

Full wwPDB X-ray Structure Validation Report (i)

Jun 7, 2020 - 04:34 am BST

PDB ID	:	6NWL
Title	:	Structure of the Ancestral Glucocorticoid Receptor 2 ligand binding domain
		in complex with hydrocortisone and PGC1a coregulator fragment
Authors	:	Liu, X.; Ortlund, E.A.
Deposited on		
$\operatorname{Resolution}$:	1.59 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

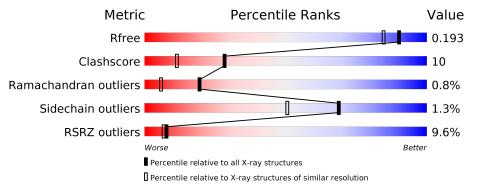
MolProbity		4.02b-467 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)		1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
$\operatorname{CCP4}$:	$7.0.044 (\mathrm{Gargrove})$
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 1.59 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries},{ m resolution\ range}({ m \AA}))$
R_{free}	130704	3398 (1.60-1.60)
Clashscore	141614	3665(1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563(1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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 <=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	А	249	9%	16%
2	В	12	92%	8%



2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 2472 atoms, of which 75 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.

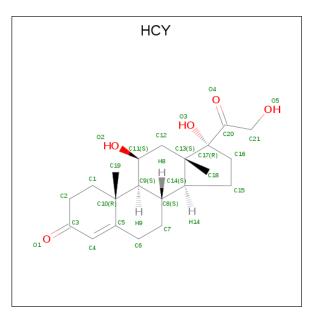
• Molecule 1 is a protein called glucocorticoid receptor.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	А	249	Total	С	Ν	Ο	S	0	19	0
_ -		- 10	2144	1383	353	389	19		10	Ū

• Molecule 2 is a protein called Peroxisome proliferator-activated receptor gamma coactivator 1-alpha.

Mol	Chain	Residues	L	Ator	\mathbf{ns}		ZeroOcc	AltConf	Trace
2	В	12	Total 88	C 61	N 14	0 13	0	0	0

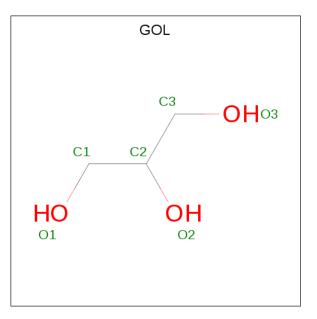
• Molecule 3 is (11alpha, 14beta)-11, 17, 21-trihydroxypregn-4-ene-3, 20-dione (three-letter code: HCY) (formula: $C_{21}H_{30}O_5$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	Δ	1	Total	С	Η	0	0	0
	Π		56	21	30	5	0	0

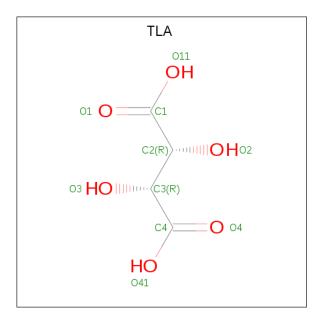


• Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

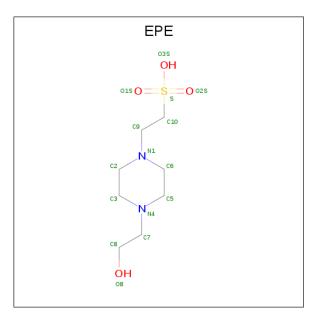
• Molecule 5 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: $C_4H_6O_6$).





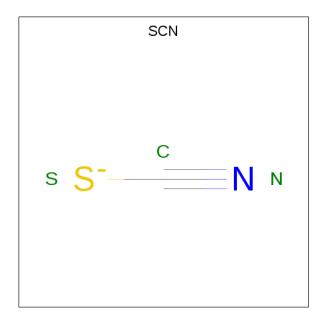
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	А	1	Total C H 14 4 4	O 6	0	0

• Molecule 6 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf			
6	А	1	Total 32		H 17			S 1	0	0

• Molecule 7 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	А	1	$\begin{array}{cccc} \mathrm{Total} & \mathrm{C} & \mathrm{N} & \mathrm{S} \\ 3 & 1 & 1 & 1 \end{array}$	0	0
7	А	1	$\begin{array}{cccc} \text{Total} & \text{C} & \text{N} & \text{S} \\ 3 & 1 & 1 & 1 \end{array}$	0	0

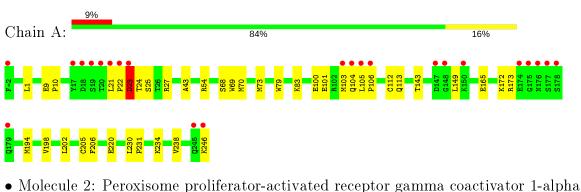
• Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	А	89	Total O 89 89	0	0
8	В	1	Total O 1 1	0	0

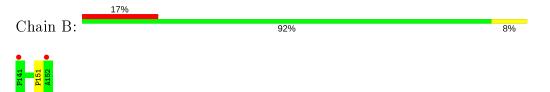


3 Residue-property plots (i)

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: glucocorticoid receptor





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants	71.76Å 96.44Å 108.19Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.42 - 1.59	Depositor
Resolution (A)	39.42 - 1.59	EDS
% Data completeness	99.4 (39.42-1.59)	Depositor
(in resolution range)	94.9(39.42 - 1.59)	EDS
R _{merge}	0.20	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.16 (at 1.59 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
D D.	0.179 , 0.193	Depositor
R, R_{free}	0.179 , 0.193	DCC
R_{free} test set	2000 reflections (4.00%)	wwPDB-VP
Wilson B-factor $(Å^2)$	27.2	Xtriage
Anisotropy	0.239	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.37, 47.8	EDS
L-test for twinning ²	$ \langle L \rangle = 0.48, \langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	2472	wwPDB-VP
Average B, all atoms $(Å^2)$	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 7.56% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: EPE, GOL, TLA, SCN, HCY

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
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.33	0/2191	0.52	0/2957
2	В	0.24	0/89	0.42	0/119
All	All	0.33	0/2280	0.51	0/3076

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	А	2144	0	2176	45	0
2	В	88	0	110	0	0
3	А	26	30	30	2	0
4	А	18	24	23	2	0
5	А	10	4	4	3	0
6	А	15	17	17	3	0
7	А	6	0	0	0	0
8	А	89	0	0	1	0
8	В	1	0	0	0	0
All	All	2397	75	2360	46	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 (46) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-1 Atom-2		Clash
		distance (Å)	overlap (Å)
1:A:100:GLU:HA	1:A:103:MET:HG3	1.44	0.99
1:A:21:LEU:HD22	1:A:22:PRO:HD2	1.54	0.87
1:A:103:MET:SD	1:A:112:CYS:HB3	2.20	0.81
1:A:100:GLU:HA	1:A:103:MET:CG	2.13	0.79
1:A:1:LEU:HD23	1:A:165:GLU:HG3	1.68	0.73
1:A:22:PRO:HG2	1:A:27[B]:ARG:NH1	2.03	0.73
1:A:101:GLU:O	1:A:104:GLN:HG2	1.90	0.70
1:A:23:ASP:HA	1:A:27[A]:ARG:NH2	2.07	0.69
1:A:220:GLU:H	1:A:220:GLU:CD	1.99	0.65
1:A:54[B]:ARG:HG2	8:A:417:HOH:O	1.95	0.65
1:A:43:ALA:HA	4:A:307:GOL:H12	1.77	0.65
1:A:83:LYS:HA	4:A:303:GOL:H11	1.81	0.63
1:A:100:GLU:HA	1:A:103:MET:SD	2.42	0.60
1:A:21:LEU:HD13	1:A:27[B]:ARG:NE	2.17	0.60
1:A:21:LEU:CD2	1:A:22:PRO:HD2	2.30	0.60
1:A:230[B]:LEU:HB3	1:A:231:PRO:HD3	1.84	0.58
1:A:79:TRP:HE1	6:A:305:EPE:H101	1.69	0.58
1:A:202:LEU:HD22	5:A:304:TLA:H3	1.86	0.58
1:A:1:LEU:HD23	1:A:165:GLU:CG	2.35	0.56
1:A:206:PHE:CG	1:A:230[B]:LEU:HD13	2.42	0.55
1:A:68:SER:HA	5:A:304:TLA:O41	2.07	0.54
1:A:194:MET:O	1:A:198[B]:VAL:HG12	2.08	0.53
1:A:246:LYS:HE2	1:A:246:LYS:HA	1.90	0.53
1:A:70:MET:HG3	1:A:198[B]:VAL:CG2	2.39	0.53
1:A:21:LEU:HD22	1:A:22:PRO:CD	2.32	0.51
1:A:22:PRO:O	1:A:24:THR:N	2.44	0.51
1:A:230[B]:LEU:HD12	1:A:234:LYS:HG2	1.94	0.50
3:A:301:HCY:H193	3:A:301:HCY:O2	2.12	0.49
1:A:143:THR:HG22	1:A:238[B]:VAL:HG21	1.94	0.49
1:A:23:ASP:HA	1:A:27[A]:ARG:HH22	1.77	0.48
1:A:25[A]:SER:OG	1:A:106:PRO:HD2	2.14	0.47
1:A:22:PRO:HG2	1:A:27[B]:ARG:HH12	1.78	0.47
1:A:22:PRO:HB2	1:A:24:THR:HG23	1.96	0.47
1:A:70:MET:HG3	1:A:198[B]:VAL:HG21	1.97	0.47
1:A:198[B]:VAL:O	1:A:198[B]:VAL:HG22	2.14	0.46
1:A:83:LYS:HE2	6:A:305:EPE:H51	1.97	0.46
1:A:173:ARG:HG2	1:A:173:ARG:O	2.15	0.46
1:A:103:MET:HE1	1:A:113:GLN:OE1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:TRP:HZ2	6:A:305:EPE:H52	1.82	0.45
1:A:69:TRP:O	1:A:73:MET:HG2	2.18	0.44
1:A:205:CYS:HA	3:A:301:HCY:O4	2.18	0.43
1:A:149[A]:LEU:N	1:A:149[A]:LEU:HD22	2.34	0.43
1:A:103:MET:SD	1:A:112:CYS:CB	3.02	0.42
1:A:143:THR:HG22	1:A:238[B]:VAL:CG2	2.49	0.42
1:A:198[B]:VAL:HG13	5:A:304:TLA:HB	1.85	0.41
1:A:9:GLU:HA	1:A:10:PRO:HD3	1.97	0.40

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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	А	266/249~(107%)	257 (97%)	8 (3%)	1 (0%)	34 15
2	В	10/12~(83%)	9~(90%)	0	1 (10%)	0 0
All	All	276/261~(106%)	266~(96%)	8 (3%)	2(1%)	19 7

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	23	ASP
2	В	151	PRO

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



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	245/228~(108%)	242~(99%)	3 (1%)	71 54
2	В	10/10~(100%)	10 (100%)	0	100 100
All	All	255/238~(107%)	252~(99%)	3 (1%)	69 54

analysed, and the total number of residues.

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	23	ASP
1	А	105	LEU
1	А	172	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

8 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	Turne	Chain	Res	Link	Bo	ond leng	ths	В	ond ang	les
	Type	Cham	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	А	307	-	$5,\!5,\!5$	0.74	0	5, 5, 5	1.05	1 (20%)
7	SCN	А	306	-	1,2,2	0.57	0	0,1,1	0.00	-
6	EPE	А	305	-	15, 15, 15	1.44	3 (20%)	$18,\!20,\!20$	1.13	2 (11%)
4	GOL	А	303	-	$5,\!5,\!5$	1.00	0	5, 5, 5	0.99	0
5	TLA	А	304	-	3,9,9	1.45	1 (33%)	$6,\!12,\!12$	1.62	2 (33%)
7	SCN	А	308	-	1,2,2	0.58	0	0,1,1	0.00	-
3	HCY	А	301	-	29,29,29	0.95	3 (10%)	$48,\!48,\!48$	0.89	<mark>1 (2%)</mark>
4	GOL	А	302	-	$5,\!5,\!5$	1.10	0	5, 5, 5	1.09	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	\mathbf{Link}	Chirals	Torsions	Rings
4	GOL	А	307	-	-	2/4/4/4	-
6	EPE	А	305	-	-	5/9/19/19	0/1/1/1
4	GOL	А	303	-	-	4/4/4/4	-
5	TLA	А	304	-	-	4/4/12/12	-
3	HCY	А	301	-	-	1/8/73/73	0/4/4/4
4	GOL	А	302	_	_	0/4/4/4	-

All (7) bond length o	outliers are listed below:
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Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\operatorname{\AA})$
6	А	305	EPE	C7-N4	2.58	1.53	1.47
6	А	305	EPE	C9-N1	2.51	1.53	1.47
5	А	304	TLA	O3-C3	-2.19	1.38	1.42
6	А	305	EPE	C10-S	2.16	1.80	1.77
3	А	301	HCY	C16-C17	2.10	1.57	1.54
3	А	301	HCY	O3-C17	-2.08	1.40	1.43
3	А	301	HCY	C10-C5	-2.07	1.48	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
3	А	301	HCY	O5-C21-C20	-2.64	105.84	112.71
5	А	304	TLA	C4-C3-C2	-2.40	107.94	113.11
6	А	305	EPE	C6-N1-C2	-2.24	103.78	108.83
6	А	305	EPE	C7-N4-C3	-2.16	105.71	111.23

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
5	А	304	TLA	C1-C2-C3	-2.07	108.66	113.11
4	А	307	GOL	C3-C2-C1	-2.01	103.88	111.70

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	А	305	EPE	C8-C7-N4-C5
6	А	305	EPE	S-C10-C9-N1
6	А	305	EPE	C9-C10-S-O1S
4	А	303	GOL	C1-C2-C3-O3
5	А	304	TLA	C1-C2-C3-C4
6	А	305	EPE	C9-C10-S-O3S
4	А	307	GOL	C1-C2-C3-O3
4	А	307	GOL	O2-C2-C3-O3
5	А	304	TLA	O2-C2-C3-O3
4	А	303	GOL	O2-C2-C3-O3
4	А	303	GOL	O1-C1-C2-C3
6	А	305	EPE	C9-C10-S-O2S
5	А	304	TLA	C1-C2-C3-O3
5	А	304	TLA	O2-C2-C3-C4
3	А	301	HCY	O4-C20-C21-O5
4	А	303	GOL	O1-C1-C2-O2

There are no ring outliers.

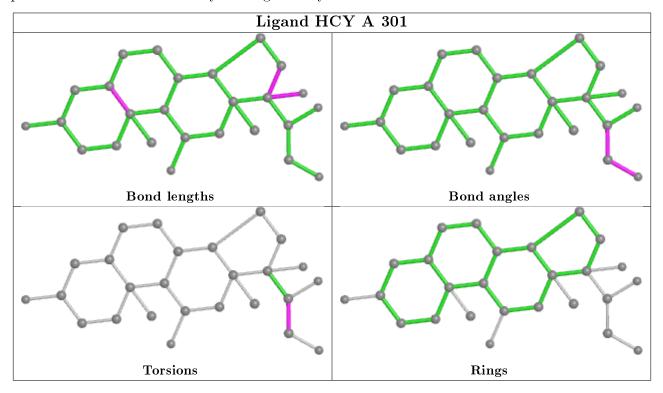
5 monomers are involved in 10 short contacts:

Mol	Chain	\mathbf{Res}	Type	Clashes	Symm-Clashes
4	А	307	GOL	1	0
6	А	305	EPE	3	0
4	А	303	GOL	1	0
5	А	304	TLA	3	0
3	А	301	HCY	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 then 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 $>$	#RSF	RZ>	$\cdot 2$	$OWAB(Å^2)$	Q<0.9
1	А	249/249~(100%)	0.40	23~(9%)	9	7	20, 30, 76, 107	0
2	В	12/12~(100%)	0.67	2(16%)	1	1	32, 44, 63, 78	0
All	All	261/261~(100%)	0.41	25~(9%)	8	7	20, 30, 76, 107	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	21	LEU	13.0
1	А	20	THR	12.1
1	А	22	PRO	9.1
1	А	18	ASP	7.5
1	А	175	GLY	6.0
2	В	152	ALA	5.2
1	А	19	SER	4.5
1	А	176	ASN	4.3
1	А	246	LYS	4.2
1	А	-2	PHE	4.0
1	А	17	TYR	3.8
1	А	177	SER	3.7
1	А	178	SER	3.4
1	А	23	ASP	3.1
2	В	141	PRO	3.0
1	А	106	PRO	3.0
1	А	174	GLU	3.0
1	А	147	ASP	2.9
1	А	104	GLN	2.5
1	А	179	GLN	2.3
1	А	150	LYS	2.3
1	А	148	GLY	2.3
1	А	103	MET	2.2
1	А	245	GLN	2.2

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Mol	Chain	\mathbf{Res}	Type	RSRZ
1	А	105	LEU	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 carbohydrates in this entry.

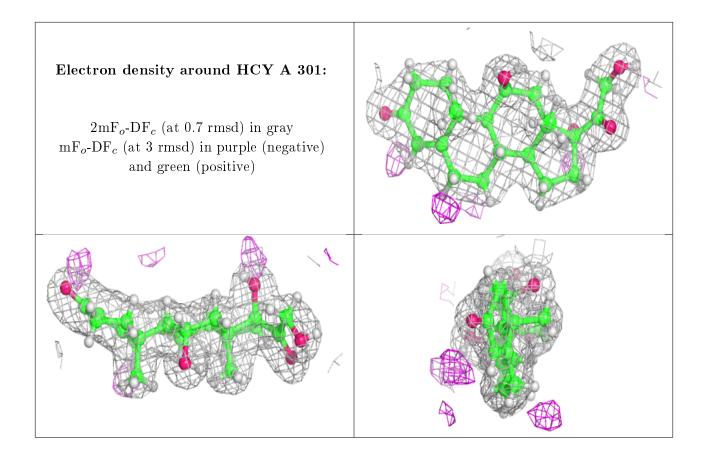
6.4 Ligands (i)

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^{th} 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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q < 0.9
4	GOL	А	303	6/6	0.66	0.24	$33,\!60,\!66,\!72$	0
5	TLA	А	304	10/10	0.74	0.33	$28,\!67,\!78,\!87$	0
7	SCN	А	306	3/3	0.79	0.19	74,74,76,77	0
6	EPE	А	305	15/15	0.79	0.38	$58,\!75,\!87,\!93$	0
4	GOL	А	302	6/6	0.82	0.18	$27,\!45,\!74,\!76$	0
4	GOL	А	307	6/6	0.88	0.20	45,72,81,87	0
7	SCN	А	308	3/3	0.90	0.21	34,34,63,87	0
3	HCY	А	301	26/26	0.95	0.07	$22,\!29,\!35,\!36$	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 (i)

There are no such residues in this entry.

