



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 09:34 am BST

PDB ID : 6QJ5  
Title : X-ray structure of PPARgamma LBD with the ligand NV1380  
Authors : Pochetti, G.; Montanari, R.; Capelli, D.  
Deposited on : 2019-01-22  
Resolution : 2.00 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](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.

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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 : 2.11  
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) : 2.11

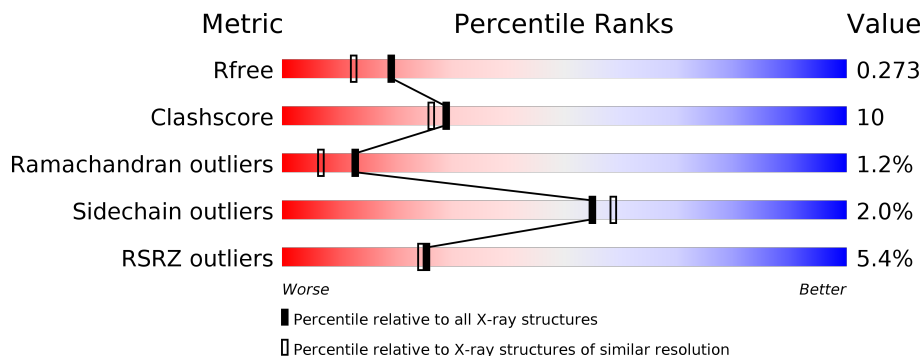
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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  $\geq 3$ , 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	304	<p>2% 66% 15% 17%</p>
1	B	304	<p>7% 68% 13% 18%</p>

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 4161 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 Peroxisome proliferator-activated receptor gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	251	2004	1294	327	373	10	0	0	0
1	B	248	1980	1280	320	370	10	0	0	0

There are 42 discrepancies between the modelled and reference sequences:

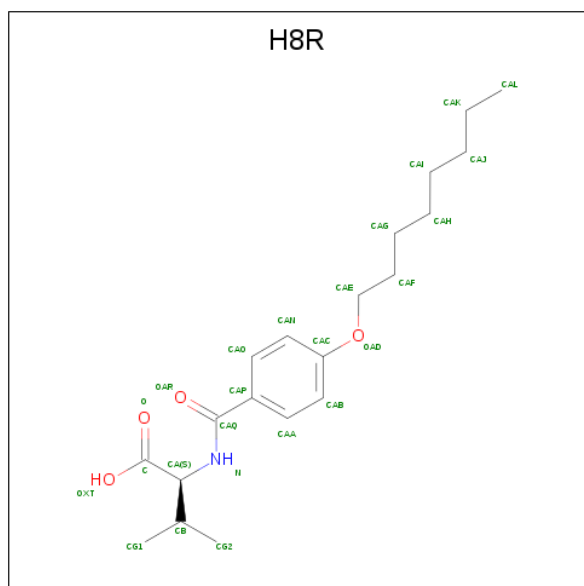
Chain	Residue	Modelled	Actual	Comment	Reference
A	174	MET	-	initiating methionine	UNP P37231
A	175	GLY	-	expression tag	UNP P37231
A	176	SER	-	expression tag	UNP P37231
A	177	SER	-	expression tag	UNP P37231
A	178	HIS	-	expression tag	UNP P37231
A	179	HIS	-	expression tag	UNP P37231
A	180	HIS	-	expression tag	UNP P37231
A	181	HIS	-	expression tag	UNP P37231
A	182	HIS	-	expression tag	UNP P37231
A	183	HIS	-	expression tag	UNP P37231
A	184	SER	-	expression tag	UNP P37231
A	185	SER	-	expression tag	UNP P37231
A	186	GLY	-	expression tag	UNP P37231
A	187	LEU	-	expression tag	UNP P37231
A	188	VAL	-	expression tag	UNP P37231
A	189	PRO	-	expression tag	UNP P37231
A	190	ARG	-	expression tag	UNP P37231
A	191	GLY	-	expression tag	UNP P37231
A	192	SER	-	expression tag	UNP P37231
A	193	HIS	-	expression tag	UNP P37231
A	194	MET	-	expression tag	UNP P37231
B	174	MET	-	initiating methionine	UNP P37231
B	175	GLY	-	expression tag	UNP P37231
B	176	SER	-	expression tag	UNP P37231
B	177	SER	-	expression tag	UNP P37231

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Chain	Residue	Modelled	Actual	Comment	Reference
B	178	HIS	-	expression tag	UNP P37231
B	179	HIS	-	expression tag	UNP P37231
B	180	HIS	-	expression tag	UNP P37231
B	181	HIS	-	expression tag	UNP P37231
B	182	HIS	-	expression tag	UNP P37231
B	183	HIS	-	expression tag	UNP P37231
B	184	SER	-	expression tag	UNP P37231
B	185	SER	-	expression tag	UNP P37231
B	186	GLY	-	expression tag	UNP P37231
B	187	LEU	-	expression tag	UNP P37231
B	188	VAL	-	expression tag	UNP P37231
B	189	PRO	-	expression tag	UNP P37231
B	190	ARG	-	expression tag	UNP P37231
B	191	GLY	-	expression tag	UNP P37231
B	192	SER	-	expression tag	UNP P37231
B	193	HIS	-	expression tag	UNP P37231
B	194	MET	-	expression tag	UNP P37231

- Molecule 2 is (2 {S})-3-methyl-2-[(4-octoxyphenyl)carbonylamino]butanoic acid (three-letter code: H8R) (formula: C<sub>20</sub>H<sub>31</sub>NO<sub>4</sub>) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	N			O
2	A	1	33	28	1	4	0	1

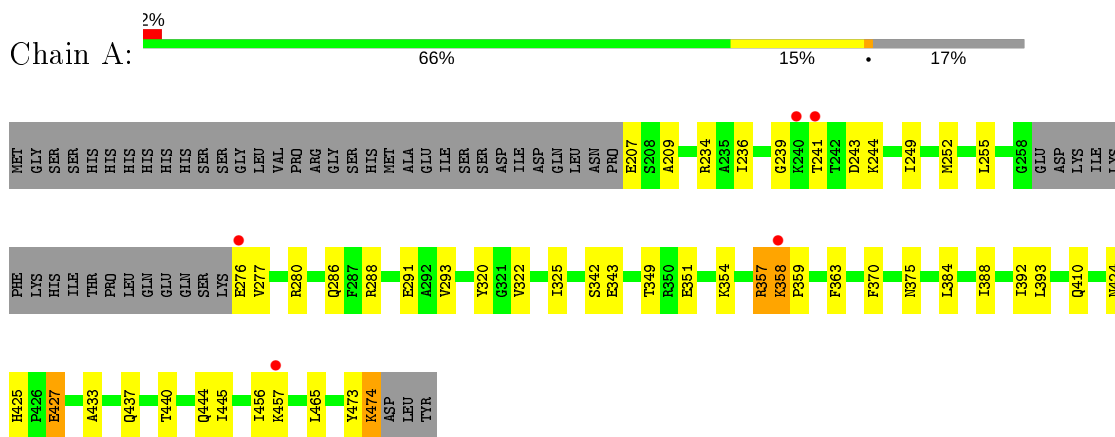
- Molecule 3 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
3	A	72	Total 72	O 72	0	0
3	B	72	Total 72	O 72	0	0

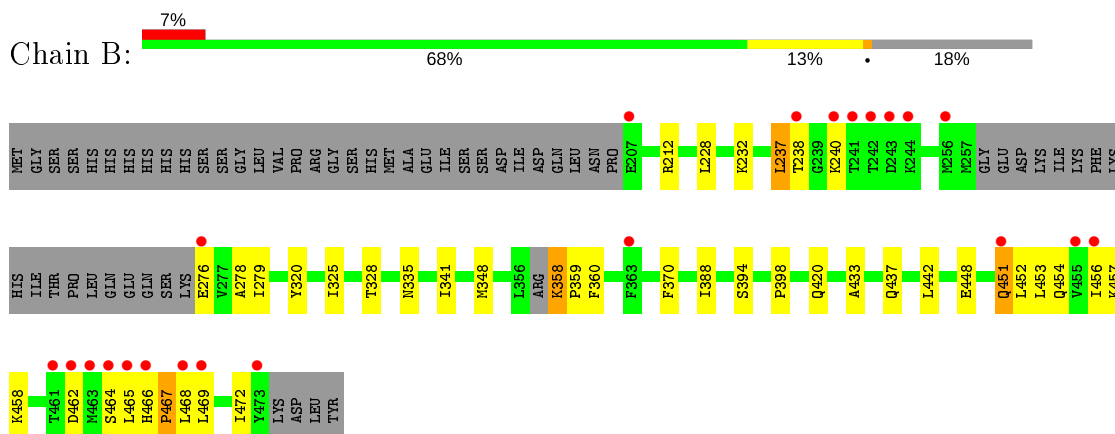
### 3 Residue-property plots [i](#)

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 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: Peroxisome proliferator-activated receptor gamma



- Molecule 1: Peroxisome proliferator-activated receptor gamma



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.60Å 61.94Å 119.40Å 90.00° 103.00° 90.00°	Depositor
Resolution (Å)	51.24 – 2.00 58.17 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.6 (51.24-2.00) 96.6 (58.17-2.00)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.35 (at 2.00Å)	Xtrriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, $R_{free}$	0.231 , 0.276 0.232 , 0.273	Depositor DCC
$R_{free}$ test set	2186 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.8	Xtrriage
Anisotropy	0.399	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 59.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4161	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.73% 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: H8R

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	0.48	0/2037	0.61	0/2745
1	B	0.42	0/2013	0.58	0/2715
All	All	0.45	0/4050	0.59	0/5460

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	2004	0	2064	52	0
1	B	1980	0	2035	26	0
2	A	33	0	0	1	0
3	A	72	0	0	1	0
3	B	72	0	0	0	0
All	All	4161	0	4099	78	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 10.

All (78) 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:363:PHE:CE2	1:A:456:ILE:HD11	2.02	0.95
1:A:241:THR:HG23	1:A:243:ASP:OD1	1.71	0.91
1:A:363:PHE:HE2	1:A:456:ILE:HD11	1.36	0.90
1:A:207:GLU:HG3	1:A:209:ALA:H	1.41	0.85
1:B:325:ILE:HD12	1:B:388:ILE:HG23	1.62	0.81
1:B:358:LYS:HB3	1:B:359:PRO:HD2	1.64	0.77
1:A:236:ILE:HG12	1:A:244:LYS:HB3	1.72	0.70
1:A:358:LYS:HB2	1:A:359:PRO:HD3	1.73	0.70
1:A:325:ILE:HG23	1:A:388:ILE:HD12	1.73	0.69
1:A:358:LYS:HB2	1:A:359:PRO:CD	2.23	0.68
1:A:293:VAL:HG22	1:A:322:VAL:HG11	1.79	0.66
1:A:440:THR:O	1:A:444:GLN:HG2	2.00	0.62
1:B:370:PHE:CZ	1:B:442:LEU:HD13	2.36	0.60
1:A:358:LYS:CB	1:A:359:PRO:CD	2.79	0.60
1:A:276:GLU:CD	1:A:357:ARG:HE	2.06	0.58
1:A:288:ARG:HH11	1:A:291:GLU:HB3	1.68	0.58
1:A:342:SER:H	2:A:501[A]:H8R:CAI	2.17	0.58
1:B:448:GLU:O	1:B:451:GLN:HG3	2.06	0.56
1:B:457:LYS:C	1:B:458:LYS:HD3	2.25	0.55
1:A:241:THR:HG22	1:A:244:LYS:H	1.72	0.55
1:A:363:PHE:CE2	1:A:456:ILE:CD1	2.85	0.54
1:A:370:PHE:HB2	1:A:445:ILE:HD11	1.90	0.54
1:A:358:LYS:CB	1:A:359:PRO:HD3	2.37	0.54
1:B:212:ARG:NH2	1:B:420:GLN:OE1	2.34	0.54
1:A:249:ILE:HD12	1:A:255:LEU:HA	1.88	0.54
1:B:237:LEU:O	1:B:240:LYS:HG2	2.08	0.54
1:A:349:THR:HG22	1:A:351:GLU:H	1.73	0.53
1:A:363:PHE:CZ	1:A:456:ILE:CD1	2.93	0.52
1:A:207:GLU:HG3	1:A:209:ALA:N	2.19	0.51
1:A:252:MET:HE1	1:A:277:VAL:HG21	1.91	0.51
1:B:276:GLU:OE2	1:B:278:ALA:HB3	2.11	0.51
1:A:320:TYR:OH	1:A:474:LYS:HE3	2.11	0.51
1:A:384:LEU:O	1:A:388:ILE:HG12	2.11	0.51
1:B:358:LYS:CB	1:B:359:PRO:HD2	2.37	0.51
1:B:320:TYR:CZ	1:B:398:PRO:HG2	2.46	0.50
1:A:241:THR:HG23	1:A:243:ASP:CG	2.33	0.49
1:A:276:GLU:OE1	1:A:357:ARG:NH2	2.46	0.48
1:A:363:PHE:CZ	1:A:456:ILE:HD11	2.48	0.48
1:B:238:THR:HG23	1:B:335:ASN:ND2	2.28	0.48
1:A:457:LYS:HD3	1:A:457:LYS:HA	1.53	0.47
1:B:465:LEU:O	1:B:467:PRO:HD3	2.14	0.47
1:B:468:LEU:O	1:B:472:ILE:HG13	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:ARG:HH22	1:A:375:ASN:ND2	2.13	0.47
1:A:354:LYS:HD2	1:A:354:LYS:O	2.15	0.46
1:A:433:ALA:O	1:A:437:GLN:HG3	2.16	0.46
1:B:276:GLU:OE2	1:B:358:LYS:HD3	2.16	0.46
1:A:349:THR:HG22	1:A:351:GLU:N	2.31	0.46
1:B:237:LEU:HB3	1:B:238:THR:H	1.58	0.46
1:A:286:GLN:NE2	1:A:465:LEU:HD12	2.31	0.45
1:B:341:ILE:HG21	1:B:348:MET:HE3	1.96	0.45
1:A:457:LYS:HZ1	1:A:465:LEU:HD13	1.80	0.45
1:A:457:LYS:NZ	1:A:465:LEU:HB2	2.32	0.45
1:B:469:LEU:HA	1:B:469:LEU:HD12	1.83	0.45
1:A:393:LEU:O	1:A:410:GLN:HB2	2.17	0.45
1:A:241:THR:HG21	1:A:244:LYS:NZ	2.30	0.44
1:A:325:ILE:HD11	1:A:392:ILE:HG12	1.97	0.44
1:A:363:PHE:CZ	1:A:456:ILE:HD12	2.53	0.44
1:A:424:ASN:HB3	1:A:425:HIS:CD2	2.53	0.44
1:B:328:THR:OG1	1:B:442:LEU:HD21	2.18	0.43
1:A:241:THR:OG1	3:A:601:HOH:O	2.21	0.43
1:A:427:GLU:H	1:A:427:GLU:CD	2.21	0.43
1:A:288:ARG:NH1	1:A:291:GLU:HB3	2.31	0.43
1:B:228:LEU:CD1	1:B:232:LYS:HG2	2.49	0.43
1:A:388:ILE:O	1:A:392:ILE:HG13	2.19	0.42
1:A:363:PHE:HZ	1:A:456:ILE:HD12	1.85	0.42
1:B:456:ILE:C	1:B:458:LYS:H	2.22	0.42
1:B:448:GLU:O	1:B:452:LEU:HD12	2.20	0.41
1:A:241:THR:HB	1:A:244:LYS:HD2	2.01	0.41
1:B:358:LYS:HB3	1:B:359:PRO:CD	2.42	0.41
1:B:454:GLN:O	1:B:458:LYS:HE3	2.20	0.41
1:B:279:ILE:HG12	1:B:360:PHE:CZ	2.56	0.41
1:B:433:ALA:O	1:B:437:GLN:HG3	2.21	0.41
1:A:241:THR:CG2	1:A:243:ASP:CG	2.89	0.41
1:B:453:LEU:HD12	1:B:453:LEU:HA	1.80	0.41
1:A:241:THR:HG21	1:A:244:LYS:HG3	2.04	0.40
1:A:293:VAL:HG22	1:A:322:VAL:CG1	2.48	0.40

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	247/304 (81%)	239 (97%)	6 (2%)	2 (1%)	19	13
1	B	244/304 (80%)	228 (93%)	12 (5%)	4 (2%)	9	4
All	All	491/608 (81%)	467 (95%)	18 (4%)	6 (1%)	13	7

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	358	LYS
1	B	358	LYS
1	B	237	LEU
1	B	467	PRO
1	A	239	GLY
1	B	466	HIS

### 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	224/273 (82%)	219 (98%)	5 (2%)	52	55
1	B	222/273 (81%)	218 (98%)	4 (2%)	59	63
All	All	446/546 (82%)	437 (98%)	9 (2%)	55	58

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	280	ARG
1	A	343	GLU
1	A	357	ARG
1	A	427	GLU
1	A	474	LYS
1	B	394	SER
1	B	451	GLN
1	B	462	ASP
1	B	464	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	466	HIS

### 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
2	H8R	A	501[B]	-	21,25,25	1.18	2 (9%)	26,31,31	1.04	3 (11%)
2	H8R	A	501[A]	-	21,25,25	1.18	2 (9%)	26,31,31	1.07	3 (11%)

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	H8R	A	501[B]	-	-	12/21/25/25	0/1/1/1
2	H8R	A	501[A]	-	-	13/21/25/25	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501[B]	H8R	CAQ-N	4.08	1.43	1.34
2	A	501[A]	H8R	CAQ-N	4.08	1.43	1.34
2	A	501[B]	H8R	OAD-CAC	2.20	1.42	1.37
2	A	501[A]	H8R	OAD-CAC	2.20	1.42	1.37

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501[B]	H8R	CA-N-CAQ	-3.01	117.45	122.28
2	A	501[A]	H8R	CA-N-CAQ	-3.01	117.45	122.28
2	A	501[B]	H8R	OAR-CAQ-N	-2.45	117.93	122.45
2	A	501[A]	H8R	OAR-CAQ-N	-2.45	117.93	122.45
2	A	501[B]	H8R	CG1-CB-CA	2.37	113.52	111.24
2	A	501[A]	H8R	CG1-CB-CA	2.37	113.52	111.24

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501[B]	H8R	C-CA-CB-CG2
2	A	501[B]	H8R	C-CA-CB-CG1
2	A	501[A]	H8R	C-CA-CB-CG2
2	A	501[A]	H8R	C-CA-CB-CG1
2	A	501[B]	H8R	N-CA-CB-CG2
2	A	501[A]	H8R	N-CA-CB-CG2

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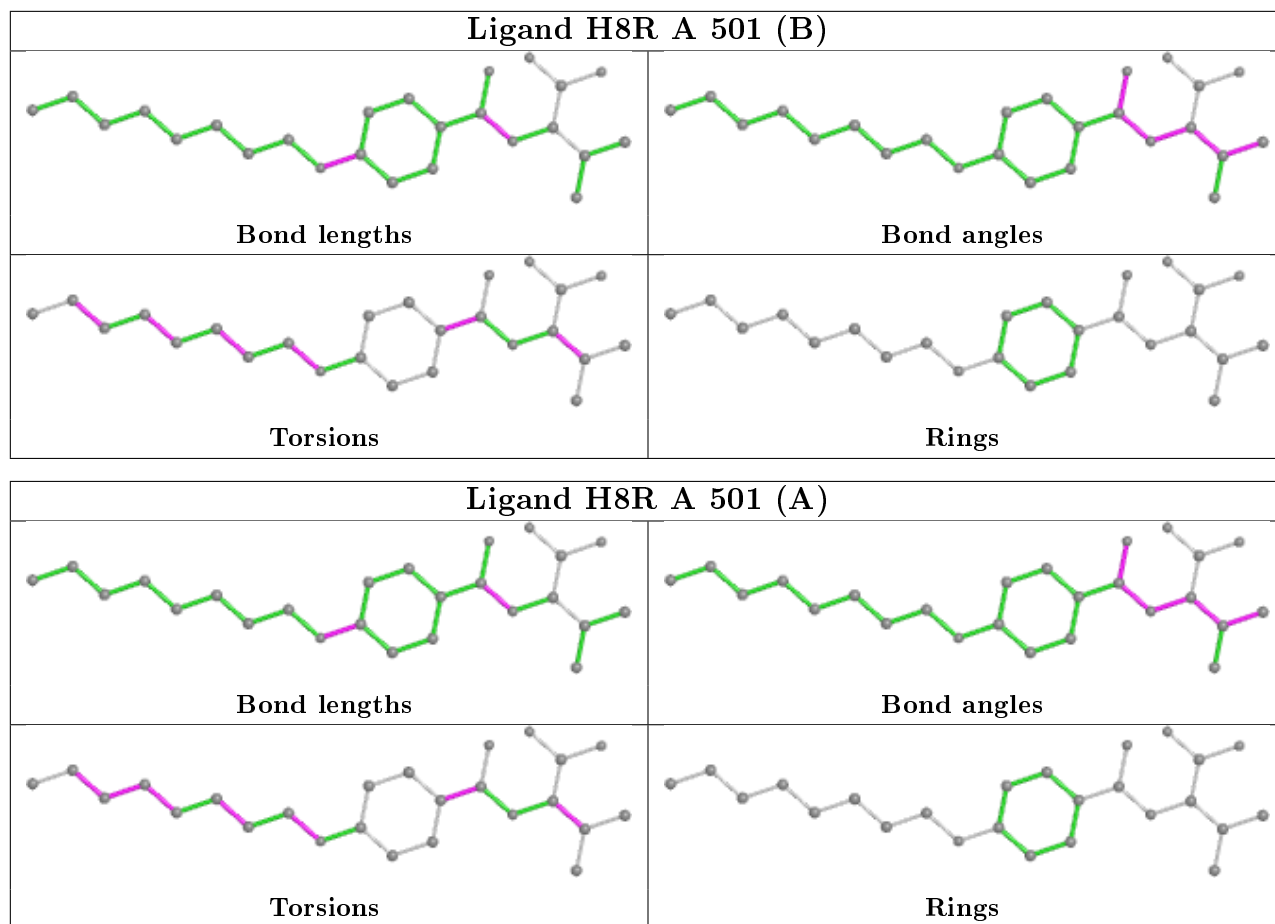
Mol	Chain	Res	Type	Atoms
2	A	501[B]	H8R	CAA-CAP-CAQ-N
2	A	501[A]	H8R	CAA-CAP-CAQ-N
2	A	501[B]	H8R	CAA-CAP-CAQ-OAR
2	A	501[A]	H8R	CAA-CAP-CAQ-OAR
2	A	501[B]	H8R	CAO-CAP-CAQ-N
2	A	501[A]	H8R	CAO-CAP-CAQ-N
2	A	501[B]	H8R	CAO-CAP-CAQ-OAR
2	A	501[A]	H8R	CAO-CAP-CAQ-OAR
2	A	501[B]	H8R	N-CA-CB-CG1
2	A	501[A]	H8R	N-CA-CB-CG1
2	A	501[B]	H8R	CAE-CAF-CAG-CAH
2	A	501[A]	H8R	CAG-CAH-CAI-CAJ
2	A	501[B]	H8R	CAI-CAJ-CAK-CAL
2	A	501[B]	H8R	CAF-CAE-OAD-CAC
2	A	501[A]	H8R	CAE-CAF-CAG-CAH
2	A	501[A]	H8R	CAI-CAJ-CAK-CAL
2	A	501[A]	H8R	CAF-CAE-OAD-CAC
2	A	501[A]	H8R	CAH-CAI-CAJ-CAK
2	A	501[B]	H8R	CAG-CAH-CAI-CAJ

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501[A]	H8R	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

### 6.1 Protein, DNA and RNA chains

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	251/304 (82%)	0.17	5 (1%) 65 63	37, 52, 71, 84	1 (0%)
1	B	248/304 (81%)	0.56	22 (8%) 9 8	37, 55, 92, 122	0
All	All	499/608 (82%)	0.37	27 (5%) 25 24	37, 53, 82, 122	1 (0%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	465	LEU	12.3
1	B	238	THR	11.4
1	B	242	THR	11.2
1	B	464	SER	8.2
1	B	463	MET	6.5
1	B	462	ASP	5.4
1	B	240	LYS	4.3
1	B	243	ASP	3.8
1	B	363	PHE	3.6
1	A	241	THR	3.5
1	B	241	THR	3.4
1	B	461	THR	3.4
1	A	358	LYS	3.4
1	B	276	GLU	3.2
1	B	256	MET	3.1
1	B	244	LYS	3.0
1	B	466	HIS	2.7
1	B	455	VAL	2.6
1	B	469	LEU	2.5
1	B	207	GLU	2.5
1	B	451	GLN	2.4
1	B	473	TYR	2.4
1	B	456	ILE	2.2
1	A	276	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	468	LEU	2.1
1	A	240	LYS	2.0
1	A	457	LYS	2.0

## 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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

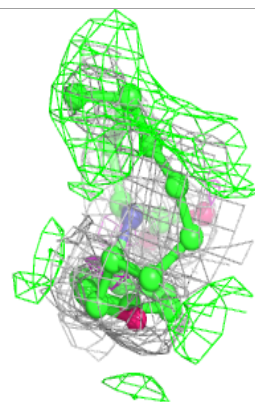
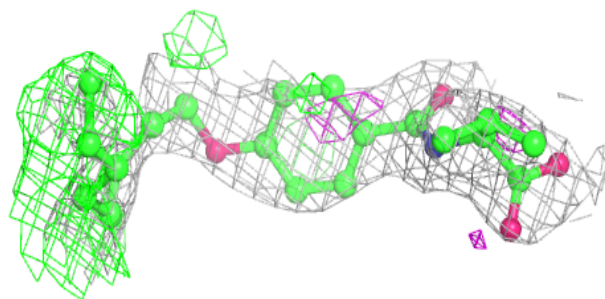
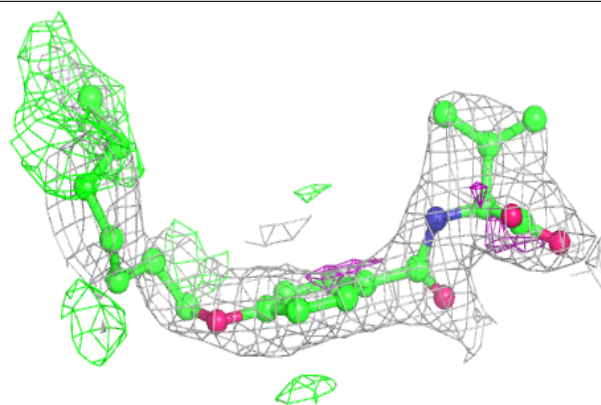
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	H8R	A	501[B]	25/25	0.69	0.29	57,64,67,70	8
2	H8R	A	501[A]	25/25	0.69	0.29	52,64,67,70	8

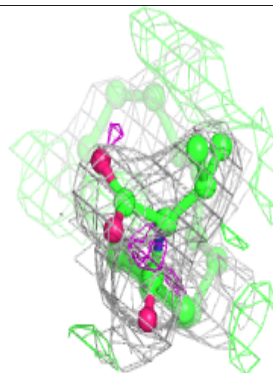
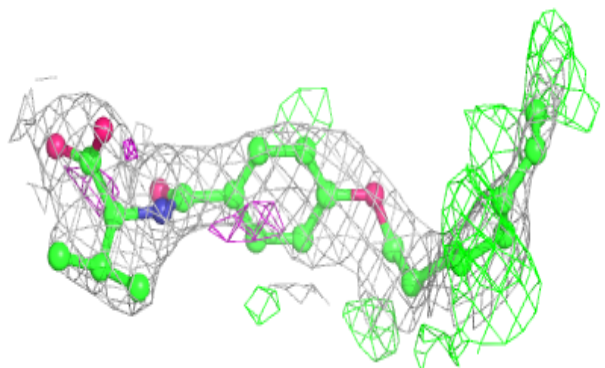
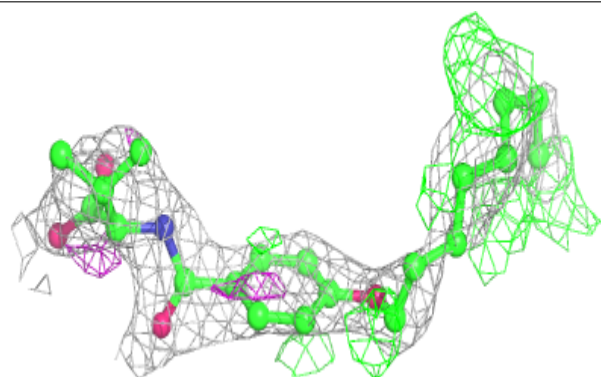
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around H8R A 501 (B):**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around H8R A 501 (A):**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers

There are no such residues in this entry.