



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 10:58 am BST

PDB ID : 1LV2
Title : Hepatocyte Nuclear Factor 4 is a Transcription Factor that Constitutively Binds Fatty Acids
Authors : Wisely, B.; Miller, A.B.; Davis, R.G.; Spitzer, T.; Shearer, B.; Moore, J.T.; Johnson, R.; Seftler, A.; Willson, T.M.; Williams, S.P.
Deposited on : 2002-05-24
Resolution : 2.70 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

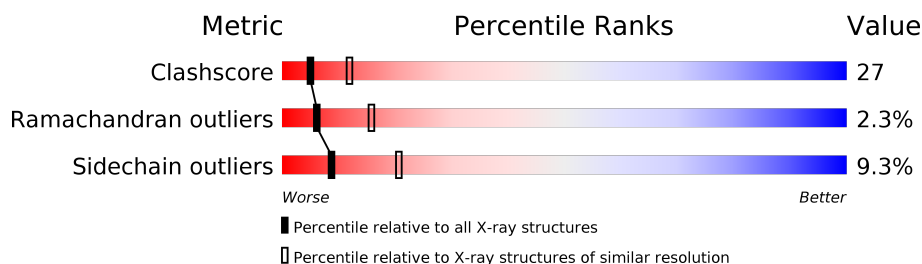
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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))
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	229	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 1806 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.

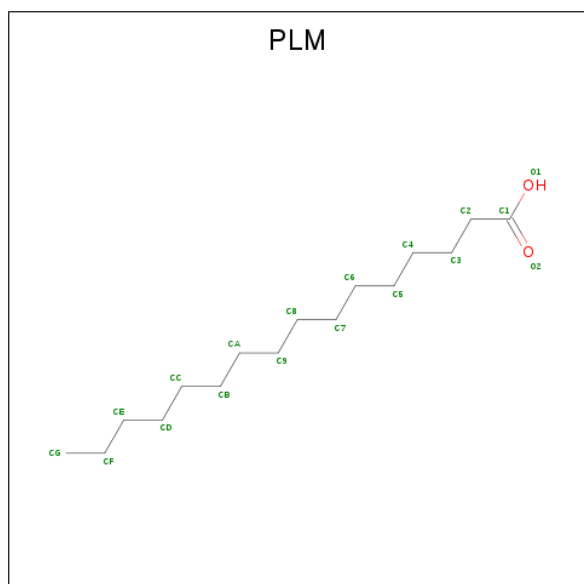
- Molecule 1 is a protein called Hepatocyte nuclear factor 4-gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	225	Total	C	N	O	S	0	0	0
			1774	1129	303	331	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	99	ALA	-	CLONING ARTIFACT	UNP Q14541
A	100	ALA	-	CLONING ARTIFACT	UNP Q14541
A	101	GLY	-	CLONING ARTIFACT	UNP Q14541
A	189	MET	ILE	CONFLICT	UNP Q14541

- Molecule 2 is PALMITIC ACID (three-letter code: PLM) (formula: C₁₆H₃₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			18	16	2		

- Molecule 3 is water.

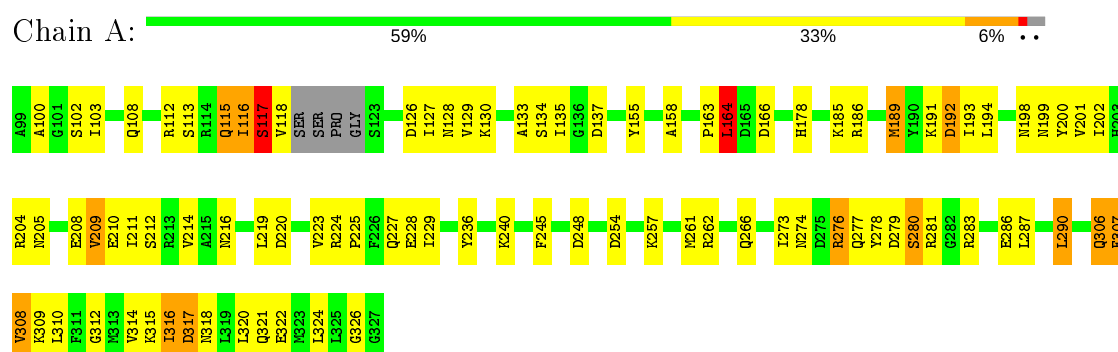
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	14	Total	O	0	0
			14	14		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

Note EDS was not executed.

- Molecule 1: Hepatocyte nuclear factor 4-gamma



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	152.71Å 152.71Å 93.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.92 – 2.70	Depositor
% Data completeness (in resolution range)	97.9 (19.92-2.70)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
Refinement program	CNS 2000	Depositor
R, R_{free}	0.245 , 0.264	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1806	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

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: PLM

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	0.62	1/1799 (0.1%)	0.75	0/2430

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
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	117	SER	C-N	17.17	1.73	1.34

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	278	TYR	Sidechain

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	1774	0	1787	98	0
2	A	18	0	31	3	0
3	A	14	0	0	2	0
All	All	1806	0	1818	98	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 27.

All (98) 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:116:ILE:CD1	1:A:116:ILE:H	1.12	1.42
1:A:117:SER:C	1:A:118:VAL:N	1.73	1.41
1:A:112:ARG:O	1:A:116:ILE:HD11	1.37	1.23
1:A:116:ILE:HD12	1:A:116:ILE:N	1.32	1.22
1:A:281:ARG:HH11	1:A:281:ARG:HG3	1.02	1.16
1:A:116:ILE:CD1	1:A:116:ILE:N	1.96	0.96
1:A:281:ARG:NH1	1:A:281:ARG:HG3	1.68	0.89
1:A:224:ARG:HB3	1:A:225:PRO:HD3	1.57	0.86
1:A:129:VAL:O	1:A:129:VAL:HG12	1.74	0.85
1:A:205:ASN:H	1:A:216:ASN:HD21	1.24	0.85
1:A:116:ILE:H	1:A:116:ILE:HD13	1.37	0.84
1:A:279:ASP:O	1:A:283:ARG:HB2	1.76	0.84
1:A:281:ARG:HH11	1:A:281:ARG:CG	1.84	0.83
1:A:318:ASN:O	1:A:322:GLU:HG3	1.77	0.83
1:A:307:PHE:CE2	1:A:308:VAL:HG23	2.15	0.82
1:A:116:ILE:H	1:A:116:ILE:HD12	0.64	0.80
1:A:126:ASP:OD1	1:A:127:ILE:N	2.15	0.80
1:A:158:ALA:HB1	1:A:261:MET:HE3	1.63	0.79
1:A:309:LYS:HB2	1:A:316:ILE:HD13	1.66	0.78
1:A:127:ILE:O	1:A:130:LYS:HG3	1.84	0.77
1:A:192:ASP:O	1:A:193:ILE:HD13	1.86	0.76
1:A:320:LEU:O	1:A:324:LEU:HB2	1.86	0.76
1:A:191:LYS:O	1:A:192:ASP:HB2	1.89	0.71
1:A:108:GLN:HG3	3:A:15:HOH:O	1.91	0.71
1:A:281:ARG:NH1	1:A:281:ARG:CG	2.46	0.69
1:A:129:VAL:O	1:A:129:VAL:CG1	2.43	0.65
1:A:245:PHE:O	1:A:262:ARG:HD3	1.95	0.65
1:A:158:ALA:HB1	1:A:261:MET:CE	2.26	0.65
1:A:306:GLN:NE2	1:A:306:GLN:HA	2.14	0.63
1:A:163:PRO:HG2	1:A:166:ASP:OD2	1.99	0.63
1:A:306:GLN:HE21	1:A:306:GLN:HA	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:LYS:HB2	1:A:316:ILE:CD1	2.30	0.62
1:A:201:VAL:CG1	1:A:202:ILE:N	2.64	0.60
1:A:306:GLN:HE21	1:A:306:GLN:CA	2.15	0.59
1:A:254:ASP:OD2	1:A:257:LYS:HB2	2.03	0.59
1:A:134:SER:H	1:A:137:ASP:HB2	1.69	0.57
1:A:204:ARG:NH2	1:A:220:ASP:OD2	2.35	0.57
1:A:316:ILE:HG22	1:A:317:ASP:O	2.05	0.57
1:A:127:ILE:HG23	1:A:128:ASN:N	2.20	0.56
1:A:135:ILE:HD11	1:A:210:GLU:HG2	1.88	0.56
1:A:126:ASP:C	1:A:126:ASP:OD1	2.44	0.55
1:A:135:ILE:CD1	1:A:210:GLU:HG2	2.37	0.54
1:A:274:ASN:HA	1:A:280:SER:OG	2.07	0.54
1:A:127:ILE:CG2	1:A:128:ASN:N	2.70	0.54
1:A:316:ILE:HG22	1:A:321:GLN:HG3	1.89	0.54
1:A:287:LEU:O	1:A:290:LEU:HB2	2.08	0.53
1:A:316:ILE:HG23	1:A:320:LEU:HB2	1.90	0.53
1:A:133:ALA:HB2	1:A:200:TYR:HB3	1.91	0.52
1:A:307:PHE:CD2	1:A:308:VAL:N	2.77	0.52
1:A:209:VAL:HA	1:A:212:SER:HB3	1.92	0.51
1:A:223:VAL:O	1:A:227:GLN:HG3	2.10	0.50
1:A:201:VAL:HG13	1:A:202:ILE:N	2.27	0.50
1:A:316:ILE:CG2	1:A:321:GLN:HG3	2.41	0.49
1:A:273:ILE:O	1:A:276:ARG:HB2	2.13	0.49
1:A:286:GLU:HA	1:A:286:GLU:OE1	2.12	0.49
1:A:317:ASP:CG	1:A:318:ASN:H	2.16	0.49
1:A:194:LEU:HD13	1:A:219:LEU:CD2	2.43	0.49
1:A:308:VAL:HG11	2:A:328:PLM:HG2	1.94	0.49
1:A:279:ASP:C	1:A:281:ARG:H	2.16	0.48
1:A:113:SER:C	1:A:116:ILE:HD13	2.32	0.48
1:A:257:LYS:O	1:A:261:MET:HG3	2.14	0.48
1:A:229:ILE:CD1	1:A:287:LEU:HD21	2.43	0.48
1:A:306:GLN:NE2	1:A:306:GLN:CA	2.73	0.48
1:A:208:GLU:O	1:A:210:GLU:N	2.47	0.47
1:A:307:PHE:CG	1:A:308:VAL:N	2.81	0.47
1:A:224:ARG:HB3	1:A:225:PRO:CD	2.38	0.47
1:A:224:ARG:O	1:A:228:GLU:HG3	2.15	0.47
1:A:178:HIS:CE1	1:A:240:LYS:HE3	2.50	0.46
1:A:317:ASP:CG	1:A:318:ASN:N	2.69	0.46
1:A:191:LYS:HA	1:A:191:LYS:HD3	1.67	0.46
1:A:314:VAL:HG12	1:A:315:LYS:N	2.31	0.45
1:A:115:GLN:C	1:A:116:ILE:HD12	2.23	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:GLN:HE21	1:A:306:GLN:C	2.18	0.45
1:A:321:GLN:O	1:A:326:GLY:N	2.40	0.45
1:A:310:LEU:HA	1:A:310:LEU:HD23	1.78	0.45
1:A:194:LEU:HD13	1:A:219:LEU:HD21	1.99	0.45
1:A:211:ILE:HB	2:A:328:PLM:HA1	1.99	0.44
1:A:229:ILE:HD11	1:A:287:LEU:HD21	1.99	0.44
1:A:198:ASN:OD1	1:A:200:TYR:HB2	2.18	0.44
1:A:279:ASP:C	1:A:281:ARG:N	2.69	0.44
1:A:201:VAL:HG13	1:A:202:ILE:H	1.82	0.44
1:A:112:ARG:HB2	1:A:155:TYR:CD2	2.52	0.44
1:A:193:ILE:HG22	1:A:194:LEU:H	1.82	0.43
1:A:205:ASN:ND2	1:A:216:ASN:OD1	2.52	0.42
1:A:205:ASN:H	1:A:216:ASN:ND2	2.05	0.42
1:A:164:LEU:HG	1:A:164:LEU:H	1.36	0.41
1:A:229:ILE:CD1	1:A:287:LEU:CD2	2.99	0.41
1:A:214:VAL:HB	2:A:328:PLM:HA2	2.02	0.41
1:A:100:ALA:HA	3:A:1:HOH:O	2.20	0.41
1:A:185:LYS:HG3	1:A:236:TYR:CZ	2.56	0.41
1:A:127:ILE:C	1:A:129:VAL:H	2.24	0.41
1:A:127:ILE:HA	1:A:130:LYS:HD2	2.02	0.41
1:A:189:MET:H	1:A:189:MET:HG2	1.50	0.41
1:A:186:ARG:HD3	1:A:186:ARG:HH11	1.60	0.41
1:A:116:ILE:N	1:A:116:ILE:HD13	2.10	0.40
1:A:191:LYS:O	1:A:192:ASP:CB	2.58	0.40
1:A:225:PRO:O	1:A:229:ILE:HG23	2.21	0.40
1:A:316:ILE:O	1:A:317:ASP:O	2.39	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	221/229 (96%)	202 (91%)	14 (6%)	5 (2%)	6	16

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	192	ASP
1	A	317	ASP
1	A	164	LEU
1	A	209	VAL
1	A	312	GLY

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	193/201 (96%)	175 (91%)	18 (9%)	9	21

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	SER
1	A	103	ILE
1	A	115	GLN
1	A	116	ILE
1	A	117	SER
1	A	164	LEU
1	A	189	MET
1	A	199	ASN
1	A	248	ASP
1	A	266	GLN
1	A	276	ARG
1	A	277	GLN
1	A	280	SER
1	A	290	LEU
1	A	306	GLN
1	A	307	PHE

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Mol	Chain	Res	Type
1	A	308	VAL
1	A	316	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	GLN
1	A	145	GLN
1	A	205	ASN
1	A	216	ASN
1	A	230	GLN
1	A	260	ASN
1	A	277	GLN
1	A	295	GLN
1	A	306	GLN
1	A	321	GLN

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 ⓘ

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
2	PLM	A	328	-	14,17,17	0.29	0	13,17,17	0.53	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
2	PLM	A	328	-	-	7/13/15/15	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	328	PLM	C1-C2-C3-C4
2	A	328	PLM	C5-C6-C7-C8
2	A	328	PLM	C7-C8-C9-CA
2	A	328	PLM	C6-C7-C8-C9
2	A	328	PLM	C9-CA-CB-CC
2	A	328	PLM	C4-C5-C6-C7
2	A	328	PLM	C3-C4-C5-C6

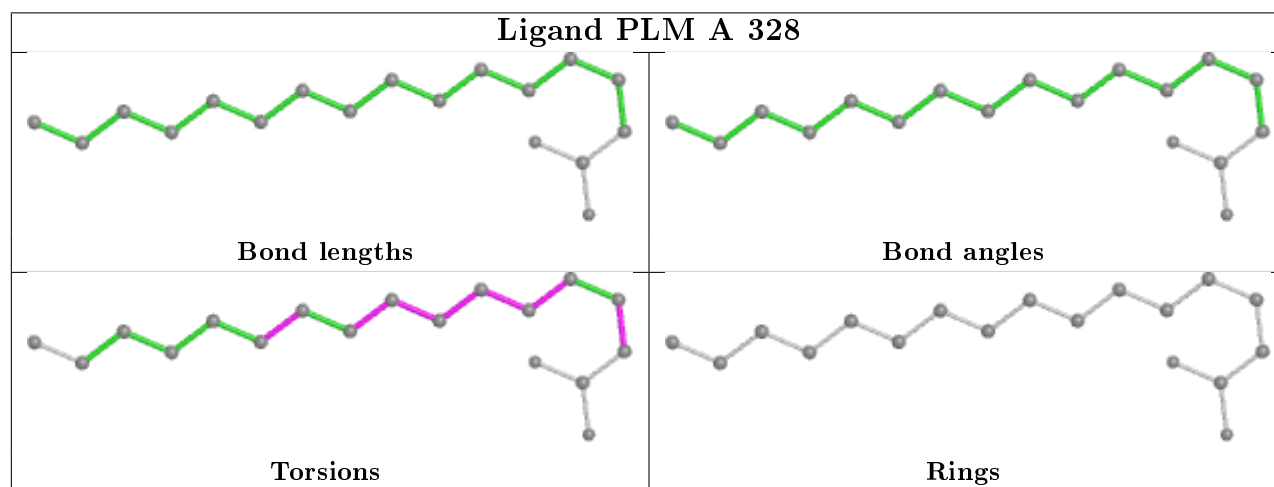
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	328	PLM	3	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	117:SER	C	118:VAL	N	1.73

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.