



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:03 PM UTC

PDB ID : 6LR9 / pdb_00006lr9
Title : HSP90 in complex with Debio0932
Authors : Cao, H.L.
Deposited on : 2020-01-15
Resolution : 2.20 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

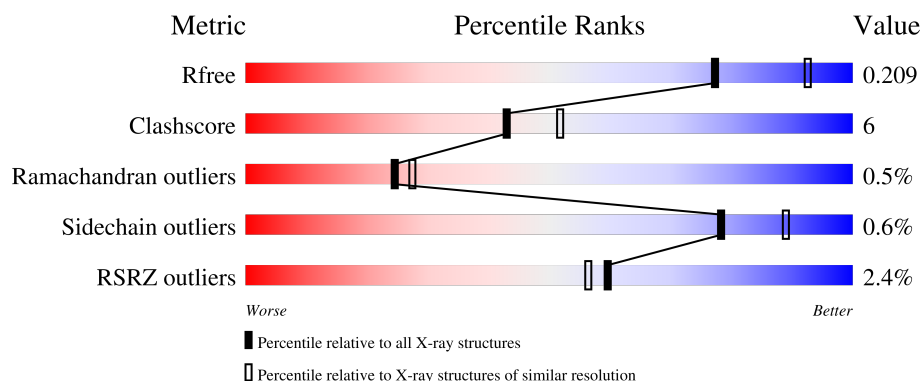
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

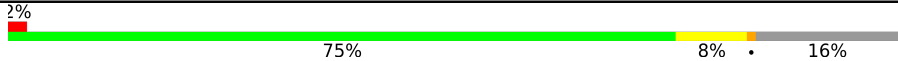
The reported resolution of this entry is 2.20 Å.

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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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 $\leq 5\%$. 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	252	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 1840 atoms, of which 8 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 Heat shock protein HSP 90-alpha.

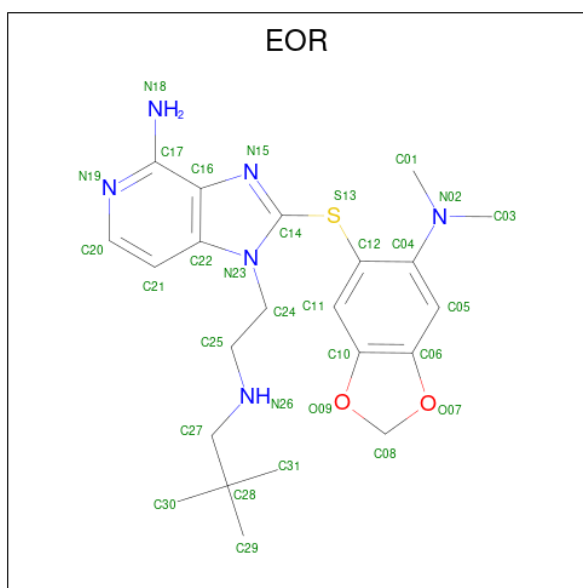
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	0	1	0
			1665	1056	274	330	5			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	initiating methionine	UNP P07900
A	-14	HIS	-	expression tag	UNP P07900
A	-13	HIS	-	expression tag	UNP P07900
A	-12	HIS	-	expression tag	UNP P07900
A	-11	HIS	-	expression tag	UNP P07900
A	-10	HIS	-	expression tag	UNP P07900
A	-9	HIS	-	expression tag	UNP P07900
A	-8	SER	-	expression tag	UNP P07900
A	-7	SER	-	expression tag	UNP P07900
A	-6	GLY	-	expression tag	UNP P07900
A	-5	VAL	-	expression tag	UNP P07900
A	-4	ASP	-	expression tag	UNP P07900
A	-3	LEU	-	expression tag	UNP P07900
A	-2	GLY	-	expression tag	UNP P07900
A	-1	THR	-	expression tag	UNP P07900
A	0	GLU	-	expression tag	UNP P07900
A	1	ASN	-	expression tag	UNP P07900
A	2	LEU	-	expression tag	UNP P07900
A	3	TYR	-	expression tag	UNP P07900
A	4	PHE	-	expression tag	UNP P07900
A	5	GLN	-	expression tag	UNP P07900
A	6	SER	-	expression tag	UNP P07900
A	7	ASN	-	expression tag	UNP P07900
A	8	ALA	-	expression tag	UNP P07900

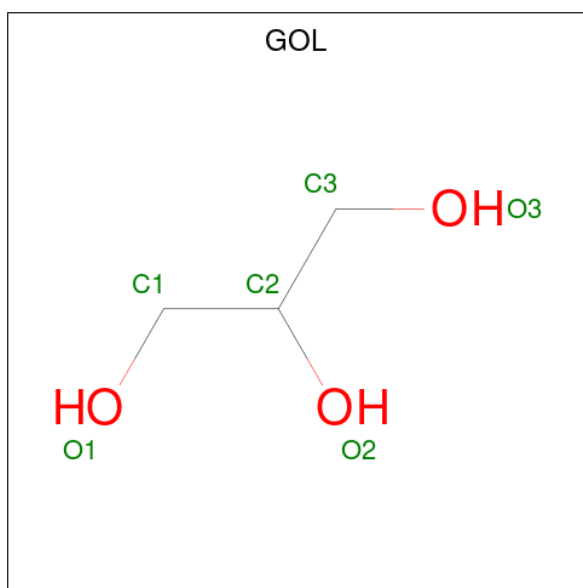
- Molecule 2 is 2-[[6-(dimethylamino)-1,3-benzodioxol-5-yl]sulfanyl]-1-[2-(2,2-dimethylpropylamino)ethyl]imidazo[4,5-c]pyridin-4-amine (CCD ID: EOR) (formula: C₂₂H₃₀N₆O₂S)

(labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			31	22	6	2	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	130	Total 130	O 130	0	0

- Molecule 1: Heat shock protein HSP 90-alpha

Residue	Position	Frequency	Conservation
ASP	1226	0.00	0.00
GLY	1227	0.00	0.00
GLU	1228	0.00	0.00
VAL	1229	0.00	0.00
ASP	1230	0.00	0.00
GLY	1231	0.00	0.00
THR	1232	0.00	0.00
GLN	1233	0.00	0.00
ASN	1234	0.00	0.00
LEU	1235	0.00	0.00
TYR	1236	0.00	0.00
PHE	1237	0.00	0.00
GLN	1238	0.00	0.00
SER	1239	0.00	0.00
ASN	1240	0.00	0.00
ALA	1241	0.00	0.00
ASP	1242	0.00	0.00
GLN	1243	0.00	0.00
PRO	1244	0.00	0.00
MET	1245	0.00	0.00
GLY	1246	0.00	0.00
GLU	1247	0.00	0.00
GLU	1248	0.00	0.00
GLU	1249	0.00	0.00
GLU	1250	0.00	0.00
GLU	1251	0.00	0.00
GLU	1252	0.00	0.00
GLU	1253	0.00	0.00
GLU	1254	0.00	0.00
GLU	1255	0.00	0.00
GLU	1256	0.00	0.00
GLU	1257	0.00	0.00
GLU	1258	0.00	0.00
GLU	1259	0.00	0.00
GLU	1260	0.00	0.00
GLU	1261	0.00	0.00
GLU	1262	0.00	0.00
GLU	1263	0.00	0.00
GLU	1264	0.00	0.00
GLU	1265	0.00	0.00
GLU	1266	0.00	0.00
GLU	1267	0.00	0.00
GLU	1268	0.00	0.00
GLU	1269	0.00	0.00
GLU	1270	0.00	0.00
GLU	1271	0.00	0.00
GLU	1272	0.00	0.00
GLU	1273	0.00	0.00
GLU	1274	0.00	0.00
GLU	1275	0.00	0.00
GLU	1276	0.00	0.00
GLU	1277	0.00	0.00
GLU	1278	0.00	0.00
GLU	1279	0.00	0.00
GLU	1280	0.00	0.00
GLU	1281	0.00	0.00
GLU	1282	0.00	0.00
GLU	1283	0.00	0.00
GLU	1284	0.00	0.00
GLU	1285	0.00	0.00
GLU	1286	0.00	0.00
GLU	1287	0.00	0.00
GLU	1288	0.00	0.00
GLU	1289	0.00	0.00
GLU	1290	0.00	0.00
GLU	1291	0.00	0.00
GLU	1292	0.00	0.00
GLU	1293	0.00	0.00
GLU	1294	0.00	0.00
GLU	1295	0.00	0.00
GLU	1296	0.00	0.00
GLU	1297	0.00	0.00
GLU	1298	0.00	0.00
GLU	1299	0.00	0.00
GLU	1300	0.00	0.00
GLU	1301	0.00	0.00
GLU	1302	0.00	0.00
GLU	1303	0.00	0.00
GLU	1304	0.00	0.00
GLU	1305	0.00	0.00
GLU	1306	0.00	0.00
GLU	1307	0.00	0.00
GLU	1308	0.00	0.00
GLU	1309	0.00	0.00
GLU	1310	0.00	0.00
GLU	1311	0.00	0.00
GLU	1312	0.00	0.00
GLU	1313	0.00	0.00
GLU	1314	0.00	0.00
GLU	1315	0.00	0.00

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	67.45Å 89.87Å 97.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.93 – 2.20 44.93 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.1 (44.93-2.20) 97.1 (44.93-2.20)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.167 , 0.209 0.169 , 0.209	Depositor DCC
R_{free} test set	1516 reflections (9.78%)	wwPDB-VP
Wilson B-factor (Å ²)	30.0	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	1840	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.71% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

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: GOL, EOR

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	0.22	0/1691	0.45	0/2280

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	1665	0	1661	21	0
2	A	31	0	0	0	0
3	A	6	8	8	0	0
4	A	130	0	0	3	2
All	All	1832	8	1669	21	2

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 6.

All (21) 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:79:ASN:HB2	1:A:92:VAL:HG13	1.64	0.79
1:A:159:GLN:HE22	1:A:178:GLU:HB2	1.55	0.72
1:A:178:GLU:HB3	1:A:179:PRO:CA	2.22	0.70
1:A:79:ASN:HB2	1:A:92:VAL:CG1	2.22	0.69
1:A:178:GLU:HB3	1:A:179:PRO:C	2.22	0.65
1:A:70:LEU:HD13	1:A:74:LYS:HD2	1.78	0.63
1:A:178:GLU:CB	1:A:179:PRO:HA	2.37	0.55
1:A:84:LYS:HG3	1:A:223:GLU:OE1	2.08	0.54
1:A:178:GLU:CB	1:A:179:PRO:CA	2.85	0.54
1:A:159:GLN:HG2	1:A:175:ASP:HB3	1.90	0.53
1:A:178:GLU:HB3	1:A:179:PRO:HA	1.91	0.53
1:A:209:LYS:HE2	4:A:518:HOH:O	2.10	0.52
1:A:115[A]:THR:HG22	1:A:119:MET:HE2	1.93	0.51
1:A:26:ILE:HD12	4:A:426:HOH:O	2.10	0.50
1:A:111:ALA:O	1:A:115[B]:THR:HG23	2.11	0.50
1:A:32:LEU:C	1:A:32:LEU:HD23	2.38	0.49
1:A:26:ILE:HG12	1:A:115[B]:THR:HG21	1.96	0.47
1:A:180:MET:SD	1:A:185:LYS:HG3	2.58	0.44
1:A:91:ILE:N	1:A:91:ILE:HD12	2.34	0.43
1:A:222:VAL:HG13	4:A:405:HOH:O	2.17	0.43
1:A:25:GLU:O	1:A:115[A]:THR:HG21	2.19	0.42

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:426:HOH:O	4:A:467:HOH:O[8_555]	1.64	0.56
4:A:459:HOH:O	4:A:529:HOH:O[2_565]	2.18	0.02

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	210/252 (83%)	205 (98%)	4 (2%)	1 (0%)	24 27

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	178	GLU

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	182/219 (83%)	181 (100%)	1 (0%)	81 90

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	VAL

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

Mol	Chain	Res	Type
1	A	123	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 oligosaccharides 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	GOL	A	302	-	5,5,5	0.51	0	5,5,5	0.20	0
2	EOR	A	301	-	34,34,34	1.87	6 (17%)	46,50,50	1.86	12 (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
3	GOL	A	302	-	-	2/4/4/4	-
2	EOR	A	301	-	-	5/16/22/22	0/4/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	EOR	C12-S13	5.46	1.83	1.77
2	A	301	EOR	C14-S13	5.13	1.83	1.75
2	A	301	EOR	C17-N18	4.46	1.45	1.34
2	A	301	EOR	C22-C16	-2.32	1.37	1.40
2	A	301	EOR	O09-C10	2.26	1.41	1.38
2	A	301	EOR	C14-N23	-2.24	1.33	1.37

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	EOR	C12-C04-N02	5.31	122.39	118.02
2	A	301	EOR	N23-C14-N15	-4.79	109.17	113.97
2	A	301	EOR	C21-C22-C16	-4.09	118.28	122.62
2	A	301	EOR	O09-C10-C11	2.63	131.35	127.86
2	A	301	EOR	C04-C12-S13	2.60	123.64	118.16
2	A	301	EOR	C20-N19-C17	2.59	121.34	117.62
2	A	301	EOR	C22-C16-N15	-2.58	107.18	110.31
2	A	301	EOR	O07-C06-C05	2.41	131.06	127.86
2	A	301	EOR	C05-C04-N02	-2.35	117.23	120.89
2	A	301	EOR	C21-C20-N19	-2.19	121.29	123.97
2	A	301	EOR	C21-C22-N23	2.17	134.92	130.42
2	A	301	EOR	C16-C22-N23	2.16	106.80	105.22

There are no chirality outliers.

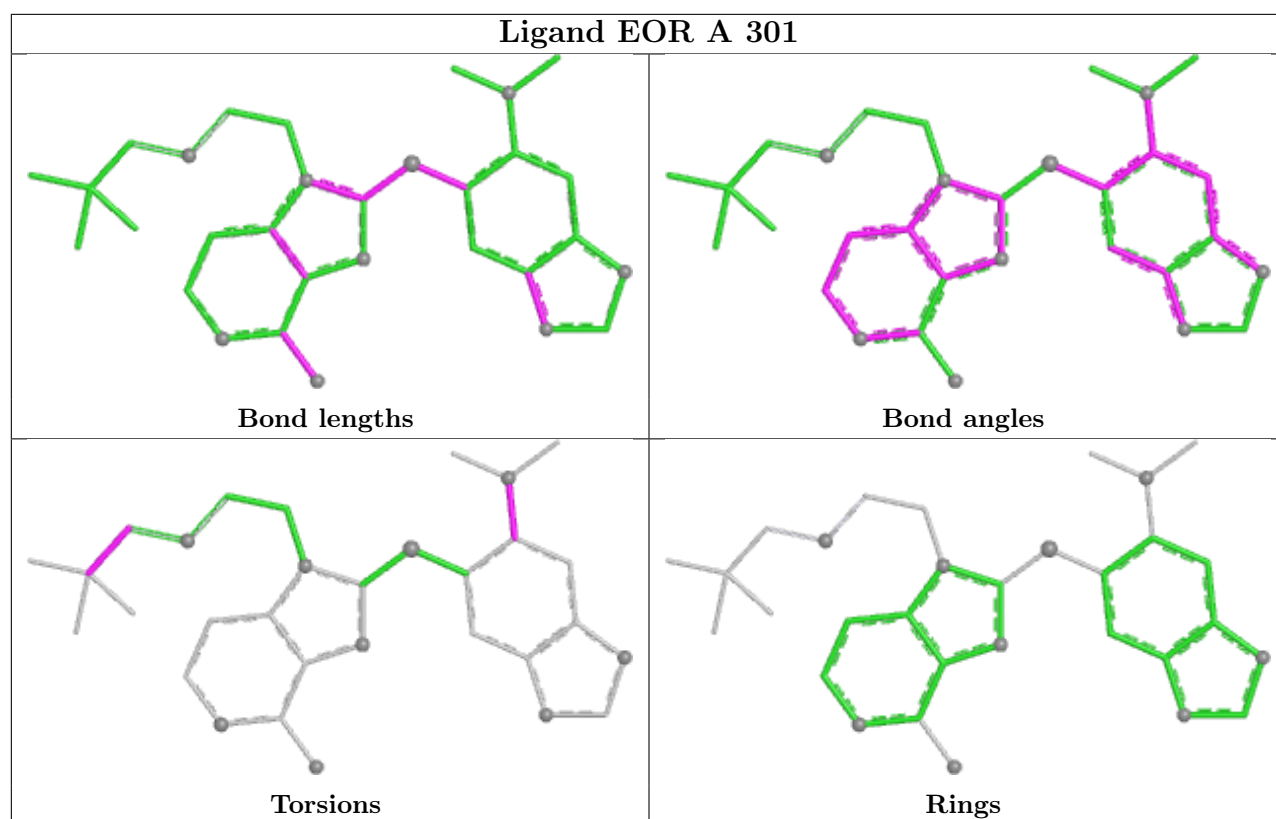
All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	302	GOL	C1-C2-C3-O3
2	A	301	EOR	N26-C27-C28-C31
2	A	301	EOR	C12-C04-N02-C01
2	A	301	EOR	N26-C27-C28-C29
2	A	301	EOR	N26-C27-C28-C30
3	A	302	GOL	O2-C2-C3-O3
2	A	301	EOR	C12-C04-N02-C03

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 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 [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, 95th 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 ²)	Q<0.9
1	A	211/252 (83%)	-0.12	5 (2%) 59 56	16, 30, 52, 81	1 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	226	ARG	3.9
1	A	176	THR	2.4
1	A	179	PRO	2.2
1	A	223	GLU	2.2
1	A	177	GLY	2.1

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](#)

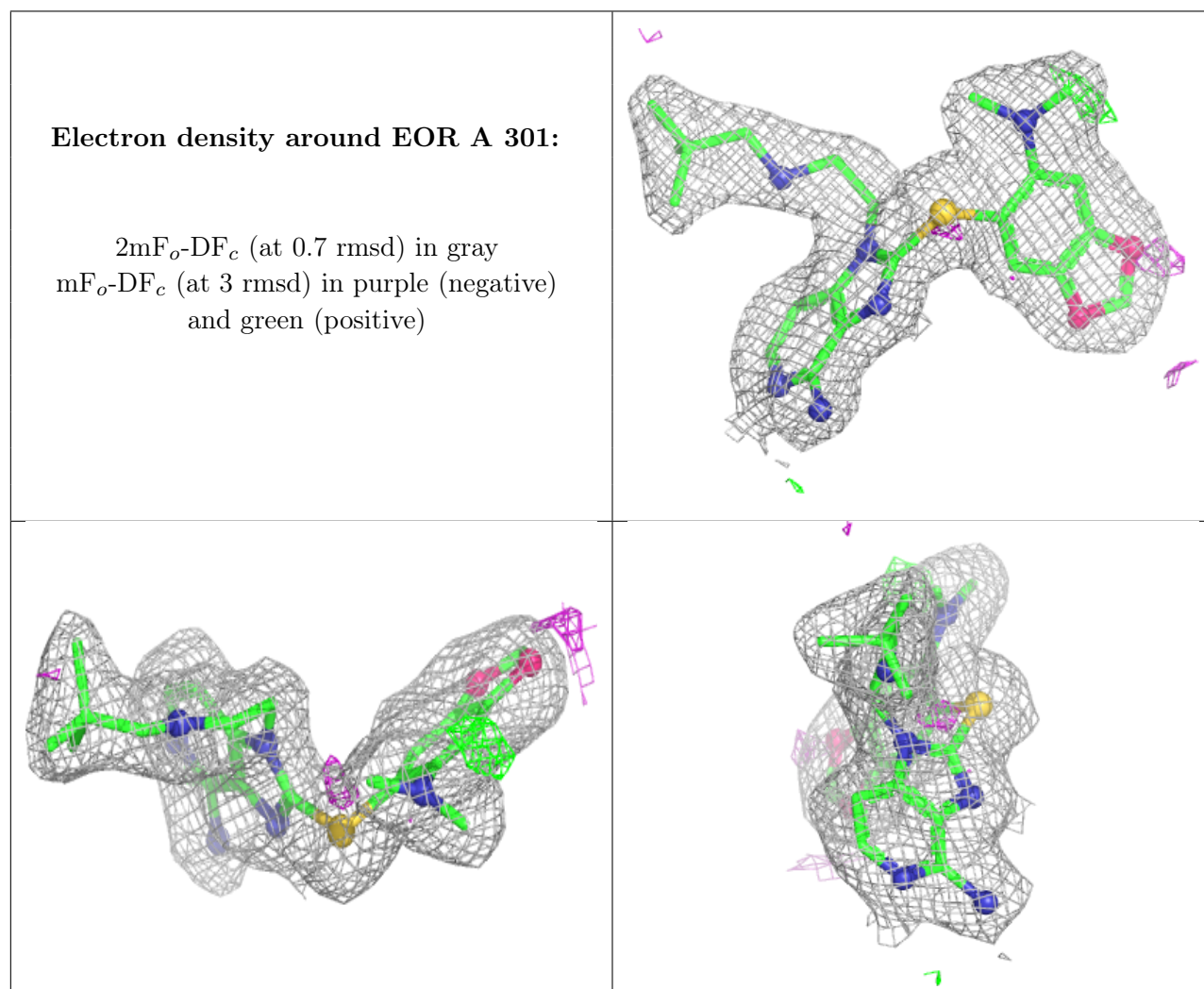
There are no oligosaccharides in this entry.

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, 95th 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 ²)	Q<0.9
3	GOL	A	302	6/6	0.94	0.13	29,35,43,43	0
2	EOR	A	301	31/31	0.96	0.07	18,25,33,37	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 ⓘ

There are no such residues in this entry.