



wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 01:00 pm BST

PDB ID : 1YUH
Title : FAB FRAGMENT
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Deposited on : 1996-01-30
Resolution : 3.00 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 ⓘ 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)
Xtrriage (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

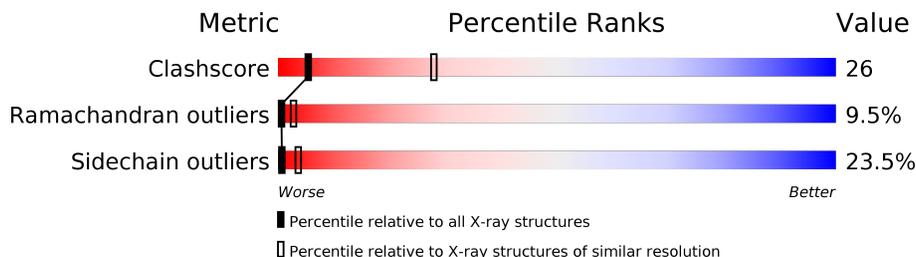
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	211	
1	L	211	
2	B	218	
2	H	218	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6530 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 88C6/12 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	211	1594	996	269	323	6	0	0	0
1	A	211	1594	996	269	323	6	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	44	ARG	HIS	CONFLICT	GB 387376
L	57	GLY	ALA	CONFLICT	GB 387376
L	160	GLU	GLN	CONFLICT	GB 387376
L	184	SER	THR	CONFLICT	GB 387376
L	192	ALA	SER	CONFLICT	GB 387376
A	44	ARG	HIS	CONFLICT	GB 387376
A	57	GLY	ALA	CONFLICT	GB 387376
A	160	GLU	GLN	CONFLICT	GB 387376
A	184	SER	THR	CONFLICT	GB 387376
A	192	ALA	SER	CONFLICT	GB 387376

- Molecule 2 is a protein called 88C6/12 FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	218	1647	1046	273	319	9	0	0	0
2	B	218	1647	1046	273	319	9	0	0	0

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	9	ALA	PRO	CONFLICT	GB 3399661
H	20	LEU	MET	CONFLICT	GB 3399661

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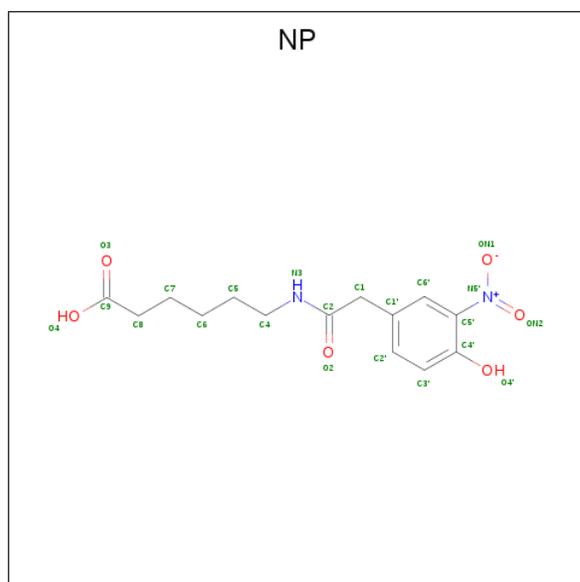
Chain	Residue	Modelled	Actual	Comment	Reference
H	33	LEU	VAL	CONFLICT	GB 3399661
H	37	ILE	VAL	CONFLICT	GB 3399661
H	40	ARG	LYS	CONFLICT	GB 3399661
H	43	ARG	GLN	CONFLICT	GB 3399661
H	50	ARG	TYR	CONFLICT	GB 3399661
H	52	ASP	ASN	CONFLICT	GB 3399661
H	54	ASN	TYR	CONFLICT	GB 3399661
H	56	VAL	ASP	CONFLICT	GB 3399661
H	57	VAL	GLY	CONFLICT	GB 3399661
H	60	PHE	TYR	CONFLICT	GB 3399661
H	66	SER	GLY	CONFLICT	GB 3399661
H	72	VAL	SER	CONFLICT	GB 3399661
H	75	PRO	SER	CONFLICT	GB 3399661
H	97	ALA	VAL	CONFLICT	GB 3399661
H	99	TYR	GLY	CONFLICT	GB 3399661
H	100	ALA	GLY	CONFLICT	GB 3399661
H	102	CYS	-	INSERTION	GB 3399661
H	?	-	TYR	DELETION	GB 3399661
H	?	-	TYR	DELETION	GB 3399661
H	?	-	ALA	DELETION	GB 3399661
H	113	THR	SER	CONFLICT	GB 3399661
H	120	ALA	LYS	CONFLICT	GB 3399661
H	163	ALA	SER	CONFLICT	GB 3399661
H	190	ALA	SER	CONFLICT	GB 3399661
H	196	GLY	GLU	CONFLICT	GB 3399661
H	210	ALA	LYS	CONFLICT	GB 3399661
B	9	ALA	PRO	CONFLICT	GB 3399661
B	20	LEU	MET	CONFLICT	GB 3399661
B	33	LEU	VAL	CONFLICT	GB 3399661
B	37	ILE	VAL	CONFLICT	GB 3399661
B	40	ARG	LYS	CONFLICT	GB 3399661
B	43	ARG	GLN	CONFLICT	GB 3399661
B	50	ARG	TYR	CONFLICT	GB 3399661
B	52	ASP	ASN	CONFLICT	GB 3399661
B	54	ASN	TYR	CONFLICT	GB 3399661
B	56	VAL	ASP	CONFLICT	GB 3399661
B	57	VAL	GLY	CONFLICT	GB 3399661
B	60	PHE	TYR	CONFLICT	GB 3399661
B	66	SER	GLY	CONFLICT	GB 3399661
B	72	VAL	SER	CONFLICT	GB 3399661
B	75	PRO	SER	CONFLICT	GB 3399661
B	97	ALA	VAL	CONFLICT	GB 3399661

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Chain	Residue	Modelled	Actual	Comment	Reference
B	99	TYR	GLY	CONFLICT	GB 3399661
B	100	ALA	GLY	CONFLICT	GB 3399661
B	102	CYS	-	INSERTION	GB 3399661
B	?	-	TYR	DELETION	GB 3399661
B	?	-	TYR	DELETION	GB 3399661
B	?	-	ALA	DELETION	GB 3399661
B	113	THR	SER	CONFLICT	GB 3399661
B	120	ALA	LYS	CONFLICT	GB 3399661
B	163	ALA	SER	CONFLICT	GB 3399661
B	190	ALA	SER	CONFLICT	GB 3399661
B	196	GLY	GLU	CONFLICT	GB 3399661
B	210	ALA	LYS	CONFLICT	GB 3399661

- Molecule 3 is 4-HYDROXY-3-NITROPHENYLACETYL-EPSILON-AMINOCAPROIC ACID (three-letter code: NP) (formula: C₁₄H₁₈N₂O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	H	1	22	14	2	6	0	0
3	B	1	22	14	2	6	0	0

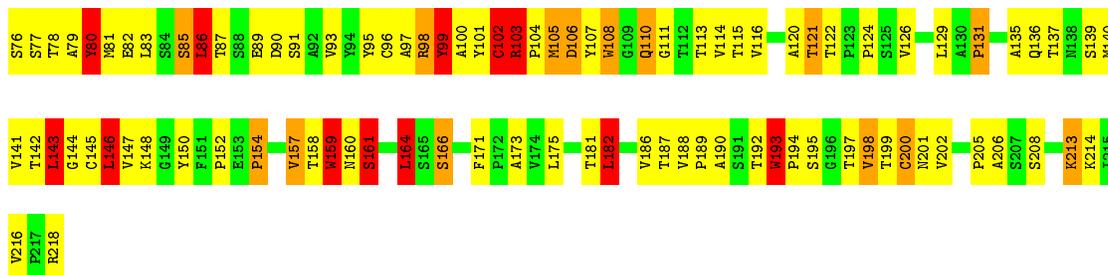
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	L	3	3	3	0	0

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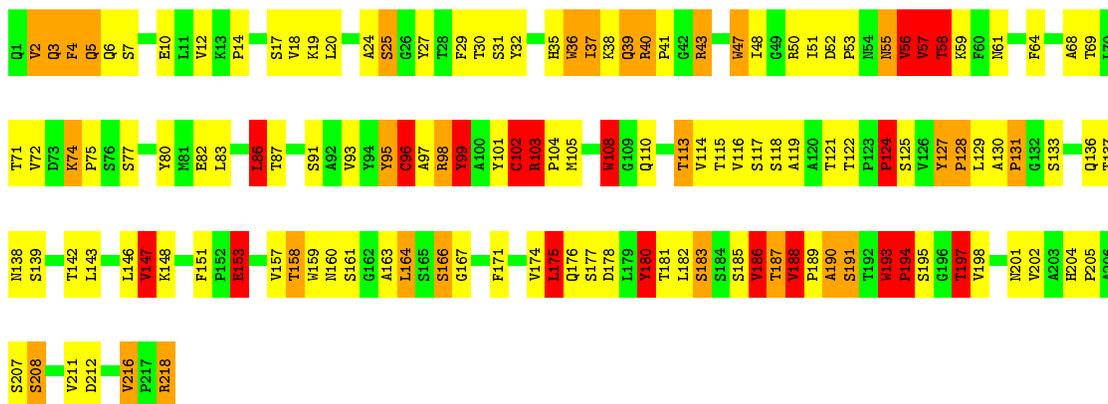
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	1	Total	O	0	0
			1	1		



• Molecule 2: 88C6/12 FAB (HEAVY CHAIN)

Chain B: 38% 40% 13% 9%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	81.20Å 86.90Å 131.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-3.00)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.190 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	6530	wwPDB-VP
Average B, all atoms (Å ²)	12.0	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: NP

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	0.93	0/1630	2.06	55/2224 (2.5%)
1	L	0.93	0/1630	2.03	59/2224 (2.7%)
2	B	0.92	0/1691	2.10	64/2311 (2.8%)
2	H	0.92	0/1691	2.06	54/2311 (2.3%)
All	All	0.92	0/6642	2.06	232/9070 (2.6%)

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	6
2	B	0	6
2	H	0	2
All	All	0	14

There are no bond length outliers.

The worst 5 of 232 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	80	TYR	CB-CG-CD2	-12.10	113.74	121.00
1	L	190	ARG	NE-CZ-NH1	10.63	125.61	120.30
2	B	98	ARG	NE-CZ-NH2	-10.58	115.01	120.30
2	H	99	TYR	CB-CG-CD1	-10.56	114.66	121.00
2	B	36	TRP	CD1-CG-CD2	10.53	114.72	106.30

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	122	PRO	Peptide
1	A	143	TYR	Peptide
1	A	41	LYS	Peptide
2	H	193	TRP	Peptide
2	H	99	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	1594	0	1538	96	0
1	L	1594	0	1538	80	0
2	B	1647	0	1622	98	0
2	H	1647	0	1622	107	0
3	B	22	0	16	2	0
3	H	22	0	16	1	0
4	H	1	0	0	0	0
4	L	3	0	0	0	0
All	All	6530	0	6352	337	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 26.

The worst 5 of 337 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:150:ASP:HB2	1:A:197:GLN:HB3	1.38	1.02
2:H:105:MET:HG2	2:H:108:TRP:HE1	1.32	0.94
2:B:39:GLN:HB3	2:B:93:VAL:HB	1.55	0.88
2:H:19:LYS:HD2	2:H:80:TYR:HB3	1.57	0.86
2:H:124:PRO:HB3	2:H:150:TYR:HB3	1.58	0.86

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	207/211 (98%)	149 (72%)	41 (20%)	17 (8%)	1	4
1	L	207/211 (98%)	164 (79%)	28 (14%)	15 (7%)	1	5
2	B	214/218 (98%)	155 (72%)	35 (16%)	24 (11%)	0	2
2	H	214/218 (98%)	167 (78%)	23 (11%)	24 (11%)	0	2
All	All	842/858 (98%)	635 (75%)	127 (15%)	80 (10%)	0	3

5 of 80 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	112	PRO
1	L	154	ASP
1	L	167	PRO
1	L	171	SER
2	H	7	SER

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	177/177 (100%)	133 (75%)	44 (25%)	0	3
1	L	177/177 (100%)	127 (72%)	50 (28%)	0	2
2	B	185/185 (100%)	143 (77%)	42 (23%)	1	4
2	H	185/185 (100%)	151 (82%)	34 (18%)	1	9
All	All	724/724 (100%)	554 (76%)	170 (24%)	1	3

5 of 170 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	158	THR
1	A	71	ASP
2	B	175	LEU
2	H	164	LEU
1	A	17	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	54	ASN
2	B	3	GLN
2	H	54	ASN
1	A	197	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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
3	NP	H	995	-	18,22,22	1.75	2 (11%)	20,28,28	10.02	6 (30%)
3	NP	B	996	-	18,22,22	1.90	2 (11%)	20,28,28	5.26	9 (45%)

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	NP	H	995	-	-	4/13/17/17	0/1/1/1
3	NP	B	996	-	-	9/13/17/17	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	996	NP	C5'-N5'	-6.40	1.34	1.45
3	H	995	NP	C5'-N5'	-5.48	1.35	1.45
3	H	995	NP	ON2-N5'	3.78	1.29	1.22
3	B	996	NP	ON2-N5'	3.28	1.28	1.22

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	995	NP	C1-C2-N3	31.16	158.28	116.19
3	H	995	NP	O2-C2-N3	-26.76	72.51	123.01
3	B	996	NP	O2-C2-C1	-18.71	79.46	122.03
3	H	995	NP	O2-C2-C1	-15.93	85.79	122.03
3	B	996	NP	C1-C2-N3	-7.78	105.68	116.19

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

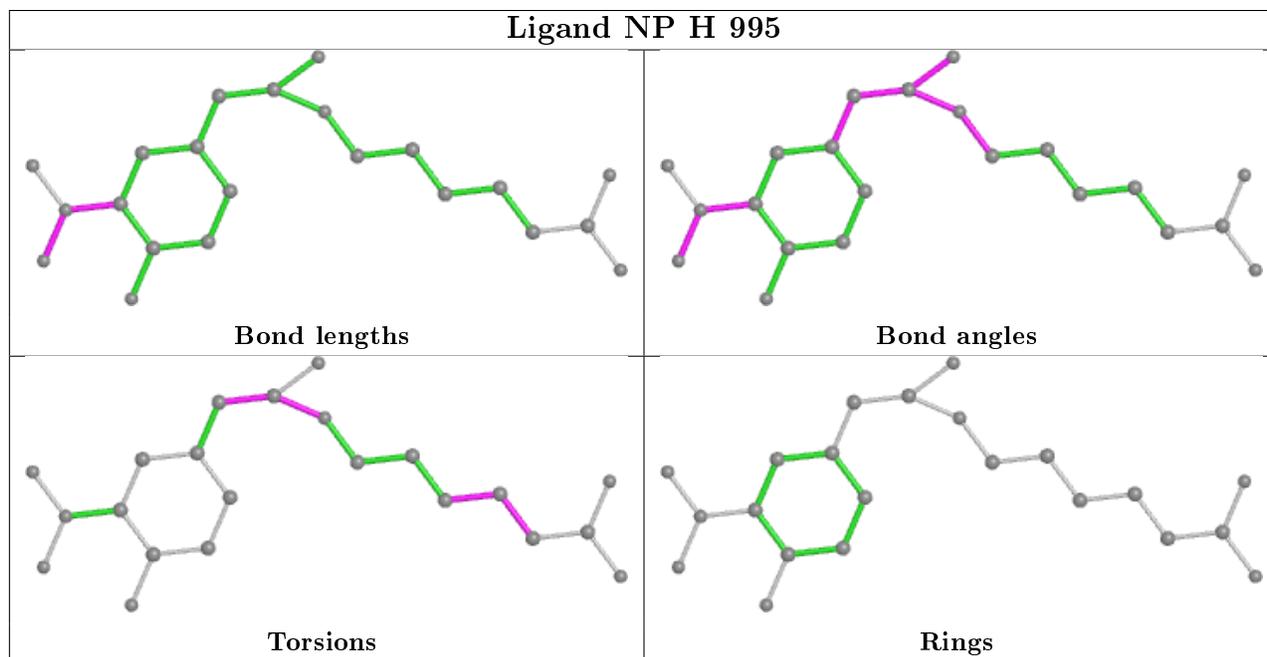
Mol	Chain	Res	Type	Atoms
3	B	996	NP	C1-C2-N3-C4
3	B	996	NP	O2-C2-N3-C4
3	B	996	NP	C6-C7-C8-C9
3	H	995	NP	O2-C2-N3-C4
3	B	996	NP	C2-C1-C1'-C2'

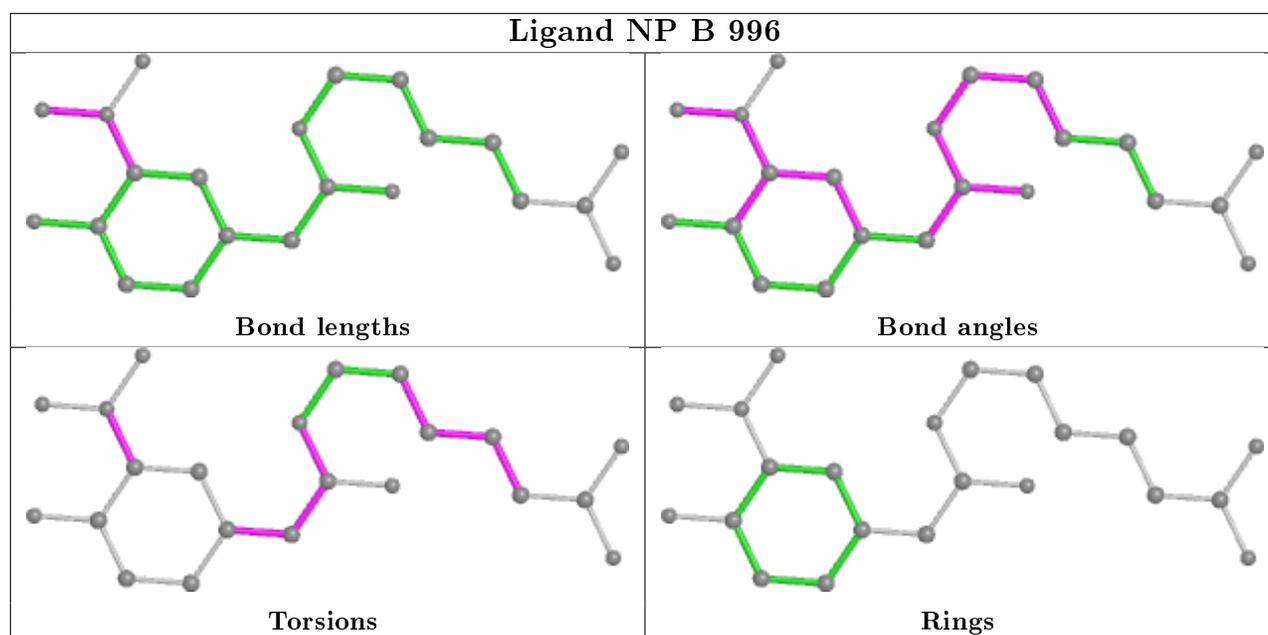
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	995	NP	1	0
3	B	996	NP	2	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
2	H	1
2	B	1
1	A	1
1	L	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	117:SER	C	118:SER	N	3.13
1	H	117:SER	C	118:SER	N	3.12
1	A	109:LEU	C	110:GLY	N	3.02
1	L	109:LEU	C	110:GLY	N	2.88

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.