	0.62	0/569	0.74	0/758
5	J	0.54	0/535	0.69	0/713
6	P	0.73	0/1010	0.78	0/1373
6	Q	0.57	0/975	0.71	0/1326
All	All	0.68	1/8328 (0.0%)	0.75	1/11223 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
6	Q	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	4066	CYS	CB-SG	5.80	1.92	1.82

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2102	ARG	NE-CZ-NH2	-6.39	117.11	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	Q	6068	ASN	Peptide
6	Q	6069	PRO	Peptide

## 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	655	0	703	16	0
1	C	647	0	687	17	1
2	B	653	0	678	25	0
2	D	706	0	732	23	1
3	E	653	0	682	16	0
3	H	658	0	686	17	0
4	F	571	0	580	11	0
4	I	590	0	602	15	0
5	G	551	0	582	15	0
5	J	527	0	549	14	0
6	P	981	0	974	15	0
6	Q	948	0	927	30	0
7	H	13	17	17	1	0
8	A	39	0	0	0	0
8	B	16	0	0	2	0
8	C	34	0	0	0	0
8	D	21	0	0	2	0
8	E	45	0	0	0	0
8	F	33	0	0	2	0
8	G	19	0	0	2	0
8	H	39	0	0	2	0
8	I	31	0	0	2	0
8	J	21	0	0	2	0
8	P	48	0	0	1	0
8	Q	26	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8525	17	8399	183	1

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 11.

The worst 5 of 183 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:D:2110:LEU:HD23	4:I:4062:VAL:HG22	1.45	0.96
2:D:2112:ASN:HB3	2:D:2113:PRO:HB3	1.51	0.92
1:C:1034:VAL:HG13	6:P:6017:THR:HG22	1.50	0.92
5:J:5008:GLU:O	5:J:5011:LYS:NZ	2.08	0.86
6:P:6132:GLU:N	6:P:6132:GLU:OE1	2.10	0.85

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1051:GLU:OE2	2:D:2055:ARG:NH1[4_556]	1.96	0.24

## 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	81/119 (68%)	79 (98%)	2 (2%)	0	100	100
1	C	80/119 (67%)	77 (96%)	3 (4%)	0	100	100
2	B	77/118 (65%)	76 (99%)	1 (1%)	0	100	100
2	D	83/118 (70%)	82 (99%)	1 (1%)	0	100	100
3	E	78/92 (85%)	77 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	H	79/92 (86%)	79 (100%)	0	0	100	100
4	F	71/86 (83%)	70 (99%)	1 (1%)	0	100	100
4	I	74/86 (86%)	73 (99%)	1 (1%)	0	100	100
5	G	70/76 (92%)	69 (99%)	1 (1%)	0	100	100
5	J	66/76 (87%)	65 (98%)	1 (2%)	0	100	100
6	P	121/129 (94%)	119 (98%)	2 (2%)	0	100	100
6	Q	117/129 (91%)	110 (94%)	7 (6%)	0	100	100
All	All	997/1240 (80%)	976 (98%)	21 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	78/101 (77%)	78 (100%)	0	100	100
1	C	77/101 (76%)	75 (97%)	2 (3%)	46	39
2	B	77/110 (70%)	75 (97%)	2 (3%)	46	39
2	D	83/110 (76%)	81 (98%)	2 (2%)	49	43
3	E	75/84 (89%)	72 (96%)	3 (4%)	31	22
3	H	76/84 (90%)	74 (97%)	2 (3%)	46	39
4	F	62/74 (84%)	61 (98%)	1 (2%)	62	60
4	I	65/74 (88%)	60 (92%)	5 (8%)	13	5
5	G	63/66 (96%)	63 (100%)	0	100	100
5	J	59/66 (89%)	59 (100%)	0	100	100
6	P	112/114 (98%)	111 (99%)	1 (1%)	78	79
6	Q	106/114 (93%)	102 (96%)	4 (4%)	33	24
All	All	933/1098 (85%)	911 (98%)	22 (2%)	52	43

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	I	4048[A]	GLU
6	Q	6032	GLU
4	I	4059	LEU
6	Q	6034	THR
3	E	3029	SER

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

Mol	Chain	Res	Type
1	C	1024	GLN
2	D	2112	ASN
3	H	3016	GLN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is 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
7	P6G	H	3101	-	12,12,18	0.56	0	11,11,17	1.43	2 (18%)

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
7	P6G	H	3101	-	-	3/10/10/16	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	H	3101	P6G	O1-C2-C3	-2.83	95.37	111.81
7	H	3101	P6G	O10-C9-C8	-2.45	99.33	110.39

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	H	3101	P6G	O10-C11-C12-O13
7	H	3101	P6G	C6-C5-O4-C3
7	H	3101	P6G	C5-C6-O7-C8

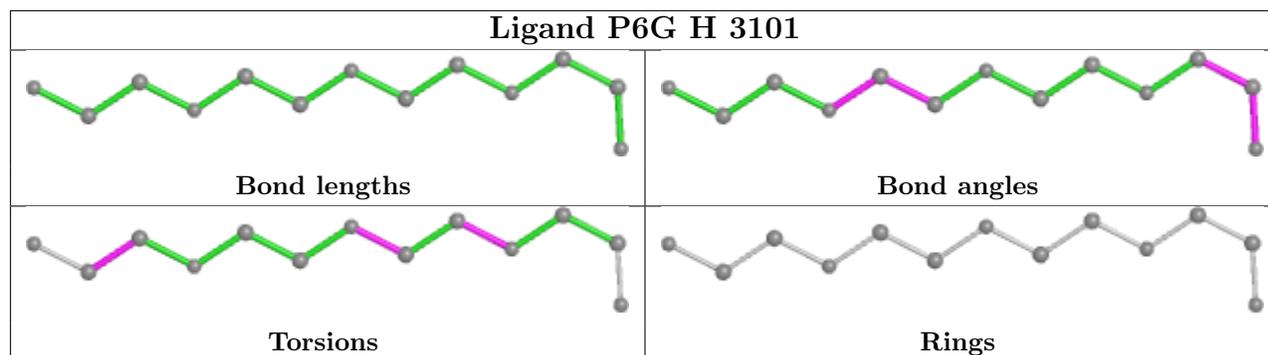
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	H	3101	P6G	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.



## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	82/119 (68%)	0.03	1 (1%) 79 81	20, 36, 59, 89	0
1	C	81/119 (68%)	0.03	1 (1%) 79 81	26, 38, 61, 106	0
2	B	80/118 (67%)	0.13	3 (3%) 40 43	23, 42, 75, 101	0
2	D	85/118 (72%)	0.41	8 (9%) 8 9	26, 41, 92, 104	0
3	E	78/92 (84%)	0.03	2 (2%) 56 58	22, 35, 65, 77	0
3	H	78/92 (84%)	-0.19	0 100 100	25, 33, 56, 69	0
4	F	73/86 (84%)	-0.23	0 100 100	23, 36, 49, 86	0
4	I	74/86 (86%)	-0.15	0 100 100	25, 38, 57, 82	0
5	G	68/76 (89%)	0.01	0 100 100	25, 39, 77, 95	0
5	J	67/76 (88%)	0.15	0 100 100	30, 46, 81, 94	0
6	P	116/129 (89%)	0.32	4 (3%) 45 48	20, 32, 70, 98	0
6	Q	120/129 (93%)	0.78	18 (15%) 2 2	27, 54, 103, 141	0
All	All	1002/1240 (80%)	0.15	37 (3%) 41 44	20, 39, 81, 141	0

The worst 5 of 37 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	Q	6049	LEU	6.9
6	Q	6011	GLU	6.6
3	E	3013	VAL	6.5
6	Q	6050	ALA	6.2
2	D	2090	VAL	6.1

### 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 [i](#)

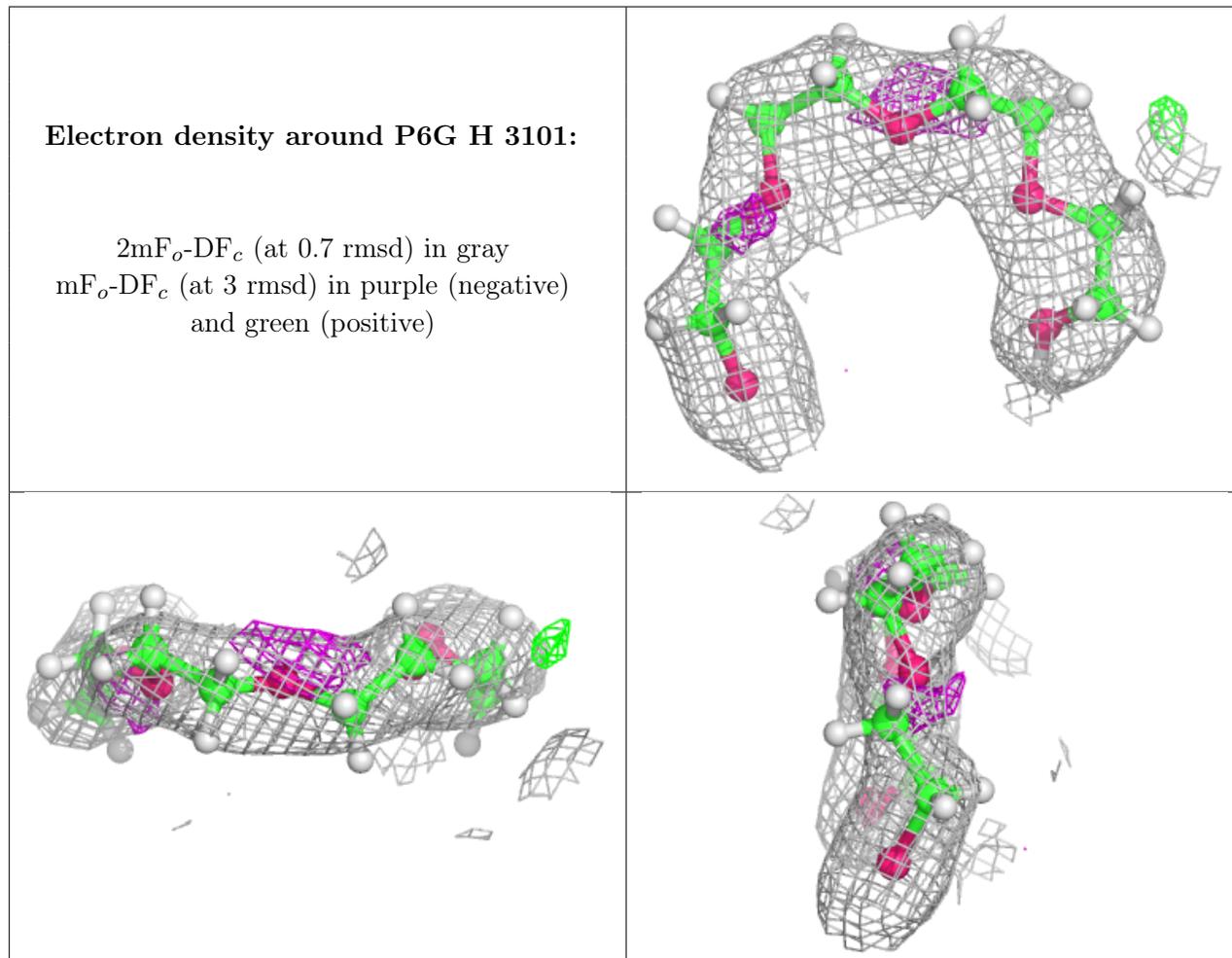
There are no monosaccharides in this entry.

### 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, 95<sup>th</sup> 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
7	P6G	H	3101	13/19	0.89	0.15	38,54,66,66	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.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.