



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 01:32 am GMT

PDB ID : 1HG4  
Title : Ultraspiracle ligand binding domain from *Drosophila melanogaster*  
Authors : Schwabe, J.W.R.; Clayton, G.M.  
Deposited on : 2000-12-12  
Resolution : 2.40 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

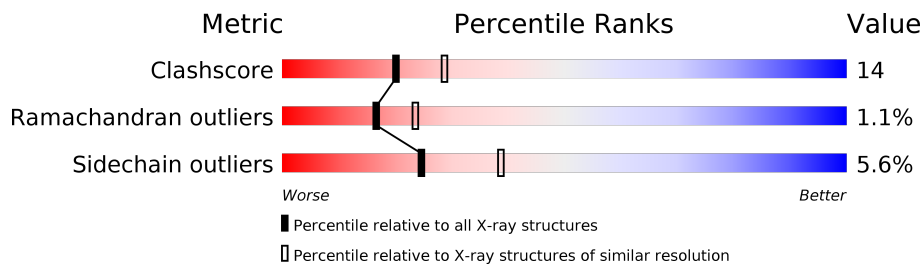
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	279	
1	B	279	
1	C	279	
1	D	279	
1	E	279	
1	F	279	

## 2 Entry composition [i](#)

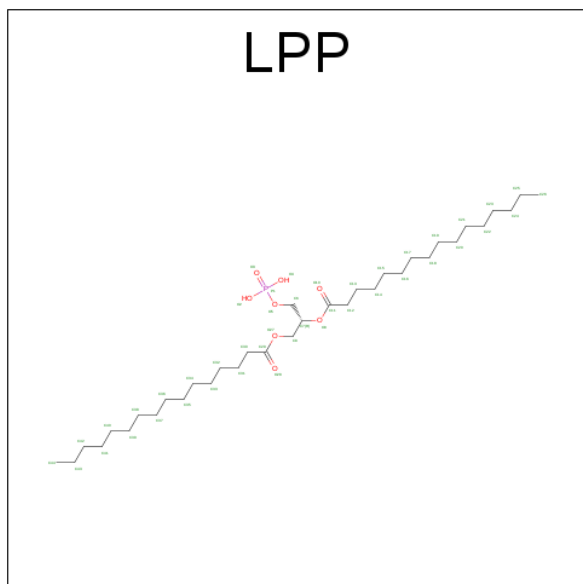
There are 3 unique types of molecules in this entry. The entry contains 11854 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ULTRASPIRACLE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	240	Total	C	N	O	S	0	0	0
			1904	1215	334	342	13			
1	B	240	Total	C	N	O	S	0	0	0
			1904	1215	334	342	13			
1	C	238	Total	C	N	O	S	0	0	0
			1893	1208	334	338	13			
1	D	238	Total	C	N	O	S	0	0	0
			1881	1202	328	338	13			
1	E	240	Total	C	N	O	S	0	0	0
			1910	1221	334	342	13			
1	F	240	Total	C	N	O	S	0	0	0
			1910	1221	334	342	13			

- Molecule 2 is 2-(HEXADECANOYLOXY)-1-[(PHOSPHONOOXY)METHYL]ETHYL HEXADECANOATE (three-letter code: LPP) (formula: C<sub>35</sub>H<sub>69</sub>O<sub>8</sub>P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			44	35	8	1		
2	B	1	Total	C	O	P	0	0
			44	35	8	1		
2	C	1	Total	C	O	P	0	0
			44	35	8	1		
2	D	1	Total	C	O	P	0	0
			44	35	8	1		
2	E	1	Total	C	O	P	0	0
			44	35	8	1		
2	F	1	Total	C	O	P	0	0
			44	35	8	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	30	Total	O	0	0
			30	30		
3	B	32	Total	O	0	0
			32	32		
3	C	32	Total	O	0	0
			32	32		
3	D	38	Total	O	0	0
			38	38		
3	E	31	Total	O	0	0
			31	31		
3	F	25	Total	O	0	0
			25	25		

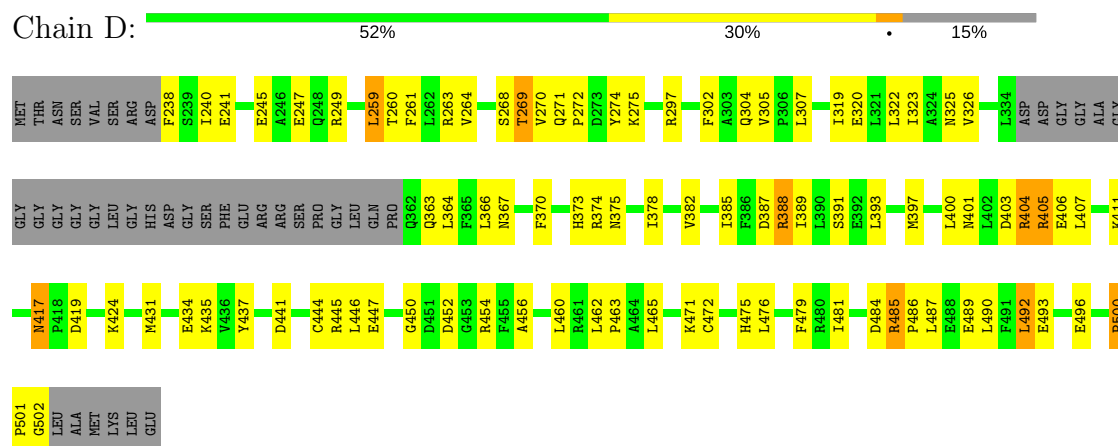


Note EDS was not executed.

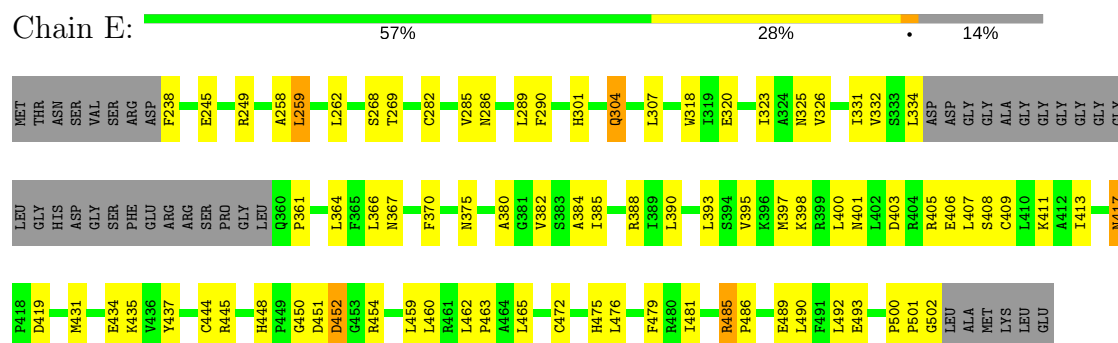
- Molecule 1: ULTRASPIRACLE



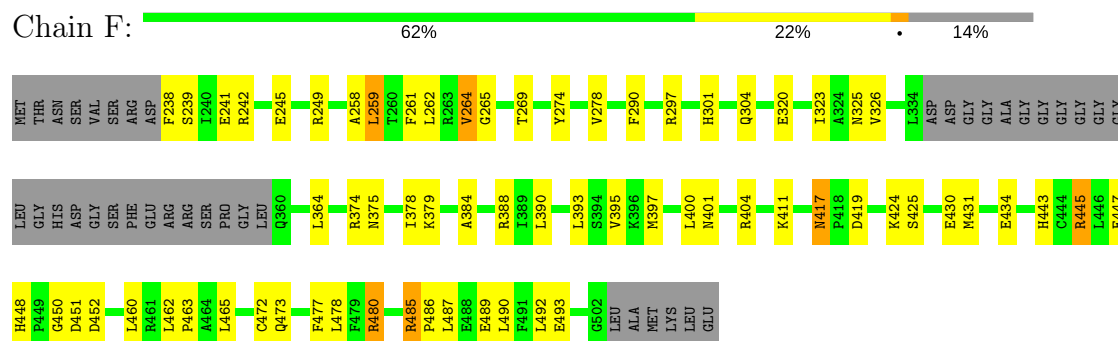
● Molecule 1: ULTRASPIRACLE



● Molecule 1: ULTRASPIRACLE



● Molecule 1: ULTRASPIRACLE



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	37.98Å 86.19Å 137.00Å 85.57° 85.94° 83.09°	Depositor
Resolution (Å)	34.00 – 2.40	Depositor
% Data completeness (in resolution range)	90.0 (34.00-2.40)	Depositor
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.248 , 0.284	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11854	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	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: LPP

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	0.41	0/1940	0.58	0/2624
1	B	0.41	0/1940	0.59	0/2624
1	C	0.40	0/1928	0.58	0/2605
1	D	0.41	0/1916	0.60	0/2591
1	E	0.41	0/1947	0.61	0/2633
1	F	0.40	0/1947	0.57	0/2633
All	All	0.41	0/11618	0.59	0/15710

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	1904	0	1928	47	0
1	B	1904	0	1928	50	0
1	C	1893	0	1924	57	0
1	D	1881	0	1902	83	0
1	E	1910	0	1935	61	0
1	F	1910	0	1935	54	0
2	A	44	0	67	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	44	0	67	2	0
2	C	44	0	67	3	0
2	D	44	0	67	7	0
2	E	44	0	67	7	0
2	F	44	0	67	3	0
3	A	30	0	0	1	0
3	B	32	0	0	1	0
3	C	32	0	0	2	0
3	D	38	0	0	4	0
3	E	31	0	0	1	0
3	F	25	0	0	3	0
All	All	11854	0	11954	333	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 14.

The worst 5 of 333 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:E:444:CYS:SG	1:E:454:ARG:HD3	1.91	1.11
1:D:500:PRO:HB2	1:D:501:PRO:HD2	1.34	1.07
1:D:444:CYS:SG	1:D:454:ARG:HD3	2.03	0.96
1:D:259:LEU:HD11	1:D:490:LEU:HD23	1.48	0.93
1:D:272:PRO:HA	1:D:275:LYS:HE3	1.53	0.90

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	236/279 (85%)	226 (96%)	9 (4%)	1 (0%)	38 54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	236/279 (85%)	223 (94%)	9 (4%)	4 (2%)	11	13
1	C	234/279 (84%)	219 (94%)	9 (4%)	6 (3%)	6	6
1	D	234/279 (84%)	217 (93%)	15 (6%)	2 (1%)	20	29
1	E	236/279 (85%)	224 (95%)	11 (5%)	1 (0%)	38	54
1	F	236/279 (85%)	221 (94%)	13 (6%)	2 (1%)	22	33
All	All	1412/1674 (84%)	1330 (94%)	66 (5%)	16 (1%)	17	23

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	266	PRO
1	F	264	VAL
1	B	260	THR
1	C	450	GLY
1	C	501	PRO

### 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	207/238 (87%)	191 (92%)	16 (8%)	15	23
1	B	207/238 (87%)	197 (95%)	10 (5%)	30	47
1	C	206/238 (87%)	200 (97%)	6 (3%)	48	68
1	D	204/238 (86%)	189 (93%)	15 (7%)	16	25
1	E	208/238 (87%)	197 (95%)	11 (5%)	26	42
1	F	208/238 (87%)	196 (94%)	12 (6%)	23	37
All	All	1240/1428 (87%)	1170 (94%)	70 (6%)	25	39

5 of 70 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	492	LEU

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Mol	Chain	Res	Type
1	D	404	ARG
1	F	445	ARG
1	D	238	PHE
1	D	271	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	367	ASN
1	D	248	GLN
1	F	367	ASN
1	C	475	HIS
1	D	304	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](#)

6 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	LPP	A	1	-	43,43,43	1.09	2 (4%)	47,48,48	1.01	1 (2%)
2	LPP	B	1	-	43,43,43	1.12	4 (9%)	47,48,48	1.01	2 (4%)
2	LPP	C	1	-	43,43,43	1.04	2 (4%)	47,48,48	1.06	3 (6%)
2	LPP	D	1	-	43,43,43	1.05	2 (4%)	47,48,48	1.02	3 (6%)
2	LPP	E	1	-	43,43,43	1.08	3 (6%)	47,48,48	0.99	3 (6%)
2	LPP	F	1	-	43,43,43	1.07	2 (4%)	47,48,48	1.02	3 (6%)

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	LPP	A	1	-	-	0/45/45/45	0/0/0/0
2	LPP	B	1	-	-	0/45/45/45	0/0/0/0
2	LPP	C	1	-	-	0/45/45/45	0/0/0/0
2	LPP	D	1	-	-	0/45/45/45	0/0/0/0
2	LPP	E	1	-	-	0/45/45/45	0/0/0/0
2	LPP	F	1	-	-	0/45/45/45	0/0/0/0

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	LPP	O27-C8	-2.14	1.40	1.45
2	E	1	LPP	P1-O2	2.02	1.63	1.54
2	B	1	LPP	P1-O2	2.03	1.63	1.54
2	C	1	LPP	P1-O3	3.23	1.61	1.50
2	D	1	LPP	P1-O3	3.25	1.61	1.50

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	LPP	C7-O9-C11	-2.69	111.53	117.88
2	E	1	LPP	C8-O27-C29	-2.58	109.37	117.13
2	F	1	LPP	C7-O9-C11	-2.48	112.00	117.88
2	C	1	LPP	C8-O27-C29	-2.39	109.95	117.13
2	F	1	LPP	C8-O27-C29	-2.27	110.30	117.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	LPP	2	0
2	B	1	LPP	2	0
2	C	1	LPP	3	0
2	D	1	LPP	7	0
2	E	1	LPP	7	0
2	F	1	LPP	3	0

## 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

### 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.