



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 06:34 PM UTC

PDB ID : 1Y9R / pdb_00001y9r
Title : Crystal structure of the human mineralocorticoid receptor ligand-binding domain bound to deoxycorticosterone and harboring the S810L mutation responsible for a severe form of hypertension
Authors : Fagart, J.; Huyet, J.; Pinon, G.M.; Rochel, M.; Mayer, C.; Rafestin-Oblin, M.E.
Deposited on : 2004-12-16
Resolution : 1.96 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 types of validation reports are described at

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

The following versions of software and data (see [references](#) ①) 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

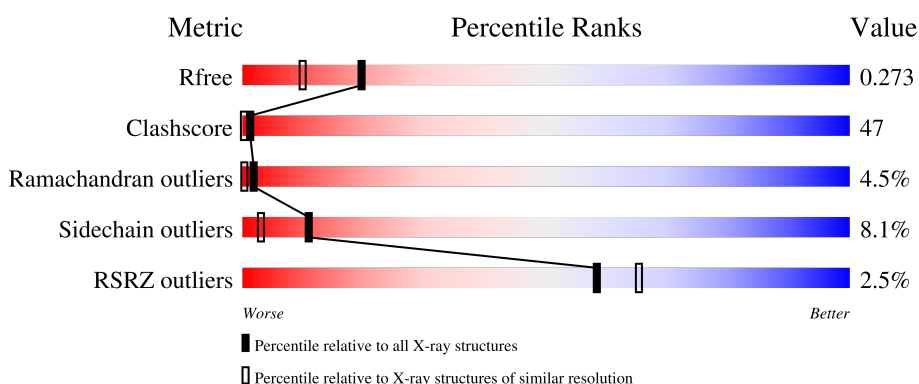
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	255	3% 26% 56% 11% • 6%
1	B	255	2% 32% 53% 9% 7%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4394 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.

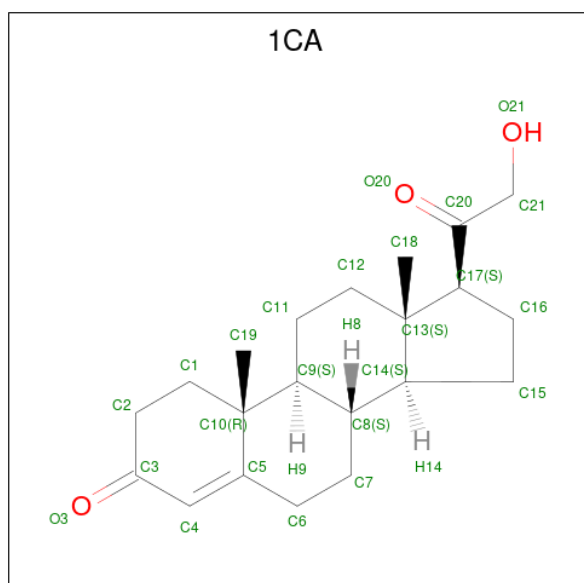
- Molecule 1 is a protein called Mineralocorticoid receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	239	Total	C	N	O	S	0	0	0
			1952	1270	317	351	14			
1	B	238	Total	C	N	O	S	0	0	0
			1933	1255	311	354	13			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	730	SER	-	cloning artifact	UNP P08235
A	810	LEU	SER	engineered mutation	UNP P08235
A	910	ALA	CYS	engineered mutation	UNP P08235
B	730	SER	-	cloning artifact	UNP P08235
B	810	LEU	SER	engineered mutation	UNP P08235
B	910	ALA	CYS	engineered mutation	UNP P08235

- Molecule 2 is DESOXYCORTICOSTERONE (CCD ID: 1CA) (formula: $C_{21}H_{30}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 24	C 21	O 3	0	0
2	B	1	Total 24	C 21	O 3	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	236	Total 236	O 236	0	0
3	B	225	Total 225	O 225	0	0

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

Chain A:

Position	Amino Acid
1	L928
2	D929
3	S930
4	M931
5	H932
6	D933
7	L934
8	V935
9	S936
10	D937
11	L938
12	L939
13	E940
14	F941
15	C942
16	F943
17	Y944
18	T945
19	E948
20	S949
21	A951
22	V954
23	E955
24	F956
25	P957
26	A958
27	N959
28	L960
29	V961
30	E962
31	I963
32	I964
33	S965
34	F966
35	Q967
36	L968
37	P969
38	K970
39	V971
40	E972
41	S973
42	A976
43	K977
44	P978
45	L979
46	V980
47	F981
48	H982
49	S983
50	L984
51	D985
52	S986
53	L987
54	Q988
55	F989
56	L992
57	T995
58	K996
59	L997
60	D997
61	L801
62	I802
63	D803
64	Y804
65	S805
66	M806
67	M807
68	C808
69	L809
70	L810
71	S811
72	L812
73	A813
74	L814
75	S815
76	H816
77	R817
78	S818
79	Y819
80	K820
81	N823
82	S824
83	Q825
84	P826
85	L827
86	Y828
87	F829
88	N835
89	N836
90	E837
91	E838
92	K839
93	M840
94	H841
95	Q842
96	S843
97	A844
98	R845
99	Y846
100	E847
101	L848
102	C849
103	Q850
104	H853
105	K854
106	L855
107	S856
108	L857
109	Q858
110	F859
111	V860
112	D863
113	L864
114	S737
115	F738
116	V739
117	M740
118	Y741
119	L742
120	E743
121	N744
122	L745
123	E746
124	F747
125	E748
126	L749
127	V750
128	Y754
129	F755
130	S756
131	K758
132	P759
133	D760
134	T761
135	A762
136	N764
137	L765
138	L766
139	S767
140	L768
141	L769
142	N770
143	A773
144	G774
145	K775
146	Q776
147	M777
148	L778
149	L779
150	V780
151	V781
152	K782
153	F783
154	K784
155	L785
156	V786
157	L787
158	F788
159	G789
160	F790
161	K791

Chain B:

32% 53% 9% 7%

SER	SER	ARG	ALA	LEU	THR	PRO	S737	P738	W739	W740	W741	L742	T745	E746	P747	E748	I749	D755	S756	S757	K758	P759	D760	T761	A762	E763	W764	T768	L769	N770	R771	L772	A773	K774	G775	Q776	M777	I778	Q779	W780	W781	K782	W783	A784	K785	W786	L787	P788	G789	T790	L793	P794	L795	T796	D797
-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	120.28Å 120.28Å 41.33Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	18.30 – 1.96 18.30 – 1.96	Depositor EDS
% Data completeness (in resolution range)	84.1 (18.30-1.96) 84.1 (18.30-1.96)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 1.96Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.229 , 0.267 0.239 , 0.273	Depositor DCC
R_{free} test set	4101 reflections (10.18%)	wwPDB-VP
Wilson B-factor (Å ²)	22.5	Xtriage
Anisotropy	0.005	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 153.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.058 for -h,-k,l 0.118 for h,-h-k,-l 0.036 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4394	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.93 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.8957e-03.*

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: 1CA

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	0/1998	1.01	11/2701 (0.4%)
1	B	0.41	0/1976	0.95	8/2668 (0.3%)
All	All	0.41	0/3974	0.98	19/5369 (0.4%)

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	1

There are no bond length outliers.

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	900	ILE	N-CA-C	-7.51	103.01	110.30
1	B	777	MET	CG-SD-CE	-6.95	85.61	100.90
1	A	848	LEU	N-CA-C	-6.39	105.61	113.41
1	A	972	GLU	N-CA-C	-6.33	105.27	112.87
1	B	757	SER	N-CA-C	-6.13	105.96	113.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	944	TYR	Sidechain

5.2 Too-close contacts ⓘ

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	1952	0	1961	195	0
1	B	1933	0	1936	174	0
2	A	24	0	30	5	0
2	B	24	0	30	5	0
3	A	236	0	0	19	0
3	B	225	0	0	26	0
All	All	4394	0	3957	371	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 47.

The worst 5 of 371 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:836:ASN:HD22	1:A:837:GLU:N	1.43	1.15
1:A:812:PHE:HB2	1:A:931:MET:HE1	1.30	1.11
1:B:872:MET:HA	1:B:875:LEU:HD12	1.35	1.06
1:B:755:ASP:HB2	1:B:758:LYS:HG2	1.37	1.03
1:A:836:ASN:ND2	1:A:837:GLU:N	2.10	0.99

There are no symmetry-related clashes.

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	235/255 (92%)	196 (83%)	29 (12%)	10 (4%)	2 0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	234/255 (92%)	197 (84%)	26 (11%)	11 (5%)	2	0
All	All	469/510 (92%)	393 (84%)	55 (12%)	21 (4%)	2	0

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	757	SER
1	A	949	SER
1	A	957	PRO
1	B	820	LYS
1	B	951	ALA

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	218/234 (93%)	198 (91%)	20 (9%)	8	2
1	B	215/234 (92%)	200 (93%)	15 (7%)	14	4
All	All	433/468 (92%)	398 (92%)	35 (8%)	11	3

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	894	GLU
1	B	908	THR
1	B	944	TYR
1	A	860	VAL
1	A	849	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	853	HIS
1	B	858	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	836	ASN
1	A	853	HIS
1	A	854	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
2	1CA	A	2001	-	27,27,27	4.88	17 (62%)	42,43,43	1.99	12 (28%)
2	1CA	B	3001	-	27,27,27	4.74	19 (70%)	42,43,43	1.82	10 (23%)

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	1CA	A	2001	-	-	0/6/64/64	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	1CA	B	3001	-	-	0/6/64/64	0/4/4/4

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001	1CA	C8-C9	10.12	1.72	1.53
2	A	2001	1CA	C10-C5	9.49	1.71	1.52
2	B	3001	1CA	C10-C9	9.04	1.70	1.56
2	A	2001	1CA	C2-C3	8.80	1.68	1.50
2	B	3001	1CA	C4-C5	8.54	1.46	1.34

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001	1CA	C17-C13-C14	-4.72	94.80	99.72
2	B	3001	1CA	C17-C13-C14	-4.51	95.01	99.72
2	B	3001	1CA	C2-C3-C4	4.31	123.27	116.73
2	A	2001	1CA	C2-C3-C4	4.09	122.94	116.73
2	A	2001	1CA	C1-C10-C9	3.75	113.70	108.74

There are no chirality outliers.

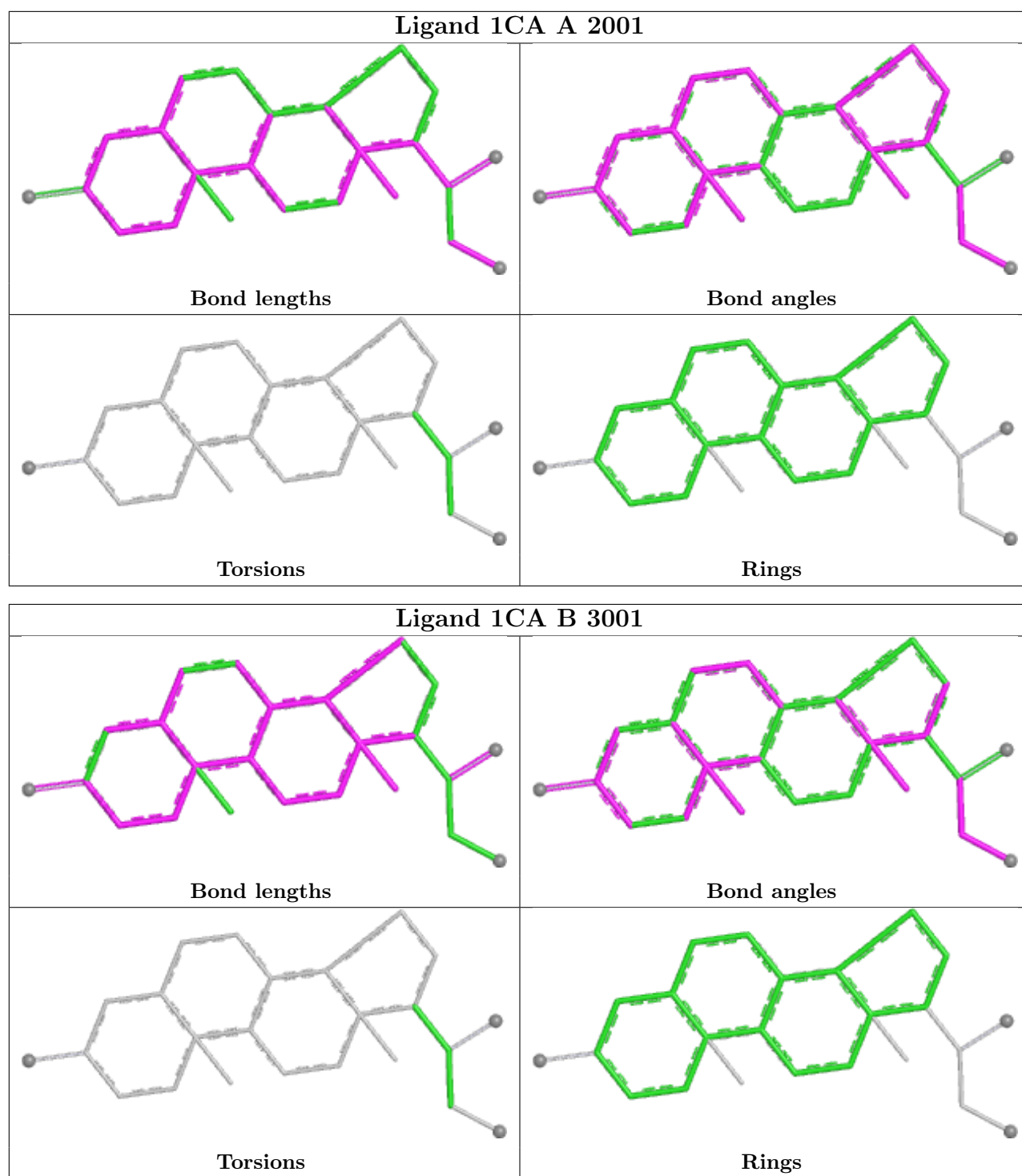
There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2001	1CA	5	0
2	B	3001	1CA	5	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 ⓘ

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	239/255 (93%)	0.39	7 (2%) 53 60	12, 23, 35, 38	0
1	B	238/255 (93%)	0.42	5 (2%) 63 70	11, 25, 36, 40	0
All	All	477/510 (93%)	0.40	12 (2%) 58 65	11, 24, 36, 40	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	761	THR	2.9
1	A	750	VAL	2.8
1	A	754	TYR	2.8
1	B	833	LEU	2.8
1	B	983	ARG	2.7

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](#)

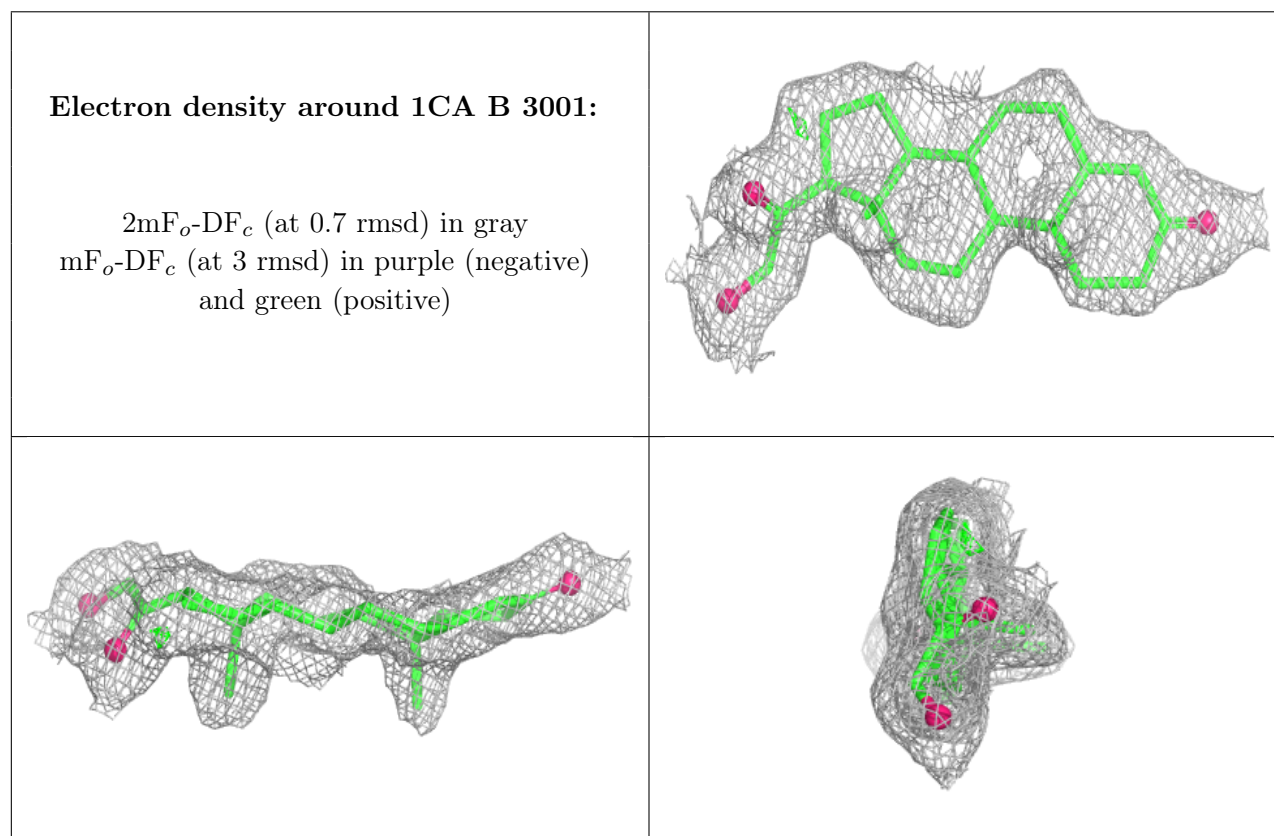
There are no oligosaccharides in this entry.

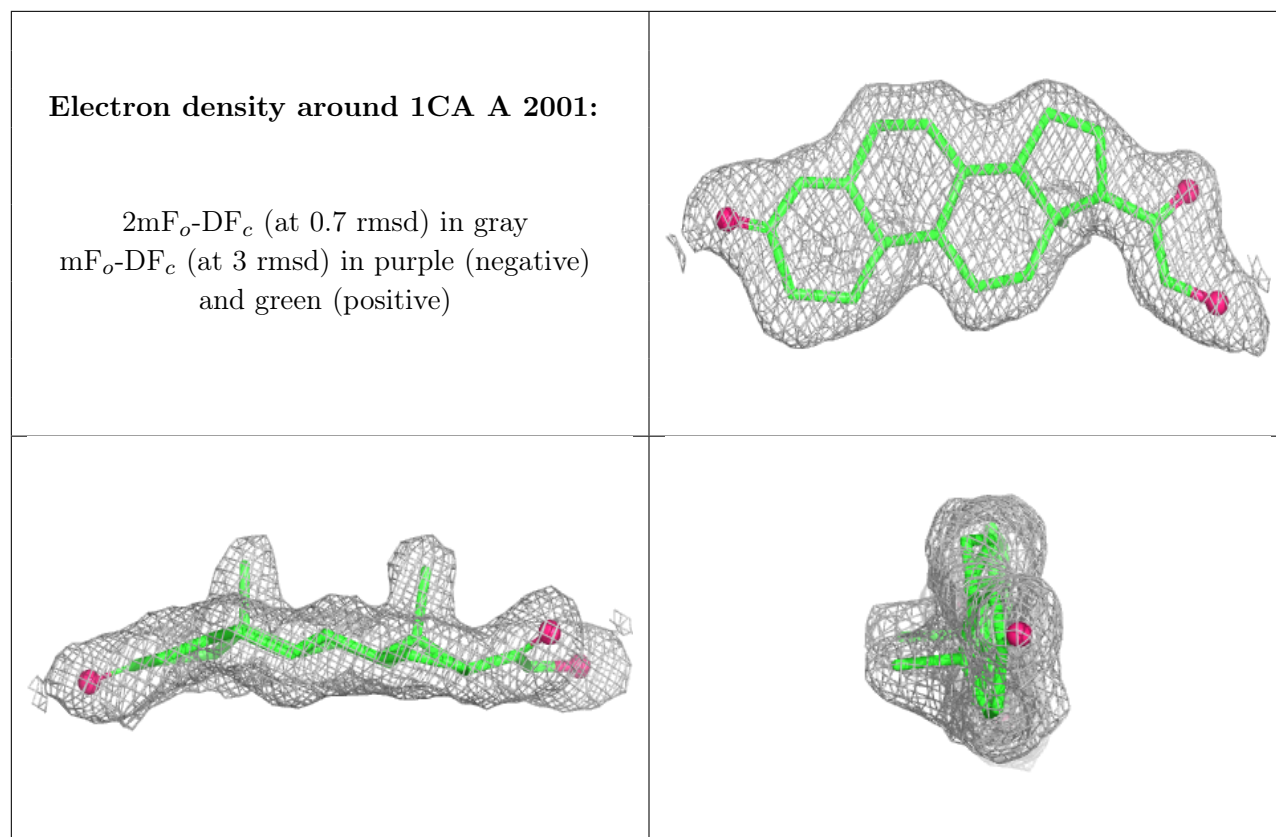
6.4 Ligands [i](#)

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($\text{\AA}^2$)	Q<0.9
2	1CA	B	3001	24/24	0.87	0.10	15,19,23,23	0
2	1CA	A	2001	24/24	0.91	0.08	18,21,24,27	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.