

wwPDB X-ray Structure Validation Summary Report (i)

Nov 19, 2023 – 06:13 PM JST

PDB ID	:	6LWD
Title	:	Crystal structure of human NEIL1(P2G, E3Q, R242) bound to duplex DNA
		containing spiroiminodihydantoin (Sp)
Authors	:	Liu, M.H.; Zhang, J.; Zhu, C.X.; Zhang, X.X.; Gao, Y.Q.; Yi, C.Q.
Deposited on	:	2020-02-07
Resolution	:	2.41 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 A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

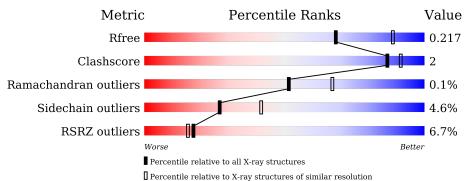
MolProbity Mogul Xtriage (Phenix) EDS	:	4.02b-467 1.8.5 (274361), CSD as541be (2020) 1.13 2.36
buster-report Percentile statistics Refmac	: : :	1.1.7 (2018) 20191225.v01 (using entries in the PDB archive December 25th 2019) 5.8.0158 7.0.044 (Gargrove)
Ideal geometry (DNA, RNA) Validation Pipeline (wwPDB-VP)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.41 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	$\begin{array}{l} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	4647(2.44-2.40)
Clashscore	141614	5161(2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074(2.44-2.40)
RSRZ outliers	127900	4543 (2.44-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	А	295	% • 85%	5% • 8%
1	D	295	83%	6% 11%
1	G	295	11% 72% 5%	23%
2	В	13	8%	8%
2	Е	13	85%	8% 8%
2	Н	13	31% 85%	15%



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Mol	Chain	Length	Quality of chain	
3	С	13	8%	15%
3	F	13	8%	8% 8%
3	Ι	13	31%	15%



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7656 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
1	Λ	270	Total	С	Ν	0	\mathbf{S}	0	0	0	
	А	270	2139	1362	391	376	10	0	0	0	
1	л	264	Total	С	Ν	0	S	0	0	0	
	D	204	2080	1325	384	361	10	0	0	0	
1	С	226	Total	С	Ν	0	S	0	0	0	
I G	220	1550	960	299	283	8	U	U	U		

• Molecule 1 is a protein called Endonuclease 8-like 1.

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	2	GLY	PRO	engineered mutation	UNP Q96FI4
А	3	GLN	GLU	engineered mutation	UNP Q96FI4
A	242	ARG	LYS	variant	UNP Q96FI4
D	2	GLY	PRO	engineered mutation	UNP Q96FI4
D	3	GLN	GLU	engineered mutation	UNP Q96FI4
D	242	ARG	LYS	variant	UNP Q96FI4
G	2	GLY	PRO	engineered mutation	UNP Q96FI4
G	3	GLN	GLU	engineered mutation	UNP Q96FI4
G	242	ARG	LYS	variant	UNP Q96FI4

• Molecule 2 is a DNA chain called DNA (5'-D(*CP*GP*TP*CP*CP*AP*(DSP)P*GP*TP* CP*TP*AP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	В	13	Total	С	Ν	Ο	Р	0	0	0
	D	10	262	125	46	79	12	0	0	
0	Е	13	Total	С	Ν	Ο	Р	0	0	0
	Ľ	10	262	125	46	79	12	0	0	0
9	Н	13	Total	С	Ν	Ο	Р	0	0	0
	11	10	262	125	46	79	12		U	0

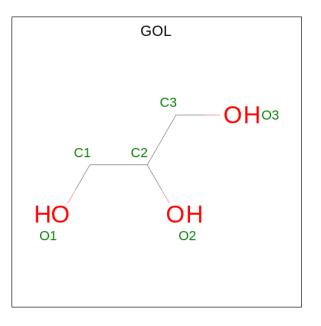
• Molecule 3 is a DNA chain called DNA (5'-D(*TP*AP*GP*AP*CP*CP*TP*GP*GP*AP*



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	13	Total	С	Ν	Ο	Р	0	0	0
0	U	10	267	127	53	75	12	0		
9	Б	13	Total	С	Ν	Ο	Р	0	0	0
0	Г	10	267	127	53	75	12	0	0	0
3	т	13	Total	С	Ν	Ο	Р	0	0	0
0	0 1	19	267	127	53	75	12	0	0	0

CP*GP*G)-3').

• Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	153	Total O 153 153	0	0
5	В	22	TotalO2222	0	0
5	С	5	Total O 5 5	0	0
5	D	91	Total O 91 91	0	0



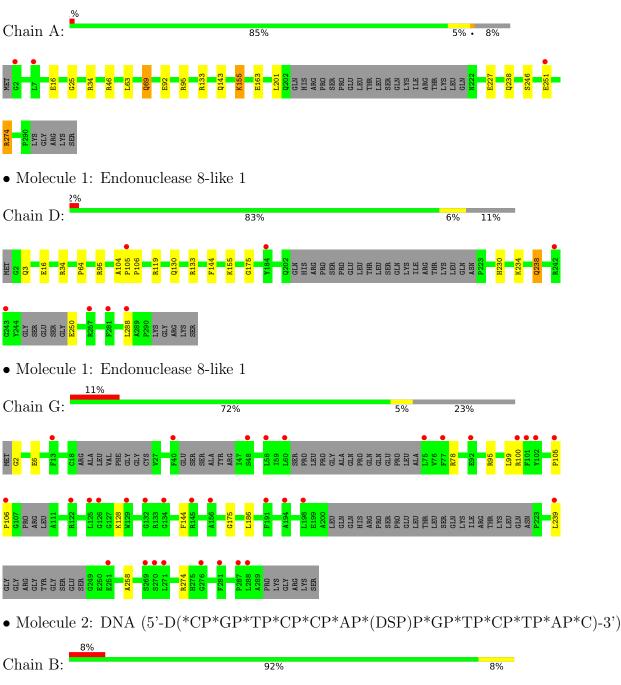
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	Е	10	Total O 10 10	0	0
5	F	7	Total O 7 7	0	0
5	G	2	Total O 2 2	0	0
5	Ι	4	Total O 4 4	0	0

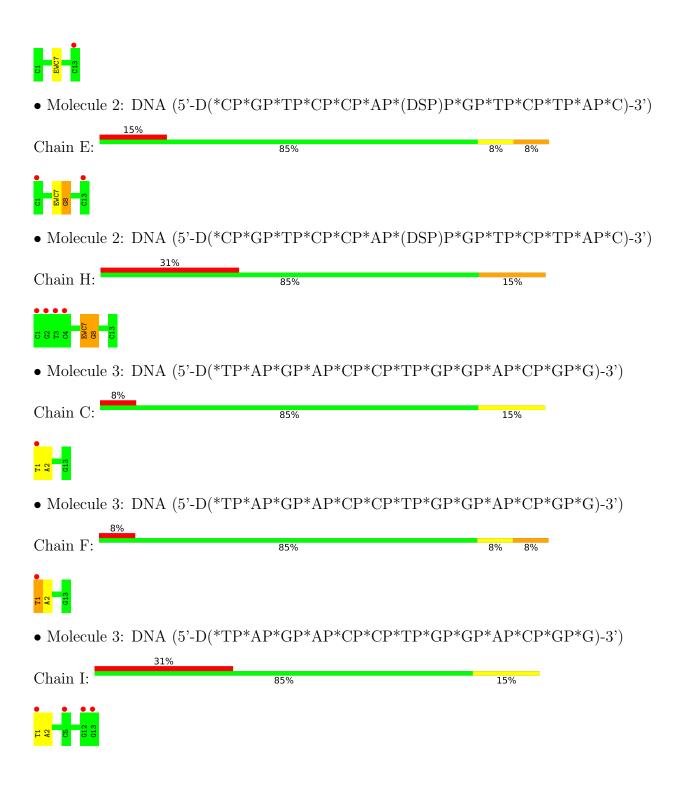


3 Residue-property plots (i)

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: Endonuclease 8-like 1





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	73.58Å 109.31Å 168.24Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.49 - 2.41	Depositor
Resolution (A)	42.46 - 2.44	EDS
% Data completeness	99.3 (42.49-2.41)	Depositor
(in resolution range)	99.4 (42.46-2.44)	EDS
R _{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$7.11 (at 2.42 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
D D.	0.211 , 0.254	Depositor
R, R_{free}	0.215 , 0.217	DCC
R_{free} test set	2606 reflections $(5.08%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	54.0	Xtriage
Anisotropy	0.541	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.33, 59.6	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	7656	wwPDB-VP
Average B, all atoms $(Å^2)$	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.99% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: EWC, GOL

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	Bo	nd lengths	Bo	ond angles
WIOI	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.86	2/2197~(0.1%)	0.83	1/2971~(0.0%)
1	D	0.68	0/2134	0.86	1/2880~(0.0%)
1	G	0.69	0/1580	0.75	0/2109
2	В	0.43	0/264	0.71	0/402
2	Ε	0.46	0/264	1.16	2/402~(0.5%)
2	Н	0.33	0/264	0.93	2/402~(0.5%)
3	С	0.44	0/300	0.78	0/462
3	F	0.45	0/300	0.83	1/462~(0.2%)
3	Ι	0.37	0/300	0.74	0/462
All	All	0.69	2/7603~(0.0%)	0.83	7/10552~(0.1%)

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.

N	Mol	Chain	#Chirality outliers	#Planarity outliers
	1	G	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	А	92	GLU	CD-OE1	18.30	1.45	1.25
1	А	92	GLU	CD-OE2	15.57	1.42	1.25

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	Ε	8	DG	O5'-P-OP1	-16.33	91.00	105.70
2	Н	8	DG	O5'-P-OP1	-10.38	96.36	105.70



Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
2	Е	8	DG	O5'-P-OP2	7.34	119.51	110.70
1	А	92	GLU	OE1-CD-OE2	6.27	130.82	123.30
2	Н	8	DG	O5'-P-OP2	6.09	118.00	110.70

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There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	105	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	А	2139	0	2107	8	0
1	D	2080	0	2043	15	0
1	G	1550	0	1294	8	0
2	В	262	0	137	0	0
2	Е	262	0	137	2	0
2	Н	262	0	137	3	0
3	С	267	0	147	1	0
3	F	267	0	147	1	0
3	Ι	267	0	147	1	0
4	А	6	0	8	0	0
5	А	153	0	0	2	0
5	В	22	0	0	0	0
5	С	5	0	0	0	0
5	D	91	0	0	0	0
5	Ε	10	0	0	0	0
5	F	7	0	0	0	0
5	G	2	0	0	0	0
5	Ι	4	0	0	0	0
All	All	7656	0	6304	29	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 29 close contacts within the same asymmetric unit are listed below, sorted by their



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:GLN:NE2	1:A:69:GLN:HA	1.96	0.80
1:A:143:GLN:OE1	5:A:401:HOH:O	2.06	0.74
1:D:238:GLN:HE21	1:D:238:GLN:HA	1.57	0.67
1:D:64:PRO:C	1:G:239:LEU:HD21	2.18	0.64
1:D:130:GLN:NE2	1:D:133:ARG:HH11	1.97	0.62

clash magnitude.

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	Perce	ntiles
1	А	266/295~(90%)	258~(97%)	8~(3%)	0	100	100
1	D	258/295~(88%)	248 (96%)	10 (4%)	0	100	100
1	G	212/295~(72%)	205~(97%)	6 (3%)	1 (0%)	29	40
All	All	736/885~(83%)	711 (97%)	24 (3%)	1 (0%)	51	67

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	106	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 side chain conformation was analysed, and the total number of residues.



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	223/247~(90%)	212~(95%)	11 (5%)	25 39
1	D	214/247~(87%)	206 (96%)	8 (4%)	34 51
1	G	127/247~(51%)	120 (94%)	7~(6%)	21 33
All	All	564/741~(76%)	538~(95%)	26~(5%)	27 42

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	144	PHE
1	D	250	GLU
1	G	144	PHE
1	D	238	GLN
1	D	288	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	А	130	GLN
1	D	70	GLN
1	D	238	GLN
1	D	130	GLN
1	А	69	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)

3 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	Turne	Chain	hain Res Link Bond lengths $C \rightarrow D M C = U C C C C C C C C C $				Bond angles			
INIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
2	EWC	В	7	2	20,26,27	2.09	8 (40%)	23,40,43	2.82	5 (21%)
2	EWC	Е	7	2	20,26,27	1.88	7 (35%)	23,40,43	2.66	5 (21%)
2	EWC	Н	7	2	20,26,27	1.90	7 (35%)	23,40,43	2.72	6 (26%)

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	EWC	В	7	2	-	3/7/56/57	0/3/3/3
2	EWC	Е	7	2	-	3/7/56/57	0/3/3/3
2	EWC	Н	7	2	-	3/7/56/57	0/3/3/3

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms		Observed(Å)	Ideal(Å)
2	В	7	EWC	C4-C5	-4.43	1.48	1.55
2	Е	7	EWC	C4-C5	-4.11	1.49	1.55
2	Н	7	EWC	C4-C5	-3.84	1.49	1.55
2	В	7	EWC	O24-C5	3.46	1.29	1.22
2	В	7	EWC	O23-C8	3.20	1.28	1.23

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	В	7	EWC	C5-N7-C8	-9.31	103.29	112.72
2	Н	7	EWC	C5-N7-C8	-9.21	103.39	112.72
2	Е	7	EWC	C5-N7-C8	-9.12	103.48	112.72
2	В	7	EWC	O23-C8-N9	-5.94	117.64	125.00
2	Н	7	EWC	O23-C8-N9	-5.30	118.43	125.00

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	В	7	EWC	O4'-C4'-C5'-O5'
2	Е	7	EWC	O4'-C4'-C5'-O5'
2	Н	7	EWC	O4'-C4'-C5'-O5'
2	В	7	EWC	C3'-C4'-C5'-O5'



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Mol	Chain	Res	Type	Atoms
2	Е	7	EWC	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Н	7	EWC	2	0

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).

ſ	Mol	Type	Chain Res		Link	Bond lengths			Bond angles		
		туре	Ullaili	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
	4	GOL	А	301	-	$5,\!5,\!5$	0.12	0	$5,\!5,\!5$	0.32	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	GOL	А	301	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

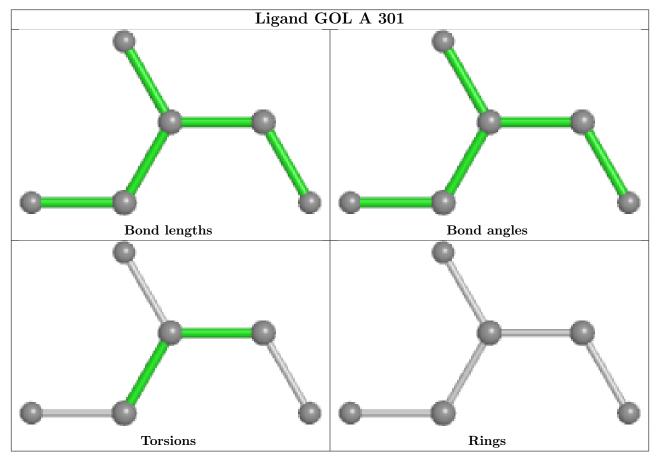
There are no torsion outliers.



There are no ring outliers.

No monomer is involved in short contacts.

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.



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^{th} 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	$OWAB(A^2)$	Q<0.9
1	А	270/295~(91%)	0.23	3 (1%) 80 78	36, 56, 89, 132	0
1	D	264/295~(89%)	0.50	7 (2%) 54 52	39, 66, 116, 143	0
1	G	226/295~(76%)	0.85	33 (14%) 2 2	70, 102, 135, 146	0
2	В	12/13~(92%)	0.27	1 (8%) 11 10	57, 96, 128, 136	0
2	Ε	12/13~(92%)	0.34	2(16%) 1 1	66, 92, 109, 125	0
2	Н	12/13~(92%)	1.37	4 (33%) 0 0	93, 116, 128, 135	0
3	С	13/13~(100%)	-0.03	1 (7%) 13 11	73, 96, 130, 150	0
3	F	13/13~(100%)	0.34	1 (7%) 13 11	54, 97, 136, 136	0
3	Ι	13/13~(100%)	0.91	4 (30%) 0 0	75, 109, 138, 143	0
All	All	835/963~(86%)	0.51	56 (6%) 17 15	36, 76, 130, 150	0

The worst 5 of 56 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	243	GLY	5.3
1	G	125	LEU	4.9
1	G	281	PHE	4.2
1	G	77	PHE	4.2
1	G	58	LEU	3.9

6.2 Non-standard residues in protein, DNA, RNA chains (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^{th} 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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
2	EWC	Н	7	24/25	0.89	0.17	98,106,112,113	0
2	EWC	Е	7	24/25	0.91	0.21	69,94,104,107	0
2	EWC	В	7	24/25	0.95	0.18	54,77,89,95	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

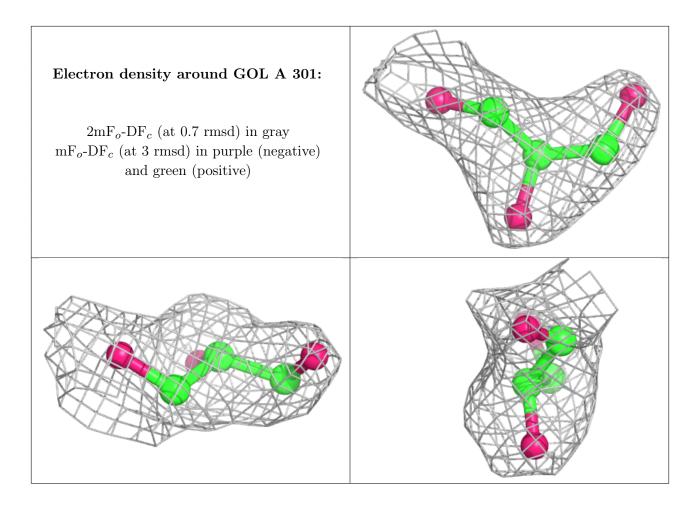
6.4 Ligands (i)

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^{th} 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	$\mathbf{B} ext{-factors}(\mathbf{\AA}^2)$	Q<0.9
4	GOL	А	301	6/6	0.91	0.28	74,75,78,79	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.

